Full wwPDB EM Validation Report ⓘ

Dec 26, 2021 – 05:39 PM JST

PDB ID	:	7WD3
EMDB ID	:	EMD-32403
Title	:	Cryo-EM structure of Drg1 in the presence of ATP/diazaborine
Deposited on	:	2021-12-21
Resolution	:	3.80 Å(reported)

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

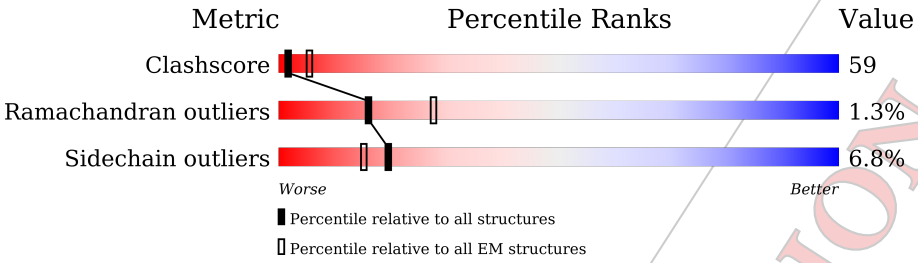
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.25

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	748	49% 42% 5% ·
1	B	748	50% 41% 6% ·
1	C	748	46% 45% 6% ·
1	D	748	50% 40% 6% ·
1	E	748	48% 43% 6% ·
1	F	748	48% 43% 6% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	A	801	X	-	X	-
2	ATP	A	803	X	-	X	-
2	ATP	B	801	X	-	X	-
2	ATP	B	803	X	-	X	-
2	ATP	C	801	X	-	X	-
2	ATP	C	803	X	-	X	-
2	ATP	D	801	X	-	X	-
2	ATP	D	803	X	-	X	-
2	ATP	E	801	X	-	X	-
2	ATP	E	803	X	-	X	-
2	ATP	F	801	X	-	X	-
2	ATP	F	803	X	-	X	-
3	NDT	A	802	X	-	X	-
3	NDT	A	804	X	-	-	-
3	NDT	B	802	X	-	X	-
3	NDT	B	804	X	-	X	-
3	NDT	C	802	X	-	X	-
3	NDT	C	804	X	-	X	-
3	NDT	D	802	X	-	X	-
3	NDT	D	804	X	-	X	-
3	NDT	E	802	X	-	X	-
3	NDT	E	804	X	-	X	-
3	NDT	F	802	X	-	X	-
3	NDT	F	804	X	-	X	-

2 Entry composition (i)

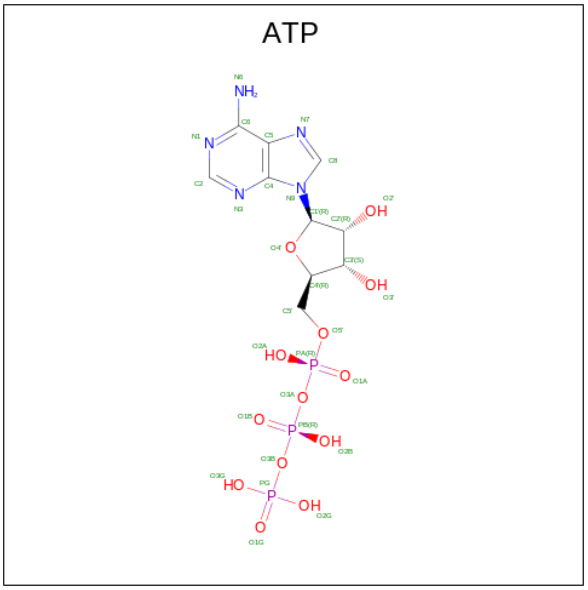
There are 3 unique types of molecules in this entry. The entry contains 34035 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATPase family gene 2 protein.

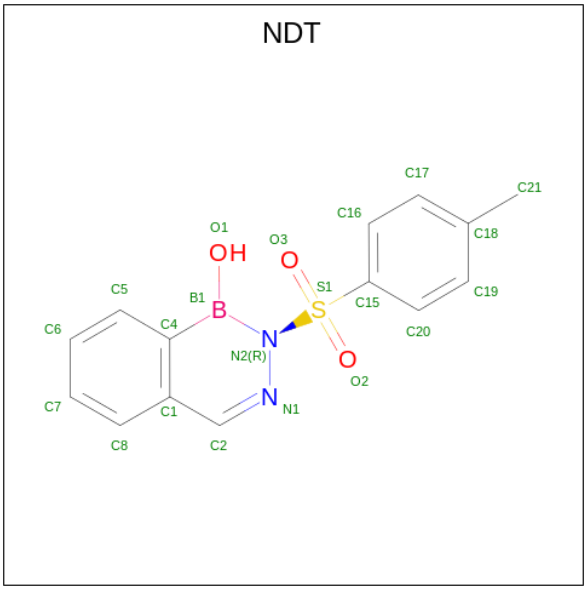
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	726	Total	C	N	O	S	0	0
			5568	3521	953	1072	22		
1	B	726	Total	C	N	O	S	0	0
			5571	3522	953	1074	22		
1	C	726	Total	C	N	O	S	0	0
			5571	3522	953	1074	22		
1	D	726	Total	C	N	O	S	0	0
			5571	3522	953	1074	22		
1	E	726	Total	C	N	O	S	0	0
			5571	3522	953	1074	22		
1	F	726	Total	C	N	O	S	0	0
			5571	3522	953	1074	22		

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			60	20	10	24	6	
2	A	1	Total	C	N	O	P	0
			60	20	10	24	6	
2	B	1	Total	C	N	O	P	0
			60	20	10	24	6	
2	B	1	Total	C	N	O	P	0
			60	20	10	24	6	
2	C	1	Total	C	N	O	P	0
			60	20	10	24	6	
2	C	1	Total	C	N	O	P	0
			60	20	10	24	6	
2	D	1	Total	C	N	O	P	0
			60	20	10	24	6	
2	D	1	Total	C	N	O	P	0
			60	20	10	24	6	
2	E	1	Total	C	N	O	P	0
			60	20	10	24	6	
2	E	1	Total	C	N	O	P	0
			60	20	10	24	6	
2	F	1	Total	C	N	O	P	0
			60	20	10	24	6	
2	F	1	Total	C	N	O	P	0
			60	20	10	24	6	

- Molecule 3 is 2-(TOLUENE-4-SULFONYL)-2H-BENZO[D][1,2,3]DIAZABORININ-1-OL (three-letter code: NDT) (formula: $C_{14}H_{13}BN_2O_3S$) (labeled as "Ligand of Interest" by depositor).



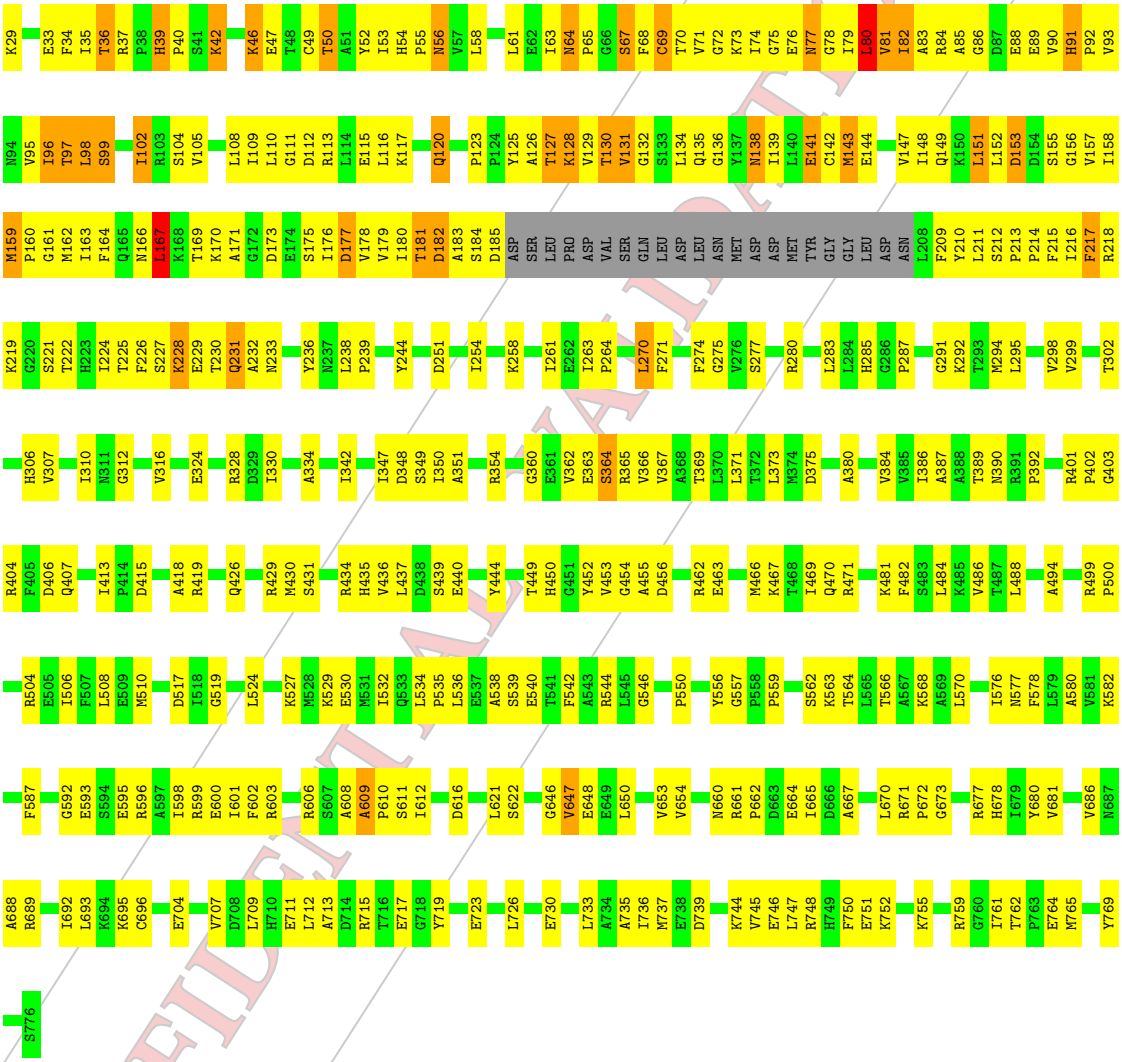
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	B	C	N	O	S	0
			42	2	28	4	6	2	
3	A	1	Total	B	C	N	O	S	0
			42	2	28	4	6	2	
3	B	1	Total	B	C	N	O	S	0
			42	2	28	4	6	2	
3	B	1	Total	B	C	N	O	S	0
			42	2	28	4	6	2	
3	C	1	Total	B	C	N	O	S	0
			42	2	28	4	6	2	
3	C	1	Total	B	C	N	O	S	0
			42	2	28	4	6	2	
3	D	1	Total	B	C	N	O	S	0
			42	2	28	4	6	2	
3	D	1	Total	B	C	N	O	S	0
			42	2	28	4	6	2	
3	E	1	Total	B	C	N	O	S	0
			42	2	28	4	6	2	
3	E	1	Total	B	C	N	O	S	0
			42	2	28	4	6	2	
3	F	1	Total	B	C	N	O	S	0
			42	2	28	4	6	2	
3	F	1	Total	B	C	N	O	S	0
			42	2	28	4	6	2	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

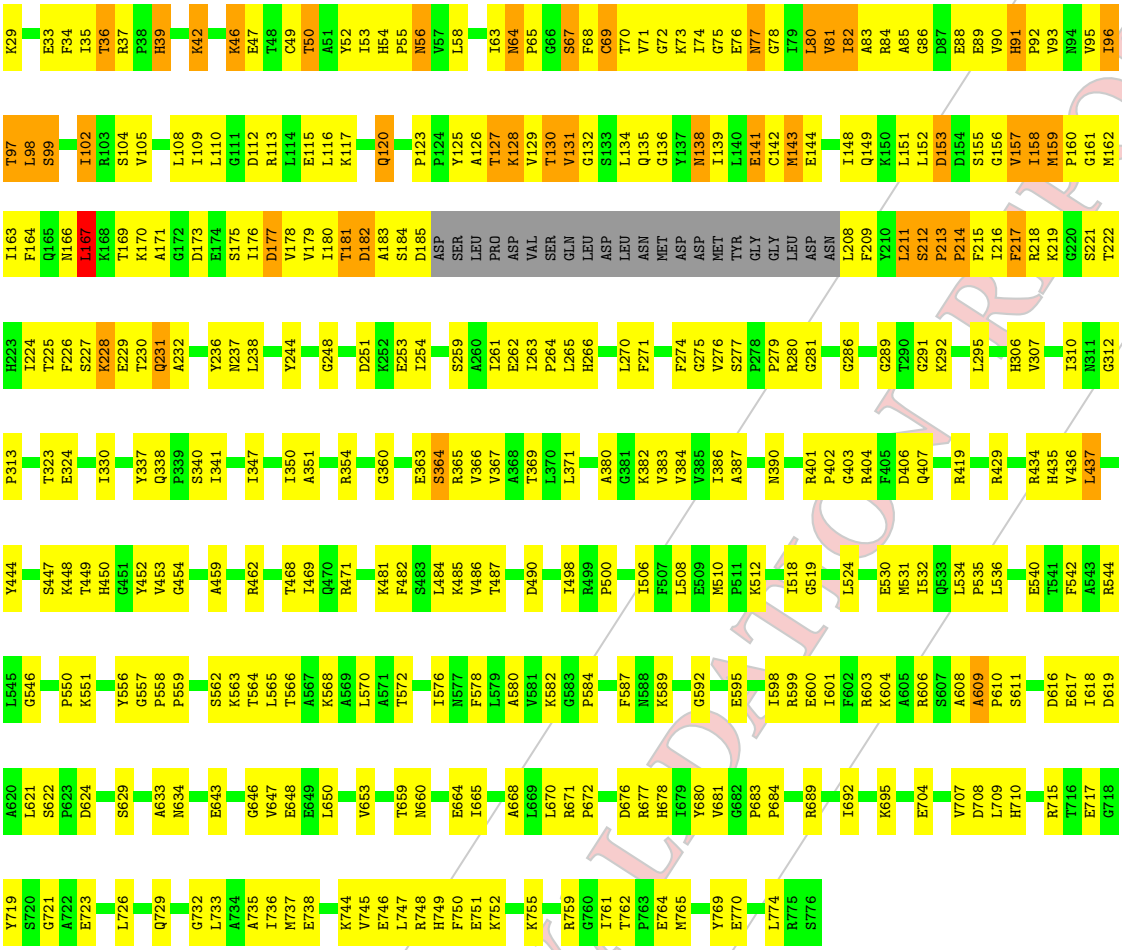
- Molecule 1: ATPase family gene 2 protein

Chain A:



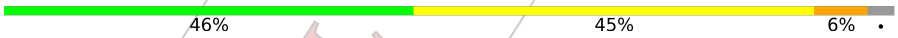
- Molecule 1: ATPase family gene 2 protein

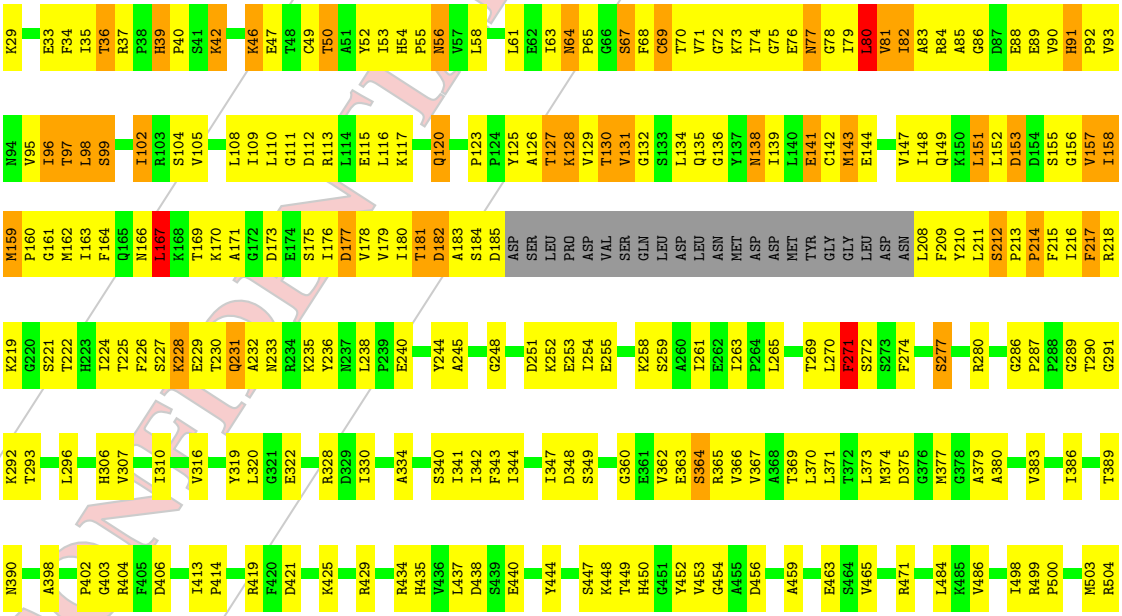
Chain B:

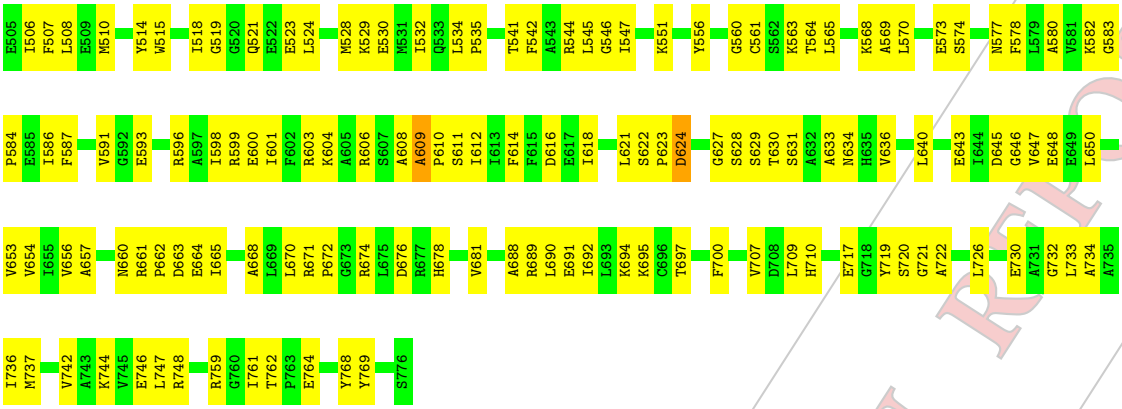


• Molecule 1: ATPase family gene 2 protein

Chain C:

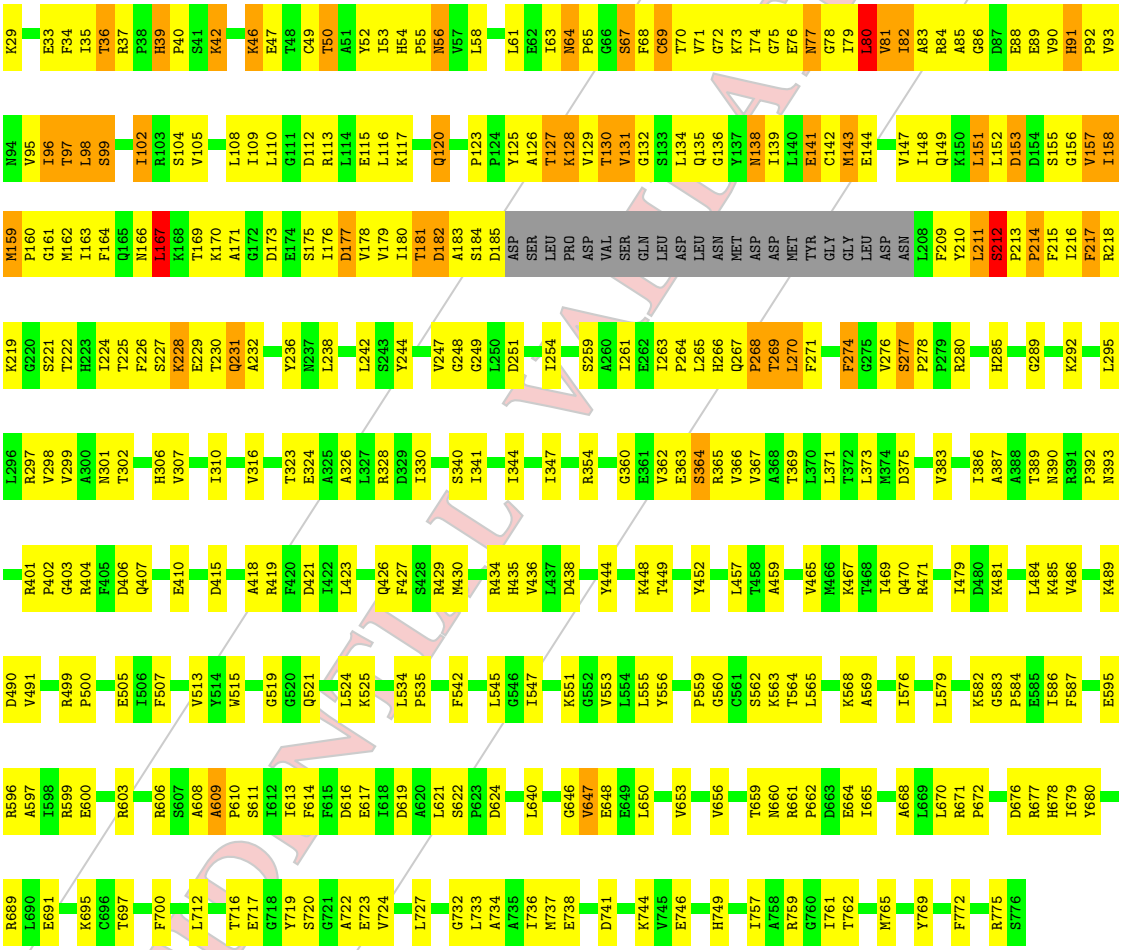






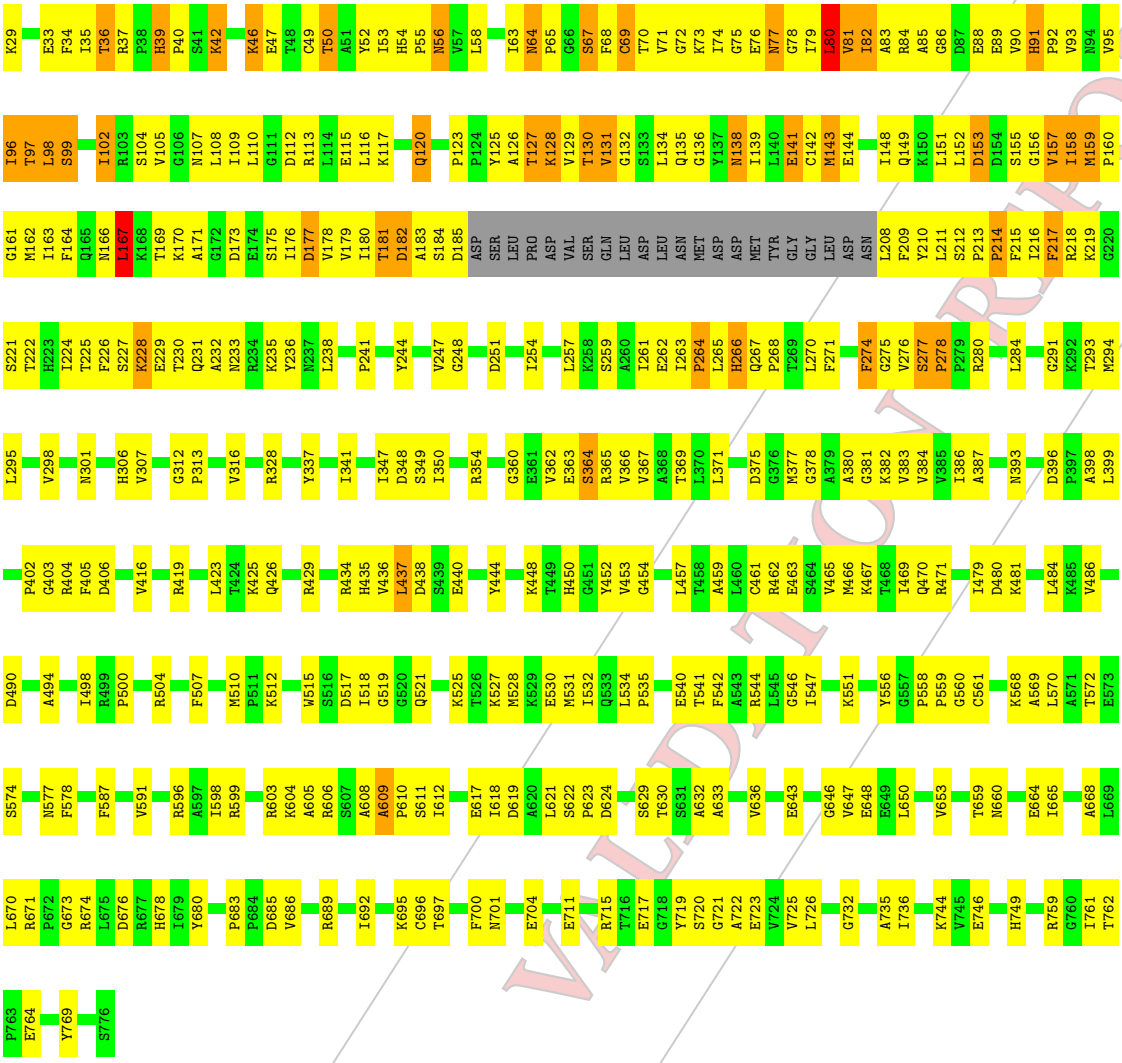
• Molecule 1: ATPase family gene 2 protein

Chain D:



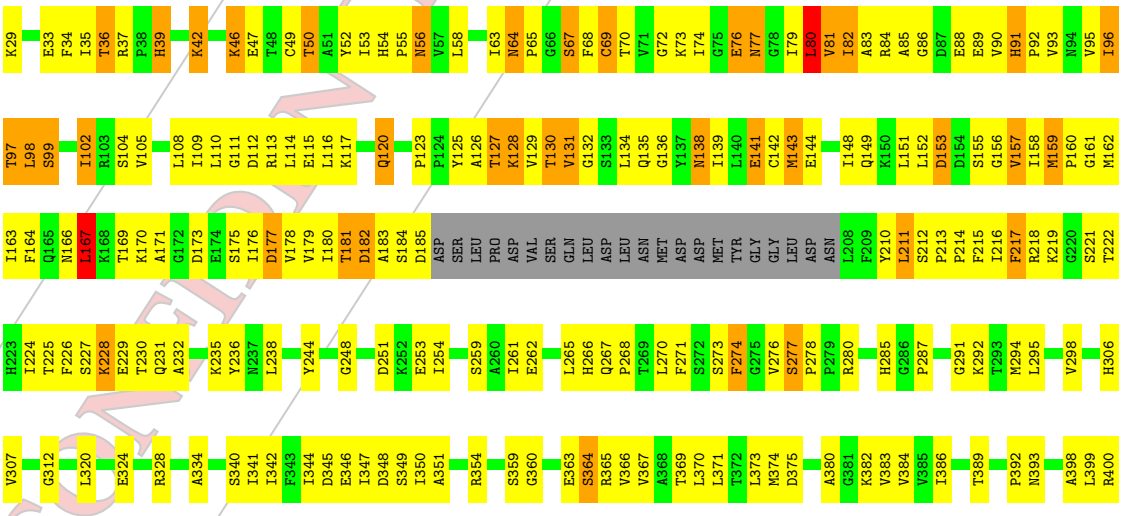
• Molecule 1: ATPase family gene 2 protein

Chain E:



• Molecule 1: ATPase family gene 2 protein

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	348781	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDT, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.32	0/5665	0.60	1/7669 (0.0%)
1	B	0.31	0/5668	0.59	1/7673 (0.0%)
1	C	0.31	0/5668	0.61	2/7673 (0.0%)
1	D	0.31	0/5668	0.61	4/7673 (0.1%)
1	E	0.30	0/5668	0.60	2/7673 (0.0%)
1	F	0.31	0/5668	0.61	1/7673 (0.0%)
All	All	0.31	0/34005	0.60	11/46034 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	268	PRO	N-CA-C	-6.35	95.60	112.10
1	E	624	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	624	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	438	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	624	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	80	LEU	CA-CB-CG	5.06	126.93	115.30
1	B	80	LEU	CA-CB-CG	5.05	126.93	115.30
1	E	80	LEU	CA-CB-CG	5.05	126.91	115.30
1	C	80	LEU	CA-CB-CG	5.05	126.91	115.30
1	F	80	LEU	CA-CB-CG	5.04	126.89	115.30
1	D	80	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5568	0	5647	685	0
1	B	5571	0	5648	712	0
1	C	5571	0	5643	685	0
1	D	5571	0	5645	656	0
1	E	5571	0	5641	662	0
1	F	5571	0	5639	703	0
2	A	60	0	20	50	0
2	B	60	0	20	45	0
2	C	60	0	20	45	0
2	D	60	0	18	38	0
2	E	60	0	20	44	0
2	F	60	0	20	45	0
3	A	42	0	24	38	0
3	B	42	0	24	56	0
3	C	42	0	24	31	0
3	D	42	0	24	48	0
3	E	42	0	21	29	0
3	F	42	0	24	25	0
All	All	34035	0	34122	4023	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

All (4023) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:ARG:CD	3:E:802:NDT:C21	1.77	1.60
1:B:721:GLY:HA3	2:B:803:ATP:C2	1.14	1.60
1:B:481:LYS:HD2	1:C:270:LEU:CD2	1.32	1.58
1:C:78:GLY:HA2	1:C:211:LEU:CG	1.31	1.57
1:F:429:ARG:NH1	3:F:802:NDT:C20	1.68	1.56
1:B:429:ARG:CZ	3:B:802:NDT:C17	1.79	1.53
1:A:159:MET:CE	1:A:182:ASP:HA	1.34	1.52
1:C:80:LEU:CD2	1:C:211:LEU:HD12	1.26	1.52
1:B:481:LYS:CD	1:C:270:LEU:CD2	1.84	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:LYS:CE	1:C:270:LEU:HD23	1.05	1.50
1:C:78:GLY:C	1:C:211:LEU:HD21	1.22	1.50
1:B:429:ARG:NH1	3:B:802:NDT:C16	1.70	1.50
1:F:160:PRO:HB3	1:F:238:LEU:CD1	1.41	1.47
1:E:429:ARG:HD2	3:E:802:NDT:C21	1.32	1.46
1:B:721:GLY:CA	2:B:803:ATP:C2	1.95	1.45
1:E:156:GLY:O	1:E:157:VAL:CG1	1.65	1.44
1:B:481:LYS:CE	1:C:270:LEU:CD2	1.87	1.44
1:D:125:TYR:CE2	1:D:218:ARG:HG3	1.53	1.43
1:D:142:CYS:SG	1:D:144:GLU:CG	2.07	1.43
1:D:142:CYS:SG	1:D:144:GLU:HG2	1.59	1.43
1:D:156:GLY:O	1:D:157:VAL:CG1	1.65	1.43
1:C:78:GLY:CA	1:C:211:LEU:CG	1.87	1.42
1:B:142:CYS:SG	1:B:144:GLU:CG	2.07	1.42
1:C:125:TYR:CE2	1:C:218:ARG:HG3	1.53	1.42
1:D:160:PRO:HB3	1:D:238:LEU:CD1	1.50	1.42
1:E:142:CYS:SG	1:E:144:GLU:HG2	1.59	1.42
1:A:211:LEU:CD2	1:A:238:LEU:HD22	1.48	1.42
1:A:142:CYS:SG	1:A:144:GLU:HG2	1.59	1.42
1:C:142:CYS:SG	1:C:144:GLU:CG	2.07	1.42
1:B:156:GLY:O	1:B:157:VAL:CG1	1.65	1.42
1:B:429:ARG:HD3	3:B:802:NDT:C21	1.47	1.42
3:A:802:NDT:H7	1:B:403:GLY:CA	1.46	1.41
1:F:142:CYS:SG	1:F:144:GLU:HG2	1.59	1.41
1:A:142:CYS:SG	1:A:144:GLU:CG	2.07	1.41
1:B:125:TYR:CE2	1:B:218:ARG:HG3	1.53	1.41
1:E:125:TYR:CE2	1:E:218:ARG:HG3	1.53	1.41
1:E:210:TYR:CE1	1:E:214:PRO:CD	2.00	1.41
1:A:125:TYR:CE2	1:A:218:ARG:HG3	1.53	1.41
1:C:156:GLY:O	1:C:157:VAL:CG1	1.65	1.41
1:F:125:TYR:CE2	1:F:218:ARG:HG3	1.53	1.41
1:C:142:CYS:SG	1:C:144:GLU:HG2	1.59	1.41
1:B:692:ILE:HD11	2:B:803:ATP:N6	1.37	1.40
1:C:160:PRO:HA	1:C:238:LEU:CD1	1.51	1.40
1:E:142:CYS:SG	1:E:144:GLU:CG	2.07	1.40
1:B:142:CYS:SG	1:B:144:GLU:HG2	1.59	1.40
1:F:142:CYS:SG	1:F:144:GLU:CG	2.07	1.40
1:F:166:ASN:ND2	1:F:169:THR:HG21	1.36	1.40
1:E:166:ASN:ND2	1:E:169:THR:HG21	1.36	1.39
1:B:159:MET:N	1:B:213:PRO:HB2	1.09	1.39
1:B:166:ASN:ND2	1:B:169:THR:HG21	1.36	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASN:ND2	1:A:169:THR:HG21	1.36	1.38
1:C:80:LEU:CD2	1:C:211:LEU:CD1	2.00	1.38
1:B:481:LYS:CD	1:C:270:LEU:CG	2.00	1.38
1:B:481:LYS:HD2	1:C:270:LEU:CG	1.50	1.37
1:C:78:GLY:N	1:C:211:LEU:CD2	1.81	1.37
1:D:166:ASN:ND2	1:D:169:THR:HG21	1.36	1.35
1:A:454:GLY:C	2:A:801:ATP:C8	1.98	1.35
3:E:802:NDT:H7	1:F:403:GLY:N	1.42	1.35
1:B:562:SER:HA	2:B:803:ATP:PA	1.65	1.34
1:C:166:ASN:ND2	1:C:169:THR:HG21	1.36	1.34
1:B:481:LYS:CD	1:C:270:LEU:HG	1.52	1.33
1:B:429:ARG:HD3	3:B:802:NDT:C18	1.55	1.33
1:E:210:TYR:CE1	1:E:214:PRO:HD3	1.03	1.32
1:A:294:MET:HE1	2:A:801:ATP:C2	1.65	1.31
1:C:80:LEU:HD23	1:C:211:LEU:CD1	1.59	1.31
1:B:218:ARG:CB	1:B:221:SER:OG	1.79	1.31
1:A:104:SER:OG	1:A:163:ILE:HD13	1.13	1.31
1:A:81:VAL:CG1	1:A:210:TYR:CE1	2.14	1.30
3:A:802:NDT:C7	1:B:403:GLY:HA2	1.59	1.30
1:B:429:ARG:NH1	3:B:802:NDT:C17	1.87	1.30
1:F:218:ARG:CB	1:F:221:SER:OG	1.79	1.30
1:A:39:HIS:HB3	1:A:97:THR:OG1	1.30	1.30
1:E:218:ARG:CB	1:E:221:SER:OG	1.79	1.30
1:C:160:PRO:CB	1:C:238:LEU:HD13	1.62	1.29
1:D:218:ARG:CB	1:D:221:SER:OG	1.79	1.29
1:A:218:ARG:CB	1:A:221:SER:OG	1.79	1.28
1:D:39:HIS:HB3	1:D:97:THR:OG1	1.29	1.28
1:A:81:VAL:CG1	1:A:210:TYR:HE1	1.47	1.28
1:A:159:MET:HE1	1:A:182:ASP:C	1.50	1.28
1:C:692:ILE:HD11	2:C:803:ATP:N6	1.45	1.28
1:D:429:ARG:NH1	3:D:802:NDT:C17	1.97	1.28
1:F:156:GLY:O	1:F:157:VAL:CG1	1.82	1.28
1:C:218:ARG:CB	1:C:221:SER:OG	1.79	1.28
1:A:104:SER:OG	1:A:163:ILE:CD1	1.82	1.27
1:D:98:LEU:O	1:D:102:ILE:HD13	1.10	1.27
3:E:804:NDT:H7	1:F:673:GLY:CA	1.61	1.27
1:B:98:LEU:O	1:B:102:ILE:HD13	1.10	1.27
1:B:104:SER:OG	1:B:163:ILE:CD1	1.82	1.27
1:C:104:SER:OG	1:C:163:ILE:CD1	1.82	1.27
1:D:104:SER:OG	1:D:163:ILE:HD13	1.13	1.27
1:F:160:PRO:CB	1:F:238:LEU:CD1	2.11	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:559:PRO:HG3	1:F:660:ASN:OD1	1.32	1.27
1:A:159:MET:HG2	1:A:236:TYR:CE1	1.70	1.27
1:B:104:SER:OG	1:B:163:ILE:HD13	1.13	1.27
1:D:429:ARG:HH22	3:D:802:NDT:C15	1.47	1.27
1:D:104:SER:OG	1:D:163:ILE:CD1	1.82	1.27
1:E:104:SER:OG	1:E:163:ILE:CD1	1.82	1.27
1:A:50:THR:OG1	1:A:84:ARG:HB2	1.35	1.26
1:A:454:GLY:O	2:A:801:ATP:C8	1.87	1.26
1:A:159:MET:CE	1:A:182:ASP:CA	2.13	1.26
1:C:104:SER:OG	1:C:163:ILE:HD13	1.13	1.26
1:C:78:GLY:N	1:C:211:LEU:HD21	1.40	1.26
1:C:160:PRO:CA	1:C:238:LEU:CD1	2.12	1.26
1:A:294:MET:CE	2:A:801:ATP:C2	2.16	1.26
1:F:104:SER:OG	1:F:163:ILE:CD1	1.82	1.26
1:A:211:LEU:HD21	1:A:238:LEU:CD2	1.66	1.26
1:D:50:THR:OG1	1:D:84:ARG:HB2	1.35	1.25
1:C:721:GLY:HA3	2:C:803:ATP:C2	1.71	1.25
1:F:104:SER:OG	1:F:163:ILE:HD13	1.13	1.25
1:A:160:PRO:CG	1:A:212:SER:OG	1.82	1.25
1:C:39:HIS:HB3	1:C:97:THR:OG1	1.30	1.25
1:A:562:SER:N	2:A:803:ATP:O1A	1.70	1.25
1:B:212:SER:CB	1:B:213:PRO:HD3	1.65	1.25
1:C:141:GLU:OE1	1:C:170:LYS:HE2	1.37	1.25
1:E:50:THR:OG1	1:E:84:ARG:HB2	1.35	1.25
1:D:268:PRO:O	1:D:269:THR:HG23	1.34	1.25
1:A:98:LEU:O	1:A:102:ILE:HD13	1.10	1.25
1:B:77:ASN:ND2	1:B:209:PHE:O	1.70	1.24
1:B:159:MET:N	1:B:213:PRO:CB	1.99	1.24
1:F:39:HIS:HB3	1:F:97:THR:OG1	1.29	1.24
1:B:39:HIS:HB3	1:B:97:THR:OG1	1.29	1.24
1:A:141:GLU:OE1	1:A:170:LYS:HE2	1.37	1.24
1:E:98:LEU:O	1:E:102:ILE:HD13	1.10	1.24
1:A:159:MET:HG3	1:A:236:TYR:CZ	1.73	1.24
1:A:159:MET:CG	1:A:236:TYR:CE1	2.20	1.24
1:C:429:ARG:HD3	3:C:802:NDT:C21	1.67	1.24
1:D:429:ARG:CZ	3:D:802:NDT:C17	2.16	1.24
1:E:39:HIS:HB3	1:E:97:THR:OG1	1.30	1.24
1:F:98:LEU:O	1:F:102:ILE:HD13	1.10	1.24
1:C:127:THR:O	1:C:184:SER:HB3	1.38	1.23
1:D:160:PRO:CB	1:D:238:LEU:CD1	2.16	1.23
1:E:104:SER:OG	1:E:163:ILE:HD13	1.13	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:ILE:HG22	1:F:212:SER:OG	1.39	1.23
1:B:218:ARG:HB2	1:B:221:SER:CB	1.69	1.23
1:C:98:LEU:O	1:C:102:ILE:HD13	1.10	1.23
1:C:125:TYR:CE2	1:C:218:ARG:CG	2.22	1.23
1:C:218:ARG:HB2	1:C:221:SER:CB	1.69	1.23
1:D:141:GLU:OE1	1:D:170:LYS:HE2	1.37	1.23
1:F:218:ARG:HB2	1:F:221:SER:CB	1.69	1.23
1:A:218:ARG:HB2	1:A:221:SER:CB	1.69	1.23
1:B:159:MET:H	1:B:213:PRO:CB	1.52	1.23
1:E:218:ARG:HB2	1:E:221:SER:CB	1.69	1.23
1:B:429:ARG:NH1	3:B:802:NDT:C15	2.00	1.22
1:B:562:SER:N	2:B:803:ATP:O1A	1.72	1.22
1:C:160:PRO:CA	1:C:238:LEU:HD11	1.67	1.22
1:D:125:TYR:CE2	1:D:218:ARG:CG	2.22	1.22
1:F:50:THR:OG1	1:F:84:ARG:HB2	1.35	1.22
1:F:141:GLU:OE1	1:F:170:LYS:HE2	1.37	1.22
1:B:429:ARG:CD	3:B:802:NDT:H213	1.70	1.21
1:E:77:ASN:O	1:E:211:LEU:CD2	1.88	1.21
1:E:125:TYR:CE2	1:E:218:ARG:CG	2.22	1.21
1:F:125:TYR:CE2	1:F:218:ARG:CG	2.22	1.21
1:A:125:TYR:CE2	1:A:218:ARG:CG	2.22	1.21
1:A:562:SER:HA	2:A:803:ATP:PA	1.79	1.21
1:B:125:TYR:CE2	1:B:218:ARG:CG	2.22	1.21
1:A:127:THR:O	1:A:184:SER:HB3	1.38	1.21
1:C:50:THR:OG1	1:C:84:ARG:HB2	1.35	1.21
1:D:218:ARG:HB2	1:D:221:SER:CB	1.69	1.21
1:F:158:ILE:CG2	1:F:212:SER:OG	1.87	1.20
1:D:160:PRO:CB	1:D:238:LEU:HD13	1.71	1.20
1:B:50:THR:OG1	1:B:84:ARG:HB2	1.35	1.20
1:B:141:GLU:OE1	1:B:170:LYS:HE2	1.36	1.20
1:D:429:ARG:HH22	3:D:802:NDT:C16	1.55	1.20
1:F:127:THR:O	1:F:184:SER:HB3	1.38	1.19
1:B:212:SER:HB2	1:B:213:PRO:CD	1.71	1.19
1:C:160:PRO:CB	1:C:238:LEU:CD1	2.19	1.19
1:E:141:GLU:OE1	1:E:170:LYS:HE2	1.37	1.19
1:F:77:ASN:O	1:F:211:LEU:HD21	1.42	1.19
1:A:673:GLY:CA	3:F:804:NDT:H7	1.73	1.19
1:F:126:ALA:O	1:F:222:THR:HB	1.42	1.19
1:A:211:LEU:CD2	1:A:238:LEU:CD2	2.19	1.18
1:E:127:THR:O	1:E:184:SER:HB3	1.38	1.18
1:B:127:THR:O	1:B:184:SER:HB3	1.38	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:MET:CG	1:A:236:TYR:CZ	2.26	1.18
1:A:158:ILE:HD13	1:A:212:SER:HB2	1.23	1.18
1:A:562:SER:HA	2:A:803:ATP:O2A	1.43	1.18
1:B:721:GLY:HA3	2:B:803:ATP:N3	1.59	1.18
1:D:127:THR:O	1:D:184:SER:HB3	1.38	1.18
1:D:562:SER:HB3	2:D:803:ATP:C2	1.79	1.18
1:A:126:ALA:O	1:A:222:THR:HB	1.42	1.17
1:E:73:LYS:HE3	1:E:112:ASP:OD2	1.44	1.17
1:B:126:ALA:O	1:B:222:THR:HB	1.42	1.17
1:E:126:ALA:O	1:E:222:THR:HB	1.42	1.17
1:B:429:ARG:CD	3:B:802:NDT:C21	2.19	1.17
1:E:159:MET:CG	1:E:236:TYR:CE1	2.18	1.17
1:F:262:GLU:OE1	1:F:266:HIS:CE1	1.98	1.17
1:E:37:ARG:HH11	1:E:306:HIS:CD2	1.60	1.17
1:C:35:ILE:HD12	1:C:113:ARG:NH1	1.60	1.16
1:D:465:VAL:HG12	1:E:271:PHE:CE1	1.79	1.16
1:B:53:ILE:O	1:B:86:GLY:HA3	1.45	1.16
3:C:802:NDT:H7	1:D:403:GLY:HA2	1.25	1.16
1:D:53:ILE:O	1:D:86:GLY:HA3	1.45	1.16
1:F:72:GLY:N	1:F:115:GLU:O	1.79	1.16
1:A:35:ILE:HD12	1:A:113:ARG:NH1	1.60	1.16
1:B:35:ILE:HD12	1:B:113:ARG:NH1	1.59	1.16
1:C:126:ALA:O	1:C:222:THR:HB	1.42	1.16
1:D:35:ILE:HD12	1:D:113:ARG:NH1	1.59	1.16
1:D:77:ASN:HD21	1:D:209:PHE:C	1.49	1.16
1:D:126:ALA:O	1:D:222:THR:HB	1.42	1.16
1:C:78:GLY:CA	1:C:211:LEU:CD1	2.25	1.15
1:E:160:PRO:HG3	1:E:238:LEU:HD11	1.21	1.15
1:A:73:LYS:HE3	1:A:112:ASP:OD2	1.44	1.15
1:B:77:ASN:OD1	1:B:209:PHE:CD1	1.99	1.15
1:C:53:ILE:O	1:C:86:GLY:HA3	1.45	1.15
1:D:563:LYS:HE3	2:D:803:ATP:O3G	1.45	1.15
1:C:160:PRO:HB3	1:C:238:LEU:CD1	1.73	1.15
1:A:462:ARG:NH1	1:B:277:SER:O	1.80	1.15
1:A:673:GLY:HA3	3:F:804:NDT:H7	1.19	1.15
1:E:159:MET:HG2	1:E:236:TYR:CE1	1.75	1.15
1:F:35:ILE:HD12	1:F:113:ARG:NH1	1.59	1.15
1:D:73:LYS:HE3	1:D:112:ASP:OD2	1.44	1.15
1:E:160:PRO:HB3	1:E:238:LEU:CD1	1.77	1.15
3:D:802:NDT:H7	1:E:403:GLY:HA2	1.19	1.14
1:F:160:PRO:CD	1:F:212:SER:OG	1.95	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LYS:HE3	1:B:112:ASP:OD2	1.44	1.14
1:C:73:LYS:HE3	1:C:112:ASP:OD2	1.44	1.14
1:E:35:ILE:HD12	1:E:113:ARG:NH1	1.60	1.14
1:E:469:ILE:HD12	1:F:270:LEU:HD21	1.27	1.14
1:B:692:ILE:HD11	2:B:803:ATP:C6	1.82	1.14
1:E:293:THR:OG1	2:E:801:ATP:O1B	1.61	1.14
1:F:563:LYS:HB2	2:F:803:ATP:O2B	1.47	1.14
1:A:81:VAL:HG12	1:A:210:TYR:CE1	1.80	1.14
1:D:271:PHE:HE2	1:D:278:PRO:CA	1.61	1.14
1:B:157:VAL:CG1	1:B:215:PHE:O	1.95	1.13
1:B:280:ARG:NH1	1:B:383:VAL:H	1.46	1.13
1:A:158:ILE:HD13	1:A:212:SER:CB	1.76	1.13
1:C:563:LYS:HG3	2:C:803:ATP:O3G	1.48	1.13
3:E:802:NDT:H7	1:F:403:GLY:CA	1.78	1.13
1:E:210:TYR:HE1	1:E:213:PRO:HA	1.14	1.13
3:B:802:NDT:C7	1:C:403:GLY:HA2	1.78	1.13
1:D:218:ARG:HB2	1:D:221:SER:OG	0.95	1.13
1:F:53:ILE:O	1:F:86:GLY:HA3	1.45	1.13
1:A:53:ILE:O	1:A:86:GLY:HA3	1.45	1.13
1:A:218:ARG:HB2	1:A:221:SER:OG	0.95	1.12
1:B:562:SER:CA	2:B:803:ATP:O1A	1.96	1.13
1:B:565:LEU:HD11	3:B:804:NDT:O2	1.47	1.12
1:C:78:GLY:HA2	1:C:211:LEU:HD23	1.13	1.12
1:A:98:LEU:O	1:A:102:ILE:CD1	1.97	1.12
1:C:160:PRO:HA	1:C:238:LEU:HD11	1.17	1.12
1:E:53:ILE:O	1:E:86:GLY:HA3	1.45	1.12
1:C:563:LYS:HE3	2:C:803:ATP:O1G	1.46	1.12
1:D:98:LEU:O	1:D:102:ILE:CD1	1.97	1.12
1:D:242:LEU:CD1	1:D:297:ARG:CG	2.27	1.12
1:D:242:LEU:HD11	1:D:297:ARG:CG	1.79	1.12
1:E:519:GLY:H	2:E:803:ATP:N6	1.47	1.12
1:C:77:ASN:O	1:C:211:LEU:HD23	1.46	1.12
1:A:159:MET:SD	1:A:182:ASP:CG	2.28	1.11
1:B:98:LEU:O	1:B:102:ILE:CD1	1.97	1.11
1:B:158:ILE:HB	1:B:213:PRO:HG2	1.32	1.11
1:E:98:LEU:O	1:E:102:ILE:CD1	1.97	1.11
1:E:561:CYS:SG	2:E:803:ATP:C2	2.43	1.11
1:E:218:ARG:HB2	1:E:221:SER:OG	0.95	1.11
1:F:160:PRO:CB	1:F:238:LEU:HD13	1.75	1.11
1:F:218:ARG:HB2	1:F:221:SER:OG	0.95	1.11
1:A:159:MET:N	1:A:160:PRO:CD	2.06	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:GLY:C	2:A:801:ATP:H8	1.41	1.11
1:B:218:ARG:HB2	1:B:221:SER:OG	0.95	1.11
1:B:469:ILE:CD1	1:C:270:LEU:HD11	1.79	1.11
1:B:695:LYS:NZ	3:B:804:NDT:C16	2.13	1.11
1:D:35:ILE:HD12	1:D:113:ARG:HH12	0.95	1.11
1:F:98:LEU:O	1:F:102:ILE:CD1	1.97	1.11
1:F:519:GLY:CA	2:F:803:ATP:HN62	1.63	1.11
1:A:159:MET:HB2	1:A:213:PRO:HG2	1.19	1.11
1:C:218:ARG:HB2	1:C:221:SER:OG	0.95	1.11
3:B:802:NDT:H7	1:C:403:GLY:CA	1.81	1.10
1:C:98:LEU:O	1:C:102:ILE:CD1	1.97	1.10
1:D:271:PHE:CE2	1:D:278:PRO:CA	2.33	1.10
1:E:35:ILE:HD12	1:E:113:ARG:HH12	0.95	1.10
1:E:469:ILE:CD1	1:F:270:LEU:HD21	1.82	1.10
1:F:158:ILE:HG22	1:F:160:PRO:HD2	1.21	1.10
1:F:160:PRO:HD2	1:F:212:SER:OG	1.51	1.10
1:A:209:PHE:CD2	1:A:210:TYR:CE2	2.39	1.10
1:B:429:ARG:CD	3:B:802:NDT:C18	2.30	1.10
1:C:79:ILE:H	1:C:211:LEU:HG	1.14	1.10
1:F:77:ASN:O	1:F:211:LEU:CD2	1.95	1.10
1:A:78:GLY:HA2	1:A:211:LEU:HB2	1.19	1.10
1:A:159:MET:SD	1:A:183:ALA:N	2.23	1.10
1:C:78:GLY:HA3	1:C:211:LEU:CD2	1.65	1.10
1:E:77:ASN:O	1:E:211:LEU:HD23	1.50	1.10
1:C:77:ASN:C	1:C:211:LEU:CD2	2.20	1.10
1:C:695:LYS:HZ1	3:C:804:NDT:C18	1.62	1.10
1:A:403:GLY:HA2	3:F:802:NDT:H7	1.25	1.10
1:F:35:ILE:HD12	1:F:113:ARG:HH12	0.95	1.10
1:F:70:THR:O	1:F:79:ILE:HD12	1.52	1.10
1:A:403:GLY:CA	3:F:802:NDT:H7	1.82	1.09
1:C:233:ASN:HD21	1:C:235:LYS:HE2	1.06	1.09
1:E:160:PRO:CG	1:E:238:LEU:HD11	1.81	1.09
1:A:53:ILE:H	1:A:86:GLY:CA	1.65	1.09
1:B:50:THR:HA	1:B:83:ALA:O	1.52	1.09
1:A:159:MET:HE2	1:A:182:ASP:HA	1.09	1.09
1:B:149:GLN:HE21	1:B:219:LYS:NZ	1.51	1.09
1:B:159:MET:HB3	1:B:213:PRO:HB3	1.35	1.09
1:E:50:THR:HA	1:E:83:ALA:O	1.52	1.09
1:C:53:ILE:H	1:C:86:GLY:CA	1.65	1.09
1:E:561:CYS:SG	2:E:803:ATP:H2	1.74	1.09
1:E:53:ILE:H	1:E:86:GLY:CA	1.65	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:PRO:HB3	1:E:238:LEU:HD12	1.33	1.08
1:F:429:ARG:NH1	3:F:802:NDT:C19	2.15	1.08
1:A:181:THR:HG22	1:A:232:ALA:HA	1.35	1.08
1:A:159:MET:CG	1:A:236:TYR:OH	2.02	1.08
1:C:79:ILE:N	1:C:211:LEU:HG	1.66	1.08
1:C:80:LEU:HD22	1:C:211:LEU:HD12	1.14	1.08
1:C:149:GLN:HE21	1:C:219:LYS:NZ	1.51	1.08
1:D:50:THR:HA	1:D:83:ALA:O	1.53	1.08
1:F:181:THR:HG22	1:F:232:ALA:HA	1.35	1.08
1:D:53:ILE:H	1:D:86:GLY:CA	1.65	1.08
1:D:271:PHE:HE2	1:D:278:PRO:N	1.51	1.08
1:E:722:ALA:HB2	2:E:803:ATP:H5'1	1.31	1.08
1:E:149:GLN:HE21	1:E:219:LYS:NZ	1.51	1.08
1:E:293:THR:CB	2:E:801:ATP:O1B	2.02	1.08
1:E:429:ARG:HD3	3:E:802:NDT:C21	1.71	1.08
1:B:35:ILE:HD12	1:B:113:ARG:HH12	0.95	1.07
1:B:53:ILE:H	1:B:86:GLY:CA	1.65	1.07
1:C:125:TYR:CD2	1:C:218:ARG:HG3	1.90	1.07
1:F:50:THR:HA	1:F:83:ALA:O	1.52	1.07
1:F:156:GLY:O	1:F:157:VAL:HG12	0.92	1.07
1:A:105:VAL:HG21	1:A:157:VAL:CG2	1.82	1.07
1:B:481:LYS:HD3	1:C:270:LEU:HG	1.16	1.07
1:B:565:LEU:CD1	3:B:804:NDT:O2	2.03	1.07
1:E:181:THR:HG22	1:E:232:ALA:HA	1.35	1.07
1:B:125:TYR:CD2	1:B:218:ARG:HG3	1.90	1.07
1:C:50:THR:HA	1:C:83:ALA:O	1.52	1.07
3:E:804:NDT:H7	1:F:673:GLY:HA2	1.23	1.07
1:F:53:ILE:H	1:F:86:GLY:CA	1.65	1.07
1:F:149:GLN:HE21	1:F:219:LYS:NZ	1.51	1.07
1:F:160:PRO:CG	1:F:238:LEU:HD11	1.84	1.07
1:A:562:SER:CA	2:A:803:ATP:O1A	2.03	1.07
1:D:149:GLN:HE21	1:D:219:LYS:NZ	1.51	1.07
1:D:481:LYS:HE2	1:E:270:LEU:HD11	1.31	1.07
3:E:802:NDT:C8	1:F:403:GLY:HA2	1.83	1.07
1:C:181:THR:HG22	1:C:232:ALA:HA	1.35	1.06
1:A:35:ILE:HD12	1:A:113:ARG:HH12	0.95	1.06
1:E:434:ARG:HD2	1:F:273:SER:HB3	1.37	1.06
1:A:159:MET:HE1	1:A:182:ASP:CA	1.81	1.06
1:D:102:ILE:H	1:D:102:ILE:HD12	1.21	1.06
1:F:125:TYR:CD2	1:F:218:ARG:HG3	1.90	1.06
1:A:81:VAL:HG12	1:A:210:TYR:HE1	0.93	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:H	1:A:102:ILE:HD12	1.21	1.06
1:A:149:GLN:HE21	1:A:219:LYS:NZ	1.51	1.06
1:A:519:GLY:H	2:A:803:ATP:N6	1.50	1.06
1:A:58:LEU:CD2	1:A:85:ALA:HB1	1.86	1.06
1:A:429:ARG:NH1	3:A:802:NDT:C16	2.18	1.06
1:D:125:TYR:CD2	1:D:218:ARG:HG3	1.90	1.06
1:A:50:THR:HA	1:A:83:ALA:O	1.52	1.05
1:C:564:THR:HB	2:C:803:ATP:O2A	1.57	1.05
1:A:128:LYS:HG2	1:A:184:SER:CB	1.86	1.05
1:A:159:MET:CB	1:A:213:PRO:HG2	1.84	1.05
1:A:166:ASN:OD1	1:A:169:THR:HG22	1.56	1.05
1:C:429:ARG:HD3	3:C:802:NDT:H212	1.34	1.05
1:D:181:THR:HG22	1:D:232:ALA:HA	1.35	1.05
1:E:125:TYR:CD2	1:E:218:ARG:HG3	1.90	1.05
1:F:73:LYS:HD2	1:F:114:LEU:CD2	1.86	1.05
1:A:125:TYR:CD2	1:A:218:ARG:HG3	1.90	1.05
1:A:159:MET:HE1	1:A:183:ALA:N	1.71	1.05
1:C:35:ILE:HD12	1:C:113:ARG:HH12	0.95	1.05
1:C:80:LEU:HD23	1:C:211:LEU:HD12	1.09	1.05
1:C:166:ASN:CG	1:C:169:THR:HG21	1.76	1.05
1:F:128:LYS:HG2	1:F:184:SER:CB	1.86	1.05
1:B:166:ASN:OD1	1:B:169:THR:HG22	1.57	1.05
1:C:692:ILE:CD1	2:C:803:ATP:N6	2.20	1.05
1:D:128:LYS:HG2	1:D:184:SER:CB	1.86	1.05
1:D:166:ASN:CG	1:D:169:THR:HG21	1.76	1.05
1:D:429:ARG:NH2	3:D:802:NDT:C16	2.20	1.05
1:F:160:PRO:HG3	1:F:238:LEU:HD11	1.35	1.05
1:B:128:LYS:HG2	1:B:184:SER:CB	1.86	1.05
1:B:181:THR:HG22	1:B:232:ALA:HA	1.35	1.05
1:D:58:LEU:CD2	1:D:85:ALA:HB1	1.86	1.05
1:D:242:LEU:HD12	1:D:297:ARG:HG3	1.32	1.05
1:B:263:ILE:HG23	1:B:264:PRO:HD3	1.37	1.04
1:D:465:VAL:CG1	1:E:271:PHE:CE1	2.39	1.04
1:E:102:ILE:H	1:E:102:ILE:HD12	1.21	1.04
1:E:166:ASN:OD1	1:E:169:THR:HG22	1.57	1.04
1:B:166:ASN:CG	1:B:169:THR:HG21	1.76	1.04
1:C:128:LYS:HG2	1:C:184:SER:CB	1.86	1.04
1:F:35:ILE:CD1	1:F:113:ARG:HH12	1.70	1.04
1:F:166:ASN:OD1	1:F:169:THR:HG22	1.57	1.04
1:A:455:ALA:N	2:A:801:ATP:H8	1.55	1.04
1:B:58:LEU:CD2	1:B:85:ALA:HB1	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:LEU:CD1	1:D:297:ARG:HG3	1.87	1.04
1:D:242:LEU:H	1:D:301:ASN:ND2	1.55	1.04
1:E:58:LEU:CD2	1:E:85:ALA:HB1	1.86	1.04
1:E:128:LYS:HG2	1:E:184:SER:CB	1.86	1.04
1:E:166:ASN:CG	1:E:169:THR:HG21	1.76	1.04
1:F:58:LEU:CD2	1:F:85:ALA:HB1	1.86	1.04
1:F:166:ASN:CG	1:F:169:THR:CG2	2.26	1.04
1:A:166:ASN:CG	1:A:169:THR:HG21	1.76	1.04
1:C:58:LEU:CD2	1:C:85:ALA:HB1	1.86	1.04
1:C:102:ILE:HD12	1:C:102:ILE:H	1.21	1.04
1:C:166:ASN:OD1	1:C:169:THR:HG22	1.57	1.04
3:A:802:NDT:H7	1:B:403:GLY:N	1.73	1.04
1:B:166:ASN:CG	1:B:169:THR:CG2	2.26	1.04
1:D:166:ASN:CG	1:D:169:THR:CG2	2.26	1.04
1:E:35:ILE:CD1	1:E:113:ARG:HH12	1.71	1.04
1:F:166:ASN:CG	1:F:169:THR:HG21	1.76	1.04
1:B:721:GLY:CA	2:B:803:ATP:H2	1.49	1.03
1:D:242:LEU:HD11	1:D:297:ARG:HG2	1.30	1.03
1:F:102:ILE:HD12	1:F:102:ILE:H	1.21	1.03
1:A:270:LEU:CD2	1:F:481:LYS:HD3	1.88	1.03
1:B:35:ILE:CD1	1:B:113:ARG:HH12	1.71	1.03
1:B:481:LYS:HD2	1:C:270:LEU:HD21	1.07	1.03
1:E:166:ASN:CG	1:E:169:THR:CG2	2.26	1.03
1:F:73:LYS:CB	1:F:114:LEU:HD23	1.88	1.03
1:A:35:ILE:CD1	1:A:113:ARG:HH12	1.71	1.03
1:C:35:ILE:CD1	1:C:113:ARG:HH12	1.71	1.03
1:C:142:CYS:SG	1:C:144:GLU:HG3	1.98	1.03
1:F:559:PRO:HG3	1:F:660:ASN:CG	1.76	1.03
1:F:624:ASP:CB	1:F:629:SER:HB2	1.89	1.03
1:A:166:ASN:CG	1:A:169:THR:CG2	2.26	1.03
1:B:481:LYS:HE2	1:C:270:LEU:HD23	1.06	1.03
1:C:160:PRO:HG3	1:C:238:LEU:HD21	1.34	1.03
1:E:39:HIS:NE2	1:E:99:SER:HB2	1.74	1.03
1:E:159:MET:HG2	1:E:236:TYR:CD1	1.92	1.03
1:F:39:HIS:NE2	1:F:99:SER:HB2	1.74	1.03
1:C:166:ASN:CG	1:C:169:THR:CG2	2.26	1.03
1:D:35:ILE:CD1	1:D:113:ARG:HH12	1.70	1.03
1:E:291:GLY:HA2	2:E:801:ATP:O1A	1.51	1.03
1:A:39:HIS:NE2	1:A:99:SER:HB2	1.74	1.02
1:B:166:ASN:ND2	1:B:169:THR:CG2	2.22	1.02
1:E:77:ASN:C	1:E:211:LEU:HD21	1.78	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:692:ILE:HD11	2:E:803:ATP:C5	1.94	1.02
1:F:160:PRO:CB	1:F:238:LEU:HD11	1.85	1.02
1:A:160:PRO:HG2	1:A:212:SER:OG	0.97	1.02
1:C:166:ASN:ND2	1:C:169:THR:CG2	2.22	1.02
1:D:142:CYS:SG	1:D:144:GLU:HG3	1.98	1.02
1:D:166:ASN:OD1	1:D:169:THR:HG22	1.57	1.02
1:F:142:CYS:SG	1:F:144:GLU:HG3	1.98	1.02
1:A:426:GLN:NE2	3:A:802:NDT:H19	1.74	1.02
1:D:50:THR:OG1	1:D:84:ARG:CB	2.08	1.02
1:D:166:ASN:ND2	1:D:169:THR:CG2	2.22	1.02
1:C:78:GLY:C	1:C:211:LEU:HD11	1.79	1.02
1:E:50:THR:OG1	1:E:84:ARG:CB	2.08	1.02
1:E:166:ASN:ND2	1:E:169:THR:CG2	2.22	1.02
1:A:426:GLN:HE22	3:A:802:NDT:C19	1.72	1.01
1:B:39:HIS:NE2	1:B:99:SER:HB2	1.74	1.01
1:B:429:ARG:CZ	3:B:802:NDT:C16	2.25	1.01
1:E:37:ARG:NH1	1:E:306:HIS:CD2	2.27	1.01
1:A:105:VAL:CG2	1:A:157:VAL:HG22	1.89	1.01
1:A:166:ASN:ND2	1:A:169:THR:CG2	2.22	1.01
1:B:692:ILE:CD1	2:B:803:ATP:C6	2.41	1.01
1:C:79:ILE:N	1:C:211:LEU:CG	2.23	1.01
1:D:39:HIS:NE2	1:D:99:SER:HB2	1.74	1.01
1:D:160:PRO:HG3	1:D:238:LEU:HD11	1.39	1.01
1:D:271:PHE:CE2	1:D:278:PRO:HA	1.92	1.01
1:D:429:ARG:NH2	3:D:802:NDT:C15	2.22	1.01
1:A:50:THR:OG1	1:A:84:ARG:CB	2.08	1.01
1:B:102:ILE:H	1:B:102:ILE:HD12	1.21	1.01
1:A:105:VAL:HG21	1:A:157:VAL:HG22	1.02	1.01
1:B:50:THR:OG1	1:B:84:ARG:CB	2.08	1.01
1:C:39:HIS:NE2	1:C:99:SER:HB2	1.74	1.01
1:C:50:THR:OG1	1:C:84:ARG:CB	2.08	1.01
1:F:50:THR:OG1	1:F:84:ARG:CB	2.08	1.01
1:F:73:LYS:HB3	1:F:114:LEU:HD23	1.01	1.01
1:B:469:ILE:HD12	1:C:270:LEU:CD1	1.89	1.00
1:E:268:PRO:HG3	1:E:382:LYS:CE	1.90	1.00
1:E:465:VAL:HG22	1:F:274:PHE:HD2	1.24	1.00
3:E:802:NDT:C7	1:F:403:GLY:CA	2.39	1.00
1:D:268:PRO:O	1:D:269:THR:CG2	2.09	1.00
1:E:80:LEU:HD23	1:E:211:LEU:HD12	1.41	1.00
1:F:73:LYS:HB3	1:F:114:LEU:CD2	1.91	1.00
1:B:429:ARG:CG	3:B:802:NDT:H213	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:ASN:ND2	1:F:169:THR:CG2	2.22	1.00
3:B:802:NDT:H7	1:C:403:GLY:HA2	1.00	1.00
1:A:519:GLY:N	2:A:803:ATP:N6	2.10	1.00
1:C:429:ARG:HD3	3:C:802:NDT:C18	1.92	1.00
1:E:210:TYR:CE1	1:E:213:PRO:HA	1.97	1.00
1:D:159:MET:HG2	1:D:236:TYR:CE1	1.96	1.00
1:E:77:ASN:ND2	1:E:209:PHE:O	1.95	0.99
1:F:163:ILE:H	1:F:163:ILE:HD12	1.26	0.99
1:A:141:GLU:OE1	1:A:170:LYS:CE	2.11	0.99
1:A:159:MET:HA	1:A:159:MET:HE3	1.40	0.99
1:E:141:GLU:OE1	1:E:170:LYS:CE	2.11	0.99
1:F:262:GLU:OE1	1:F:266:HIS:ND1	1.93	0.99
1:A:149:GLN:HE21	1:A:219:LYS:HZ1	1.09	0.99
1:E:692:ILE:HD13	2:E:803:ATP:C6	1.97	0.99
1:A:142:CYS:SG	1:A:144:GLU:HG3	1.98	0.99
1:D:104:SER:HG	1:D:163:ILE:CD1	1.65	0.99
1:F:128:LYS:N	1:F:222:THR:OG1	1.96	0.99
1:B:163:ILE:HD12	1:B:163:ILE:H	1.26	0.99
1:C:78:GLY:HA3	1:C:211:LEU:CD1	1.88	0.99
1:D:39:HIS:CB	1:D:97:THR:OG1	2.11	0.99
1:E:37:ARG:HD3	1:E:337:TYR:CE2	1.98	0.99
1:F:141:GLU:OE1	1:F:170:LYS:CE	2.11	0.99
1:B:142:CYS:SG	1:B:144:GLU:HG3	1.98	0.99
1:B:481:LYS:HE3	1:C:270:LEU:HD23	1.03	0.99
1:A:158:ILE:CD1	1:A:212:SER:HB2	1.65	0.98
1:A:159:MET:CE	1:A:183:ALA:N	2.25	0.98
3:A:802:NDT:H7	1:B:403:GLY:HA2	1.01	0.98
1:D:160:PRO:CG	1:D:238:LEU:HD11	1.93	0.98
3:E:804:NDT:H7	1:F:673:GLY:HA3	1.37	0.98
1:A:39:HIS:CB	1:A:97:THR:OG1	2.11	0.98
1:A:128:LYS:HG2	1:A:184:SER:HB2	1.45	0.98
1:A:159:MET:SD	1:A:236:TYR:OH	2.20	0.98
1:B:159:MET:CG	1:B:236:TYR:CE1	2.34	0.98
1:B:692:ILE:CD1	2:B:803:ATP:N6	2.27	0.98
1:D:128:LYS:HG2	1:D:184:SER:HB2	1.45	0.98
1:D:560:GLY:N	2:D:803:ATP:O2B	1.96	0.98
1:C:128:LYS:N	1:C:222:THR:OG1	1.96	0.98
1:E:142:CYS:SG	1:E:144:GLU:HG3	1.98	0.98
1:E:39:HIS:CB	1:E:97:THR:OG1	2.11	0.98
1:B:128:LYS:N	1:B:222:THR:OG1	1.96	0.98
1:B:562:SER:HA	2:B:803:ATP:O1A	1.58	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:PRO:HG2	1:D:216:ILE:HD11	1.46	0.98
1:C:105:VAL:HG21	1:C:162:MET:HG2	1.46	0.98
1:E:54:HIS:CD2	1:E:93:VAL:HG22	1.99	0.98
1:F:563:LYS:CB	2:F:803:ATP:O2B	2.10	0.98
1:A:128:LYS:N	1:A:222:THR:OG1	1.96	0.98
1:B:141:GLU:OE1	1:B:170:LYS:CE	2.11	0.98
1:D:128:LYS:N	1:D:222:THR:OG1	1.96	0.98
1:F:54:HIS:CD2	1:F:93:VAL:HG22	1.99	0.98
1:A:163:ILE:H	1:A:163:ILE:HD12	1.26	0.98
1:C:123:PRO:HG2	1:C:216:ILE:HD11	1.46	0.98
1:D:141:GLU:OE1	1:D:170:LYS:CE	2.11	0.98
1:E:163:ILE:H	1:E:163:ILE:HD12	1.26	0.98
1:A:123:PRO:HG2	1:A:216:ILE:HD11	1.46	0.97
1:B:160:PRO:HA	1:B:238:LEU:CD1	1.93	0.97
1:B:562:SER:CA	2:B:803:ATP:PA	2.52	0.97
3:E:802:NDT:H8	1:F:403:GLY:HA2	1.42	0.97
1:F:519:GLY:H	2:F:803:ATP:N6	1.60	0.97
1:A:141:GLU:CG	1:A:171:ALA:H	1.76	0.97
1:D:163:ILE:H	1:D:163:ILE:HD12	1.26	0.97
1:F:210:TYR:CE1	1:F:213:PRO:C	2.19	0.97
1:B:39:HIS:CB	1:B:97:THR:OG1	2.11	0.97
1:C:39:HIS:CB	1:C:97:THR:OG1	2.11	0.97
1:C:77:ASN:O	1:C:211:LEU:CD2	2.07	0.97
1:C:692:ILE:HD11	2:C:803:ATP:HN62	1.20	0.97
3:D:802:NDT:H7	1:E:403:GLY:CA	1.93	0.97
1:B:54:HIS:CD2	1:B:93:VAL:HG22	1.99	0.97
1:D:105:VAL:HG21	1:D:162:MET:HG2	1.46	0.97
1:C:141:GLU:OE1	1:C:170:LYS:CE	2.11	0.97
1:B:128:LYS:HG2	1:B:184:SER:HB2	1.45	0.97
1:B:212:SER:HB2	1:B:213:PRO:HD3	0.97	0.97
1:E:128:LYS:N	1:E:222:THR:OG1	1.96	0.97
1:F:429:ARG:NH1	3:F:802:NDT:H20	1.77	0.97
1:E:722:ALA:HB2	2:E:803:ATP:C5'	1.93	0.97
1:B:562:SER:HA	2:B:803:ATP:O2A	1.64	0.97
1:D:77:ASN:HD21	1:D:209:PHE:CA	1.77	0.97
1:A:218:ARG:HH21	1:A:218:ARG:HA	1.27	0.97
3:A:802:NDT:C7	1:B:403:GLY:CA	2.26	0.97
1:D:54:HIS:CD2	1:D:93:VAL:HG22	1.99	0.97
1:D:722:ALA:CB	3:D:804:NDT:H5	1.94	0.97
1:B:218:ARG:HH21	1:B:218:ARG:HA	1.27	0.96
1:C:160:PRO:HB3	1:C:238:LEU:HD13	0.98	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ARG:HH21	1:D:218:ARG:HA	1.27	0.96
1:E:218:ARG:HH21	1:E:218:ARG:HA	1.27	0.96
1:B:105:VAL:HG21	1:B:162:MET:HG2	1.46	0.96
1:B:159:MET:HG2	1:B:236:TYR:CE1	1.96	0.96
1:E:123:PRO:HG2	1:E:216:ILE:HD11	1.46	0.96
1:A:54:HIS:CD2	1:A:93:VAL:HG22	1.99	0.96
3:E:802:NDT:C7	1:F:403:GLY:HA2	1.95	0.96
1:F:39:HIS:CB	1:F:97:THR:OG1	2.11	0.96
1:C:128:LYS:HG2	1:C:184:SER:HB2	1.45	0.96
1:F:73:LYS:HD2	1:F:114:LEU:HD21	1.46	0.96
1:A:562:SER:HA	2:A:803:ATP:O1A	1.64	0.96
1:D:46:LYS:HE3	1:D:46:LYS:HA	1.48	0.96
1:A:159:MET:N	1:A:160:PRO:HD2	1.77	0.96
1:C:54:HIS:CD2	1:C:93:VAL:HG22	1.99	0.95
1:F:128:LYS:HG2	1:F:184:SER:HB2	1.45	0.95
1:F:149:GLN:NE2	1:F:219:LYS:HZ1	1.64	0.95
1:A:159:MET:HG2	1:A:236:TYR:HE1	1.15	0.95
1:C:695:LYS:NZ	3:C:804:NDT:C18	2.28	0.95
1:F:158:ILE:CG2	1:F:212:SER:HG	1.78	0.95
1:B:429:ARG:NH1	3:B:802:NDT:C18	2.29	0.95
1:C:163:ILE:H	1:C:163:ILE:HD12	1.26	0.95
1:B:280:ARG:NH2	1:B:380:ALA:O	1.99	0.95
1:B:469:ILE:HD12	1:C:270:LEU:HD11	0.98	0.95
1:D:82:ILE:H	1:D:82:ILE:HD12	1.32	0.95
1:F:559:PRO:CG	1:F:660:ASN:OD1	2.15	0.95
1:C:156:GLY:C	1:C:157:VAL:HG12	1.87	0.95
1:F:105:VAL:HG21	1:F:162:MET:HG2	1.46	0.95
1:A:80:LEU:HB3	1:A:158:ILE:HD11	1.46	0.95
1:E:212:SER:OG	1:E:238:LEU:HD11	1.66	0.95
1:F:141:GLU:CG	1:F:171:ALA:N	2.30	0.95
1:F:218:ARG:HA	1:F:218:ARG:HH21	1.27	0.95
1:A:141:GLU:CG	1:A:171:ALA:N	2.30	0.95
1:A:159:MET:CE	1:A:182:ASP:C	2.32	0.95
1:D:156:GLY:C	1:D:157:VAL:HG12	1.87	0.95
1:F:125:TYR:HE2	1:F:218:ARG:CG	1.71	0.95
1:E:267:GLN:OE1	1:E:270:LEU:HD12	1.67	0.94
1:E:105:VAL:HG21	1:E:162:MET:HG2	1.46	0.94
1:E:128:LYS:HG2	1:E:184:SER:HB2	1.45	0.94
1:E:156:GLY:C	1:E:157:VAL:HG12	1.87	0.94
1:A:105:VAL:CG1	1:A:158:ILE:HD12	1.96	0.94
1:D:141:GLU:CG	1:D:171:ALA:N	2.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:GLU:CG	1:C:171:ALA:N	2.30	0.94
1:E:141:GLU:CG	1:E:171:ALA:N	2.30	0.94
1:F:123:PRO:HG2	1:F:216:ILE:HD11	1.46	0.94
1:B:481:LYS:HE3	1:C:270:LEU:CD2	1.74	0.94
1:C:218:ARG:HA	1:C:218:ARG:HH21	1.27	0.94
1:A:46:LYS:HA	1:A:46:LYS:HE3	1.48	0.94
1:A:105:VAL:HG21	1:A:162:MET:HG2	1.46	0.94
1:A:673:GLY:HA3	3:F:804:NDT:C7	1.96	0.94
1:B:156:GLY:C	1:B:157:VAL:HG12	1.87	0.94
1:D:562:SER:CB	2:D:803:ATP:C2	2.51	0.94
1:E:264:PRO:CD	1:E:266:HIS:CE1	2.51	0.94
1:F:160:PRO:HD2	1:F:212:SER:HG	1.21	0.94
1:C:46:LYS:HA	1:C:46:LYS:HE3	1.48	0.94
1:E:105:VAL:CG2	1:E:162:MET:HG2	1.98	0.94
1:F:105:VAL:CG2	1:F:162:MET:HG2	1.98	0.94
1:B:123:PRO:HG2	1:B:216:ILE:HD11	1.46	0.94
1:A:519:GLY:N	2:A:803:ATP:HN61	1.67	0.93
1:B:82:ILE:H	1:B:82:ILE:HD12	1.32	0.93
1:E:160:PRO:CB	1:E:238:LEU:CD1	2.46	0.93
1:B:105:VAL:CG2	1:B:162:MET:HG2	1.98	0.93
1:F:519:GLY:CA	2:F:803:ATP:N6	2.29	0.93
1:C:105:VAL:CG2	1:C:162:MET:HG2	1.98	0.93
1:B:149:GLN:NE2	1:B:219:LYS:HZ1	1.66	0.93
1:C:149:GLN:HE21	1:C:219:LYS:HZ1	0.96	0.93
1:D:429:ARG:NH2	3:D:802:NDT:C17	2.30	0.93
1:E:125:TYR:HE2	1:E:218:ARG:CG	1.71	0.93
1:B:692:ILE:HD11	2:B:803:ATP:HN62	1.32	0.93
1:C:695:LYS:HE2	3:C:804:NDT:C17	1.99	0.93
1:F:519:GLY:N	2:F:803:ATP:N6	2.15	0.93
1:D:149:GLN:HE21	1:D:219:LYS:HZ1	0.97	0.93
1:E:46:LYS:HA	1:E:46:LYS:HE3	1.48	0.93
1:F:70:THR:C	1:F:79:ILE:HD12	1.81	0.93
1:B:141:GLU:CG	1:B:171:ALA:N	2.30	0.93
1:C:695:LYS:CE	3:C:804:NDT:C17	2.47	0.93
1:B:141:GLU:CD	1:B:171:ALA:H	1.73	0.93
1:A:105:VAL:CG2	1:A:162:MET:HG2	1.98	0.92
1:B:263:ILE:HG12	1:B:271:PHE:HE1	1.32	0.92
1:E:80:LEU:HD23	1:E:211:LEU:CD1	1.99	0.92
1:E:82:ILE:HD12	1:E:82:ILE:H	1.32	0.92
1:B:160:PRO:HB3	1:B:238:LEU:HD13	1.51	0.92
1:C:58:LEU:HD22	1:C:85:ALA:HB1	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:LEU:HD22	1:E:85:ALA:HB1	1.51	0.92
1:A:82:ILE:H	1:A:82:ILE:HD12	1.32	0.92
1:A:159:MET:SD	1:A:182:ASP:HA	2.09	0.92
1:E:141:GLU:CD	1:E:171:ALA:H	1.73	0.92
1:B:429:ARG:CZ	3:B:802:NDT:H17	1.99	0.92
1:D:105:VAL:CG2	1:D:162:MET:HG2	1.98	0.92
1:D:125:TYR:HE2	1:D:218:ARG:CG	1.71	0.92
1:D:242:LEU:H	1:D:301:ASN:HD22	1.12	0.92
1:F:46:LYS:HA	1:F:46:LYS:HE3	1.48	0.92
1:C:695:LYS:NZ	3:C:804:NDT:C17	2.33	0.92
3:D:802:NDT:C7	1:E:403:GLY:HA2	1.98	0.92
1:D:141:GLU:CD	1:D:171:ALA:H	1.73	0.92
1:F:82:ILE:H	1:F:82:ILE:HD12	1.32	0.92
1:D:248:GLY:H	2:D:801:ATP:N6	1.68	0.92
1:B:46:LYS:HA	1:B:46:LYS:HE3	1.48	0.92
1:C:141:GLU:CD	1:C:171:ALA:H	1.73	0.92
1:C:291:GLY:HA2	2:C:801:ATP:O1A	1.70	0.92
1:B:695:LYS:HZ3	3:B:804:NDT:C16	1.75	0.92
1:C:78:GLY:C	1:C:211:LEU:CG	2.28	0.92
1:C:141:GLU:CG	1:C:171:ALA:H	1.76	0.92
1:A:81:VAL:HG11	1:A:210:TYR:CE1	2.04	0.91
1:A:211:LEU:HD23	1:A:238:LEU:CD2	2.00	0.91
1:B:35:ILE:CD1	1:B:113:ARG:NH1	2.32	0.91
1:C:78:GLY:C	1:C:211:LEU:CD1	2.38	0.91
1:C:82:ILE:H	1:C:82:ILE:HD12	1.32	0.91
1:F:104:SER:HG	1:F:163:ILE:CD1	1.72	0.91
1:D:156:GLY:O	1:D:157:VAL:HG12	0.73	0.91
1:B:157:VAL:HG12	1:B:215:PHE:O	1.69	0.91
1:D:248:GLY:H	2:D:801:ATP:HN62	1.16	0.91
1:E:465:VAL:HG12	1:F:271:PHE:CE1	2.05	0.91
1:A:104:SER:HG	1:A:163:ILE:HD13	1.12	0.91
1:B:125:TYR:HE2	1:B:218:ARG:CG	1.71	0.91
1:C:78:GLY:CA	1:C:211:LEU:CD2	0.92	0.91
1:C:156:GLY:O	1:C:157:VAL:HG12	0.73	0.91
1:C:78:GLY:C	1:C:211:LEU:CD2	1.97	0.91
1:D:141:GLU:CG	1:D:171:ALA:H	1.76	0.91
1:D:271:PHE:CZ	1:D:277:SER:O	2.23	0.91
1:E:37:ARG:HD3	1:E:337:TYR:CD2	2.06	0.91
1:F:141:GLU:CD	1:F:171:ALA:H	1.73	0.91
1:B:156:GLY:O	1:B:157:VAL:HG12	0.73	0.91
1:F:519:GLY:H	2:F:803:ATP:HN61	1.06	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:CYS:O	1:D:82:ILE:HD12	1.71	0.90
1:D:271:PHE:CE2	1:D:277:SER:C	2.44	0.90
1:E:69:CYS:O	1:E:82:ILE:HD12	1.71	0.90
1:A:141:GLU:CD	1:A:171:ALA:H	1.73	0.90
1:B:429:ARG:HG2	3:B:802:NDT:H213	1.50	0.90
1:F:58:LEU:HD22	1:F:85:ALA:HB1	1.51	0.90
1:E:156:GLY:O	1:E:157:VAL:HG12	0.73	0.90
1:B:69:CYS:O	1:B:82:ILE:HD12	1.71	0.90
1:E:35:ILE:CD1	1:E:113:ARG:NH1	2.32	0.90
1:B:695:LYS:HZ1	3:B:804:NDT:C17	1.85	0.90
1:D:266:HIS:C	1:D:268:PRO:CD	2.40	0.90
1:A:481:LYS:HD3	1:B:270:LEU:HG	1.52	0.90
1:D:429:ARG:NH1	3:D:802:NDT:H17	1.82	0.90
1:F:559:PRO:CG	1:F:660:ASN:HD21	1.85	0.90
1:A:69:CYS:O	1:A:82:ILE:HD12	1.71	0.90
1:B:58:LEU:HD22	1:B:85:ALA:HB1	1.52	0.90
1:D:160:PRO:CB	1:D:238:LEU:HD11	1.98	0.90
1:C:80:LEU:HD23	1:C:211:LEU:HD11	1.54	0.90
1:D:429:ARG:CZ	3:D:802:NDT:C18	2.50	0.90
1:E:125:TYR:CD2	1:E:218:ARG:CG	2.51	0.90
1:D:58:LEU:HD22	1:D:85:ALA:HB1	1.52	0.89
1:D:123:PRO:HG2	1:D:216:ILE:CD1	2.03	0.89
1:A:58:LEU:HD22	1:A:85:ALA:HB1	1.52	0.89
1:C:69:CYS:O	1:C:82:ILE:HD12	1.71	0.89
1:D:429:ARG:NH2	3:D:802:NDT:C20	2.35	0.89
1:A:123:PRO:HG2	1:A:216:ILE:CD1	2.03	0.89
1:B:123:PRO:HG2	1:B:216:ILE:CD1	2.03	0.89
1:B:158:ILE:C	1:B:213:PRO:HB2	1.92	0.89
1:F:262:GLU:CD	1:F:266:HIS:ND1	2.25	0.89
1:A:294:MET:HE1	2:A:801:ATP:N1	1.88	0.89
1:E:77:ASN:OD1	1:E:208:LEU:O	1.91	0.89
1:F:125:TYR:CD2	1:F:218:ARG:CG	2.51	0.89
1:F:159:MET:HG3	1:F:236:TYR:CE2	2.07	0.89
1:A:159:MET:HG3	1:A:236:TYR:CE1	1.96	0.89
1:A:429:ARG:HH12	3:A:802:NDT:C16	1.82	0.89
1:C:58:LEU:HD21	1:C:85:ALA:CB	2.03	0.89
1:C:123:PRO:HG2	1:C:216:ILE:CD1	2.03	0.89
1:D:58:LEU:HD21	1:D:85:ALA:CB	2.03	0.89
1:F:69:CYS:O	1:F:82:ILE:HD12	1.71	0.89
1:D:481:LYS:CE	1:E:270:LEU:HD11	1.96	0.89
1:B:125:TYR:CD2	1:B:218:ARG:CG	2.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:MET:CG	1:D:236:TYR:CE1	2.34	0.89
1:A:125:TYR:CD2	1:A:218:ARG:CG	2.51	0.89
1:B:429:ARG:CZ	3:B:802:NDT:C18	2.51	0.89
1:E:58:LEU:HD21	1:E:85:ALA:CB	2.03	0.89
1:A:58:LEU:HD21	1:A:85:ALA:CB	2.03	0.89
1:C:125:TYR:CD2	1:C:218:ARG:CG	2.51	0.89
1:A:109:ILE:HD12	1:A:307:VAL:HG21	1.54	0.88
1:A:430:MET:HG2	1:B:274:PHE:O	1.72	0.88
1:C:58:LEU:HD21	1:C:85:ALA:HB1	1.55	0.88
1:E:264:PRO:CD	1:E:266:HIS:HE1	1.85	0.88
1:E:465:VAL:HG22	1:F:274:PHE:CD2	2.09	0.88
1:A:53:ILE:H	1:A:86:GLY:HA3	1.39	0.88
1:C:35:ILE:CD1	1:C:113:ARG:NH1	2.32	0.88
1:D:481:LYS:HE2	1:E:270:LEU:CD1	2.04	0.88
1:A:53:ILE:HD13	1:A:116:LEU:HD22	1.55	0.88
1:F:123:PRO:HG2	1:F:216:ILE:CD1	2.03	0.88
1:C:53:ILE:N	1:C:86:GLY:CA	2.36	0.88
1:D:53:ILE:H	1:D:86:GLY:HA3	1.39	0.88
1:D:70:THR:HG22	1:D:81:VAL:HG12	1.56	0.88
1:E:123:PRO:HG2	1:E:216:ILE:CD1	2.03	0.88
1:C:233:ASN:HD21	1:C:235:LYS:CE	1.86	0.88
1:C:374:MET:HA	1:C:377:MET:HG3	1.55	0.88
1:D:53:ILE:HD13	1:D:116:LEU:HD22	1.55	0.88
1:D:53:ILE:N	1:D:86:GLY:CA	2.36	0.88
1:E:519:GLY:N	2:E:803:ATP:N6	2.21	0.88
1:F:58:LEU:HD21	1:F:85:ALA:HB1	1.55	0.88
1:A:53:ILE:N	1:A:86:GLY:CA	2.36	0.88
1:B:159:MET:HG2	1:B:236:TYR:CD1	2.09	0.88
1:D:159:MET:HG2	1:D:236:TYR:CD1	2.09	0.88
1:A:70:THR:HG22	1:A:81:VAL:HG12	1.56	0.88
1:F:159:MET:HB3	1:F:213:PRO:HG2	1.55	0.88
1:A:426:GLN:CD	3:A:802:NDT:H19	1.93	0.88
1:B:53:ILE:N	1:B:86:GLY:CA	2.36	0.88
1:E:141:GLU:CG	1:E:171:ALA:H	1.76	0.88
1:F:159:MET:HE2	1:F:159:MET:O	1.74	0.88
1:F:624:ASP:HB3	1:F:629:SER:HB2	1.54	0.88
1:A:160:PRO:HG3	1:A:238:LEU:HD11	1.55	0.87
1:D:125:TYR:CD2	1:D:218:ARG:CG	2.51	0.87
1:E:79:ILE:H	1:E:211:LEU:HG	1.39	0.87
1:E:248:GLY:H	2:E:801:ATP:HN62	1.15	0.87
1:F:53:ILE:N	1:F:86:GLY:CA	2.36	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ASN:ND2	1:D:209:PHE:C	2.27	0.87
1:A:35:ILE:CD1	1:A:113:ARG:NH1	2.32	0.87
1:F:159:MET:CB	1:F:213:PRO:HG2	2.03	0.87
1:A:53:ILE:HD13	1:A:116:LEU:CD2	2.05	0.87
1:A:105:VAL:CG2	1:A:157:VAL:CG2	2.51	0.87
1:B:58:LEU:HD21	1:B:85:ALA:CB	2.03	0.87
1:E:58:LEU:HD21	1:E:85:ALA:HB1	1.55	0.87
1:F:58:LEU:HD21	1:F:85:ALA:CB	2.03	0.87
1:B:280:ARG:HH12	1:B:382:LYS:HA	1.37	0.87
1:C:53:ILE:N	1:C:86:GLY:HA3	1.90	0.87
1:D:77:ASN:ND2	1:D:77:ASN:O	2.08	0.87
1:E:53:ILE:N	1:E:86:GLY:CA	2.36	0.87
1:A:125:TYR:HE2	1:A:218:ARG:CG	1.71	0.87
1:B:429:ARG:HH11	3:B:802:NDT:C19	1.87	0.87
1:E:53:ILE:N	1:E:86:GLY:HA3	1.90	0.87
1:E:70:THR:HG22	1:E:81:VAL:HG12	1.56	0.87
1:F:53:ILE:H	1:F:86:GLY:HA3	1.39	0.87
1:B:721:GLY:HA2	2:B:803:ATP:C2	2.06	0.87
1:D:77:ASN:OD1	1:D:209:PHE:CB	2.22	0.87
1:D:429:ARG:HH12	3:D:802:NDT:C16	1.86	0.87
1:F:53:ILE:N	1:F:86:GLY:HA3	1.90	0.87
1:F:53:ILE:HD13	1:F:116:LEU:HD22	1.55	0.87
1:B:695:LYS:HZ1	3:B:804:NDT:C16	1.84	0.87
1:C:123:PRO:HG2	1:C:216:ILE:CG1	2.05	0.87
1:D:123:PRO:HG2	1:D:216:ILE:CG1	2.05	0.87
1:C:125:TYR:HE2	1:C:218:ARG:CG	1.71	0.87
1:D:58:LEU:HD21	1:D:85:ALA:HB1	1.55	0.87
1:F:160:PRO:HD3	1:F:213:PRO:HD2	1.55	0.87
1:F:160:PRO:HG2	1:F:212:SER:HB2	1.56	0.87
1:A:481:LYS:HD3	1:B:270:LEU:CD1	2.05	0.86
1:A:519:GLY:H	2:A:803:ATP:HN61	0.88	0.86
1:B:53:ILE:N	1:B:86:GLY:HA3	1.90	0.86
1:B:53:ILE:HD13	1:B:116:LEU:HD22	1.55	0.86
1:C:126:ALA:O	1:C:222:THR:CB	2.23	0.86
1:E:53:ILE:HD13	1:E:116:LEU:CD2	2.05	0.86
1:F:559:PRO:HB3	1:F:660:ASN:ND2	1.90	0.86
1:A:53:ILE:N	1:A:86:GLY:HA3	1.90	0.86
1:B:143:MET:CE	1:B:143:MET:H	1.89	0.86
1:C:78:GLY:CA	1:C:211:LEU:HD21	0.71	0.86
1:B:58:LEU:HD21	1:B:85:ALA:HB1	1.55	0.86
1:D:53:ILE:N	1:D:86:GLY:HA3	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:LEU:HD12	1:D:297:ARG:CG	1.98	0.86
1:B:141:GLU:CG	1:B:171:ALA:H	1.76	0.86
1:C:70:THR:HG22	1:C:81:VAL:HG12	1.56	0.86
1:F:70:THR:HG22	1:F:81:VAL:HG12	1.56	0.86
1:F:123:PRO:HG2	1:F:216:ILE:CG1	2.05	0.86
1:A:211:LEU:HD23	1:A:238:LEU:HD21	1.57	0.86
1:B:53:ILE:HD13	1:B:116:LEU:CD2	2.05	0.86
1:B:126:ALA:O	1:B:222:THR:CB	2.23	0.86
1:B:263:ILE:CG2	1:B:264:PRO:HD3	2.04	0.86
1:C:53:ILE:HD13	1:C:116:LEU:HD22	1.55	0.86
1:E:123:PRO:HG2	1:E:216:ILE:CG1	2.05	0.86
1:F:519:GLY:C	2:F:803:ATP:HN62	1.78	0.86
1:F:624:ASP:HB2	1:F:629:SER:HB2	1.57	0.86
1:A:436:VAL:HG12	1:A:486:VAL:O	1.74	0.86
1:B:77:ASN:ND2	1:B:77:ASN:O	2.08	0.86
1:D:53:ILE:HD13	1:D:116:LEU:CD2	2.05	0.86
1:D:128:LYS:HG2	1:D:184:SER:HB3	1.58	0.86
1:E:53:ILE:H	1:E:86:GLY:HA3	1.39	0.86
1:E:77:ASN:O	1:E:77:ASN:ND2	2.08	0.86
1:F:35:ILE:CD1	1:F:113:ARG:NH1	2.32	0.86
1:F:73:LYS:HE3	1:F:112:ASP:OD2	1.74	0.86
1:A:128:LYS:HG2	1:A:184:SER:HB3	1.58	0.86
1:B:128:LYS:HG2	1:B:184:SER:HB3	1.58	0.86
1:B:481:LYS:CD	1:C:270:LEU:HD21	1.74	0.86
1:C:160:PRO:HG3	1:C:238:LEU:CD2	2.06	0.86
1:F:53:ILE:HD13	1:F:116:LEU:CD2	2.05	0.86
1:A:158:ILE:C	1:A:160:PRO:HD2	1.86	0.86
1:A:294:MET:SD	2:A:801:ATP:C2	2.68	0.86
1:D:35:ILE:CD1	1:D:113:ARG:NH1	2.32	0.86
1:D:54:HIS:CD2	1:D:93:VAL:CG2	2.59	0.86
1:A:58:LEU:HD21	1:A:85:ALA:HB1	1.55	0.86
1:A:562:SER:CA	2:A:803:ATP:PA	2.62	0.86
1:C:53:ILE:HD13	1:C:116:LEU:CD2	2.05	0.86
1:E:53:ILE:HD13	1:E:116:LEU:HD22	1.55	0.86
1:E:126:ALA:O	1:E:222:THR:CB	2.23	0.86
1:E:264:PRO:HD3	1:E:266:HIS:HE1	1.40	0.86
1:E:79:ILE:N	1:E:211:LEU:HG	1.89	0.85
1:F:54:HIS:CD2	1:F:93:VAL:CG2	2.59	0.85
1:B:70:THR:HG22	1:B:81:VAL:HG12	1.56	0.85
1:B:123:PRO:HG2	1:B:216:ILE:CG1	2.05	0.85
1:E:77:ASN:HD21	1:E:209:PHE:C	1.80	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASN:HB3	1:A:236:TYR:HE2	1.41	0.85
1:B:104:SER:HG	1:B:163:ILE:HD13	1.03	0.85
1:D:143:MET:CE	1:D:143:MET:H	1.89	0.85
1:C:143:MET:H	1:C:143:MET:CE	1.89	0.85
1:F:143:MET:CE	1:F:143:MET:H	1.88	0.85
1:A:77:ASN:O	1:A:77:ASN:ND2	2.08	0.85
1:A:126:ALA:O	1:A:222:THR:CB	2.23	0.85
1:B:53:ILE:H	1:B:86:GLY:HA3	1.39	0.85
1:B:429:ARG:NH2	3:B:802:NDT:C17	2.39	0.85
1:B:429:ARG:NE	3:B:802:NDT:C17	2.38	0.85
1:D:271:PHE:CE2	1:D:278:PRO:N	2.42	0.85
1:D:429:ARG:HH12	3:D:802:NDT:C17	1.85	0.85
1:F:126:ALA:O	1:F:222:THR:CB	2.23	0.85
1:C:53:ILE:H	1:C:86:GLY:HA3	1.39	0.85
1:C:77:ASN:O	1:C:77:ASN:ND2	2.08	0.85
1:D:268:PRO:C	1:D:269:THR:HG23	1.97	0.85
1:F:559:PRO:HG3	1:F:660:ASN:ND2	1.91	0.85
1:E:39:HIS:HB3	1:E:97:THR:CB	2.06	0.85
1:E:160:PRO:CG	1:E:238:LEU:CD1	2.54	0.85
1:F:104:SER:HG	1:F:163:ILE:HD13	0.80	0.85
1:A:143:MET:CE	1:A:143:MET:H	1.89	0.85
1:C:128:LYS:HG2	1:C:184:SER:HB3	1.58	0.85
1:C:149:GLN:NE2	1:C:219:LYS:HZ1	1.75	0.85
1:E:54:HIS:CD2	1:E:93:VAL:CG2	2.59	0.85
1:E:434:ARG:CD	1:F:273:SER:HB3	2.06	0.85
1:F:39:HIS:HB3	1:F:97:THR:CB	2.06	0.85
1:D:126:ALA:O	1:D:222:THR:CB	2.23	0.85
1:E:143:MET:H	1:E:143:MET:CE	1.88	0.85
1:E:465:VAL:CG2	1:F:274:PHE:HD2	1.90	0.85
1:C:54:HIS:CD2	1:C:93:VAL:CG2	2.59	0.85
1:D:39:HIS:HB3	1:D:97:THR:CB	2.06	0.85
3:A:802:NDT:C8	1:B:403:GLY:HA2	2.06	0.84
1:B:159:MET:CB	1:B:213:PRO:HB3	2.06	0.84
1:C:39:HIS:HB3	1:C:97:THR:CB	2.06	0.84
1:E:149:GLN:HE21	1:E:219:LYS:HZ1	1.22	0.84
1:A:39:HIS:HB3	1:A:97:THR:CB	2.06	0.84
1:F:158:ILE:HG22	1:F:160:PRO:CD	2.06	0.84
1:B:54:HIS:CD2	1:B:93:VAL:CG2	2.59	0.84
1:C:564:THR:CB	2:C:803:ATP:O2A	2.24	0.84
1:D:481:LYS:CE	1:E:270:LEU:CD1	2.56	0.84
1:A:123:PRO:HG2	1:A:216:ILE:CG1	2.05	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLN:HE21	1:B:219:LYS:HZ1	0.86	0.84
1:C:104:SER:HG	1:C:163:ILE:HD13	1.01	0.84
1:B:125:TYR:CE2	1:B:218:ARG:CD	2.61	0.84
1:C:429:ARG:HB3	3:C:802:NDT:H212	1.57	0.84
1:A:125:TYR:CE2	1:A:218:ARG:CD	2.61	0.84
1:E:104:SER:HG	1:E:163:ILE:CD1	1.77	0.84
1:F:160:PRO:HG2	1:F:212:SER:CB	2.07	0.84
1:E:37:ARG:CD	1:E:337:TYR:CE2	2.60	0.84
1:E:692:ILE:CD1	2:E:803:ATP:C6	2.59	0.84
1:E:128:LYS:HG2	1:E:184:SER:HB3	1.58	0.83
1:F:158:ILE:CG2	1:F:160:PRO:HD2	2.08	0.83
1:B:39:HIS:HB3	1:B:97:THR:CB	2.06	0.83
1:B:429:ARG:NH1	3:B:802:NDT:C20	2.40	0.83
1:E:159:MET:HB3	1:E:213:PRO:HG2	1.60	0.83
1:A:54:HIS:CD2	1:A:93:VAL:CG2	2.59	0.83
1:A:519:GLY:C	2:A:803:ATP:HN62	1.80	0.83
1:C:79:ILE:N	1:C:211:LEU:CD2	2.41	0.83
1:C:519:GLY:O	2:C:803:ATP:N6	2.11	0.83
2:D:803:ATP:H3'	3:D:804:NDT:C5	2.09	0.83
1:E:149:GLN:HE21	1:E:219:LYS:HZ2	1.25	0.83
1:E:519:GLY:H	2:E:803:ATP:HN61	1.22	0.83
1:F:159:MET:HB3	1:F:213:PRO:CG	2.09	0.83
1:B:279:PRO:HG3	1:B:407:GLN:HE21	1.43	0.83
1:F:54:HIS:ND1	1:F:55:PRO:HD2	1.94	0.83
1:F:158:ILE:HG21	1:F:212:SER:OG	1.75	0.83
2:C:803:ATP:H3'	3:C:804:NDT:C5	2.09	0.83
1:D:149:GLN:NE2	1:D:219:LYS:HZ1	1.75	0.83
1:A:54:HIS:ND1	1:A:55:PRO:HD2	1.94	0.83
1:D:159:MET:HB3	1:D:213:PRO:HG2	1.60	0.83
1:F:128:LYS:HG2	1:F:184:SER:HB3	1.58	0.83
1:F:625:ARG:NH2	1:F:666:ASP:OD1	2.12	0.83
1:C:248:GLY:H	2:C:801:ATP:N6	1.75	0.83
1:E:79:ILE:H	1:E:211:LEU:CG	1.87	0.83
1:E:125:TYR:CE2	1:E:218:ARG:CD	2.61	0.83
1:F:125:TYR:CE2	1:F:218:ARG:CD	2.61	0.83
1:F:141:GLU:CG	1:F:171:ALA:H	1.76	0.82
1:C:125:TYR:CE2	1:C:218:ARG:CD	2.61	0.82
1:C:125:TYR:HE2	1:C:218:ARG:HG3	1.02	0.82
1:D:125:TYR:CE2	1:D:218:ARG:CD	2.61	0.82
1:E:125:TYR:HE2	1:E:218:ARG:HG3	1.02	0.82
1:E:293:THR:HB	2:E:801:ATP:O1B	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:GLY:C	2:A:801:ATP:N7	2.31	0.82
1:C:54:HIS:ND1	1:C:55:PRO:HD2	1.93	0.82
1:C:159:MET:HB3	1:C:213:PRO:HG2	1.60	0.82
1:B:54:HIS:ND1	1:B:55:PRO:HD2	1.93	0.82
1:C:160:PRO:HA	1:C:238:LEU:HD12	1.62	0.82
1:E:54:HIS:ND1	1:E:55:PRO:HD2	1.93	0.82
1:A:426:GLN:OE1	3:A:802:NDT:H19	1.79	0.82
1:B:160:PRO:HA	1:B:238:LEU:HD11	1.60	0.82
1:D:563:LYS:HE2	2:D:803:ATP:O1G	1.79	0.82
1:D:54:HIS:ND1	1:D:55:PRO:HD2	1.93	0.82
1:D:429:ARG:NH1	3:D:802:NDT:C16	2.43	0.82
1:A:78:GLY:CA	1:A:211:LEU:HB2	2.07	0.81
1:D:266:HIS:C	1:D:268:PRO:HD3	2.00	0.81
1:D:267:GLN:N	1:D:268:PRO:CD	2.42	0.81
1:F:125:TYR:HE2	1:F:218:ARG:HG3	1.02	0.81
1:B:429:ARG:HH11	3:B:802:NDT:C20	1.93	0.81
1:B:695:LYS:NZ	3:B:804:NDT:C17	2.42	0.81
1:D:271:PHE:CZ	1:D:278:PRO:HA	2.15	0.81
1:D:429:ARG:NH2	3:D:802:NDT:C18	2.43	0.81
1:F:160:PRO:HB3	1:F:238:LEU:HD13	0.83	0.81
1:A:426:GLN:HE22	3:A:802:NDT:H19	1.33	0.81
1:A:481:LYS:HD3	1:B:270:LEU:CG	2.09	0.81
1:D:141:GLU:HG2	1:D:171:ALA:N	1.94	0.81
1:F:563:LYS:HB3	2:F:803:ATP:O1B	1.80	0.81
1:C:141:GLU:HG2	1:C:171:ALA:N	1.94	0.81
1:C:429:ARG:CD	3:C:802:NDT:H212	2.10	0.81
1:D:125:TYR:HE2	1:D:218:ARG:HG3	1.02	0.81
1:D:160:PRO:CG	1:D:238:LEU:CD1	2.56	0.81
1:D:244:TYR:HD1	1:D:254:ILE:HD11	1.46	0.81
1:C:212:SER:OG	1:C:238:LEU:HD21	1.81	0.80
1:C:429:ARG:CD	3:C:802:NDT:C18	2.59	0.80
1:D:29:LYS:HD3	1:D:56:ASN:OD1	1.72	0.80
1:E:429:ARG:NE	3:E:802:NDT:C21	2.35	0.80
1:E:692:ILE:CD1	2:E:803:ATP:C5	2.63	0.80
1:E:262:GLU:HG3	1:E:266:HIS:CG	2.15	0.80
1:B:159:MET:HB3	1:B:213:PRO:CB	2.11	0.80
1:A:166:ASN:HD21	1:A:169:THR:HG21	1.45	0.80
1:A:233:ASN:HB3	1:A:236:TYR:CE2	2.17	0.80
1:A:429:ARG:NH1	3:A:802:NDT:C17	2.44	0.80
1:D:471:ARG:HE	1:D:484:LEU:HD21	1.45	0.80
1:F:559:PRO:CB	1:F:660:ASN:HD21	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TYR:HE2	1:A:218:ARG:HG3	1.02	0.80
1:B:29:LYS:HD3	1:B:56:ASN:OD1	1.72	0.80
1:B:160:PRO:HG3	1:B:238:LEU:HD21	1.62	0.80
1:E:155:SER:OG	1:E:156:GLY:N	2.14	0.80
1:B:141:GLU:HG2	1:B:171:ALA:N	1.94	0.80
1:C:233:ASN:HB3	1:C:236:TYR:CD2	2.16	0.80
1:A:141:GLU:OE2	1:A:171:ALA:N	2.15	0.80
1:A:159:MET:SD	1:A:182:ASP:OD1	2.38	0.80
1:A:429:ARG:HH11	3:A:802:NDT:C17	1.94	0.80
1:A:455:ALA:CA	2:A:801:ATP:H8	1.93	0.80
1:B:125:TYR:HE2	1:B:218:ARG:HG3	1.02	0.80
1:D:429:ARG:NH2	3:D:802:NDT:C19	2.45	0.79
1:A:158:ILE:C	1:A:160:PRO:CD	2.48	0.79
1:A:519:GLY:CA	2:A:803:ATP:N6	2.45	0.79
1:B:481:LYS:HE3	1:C:270:LEU:CG	2.11	0.79
1:B:721:GLY:CA	2:B:803:ATP:N3	2.29	0.79
1:C:233:ASN:ND2	1:C:235:LYS:HE2	1.92	0.79
1:B:280:ARG:NH1	1:B:383:VAL:N	2.28	0.79
1:D:242:LEU:N	1:D:301:ASN:HD22	1.79	0.79
1:F:141:GLU:OE2	1:F:171:ALA:N	2.15	0.79
1:F:155:SER:OG	1:F:156:GLY:N	2.15	0.79
1:D:266:HIS:C	1:D:268:PRO:HD2	2.03	0.79
1:E:104:SER:HG	1:E:163:ILE:HD13	0.87	0.79
1:E:210:TYR:HE1	1:E:213:PRO:CA	1.94	0.79
3:E:802:NDT:C8	1:F:403:GLY:CA	2.59	0.79
1:A:562:SER:CA	2:A:803:ATP:O2A	2.29	0.79
1:C:141:GLU:OE2	1:C:171:ALA:N	2.15	0.79
1:D:49:CYS:O	1:D:82:ILE:HB	1.83	0.79
1:D:141:GLU:OE2	1:D:171:ALA:N	2.15	0.79
1:B:155:SER:OG	1:B:156:GLY:N	2.15	0.79
1:D:562:SER:HB3	2:D:803:ATP:N1	1.98	0.79
1:E:363:GLU:O	1:E:366:VAL:N	2.16	0.79
1:D:160:PRO:HB3	1:D:238:LEU:HD13	0.81	0.79
1:B:141:GLU:OE2	1:B:171:ALA:N	2.15	0.79
1:B:481:LYS:CE	1:C:270:LEU:CG	2.48	0.79
1:A:49:CYS:O	1:A:82:ILE:HB	1.83	0.79
1:A:155:SER:OG	1:A:156:GLY:N	2.16	0.79
1:E:268:PRO:HG3	1:E:382:LYS:HE2	1.64	0.79
1:C:402:PRO:HA	1:C:406:ASP:HB3	1.63	0.79
1:E:212:SER:OG	1:E:238:LEU:CD1	2.31	0.79
1:E:248:GLY:H	2:E:801:ATP:N6	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PRO:CA	1:C:238:LEU:HD13	1.97	0.78
1:A:105:VAL:HG11	1:A:158:ILE:HD12	1.64	0.78
1:E:465:VAL:HG12	1:F:271:PHE:HE1	1.46	0.78
1:A:270:LEU:CG	1:F:481:LYS:HD3	2.13	0.78
1:F:109:ILE:HD12	1:F:307:VAL:HG21	1.65	0.78
1:B:166:ASN:HD21	1:B:169:THR:HG21	1.45	0.78
1:D:42:LYS:HE2	1:D:42:LYS:N	1.99	0.78
1:F:53:ILE:H	1:F:86:GLY:N	1.81	0.78
1:A:42:LYS:HE2	1:A:42:LYS:N	1.99	0.78
1:A:159:MET:SD	1:A:182:ASP:CA	2.71	0.78
1:B:161:GLY:HA3	1:B:179:VAL:HG13	1.66	0.78
1:F:42:LYS:HE2	1:F:42:LYS:N	1.99	0.78
1:A:149:GLN:NE2	1:A:219:LYS:NZ	2.32	0.78
1:B:159:MET:CA	1:B:213:PRO:HB2	2.14	0.78
1:D:465:VAL:HG12	1:E:271:PHE:CZ	2.17	0.78
1:E:141:GLU:HG2	1:E:171:ALA:N	1.94	0.78
1:F:149:GLN:HE21	1:F:219:LYS:HZ1	0.83	0.78
1:F:160:PRO:CG	1:F:212:SER:OG	2.31	0.78
1:C:561:CYS:O	2:C:803:ATP:C2	2.37	0.78
1:B:160:PRO:CB	1:B:238:LEU:HD13	2.14	0.78
1:F:142:CYS:SG	1:F:144:GLU:OE1	2.42	0.78
1:A:53:ILE:H	1:A:86:GLY:N	1.81	0.78
1:C:53:ILE:H	1:C:86:GLY:N	1.81	0.78
1:E:49:CYS:O	1:E:82:ILE:HB	1.83	0.78
1:E:53:ILE:H	1:E:86:GLY:N	1.81	0.78
1:F:166:ASN:HD21	1:F:169:THR:HG21	1.45	0.78
1:C:49:CYS:O	1:C:82:ILE:HB	1.83	0.77
1:E:141:GLU:OE2	1:E:171:ALA:N	2.15	0.77
1:F:624:ASP:HA	1:F:629:SER:OG	1.84	0.77
1:A:161:GLY:HA3	1:A:179:VAL:HG13	1.66	0.77
1:B:49:CYS:O	1:B:82:ILE:HB	1.83	0.77
1:B:142:CYS:SG	1:B:144:GLU:OE1	2.42	0.77
1:C:155:SER:OG	1:C:156:GLY:N	2.14	0.77
1:C:695:LYS:HE2	3:C:804:NDT:H17	1.66	0.77
1:D:142:CYS:SG	1:D:144:GLU:OE1	2.42	0.77
1:E:42:LYS:N	1:E:42:LYS:HE2	1.99	0.77
1:E:166:ASN:HD21	1:E:169:THR:HG21	1.46	0.77
1:F:49:CYS:O	1:F:82:ILE:HB	1.83	0.77
1:F:363:GLU:O	1:F:366:VAL:N	2.17	0.77
1:A:46:LYS:HE3	1:A:46:LYS:CA	2.15	0.77
1:C:142:CYS:SG	1:C:144:GLU:CD	2.62	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:GLN:N	1:D:268:PRO:HD3	2.00	0.77
1:E:53:ILE:O	1:E:86:GLY:CA	2.32	0.77
1:E:436:VAL:O	1:E:437:LEU:HD13	1.84	0.77
1:F:42:LYS:HE2	1:F:42:LYS:H	1.50	0.77
1:F:142:CYS:SG	1:F:144:GLU:CD	2.62	0.77
1:F:160:PRO:CD	1:F:212:SER:HG	1.86	0.77
1:F:559:PRO:CG	1:F:660:ASN:ND2	2.44	0.77
1:B:53:ILE:H	1:B:86:GLY:N	1.81	0.77
1:D:142:CYS:SG	1:D:144:GLU:CD	2.62	0.77
1:B:35:ILE:CG1	1:B:113:ARG:NH1	2.48	0.77
1:B:158:ILE:HB	1:B:213:PRO:CG	2.14	0.77
1:D:53:ILE:H	1:D:86:GLY:N	1.81	0.77
1:E:42:LYS:HE2	1:E:42:LYS:H	1.50	0.77
1:E:471:ARG:HE	1:E:484:LEU:HD21	1.50	0.77
1:B:42:LYS:HE2	1:B:42:LYS:H	1.50	0.77
1:D:161:GLY:HA3	1:D:179:VAL:HG13	1.66	0.77
1:E:35:ILE:CG1	1:E:113:ARG:NH1	2.48	0.77
1:A:158:ILE:HD13	1:A:212:SER:OG	1.83	0.77
1:C:721:GLY:CA	2:C:803:ATP:C2	2.63	0.77
1:F:141:GLU:HG2	1:F:171:ALA:N	1.94	0.77
1:A:35:ILE:CG1	1:A:113:ARG:NH1	2.48	0.77
1:B:42:LYS:HE2	1:B:42:LYS:N	1.99	0.77
1:B:363:GLU:O	1:B:366:VAL:N	2.17	0.77
1:C:42:LYS:H	1:C:42:LYS:HE2	1.50	0.77
1:C:371:LEU:O	1:C:375:ASP:HB2	1.85	0.77
1:A:142:CYS:SG	1:A:144:GLU:CD	2.62	0.77
1:B:429:ARG:HD3	3:B:802:NDT:H211	1.64	0.77
1:C:42:LYS:HE2	1:C:42:LYS:N	1.99	0.77
1:C:78:GLY:HA3	1:C:211:LEU:HD13	1.66	0.77
1:C:161:GLY:HA3	1:C:179:VAL:HG13	1.66	0.77
1:D:242:LEU:HB3	1:D:298:VAL:HG22	1.65	0.77
1:E:142:CYS:SG	1:E:144:GLU:CD	2.62	0.77
1:E:142:CYS:SG	1:E:144:GLU:OE1	2.42	0.77
1:F:35:ILE:CG1	1:F:113:ARG:NH1	2.47	0.77
1:D:160:PRO:HG3	1:D:238:LEU:CD1	2.15	0.77
1:C:320:LEU:H	1:C:320:LEU:HD22	1.50	0.76
1:F:46:LYS:HE3	1:F:46:LYS:CA	2.15	0.76
1:F:292:LYS:CE	2:F:801:ATP:O3G	2.33	0.76
1:A:159:MET:HG2	1:A:236:TYR:CZ	2.05	0.76
1:C:35:ILE:CG1	1:C:113:ARG:NH1	2.47	0.76
1:D:65:PRO:HA	1:D:85:ALA:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:668:ALA:HA	1:D:671:ARG:HH12	1.50	0.76
1:A:270:LEU:HG	1:F:481:LYS:HD3	1.67	0.76
1:C:46:LYS:HE3	1:C:46:LYS:CA	2.15	0.76
1:C:127:THR:O	1:C:184:SER:CB	2.29	0.76
1:E:46:LYS:HE3	1:E:46:LYS:CA	2.15	0.76
1:E:519:GLY:N	2:E:803:ATP:HN62	1.83	0.76
1:A:65:PRO:HA	1:A:85:ALA:HB2	1.67	0.76
1:B:157:VAL:HG11	1:B:215:PHE:O	1.85	0.76
1:B:454:GLY:HA3	2:B:801:ATP:C2	2.21	0.76
1:A:142:CYS:SG	1:A:144:GLU:OE1	2.42	0.76
1:B:142:CYS:SG	1:B:144:GLU:CD	2.62	0.76
1:C:80:LEU:HD21	1:C:211:LEU:CD1	2.13	0.76
1:D:35:ILE:CG1	1:D:113:ARG:NH1	2.47	0.76
1:D:271:PHE:HE2	1:D:277:SER:C	1.83	0.76
1:E:161:GLY:HA3	1:E:179:VAL:HG13	1.66	0.76
1:F:161:GLY:HA3	1:F:179:VAL:HG13	1.66	0.76
1:C:142:CYS:SG	1:C:144:GLU:OE1	2.42	0.76
1:D:77:ASN:CG	1:D:209:PHE:HB2	2.06	0.76
1:A:141:GLU:HG2	1:A:171:ALA:N	1.94	0.76
1:A:454:GLY:CA	2:A:801:ATP:N7	2.48	0.76
1:B:46:LYS:HE3	1:B:46:LYS:CA	2.15	0.76
1:B:437:LEU:HD22	1:B:437:LEU:N	2.01	0.76
1:E:39:HIS:NE2	1:E:99:SER:CB	2.49	0.76
1:A:218:ARG:CA	1:A:221:SER:OG	2.34	0.76
1:D:42:LYS:HE2	1:D:42:LYS:H	1.50	0.76
1:E:149:GLN:NE2	1:E:219:LYS:NZ	2.32	0.76
1:E:437:LEU:HD22	1:E:437:LEU:N	2.01	0.76
1:F:29:LYS:HD3	1:F:56:ASN:OD1	1.72	0.76
1:F:561:CYS:CB	1:F:721:GLY:H	1.99	0.76
1:A:73:LYS:HD2	1:A:108:LEU:HD23	1.68	0.75
1:B:429:ARG:NE	3:B:802:NDT:C18	2.48	0.75
1:A:294:MET:SD	2:A:801:ATP:H2	2.08	0.75
1:C:79:ILE:H	1:C:211:LEU:CG	1.92	0.75
1:C:471:ARG:HE	1:C:484:LEU:HD21	1.51	0.75
1:E:78:GLY:N	1:E:211:LEU:HD21	1.67	0.75
3:E:804:NDT:C7	1:F:673:GLY:HA3	2.15	0.75
1:A:65:PRO:HA	1:A:85:ALA:CB	2.17	0.75
1:A:426:GLN:HE22	3:A:802:NDT:C20	1.98	0.75
1:B:617:GLU:OE2	2:B:803:ATP:O3G	2.04	0.75
1:D:65:PRO:HA	1:D:85:ALA:CB	2.17	0.75
1:D:73:LYS:HD2	1:D:108:LEU:HD23	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:ILE:HG22	1:F:212:SER:HG	1.36	0.75
1:F:561:CYS:HB3	1:F:721:GLY:H	1.50	0.75
1:A:127:THR:O	1:A:184:SER:CB	2.29	0.75
1:B:280:ARG:HH11	1:B:383:VAL:H	1.31	0.75
1:C:65:PRO:HA	1:C:85:ALA:HB2	1.67	0.75
1:D:39:HIS:NE2	1:D:99:SER:CB	2.49	0.75
1:D:64:ASN:O	1:D:67:SER:OG	2.04	0.75
1:D:218:ARG:CA	1:D:221:SER:OG	2.34	0.75
1:D:224:ILE:N	1:D:224:ILE:HD12	2.02	0.75
1:F:39:HIS:NE2	1:F:99:SER:CB	2.49	0.75
1:A:53:ILE:O	1:A:86:GLY:CA	2.32	0.75
1:B:65:PRO:HA	1:B:85:ALA:HB2	1.67	0.75
1:B:471:ARG:HE	1:B:484:LEU:HD21	1.52	0.75
1:C:218:ARG:CA	1:C:221:SER:OG	2.34	0.75
1:D:46:LYS:HE3	1:D:46:LYS:CA	2.15	0.75
1:C:561:CYS:O	2:C:803:ATP:N3	2.19	0.75
1:E:268:PRO:HG3	1:E:382:LYS:NZ	2.02	0.75
1:A:39:HIS:NE2	1:A:99:SER:CB	2.49	0.75
1:B:65:PRO:HA	1:B:85:ALA:CB	2.17	0.75
1:C:130:THR:HG22	1:C:182:ASP:O	1.87	0.75
1:D:155:SER:OG	1:D:156:GLY:N	2.15	0.75
1:B:263:ILE:HG12	1:B:271:PHE:CE1	2.21	0.75
1:E:262:GLU:OE1	1:E:266:HIS:HD2	1.70	0.75
1:A:149:GLN:NE2	1:A:219:LYS:HZ1	1.85	0.75
1:E:65:PRO:HA	1:E:85:ALA:HB2	1.67	0.75
1:E:130:THR:HG22	1:E:182:ASP:O	1.87	0.75
1:A:42:LYS:HE2	1:A:42:LYS:H	1.50	0.74
3:A:802:NDT:C21	1:B:276:VAL:HG12	2.17	0.74
1:C:65:PRO:HA	1:C:85:ALA:CB	2.17	0.74
1:C:78:GLY:HA3	1:C:211:LEU:HD22	1.40	0.74
1:E:64:ASN:O	1:E:67:SER:OG	2.04	0.74
1:F:224:ILE:N	1:F:224:ILE:HD12	2.02	0.74
1:F:64:ASN:O	1:F:67:SER:OG	2.04	0.74
1:A:224:ILE:N	1:A:224:ILE:HD12	2.02	0.74
1:C:224:ILE:HD12	1:C:224:ILE:N	2.02	0.74
1:E:218:ARG:CA	1:E:221:SER:OG	2.34	0.74
1:A:280:ARG:NH2	1:A:380:ALA:O	2.21	0.74
1:A:469:ILE:HD11	1:B:270:LEU:HD21	1.70	0.74
1:B:77:ASN:OD1	1:B:209:PHE:HD1	1.67	0.74
1:B:224:ILE:HD12	1:B:224:ILE:N	2.02	0.74
1:B:263:ILE:HG23	1:B:264:PRO:CD	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:GLY:N	1:C:211:LEU:HD22	1.68	0.74
1:D:166:ASN:HD21	1:D:169:THR:HG21	1.46	0.74
1:F:163:ILE:HD12	1:F:163:ILE:N	2.02	0.74
1:F:559:PRO:HB3	1:F:660:ASN:HD21	1.50	0.74
1:B:39:HIS:NE2	1:B:99:SER:CB	2.49	0.74
1:B:218:ARG:CA	1:B:221:SER:OG	2.34	0.74
1:C:39:HIS:NE2	1:C:99:SER:CB	2.49	0.74
1:D:130:THR:HG22	1:D:182:ASP:O	1.87	0.74
1:E:29:LYS:HD3	1:E:56:ASN:OD1	1.72	0.74
1:F:65:PRO:HA	1:F:85:ALA:HB2	1.67	0.74
1:F:65:PRO:HA	1:F:85:ALA:CB	2.17	0.74
1:C:163:ILE:HD12	1:C:163:ILE:N	2.02	0.74
1:D:177:ASP:N	1:D:177:ASP:OD1	2.20	0.74
1:E:224:ILE:HD12	1:E:224:ILE:N	2.02	0.74
1:F:159:MET:CE	1:F:159:MET:HA	2.17	0.74
1:B:130:THR:HG22	1:B:182:ASP:O	1.87	0.74
1:B:429:ARG:NH2	3:B:802:NDT:C16	2.50	0.74
1:E:465:VAL:CG1	1:F:271:PHE:CE1	2.71	0.74
1:A:130:THR:HG22	1:A:182:ASP:O	1.87	0.74
1:A:166:ASN:CG	1:A:169:THR:HG22	2.00	0.74
1:B:73:LYS:HD2	1:B:108:LEU:HD23	1.69	0.74
1:E:65:PRO:HA	1:E:85:ALA:CB	2.17	0.74
1:E:160:PRO:HG3	1:E:238:LEU:CD1	2.12	0.74
1:F:166:ASN:OD1	1:F:169:THR:CG2	2.30	0.74
1:F:218:ARG:CA	1:F:221:SER:OG	2.34	0.74
1:A:29:LYS:HD3	1:A:56:ASN:OD1	1.72	0.74
1:B:35:ILE:HB	1:B:113:ARG:NH1	2.03	0.74
1:C:280:ARG:NH2	1:C:380:ALA:O	2.21	0.74
1:C:692:ILE:HD11	2:C:803:ATP:HN61	1.53	0.74
1:A:673:GLY:N	3:F:804:NDT:H7	2.03	0.74
1:B:177:ASP:N	1:B:177:ASP:OD1	2.20	0.74
1:B:429:ARG:HD3	3:B:802:NDT:C19	2.18	0.74
1:D:465:VAL:HG11	1:E:271:PHE:CE1	2.21	0.74
1:E:166:ASN:HD22	1:E:176:ILE:H	1.36	0.74
1:D:427:PHE:O	1:D:430:MET:HG2	1.88	0.73
1:E:218:ARG:HH21	1:E:218:ARG:CA	2.01	0.73
1:F:519:GLY:HA3	2:F:803:ATP:HN62	1.50	0.73
1:A:519:GLY:CA	2:A:803:ATP:HN62	1.99	0.73
1:E:73:LYS:HD2	1:E:108:LEU:HD23	1.69	0.73
3:E:802:NDT:H7	1:F:402:PRO:C	2.08	0.73
1:F:127:THR:O	1:F:184:SER:CB	2.29	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:HD23	1:A:211:LEU:O	1.88	0.73
1:C:73:LYS:HD2	1:C:108:LEU:HD23	1.69	0.73
1:D:35:ILE:HB	1:D:113:ARG:NH1	2.03	0.73
1:E:426:GLN:NE2	1:E:461:CYS:SG	2.61	0.73
1:F:563:LYS:HB3	2:F:803:ATP:PB	2.28	0.73
1:B:166:ASN:HD22	1:B:176:ILE:H	1.36	0.73
1:D:722:ALA:HB1	3:D:804:NDT:C5	2.18	0.73
1:E:35:ILE:HB	1:E:113:ARG:NH1	2.03	0.73
1:A:159:MET:CB	1:A:213:PRO:CG	2.66	0.73
1:A:177:ASP:N	1:A:177:ASP:OD1	2.20	0.73
1:B:218:ARG:HH21	1:B:218:ARG:CA	2.01	0.73
1:D:53:ILE:O	1:D:86:GLY:CA	2.32	0.73
1:F:166:ASN:HD22	1:F:176:ILE:H	1.36	0.73
1:F:218:ARG:HH21	1:F:218:ARG:CA	2.01	0.73
1:B:280:ARG:HD2	1:B:383:VAL:O	1.88	0.73
1:C:35:ILE:HB	1:C:113:ARG:NH1	2.03	0.73
1:D:163:ILE:HD12	1:D:163:ILE:N	2.02	0.73
1:D:166:ASN:CG	1:D:169:THR:HG22	2.01	0.73
1:D:429:ARG:CZ	3:D:802:NDT:C16	2.63	0.73
1:F:72:GLY:HA3	1:F:115:GLU:HB2	1.69	0.73
1:A:35:ILE:HB	1:A:113:ARG:NH1	2.03	0.73
1:A:455:ALA:N	2:A:801:ATP:C8	2.43	0.73
1:D:363:GLU:O	1:D:366:VAL:N	2.20	0.73
1:E:37:ARG:CD	1:E:337:TYR:CD2	2.72	0.73
1:A:440:GLU:OE1	1:A:440:GLU:N	2.18	0.73
1:C:166:ASN:HD22	1:C:176:ILE:H	1.36	0.73
1:E:50:THR:OG1	1:E:84:ARG:CD	2.37	0.73
1:A:50:THR:OG1	1:A:84:ARG:HD2	1.89	0.73
1:B:64:ASN:O	1:B:67:SER:OG	2.04	0.73
1:C:128:LYS:CG	1:C:184:SER:HB2	2.19	0.73
1:C:271:PHE:CE1	1:C:277:SER:N	2.46	0.73
1:D:563:LYS:HB2	2:D:803:ATP:O1B	1.89	0.73
1:D:722:ALA:CB	3:D:804:NDT:C5	2.67	0.73
1:F:160:PRO:HG3	1:F:238:LEU:CD1	2.15	0.73
1:B:50:THR:OG1	1:B:84:ARG:CD	2.37	0.72
1:B:163:ILE:HD12	1:B:163:ILE:N	2.02	0.72
1:C:50:THR:OG1	1:C:84:ARG:CD	2.37	0.72
1:D:77:ASN:OD1	1:D:209:PHE:HB2	1.87	0.72
1:F:50:THR:OG1	1:F:84:ARG:HD2	1.89	0.72
1:A:271:PHE:CZ	1:A:277:SER:O	2.42	0.72
1:A:431:SER:O	1:A:435:HIS:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:THR:OG1	1:B:84:ARG:HD2	1.89	0.72
1:B:160:PRO:CA	1:B:238:LEU:CD1	2.66	0.72
1:C:177:ASP:OD1	1:C:177:ASP:N	2.20	0.72
1:D:128:LYS:CG	1:D:184:SER:HB2	2.19	0.72
1:F:130:THR:HG22	1:F:182:ASP:O	1.87	0.72
1:D:77:ASN:OD1	1:D:209:PHE:HB3	1.90	0.72
1:E:50:THR:OG1	1:E:84:ARG:HD2	1.89	0.72
1:F:35:ILE:HB	1:F:113:ARG:NH1	2.03	0.72
1:F:375:ASP:OD2	1:F:404:ARG:NH2	2.22	0.72
1:A:98:LEU:C	1:A:102:ILE:HD13	2.08	0.72
1:B:77:ASN:HD21	1:B:209:PHE:C	1.93	0.72
1:C:64:ASN:O	1:C:67:SER:OG	2.04	0.72
1:D:50:THR:OG1	1:D:84:ARG:HD2	1.89	0.72
1:F:280:ARG:NH2	1:F:380:ALA:O	2.22	0.72
1:A:163:ILE:HD12	1:A:163:ILE:N	2.02	0.72
1:D:271:PHE:CE2	1:D:278:PRO:CB	2.71	0.72
1:F:559:PRO:CB	1:F:660:ASN:ND2	2.51	0.72
1:A:402:PRO:HA	1:A:406:ASP:HB3	1.71	0.72
1:B:128:LYS:CG	1:B:184:SER:HB2	2.19	0.72
1:C:149:GLN:NE2	1:C:219:LYS:NZ	2.32	0.72
1:E:402:PRO:HA	1:E:406:ASP:HB3	1.72	0.72
1:F:50:THR:OG1	1:F:84:ARG:CD	2.37	0.72
1:F:177:ASP:OD1	1:F:177:ASP:N	2.21	0.72
1:D:166:ASN:HD22	1:D:176:ILE:H	1.36	0.72
1:D:218:ARG:HH21	1:D:218:ARG:CA	2.01	0.72
1:B:53:ILE:O	1:B:86:GLY:CA	2.32	0.72
1:C:563:LYS:CG	2:C:803:ATP:O3G	2.34	0.72
1:D:37:ARG:NH1	1:D:306:HIS:ND1	2.37	0.72
1:D:722:ALA:HB1	3:D:804:NDT:C6	2.20	0.72
1:C:78:GLY:CA	1:C:211:LEU:HD23	1.82	0.72
1:E:210:TYR:HE1	1:E:214:PRO:HD3	0.90	0.72
1:C:167:LEU:HD22	1:C:167:LEU:H	1.55	0.72
1:D:50:THR:OG1	1:D:84:ARG:CD	2.37	0.72
1:D:143:MET:H	1:D:143:MET:HE3	1.53	0.72
1:D:242:LEU:CD1	1:D:297:ARG:CB	2.68	0.72
1:D:559:PRO:HB3	1:D:660:ASN:HD21	1.55	0.72
1:E:58:LEU:CD2	1:E:85:ALA:CB	2.64	0.72
1:A:128:LYS:CG	1:A:184:SER:HB2	2.19	0.71
1:A:158:ILE:CD1	1:A:212:SER:CB	2.43	0.71
1:A:270:LEU:HD21	1:F:481:LYS:HD3	1.71	0.71
1:C:269:THR:HA	1:C:272:SER:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:PHE:CE2	1:D:277:SER:O	2.42	0.71
1:A:50:THR:OG1	1:A:84:ARG:CD	2.37	0.71
1:C:69:CYS:O	1:C:82:ILE:CD1	2.38	0.71
1:D:69:CYS:O	1:D:82:ILE:CD1	2.38	0.71
1:E:37:ARG:HG3	1:E:337:TYR:HE2	1.54	0.71
1:E:80:LEU:CD2	1:E:211:LEU:CD1	2.68	0.71
1:E:438:ASP:OD1	1:E:440:GLU:N	2.23	0.71
1:E:466:MET:SD	1:F:271:PHE:HZ	2.12	0.71
3:E:804:NDT:C7	1:F:673:GLY:HA2	2.14	0.71
1:F:70:THR:O	1:F:79:ILE:CD1	2.33	0.71
1:F:561:CYS:HB3	1:F:721:GLY:N	2.05	0.71
1:B:166:ASN:O	1:B:167:LEU:C	2.29	0.71
1:C:50:THR:OG1	1:C:84:ARG:HD2	1.89	0.71
2:C:803:ATP:H8	3:C:804:NDT:O2	1.74	0.71
1:E:177:ASP:OD1	1:E:177:ASP:N	2.20	0.71
1:A:159:MET:HE2	1:A:182:ASP:CA	1.98	0.71
1:A:218:ARG:HH21	1:A:218:ARG:CA	2.01	0.71
1:C:218:ARG:HH21	1:C:218:ARG:CA	2.01	0.71
1:F:69:CYS:O	1:F:82:ILE:CD1	2.38	0.71
1:F:248:GLY:H	2:F:801:ATP:N6	1.88	0.71
1:A:69:CYS:O	1:A:82:ILE:CD1	2.38	0.71
1:A:166:ASN:HD22	1:A:176:ILE:H	1.36	0.71
1:A:431:SER:O	1:A:435:HIS:CD2	2.43	0.71
1:B:518:ILE:HD11	1:B:565:LEU:HD22	1.73	0.71
1:D:163:ILE:CD1	1:D:163:ILE:H	2.02	0.71
1:F:210:TYR:HE1	1:F:213:PRO:C	1.92	0.71
1:F:624:ASP:CB	1:F:629:SER:CB	2.67	0.71
1:A:270:LEU:O	1:A:270:LEU:HD22	1.90	0.71
1:B:127:THR:O	1:B:184:SER:CB	2.29	0.71
1:E:127:THR:O	1:E:184:SER:CB	2.29	0.71
1:F:419:ARG:NE	1:F:449:THR:O	2.24	0.71
1:D:242:LEU:CB	1:D:301:ASN:HD22	2.04	0.71
1:E:167:LEU:HD22	1:E:167:LEU:H	1.55	0.71
1:F:160:PRO:CG	1:F:238:LEU:CD1	2.54	0.71
1:A:166:ASN:O	1:A:167:LEU:C	2.29	0.71
1:B:166:ASN:OD1	1:B:169:THR:CG2	2.30	0.71
1:B:429:ARG:NH1	3:B:802:NDT:C19	2.53	0.71
1:B:558:PRO:HG2	1:B:683:PRO:HD3	1.71	0.71
1:C:79:ILE:N	1:C:211:LEU:HD21	2.01	0.71
1:B:236:TYR:HB2	1:B:238:LEU:HG	1.73	0.71
1:F:167:LEU:H	1:F:167:LEU:HD22	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:CYS:O	1:B:82:ILE:CD1	2.38	0.71
1:D:167:LEU:H	1:D:167:LEU:HD22	1.55	0.71
1:E:69:CYS:O	1:E:82:ILE:CD1	2.38	0.71
1:A:64:ASN:O	1:A:67:SER:OG	2.04	0.70
1:E:163:ILE:HD12	1:E:163:ILE:N	2.02	0.70
1:E:166:ASN:O	1:E:167:LEU:C	2.29	0.70
1:F:210:TYR:CD1	1:F:213:PRO:CA	2.73	0.70
1:A:102:ILE:CD1	1:A:102:ILE:H	1.96	0.70
1:B:109:ILE:HD12	1:B:307:VAL:HG21	1.71	0.70
1:D:244:TYR:CE2	1:D:302:THR:HG21	2.26	0.70
1:A:270:LEU:CD2	1:F:481:LYS:CD	2.68	0.70
1:E:107:ASN:CG	1:E:241:PRO:HD3	2.12	0.70
1:E:429:ARG:HD2	3:E:802:NDT:C18	2.18	0.70
1:A:167:LEU:H	1:A:167:LEU:HD22	1.55	0.70
1:D:551:LYS:HZ1	1:D:650:LEU:HB2	1.56	0.70
1:E:128:LYS:CG	1:E:184:SER:HB2	2.19	0.70
1:E:262:GLU:CG	1:E:266:HIS:CG	2.67	0.70
1:A:159:MET:N	1:A:160:PRO:HD3	2.04	0.70
1:B:143:MET:H	1:B:143:MET:HE3	1.56	0.70
1:C:77:ASN:C	1:C:211:LEU:HD23	2.00	0.70
1:E:721:GLY:HA3	2:E:803:ATP:C2	2.26	0.70
1:F:563:LYS:CE	1:F:659:THR:O	2.39	0.70
1:A:294:MET:HE2	2:A:801:ATP:C2	2.23	0.70
1:C:76:GLU:HG3	1:C:76:GLU:O	1.91	0.70
1:C:510:MET:HB3	1:C:568:LYS:HD2	1.72	0.70
1:A:211:LEU:HD21	1:A:238:LEU:HD22	0.73	0.70
1:B:76:GLU:HG3	1:B:76:GLU:O	1.91	0.70
1:D:127:THR:O	1:D:184:SER:CB	2.29	0.70
3:E:802:NDT:H8	1:F:403:GLY:CA	2.20	0.70
1:B:159:MET:CA	1:B:213:PRO:CB	2.68	0.70
1:C:452:TYR:CZ	1:C:500:PRO:HG3	2.27	0.70
1:D:166:ASN:O	1:D:167:LEU:C	2.29	0.70
1:D:427:PHE:O	1:D:430:MET:CG	2.39	0.70
1:E:184:SER:O	1:E:185:ASP:HB3	1.92	0.70
1:E:265:LEU:HD11	1:E:384:VAL:HG12	1.72	0.70
1:F:291:GLY:N	2:F:801:ATP:O1A	2.25	0.70
1:A:149:GLN:HE21	1:A:219:LYS:HZ2	1.38	0.70
1:A:429:ARG:HH11	3:A:802:NDT:C16	2.03	0.70
1:B:167:LEU:HD22	1:B:167:LEU:H	1.54	0.70
1:C:80:LEU:CD2	1:C:211:LEU:HD11	2.10	0.70
1:D:270:LEU:C	1:D:270:LEU:HD13	2.11	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:LYS:HE3	1:C:270:LEU:CB	2.21	0.70
1:C:233:ASN:HB3	1:C:236:TYR:CE2	2.27	0.70
1:C:291:GLY:CA	2:C:801:ATP:O1A	2.39	0.70
1:E:481:LYS:HD3	1:F:270:LEU:HD13	1.74	0.70
1:F:77:ASN:N	1:F:77:ASN:HD22	1.89	0.70
1:F:163:ILE:CD1	1:F:163:ILE:H	2.02	0.70
1:D:465:VAL:HG11	1:E:271:PHE:CD1	2.27	0.69
1:A:143:MET:H	1:A:143:MET:HE3	1.56	0.69
1:A:184:SER:O	1:A:185:ASP:HB3	1.92	0.69
1:A:471:ARG:HE	1:A:484:LEU:HD21	1.56	0.69
1:B:208:LEU:HD12	1:B:208:LEU:N	2.06	0.69
1:D:79:ILE:C	1:D:211:LEU:HD11	2.13	0.69
1:D:218:ARG:HB2	1:D:221:SER:HB3	1.72	0.69
1:E:163:ILE:CD1	1:E:163:ILE:H	2.03	0.69
1:A:426:GLN:NE2	3:A:802:NDT:C19	2.42	0.69
1:B:692:ILE:HD13	2:B:803:ATP:C6	2.26	0.69
1:C:166:ASN:O	1:C:167:LEU:C	2.29	0.69
1:D:149:GLN:NE2	1:D:219:LYS:NZ	2.32	0.69
1:D:242:LEU:HB2	1:D:301:ASN:HD22	1.57	0.69
1:E:37:ARG:CZ	1:E:337:TYR:HD2	2.05	0.69
1:A:58:LEU:CD2	1:A:85:ALA:CB	2.64	0.69
1:A:209:PHE:CD2	1:A:210:TYR:HE2	2.07	0.69
1:A:363:GLU:O	1:A:366:VAL:N	2.23	0.69
1:E:77:ASN:OD1	1:E:209:PHE:HA	1.92	0.69
1:F:73:LYS:HB2	1:F:113:ARG:O	1.92	0.69
2:A:801:ATP:O3'	3:A:802:NDT:O3	2.06	0.69
1:B:98:LEU:C	1:B:102:ILE:HD13	2.09	0.69
1:B:149:GLN:NE2	1:B:219:LYS:NZ	2.32	0.69
1:B:156:GLY:O	1:B:215:PHE:O	2.10	0.69
1:F:624:ASP:O	1:F:628:SER:N	2.24	0.69
1:B:126:ALA:HB2	1:B:215:PHE:HB3	1.75	0.69
1:B:166:ASN:CG	1:B:169:THR:HG22	2.01	0.69
1:A:76:GLU:HG3	1:A:76:GLU:O	1.91	0.69
1:C:166:ASN:HD21	1:C:169:THR:HG21	1.46	0.69
1:A:218:ARG:HB2	1:A:221:SER:HB3	1.72	0.69
1:A:402:PRO:HB3	1:F:459:ALA:HB2	1.74	0.69
1:A:454:GLY:HA3	2:A:801:ATP:N7	2.06	0.69
1:C:53:ILE:O	1:C:86:GLY:CA	2.32	0.69
1:C:290:THR:O	2:C:801:ATP:C2	2.46	0.69
1:C:419:ARG:NE	1:C:449:THR:O	2.26	0.69
1:D:39:HIS:CE1	1:D:99:SER:HB2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:722:ALA:HB1	3:D:804:NDT:H5	1.75	0.69
1:F:128:LYS:CG	1:F:184:SER:HB2	2.19	0.69
1:F:166:ASN:O	1:F:167:LEU:C	2.29	0.69
1:A:39:HIS:CE1	1:A:99:SER:HB2	2.28	0.69
1:D:148:ILE:HG22	1:D:152:LEU:HD23	1.75	0.69
1:E:76:GLU:HG3	1:E:76:GLU:O	1.91	0.69
1:F:759:ARG:NH1	1:F:761:ILE:O	2.26	0.69
2:B:801:ATP:H8	3:B:802:NDT:O2	1.76	0.69
1:D:76:GLU:O	1:D:76:GLU:HG3	1.91	0.69
1:D:77:ASN:ND2	1:D:209:PHE:CA	2.56	0.69
1:D:159:MET:CB	1:D:213:PRO:HG2	2.23	0.69
1:E:39:HIS:CE1	1:E:99:SER:HB2	2.28	0.69
1:E:466:MET:SD	1:F:271:PHE:CZ	2.86	0.69
1:F:39:HIS:CE1	1:F:99:SER:HB2	2.28	0.69
1:F:184:SER:O	1:F:185:ASP:HB3	1.92	0.69
1:B:721:GLY:HA3	2:B:803:ATP:H2	0.87	0.68
1:B:39:HIS:CE1	1:B:99:SER:HB2	2.28	0.68
1:C:29:LYS:HD3	1:C:56:ASN:OD1	1.72	0.68
1:C:320:LEU:HD22	1:C:320:LEU:N	2.07	0.68
1:F:53:ILE:O	1:F:86:GLY:CA	2.32	0.68
1:A:157:VAL:CG1	1:A:180:ILE:HD12	2.24	0.68
1:B:37:ARG:NH1	1:B:306:HIS:ND1	2.40	0.68
1:C:39:HIS:CE1	1:C:99:SER:HB2	2.28	0.68
2:C:801:ATP:H3'	3:C:802:NDT:C5	2.24	0.68
1:D:271:PHE:CE2	1:D:278:PRO:HB3	2.29	0.68
1:D:58:LEU:HD12	1:D:63:ILE:HD11	1.76	0.68
1:E:452:TYR:CZ	1:E:500:PRO:HG3	2.28	0.68
1:C:363:GLU:O	1:C:366:VAL:N	2.25	0.68
1:F:54:HIS:HD2	1:F:93:VAL:HA	1.59	0.68
1:F:160:PRO:HG2	1:F:212:SER:OG	1.93	0.68
1:A:148:ILE:HG22	1:A:152:LEU:HD23	1.75	0.68
1:B:429:ARG:CG	3:B:802:NDT:C21	2.67	0.68
1:B:519:GLY:O	2:B:803:ATP:N6	2.26	0.68
1:E:138:ASN:CB	1:E:228:LYS:HB3	2.24	0.68
1:E:159:MET:CB	1:E:213:PRO:HG2	2.23	0.68
1:F:58:LEU:HD12	1:F:63:ILE:HD11	1.76	0.68
1:A:81:VAL:CG1	1:A:210:TYR:CD1	2.75	0.68
1:B:37:ARG:HD3	1:B:337:TYR:CD2	2.28	0.68
1:B:212:SER:CB	1:B:213:PRO:CD	2.44	0.68
1:C:148:ILE:HG22	1:C:152:LEU:HD23	1.75	0.68
1:C:438:ASP:HB3	1:C:440:GLU:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:GLY:HA3	1:E:78:GLY:O	1.94	0.68
1:A:58:LEU:CD1	1:A:63:ILE:HG13	2.24	0.68
1:B:54:HIS:HD2	1:B:93:VAL:HA	1.59	0.68
1:B:110:LEU:O	1:B:307:VAL:HG22	1.94	0.68
1:B:163:ILE:CD1	1:B:163:ILE:H	2.03	0.68
1:B:184:SER:O	1:B:185:ASP:HB3	1.92	0.68
1:C:143:MET:H	1:C:143:MET:HE3	1.57	0.68
1:C:184:SER:O	1:C:185:ASP:HB3	1.92	0.68
1:E:58:LEU:HD12	1:E:63:ILE:HD11	1.76	0.68
1:E:77:ASN:ND2	1:E:209:PHE:C	2.44	0.68
1:A:54:HIS:HD2	1:A:93:VAL:HA	1.59	0.68
1:B:280:ARG:HH12	1:B:382:LYS:CA	2.06	0.68
1:D:138:ASN:CB	1:D:228:LYS:HB3	2.24	0.68
1:B:429:ARG:HH11	3:B:802:NDT:C18	2.01	0.68
1:B:622:SER:HB2	1:B:665:ILE:HA	1.75	0.68
1:B:695:LYS:CE	3:B:804:NDT:C17	2.72	0.68
1:C:58:LEU:CD1	1:C:63:ILE:HG13	2.24	0.68
1:E:264:PRO:HD2	1:E:266:HIS:CE1	2.29	0.68
1:F:148:ILE:HG22	1:F:152:LEU:HD23	1.75	0.68
1:A:138:ASN:CB	1:A:228:LYS:HB3	2.24	0.67
1:C:306:HIS:O	1:C:340:SER:HA	1.94	0.67
1:D:58:LEU:CD1	1:D:63:ILE:HG13	2.24	0.67
1:D:104:SER:HG	1:D:163:ILE:HD13	0.71	0.67
1:A:72:GLY:HA3	1:A:78:GLY:O	1.94	0.67
1:B:156:GLY:O	1:B:157:VAL:CB	2.42	0.67
1:D:160:PRO:CA	1:D:238:LEU:CD1	2.72	0.67
1:D:722:ALA:HB2	3:D:804:NDT:H5	1.75	0.67
1:E:58:LEU:CD1	1:E:63:ILE:HG13	2.24	0.67
2:E:803:ATP:H8	3:E:804:NDT:O2	1.77	0.67
1:B:58:LEU:CD1	1:B:63:ILE:HG13	2.24	0.67
1:D:54:HIS:HD2	1:D:93:VAL:HA	1.59	0.67
1:E:54:HIS:HD2	1:E:93:VAL:HA	1.59	0.67
1:F:402:PRO:HA	1:F:406:ASP:HB3	1.75	0.67
1:F:559:PRO:O	2:F:803:ATP:O2B	2.12	0.67
1:A:159:MET:HE3	1:A:159:MET:CA	2.19	0.67
1:C:159:MET:CB	1:C:213:PRO:HG2	2.23	0.67
1:C:166:ASN:OD1	1:C:169:THR:CG2	2.30	0.67
1:F:138:ASN:CB	1:F:228:LYS:HB3	2.24	0.67
1:B:72:GLY:HA3	1:B:78:GLY:O	1.94	0.67
1:B:138:ASN:CB	1:B:228:LYS:HB3	2.24	0.67
1:B:148:ILE:HG22	1:B:152:LEU:HD23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:HIS:HD2	1:C:93:VAL:HA	1.59	0.67
1:C:138:ASN:HB3	1:C:228:LYS:HB3	1.77	0.67
1:C:156:GLY:O	1:C:157:VAL:CB	2.42	0.67
1:C:561:CYS:HB2	2:C:803:ATP:C2	2.29	0.67
1:C:692:ILE:CG1	2:C:803:ATP:N6	2.58	0.67
1:F:159:MET:CG	1:F:236:TYR:CE2	2.36	0.67
1:A:138:ASN:HB3	1:A:228:LYS:HB3	1.77	0.67
1:A:159:MET:H	1:A:160:PRO:CD	2.04	0.67
1:A:564:THR:HG21	2:A:803:ATP:O3G	1.95	0.67
1:B:58:LEU:HD12	1:B:63:ILE:HD11	1.76	0.67
1:B:751:GLU:HG3	1:B:755:LYS:HZ3	1.59	0.67
1:C:78:GLY:CA	1:C:211:LEU:HD22	1.15	0.67
1:F:58:LEU:CD1	1:F:63:ILE:HG13	2.24	0.67
1:F:623:PRO:HG3	1:F:664:GLU:HB3	1.76	0.67
1:B:134:LEU:HD13	1:B:134:LEU:O	1.95	0.67
1:B:159:MET:H	1:B:213:PRO:HB2	0.84	0.67
1:C:72:GLY:HA3	1:C:78:GLY:O	1.94	0.67
1:D:132:GLY:HA2	1:D:227:SER:O	1.95	0.67
1:D:134:LEU:O	1:D:134:LEU:HD13	1.95	0.67
1:E:559:PRO:HG3	1:E:660:ASN:HD21	1.59	0.67
1:C:98:LEU:C	1:C:102:ILE:HD13	2.08	0.67
1:D:184:SER:O	1:D:185:ASP:HB3	1.92	0.67
1:E:241:PRO:HB2	1:E:301:ASN:HB3	1.77	0.67
1:A:157:VAL:HG11	1:A:180:ILE:HD12	1.75	0.67
1:B:132:GLY:HA2	1:B:227:SER:O	1.95	0.67
1:B:280:ARG:HH12	1:B:383:VAL:H	1.40	0.67
1:E:148:ILE:HG22	1:E:152:LEU:HD23	1.75	0.67
2:F:801:ATP:H8	3:F:802:NDT:O3	1.76	0.67
1:A:181:THR:HG22	1:A:232:ALA:CA	2.20	0.67
1:E:156:GLY:O	1:E:157:VAL:CB	2.42	0.67
1:E:218:ARG:CB	1:E:221:SER:CB	2.62	0.67
1:F:519:GLY:HA3	2:F:803:ATP:N6	2.06	0.67
1:A:419:ARG:NE	1:A:449:THR:O	2.28	0.66
1:C:58:LEU:HD12	1:C:63:ILE:HD11	1.76	0.66
1:D:98:LEU:C	1:D:102:ILE:HD13	2.09	0.66
1:E:436:VAL:C	1:E:437:LEU:HD13	2.16	0.66
1:F:363:GLU:HG2	1:F:364:SER:H	1.58	0.66
1:B:481:LYS:HE3	1:C:270:LEU:HB2	1.78	0.66
1:B:704:GLU:HB3	1:B:744:LYS:HD3	1.76	0.66
1:C:181:THR:CG2	1:C:232:ALA:HA	2.21	0.66
1:D:49:CYS:HA	1:D:82:ILE:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:GLY:HA2	1:E:227:SER:O	1.95	0.66
1:E:263:ILE:HD11	1:E:271:PHE:CE2	2.30	0.66
1:F:132:GLY:HA2	1:F:227:SER:O	1.95	0.66
1:F:725:VAL:HG21	3:F:804:NDT:O1	1.95	0.66
1:C:691:GLU:HA	1:C:694:LYS:HE2	1.75	0.66
1:D:270:LEU:HD13	1:D:270:LEU:O	1.95	0.66
1:E:462:ARG:HB2	1:F:276:VAL:HG21	1.77	0.66
1:A:58:LEU:HD12	1:A:63:ILE:HD11	1.76	0.66
1:A:132:GLY:HA2	1:A:227:SER:O	1.95	0.66
1:B:263:ILE:HD12	1:B:263:ILE:O	1.96	0.66
1:C:109:ILE:HD12	1:C:307:VAL:HG21	1.76	0.66
1:F:160:PRO:CA	1:F:238:LEU:CD1	2.73	0.66
1:A:49:CYS:HA	1:A:82:ILE:HG22	1.77	0.66
1:A:159:MET:HB3	1:A:213:PRO:HD2	1.77	0.66
1:D:138:ASN:HB3	1:D:228:LYS:HB3	1.77	0.66
1:E:109:ILE:HD12	1:E:307:VAL:HG21	1.78	0.66
1:E:558:PRO:HG2	1:E:683:PRO:HD3	1.77	0.66
1:C:360:GLY:N	1:C:363:GLU:OE1	2.29	0.66
1:D:181:THR:HG22	1:D:232:ALA:CA	2.20	0.66
1:E:262:GLU:CD	1:E:266:HIS:CD2	2.68	0.66
2:E:801:ATP:H8	3:E:802:NDT:O2	1.78	0.66
1:C:563:LYS:HE3	2:C:803:ATP:PG	2.36	0.66
1:C:627:GLY:O	1:C:628:SER:HB2	1.96	0.66
1:C:744:LYS:HE2	1:C:746:GLU:HG2	1.78	0.66
3:C:802:NDT:H7	1:D:403:GLY:CA	2.16	0.66
1:E:166:ASN:OD1	1:E:169:THR:CG2	2.30	0.66
1:A:81:VAL:HG13	1:A:210:TYR:CE1	2.27	0.66
1:B:419:ARG:NE	1:B:449:THR:O	2.28	0.66
1:C:125:TYR:CD2	1:C:218:ARG:HG2	2.31	0.66
1:D:744:LYS:HE2	1:D:746:GLU:HG2	1.77	0.66
1:F:159:MET:HA	1:F:159:MET:HE3	1.77	0.66
1:A:35:ILE:HD12	1:A:113:ARG:CZ	2.26	0.66
1:B:746:GLU:OE1	1:B:748:ARG:NE	2.28	0.66
2:D:801:ATP:H3'	3:D:802:NDT:C5	2.26	0.66
1:A:134:LEU:HB3	1:A:177:ASP:HB2	1.78	0.66
1:A:209:PHE:CD2	1:A:210:TYR:CD2	2.83	0.66
1:B:58:LEU:CD2	1:B:85:ALA:CB	2.64	0.66
1:B:434:ARG:HH21	1:B:482:PHE:HB3	1.61	0.66
1:C:138:ASN:CB	1:C:228:LYS:HB3	2.24	0.66
1:D:280:ARG:HH21	1:D:383:VAL:H	1.44	0.66
1:F:125:TYR:CD2	1:F:218:ARG:HG2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:149:GLN:NE2	1:F:219:LYS:NZ	2.32	0.66
1:F:563:LYS:HE3	1:F:659:THR:O	1.96	0.66
1:C:117:LYS:HB2	1:C:117:LYS:NZ	2.11	0.65
1:D:72:GLY:HA3	1:D:78:GLY:O	1.94	0.65
1:D:109:ILE:HD12	1:D:307:VAL:HG21	1.78	0.65
1:F:49:CYS:HA	1:F:82:ILE:HG22	1.77	0.65
1:B:160:PRO:HG3	1:B:238:LEU:CD2	2.27	0.65
1:C:49:CYS:HA	1:C:82:ILE:HG22	1.77	0.65
1:F:429:ARG:NH1	3:F:802:NDT:C15	2.59	0.65
1:A:134:LEU:O	1:A:134:LEU:HD13	1.95	0.65
1:B:323:THR:OG1	1:B:365:ARG:NH2	2.29	0.65
1:C:77:ASN:ND2	1:C:209:PHE:O	2.30	0.65
1:D:270:LEU:O	1:D:270:LEU:HD22	1.95	0.65
1:E:98:LEU:C	1:E:102:ILE:HD13	2.08	0.65
1:E:102:ILE:CD1	1:E:102:ILE:H	1.96	0.65
1:F:130:THR:HG23	1:F:182:ASP:H	1.62	0.65
1:F:134:LEU:O	1:F:134:LEU:HD13	1.95	0.65
1:A:117:LYS:HB2	1:A:117:LYS:NZ	2.11	0.65
1:B:117:LYS:HB2	1:B:117:LYS:NZ	2.11	0.65
1:B:160:PRO:HA	1:B:238:LEU:HD13	1.76	0.65
1:B:160:PRO:CA	1:B:238:LEU:HD13	2.27	0.65
1:D:563:LYS:HE3	2:D:803:ATP:PG	2.36	0.65
1:F:507:PHE:CE2	1:F:604:LYS:HD3	2.32	0.65
1:A:152:LEU:HD12	1:A:153:ASP:HB3	1.79	0.65
1:A:360:GLY:N	1:A:363:GLU:OE1	2.29	0.65
1:B:68:PHE:O	1:B:120:GLN:HG2	1.97	0.65
1:B:736:ILE:HG21	1:C:545:LEU:HD21	1.78	0.65
1:E:134:LEU:HD13	1:E:134:LEU:O	1.95	0.65
1:F:68:PHE:O	1:F:120:GLN:HG2	1.97	0.65
1:A:105:VAL:HG12	1:A:158:ILE:HD12	1.77	0.65
1:B:49:CYS:HA	1:B:82:ILE:HG22	1.77	0.65
1:B:469:ILE:CD1	1:C:270:LEU:CD1	2.62	0.65
1:C:623:PRO:HB3	1:C:664:GLU:HB2	1.78	0.65
1:D:117:LYS:HB2	1:D:117:LYS:NZ	2.11	0.65
1:D:268:PRO:O	1:D:269:THR:CB	2.44	0.65
1:E:68:PHE:O	1:E:120:GLN:HG2	1.97	0.65
1:E:152:LEU:HD12	1:E:153:ASP:HB3	1.79	0.65
1:E:159:MET:HB3	1:E:213:PRO:CG	2.27	0.65
1:F:138:ASN:HB3	1:F:228:LYS:HB3	1.77	0.65
1:F:563:LYS:HB3	2:F:803:ATP:O2B	1.96	0.65
1:B:130:THR:HG23	1:B:182:ASP:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:GLU:OE2	1:B:266:HIS:CD2	2.50	0.65
1:C:132:GLY:HA2	1:C:227:SER:O	1.95	0.65
1:C:160:PRO:CB	1:C:238:LEU:HD11	2.03	0.65
1:C:622:SER:HB2	1:C:665:ILE:HA	1.77	0.65
1:D:277:SER:HB3	1:D:278:PRO:CD	2.26	0.65
1:D:722:ALA:HB1	3:D:804:NDT:H6	1.78	0.65
1:E:622:SER:HB2	1:E:665:ILE:HA	1.77	0.65
1:F:152:LEU:HD12	1:F:153:ASP:HB3	1.79	0.65
1:B:138:ASN:HB3	1:B:228:LYS:HB3	1.77	0.65
1:C:134:LEU:O	1:C:134:LEU:HD13	1.95	0.65
1:C:429:ARG:CB	3:C:802:NDT:H212	2.26	0.65
1:C:534:LEU:HB2	1:C:535:PRO:HD3	1.78	0.65
1:C:564:THR:HB	2:C:803:ATP:PA	2.37	0.65
1:F:156:GLY:C	1:F:157:VAL:HG12	2.03	0.65
1:A:123:PRO:HG2	1:A:216:ILE:HG13	1.79	0.65
1:B:139:ILE:HG23	1:B:226:PHE:HE1	1.62	0.65
1:B:721:GLY:C	2:B:803:ATP:N3	2.49	0.65
1:C:134:LEU:HB3	1:C:177:ASP:HB2	1.78	0.65
1:C:507:PHE:CE2	1:C:604:LYS:HD3	2.32	0.65
1:E:138:ASN:HB3	1:E:228:LYS:HB3	1.77	0.65
1:E:604:LYS:O	1:E:608:ALA:HB2	1.97	0.65
1:A:130:THR:HG23	1:A:182:ASP:H	1.62	0.65
1:C:35:ILE:HD12	1:C:113:ARG:CZ	2.26	0.65
1:C:159:MET:HB3	1:C:213:PRO:CG	2.27	0.65
1:D:68:PHE:O	1:D:120:GLN:HG2	1.97	0.65
1:D:134:LEU:HB3	1:D:177:ASP:HB2	1.78	0.65
1:E:130:THR:HG23	1:E:182:ASP:H	1.62	0.65
1:F:98:LEU:C	1:F:102:ILE:HD13	2.08	0.65
1:F:692:ILE:HD11	2:F:803:ATP:N1	2.11	0.65
1:B:134:LEU:HB3	1:B:177:ASP:HB2	1.78	0.64
1:C:53:ILE:CD1	1:C:116:LEU:HD21	2.28	0.64
1:C:78:GLY:HA2	1:C:211:LEU:CD2	0.28	0.64
1:C:117:LYS:HB2	1:C:117:LYS:HZ3	1.61	0.64
1:C:609:ALA:HB1	1:C:610:PRO:HD2	1.79	0.64
1:D:159:MET:HB3	1:D:213:PRO:CG	2.27	0.64
1:F:359:SER:OG	1:F:363:GLU:OE1	2.10	0.64
1:A:68:PHE:O	1:A:120:GLN:HG2	1.97	0.64
1:A:139:ILE:HG23	1:A:226:PHE:HE1	1.62	0.64
1:B:53:ILE:CD1	1:B:116:LEU:HD21	2.27	0.64
1:B:89:GLU:OE1	1:B:89:GLU:HA	1.97	0.64
1:C:152:LEU:HD12	1:C:153:ASP:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:VAL:HG12	1:C:180:ILE:N	2.12	0.64
1:C:515:TRP:HE1	1:C:573:GLU:HG3	1.62	0.64
1:C:545:LEU:HD23	1:C:547:ILE:HD12	1.78	0.64
1:D:123:PRO:HG2	1:D:216:ILE:HG13	1.79	0.64
1:E:89:GLU:OE1	1:E:89:GLU:HA	1.97	0.64
1:F:181:THR:HG22	1:F:232:ALA:CA	2.20	0.64
1:A:209:PHE:CE2	1:A:210:TYR:CE2	2.86	0.64
1:A:670:LEU:HD11	1:A:678:HIS:CE1	2.32	0.64
1:B:565:LEU:HD13	3:B:804:NDT:O2	1.95	0.64
1:D:125:TYR:CD2	1:D:218:ARG:HG2	2.31	0.64
1:E:49:CYS:HA	1:E:82:ILE:HG22	1.77	0.64
1:E:158:ILE:HG22	1:E:213:PRO:O	1.98	0.64
1:F:134:LEU:HB3	1:F:177:ASP:HB2	1.78	0.64
1:A:110:LEU:O	1:A:307:VAL:HG22	1.97	0.64
1:B:179:VAL:HG12	1:B:180:ILE:N	2.12	0.64
1:C:126:ALA:HB2	1:C:215:PHE:CB	2.28	0.64
1:E:149:GLN:NE2	1:E:219:LYS:HZ2	1.92	0.64
1:E:465:VAL:HG11	1:F:271:PHE:CD1	2.32	0.64
1:A:126:ALA:HB2	1:A:215:PHE:CB	2.28	0.64
1:A:159:MET:CE	1:A:159:MET:HA	2.22	0.64
1:A:481:LYS:HE2	1:B:270:LEU:HD12	1.79	0.64
1:A:664:GLU:OE1	1:A:664:GLU:N	2.31	0.64
1:B:270:LEU:HD23	1:B:270:LEU:C	2.17	0.64
1:C:68:PHE:O	1:C:120:GLN:HG2	1.97	0.64
1:C:89:GLU:OE1	1:C:89:GLU:HA	1.97	0.64
1:D:53:ILE:CD1	1:D:116:LEU:HD21	2.28	0.64
1:E:53:ILE:CD1	1:E:116:LEU:HD21	2.27	0.64
1:F:53:ILE:C	1:F:86:GLY:HA3	2.18	0.64
1:F:73:LYS:HB3	1:F:114:LEU:HA	1.78	0.64
1:F:181:THR:CG2	1:F:232:ALA:HA	2.21	0.64
1:A:125:TYR:HE2	1:A:218:ARG:CD	2.05	0.64
1:C:130:THR:HG23	1:C:182:ASP:H	1.62	0.64
1:E:166:ASN:HB3	1:E:175:SER:HB2	1.80	0.64
1:E:247:VAL:O	1:E:425:LYS:NZ	2.29	0.64
1:F:53:ILE:CD1	1:F:116:LEU:HD21	2.28	0.64
1:A:481:LYS:CE	1:B:270:LEU:HD12	2.28	0.64
1:B:102:ILE:CD1	1:B:102:ILE:H	1.96	0.64
1:B:160:PRO:CA	1:B:238:LEU:HD11	2.27	0.64
1:B:481:LYS:HE2	1:C:270:LEU:CD2	1.91	0.64
1:E:181:THR:CG2	1:E:232:ALA:HA	2.22	0.64
1:F:564:THR:HG21	1:F:616:ASP:OD1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PRO:HG2	1:B:216:ILE:HG13	1.79	0.64
1:B:125:TYR:CD2	1:B:218:ARG:HG2	2.31	0.64
1:D:179:VAL:HG12	1:D:180:ILE:N	2.12	0.64
1:D:363:GLU:HG2	1:D:364:SER:H	1.62	0.64
1:F:179:VAL:HG12	1:F:180:ILE:N	2.12	0.64
1:F:435:HIS:HB2	1:F:486:VAL:HB	1.78	0.64
1:F:622:SER:OG	1:F:623:PRO:HD3	1.97	0.64
1:A:179:VAL:HG12	1:A:180:ILE:N	2.12	0.64
1:C:139:ILE:HG23	1:C:226:PHE:HE1	1.62	0.64
1:E:126:ALA:HB2	1:E:215:PHE:CB	2.28	0.64
1:F:126:ALA:HB2	1:F:215:PHE:CB	2.28	0.64
1:F:452:TYR:CZ	1:F:500:PRO:HG3	2.33	0.64
1:B:125:TYR:HE2	1:B:218:ARG:CD	2.05	0.64
1:B:181:THR:HG22	1:B:232:ALA:CA	2.20	0.64
1:D:117:LYS:HB2	1:D:117:LYS:HZ3	1.62	0.64
1:D:125:TYR:CE2	1:D:218:ARG:HD3	2.32	0.64
1:D:274:PHE:H	1:D:274:PHE:HD1	1.46	0.64
1:E:37:ARG:NE	1:E:337:TYR:CD2	2.66	0.64
1:E:53:ILE:C	1:E:86:GLY:HA3	2.18	0.64
1:F:166:ASN:HB3	1:F:175:SER:HB2	1.80	0.64
1:A:455:ALA:HA	2:A:801:ATP:H8	1.62	0.63
1:B:158:ILE:HG23	1:B:214:PRO:HA	1.80	0.63
1:E:73:LYS:CE	1:E:112:ASP:OD2	2.36	0.63
1:E:117:LYS:HZ3	1:E:117:LYS:HB2	1.61	0.63
1:E:277:SER:HB3	1:E:278:PRO:CD	2.28	0.63
1:F:73:LYS:CB	1:F:113:ARG:O	2.46	0.63
1:F:143:MET:H	1:F:143:MET:HE3	1.63	0.63
2:A:803:ATP:H3'	3:A:804:NDT:C5	2.28	0.63
1:C:158:ILE:HG22	1:C:213:PRO:O	1.98	0.63
1:C:181:THR:HG22	1:C:232:ALA:CA	2.20	0.63
1:D:126:ALA:HB2	1:D:215:PHE:CB	2.28	0.63
1:D:166:ASN:OD1	1:D:169:THR:CG2	2.30	0.63
1:D:166:ASN:HB3	1:D:175:SER:HB2	1.80	0.63
1:D:697:THR:HA	1:D:700:PHE:HD2	1.62	0.63
1:E:280:ARG:NH2	1:E:380:ALA:O	2.27	0.63
1:B:532:ILE:HG21	1:B:570:LEU:HD11	1.79	0.63
1:E:125:TYR:CE2	1:E:218:ARG:HD3	2.32	0.63
1:F:125:TYR:CE2	1:F:218:ARG:HD3	2.33	0.63
1:F:471:ARG:HE	1:F:484:LEU:HD21	1.63	0.63
1:F:519:GLY:O	2:F:803:ATP:N6	2.31	0.63
1:B:212:SER:HB3	1:B:213:PRO:HD3	1.74	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ASN:HB3	1:C:175:SER:HB2	1.80	0.63
1:C:435:HIS:ND1	1:C:437:LEU:HG	2.12	0.63
1:D:35:ILE:HD12	1:D:113:ARG:CZ	2.26	0.63
1:E:134:LEU:HB3	1:E:177:ASP:HB2	1.78	0.63
1:A:371:LEU:O	1:A:375:ASP:HB2	1.99	0.63
1:A:469:ILE:HD12	1:B:270:LEU:HD11	1.79	0.63
1:C:695:LYS:HZ3	3:C:804:NDT:C17	2.10	0.63
1:E:143:MET:H	1:E:143:MET:HE3	1.63	0.63
1:E:181:THR:HG22	1:E:232:ALA:CA	2.20	0.63
1:F:117:LYS:HB2	1:F:117:LYS:NZ	2.11	0.63
1:B:166:ASN:HB3	1:B:175:SER:HB2	1.80	0.63
1:C:125:TYR:HE2	1:C:218:ARG:CD	2.05	0.63
1:D:110:LEU:CB	1:D:306:HIS:HA	2.28	0.63
1:D:152:LEU:HD12	1:D:153:ASP:HB3	1.79	0.63
1:E:179:VAL:HG12	1:E:180:ILE:N	2.12	0.63
1:E:561:CYS:CB	2:E:803:ATP:C2	2.81	0.63
1:F:89:GLU:OE1	1:F:89:GLU:HA	1.97	0.63
1:A:160:PRO:HG3	1:A:238:LEU:CD1	2.28	0.63
1:A:436:VAL:CG1	1:A:486:VAL:O	2.45	0.63
1:B:117:LYS:HB2	1:B:117:LYS:HZ3	1.64	0.63
1:B:735:ALA:HB2	1:B:745:VAL:HG23	1.81	0.63
1:E:80:LEU:CD2	1:E:211:LEU:HD13	2.28	0.63
1:E:123:PRO:HG2	1:E:216:ILE:HG13	1.79	0.63
1:F:102:ILE:HD12	1:F:102:ILE:N	2.05	0.63
1:F:110:LEU:O	1:F:307:VAL:HG22	1.99	0.63
1:F:139:ILE:HG23	1:F:226:PHE:HE1	1.62	0.63
1:B:35:ILE:HD12	1:B:113:ARG:CZ	2.26	0.63
1:B:98:LEU:H	1:B:98:LEU:CD2	2.12	0.63
1:C:49:CYS:O	1:C:82:ILE:CB	2.47	0.63
1:D:242:LEU:CD1	1:D:297:ARG:HB3	2.29	0.63
1:D:562:SER:N	2:D:803:ATP:C2	2.67	0.63
1:E:139:ILE:HG23	1:E:226:PHE:HE1	1.62	0.63
1:A:89:GLU:OE1	1:A:89:GLU:HA	1.97	0.63
1:B:152:LEU:HD12	1:B:153:ASP:HB3	1.79	0.63
1:D:139:ILE:HG23	1:D:226:PHE:HE1	1.62	0.63
1:D:563:LYS:CE	2:D:803:ATP:O3G	2.36	0.63
1:F:98:LEU:H	1:F:98:LEU:CD2	2.12	0.63
1:F:266:HIS:C	1:F:268:PRO:HD3	2.19	0.63
1:F:751:GLU:HG3	1:F:755:LYS:HZ3	1.63	0.63
1:A:53:ILE:CD1	1:A:116:LEU:HD21	2.28	0.62
1:A:166:ASN:O	1:A:167:LEU:O	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ILE:HD12	1:B:82:ILE:N	2.07	0.62
1:B:105:VAL:HG13	1:B:160:PRO:HB2	1.81	0.62
1:D:402:PRO:HA	1:D:406:ASP:HB3	1.79	0.62
1:E:82:ILE:HD12	1:E:82:ILE:N	2.07	0.62
1:E:229:GLU:HG2	1:E:229:GLU:O	1.99	0.62
1:F:35:ILE:HD12	1:F:113:ARG:CZ	2.26	0.62
1:F:49:CYS:O	1:F:82:ILE:CB	2.47	0.62
1:F:159:MET:HB2	1:F:213:PRO:HG2	1.81	0.62
1:A:166:ASN:HB3	1:A:175:SER:HB2	1.80	0.62
1:B:49:CYS:O	1:B:82:ILE:CB	2.47	0.62
1:C:125:TYR:CE2	1:C:218:ARG:HD3	2.32	0.62
1:D:58:LEU:CD2	1:D:85:ALA:CB	2.64	0.62
1:F:166:ASN:O	1:F:167:LEU:O	2.17	0.62
1:B:102:ILE:HD12	1:B:102:ILE:N	2.05	0.62
1:B:291:GLY:N	2:B:801:ATP:O1A	2.32	0.62
1:B:510:MET:HB3	1:B:568:LYS:HD2	1.81	0.62
1:C:532:ILE:HG21	1:C:570:LEU:HD11	1.81	0.62
1:D:130:THR:HG23	1:D:182:ASP:H	1.62	0.62
1:A:149:GLN:HA	1:A:152:LEU:HG	1.82	0.62
1:C:166:ASN:O	1:C:167:LEU:O	2.17	0.62
1:D:166:ASN:O	1:D:167:LEU:O	2.17	0.62
1:D:719:TYR:CD1	1:D:759:ARG:HB3	2.34	0.62
1:F:622:SER:HB2	1:F:665:ILE:HA	1.80	0.62
1:A:270:LEU:HD23	1:F:481:LYS:HD3	1.81	0.62
1:A:294:MET:HE2	2:A:801:ATP:N3	2.14	0.62
1:A:437:LEU:HD21	1:A:488:LEU:N	2.15	0.62
1:C:163:ILE:CG2	1:C:177:ASP:HB3	2.30	0.62
1:D:98:LEU:H	1:D:98:LEU:CD2	2.12	0.62
1:D:163:ILE:CG2	1:D:177:ASP:HB3	2.30	0.62
1:E:35:ILE:HD12	1:E:113:ARG:CZ	2.26	0.62
1:E:519:GLY:CA	2:E:803:ATP:HN62	2.11	0.62
1:F:77:ASN:HD22	1:F:77:ASN:H	1.46	0.62
1:F:229:GLU:HG2	1:F:229:GLU:O	2.00	0.62
1:F:435:HIS:CE1	1:F:437:LEU:HB2	2.35	0.62
1:F:624:ASP:O	1:F:628:SER:CA	2.47	0.62
1:A:110:LEU:CB	1:A:306:HIS:HA	2.29	0.62
1:A:125:TYR:CD2	1:A:218:ARG:HG2	2.31	0.62
1:B:166:ASN:O	1:B:167:LEU:O	2.17	0.62
2:E:801:ATP:H3'	3:E:802:NDT:C5	2.30	0.62
1:F:157:VAL:O	1:F:157:VAL:HG22	2.00	0.62
1:F:210:TYR:CE1	1:F:213:PRO:CA	2.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ILE:C	1:B:86:GLY:HA3	2.18	0.62
1:B:125:TYR:CE2	1:B:218:ARG:HD3	2.32	0.62
1:B:229:GLU:O	1:B:229:GLU:HG2	2.00	0.62
1:C:105:VAL:HG13	1:C:160:PRO:HB2	1.81	0.62
1:C:293:THR:HB	2:C:801:ATP:O2A	1.98	0.62
1:D:158:ILE:HG22	1:D:213:PRO:O	1.98	0.62
1:D:229:GLU:O	1:D:229:GLU:HG2	1.99	0.62
1:F:123:PRO:HG2	1:F:216:ILE:HG13	1.79	0.62
1:F:125:TYR:HE2	1:F:218:ARG:CD	2.05	0.62
1:C:228:LYS:O	1:C:228:LYS:HD3	2.00	0.62
1:C:248:GLY:H	2:C:801:ATP:HN62	1.48	0.62
1:D:49:CYS:O	1:D:82:ILE:CB	2.47	0.62
1:D:53:ILE:CD1	1:D:116:LEU:CD2	2.78	0.62
1:D:89:GLU:OE1	1:D:89:GLU:HA	1.97	0.62
1:D:218:ARG:NH2	1:D:218:ARG:HB3	2.15	0.62
1:E:166:ASN:O	1:E:167:LEU:O	2.17	0.62
1:E:609:ALA:HB1	1:E:610:PRO:HD2	1.81	0.62
1:F:105:VAL:HG13	1:F:160:PRO:HB2	1.81	0.62
1:F:218:ARG:NH2	1:F:218:ARG:HB3	2.15	0.62
1:A:218:ARG:NH2	1:A:218:ARG:HB3	2.15	0.62
1:C:218:ARG:CB	1:C:221:SER:CB	2.62	0.62
1:D:77:ASN:ND2	1:D:209:PHE:HB2	2.14	0.62
1:E:218:ARG:HB2	1:E:221:SER:HB3	1.72	0.62
1:A:81:VAL:HG13	1:A:210:TYR:CD1	2.34	0.62
1:A:452:TYR:CZ	1:A:500:PRO:HG3	2.34	0.62
1:B:218:ARG:CB	1:B:221:SER:CB	2.62	0.62
1:D:74:ILE:O	1:D:74:ILE:HG23	2.00	0.62
1:D:102:ILE:HD12	1:D:102:ILE:N	2.05	0.62
2:D:803:ATP:H3'	3:D:804:NDT:C4	2.29	0.62
1:F:218:ARG:CB	1:F:221:SER:CB	2.62	0.62
1:A:105:VAL:HG13	1:A:160:PRO:HB2	1.81	0.61
1:A:125:TYR:CE2	1:A:218:ARG:HD3	2.32	0.61
1:A:228:LYS:O	1:A:228:LYS:HD3	2.00	0.61
1:B:157:VAL:HG22	1:B:157:VAL:O	2.00	0.61
1:C:229:GLU:HG2	1:C:229:GLU:O	2.00	0.61
1:D:79:ILE:C	1:D:211:LEU:CD1	2.69	0.61
1:D:560:GLY:H	2:D:803:ATP:PB	2.23	0.61
1:E:105:VAL:HG13	1:E:160:PRO:HB2	1.81	0.61
1:E:157:VAL:HG22	1:E:157:VAL:O	2.00	0.61
1:E:160:PRO:CB	1:E:238:LEU:HD12	2.17	0.61
1:F:110:LEU:HB3	1:F:306:HIS:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HB3	1:A:306:HIS:HA	1.81	0.61
1:A:455:ALA:HA	2:A:801:ATP:C8	2.35	0.61
1:C:759:ARG:HB2	1:C:761:ILE:HG22	1.81	0.61
1:D:53:ILE:C	1:D:86:GLY:HA3	2.18	0.61
1:D:149:GLN:HA	1:D:152:LEU:HG	1.82	0.61
1:D:181:THR:CG2	1:D:232:ALA:HA	2.22	0.61
1:E:98:LEU:CD2	1:E:98:LEU:H	2.12	0.61
1:E:360:GLY:N	1:E:363:GLU:OE1	2.31	0.61
1:F:564:THR:O	1:F:564:THR:HG22	2.00	0.61
1:A:163:ILE:CD1	1:A:163:ILE:H	2.03	0.61
1:A:218:ARG:CB	1:A:221:SER:CB	2.62	0.61
1:B:149:GLN:HA	1:B:152:LEU:HG	1.82	0.61
1:C:157:VAL:O	1:C:157:VAL:HG22	2.00	0.61
1:C:163:ILE:CD1	1:C:163:ILE:H	2.02	0.61
1:C:320:LEU:H	1:C:320:LEU:CD2	2.12	0.61
1:E:125:TYR:CD2	1:E:218:ARG:HG2	2.31	0.61
1:E:218:ARG:NH2	1:E:218:ARG:HB3	2.15	0.61
1:F:228:LYS:O	1:F:228:LYS:HD3	2.00	0.61
1:F:593:GLU:OE2	1:F:596:ARG:NH2	2.25	0.61
1:F:692:ILE:CG1	2:F:803:ATP:C6	2.83	0.61
1:A:98:LEU:H	1:A:98:LEU:CD2	2.12	0.61
1:A:209:PHE:HD2	1:A:210:TYR:CE2	2.09	0.61
1:A:229:GLU:O	1:A:229:GLU:HG2	1.99	0.61
1:A:733:LEU:HD11	1:B:550:PRO:HG3	1.82	0.61
1:B:163:ILE:CG2	1:B:177:ASP:HB3	2.30	0.61
1:C:149:GLN:HA	1:C:152:LEU:HG	1.82	0.61
1:D:228:LYS:O	1:D:228:LYS:HD3	2.00	0.61
1:E:49:CYS:O	1:E:82:ILE:CB	2.47	0.61
1:E:577:ASN:O	1:E:611:SER:OG	2.16	0.61
1:F:218:ARG:HB2	1:F:221:SER:HB3	1.72	0.61
1:A:49:CYS:O	1:A:82:ILE:CB	2.47	0.61
1:A:53:ILE:CD1	1:A:116:LEU:CD2	2.78	0.61
1:B:159:MET:HE3	1:B:183:ALA:H	1.65	0.61
1:C:82:ILE:HD12	1:C:82:ILE:N	2.07	0.61
1:D:105:VAL:HG13	1:D:160:PRO:HB2	1.81	0.61
1:D:266:HIS:O	1:D:268:PRO:HD2	2.00	0.61
1:D:328:ARG:HG2	1:D:373:LEU:HD21	1.83	0.61
1:E:262:GLU:CD	1:E:266:HIS:HB3	2.20	0.61
1:F:73:LYS:CE	1:F:112:ASP:OD2	2.45	0.61
1:F:74:ILE:HG23	1:F:74:ILE:O	2.01	0.61
1:B:53:ILE:CD1	1:B:116:LEU:CD2	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ARG:NH2	1:C:218:ARG:HB3	2.15	0.61
1:C:518:ILE:HD11	1:C:569:ALA:HB2	1.82	0.61
1:E:77:ASN:CG	1:E:208:LEU:O	2.38	0.61
1:E:268:PRO:HB3	1:E:381:GLY:O	2.01	0.61
1:B:74:ILE:HG23	1:B:74:ILE:O	2.00	0.61
1:B:600:GLU:HG3	1:B:603:ARG:HH21	1.65	0.61
1:E:149:GLN:HA	1:E:152:LEU:HG	1.82	0.61
1:F:53:ILE:CD1	1:F:116:LEU:CD2	2.78	0.61
1:F:82:ILE:HD12	1:F:82:ILE:N	2.07	0.61
1:A:53:ILE:C	1:A:86:GLY:HA3	2.18	0.61
1:A:74:ILE:HG23	1:A:74:ILE:O	2.00	0.61
1:A:166:ASN:OD1	1:A:169:THR:CG2	2.30	0.61
1:A:609:ALA:HB1	1:A:610:PRO:HD2	1.82	0.61
2:A:803:ATP:H8	3:A:804:NDT:O3	1.84	0.61
1:B:160:PRO:CB	1:B:238:LEU:CD1	2.78	0.61
1:B:218:ARG:NH2	1:B:218:ARG:HB3	2.15	0.61
1:E:117:LYS:HB2	1:E:117:LYS:NZ	2.11	0.61
1:E:228:LYS:O	1:E:228:LYS:HD3	2.00	0.61
1:E:434:ARG:CD	1:F:273:SER:CB	2.78	0.61
1:F:72:GLY:CA	1:F:115:GLU:HB2	2.30	0.61
1:F:158:ILE:HG21	1:F:212:SER:CB	2.30	0.61
1:F:163:ILE:CG2	1:F:177:ASP:HB3	2.30	0.61
1:A:163:ILE:CG2	1:A:177:ASP:HB3	2.30	0.61
2:A:801:ATP:H1'	3:A:802:NDT:H5	1.83	0.61
1:B:481:LYS:CB	1:C:270:LEU:HD21	2.31	0.61
2:C:803:ATP:H3'	3:C:804:NDT:C4	2.29	0.61
2:D:801:ATP:H3'	3:D:802:NDT:C4	2.31	0.61
1:A:159:MET:SD	1:A:182:ASP:OD2	2.58	0.61
1:B:158:ILE:CG2	1:B:214:PRO:HA	2.30	0.61
1:F:746:GLU:OE1	1:F:748:ARG:NE	2.32	0.61
1:C:98:LEU:H	1:C:98:LEU:CD2	2.12	0.60
1:C:123:PRO:HG2	1:C:216:ILE:HG13	1.79	0.60
1:F:160:PRO:CA	1:F:238:LEU:HD11	2.31	0.60
1:B:228:LYS:O	1:B:228:LYS:HD3	2.00	0.60
1:C:53:ILE:C	1:C:86:GLY:HA3	2.18	0.60
1:C:111:GLY:CA	1:C:306:HIS:CE1	2.84	0.60
1:C:290:THR:O	2:C:801:ATP:H2	1.83	0.60
1:D:264:PRO:O	1:D:268:PRO:HB3	2.02	0.60
1:F:35:ILE:CB	1:F:113:ARG:NH1	2.64	0.60
1:F:149:GLN:HA	1:F:152:LEU:HG	1.82	0.60
1:F:159:MET:HG2	1:F:236:TYR:CE1	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:MET:CE	2:A:801:ATP:N3	2.64	0.60
1:A:726:LEU:HD22	1:B:672:PRO:HB3	1.82	0.60
1:B:664:GLU:N	1:B:664:GLU:OE2	2.33	0.60
1:D:35:ILE:CB	1:D:113:ARG:NH1	2.64	0.60
1:E:210:TYR:HE1	1:E:214:PRO:CD	1.70	0.60
1:B:211:LEU:HD22	1:B:211:LEU:N	2.17	0.60
1:B:263:ILE:CG1	1:B:271:PHE:HE1	2.10	0.60
1:B:609:ALA:HB1	1:B:610:PRO:HD2	1.81	0.60
1:C:166:ASN:CG	1:C:169:THR:HG22	2.01	0.60
1:E:74:ILE:HG23	1:E:74:ILE:O	2.00	0.60
1:E:125:TYR:HE2	1:E:218:ARG:CD	2.05	0.60
1:E:126:ALA:HB2	1:E:215:PHE:HB3	1.84	0.60
1:E:163:ILE:CG2	1:E:177:ASP:HB3	2.30	0.60
1:E:542:PHE:O	1:E:546:GLY:N	2.34	0.60
1:F:159:MET:CB	1:F:213:PRO:CG	2.73	0.60
1:C:74:ILE:HG23	1:C:74:ILE:O	2.00	0.60
1:C:126:ALA:HB2	1:C:215:PHE:HB3	1.84	0.60
1:C:719:TYR:CD1	1:C:759:ARG:HB3	2.37	0.60
1:E:102:ILE:HD12	1:E:102:ILE:N	2.05	0.60
1:E:139:ILE:O	1:E:139:ILE:HG22	2.01	0.60
1:E:469:ILE:CG1	1:F:270:LEU:HD21	2.31	0.60
1:E:670:LEU:HD11	1:E:678:HIS:CE1	2.37	0.60
3:E:802:NDT:C7	1:F:403:GLY:N	2.38	0.60
1:A:49:CYS:O	1:A:82:ILE:CG2	2.50	0.60
1:B:49:CYS:O	1:B:82:ILE:CG2	2.50	0.60
1:C:49:CYS:O	1:C:82:ILE:CG2	2.50	0.60
1:C:88:GLU:HG2	1:C:90:VAL:HG12	1.83	0.60
1:E:88:GLU:HG2	1:E:90:VAL:HG12	1.83	0.60
1:E:465:VAL:CG2	1:F:274:PHE:CD2	2.78	0.60
1:F:267:GLN:N	1:F:268:PRO:HD3	2.17	0.60
1:F:609:ALA:HB1	1:F:610:PRO:HD2	1.82	0.60
1:A:126:ALA:HB2	1:A:215:PHE:HB3	1.84	0.60
1:B:695:LYS:HZ3	3:B:804:NDT:H16	1.61	0.60
1:C:726:LEU:HD22	1:D:672:PRO:HB3	1.82	0.60
1:E:149:GLN:NE2	1:E:219:LYS:HZ1	1.97	0.60
1:E:465:VAL:CG1	1:F:271:PHE:CD1	2.85	0.60
1:F:244:TYR:CD1	1:F:254:ILE:HD11	2.37	0.60
1:A:274:PHE:CD1	1:F:434:ARG:HD3	2.37	0.60
1:B:218:ARG:HB2	1:B:221:SER:HB3	1.72	0.60
1:C:35:ILE:CB	1:C:113:ARG:NH1	2.64	0.60
1:C:160:PRO:CG	1:C:238:LEU:CD2	2.78	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:TYR:HE2	1:D:218:ARG:CD	2.05	0.60
1:D:157:VAL:O	1:D:157:VAL:HG22	2.00	0.60
1:A:35:ILE:CB	1:A:113:ARG:NH1	2.64	0.60
1:B:52:TYR:CA	1:B:86:GLY:HA2	2.32	0.60
1:C:52:TYR:CA	1:C:86:GLY:HA2	2.32	0.60
1:C:218:ARG:HB2	1:C:221:SER:HB3	1.72	0.60
1:D:126:ALA:HB2	1:D:215:PHE:HB3	1.84	0.60
1:E:53:ILE:CD1	1:E:116:LEU:CD2	2.78	0.60
1:F:126:ALA:HB2	1:F:215:PHE:HB3	1.84	0.60
1:B:35:ILE:CB	1:B:113:ARG:NH1	2.64	0.59
1:B:270:LEU:HD23	1:B:270:LEU:O	2.02	0.59
1:D:88:GLU:HG2	1:D:90:VAL:HG12	1.84	0.59
2:D:801:ATP:H8	3:D:802:NDT:O2	1.84	0.59
1:E:49:CYS:O	1:E:82:ILE:CG2	2.50	0.59
1:F:532:ILE:HD13	1:F:570:LEU:HD11	1.82	0.59
1:F:624:ASP:HB3	1:F:629:SER:CB	2.29	0.59
1:F:719:TYR:CD1	1:F:759:ARG:HB3	2.37	0.59
1:A:88:GLU:HG2	1:A:90:VAL:HG12	1.84	0.59
1:A:363:GLU:HG2	1:A:364:SER:H	1.67	0.59
1:A:719:TYR:HB3	1:A:723:GLU:HB2	1.84	0.59
1:B:139:ILE:O	1:B:139:ILE:HG22	2.01	0.59
1:C:363:GLU:HG2	1:C:364:SER:H	1.67	0.59
1:D:423:LEU:HD21	1:D:457:LEU:HD12	1.84	0.59
1:D:426:GLN:OE1	3:D:802:NDT:H19	2.02	0.59
1:D:452:TYR:CE1	1:D:500:PRO:HG3	2.37	0.59
1:E:261:ILE:HD13	1:E:386:ILE:HD11	1.85	0.59
1:F:49:CYS:O	1:F:82:ILE:CG2	2.50	0.59
1:F:563:LYS:HE2	1:F:659:THR:C	2.23	0.59
1:D:49:CYS:O	1:D:82:ILE:CG2	2.50	0.59
1:D:110:LEU:HB3	1:D:306:HIS:HA	1.83	0.59
1:D:139:ILE:O	1:D:139:ILE:HG22	2.01	0.59
1:A:52:TYR:CA	1:A:86:GLY:HA2	2.32	0.59
1:A:401:ARG:HB2	1:A:404:ARG:HD3	1.84	0.59
1:A:426:GLN:OE1	3:A:802:NDT:H211	2.01	0.59
1:C:746:GLU:OE1	1:C:748:ARG:NE	2.35	0.59
1:D:609:ALA:HB1	1:D:610:PRO:HD2	1.83	0.59
1:E:534:LEU:HB2	1:E:535:PRO:HD3	1.84	0.59
1:F:139:ILE:HG22	1:F:139:ILE:O	2.01	0.59
1:D:52:TYR:CA	1:D:86:GLY:HA2	2.32	0.59
1:F:680:TYR:HE1	1:F:769:TYR:HB3	1.68	0.59
1:B:110:LEU:HB3	1:B:306:HIS:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:THR:O	1:B:225:THR:OG1	2.19	0.59
1:B:363:GLU:HG2	1:B:364:SER:H	1.67	0.59
1:C:139:ILE:HG22	1:C:139:ILE:O	2.01	0.59
1:C:624:ASP:HB3	1:C:629:SER:OG	2.02	0.59
1:E:139:ILE:HG23	1:E:226:PHE:CE1	2.38	0.59
1:F:52:TYR:CA	1:F:86:GLY:HA2	2.32	0.59
1:F:134:LEU:HD13	1:F:134:LEU:C	2.23	0.59
1:F:564:THR:N	2:F:803:ATP:O2A	2.33	0.59
1:D:110:LEU:O	1:D:307:VAL:HG22	2.01	0.59
1:E:363:GLU:HG2	1:E:364:SER:H	1.67	0.59
1:F:139:ILE:HG23	1:F:226:PHE:CE1	2.38	0.59
1:F:277:SER:HB3	1:F:278:PRO:HD2	1.83	0.59
1:A:54:HIS:CD2	1:A:93:VAL:HA	2.38	0.59
1:A:139:ILE:O	1:A:139:ILE:HG22	2.02	0.59
1:A:270:LEU:HD23	1:F:481:LYS:CD	2.31	0.59
1:A:436:VAL:HG13	1:A:436:VAL:O	2.03	0.59
1:A:673:GLY:CA	3:F:804:NDT:C7	2.63	0.59
1:B:88:GLU:HG2	1:B:90:VAL:HG12	1.83	0.59
1:B:733:LEU:O	1:B:737:MET:HG2	2.02	0.59
2:C:801:ATP:H3'	3:C:802:NDT:C4	2.32	0.59
1:D:71:VAL:O	1:D:71:VAL:HG23	2.03	0.59
1:D:139:ILE:HG23	1:D:226:PHE:CE1	2.38	0.59
1:D:344:ILE:HG22	1:D:347:ILE:HG22	1.83	0.59
1:E:35:ILE:CB	1:E:113:ARG:NH1	2.64	0.59
1:E:37:ARG:CZ	1:E:337:TYR:CD2	2.86	0.59
1:E:623:PRO:HB3	1:E:664:GLU:HB2	1.83	0.59
1:F:73:LYS:NZ	1:F:108:LEU:HA	2.17	0.59
1:F:79:ILE:O	1:F:80:LEU:HG	2.02	0.59
1:F:110:LEU:CB	1:F:306:HIS:HA	2.32	0.59
1:A:139:ILE:HG23	1:A:226:PHE:CE1	2.38	0.59
1:A:746:GLU:OE1	1:A:748:ARG:NE	2.34	0.59
1:C:134:LEU:HD13	1:C:134:LEU:C	2.23	0.59
1:F:158:ILE:HG23	1:F:210:TYR:HE1	1.67	0.59
1:A:158:ILE:CG2	1:A:159:MET:N	2.60	0.59
1:A:181:THR:CG2	1:A:232:ALA:HA	2.22	0.59
1:A:542:PHE:O	1:A:546:GLY:N	2.35	0.59
1:C:561:CYS:HB2	2:C:803:ATP:N3	2.17	0.59
1:E:134:LEU:HD13	1:E:134:LEU:C	2.23	0.59
1:F:88:GLU:HG2	1:F:90:VAL:HG12	1.84	0.59
1:A:218:ARG:HA	1:A:218:ARG:NH2	2.10	0.58
1:A:715:ARG:NH2	1:A:751:GLU:OE1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:THR:CG2	1:B:232:ALA:HA	2.21	0.58
1:B:481:LYS:HD2	1:C:270:LEU:CD1	2.28	0.58
1:D:244:TYR:CD1	1:D:254:ILE:HD11	2.33	0.58
1:E:274:PHE:H	1:E:274:PHE:HD2	1.49	0.58
1:F:670:LEU:HD11	1:F:678:HIS:CE1	2.38	0.58
1:A:519:GLY:O	2:A:803:ATP:N6	2.30	0.58
1:B:77:ASN:OD1	1:B:209:PHE:CG	2.56	0.58
1:B:134:LEU:HD13	1:B:134:LEU:C	2.23	0.58
1:B:312:GLY:HA2	1:B:350:ILE:HD11	1.85	0.58
1:C:58:LEU:CD2	1:C:85:ALA:CB	2.64	0.58
1:C:110:LEU:CB	1:C:306:HIS:HA	2.33	0.58
1:D:261:ILE:HD11	1:D:386:ILE:HD11	1.85	0.58
1:F:434:ARG:HH12	1:F:482:PHE:HD1	1.51	0.58
1:A:719:TYR:CD1	1:A:759:ARG:HB3	2.38	0.58
1:B:139:ILE:HG23	1:B:226:PHE:CE1	2.38	0.58
1:D:271:PHE:CD2	1:D:278:PRO:HB3	2.38	0.58
1:D:563:LYS:CE	2:D:803:ATP:PG	2.92	0.58
1:E:606:ARG:NH2	1:E:648:GLU:OE1	2.33	0.58
1:A:134:LEU:HD13	1:A:134:LEU:C	2.23	0.58
1:A:141:GLU:HG2	1:A:170:LYS:C	1.98	0.58
1:C:53:ILE:HD13	1:C:116:LEU:HD21	1.85	0.58
1:D:134:LEU:HD13	1:D:134:LEU:C	2.23	0.58
1:E:52:TYR:CA	1:E:86:GLY:HA2	2.32	0.58
1:E:393:ASN:HB3	1:E:596:ARG:HH21	1.69	0.58
1:F:285:HIS:NE2	1:F:410:GLU:OE2	2.37	0.58
1:B:54:HIS:CD2	1:B:93:VAL:HA	2.38	0.58
1:B:429:ARG:NE	3:B:802:NDT:H213	2.16	0.58
1:C:110:LEU:HB3	1:C:306:HIS:HA	1.84	0.58
1:C:293:THR:OG1	2:C:801:ATP:O3G	2.15	0.58
1:D:360:GLY:N	1:D:363:GLU:OE1	2.35	0.58
1:F:274:PHE:HD1	1:F:274:PHE:H	1.50	0.58
1:F:519:GLY:N	2:F:803:ATP:HN61	1.82	0.58
1:A:158:ILE:C	1:A:160:PRO:N	2.53	0.58
1:B:110:LEU:CB	1:B:306:HIS:HA	2.33	0.58
1:B:178:VAL:HG23	1:B:178:VAL:O	2.04	0.58
1:B:670:LEU:HD11	1:B:678:HIS:CE1	2.38	0.58
1:E:71:VAL:HG23	1:E:71:VAL:O	2.03	0.58
1:E:617:GLU:OE2	2:E:803:ATP:O1G	2.20	0.58
1:A:46:LYS:H	1:A:46:LYS:HD2	1.69	0.58
1:C:73:LYS:CE	1:C:112:ASP:OD2	2.36	0.58
1:C:139:ILE:HG23	1:C:226:PHE:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:692:ILE:CG1	2:C:803:ATP:HN61	2.16	0.58
1:D:54:HIS:CD2	1:D:93:VAL:HA	2.38	0.58
1:D:218:ARG:CB	1:D:221:SER:CB	2.62	0.58
1:F:363:GLU:O	1:F:365:ARG:N	2.36	0.58
1:A:35:ILE:HB	1:A:113:ARG:HH11	1.69	0.58
1:A:159:MET:HE2	1:A:159:MET:O	2.03	0.58
1:A:178:VAL:O	1:A:178:VAL:HG23	2.04	0.58
1:C:650:LEU:HB3	1:C:653:VAL:HG22	1.86	0.58
1:F:159:MET:CE	1:F:181:THR:O	2.50	0.58
1:A:71:VAL:O	1:A:71:VAL:HG23	2.03	0.58
1:A:622:SER:HB2	1:A:665:ILE:HA	1.86	0.58
1:B:46:LYS:N	1:B:46:LYS:HD2	2.19	0.58
1:B:71:VAL:HG23	1:B:71:VAL:O	2.03	0.58
1:B:532:ILE:HD13	1:B:570:LEU:HD11	1.86	0.58
1:C:688:ALA:O	1:C:692:ILE:HD12	2.03	0.58
1:D:722:ALA:CA	3:D:804:NDT:H5	2.34	0.58
1:E:46:LYS:HD2	1:E:46:LYS:N	2.19	0.58
1:E:46:LYS:HD2	1:E:46:LYS:H	1.69	0.58
1:E:680:TYR:HE1	1:E:769:TYR:HB3	1.67	0.58
1:A:130:THR:CG2	1:A:182:ASP:O	2.52	0.57
1:C:54:HIS:CD2	1:C:93:VAL:HA	2.38	0.57
1:C:166:ASN:ND2	1:C:176:ILE:H	2.02	0.57
1:D:46:LYS:N	1:D:46:LYS:HD2	2.19	0.57
1:E:37:ARG:CG	1:E:337:TYR:CE2	2.87	0.57
1:F:46:LYS:N	1:F:46:LYS:HD2	2.19	0.57
1:F:178:VAL:HG23	1:F:178:VAL:O	2.04	0.57
1:A:209:PHE:HD2	1:A:210:TYR:CD2	2.22	0.57
1:B:77:ASN:HD22	1:B:77:ASN:C	2.06	0.57
1:C:71:VAL:HG23	1:C:71:VAL:O	2.03	0.57
1:C:695:LYS:HZ1	3:C:804:NDT:C21	2.17	0.57
3:C:802:NDT:C7	1:D:403:GLY:HA2	2.18	0.57
1:E:35:ILE:HB	1:E:113:ARG:HH11	1.69	0.57
1:E:469:ILE:HD12	1:F:270:LEU:CD2	2.18	0.57
1:F:58:LEU:CD2	1:F:85:ALA:CB	2.64	0.57
1:A:211:LEU:HD23	1:A:211:LEU:C	2.23	0.57
1:A:707:VAL:HG12	1:A:747:LEU:HD12	1.86	0.57
1:B:73:LYS:CE	1:B:112:ASP:OD2	2.36	0.57
1:C:46:LYS:HD2	1:C:46:LYS:N	2.19	0.57
1:C:53:ILE:CD1	1:C:116:LEU:CD2	2.78	0.57
1:C:159:MET:HE3	1:C:183:ALA:H	1.68	0.57
1:D:130:THR:CG2	1:D:182:ASP:O	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:VAL:HG23	1:D:178:VAL:O	2.04	0.57
1:D:521:GLN:HE21	1:D:524:LEU:HD13	1.69	0.57
1:E:166:ASN:ND2	1:E:176:ILE:H	2.02	0.57
1:E:178:VAL:HG23	1:E:178:VAL:O	2.04	0.57
1:F:367:VAL:O	1:F:371:LEU:HG	2.04	0.57
1:F:619:ASP:HA	1:F:622:SER:OG	2.03	0.57
1:A:46:LYS:HD2	1:A:46:LYS:N	2.19	0.57
1:A:160:PRO:CG	1:A:238:LEU:HD11	2.31	0.57
1:A:680:TYR:HE1	1:A:769:TYR:HB3	1.69	0.57
3:A:802:NDT:H212	1:B:276:VAL:HG12	1.86	0.57
1:C:630:THR:O	1:C:633:ALA:N	2.36	0.57
1:F:46:LYS:HD2	1:F:46:LYS:H	1.69	0.57
1:A:166:ASN:ND2	1:A:176:ILE:H	2.02	0.57
1:B:35:ILE:HB	1:B:113:ARG:HH11	1.69	0.57
1:B:155:SER:HG	1:B:156:GLY:H	1.50	0.57
1:E:465:VAL:HG13	1:F:274:PHE:CD2	2.38	0.57
1:E:527:LYS:O	1:E:531:MET:HG2	2.04	0.57
1:F:285:HIS:ND1	1:F:392:PRO:HG3	2.20	0.57
1:B:281:GLY:O	1:B:407:GLN:HB2	2.05	0.57
1:C:46:LYS:HD2	1:C:46:LYS:H	1.69	0.57
1:D:149:GLN:HE21	1:D:219:LYS:HZ2	1.50	0.57
1:D:271:PHE:HZ	1:D:277:SER:O	1.80	0.57
1:E:37:ARG:HG3	1:E:337:TYR:CE2	2.36	0.57
1:F:341:ILE:HG23	1:F:384:VAL:HG23	1.87	0.57
1:B:130:THR:CG2	1:B:182:ASP:O	2.53	0.57
1:C:131:VAL:HG13	1:C:226:PHE:HA	1.87	0.57
1:C:178:VAL:HG23	1:C:178:VAL:O	2.04	0.57
1:C:233:ASN:HB3	1:C:236:TYR:HD2	1.67	0.57
1:E:131:VAL:HG13	1:E:226:PHE:HA	1.87	0.57
1:F:111:GLY:CA	1:F:306:HIS:CE1	2.88	0.57
1:C:292:LYS:NZ	1:C:390:ASN:HA	2.20	0.57
1:F:166:ASN:CG	1:F:169:THR:HG22	2.01	0.57
1:B:104:SER:HG	1:B:163:ILE:CD1	1.89	0.57
1:B:719:TYR:HB3	1:B:723:GLU:HB2	1.86	0.57
1:E:268:PRO:CG	1:E:382:LYS:HE2	2.34	0.57
1:F:759:ARG:HB2	1:F:761:ILE:HG22	1.86	0.57
1:A:244:TYR:CD1	1:A:254:ILE:HD11	2.40	0.57
1:A:454:GLY:O	2:A:801:ATP:N7	2.33	0.57
1:B:292:LYS:NZ	1:B:390:ASN:HA	2.20	0.57
1:B:589:LYS:HD2	1:C:591:VAL:HG11	1.87	0.57
1:B:759:ARG:NH1	1:B:761:ILE:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:ASP:O	1:C:425:LYS:HG2	2.05	0.57
1:E:37:ARG:NH1	1:E:306:HIS:CG	2.73	0.57
1:E:218:ARG:HA	1:E:218:ARG:NH2	2.10	0.57
1:F:54:HIS:CD2	1:F:93:VAL:HA	2.38	0.57
1:F:166:ASN:ND2	1:F:176:ILE:H	2.02	0.57
1:F:556:TYR:HE1	1:F:678:HIS:HB3	1.68	0.57
1:A:82:ILE:HD12	1:A:82:ILE:N	2.07	0.56
1:A:138:ASN:OD1	1:A:228:LYS:HG2	2.05	0.56
1:D:46:LYS:HD2	1:D:46:LYS:H	1.69	0.56
1:D:248:GLY:N	2:D:801:ATP:N6	2.49	0.56
1:E:244:TYR:CD1	1:E:254:ILE:HD11	2.40	0.56
1:E:719:TYR:CD1	1:E:759:ARG:HB3	2.40	0.56
1:A:34:PHE:HB3	1:A:96:ILE:CG2	2.36	0.56
1:A:328:ARG:HG2	1:A:373:LEU:HD21	1.87	0.56
1:A:647:VAL:HG21	1:F:508:LEU:HD21	1.85	0.56
1:D:35:ILE:HB	1:D:113:ARG:HH11	1.69	0.56
1:D:274:PHE:CD1	1:D:274:PHE:N	2.73	0.56
1:F:73:LYS:CD	1:F:114:LEU:CD2	2.75	0.56
1:F:453:VAL:HG22	1:F:454:GLY:H	1.70	0.56
1:A:426:GLN:OE1	3:A:802:NDT:C19	2.51	0.56
1:A:689:ARG:NH1	1:A:713:ALA:O	2.38	0.56
1:B:46:LYS:HD2	1:B:46:LYS:H	1.69	0.56
1:B:138:ASN:OD1	1:B:228:LYS:HG2	2.05	0.56
1:C:138:ASN:OD1	1:C:228:LYS:HG2	2.05	0.56
1:D:71:VAL:HG12	1:D:116:LEU:HD13	1.87	0.56
1:D:156:GLY:O	1:D:157:VAL:CB	2.42	0.56
1:E:34:PHE:HB3	1:E:96:ILE:CG2	2.36	0.56
1:E:53:ILE:HD13	1:E:116:LEU:HD21	1.86	0.56
1:E:54:HIS:CD2	1:E:93:VAL:HA	2.38	0.56
1:E:138:ASN:OD1	1:E:228:LYS:HG2	2.06	0.56
1:E:274:PHE:CD2	1:E:274:PHE:N	2.73	0.56
1:E:423:LEU:HD21	1:E:457:LEU:HD22	1.88	0.56
1:F:34:PHE:HB3	1:F:96:ILE:CG2	2.35	0.56
1:F:73:LYS:NZ	1:F:108:LEU:CA	2.68	0.56
1:F:131:VAL:HG13	1:F:226:PHE:HA	1.87	0.56
1:F:274:PHE:N	1:F:274:PHE:CD1	2.73	0.56
1:F:434:ARG:HH21	1:F:485:LYS:HA	1.71	0.56
1:F:664:GLU:OE1	1:F:664:GLU:N	2.38	0.56
1:A:131:VAL:HG13	1:A:226:PHE:HA	1.87	0.56
1:B:91:HIS:ND1	1:B:91:HIS:O	2.39	0.56
1:C:34:PHE:HB3	1:C:96:ILE:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:ASN:OD1	1:F:228:LYS:HG2	2.05	0.56
1:A:347:ILE:HG22	1:A:389:THR:HB	1.88	0.56
1:D:138:ASN:OD1	1:D:228:LYS:HG2	2.05	0.56
1:D:242:LEU:HB2	1:D:301:ASN:ND2	2.21	0.56
1:A:163:ILE:HG22	1:A:177:ASP:HB3	1.88	0.56
1:C:71:VAL:HG12	1:C:116:LEU:HD13	1.87	0.56
1:C:347:ILE:HG22	1:C:389:THR:HB	1.86	0.56
1:D:292:LYS:NZ	1:D:390:ASN:HA	2.20	0.56
1:E:37:ARG:NE	1:E:337:TYR:HD2	2.02	0.56
1:E:720:SER:H	1:E:723:GLU:HB3	1.71	0.56
1:F:35:ILE:HB	1:F:113:ARG:HH11	1.69	0.56
1:F:444:TYR:O	1:F:447:SER:OG	2.20	0.56
1:F:604:LYS:O	1:F:608:ALA:HB2	2.06	0.56
1:F:725:VAL:HG11	3:F:804:NDT:C4	2.35	0.56
1:C:58:LEU:HD12	1:C:63:ILE:CD1	2.36	0.56
1:C:212:SER:OG	1:C:238:LEU:CD2	2.47	0.56
1:D:166:ASN:ND2	1:D:176:ILE:H	2.02	0.56
1:E:606:ARG:HH21	1:E:650:LEU:HD11	1.71	0.56
1:A:71:VAL:HG12	1:A:116:LEU:HD13	1.87	0.56
1:A:159:MET:HB3	1:A:213:PRO:HG2	1.81	0.56
1:B:166:ASN:ND2	1:B:176:ILE:H	2.02	0.56
1:B:263:ILE:CG1	1:B:271:PHE:CE1	2.86	0.56
1:B:462:ARG:NH1	1:C:277:SER:O	2.39	0.56
2:C:801:ATP:H8	3:C:802:NDT:O2	1.88	0.56
1:E:435:HIS:HB2	1:E:486:VAL:HB	1.87	0.56
1:E:697:THR:HA	1:E:700:PHE:HD2	1.71	0.56
1:F:127:THR:HG23	1:F:184:SER:O	2.06	0.56
1:F:708:ASP:HB2	1:F:710:HIS:CE1	2.41	0.56
1:A:127:THR:HG23	1:A:184:SER:O	2.06	0.56
1:A:159:MET:HG2	1:A:236:TYR:OH	1.94	0.56
1:C:91:HIS:ND1	1:C:91:HIS:O	2.39	0.56
1:C:130:THR:CG2	1:C:182:ASP:O	2.52	0.56
1:A:91:HIS:ND1	1:A:91:HIS:O	2.39	0.56
1:B:75:GLY:N	1:B:115:GLU:OE2	2.39	0.56
1:B:127:THR:HG23	1:B:184:SER:O	2.06	0.56
1:B:244:TYR:CD1	1:B:254:ILE:HD11	2.41	0.56
1:E:262:GLU:HG3	1:E:266:HIS:CB	2.36	0.56
1:E:530:GLU:O	1:E:534:LEU:HG	2.05	0.56
1:F:70:THR:C	1:F:79:ILE:CD1	2.66	0.56
1:F:692:ILE:HG12	2:F:803:ATP:C6	2.41	0.56
1:B:34:PHE:HB3	1:B:96:ILE:CG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:VAL:HG13	1:B:226:PHE:HA	1.87	0.55
1:B:559:PRO:HG3	1:B:660:ASN:HD21	1.72	0.55
1:C:759:ARG:NH1	1:C:761:ILE:O	2.39	0.55
1:D:127:THR:HG23	1:D:184:SER:O	2.06	0.55
1:D:435:HIS:HB2	1:D:486:VAL:HB	1.87	0.55
1:D:556:TYR:HE1	1:D:678:HIS:HB3	1.70	0.55
1:E:453:VAL:HG22	1:E:454:GLY:H	1.71	0.55
1:E:560:GLY:O	2:E:803:ATP:O1A	2.23	0.55
1:F:76:GLU:OE1	1:F:76:GLU:HA	2.06	0.55
1:F:91:HIS:ND1	1:F:91:HIS:O	2.39	0.55
1:F:686:VAL:HG12	1:F:689:ARG:HH12	1.72	0.55
1:A:159:MET:HB3	1:A:213:PRO:CG	2.35	0.55
1:A:434:ARG:NH1	1:A:434:ARG:HA	2.21	0.55
1:B:71:VAL:HG12	1:B:116:LEU:HD13	1.87	0.55
1:C:75:GLY:N	1:C:115:GLU:OE2	2.39	0.55
1:C:78:GLY:CA	1:C:211:LEU:HD11	2.15	0.55
1:D:90:VAL:HG22	1:D:90:VAL:O	2.07	0.55
1:E:91:HIS:ND1	1:E:91:HIS:O	2.39	0.55
1:E:130:THR:CG2	1:E:182:ASP:O	2.52	0.55
2:E:801:ATP:H3'	3:E:802:NDT:C4	2.36	0.55
1:A:58:LEU:HD12	1:A:63:ILE:CD1	2.36	0.55
1:B:163:ILE:HG22	1:B:177:ASP:HB3	1.88	0.55
1:B:367:VAL:O	1:B:371:LEU:HG	2.06	0.55
1:B:452:TYR:CZ	1:B:500:PRO:HG3	2.40	0.55
1:B:762:THR:HG23	1:B:764:GLU:HG3	1.87	0.55
1:C:35:ILE:HB	1:C:113:ARG:HH11	1.69	0.55
1:C:65:PRO:O	1:C:84:ARG:HA	2.07	0.55
1:C:155:SER:HG	1:C:156:GLY:H	1.50	0.55
1:C:459:ALA:HB2	1:D:402:PRO:HB3	1.88	0.55
1:C:707:VAL:HG12	1:C:747:LEU:HD12	1.87	0.55
1:D:163:ILE:HG22	1:D:177:ASP:HB3	1.88	0.55
1:D:244:TYR:CZ	1:D:302:THR:HG21	2.41	0.55
1:D:444:TYR:CZ	1:D:448:LYS:HE2	2.41	0.55
1:E:58:LEU:HD12	1:E:63:ILE:CD1	2.36	0.55
1:F:37:ARG:CG	1:F:95:VAL:HG21	2.36	0.55
1:F:210:TYR:CD1	1:F:213:PRO:HA	2.42	0.55
1:F:508:LEU:HD23	1:F:582:LYS:HZ1	1.71	0.55
1:F:532:ILE:HG21	1:F:570:LEU:HD11	1.88	0.55
1:F:582:LYS:HA	1:F:616:ASP:HB3	1.88	0.55
1:A:225:THR:OG1	1:A:225:THR:O	2.19	0.55
1:A:292:LYS:NZ	1:A:390:ASN:HA	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ARG:HH12	1:B:383:VAL:N	2.00	0.55
1:C:163:ILE:HG22	1:C:177:ASP:HB3	1.88	0.55
1:E:37:ARG:CG	1:E:95:VAL:HG21	2.36	0.55
1:E:90:VAL:O	1:E:90:VAL:HG22	2.07	0.55
1:F:58:LEU:HD12	1:F:63:ILE:CD1	2.36	0.55
1:F:158:ILE:HG21	1:F:212:SER:HG	1.57	0.55
1:A:37:ARG:CG	1:A:95:VAL:HG21	2.36	0.55
1:A:65:PRO:O	1:A:84:ARG:HA	2.07	0.55
1:A:481:LYS:CD	1:B:270:LEU:CD1	2.84	0.55
1:A:481:LYS:CD	1:B:270:LEU:HG	2.31	0.55
1:A:562:SER:OG	2:A:803:ATP:N3	2.39	0.55
1:B:436:VAL:O	1:B:436:VAL:HG13	2.05	0.55
1:B:676:ASP:O	1:B:678:HIS:ND1	2.37	0.55
1:C:444:TYR:O	1:C:447:SER:OG	2.20	0.55
1:D:65:PRO:O	1:D:84:ARG:HA	2.07	0.55
1:D:75:GLY:N	1:D:115:GLU:OE2	2.39	0.55
1:D:91:HIS:O	1:D:91:HIS:ND1	2.39	0.55
1:D:131:VAL:HG13	1:D:226:PHE:HA	1.87	0.55
1:A:75:GLY:N	1:A:115:GLU:OE2	2.39	0.55
1:B:58:LEU:HD12	1:B:63:ILE:CD1	2.36	0.55
1:B:77:ASN:CG	1:B:209:PHE:O	2.41	0.55
1:B:81:VAL:CG1	1:B:211:LEU:HD12	2.36	0.55
1:C:78:GLY:HA2	1:C:211:LEU:HD22	0.93	0.55
1:C:721:GLY:HA3	2:C:803:ATP:N3	2.21	0.55
1:D:34:PHE:HB3	1:D:96:ILE:CG2	2.36	0.55
1:D:160:PRO:CA	1:D:238:LEU:HD11	2.36	0.55
2:D:803:ATP:H8	3:D:804:NDT:O2	1.89	0.55
1:E:75:GLY:N	1:E:115:GLU:OE2	2.39	0.55
1:E:454:GLY:HA3	2:E:801:ATP:C2	2.42	0.55
1:F:291:GLY:CA	2:F:801:ATP:O1A	2.55	0.55
1:F:563:LYS:N	2:F:803:ATP:O1A	2.38	0.55
1:A:90:VAL:HG22	1:A:90:VAL:O	2.07	0.55
1:B:291:GLY:CA	2:B:801:ATP:O1A	2.55	0.55
1:B:434:ARG:NH2	1:B:482:PHE:HB3	2.21	0.55
1:B:650:LEU:HB3	1:B:653:VAL:HG22	1.89	0.55
1:C:733:LEU:HD23	1:C:736:ILE:HD11	1.89	0.55
1:D:268:PRO:C	1:D:269:THR:CG2	2.69	0.55
1:D:563:LYS:CE	2:D:803:ATP:O1G	2.50	0.55
1:E:159:MET:HE3	1:E:183:ALA:H	1.72	0.55
1:F:90:VAL:HG22	1:F:90:VAL:O	2.07	0.55
1:B:65:PRO:O	1:B:84:ARG:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLY:H	2:B:801:ATP:N6	2.04	0.55
1:C:646:GLY:O	1:C:648:GLU:N	2.39	0.55
1:E:127:THR:HG23	1:E:184:SER:O	2.06	0.55
2:F:801:ATP:H3'	3:F:802:NDT:C4	2.36	0.55
1:A:519:GLY:N	2:A:803:ATP:HN62	2.00	0.55
1:C:690:LEU:O	1:C:694:LYS:HG3	2.07	0.55
1:D:58:LEU:HD12	1:D:63:ILE:CD1	2.36	0.55
1:D:79:ILE:CA	1:D:211:LEU:HD11	2.37	0.55
1:D:79:ILE:N	1:D:211:LEU:HD11	2.19	0.55
1:D:159:MET:HE3	1:D:183:ALA:H	1.72	0.55
1:F:117:LYS:HB2	1:F:117:LYS:HZ3	1.72	0.55
1:C:102:ILE:HD12	1:C:102:ILE:N	2.05	0.55
1:D:37:ARG:CG	1:D:95:VAL:HG21	2.36	0.55
1:D:277:SER:HB3	1:D:278:PRO:HD2	1.88	0.55
1:D:565:LEU:HD13	3:D:804:NDT:O3	2.07	0.55
1:F:130:THR:CG2	1:F:182:ASP:O	2.52	0.55
1:A:401:ARG:HE	1:A:402:PRO:HD2	1.72	0.54
1:B:341:ILE:HG23	1:B:384:VAL:HG23	1.89	0.54
1:C:39:HIS:ND1	1:C:39:HIS:O	2.41	0.54
1:D:247:VAL:HA	2:D:801:ATP:N6	2.22	0.54
1:E:65:PRO:O	1:E:84:ARG:HA	2.07	0.54
1:E:762:THR:HG23	1:E:764:GLU:HG3	1.90	0.54
1:F:287:PRO:HG2	1:F:413:ILE:HG23	1.89	0.54
1:F:374:MET:SD	1:F:404:ARG:HB2	2.47	0.54
1:F:508:LEU:HD23	1:F:582:LYS:NZ	2.22	0.54
1:A:39:HIS:ND1	1:A:39:HIS:O	2.41	0.54
1:A:77:ASN:HD22	1:A:77:ASN:C	2.06	0.54
1:C:593:GLU:OE2	1:C:596:ARG:NH2	2.30	0.54
2:D:803:ATP:C3'	3:D:804:NDT:C4	2.86	0.54
1:E:39:HIS:ND1	1:E:39:HIS:O	2.41	0.54
1:E:71:VAL:HG12	1:E:116:LEU:HD13	1.87	0.54
1:E:262:GLU:OE1	1:E:266:HIS:CD2	2.56	0.54
1:F:76:GLU:O	1:F:211:LEU:HD11	2.06	0.54
1:A:508:LEU:HD23	1:A:582:LYS:NZ	2.22	0.54
1:B:37:ARG:CG	1:B:95:VAL:HG21	2.36	0.54
1:B:50:THR:HG1	1:B:84:ARG:CB	2.20	0.54
1:D:77:ASN:HD22	1:D:77:ASN:C	2.06	0.54
1:D:224:ILE:HD12	1:D:224:ILE:H	1.71	0.54
1:D:366:VAL:HA	1:D:369:THR:HG22	1.88	0.54
1:F:73:LYS:HD2	1:F:114:LEU:HD23	1.86	0.54
1:A:58:LEU:HD12	1:A:63:ILE:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD22	1:A:167:LEU:N	2.22	0.54
1:A:587:PHE:HZ	1:A:621:LEU:HA	1.73	0.54
1:B:39:HIS:O	1:B:39:HIS:ND1	2.41	0.54
1:B:224:ILE:HD12	1:B:224:ILE:H	1.71	0.54
1:B:719:TYR:CD1	1:B:759:ARG:HB3	2.43	0.54
1:C:90:VAL:O	1:C:90:VAL:HG22	2.07	0.54
1:D:158:ILE:HB	1:D:160:PRO:HD2	1.89	0.54
1:F:39:HIS:ND1	1:F:39:HIS:O	2.41	0.54
1:F:218:ARG:HA	1:F:218:ARG:NH2	2.10	0.54
1:A:117:LYS:HB2	1:A:117:LYS:HZ3	1.70	0.54
1:A:751:GLU:HG3	1:A:755:LYS:HZ3	1.72	0.54
1:D:73:LYS:CE	1:D:112:ASP:OD2	2.36	0.54
1:D:285:HIS:NE2	1:D:410:GLU:HG2	2.22	0.54
1:E:462:ARG:CB	1:F:276:VAL:HG21	2.38	0.54
1:F:156:GLY:O	1:F:157:VAL:CB	2.53	0.54
1:F:167:LEU:HD22	1:F:167:LEU:N	2.22	0.54
1:B:363:GLU:O	1:B:365:ARG:N	2.40	0.54
1:B:481:LYS:HB3	1:C:270:LEU:HD21	1.89	0.54
1:C:37:ARG:CG	1:C:95:VAL:HG21	2.36	0.54
1:C:542:PHE:O	1:C:546:GLY:N	2.33	0.54
1:C:670:LEU:HD11	1:C:678:HIS:CE1	2.42	0.54
1:E:128:LYS:N	1:E:222:THR:HG1	2.05	0.54
1:E:377:MET:HE1	1:E:383:VAL:HG21	1.90	0.54
1:F:733:LEU:O	1:F:737:MET:HG2	2.08	0.54
1:A:224:ILE:HD12	1:A:224:ILE:H	1.71	0.54
1:A:481:LYS:HZ3	1:B:270:LEU:HB2	1.72	0.54
1:A:744:LYS:HE2	1:A:746:GLU:HG2	1.90	0.54
1:C:78:GLY:HA2	1:C:211:LEU:CB	2.28	0.54
1:C:556:TYR:HE1	1:C:678:HIS:HB3	1.73	0.54
1:D:39:HIS:ND1	1:D:39:HIS:O	2.41	0.54
1:E:158:ILE:HB	1:E:160:PRO:HD2	1.89	0.54
1:F:744:LYS:HE2	1:F:746:GLU:HG2	1.89	0.54
1:B:158:ILE:HB	1:B:160:PRO:HD2	1.89	0.54
1:B:354:ARG:HD3	1:B:364:SER:HB3	1.90	0.54
1:C:167:LEU:HD22	1:C:167:LEU:N	2.22	0.54
1:C:435:HIS:HB2	1:C:486:VAL:HB	1.89	0.54
1:C:563:LYS:CE	2:C:803:ATP:O1G	2.39	0.54
1:D:671:ARG:HG3	1:D:672:PRO:HD2	1.90	0.54
1:D:689:ARG:HG2	1:D:724:VAL:HG21	1.90	0.54
1:E:73:LYS:HD2	1:E:108:LEU:CD2	2.38	0.54
1:F:159:MET:CE	1:F:159:MET:CA	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:ILE:HD12	1:F:224:ILE:H	1.71	0.54
1:F:426:GLN:OE1	1:F:458:THR:OG1	2.17	0.54
1:A:160:PRO:HB3	1:A:238:LEU:HD12	1.90	0.54
1:A:291:GLY:HA2	2:A:801:ATP:O2A	2.08	0.54
1:B:90:VAL:O	1:B:90:VAL:HG22	2.07	0.54
1:C:104:SER:HG	1:C:163:ILE:CD1	1.88	0.54
1:C:127:THR:HG23	1:C:184:SER:O	2.06	0.54
1:D:259:SER:O	1:D:263:ILE:HG12	2.08	0.54
1:D:289:GLY:HA2	2:D:801:ATP:O2B	2.08	0.54
1:E:110:LEU:CB	1:E:306:HIS:HA	2.38	0.54
1:B:437:LEU:HD22	1:B:437:LEU:H	1.73	0.54
1:E:463:GLU:HB3	1:E:494:ALA:HB1	1.89	0.54
1:F:105:VAL:CG2	1:F:162:MET:CG	2.82	0.54
1:F:348:ASP:OD1	1:F:349:SER:N	2.41	0.54
1:A:54:HIS:HD2	1:A:93:VAL:CA	2.21	0.53
1:A:160:PRO:CG	1:A:238:LEU:CD1	2.87	0.53
1:B:159:MET:H	1:B:213:PRO:CA	2.16	0.53
1:B:167:LEU:HD22	1:B:167:LEU:N	2.22	0.53
1:C:158:ILE:HB	1:C:160:PRO:HD2	1.89	0.53
1:E:163:ILE:HG22	1:E:177:ASP:HB3	1.88	0.53
1:E:722:ALA:HB2	2:E:803:ATP:H5'2	1.86	0.53
1:E:725:VAL:HG21	2:E:803:ATP:H1'	1.89	0.53
1:F:65:PRO:O	1:F:84:ARG:HA	2.07	0.53
1:A:159:MET:HB3	1:A:213:PRO:CD	2.37	0.53
1:B:160:PRO:HB3	1:B:238:LEU:CD1	2.29	0.53
1:B:360:GLY:N	1:B:363:GLU:OE1	2.40	0.53
2:C:803:ATP:C3'	3:C:804:NDT:C4	2.86	0.53
1:D:58:LEU:HD12	1:D:63:ILE:CG1	2.38	0.53
1:F:58:LEU:HD12	1:F:63:ILE:CG1	2.38	0.53
1:B:692:ILE:CD1	2:B:803:ATP:N1	2.71	0.53
2:B:801:ATP:H3'	3:B:802:NDT:C4	2.39	0.53
1:D:560:GLY:HA2	2:D:803:ATP:H5'1	1.90	0.53
1:F:292:LYS:HE3	2:F:801:ATP:O3G	2.07	0.53
1:A:406:ASP:OD1	1:A:407:GLN:N	2.41	0.53
1:F:540:GLU:HG2	1:F:544:ARG:HH12	1.73	0.53
1:B:58:LEU:HD12	1:B:63:ILE:CG1	2.38	0.53
1:C:54:HIS:CD2	1:C:93:VAL:HG23	2.44	0.53
1:D:565:LEU:CD1	3:D:804:NDT:O3	2.57	0.53
1:B:53:ILE:HD13	1:B:116:LEU:HD21	1.85	0.53
1:B:159:MET:CA	1:B:213:PRO:HB3	2.36	0.53
1:B:228:LYS:HD3	1:B:228:LYS:C	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:TYR:O	1:B:447:SER:OG	2.20	0.53
1:B:459:ALA:HB2	1:C:402:PRO:HB3	1.91	0.53
1:B:542:PHE:O	1:B:546:GLY:N	2.40	0.53
1:C:54:HIS:HD2	1:C:93:VAL:CA	2.21	0.53
1:C:123:PRO:CG	1:C:216:ILE:CG1	2.85	0.53
1:C:141:GLU:HG2	1:C:170:LYS:C	1.98	0.53
1:D:211:LEU:O	1:D:238:LEU:HD22	2.08	0.53
1:D:347:ILE:HG21	1:D:387:ALA:HB1	1.90	0.53
1:D:363:GLU:O	1:D:365:ARG:N	2.42	0.53
1:E:167:LEU:HD22	1:E:167:LEU:N	2.22	0.53
1:E:519:GLY:C	2:E:803:ATP:HN62	2.12	0.53
1:F:163:ILE:HG22	1:F:177:ASP:HB3	1.88	0.53
1:F:563:LYS:CE	1:F:659:THR:C	2.77	0.53
1:A:73:LYS:CE	1:A:112:ASP:OD2	2.36	0.53
1:A:688:ALA:O	1:A:692:ILE:HD12	2.08	0.53
1:B:159:MET:CB	1:B:213:PRO:CB	2.78	0.53
1:C:58:LEU:HD12	1:C:63:ILE:CG1	2.38	0.53
1:C:228:LYS:HD3	1:C:228:LYS:C	2.29	0.53
1:D:102:ILE:CD1	1:D:102:ILE:H	1.96	0.53
1:D:242:LEU:HD12	1:D:297:ARG:C	2.29	0.53
1:E:224:ILE:HD12	1:E:224:ILE:H	1.71	0.53
1:A:463:GLU:HB3	1:A:494:ALA:HB1	1.90	0.53
1:A:517:ASP:OD2	1:A:695:LYS:NZ	2.42	0.53
1:E:58:LEU:HD12	1:E:63:ILE:CG1	2.38	0.53
1:E:465:VAL:HG13	1:F:274:PHE:CE2	2.44	0.53
1:A:271:PHE:HZ	1:A:277:SER:O	1.89	0.53
1:A:559:PRO:HB3	1:A:660:ASN:HD21	1.74	0.53
1:A:704:GLU:HB3	1:A:744:LYS:HD3	1.91	0.53
1:C:721:GLY:HA3	2:C:803:ATP:N1	2.20	0.53
1:D:228:LYS:HD3	1:D:228:LYS:C	2.29	0.53
1:E:363:GLU:O	1:E:365:ARG:N	2.42	0.53
2:E:803:ATP:H3'	3:E:804:NDT:C4	2.38	0.53
1:F:347:ILE:HG22	1:F:389:THR:HB	1.91	0.53
1:B:436:VAL:O	1:B:436:VAL:HG22	2.07	0.53
1:C:508:LEU:HD11	1:D:647:VAL:HG21	1.91	0.53
1:D:218:ARG:HA	1:D:218:ARG:NH2	2.10	0.53
1:D:371:LEU:O	1:D:375:ASP:HB2	2.08	0.53
1:D:619:ASP:HB3	1:D:659:THR:OG1	2.09	0.53
1:F:371:LEU:O	1:F:375:ASP:HB2	2.09	0.53
1:F:650:LEU:HB3	1:F:653:VAL:HG22	1.90	0.53
2:F:801:ATP:H3'	3:F:802:NDT:C5	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:PRO:HA	1:A:85:ALA:HB3	1.91	0.52
1:A:532:ILE:HD13	1:A:570:LEU:HD11	1.90	0.52
1:B:512:LYS:HG3	1:B:572:THR:HG23	1.91	0.52
1:C:111:GLY:HA2	1:C:306:HIS:CE1	2.44	0.52
1:D:126:ALA:HB2	1:D:215:PHE:HB2	1.91	0.52
1:D:323:THR:OG1	1:D:324:GLU:OE2	2.27	0.52
1:F:72:GLY:C	1:F:115:GLU:HB2	2.29	0.52
1:F:161:GLY:HA3	1:F:179:VAL:CG1	2.39	0.52
1:F:210:TYR:O	1:F:211:LEU:HB2	2.09	0.52
1:F:225:THR:O	1:F:225:THR:OG1	2.19	0.52
1:F:328:ARG:HG2	1:F:373:LEU:HD21	1.91	0.52
1:F:751:GLU:HG3	1:F:755:LYS:NZ	2.24	0.52
1:A:98:LEU:CD2	1:A:98:LEU:N	2.72	0.52
1:A:105:VAL:HG11	1:A:158:ILE:CD1	2.37	0.52
1:B:54:HIS:HD2	1:B:93:VAL:CA	2.21	0.52
1:B:98:LEU:CD2	1:B:98:LEU:N	2.72	0.52
1:B:578:PHE:HE2	1:B:580:ALA:HB2	1.75	0.52
1:C:77:ASN:C	1:C:77:ASN:HD22	2.06	0.52
1:C:434:ARG:NH1	1:C:434:ARG:HA	2.25	0.52
1:D:82:ILE:HD12	1:D:82:ILE:N	2.07	0.52
1:D:247:VAL:HA	2:D:801:ATP:HN61	1.74	0.52
1:D:732:GLY:HA3	1:E:547:ILE:HD11	1.91	0.52
1:E:54:HIS:HD2	1:E:93:VAL:CA	2.21	0.52
1:A:104:SER:CB	1:A:163:ILE:HD13	2.30	0.52
1:A:453:VAL:HG22	1:A:454:GLY:H	1.75	0.52
2:A:803:ATP:H3'	3:A:804:NDT:C4	2.39	0.52
1:D:73:LYS:HD2	1:D:108:LEU:CD2	2.38	0.52
1:D:141:GLU:OE1	1:D:170:LYS:CD	2.54	0.52
1:E:591:VAL:HG22	1:E:632:ALA:HB2	1.90	0.52
1:F:46:LYS:N	1:F:46:LYS:CD	2.73	0.52
1:F:54:HIS:HD2	1:F:93:VAL:CA	2.21	0.52
1:F:228:LYS:HD3	1:F:228:LYS:C	2.29	0.52
1:F:351:ALA:HB1	1:F:367:VAL:HG22	1.91	0.52
1:F:534:LEU:HB2	1:F:535:PRO:HD3	1.91	0.52
1:A:126:ALA:HB2	1:A:215:PHE:HB2	1.91	0.52
1:E:540:GLU:HG2	1:E:544:ARG:HH12	1.73	0.52
1:F:98:LEU:O	1:F:102:ILE:CG1	2.58	0.52
1:B:35:ILE:CG1	1:B:113:ARG:HH12	2.18	0.52
1:B:259:SER:O	1:B:263:ILE:HG22	2.10	0.52
1:B:429:ARG:NH2	3:B:802:NDT:H17	2.19	0.52
1:B:530:GLU:O	1:B:534:LEU:HG	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:751:GLU:HG3	1:B:755:LYS:NZ	2.24	0.52
1:C:514:TYR:O	1:C:518:ILE:HG12	2.09	0.52
1:E:218:ARG:CB	1:E:218:ARG:NH2	2.73	0.52
1:F:762:THR:O	1:F:765:MET:HG2	2.09	0.52
1:A:218:ARG:CB	1:A:218:ARG:NH2	2.73	0.52
1:B:73:LYS:HD2	1:B:108:LEU:CD2	2.38	0.52
1:B:253:GLU:N	1:B:253:GLU:OE2	2.43	0.52
1:D:64:ASN:N	1:D:64:ASN:OD1	2.43	0.52
1:E:64:ASN:OD1	1:E:64:ASN:N	2.43	0.52
1:E:689:ARG:CZ	1:E:717:GLU:HA	2.40	0.52
1:F:98:LEU:CD2	1:F:98:LEU:N	2.72	0.52
1:B:52:TYR:HA	1:B:86:GLY:HA2	1.92	0.52
2:B:803:ATP:H8	3:B:804:NDT:O3	1.92	0.52
1:C:561:CYS:SG	1:C:720:SER:HB2	2.49	0.52
1:D:65:PRO:HA	1:D:85:ALA:HB3	1.91	0.52
1:D:77:ASN:ND2	1:D:209:PHE:CB	2.73	0.52
1:E:54:HIS:CD2	1:E:93:VAL:HG23	2.44	0.52
1:A:532:ILE:HG21	1:A:570:LEU:HD11	1.92	0.52
1:A:534:LEU:HB2	1:A:535:PRO:HD3	1.91	0.52
1:B:668:ALA:HA	1:B:671:ARG:HH12	1.75	0.52
3:B:802:NDT:C7	1:C:403:GLY:CA	2.62	0.52
1:C:73:LYS:HD2	1:C:108:LEU:CD2	2.38	0.52
1:C:582:LYS:HA	1:C:616:ASP:HB3	1.92	0.52
3:D:802:NDT:H7	1:E:403:GLY:N	2.25	0.52
1:E:46:LYS:CA	1:E:46:LYS:CE	2.85	0.52
1:E:104:SER:CB	1:E:163:ILE:HD13	2.30	0.52
1:F:123:PRO:CG	1:F:216:ILE:CG1	2.85	0.52
1:F:306:HIS:O	1:F:340:SER:HA	2.09	0.52
1:F:590:TYR:HB3	1:F:593:GLU:HB2	1.92	0.52
1:A:46:LYS:N	1:A:46:LYS:CD	2.73	0.52
1:A:434:ARG:NH2	1:A:482:PHE:HA	2.24	0.52
1:B:65:PRO:HA	1:B:85:ALA:HB3	1.91	0.52
1:C:224:ILE:HD12	1:C:224:ILE:H	1.71	0.52
1:D:80:LEU:N	1:D:211:LEU:CD1	2.73	0.52
1:E:65:PRO:HA	1:E:85:ALA:HB3	1.91	0.52
1:E:110:LEU:O	1:E:307:VAL:HG22	2.08	0.52
1:E:228:LYS:HD3	1:E:228:LYS:C	2.29	0.52
1:F:688:ALA:O	1:F:692:ILE:HD12	2.10	0.52
1:A:73:LYS:HD2	1:A:108:LEU:CD2	2.38	0.52
1:A:82:ILE:H	1:A:82:ILE:CD1	2.11	0.52
1:A:466:MET:CE	1:B:271:PHE:HZ	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LYS:N	1:B:46:LYS:CD	2.72	0.52
1:B:237:ASN:HB2	1:C:379:ALA:HB3	1.91	0.52
2:B:801:ATP:H3'	3:B:802:NDT:C5	2.40	0.52
1:C:584:PRO:HA	1:C:587:PHE:HD2	1.75	0.52
1:D:46:LYS:N	1:D:46:LYS:CD	2.73	0.52
1:D:306:HIS:O	1:D:340:SER:HA	2.09	0.52
1:D:401:ARG:HG2	1:D:402:PRO:HD2	1.92	0.52
1:E:46:LYS:N	1:E:46:LYS:CD	2.73	0.52
1:E:126:ALA:HB2	1:E:215:PHE:HB2	1.91	0.52
1:F:65:PRO:HA	1:F:85:ALA:HB3	1.91	0.52
1:A:98:LEU:O	1:A:102:ILE:CG1	2.58	0.51
1:A:762:THR:HG23	1:A:764:GLU:HG3	1.92	0.51
1:B:64:ASN:N	1:B:64:ASN:OD1	2.43	0.51
1:B:218:ARG:CB	1:B:218:ARG:NH2	2.73	0.51
1:B:629:SER:HB3	1:B:633:ALA:HB3	1.92	0.51
1:C:77:ASN:C	1:C:211:LEU:HD22	2.06	0.51
1:C:105:VAL:CG2	1:C:162:MET:CG	2.82	0.51
1:C:160:PRO:CG	1:C:238:LEU:HD11	2.39	0.51
1:C:218:ARG:HA	1:C:218:ARG:NH2	2.10	0.51
1:D:34:PHE:HB3	1:D:96:ILE:HG22	1.92	0.51
1:D:584:PRO:HD3	1:D:617:GLU:HB2	1.92	0.51
1:A:159:MET:SD	1:A:182:ASP:CB	2.99	0.51
1:A:436:VAL:O	1:A:436:VAL:HG22	2.10	0.51
1:A:536:LEU:HD22	1:A:576:ILE:HD11	1.92	0.51
1:C:46:LYS:N	1:C:46:LYS:CD	2.73	0.51
1:C:218:ARG:CB	1:C:218:ARG:NH2	2.73	0.51
1:C:245:ALA:O	1:C:425:LYS:NZ	2.22	0.51
1:D:278:PRO:O	1:D:280:ARG:HD3	2.11	0.51
1:E:518:ILE:HD11	1:E:569:ALA:HB2	1.91	0.51
1:E:519:GLY:CA	2:E:803:ATP:N6	2.72	0.51
1:E:704:GLU:HB3	1:E:744:LYS:HD3	1.92	0.51
1:F:64:ASN:OD1	1:F:64:ASN:N	2.43	0.51
1:F:160:PRO:CG	1:F:212:SER:HG	2.16	0.51
1:F:438:ASP:OD1	1:F:438:ASP:N	2.44	0.51
1:A:34:PHE:HB3	1:A:96:ILE:HG22	1.92	0.51
1:A:228:LYS:HD3	1:A:228:LYS:C	2.29	0.51
1:C:64:ASN:OD1	1:C:64:ASN:N	2.43	0.51
1:C:126:ALA:HB2	1:C:215:PHE:HB2	1.91	0.51
1:D:98:LEU:CD2	1:D:98:LEU:N	2.72	0.51
1:D:160:PRO:HA	1:D:238:LEU:CD1	2.39	0.51
1:D:559:PRO:HA	2:D:803:ATP:O2B	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:570:LEU:O	1:E:574:SER:OG	2.20	0.51
1:F:73:LYS:CB	1:F:114:LEU:HA	2.40	0.51
1:F:218:ARG:CB	1:F:218:ARG:NH2	2.73	0.51
1:F:346:GLU:OE2	2:F:801:ATP:O2G	2.29	0.51
1:F:399:LEU:HA	1:F:404:ARG:HD2	1.91	0.51
1:A:530:GLU:O	1:A:534:LEU:HG	2.10	0.51
1:A:739:ASP:OD1	1:A:739:ASP:N	2.42	0.51
3:A:802:NDT:H212	1:B:276:VAL:CG1	2.41	0.51
1:B:123:PRO:CG	1:B:216:ILE:CG1	2.85	0.51
1:D:218:ARG:CB	1:D:218:ARG:NH2	2.73	0.51
1:D:274:PHE:HB2	1:D:276:VAL:HG22	1.92	0.51
1:D:650:LEU:HB3	1:D:653:VAL:HG22	1.92	0.51
1:E:161:GLY:HA3	1:E:179:VAL:CG1	2.39	0.51
1:F:563:LYS:NZ	1:F:660:ASN:OD1	2.20	0.51
1:A:64:ASN:N	1:A:64:ASN:OD1	2.43	0.51
2:A:801:ATP:N3	2:A:801:ATP:C2'	2.73	0.51
1:B:624:ASP:OD1	1:B:634:ASN:CG	2.49	0.51
1:C:65:PRO:HA	1:C:85:ALA:HB3	1.91	0.51
1:C:98:LEU:CD2	1:C:98:LEU:N	2.72	0.51
1:C:564:THR:CG2	2:C:803:ATP:O2A	2.57	0.51
1:D:545:LEU:HB3	1:D:547:ILE:HG13	1.92	0.51
1:F:77:ASN:O	1:F:211:LEU:HD22	2.02	0.51
1:A:52:TYR:HA	1:A:86:GLY:HA2	1.92	0.51
1:A:160:PRO:HB3	1:A:238:LEU:CD1	2.40	0.51
1:A:707:VAL:HG23	1:A:709:LEU:HD22	1.91	0.51
1:B:435:HIS:HB2	1:B:486:VAL:HB	1.91	0.51
1:D:469:ILE:HG13	1:E:271:PHE:CE2	2.45	0.51
1:E:264:PRO:N	1:E:266:HIS:CE1	2.76	0.51
1:E:265:LEU:HD11	1:E:384:VAL:CG1	2.41	0.51
1:F:559:PRO:O	2:F:803:ATP:PB	2.68	0.51
1:B:161:GLY:HA3	1:B:179:VAL:CG1	2.39	0.51
1:C:98:LEU:O	1:C:102:ILE:CG1	2.58	0.51
1:C:149:GLN:HE21	1:C:219:LYS:HZ2	1.50	0.51
1:C:208:LEU:HD23	1:C:208:LEU:C	2.31	0.51
1:C:251:ASP:O	1:C:254:ILE:HG22	2.11	0.51
1:D:54:HIS:HD2	1:D:93:VAL:CA	2.21	0.51
1:D:104:SER:CB	1:D:163:ILE:HD13	2.30	0.51
1:D:105:VAL:CG2	1:D:162:MET:CG	2.82	0.51
1:D:166:ASN:HD21	1:D:169:THR:CG2	2.13	0.51
1:E:52:TYR:HA	1:E:86:GLY:HA2	1.92	0.51
1:E:224:ILE:N	1:E:224:ILE:CD1	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:GLN:OE1	1:E:270:LEU:CD1	2.51	0.51
1:E:470:GLN:NE2	1:F:259:SER:OG	2.44	0.51
1:F:54:HIS:CD2	1:F:93:VAL:HG23	2.44	0.51
1:F:587:PHE:HZ	1:F:621:LEU:HA	1.75	0.51
1:A:159:MET:CE	1:A:159:MET:CA	2.86	0.51
1:B:159:MET:HG2	1:B:236:TYR:CG	2.45	0.51
1:B:291:GLY:HA2	2:B:801:ATP:O1A	2.11	0.51
1:C:34:PHE:HB3	1:C:96:ILE:HG22	1.92	0.51
1:C:224:ILE:N	1:C:224:ILE:CD1	2.73	0.51
1:C:316:VAL:HG13	1:C:362:VAL:HG11	1.93	0.51
1:D:42:LYS:N	1:D:42:LYS:CE	2.73	0.51
1:D:52:TYR:HA	1:D:86:GLY:HA2	1.92	0.51
1:D:52:TYR:HB3	1:D:86:GLY:HA2	1.93	0.51
1:D:427:PHE:O	1:D:430:MET:HG3	2.09	0.51
1:D:741:ASP:OD1	1:E:544:ARG:NH2	2.43	0.51
1:E:52:TYR:HB3	1:E:86:GLY:HA2	1.93	0.51
1:F:606:ARG:HH21	1:F:650:LEU:HD11	1.75	0.51
1:A:582:LYS:HA	1:A:616:ASP:HB3	1.93	0.51
1:A:600:GLU:OE2	1:A:603:ARG:NH2	2.27	0.51
1:C:328:ARG:HG2	1:C:373:LEU:HD21	1.93	0.51
1:D:54:HIS:ND1	1:D:55:PRO:CD	2.72	0.51
1:E:123:PRO:CG	1:E:216:ILE:CG1	2.85	0.51
1:E:650:LEU:HB3	1:E:653:VAL:HG22	1.92	0.51
1:F:52:TYR:HA	1:F:86:GLY:HA2	1.92	0.51
1:F:624:ASP:O	1:F:628:SER:HA	2.09	0.51
1:A:149:GLN:NE2	1:A:219:LYS:HZ2	2.04	0.51
1:A:159:MET:HB3	1:A:160:PRO:HD3	1.93	0.51
1:B:211:LEU:CB	1:B:214:PRO:HG3	2.40	0.51
1:B:261:ILE:HD11	1:B:384:VAL:HG21	1.93	0.51
1:B:261:ILE:HD13	1:B:386:ILE:HD11	1.93	0.51
1:C:587:PHE:HZ	1:C:621:LEU:HA	1.76	0.51
1:C:730:GLU:OE2	1:D:677:ARG:NH1	2.42	0.51
1:E:77:ASN:C	1:E:77:ASN:HD22	2.06	0.51
1:E:98:LEU:CD2	1:E:98:LEU:N	2.72	0.51
1:F:52:TYR:HB3	1:F:86:GLY:HA2	1.93	0.51
1:F:530:GLU:O	1:F:534:LEU:HG	2.11	0.51
1:F:721:GLY:HA3	2:F:803:ATP:C2	2.46	0.51
1:A:275:GLY:C	3:F:802:NDT:H213	2.31	0.50
1:A:440:GLU:O	1:A:444:TYR:N	2.36	0.50
1:B:599:ARG:NH1	1:B:643:GLU:OE2	2.43	0.50
1:C:271:PHE:HE1	1:C:277:SER:N	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:LYS:O	1:C:608:ALA:HB2	2.11	0.50
1:C:646:GLY:C	1:C:648:GLU:H	2.14	0.50
1:D:98:LEU:O	1:D:102:ILE:CG1	2.58	0.50
1:E:184:SER:O	1:E:185:ASP:CB	2.59	0.50
1:F:54:HIS:ND1	1:F:55:PRO:CD	2.72	0.50
1:B:34:PHE:HB3	1:B:96:ILE:HG22	1.92	0.50
1:B:286:GLY:O	1:B:292:LYS:NZ	2.37	0.50
1:B:707:VAL:HG12	1:B:747:LEU:HD12	1.92	0.50
1:C:251:ASP:O	1:C:255:GLU:HG2	2.10	0.50
1:D:167:LEU:HD22	1:D:167:LEU:N	2.22	0.50
1:F:261:ILE:HD13	1:F:386:ILE:HD11	1.92	0.50
1:A:52:TYR:HB3	1:A:86:GLY:HA2	1.93	0.50
1:A:102:ILE:HD12	1:A:102:ILE:N	2.05	0.50
1:A:123:PRO:CG	1:A:216:ILE:CG1	2.85	0.50
1:A:271:PHE:CZ	1:A:277:SER:C	2.81	0.50
1:C:52:TYR:HA	1:C:86:GLY:HA2	1.92	0.50
1:D:680:TYR:HE1	1:D:769:TYR:HB3	1.76	0.50
1:E:218:ARG:HB3	1:E:218:ARG:CZ	2.41	0.50
1:E:722:ALA:CB	2:E:803:ATP:C5'	2.80	0.50
1:F:126:ALA:HB2	1:F:215:PHE:HB2	1.91	0.50
1:F:184:SER:O	1:F:185:ASP:CB	2.59	0.50
1:A:129:VAL:HG23	1:A:129:VAL:O	2.12	0.50
1:B:534:LEU:HB3	1:B:542:PHE:HZ	1.77	0.50
1:C:79:ILE:N	1:C:211:LEU:CD1	2.71	0.50
1:D:37:ARG:HH11	1:D:306:HIS:CG	2.29	0.50
1:E:276:VAL:HG23	1:E:277:SER:N	2.26	0.50
1:E:726:LEU:HD22	1:F:672:PRO:HB3	1.93	0.50
1:F:559:PRO:HA	1:F:563:LYS:HD2	1.93	0.50
1:F:715:ARG:NH2	1:F:751:GLU:OE1	2.44	0.50
1:A:98:LEU:H	1:A:98:LEU:HD22	1.77	0.50
1:B:98:LEU:H	1:B:98:LEU:HD22	1.77	0.50
1:B:208:LEU:N	1:B:208:LEU:CD1	2.73	0.50
1:D:218:ARG:HB3	1:D:218:ARG:CZ	2.41	0.50
1:D:470:GLN:OE1	1:E:259:SER:OG	2.26	0.50
1:E:42:LYS:N	1:E:42:LYS:CE	2.73	0.50
2:E:801:ATP:O2B	2:E:801:ATP:H5'2	2.12	0.50
1:F:111:GLY:HA2	1:F:306:HIS:CE1	2.47	0.50
1:F:274:PHE:HD1	1:F:274:PHE:N	2.08	0.50
1:F:542:PHE:O	1:F:546:GLY:N	2.44	0.50
1:C:218:ARG:HB3	1:C:218:ARG:CZ	2.42	0.50
1:E:98:LEU:H	1:E:98:LEU:HD22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:551:LYS:NZ	1:E:650:LEU:H	2.10	0.50
1:F:34:PHE:HB3	1:F:96:ILE:HG22	1.92	0.50
1:F:159:MET:CG	1:F:236:TYR:CE1	2.58	0.50
1:B:646:GLY:O	1:B:648:GLU:N	2.45	0.50
1:C:225:THR:O	1:C:225:THR:OG1	2.19	0.50
1:C:578:PHE:CE2	1:C:580:ALA:HB2	2.46	0.50
1:D:35:ILE:HG23	1:D:35:ILE:O	2.12	0.50
1:D:129:VAL:HG23	1:D:129:VAL:O	2.12	0.50
1:E:313:PRO:O	1:F:365:ARG:NH2	2.45	0.50
2:E:801:ATP:O1A	2:E:801:ATP:H4'	2.12	0.50
1:F:76:GLU:O	1:F:211:LEU:CD1	2.60	0.50
1:F:129:VAL:HG23	1:F:129:VAL:O	2.12	0.50
1:B:54:HIS:CD2	1:B:93:VAL:HG23	2.44	0.50
1:B:759:ARG:HB2	1:B:761:ILE:HG22	1.93	0.50
1:D:37:ARG:HH12	1:D:306:HIS:HB2	1.77	0.50
1:D:225:THR:O	1:D:225:THR:OG1	2.19	0.50
1:D:722:ALA:HA	3:D:804:NDT:H5	1.93	0.50
1:E:419:ARG:CZ	1:E:450:HIS:HA	2.42	0.50
1:E:668:ALA:HA	1:E:671:ARG:HH12	1.77	0.50
1:F:72:GLY:CA	1:F:115:GLU:O	2.57	0.50
1:F:218:ARG:HB3	1:F:218:ARG:CZ	2.41	0.50
1:A:184:SER:O	1:A:185:ASP:CB	2.59	0.50
1:B:587:PHE:HZ	1:B:621:LEU:HA	1.77	0.50
1:C:334:ALA:HB2	1:C:342:ILE:HD11	1.93	0.50
1:E:398:ALA:O	1:E:404:ARG:NH2	2.42	0.50
1:E:605:ALA:HB1	1:E:653:VAL:HG11	1.93	0.50
1:F:42:LYS:N	1:F:42:LYS:CE	2.73	0.50
1:F:143:MET:SD	1:F:144:GLU:N	2.85	0.50
1:A:42:LYS:N	1:A:42:LYS:CE	2.73	0.49
1:A:481:LYS:NZ	1:B:270:LEU:HB2	2.27	0.49
1:A:556:TYR:HE1	1:A:678:HIS:HB3	1.75	0.49
1:B:35:ILE:HG23	1:B:35:ILE:O	2.12	0.49
1:B:68:PHE:O	1:B:120:GLN:CG	2.60	0.49
1:B:695:LYS:HE2	3:B:804:NDT:H17	1.94	0.49
1:C:695:LYS:HZ3	3:C:804:NDT:C16	2.25	0.49
1:D:242:LEU:HD12	1:D:297:ARG:CB	2.37	0.49
1:E:143:MET:SD	1:E:144:GLU:N	2.85	0.49
1:E:721:GLY:HA3	2:E:803:ATP:H2	1.73	0.49
1:F:79:ILE:C	1:F:80:LEU:HD23	2.33	0.49
1:C:104:SER:CB	1:C:163:ILE:HD13	2.30	0.49
1:D:98:LEU:H	1:D:98:LEU:HD22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:PRO:C	2:D:803:ATP:O2B	2.49	0.49
1:E:685:ASP:OD1	1:E:686:VAL:N	2.38	0.49
1:E:759:ARG:HB2	1:E:761:ILE:HG22	1.94	0.49
1:F:393:ASN:HA	1:F:400:ARG:HH22	1.78	0.49
1:F:510:MET:HB3	1:F:568:LYS:HG3	1.93	0.49
1:F:712:LEU:O	1:F:716:THR:HG22	2.13	0.49
1:A:143:MET:SD	1:A:144:GLU:N	2.85	0.49
1:A:434:ARG:HH22	1:A:482:PHE:HA	1.76	0.49
1:A:693:LEU:HA	1:A:696:CYS:SG	2.52	0.49
1:B:534:LEU:HB2	1:B:535:PRO:HD3	1.93	0.49
1:C:561:CYS:HB2	1:C:722:ALA:H	1.77	0.49
1:C:621:LEU:HD13	1:C:640:LEU:HD21	1.94	0.49
1:D:759:ARG:HB2	1:D:761:ILE:HG22	1.94	0.49
1:E:35:ILE:HG23	1:E:35:ILE:O	2.12	0.49
1:F:68:PHE:O	1:F:120:GLN:CG	2.60	0.49
1:F:98:LEU:H	1:F:98:LEU:HD22	1.77	0.49
1:F:262:GLU:OE2	1:F:266:HIS:CG	2.65	0.49
1:F:398:ALA:O	1:F:404:ARG:NH1	2.45	0.49
1:F:707:VAL:HG12	1:F:747:LEU:HD12	1.95	0.49
1:F:733:LEU:HA	1:F:736:ILE:HG12	1.94	0.49
1:A:138:ASN:HB3	1:A:228:LYS:CB	2.42	0.49
1:A:161:GLY:HA3	1:A:179:VAL:CG1	2.39	0.49
1:A:218:ARG:HB3	1:A:218:ARG:CZ	2.42	0.49
1:A:735:ALA:HB2	1:A:745:VAL:HG23	1.94	0.49
1:B:217:PHE:C	1:B:217:PHE:CD2	2.86	0.49
1:C:68:PHE:O	1:C:120:GLN:CG	2.60	0.49
1:D:141:GLU:HG2	1:D:170:LYS:C	1.98	0.49
1:E:37:ARG:NH1	1:E:306:HIS:HD2	2.00	0.49
1:F:102:ILE:CD1	1:F:102:ILE:H	1.96	0.49
1:A:529:LYS:HA	1:A:532:ILE:HG12	1.94	0.49
1:B:54:HIS:ND1	1:B:55:PRO:CD	2.72	0.49
1:B:129:VAL:HG23	1:B:129:VAL:O	2.12	0.49
1:B:218:ARG:HB3	1:B:218:ARG:CZ	2.42	0.49
1:B:584:PRO:HD3	1:B:617:GLU:HB2	1.95	0.49
1:C:82:ILE:H	1:C:82:ILE:CD1	2.11	0.49
1:C:98:LEU:H	1:C:98:LEU:HD22	1.77	0.49
1:C:129:VAL:HG23	1:C:129:VAL:O	2.12	0.49
1:C:217:PHE:CD2	1:C:217:PHE:C	2.86	0.49
1:C:248:GLY:H	2:C:801:ATP:HN61	1.55	0.49
1:D:218:ARG:CA	1:D:218:ARG:NH2	2.74	0.49
1:E:34:PHE:HB3	1:E:96:ILE:HG22	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PHE:O	1:A:177:ASP:HA	2.13	0.49
1:B:453:VAL:HG22	1:B:454:GLY:H	1.76	0.49
3:B:802:NDT:H7	1:C:403:GLY:N	2.23	0.49
1:C:35:ILE:O	1:C:35:ILE:HG23	2.12	0.49
1:C:52:TYR:HB3	1:C:86:GLY:HA2	1.93	0.49
1:C:75:GLY:H	1:C:115:GLU:CD	2.16	0.49
1:C:367:VAL:O	1:C:371:LEU:HG	2.13	0.49
1:E:217:PHE:C	1:E:217:PHE:CD2	2.86	0.49
1:F:135:GLN:HE21	1:F:136:GLY:H	1.60	0.49
1:F:138:ASN:HB3	1:F:228:LYS:CB	2.42	0.49
1:A:612:ILE:HG22	1:A:654:VAL:HB	1.95	0.49
1:A:689:ARG:CZ	1:A:717:GLU:HA	2.43	0.49
1:B:52:TYR:HB3	1:B:86:GLY:HA2	1.93	0.49
1:B:143:MET:SD	1:B:144:GLU:N	2.85	0.49
1:C:320:LEU:N	1:C:320:LEU:CD2	2.75	0.49
1:C:578:PHE:HD1	1:C:612:ILE:HD11	1.77	0.49
1:D:54:HIS:CD2	1:D:93:VAL:HG23	2.44	0.49
1:E:75:GLY:H	1:E:115:GLU:CD	2.16	0.49
1:A:75:GLY:H	1:A:115:GLU:CD	2.16	0.49
1:B:138:ASN:HB3	1:B:228:LYS:CB	2.42	0.49
1:B:159:MET:HE3	1:B:183:ALA:N	2.28	0.49
1:B:366:VAL:HA	1:B:369:THR:HG22	1.95	0.49
1:B:444:TYR:CZ	1:B:448:LYS:HE2	2.48	0.49
1:C:363:GLU:O	1:C:365:ARG:N	2.46	0.49
1:D:75:GLY:H	1:D:115:GLU:CD	2.16	0.49
1:D:161:GLY:HA3	1:D:179:VAL:CG1	2.39	0.49
1:D:393:ASN:HB3	1:D:596:ARG:HH21	1.78	0.49
1:E:257:LEU:HD12	1:E:284:LEU:HD21	1.95	0.49
1:E:444:TYR:CZ	1:E:448:LYS:HE2	2.47	0.49
1:A:593:GLU:O	1:A:596:ARG:HG3	2.13	0.49
1:B:646:GLY:C	1:B:648:GLU:H	2.16	0.49
1:C:135:GLN:HE21	1:C:136:GLY:H	1.60	0.49
1:C:444:TYR:CZ	1:C:448:LYS:HE2	2.48	0.49
1:D:37:ARG:NH1	1:D:306:HIS:CG	2.81	0.49
1:D:534:LEU:HB2	1:D:535:PRO:HD3	1.94	0.49
1:E:68:PHE:O	1:E:120:GLN:CG	2.60	0.49
1:E:135:GLN:HE21	1:E:136:GLY:H	1.60	0.49
1:E:692:ILE:HD11	2:E:803:ATP:N7	2.24	0.49
1:A:35:ILE:HG23	1:A:35:ILE:O	2.12	0.49
1:A:354:ARG:HD3	1:A:364:SER:HB3	1.95	0.49
1:A:751:GLU:HG3	1:A:755:LYS:NZ	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLY:C	1:B:157:VAL:CG1	2.59	0.49
1:C:419:ARG:CZ	1:C:450:HIS:HA	2.43	0.49
1:E:39:HIS:CE1	1:E:47:GLU:HB2	2.48	0.49
1:F:507:PHE:HE2	1:F:604:LYS:HD3	1.76	0.49
1:A:39:HIS:CE1	1:A:47:GLU:HB2	2.48	0.48
1:A:142:CYS:N	1:A:170:LYS:NZ	2.61	0.48
1:A:217:PHE:CD2	1:A:217:PHE:C	2.86	0.48
1:A:310:ILE:HD11	1:A:330:ILE:HG21	1.95	0.48
1:A:334:ALA:HB2	1:A:342:ILE:HD11	1.95	0.48
1:A:540:GLU:HG2	1:A:544:ARG:HH12	1.78	0.48
1:A:550:PRO:HB3	1:A:677:ARG:HH12	1.78	0.48
1:B:135:GLN:HE21	1:B:136:GLY:H	1.60	0.48
1:B:606:ARG:HH21	1:B:650:LEU:HD11	1.77	0.48
1:C:231:GLN:NE2	1:C:240:GLU:OE2	2.46	0.48
1:C:762:THR:HG23	1:C:764:GLU:HG3	1.95	0.48
1:D:217:PHE:CD2	1:D:217:PHE:C	2.86	0.48
1:D:242:LEU:CB	1:D:301:ASN:ND2	2.73	0.48
1:E:142:CYS:N	1:E:170:LYS:NZ	2.61	0.48
1:A:371:LEU:HD22	1:A:404:ARG:HE	1.76	0.48
1:B:46:LYS:CA	1:B:46:LYS:CE	2.85	0.48
1:B:141:GLU:HG2	1:B:170:LYS:C	1.98	0.48
1:B:218:ARG:HA	1:B:218:ARG:NH2	2.10	0.48
1:D:123:PRO:CG	1:D:216:ILE:HG13	2.43	0.48
1:E:129:VAL:O	1:E:129:VAL:HG23	2.12	0.48
1:E:138:ASN:HB3	1:E:228:LYS:CB	2.42	0.48
1:F:39:HIS:CE1	1:F:47:GLU:HB2	2.48	0.48
1:F:160:PRO:HA	1:F:238:LEU:CD1	2.43	0.48
1:F:179:VAL:CG1	1:F:180:ILE:N	2.77	0.48
1:F:268:PRO:HG2	1:F:382:LYS:HE2	1.95	0.48
1:A:160:PRO:HG3	1:A:212:SER:OG	2.02	0.48
1:A:312:GLY:HA2	1:A:350:ILE:HD11	1.95	0.48
1:B:158:ILE:CG2	1:B:214:PRO:CA	2.92	0.48
1:B:164:PHE:O	1:B:177:ASP:HA	2.13	0.48
1:D:251:ASP:HA	1:D:254:ILE:HG22	1.94	0.48
1:E:164:PHE:O	1:E:177:ASP:HA	2.13	0.48
1:F:393:ASN:HA	1:F:400:ARG:NH2	2.28	0.48
1:A:58:LEU:HD11	1:A:63:ILE:HG13	1.96	0.48
1:A:68:PHE:O	1:A:120:GLN:CG	2.60	0.48
1:A:470:GLN:OE1	1:B:259:SER:OG	2.24	0.48
1:B:37:ARG:HD2	1:B:306:HIS:CE1	2.48	0.48
1:B:179:VAL:CG1	1:B:180:ILE:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:LEU:N	1:B:437:LEU:CD2	2.73	0.48
1:B:452:TYR:CE2	1:B:500:PRO:HG3	2.49	0.48
1:B:578:PHE:CE2	1:B:580:ALA:HB2	2.48	0.48
1:C:560:GLY:H	1:C:563:LYS:HE2	1.78	0.48
1:C:689:ARG:CZ	1:C:717:GLU:HA	2.43	0.48
1:D:68:PHE:O	1:D:120:GLN:CG	2.60	0.48
1:E:141:GLU:OE1	1:E:170:LYS:CD	2.54	0.48
1:A:135:GLN:HE21	1:A:136:GLY:H	1.60	0.48
1:B:42:LYS:N	1:B:42:LYS:CE	2.73	0.48
1:B:98:LEU:O	1:B:102:ILE:CG1	2.58	0.48
1:C:244:TYR:CD1	1:C:254:ILE:HD11	2.47	0.48
1:D:354:ARG:HD3	1:D:364:SER:HB3	1.94	0.48
1:E:98:LEU:O	1:E:102:ILE:CG1	2.58	0.48
1:E:153:ASP:H	1:E:217:PHE:HD2	1.61	0.48
1:E:462:ARG:HB2	1:F:276:VAL:CG2	2.43	0.48
1:E:660:ASN:O	1:E:769:TYR:OH	2.26	0.48
1:F:35:ILE:HG23	1:F:35:ILE:O	2.12	0.48
1:F:164:PHE:O	1:F:177:ASP:HA	2.13	0.48
1:F:179:VAL:HG12	1:F:180:ILE:H	1.79	0.48
1:F:366:VAL:O	1:F:369:THR:HG22	2.13	0.48
1:A:466:MET:HE2	1:B:271:PHE:HZ	1.77	0.48
1:B:310:ILE:HD11	1:B:330:ILE:HG21	1.96	0.48
1:C:50:THR:HG1	1:C:84:ARG:CB	2.20	0.48
1:C:138:ASN:HB3	1:C:228:LYS:CB	2.42	0.48
1:C:143:MET:SD	1:C:144:GLU:N	2.85	0.48
1:C:164:PHE:O	1:C:177:ASP:HA	2.13	0.48
1:D:58:LEU:HD11	1:D:63:ILE:HG13	1.96	0.48
1:D:164:PHE:O	1:D:177:ASP:HA	2.13	0.48
1:D:434:ARG:O	1:D:485:LYS:HB2	2.14	0.48
1:D:621:LEU:HD13	1:D:640:LEU:HD21	1.95	0.48
1:A:54:HIS:ND1	1:A:55:PRO:CD	2.72	0.48
1:C:161:GLY:HA3	1:C:179:VAL:CG1	2.39	0.48
1:D:143:MET:SD	1:D:144:GLU:N	2.85	0.48
1:D:297:ARG:NH1	1:D:301:ASN:OD1	2.46	0.48
1:E:107:ASN:OD1	1:E:241:PRO:HD3	2.13	0.48
1:E:179:VAL:HG12	1:E:180:ILE:H	1.79	0.48
1:E:261:ILE:HD11	1:E:384:VAL:HG11	1.95	0.48
1:E:264:PRO:HD3	1:E:266:HIS:CE1	2.28	0.48
1:F:160:PRO:CG	1:F:212:SER:CB	2.85	0.48
1:F:210:TYR:C	1:F:212:SER:H	2.17	0.48
1:A:578:PHE:HE2	1:A:580:ALA:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:THR:HG21	1:B:485:LYS:O	2.13	0.48
1:B:540:GLU:HG2	1:B:544:ARG:HH12	1.79	0.48
1:D:138:ASN:HB3	1:D:228:LYS:CB	2.42	0.48
1:D:563:LYS:HB2	2:D:803:ATP:O3G	2.14	0.48
1:E:179:VAL:CG1	1:E:180:ILE:N	2.77	0.48
1:E:377:MET:SD	1:E:378:GLY:N	2.87	0.48
1:F:153:ASP:H	1:F:217:PHE:HD2	1.61	0.48
1:B:75:GLY:H	1:B:115:GLU:CD	2.16	0.48
1:C:33:GLU:OE1	1:C:33:GLU:N	2.47	0.48
1:C:218:ARG:CA	1:C:218:ARG:NH2	2.74	0.48
1:D:135:GLN:HE21	1:D:136:GLY:H	1.60	0.48
1:D:184:SER:O	1:D:185:ASP:CB	2.59	0.48
1:D:209:PHE:HD1	1:D:209:PHE:O	1.97	0.48
1:D:242:LEU:CA	1:D:301:ASN:HD22	2.26	0.48
1:F:217:PHE:CD2	1:F:217:PHE:C	2.86	0.48
1:F:363:GLU:O	1:F:366:VAL:HG12	2.14	0.48
1:A:79:ILE:HB	1:A:210:TYR:CD1	2.48	0.48
1:A:508:LEU:HD23	1:A:582:LYS:HZ3	1.77	0.48
1:A:563:LYS:O	1:A:566:THR:OG1	2.28	0.48
1:B:105:VAL:CG2	1:B:162:MET:CG	2.82	0.48
1:B:153:ASP:H	1:B:217:PHE:HD2	1.61	0.48
1:B:562:SER:HB2	2:B:803:ATP:H4'	1.96	0.48
1:C:153:ASP:H	1:C:217:PHE:HD2	1.62	0.48
1:D:265:LEU:O	1:D:268:PRO:HG3	2.13	0.48
1:E:33:GLU:OE1	1:E:33:GLU:N	2.47	0.48
1:F:561:CYS:CB	1:F:721:GLY:N	2.70	0.48
1:F:707:VAL:HG23	1:F:709:LEU:HD22	1.95	0.48
1:A:261:ILE:HD13	1:A:386:ILE:HD11	1.96	0.47
1:A:324:GLU:HB2	1:A:328:ARG:HH21	1.78	0.47
1:A:577:ASN:O	1:A:611:SER:OG	2.25	0.47
1:A:712:LEU:HD11	1:A:750:PHE:CD2	2.49	0.47
1:B:104:SER:CB	1:B:163:ILE:HD13	2.30	0.47
1:C:54:HIS:ND1	1:C:55:PRO:CD	2.72	0.47
1:C:280:ARG:NH1	1:C:383:VAL:O	2.45	0.47
1:D:179:VAL:CG1	1:D:180:ILE:N	2.76	0.47
1:D:429:ARG:HH21	3:D:802:NDT:C20	2.21	0.47
1:D:436:VAL:HG13	1:D:436:VAL:O	2.14	0.47
1:D:606:ARG:HH21	1:D:650:LEU:HD11	1.78	0.47
1:F:142:CYS:N	1:F:170:LYS:NZ	2.61	0.47
1:B:39:HIS:CE1	1:B:47:GLU:HB2	2.48	0.47
1:B:123:PRO:CG	1:B:216:ILE:HG13	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:HIS:CE1	1:C:47:GLU:HB2	2.49	0.47
1:C:210:TYR:CZ	1:C:214:PRO:HG3	2.48	0.47
1:C:252:LYS:HG3	1:C:253:GLU:OE1	2.15	0.47
1:D:33:GLU:OE1	1:D:33:GLU:N	2.47	0.47
1:F:159:MET:O	1:F:180:ILE:O	2.31	0.47
2:F:803:ATP:H8	3:F:804:NDT:O3	1.97	0.47
1:A:504:ARG:HH12	1:A:506:ILE:HD13	1.80	0.47
1:B:715:ARG:NH2	1:B:751:GLU:OE1	2.47	0.47
1:C:58:LEU:HD11	1:C:63:ILE:HG13	1.96	0.47
1:C:692:ILE:HG12	2:C:803:ATP:N6	2.28	0.47
1:D:738:GLU:HG3	1:D:749:HIS:HE2	1.79	0.47
1:F:689:ARG:CZ	1:F:717:GLU:HA	2.43	0.47
1:A:33:GLU:OE1	1:A:33:GLU:N	2.47	0.47
1:A:179:VAL:HG12	1:A:180:ILE:H	1.79	0.47
1:A:363:GLU:O	1:A:365:ARG:N	2.46	0.47
1:A:711:GLU:OE2	1:A:715:ARG:NH1	2.43	0.47
1:B:406:ASP:OD1	1:B:406:ASP:N	2.47	0.47
1:B:531:MET:O	1:B:535:PRO:HD3	2.15	0.47
1:B:618:ILE:HG22	1:B:659:THR:HB	1.97	0.47
1:B:729:GLN:HB3	1:C:547:ILE:HG23	1.96	0.47
1:C:662:PRO:HD2	1:C:768:TYR:HE2	1.79	0.47
1:D:39:HIS:CE1	1:D:47:GLU:HB2	2.48	0.47
1:D:46:LYS:CA	1:D:46:LYS:CE	2.85	0.47
1:D:159:MET:HG2	1:D:236:TYR:CG	2.45	0.47
1:D:179:VAL:HG12	1:D:180:ILE:H	1.79	0.47
1:D:363:GLU:O	1:D:366:VAL:HG22	2.14	0.47
1:A:54:HIS:CD2	1:A:93:VAL:HG23	2.44	0.47
1:B:33:GLU:N	1:B:33:GLU:OE1	2.47	0.47
1:B:141:GLU:OE1	1:B:170:LYS:CD	2.54	0.47
1:B:770:GLU:O	1:B:774:LEU:HG	2.15	0.47
1:C:577:ASN:O	1:C:611:SER:OG	2.21	0.47
1:C:660:ASN:O	1:C:769:TYR:OH	2.17	0.47
1:D:153:ASP:H	1:D:217:PHE:HD2	1.61	0.47
1:D:563:LYS:NZ	1:D:659:THR:O	2.35	0.47
1:E:578:PHE:HD1	1:E:612:ILE:HD11	1.79	0.47
1:E:700:PHE:HE1	1:F:545:LEU:HD23	1.79	0.47
1:F:33:GLU:OE1	1:F:33:GLU:N	2.47	0.47
1:F:618:ILE:HG22	1:F:659:THR:HB	1.95	0.47
1:A:179:VAL:CG1	1:A:180:ILE:N	2.76	0.47
3:A:802:NDT:H7	1:B:402:PRO:C	2.33	0.47
1:B:550:PRO:O	1:B:551:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:VAL:CG1	1:C:180:ILE:N	2.76	0.47
1:C:551:LYS:NZ	1:C:645:ASP:OD1	2.41	0.47
1:C:668:ALA:HA	1:C:671:ARG:HH22	1.80	0.47
1:D:77:ASN:HD21	1:D:209:PHE:HA	1.74	0.47
1:D:292:LYS:HE3	2:D:801:ATP:O1G	2.14	0.47
1:A:123:PRO:CG	1:A:216:ILE:HG13	2.43	0.47
1:A:270:LEU:HD22	1:A:270:LEU:C	2.35	0.47
1:A:527:LYS:O	1:A:530:GLU:HB3	2.14	0.47
2:A:803:ATP:C3'	3:A:804:NDT:C4	2.93	0.47
1:B:184:SER:O	1:B:185:ASP:CB	2.59	0.47
1:C:519:GLY:HA3	1:C:692:ILE:HG13	1.96	0.47
1:C:563:LYS:NZ	1:C:660:ASN:HA	2.30	0.47
1:C:599:ARG:NH1	1:C:643:GLU:OE2	2.48	0.47
1:C:661:ARG:NH1	1:C:664:GLU:HB3	2.29	0.47
1:D:210:TYR:C	1:D:212:SER:N	2.68	0.47
2:D:801:ATP:C3'	3:D:802:NDT:C4	2.93	0.47
1:E:434:ARG:HD3	1:F:273:SER:CB	2.44	0.47
1:E:517:ASP:OD1	1:E:695:LYS:NZ	2.30	0.47
1:E:676:ASP:O	1:E:678:HIS:ND1	2.43	0.47
1:F:563:LYS:HE2	1:F:659:THR:O	2.15	0.47
1:A:158:ILE:CG2	1:A:159:MET:H	2.24	0.47
1:C:123:PRO:CG	1:C:216:ILE:HG13	2.43	0.47
1:C:166:ASN:HD21	1:C:169:THR:CG2	2.13	0.47
1:C:233:ASN:HD22	1:C:236:TYR:HE2	1.62	0.47
1:D:77:ASN:ND2	1:D:209:PHE:O	2.47	0.47
1:D:465:VAL:HG22	1:E:274:PHE:CD1	2.49	0.47
1:E:711:GLU:OE2	1:E:715:ARG:NH1	2.42	0.47
1:F:454:GLY:HA3	2:F:801:ATP:C2	2.50	0.47
1:C:210:TYR:CE2	1:C:214:PRO:HG3	2.50	0.47
2:C:801:ATP:C3'	3:C:802:NDT:C4	2.92	0.47
1:D:367:VAL:O	1:D:371:LEU:HG	2.14	0.47
1:D:661:ARG:HG2	1:D:664:GLU:HG3	1.96	0.47
1:D:720:SER:H	1:D:723:GLU:HB2	1.80	0.47
1:E:53:ILE:N	1:E:86:GLY:HA2	2.28	0.47
1:E:117:LYS:NZ	1:E:117:LYS:CB	2.77	0.47
1:E:556:TYR:HE1	1:E:678:HIS:HB3	1.80	0.47
1:E:587:PHE:HZ	1:E:621:LEU:HA	1.79	0.47
1:F:735:ALA:HB2	1:F:745:VAL:HG23	1.95	0.47
1:A:550:PRO:HB3	1:A:677:ARG:NH1	2.30	0.47
1:C:287:PRO:HG2	1:C:413:ILE:HG23	1.97	0.47
1:C:437:LEU:HD21	1:C:486:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:TYR:CE1	1:D:678:HIS:HB3	2.50	0.47
1:E:37:ARG:HG2	1:E:95:VAL:CG2	2.45	0.47
1:F:334:ALA:HB2	1:F:342:ILE:HD11	1.97	0.47
1:F:722:ALA:HA	3:F:804:NDT:H5	1.97	0.47
1:A:37:ARG:HG2	1:A:95:VAL:CG2	2.45	0.46
1:A:53:ILE:N	1:A:86:GLY:HA2	2.28	0.46
1:A:686:VAL:HG12	1:A:689:ARG:HH12	1.80	0.46
1:C:109:ILE:HD12	1:C:307:VAL:CG2	2.45	0.46
1:D:210:TYR:C	1:D:212:SER:H	2.17	0.46
1:D:371:LEU:HD22	1:D:404:ARG:HG2	1.97	0.46
1:D:459:ALA:HB2	1:E:402:PRO:HB3	1.97	0.46
1:D:670:LEU:HD11	1:D:678:HIS:CE1	2.50	0.46
1:E:159:MET:HE2	1:E:182:ASP:HA	1.05	0.46
1:E:341:ILE:HG23	1:E:384:VAL:HG13	1.96	0.46
1:E:459:ALA:HB1	1:E:498:ILE:HD11	1.97	0.46
1:F:158:ILE:CG2	1:F:212:SER:CB	2.86	0.46
1:F:559:PRO:O	2:F:803:ATP:O3B	2.33	0.46
1:A:39:HIS:C	1:A:39:HIS:HD1	2.19	0.46
1:A:270:LEU:C	1:A:270:LEU:HD13	2.36	0.46
1:A:469:ILE:CD1	1:B:270:LEU:HD11	2.44	0.46
1:A:752:LYS:HA	1:A:755:LYS:HE2	1.97	0.46
3:A:802:NDT:C8	1:B:403:GLY:CA	2.85	0.46
1:C:156:GLY:C	1:C:157:VAL:CG1	2.59	0.46
1:E:241:PRO:HA	1:E:301:ASN:ND2	2.30	0.46
1:E:312:GLY:HA2	1:E:350:ILE:HD11	1.98	0.46
1:E:689:ARG:O	1:E:692:ILE:HG22	2.15	0.46
1:F:467:LYS:HB2	1:F:490:ASP:OD1	2.14	0.46
1:A:153:ASP:H	1:A:217:PHE:HD2	1.62	0.46
1:B:37:ARG:HD3	1:B:337:TYR:CE2	2.50	0.46
1:B:454:GLY:HA3	2:B:801:ATP:H2	1.77	0.46
1:B:508:LEU:HD23	1:B:582:LYS:NZ	2.31	0.46
1:B:689:ARG:CZ	1:B:717:GLU:HA	2.45	0.46
1:C:42:LYS:N	1:C:42:LYS:CE	2.73	0.46
1:C:53:ILE:N	1:C:86:GLY:HA2	2.28	0.46
1:D:37:ARG:HD2	1:D:306:HIS:CE1	2.49	0.46
1:D:53:ILE:N	1:D:86:GLY:HA2	2.28	0.46
1:F:37:ARG:HG2	1:F:95:VAL:CG2	2.45	0.46
1:F:73:LYS:CA	1:F:114:LEU:HA	2.45	0.46
1:F:524:LEU:HD22	1:F:681:VAL:HG23	1.97	0.46
1:A:218:ARG:CB	1:A:218:ARG:HH21	2.28	0.46
1:A:598:ILE:HA	1:A:601:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ARG:CB	1:B:218:ARG:HH21	2.28	0.46
1:B:419:ARG:CZ	1:B:450:HIS:HA	2.44	0.46
1:B:592:GLY:HA2	1:B:595:GLU:HB3	1.98	0.46
1:C:79:ILE:HB	1:C:210:TYR:CD1	2.51	0.46
1:D:37:ARG:HG2	1:D:95:VAL:CG2	2.46	0.46
1:D:142:CYS:N	1:D:170:LYS:NZ	2.61	0.46
1:E:291:GLY:CA	2:E:801:ATP:O1A	2.42	0.46
1:E:354:ARG:HD3	1:E:364:SER:HB3	1.96	0.46
1:E:436:VAL:O	1:E:436:VAL:HG13	2.16	0.46
1:E:646:GLY:O	1:E:648:GLU:N	2.48	0.46
1:F:46:LYS:CA	1:F:46:LYS:CE	2.85	0.46
1:F:629:SER:HB3	1:F:633:ALA:CB	2.45	0.46
1:A:49:CYS:O	1:A:82:ILE:HG22	2.16	0.46
1:A:80:LEU:HB3	1:A:158:ILE:CD1	2.33	0.46
1:B:157:VAL:HG13	1:B:215:PHE:O	2.06	0.46
1:B:363:GLU:O	1:B:366:VAL:HG12	2.16	0.46
1:B:481:LYS:CG	1:C:270:LEU:HD21	2.43	0.46
1:C:39:HIS:HD1	1:C:39:HIS:C	2.19	0.46
1:C:348:ASP:OD1	1:C:349:SER:N	2.48	0.46
1:C:370:LEU:O	1:C:374:MET:HG3	2.15	0.46
1:C:453:VAL:HG22	1:C:454:GLY:H	1.80	0.46
1:D:49:CYS:O	1:D:82:ILE:HG22	2.16	0.46
1:D:734:ALA:HA	1:D:737:MET:CE	2.45	0.46
1:F:73:LYS:HA	1:F:114:LEU:HA	1.96	0.46
1:A:110:LEU:HB2	1:A:306:HIS:HA	1.98	0.46
1:A:111:GLY:CA	1:A:306:HIS:CE1	2.99	0.46
1:B:37:ARG:HG2	1:B:95:VAL:CG2	2.46	0.46
1:B:39:HIS:HD1	1:B:39:HIS:C	2.19	0.46
1:B:668:ALA:HA	1:B:671:ARG:NH1	2.31	0.46
1:C:289:GLY:HA2	2:C:801:ATP:O3A	2.13	0.46
1:C:598:ILE:HA	1:C:601:ILE:HG22	1.98	0.46
1:D:99:SER:CB	1:D:102:ILE:CD1	2.94	0.46
1:D:123:PRO:CG	1:D:216:ILE:CG1	2.85	0.46
1:E:54:HIS:ND1	1:E:55:PRO:CD	2.72	0.46
1:E:74:ILE:HD12	1:E:74:ILE:HA	1.73	0.46
1:E:251:ASP:HA	1:E:254:ILE:HG22	1.97	0.46
1:E:686:VAL:HG12	1:E:689:ARG:HH12	1.80	0.46
1:F:752:LYS:HA	1:F:755:LYS:HE2	1.96	0.46
3:A:802:NDT:C21	1:B:276:VAL:CG1	2.91	0.46
1:B:347:ILE:HG21	1:B:387:ALA:HB1	1.96	0.46
1:B:735:ALA:HA	1:B:749:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:GLU:O	1:C:596:ARG:HG3	2.14	0.46
1:C:630:THR:O	1:C:631:SER:C	2.51	0.46
1:C:668:ALA:HA	1:C:671:ARG:NH2	2.31	0.46
1:D:52:TYR:CB	1:D:86:GLY:HA2	2.46	0.46
1:D:80:LEU:N	1:D:211:LEU:HG	2.30	0.46
1:D:266:HIS:CA	1:D:268:PRO:HD3	2.45	0.46
1:D:280:ARG:HH21	1:D:383:VAL:N	2.10	0.46
1:D:551:LYS:NZ	1:D:650:LEU:H	2.13	0.46
1:D:587:PHE:HZ	1:D:621:LEU:HA	1.80	0.46
1:E:77:ASN:ND2	1:E:208:LEU:O	2.48	0.46
1:E:91:HIS:HA	1:E:92:PRO:HD3	1.69	0.46
1:E:598:ILE:HD11	1:E:636:VAL:HG13	1.98	0.46
1:E:646:GLY:C	1:E:648:GLU:H	2.19	0.46
1:F:248:GLY:H	2:F:801:ATP:HN62	1.60	0.46
1:A:52:TYR:CB	1:A:86:GLY:HA2	2.46	0.46
1:A:233:ASN:O	1:A:236:TYR:HD2	1.99	0.46
1:A:275:GLY:O	3:F:802:NDT:C21	2.64	0.46
1:B:143:MET:SD	1:B:143:MET:N	2.89	0.46
1:C:104:SER:OG	1:C:163:ILE:HD12	2.02	0.46
1:D:141:GLU:OE2	1:D:171:ALA:O	2.34	0.46
1:E:160:PRO:HB3	1:E:238:LEU:HD13	1.85	0.46
1:E:248:GLY:N	2:E:801:ATP:N6	2.57	0.46
1:E:262:GLU:OE2	1:E:266:HIS:HB3	2.16	0.46
1:E:619:ASP:HB3	1:E:659:THR:OG1	2.16	0.46
1:F:99:SER:CB	1:F:102:ILE:CD1	2.94	0.46
1:F:292:LYS:HE2	2:F:801:ATP:O3G	2.15	0.46
1:F:689:ARG:NH1	1:F:713:ALA:O	2.49	0.46
1:A:141:GLU:OE2	1:A:171:ALA:O	2.34	0.46
1:A:261:ILE:HD11	1:A:384:VAL:HG21	1.97	0.46
1:A:462:ARG:HD3	1:B:279:PRO:HD3	1.98	0.46
1:B:158:ILE:HG22	1:B:214:PRO:CA	2.36	0.46
1:C:141:GLU:OE2	1:C:171:ALA:O	2.34	0.46
1:C:398:ALA:O	1:C:404:ARG:NH2	2.49	0.46
1:D:39:HIS:C	1:D:39:HIS:HD1	2.19	0.46
1:D:54:HIS:HD2	1:D:93:VAL:CG2	2.25	0.46
1:D:265:LEU:HD11	1:D:341:ILE:HD11	1.98	0.46
1:E:123:PRO:CG	1:E:216:ILE:HG13	2.43	0.46
1:E:143:MET:SD	1:E:143:MET:N	2.89	0.46
1:E:166:ASN:HD21	1:E:169:THR:CG2	2.13	0.46
1:F:58:LEU:HD11	1:F:63:ILE:HG13	1.96	0.46
1:F:123:PRO:CG	1:F:216:ILE:HG13	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:ASP:HA	1:F:254:ILE:HG22	1.98	0.46
1:F:561:CYS:SG	1:F:684:PRO:HD3	2.55	0.46
1:B:276:VAL:O	1:B:276:VAL:HG23	2.16	0.46
1:B:452:TYR:HE1	1:B:498:ILE:HG23	1.79	0.46
1:D:159:MET:HE2	1:D:182:ASP:HA	1.05	0.46
1:E:77:ASN:OD1	1:E:208:LEU:C	2.54	0.46
1:E:99:SER:CB	1:E:102:ILE:CD1	2.94	0.46
1:E:746:GLU:HB2	1:E:749:HIS:ND1	2.31	0.46
1:F:265:LEU:HA	1:F:382:LYS:HB2	1.98	0.46
1:A:141:GLU:OE2	1:A:171:ALA:CA	2.64	0.45
1:A:466:MET:HE2	1:B:271:PHE:CZ	2.51	0.45
1:A:534:LEU:HB3	1:A:542:PHE:HZ	1.81	0.45
1:B:58:LEU:HD11	1:B:63:ILE:HG13	1.96	0.45
1:C:159:MET:HE3	1:C:183:ALA:N	2.30	0.45
1:C:179:VAL:HG12	1:C:180:ILE:H	1.79	0.45
1:D:58:LEU:CD1	1:D:63:ILE:CG1	2.94	0.45
1:D:211:LEU:HD23	1:D:211:LEU:N	2.31	0.45
1:D:505:GLU:OE1	1:D:507:PHE:HB3	2.16	0.45
1:D:595:GLU:O	1:D:599:ARG:HG2	2.17	0.45
1:E:276:VAL:CG2	1:E:277:SER:N	2.78	0.45
1:F:143:MET:SD	1:F:143:MET:N	2.89	0.45
1:F:598:ILE:O	1:F:601:ILE:HG22	2.15	0.45
3:A:802:NDT:H212	1:B:275:GLY:O	2.15	0.45
1:B:37:ARG:HH12	1:B:306:HIS:HB2	1.80	0.45
1:B:692:ILE:HD13	2:B:803:ATP:N1	2.31	0.45
1:B:745:VAL:HG13	1:B:750:PHE:CZ	2.52	0.45
1:D:419:ARG:NE	1:D:449:THR:O	2.50	0.45
1:D:564:THR:HB	2:D:803:ATP:O2A	2.16	0.45
1:E:39:HIS:HD1	1:E:39:HIS:C	2.19	0.45
1:F:39:HIS:HD1	1:F:39:HIS:C	2.19	0.45
1:F:141:GLU:OE2	1:F:171:ALA:O	2.34	0.45
1:F:668:ALA:HA	1:F:671:ARG:HH22	1.80	0.45
1:A:419:ARG:CZ	1:A:450:HIS:HA	2.46	0.45
1:B:58:LEU:CD1	1:B:63:ILE:CG1	2.94	0.45
1:C:218:ARG:CB	1:C:218:ARG:HH21	2.28	0.45
1:C:310:ILE:HD11	1:C:330:ILE:HG21	1.98	0.45
1:C:736:ILE:HG21	1:D:545:LEU:HD21	1.98	0.45
1:D:141:GLU:OE2	1:D:171:ALA:CA	2.64	0.45
1:E:50:THR:HG1	1:E:84:ARG:CB	2.26	0.45
1:E:141:GLU:OE2	1:E:171:ALA:CA	2.64	0.45
1:E:467:LYS:HB3	1:E:490:ASP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:GLU:OE2	1:F:171:ALA:CA	2.64	0.45
1:F:519:GLY:HA2	1:F:691:GLU:OE1	2.16	0.45
1:A:99:SER:CB	1:A:102:ILE:CD1	2.94	0.45
1:A:105:VAL:HG23	1:A:157:VAL:CG2	2.42	0.45
1:A:299:VAL:HA	1:A:302:THR:HG22	1.98	0.45
1:A:662:PRO:HD3	1:A:769:TYR:HE1	1.81	0.45
1:B:52:TYR:CB	1:B:86:GLY:HA2	2.46	0.45
1:C:37:ARG:CG	1:C:95:VAL:CG2	2.95	0.45
1:C:49:CYS:O	1:C:82:ILE:HG22	2.16	0.45
1:D:582:LYS:HA	1:D:616:ASP:HB3	1.99	0.45
1:E:110:LEU:HB3	1:E:306:HIS:HA	1.97	0.45
1:E:141:GLU:OE2	1:E:171:ALA:O	2.34	0.45
1:E:241:PRO:CA	1:E:301:ASN:ND2	2.80	0.45
1:E:561:CYS:HA	2:E:803:ATP:O2A	2.16	0.45
1:F:79:ILE:HG12	1:F:211:LEU:HD21	1.98	0.45
1:F:578:PHE:HE2	1:F:580:ALA:HB2	1.81	0.45
1:A:105:VAL:CG2	1:A:162:MET:CG	2.82	0.45
1:A:415:ASP:OD1	1:A:418:ALA:N	2.34	0.45
1:C:52:TYR:CB	1:C:86:GLY:HA2	2.46	0.45
1:C:99:SER:CB	1:C:102:ILE:CD1	2.94	0.45
1:C:142:CYS:N	1:C:170:LYS:NZ	2.61	0.45
1:C:296:LEU:HD23	1:C:343:PHE:HB3	1.98	0.45
1:C:316:VAL:HG12	1:D:365:ARG:HH22	1.81	0.45
1:D:211:LEU:O	1:D:238:LEU:CD2	2.65	0.45
1:D:515:TRP:CZ3	1:D:525:LYS:HG2	2.52	0.45
1:D:622:SER:HB2	1:D:665:ILE:HA	1.97	0.45
1:E:52:TYR:CB	1:E:86:GLY:HA2	2.46	0.45
1:E:158:ILE:H	1:E:158:ILE:HG12	1.52	0.45
1:F:159:MET:HE2	1:F:159:MET:CA	2.46	0.45
1:A:429:ARG:HH12	3:A:802:NDT:H16	1.75	0.45
1:B:141:GLU:OE2	1:B:171:ALA:O	2.34	0.45
1:B:604:LYS:O	1:B:608:ALA:HB2	2.16	0.45
1:C:37:ARG:HG2	1:C:95:VAL:CG2	2.46	0.45
1:C:130:THR:HG23	1:C:182:ASP:N	2.31	0.45
1:C:141:GLU:OE2	1:C:171:ALA:CA	2.64	0.45
1:C:159:MET:HE2	1:C:182:ASP:HA	1.02	0.45
1:D:50:THR:OG1	1:D:84:ARG:CG	2.65	0.45
1:D:143:MET:SD	1:D:143:MET:N	2.89	0.45
1:D:772:PHE:HE1	1:D:775:ARG:HH21	1.64	0.45
1:A:481:LYS:CD	1:B:270:LEU:HD12	2.45	0.45
1:B:37:ARG:CG	1:B:95:VAL:CG2	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:GLU:OE2	1:B:171:ALA:CA	2.64	0.45
1:B:141:GLU:HG3	1:B:171:ALA:N	2.18	0.45
1:B:157:VAL:CG1	1:B:215:PHE:C	2.79	0.45
1:B:179:VAL:HG12	1:B:180:ILE:H	1.79	0.45
1:C:429:ARG:CD	3:C:802:NDT:C21	2.61	0.45
1:D:499:ARG:NH1	1:E:603:ARG:HG3	2.32	0.45
1:D:600:GLU:HA	1:D:603:ARG:HG3	1.98	0.45
1:D:606:ARG:NH2	1:D:648:GLU:OE1	2.46	0.45
1:E:49:CYS:O	1:E:82:ILE:HG22	2.16	0.45
1:E:371:LEU:O	1:E:375:ASP:HB2	2.17	0.45
1:F:37:ARG:CG	1:F:95:VAL:CG2	2.95	0.45
1:F:49:CYS:O	1:F:82:ILE:HG22	2.16	0.45
1:F:218:ARG:CB	1:F:218:ARG:HH21	2.28	0.45
1:F:399:LEU:HD22	1:F:405:PHE:CE2	2.52	0.45
1:B:98:LEU:H	1:B:98:LEU:HD23	1.82	0.45
1:B:436:VAL:HB	1:B:485:LYS:HD2	1.99	0.45
1:B:506:ILE:HD11	1:B:604:LYS:NZ	2.32	0.45
1:C:98:LEU:H	1:C:98:LEU:HD23	1.82	0.45
1:E:159:MET:HE3	1:E:183:ALA:N	2.32	0.45
1:E:512:LYS:HG3	1:E:572:THR:HG23	1.99	0.45
1:A:39:HIS:HA	1:A:40:PRO:HD3	1.55	0.45
1:B:351:ALA:HB1	1:B:367:VAL:HG22	1.99	0.45
1:B:556:TYR:HE1	1:B:678:HIS:HB3	1.82	0.45
2:B:803:ATP:C8	3:B:804:NDT:O3	2.70	0.45
1:D:138:ASN:HB2	1:D:228:LYS:HB3	1.99	0.45
1:D:217:PHE:CD2	1:D:217:PHE:O	2.70	0.45
2:E:801:ATP:C3'	3:E:802:NDT:C4	2.94	0.45
1:F:91:HIS:HA	1:F:92:PRO:HD3	1.69	0.45
1:F:98:LEU:H	1:F:98:LEU:HD23	1.82	0.45
1:F:134:LEU:C	1:F:134:LEU:CD1	2.85	0.45
1:F:141:GLU:HG3	1:F:171:ALA:N	2.18	0.45
1:A:143:MET:SD	1:A:143:MET:N	2.89	0.45
1:B:99:SER:CB	1:B:102:ILE:CD1	2.94	0.45
1:B:251:ASP:HA	1:B:254:ILE:HG22	1.98	0.45
1:C:143:MET:SD	1:C:143:MET:N	2.89	0.45
1:C:217:PHE:CD2	1:C:217:PHE:O	2.70	0.45
1:C:499:ARG:HH21	1:C:500:PRO:HD2	1.81	0.45
1:D:363:GLU:HG2	1:D:364:SER:N	2.31	0.45
1:D:583:GLY:HA3	1:D:617:GLU:O	2.17	0.45
1:F:399:LEU:HD23	1:F:404:ARG:HD3	1.99	0.45
1:A:37:ARG:CG	1:A:95:VAL:CG2	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASN:HB2	1:A:228:LYS:HB3	1.99	0.44
1:A:759:ARG:HB2	1:A:761:ILE:HG22	1.98	0.44
1:B:37:ARG:HH11	1:B:306:HIS:CG	2.32	0.44
1:B:142:CYS:N	1:B:170:LYS:NZ	2.61	0.44
1:C:159:MET:HB3	1:C:213:PRO:HD2	1.99	0.44
1:C:167:LEU:O	1:C:175:SER:HB3	2.17	0.44
1:C:271:PHE:O	1:C:271:PHE:CD1	2.70	0.44
1:D:130:THR:HG23	1:D:182:ASP:N	2.31	0.44
1:D:167:LEU:N	1:D:167:LEU:CD2	2.80	0.44
1:D:209:PHE:O	1:D:209:PHE:CD1	2.70	0.44
1:E:141:GLU:HG2	1:E:170:LYS:C	1.98	0.44
1:E:167:LEU:N	1:E:167:LEU:CD2	2.80	0.44
1:F:167:LEU:O	1:F:175:SER:HB3	2.17	0.44
1:F:265:LEU:HD21	1:F:384:VAL:HG22	1.99	0.44
1:A:211:LEU:CD2	1:A:211:LEU:C	2.85	0.44
1:A:751:GLU:C	1:A:755:LYS:HZ3	2.20	0.44
1:B:217:PHE:CD2	1:B:217:PHE:O	2.70	0.44
1:B:224:ILE:N	1:B:224:ILE:CD1	2.73	0.44
1:B:434:ARG:HD3	1:C:274:PHE:CD1	2.52	0.44
1:B:532:ILE:O	1:B:535:PRO:HD2	2.18	0.44
1:C:37:ARG:HG3	1:C:95:VAL:HG21	1.99	0.44
1:C:167:LEU:N	1:C:167:LEU:CD2	2.80	0.44
1:C:270:LEU:HD13	1:C:270:LEU:C	2.38	0.44
1:C:541:THR:HA	1:C:544:ARG:CZ	2.48	0.44
1:C:600:GLU:HA	1:C:603:ARG:HG2	1.99	0.44
1:C:707:VAL:HG23	1:C:709:LEU:HD22	1.98	0.44
1:D:347:ILE:HG12	1:D:389:THR:HB	1.98	0.44
1:E:159:MET:HB3	1:E:213:PRO:HD2	1.99	0.44
1:E:225:THR:O	1:E:225:THR:OG1	2.19	0.44
1:E:561:CYS:SG	1:E:721:GLY:HA3	2.58	0.44
1:F:253:GLU:HG2	1:F:410:GLU:O	2.17	0.44
2:F:803:ATP:C8	3:F:804:NDT:O3	2.71	0.44
1:A:50:THR:HG1	1:A:84:ARG:CB	2.25	0.44
1:B:74:ILE:HD12	1:B:74:ILE:HA	1.72	0.44
1:D:37:ARG:CG	1:D:95:VAL:CG2	2.95	0.44
1:D:77:ASN:CG	1:D:209:PHE:CB	2.73	0.44
1:D:104:SER:OG	1:D:163:ILE:HD12	2.02	0.44
1:D:159:MET:CE	1:D:183:ALA:H	2.31	0.44
1:D:213:PRO:HA	1:D:214:PRO:HD3	1.88	0.44
1:E:39:HIS:HA	1:E:40:PRO:HD3	1.55	0.44
1:E:98:LEU:H	1:E:98:LEU:HD23	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:GLY:C	1:E:157:VAL:CG1	2.59	0.44
1:E:167:LEU:O	1:E:175:SER:HB3	2.17	0.44
1:F:50:THR:OG1	1:F:84:ARG:CG	2.65	0.44
1:F:224:ILE:N	1:F:224:ILE:CD1	2.73	0.44
1:F:434:ARG:O	1:F:485:LYS:HB2	2.18	0.44
1:F:434:ARG:HH22	1:F:482:PHE:HA	1.82	0.44
1:F:591:VAL:HG22	1:F:632:ALA:HB2	1.99	0.44
1:A:167:LEU:N	1:A:167:LEU:CD2	2.80	0.44
1:A:434:ARG:HA	1:A:434:ARG:CZ	2.48	0.44
1:B:680:TYR:HE1	1:B:769:TYR:HB3	1.82	0.44
1:C:80:LEU:HD22	1:C:211:LEU:CD1	2.04	0.44
1:C:134:LEU:C	1:C:134:LEU:CD1	2.85	0.44
1:C:258:LYS:HE3	1:C:258:LYS:HB2	1.84	0.44
1:D:218:ARG:CB	1:D:218:ARG:HH21	2.28	0.44
1:D:733:LEU:HA	1:D:736:ILE:HG12	2.00	0.44
1:E:37:ARG:HG2	1:E:95:VAL:HG23	2.00	0.44
1:E:58:LEU:HD11	1:E:63:ILE:HG13	1.96	0.44
1:F:37:ARG:HG2	1:F:95:VAL:HG23	2.00	0.44
1:F:52:TYR:CB	1:F:86:GLY:HA2	2.46	0.44
1:F:166:ASN:HD21	1:F:169:THR:CG2	2.13	0.44
1:F:444:TYR:CZ	1:F:448:LYS:HE2	2.53	0.44
1:A:134:LEU:C	1:A:134:LEU:CD1	2.85	0.44
1:A:440:GLU:H	1:A:440:GLU:CD	2.11	0.44
1:B:738:GLU:CD	1:B:749:HIS:HE2	2.21	0.44
1:B:762:THR:H	1:B:765:MET:HE2	1.83	0.44
1:C:39:HIS:HA	1:C:40:PRO:HD3	1.55	0.44
1:C:528:MET:CE	1:C:570:LEU:HD13	2.48	0.44
1:D:167:LEU:O	1:D:175:SER:HB3	2.17	0.44
1:D:689:ARG:CZ	1:D:717:GLU:HA	2.46	0.44
1:E:37:ARG:CG	1:E:95:VAL:CG2	2.95	0.44
1:E:274:PHE:HD2	1:E:274:PHE:N	2.11	0.44
1:E:534:LEU:HB3	1:E:542:PHE:HZ	1.82	0.44
1:F:37:ARG:HG3	1:F:95:VAL:HG21	1.99	0.44
1:F:167:LEU:N	1:F:167:LEU:CD2	2.81	0.44
1:F:324:GLU:HB2	1:F:328:ARG:HH21	1.83	0.44
1:A:37:ARG:HG3	1:A:95:VAL:HG21	1.99	0.44
1:A:70:THR:CG2	1:A:210:TYR:CE1	3.00	0.44
1:A:217:PHE:CD2	1:A:217:PHE:O	2.70	0.44
1:B:134:LEU:C	1:B:134:LEU:CD1	2.85	0.44
1:B:562:SER:O	1:B:566:THR:HG23	2.18	0.44
1:C:261:ILE:HD11	1:C:386:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:MET:SD	1:C:404:ARG:HG3	2.57	0.44
1:D:583:GLY:O	1:D:586:ILE:HG12	2.18	0.44
1:E:105:VAL:CG2	1:E:162:MET:CG	2.82	0.44
1:E:262:GLU:O	1:E:266:HIS:N	2.44	0.44
1:E:532:ILE:HG21	1:E:570:LEU:HD11	2.00	0.44
1:F:53:ILE:N	1:F:86:GLY:HA2	2.28	0.44
1:F:366:VAL:O	1:F:370:LEU:HD23	2.17	0.44
1:F:487:THR:HG23	1:F:490:ASP:H	1.83	0.44
1:F:593:GLU:O	1:F:596:ARG:HG3	2.18	0.44
1:A:141:GLU:OE1	1:A:170:LYS:CD	2.54	0.44
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.81	0.44
1:A:650:LEU:HB3	1:A:653:VAL:HG22	1.99	0.44
1:A:672:PRO:C	3:F:804:NDT:H7	2.38	0.44
1:B:138:ASN:HB2	1:B:228:LYS:HB3	1.99	0.44
1:B:167:LEU:N	1:B:167:LEU:CD2	2.80	0.44
1:B:562:SER:HB3	2:B:803:ATP:O4'	2.18	0.44
1:C:37:ARG:HG2	1:C:95:VAL:HG23	2.00	0.44
1:C:530:GLU:O	1:C:534:LEU:HG	2.17	0.44
1:E:465:VAL:CG1	1:F:274:PHE:CD2	3.00	0.44
1:F:614:PHE:HA	1:F:656:VAL:O	2.18	0.44
1:A:50:THR:OG1	1:A:84:ARG:CG	2.65	0.44
1:A:592:GLY:HA2	1:A:595:GLU:HB3	2.00	0.44
1:B:37:ARG:NH1	1:B:306:HIS:CG	2.86	0.44
1:B:684:PRO:HG3	2:B:803:ATP:N1	2.32	0.44
1:D:134:LEU:C	1:D:134:LEU:CD1	2.85	0.44
1:D:513:VAL:HG12	1:D:568:LYS:HB3	1.99	0.44
1:D:553:VAL:HA	1:D:677:ARG:HB2	2.00	0.44
1:D:596:ARG:O	1:D:600:GLU:OE1	2.36	0.44
1:E:141:GLU:HG3	1:E:171:ALA:N	2.18	0.44
1:E:399:LEU:HD22	1:E:405:PHE:CE2	2.52	0.44
1:E:559:PRO:HG3	1:E:660:ASN:ND2	2.29	0.44
1:F:437:LEU:HD23	1:F:437:LEU:HA	1.91	0.44
1:A:167:LEU:O	1:A:175:SER:HB3	2.17	0.44
1:A:670:LEU:HD11	1:A:678:HIS:HE1	1.80	0.44
1:B:49:CYS:O	1:B:82:ILE:HG22	2.16	0.44
1:B:50:THR:OG1	1:B:84:ARG:CG	2.65	0.44
1:B:606:ARG:NH2	1:B:648:GLU:OE1	2.46	0.44
1:D:39:HIS:HA	1:D:40:PRO:HD3	1.55	0.44
1:E:366:VAL:HA	1:E:369:THR:HG22	1.99	0.44
1:A:564:THR:CG2	2:A:803:ATP:O3G	2.64	0.43
1:B:265:LEU:HD11	1:B:341:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:HIS:HB3	1:C:97:THR:HB	1.98	0.43
1:C:500:PRO:HB2	1:C:503:MET:HE3	1.99	0.43
1:D:37:ARG:HG2	1:D:95:VAL:HG23	2.00	0.43
1:D:149:GLN:HA	1:D:152:LEU:CG	2.48	0.43
1:D:159:MET:HB3	1:D:213:PRO:HD2	1.99	0.43
1:E:77:ASN:OD1	1:E:209:PHE:CA	2.63	0.43
1:E:159:MET:CE	1:E:183:ALA:H	2.31	0.43
1:E:218:ARG:CB	1:E:218:ARG:HH21	2.28	0.43
1:E:434:ARG:HD3	1:F:273:SER:HB2	2.00	0.43
1:F:506:ILE:HG23	1:F:507:PHE:CD1	2.53	0.43
1:F:730:GLU:O	1:F:733:LEU:HG	2.18	0.43
1:B:676:ASP:HB3	1:B:677:ARG:NH1	2.33	0.43
1:C:46:LYS:CA	1:C:46:LYS:CE	2.85	0.43
1:C:233:ASN:ND2	1:C:235:LYS:CE	2.66	0.43
1:C:374:MET:HA	1:C:377:MET:CG	2.37	0.43
1:C:465:VAL:HG21	1:D:276:VAL:HG21	2.01	0.43
1:C:528:MET:O	1:C:532:ILE:HG23	2.18	0.43
1:D:646:GLY:O	1:D:647:VAL:HG12	2.18	0.43
1:E:37:ARG:HG3	1:E:95:VAL:HG21	1.99	0.43
1:F:105:VAL:HG23	1:F:162:MET:HA	2.00	0.43
1:A:70:THR:HG22	1:A:210:TYR:HE1	1.83	0.43
1:A:348:ASP:OD1	1:A:349:SER:N	2.51	0.43
1:A:452:TYR:CE2	1:A:500:PRO:HG3	2.53	0.43
3:A:802:NDT:H211	1:B:276:VAL:HG12	1.96	0.43
1:B:92:PRO:HD2	1:B:95:VAL:HG11	2.00	0.43
1:B:429:ARG:HG2	3:B:802:NDT:C21	2.33	0.43
1:B:459:ALA:HB1	1:B:498:ILE:HD11	2.00	0.43
1:D:597:ALA:HA	1:D:600:GLU:CD	2.37	0.43
1:E:507:PHE:CE2	1:E:604:LYS:HD3	2.53	0.43
1:F:79:ILE:O	1:F:80:LEU:CG	2.67	0.43
1:A:37:ARG:HG2	1:A:95:VAL:HG23	2.00	0.43
1:A:455:ALA:CA	2:A:801:ATP:C8	2.85	0.43
1:B:167:LEU:O	1:B:175:SER:HB3	2.17	0.43
1:B:289:GLY:N	2:B:801:ATP:O1B	2.48	0.43
1:C:435:HIS:HA	1:C:486:VAL:H	1.83	0.43
1:C:583:GLY:O	1:C:586:ILE:HG12	2.18	0.43
1:C:676:ASP:O	1:C:678:HIS:ND1	2.48	0.43
1:D:159:MET:HE3	1:D:183:ALA:N	2.32	0.43
1:D:242:LEU:HG	1:D:301:ASN:ND2	2.33	0.43
1:D:695:LYS:HE2	3:D:804:NDT:H212	2.00	0.43
1:E:92:PRO:HD2	1:E:95:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:PHE:CD2	1:E:217:PHE:O	2.70	0.43
1:E:452:TYR:CE2	1:E:498:ILE:HG23	2.54	0.43
1:E:479:ILE:HG13	1:E:480:ASP:N	2.34	0.43
1:E:671:ARG:HH11	1:E:674:ARG:NH1	2.16	0.43
2:E:803:ATP:H3'	3:E:804:NDT:C5	2.49	0.43
1:A:646:GLY:O	1:A:647:VAL:HG12	2.19	0.43
1:B:37:ARG:HG3	1:B:95:VAL:HG21	2.00	0.43
1:B:708:ASP:HB2	1:B:710:HIS:CE1	2.54	0.43
1:C:138:ASN:HB2	1:C:228:LYS:HB3	1.99	0.43
1:C:159:MET:HB3	1:C:213:PRO:CD	2.49	0.43
1:C:695:LYS:CE	3:C:804:NDT:H17	2.31	0.43
1:D:266:HIS:N	1:D:268:PRO:HD3	2.33	0.43
1:E:128:LYS:HG3	1:E:128:LYS:O	2.19	0.43
1:E:366:VAL:O	1:E:369:THR:HG22	2.19	0.43
1:E:629:SER:HB3	1:E:633:ALA:CB	2.48	0.43
1:F:160:PRO:HD3	1:F:212:SER:OG	2.06	0.43
1:F:217:PHE:CD2	1:F:217:PHE:O	2.70	0.43
1:F:344:ILE:HG21	1:F:347:ILE:HD13	2.00	0.43
1:F:692:ILE:HD11	2:F:803:ATP:C6	2.53	0.43
1:B:53:ILE:N	1:B:86:GLY:HA2	2.28	0.43
1:B:130:THR:HG23	1:B:182:ASP:N	2.31	0.43
1:B:295:LEU:HA	1:B:295:LEU:HD23	1.83	0.43
1:B:624:ASP:OD1	1:B:634:ASN:HA	2.18	0.43
1:C:141:GLU:OE1	1:C:170:LYS:CD	2.54	0.43
1:C:524:LEU:HD13	1:C:681:VAL:HG23	1.99	0.43
1:C:690:LEU:HD12	1:C:710:HIS:HA	2.01	0.43
1:D:77:ASN:O	1:D:211:LEU:HD23	2.18	0.43
1:D:128:LYS:HG3	1:D:128:LYS:O	2.19	0.43
1:D:285:HIS:CG	1:D:392:PRO:HG3	2.53	0.43
1:E:50:THR:OG1	1:E:84:ARG:CG	2.65	0.43
1:E:105:VAL:HG23	1:E:162:MET:HA	2.00	0.43
1:E:149:GLN:HA	1:E:152:LEU:CG	2.48	0.43
1:F:577:ASN:O	1:F:611:SER:OG	2.20	0.43
1:A:98:LEU:H	1:A:98:LEU:HD23	1.82	0.43
1:A:274:PHE:CE1	1:F:434:ARG:HD3	2.54	0.43
1:B:105:VAL:HG23	1:B:162:MET:HA	2.00	0.43
1:B:128:LYS:HG3	1:B:128:LYS:O	2.19	0.43
1:C:213:PRO:HB2	1:C:215:PHE:CZ	2.54	0.43
1:C:366:VAL:O	1:C:369:THR:HG22	2.19	0.43
1:C:463:GLU:HG3	1:C:498:ILE:HD13	2.00	0.43
1:C:598:ILE:HD11	1:C:636:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LEU:HD13	1:D:61:LEU:HA	1.92	0.43
1:D:80:LEU:N	1:D:211:LEU:HD12	2.34	0.43
1:D:213:PRO:HB2	1:D:215:PHE:CZ	2.54	0.43
1:F:345:ASP:HB3	1:F:346:GLU:OE1	2.19	0.43
1:F:662:PRO:HB2	1:F:772:PHE:CZ	2.53	0.43
1:A:128:LYS:O	1:A:128:LYS:HG3	2.19	0.43
1:A:218:ARG:CA	1:A:218:ARG:NH2	2.74	0.43
1:A:285:HIS:HB2	1:A:392:PRO:HG3	2.00	0.43
1:A:593:GLU:OE2	1:A:596:ARG:NH2	2.46	0.43
1:A:660:ASN:O	1:A:769:TYR:OH	2.22	0.43
1:B:37:ARG:HG2	1:B:95:VAL:HG23	2.00	0.43
1:B:218:ARG:CA	1:B:218:ARG:NH2	2.74	0.43
1:C:77:ASN:O	1:C:211:LEU:HD22	2.02	0.43
1:D:159:MET:HB3	1:D:213:PRO:CD	2.49	0.43
1:D:299:VAL:HA	1:D:302:THR:HG22	2.00	0.43
1:E:134:LEU:C	1:E:134:LEU:CD1	2.85	0.43
1:E:159:MET:HB3	1:E:213:PRO:CD	2.49	0.43
1:E:241:PRO:CB	1:E:301:ASN:ND2	2.81	0.43
1:F:39:HIS:HB3	1:F:97:THR:HB	1.98	0.43
1:F:99:SER:HB3	1:F:102:ILE:HD11	2.01	0.43
1:F:128:LYS:O	1:F:128:LYS:HG3	2.19	0.43
1:F:141:GLU:HG2	1:F:170:LYS:C	1.98	0.43
1:A:91:HIS:ND1	1:A:91:HIS:C	2.73	0.43
1:A:213:PRO:HB2	1:A:215:PHE:CZ	2.54	0.43
1:A:365:ARG:HG3	1:A:366:VAL:N	2.33	0.43
1:B:159:MET:CE	1:B:183:ALA:H	2.31	0.43
1:B:551:LYS:NZ	1:B:650:LEU:H	2.17	0.43
1:C:35:ILE:HG13	1:C:113:ARG:NH1	2.33	0.43
1:D:37:ARG:HG3	1:D:95:VAL:HG21	1.99	0.43
1:D:159:MET:O	1:D:180:ILE:O	2.37	0.43
1:D:619:ASP:HB2	1:D:664:GLU:OE1	2.19	0.43
1:E:99:SER:HB3	1:E:102:ILE:HD11	2.01	0.43
1:E:233:ASN:HB3	1:E:236:TYR:CE2	2.54	0.43
1:A:56:ASN:C	1:A:56:ASN:ND2	2.72	0.43
1:A:82:ILE:CD1	1:A:82:ILE:N	2.72	0.43
1:A:92:PRO:HD2	1:A:95:VAL:HG11	2.00	0.43
1:A:606:ARG:HE	1:A:650:LEU:HD21	1.83	0.43
1:A:730:GLU:HA	1:A:733:LEU:HD12	2.00	0.43
1:C:208:LEU:C	1:C:208:LEU:CD2	2.87	0.43
1:C:366:VAL:HA	1:C:369:THR:HG22	2.01	0.43
1:C:414:PRO:O	1:C:419:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:GLN:OE1	1:C:523:GLU:HB3	2.19	0.43
1:D:74:ILE:HD12	1:D:74:ILE:HA	1.72	0.43
1:D:80:LEU:H	1:D:211:LEU:HG	1.83	0.43
1:D:469:ILE:HG21	1:E:263:ILE:HD12	1.99	0.43
1:E:265:LEU:CD2	1:E:382:LYS:C	2.87	0.43
1:F:56:ASN:ND2	1:F:56:ASN:C	2.72	0.43
1:F:159:MET:HE2	1:F:159:MET:HA	1.98	0.43
1:A:70:THR:HG22	1:A:210:TYR:CE1	2.54	0.42
1:A:141:GLU:HG3	1:A:171:ALA:N	2.18	0.42
1:A:466:MET:CE	1:B:271:PHE:CZ	3.02	0.42
1:B:56:ASN:ND2	1:B:56:ASN:C	2.73	0.42
1:B:557:GLY:HA3	1:B:681:VAL:HG13	2.00	0.42
1:C:56:ASN:ND2	1:C:56:ASN:C	2.72	0.42
1:C:159:MET:CE	1:C:183:ALA:H	2.31	0.42
1:C:736:ILE:HG22	1:C:742:VAL:HG22	2.01	0.42
1:E:35:ILE:HG13	1:E:113:ARG:NH1	2.33	0.42
1:E:56:ASN:ND2	1:E:56:ASN:C	2.72	0.42
1:E:91:HIS:ND1	1:E:91:HIS:C	2.73	0.42
1:E:213:PRO:HB2	1:E:215:PHE:CZ	2.54	0.42
1:E:276:VAL:O	1:E:277:SER:CB	2.67	0.42
1:E:452:TYR:HE2	1:E:498:ILE:HG23	1.84	0.42
1:E:459:ALA:HB2	1:F:402:PRO:HB3	1.99	0.42
1:F:35:ILE:CB	1:F:113:ARG:HH11	2.32	0.42
1:F:91:HIS:ND1	1:F:91:HIS:C	2.73	0.42
1:A:104:SER:HG	1:A:163:ILE:CD1	1.95	0.42
1:A:556:TYR:CE1	1:A:678:HIS:HB3	2.53	0.42
1:A:576:ILE:HG22	1:A:611:SER:HA	2.01	0.42
1:B:211:LEU:HG	1:B:214:PRO:HG3	2.01	0.42
1:C:319:TYR:HB2	1:C:322:GLU:HB2	2.01	0.42
1:C:614:PHE:HA	1:C:656:VAL:O	2.19	0.42
1:E:218:ARG:CA	1:E:218:ARG:NH2	2.74	0.42
1:E:629:SER:HB3	1:E:633:ALA:HB3	2.00	0.42
1:E:722:ALA:CB	2:E:803:ATP:H5'2	2.49	0.42
1:F:521:GLN:OE1	1:F:521:GLN:N	2.52	0.42
1:F:562:SER:CA	2:F:803:ATP:O1A	2.67	0.42
1:A:499:ARG:NH1	1:B:603:ARG:HG3	2.34	0.42
1:A:595:GLU:OE2	1:A:599:ARG:NH2	2.51	0.42
1:B:429:ARG:HH22	3:B:802:NDT:C16	2.28	0.42
1:C:92:PRO:HD2	1:C:95:VAL:HG11	2.00	0.42
1:C:149:GLN:HA	1:C:152:LEU:CG	2.48	0.42
1:C:159:MET:O	1:C:180:ILE:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PRO:CG	1:C:238:LEU:CD1	2.90	0.42
1:D:242:LEU:N	1:D:301:ASN:ND2	2.38	0.42
2:D:801:ATP:C8	3:D:802:NDT:O2	2.70	0.42
1:E:82:ILE:CD1	1:E:82:ILE:N	2.73	0.42
1:E:99:SER:CB	1:E:102:ILE:HD11	2.49	0.42
1:E:316:VAL:HG13	1:E:362:VAL:HG21	2.00	0.42
1:F:92:PRO:HD2	1:F:95:VAL:HG11	2.00	0.42
1:F:99:SER:CB	1:F:102:ILE:HD11	2.50	0.42
1:F:354:ARG:HD3	1:F:364:SER:HB3	2.01	0.42
1:F:534:LEU:HB3	1:F:542:PHE:HZ	1.84	0.42
1:A:78:GLY:HA2	1:A:211:LEU:CB	2.14	0.42
1:A:99:SER:CB	1:A:102:ILE:HD11	2.50	0.42
1:A:149:GLN:HA	1:A:152:LEU:CG	2.48	0.42
1:A:157:VAL:N	1:A:162:MET:SD	2.61	0.42
1:A:452:TYR:HD1	1:A:456:ASP:HB3	1.85	0.42
1:B:39:HIS:ND1	1:B:39:HIS:C	2.73	0.42
1:B:104:SER:OG	1:B:163:ILE:HD12	2.02	0.42
1:B:120:GLN:NE2	1:B:120:GLN:C	2.73	0.42
1:B:149:GLN:HA	1:B:152:LEU:CG	2.48	0.42
1:B:452:TYR:CE1	1:B:498:ILE:HG23	2.54	0.42
1:B:524:LEU:HD21	1:B:681:VAL:HA	2.01	0.42
1:B:559:PRO:HG3	1:B:660:ASN:ND2	2.34	0.42
1:C:286:GLY:O	1:C:292:LYS:NZ	2.41	0.42
2:C:801:ATP:C8	3:C:802:NDT:O2	2.70	0.42
1:D:92:PRO:HD2	1:D:95:VAL:HG11	2.00	0.42
1:D:110:LEU:HB2	1:D:306:HIS:HA	1.99	0.42
1:D:231:GLN:HE21	1:D:231:GLN:HB2	1.58	0.42
2:D:803:ATP:C8	3:D:804:NDT:O2	2.71	0.42
1:F:218:ARG:CA	1:F:218:ARG:NH2	2.74	0.42
1:F:276:VAL:HG13	1:F:277:SER:N	2.35	0.42
1:F:291:GLY:HA2	2:F:801:ATP:O1A	2.19	0.42
1:F:320:LEU:HD12	1:F:365:ARG:NE	2.35	0.42
1:F:559:PRO:CG	1:F:660:ASN:CG	2.61	0.42
1:F:598:ILE:HD11	1:F:636:VAL:HG13	1.99	0.42
1:B:91:HIS:ND1	1:B:91:HIS:C	2.73	0.42
1:B:159:MET:HE2	1:B:182:ASP:HA	1.00	0.42
1:B:313:PRO:HB2	1:C:365:ARG:HG2	2.00	0.42
1:D:132:GLY:O	1:D:179:VAL:HB	2.19	0.42
1:D:415:ASP:OD1	1:D:418:ALA:N	2.33	0.42
1:E:132:GLY:O	1:E:179:VAL:HB	2.19	0.42
1:E:515:TRP:CZ3	1:E:525:LYS:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:LYS:HZ1	1:F:108:LEU:HA	1.85	0.42
1:F:88:GLU:CG	1:F:90:VAL:HG12	2.49	0.42
1:F:228:LYS:HB2	1:F:228:LYS:HE3	1.79	0.42
1:F:268:PRO:CG	1:F:382:LYS:HE2	2.49	0.42
1:B:132:GLY:O	1:B:179:VAL:HB	2.19	0.42
1:B:228:LYS:HB2	1:B:228:LYS:HE3	1.80	0.42
1:B:617:GLU:OE2	2:B:803:ATP:PG	2.77	0.42
2:B:803:ATP:C2'	3:B:804:NDT:S1	3.07	0.42
1:C:39:HIS:CB	1:C:97:THR:CB	2.90	0.42
1:C:120:GLN:NE2	1:C:120:GLN:C	2.73	0.42
1:C:624:ASP:CB	1:C:629:SER:OG	2.63	0.42
1:D:268:PRO:O	1:D:269:THR:OG1	2.32	0.42
1:D:289:GLY:CA	2:D:801:ATP:O2B	2.66	0.42
1:D:555:LEU:HD13	1:D:679:ILE:HB	2.01	0.42
1:D:646:GLY:C	1:D:648:GLU:H	2.21	0.42
1:E:39:HIS:ND1	1:E:39:HIS:C	2.73	0.42
1:E:159:MET:O	1:E:180:ILE:O	2.37	0.42
1:E:277:SER:HB3	1:E:278:PRO:HD2	2.01	0.42
1:E:348:ASP:OD1	1:E:349:SER:N	2.52	0.42
1:E:603:ARG:NH2	1:E:604:LYS:HB2	2.35	0.42
3:E:804:NDT:C7	1:F:673:GLY:CA	2.58	0.42
1:F:132:GLY:O	1:F:179:VAL:HB	2.19	0.42
1:A:149:GLN:HA	1:A:152:LEU:CD2	2.50	0.42
1:A:602:PHE:O	1:A:606:ARG:HG3	2.20	0.42
3:A:802:NDT:H8	1:B:403:GLY:HA2	1.96	0.42
1:B:127:THR:HA	1:B:222:THR:OG1	2.20	0.42
1:B:236:TYR:CB	1:B:238:LEU:HG	2.46	0.42
1:B:338:GLN:OE1	1:B:382:LYS:N	2.51	0.42
1:B:564:THR:O	1:B:568:LYS:HG3	2.20	0.42
1:C:105:VAL:HG23	1:C:162:MET:HA	2.00	0.42
1:C:606:ARG:NH1	1:C:648:GLU:OE1	2.46	0.42
1:D:99:SER:HB3	1:D:102:ILE:HD11	2.01	0.42
1:D:159:MET:N	1:D:160:PRO:CD	2.83	0.42
1:D:479:ILE:HD12	1:D:479:ILE:HA	1.93	0.42
1:E:138:ASN:HB2	1:E:228:LYS:HB3	1.99	0.42
1:E:159:MET:N	1:E:160:PRO:CD	2.83	0.42
1:F:598:ILE:HA	1:F:601:ILE:HG22	2.00	0.42
1:A:270:LEU:HG	1:F:481:LYS:CD	2.44	0.42
1:A:274:PHE:CE2	1:F:465:VAL:HG13	2.55	0.42
1:B:99:SER:HB3	1:B:102:ILE:HD11	2.01	0.42
1:B:598:ILE:O	1:B:601:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:LYS:HE2	3:B:804:NDT:C17	2.45	0.42
1:B:721:GLY:N	2:B:803:ATP:H2	2.09	0.42
1:C:37:ARG:HH12	1:C:306:HIS:HB2	1.85	0.42
1:D:99:SER:CB	1:D:102:ILE:HD11	2.50	0.42
1:D:563:LYS:HE2	2:D:803:ATP:PG	2.58	0.42
1:D:597:ALA:HA	1:D:600:GLU:OE2	2.20	0.42
1:E:127:THR:HA	1:E:222:THR:OG1	2.20	0.42
1:E:363:GLU:HG2	1:E:364:SER:N	2.33	0.42
1:E:732:GLY:O	1:E:736:ILE:HG23	2.20	0.42
1:F:39:HIS:ND1	1:F:39:HIS:C	2.73	0.42
1:F:623:PRO:CG	1:F:664:GLU:HB3	2.47	0.42
1:F:708:ASP:O	1:F:710:HIS:ND1	2.52	0.42
1:A:99:SER:HB3	1:A:102:ILE:HD11	2.01	0.42
1:A:132:GLY:O	1:A:179:VAL:HB	2.19	0.42
1:A:403:GLY:HA2	3:F:802:NDT:C7	2.19	0.42
1:A:467:LYS:HD3	1:A:467:LYS:HA	1.85	0.42
1:B:99:SER:CB	1:B:102:ILE:HD11	2.49	0.42
1:B:159:MET:N	1:B:160:PRO:CD	2.83	0.42
1:B:324:GLU:OE2	1:B:365:ARG:NE	2.52	0.42
1:B:707:VAL:HG23	1:B:709:LEU:HD22	2.00	0.42
1:C:608:ALA:O	1:C:609:ALA:HB3	2.20	0.42
1:C:612:ILE:HG22	1:C:654:VAL:HB	2.01	0.42
1:C:733:LEU:HA	1:C:736:ILE:HG12	2.02	0.42
1:D:39:HIS:ND1	1:D:39:HIS:C	2.73	0.42
1:D:326:ALA:O	1:D:330:ILE:HG13	2.19	0.42
1:D:513:VAL:O	1:D:569:ALA:HA	2.20	0.42
1:D:712:LEU:O	1:D:716:THR:HG22	2.19	0.42
1:E:120:GLN:NE2	1:E:120:GLN:C	2.73	0.42
1:F:479:ILE:HG13	1:F:480:ASP:N	2.35	0.42
1:A:105:VAL:HG23	1:A:162:MET:HA	2.00	0.42
1:A:238:LEU:HB3	1:A:239:PRO:HD2	2.01	0.42
1:A:646:GLY:C	1:A:648:GLU:H	2.23	0.42
1:B:35:ILE:HG13	1:B:113:ARG:NH1	2.33	0.42
1:B:149:GLN:HA	1:B:152:LEU:CD2	2.50	0.42
1:B:338:GLN:HG3	1:B:382:LYS:HG2	2.00	0.42
1:B:684:PRO:HG3	2:B:803:ATP:C2	2.55	0.42
1:C:128:LYS:HG3	1:C:128:LYS:O	2.19	0.42
1:C:138:ASN:C	1:C:138:ASN:HD22	2.22	0.42
1:C:529:LYS:HA	1:C:532:ILE:HG12	2.01	0.42
1:D:105:VAL:HG23	1:D:162:MET:HA	2.00	0.42
1:D:120:GLN:NE2	1:D:120:GLN:C	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:GLN:HA	1:D:152:LEU:CD2	2.50	0.42
1:D:249:GLY:N	1:D:421:ASP:OD2	2.52	0.42
1:D:429:ARG:HH21	3:D:802:NDT:C19	2.28	0.42
1:E:367:VAL:HG11	1:E:396:ASP:OD2	2.20	0.42
1:A:46:LYS:CA	1:A:46:LYS:CE	2.85	0.41
1:A:126:ALA:O	1:A:222:THR:CG2	2.68	0.41
1:A:263:ILE:HG23	1:A:264:PRO:HD3	2.01	0.41
2:A:801:ATP:H3'	3:A:802:NDT:N2	2.35	0.41
1:B:382:LYS:HE2	1:B:382:LYS:HB3	1.89	0.41
1:B:576:ILE:HG22	1:B:611:SER:HA	2.01	0.41
1:C:506:ILE:HG23	1:C:507:PHE:CD1	2.54	0.41
1:C:663:ASP:OD2	1:C:768:TYR:OH	2.30	0.41
1:C:671:ARG:HH11	1:C:674:ARG:NH1	2.18	0.41
1:D:126:ALA:O	1:D:222:THR:CG2	2.68	0.41
1:D:489:LYS:HE2	1:D:489:LYS:HB3	1.79	0.41
1:D:723:GLU:O	1:D:727:LEU:HD23	2.19	0.41
1:E:347:ILE:HG21	1:E:387:ALA:HB1	2.02	0.41
1:E:521:GLN:O	1:E:525:LYS:HG3	2.19	0.41
1:F:129:VAL:HA	1:F:183:ALA:HA	2.02	0.41
1:F:159:MET:HE2	1:F:159:MET:C	2.36	0.41
1:F:762:THR:HG22	1:F:765:MET:SD	2.60	0.41
1:B:138:ASN:HD22	1:B:138:ASN:C	2.22	0.41
1:B:487:THR:HG23	1:B:490:ASP:H	1.85	0.41
1:C:39:HIS:ND1	1:C:39:HIS:C	2.73	0.41
1:C:102:ILE:CD1	1:C:102:ILE:H	1.96	0.41
1:C:129:VAL:HA	1:C:183:ALA:HA	2.02	0.41
1:C:132:GLY:O	1:C:179:VAL:HB	2.19	0.41
1:C:565:LEU:HD11	3:C:804:NDT:O3	2.20	0.41
1:C:618:ILE:HB	1:C:657:ALA:HB1	2.01	0.41
1:C:661:ARG:HH12	1:C:664:GLU:HB3	1.85	0.41
1:C:697:THR:HA	1:C:700:PHE:HD2	1.85	0.41
1:C:732:GLY:O	1:C:736:ILE:HG23	2.20	0.41
1:D:35:ILE:HG13	1:D:113:ARG:NH1	2.33	0.41
1:D:56:ASN:C	1:D:56:ASN:ND2	2.73	0.41
1:D:91:HIS:ND1	1:D:91:HIS:C	2.73	0.41
1:D:127:THR:HA	1:D:222:THR:OG1	2.20	0.41
1:D:490:ASP:OD1	1:D:491:VAL:N	2.53	0.41
1:D:727:LEU:HD21	1:D:757:ILE:HG21	2.01	0.41
1:E:382:LYS:HE2	1:E:382:LYS:HB3	1.82	0.41
1:F:74:ILE:HD12	1:F:74:ILE:HA	1.88	0.41
1:F:82:ILE:CG2	1:F:102:ILE:HG21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:149:GLN:HA	1:F:152:LEU:CD2	2.50	0.41
1:F:366:VAL:HA	1:F:369:THR:HG22	2.02	0.41
1:A:39:HIS:ND1	1:A:39:HIS:C	2.73	0.41
1:A:127:THR:HA	1:A:222:THR:OG1	2.20	0.41
1:A:351:ALA:HB1	1:A:367:VAL:HG22	2.02	0.41
1:A:510:MET:HB3	1:A:568:LYS:HD2	2.01	0.41
1:B:306:HIS:O	1:B:340:SER:HA	2.18	0.41
1:B:726:LEU:HD22	1:C:672:PRO:HB3	2.02	0.41
1:C:54:HIS:HA	1:C:55:PRO:HD3	1.95	0.41
1:C:91:HIS:ND1	1:C:91:HIS:C	2.73	0.41
1:C:127:THR:HA	1:C:222:THR:OG1	2.20	0.41
1:C:231:GLN:HE21	1:C:231:GLN:HB2	1.58	0.41
1:D:129:VAL:HA	1:D:183:ALA:HA	2.02	0.41
1:D:576:ILE:HG22	1:D:611:SER:HA	2.02	0.41
1:D:662:PRO:HD3	1:D:769:TYR:HE1	1.85	0.41
1:E:88:GLU:CG	1:E:90:VAL:HG12	2.49	0.41
1:A:74:ILE:HA	1:A:74:ILE:HD12	1.73	0.41
1:A:82:ILE:CG2	1:A:102:ILE:HG21	2.51	0.41
1:A:158:ILE:O	1:A:160:PRO:O	2.38	0.41
1:C:36:THR:HG22	1:C:112:ASP:O	2.21	0.41
1:C:99:SER:CB	1:C:102:ILE:HD11	2.50	0.41
1:C:270:LEU:HD13	1:C:270:LEU:O	2.21	0.41
1:C:692:ILE:CD1	2:C:803:ATP:HN61	2.15	0.41
1:D:160:PRO:HD2	1:D:212:SER:HB3	1.40	0.41
1:D:316:VAL:HG13	1:D:362:VAL:HG21	2.02	0.41
1:D:579:LEU:HB2	1:D:613:ILE:HD12	2.03	0.41
1:E:696:CYS:SG	1:E:725:VAL:HG22	2.59	0.41
1:F:149:GLN:HA	1:F:152:LEU:CG	2.48	0.41
1:F:280:ARG:HD2	1:F:383:VAL:O	2.20	0.41
1:F:670:LEU:HD12	1:F:670:LEU:HA	1.87	0.41
1:A:120:GLN:C	1:A:120:GLN:NE2	2.73	0.41
1:A:283:LEU:HD12	1:A:387:ALA:O	2.20	0.41
1:A:316:VAL:HG13	1:A:362:VAL:HG21	2.02	0.41
2:A:803:ATP:C8	3:A:804:NDT:O3	2.70	0.41
1:C:159:MET:N	1:C:160:PRO:CD	2.83	0.41
1:C:259:SER:O	1:C:263:ILE:HG12	2.21	0.41
1:C:624:ASP:OD2	1:C:634:ASN:HA	2.20	0.41
1:D:36:THR:HG22	1:D:112:ASP:O	2.21	0.41
1:D:98:LEU:H	1:D:98:LEU:HD23	1.82	0.41
1:D:469:ILE:HG13	1:E:271:PHE:HE2	1.85	0.41
1:D:551:LYS:HZ2	1:D:650:LEU:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:762:THR:HG23	1:D:765:MET:H	1.85	0.41
1:E:39:HIS:HB3	1:E:97:THR:HB	1.98	0.41
1:E:123:PRO:CG	1:E:216:ILE:HD11	2.34	0.41
1:E:149:GLN:HA	1:E:152:LEU:CD2	2.50	0.41
1:E:228:LYS:HB2	1:E:228:LYS:HE3	1.80	0.41
1:E:406:ASP:N	1:E:406:ASP:OD1	2.53	0.41
1:E:510:MET:HB3	1:E:568:LYS:HD3	2.01	0.41
1:F:120:GLN:NE2	1:F:120:GLN:C	2.73	0.41
1:F:127:THR:HA	1:F:222:THR:OG1	2.20	0.41
1:F:608:ALA:O	1:F:609:ALA:HB3	2.21	0.41
1:A:129:VAL:HA	1:A:183:ALA:HA	2.02	0.41
1:A:138:ASN:C	1:A:138:ASN:HD22	2.22	0.41
1:A:258:LYS:HE3	1:A:258:LYS:HB2	1.91	0.41
1:B:159:MET:O	1:B:180:ILE:O	2.37	0.41
1:B:231:GLN:HE21	1:B:231:GLN:HB2	1.58	0.41
1:B:270:LEU:C	1:B:270:LEU:CD2	2.86	0.41
1:C:99:SER:HB3	1:C:102:ILE:HD11	2.01	0.41
1:C:587:PHE:CZ	1:C:621:LEU:HA	2.55	0.41
1:C:697:THR:O	1:C:700:PHE:N	2.54	0.41
1:D:429:ARG:HH12	3:D:802:NDT:H16	1.78	0.41
1:D:614:PHE:HA	1:D:656:VAL:O	2.20	0.41
1:D:676:ASP:O	1:D:678:HIS:ND1	2.48	0.41
1:E:82:ILE:CG2	1:E:102:ILE:HG21	2.51	0.41
1:F:183:ALA:HB3	1:F:215:PHE:CD2	2.56	0.41
1:F:261:ILE:HD11	1:F:384:VAL:HG21	2.02	0.41
1:F:292:LYS:NZ	2:F:801:ATP:O3G	2.53	0.41
1:A:123:PRO:CG	1:A:216:ILE:HD11	2.34	0.41
1:A:557:GLY:N	1:A:563:LYS:HZ3	2.18	0.41
1:A:667:ALA:O	1:A:671:ARG:HG3	2.21	0.41
1:A:762:THR:HG22	1:A:765:MET:HE2	2.02	0.41
1:B:42:LYS:N	1:B:42:LYS:CD	2.84	0.41
1:B:759:ARG:H	1:B:759:ARG:HG2	1.74	0.41
1:C:141:GLU:HG3	1:C:171:ALA:N	2.18	0.41
3:D:802:NDT:H212	1:E:275:GLY:C	2.40	0.41
1:E:36:THR:HG22	1:E:112:ASP:O	2.21	0.41
1:E:71:VAL:HG12	1:E:116:LEU:CD1	2.50	0.41
1:F:130:THR:HG23	1:F:182:ASP:N	2.31	0.41
1:F:235:LYS:HB2	1:F:235:LYS:HE3	1.76	0.41
1:F:730:GLU:HA	1:F:733:LEU:HG	2.03	0.41
2:F:801:ATP:C3'	3:F:802:NDT:C4	2.99	0.41
1:A:183:ALA:HB3	1:A:215:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ILE:H	1:B:158:ILE:HG12	1.52	0.41
2:B:801:ATP:C3'	3:B:802:NDT:C4	2.98	0.41
1:C:117:LYS:NZ	1:C:117:LYS:CB	2.77	0.41
1:C:661:ARG:HD3	1:C:768:TYR:OH	2.21	0.41
1:F:42:LYS:N	1:F:42:LYS:CD	2.84	0.41
1:F:58:LEU:HG	1:F:63:ILE:O	2.21	0.41
1:F:77:ASN:N	1:F:77:ASN:ND2	2.60	0.41
1:F:295:LEU:HD23	1:F:295:LEU:HA	1.88	0.41
1:A:42:LYS:N	1:A:42:LYS:CD	2.84	0.41
1:A:58:LEU:HG	1:A:63:ILE:O	2.21	0.41
1:A:251:ASP:HA	1:A:254:ILE:HG22	2.02	0.41
1:A:287:PRO:HG2	1:A:413:ILE:HG23	2.03	0.41
1:A:366:VAL:O	1:A:369:THR:HG22	2.21	0.41
1:A:524:LEU:HD21	1:A:681:VAL:HA	2.03	0.41
1:A:608:ALA:O	1:A:609:ALA:HB3	2.21	0.41
1:A:661:ARG:HB3	1:A:664:GLU:OE1	2.20	0.41
1:A:736:ILE:HG13	1:A:737:MET:N	2.36	0.41
1:B:262:GLU:O	1:B:266:HIS:HB2	2.21	0.41
1:B:587:PHE:CZ	1:B:621:LEU:HA	2.56	0.41
1:B:619:ASP:HB3	1:B:659:THR:OG1	2.21	0.41
1:C:42:LYS:N	1:C:42:LYS:CD	2.84	0.41
1:C:58:LEU:HG	1:C:63:ILE:O	2.21	0.41
1:C:91:HIS:HA	1:C:92:PRO:HD3	1.69	0.41
1:C:149:GLN:HA	1:C:152:LEU:CD2	2.50	0.41
1:C:265:LEU:HD11	1:C:341:ILE:HD11	2.01	0.41
1:C:344:ILE:HG21	1:C:347:ILE:HD13	2.02	0.41
1:C:734:ALA:O	1:C:737:MET:HG3	2.21	0.41
1:D:158:ILE:H	1:D:158:ILE:HG12	1.52	0.41
1:D:646:GLY:O	1:D:648:GLU:N	2.54	0.41
1:D:660:ASN:O	1:D:769:TYR:OH	2.32	0.41
1:E:42:LYS:N	1:E:42:LYS:CD	2.84	0.41
1:E:58:LEU:HG	1:E:63:ILE:O	2.21	0.41
1:E:126:ALA:O	1:E:222:THR:CG2	2.68	0.41
1:E:129:VAL:HA	1:E:183:ALA:HA	2.02	0.41
1:E:183:ALA:HB3	1:E:215:PHE:CD2	2.56	0.41
1:E:294:MET:O	1:E:298:VAL:HG23	2.21	0.41
1:E:367:VAL:O	1:E:371:LEU:HG	2.21	0.41
1:E:435:HIS:HB2	1:E:437:LEU:HD21	1.28	0.41
1:E:528:MET:O	1:E:532:ILE:HG23	2.21	0.41
1:E:541:THR:HA	1:E:544:ARG:CZ	2.51	0.41
1:E:735:ALA:HA	1:E:749:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:LYS:HE3	1:F:112:ASP:CG	2.41	0.41
1:F:550:PRO:HB2	1:F:677:ARG:NH2	2.36	0.41
1:A:130:THR:HG23	1:A:182:ASP:N	2.31	0.41
1:B:36:THR:HG22	1:B:112:ASP:O	2.21	0.41
1:B:135:GLN:HA	1:B:135:GLN:NE2	2.37	0.41
1:B:261:ILE:HD12	1:B:261:ILE:HA	1.95	0.41
1:B:606:ARG:NH2	1:B:650:LEU:HD11	2.36	0.41
1:D:176:ILE:O	1:D:176:ILE:HG13	2.21	0.41
1:E:532:ILE:HD13	1:E:570:LEU:HD11	2.03	0.41
1:E:534:LEU:HB3	1:E:542:PHE:CZ	2.56	0.41
1:F:36:THR:HG22	1:F:112:ASP:O	2.21	0.41
1:F:135:GLN:NE2	1:F:135:GLN:HA	2.36	0.41
1:F:527:LYS:HB3	1:F:531:MET:HE1	2.02	0.41
1:A:36:THR:HG22	1:A:112:ASP:O	2.21	0.40
1:A:88:GLU:CG	1:A:90:VAL:HG12	2.49	0.40
1:B:54:HIS:HD2	1:B:93:VAL:CG2	2.25	0.40
1:B:166:ASN:HD21	1:B:169:THR:CG2	2.13	0.40
1:B:695:LYS:CE	3:B:804:NDT:H17	2.48	0.40
1:C:176:ILE:O	1:C:176:ILE:HG13	2.21	0.40
1:C:184:SER:O	1:C:185:ASP:CB	2.59	0.40
1:D:406:ASP:OD1	1:D:407:GLN:N	2.54	0.40
1:D:465:VAL:CG1	1:E:271:PHE:CZ	2.91	0.40
1:D:662:PRO:HD3	1:D:769:TYR:CE1	2.55	0.40
1:D:722:ALA:N	2:D:803:ATP:H1'	2.35	0.40
1:E:58:LEU:HD12	1:E:63:ILE:HG13	1.98	0.40
1:E:98:LEU:N	1:E:98:LEU:HD22	2.36	0.40
1:E:608:ALA:O	1:E:609:ALA:HB3	2.21	0.40
1:F:138:ASN:H	1:F:138:ASN:HD22	1.69	0.40
1:F:294:MET:O	1:F:298:VAL:HG23	2.21	0.40
1:F:646:GLY:C	1:F:648:GLU:H	2.24	0.40
2:F:803:ATP:C2'	3:F:804:NDT:S1	3.09	0.40
1:A:53:ILE:CA	1:A:86:GLY:HA3	2.51	0.40
1:A:91:HIS:HA	1:A:92:PRO:HD3	1.69	0.40
1:A:135:GLN:NE2	1:A:135:GLN:HA	2.36	0.40
1:B:58:LEU:HG	1:B:63:ILE:O	2.21	0.40
1:B:129:VAL:HA	1:B:183:ALA:HA	2.02	0.40
1:B:401:ARG:NH1	1:B:404:ARG:HH22	2.19	0.40
1:B:402:PRO:HA	1:B:406:ASP:HB3	2.03	0.40
1:B:536:LEU:HD11	1:B:576:ILE:HG12	2.03	0.40
1:B:557:GLY:N	1:B:563:LYS:HZ3	2.19	0.40
1:D:82:ILE:CG2	1:D:102:ILE:HG21	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ASN:O	1:D:169:THR:CG2	2.69	0.40
1:D:534:LEU:HB3	1:D:542:PHE:HZ	1.86	0.40
1:E:135:GLN:NE2	1:E:135:GLN:HA	2.36	0.40
1:E:481:LYS:H	1:E:481:LYS:HG3	1.70	0.40
1:E:599:ARG:NH1	1:E:643:GLU:OE2	2.55	0.40
1:E:697:THR:O	1:E:697:THR:HG22	2.21	0.40
1:E:701:ASN:HD22	1:E:704:GLU:CD	2.25	0.40
1:F:123:PRO:CG	1:F:216:ILE:HD11	2.34	0.40
1:A:61:LEU:HD13	1:A:61:LEU:HA	1.92	0.40
1:A:138:ASN:N	1:A:138:ASN:ND2	2.70	0.40
1:A:292:LYS:HZ2	1:A:390:ASN:HA	1.86	0.40
1:B:71:VAL:HG12	1:B:116:LEU:CD1	2.50	0.40
1:C:82:ILE:CG2	1:C:102:ILE:HG21	2.51	0.40
1:C:88:GLU:CG	1:C:90:VAL:HG12	2.49	0.40
1:C:138:ASN:HD22	1:C:138:ASN:H	1.69	0.40
1:C:570:LEU:O	1:C:574:SER:OG	2.27	0.40
1:D:310:ILE:CD1	1:D:344:ILE:HG23	2.52	0.40
1:D:608:ALA:O	1:D:609:ALA:HB3	2.21	0.40
3:D:804:NDT:H7	1:E:673:GLY:HA3	2.03	0.40
1:E:416:VAL:HG22	1:E:419:ARG:NH2	2.36	0.40
1:E:426:GLN:OE1	3:E:802:NDT:H17	2.22	0.40
1:E:618:ILE:HG22	1:E:659:THR:HB	2.03	0.40
1:F:360:GLY:N	1:F:363:GLU:OE1	2.54	0.40
1:F:578:PHE:CE2	1:F:580:ALA:HB2	2.56	0.40
1:A:46:LYS:N	1:A:46:LYS:CE	2.85	0.40
1:A:147:VAL:HG12	1:A:151:LEU:HD22	2.04	0.40
1:A:166:ASN:O	1:A:169:THR:CG2	2.69	0.40
1:A:294:MET:O	1:A:298:VAL:HG23	2.21	0.40
1:B:732:GLY:HA3	1:C:547:ILE:HD11	2.03	0.40
1:C:50:THR:OG1	1:C:84:ARG:CG	2.65	0.40
1:C:110:LEU:O	1:C:307:VAL:HG22	2.21	0.40
1:C:126:ALA:O	1:C:222:THR:CG2	2.68	0.40
1:C:147:VAL:HG12	1:C:151:LEU:HD22	2.04	0.40
1:C:179:VAL:CG1	1:C:180:ILE:H	2.35	0.40
1:C:213:PRO:HA	1:C:214:PRO:HD3	1.88	0.40
1:C:231:GLN:H	1:C:231:GLN:HG3	1.77	0.40
1:C:452:TYR:HD2	1:C:456:ASP:HB3	1.86	0.40
1:C:606:ARG:HH21	1:C:650:LEU:HD11	1.86	0.40
1:D:53:ILE:CA	1:D:86:GLY:HA3	2.51	0.40
1:D:242:LEU:HB2	1:D:298:VAL:HA	2.04	0.40
1:D:295:LEU:HD23	1:D:295:LEU:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:LYS:HD3	1:D:467:LYS:HA	1.83	0.40
1:D:471:ARG:NE	1:D:484:LEU:HD21	2.24	0.40
1:E:46:LYS:N	1:E:46:LYS:CE	2.85	0.40
1:E:130:THR:HG23	1:E:182:ASP:N	2.31	0.40
1:E:138:ASN:C	1:E:138:ASN:HD22	2.23	0.40
1:E:295:LEU:HD23	1:E:295:LEU:HA	1.92	0.40
1:F:138:ASN:HB2	1:F:228:LYS:HB3	1.99	0.40
1:F:583:GLY:O	1:F:586:ILE:HG12	2.20	0.40
1:A:105:VAL:HG11	1:A:158:ILE:CG1	2.51	0.40
1:A:179:VAL:CG1	1:A:180:ILE:H	2.35	0.40
1:A:231:GLN:HE21	1:A:231:GLN:HB2	1.58	0.40
1:A:263:ILE:CG2	1:A:264:PRO:HD3	2.52	0.40
1:A:534:LEU:O	1:A:538:ALA:HB3	2.21	0.40
1:A:539:SER:HA	1:A:542:PHE:CD2	2.55	0.40
1:A:606:ARG:NH2	1:A:650:LEU:HD11	2.36	0.40
1:A:662:PRO:HD3	1:A:769:TYR:CE1	2.56	0.40
1:B:54:HIS:HA	1:B:55:PRO:HD3	1.95	0.40
1:B:117:LYS:NZ	1:B:117:LYS:CB	2.77	0.40
1:B:157:VAL:HG11	1:B:215:PHE:C	2.42	0.40
1:B:166:ASN:O	1:B:169:THR:CG2	2.69	0.40
1:B:176:ILE:HG13	1:B:176:ILE:O	2.21	0.40
1:B:562:SER:CB	2:B:803:ATP:H4'	2.52	0.40
1:B:582:LYS:HA	1:B:616:ASP:HB3	2.03	0.40
1:B:752:LYS:HA	1:B:755:LYS:HE2	2.02	0.40
1:C:61:LEU:HD13	1:C:61:LEU:HA	1.92	0.40
1:C:600:GLU:O	1:C:603:ARG:HG2	2.22	0.40
1:D:147:VAL:HG12	1:D:151:LEU:HD22	2.04	0.40
1:D:183:ALA:HB3	1:D:215:PHE:CD2	2.56	0.40
1:D:519:GLY:HA2	1:D:691:GLU:OE1	2.22	0.40
1:E:138:ASN:HD22	1:E:138:ASN:H	1.69	0.40
1:E:235:LYS:HE3	1:E:235:LYS:HB2	1.76	0.40
1:F:46:LYS:N	1:F:46:LYS:CE	2.85	0.40
1:F:166:ASN:O	1:F:169:THR:CG2	2.69	0.40
1:F:312:GLY:HA2	1:F:350:ILE:HD11	2.02	0.40
1:F:414:PRO:HB2	1:F:419:ARG:HG3	2.03	0.40
1:F:423:LEU:HD23	1:F:423:LEU:HA	1.94	0.40
1:F:562:SER:HA	2:F:803:ATP:O1A	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	722/748 (96%)	655 (91%)	60 (8%)	7 (1%)	15	52
1	B	722/748 (96%)	661 (92%)	52 (7%)	9 (1%)	13	50
1	C	722/748 (96%)	653 (90%)	60 (8%)	9 (1%)	13	50
1	D	722/748 (96%)	654 (91%)	58 (8%)	10 (1%)	11	46
1	E	722/748 (96%)	655 (91%)	56 (8%)	11 (2%)	10	46
1	F	722/748 (96%)	654 (91%)	57 (8%)	11 (2%)	10	46
All	All	4332/4488 (96%)	3932 (91%)	343 (8%)	57 (1%)	16	48

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	LEU
1	A	439	SER
1	A	609	ALA
1	B	167	LEU
1	B	212	SER
1	B	213	PRO
1	B	609	ALA
1	B	647	VAL
1	C	167	LEU
1	C	609	ALA
1	C	647	VAL
1	D	167	LEU
1	D	609	ALA
1	D	647	VAL
1	E	167	LEU
1	E	277	SER
1	E	609	ALA
1	E	647	VAL
1	F	167	LEU
1	F	609	ALA

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Mol	Chain	Res	Type
1	F	647	VAL
1	A	364	SER
1	A	647	VAL
1	B	364	SER
1	C	271	PHE
1	C	364	SER
1	D	269	THR
1	D	364	SER
1	E	364	SER
1	E	630	THR
1	F	157	VAL
1	F	364	SER
1	F	630	THR
1	A	128	LYS
1	B	128	LYS
1	B	157	VAL
1	B	214	PRO
1	C	128	LYS
1	C	157	VAL
1	D	128	LYS
1	D	157	VAL
1	E	128	LYS
1	E	157	VAL
1	F	128	LYS
1	A	214	PRO
1	C	214	PRO
1	D	214	PRO
1	E	214	PRO
1	E	278	PRO
1	F	211	LEU
1	F	277	SER
1	C	277	SER
1	D	277	SER
1	E	264	PRO
1	F	623	PRO
1	D	212	SER
1	F	214	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	611/632 (97%)	572 (94%)	39 (6%)	17	48
1	B	612/632 (97%)	571 (93%)	41 (7%)	16	47
1	C	612/632 (97%)	570 (93%)	42 (7%)	15	46
1	D	612/632 (97%)	569 (93%)	43 (7%)	15	46
1	E	612/632 (97%)	568 (93%)	44 (7%)	14	45
1	F	612/632 (97%)	570 (93%)	42 (7%)	15	46
All	All	3671/3792 (97%)	3420 (93%)	251 (7%)	19	47

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	39	HIS
1	A	42	LYS
1	A	46	LYS
1	A	50	THR
1	A	56	ASN
1	A	64	ASN
1	A	67	SER
1	A	69	CYS
1	A	77	ASN
1	A	80	LEU
1	A	81	VAL
1	A	82	ILE
1	A	91	HIS
1	A	96	ILE
1	A	97	THR
1	A	98	LEU
1	A	99	SER
1	A	102	ILE
1	A	120	GLN
1	A	127	THR
1	A	130	THR
1	A	131	VAL
1	A	138	ASN
1	A	141	GLU
1	A	143	MET

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Mol	Chain	Res	Type
1	A	151	LEU
1	A	153	ASP
1	A	159	MET
1	A	167	LEU
1	A	173	ASP
1	A	177	ASP
1	A	181	THR
1	A	182	ASP
1	A	217	PHE
1	A	228	LYS
1	A	230	THR
1	A	231	GLN
1	A	270	LEU
1	B	36	THR
1	B	39	HIS
1	B	42	LYS
1	B	46	LYS
1	B	50	THR
1	B	56	ASN
1	B	64	ASN
1	B	67	SER
1	B	69	CYS
1	B	77	ASN
1	B	80	LEU
1	B	81	VAL
1	B	82	ILE
1	B	91	HIS
1	B	96	ILE
1	B	97	THR
1	B	98	LEU
1	B	99	SER
1	B	102	ILE
1	B	120	GLN
1	B	127	THR
1	B	130	THR
1	B	131	VAL
1	B	138	ASN
1	B	141	GLU
1	B	143	MET
1	B	151	LEU
1	B	153	ASP
1	B	158	ILE

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Mol	Chain	Res	Type
1	B	159	MET
1	B	167	LEU
1	B	173	ASP
1	B	177	ASP
1	B	181	THR
1	B	182	ASP
1	B	211	LEU
1	B	217	PHE
1	B	228	LYS
1	B	230	THR
1	B	231	GLN
1	B	437	LEU
1	C	36	THR
1	C	39	HIS
1	C	42	LYS
1	C	46	LYS
1	C	50	THR
1	C	56	ASN
1	C	64	ASN
1	C	67	SER
1	C	69	CYS
1	C	77	ASN
1	C	80	LEU
1	C	81	VAL
1	C	82	ILE
1	C	91	HIS
1	C	96	ILE
1	C	97	THR
1	C	98	LEU
1	C	99	SER
1	C	102	ILE
1	C	120	GLN
1	C	127	THR
1	C	130	THR
1	C	131	VAL
1	C	138	ASN
1	C	141	GLU
1	C	143	MET
1	C	151	LEU
1	C	153	ASP
1	C	158	ILE
1	C	159	MET

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Mol	Chain	Res	Type
1	C	167	LEU
1	C	173	ASP
1	C	177	ASP
1	C	181	THR
1	C	182	ASP
1	C	212	SER
1	C	217	PHE
1	C	228	LYS
1	C	230	THR
1	C	231	GLN
1	C	271	PHE
1	C	504	ARG
1	D	36	THR
1	D	39	HIS
1	D	42	LYS
1	D	46	LYS
1	D	50	THR
1	D	56	ASN
1	D	64	ASN
1	D	67	SER
1	D	69	CYS
1	D	77	ASN
1	D	80	LEU
1	D	81	VAL
1	D	82	ILE
1	D	91	HIS
1	D	96	ILE
1	D	97	THR
1	D	98	LEU
1	D	99	SER
1	D	102	ILE
1	D	120	GLN
1	D	127	THR
1	D	130	THR
1	D	131	VAL
1	D	138	ASN
1	D	141	GLU
1	D	143	MET
1	D	151	LEU
1	D	153	ASP
1	D	158	ILE
1	D	159	MET

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Mol	Chain	Res	Type
1	D	167	LEU
1	D	173	ASP
1	D	177	ASP
1	D	181	THR
1	D	182	ASP
1	D	211	LEU
1	D	212	SER
1	D	217	PHE
1	D	228	LYS
1	D	230	THR
1	D	231	GLN
1	D	270	LEU
1	D	274	PHE
1	E	36	THR
1	E	39	HIS
1	E	42	LYS
1	E	46	LYS
1	E	50	THR
1	E	56	ASN
1	E	64	ASN
1	E	67	SER
1	E	69	CYS
1	E	77	ASN
1	E	80	LEU
1	E	81	VAL
1	E	82	ILE
1	E	91	HIS
1	E	96	ILE
1	E	97	THR
1	E	98	LEU
1	E	99	SER
1	E	102	ILE
1	E	120	GLN
1	E	127	THR
1	E	130	THR
1	E	131	VAL
1	E	138	ASN
1	E	141	GLU
1	E	143	MET
1	E	151	LEU
1	E	153	ASP
1	E	158	ILE

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Mol	Chain	Res	Type
1	E	159	MET
1	E	167	LEU
1	E	173	ASP
1	E	177	ASP
1	E	181	THR
1	E	182	ASP
1	E	217	PHE
1	E	228	LYS
1	E	230	THR
1	E	231	GLN
1	E	266	HIS
1	E	274	PHE
1	E	328	ARG
1	E	437	LEU
1	E	504	ARG
1	F	36	THR
1	F	39	HIS
1	F	42	LYS
1	F	46	LYS
1	F	50	THR
1	F	56	ASN
1	F	64	ASN
1	F	67	SER
1	F	69	CYS
1	F	76	GLU
1	F	77	ASN
1	F	80	LEU
1	F	81	VAL
1	F	82	ILE
1	F	91	HIS
1	F	96	ILE
1	F	97	THR
1	F	98	LEU
1	F	99	SER
1	F	102	ILE
1	F	120	GLN
1	F	127	THR
1	F	130	THR
1	F	131	VAL
1	F	138	ASN
1	F	141	GLU
1	F	143	MET

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Mol	Chain	Res	Type
1	F	151	LEU
1	F	153	ASP
1	F	159	MET
1	F	167	LEU
1	F	173	ASP
1	F	177	ASP
1	F	181	THR
1	F	182	ASP
1	F	217	PHE
1	F	228	LYS
1	F	230	THR
1	F	231	GLN
1	F	274	PHE
1	F	438	ASP
1	F	677	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	120	GLN
1	A	135	GLN
1	A	149	GLN
1	A	166	ASN
1	A	231	GLN
1	A	237	ASN
1	A	435	HIS
1	B	54	HIS
1	B	120	GLN
1	B	135	GLN
1	B	149	GLN
1	B	166	ASN
1	B	231	GLN
1	B	266	HIS
1	B	407	GLN
1	C	54	HIS
1	C	77	ASN
1	C	120	GLN
1	C	135	GLN
1	C	149	GLN
1	C	166	ASN
1	C	231	GLN

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Mol	Chain	Res	Type
1	C	233	ASN
1	D	54	HIS
1	D	77	ASN
1	D	120	GLN
1	D	135	GLN
1	D	149	GLN
1	D	166	ASN
1	D	231	GLN
1	D	237	ASN
1	D	301	ASN
1	E	54	HIS
1	E	120	GLN
1	E	135	GLN
1	E	149	GLN
1	E	166	ASN
1	E	231	GLN
1	E	237	ASN
1	E	301	ASN
1	E	306	HIS
1	E	426	GLN
1	F	54	HIS
1	F	77	ASN
1	F	120	GLN
1	F	135	GLN
1	F	149	GLN
1	F	166	ASN
1	F	231	GLN
1	F	237	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ATP	F	801	3	26,32,33	4.00	10 (38%)	30,50,52	1.68	4 (13%)
2	ATP	B	803	3	26,32,33	4.00	10 (38%)	30,50,52	1.66	5 (16%)
3	NDT	D	804	2	22,23,23	6.93	18 (81%)	25,34,34	3.00	9 (36%)
2	ATP	E	801	3	26,32,33	4.00	10 (38%)	30,50,52	1.51	3 (10%)
2	ATP	F	803	3	26,32,33	4.00	10 (38%)	30,50,52	1.51	3 (10%)
3	NDT	B	802	2	22,23,23	6.92	18 (81%)	25,34,34	3.00	9 (36%)
2	ATP	C	801	3	26,32,33	3.99	10 (38%)	30,50,52	1.50	3 (10%)
3	NDT	F	802	2	22,23,23	6.93	18 (81%)	25,34,34	2.99	9 (36%)
3	NDT	D	802	2	22,23,23	6.91	18 (81%)	25,34,34	3.00	9 (36%)
3	NDT	A	804	2	22,23,23	6.93	18 (81%)	25,34,34	3.00	9 (36%)
2	ATP	D	801	3	26,32,33	4.00	10 (38%)	30,50,52	1.67	4 (13%)
3	NDT	F	804	2	22,23,23	6.94	18 (81%)	25,34,34	2.99	9 (36%)
3	NDT	A	802	2	22,23,23	6.92	18 (81%)	25,34,34	2.99	9 (36%)
3	NDT	C	802	2,1	22,23,23	6.92	18 (81%)	25,34,34	3.01	9 (36%)
2	ATP	B	801	3	26,32,33	4.01	10 (38%)	30,50,52	1.66	4 (13%)
2	ATP	D	803	3,1	26,32,33	4.03	10 (38%)	30,50,52	1.48	3 (10%)
3	NDT	E	804	2	22,23,23	6.92	18 (81%)	25,34,34	2.99	9 (36%)
2	ATP	A	801	3	26,32,33	3.99	10 (38%)	30,50,52	1.74	7 (23%)
2	ATP	E	803	3	26,32,33	3.99	10 (38%)	30,50,52	1.53	4 (13%)
2	ATP	A	803	3	26,32,33	4.01	10 (38%)	30,50,52	1.65	4 (13%)
3	NDT	C	804	2	22,23,23	6.93	18 (81%)	25,34,34	3.00	9 (36%)
3	NDT	E	802	2,1	22,23,23	6.93	18 (81%)	25,34,34	3.01	9 (36%)
2	ATP	C	803	3	26,32,33	4.02	10 (38%)	30,50,52	1.48	3 (10%)
3	NDT	B	804	2	22,23,23	6.93	18 (81%)	25,34,34	2.99	9 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	F	801	3	2/2/6/7	4/18/34/38	0/3/3/3
2	ATP	B	803	3	2/2/6/7	3/18/34/38	0/3/3/3
3	NDT	D	804	2	1/1/3/4	1/9/25/25	0/3/3/3
2	ATP	E	801	3	2/2/6/7	8/18/34/38	0/3/3/3
2	ATP	F	803	3	2/2/6/7	4/18/34/38	0/3/3/3
3	NDT	B	802	2	1/1/3/4	0/9/25/25	0/3/3/3
2	ATP	C	801	3	2/2/6/7	4/18/34/38	0/3/3/3
3	NDT	F	802	2	1/1/3/4	2/9/25/25	0/3/3/3
3	NDT	D	802	2	1/1/3/4	0/9/25/25	0/3/3/3
3	NDT	A	804	2	1/1/3/4	0/9/25/25	0/3/3/3
2	ATP	D	801	3	2/2/6/7	6/18/34/38	0/3/3/3
3	NDT	F	804	2	1/1/3/4	2/9/25/25	0/3/3/3
3	NDT	A	802	2	1/1/3/4	3/9/25/25	0/3/3/3
3	NDT	C	802	2,1	1/1/3/4	0/9/25/25	0/3/3/3
2	ATP	B	801	3	2/2/6/7	7/18/34/38	0/3/3/3
2	ATP	D	803	3,1	2/2/6/7	3/18/34/38	0/3/3/3
3	NDT	E	804	2	1/1/3/4	0/9/25/25	0/3/3/3
2	ATP	A	801	3	2/2/6/7	8/18/34/38	0/3/3/3
2	ATP	E	803	3	2/2/6/7	4/18/34/38	0/3/3/3
2	ATP	A	803	3	2/2/6/7	5/18/34/38	0/3/3/3
3	NDT	C	804	2	1/1/3/4	2/9/25/25	0/3/3/3
3	NDT	E	802	2,1	1/1/3/4	0/9/25/25	0/3/3/3
2	ATP	C	803	3	2/2/6/7	6/18/34/38	0/3/3/3
3	NDT	B	804	2	1/1/3/4	2/9/25/25	0/3/3/3

All (336) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	804	NDT	C2-N1	17.03	1.49	1.29
3	C	802	NDT	C2-N1	17.02	1.49	1.29
3	E	802	NDT	C2-N1	17.02	1.49	1.29
3	F	802	NDT	C2-N1	17.01	1.49	1.29
3	A	802	NDT	C2-N1	16.99	1.49	1.29
3	C	804	NDT	C2-N1	16.98	1.49	1.29
3	B	802	NDT	C2-N1	16.97	1.49	1.29
3	A	804	NDT	C2-N1	16.97	1.49	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	804	NDT	C2-N1	16.97	1.49	1.29
3	D	802	NDT	C2-N1	16.95	1.49	1.29
3	E	804	NDT	C2-N1	16.95	1.49	1.29
3	D	804	NDT	C2-N1	16.95	1.49	1.29
2	C	803	ATP	C4-N3	10.38	1.50	1.35
2	D	803	ATP	C4-N3	10.31	1.49	1.35
2	B	803	ATP	C4-N3	10.30	1.49	1.35
2	A	803	ATP	C4-N3	10.29	1.49	1.35
2	A	801	ATP	C4-N3	10.25	1.49	1.35
2	B	801	ATP	C4-N3	10.24	1.49	1.35
2	E	803	ATP	C4-N3	10.23	1.49	1.35
2	F	803	ATP	C4-N3	10.22	1.49	1.35
2	E	801	ATP	C4-N3	10.21	1.49	1.35
2	D	801	ATP	C4-N3	10.20	1.49	1.35
2	F	801	ATP	C4-N3	10.20	1.49	1.35
2	C	801	ATP	C4-N3	10.19	1.49	1.35
3	C	804	NDT	N2-N1	10.13	1.50	1.39
3	F	802	NDT	N2-N1	10.10	1.50	1.39
3	F	804	NDT	N2-N1	10.09	1.50	1.39
3	D	804	NDT	N2-N1	10.08	1.50	1.39
3	A	804	NDT	N2-N1	10.07	1.50	1.39
3	B	804	NDT	N2-N1	10.07	1.50	1.39
3	E	804	NDT	N2-N1	10.04	1.50	1.39
3	A	802	NDT	N2-N1	10.04	1.50	1.39
3	E	802	NDT	N2-N1	10.04	1.50	1.39
3	B	802	NDT	N2-N1	10.03	1.50	1.39
3	C	802	NDT	N2-N1	10.01	1.50	1.39
3	D	802	NDT	N2-N1	9.99	1.50	1.39
3	B	804	NDT	C5-C4	9.52	1.55	1.40
3	F	804	NDT	C5-C4	9.51	1.55	1.40
3	A	804	NDT	C5-C4	9.50	1.55	1.40
3	E	804	NDT	C5-C4	9.49	1.55	1.40
3	C	802	NDT	C5-C4	9.48	1.55	1.40
3	D	802	NDT	C5-C4	9.48	1.55	1.40
3	C	804	NDT	C5-C4	9.47	1.55	1.40
3	A	802	NDT	C5-C4	9.46	1.55	1.40
3	F	802	NDT	C5-C4	9.46	1.55	1.40
3	B	802	NDT	C5-C4	9.44	1.55	1.40
3	E	802	NDT	C5-C4	9.43	1.55	1.40
3	D	804	NDT	C5-C4	9.40	1.54	1.40
3	D	804	NDT	C16-C15	9.24	1.53	1.38
3	C	804	NDT	C16-C15	9.18	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	NDT	C16-C15	9.17	1.53	1.38
3	A	802	NDT	C16-C15	9.16	1.53	1.38
3	E	804	NDT	C16-C15	9.16	1.53	1.38
3	F	804	NDT	C16-C15	9.16	1.53	1.38
3	F	802	NDT	C16-C15	9.16	1.53	1.38
3	B	804	NDT	C16-C15	9.16	1.53	1.38
3	B	802	NDT	C16-C15	9.16	1.53	1.38
3	A	804	NDT	C16-C15	9.15	1.53	1.38
3	C	802	NDT	C16-C15	9.12	1.53	1.38
3	E	802	NDT	C16-C15	9.11	1.53	1.38
3	A	804	NDT	C20-C15	9.08	1.53	1.38
3	E	804	NDT	C20-C15	9.06	1.53	1.38
3	D	802	NDT	C20-C15	9.05	1.53	1.38
3	A	802	NDT	C20-C15	9.04	1.53	1.38
3	F	804	NDT	C20-C15	9.04	1.53	1.38
3	C	802	NDT	C20-C15	9.03	1.53	1.38
3	E	802	NDT	C20-C15	9.03	1.53	1.38
3	B	804	NDT	C20-C15	9.02	1.53	1.38
3	C	804	NDT	C20-C15	9.02	1.53	1.38
3	B	802	NDT	C20-C15	9.01	1.53	1.38
3	D	804	NDT	C20-C15	9.00	1.53	1.38
3	F	802	NDT	C20-C15	8.97	1.52	1.38
2	D	803	ATP	C2-N3	8.83	1.46	1.32
2	F	801	ATP	C2-N3	8.79	1.46	1.32
2	C	801	ATP	C2-N3	8.78	1.46	1.32
2	B	801	ATP	C2-N3	8.77	1.46	1.32
2	A	803	ATP	C2-N3	8.77	1.46	1.32
2	F	803	ATP	C2-N3	8.77	1.46	1.32
2	C	803	ATP	C2-N3	8.76	1.46	1.32
2	B	803	ATP	C2-N3	8.76	1.46	1.32
2	A	801	ATP	C2-N3	8.75	1.46	1.32
2	E	803	ATP	C2-N3	8.75	1.46	1.32
2	E	801	ATP	C2-N3	8.73	1.46	1.32
2	D	801	ATP	C2-N3	8.73	1.46	1.32
3	E	802	NDT	C8-C1	8.19	1.55	1.41
3	C	804	NDT	C8-C1	8.17	1.55	1.41
3	D	804	NDT	C8-C1	8.16	1.55	1.41
3	F	804	NDT	C8-C1	8.16	1.55	1.41
3	C	802	NDT	C8-C1	8.16	1.55	1.41
3	F	802	NDT	C8-C1	8.15	1.55	1.41
3	A	804	NDT	C8-C1	8.14	1.55	1.41
3	B	802	NDT	C8-C1	8.14	1.55	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	804	NDT	C8-C1	8.14	1.55	1.41
3	E	804	NDT	C8-C1	8.13	1.55	1.41
3	A	802	NDT	C8-C1	8.12	1.55	1.41
3	D	802	NDT	C8-C1	8.11	1.55	1.41
3	D	804	NDT	C20-C19	8.02	1.53	1.38
3	E	802	NDT	C20-C19	7.99	1.53	1.38
3	B	802	NDT	C20-C19	7.98	1.53	1.38
3	F	802	NDT	C20-C19	7.98	1.53	1.38
3	E	804	NDT	C20-C19	7.97	1.53	1.38
3	F	804	NDT	C20-C19	7.97	1.53	1.38
3	C	802	NDT	C20-C19	7.97	1.53	1.38
3	B	804	NDT	C20-C19	7.97	1.53	1.38
3	A	802	NDT	C20-C19	7.97	1.53	1.38
3	A	804	NDT	C20-C19	7.96	1.53	1.38
3	C	804	NDT	C20-C19	7.95	1.53	1.38
3	D	802	NDT	C20-C19	7.93	1.53	1.38
3	A	802	NDT	C17-C16	7.89	1.53	1.38
3	B	802	NDT	C17-C16	7.87	1.53	1.38
3	C	804	NDT	C17-C16	7.86	1.53	1.38
3	D	804	NDT	C17-C16	7.86	1.53	1.38
3	E	804	NDT	C17-C16	7.86	1.53	1.38
3	F	802	NDT	C17-C16	7.85	1.53	1.38
3	A	804	NDT	C17-C16	7.85	1.53	1.38
3	B	804	NDT	C17-C16	7.85	1.53	1.38
3	C	802	NDT	C17-C16	7.85	1.53	1.38
3	F	804	NDT	C17-C16	7.84	1.53	1.38
3	E	802	NDT	C17-C16	7.83	1.53	1.38
3	D	802	NDT	C17-C16	7.82	1.53	1.38
2	B	801	ATP	C3'-C4'	-7.31	1.32	1.53
2	D	801	ATP	C3'-C4'	-7.29	1.33	1.53
2	F	801	ATP	C3'-C4'	-7.28	1.33	1.53
2	B	803	ATP	C3'-C4'	-7.27	1.33	1.53
2	A	801	ATP	C3'-C4'	-7.27	1.33	1.53
2	F	803	ATP	C3'-C4'	-7.26	1.33	1.53
2	C	801	ATP	C3'-C4'	-7.26	1.33	1.53
2	E	803	ATP	C3'-C4'	-7.24	1.33	1.53
2	A	803	ATP	C3'-C4'	-7.23	1.33	1.53
2	E	801	ATP	C3'-C4'	-7.20	1.33	1.53
2	C	803	ATP	C3'-C4'	-7.16	1.33	1.53
2	D	803	ATP	C3'-C4'	-7.15	1.33	1.53
2	D	803	ATP	O4'-C4'	6.70	1.60	1.45
2	C	803	ATP	O4'-C4'	6.68	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	ATP	O4'-C4'	6.67	1.59	1.45
2	B	801	ATP	O4'-C4'	6.66	1.59	1.45
2	F	801	ATP	O4'-C4'	6.60	1.59	1.45
2	F	803	ATP	O4'-C4'	6.59	1.59	1.45
2	C	801	ATP	O4'-C4'	6.59	1.59	1.45
2	A	803	ATP	O4'-C4'	6.57	1.59	1.45
2	D	801	ATP	O4'-C4'	6.57	1.59	1.45
3	E	802	NDT	C7-C8	6.53	1.52	1.38
3	D	802	NDT	C7-C8	6.52	1.52	1.38
3	B	802	NDT	C7-C8	6.52	1.52	1.38
3	A	802	NDT	C7-C8	6.52	1.52	1.38
3	D	804	NDT	C7-C8	6.51	1.52	1.38
3	F	804	NDT	C7-C8	6.51	1.52	1.38
3	E	804	NDT	C7-C8	6.51	1.52	1.38
3	B	804	NDT	C7-C8	6.50	1.52	1.38
3	A	804	NDT	C7-C8	6.50	1.52	1.38
3	C	804	NDT	C7-C8	6.50	1.52	1.38
3	F	802	NDT	C7-C8	6.50	1.52	1.38
3	C	802	NDT	C7-C8	6.49	1.52	1.38
2	B	803	ATP	O4'-C4'	6.49	1.59	1.45
2	E	803	ATP	O4'-C4'	6.48	1.59	1.45
2	A	801	ATP	O4'-C4'	6.45	1.59	1.45
3	D	804	NDT	C6-C5	6.42	1.52	1.38
3	C	804	NDT	C6-C5	6.40	1.52	1.38
3	F	804	NDT	C6-C5	6.39	1.52	1.38
3	E	802	NDT	C6-C5	6.38	1.52	1.38
3	B	802	NDT	C6-C5	6.37	1.52	1.38
3	D	802	NDT	C6-C5	6.37	1.52	1.38
3	A	804	NDT	C6-C5	6.36	1.52	1.38
3	B	804	NDT	C6-C5	6.36	1.52	1.38
3	A	802	NDT	C6-C5	6.36	1.52	1.38
3	F	802	NDT	C6-C5	6.36	1.52	1.38
3	C	802	NDT	C6-C5	6.35	1.52	1.38
3	E	804	NDT	C6-C5	6.33	1.52	1.38
2	D	803	ATP	C2'-C1'	-5.62	1.36	1.52
2	D	803	ATP	C2-N1	5.59	1.44	1.33
2	C	803	ATP	C2'-C1'	-5.58	1.36	1.52
2	E	801	ATP	C2'-C1'	-5.58	1.36	1.52
2	F	803	ATP	C2-N1	5.56	1.44	1.33
2	D	801	ATP	C2-N1	5.54	1.44	1.33
2	B	803	ATP	C2-N1	5.53	1.44	1.33
2	B	801	ATP	C2'-C1'	-5.52	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ATP	C2'-C1'	-5.52	1.37	1.52
2	E	803	ATP	C2-N1	5.51	1.44	1.33
2	C	803	ATP	C2-N1	5.51	1.44	1.33
2	A	803	ATP	C2-N1	5.51	1.44	1.33
2	D	801	ATP	C2'-C1'	-5.51	1.37	1.52
2	E	801	ATP	C2-N1	5.51	1.44	1.33
2	F	801	ATP	C2-N1	5.50	1.44	1.33
2	F	801	ATP	C2'-C1'	-5.50	1.37	1.52
2	B	801	ATP	C2-N1	5.49	1.44	1.33
2	A	803	ATP	O4'-C1'	5.47	1.54	1.42
2	A	803	ATP	C2'-C1'	-5.47	1.37	1.52
2	B	803	ATP	C2'-C1'	-5.47	1.37	1.52
2	F	803	ATP	C2'-C1'	-5.46	1.37	1.52
2	A	801	ATP	C2-N1	5.46	1.44	1.33
2	C	803	ATP	O4'-C1'	5.46	1.54	1.42
2	C	801	ATP	C2-N1	5.45	1.44	1.33
2	E	801	ATP	O4'-C1'	5.45	1.54	1.42
2	E	803	ATP	C2'-C1'	-5.45	1.37	1.52
2	D	803	ATP	O4'-C1'	5.45	1.54	1.42
2	F	803	ATP	O4'-C1'	5.44	1.54	1.42
2	D	801	ATP	O4'-C1'	5.44	1.54	1.42
2	B	801	ATP	O4'-C1'	5.42	1.54	1.42
2	E	803	ATP	O4'-C1'	5.42	1.54	1.42
2	C	801	ATP	O4'-C1'	5.41	1.54	1.42
2	B	803	ATP	O4'-C1'	5.41	1.54	1.42
2	A	801	ATP	C2'-C1'	-5.41	1.37	1.52
2	F	801	ATP	O4'-C1'	5.39	1.54	1.42
3	F	802	NDT	C7-C6	5.29	1.52	1.38
3	B	804	NDT	C7-C6	5.28	1.52	1.38
3	D	802	NDT	C7-C6	5.27	1.52	1.38
3	B	802	NDT	C7-C6	5.27	1.52	1.38
3	A	802	NDT	C7-C6	5.27	1.52	1.38
3	A	804	NDT	C7-C6	5.27	1.52	1.38
3	C	802	NDT	C7-C6	5.26	1.52	1.38
3	E	802	NDT	C7-C6	5.26	1.52	1.38
3	E	804	NDT	C7-C6	5.26	1.52	1.38
3	C	804	NDT	C7-C6	5.26	1.52	1.38
3	F	804	NDT	C7-C6	5.26	1.51	1.38
2	A	801	ATP	O4'-C1'	5.26	1.54	1.42
3	D	804	NDT	C7-C6	5.22	1.51	1.38
3	D	802	NDT	C17-C18	5.17	1.53	1.38
3	B	804	NDT	C17-C18	5.17	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	804	NDT	C17-C18	5.17	1.53	1.38
3	A	804	NDT	C17-C18	5.17	1.53	1.38
3	F	802	NDT	C19-C18	5.16	1.53	1.38
3	C	804	NDT	C19-C18	5.16	1.53	1.38
3	A	802	NDT	C17-C18	5.16	1.53	1.38
3	E	804	NDT	C17-C18	5.16	1.53	1.38
3	F	802	NDT	C17-C18	5.16	1.53	1.38
3	D	804	NDT	C17-C18	5.16	1.53	1.38
3	E	804	NDT	C19-C18	5.15	1.53	1.38
3	B	802	NDT	C17-C18	5.15	1.53	1.38
3	A	804	NDT	C19-C18	5.15	1.53	1.38
3	C	802	NDT	C19-C18	5.15	1.53	1.38
3	F	804	NDT	C19-C18	5.15	1.53	1.38
3	E	802	NDT	C17-C18	5.15	1.53	1.38
3	F	804	NDT	C17-C18	5.15	1.53	1.38
3	C	802	NDT	C17-C18	5.14	1.53	1.38
3	E	802	NDT	C19-C18	5.14	1.53	1.38
3	B	804	NDT	C19-C18	5.14	1.53	1.38
3	B	802	NDT	C19-C18	5.14	1.53	1.38
3	D	802	NDT	C19-C18	5.14	1.53	1.38
3	D	804	NDT	C19-C18	5.12	1.53	1.38
3	A	802	NDT	C19-C18	5.11	1.53	1.38
3	F	802	NDT	C15-S1	4.26	1.82	1.76
3	C	804	NDT	C15-S1	4.25	1.82	1.76
3	E	802	NDT	C15-S1	4.23	1.82	1.76
3	B	804	NDT	C15-S1	4.23	1.82	1.76
3	B	802	NDT	C15-S1	4.22	1.82	1.76
3	E	804	NDT	C15-S1	4.21	1.82	1.76
3	C	802	NDT	C15-S1	4.21	1.82	1.76
3	A	804	NDT	C15-S1	4.21	1.82	1.76
3	A	802	NDT	C15-S1	4.21	1.82	1.76
3	D	802	NDT	C15-S1	4.20	1.82	1.76
3	D	804	NDT	C15-S1	4.20	1.82	1.76
3	F	804	NDT	C15-S1	4.19	1.82	1.76
2	A	801	ATP	C2'-C3'	4.15	1.63	1.52
2	B	803	ATP	C2'-C3'	3.95	1.63	1.52
2	E	803	ATP	C2'-C3'	3.94	1.63	1.52
2	F	801	ATP	C2'-C3'	3.93	1.63	1.52
2	F	803	ATP	C2'-C3'	3.91	1.63	1.52
2	B	801	ATP	C2'-C3'	3.90	1.63	1.52
2	D	801	ATP	C2'-C3'	3.90	1.63	1.52
2	C	803	ATP	C2'-C3'	3.88	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	803	ATP	C2'-C3'	3.87	1.63	1.52
2	A	803	ATP	C2'-C3'	3.87	1.63	1.52
2	E	801	ATP	C2'-C3'	3.85	1.63	1.52
2	C	801	ATP	C2'-C3'	3.84	1.63	1.52
3	D	804	NDT	C1-C4	3.32	1.45	1.42
3	A	802	NDT	C1-C4	3.28	1.45	1.42
3	C	804	NDT	C1-C4	3.25	1.45	1.42
3	E	802	NDT	C1-C4	3.24	1.45	1.42
3	E	804	NDT	C1-C4	3.24	1.45	1.42
3	B	804	NDT	C1-C4	3.23	1.45	1.42
3	F	802	NDT	C1-C4	3.22	1.45	1.42
3	F	804	NDT	C1-C4	3.22	1.45	1.42
3	A	804	NDT	C1-C4	3.22	1.45	1.42
3	D	802	NDT	C1-C4	3.21	1.45	1.42
3	C	802	NDT	C1-C4	3.21	1.45	1.42
3	B	802	NDT	C1-C4	3.17	1.45	1.42
3	E	804	NDT	O3-S1	3.00	1.46	1.43
3	E	802	NDT	O3-S1	2.99	1.46	1.43
3	A	804	NDT	O3-S1	2.98	1.46	1.43
3	D	802	NDT	O3-S1	2.97	1.46	1.43
3	F	804	NDT	O3-S1	2.96	1.46	1.43
3	C	804	NDT	O3-S1	2.94	1.46	1.43
3	C	802	NDT	O3-S1	2.94	1.46	1.43
3	B	802	NDT	O3-S1	2.93	1.46	1.43
3	B	804	NDT	O3-S1	2.92	1.46	1.43
3	D	804	NDT	O3-S1	2.92	1.46	1.43
2	B	803	ATP	C6-N6	2.90	1.44	1.34
2	C	803	ATP	C6-N6	2.90	1.44	1.34
3	F	802	NDT	O3-S1	2.89	1.46	1.43
2	E	803	ATP	C6-N6	2.89	1.44	1.34
2	A	803	ATP	C6-N6	2.89	1.44	1.34
2	E	801	ATP	C6-N6	2.89	1.44	1.34
2	F	803	ATP	C6-N6	2.88	1.44	1.34
2	D	803	ATP	C6-N6	2.88	1.44	1.34
2	D	801	ATP	C6-N6	2.88	1.44	1.34
2	F	801	ATP	C6-N6	2.88	1.44	1.34
3	A	802	NDT	O3-S1	2.86	1.46	1.43
3	D	804	NDT	O2-S1	2.86	1.46	1.43
2	B	801	ATP	C6-N6	2.86	1.44	1.34
2	A	801	ATP	C6-N6	2.86	1.44	1.34
2	C	801	ATP	C6-N6	2.86	1.44	1.34
3	B	804	NDT	O2-S1	2.84	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	NDT	O2-S1	2.81	1.46	1.43
3	F	804	NDT	O2-S1	2.81	1.46	1.43
3	B	802	NDT	O2-S1	2.79	1.46	1.43
3	E	804	NDT	O2-S1	2.79	1.46	1.43
3	A	802	NDT	O2-S1	2.78	1.46	1.43
3	C	804	NDT	O2-S1	2.77	1.46	1.43
3	F	802	NDT	O2-S1	2.76	1.46	1.43
2	C	803	ATP	C6-C5	2.74	1.53	1.43
2	A	803	ATP	C6-C5	2.74	1.53	1.43
2	E	803	ATP	C6-C5	2.73	1.53	1.43
3	D	802	NDT	O2-S1	2.73	1.46	1.43
2	F	803	ATP	C6-C5	2.73	1.53	1.43
2	D	801	ATP	C6-C5	2.72	1.53	1.43
2	B	803	ATP	C6-C5	2.72	1.53	1.43
2	E	801	ATP	C6-C5	2.72	1.53	1.43
2	A	801	ATP	C6-C5	2.71	1.53	1.43
2	F	801	ATP	C6-C5	2.71	1.53	1.43
2	B	801	ATP	C6-C5	2.70	1.53	1.43
2	D	803	ATP	C6-C5	2.70	1.53	1.43
2	C	801	ATP	C6-C5	2.70	1.53	1.43
3	E	802	NDT	O2-S1	2.66	1.46	1.43
3	C	802	NDT	O2-S1	2.65	1.46	1.43
3	E	802	NDT	S1-N2	2.43	1.72	1.67
3	A	802	NDT	S1-N2	2.43	1.72	1.67
3	D	804	NDT	S1-N2	2.42	1.72	1.67
3	A	804	NDT	S1-N2	2.42	1.72	1.67
3	B	802	NDT	S1-N2	2.42	1.72	1.67
3	E	804	NDT	S1-N2	2.41	1.72	1.67
3	C	804	NDT	S1-N2	2.40	1.72	1.67
3	B	804	NDT	S1-N2	2.40	1.72	1.67
3	C	802	NDT	S1-N2	2.39	1.72	1.67
3	D	802	NDT	S1-N2	2.39	1.72	1.67
3	F	804	NDT	S1-N2	2.39	1.72	1.67
3	F	802	NDT	S1-N2	2.36	1.72	1.67

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	802	NDT	O3-S1-O2	-11.38	101.08	119.52
3	D	802	NDT	O3-S1-O2	-11.37	101.10	119.52
3	B	802	NDT	O3-S1-O2	-11.36	101.11	119.52
3	C	802	NDT	O3-S1-O2	-11.35	101.13	119.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	NDT	O3-S1-O2	-11.34	101.15	119.52
3	E	804	NDT	O3-S1-O2	-11.33	101.16	119.52
3	A	804	NDT	O3-S1-O2	-11.33	101.17	119.52
3	D	804	NDT	O3-S1-O2	-11.31	101.19	119.52
3	C	804	NDT	O3-S1-O2	-11.31	101.20	119.52
3	F	802	NDT	O3-S1-O2	-11.29	101.23	119.52
3	B	804	NDT	O3-S1-O2	-11.27	101.26	119.52
3	F	804	NDT	O3-S1-O2	-11.24	101.31	119.52
2	D	803	ATP	N3-C2-N1	-5.72	119.74	128.68
2	F	803	ATP	N3-C2-N1	-5.71	119.75	128.68
2	B	803	ATP	N3-C2-N1	-5.71	119.76	128.68
2	E	801	ATP	N3-C2-N1	-5.70	119.76	128.68
2	E	803	ATP	N3-C2-N1	-5.70	119.76	128.68
2	D	801	ATP	N3-C2-N1	-5.70	119.77	128.68
2	A	803	ATP	N3-C2-N1	-5.68	119.80	128.68
2	C	801	ATP	N3-C2-N1	-5.68	119.80	128.68
2	F	801	ATP	N3-C2-N1	-5.68	119.80	128.68
2	C	803	ATP	N3-C2-N1	-5.68	119.80	128.68
2	B	801	ATP	N3-C2-N1	-5.67	119.82	128.68
2	A	801	ATP	N3-C2-N1	-5.64	119.86	128.68
3	E	802	NDT	C1-C2-N1	-5.03	119.20	125.88
3	A	804	NDT	C1-C2-N1	-5.02	119.22	125.88
3	A	802	NDT	C1-C2-N1	-5.01	119.23	125.88
3	F	802	NDT	C1-C2-N1	-5.00	119.24	125.88
3	F	804	NDT	C1-C2-N1	-4.99	119.25	125.88
3	C	802	NDT	C1-C2-N1	-4.99	119.26	125.88
3	D	802	NDT	C1-C2-N1	-4.98	119.26	125.88
3	D	804	NDT	C1-C2-N1	-4.98	119.27	125.88
3	B	802	NDT	C1-C2-N1	-4.97	119.28	125.88
3	E	804	NDT	C1-C2-N1	-4.97	119.29	125.88
3	B	804	NDT	C1-C2-N1	-4.97	119.29	125.88
3	C	804	NDT	C1-C2-N1	-4.96	119.30	125.88
3	C	804	NDT	S1-N2-N1	4.31	119.92	110.44
3	B	804	NDT	S1-N2-N1	4.28	119.84	110.44
3	D	804	NDT	S1-N2-N1	4.28	119.84	110.44
3	F	804	NDT	S1-N2-N1	4.24	119.77	110.44
3	C	802	NDT	S1-N2-N1	4.24	119.77	110.44
3	A	802	NDT	S1-N2-N1	4.22	119.72	110.44
3	D	802	NDT	S1-N2-N1	4.18	119.64	110.44
3	E	804	NDT	S1-N2-N1	4.16	119.58	110.44
3	F	802	NDT	S1-N2-N1	4.15	119.57	110.44
3	B	802	NDT	S1-N2-N1	4.15	119.56	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	802	NDT	S1-N2-N1	4.12	119.49	110.44
3	A	804	NDT	S1-N2-N1	4.11	119.49	110.44
2	D	801	ATP	O2B-PB-O1B	3.99	131.98	112.24
2	A	801	ATP	O2B-PB-O1B	3.99	131.95	112.24
2	B	803	ATP	O2B-PB-O1B	3.99	131.95	112.24
2	A	803	ATP	O2B-PB-O1B	3.98	131.91	112.24
2	F	801	ATP	O2B-PB-O1B	3.96	131.81	112.24
2	B	801	ATP	O2B-PB-O1B	3.94	131.74	112.24
3	E	802	NDT	C4-C1-C2	3.34	120.56	118.20
3	C	802	NDT	C4-C1-C2	3.32	120.55	118.20
3	D	804	NDT	C4-C1-C2	3.32	120.54	118.20
3	F	804	NDT	C4-C1-C2	3.30	120.53	118.20
3	F	802	NDT	C4-C1-C2	3.28	120.52	118.20
3	A	802	NDT	C4-C1-C2	3.27	120.51	118.20
3	B	804	NDT	C4-C1-C2	3.27	120.50	118.20
3	C	804	NDT	C4-C1-C2	3.26	120.50	118.20
3	D	802	NDT	C4-C1-C2	3.24	120.49	118.20
3	B	802	NDT	C4-C1-C2	3.23	120.48	118.20
3	A	804	NDT	C4-C1-C2	3.22	120.48	118.20
3	A	804	NDT	B1-C4-C5	-3.21	119.94	123.89
3	E	804	NDT	C4-C1-C2	3.20	120.46	118.20
3	B	802	NDT	B1-C4-C5	-3.20	119.95	123.89
3	C	804	NDT	B1-C4-C5	-3.18	119.97	123.89
3	F	804	NDT	B1-C4-C5	-3.17	119.97	123.89
3	F	802	NDT	B1-C4-C5	-3.16	119.99	123.89
3	D	802	NDT	B1-C4-C5	-3.16	119.99	123.89
3	B	804	NDT	B1-C4-C5	-3.15	120.01	123.89
3	E	804	NDT	B1-C4-C5	-3.15	120.01	123.89
3	E	802	NDT	B1-C4-C5	-3.14	120.02	123.89
3	C	802	NDT	B1-C4-C5	-3.13	120.03	123.89
3	D	804	NDT	B1-C4-C5	-3.11	120.05	123.89
3	A	802	NDT	B1-C4-C5	-3.05	120.13	123.89
2	E	801	ATP	PA-O3A-PB	-2.97	122.64	132.83
2	C	801	ATP	PA-O3A-PB	-2.96	122.67	132.83
2	E	801	ATP	PB-O3B-PG	-2.90	122.88	132.83
2	F	801	ATP	PA-O3A-PB	-2.86	123.01	132.83
2	B	801	ATP	PA-O3A-PB	-2.86	123.02	132.83
2	A	801	ATP	PB-O3B-PG	-2.85	123.03	132.83
2	A	801	ATP	PA-O3A-PB	-2.85	123.04	132.83
2	F	801	ATP	PB-O3B-PG	-2.82	123.14	132.83
2	A	803	ATP	PB-O3B-PG	-2.82	123.15	132.83
2	B	801	ATP	PB-O3B-PG	-2.81	123.19	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	ATP	PA-O3A-PB	-2.77	123.33	132.83
2	A	803	ATP	PA-O3A-PB	-2.77	123.33	132.83
2	C	801	ATP	PB-O3B-PG	-2.77	123.33	132.83
2	E	803	ATP	PA-O3A-PB	-2.74	123.41	132.83
2	F	803	ATP	PA-O3A-PB	-2.74	123.44	132.83
2	B	803	ATP	PB-O3B-PG	-2.71	123.53	132.83
2	F	803	ATP	PB-O3B-PG	-2.70	123.56	132.83
2	E	803	ATP	PB-O3B-PG	-2.70	123.57	132.83
2	D	803	ATP	PA-O3A-PB	-2.69	123.60	132.83
2	C	803	ATP	PA-O3A-PB	-2.68	123.62	132.83
2	C	803	ATP	PB-O3B-PG	-2.67	123.65	132.83
2	D	803	ATP	PB-O3B-PG	-2.67	123.67	132.83
2	D	801	ATP	PB-O3B-PG	-2.65	123.73	132.83
2	B	803	ATP	PA-O3A-PB	-2.63	123.82	132.83
3	D	804	NDT	C5-C4-C1	2.61	120.21	117.10
3	C	804	NDT	C5-C4-C1	2.61	120.20	117.10
3	B	804	NDT	O2-S1-C15	2.60	111.33	108.05
3	F	804	NDT	O2-S1-C15	2.58	111.31	108.05
3	B	802	NDT	C5-C4-C1	2.57	120.16	117.10
3	B	804	NDT	C5-C4-C1	2.57	120.16	117.10
3	F	804	NDT	C5-C4-C1	2.57	120.16	117.10
3	F	802	NDT	C5-C4-C1	2.55	120.14	117.10
3	D	802	NDT	C5-C4-C1	2.54	120.13	117.10
3	C	802	NDT	C5-C4-C1	2.54	120.12	117.10
3	D	804	NDT	O3-S1-C15	2.54	111.26	108.05
3	E	804	NDT	C5-C4-C1	2.54	120.12	117.10
3	C	804	NDT	O3-S1-C15	2.53	111.25	108.05
3	A	804	NDT	C5-C4-C1	2.53	120.11	117.10
2	A	801	ATP	C4'-O4'-C1'	-2.53	103.35	109.45
3	E	802	NDT	O2-S1-C15	2.53	111.24	108.05
3	A	802	NDT	O3-S1-C15	2.53	111.24	108.05
3	C	802	NDT	O2-S1-C15	2.52	111.23	108.05
3	E	802	NDT	C5-C4-C1	2.51	120.09	117.10
3	D	802	NDT	O3-S1-C15	2.51	111.22	108.05
3	C	804	NDT	O2-S1-C15	2.50	111.21	108.05
3	F	802	NDT	O2-S1-C15	2.50	111.21	108.05
3	E	804	NDT	O3-S1-C15	2.49	111.19	108.05
3	C	802	NDT	O3-S1-C15	2.49	111.19	108.05
3	B	802	NDT	O3-S1-C15	2.48	111.19	108.05
3	D	804	NDT	O2-S1-C15	2.48	111.19	108.05
3	A	804	NDT	O3-S1-C15	2.48	111.19	108.05
3	A	802	NDT	O2-S1-C15	2.48	111.18	108.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	802	NDT	O3-S1-C15	2.47	111.17	108.05
3	A	802	NDT	C5-C4-C1	2.47	120.04	117.10
3	E	804	NDT	O2-S1-C15	2.45	111.15	108.05
3	D	802	NDT	O2-S1-C15	2.44	111.14	108.05
3	A	804	NDT	O2-S1-C15	2.44	111.13	108.05
3	F	802	NDT	O3-S1-C15	2.39	111.06	108.05
3	B	804	NDT	O3-S1-C15	2.37	111.05	108.05
3	B	802	NDT	O2-S1-C15	2.37	111.04	108.05
3	F	804	NDT	O3-S1-C15	2.36	111.03	108.05
3	E	802	NDT	C8-C1-C2	-2.11	118.43	121.83
2	B	803	ATP	C4'-O4'-C1'	-2.10	104.38	109.45
3	C	802	NDT	C8-C1-C2	-2.09	118.46	121.83
3	A	802	NDT	C8-C1-C2	-2.08	118.47	121.83
2	E	803	ATP	C4'-O4'-C1'	-2.08	104.43	109.45
3	F	802	NDT	C8-C1-C2	-2.07	118.49	121.83
3	F	804	NDT	C8-C1-C2	-2.07	118.50	121.83
3	D	802	NDT	C8-C1-C2	-2.06	118.50	121.83
2	A	801	ATP	C3'-C2'-C1'	2.06	107.70	102.54
3	A	804	NDT	C8-C1-C2	-2.06	118.51	121.83
3	B	802	NDT	C8-C1-C2	-2.05	118.52	121.83
3	B	804	NDT	C8-C1-C2	-2.05	118.52	121.83
3	E	804	NDT	C8-C1-C2	-2.04	118.53	121.83
2	A	801	ATP	C2'-C1'-N9	-2.04	109.57	114.27
3	C	804	NDT	C8-C1-C2	-2.03	118.56	121.83
3	D	804	NDT	C8-C1-C2	-2.02	118.57	121.83

All (36) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	801	ATP	C4'
2	A	801	ATP	C3'
2	A	803	ATP	C4'
2	A	803	ATP	C3'
2	B	801	ATP	C4'
2	B	801	ATP	C3'
2	B	803	ATP	C4'
2	B	803	ATP	C3'
2	C	801	ATP	C4'
2	C	801	ATP	C3'
2	C	803	ATP	C4'
2	C	803	ATP	C3'
2	D	801	ATP	C4'

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Mol	Chain	Res	Type	Atom
2	D	801	ATP	C3'
2	D	803	ATP	C4'
2	D	803	ATP	C3'
2	E	801	ATP	C4'
2	E	801	ATP	C3'
2	E	803	ATP	C4'
2	E	803	ATP	C3'
2	F	801	ATP	C4'
2	F	801	ATP	C3'
2	F	803	ATP	C4'
2	F	803	ATP	C3'
3	A	802	NDT	N2
3	A	804	NDT	N2
3	B	802	NDT	N2
3	B	804	NDT	N2
3	C	802	NDT	N2
3	C	804	NDT	N2
3	D	802	NDT	N2
3	D	804	NDT	N2
3	E	802	NDT	N2
3	E	804	NDT	N2
3	F	802	NDT	N2
3	F	804	NDT	N2

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ATP	C5'-O5'-PA-O2A
2	A	801	ATP	C5'-O5'-PA-O3A
2	A	801	ATP	C3'-C4'-C5'-O5'
2	A	803	ATP	PB-O3B-PG-O2G
2	A	803	ATP	PB-O3B-PG-O3G
2	B	801	ATP	C3'-C4'-C5'-O5'
2	D	801	ATP	C5'-O5'-PA-O1A
2	D	801	ATP	C5'-O5'-PA-O2A
2	E	801	ATP	C5'-O5'-PA-O1A
2	E	801	ATP	C4'-C5'-O5'-PA
2	E	803	ATP	O4'-C4'-C5'-O5'
2	F	801	ATP	C3'-C4'-C5'-O5'
2	F	803	ATP	C5'-O5'-PA-O1A
2	F	803	ATP	C3'-C4'-C5'-O5'
3	B	804	NDT	N1-N2-S1-O2

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Mol	Chain	Res	Type	Atoms
3	B	804	NDT	N1-N2-S1-C15
3	C	804	NDT	N1-N2-S1-O3
3	C	804	NDT	N1-N2-S1-C15
3	D	804	NDT	N1-N2-S1-O3
3	F	804	NDT	N1-N2-S1-O2
3	F	804	NDT	N1-N2-S1-C15
2	B	801	ATP	O4'-C4'-C5'-O5'
2	C	801	ATP	O4'-C4'-C5'-O5'
2	C	801	ATP	C3'-C4'-C5'-O5'
2	C	803	ATP	O4'-C4'-C5'-O5'
2	C	803	ATP	C3'-C4'-C5'-O5'
2	D	801	ATP	O4'-C4'-C5'-O5'
2	D	801	ATP	C3'-C4'-C5'-O5'
2	D	803	ATP	O4'-C4'-C5'-O5'
2	D	803	ATP	C3'-C4'-C5'-O5'
2	E	803	ATP	C3'-C4'-C5'-O5'
2	F	801	ATP	O4'-C4'-C5'-O5'
2	A	801	ATP	O4'-C4'-C5'-O5'
2	A	803	ATP	C3'-C4'-C5'-O5'
2	E	801	ATP	C3'-C4'-C5'-O5'
2	F	803	ATP	O4'-C4'-C5'-O5'
2	B	803	ATP	C3'-C4'-C5'-O5'
2	E	801	ATP	O4'-C4'-C5'-O5'
2	E	803	ATP	C4'-C5'-O5'-PA
2	A	803	ATP	O4'-C4'-C5'-O5'
2	A	801	ATP	C4'-C5'-O5'-PA
2	C	801	ATP	C4'-C5'-O5'-PA
2	D	803	ATP	C4'-C5'-O5'-PA
2	A	803	ATP	C4'-C5'-O5'-PA
2	F	801	ATP	C4'-C5'-O5'-PA
2	B	801	ATP	PB-O3B-PG-O3G
2	B	803	ATP	PB-O3B-PG-O2G
2	B	803	ATP	PB-O3B-PG-O3G
2	C	803	ATP	PB-O3B-PG-O3G
2	B	801	ATP	C5'-O5'-PA-O3A
2	E	801	ATP	C5'-O5'-PA-O3A
3	A	802	NDT	N1-N2-S1-O3
2	F	803	ATP	PG-O3B-PB-O1B
2	B	801	ATP	C4'-C5'-O5'-PA
2	C	803	ATP	C4'-C5'-O5'-PA
2	B	801	ATP	C5'-O5'-PA-O1A
2	E	801	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	D	801	ATP	C4'-C5'-O5'-PA
2	E	801	ATP	PA-O3A-PB-O2B
2	A	801	ATP	PB-O3B-PG-O1G
2	E	803	ATP	PA-O3A-PB-O1B
3	A	802	NDT	C16-C15-S1-O3
3	A	802	NDT	C20-C15-S1-O3
3	F	802	NDT	C20-C15-S1-O3
3	F	802	NDT	C16-C15-S1-O3
2	A	801	ATP	PB-O3B-PG-O2G
2	A	801	ATP	PB-O3B-PG-O3G
2	C	803	ATP	PB-O3B-PG-O2G
2	D	801	ATP	C5'-O5'-PA-O3A
2	C	803	ATP	PA-O3A-PB-O2B
2	E	801	ATP	PA-O3A-PB-O1B
2	B	801	ATP	C5'-O5'-PA-O2A
2	C	801	ATP	C5'-O5'-PA-O1A
2	F	801	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

24 monomers are involved in 446 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	801	ATP	15	0
2	B	803	ATP	34	0
3	D	804	NDT	18	0
2	E	801	ATP	15	0
2	F	803	ATP	30	0
3	B	802	NDT	40	0
2	C	801	ATP	15	0
3	F	802	NDT	13	0
3	D	802	NDT	30	0
3	A	804	NDT	5	0
2	D	801	ATP	13	0
3	F	804	NDT	12	0
3	A	802	NDT	33	0
3	C	802	NDT	16	0
2	B	801	ATP	11	0
2	D	803	ATP	25	0
3	E	804	NDT	9	0
2	A	801	ATP	26	0
2	E	803	ATP	29	0
2	A	803	ATP	24	0

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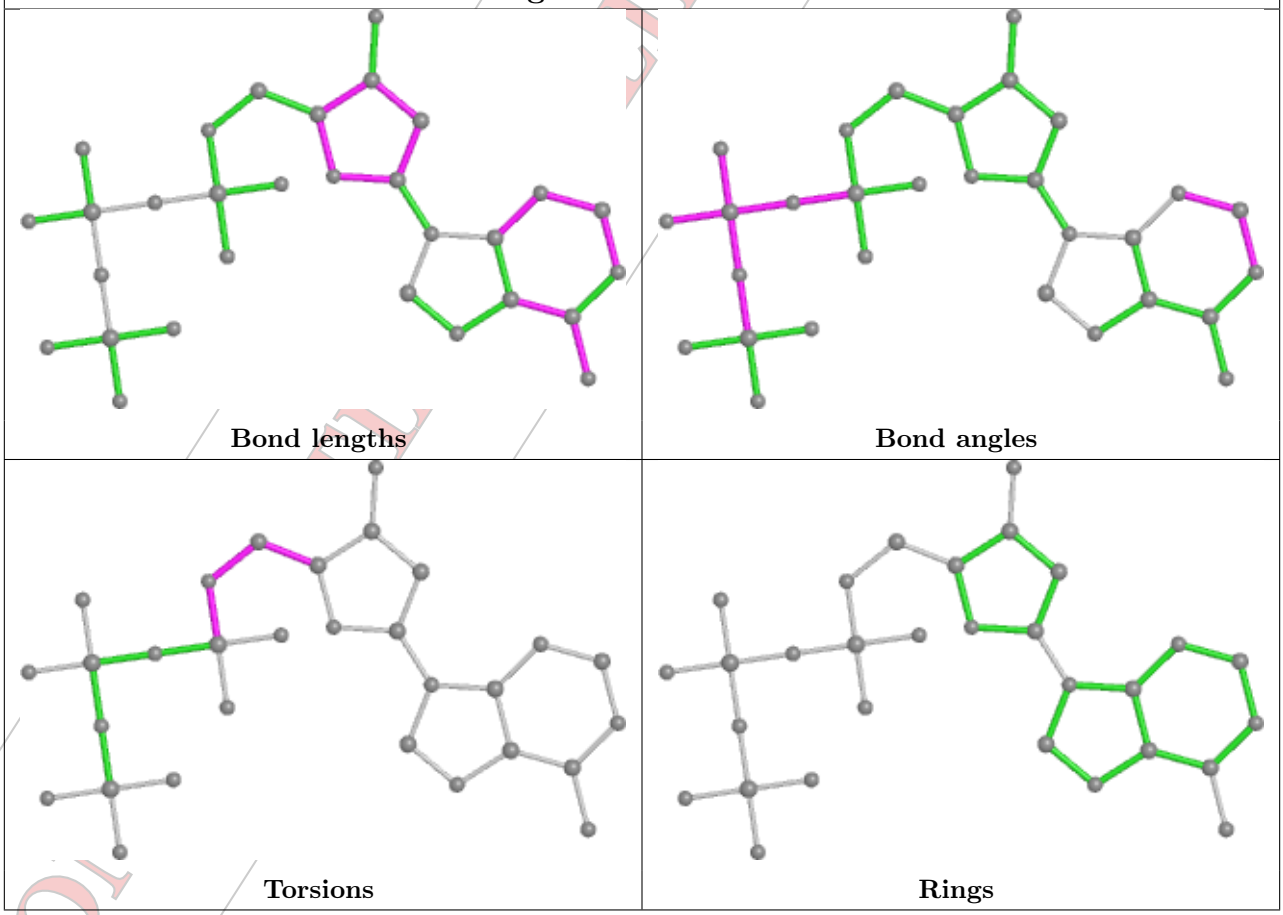
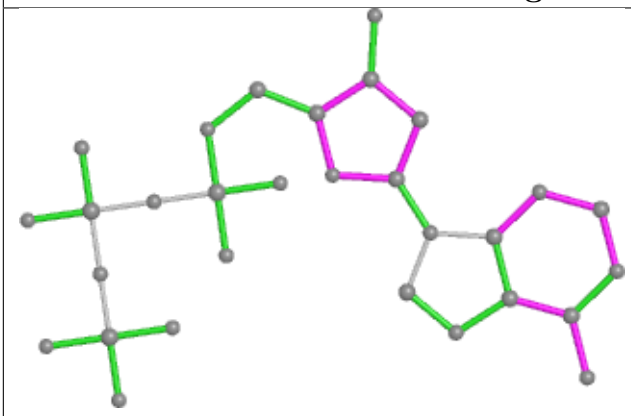
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	804	NDT	15	0
3	E	802	NDT	20	0
2	C	803	ATP	30	0
3	B	804	NDT	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

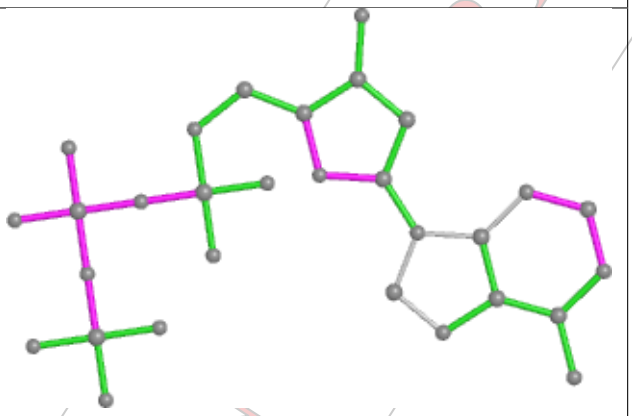
Ligand ATP F 801



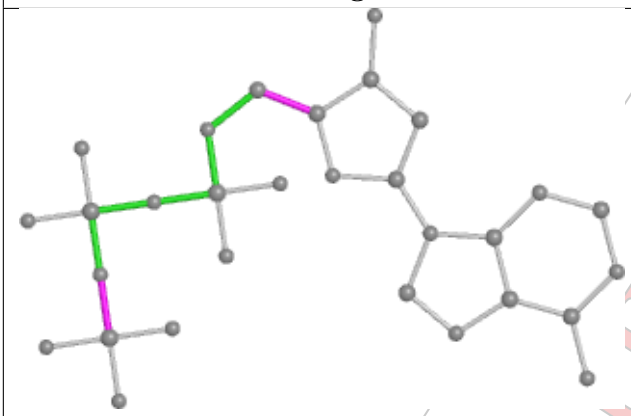
Ligand ATP B 803



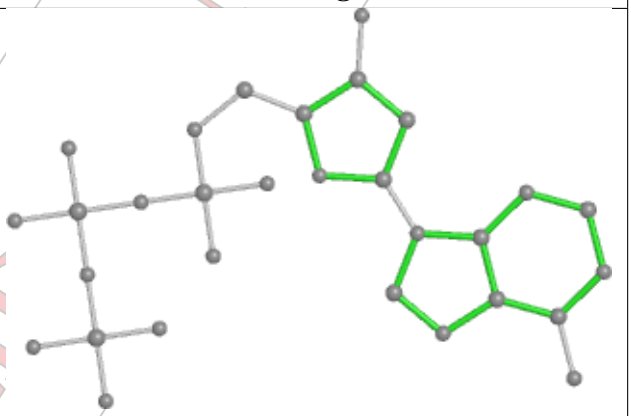
Bond lengths



Bond angles

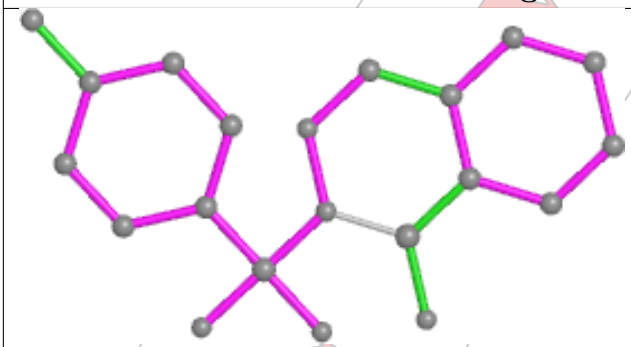


Torsions

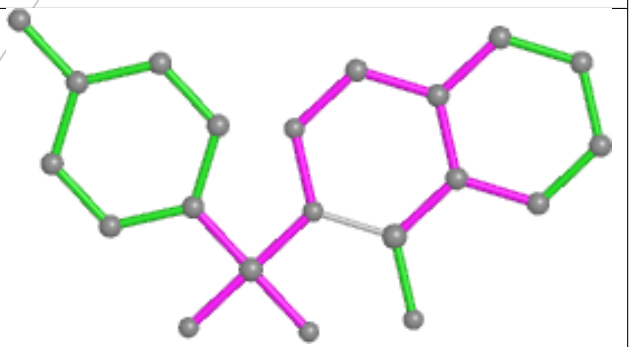


Rings

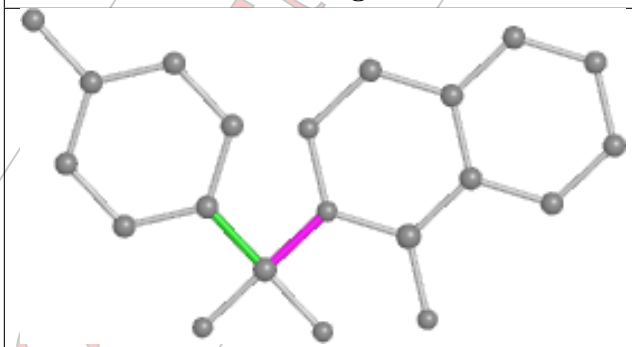
Ligand NDT D 804



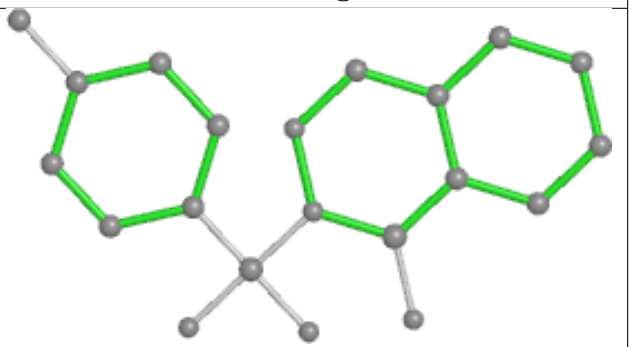
Bond lengths



Bond angles

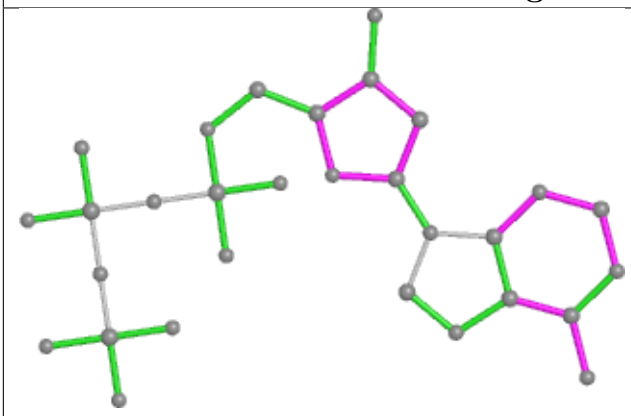


Torsions

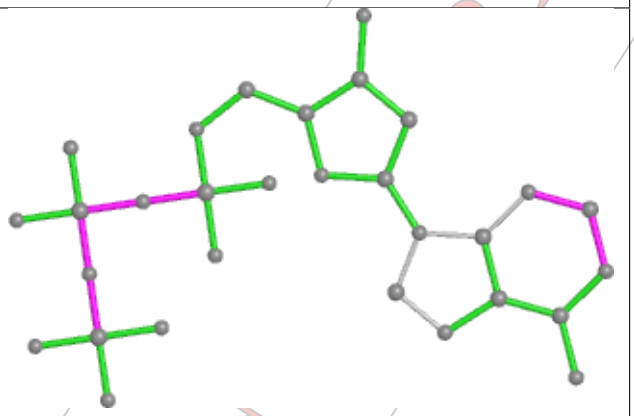


Rings

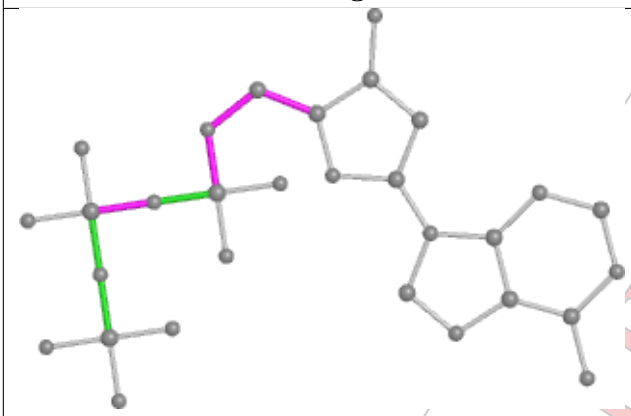
Ligand ATP E 801



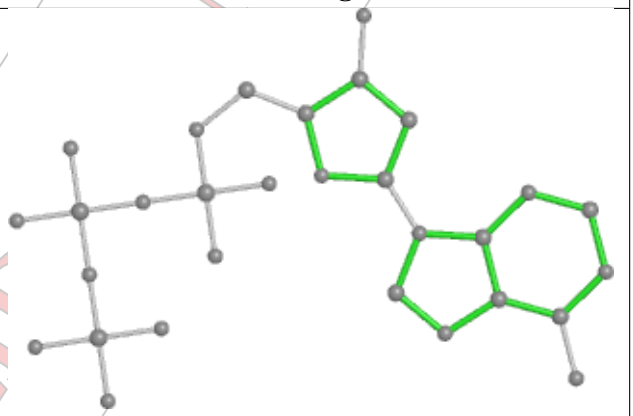
Bond lengths



Bond angles

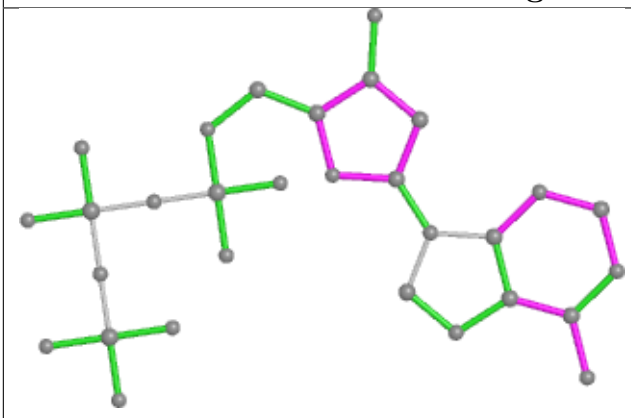


Torsions



Rings

Ligand ATP F 803



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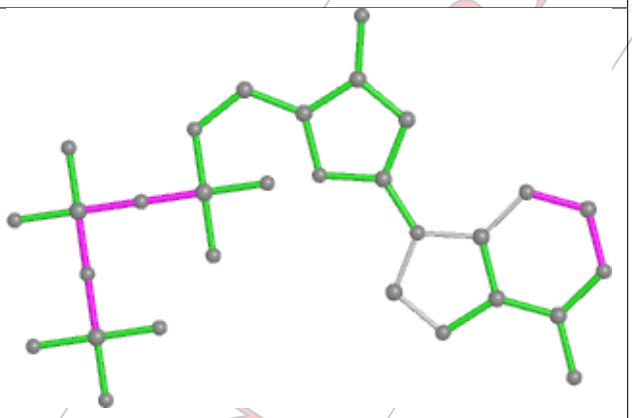

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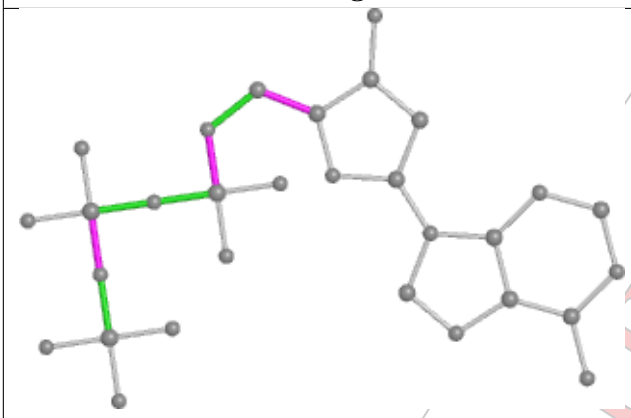

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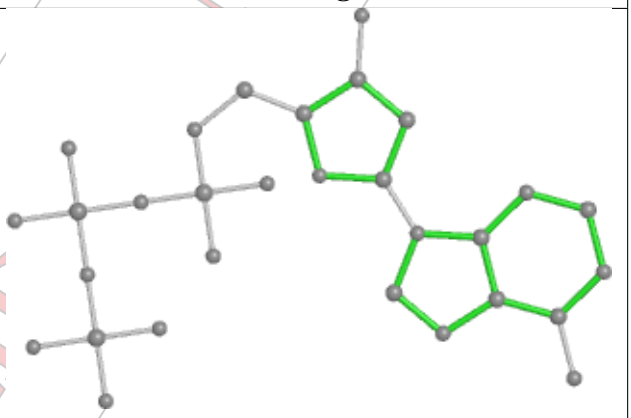
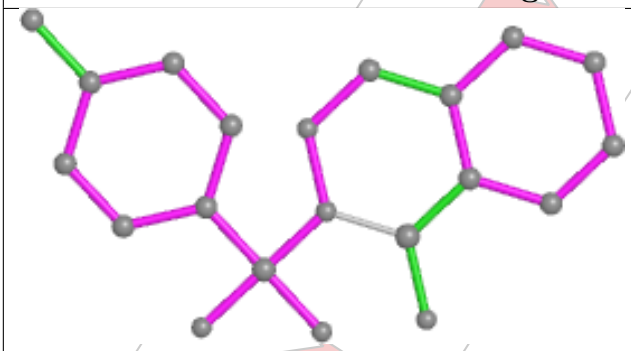


Rings

Ligand NDT B 802



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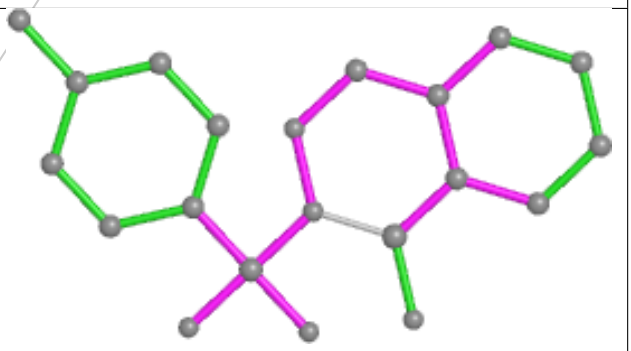

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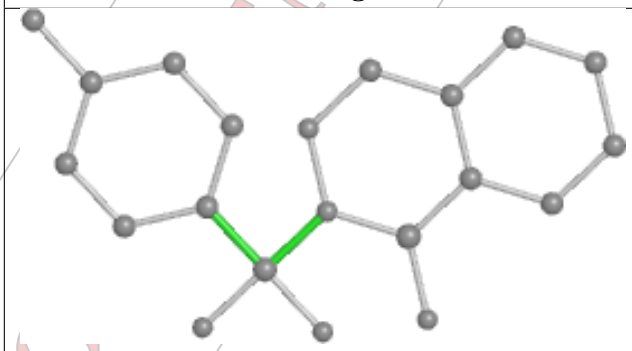

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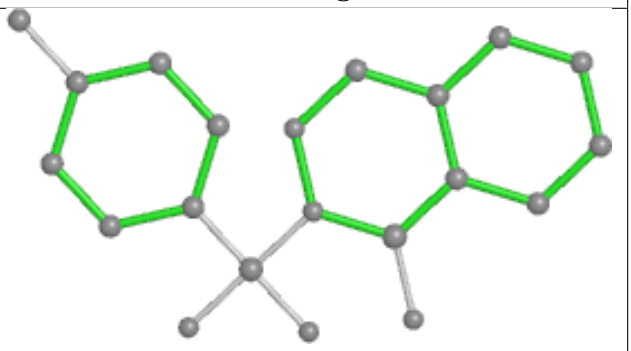
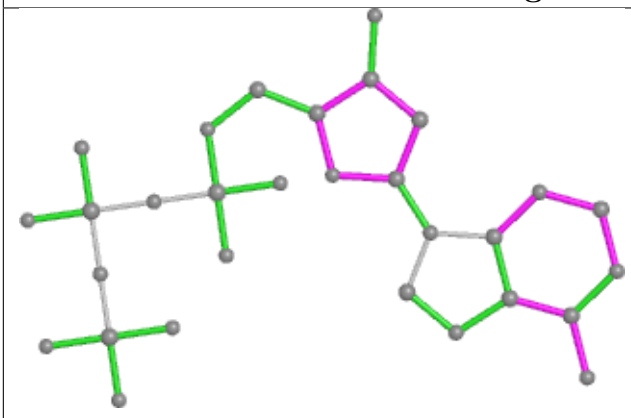


Rings

Ligand ATP C 801



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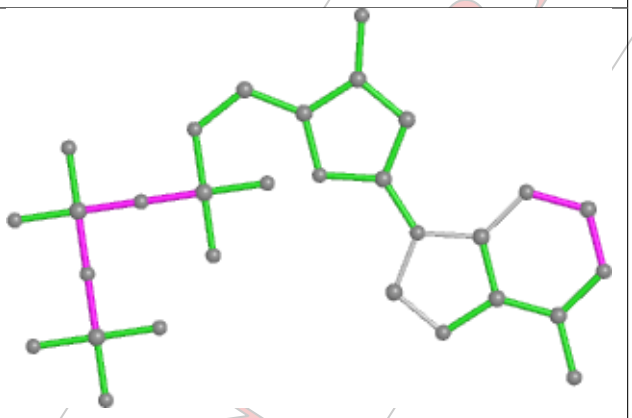

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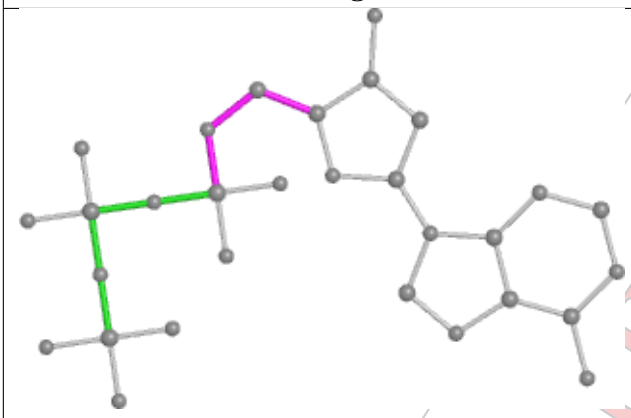

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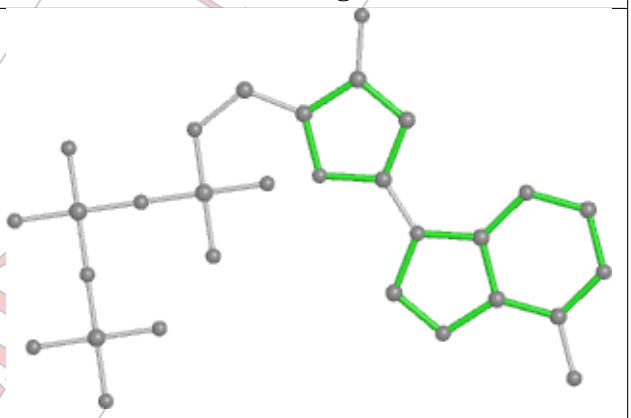
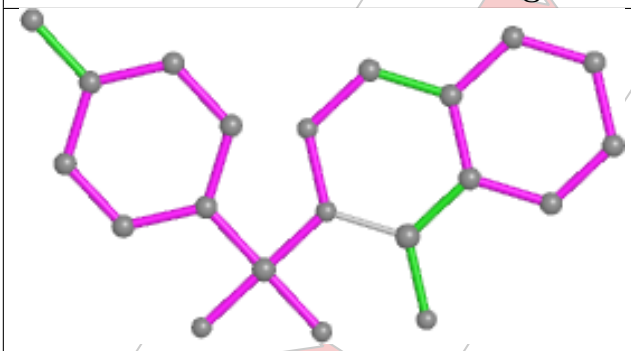


Rings

Ligand NDT F 802



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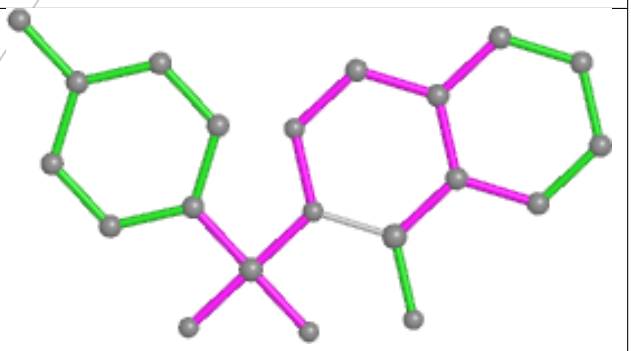
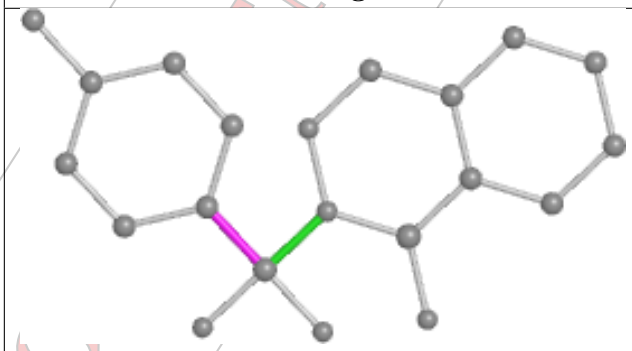


Bond angles



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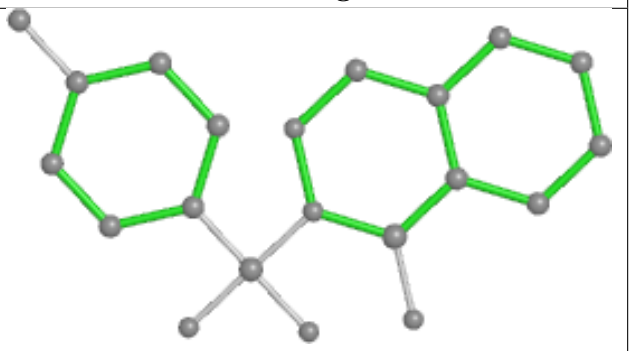
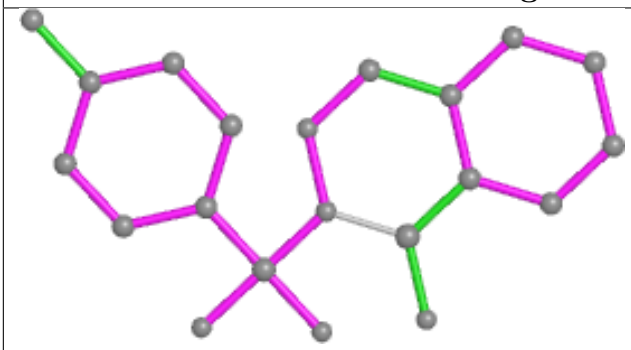


Rings

Ligand NDT D 802



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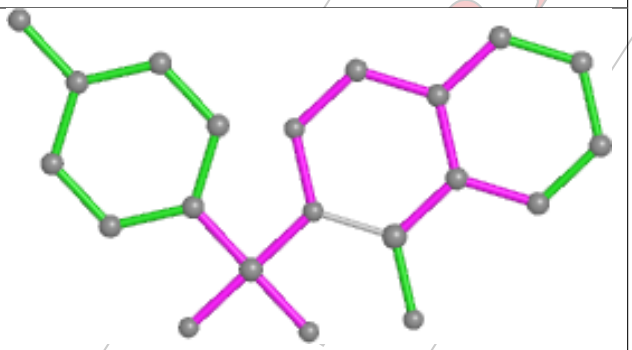

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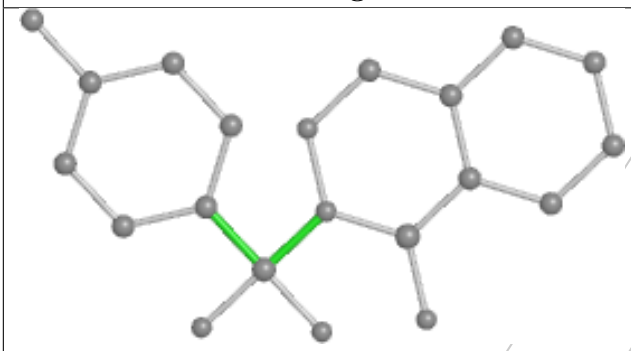

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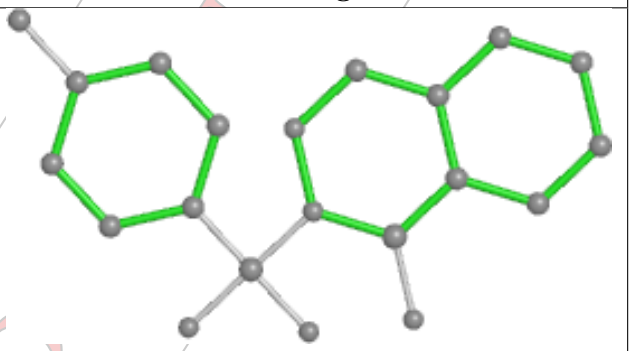
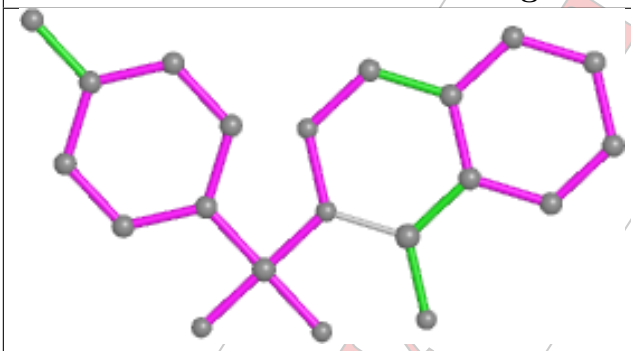


Rings

Ligand NDT A 804



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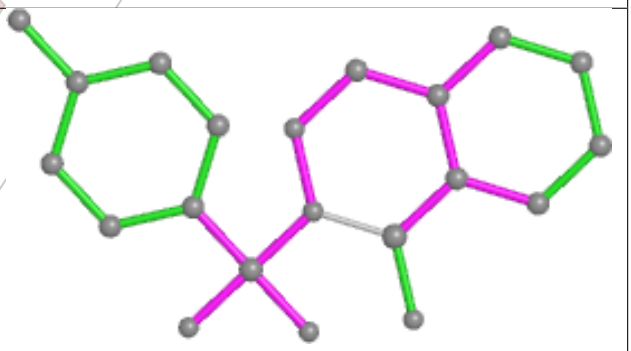

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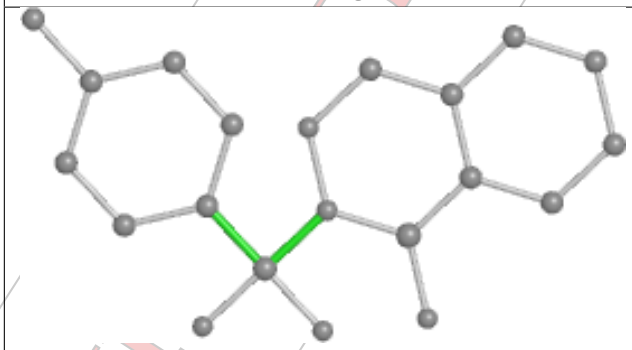

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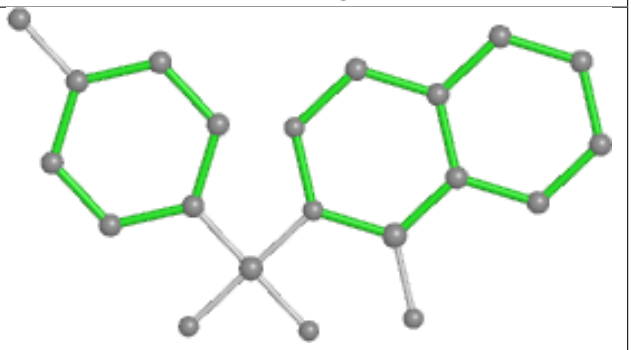
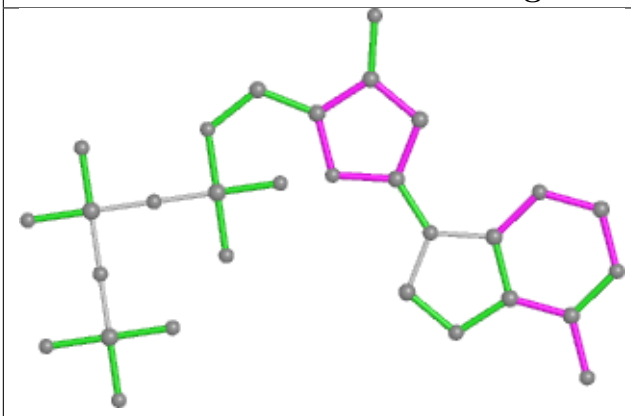


Rings

Ligand ATP D 801



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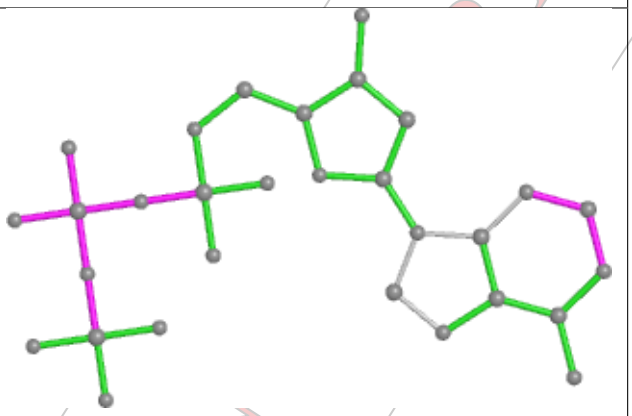

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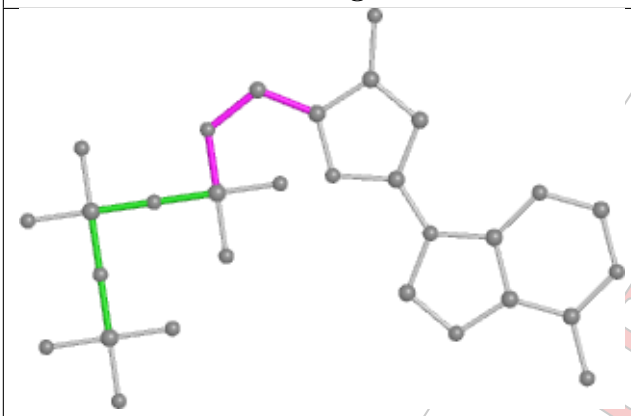

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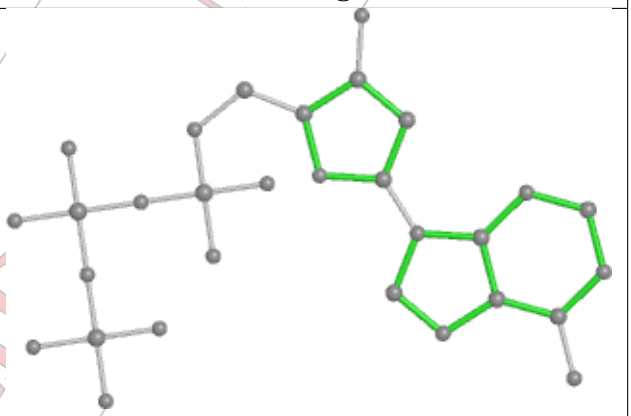
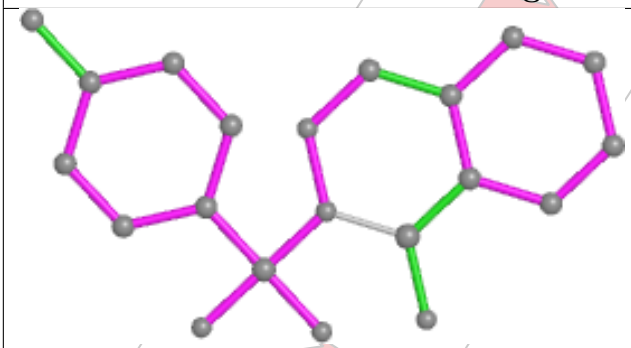


Rings

Ligand NDT F 804



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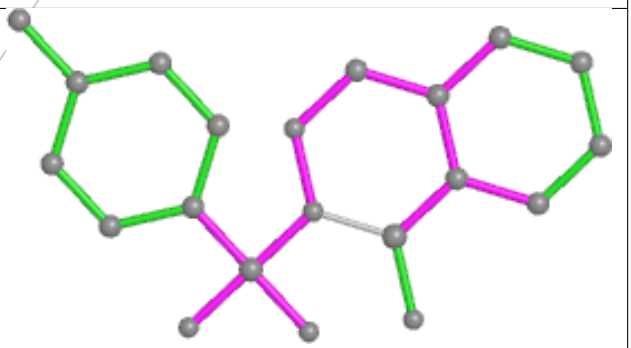
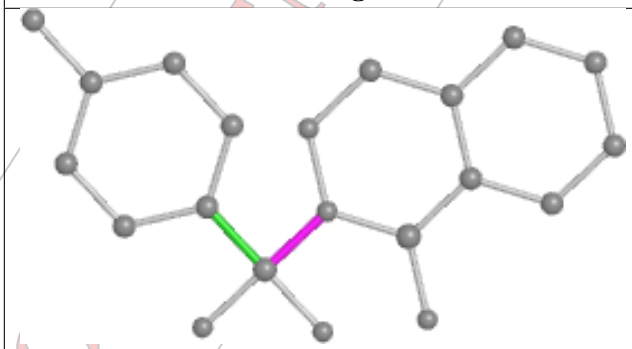


Bond angles



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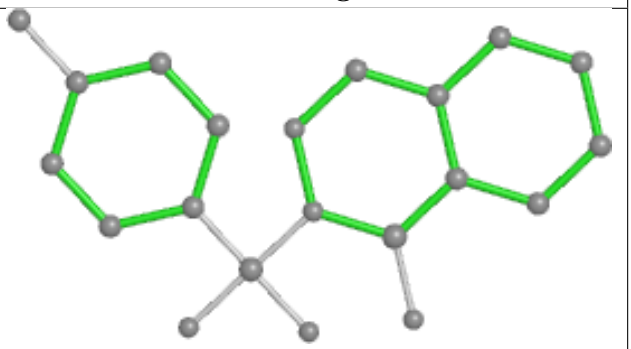
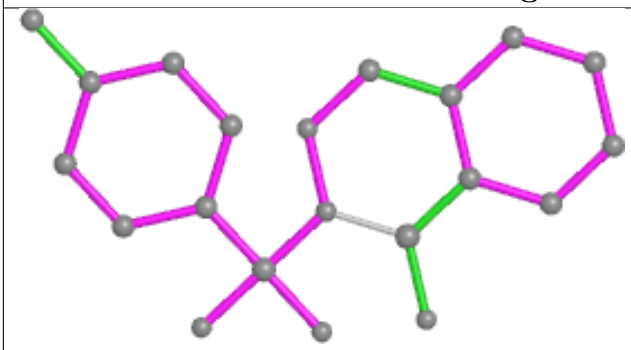


Rings

Ligand NDT A 802



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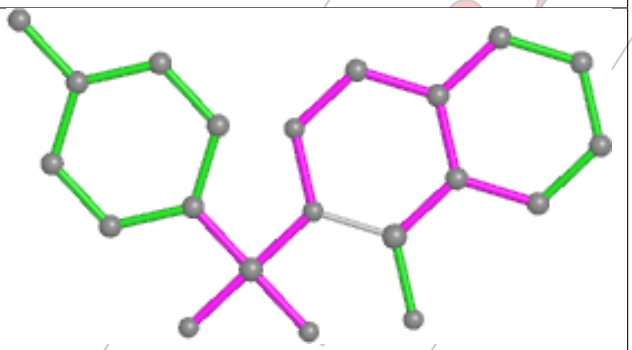
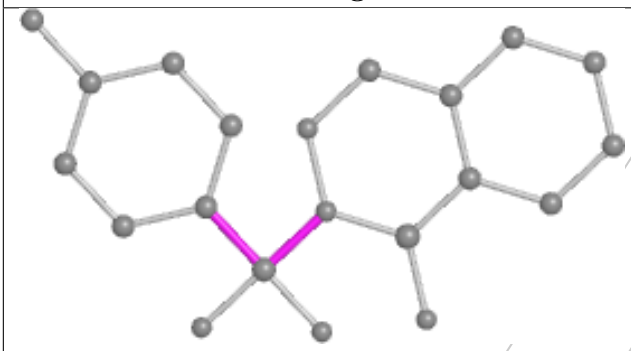


Bond angles



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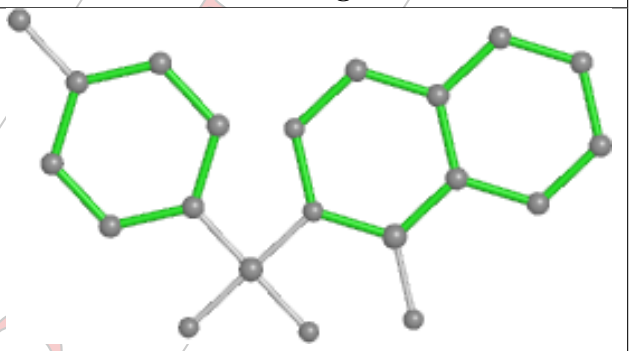
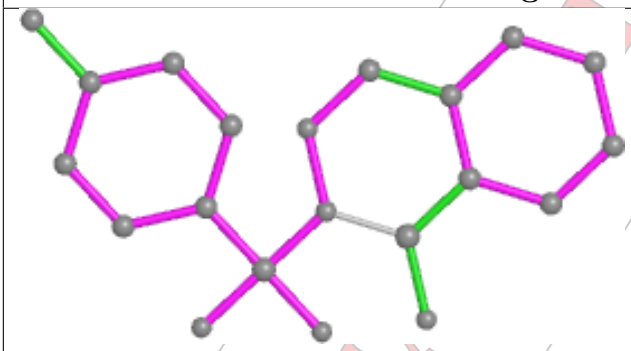


Rings

Ligand NDT C 802



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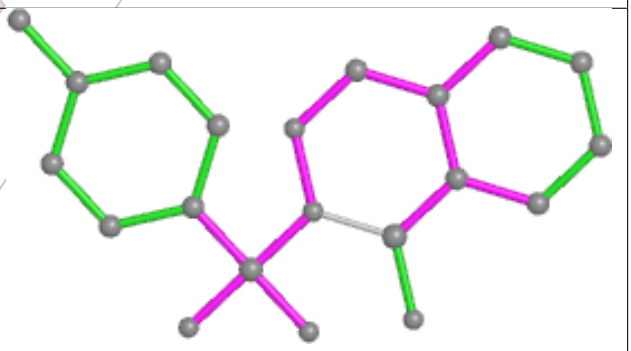
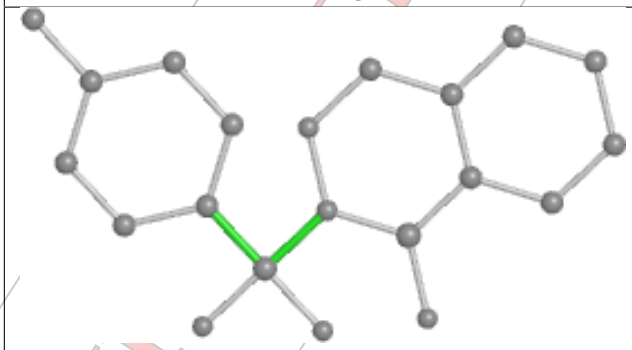


Bond angles



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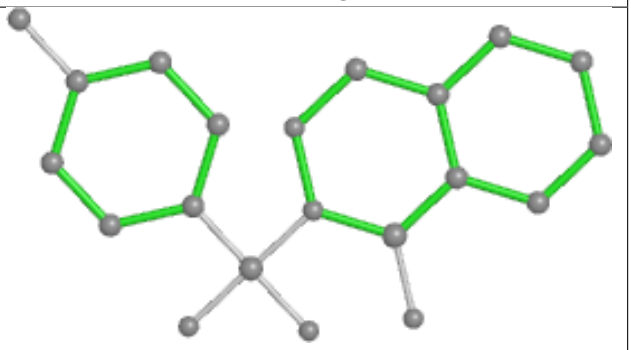
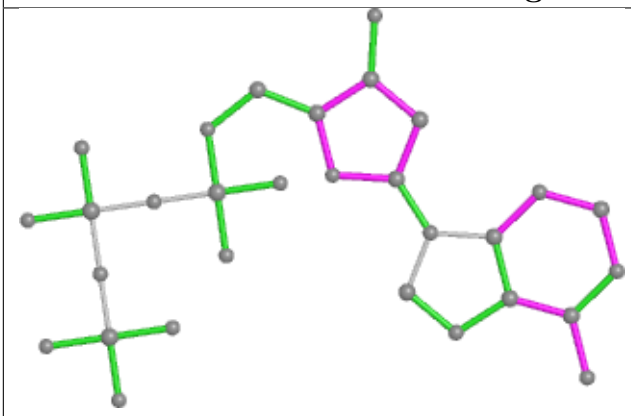


Rings

Ligand ATP B 801



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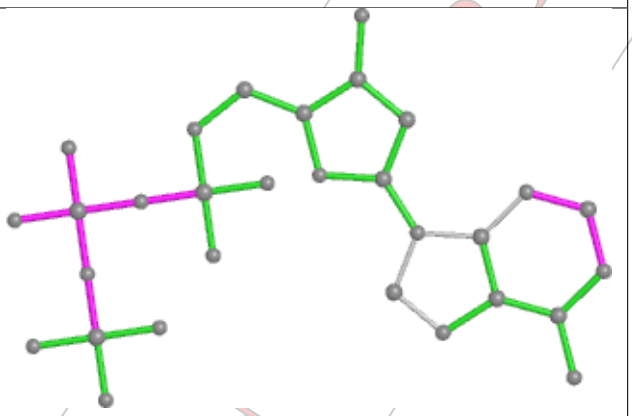

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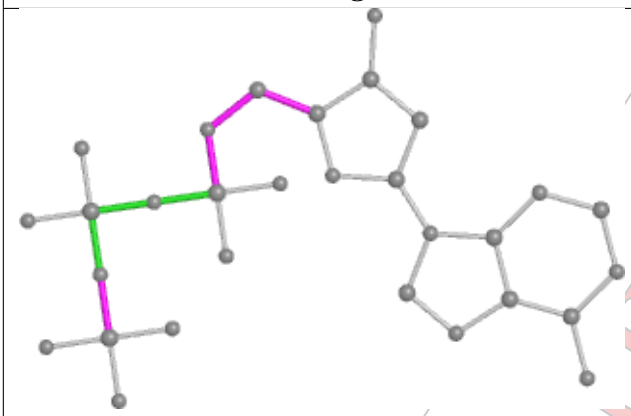

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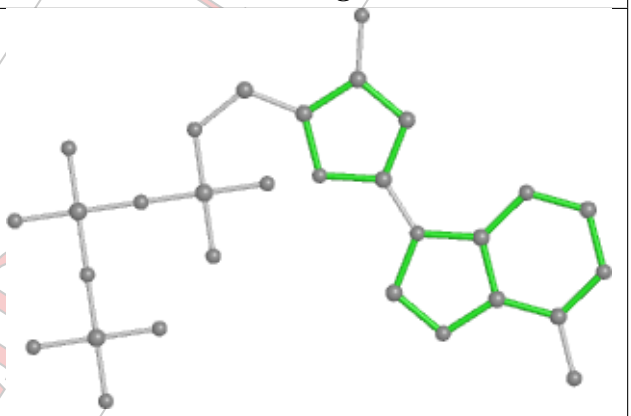
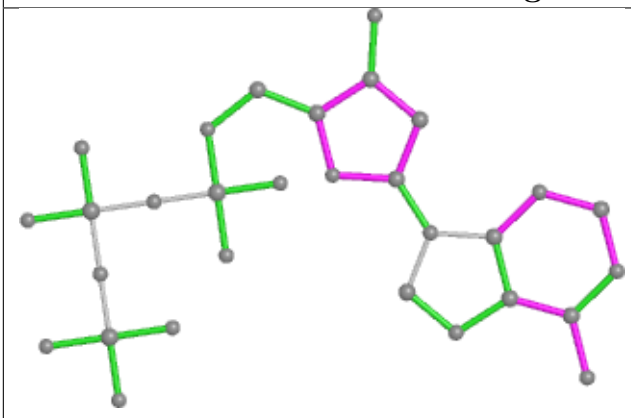


Rings

Ligand ATP D 803



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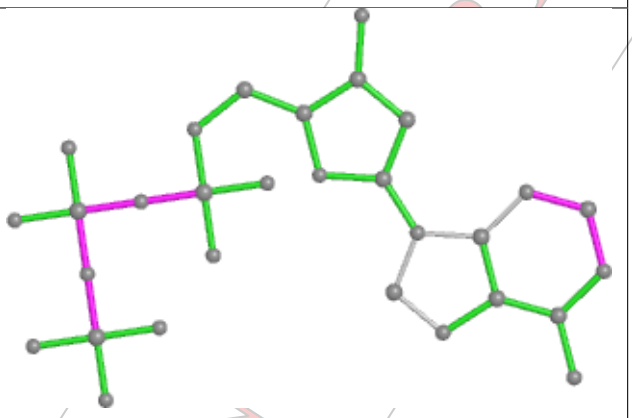
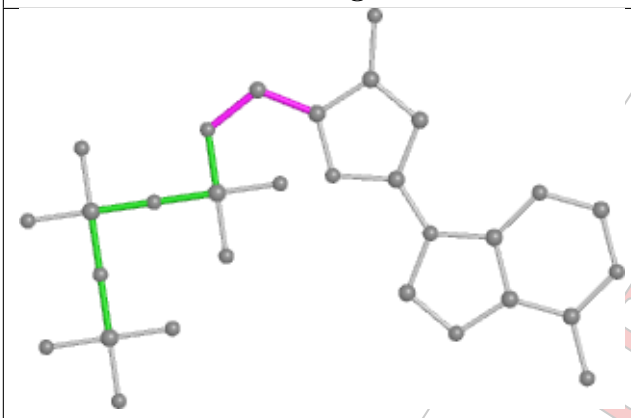


Bond angles



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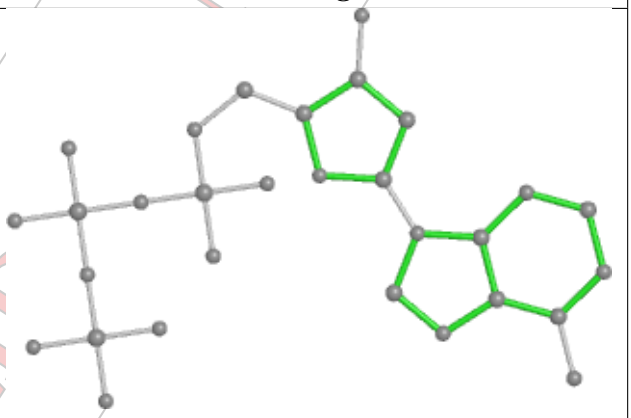
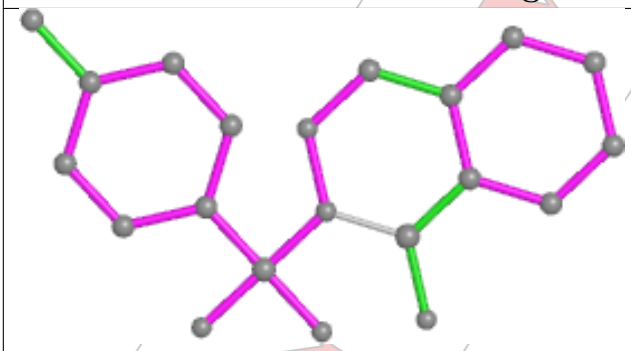


Rings

Ligand NDT E 804



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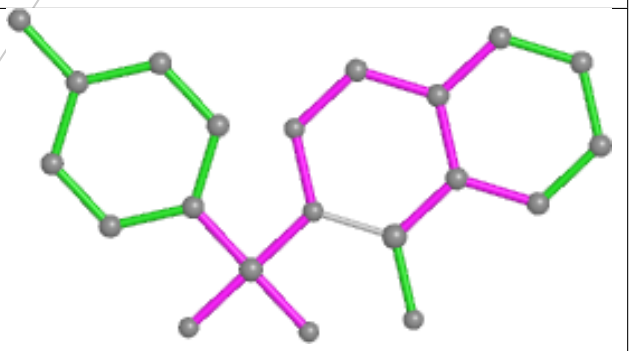
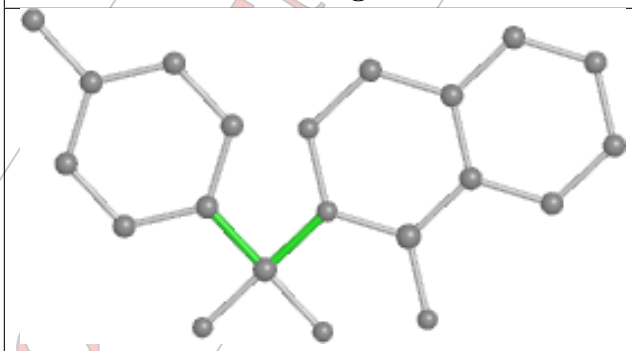
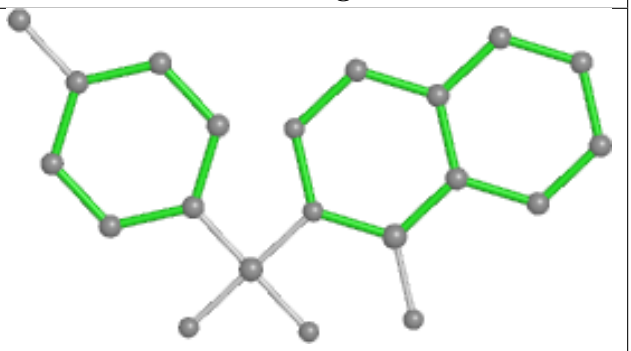


Bond angles

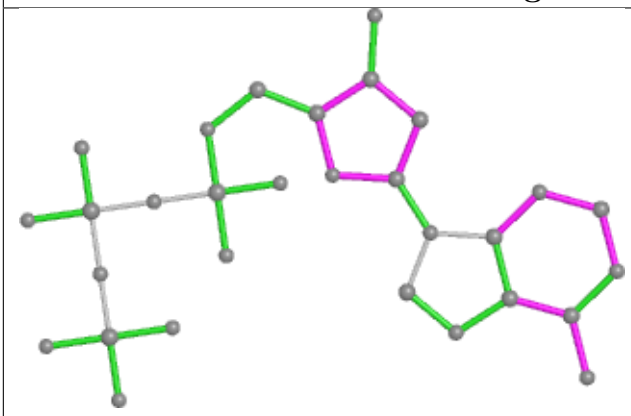


Torsions



Rings

Ligand ATP A 801



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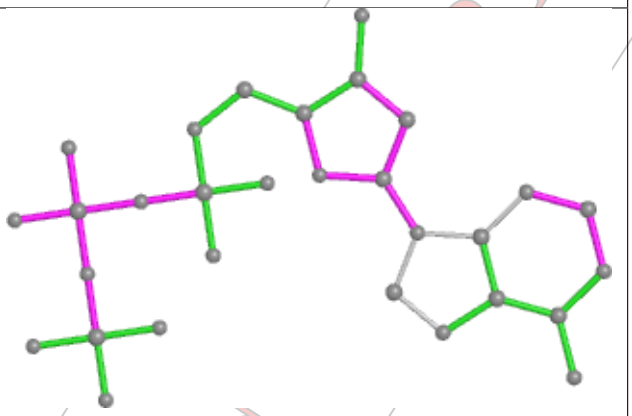
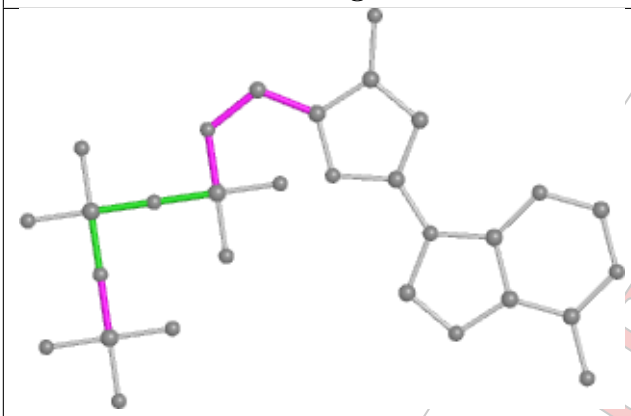
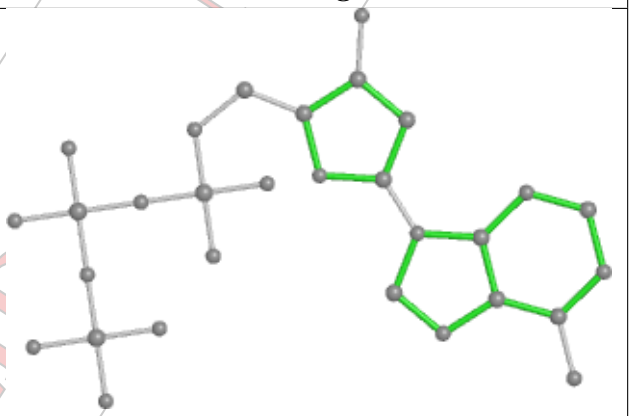


Bond angles

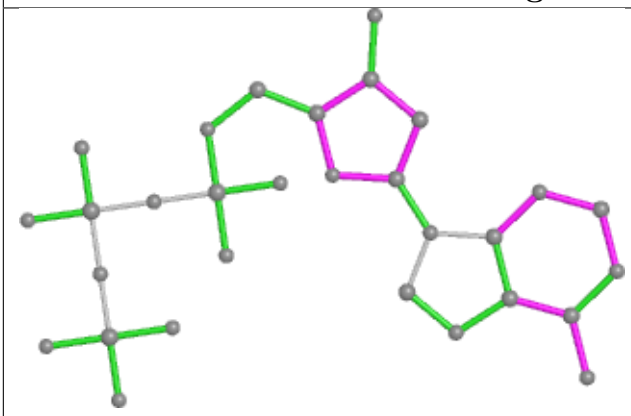


Torsions

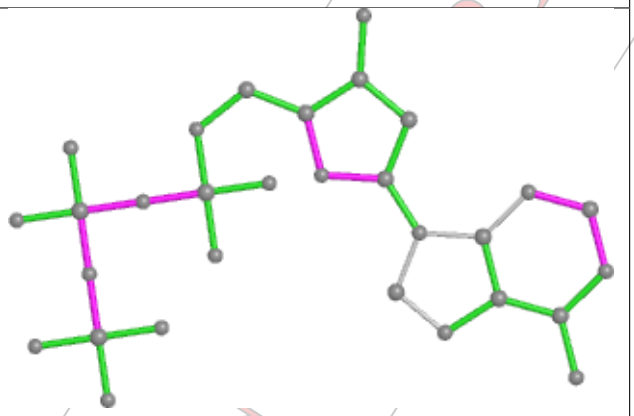


Rings

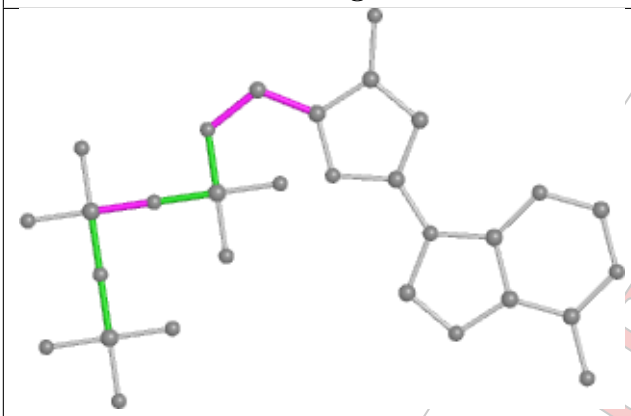
Ligand ATP E 803



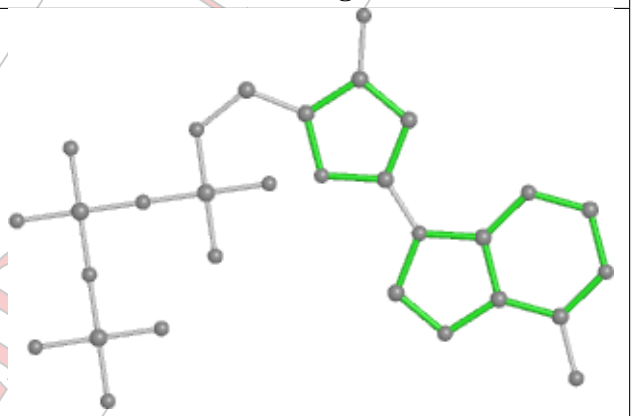
Bond lengths



Bond angles

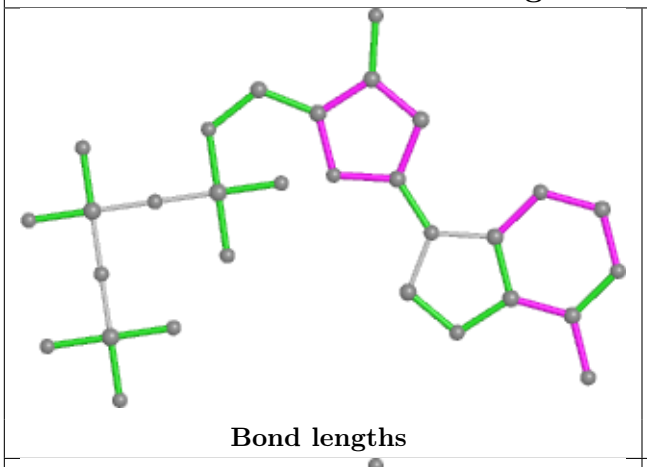


Torsions



Rings

Ligand ATP A 803



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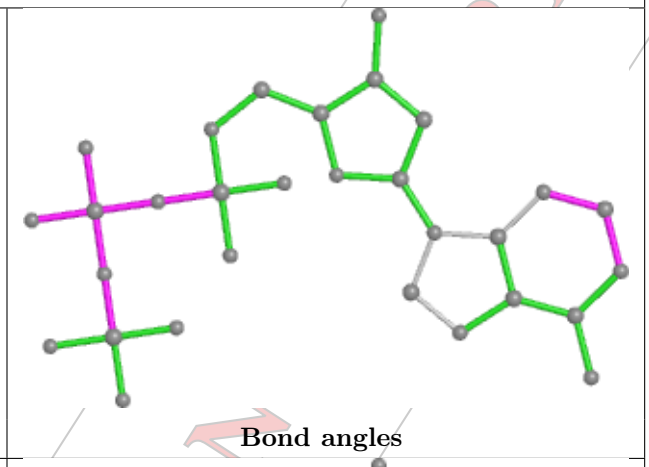
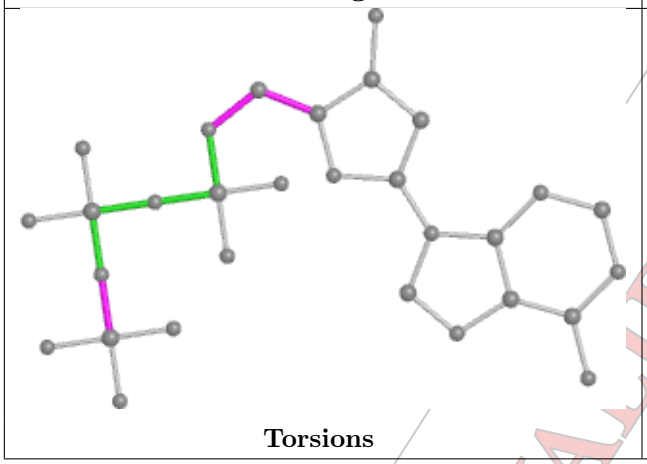
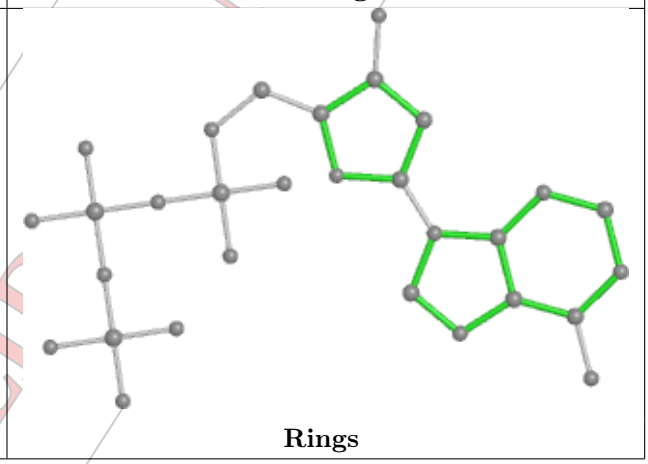


Bond angles

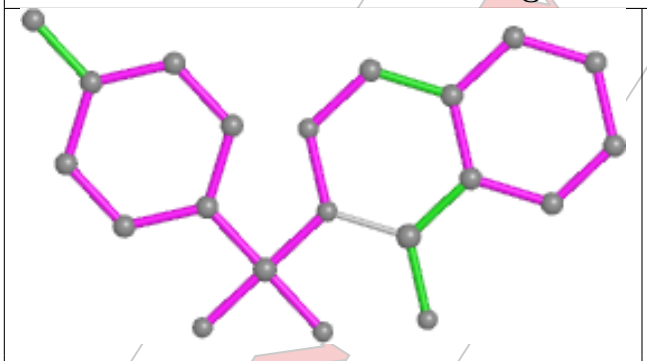


Torsions

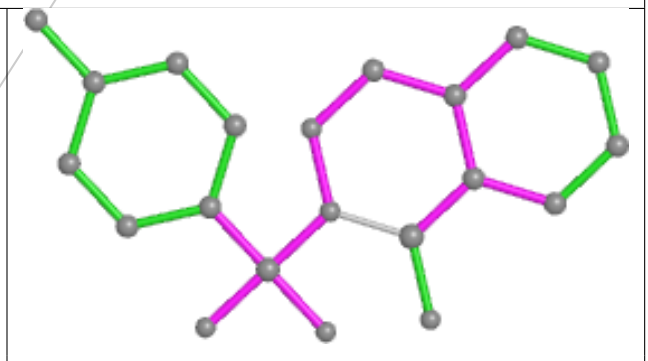


Rings

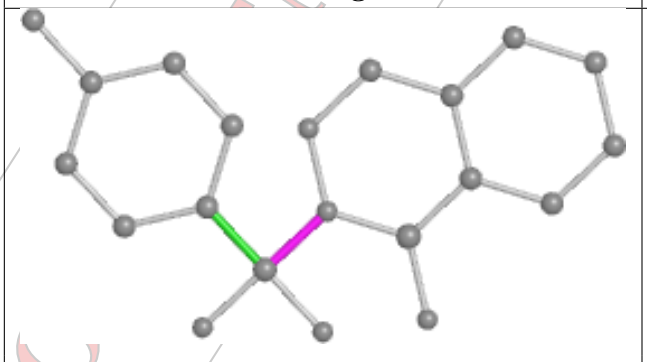
Ligand NDT C 804



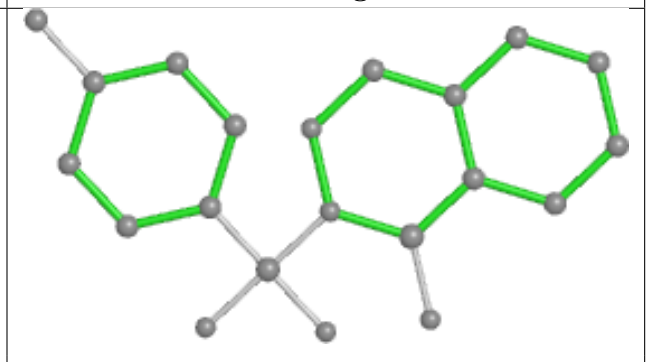
Bond lengths



Bond angles

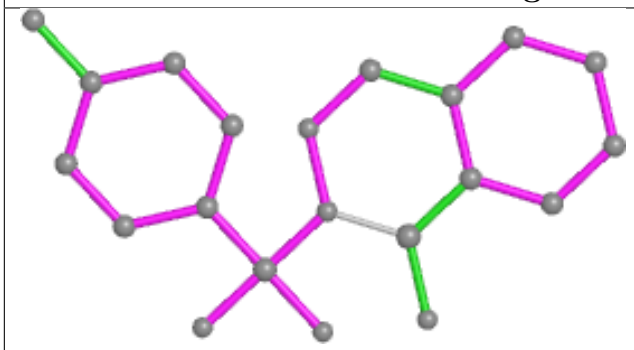


Torsions

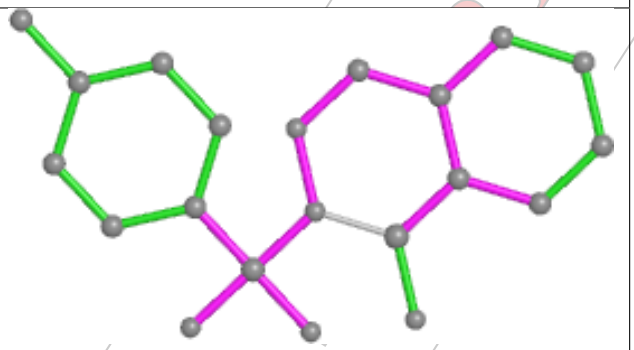


Rings

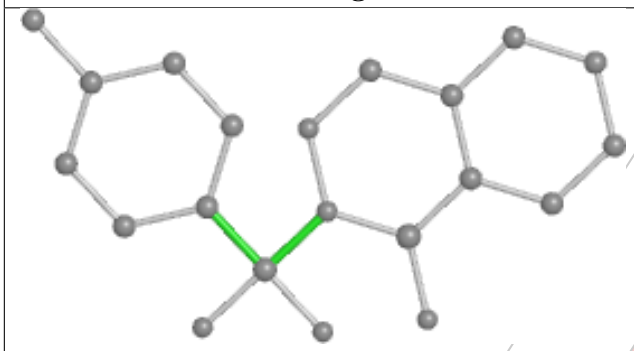
Ligand NDT E 802



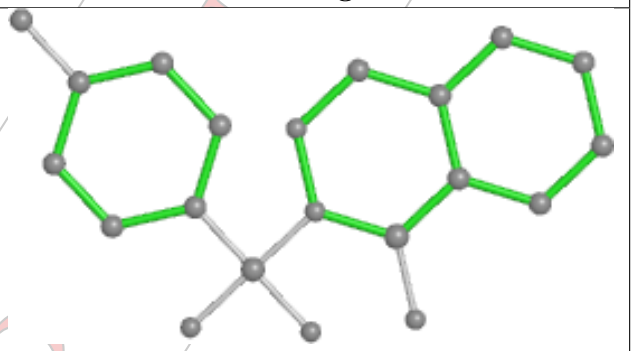
Bond lengths



Bond angles

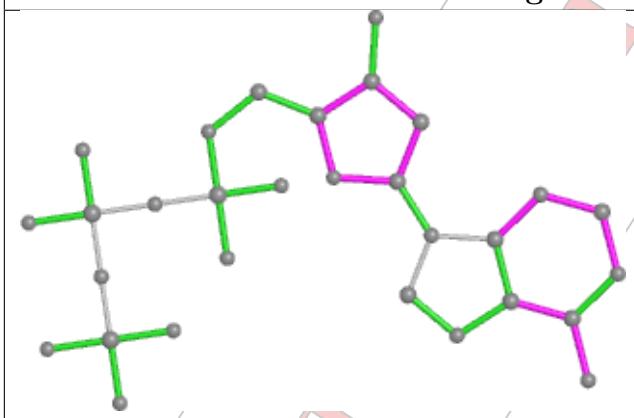


Torsions

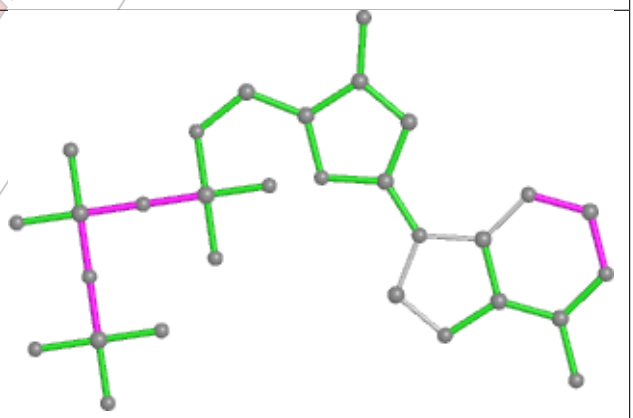


Rings

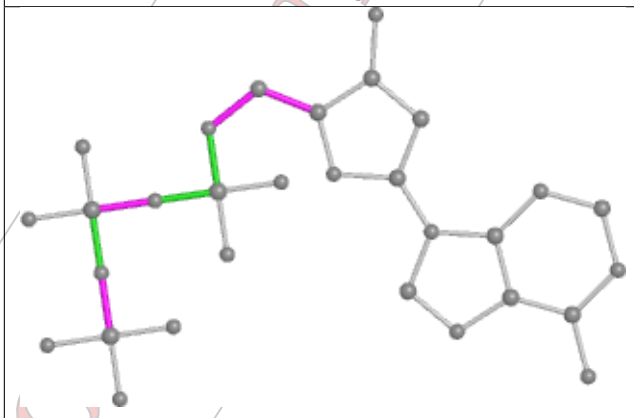
Ligand ATP C 803



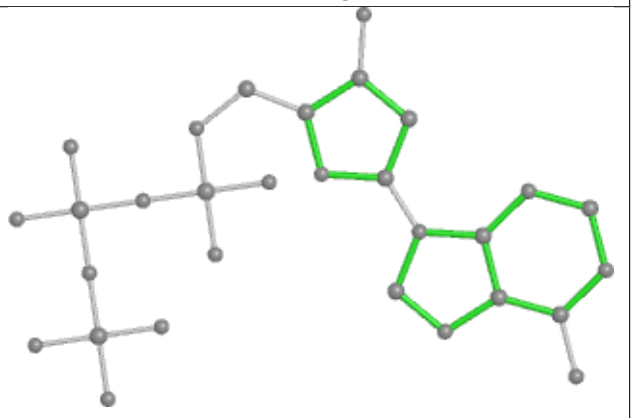
Bond lengths



Bond angles

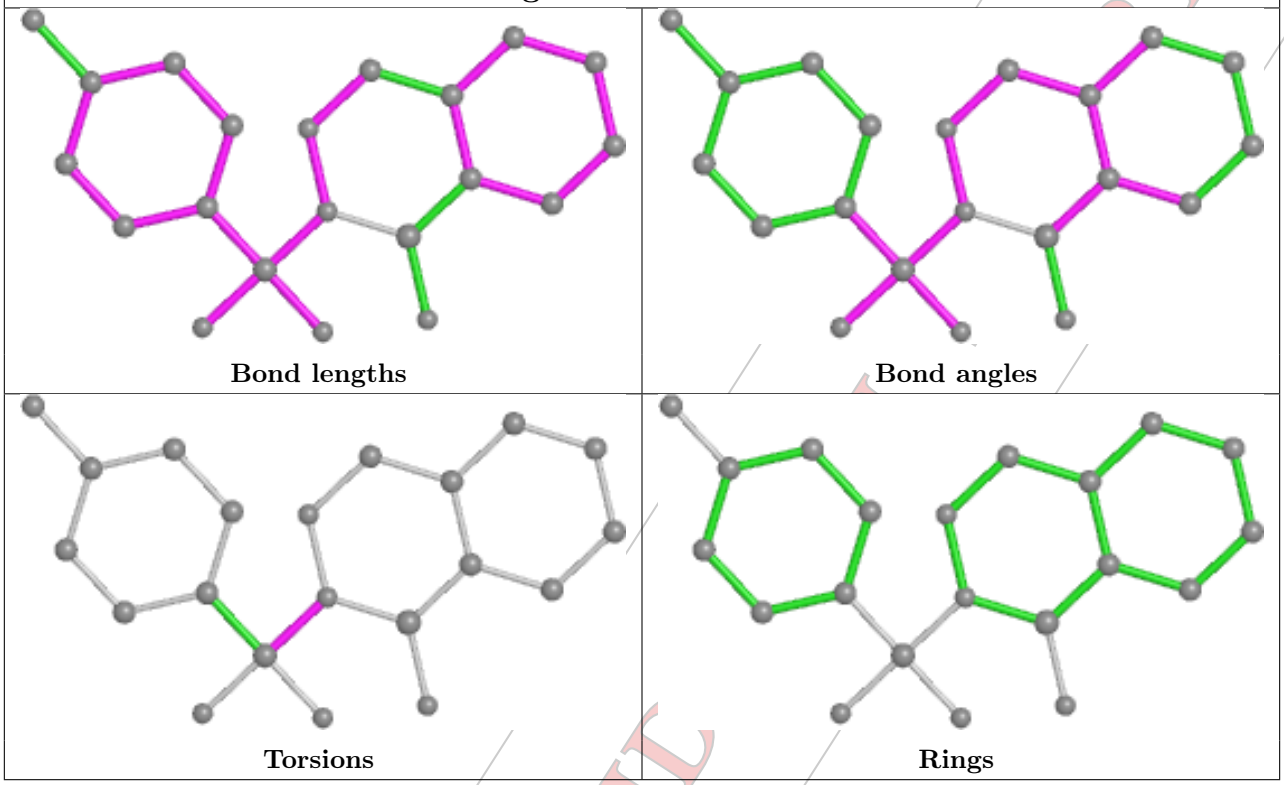


Torsions



Rings

Ligand NDT B 804



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.