Preliminary Full wwPDB EM Validation Report ⓘ

Aug 12, 2022 – 04:29 PM JST

Deposition ID : D_1300031551

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

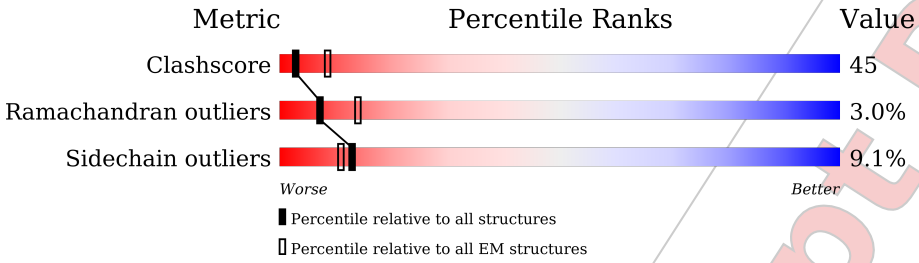
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 unknown.

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	22% 44% 42% 12% ·
2	B	229	31% 52% 40% 7% ·
3	C	228	31% 52% 37% 7% ·
4	D	225	24% 61% 35% ·
4	E	225	22% 53% 41% 5% ·
4	F	225	24% 52% 39% 5% ·
4	G	225	22% 60% 36% · ·
4	H	225	24% 58% 32% 7% ·

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Mol	Chain	Length	Quality of chain
5	J	106	60% 35% 5%
6	K	233	21% 42% 44% 12%
7	L	233	38% 49% 40% 9%
8	P	495	31% 51% 38% 10%
9	R	101	62% 44% 48% 9%
10	S	103	35% 42% 49% 10%
11	U	103	42% 43% 50% 5%
12	V	106	75% 58% 40%
13	I	2	100%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 25675 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	232	1800	1131	304	356	9	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	229	1783	1122	301	352	8	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	228	1777	1119	300	350	8	0	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	225	1757	1108	297	344	8	0	0
4	E	225	1757	1108	297	344	8	0	0
4	F	225	1757	1108	297	344	8	0	0
4	G	225	1756	1108	297	343	8	0	0
4	H	233	1812	1140	305	358	9	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	106	Total	C	N	O	S	0	0
			851	528	150	166	7		

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	233	Total	C	N	O	S	0	0
			1812	1140	305	358	9		

- Molecule 7 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	233	Total	C	N	O	S	0	0
			1812	1140	305	358	9		

- Molecule 8 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	495	Total	C	N	O	S	0	0
			3851	2431	670	731	19		

- Molecule 9 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	101	Total	C	N	O	S	0	0
			766	480	132	147	7		

- Molecule 10 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	103	Total	C	N	O	S	0	0
			785	492	137	149	7		

- Molecule 11 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	101	Total	C	N	O	S	0	0
			766	480	132	147	7		

- Molecule 12 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	V	106	805	504	140	154	7	0	0

- Molecule 13 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

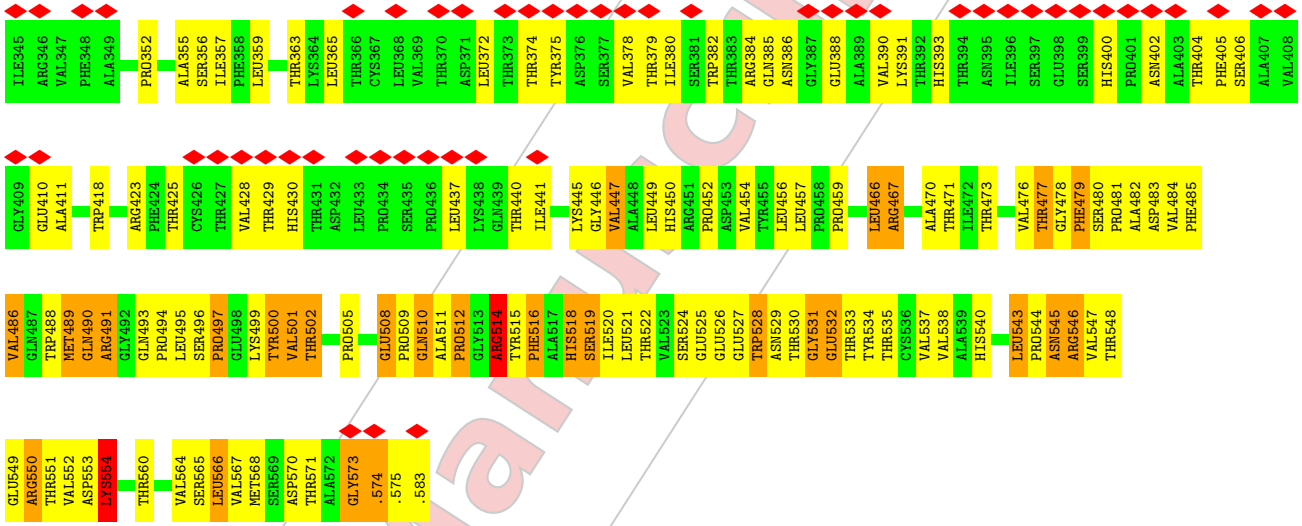
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	I	2	28	16	2	10	0	0

3 Residue-property plots (i)

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

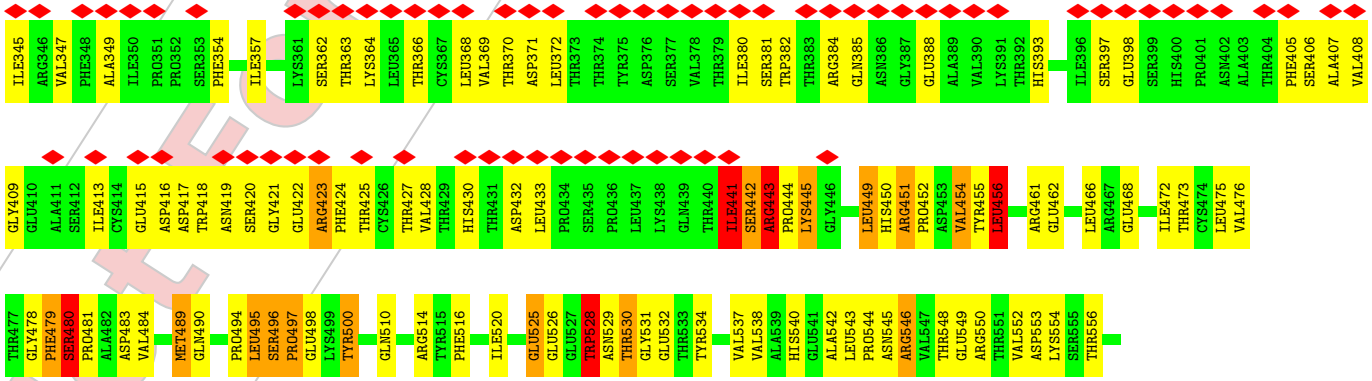
- Molecule 1:

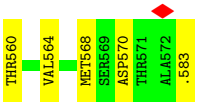
Chain A:



- Molecule 2:

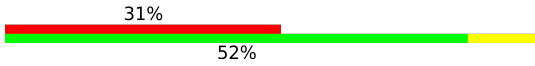
Chain B:

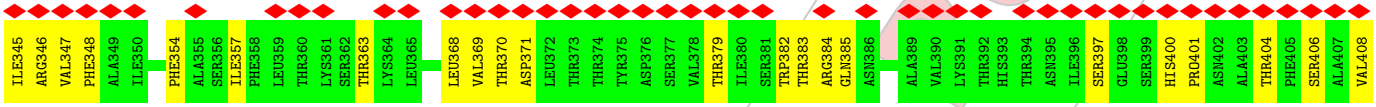


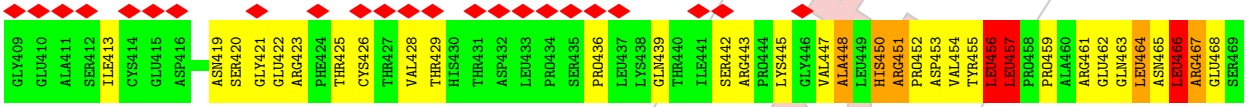


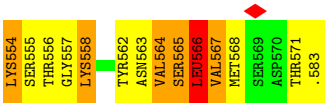
• Molecule 3:

Chain C:



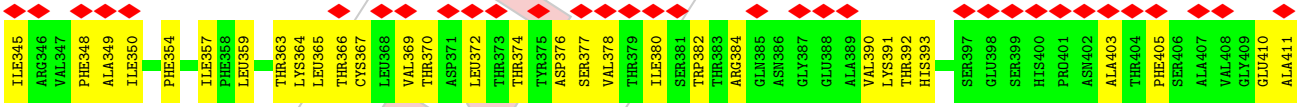


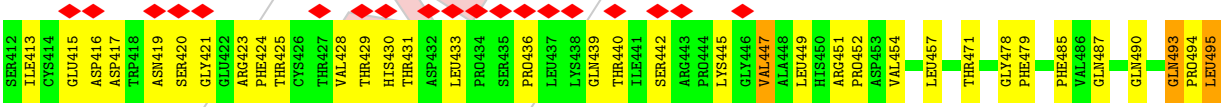




• Molecule 4:

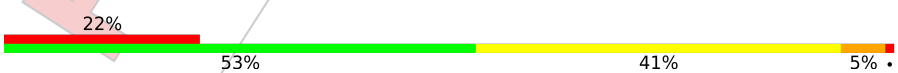
Chain D:

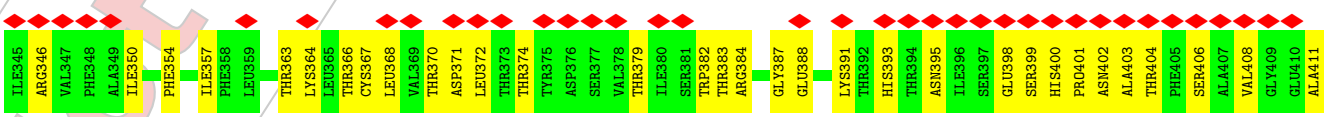


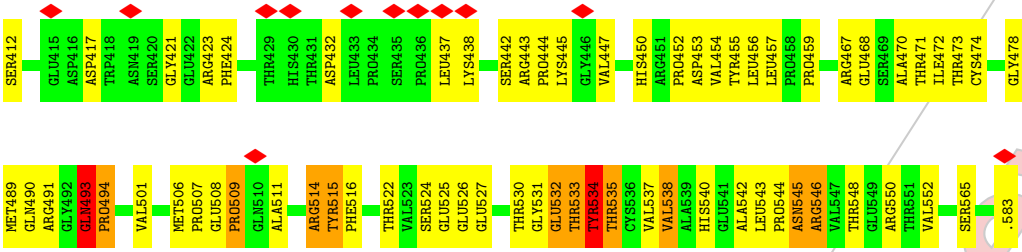


• Molecule 4:

Chain E:

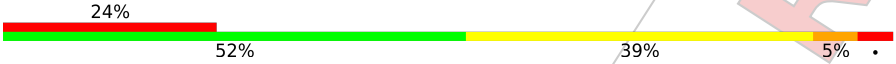


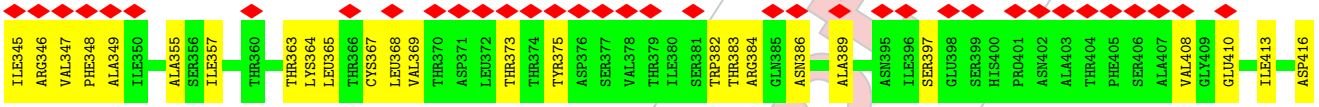




• Molecule 4:

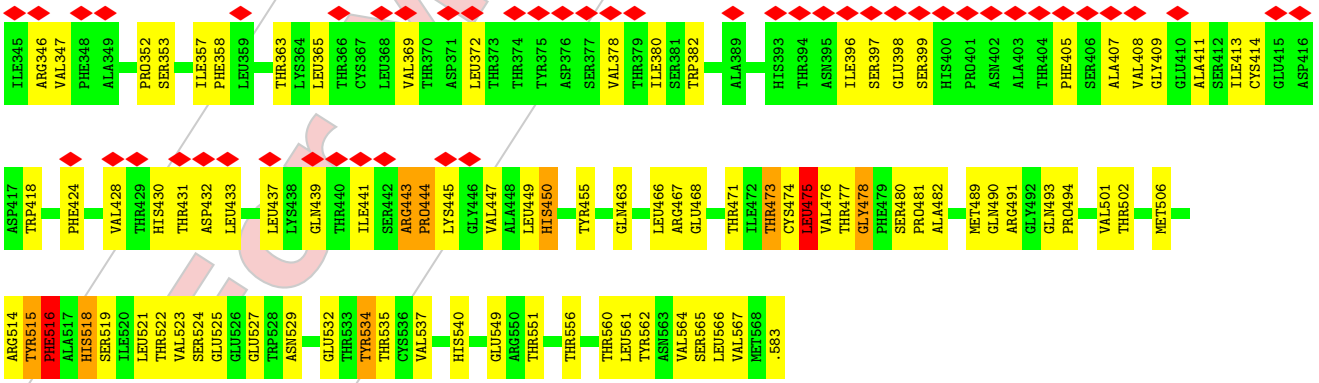
Chain F:





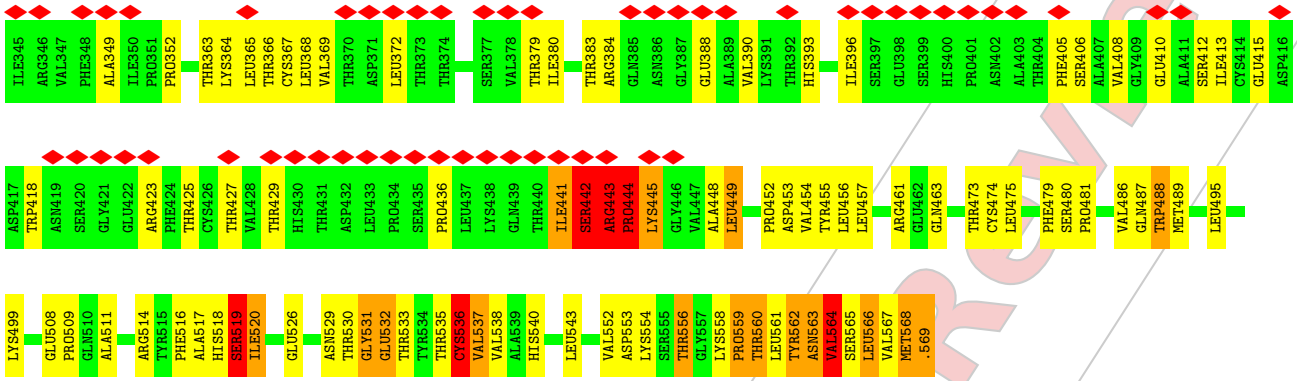
• Molecule 4:

Chain G:



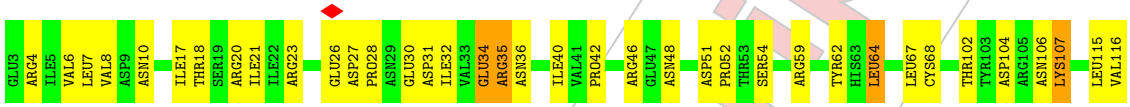
• Molecule 4:

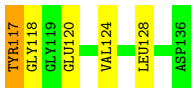
Chain H:



• Molecule 5:

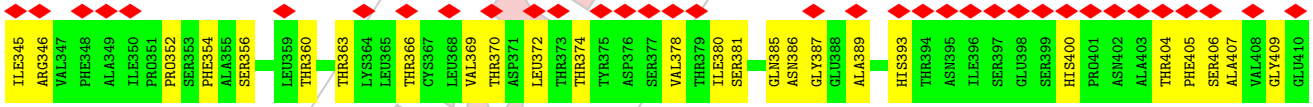
Chain J:

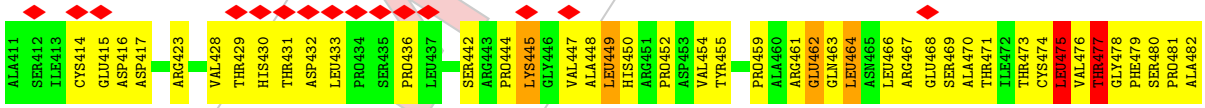


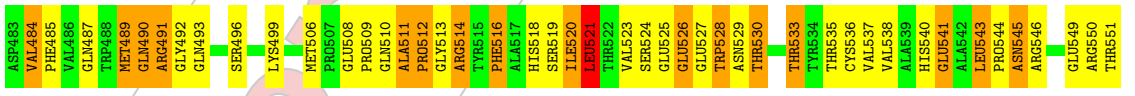


• Molecule 6:

Chain K:

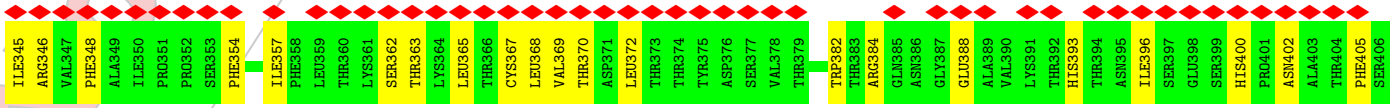


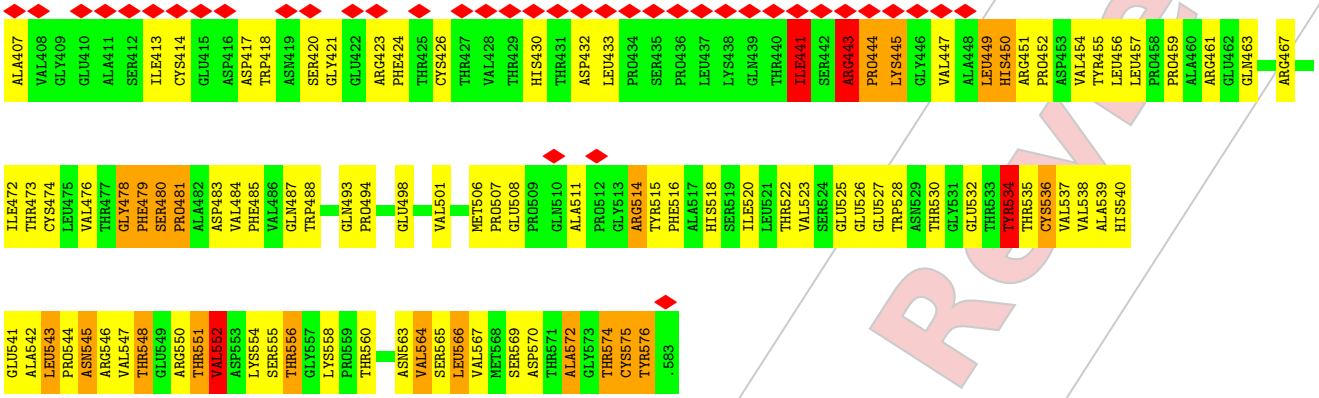




• Molecule 7:

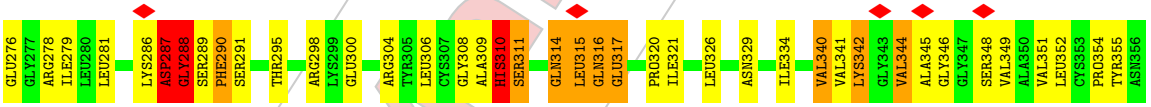
Chain L:

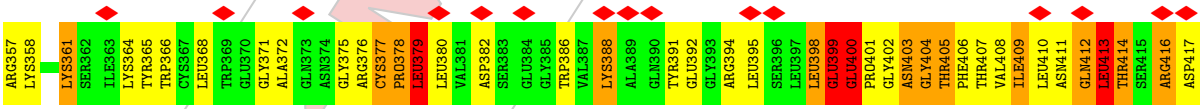


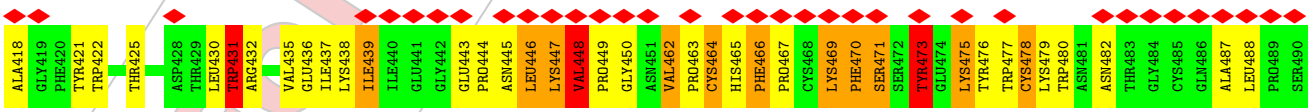


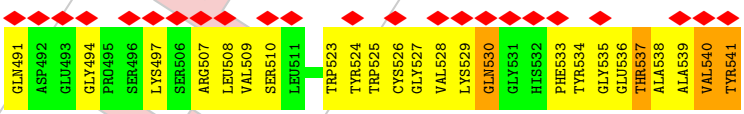
- Molecule 8:

Chain P:



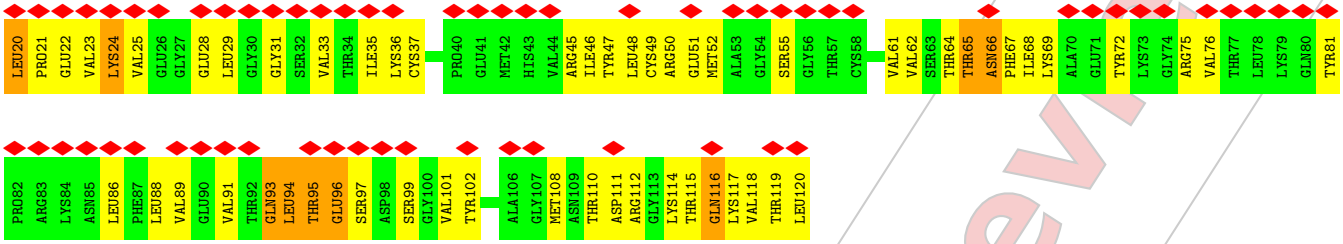






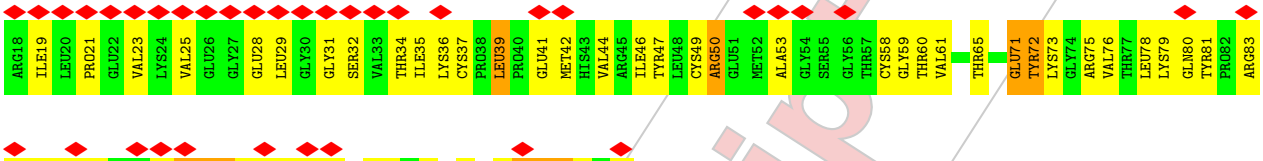
- Molecule 9:

Chain R:



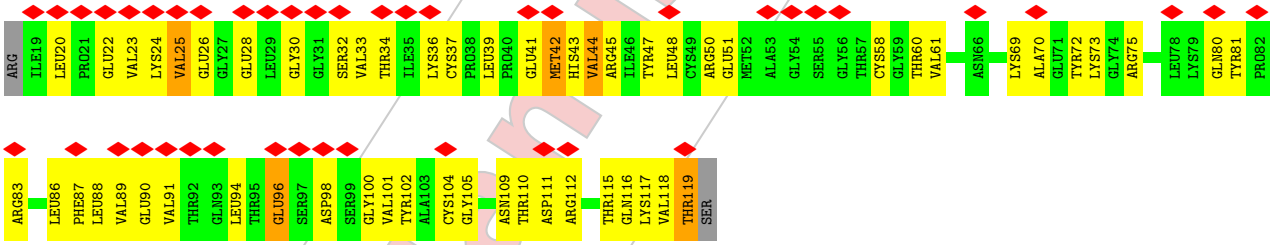
• Molecule 10:

Chain S:



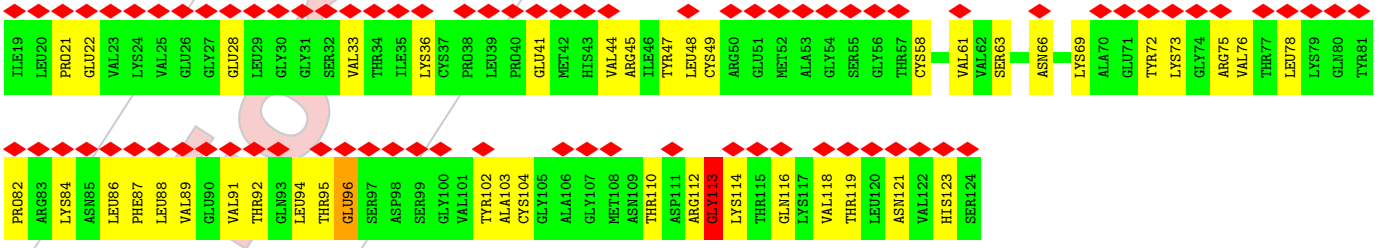
• Molecule 11:

Chain U:



• Molecule 12:

Chain V:



• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	2.308	Depositor
Minimum map value	-1.208	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.32	17/1831 (0.9%)	0.96	8/2508 (0.3%)
2	B	1.23	13/1814 (0.7%)	0.92	6/2485 (0.2%)
3	C	0.94	3/1808 (0.2%)	0.85	8/2476 (0.3%)
4	D	0.63	1/1788 (0.1%)	0.67	1/2449 (0.0%)
4	E	0.78	3/1788 (0.2%)	0.80	5/2449 (0.2%)
4	F	0.78	3/1788 (0.2%)	0.84	5/2449 (0.2%)
4	G	0.88	6/1787 (0.3%)	0.79	4/2447 (0.2%)
4	H	0.94	12/1844 (0.7%)	0.81	7/2526 (0.3%)
5	J	0.78	1/864 (0.1%)	0.82	2/1173 (0.2%)
6	K	1.00	5/1844 (0.3%)	0.89	6/2526 (0.2%)
7	L	0.75	5/1844 (0.3%)	0.84	7/2526 (0.3%)
8	P	0.61	6/3935 (0.2%)	0.77	6/5333 (0.1%)
9	R	0.37	0/776	0.72	1/1046 (0.1%)
10	S	0.42	0/795	0.74	0/1071
11	U	0.41	0/776	0.75	0/1046
12	V	0.31	0/816	0.61	1/1101 (0.1%)
All	All	0.85	75/26098 (0.3%)	0.82	67/35611 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	3
4	E	0	1
4	G	1	0
4	H	0	1
8	P	0	2
All	All	1	7

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	455	TYR	CB-CG	-8.64	1.38	1.51
8	P	404	GLY	C-N	8.12	1.52	1.34
1	A	515	TYR	CE1-CZ	-7.66	1.28	1.38
2	B	534	TYR	CE1-CZ	-7.47	1.28	1.38
7	L	576	TYR	CE2-CZ	-6.95	1.29	1.38
2	B	534	TYR	CB-CG	-6.83	1.41	1.51
2	B	455	TYR	CB-CG	-6.73	1.41	1.51
2	B	500	TYR	CE1-CZ	-6.69	1.29	1.38
4	E	534	TYR	CB-CG	-6.63	1.41	1.51
1	A	500	TYR	CE1-CZ	-6.57	1.30	1.38
1	A	515	TYR	CG-CD1	-6.53	1.30	1.39
4	H	488	TRP	CD2-CE2	-6.51	1.33	1.41
1	A	479	PHE	CG-CD2	-6.43	1.29	1.38
5	J	62	TYR	CE1-CZ	-6.22	1.30	1.38
8	P	60	TYR	CB-CG	-6.19	1.42	1.51
1	A	500	TYR	CG-CD2	-6.19	1.31	1.39
2	B	479	PHE	CG-CD1	-6.17	1.29	1.38
4	H	562	TYR	CB-CG	-6.15	1.42	1.51
4	H	562	TYR	CE1-CZ	-6.00	1.30	1.38
4	G	515	TYR	CB-CG	-5.87	1.42	1.51
4	H	517	ALA	C-O	-5.84	1.12	1.23
8	P	60	TYR	CE1-CZ	-5.83	1.30	1.38
8	P	60	TYR	CG-CD2	-5.82	1.31	1.39
2	B	525	GLU	CD-OE2	-5.79	1.19	1.25
4	H	562	TYR	CG-CD2	-5.76	1.31	1.39
4	E	515	TYR	CB-CG	-5.76	1.43	1.51
1	A	479	PHE	CG-CD1	-5.74	1.30	1.38
4	H	488	TRP	CZ3-CH2	-5.70	1.30	1.40
2	B	455	TYR	C-O	-5.62	1.12	1.23
2	B	455	TYR	CE1-CZ	-5.59	1.31	1.38
2	B	500	TYR	CG-CD1	-5.59	1.31	1.39
2	B	534	TYR	CG-CD1	-5.58	1.31	1.39
4	H	536	CYS	C-O	-5.58	1.12	1.23
6	K	562	TYR	CB-CG	-5.56	1.43	1.51
2	B	528	TRP	CE3-CZ3	-5.56	1.28	1.38
1	A	515	TYR	CB-CG	-5.50	1.43	1.51
4	G	475	LEU	C-O	-5.50	1.12	1.23
3	C	455	TYR	CE1-CZ	-5.47	1.31	1.38
1	A	516	PHE	C-O	-5.43	1.13	1.23
1	A	500	TYR	CE2-CZ	-5.43	1.31	1.38
4	F	479	PHE	CG-CD1	-5.43	1.30	1.38
7	L	576	TYR	CG-CD2	-5.42	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	500	TYR	CB-CG	-5.42	1.43	1.51
4	G	515	TYR	CG-CD2	-5.42	1.32	1.39
4	H	537	VAL	C-O	-5.42	1.13	1.23
4	H	488	TRP	CE3-CZ3	-5.41	1.29	1.38
4	G	562	TYR	C-O	-5.39	1.13	1.23
4	G	534	TYR	CB-CG	-5.31	1.43	1.51
1	A	516	PHE	CG-CD2	-5.30	1.30	1.38
1	A	479	PHE	CB-CG	-5.30	1.42	1.51
6	K	475	LEU	C-O	-5.27	1.13	1.23
7	L	576	TYR	CB-CG	-5.27	1.43	1.51
1	A	479	PHE	C-O	-5.26	1.13	1.23
4	F	500	TYR	CE1-CZ	-5.23	1.31	1.38
8	P	60	TYR	CE2-CZ	-5.15	1.31	1.38
4	G	474	CYS	C-O	-5.14	1.13	1.23
6	K	562	TYR	CE1-CZ	-5.14	1.31	1.38
4	H	487	GLN	C-O	-5.14	1.13	1.23
7	L	565	SER	C-O	-5.14	1.13	1.23
4	D	534	TYR	CB-CG	-5.13	1.44	1.51
4	E	515	TYR	CG-CD1	-5.11	1.32	1.39
2	B	528	TRP	CB-CG	-5.09	1.41	1.50
4	F	548	THR	C-O	-5.09	1.13	1.23
4	H	562	TYR	C-O	-5.07	1.13	1.23
6	K	565	SER	C-O	-5.06	1.13	1.23
1	A	528	TRP	CB-CG	-5.06	1.41	1.50
1	A	500	TYR	CG-CD1	-5.05	1.32	1.39
2	B	544	PRO	CA-C	-5.04	1.42	1.52
1	A	515	TYR	CE2-CZ	-5.04	1.32	1.38
6	K	528	TRP	CE3-CZ3	-5.03	1.29	1.38
8	P	431	TRP	CB-CG	-5.03	1.41	1.50
3	C	455	TYR	CG-CD2	-5.02	1.32	1.39
4	H	519	SER	CA-CB	-5.01	1.45	1.52
1	A	546	ARG	C-O	-5.01	1.13	1.23
7	L	576	TYR	CE1-CZ	-5.00	1.32	1.38

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	480	SER	C-N-CD	-11.81	94.61	120.60
8	P	404	GLY	C-N-CA	11.12	149.50	121.70
7	L	551	THR	N-CA-C	9.32	136.17	111.00
7	L	552	VAL	CB-CA-C	-8.80	94.68	111.40
4	H	443	ARG	N-CA-CB	8.33	125.60	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	404	GLY	CA-C-O	-7.98	106.23	120.60
4	G	478	GLY	N-CA-C	7.92	132.90	113.10
4	F	443	ARG	C-N-CD	-7.81	103.41	120.60
2	B	495	LEU	CB-CG-CD2	-7.60	98.08	111.00
4	E	533	THR	N-CA-C	7.33	130.80	111.00
3	C	564	VAL	CB-CA-C	-7.28	97.57	111.40
9	R	66	ASN	N-CA-C	6.95	129.76	111.00
5	J	118	GLY	N-CA-C	-6.87	95.91	113.10
3	C	457	LEU	CB-CG-CD1	-6.83	99.39	111.00
1	A	480	SER	C-N-CA	6.78	150.47	122.00
6	K	449	LEU	N-CA-C	6.74	129.21	111.00
4	G	564	VAL	CB-CA-C	-6.62	98.81	111.40
6	K	566	LEU	CB-CG-CD2	-6.35	100.20	111.00
4	E	493	GLN	C-N-CD	-6.32	106.69	120.60
7	L	564	VAL	CB-CA-C	-6.31	99.42	111.40
4	G	518	HIS	CB-CA-C	-6.18	98.04	110.40
6	K	564	VAL	CB-CA-C	-6.18	99.66	111.40
2	B	443	ARG	N-CA-C	-6.18	94.33	111.00
3	C	480	SER	C-N-CD	-6.16	107.05	120.60
4	H	520	ILE	CG1-CB-CG2	-6.09	98.00	111.40
3	C	456	LEU	CB-CG-CD1	-6.06	100.70	111.00
4	H	441	ILE	CA-C-N	-6.05	103.90	117.20
4	G	516	PHE	CB-CG-CD2	6.03	125.02	120.80
4	D	538	VAL	CB-CA-C	-6.00	100.00	111.40
7	L	575	CYS	CA-CB-SG	-5.97	103.25	114.00
1	A	447	VAL	CB-CA-C	-5.89	100.20	111.40
2	B	489	MET	CB-CA-C	-5.88	98.64	110.40
4	F	448	ALA	N-CA-C	5.84	126.76	111.00
2	B	456	LEU	CB-CG-CD1	-5.83	101.10	111.00
6	K	477	THR	N-CA-C	5.79	126.63	111.00
1	A	554	LYS	N-CA-C	5.68	126.34	111.00
4	H	564	VAL	CB-CA-C	-5.62	100.72	111.40
4	F	520	ILE	CB-CA-C	-5.56	100.47	111.60
4	H	563	ASN	CB-CA-C	5.54	121.48	110.40
2	B	496	SER	C-N-CD	-5.54	108.42	120.60
7	L	566	LEU	CB-CG-CD1	-5.54	101.59	111.00
7	L	572	ALA	N-CA-C	-5.53	96.06	111.00
3	C	482	ALA	N-CA-C	5.51	125.87	111.00
1	A	489	MET	CB-CG-SD	-5.50	95.89	112.40
4	H	441	ILE	C-N-CA	5.49	135.43	121.70
2	B	456	LEU	CA-CB-CG	5.47	127.89	115.30
4	E	534	TYR	N-CA-C	5.43	125.65	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	34	GLU	CB-CA-C	-5.41	99.57	110.40
7	L	552	VAL	N-CA-C	5.39	125.56	111.00
3	C	531	GLY	N-CA-C	5.38	126.54	113.10
4	E	531	GLY	N-CA-C	-5.35	99.73	113.10
4	H	520	ILE	CB-CA-C	-5.32	100.95	111.60
8	P	288	GLY	N-CA-C	-5.30	99.86	113.10
8	P	60	TYR	N-CA-CB	5.28	120.10	110.60
4	E	546	ARG	N-CA-C	5.27	125.23	111.00
1	A	514	ARG	CB-CA-C	-5.26	99.88	110.40
12	V	113	GLY	N-CA-C	5.24	126.19	113.10
6	K	536	CYS	N-CA-CB	-5.23	101.18	110.60
1	A	486	VAL	CB-CA-C	-5.20	101.52	111.40
6	K	521	LEU	CB-CG-CD2	5.18	119.80	111.00
3	C	525	GLU	N-CA-C	5.16	124.93	111.00
8	P	310	HIS	N-CA-C	-5.10	97.22	111.00
3	C	566	LEU	CB-CA-C	-5.06	100.59	110.20
8	P	448	VAL	N-CA-C	5.03	124.57	111.00
4	F	449	LEU	N-CA-C	5.01	124.53	111.00
4	F	547	VAL	CG1-CB-CG2	-5.01	102.89	110.90
1	A	449	LEU	CB-CG-CD2	-5.00	102.50	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	583	NAG	C1

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	452	PRO	Mainchain
3	C	464	LEU	Mainchain
3	C	480	SER	Peptide
4	E	480	SER	Peptide
4	H	441	ILE	Mainchain
8	P	376	ARG	Mainchain
8	P	400	GLU	Peptide

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	1800	0	1754	175	0
2	B	1783	0	1738	186	0
3	C	1777	0	1737	136	0
4	D	1757	0	1721	93	0
4	E	1757	0	1723	139	0
4	F	1757	0	1715	149	0
4	G	1756	0	1721	99	0
4	H	1812	0	1764	110	0
5	J	851	0	842	81	0
6	K	1812	0	1766	197	0
7	L	1812	0	1764	271	0
8	P	3851	0	3755	526	0
9	R	766	0	784	91	0
10	S	785	0	808	90	0
11	U	766	0	784	60	0
12	V	805	0	821	49	0
13	I	28	0	25	6	0
All	All	25675	0	25222	2274	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 45.

All (2274) 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)
4:F:482:ALA:HB2	4:F:515:TYR:CD2	1.29	1.63
9:R:20:LEU:HD21	9:R:117:LYS:CG	1.17	1.62
1:A:359:LEU:HD12	5:J:117:TYR:CD2	1.09	1.58
9:R:20:LEU:CD2	9:R:117:LYS:HG3	1.16	1.57
2:B:421:GLY:CA	2:B:445:LYS:CE	1.81	1.56
8:P:395:LEU:CD1	8:P:410:LEU:HD13	1.29	1.56
7:L:540:HIS:CB	7:L:543:LEU:HD21	1.18	1.56
8:P:395:LEU:HD13	8:P:410:LEU:CD1	1.36	1.55
8:P:131:THR:CG2	8:P:188:VAL:HG22	1.23	1.54
7:L:450:HIS:H	7:L:480:SER:CB	1.19	1.54
1:A:359:LEU:CD1	5:J:117:TYR:HD2	1.14	1.53
8:P:131:THR:HG21	8:P:188:VAL:CG2	1.34	1.53
8:P:466:PHE:CE2	8:P:507:ARG:HG3	1.39	1.51
7:L:540:HIS:CA	7:L:543:LEU:CD2	1.86	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:482:ALA:CB	4:F:515:TYR:CD2	1.92	1.51
3:C:563:ASN:ND2	3:C:583:NAG:C1	1.70	1.50
10:S:39:LEU:HD13	10:S:87:PHE:CD1	1.46	1.49
2:B:421:GLY:HA2	2:B:445:LYS:CE	1.39	1.45
8:P:278:ARG:O	8:P:422:TRP:CZ2	1.66	1.45
4:F:535:THR:HG22	4:F:551:THR:CG2	1.43	1.45
8:P:448:VAL:HB	8:P:449:PRO:CD	1.14	1.45
8:P:477:TRP:CH2	8:P:524:TYR:CD1	2.02	1.45
10:S:31:GLY:C	10:S:94:LEU:HD23	1.09	1.45
7:L:540:HIS:CB	7:L:543:LEU:CD2	1.95	1.45
7:L:540:HIS:HB3	7:L:543:LEU:CD2	1.46	1.43
8:P:446:LEU:CA	8:P:465:HIS:O	1.66	1.43
6:K:450:HIS:CD2	6:K:514:ARG:HH12	1.36	1.43
6:K:464:LEU:CD1	6:K:525:GLU:OE2	1.64	1.43
7:L:511:ALA:HB3	7:L:514:ARG:CD	1.51	1.41
7:L:540:HIS:N	7:L:543:LEU:HD23	1.35	1.40
8:P:345:ALA:C	8:P:413:LEU:HD12	1.34	1.40
4:H:554:LYS:HZ3	4:H:558:LYS:NZ	1.03	1.38
4:E:489:MET:SD	4:E:494:PRO:HD3	1.65	1.37
4:H:554:LYS:NZ	4:H:558:LYS:NZ	1.71	1.37
7:L:424:PHE:N	7:L:441:ILE:HD11	1.36	1.36
8:P:477:TRP:HH2	8:P:524:TYR:CD1	1.36	1.36
7:L:424:PHE:CB	7:L:441:ILE:HD11	1.54	1.35
2:B:421:GLY:CA	2:B:445:LYS:HE3	0.88	1.35
4:F:560:THR:O	4:G:560:THR:HG22	1.25	1.35
8:P:131:THR:CG2	8:P:188:VAL:CG2	1.97	1.35
4:E:450:HIS:CG	4:E:514:ARG:NH2	1.95	1.34
8:P:340:VAL:CG1	8:P:436:GLU:HB3	1.54	1.34
10:S:39:LEU:CD1	10:S:87:PHE:CE1	2.08	1.34
8:P:346:GLY:N	8:P:413:LEU:CG	1.88	1.34
7:L:421:GLY:O	7:L:443:ARG:NH1	1.59	1.33
10:S:31:GLY:C	10:S:94:LEU:CD2	1.95	1.32
1:A:356:SER:CA	5:J:117:TYR:OH	1.77	1.32
4:F:482:ALA:CB	4:F:515:TYR:HD2	1.29	1.32
8:P:446:LEU:HD21	8:P:537:THR:O	1.17	1.32
8:P:368:LEU:N	8:P:378:PRO:HD2	1.46	1.31
7:L:424:PHE:CB	7:L:441:ILE:CD1	2.09	1.30
7:L:450:HIS:N	7:L:480:SER:CB	1.94	1.30
7:L:424:PHE:HB2	7:L:441:ILE:CD1	1.61	1.30
7:L:511:ALA:HB3	7:L:514:ARG:CG	1.60	1.30
8:P:448:VAL:CB	8:P:449:PRO:CD	2.01	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:450:HIS:ND1	4:E:514:ARG:NH2	1.75	1.30
8:P:446:LEU:CD2	8:P:537:THR:O	1.79	1.30
8:P:466:PHE:HE2	8:P:507:ARG:CG	1.46	1.29
10:S:31:GLY:O	10:S:94:LEU:HD23	1.25	1.29
7:L:424:PHE:CA	7:L:441:ILE:HD11	1.62	1.29
8:P:251:PHE:CE1	8:P:308:GLY:O	1.86	1.28
3:C:508:GLU:HG2	3:C:509:PRO:CD	1.61	1.28
8:P:477:TRP:CZ2	8:P:524:TYR:HB3	1.67	1.27
4:D:421:GLY:HA2	4:D:445:LYS:CE	1.66	1.26
7:L:424:PHE:N	7:L:441:ILE:CD1	1.99	1.26
8:P:261:CYS:CB	8:P:315:LEU:HD23	1.66	1.25
10:S:29:LEU:CD2	10:S:95:THR:HG23	1.66	1.24
7:L:540:HIS:C	7:L:543:LEU:CD2	2.05	1.24
2:B:382:TRP:CH2	2:B:441:ILE:HD11	1.72	1.23
8:P:447:LYS:HG2	8:P:465:HIS:CB	1.68	1.23
2:B:421:GLY:HA3	2:B:445:LYS:CD	1.68	1.22
4:G:523:VAL:HG21	4:G:534:TYR:OH	1.32	1.22
7:L:450:HIS:HB2	7:L:480:SER:OG	1.07	1.22
7:L:450:HIS:CB	7:L:480:SER:OG	1.87	1.22
7:L:479:PHE:CB	7:L:515:TYR:O	1.87	1.22
8:P:278:ARG:O	8:P:422:TRP:HZ2	0.94	1.22
4:F:535:THR:CG2	4:F:551:THR:HG22	1.69	1.22
7:L:456:LEU:HD23	7:L:552:VAL:CG2	1.68	1.22
10:S:39:LEU:CD1	10:S:87:PHE:CD1	2.22	1.21
1:A:356:SER:CB	5:J:117:TYR:OH	1.87	1.21
6:K:509:PRO:CG	7:L:501:VAL:HG21	1.69	1.21
7:L:479:PHE:HB2	7:L:515:TYR:O	1.05	1.20
10:S:37:CYS:CB	10:S:116:GLN:OE1	1.88	1.20
8:P:448:VAL:CB	8:P:449:PRO:HD2	1.64	1.20
4:D:490:GLN:OE1	4:D:532:GLU:HB3	1.41	1.20
7:L:540:HIS:N	7:L:543:LEU:CD2	1.94	1.20
3:C:461:ARG:NH1	3:C:465:ASN:HD21	1.40	1.19
5:J:21:ILE:CD1	7:L:555:SER:HB3	1.71	1.19
6:K:463:GLN:HB2	7:L:455:TYR:CZ	1.77	1.18
8:P:466:PHE:CE2	8:P:507:ARG:CG	2.24	1.17
6:K:354:PHE:HE1	6:K:541:GLU:N	1.42	1.16
8:P:261:CYS:SG	8:P:315:LEU:HD23	0.64	1.16
8:P:421:TYR:CE1	8:P:437:ILE:HD12	1.79	1.16
10:S:37:CYS:HA	10:S:116:GLN:OE1	1.45	1.16
8:P:368:LEU:H	8:P:378:PRO:CD	1.59	1.16
8:P:345:ALA:C	8:P:413:LEU:CD1	2.13	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:493:GLN:HB2	4:E:494:PRO:HD2	1.20	1.15
7:L:540:HIS:CA	7:L:543:LEU:HD21	1.59	1.15
7:L:511:ALA:HB3	7:L:514:ARG:HD2	1.26	1.15
7:L:540:HIS:C	7:L:543:LEU:HD22	1.63	1.15
6:K:511:ALA:HB1	6:K:512:PRO:CD	1.72	1.15
8:P:261:CYS:SG	8:P:315:LEU:CG	2.35	1.14
4:F:482:ALA:CB	4:F:515:TYR:CE2	2.30	1.13
7:L:424:PHE:H	7:L:441:ILE:CD1	1.58	1.13
4:E:543:LEU:HD23	4:E:544:PRO:HD3	1.30	1.13
6:K:509:PRO:HG3	7:L:501:VAL:HG21	1.17	1.13
8:P:450:GLY:HA3	8:P:540:VAL:HG12	1.29	1.13
2:B:480:SER:OG	2:B:481:PRO:HD3	1.47	1.12
1:A:514:ARG:HB3	1:A:514:ARG:HH11	1.11	1.12
2:B:418:TRP:CE3	2:B:443:ARG:HD2	1.79	1.12
10:S:37:CYS:CA	10:S:116:GLN:OE1	1.97	1.12
8:P:345:ALA:HA	8:P:413:LEU:HB2	1.17	1.11
8:P:261:CYS:SG	8:P:315:LEU:CD2	1.19	1.11
3:C:508:GLU:HG2	3:C:509:PRO:HD3	1.33	1.10
8:P:250:LYS:HG2	8:P:309:ALA:HB2	1.33	1.10
8:P:346:GLY:N	8:P:413:LEU:CB	2.14	1.10
9:R:75:ARG:NH2	9:R:95:THR:OG1	1.84	1.10
4:F:524:SER:HG	4:F:527:GLU:HB2	1.16	1.10
6:K:464:LEU:HD12	6:K:525:GLU:OE2	1.44	1.10
11:U:22:GLU:HB2	11:U:119:THR:O	1.51	1.10
1:A:478:GLY:O	1:A:514:ARG:NH1	1.83	1.10
7:L:540:HIS:H	7:L:543:LEU:CD2	1.57	1.10
8:P:411:ASN:HB3	8:P:537:THR:OG1	1.47	1.10
8:P:445:ASN:O	8:P:466:PHE:HA	1.51	1.10
9:R:116:GLN:HE22	9:R:118:VAL:CG2	1.64	1.10
8:P:475:LYS:HB2	8:P:507:ARG:HD2	1.20	1.09
1:A:493:GLN:HB2	1:A:494:PRO:HD2	1.25	1.09
2:B:461:ARG:HH21	7:L:570:ASP:CG	1.54	1.09
6:K:464:LEU:HD11	6:K:525:GLU:OE2	1.47	1.09
1:A:356:SER:HB2	5:J:117:TYR:OH	1.44	1.09
2:B:421:GLY:HA3	2:B:445:LYS:CE	1.55	1.09
3:C:508:GLU:HG2	3:C:509:PRO:HD2	1.27	1.09
6:K:563:ASN:HD21	6:K:583:NAG:C1	1.63	1.09
9:R:61:VAL:HG21	9:R:72:TYR:CD2	1.87	1.08
2:B:480:SER:HG	2:B:481:PRO:HD3	1.00	1.08
7:L:540:HIS:O	7:L:543:LEU:CD2	2.01	1.08
8:P:448:VAL:CG2	8:P:449:PRO:HD2	1.82	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:447:LYS:HG2	8:P:465:HIS:HB3	1.30	1.08
6:K:450:HIS:CD2	6:K:514:ARG:NH1	2.20	1.07
8:P:131:THR:HG23	8:P:188:VAL:HA	1.32	1.07
9:R:61:VAL:HG21	9:R:72:TYR:HD2	1.11	1.07
4:D:421:GLY:CA	4:D:445:LYS:CE	2.33	1.07
8:P:251:PHE:CD1	8:P:308:GLY:O	2.07	1.07
10:S:39:LEU:HD13	10:S:87:PHE:CE1	1.82	1.07
7:L:450:HIS:N	7:L:480:SER:HB2	1.58	1.07
4:F:482:ALA:HB2	4:F:515:TYR:CE2	1.88	1.07
9:R:22:GLU:HA	9:R:117:LYS:O	1.54	1.07
1:A:356:SER:HA	5:J:117:TYR:OH	1.55	1.07
4:E:421:GLY:HA3	4:E:445:LYS:HE3	1.36	1.07
4:F:482:ALA:HB1	4:F:515:TYR:HD2	1.16	1.06
7:L:511:ALA:CB	7:L:514:ARG:CD	2.31	1.06
4:D:420:SER:C	4:D:445:LYS:HZ2	1.56	1.06
6:K:527:GLU:HA	6:K:530:THR:OG1	1.55	1.06
7:L:450:HIS:N	7:L:480:SER:OG	1.85	1.06
7:L:424:PHE:H	7:L:441:ILE:CG1	1.69	1.06
9:R:50:ARG:HD2	9:R:72:TYR:OH	1.56	1.06
6:K:354:PHE:CE1	6:K:541:GLU:N	2.24	1.06
8:P:340:VAL:CG1	8:P:436:GLU:CB	2.34	1.06
4:E:454:VAL:HG21	4:E:538:VAL:HG21	1.37	1.05
4:E:450:HIS:CG	4:E:514:ARG:HH22	1.68	1.05
4:E:508:GLU:OE1	4:E:509:PRO:HD2	1.55	1.05
6:K:454:VAL:CG2	6:K:538:VAL:HG21	1.85	1.05
7:L:511:ALA:CB	7:L:514:ARG:HD2	1.86	1.05
8:P:243:PRO:O	8:P:246:ALA:CB	2.04	1.05
8:P:261:CYS:SG	8:P:315:LEU:HD21	1.91	1.05
4:F:450:HIS:HD2	4:F:514:ARG:CZ	1.68	1.05
2:B:421:GLY:HA3	2:B:445:LYS:HD3	1.36	1.04
7:L:443:ARG:N	7:L:444:PRO:HD3	1.67	1.04
8:P:477:TRP:CZ2	8:P:524:TYR:CB	2.40	1.04
3:C:508:GLU:CG	3:C:509:PRO:HD3	1.87	1.04
7:L:456:LEU:CD2	7:L:552:VAL:CG2	2.34	1.04
4:E:450:HIS:CE1	4:E:514:ARG:HH12	1.75	1.04
8:P:448:VAL:HB	8:P:449:PRO:HD2	1.07	1.04
8:P:345:ALA:CA	8:P:413:LEU:HB2	1.87	1.03
5:J:21:ILE:HD11	7:L:555:SER:HB3	1.08	1.03
8:P:395:LEU:HB2	8:P:410:LEU:HD11	1.40	1.03
8:P:346:GLY:H	8:P:413:LEU:CB	1.69	1.03
9:R:22:GLU:OE1	9:R:101:VAL:HG13	1.57	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:46:ILE:H	9:R:64:THR:CG2	1.72	1.03
2:B:478:GLY:O	2:B:514:ARG:HG3	1.59	1.02
6:K:509:PRO:CG	7:L:501:VAL:CG2	2.35	1.02
7:L:456:LEU:CD2	7:L:552:VAL:HG22	1.89	1.02
4:E:489:MET:SD	4:E:494:PRO:CD	2.47	1.02
4:E:543:LEU:HD23	4:E:544:PRO:CD	1.89	1.02
3:C:566:LEU:H	3:C:566:LEU:HD12	1.23	1.02
8:P:368:LEU:H	8:P:378:PRO:HD2	0.89	1.02
8:P:368:LEU:HB2	8:P:378:PRO:CG	1.90	1.02
9:R:116:GLN:NE2	9:R:118:VAL:HG23	1.74	1.02
3:C:451:ARG:HB3	3:C:451:ARG:HH11	1.20	1.02
4:G:501:VAL:HG21	4:H:509:PRO:HD3	1.42	1.01
5:J:27:ASP:HB2	5:J:28:PRO:CD	1.90	1.01
8:P:418:ALA:HB2	8:P:439:ILE:HD13	1.43	1.01
8:P:462:VAL:HG12	8:P:540:VAL:HG11	1.36	1.01
4:F:524:SER:OG	4:F:527:GLU:HB2	1.61	1.01
8:P:340:VAL:HG12	8:P:436:GLU:O	1.60	1.01
2:B:382:TRP:HH2	2:B:441:ILE:HD11	1.08	1.01
6:K:354:PHE:HZ	6:K:546:ARG:HD3	1.26	1.01
7:L:421:GLY:O	7:L:443:ARG:CZ	2.06	1.01
10:S:29:LEU:HD23	10:S:95:THR:HG23	1.42	1.01
3:C:461:ARG:NH1	3:C:465:ASN:ND2	2.08	1.01
5:J:115:LEU:HD12	5:J:124:VAL:HG21	1.38	1.01
6:K:509:PRO:HG2	7:L:501:VAL:CG2	1.90	1.01
8:P:446:LEU:CD2	8:P:538:ALA:HB2	1.89	1.01
4:E:450:HIS:CD2	4:E:514:ARG:NH1	2.29	1.00
4:F:450:HIS:CD2	4:F:514:ARG:CZ	2.42	1.00
6:K:484:VAL:HG23	6:K:540:HIS:HB2	1.43	1.00
6:K:511:ALA:HB1	6:K:512:PRO:HD3	1.01	1.00
9:R:20:LEU:CD2	9:R:117:LYS:CG	1.96	1.00
2:B:418:TRP:CE3	2:B:443:ARG:CD	2.44	1.00
8:P:447:LYS:H	8:P:465:HIS:H	1.03	1.00
7:L:424:PHE:CG	7:L:441:ILE:HD11	1.96	1.00
1:A:456:LEU:HD11	1:A:550:ARG:O	1.59	1.00
8:P:414:THR:OG1	8:P:417:ASP:OD2	1.80	1.00
8:P:447:LYS:HG2	8:P:465:HIS:HB2	1.42	1.00
3:C:457:LEU:HD12	3:C:473:THR:OG1	1.62	1.00
8:P:391:TYR:OH	8:P:416:ARG:NH1	1.95	0.99
8:P:450:GLY:CA	8:P:540:VAL:HG12	1.92	0.99
8:P:131:THR:CG2	8:P:188:VAL:HA	1.92	0.99
2:B:451:ARG:HG2	2:B:542:ALA:O	1.60	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:527:GLU:O	6:K:530:THR:OG1	1.80	0.99
4:D:421:GLY:HA2	4:D:445:LYS:HE2	1.42	0.99
4:E:421:GLY:HA3	4:E:445:LYS:CE	1.91	0.99
4:E:493:GLN:CB	4:E:494:PRO:HD2	1.77	0.99
7:L:424:PHE:CG	7:L:441:ILE:CD1	2.46	0.99
4:D:421:GLY:CA	4:D:445:LYS:NZ	2.26	0.99
7:L:456:LEU:HD23	7:L:552:VAL:HG22	1.01	0.99
4:E:450:HIS:CG	4:E:514:ARG:CZ	2.46	0.98
8:P:131:THR:HG23	8:P:188:VAL:HG22	1.42	0.98
10:S:29:LEU:HD22	10:S:95:THR:HG23	1.43	0.98
3:C:508:GLU:CG	3:C:509:PRO:CD	2.40	0.98
4:E:508:GLU:OE1	4:E:509:PRO:CD	2.11	0.98
6:K:511:ALA:CB	6:K:512:PRO:HD3	1.89	0.98
8:P:447:LYS:CG	8:P:465:HIS:HB3	1.92	0.98
3:C:482:ALA:HB2	3:C:515:TYR:CD1	1.97	0.98
2:B:450:HIS:O	2:B:542:ALA:CB	2.12	0.98
4:D:421:GLY:N	4:D:445:LYS:NZ	2.12	0.98
1:A:502:THR:HB	1:A:519:SER:HB2	1.46	0.97
9:R:116:GLN:HE22	9:R:118:VAL:HG23	1.23	0.97
4:H:526:GLU:O	4:H:530:THR:HG23	1.64	0.97
8:P:368:LEU:HB2	8:P:378:PRO:CD	1.94	0.97
8:P:447:LYS:H	8:P:465:HIS:N	1.62	0.97
1:A:355:ALA:O	5:J:117:TYR:HE2	1.48	0.97
6:K:527:GLU:CA	6:K:530:THR:OG1	2.12	0.97
5:J:21:ILE:HD11	7:L:555:SER:CB	1.93	0.97
10:S:31:GLY:HA3	10:S:94:LEU:HD21	1.47	0.97
6:K:450:HIS:CG	6:K:514:ARG:HH12	1.82	0.96
8:P:340:VAL:HG13	8:P:436:GLU:CB	1.92	0.96
8:P:243:PRO:O	8:P:246:ALA:HB3	1.63	0.96
2:B:421:GLY:HA3	2:B:445:LYS:HE3	1.09	0.96
11:U:50:ARG:NH1	11:U:100:GLY:HA3	1.79	0.96
8:P:395:LEU:CD1	8:P:410:LEU:CD1	2.13	0.96
4:E:450:HIS:CE1	4:E:514:ARG:HH22	1.83	0.96
8:P:345:ALA:O	8:P:413:LEU:HD12	1.65	0.95
8:P:477:TRP:CH2	8:P:524:TYR:HD1	1.62	0.95
8:P:342:LYS:HB3	8:P:438:LYS:HB3	1.45	0.95
8:P:445:ASN:O	8:P:467:PRO:HD3	1.66	0.95
9:R:61:VAL:CG2	9:R:72:TYR:HD2	1.77	0.95
4:E:454:VAL:CG2	4:E:538:VAL:HG21	1.96	0.95
4:E:450:HIS:NE2	4:E:514:ARG:NH1	2.13	0.95
2:B:418:TRP:HZ2	2:B:444:PRO:CD	1.78	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:22:GLU:CG	11:U:119:THR:HG23	1.96	0.95
6:K:510:GLN:CG	7:L:522:THR:HG21	1.97	0.95
7:L:543:LEU:HB2	7:L:546:ARG:HA	1.46	0.95
8:P:477:TRP:CZ2	8:P:524:TYR:CG	2.54	0.95
8:P:477:TRP:CZ2	8:P:524:TYR:CD1	2.54	0.94
2:B:418:TRP:CZ2	2:B:444:PRO:CD	2.47	0.94
6:K:527:GLU:C	6:K:530:THR:HG1	1.70	0.94
7:L:487:GLN:O	7:L:537:VAL:HG12	1.66	0.94
7:L:540:HIS:O	7:L:543:LEU:HD23	1.67	0.94
10:S:29:LEU:CD2	10:S:95:THR:CG2	2.44	0.94
4:F:450:HIS:HD2	4:F:514:ARG:NH2	1.64	0.94
7:L:424:PHE:HB2	7:L:441:ILE:HD13	1.46	0.94
8:P:366:TRP:CE2	8:P:408:VAL:HG21	2.03	0.94
8:P:450:GLY:HA3	8:P:540:VAL:CG1	1.97	0.94
8:P:340:VAL:HG13	8:P:436:GLU:HB3	0.96	0.94
7:L:443:ARG:H	7:L:444:PRO:HD3	1.34	0.93
3:C:526:GLU:O	3:C:530:THR:HG23	1.67	0.93
6:K:563:ASN:ND2	6:K:583:NAG:C1	2.31	0.93
6:K:454:VAL:HG21	6:K:538:VAL:HG21	1.47	0.93
3:C:457:LEU:CD1	3:C:473:THR:OG1	2.17	0.93
4:E:450:HIS:HD1	4:E:514:ARG:HH22	1.11	0.93
8:P:446:LEU:HA	8:P:465:HIS:O	0.75	0.93
8:P:477:TRP:HZ2	8:P:524:TYR:CB	1.81	0.93
3:C:461:ARG:HH12	3:C:465:ASN:ND2	1.63	0.93
8:P:446:LEU:HA	8:P:465:HIS:C	1.88	0.93
10:S:31:GLY:CA	10:S:94:LEU:CD2	2.47	0.92
8:P:278:ARG:O	8:P:422:TRP:CH2	2.21	0.92
8:P:446:LEU:H	8:P:446:LEU:HD12	1.33	0.92
2:B:450:HIS:O	2:B:542:ALA:HB3	1.68	0.92
9:R:111:ASP:O	9:R:114:LYS:CE	2.18	0.92
10:S:39:LEU:CD1	10:S:87:PHE:HE1	1.77	0.92
1:A:359:LEU:CD1	5:J:117:TYR:CD2	2.04	0.92
4:H:554:LYS:NZ	4:H:558:LYS:HZ2	1.50	0.92
6:K:516:PHE:CE2	7:L:520:ILE:HD13	2.04	0.92
7:L:424:PHE:H	7:L:441:ILE:HG13	1.32	0.92
9:R:116:GLN:NE2	9:R:118:VAL:CG2	2.32	0.92
1:A:359:LEU:HD13	5:J:117:TYR:HB3	1.50	0.92
8:P:448:VAL:HB	8:P:449:PRO:HD3	0.92	0.91
8:P:479:LYS:HG2	8:P:524:TYR:CE1	2.05	0.91
7:L:479:PHE:CZ	7:L:484:VAL:HG11	2.05	0.91
7:L:540:HIS:O	7:L:543:LEU:HD22	1.65	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:39:LEU:HD12	10:S:87:PHE:CE1	2.04	0.91
6:K:510:GLN:HG2	7:L:522:THR:HG21	1.52	0.91
4:F:365:LEU:O	4:F:410:GLU:HA	1.68	0.91
8:P:131:THR:HG23	8:P:188:VAL:CA	1.99	0.91
8:P:529:LYS:CE	8:P:534:TYR:HE2	1.82	0.91
8:P:411:ASN:ND2	8:P:525:TRP:CZ2	2.39	0.91
4:F:502:THR:OG1	4:F:519:SER:CB	2.18	0.91
5:J:28:PRO:HG3	7:L:467:ARG:CZ	1.99	0.91
4:E:482:ALA:CB	4:E:515:TYR:HE2	1.83	0.90
10:S:31:GLY:CA	10:S:94:LEU:HD23	2.01	0.90
6:K:445:LYS:HA	6:K:445:LYS:CE	2.02	0.90
8:P:475:LYS:CB	8:P:507:ARG:HD2	2.00	0.90
9:R:46:ILE:H	9:R:64:THR:HG23	1.35	0.90
6:K:450:HIS:CG	6:K:514:ARG:NH1	2.38	0.90
7:L:450:HIS:H	7:L:480:SER:HB2	0.76	0.90
2:B:461:ARG:NH2	7:L:570:ASP:OD2	2.05	0.90
8:P:346:GLY:N	8:P:413:LEU:HB2	1.86	0.90
4:D:420:SER:C	4:D:445:LYS:NZ	2.26	0.90
4:G:450:HIS:HD2	4:G:514:ARG:NH2	1.68	0.90
7:L:424:PHE:HB2	7:L:441:ILE:CG1	2.01	0.90
8:P:448:VAL:CB	8:P:449:PRO:HD3	1.81	0.90
11:U:22:GLU:CB	11:U:119:THR:HG23	2.01	0.90
7:L:540:HIS:HB3	7:L:543:LEU:HD21	0.90	0.90
2:B:451:ARG:HG2	2:B:542:ALA:C	1.93	0.89
8:P:477:TRP:HH2	8:P:524:TYR:CE1	1.89	0.89
4:H:554:LYS:CE	4:H:558:LYS:HZ2	1.85	0.89
8:P:395:LEU:HB2	8:P:410:LEU:CD1	2.02	0.89
8:P:445:ASN:OD1	8:P:467:PRO:HG2	1.71	0.89
4:E:526:GLU:O	4:E:530:THR:HG23	1.73	0.89
9:R:25:VAL:HG11	9:R:33:VAL:HG13	1.54	0.89
6:K:511:ALA:CB	6:K:512:PRO:CD	2.46	0.89
10:S:117:LYS:HD3	10:S:117:LYS:N	1.87	0.89
1:A:355:ALA:C	5:J:117:TYR:HE2	1.75	0.89
2:B:419:ASN:C	2:B:443:ARG:NH1	2.25	0.89
8:P:529:LYS:HG3	8:P:534:TYR:CE2	2.08	0.89
4:F:450:HIS:ND1	4:F:480:SER:CB	2.30	0.88
6:K:510:GLN:HG3	7:L:522:THR:CG2	2.03	0.88
7:L:540:HIS:H	7:L:543:LEU:HD23	0.84	0.88
4:F:482:ALA:HB3	4:F:515:TYR:CE2	2.08	0.88
6:K:510:GLN:CG	7:L:522:THR:CG2	2.50	0.88
8:P:366:TRP:CZ3	8:P:380:LEU:HD12	2.08	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:481:PRO:HD2	2:B:540:HIS:NE2	1.89	0.88
7:L:511:ALA:CB	7:L:514:ARG:CG	2.50	0.88
8:P:345:ALA:CA	8:P:413:LEU:HD12	1.98	0.88
1:A:356:SER:HB2	5:J:117:TYR:HH	1.37	0.87
4:E:527:GLU:O	4:E:530:THR:OG1	1.92	0.87
1:A:554:LYS:O	1:A:554:LYS:NZ	2.08	0.87
2:B:545:ASN:O	2:B:545:ASN:ND2	2.06	0.87
8:P:529:LYS:NZ	8:P:534:TYR:CE2	2.43	0.87
4:H:554:LYS:CE	4:H:558:LYS:NZ	2.37	0.87
8:P:357:ARG:NH2	8:P:403:ASN:HD22	1.72	0.87
8:P:470:PHE:HE2	8:P:528:VAL:HG11	1.39	0.87
10:S:39:LEU:HD11	10:S:87:PHE:HE1	1.38	0.87
8:P:131:THR:CG2	8:P:188:VAL:CA	2.52	0.87
10:S:39:LEU:HD13	10:S:87:PHE:HD1	1.07	0.87
1:A:493:GLN:OE1	1:A:493:GLN:N	2.07	0.87
4:F:450:HIS:CD2	4:F:514:ARG:NH1	2.43	0.87
10:S:37:CYS:HB2	10:S:116:GLN:OE1	1.72	0.87
1:A:493:GLN:CB	1:A:494:PRO:HD2	1.94	0.87
3:C:564:VAL:HG21	4:H:566:LEU:HD21	1.55	0.87
7:L:545:ASN:ND2	7:L:545:ASN:O	2.07	0.87
7:L:540:HIS:CA	7:L:543:LEU:HD23	1.74	0.87
6:K:445:LYS:HA	6:K:445:LYS:HE3	1.57	0.86
4:F:480:SER:HB2	4:F:481:PRO:HD2	1.56	0.86
8:P:411:ASN:ND2	8:P:525:TRP:CE2	2.42	0.86
8:P:529:LYS:HG3	8:P:534:TYR:CD2	2.09	0.86
4:F:535:THR:CG2	4:F:551:THR:CG2	2.37	0.86
8:P:418:ALA:HB2	8:P:439:ILE:CD1	2.03	0.86
4:G:357:ILE:HD12	4:G:363:THR:HG22	1.57	0.86
8:P:278:ARG:C	8:P:422:TRP:HZ2	1.78	0.86
8:P:412:GLN:NE2	8:P:412:GLN:O	2.08	0.86
8:P:357:ARG:HH21	8:P:403:ASN:HD22	1.20	0.86
2:B:451:ARG:CG	2:B:542:ALA:O	2.24	0.86
3:C:451:ARG:HH11	3:C:451:ARG:CB	1.87	0.86
8:P:418:ALA:HA	8:P:439:ILE:HD11	1.56	0.86
8:P:446:LEU:HD22	8:P:538:ALA:HB2	1.56	0.86
4:E:506:MET:HG2	4:E:507:PRO:HD2	1.58	0.85
6:K:354:PHE:CZ	6:K:546:ARG:HD3	2.10	0.85
9:R:111:ASP:O	9:R:114:LYS:HE3	1.76	0.85
8:P:264:VAL:HG13	8:P:275:PHE:CD2	2.11	0.85
8:P:471:SER:O	8:P:475:LYS:NZ	2.09	0.85
8:P:395:LEU:HD12	8:P:409:ILE:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:CD1	1:A:550:ARG:O	2.25	0.85
4:D:421:GLY:N	4:D:445:LYS:HZ1	1.74	0.85
4:E:511:ALA:HB1	4:E:514:ARG:HG3	1.57	0.85
2:B:478:GLY:O	2:B:514:ARG:CG	2.25	0.85
8:P:253:CYS:SG	8:P:315:LEU:HB3	2.16	0.85
8:P:357:ARG:HH21	8:P:403:ASN:ND2	1.74	0.85
6:K:516:PHE:CE2	7:L:520:ILE:CD1	2.59	0.85
4:G:523:VAL:HG21	4:G:534:TYR:HH	1.42	0.85
3:C:482:ALA:HB2	3:C:515:TYR:CE1	2.11	0.84
3:C:525:GLU:N	3:C:525:GLU:OE1	2.10	0.84
4:H:583:NAG:H61	6:K:583:NAG:H61	1.58	0.84
8:P:447:LYS:HB2	8:P:464:CYS:C	1.98	0.84
4:D:421:GLY:CA	4:D:445:LYS:HE3	2.07	0.84
4:E:493:GLN:HB2	4:E:494:PRO:CD	2.08	0.84
4:G:443:ARG:O	4:G:443:ARG:NE	2.09	0.84
4:H:554:LYS:NZ	4:H:558:LYS:HZ1	1.53	0.84
4:G:525:GLU:OE2	4:G:529:ASN:ND2	2.10	0.84
5:J:27:ASP:HB2	5:J:28:PRO:HD3	1.57	0.84
6:K:463:GLN:HB2	7:L:455:TYR:CE2	2.13	0.84
4:F:502:THR:OG1	4:F:519:SER:HA	1.77	0.84
2:B:421:GLY:C	2:B:445:LYS:HE3	1.97	0.84
9:R:29:LEU:O	9:R:94:LEU:O	1.96	0.84
4:E:491:ARG:HD3	12:V:44:VAL:HG11	1.59	0.83
4:H:475:LEU:HD13	4:H:518:HIS:CE1	2.13	0.83
7:L:479:PHE:HZ	7:L:484:VAL:HG11	1.43	0.83
1:A:518:HIS:HE1	2:B:520:ILE:CG2	1.91	0.83
2:B:418:TRP:CZ2	2:B:444:PRO:HD3	2.10	0.83
1:A:491:ARG:HH11	1:A:491:ARG:HG2	1.42	0.83
3:C:480:SER:O	3:C:540:HIS:CE1	2.31	0.83
4:E:421:GLY:CA	4:E:445:LYS:HE2	2.09	0.83
7:L:540:HIS:HB2	7:L:543:LEU:HD21	1.57	0.83
7:L:511:ALA:HB3	7:L:514:ARG:HG3	1.59	0.83
8:P:131:THR:HG21	8:P:188:VAL:HG23	1.57	0.83
6:K:509:PRO:HG2	7:L:501:VAL:HG23	1.60	0.83
8:P:439:ILE:H	8:P:439:ILE:HD12	1.42	0.83
7:L:443:ARG:N	7:L:444:PRO:CD	2.42	0.82
7:L:540:HIS:HB3	7:L:543:LEU:HD22	1.60	0.82
8:P:395:LEU:CB	8:P:410:LEU:CD1	2.55	0.82
6:K:509:PRO:HG3	7:L:501:VAL:CG2	2.01	0.82
3:C:526:GLU:O	3:C:530:THR:CG2	2.27	0.82
6:K:516:PHE:CD2	7:L:520:ILE:HD13	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:20:LEU:HD23	9:R:117:LYS:CG	2.10	0.82
1:A:514:ARG:HH11	1:A:514:ARG:CB	1.91	0.82
2:B:443:ARG:HG2	2:B:443:ARG:HH11	1.43	0.82
7:L:481:PRO:HD2	7:L:540:HIS:HE2	1.45	0.82
3:C:527:GLU:O	3:C:532:GLU:HG2	1.80	0.82
8:P:475:LYS:CE	8:P:475:LYS:H	1.93	0.82
1:A:356:SER:N	5:J:117:TYR:OH	2.13	0.82
5:J:27:ASP:CB	5:J:28:PRO:CD	2.55	0.82
8:P:366:TRP:CE3	8:P:380:LEU:HD12	2.15	0.82
7:L:450:HIS:HB2	7:L:480:SER:HG	0.85	0.81
1:A:355:ALA:C	5:J:117:TYR:CE2	2.53	0.81
2:B:451:ARG:NH1	2:B:451:ARG:HB2	1.95	0.81
8:P:525:TRP:CZ3	8:P:537:THR:HG21	2.14	0.81
4:F:480:SER:HB2	4:F:481:PRO:CD	2.10	0.81
8:P:446:LEU:HD23	8:P:538:ALA:HB2	1.62	0.81
8:P:523:TRP:CZ3	8:P:539:ALA:HB1	2.14	0.81
8:P:529:LYS:HE2	8:P:534:TYR:HE2	1.43	0.81
4:E:421:GLY:CA	4:E:445:LYS:CE	2.58	0.81
2:B:449:LEU:HA	2:B:480:SER:OG	1.81	0.81
8:P:344:VAL:HG22	8:P:413:LEU:CD1	2.10	0.81
8:P:345:ALA:HA	8:P:413:LEU:CB	2.06	0.81
4:F:535:THR:HG22	4:F:551:THR:HG21	1.58	0.81
6:K:510:GLN:HG3	7:L:522:THR:HG23	1.63	0.81
7:L:479:PHE:O	7:L:515:TYR:HB2	1.81	0.81
8:P:525:TRP:CE3	8:P:537:THR:HG21	2.16	0.81
9:R:46:ILE:H	9:R:64:THR:HG21	1.46	0.81
4:D:493:GLN:OE1	4:D:493:GLN:N	2.14	0.81
4:E:543:LEU:CD2	4:E:544:PRO:HD2	2.11	0.81
4:E:543:LEU:CD2	4:E:544:PRO:CD	2.58	0.81
4:F:523:VAL:HG11	4:F:534:TYR:CZ	2.15	0.81
6:K:454:VAL:HG22	6:K:538:VAL:HG21	1.61	0.81
1:A:533:THR:HA	1:A:553:ASP:HB3	1.62	0.81
4:F:450:HIS:CD2	4:F:514:ARG:NH2	2.47	0.81
8:P:462:VAL:HB	8:P:509:VAL:HB	1.62	0.81
4:D:421:GLY:HA2	4:D:445:LYS:NZ	1.93	0.81
10:S:39:LEU:HD11	10:S:87:PHE:CE1	2.10	0.81
1:A:482:ALA:O	1:A:505:PRO:HG2	1.79	0.80
8:P:446:LEU:HD23	8:P:537:THR:O	1.79	0.80
8:P:412:GLN:HE22	8:P:414:THR:HG23	1.47	0.80
9:R:61:VAL:CG2	9:R:72:TYR:CD2	2.59	0.80
2:B:420:SER:N	2:B:443:ARG:CZ	2.41	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:GLN:NE2	1:A:510:GLN:H	1.78	0.80
5:J:27:ASP:HB2	5:J:28:PRO:HD2	1.61	0.80
4:F:524:SER:OG	4:F:527:GLU:CB	2.29	0.80
6:K:563:ASN:HB3	7:L:563:ASN:HA	1.64	0.80
1:A:356:SER:HA	5:J:117:TYR:CZ	2.15	0.80
6:K:527:GLU:C	6:K:530:THR:OG1	2.17	0.80
8:P:411:ASN:HB3	8:P:537:THR:CB	2.12	0.80
8:P:418:ALA:CA	8:P:439:ILE:HD11	2.12	0.80
8:P:479:LYS:CG	8:P:524:TYR:CE1	2.65	0.80
7:L:479:PHE:CZ	7:L:484:VAL:CG1	2.64	0.80
8:P:261:CYS:SG	8:P:315:LEU:HD22	1.36	0.80
10:S:32:SER:N	10:S:94:LEU:HD23	1.95	0.80
8:P:348:SER:CB	8:P:537:THR:OG1	2.30	0.80
2:B:480:SER:CB	2:B:481:PRO:HD3	2.12	0.79
4:G:450:HIS:CD2	4:G:514:ARG:CZ	2.65	0.79
7:L:450:HIS:CA	7:L:480:SER:OG	2.29	0.79
7:L:479:PHE:HB3	7:L:515:TYR:CB	2.12	0.79
8:P:131:THR:HG22	8:P:187:VAL:O	1.81	0.79
1:A:514:ARG:HB3	1:A:514:ARG:NH1	1.95	0.79
7:L:424:PHE:CB	7:L:441:ILE:HD13	2.07	0.79
7:L:443:ARG:H	7:L:444:PRO:CD	1.93	0.79
8:P:248:VAL:CG1	8:P:311:SER:H	1.95	0.79
4:E:482:ALA:HB2	4:E:515:TYR:HE2	1.46	0.78
8:P:355:TYR:CE1	8:P:405:THR:N	2.51	0.78
4:E:454:VAL:HG21	4:E:538:VAL:CG2	2.13	0.78
8:P:131:THR:HG23	8:P:188:VAL:CB	2.12	0.78
4:G:501:VAL:CG2	4:H:509:PRO:HD3	2.13	0.78
6:K:543:LEU:HD12	6:K:543:LEU:H	1.48	0.78
8:P:475:LYS:H	8:P:475:LYS:CD	1.96	0.78
2:B:354:PHE:HZ	2:B:546:ARG:HG2	1.46	0.78
2:B:461:ARG:NH2	7:L:570:ASP:OD1	2.17	0.78
1:A:535:THR:HG22	1:A:551:THR:HB	1.65	0.78
7:L:479:PHE:HB3	7:L:515:TYR:HB2	1.64	0.78
8:P:342:LYS:CE	8:P:438:LYS:HE2	2.14	0.78
10:S:75:ARG:O	10:S:92:THR:HG23	1.84	0.78
1:A:359:LEU:CD1	5:J:117:TYR:HB3	2.13	0.78
2:B:454:VAL:HG22	2:B:550:ARG:HG3	1.66	0.78
4:G:450:HIS:HD2	4:G:514:ARG:CZ	1.95	0.78
4:H:583:NAG:H83	4:H:583:NAG:O3	1.84	0.78
8:P:413:LEU:HD23	8:P:413:LEU:H	1.49	0.77
8:P:471:SER:HA	8:P:475:LYS:HZ3	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:479:PHE:CZ	7:L:484:VAL:HB	2.19	0.77
8:P:287:ASP:OD1	8:P:287:ASP:N	2.17	0.77
2:B:418:TRP:O	2:B:443:ARG:NH1	2.13	0.77
8:P:479:LYS:CG	8:P:524:TYR:HE1	1.96	0.77
4:G:523:VAL:CG2	4:G:534:TYR:OH	2.26	0.77
8:P:346:GLY:N	8:P:413:LEU:CD1	2.41	0.77
9:R:20:LEU:HD21	9:R:117:LYS:CB	2.14	0.77
10:S:31:GLY:CA	10:S:94:LEU:HD21	2.13	0.77
8:P:131:THR:CG2	8:P:188:VAL:CB	2.63	0.77
8:P:346:GLY:H	8:P:413:LEU:HB2	1.45	0.77
8:P:446:LEU:HD22	8:P:538:ALA:CB	2.15	0.77
8:P:348:SER:OG	8:P:537:THR:OG1	2.02	0.77
8:P:361:LYS:HG2	8:P:364:LYS:HE2	1.64	0.77
8:P:132:ILE:HD13	8:P:187:VAL:HG23	1.66	0.77
8:P:529:LYS:CE	8:P:534:TYR:CE2	2.67	0.77
1:A:491:ARG:NH1	1:A:491:ARG:O	2.19	0.77
8:P:134:CYS:HB2	8:P:185:PHE:HD2	1.50	0.77
10:S:31:GLY:O	10:S:94:LEU:CD2	2.17	0.77
4:E:346:ARG:HE	4:E:371:ASP:HB2	1.49	0.76
4:E:516:PHE:CZ	4:F:520:ILE:HD11	2.20	0.76
4:H:365:LEU:HD11	4:H:418:TRP:HZ2	1.50	0.76
6:K:510:GLN:HG2	7:L:522:THR:CG2	2.12	0.76
4:D:364:LYS:HD2	4:D:410:GLU:HG3	1.65	0.76
7:L:514:ARG:HB3	7:L:514:ARG:HH11	1.48	0.76
8:P:348:SER:HB3	8:P:536:GLU:HB2	1.66	0.76
7:L:424:PHE:N	7:L:441:ILE:CG1	2.42	0.76
9:R:20:LEU:CD2	9:R:117:LYS:CB	2.63	0.76
8:P:466:PHE:CD2	8:P:507:ARG:HG3	2.16	0.76
8:P:391:TYR:HH	8:P:416:ARG:HH12	1.32	0.76
8:P:425:THR:O	8:P:430:LEU:HD21	1.85	0.76
9:R:23:VAL:HB	9:R:118:VAL:HG13	1.66	0.76
7:L:514:ARG:HH11	7:L:514:ARG:CB	1.98	0.76
8:P:450:GLY:N	8:P:540:VAL:HG12	2.00	0.76
8:P:345:ALA:C	8:P:413:LEU:CG	2.47	0.76
4:E:450:HIS:CE1	4:E:514:ARG:NH1	2.49	0.76
4:F:450:HIS:HE2	4:F:514:ARG:HH12	1.34	0.76
8:P:43:ARG:HG2	8:P:43:ARG:HH11	1.50	0.76
4:G:471:THR:HG22	4:G:522:THR:HG22	1.67	0.76
1:A:550:ARG:HG2	1:A:550:ARG:HH11	1.51	0.75
8:P:243:PRO:HA	8:P:246:ALA:HB2	1.66	0.75
4:D:421:GLY:HA3	4:D:445:LYS:HE3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:554:LYS:HZ3	4:H:558:LYS:HZ3	1.26	0.75
8:P:462:VAL:CG2	8:P:509:VAL:O	2.35	0.75
7:L:467:ARG:NH1	7:L:525:GLU:OE1	2.20	0.75
8:P:368:LEU:N	8:P:378:PRO:CD	2.28	0.75
8:P:525:TRP:CE3	8:P:537:THR:CG2	2.68	0.75
1:A:524:SER:OG	1:A:527:GLU:HB2	1.87	0.75
7:L:450:HIS:HB2	7:L:480:SER:CB	2.15	0.75
7:L:532:GLU:HB2	7:L:534:TYR:CE2	2.22	0.75
10:S:71:GLU:N	10:S:71:GLU:OE1	2.19	0.75
4:G:537:VAL:HG22	4:G:549:GLU:HG2	1.68	0.75
4:H:554:LYS:HZ3	4:H:558:LYS:HZ1	0.76	0.75
1:A:355:ALA:O	5:J:117:TYR:CE2	2.39	0.75
8:P:357:ARG:NH2	8:P:403:ASN:ND2	2.32	0.75
1:A:359:LEU:HD12	5:J:117:TYR:CG	2.07	0.75
4:E:483:ASP:O	4:E:540:HIS:ND1	2.19	0.75
4:F:449:LEU:HA	4:F:481:PRO:HD3	1.67	0.75
4:F:502:THR:OG1	4:F:519:SER:CA	2.35	0.75
10:S:29:LEU:HD23	10:S:95:THR:CG2	2.14	0.75
4:F:423:ARG:HA	4:F:441:ILE:O	1.87	0.74
4:F:560:THR:O	4:G:560:THR:CG2	2.21	0.74
8:P:411:ASN:CB	8:P:537:THR:OG1	2.32	0.74
2:B:454:VAL:HG11	2:B:538:VAL:HG11	1.68	0.74
4:E:471:THR:HG22	4:E:522:THR:HG22	1.68	0.74
10:S:37:CYS:HB3	10:S:116:GLN:OE1	1.84	0.74
13:I:1:NAG:C1	13:I:1:NAG:H82	2.18	0.74
7:L:424:PHE:CG	7:L:441:ILE:HD13	2.18	0.74
8:P:361:LYS:O	8:P:361:LYS:HE3	1.87	0.74
8:P:450:GLY:CA	8:P:540:VAL:CG1	2.61	0.74
8:P:466:PHE:HE2	8:P:507:ARG:CB	2.00	0.74
13:I:1:NAG:O4	13:I:1:NAG:N2	2.17	0.74
2:B:466:LEU:HB3	2:B:468:GLU:HG3	1.70	0.74
6:K:463:GLN:CB	7:L:455:TYR:CZ	2.67	0.74
8:P:43:ARG:HG2	8:P:43:ARG:NH1	2.01	0.74
4:D:514:ARG:HH11	12:V:66:ASN:ND2	1.85	0.74
4:E:450:HIS:CD2	4:E:514:ARG:CZ	2.68	0.74
8:P:342:LYS:HB3	8:P:438:LYS:CB	2.18	0.74
7:L:424:PHE:HB2	7:L:441:ILE:HG12	1.69	0.74
8:P:446:LEU:CD2	8:P:538:ALA:CB	2.65	0.74
8:P:477:TRP:HZ2	8:P:524:TYR:CG	1.96	0.74
8:P:264:VAL:HG12	8:P:265:VAL:HG23	1.69	0.73
8:P:340:VAL:HG12	8:P:436:GLU:C	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:395:LEU:HA	8:P:410:LEU:HD12	1.70	0.73
12:V:21:PRO:HD2	12:V:116:GLN:HG3	1.69	0.73
4:E:450:HIS:CB	4:E:514:ARG:NH2	2.51	0.73
8:P:368:LEU:CB	8:P:378:PRO:CD	2.66	0.73
9:R:25:VAL:HG11	9:R:33:VAL:CG1	2.16	0.73
8:P:243:PRO:O	8:P:246:ALA:HB2	1.84	0.73
4:F:482:ALA:HB3	4:F:515:TYR:HE2	1.50	0.73
7:L:479:PHE:HZ	7:L:484:VAL:CG1	1.99	0.73
8:P:281:LEU:HD11	8:P:290:PHE:HE2	1.52	0.73
8:P:446:LEU:HD12	8:P:446:LEU:N	2.03	0.73
7:L:421:GLY:O	7:L:443:ARG:NH2	2.22	0.73
8:P:361:LYS:HG2	8:P:364:LYS:CE	2.17	0.73
4:F:450:HIS:NE2	4:F:514:ARG:NH1	2.35	0.73
8:P:348:SER:HB2	8:P:537:THR:OG1	1.88	0.73
1:A:485:PHE:HE2	5:J:115:LEU:HD22	1.53	0.73
2:B:490:GLN:HG3	2:B:490:GLN:O	1.88	0.73
6:K:518:HIS:CE1	7:L:518:HIS:ND1	2.57	0.73
8:P:265:VAL:HG21	8:P:279:ILE:HG21	1.71	0.73
9:R:31:GLY:O	9:R:94:LEU:HD13	1.88	0.73
3:C:456:LEU:HD12	3:C:550:ARG:HB2	1.71	0.73
4:D:514:ARG:HD3	4:D:514:ARG:N	2.02	0.73
4:D:514:ARG:NH2	4:D:514:ARG:HG2	2.02	0.73
4:E:543:LEU:HD22	4:E:544:PRO:HD2	1.70	0.73
8:P:398:LEU:HD11	8:P:409:ILE:HG13	1.69	0.73
9:R:75:ARG:HG2	9:R:75:ARG:O	1.89	0.73
10:S:35:ILE:HG12	10:S:118:VAL:HG21	1.70	0.73
2:B:480:SER:OG	2:B:481:PRO:CD	2.34	0.73
3:C:467:ARG:HD3	3:C:467:ARG:N	2.03	0.73
10:S:72:TYR:HB3	10:S:76:VAL:HG21	1.70	0.73
4:F:535:THR:HG22	4:F:551:THR:HG22	0.75	0.72
8:P:342:LYS:HE2	8:P:438:LYS:HE2	1.69	0.72
8:P:471:SER:CA	8:P:475:LYS:HZ3	2.02	0.72
3:C:461:ARG:HH12	3:C:465:ASN:HD21	0.78	0.72
4:E:493:GLN:NE2	4:E:493:GLN:H	1.87	0.72
1:A:488:TRP:HE1	1:A:519:SER:HG	1.37	0.72
7:L:479:PHE:CZ	7:L:484:VAL:CB	2.72	0.72
3:C:554:LYS:O	3:C:554:LYS:HG2	1.89	0.72
7:L:540:HIS:C	7:L:543:LEU:HD23	1.88	0.72
3:C:421:GLY:O	3:C:423:ARG:NH2	2.23	0.72
3:C:454:VAL:HG22	3:C:538:VAL:HG21	1.71	0.72
5:J:64:LEU:HD22	5:J:64:LEU:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:479:LYS:HG2	8:P:524:TYR:CD1	2.24	0.72
10:S:32:SER:N	10:S:94:LEU:CD2	2.51	0.72
7:L:540:HIS:N	7:L:543:LEU:HD21	1.85	0.72
8:P:450:GLY:N	8:P:540:VAL:CG1	2.53	0.72
11:U:22:GLU:O	11:U:22:GLU:HG2	1.89	0.72
6:K:471:THR:HG23	6:K:520:ILE:HG13	1.71	0.72
4:F:348:PHE:H	4:F:369:VAL:HG13	1.53	0.71
8:P:132:ILE:N	8:P:132:ILE:HD12	2.05	0.71
10:S:39:LEU:HD22	10:S:86:LEU:N	2.04	0.71
8:P:439:ILE:HD12	8:P:439:ILE:N	2.05	0.71
8:P:447:LYS:HB2	8:P:465:HIS:N	2.04	0.71
4:E:506:MET:CG	4:E:507:PRO:HD2	2.19	0.71
6:K:484:VAL:HG23	6:K:540:HIS:CB	2.20	0.71
12:V:76:VAL:HG12	12:V:91:VAL:HG22	1.72	0.71
7:L:527:GLU:HB3	7:L:534:TYR:OH	1.89	0.71
7:L:479:PHE:HZ	7:L:484:VAL:CB	2.03	0.71
4:G:430:HIS:CD2	4:G:431:THR:H	2.09	0.71
4:H:365:LEU:HD22	4:H:413:ILE:HD13	1.73	0.71
6:K:553:ASP:OD2	6:K:554:LYS:N	2.23	0.71
3:C:371:ASP:H	3:C:404:THR:HG23	1.55	0.71
4:G:428:VAL:H	4:G:437:LEU:HB3	1.55	0.71
8:P:340:VAL:HG12	8:P:436:GLU:CB	2.20	0.71
6:K:540:HIS:O	6:K:543:LEU:HD12	1.91	0.71
8:P:418:ALA:CB	8:P:439:ILE:CD1	2.69	0.71
4:G:506:MET:CE	4:G:516:PHE:HE2	2.03	0.71
6:K:354:PHE:CE1	6:K:541:GLU:HB3	2.26	0.71
4:D:478:GLY:HA2	4:D:514:ARG:HB3	1.72	0.70
4:F:441:ILE:HG22	4:F:443:ARG:H	1.56	0.70
4:F:449:LEU:HA	4:F:481:PRO:CD	2.20	0.70
7:L:456:LEU:HG	7:L:552:VAL:HG21	1.73	0.70
1:A:356:SER:HA	5:J:117:TYR:CE2	2.26	0.70
1:A:550:ARG:HG2	1:A:550:ARG:NH1	2.03	0.70
11:U:22:GLU:CB	11:U:119:THR:CG2	2.68	0.70
1:A:357:ILE:HG12	1:A:363:THR:HG22	1.73	0.70
2:B:454:VAL:HG11	2:B:538:VAL:CG1	2.21	0.70
8:P:368:LEU:HD12	8:P:378:PRO:HG2	1.72	0.70
8:P:529:LYS:CG	8:P:534:TYR:CE2	2.73	0.70
4:E:372:LEU:HD12	4:E:432:ASP:HB3	1.74	0.70
8:P:421:TYR:CD1	8:P:437:ILE:HD12	2.26	0.70
11:U:37:CYS:HB3	11:U:87:PHE:HB3	1.73	0.70
4:F:543:LEU:HD23	4:F:544:PRO:HD2	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:583:NAG:C3	4:G:583:NAG:H83	2.21	0.70
8:P:466:PHE:CD2	8:P:507:ARG:CG	2.74	0.70
10:S:99:SER:HB2	10:S:120:LEU:O	1.91	0.70
4:H:418:TRP:HB3	4:H:443:ARG:HB2	1.72	0.70
5:J:21:ILE:HD13	7:L:554:LYS:HG2	1.74	0.70
8:P:529:LYS:HE2	8:P:534:TYR:CE2	2.26	0.70
2:B:461:ARG:NH2	7:L:570:ASP:CG	2.38	0.70
3:C:566:LEU:HD12	3:C:566:LEU:N	2.01	0.70
4:F:550:ARG:HG2	4:F:550:ARG:NH1	2.05	0.70
8:P:134:CYS:HB2	8:P:185:PHE:CD2	2.26	0.70
8:P:471:SER:HB2	8:P:475:LYS:NZ	2.07	0.70
6:K:381:SER:HB3	6:K:389:ALA:HB1	1.74	0.70
8:P:479:LYS:HB2	8:P:488:LEU:HD13	1.74	0.70
4:G:532:GLU:OE1	4:G:532:GLU:HA	1.90	0.70
3:C:566:LEU:HD13	4:D:566:LEU:HD23	1.74	0.69
8:P:247:ASN:OD1	8:P:247:ASN:N	2.24	0.69
12:V:45:ARG:NH2	12:V:110:THR:OG1	2.25	0.69
8:P:131:THR:HG22	8:P:187:VAL:C	2.12	0.69
8:P:418:ALA:CA	8:P:439:ILE:CD1	2.69	0.69
8:P:471:SER:CA	8:P:475:LYS:NZ	2.55	0.69
1:A:356:SER:CB	5:J:117:TYR:HH	1.97	0.69
8:P:306:LEU:HD22	8:P:321:ILE:HD12	1.74	0.69
11:U:22:GLU:HG3	11:U:119:THR:HG23	1.72	0.69
11:U:33:VAL:HG12	11:U:94:LEU:HD11	1.75	0.69
8:P:413:LEU:HD23	8:P:413:LEU:N	2.06	0.69
7:L:354:PHE:HA	7:L:357:ILE:HG12	1.75	0.69
7:L:508:GLU:OE1	7:L:508:GLU:HA	1.92	0.69
9:R:116:GLN:HE22	9:R:118:VAL:HG22	1.53	0.69
4:E:508:GLU:OE1	4:E:509:PRO:HD3	1.93	0.69
10:S:61:VAL:CG1	10:S:72:TYR:CD1	2.76	0.69
8:P:446:LEU:HB3	8:P:466:PHE:CD1	2.27	0.69
8:P:462:VAL:HB	8:P:509:VAL:O	1.92	0.69
9:R:47:TYR:HE2	9:R:49:CYS:HB2	1.57	0.69
3:C:564:VAL:CG2	4:H:566:LEU:HD21	2.23	0.69
3:C:568:MET:HE2	4:H:562:TYR:CD1	2.28	0.69
6:K:464:LEU:CD1	6:K:525:GLU:CD	2.59	0.69
8:P:149:LYS:HD2	8:P:151:ILE:CG2	2.22	0.69
8:P:340:VAL:HG12	8:P:436:GLU:HB3	1.69	0.69
8:P:446:LEU:HD21	8:P:537:THR:C	2.12	0.69
8:P:447:LYS:CG	8:P:465:HIS:CB	2.55	0.69
3:C:451:ARG:HB3	3:C:451:ARG:NH1	2.03	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:GLY:HA2	2:B:445:LYS:NZ	2.08	0.69
4:H:456:LEU:HD22	4:H:552:VAL:HB	1.75	0.68
10:S:61:VAL:HG11	10:S:72:TYR:CD1	2.27	0.68
2:B:443:ARG:HH11	2:B:443:ARG:CG	2.06	0.68
5:J:30:GLU:OE1	5:J:30:GLU:HA	1.92	0.68
10:S:72:TYR:HB3	10:S:76:VAL:CG2	2.24	0.68
3:C:457:LEU:HD13	4:D:457:LEU:HD23	1.75	0.68
6:K:454:VAL:HG21	6:K:538:VAL:CG2	2.21	0.68
7:L:424:PHE:O	7:L:441:ILE:HG12	1.93	0.68
6:K:566:LEU:HD23	6:K:566:LEU:O	1.94	0.68
8:P:345:ALA:C	8:P:413:LEU:HB2	2.13	0.68
9:R:75:ARG:HH22	9:R:95:THR:HG1	1.36	0.68
7:L:487:GLN:HB3	7:L:537:VAL:CG1	2.24	0.68
8:P:244:GLU:H	8:P:244:GLU:CD	1.97	0.68
8:P:476:TYR:CD1	8:P:527:GLY:O	2.46	0.68
5:J:64:LEU:HD22	5:J:64:LEU:H	1.59	0.68
6:K:509:PRO:HG2	7:L:501:VAL:HG21	1.54	0.68
6:K:561:LEU:HG	6:K:561:LEU:O	1.93	0.68
1:A:554:LYS:HZ2	1:A:554:LYS:C	1.95	0.68
4:F:543:LEU:HD13	4:F:548:THR:HG22	1.75	0.68
8:P:526:CYS:O	8:P:538:ALA:CB	2.42	0.68
10:S:76:VAL:HG22	10:S:91:VAL:HG22	1.75	0.68
4:E:357:ILE:HG22	4:E:363:THR:HA	1.76	0.67
4:F:549:GLU:O	4:F:549:GLU:HG2	1.94	0.67
8:P:149:LYS:HD2	8:P:151:ILE:HG22	1.75	0.67
10:S:71:GLU:CD	10:S:71:GLU:H	1.95	0.67
1:A:518:HIS:CE1	2:B:520:ILE:CG2	2.76	0.67
7:L:384:ARG:HD3	7:L:388:GLU:HB3	1.77	0.67
7:L:511:ALA:HB3	7:L:514:ARG:HG2	1.71	0.67
8:P:344:VAL:HG22	8:P:413:LEU:HD11	1.74	0.67
11:U:70:ALA:HA	11:U:73:LYS:HE2	1.76	0.67
2:B:418:TRP:HZ2	2:B:444:PRO:HD2	1.60	0.67
4:E:452:PRO:HD2	4:E:543:LEU:HG	1.76	0.67
4:F:349:ALA:HA	4:F:367:CYS:HA	1.76	0.67
7:L:540:HIS:CB	7:L:543:LEU:HD22	2.08	0.67
8:P:526:CYS:O	8:P:538:ALA:HB3	1.94	0.67
3:C:480:SER:O	3:C:540:HIS:NE2	2.26	0.67
8:P:395:LEU:CG	8:P:410:LEU:CD1	2.71	0.67
1:A:471:THR:HG22	1:A:522:THR:HG22	1.75	0.67
1:A:583:NAG:H5	2:B:583:NAG:H4	1.76	0.67
2:B:419:ASN:C	2:B:443:ARG:CZ	2.63	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:456:LEU:CD1	3:C:550:ARG:HB2	2.25	0.67
5:J:4:ARG:HG2	5:J:20:ARG:HD3	1.76	0.67
8:P:261:CYS:SG	8:P:315:LEU:CB	2.82	0.67
8:P:342:LYS:CB	8:P:438:LYS:O	2.43	0.67
8:P:346:GLY:H	8:P:413:LEU:CA	2.08	0.67
8:P:348:SER:HB3	8:P:537:THR:H	1.57	0.67
2:B:450:HIS:C	2:B:542:ALA:CB	2.63	0.67
4:G:450:HIS:CD2	4:G:514:ARG:NH2	2.59	0.67
4:G:516:PHE:CE1	4:H:520:ILE:HD12	2.30	0.67
8:P:135:PRO:O	8:P:204:ALA:HB3	1.94	0.67
2:B:382:TRP:CZ3	2:B:441:ILE:HD11	2.28	0.67
4:F:450:HIS:HB2	4:F:480:SER:N	2.10	0.67
8:P:131:THR:CG2	8:P:188:VAL:HG23	2.18	0.67
4:G:524:SER:HB3	4:G:527:GLU:HG3	1.75	0.66
11:U:102:TYR:HB2	11:U:118:VAL:HG23	1.77	0.66
8:P:352:LEU:HD23	8:P:406:PHE:O	1.96	0.66
8:P:395:LEU:CG	8:P:410:LEU:HD13	2.22	0.66
7:L:473:THR:HG22	7:L:520:ILE:HG22	1.75	0.66
8:P:261:CYS:SG	8:P:315:LEU:HB3	2.34	0.66
3:C:345:ILE:N	3:C:370:THR:O	2.29	0.66
7:L:479:PHE:CE2	7:L:484:VAL:HG11	2.30	0.66
8:P:480:TRP:CH2	8:P:482:ASN:HB3	2.31	0.66
2:B:354:PHE:CZ	2:B:546:ARG:HG2	2.28	0.66
4:F:383:THR:HG1	4:F:425:THR:HG1	1.35	0.66
8:P:368:LEU:HB2	8:P:378:PRO:HG2	1.76	0.66
11:U:22:GLU:HB3	11:U:119:THR:CG2	2.26	0.66
2:B:362:SER:OG	2:B:364:LYS:NZ	2.24	0.66
3:C:466:LEU:HD21	12:V:45:ARG:NE	2.11	0.66
8:P:132:ILE:HD12	8:P:132:ILE:H	1.60	0.66
1:A:538:VAL:CG2	1:A:548:THR:CG2	2.74	0.66
4:G:583:NAG:H83	4:G:583:NAG:O3	1.96	0.66
8:P:475:LYS:H	8:P:475:LYS:HE2	1.59	0.66
4:H:368:LEU:HB2	4:H:406:SER:HB2	1.76	0.66
2:B:418:TRP:HZ2	2:B:444:PRO:HD3	1.48	0.66
4:F:502:THR:OG1	4:F:519:SER:OG	2.06	0.66
2:B:564:VAL:HG22	3:C:564:VAL:HA	1.78	0.65
4:E:482:ALA:HB2	4:E:515:TYR:CE2	2.29	0.65
4:E:482:ALA:HA	4:E:515:TYR:CE2	2.30	0.65
2:B:430:HIS:ND1	2:B:432:ASP:OD1	2.25	0.65
4:G:380:ILE:HD13	4:G:409:GLY:HA3	1.78	0.65
8:P:368:LEU:CA	8:P:378:PRO:CD	2.74	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:535:THR:HG22	6:K:551:THR:OG1	1.96	0.65
1:A:483:ASP:O	1:A:540:HIS:HD2	1.79	0.65
2:B:451:ARG:HA	2:B:542:ALA:HB3	1.77	0.65
3:C:568:MET:CE	4:H:562:TYR:HD1	2.09	0.65
4:E:545:ASN:OD1	4:E:545:ASN:N	2.25	0.65
4:F:523:VAL:CG1	4:F:534:TYR:CZ	2.80	0.65
5:J:21:ILE:CG1	7:L:555:SER:HB3	2.25	0.65
4:D:514:ARG:HG2	4:D:514:ARG:HH21	1.62	0.65
2:B:480:SER:CB	2:B:481:PRO:CD	2.70	0.65
8:P:529:LYS:CG	8:P:534:TYR:CD2	2.79	0.65
2:B:419:ASN:C	2:B:443:ARG:HH12	1.99	0.65
4:E:421:GLY:CA	4:E:445:LYS:HE3	2.21	0.65
7:L:424:PHE:O	7:L:441:ILE:CG1	2.45	0.65
8:P:368:LEU:CA	8:P:378:PRO:HD2	2.25	0.65
8:P:462:VAL:CG1	8:P:540:VAL:HG11	2.21	0.65
8:P:477:TRP:CE2	8:P:524:TYR:HB3	2.30	0.65
4:D:391:LYS:NZ	4:D:392:THR:O	2.29	0.65
3:C:508:GLU:HG3	3:C:509:PRO:HD3	1.79	0.64
7:L:546:ARG:HG2	7:L:546:ARG:O	1.97	0.64
8:P:340:VAL:CG1	8:P:436:GLU:CG	2.74	0.64
11:U:22:GLU:HB2	11:U:119:THR:N	2.12	0.64
1:A:540:HIS:HB3	1:A:543:LEU:HD12	1.78	0.64
4:G:397:SER:HB3	4:G:408:VAL:HG23	1.79	0.64
8:P:394:ARG:NH1	8:P:414:THR:OG1	2.30	0.64
8:P:462:VAL:HG23	8:P:509:VAL:O	1.96	0.64
10:S:39:LEU:CD2	10:S:85:ASN:HA	2.27	0.64
11:U:22:GLU:HA	11:U:118:VAL:HA	1.77	0.64
1:A:459:PRO:CG	1:A:470:ALA:HB1	2.28	0.64
4:F:546:ARG:HH11	4:F:546:ARG:CG	2.10	0.64
4:H:372:LEU:HD11	4:H:405:PHE:HB2	1.80	0.64
5:J:27:ASP:CB	5:J:28:PRO:HD2	2.26	0.64
8:P:264:VAL:CG2	8:P:275:PHE:HE2	2.10	0.64
8:P:470:PHE:HE2	8:P:528:VAL:CG1	2.10	0.64
4:E:450:HIS:CE1	4:E:514:ARG:NH2	2.54	0.64
4:G:346:ARG:NH1	4:G:347:VAL:O	2.31	0.64
4:G:556:THR:O	4:H:461:ARG:NH2	2.30	0.64
6:K:464:LEU:HD13	6:K:525:GLU:OE2	1.91	0.64
8:P:471:SER:HB2	8:P:475:LYS:HZ2	1.62	0.64
6:K:452:PRO:HG3	6:K:479:PHE:HB3	1.78	0.64
6:K:518:HIS:ND1	7:L:518:HIS:ND1	2.45	0.64
8:P:448:VAL:HG23	8:P:449:PRO:HD2	1.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:22:GLU:CB	11:U:119:THR:O	2.37	0.64
4:E:482:ALA:HA	4:E:515:TYR:CD2	2.33	0.64
7:L:367:CYS:HB2	7:L:382:TRP:HE3	1.63	0.64
8:P:526:CYS:HB3	8:P:538:ALA:HB3	1.79	0.64
7:L:527:GLU:O	7:L:530:THR:OG1	2.15	0.64
11:U:50:ARG:HH12	11:U:100:GLY:HA3	1.62	0.64
1:A:485:PHE:HE2	5:J:115:LEU:CD2	2.11	0.64
4:E:516:PHE:CE2	4:F:520:ILE:HD11	2.33	0.64
4:F:482:ALA:HB1	4:F:515:TYR:CD2	1.99	0.64
6:K:521:LEU:HD23	6:K:521:LEU:O	1.97	0.64
8:P:314:GLN:CA	8:P:314:GLN:HE21	2.09	0.64
9:R:48:LEU:HD11	9:R:102:TYR:HB3	1.79	0.64
3:C:419:ASN:O	3:C:443:ARG:NH1	2.30	0.63
6:K:516:PHE:CD2	7:L:520:ILE:CD1	2.79	0.63
8:P:250:LYS:HG2	8:P:309:ALA:CB	2.20	0.63
4:F:368:LEU:HD12	4:F:408:VAL:HA	1.78	0.63
7:L:537:VAL:HA	7:L:548:THR:O	1.99	0.63
8:P:525:TRP:HA	8:P:538:ALA:O	1.98	0.63
9:R:21:PRO:O	9:R:117:LYS:O	2.14	0.63
9:R:46:ILE:HG22	9:R:64:THR:CG2	2.28	0.63
13:I:2:NAG:O7	13:I:2:NAG:O3	2.12	0.63
3:C:383:THR:HG1	3:C:425:THR:HG1	1.47	0.63
4:H:384:ARG:HH21	4:H:390:VAL:HG22	1.61	0.63
6:K:469:SER:CA	6:K:525:GLU:HB2	2.29	0.63
7:L:451:ARG:NH1	7:L:544:PRO:HG3	2.13	0.63
1:A:566:LEU:HD13	1:A:566:LEU:N	2.13	0.63
8:P:494:GLY:O	8:P:507:ARG:NH2	2.30	0.63
1:A:502:THR:HA	1:A:519:SER:HA	1.80	0.63
3:C:457:LEU:HD11	3:C:473:THR:OG1	1.98	0.63
4:D:471:THR:HG22	4:D:522:THR:HG22	1.79	0.63
2:B:347:VAL:HG11	2:B:428:VAL:HG21	1.80	0.63
3:C:369:VAL:O	3:C:406:SER:HA	1.99	0.63
6:K:518:HIS:ND1	7:L:518:HIS:CE1	2.66	0.63
6:K:540:HIS:O	6:K:543:LEU:CD1	2.47	0.63
8:P:131:THR:HG21	8:P:188:VAL:HG22	0.63	0.63
4:F:346:ARG:HH21	4:F:348:PHE:HA	1.64	0.63
8:P:151:ILE:C	8:P:151:ILE:HD12	2.19	0.63
11:U:41:GLU:C	11:U:43:HIS:H	2.02	0.63
1:A:493:GLN:HB2	1:A:494:PRO:CD	2.15	0.63
5:J:35:ARG:HG2	5:J:35:ARG:HH11	1.64	0.63
7:L:511:ALA:CB	7:L:514:ARG:NE	2.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:131:THR:HG23	8:P:188:VAL:CG2	2.02	0.63
8:P:264:VAL:HG22	8:P:275:PHE:HE2	1.64	0.63
8:P:334:ILE:HG23	8:P:431:TRP:CZ3	2.34	0.63
7:L:538:VAL:HG13	7:L:548:THR:OG1	1.98	0.62
8:P:345:ALA:CA	8:P:413:LEU:CB	2.72	0.62
10:S:41:GLU:HA	10:S:41:GLU:OE2	1.99	0.62
12:V:28:GLU:C	12:V:96:GLU:OE1	2.37	0.62
5:J:10:ASN:HD22	5:J:67:LEU:HD22	1.65	0.62
8:P:398:LEU:N	8:P:398:LEU:HD12	2.13	0.62
9:R:20:LEU:CD2	9:R:117:LYS:HG2	2.20	0.62
11:U:25:VAL:HG23	11:U:25:VAL:O	1.99	0.62
2:B:423:ARG:NH1	2:B:425:THR:OG1	2.33	0.62
3:C:451:ARG:HH11	3:C:451:ARG:CG	2.11	0.62
1:A:537:VAL:HG22	1:A:549:GLU:HB3	1.81	0.62
1:A:570:ASP:HB2	9:R:112:ARG:HH22	1.64	0.62
3:C:568:MET:CE	4:H:562:TYR:CD1	2.81	0.62
4:F:449:LEU:HD22	4:F:449:LEU:H	1.64	0.62
8:P:361:LYS:CG	8:P:364:LYS:HE2	2.30	0.62
4:D:354:PHE:HA	4:D:357:ILE:HG22	1.81	0.62
4:F:543:LEU:HD22	4:F:548:THR:CG2	2.28	0.62
8:P:43:ARG:HH11	8:P:43:ARG:CG	2.13	0.62
8:P:464:CYS:O	8:P:507:ARG:O	2.17	0.62
8:P:466:PHE:CE2	8:P:507:ARG:CB	2.79	0.62
4:E:482:ALA:CB	4:E:515:TYR:CE2	2.76	0.62
4:H:560:THR:HB	6:K:560:THR:O	1.99	0.62
3:C:454:VAL:CG2	3:C:538:VAL:HG21	2.29	0.62
1:A:538:VAL:HG23	1:A:548:THR:HG22	1.80	0.62
2:B:443:ARG:HD3	2:B:443:ARG:N	2.15	0.62
4:F:450:HIS:ND1	4:F:480:SER:HB3	2.11	0.62
4:F:545:ASN:HB3	4:G:358:PHE:HZ	1.64	0.62
6:K:378:VAL:HG12	6:K:431:THR:HG23	1.81	0.62
1:A:566:LEU:HD13	1:A:566:LEU:H	1.64	0.62
3:C:563:ASN:HD22	3:C:583:NAG:C1	2.03	0.62
8:P:471:SER:CB	8:P:475:LYS:NZ	2.63	0.62
4:E:450:HIS:HB3	4:E:514:ARG:NH2	2.15	0.62
7:L:543:LEU:HD22	7:L:543:LEU:H	1.64	0.62
9:R:111:ASP:O	9:R:114:LYS:CD	2.47	0.62
8:P:398:LEU:HD11	8:P:409:ILE:CG1	2.30	0.61
9:R:86:LEU:HD23	9:R:88:LEU:HD21	1.82	0.61
5:J:8:VAL:HG11	5:J:68:CYS:HA	1.81	0.61
7:L:484:VAL:HG13	7:L:484:VAL:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:366:TRP:NE1	8:P:408:VAL:HG21	2.14	0.61
8:P:418:ALA:CB	8:P:439:ILE:HD13	2.25	0.61
2:B:354:PHE:HA	2:B:357:ILE:HG22	1.82	0.61
6:K:469:SER:N	6:K:525:GLU:HB2	2.15	0.61
6:K:546:ARG:O	6:K:546:ARG:HG2	2.00	0.61
8:P:529:LYS:HG3	8:P:534:TYR:HD2	1.65	0.61
10:S:31:GLY:HA3	10:S:94:LEU:CD2	2.15	0.61
1:A:508:GLU:HG2	1:A:509:PRO:HD2	1.80	0.61
2:B:445:LYS:CA	2:B:445:LYS:HZ3	2.13	0.61
8:P:529:LYS:HG3	8:P:534:TYR:HE2	1.62	0.61
2:B:345:ILE:HG22	2:B:372:LEU:HD13	1.82	0.61
4:E:459:PRO:HG3	4:E:470:ALA:HB1	1.82	0.61
9:R:46:ILE:O	9:R:64:THR:HG23	2.00	0.61
9:R:76:VAL:HG12	9:R:91:VAL:HG22	1.82	0.61
4:H:481:PRO:HB2	4:H:540:HIS:HE2	1.66	0.61
5:J:6:VAL:HA	5:J:18:THR:HG22	1.83	0.61
4:E:483:ASP:O	4:E:540:HIS:CE1	2.54	0.61
4:E:491:ARG:CD	12:V:44:VAL:HG11	2.29	0.61
4:F:430:HIS:ND1	4:F:432:ASP:OD2	2.34	0.61
3:C:566:LEU:HD21	4:H:564:VAL:HG11	1.81	0.61
8:P:264:VAL:HG13	8:P:275:PHE:CE2	2.35	0.61
8:P:462:VAL:HB	8:P:509:VAL:CB	2.30	0.61
8:P:466:PHE:CD1	8:P:470:PHE:CZ	2.83	0.61
1:A:356:SER:CA	5:J:117:TYR:CZ	2.76	0.61
1:A:518:HIS:CE1	2:B:520:ILE:HG21	2.36	0.61
5:J:106:ASN:HA	8:P:29:VAL:HG21	1.83	0.61
8:P:342:LYS:HA	8:P:438:LYS:O	2.00	0.61
8:P:342:LYS:HE3	8:P:438:LYS:HE2	1.82	0.61
11:U:94:LEU:C	11:U:96:GLU:H	2.04	0.61
2:B:510:GLN:HA	2:B:510:GLN:OE1	2.01	0.61
4:F:427:THR:HG23	4:F:438:LYS:HB3	1.82	0.61
6:K:540:HIS:HB3	6:K:543:LEU:HD11	1.83	0.61
8:P:418:ALA:HA	8:P:439:ILE:CD1	2.27	0.61
1:A:490:GLN:HB3	1:A:495:LEU:HD21	1.83	0.60
1:A:518:HIS:HE1	2:B:520:ILE:HG21	1.63	0.60
4:G:506:MET:HE2	4:G:516:PHE:HE2	1.66	0.60
4:H:384:ARG:HE	4:H:390:VAL:HG22	1.66	0.60
5:J:115:LEU:HD12	5:J:124:VAL:CG2	2.24	0.60
12:V:112:ARG:HB3	12:V:112:ARG:CZ	2.31	0.60
1:A:567:VAL:O	1:A:567:VAL:HG12	2.02	0.60
8:P:276:GLU:OE1	8:P:372:ALA:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:49:CYS:N	10:S:103:ALA:O	2.33	0.60
3:C:467:ARG:HD3	3:C:467:ARG:H	1.66	0.60
3:C:482:ALA:HB2	3:C:515:TYR:CG	2.35	0.60
4:F:524:SER:OG	4:F:527:GLU:CG	2.50	0.60
4:G:352:PRO:HB2	4:G:357:ILE:HD11	1.83	0.60
6:K:484:VAL:CG2	6:K:540:HIS:HB2	2.25	0.60
7:L:443:ARG:HD3	7:L:443:ARG:C	2.21	0.60
7:L:537:VAL:HG23	7:L:548:THR:O	2.01	0.60
11:U:39:LEU:O	11:U:39:LEU:HD23	2.02	0.60
4:H:532:GLU:O	4:H:553:ASP:CB	2.49	0.60
7:L:538:VAL:CG1	7:L:548:THR:OG1	2.50	0.60
2:B:421:GLY:HA2	2:B:445:LYS:HE3	0.60	0.60
4:E:447:VAL:O	4:E:447:VAL:HG13	2.01	0.60
4:F:490:GLN:NE2	4:F:532:GLU:OE1	2.33	0.60
4:G:467:ARG:HH11	4:G:467:ARG:HG3	1.67	0.60
4:H:418:TRP:O	4:H:442:SER:O	2.18	0.60
8:P:466:PHE:HE2	8:P:507:ARG:HG3	0.72	0.60
12:V:95:THR:HG22	12:V:95:THR:O	2.02	0.60
1:A:516:PHE:CE1	2:B:520:ILE:HD11	2.37	0.60
7:L:479:PHE:CE2	7:L:484:VAL:CG1	2.85	0.60
8:P:462:VAL:CB	8:P:509:VAL:O	2.49	0.60
3:C:347:VAL:O	3:C:439:GLN:NE2	2.34	0.60
3:C:471:THR:HG22	3:C:522:THR:HG22	1.82	0.60
7:L:424:PHE:CA	7:L:441:ILE:CG1	2.78	0.60
7:L:480:SER:CB	7:L:481:PRO:HD3	2.32	0.60
7:L:543:LEU:CB	7:L:546:ARG:HA	2.27	0.60
8:P:366:TRP:O	8:P:379:LEU:HA	2.02	0.60
9:R:21:PRO:O	9:R:117:LYS:HB2	2.01	0.60
11:U:81:TYR:HD1	11:U:86:LEU:HB2	1.65	0.60
4:D:449:LEU:HB3	4:D:542:ALA:HB2	1.82	0.60
7:L:423:ARG:NH2	7:L:444:PRO:HB3	2.17	0.60
10:S:39:LEU:HD12	10:S:87:PHE:CD1	2.31	0.60
4:E:399:SER:HB3	4:E:403:ALA:HA	1.82	0.60
4:F:480:SER:CB	4:F:481:PRO:CD	2.80	0.60
7:L:417:ASP:OD2	7:L:418:TRP:N	2.35	0.60
2:B:385:GLN:NE2	2:B:422:GLU:O	2.32	0.59
5:J:48:ASN:HB3	5:J:51:ASP:HB3	1.84	0.59
8:P:348:SER:CB	8:P:537:THR:H	2.15	0.59
1:A:491:ARG:HG2	1:A:491:ARG:NH1	2.14	0.59
4:G:583:NAG:H83	4:G:583:NAG:H3	1.83	0.59
10:S:61:VAL:HG11	10:S:72:TYR:HD1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:GLU:O	1:A:553:ASP:HB2	2.02	0.59
8:P:447:LYS:N	8:P:465:HIS:H	1.86	0.59
11:U:50:ARG:HH11	11:U:100:GLY:HA3	1.65	0.59
4:E:493:GLN:H	4:E:493:GLN:HE21	1.50	0.59
8:P:122:TYR:CE2	8:P:132:ILE:HG23	2.38	0.59
8:P:131:THR:HG22	8:P:188:VAL:HA	1.83	0.59
8:P:341:VAL:HG23	8:P:341:VAL:O	2.01	0.59
2:B:418:TRP:CH2	2:B:444:PRO:HD3	2.38	0.59
4:E:478:GLY:HA2	4:E:514:ARG:HB3	1.83	0.59
8:P:128:ARG:HE	8:P:320:PRO:HB3	1.67	0.59
8:P:248:VAL:HG12	8:P:311:SER:H	1.66	0.59
1:A:551:THR:HG23	1:A:551:THR:O	2.02	0.59
4:F:543:LEU:CD2	4:F:548:THR:HG21	2.32	0.59
5:J:42:PRO:HG3	5:J:102:THR:HG22	1.85	0.59
7:L:574:THR:HG23	7:L:574:THR:O	2.01	0.59
8:P:281:LEU:HD11	8:P:290:PHE:CE2	2.35	0.59
8:P:342:LYS:HE2	8:P:438:LYS:CE	2.32	0.59
8:P:342:LYS:CA	8:P:438:LYS:O	2.51	0.59
8:P:523:TRP:CH2	8:P:539:ALA:HB1	2.37	0.59
3:C:567:VAL:O	3:C:567:VAL:HG22	2.03	0.59
4:F:550:ARG:HG2	4:F:550:ARG:HH11	1.66	0.59
8:P:132:ILE:CD1	8:P:187:VAL:HG23	2.33	0.59
2:B:443:ARG:HD3	2:B:443:ARG:O	2.02	0.59
4:E:374:THR:OG1	4:E:398:GLU:O	2.18	0.59
4:E:493:GLN:CB	4:E:494:PRO:CD	2.64	0.59
7:L:537:VAL:HG13	7:L:537:VAL:O	2.02	0.59
8:P:43:ARG:HG2	8:P:43:ARG:O	2.03	0.59
8:P:361:LYS:CB	8:P:364:LYS:HE2	2.33	0.59
12:V:28:GLU:CA	12:V:96:GLU:OE1	2.51	0.59
1:A:493:GLN:CB	1:A:494:PRO:CD	2.73	0.59
7:L:363:THR:HG21	7:L:418:TRP:HB2	1.85	0.59
10:S:23:VAL:HB	10:S:35:ILE:HD13	1.85	0.59
11:U:101:VAL:O	11:U:101:VAL:HG13	2.02	0.59
4:E:456:LEU:HD23	4:E:552:VAL:HG12	1.83	0.58
4:G:468:GLU:HG2	10:S:60:THR:HG21	1.85	0.58
5:J:40:ILE:HD13	6:K:574:THR:HG21	1.83	0.58
8:P:159:ILE:HD11	8:P:173:ILE:HG21	1.85	0.58
9:R:20:LEU:CD2	9:R:117:LYS:HB2	2.33	0.58
11:U:41:GLU:OE1	11:U:41:GLU:HA	2.03	0.58
12:V:94:LEU:HD23	12:V:96:GLU:HG2	1.84	0.58
3:C:368:LEU:HD11	3:C:406:SER:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:565:SER:HB3	4:E:583:NAG:H62	1.85	0.58
4:F:545:ASN:HB3	4:G:358:PHE:CZ	2.38	0.58
8:P:149:LYS:O	8:P:155:PRO:HA	2.03	0.58
3:C:565:SER:O	3:C:565:SER:OG	2.17	0.58
4:E:354:PHE:HA	4:E:357:ILE:HG12	1.85	0.58
4:G:467:ARG:HH11	4:G:467:ARG:CG	2.16	0.58
8:P:445:ASN:O	8:P:467:PRO:CD	2.48	0.58
8:P:35:LYS:HB2	8:P:52:SER:HB2	1.85	0.58
8:P:122:TYR:HE2	8:P:132:ILE:HG23	1.68	0.58
8:P:131:THR:HG22	8:P:188:VAL:CA	2.33	0.58
8:P:528:VAL:HG13	8:P:535:GLY:HA3	1.85	0.58
9:R:20:LEU:CG	9:R:117:LYS:HG3	2.22	0.58
9:R:111:ASP:O	9:R:114:LYS:HD2	2.03	0.58
10:S:94:LEU:HD12	10:S:94:LEU:O	2.02	0.58
2:B:451:ARG:HB2	2:B:451:ARG:HH11	1.68	0.58
4:G:378:VAL:HG21	4:G:405:PHE:CE2	2.38	0.58
8:P:398:LEU:CD1	8:P:407:THR:O	2.52	0.58
9:R:45:ARG:NH2	9:R:110:THR:OG1	2.37	0.58
11:U:104:CYS:HB2	11:U:116:GLN:HG2	1.84	0.58
7:L:400:HIS:CE1	7:L:405:PHE:HA	2.38	0.58
8:P:189:ILE:HG23	8:P:192:LEU:HD11	1.85	0.58
8:P:476:TYR:CD1	8:P:529:LYS:HB2	2.38	0.58
2:B:423:ARG:HA	2:B:442:SER:HB2	1.86	0.58
4:F:449:LEU:HA	4:F:480:SER:HB2	1.84	0.58
4:H:562:TYR:CD2	4:H:562:TYR:N	2.71	0.58
6:K:520:ILE:O	6:K:520:ILE:HG23	2.03	0.58
7:L:430:HIS:CE1	7:L:432:ASP:HB3	2.37	0.58
12:V:22:GLU:HA	12:V:118:VAL:HA	1.84	0.58
1:A:393:HIS:HA	1:A:410:GLU:HB3	1.84	0.58
4:D:421:GLY:N	4:D:445:LYS:HZ2	1.82	0.58
2:B:454:VAL:HB	2:B:476:VAL:HG12	1.85	0.58
3:C:459:PRO:HD3	3:C:472:ILE:HG12	1.85	0.58
4:F:563:ASN:OD1	4:F:583:NAG:N2	2.36	0.58
5:J:31:ASP:HB2	7:L:554:LYS:NZ	2.19	0.58
6:K:545:ASN:ND2	6:K:545:ASN:H	2.00	0.58
7:L:424:PHE:CA	7:L:441:ILE:CD1	2.45	0.58
7:L:540:HIS:ND1	7:L:542:ALA:HB3	2.18	0.58
1:A:356:SER:N	5:J:117:TYR:HH	2.00	0.58
4:E:537:VAL:O	4:E:537:VAL:HG12	2.03	0.58
4:H:393:HIS:HB2	4:H:396:ILE:HD11	1.86	0.58
6:K:448:ALA:HB1	6:K:481:PRO:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:314:GLN:HE21	8:P:314:GLN:HA	1.69	0.58
9:R:47:TYR:CE2	9:R:49:CYS:HB2	2.38	0.58
10:S:99:SER:CB	10:S:120:LEU:HB3	2.34	0.58
12:V:84:LYS:HE3	12:V:86:LEU:HD23	1.86	0.58
3:C:567:VAL:HB	4:D:567:VAL:HG13	1.86	0.57
5:J:116:VAL:O	5:J:116:VAL:HG22	2.04	0.57
6:K:354:PHE:CE1	6:K:541:GLU:CA	2.87	0.57
7:L:367:CYS:HB2	7:L:382:TRP:CE3	2.38	0.57
7:L:450:HIS:CA	7:L:480:SER:CB	2.81	0.57
7:L:450:HIS:NE2	9:R:65:THR:HG22	2.18	0.57
8:P:398:LEU:HD13	8:P:407:THR:O	2.03	0.57
2:B:450:HIS:O	2:B:542:ALA:HB2	2.03	0.57
4:H:445:LYS:HA	4:H:445:LYS:HE3	1.86	0.57
8:P:314:GLN:HE21	8:P:314:GLN:N	2.02	0.57
9:R:46:ILE:N	9:R:64:THR:HG21	2.18	0.57
4:E:524:SER:OG	4:E:527:GLU:OE1	2.22	0.57
4:E:535:THR:CG2	4:E:550:ARG:O	2.52	0.57
4:H:364:LYS:HE3	4:H:410:GLU:HB3	1.87	0.57
8:P:529:LYS:NZ	8:P:534:TYR:CZ	2.71	0.57
3:C:556:THR:O	3:C:556:THR:HG22	2.04	0.57
4:D:349:ALA:HB2	4:D:439:GLN:HG3	1.85	0.57
4:D:377:SER:O	4:D:431:THR:OG1	2.22	0.57
5:J:36:ASN:ND2	7:L:563:ASN:OD1	2.37	0.57
5:J:116:VAL:O	5:J:116:VAL:HG13	2.05	0.57
11:U:102:TYR:HB2	11:U:118:VAL:CG2	2.34	0.57
1:A:489:MET:CE	1:A:537:VAL:HG21	2.33	0.57
5:J:52:PRO:HG3	5:J:128:LEU:HD21	1.86	0.57
7:L:540:HIS:ND1	7:L:542:ALA:CB	2.67	0.57
6:K:366:THR:HG23	6:K:409:GLY:H	1.69	0.57
6:K:476:VAL:O	6:K:476:VAL:HG12	2.04	0.57
1:A:491:ARG:HG2	1:A:491:ARG:O	2.04	0.57
6:K:521:LEU:HD23	6:K:521:LEU:C	2.25	0.57
8:P:475:LYS:HE2	8:P:475:LYS:N	2.20	0.57
1:A:488:TRP:NE1	1:A:519:SER:OG	2.24	0.57
1:A:491:ARG:HH11	1:A:491:ARG:CG	2.16	0.57
4:D:534:TYR:N	4:D:534:TYR:CD1	2.73	0.57
4:E:400:HIS:HB3	4:E:404:THR:H	1.69	0.57
7:L:543:LEU:HD13	7:L:543:LEU:N	2.19	0.57
8:P:201:LEU:HD13	8:P:214:ASN:HA	1.86	0.57
8:P:541:TYR:N	8:P:541:TYR:CD1	2.73	0.57
1:A:501:VAL:HG13	1:A:501:VAL:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:452:PRO:HD2	4:F:543:LEU:HG	1.86	0.57
4:G:398:GLU:HG3	4:G:399:SER:H	1.70	0.57
4:G:475:LEU:HG	4:G:475:LEU:O	2.04	0.57
7:L:534:TYR:CD2	7:L:534:TYR:N	2.73	0.57
8:P:147:LEU:HB3	8:P:159:ILE:HB	1.86	0.57
8:P:368:LEU:HB2	8:P:378:PRO:HD3	1.83	0.57
1:A:359:LEU:CD1	5:J:117:TYR:CB	2.82	0.57
1:A:489:MET:CE	1:A:537:VAL:CG2	2.83	0.57
3:C:566:LEU:H	3:C:566:LEU:CD1	2.01	0.57
4:F:548:THR:HG23	4:F:548:THR:O	2.05	0.57
11:U:22:GLU:HB2	11:U:119:THR:C	2.22	0.57
4:D:374:THR:HG22	4:D:403:ALA:HB1	1.85	0.56
4:G:363:THR:HG21	4:G:418:TRP:HB3	1.86	0.56
1:A:520:ILE:HD13	2:B:475:LEU:HD11	1.87	0.56
4:D:454:VAL:HG21	4:D:538:VAL:HG21	1.87	0.56
4:E:489:MET:SD	4:E:493:GLN:HA	2.45	0.56
4:H:568:MET:O	4:H:570:ASP:N	2.38	0.56
6:K:452:PRO:HD2	6:K:543:LEU:HG	1.86	0.56
13:I:2:NAG:O6	13:I:2:NAG:O4	2.02	0.56
2:B:484:VAL:HG13	2:B:484:VAL:O	2.05	0.56
4:E:364:LYS:NZ	4:E:412:SER:OG	2.31	0.56
6:K:477:THR:HG22	6:K:516:PHE:HB2	1.86	0.56
8:P:523:TRP:HZ3	8:P:539:ALA:HB1	1.68	0.56
9:R:35:ILE:HD12	9:R:118:VAL:HG11	1.87	0.56
10:S:72:TYR:HD2	10:S:72:TYR:N	2.03	0.56
11:U:22:GLU:HB3	11:U:119:THR:HG22	1.86	0.56
11:U:118:VAL:HG23	11:U:118:VAL:O	2.04	0.56
1:A:501:VAL:O	1:A:501:VAL:HG22	2.03	0.56
3:C:486:VAL:HG22	3:C:538:VAL:HG22	1.87	0.56
4:E:437:LEU:HG	4:E:438:LYS:H	1.69	0.56
4:G:396:ILE:HD11	4:G:407:ALA:HB1	1.88	0.56
4:G:467:ARG:O	10:S:60:THR:HG22	2.06	0.56
4:H:456:LEU:HD12	4:H:536:CYS:HB3	1.86	0.56
8:P:149:LYS:CD	8:P:151:ILE:HG22	2.34	0.56
4:H:479:PHE:HB2	4:H:540:HIS:CE1	2.41	0.56
6:K:478:GLY:HA2	6:K:514:ARG:HB3	1.86	0.56
3:C:508:GLU:CG	3:C:509:PRO:HD2	2.17	0.56
4:D:367:CYS:HB3	4:D:382:TRP:CZ2	2.40	0.56
4:H:452:PRO:HD2	4:H:543:LEU:HG	1.88	0.56
6:K:560:THR:O	6:K:560:THR:HG23	2.05	0.56
8:P:315:LEU:HG	8:P:315:LEU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:407:THR:O	8:P:407:THR:HG22	2.06	0.56
2:B:564:VAL:CG2	3:C:564:VAL:HA	2.35	0.56
4:D:369:VAL:HG11	4:D:378:VAL:HG21	1.87	0.56
4:D:429:THR:HB	4:D:436:PRO:HA	1.87	0.56
4:E:367:CYS:H	4:E:382:TRP:HH2	1.52	0.56
8:P:286:LYS:C	8:P:286:LYS:HD3	2.26	0.56
11:U:51:GLU:HA	11:U:58:CYS:HA	1.88	0.56
1:A:450:HIS:N	1:A:450:HIS:CD2	2.72	0.56
4:G:501:VAL:O	4:G:501:VAL:HG12	2.06	0.56
4:G:502:THR:HG23	4:G:502:THR:O	2.04	0.56
5:J:64:LEU:H	5:J:64:LEU:CD2	2.18	0.56
8:P:366:TRP:CZ2	8:P:408:VAL:HG21	2.41	0.56
8:P:431:TRP:N	8:P:431:TRP:CD1	2.72	0.56
8:P:462:VAL:CB	8:P:509:VAL:HB	2.34	0.56
9:R:91:VAL:HG12	9:R:93:GLN:O	2.06	0.56
4:D:380:ILE:HD12	4:D:393:HIS:CD2	2.41	0.56
6:K:510:GLN:CG	7:L:522:THR:HG23	2.27	0.56
7:L:487:GLN:HB3	7:L:537:VAL:HG11	1.88	0.56
8:P:471:SER:C	8:P:475:LYS:NZ	2.59	0.56
9:R:20:LEU:HD22	9:R:20:LEU:C	2.26	0.56
10:S:34:THR:HB	10:S:88:LEU:HD11	1.88	0.56
1:A:564:VAL:HG22	2:B:564:VAL:HA	1.88	0.56
6:K:535:THR:HA	6:K:550:ARG:O	2.06	0.56
7:L:452:PRO:HB3	7:L:479:PHE:HD1	1.71	0.56
4:G:506:MET:HE3	4:G:516:PHE:HE2	1.71	0.55
5:J:21:ILE:CD1	7:L:555:SER:CB	2.65	0.55
8:P:250:LYS:HA	8:P:309:ALA:HA	1.87	0.55
10:S:61:VAL:HG13	10:S:72:TYR:CD1	2.41	0.55
2:B:449:LEU:HA	2:B:480:SER:HG	1.72	0.55
4:H:532:GLU:O	4:H:553:ASP:HB3	2.05	0.55
5:J:17:ILE:HD11	5:J:64:LEU:HD12	1.87	0.55
6:K:380:ILE:HB	6:K:393:HIS:HD2	1.71	0.55
8:P:421:TYR:CZ	8:P:437:ILE:HD12	2.37	0.55
2:B:451:ARG:CB	2:B:451:ARG:CZ	2.84	0.55
3:C:478:GLY:HA2	3:C:514:ARG:HG2	1.89	0.55
4:E:491:ARG:HG2	12:V:44:VAL:HG11	1.88	0.55
4:G:516:PHE:C	4:G:516:PHE:CD2	2.80	0.55
4:H:443:ARG:N	4:H:444:PRO:HD3	2.22	0.55
4:H:554:LYS:HE2	4:H:558:LYS:NZ	2.21	0.55
8:P:469:LYS:HG2	8:P:469:LYS:O	2.05	0.55
9:R:61:VAL:HG21	9:R:72:TYR:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:529:ASN:C	4:H:531:GLY:H	2.10	0.55
7:L:369:VAL:HG12	7:L:372:LEU:HD21	1.88	0.55
8:P:317:GLU:N	8:P:317:GLU:OE2	2.39	0.55
8:P:491:GLN:HE22	8:P:510:SER:HB2	1.72	0.55
2:B:553:ASP:OD1	2:B:554:LYS:N	2.36	0.55
8:P:395:LEU:CA	8:P:410:LEU:HD12	2.35	0.55
10:S:23:VAL:HG22	10:S:25:VAL:HG23	1.89	0.55
1:A:356:SER:N	5:J:117:TYR:CE2	2.75	0.55
1:A:574:THR:HA	6:K:461:ARG:NH1	2.21	0.55
2:B:461:ARG:CZ	7:L:570:ASP:OD2	2.55	0.55
3:C:423:ARG:HE	3:C:442:SER:HB3	1.71	0.55
5:J:21:ILE:CD1	7:L:554:LYS:HG2	2.37	0.55
7:L:424:PHE:N	7:L:441:ILE:HG13	2.10	0.55
7:L:424:PHE:CD2	7:L:441:ILE:HD13	2.41	0.55
7:L:450:HIS:CB	7:L:480:SER:CB	2.78	0.55
7:L:511:ALA:O	7:L:514:ARG:CG	2.55	0.55
8:P:38:CYS:SG	8:P:91:LYS:HB2	2.47	0.55
8:P:450:GLY:H	8:P:540:VAL:HG12	1.67	0.55
2:B:454:VAL:CG1	2:B:538:VAL:HG11	2.36	0.55
4:H:443:ARG:N	4:H:444:PRO:CD	2.68	0.55
7:L:508:GLU:CG	7:L:514:ARG:HB2	2.36	0.55
7:L:508:GLU:HG3	7:L:514:ARG:HB2	1.89	0.55
7:L:511:ALA:CB	7:L:514:ARG:HG2	2.34	0.55
8:P:249:ALA:O	8:P:309:ALA:HA	2.06	0.55
8:P:371:GLY:H	8:P:375:GLY:HA2	1.72	0.55
2:B:445:LYS:HZ3	2:B:445:LYS:N	2.05	0.55
4:D:384:ARG:NH1	4:D:390:VAL:HA	2.22	0.55
10:S:72:TYR:N	10:S:72:TYR:CD2	2.72	0.55
1:A:423:ARG:HE	1:A:440:THR:HG23	1.71	0.55
3:C:454:VAL:HG13	3:C:474:CYS:SG	2.46	0.55
4:D:369:VAL:HB	4:D:428:VAL:HG11	1.89	0.55
4:E:450:HIS:CE1	4:E:514:ARG:CZ	2.90	0.55
4:F:520:ILE:O	4:F:520:ILE:HG13	2.05	0.55
6:K:563:ASN:HB3	7:L:563:ASN:CA	2.35	0.55
8:P:39:ARG:HB2	8:P:49:LEU:HD11	1.87	0.55
13:I:1:NAG:C1	13:I:1:NAG:C8	2.85	0.55
2:B:422:GLU:H	2:B:443:ARG:HE	1.55	0.55
2:B:430:HIS:CE1	2:B:433:LEU:HB2	2.42	0.55
4:H:454:VAL:HG21	4:H:538:VAL:HG21	1.89	0.55
5:J:35:ARG:HH11	5:J:35:ARG:CG	2.19	0.55
6:K:354:PHE:CE1	6:K:541:GLU:CB	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:537:VAL:HG22	4:F:549:GLU:HB3	1.89	0.54
4:H:568:MET:O	4:H:569:SER:C	2.45	0.54
6:K:535:THR:CG2	6:K:551:THR:OG1	2.54	0.54
6:K:571:THR:O	6:K:572:ALA:C	2.45	0.54
8:P:471:SER:C	8:P:475:LYS:HZ1	2.05	0.54
1:A:400:HIS:ND1	1:A:402:ASN:OD1	2.39	0.54
4:G:476:VAL:O	4:G:476:VAL:HG12	2.06	0.54
6:K:496:SER:HG	6:K:499:LYS:HZ3	1.49	0.54
10:S:39:LEU:O	10:S:39:LEU:HD23	2.07	0.54
1:A:391:LYS:HA	1:A:391:LYS:HE3	1.90	0.54
4:E:454:VAL:HG22	4:E:538:VAL:HG21	1.87	0.54
4:E:479:PHE:HB2	4:E:540:HIS:CE1	2.41	0.54
6:K:464:LEU:HD11	6:K:525:GLU:CD	2.24	0.54
3:C:346:ARG:HG2	3:C:371:ASP:OD1	2.08	0.54
4:G:463:GLN:HG2	4:H:455:TYR:CZ	2.42	0.54
6:K:481:PRO:HG2	6:K:541:GLU:OE2	2.06	0.54
8:P:425:THR:O	8:P:430:LEU:CD2	2.54	0.54
3:C:419:ASN:OD1	3:C:420:SER:N	2.40	0.54
7:L:523:VAL:HG11	7:L:534:TYR:HE1	1.71	0.54
8:P:361:LYS:HB3	8:P:364:LYS:HE2	1.90	0.54
8:P:446:LEU:C	8:P:465:HIS:O	2.41	0.54
8:P:447:LYS:N	8:P:465:HIS:N	2.46	0.54
8:P:450:GLY:H	8:P:540:VAL:CG1	2.20	0.54
9:R:99:SER:HB2	9:R:120:LEU:HB2	1.89	0.54
4:F:348:PHE:HB3	4:F:369:VAL:HA	1.90	0.54
6:K:512:PRO:HD2	6:K:514:ARG:HG2	1.90	0.54
7:L:354:PHE:CD2	7:L:546:ARG:NH2	2.75	0.54
7:L:414:CYS:SG	8:P:497:LYS:NZ	2.75	0.54
8:P:263:VAL:HG21	8:P:314:GLN:NE2	2.23	0.54
8:P:399:GLU:O	8:P:406:PHE:HA	2.08	0.54
8:P:450:GLY:HA2	8:P:463:PRO:HD2	1.90	0.54
9:R:116:GLN:NE2	9:R:116:GLN:O	2.41	0.54
1:A:566:LEU:N	1:A:566:LEU:CD1	2.70	0.54
2:B:418:TRP:CE3	2:B:443:ARG:HD3	2.40	0.54
2:B:476:VAL:HG23	2:B:479:PHE:HE1	1.73	0.54
4:D:364:LYS:HA	4:D:411:ALA:O	2.08	0.54
4:E:482:ALA:CA	4:E:515:TYR:CE2	2.91	0.54
7:L:481:PRO:HD2	7:L:540:HIS:NE2	2.20	0.54
8:P:289:SER:O	8:P:289:SER:OG	2.20	0.54
12:V:61:VAL:HA	12:V:69:LYS:HB2	1.90	0.54
4:F:486:VAL:HG22	4:F:538:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:456:LEU:CG	7:L:552:VAL:HG21	2.35	0.54
8:P:462:VAL:HG11	8:P:509:VAL:CG1	2.37	0.54
4:D:454:VAL:CG2	4:D:538:VAL:HG21	2.38	0.54
8:P:473:TYR:CD2	8:P:473:TYR:N	2.76	0.54
2:B:531:GLY:HA2	2:B:554:LYS:HB2	1.90	0.54
3:C:448:ALA:O	3:C:481:PRO:HD3	2.08	0.54
7:L:456:LEU:CG	7:L:552:VAL:CG2	2.85	0.54
8:P:314:GLN:HA	8:P:314:GLN:NE2	2.23	0.54
4:D:487:GLN:NE2	4:D:494:PRO:HB3	2.22	0.53
2:B:473:THR:HG22	2:B:520:ILE:HG22	1.90	0.53
4:F:502:THR:O	4:F:502:THR:HG22	2.08	0.53
4:H:445:LYS:HA	4:H:445:LYS:CE	2.38	0.53
7:L:346:ARG:HG2	7:L:370:THR:H	1.73	0.53
8:P:264:VAL:HG13	8:P:275:PHE:HD2	1.66	0.53
8:P:264:VAL:CG1	8:P:275:PHE:CE2	2.91	0.53
8:P:366:TRP:CZ3	8:P:380:LEU:CD1	2.87	0.53
9:R:22:GLU:HG3	9:R:119:THR:HG22	1.90	0.53
1:A:489:MET:HE1	1:A:537:VAL:CG2	2.38	0.53
1:A:538:VAL:HG22	1:A:548:THR:CG2	2.38	0.53
3:C:457:LEU:CD1	4:D:457:LEU:HD23	2.38	0.53
4:F:449:LEU:CA	4:F:480:SER:HB2	2.37	0.53
6:K:463:GLN:HB2	7:L:455:TYR:CE1	2.37	0.53
8:P:445:ASN:OD1	8:P:467:PRO:CG	2.51	0.53
2:B:419:ASN:CA	2:B:443:ARG:NH1	2.72	0.53
8:P:121:VAL:HA	8:P:216:ASP:HB3	1.90	0.53
8:P:541:TYR:N	8:P:541:TYR:HD1	2.06	0.53
11:U:105:GLY:HA2	11:U:115:THR:HG23	1.90	0.53
8:P:24:TYR:CD2	8:P:30:ASN:HB3	2.43	0.53
8:P:355:TYR:CD1	8:P:405:THR:HA	2.44	0.53
8:P:447:LYS:HE2	8:P:465:HIS:CG	2.44	0.53
1:A:384:ARG:NH1	1:A:388:GLU:OE2	2.42	0.53
1:A:483:ASP:O	1:A:540:HIS:CD2	2.62	0.53
3:C:457:LEU:CD1	3:C:473:THR:HG1	2.21	0.53
3:C:473:THR:HG22	3:C:520:ILE:HG22	1.91	0.53
6:K:562:TYR:N	6:K:562:TYR:HD1	2.06	0.53
8:P:37:TRP:HB3	8:P:50:ILE:HG22	1.89	0.53
8:P:134:CYS:O	8:P:185:PHE:HB3	2.09	0.53
8:P:197:ALA:HB2	8:P:219:VAL:HG13	1.91	0.53
8:P:477:TRP:HD1	8:P:526:CYS:HB2	1.74	0.53
4:E:383:THR:HB	4:E:387:GLY:HA2	1.91	0.53
4:E:482:ALA:CA	4:E:515:TYR:HE2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:355:TYR:HE1	8:P:405:THR:O	1.92	0.53
2:B:382:TRP:HH2	2:B:441:ILE:CD1	2.00	0.53
2:B:418:TRP:CE3	2:B:442:SER:OG	2.61	0.53
3:C:477:THR:OG1	3:C:508:GLU:OE2	2.26	0.53
4:G:482:ALA:HB2	4:G:515:TYR:CE2	2.44	0.53
6:K:491:ARG:O	6:K:493:GLN:N	2.41	0.53
8:P:447:LYS:CD	8:P:465:HIS:HB3	2.37	0.53
3:C:506:MET:HG3	3:C:507:PRO:HD2	1.91	0.53
6:K:480:SER:HB2	6:K:481:PRO:HD3	1.91	0.53
8:P:479:LYS:HG3	8:P:524:TYR:HE1	1.73	0.53
1:A:459:PRO:HG2	1:A:470:ALA:HB1	1.90	0.53
1:A:538:VAL:CG2	1:A:548:THR:HG22	2.38	0.53
4:F:471:THR:HG22	4:F:522:THR:HG23	1.91	0.53
8:P:340:VAL:HG11	8:P:436:GLU:CD	2.29	0.53
9:R:46:ILE:N	9:R:64:THR:HG23	2.15	0.53
10:S:39:LEU:CD2	10:S:85:ASN:C	2.78	0.53
2:B:489:MET:HG2	2:B:494:PRO:HA	1.91	0.52
3:C:426:CYS:HB3	3:C:439:GLN:HB2	1.91	0.52
4:E:480:SER:O	4:E:480:SER:OG	2.25	0.52
4:G:481:PRO:HD2	4:G:540:HIS:CE1	2.44	0.52
4:G:482:ALA:HB2	4:G:515:TYR:CZ	2.44	0.52
7:L:511:ALA:HB2	7:L:514:ARG:HD2	1.81	0.52
8:P:8:GLU:OE1	8:P:8:GLU:N	2.42	0.52
8:P:463:PRO:HA	8:P:508:LEU:HD12	1.91	0.52
9:R:22:GLU:OE1	9:R:101:VAL:CG1	2.44	0.52
10:S:75:ARG:HG3	10:S:91:VAL:HG13	1.90	0.52
11:U:36:LYS:HA	11:U:88:LEU:HD23	1.90	0.52
1:A:466:LEU:N	1:A:466:LEU:CD1	2.72	0.52
1:A:489:MET:HG2	1:A:494:PRO:HA	1.91	0.52
1:A:538:VAL:HG22	1:A:548:THR:HG23	1.91	0.52
4:E:535:THR:HG22	4:E:550:ARG:O	2.10	0.52
6:K:356:SER:O	6:K:360:THR:OG1	2.25	0.52
6:K:508:GLU:HG3	6:K:514:ARG:HB2	1.89	0.52
6:K:562:TYR:N	6:K:562:TYR:CD1	2.71	0.52
1:A:508:GLU:HG2	1:A:509:PRO:CD	2.40	0.52
4:F:456:LEU:HD11	4:F:536:CYS:HB3	1.91	0.52
6:K:480:SER:HA	6:K:513:GLY:O	2.09	0.52
7:L:449:LEU:HA	7:L:480:SER:HB3	1.89	0.52
3:C:466:LEU:HD21	12:V:45:ARG:CZ	2.39	0.52
7:L:556:THR:O	7:L:556:THR:HG23	2.10	0.52
8:P:196:ASP:O	8:P:200:TYR:OH	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:344:VAL:HG21	8:P:444:PRO:HA	1.92	0.52
8:P:470:PHE:CZ	8:P:528:VAL:HB	2.43	0.52
8:P:491:GLN:NE2	8:P:510:SER:HB2	2.24	0.52
4:F:449:LEU:N	4:F:449:LEU:CD2	2.73	0.52
4:F:453:ASP:OD2	4:F:455:TYR:OH	2.21	0.52
5:J:35:ARG:CG	5:J:35:ARG:NH1	2.70	0.52
7:L:430:HIS:HE1	7:L:432:ASP:HB3	1.74	0.52
11:U:48:LEU:HB2	11:U:89:VAL:HG11	1.91	0.52
6:K:558:LYS:NZ	7:L:461:ARG:HE	2.06	0.52
9:R:37:CYS:HA	9:R:116:GLN:HG3	1.91	0.52
2:B:345:ILE:N	2:B:370:THR:O	2.43	0.52
7:L:456:LEU:CD2	7:L:552:VAL:HG21	2.32	0.52
9:R:25:VAL:HB	9:R:120:LEU:HG	1.91	0.52
2:B:454:VAL:HG22	2:B:550:ARG:CG	2.38	0.52
3:C:451:ARG:NH1	3:C:451:ARG:CG	2.72	0.52
7:L:450:HIS:CE1	9:R:65:THR:HG22	2.45	0.52
8:P:261:CYS:O	8:P:263:VAL:N	2.43	0.52
5:J:40:ILE:CD1	6:K:574:THR:HG21	2.39	0.52
6:K:565:SER:O	6:K:565:SER:OG	2.19	0.52
8:P:314:GLN:CA	8:P:314:GLN:NE2	2.72	0.52
11:U:22:GLU:CB	11:U:119:THR:N	2.72	0.52
1:A:489:MET:HE1	1:A:537:VAL:HG21	1.91	0.52
4:E:493:GLN:NE2	4:E:493:GLN:N	2.58	0.52
4:F:449:LEU:HD22	4:F:449:LEU:N	2.25	0.52
7:L:526:GLU:O	7:L:530:THR:HG23	2.10	0.52
1:A:356:SER:CA	5:J:117:TYR:CE2	2.92	0.51
4:E:368:LEU:HD21	4:E:406:SER:HB2	1.92	0.51
4:F:474:CYS:HB2	4:F:488:TRP:CZ2	2.45	0.51
6:K:450:HIS:NE2	6:K:514:ARG:NH1	2.54	0.51
8:P:227:VAL:HG23	8:P:326:LEU:HA	1.92	0.51
1:A:518:HIS:HE1	2:B:520:ILE:HG23	1.70	0.51
1:A:535:THR:HG22	1:A:551:THR:CB	2.37	0.51
4:E:467:ARG:HD3	4:E:525:GLU:HG3	1.92	0.51
7:L:354:PHE:HD2	7:L:546:ARG:HH21	1.55	0.51
8:P:63:ARG:NH2	8:P:86:ASP:OD2	2.41	0.51
8:P:355:TYR:CE1	8:P:405:THR:CA	2.93	0.51
8:P:525:TRP:CE3	8:P:537:THR:HG22	2.44	0.51
10:S:79:LYS:HD3	10:S:80:GLN:H	1.75	0.51
1:A:564:VAL:CG2	2:B:564:VAL:HA	2.40	0.51
3:C:429:THR:HG22	3:C:436:PRO:HB3	1.92	0.51
4:H:495:LEU:HD22	4:H:499:LYS:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:518:HIS:ND1	7:L:518:HIS:CG	2.78	0.51
1:A:467:ARG:HG3	1:A:525:GLU:OE1	2.11	0.51
3:C:466:LEU:CD2	12:V:45:ARG:CZ	2.88	0.51
4:D:562:TYR:CE1	4:H:568:MET:SD	3.04	0.51
4:F:373:THR:HB	4:F:375:TYR:HE1	1.75	0.51
8:P:361:LYS:HG2	8:P:364:LYS:HE3	1.91	0.51
8:P:450:GLY:N	8:P:540:VAL:HG13	2.26	0.51
4:E:453:ASP:OD2	4:E:455:TYR:OH	2.27	0.51
4:F:543:LEU:HD22	4:F:548:THR:HG21	1.92	0.51
4:G:518:HIS:NE2	4:H:520:ILE:HD11	2.25	0.51
8:P:295:THR:HG22	8:P:432:ARG:HB2	1.93	0.51
8:P:361:LYS:HD2	8:P:361:LYS:C	2.30	0.51
8:P:525:TRP:CZ3	8:P:537:THR:CG2	2.92	0.51
12:V:112:ARG:CB	12:V:112:ARG:NH1	2.73	0.51
2:B:349:ALA:HB1	2:B:441:ILE:HG12	1.92	0.51
3:C:482:ALA:CB	3:C:515:TYR:CE1	2.91	0.51
4:F:546:ARG:CG	4:F:546:ARG:NH1	2.72	0.51
5:J:28:PRO:HG3	7:L:467:ARG:NH2	2.24	0.51
6:K:423:ARG:HG3	6:K:442:SER:HB2	1.93	0.51
8:P:127:GLY:N	8:P:192:LEU:O	2.35	0.51
2:B:441:ILE:HD12	2:B:442:SER:H	1.76	0.51
2:B:443:ARG:CD	2:B:443:ARG:N	2.71	0.51
2:B:445:LYS:NZ	2:B:445:LYS:CB	2.72	0.51
2:B:498:GLU:O	2:B:498:GLU:HG2	2.11	0.51
4:H:453:ASP:OD1	4:H:455:TYR:OH	2.18	0.51
6:K:510:GLN:OE1	6:K:510:GLN:HA	2.09	0.51
8:P:368:LEU:CD1	8:P:378:PRO:HG2	2.39	0.51
1:A:380:ILE:H	1:A:393:HIS:CD2	2.29	0.51
4:D:421:GLY:CA	4:D:445:LYS:HZ1	2.10	0.51
4:G:352:PRO:HD3	4:G:365:LEU:HD13	1.92	0.51
8:P:132:ILE:HD12	8:P:187:VAL:O	2.11	0.51
8:P:239:CYS:HB2	8:P:290:PHE:CE1	2.46	0.51
8:P:248:VAL:HG12	8:P:311:SER:N	2.26	0.51
4:G:516:PHE:C	4:G:516:PHE:HD2	2.14	0.51
7:L:514:ARG:CA	7:L:514:ARG:NH1	2.73	0.51
8:P:60:TYR:HB3	8:P:64:ALA:HB3	1.93	0.51
8:P:368:LEU:CG	8:P:378:PRO:HG2	2.40	0.51
8:P:391:TYR:N	8:P:391:TYR:CD1	2.79	0.51
10:S:29:LEU:HD22	10:S:95:THR:CG2	2.27	0.51
11:U:72:TYR:HA	11:U:75:ARG:HD3	1.92	0.51
1:A:400:HIS:HD2	1:A:406:SER:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:365:LEU:HD23	7:L:413:ILE:HD11	1.93	0.51
4:D:393:HIS:CD2	4:D:393:HIS:H	2.27	0.50
4:G:502:THR:HA	4:G:519:SER:HA	1.93	0.50
7:L:523:VAL:HG11	7:L:534:TYR:CE1	2.46	0.50
7:L:540:HIS:HB3	7:L:543:LEU:CG	2.32	0.50
8:P:446:LEU:CD2	8:P:538:ALA:CA	2.90	0.50
8:P:470:PHE:O	8:P:473:TYR:CE2	2.64	0.50
6:K:537:VAL:HG12	6:K:549:GLU:HG2	1.93	0.50
8:P:253:CYS:HB2	8:P:306:LEU:HB2	1.93	0.50
1:A:477:THR:HG22	1:A:508:GLU:OE2	2.12	0.50
4:G:450:HIS:CD2	4:G:514:ARG:NH1	2.80	0.50
5:J:21:ILE:CG1	7:L:555:SER:CB	2.90	0.50
8:P:243:PRO:CA	8:P:246:ALA:HB2	2.37	0.50
8:P:464:CYS:O	8:P:507:ARG:C	2.50	0.50
8:P:529:LYS:CG	8:P:534:TYR:HE2	2.17	0.50
9:R:28:GLU:HG3	9:R:29:LEU:H	1.76	0.50
11:U:48:LEU:HD22	11:U:89:VAL:HG21	1.93	0.50
3:C:384:ARG:NH2	3:C:422:GLU:O	2.44	0.50
4:E:484:VAL:O	4:E:484:VAL:HG13	2.12	0.50
4:F:523:VAL:CG1	4:F:534:TYR:OH	2.60	0.50
4:H:365:LEU:HD11	4:H:418:TRP:CZ2	2.40	0.50
6:K:477:THR:CG2	6:K:516:PHE:HB2	2.41	0.50
1:A:384:ARG:HG2	1:A:385:GLN:H	1.77	0.50
1:A:459:PRO:CB	1:A:470:ALA:HB1	2.41	0.50
1:A:516:PHE:C	1:A:516:PHE:CD2	2.85	0.50
2:B:418:TRP:HE3	2:B:443:ARG:HD2	1.61	0.50
2:B:368:LEU:HG	2:B:406:SER:HA	1.94	0.50
4:F:545:ASN:N	4:F:545:ASN:ND2	2.58	0.50
6:K:430:HIS:CD2	6:K:432:ASP:HB2	2.47	0.50
6:K:490:GLN:O	6:K:490:GLN:HG3	2.10	0.50
8:P:448:VAL:HG23	8:P:463:PRO:CG	2.41	0.50
8:P:470:PHE:O	8:P:473:TYR:CD2	2.64	0.50
12:V:48:LEU:HD21	12:V:102:TYR:CG	2.47	0.50
1:A:560:THR:O	2:B:560:THR:N	2.43	0.50
2:B:362:SER:HG	2:B:364:LYS:HZ2	1.51	0.50
7:L:511:ALA:O	7:L:514:ARG:HG2	2.11	0.50
8:P:148:TYR:HD2	8:P:202:CYS:HA	1.77	0.50
8:P:478:CYS:HA	8:P:487:ALA:HA	1.93	0.50
5:J:115:LEU:CD1	5:J:124:VAL:HG21	2.25	0.50
8:P:27:THR:OG1	8:P:30:ASN:OD1	2.27	0.50
8:P:245:VAL:HG11	8:P:320:PRO:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:351:VAL:HG11	8:P:435:VAL:HG11	1.94	0.50
2:B:381:SER:OG	2:B:427:THR:OG1	2.28	0.50
2:B:445:LYS:HZ3	2:B:445:LYS:CB	2.25	0.50
4:D:514:ARG:HH11	12:V:66:ASN:HD21	1.60	0.50
8:P:526:CYS:O	8:P:538:ALA:HB2	2.11	0.50
9:R:36:LYS:HE2	9:R:86:LEU:HG	1.93	0.50
1:A:359:LEU:CD1	5:J:117:TYR:CG	2.81	0.49
3:C:456:LEU:HD11	3:C:536:CYS:HB3	1.93	0.49
4:G:467:ARG:HD3	4:G:525:GLU:OE1	2.12	0.49
6:K:510:GLN:HG3	7:L:522:THR:HG21	1.72	0.49
8:P:476:TYR:O	8:P:527:GLY:N	2.45	0.49
3:C:484:VAL:O	3:C:484:VAL:HG13	2.11	0.49
4:D:500:TYR:C	4:D:500:TYR:CD1	2.85	0.49
4:F:500:TYR:CD1	4:F:500:TYR:C	2.84	0.49
4:H:480:SER:HB3	4:H:481:PRO:HD3	1.94	0.49
5:J:117:TYR:CD1	5:J:117:TYR:C	2.85	0.49
6:K:464:LEU:HD13	6:K:525:GLU:CG	2.42	0.49
6:K:473:THR:O	6:K:473:THR:HG22	2.12	0.49
6:K:479:PHE:HB2	6:K:540:HIS:CE1	2.47	0.49
8:P:24:TYR:HD2	8:P:30:ASN:HB3	1.75	0.49
8:P:99:ARG:HG3	8:P:99:ARG:O	2.11	0.49
8:P:290:PHE:CD1	8:P:290:PHE:C	2.85	0.49
8:P:368:LEU:CA	8:P:378:PRO:HD3	2.42	0.49
11:U:34:THR:HG22	11:U:90:GLU:HG3	1.94	0.49
1:A:489:MET:HB2	1:A:535:THR:OG1	2.13	0.49
2:B:424:PHE:H	2:B:442:SER:HB2	1.76	0.49
6:K:459:PRO:HG3	6:K:470:ALA:HB1	1.95	0.49
9:R:81:TYR:HB2	9:R:86:LEU:HB2	1.95	0.49
1:A:485:PHE:CE2	5:J:115:LEU:HD22	2.41	0.49
7:L:484:VAL:HA	7:L:539:ALA:O	2.12	0.49
8:P:466:PHE:CE2	8:P:507:ARG:HB2	2.47	0.49
1:A:457:LEU:HB2	1:A:473:THR:CG2	2.42	0.49
2:B:496:SER:HB2	2:B:497:PRO:HD2	1.95	0.49
3:C:480:SER:O	3:C:540:HIS:HE1	1.93	0.49
4:F:345:ILE:HG22	4:F:437:LEU:HD21	1.94	0.49
8:P:310:HIS:CE1	8:P:316:GLN:HB2	2.47	0.49
11:U:50:ARG:NH1	11:U:100:GLY:CA	2.64	0.49
2:B:543:LEU:HD11	2:B:548:THR:HG22	1.95	0.49
4:E:514:ARG:NH1	4:E:514:ARG:HG2	2.27	0.49
4:G:489:MET:HA	4:G:494:PRO:HA	1.94	0.49
7:L:514:ARG:CB	7:L:514:ARG:NH1	2.72	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:351:VAL:HB	8:P:408:VAL:HG22	1.95	0.49
12:V:78:LEU:HB2	12:V:87:PHE:CE1	2.47	0.49
3:C:363:THR:OG1	3:C:413:ILE:O	2.30	0.49
6:K:463:GLN:O	6:K:463:GLN:HG2	2.09	0.49
9:R:50:ARG:NH1	9:R:51:GLU:O	2.45	0.49
10:S:46:ILE:HD13	10:S:87:PHE:CD2	2.47	0.49
12:V:75:ARG:NH2	12:V:95:THR:H	2.11	0.49
2:B:423:ARG:CA	2:B:442:SER:HB2	2.43	0.49
3:C:502:THR:HA	3:C:519:SER:HA	1.94	0.49
4:D:376:ASP:HB3	4:D:430:HIS:NE2	2.28	0.49
4:D:376:ASP:OD1	4:D:377:SER:N	2.45	0.49
4:E:514:ARG:HG2	4:E:514:ARG:HH11	1.78	0.49
4:G:378:VAL:HG21	4:G:405:PHE:HE2	1.77	0.49
4:G:565:SER:O	4:G:565:SER:OG	2.24	0.49
4:G:583:NAG:C3	4:G:583:NAG:C8	2.85	0.49
6:K:380:ILE:HB	6:K:393:HIS:CD2	2.48	0.49
11:U:32:SER:HA	11:U:91:VAL:O	2.13	0.49
1:A:423:ARG:CZ	1:A:425:THR:HB	2.43	0.49
2:B:418:TRP:CH2	2:B:444:PRO:CD	2.94	0.49
2:B:481:PRO:HD2	2:B:540:HIS:CE1	2.48	0.49
2:B:537:VAL:HG12	2:B:549:GLU:HG2	1.95	0.49
3:C:463:GLN:O	3:C:466:LEU:HB2	2.12	0.49
4:E:511:ALA:CB	4:E:514:ARG:HG3	2.38	0.49
4:F:397:SER:H	4:F:408:VAL:HG22	1.77	0.49
8:P:340:VAL:HG11	8:P:436:GLU:CG	2.43	0.49
8:P:368:LEU:CB	8:P:378:PRO:CG	2.78	0.49
8:P:400:GLU:HA	8:P:402:GLY:N	2.27	0.49
2:B:354:PHE:CZ	2:B:546:ARG:CG	2.96	0.49
6:K:533:THR:HG22	6:K:551:THR:CG2	2.43	0.49
6:K:346:ARG:O	6:K:370:THR:OG1	2.24	0.48
6:K:487:GLN:HB3	6:K:537:VAL:HG23	1.95	0.48
8:P:263:VAL:HG21	8:P:314:GLN:HE22	1.78	0.48
4:F:561:LEU:HD12	4:F:561:LEU:HA	1.52	0.48
4:H:572:ALA:HB3	4:H:574:THR:HG22	1.93	0.48
6:K:463:GLN:HA	6:K:466:LEU:HD23	1.93	0.48
10:S:50:ARG:N	10:S:59:GLY:O	2.45	0.48
3:C:481:PRO:O	3:C:481:PRO:HG2	2.13	0.48
4:D:510:GLN:OE1	4:D:510:GLN:HA	2.14	0.48
6:K:386:ASN:OD1	6:K:387:GLY:N	2.46	0.48
6:K:545:ASN:ND2	6:K:545:ASN:N	2.60	0.48
8:P:29:VAL:O	8:P:33:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:395:LEU:CB	8:P:410:LEU:HD11	2.20	0.48
8:P:411:ASN:ND2	8:P:525:TRP:CH2	2.81	0.48
10:S:39:LEU:HD23	10:S:85:ASN:HA	1.94	0.48
10:S:49:CYS:HB3	10:S:58:CYS:HB2	1.44	0.48
1:A:428:VAL:HG22	1:A:437:LEU:H	1.78	0.48
2:B:363:THR:HG1	2:B:413:ILE:H	1.60	0.48
4:E:459:PRO:HD3	4:E:472:ILE:HG13	1.96	0.48
4:G:491:ARG:HD2	11:U:44:VAL:HG11	1.95	0.48
7:L:538:VAL:HG12	7:L:548:THR:HB	1.94	0.48
8:P:251:PHE:CZ	8:P:308:GLY:O	2.58	0.48
8:P:286:LYS:HD3	8:P:286:LYS:O	2.12	0.48
11:U:50:ARG:HH12	11:U:100:GLY:CA	2.24	0.48
4:D:493:GLN:H	4:D:493:GLN:CD	2.09	0.48
4:F:470:ALA:HB3	4:F:523:VAL:HG23	1.95	0.48
4:F:554:LYS:O	4:F:554:LYS:HD3	2.13	0.48
7:L:540:HIS:HB3	7:L:543:LEU:CD1	2.44	0.48
11:U:37:CYS:HB3	11:U:87:PHE:O	2.13	0.48
12:V:86:LEU:HD12	12:V:87:PHE:H	1.79	0.48
2:B:357:ILE:HD11	2:B:415:GLU:HG3	1.95	0.48
3:C:566:LEU:HD13	4:D:566:LEU:CD2	2.43	0.48
4:E:508:GLU:HB2	4:E:514:ARG:O	2.14	0.48
8:P:366:TRP:O	8:P:380:LEU:N	2.45	0.48
2:B:380:ILE:HG12	2:B:428:VAL:HG22	1.95	0.48
4:E:367:CYS:N	4:E:382:TRP:HH2	2.11	0.48
4:G:467:ARG:CG	4:G:467:ARG:NH1	2.72	0.48
6:K:467:ARG:NH2	9:R:111:ASP:OD1	2.46	0.48
8:P:447:LYS:HB2	8:P:464:CYS:CA	2.44	0.48
4:E:491:ARG:CG	12:V:44:VAL:HG11	2.44	0.48
4:F:416:ASP:O	4:F:420:SER:HB3	2.13	0.48
4:H:565:SER:HB3	6:K:565:SER:HB2	1.96	0.48
7:L:345:ILE:HA	7:L:433:LEU:HD11	1.96	0.48
7:L:576:TYR:HD2	7:L:576:TYR:N	2.10	0.48
11:U:20:LEU:HG	11:U:117:LYS:HB2	1.94	0.48
11:U:80:GLN:OE1	11:U:87:PHE:HD1	1.95	0.48
4:D:514:ARG:HH21	4:D:514:ARG:CG	2.23	0.48
4:F:363:THR:OG1	4:F:413:ILE:O	2.32	0.48
4:H:514:ARG:HH12	10:S:65:THR:HG23	1.79	0.48
4:H:554:LYS:HZ2	4:H:558:LYS:HZ2	1.52	0.48
4:H:554:LYS:HZ2	4:H:558:LYS:NZ	1.94	0.48
10:S:78:LEU:HD11	10:S:87:PHE:HD2	1.78	0.48
12:V:47:TYR:OH	12:V:113:GLY:HA3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:GLY:HA2	1:A:554:LYS:HB2	1.96	0.48
2:B:461:ARG:HH22	6:K:570:ASP:HB3	1.79	0.48
2:B:472:ILE:HG21	2:B:552:VAL:HG11	1.96	0.48
4:D:348:PHE:HD2	4:D:370:THR:HB	1.79	0.48
2:B:476:VAL:HG11	2:B:538:VAL:HG21	1.96	0.47
3:C:379:THR:HB	3:C:429:THR:OG1	2.14	0.47
4:D:535:THR:HG22	4:D:551:THR:HB	1.96	0.47
9:R:47:TYR:OH	9:R:110:THR:O	2.32	0.47
9:R:62:VAL:HG12	9:R:68:ILE:HG22	1.94	0.47
4:D:384:ARG:HH11	4:D:390:VAL:HA	1.79	0.47
4:E:457:LEU:HB2	4:E:473:THR:CG2	2.44	0.47
4:E:489:MET:SD	4:E:494:PRO:N	2.87	0.47
7:L:449:LEU:CA	7:L:480:SER:HB3	2.44	0.47
8:P:120:LYS:O	8:P:216:ASP:N	2.47	0.47
8:P:445:ASN:CB	8:P:536:GLU:OE2	2.62	0.47
9:R:46:ILE:HG22	9:R:64:THR:HG21	1.95	0.47
10:S:105:GLY:HA3	10:S:114:LYS:HA	1.95	0.47
4:D:359:LEU:HD21	4:D:485:PHE:CZ	2.48	0.47
6:K:445:LYS:CE	6:K:445:LYS:CA	2.84	0.47
8:P:466:PHE:CD2	8:P:466:PHE:N	2.82	0.47
9:R:95:THR:C	9:R:97:SER:H	2.17	0.47
2:B:347:VAL:HG22	2:B:369:VAL:HG22	1.96	0.47
3:C:382:TRP:CH2	3:C:426:CYS:HB2	2.50	0.47
12:V:75:ARG:HG3	12:V:76:VAL:HG13	1.97	0.47
1:A:510:GLN:H	1:A:510:GLN:CD	2.18	0.47
2:B:397:SER:OG	2:B:398:GLU:N	2.46	0.47
4:D:493:GLN:HA	4:D:494:PRO:HD2	1.45	0.47
4:F:347:VAL:HG11	4:F:428:VAL:HB	1.97	0.47
5:J:42:PRO:HG3	5:J:102:THR:CG2	2.43	0.47
6:K:529:ASN:HA	6:K:554:LYS:HD3	1.97	0.47
6:K:556:THR:HG23	6:K:556:THR:O	2.14	0.47
7:L:424:PHE:CD1	7:L:441:ILE:HD11	2.46	0.47
7:L:452:PRO:HB3	7:L:479:PHE:CD1	2.48	0.47
7:L:480:SER:HB2	7:L:481:PRO:HD3	1.97	0.47
1:A:402:ASN:OD1	1:A:404:THR:OG1	2.22	0.47
1:A:466:LEU:N	1:A:466:LEU:HD13	2.29	0.47
4:E:490:GLN:HB3	4:E:534:TYR:HA	1.96	0.47
4:F:545:ASN:CB	4:G:358:PHE:HZ	2.27	0.47
4:G:443:ARG:HA	4:G:444:PRO:HD2	1.52	0.47
4:G:473:THR:O	4:G:473:THR:OG1	2.23	0.47
4:H:379:THR:HG21	4:H:429:THR:OG1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:526:GLU:HA	6:K:529:ASN:OD1	2.14	0.47
7:L:417:ASP:O	7:L:420:SER:OG	2.31	0.47
1:A:491:ARG:NH1	1:A:491:ARG:CG	2.73	0.47
2:B:451:ARG:NH1	2:B:451:ARG:CB	2.72	0.47
3:C:526:GLU:CD	3:C:526:GLU:H	2.17	0.47
3:C:533:THR:O	3:C:552:VAL:O	2.33	0.47
4:G:468:GLU:O	4:G:525:GLU:HB2	2.15	0.47
6:K:416:ASP:OD1	6:K:417:ASP:N	2.47	0.47
8:P:56:VAL:O	8:P:56:VAL:HG23	2.14	0.47
8:P:445:ASN:HB2	8:P:536:GLU:OE2	2.14	0.47
10:S:81:TYR:HB3	10:S:84:LYS:HB2	1.96	0.47
11:U:22:GLU:CD	11:U:119:THR:HG23	2.33	0.47
4:E:489:MET:O	4:E:535:THR:CB	2.63	0.47
4:H:552:VAL:HG13	4:H:556:THR:HG21	1.95	0.47
5:J:21:ILE:HD11	7:L:555:SER:CA	2.44	0.47
8:P:526:CYS:CB	8:P:538:ALA:HB3	2.44	0.47
10:S:39:LEU:HD21	10:S:41:GLU:HG2	1.97	0.47
4:E:350:ILE:HB	4:E:366:THR:HB	1.96	0.47
4:F:452:PRO:HD3	4:F:540:HIS:HD2	1.79	0.47
4:H:364:LYS:HB3	4:H:410:GLU:HB3	1.96	0.47
6:K:558:LYS:HG2	6:K:558:LYS:O	2.15	0.47
8:P:462:VAL:HG11	8:P:509:VAL:HG12	1.97	0.47
8:P:466:PHE:CD1	8:P:470:PHE:HZ	2.31	0.47
4:G:413:ILE:HD13	4:G:424:PHE:HZ	1.79	0.47
4:H:384:ARG:HD2	4:H:388:GLU:HB2	1.97	0.47
6:K:537:VAL:CG1	6:K:549:GLU:HG2	2.44	0.47
8:P:143:LYS:O	8:P:145:LYS:HG3	2.14	0.47
9:R:52:MET:HE1	9:R:69:LYS:NZ	2.30	0.47
10:S:105:GLY:HA2	10:S:115:THR:HG23	1.96	0.47
12:V:121:ASN:HD21	12:V:123:HIS:HB3	1.79	0.47
1:A:514:ARG:HH11	1:A:514:ARG:CG	2.28	0.46
4:F:546:ARG:HH11	4:F:546:ARG:HG3	1.79	0.46
4:G:493:GLN:HG2	11:U:42:MET:O	2.15	0.46
4:G:521:LEU:HD21	4:G:534:TYR:CE2	2.50	0.46
4:H:474:CYS:HB2	4:H:488:TRP:CZ2	2.50	0.46
6:K:528:TRP:HH2	6:K:552:VAL:HG22	1.79	0.46
7:L:423:ARG:HH21	7:L:444:PRO:HB3	1.80	0.46
7:L:445:LYS:H	7:L:445:LYS:HG3	1.48	0.46
8:P:462:VAL:O	8:P:509:VAL:N	2.47	0.46
4:E:423:ARG:HA	4:E:442:SER:HB3	1.96	0.46
4:E:467:ARG:NH1	11:U:111:ASP:OD2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:464:LEU:HD13	6:K:464:LEU:HA	1.60	0.46
8:P:224:PRO:HG3	8:P:304:ARG:HH12	1.80	0.46
8:P:352:LEU:HD21	8:P:401:PRO:HG2	1.97	0.46
4:E:468:GLU:OE2	11:U:45:ARG:NH1	2.43	0.46
4:F:449:LEU:HA	4:F:481:PRO:HD2	1.97	0.46
7:L:478:GLY:O	7:L:515:TYR:N	2.39	0.46
8:P:38:CYS:HB2	8:P:46:CYS:HB3	1.52	0.46
9:R:45:ARG:HA	9:R:64:THR:OG1	2.16	0.46
10:S:79:LYS:HD3	10:S:80:GLN:N	2.30	0.46
11:U:39:LEU:HD23	11:U:39:LEU:C	2.35	0.46
4:G:363:THR:OG1	4:G:413:ILE:HG13	2.15	0.46
6:K:414:CYS:SG	6:K:415:GLU:N	2.88	0.46
10:S:39:LEU:CD2	10:S:85:ASN:CA	2.94	0.46
2:B:568:MET:HE2	6:K:562:TYR:CE2	2.51	0.46
4:E:535:THR:HG23	4:E:550:ARG:O	2.15	0.46
4:G:382:TRP:CG	4:G:411:ALA:HB2	2.50	0.46
4:H:532:GLU:O	4:H:553:ASP:HB2	2.14	0.46
8:P:365:TYR:CE1	8:P:379:LEU:HD13	2.50	0.46
8:P:395:LEU:CB	8:P:410:LEU:HD12	2.41	0.46
9:R:22:GLU:CG	9:R:119:THR:HG22	2.45	0.46
1:A:575:CYS:CB	5:J:7:LEU:HD23	2.46	0.46
2:B:418:TRP:HA	2:B:443:ARG:HD2	1.76	0.46
4:F:479:PHE:CD1	4:F:479:PHE:N	2.84	0.46
4:F:506:MET:O	4:F:516:PHE:CE2	2.68	0.46
4:G:535:THR:HG22	4:G:551:THR:OG1	2.15	0.46
4:H:571:THR:O	4:H:572:ALA:HB3	2.15	0.46
6:K:484:VAL:HG23	6:K:540:HIS:CG	2.49	0.46
7:L:451:ARG:HH12	7:L:544:PRO:HG3	1.80	0.46
8:P:30:ASN:O	8:P:35:LYS:NZ	2.34	0.46
12:V:36:LYS:HG2	12:V:86:LEU:CD1	2.46	0.46
12:V:47:TYR:HA	12:V:63:SER:HA	1.97	0.46
12:V:86:LEU:HG	12:V:88:LEU:HD22	1.97	0.46
2:B:570:ASP:HB2	3:C:571:THR:HA	1.97	0.46
4:F:496:SER:OG	4:F:499:LYS:NZ	2.48	0.46
4:F:502:THR:OG1	4:F:519:SER:HB2	2.08	0.46
4:H:352:PRO:HD2	4:H:418:TRP:CH2	2.51	0.46
6:K:574:THR:OG1	6:K:575:CYS:N	2.49	0.46
8:P:344:VAL:HG21	8:P:443:GLU:O	2.16	0.46
1:A:390:VAL:HG13	1:A:391:LYS:N	2.31	0.46
2:B:568:MET:HE3	7:L:564:VAL:HG21	1.98	0.46
4:D:423:ARG:HD3	4:D:440:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:372:LEU:HD11	4:G:433:LEU:HB2	1.97	0.46
4:H:554:LYS:CE	4:H:558:LYS:HZ1	2.14	0.46
7:L:457:LEU:HB2	7:L:473:THR:OG1	2.15	0.46
8:P:351:VAL:CG1	8:P:435:VAL:HG11	2.46	0.46
8:P:368:LEU:HB2	8:P:378:PRO:HG3	1.89	0.46
8:P:450:GLY:HA2	8:P:462:VAL:HA	1.97	0.46
12:V:28:GLU:O	12:V:94:LEU:HB3	2.15	0.46
4:D:382:TRP:CZ3	4:D:424:PHE:HB3	2.51	0.46
4:E:443:ARG:HG3	4:E:444:PRO:HD2	1.97	0.46
4:E:481:PRO:HD2	4:E:540:HIS:CE1	2.51	0.46
4:E:509:PRO:HG3	4:F:501:VAL:HG12	1.97	0.46
4:G:443:ARG:C	4:G:443:ARG:CD	2.84	0.46
4:H:554:LYS:NZ	4:H:558:LYS:HZ3	1.90	0.46
6:K:470:ALA:HB3	6:K:523:VAL:HG12	1.97	0.46
6:K:481:PRO:CG	6:K:541:GLU:OE2	2.63	0.46
7:L:506:MET:HB3	7:L:507:PRO:HD2	1.97	0.46
8:P:275:PHE:HB3	8:P:279:ILE:HD12	1.98	0.46
9:R:35:ILE:HB	9:R:89:VAL:HB	1.98	0.46
10:S:39:LEU:HG	10:S:41:GLU:HG2	1.98	0.46
12:V:72:TYR:HA	12:V:75:ARG:HD3	1.97	0.46
4:D:363:THR:OG1	4:D:413:ILE:O	2.30	0.46
4:H:486:VAL:HG11	4:H:519:SER:OG	2.16	0.46
6:K:516:PHE:CD1	6:K:516:PHE:C	2.88	0.46
6:K:528:TRP:CD1	6:K:528:TRP:O	2.69	0.46
7:L:424:PHE:O	7:L:441:ILE:HG13	2.14	0.46
7:L:543:LEU:HA	7:L:544:PRO:HD3	1.51	0.46
8:P:237:PHE:O	8:P:291:SER:HA	2.16	0.46
8:P:368:LEU:C	8:P:378:PRO:HD3	2.36	0.46
10:S:61:VAL:HG13	10:S:72:TYR:CG	2.51	0.46
4:E:400:HIS:CD2	4:E:402:ASN:H	2.34	0.45
4:F:500:TYR:CD1	4:F:500:TYR:O	2.69	0.45
7:L:540:HIS:CE1	7:L:542:ALA:HB2	2.51	0.45
8:P:271:ARG:HB2	8:P:372:ALA:HB3	1.97	0.45
9:R:46:ILE:HG22	9:R:64:THR:HG22	1.99	0.45
1:A:352:PRO:HD3	1:A:365:LEU:HD23	1.97	0.45
2:B:385:GLN:NE2	2:B:423:ARG:HB3	2.31	0.45
3:C:555:SER:HA	3:C:558:LYS:HD2	1.96	0.45
6:K:378:VAL:HG23	6:K:380:ILE:HG12	1.97	0.45
7:L:382:TRP:CZ3	7:L:426:CYS:HB2	2.51	0.45
8:P:368:LEU:CB	8:P:378:PRO:HG2	2.43	0.45
10:S:36:LYS:HD3	10:S:86:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:102:TYR:N	10:S:118:VAL:O	2.34	0.45
1:A:356:SER:N	5:J:117:TYR:CZ	2.84	0.45
1:A:400:HIS:HB3	1:A:404:THR:H	1.82	0.45
1:A:476:VAL:O	1:A:516:PHE:HA	2.16	0.45
1:A:516:PHE:CD2	1:A:516:PHE:O	2.69	0.45
1:A:565:SER:HB2	5:J:59:ARG:HA	1.99	0.45
2:B:382:TRP:CE3	2:B:424:PHE:HB3	2.52	0.45
4:D:363:THR:OG1	4:D:363:THR:O	2.34	0.45
4:E:501:VAL:HG21	4:F:509:PRO:HD3	1.99	0.45
4:F:477:THR:HG22	4:F:516:PHE:HB2	1.98	0.45
4:F:481:PRO:HG2	4:F:481:PRO:O	2.16	0.45
4:H:418:TRP:HE3	4:H:443:ARG:HB2	1.80	0.45
7:L:372:LEU:HG	7:L:407:ALA:HB3	1.96	0.45
8:P:94:LEU:HB2	8:P:101:LEU:HD23	1.99	0.45
11:U:41:GLU:C	11:U:43:HIS:N	2.69	0.45
12:V:48:LEU:HD13	12:V:89:VAL:HG11	1.97	0.45
4:E:379:THR:HB	4:E:393:HIS:HB3	1.99	0.45
7:L:456:LEU:HD11	7:L:488:TRP:CH2	2.52	0.45
7:L:493:GLN:NE2	7:L:494:PRO:O	2.49	0.45
7:L:514:ARG:HH11	7:L:514:ARG:CA	2.30	0.45
7:L:514:ARG:NH1	7:L:514:ARG:HA	2.31	0.45
8:P:491:GLN:O	8:P:507:ARG:NH1	2.49	0.45
2:B:432:ASP:OD1	2:B:432:ASP:N	2.50	0.45
3:C:526:GLU:O	3:C:530:THR:HG21	2.15	0.45
4:E:489:MET:CE	4:E:494:PRO:HD3	2.44	0.45
4:F:383:THR:OG1	4:F:425:THR:OG1	2.12	0.45
4:H:454:VAL:CG2	4:H:538:VAL:HG21	2.47	0.45
10:S:47:TYR:CZ	10:S:110:THR:HA	2.51	0.45
11:U:94:LEU:C	11:U:96:GLU:N	2.69	0.45
12:V:112:ARG:CZ	12:V:112:ARG:CB	2.94	0.45
1:A:378:VAL:HG12	1:A:393:HIS:NE2	2.32	0.45
2:B:418:TRP:HE3	2:B:442:SER:HG	1.62	0.45
3:C:566:LEU:HD22	4:H:564:VAL:HG21	1.99	0.45
4:G:365:LEU:HB2	4:G:411:ALA:HB3	1.98	0.45
4:G:490:GLN:NE2	4:G:532:GLU:OE2	2.30	0.45
4:H:383:THR:HA	4:H:390:VAL:HG23	1.99	0.45
6:K:516:PHE:CE2	7:L:520:ILE:HD11	2.46	0.45
8:P:136:PHE:O	8:P:136:PHE:CD2	2.70	0.45
8:P:413:LEU:H	8:P:413:LEU:CD2	2.07	0.45
1:A:485:PHE:CD2	1:A:485:PHE:O	2.70	0.45
1:A:510:GLN:H	1:A:510:GLN:HE21	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:528:TRP:O	2:B:528:TRP:CG	2.69	0.45
4:G:481:PRO:HD2	4:G:540:HIS:HE1	1.81	0.45
6:K:485:PHE:O	6:K:485:PHE:CD1	2.70	0.45
7:L:372:LEU:HB2	7:L:405:PHE:O	2.17	0.45
8:P:272:ALA:HA	8:P:273:PRO:HD3	1.57	0.45
8:P:382:ASP:OD1	8:P:386:TRP:N	2.48	0.45
2:B:345:ILE:HA	2:B:372:LEU:HB2	1.99	0.45
4:D:416:ASP:OD2	4:D:417:ASP:N	2.50	0.45
4:F:449:LEU:CA	4:F:480:SER:CB	2.93	0.45
4:F:523:VAL:HG11	4:F:534:TYR:OH	2.16	0.45
4:F:543:LEU:CD2	4:F:548:THR:CG2	2.94	0.45
6:K:468:GLU:HA	9:R:67:PHE:CE2	2.51	0.45
8:P:290:PHE:CD1	8:P:290:PHE:O	2.69	0.45
4:D:421:GLY:CA	4:D:445:LYS:HZ2	2.12	0.45
4:D:495:LEU:HD22	4:D:495:LEU:HA	1.70	0.45
4:H:560:THR:CB	6:K:560:THR:O	2.65	0.45
8:P:448:VAL:HG23	8:P:463:PRO:HG3	1.99	0.45
9:R:35:ILE:O	9:R:88:LEU:HA	2.17	0.45
1:A:500:TYR:HA	1:A:520:ILE:O	2.17	0.45
4:E:384:ARG:HD3	4:E:388:GLU:HB3	1.99	0.45
4:E:543:LEU:HD13	4:E:548:THR:OG1	2.15	0.45
4:F:536:CYS:O	4:F:549:GLU:HB2	2.17	0.45
6:K:485:PHE:O	6:K:485:PHE:CG	2.69	0.45
8:P:99:ARG:HA	8:P:99:ARG:HD3	1.58	0.45
8:P:173:ILE:HD13	8:P:189:ILE:HB	1.99	0.45
8:P:243:PRO:O	8:P:246:ALA:N	2.50	0.45
8:P:345:ALA:CA	8:P:413:LEU:CD1	2.74	0.45
12:V:36:LYS:HG2	12:V:86:LEU:HD11	1.98	0.45
2:B:500:TYR:HA	2:B:520:ILE:O	2.17	0.44
3:C:384:ARG:HG3	3:C:385:GLN:N	2.32	0.44
3:C:568:MET:CE	6:K:564:VAL:HG21	2.47	0.44
4:G:372:LEU:HD21	4:G:433:LEU:HD12	1.97	0.44
4:G:480:SER:OG	4:G:481:PRO:HD3	2.16	0.44
6:K:566:LEU:HD23	6:K:566:LEU:C	2.37	0.44
8:P:127:GLY:HA2	8:P:191:GLN:HA	1.99	0.44
8:P:149:LYS:HG2	8:P:200:TYR:CE1	2.52	0.44
8:P:526:CYS:HB3	8:P:538:ALA:CB	2.45	0.44
2:B:418:TRP:CZ2	2:B:444:PRO:HD2	2.42	0.44
2:B:451:ARG:HB2	2:B:451:ARG:CZ	2.45	0.44
2:B:528:TRP:O	2:B:528:TRP:CD2	2.70	0.44
3:C:509:PRO:HG2	4:D:522:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:384:ARG:HB3	4:F:386:ASN:OD1	2.17	0.44
4:F:471:THR:CG2	4:F:522:THR:HG23	2.47	0.44
4:G:363:THR:OG1	4:G:414:CYS:O	2.29	0.44
5:J:117:TYR:CG	5:J:117:TYR:O	2.69	0.44
8:P:149:LYS:HD2	8:P:151:ILE:HG21	1.99	0.44
8:P:310:HIS:O	8:P:310:HIS:CG	2.70	0.44
9:R:20:LEU:CD2	9:R:20:LEU:C	2.86	0.44
11:U:47:TYR:CE2	11:U:110:THR:HG23	2.53	0.44
1:A:514:ARG:CD	1:A:514:ARG:N	2.78	0.44
1:A:528:TRP:O	1:A:528:TRP:CG	2.70	0.44
2:B:366:THR:HB	2:B:408:VAL:HG23	1.99	0.44
2:B:461:ARG:NE	7:L:570:ASP:OD2	2.51	0.44
4:D:423:ARG:HH11	4:D:425:THR:HB	1.83	0.44
4:E:540:HIS:CD2	4:E:542:ALA:H	2.34	0.44
4:G:506:MET:HE2	4:G:516:PHE:CE2	2.51	0.44
4:H:573:GLY:O	4:H:574:THR:C	2.56	0.44
6:K:476:VAL:HG12	6:K:479:PHE:CD1	2.53	0.44
8:P:151:ILE:HD12	8:P:152:GLY:N	2.32	0.44
8:P:361:LYS:C	8:P:361:LYS:CD	2.85	0.44
8:P:439:ILE:CD1	8:P:439:ILE:H	2.22	0.44
12:V:104:CYS:HB2	12:V:116:GLN:HB3	1.98	0.44
1:A:372:LEU:HD21	1:A:405:PHE:HD2	1.83	0.44
1:A:386:ASN:OD1	1:A:388:GLU:HG2	2.17	0.44
4:D:452:PRO:HG3	4:D:479:PHE:HB3	1.97	0.44
4:E:417:ASP:HB3	4:E:424:PHE:CZ	2.52	0.44
4:F:456:LEU:HD13	4:F:550:ARG:HB2	1.99	0.44
4:H:367:CYS:HB2	4:H:380:ILE:HG13	1.99	0.44
6:K:345:ILE:HG22	6:K:372:LEU:HD21	1.98	0.44
6:K:428:VAL:HG12	6:K:430:HIS:HB2	2.00	0.44
7:L:511:ALA:O	7:L:514:ARG:HG3	2.16	0.44
8:P:31:ARG:HD2	8:P:70:PRO:HB3	1.98	0.44
8:P:287:ASP:HB2	8:P:288:GLY:H	1.47	0.44
8:P:368:LEU:CB	8:P:378:PRO:HD2	2.43	0.44
8:P:411:ASN:HD22	8:P:537:THR:HG21	1.83	0.44
8:P:418:ALA:N	8:P:439:ILE:HD11	2.31	0.44
10:S:99:SER:HB2	10:S:120:LEU:HB3	1.98	0.44
11:U:22:GLU:HB2	11:U:119:THR:CA	2.47	0.44
3:C:454:VAL:CG1	3:C:474:CYS:SG	3.05	0.44
3:C:459:PRO:HG3	3:C:470:ALA:HB1	2.00	0.44
4:D:350:ILE:HB	4:D:366:THR:OG1	2.17	0.44
4:E:391:LYS:HG3	4:E:412:SER:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:347:VAL:HG22	4:G:369:VAL:HG13	1.99	0.44
4:H:575:CYS:HB2	6:K:575:CYS:HB3	1.61	0.44
8:P:471:SER:HA	8:P:475:LYS:NZ	2.22	0.44
10:S:97:SER:O	10:S:97:SER:OG	2.29	0.44
3:C:371:ASP:N	3:C:404:THR:HG23	2.29	0.44
3:C:447:VAL:HG11	3:C:481:PRO:HB3	1.99	0.44
4:F:445:LYS:HB3	4:F:445:LYS:HE2	1.44	0.44
4:F:491:ARG:HE	4:F:491:ARG:HB2	1.58	0.44
4:F:554:LYS:C	4:F:554:LYS:CD	2.85	0.44
6:K:493:GLN:HG3	10:S:44:VAL:HG22	2.00	0.44
4:F:383:THR:HG22	4:F:389:ALA:HA	1.99	0.44
4:F:430:HIS:HB3	4:F:433:LEU:HB2	2.00	0.44
4:F:501:VAL:O	4:F:501:VAL:HG22	2.17	0.44
10:S:28:GLU:O	10:S:94:LEU:HG	2.18	0.44
12:V:112:ARG:NH1	12:V:112:ARG:HB2	2.33	0.44
2:B:405:PHE:CE2	2:B:407:ALA:HB2	2.52	0.44
3:C:346:ARG:HH21	3:C:348:PHE:HB2	1.82	0.44
4:D:447:VAL:O	4:D:447:VAL:HG22	2.18	0.44
4:E:511:ALA:HB1	4:E:514:ARG:CG	2.39	0.44
4:H:562:TYR:H	4:H:562:TYR:HD2	1.64	0.44
6:K:462:GLU:HB3	7:L:455:TYR:HE1	1.83	0.44
8:P:286:LYS:C	8:P:286:LYS:CD	2.85	0.44
12:V:41:GLU:OE1	12:V:82:PRO:HB3	2.18	0.44
1:A:390:VAL:O	1:A:391:LYS:HD2	2.18	0.44
2:B:393:HIS:CD2	2:B:409:GLY:HA3	2.52	0.44
4:D:345:ILE:HB	4:D:372:LEU:HD13	2.00	0.43
4:H:558:LYS:HA	4:H:559:PRO:HD3	1.79	0.43
6:K:385:GLN:HE21	6:K:423:ARG:H	1.66	0.43
8:P:47:ILE:HG13	8:P:47:ILE:O	2.17	0.43
9:R:36:LYS:O	9:R:116:GLN:HG3	2.18	0.43
9:R:46:ILE:N	9:R:64:THR:CG2	2.57	0.43
2:B:478:GLY:O	2:B:514:ARG:HG2	2.14	0.43
2:B:481:PRO:CD	2:B:540:HIS:NE2	2.72	0.43
4:E:382:TRP:CD2	4:E:411:ALA:HB2	2.53	0.43
10:S:19:ILE:HG22	10:S:21:PRO:HD3	2.00	0.43
12:V:49:CYS:HB3	12:V:103:ALA:HB3	2.00	0.43
1:A:514:ARG:NH1	1:A:514:ARG:CG	2.77	0.43
2:B:345:ILE:N	2:B:371:ASP:HB3	2.33	0.43
4:G:450:HIS:ND1	4:G:450:HIS:N	2.66	0.43
6:K:374:THR:HA	6:K:405:PHE:HB2	1.99	0.43
6:K:380:ILE:CG2	6:K:409:GLY:HA2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:ALA:CB	2:B:441:ILE:HG12	2.48	0.43
4:G:516:PHE:CZ	4:H:520:ILE:HD12	2.54	0.43
7:L:487:GLN:C	7:L:537:VAL:HG12	2.37	0.43
8:P:149:LYS:H	8:P:155:PRO:HB3	1.84	0.43
8:P:243:PRO:C	8:P:246:ALA:HB2	2.39	0.43
9:R:50:ARG:HG2	9:R:50:ARG:HH11	1.82	0.43
1:A:352:PRO:HD2	1:A:418:TRP:CH2	2.53	0.43
1:A:499:LYS:HB3	1:A:521:LEU:HD12	2.01	0.43
3:C:508:GLU:CB	3:C:509:PRO:CD	2.90	0.43
3:C:562:TYR:CD2	4:H:568:MET:HE2	2.54	0.43
4:E:354:PHE:HD1	4:E:357:ILE:HD11	1.84	0.43
4:F:450:HIS:HE2	4:F:514:ARG:NH1	1.99	0.43
4:H:457:LEU:HB2	4:H:473:THR:OG1	2.19	0.43
6:K:490:GLN:OE1	6:K:491:ARG:N	2.51	0.43
7:L:569:SER:HB3	7:L:572:ALA:HB2	1.99	0.43
8:P:345:ALA:O	8:P:413:LEU:CD1	2.46	0.43
9:R:22:GLU:HA	9:R:117:LYS:C	2.35	0.43
9:R:52:MET:CE	9:R:69:LYS:NZ	2.81	0.43
1:A:456:LEU:HD12	1:A:550:ARG:O	2.15	0.43
4:E:534:TYR:CD2	4:E:534:TYR:N	2.85	0.43
7:L:430:HIS:CE1	7:L:432:ASP:CB	3.01	0.43
8:P:477:TRP:CD1	8:P:526:CYS:HB2	2.52	0.43
1:A:374:THR:HG22	1:A:405:PHE:HB2	2.01	0.43
1:A:467:ARG:HE	1:A:467:ARG:HB2	1.38	0.43
4:D:451:ARG:HH12	4:D:544:PRO:HD3	1.83	0.43
4:H:583:NAG:C6	6:K:583:NAG:H61	2.37	0.43
5:J:32:ILE:HG23	7:L:560:THR:HB	2.00	0.43
5:J:46:ARG:HD2	5:J:54:SER:O	2.19	0.43
6:K:405:PHE:CE2	6:K:407:ALA:HB2	2.53	0.43
6:K:521:LEU:C	6:K:521:LEU:CD2	2.85	0.43
7:L:450:HIS:CA	7:L:480:SER:HB2	2.40	0.43
8:P:253:CYS:SG	8:P:315:LEU:CB	2.99	0.43
2:B:405:PHE:CZ	2:B:407:ALA:HB2	2.54	0.43
2:B:454:VAL:HG22	2:B:454:VAL:O	2.18	0.43
2:B:496:SER:CB	2:B:497:PRO:HD2	2.42	0.43
2:B:549:GLU:O	2:B:550:ARG:NH1	2.42	0.43
4:D:380:ILE:HD12	4:D:393:HIS:CG	2.54	0.43
4:D:384:ARG:HD3	4:D:390:VAL:HG22	2.01	0.43
4:F:447:VAL:HG21	4:F:481:PRO:HB3	2.01	0.43
4:G:353:SER:O	4:G:357:ILE:HG12	2.18	0.43
8:P:148:TYR:HB3	8:P:155:PRO:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:150:GLN:OE1	8:P:201:LEU:HD23	2.18	0.43
8:P:466:PHE:CE2	8:P:475:LYS:HB3	2.53	0.43
2:B:552:VAL:HG23	2:B:556:THR:HG21	2.00	0.43
3:C:450:HIS:ND1	3:C:450:HIS:N	2.67	0.43
4:D:485:PHE:HB3	4:D:539:ALA:HB3	2.00	0.43
4:F:535:THR:CG2	4:F:551:THR:HG21	2.30	0.43
4:H:520:ILE:HG21	4:H:520:ILE:HD13	1.59	0.43
8:P:128:ARG:HD3	8:P:128:ARG:HA	1.77	0.43
8:P:410:LEU:HD12	8:P:410:LEU:HA	1.88	0.43
8:P:480:TRP:O	8:P:480:TRP:CE3	2.72	0.43
1:A:526:GLU:O	1:A:530:THR:N	2.52	0.43
3:C:451:ARG:O	3:C:451:ARG:HG3	2.19	0.43
4:E:400:HIS:CG	4:E:401:PRO:HD2	2.54	0.43
4:F:529:ASN:OD1	4:F:530:THR:N	2.52	0.43
4:G:347:VAL:HG22	4:G:369:VAL:HA	2.00	0.43
4:G:567:VAL:O	4:H:568:MET:HG2	2.19	0.43
6:K:455:TYR:CZ	7:L:463:GLN:HB3	2.54	0.43
8:P:298:ARG:NH2	8:P:300:GLU:OE2	2.52	0.43
2:B:530:THR:O	2:B:530:THR:CG2	2.67	0.42
4:E:526:GLU:HG2	4:E:527:GLU:OE1	2.19	0.42
4:F:355:ALA:HA	4:F:485:PHE:HB2	2.00	0.42
6:K:450:HIS:CE1	6:K:514:ARG:NH1	2.87	0.42
7:L:550:ARG:HD3	7:L:550:ARG:HA	1.61	0.42
8:P:290:PHE:H	8:P:290:PHE:HD1	1.66	0.42
9:R:45:ARG:HD3	9:R:108:MET:HE2	2.01	0.42
9:R:46:ILE:CG2	9:R:64:THR:CG2	2.96	0.42
1:A:496:SER:O	1:A:496:SER:OG	2.28	0.42
2:B:384:ARG:HE	2:B:388:GLU:HB2	1.84	0.42
2:B:450:HIS:C	2:B:542:ALA:HB1	2.39	0.42
3:C:466:LEU:CD2	12:V:45:ARG:NH2	2.82	0.42
4:E:395:ASN:HB3	4:E:408:VAL:HB	2.00	0.42
4:F:524:SER:OG	4:F:527:GLU:CD	2.58	0.42
4:F:543:LEU:HD21	4:F:548:THR:HG21	1.99	0.42
4:H:448:ALA:HB3	4:H:480:SER:OG	2.19	0.42
5:J:21:ILE:HG13	7:L:555:SER:CB	2.48	0.42
6:K:429:THR:HA	6:K:436:PRO:HB3	2.01	0.42
6:K:475:LEU:O	6:K:475:LEU:HG	2.19	0.42
6:K:554:LYS:HB3	6:K:554:LYS:HE3	1.81	0.42
11:U:28:GLU:HG3	11:U:30:GLY:H	1.84	0.42
2:B:452:PRO:HG2	2:B:452:PRO:O	2.19	0.42
2:B:478:GLY:HA2	2:B:514:ARG:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:457:LEU:HB2	4:E:473:THR:HG23	2.02	0.42
8:P:334:ILE:HG23	8:P:431:TRP:CE3	2.54	0.42
3:C:347:VAL:HG22	3:C:369:VAL:HG23	2.01	0.42
4:E:474:CYS:HB2	4:E:488:TRP:CZ2	2.54	0.42
4:E:543:LEU:HD23	4:E:543:LEU:HA	1.61	0.42
4:F:357:ILE:HG12	4:F:363:THR:HG22	2.00	0.42
4:F:449:LEU:H	4:F:449:LEU:CD2	2.30	0.42
4:H:445:LYS:HE2	4:H:445:LYS:HB3	1.56	0.42
4:H:481:PRO:HD2	4:H:540:HIS:CE1	2.55	0.42
4:H:516:PHE:CD2	4:H:516:PHE:C	2.93	0.42
8:P:530:GLN:NE2	8:P:530:GLN:C	2.73	0.42
9:R:48:LEU:HD22	9:R:89:VAL:HG21	2.01	0.42
1:A:520:ILE:HD12	2:B:516:PHE:CE2	2.54	0.42
2:B:540:HIS:O	2:B:543:LEU:HB2	2.19	0.42
3:C:459:PRO:HD2	3:C:528:TRP:CZ2	2.54	0.42
4:D:508:GLU:HB3	4:D:514:ARG:O	2.19	0.42
4:F:364:LYS:HD2	4:F:364:LYS:HA	1.79	0.42
4:G:413:ILE:HD13	4:G:424:PHE:CZ	2.54	0.42
4:G:561:LEU:HA	4:G:561:LEU:HD23	1.76	0.42
5:J:107:LYS:HB3	5:J:107:LYS:HE3	1.54	0.42
6:K:479:PHE:CD2	6:K:482:ALA:HA	2.55	0.42
7:L:476:VAL:O	7:L:516:PHE:HA	2.20	0.42
8:P:357:ARG:HG2	8:P:404:GLY:HA3	2.01	0.42
8:P:447:LYS:HD3	8:P:447:LYS:HA	1.37	0.42
10:S:19:ILE:HG22	10:S:21:PRO:CD	2.49	0.42
10:S:39:LEU:HD23	10:S:85:ASN:CA	2.49	0.42
10:S:39:LEU:HD23	10:S:85:ASN:C	2.39	0.42
1:A:375:TYR:HD2	1:A:430:HIS:CE1	2.38	0.42
1:A:375:TYR:HB2	1:A:430:HIS:NE2	2.35	0.42
1:A:511:ALA:HA	1:A:512:PRO:HD2	1.59	0.42
1:A:532:GLU:O	1:A:553:ASP:CB	2.67	0.42
2:B:466:LEU:O	8:P:34:ARG:NH1	2.51	0.42
3:C:400:HIS:CG	3:C:401:PRO:HD2	2.54	0.42
4:D:423:ARG:HA	4:D:442:SER:HB2	2.02	0.42
4:D:429:THR:OG1	4:D:433:LEU:O	2.38	0.42
4:F:449:LEU:N	4:F:481:PRO:HD3	2.34	0.42
4:F:506:MET:O	4:F:516:PHE:CD2	2.73	0.42
4:H:415:GLU:O	4:H:418:TRP:HB2	2.20	0.42
4:H:536:CYS:O	4:H:536:CYS:SG	2.77	0.42
4:H:558:LYS:HB2	6:K:559:PRO:HG2	2.00	0.42
6:K:518:HIS:CE1	7:L:518:HIS:CG	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:377:CYS:O	8:P:377:CYS:SG	2.78	0.42
8:P:395:LEU:CD1	8:P:410:LEU:HD12	2.35	0.42
8:P:462:VAL:HB	8:P:509:VAL:C	2.38	0.42
6:K:464:LEU:CD1	6:K:525:GLU:CG	2.97	0.42
7:L:474:CYS:HB2	7:L:488:TRP:CZ2	2.55	0.42
8:P:264:VAL:HG22	8:P:275:PHE:CE2	2.49	0.42
8:P:471:SER:HB2	8:P:475:LYS:HZ3	1.83	0.42
9:R:111:ASP:O	9:R:114:LYS:HE2	2.15	0.42
9:R:116:GLN:NE2	9:R:116:GLN:C	2.73	0.42
11:U:61:VAL:HG12	11:U:69:LYS:HD2	2.02	0.42
2:B:479:PHE:CD1	2:B:479:PHE:N	2.86	0.42
2:B:543:LEU:HA	2:B:543:LEU:HD23	1.40	0.42
4:E:370:THR:HG22	4:E:371:ASP:N	2.35	0.42
4:H:384:ARG:HE	4:H:390:VAL:CG2	2.31	0.42
6:K:405:PHE:HE2	6:K:407:ALA:HB2	1.85	0.42
6:K:476:VAL:O	6:K:479:PHE:HE1	2.02	0.42
6:K:489:MET:HE2	6:K:489:MET:HB2	1.75	0.42
7:L:400:HIS:HE1	7:L:405:PHE:HA	1.82	0.42
7:L:445:LYS:HB2	7:L:445:LYS:HE2	1.70	0.42
8:P:526:CYS:CA	8:P:538:ALA:HB3	2.50	0.42
11:U:37:CYS:CB	11:U:87:PHE:O	2.68	0.42
2:B:568:MET:HB3	3:C:568:MET:HG2	2.02	0.42
3:C:466:LEU:HD23	12:V:45:ARG:NH2	2.34	0.42
4:E:515:TYR:CD1	4:E:515:TYR:N	2.83	0.42
4:F:461:ARG:HD3	4:F:461:ARG:HA	1.79	0.42
4:H:529:ASN:C	4:H:531:GLY:N	2.73	0.42
6:K:400:HIS:HB3	6:K:404:THR:O	2.20	0.42
8:P:412:GLN:NE2	8:P:412:GLN:C	2.73	0.42
12:V:86:LEU:HD12	12:V:87:PHE:N	2.35	0.42
1:A:484:VAL:O	1:A:484:VAL:HG13	2.16	0.42
1:A:486:VAL:HG22	1:A:538:VAL:HG12	2.02	0.42
1:A:496:SER:HA	1:A:497:PRO:HD3	1.75	0.42
1:A:543:LEU:HD23	1:A:544:PRO:HD2	2.02	0.42
2:B:500:TYR:CD1	2:B:500:TYR:N	2.86	0.42
3:C:461:ARG:NH1	3:C:465:ASN:CG	2.69	0.42
4:F:523:VAL:HB	4:F:524:SER:H	1.41	0.42
4:H:423:ARG:HH11	4:H:425:THR:HB	1.85	0.42
7:L:372:LEU:HD23	7:L:407:ALA:H	1.85	0.42
2:B:445:LYS:NZ	2:B:445:LYS:CA	2.82	0.41
3:C:454:VAL:CG2	3:C:538:VAL:CG2	2.98	0.41
4:F:536:CYS:O	4:F:549:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:427:THR:OG1	4:H:436:PRO:HB3	2.20	0.41
6:K:369:VAL:O	6:K:406:SER:HA	2.21	0.41
8:P:148:TYR:CE2	8:P:203:GLN:HG2	2.55	0.41
10:S:49:CYS:HB2	10:S:103:ALA:HB3	2.01	0.41
11:U:104:CYS:O	11:U:115:THR:N	2.33	0.41
1:A:382:TRP:CD1	1:A:411:ALA:HB2	2.54	0.41
3:C:568:MET:HE1	6:K:564:VAL:HG21	2.01	0.41
4:G:365:LEU:HG	4:G:424:PHE:CD2	2.55	0.41
11:U:81:TYR:OH	11:U:88:LEU:HD12	2.20	0.41
12:V:75:ARG:O	12:V:92:THR:N	2.53	0.41
1:A:379:THR:H	1:A:429:THR:HB	1.84	0.41
1:A:495:LEU:CD1	1:A:521:LEU:HD11	2.50	0.41
2:B:525:GLU:O	2:B:525:GLU:CG	2.68	0.41
3:C:423:ARG:HE	3:C:442:SER:CB	2.33	0.41
3:C:462:GLU:O	3:C:465:ASN:HB2	2.20	0.41
3:C:467:ARG:N	3:C:467:ARG:CD	2.72	0.41
4:G:489:MET:SD	4:G:537:VAL:HG21	2.60	0.41
12:V:33:VAL:HG22	12:V:91:VAL:HB	2.01	0.41
2:B:430:HIS:HE1	2:B:433:LEU:HB2	1.85	0.41
2:B:483:ASP:O	2:B:540:HIS:HD2	2.03	0.41
4:D:533:THR:HA	4:D:552:VAL:O	2.21	0.41
4:E:370:THR:HG22	4:E:371:ASP:H	1.86	0.41
4:E:467:ARG:O	11:U:60:THR:HB	2.20	0.41
4:E:481:PRO:HD2	4:E:540:HIS:NE2	2.35	0.41
4:E:532:GLU:HB3	4:E:534:TYR:CE2	2.56	0.41
4:G:439:GLN:HG3	4:G:441:ILE:HG23	2.01	0.41
5:J:31:ASP:HB2	7:L:554:LYS:HZ3	1.84	0.41
5:J:104:ASP:HB3	5:J:107:LYS:HB2	2.03	0.41
7:L:354:PHE:CG	7:L:541:GLU:HB3	2.55	0.41
7:L:400:HIS:CD2	7:L:402:ASN:HB2	2.55	0.41
7:L:528:TRP:CH2	7:L:554:LYS:HA	2.55	0.41
7:L:556:THR:O	7:L:556:THR:CG2	2.69	0.41
8:P:25:PRO:HB3	8:P:329:ASN:HD21	1.86	0.41
8:P:479:LYS:CE	8:P:524:TYR:HE1	2.34	0.41
10:S:39:LEU:CD2	10:S:41:GLU:HG2	2.51	0.41
2:B:416:ASP:OD1	2:B:417:ASP:N	2.54	0.41
3:C:466:LEU:CD2	3:C:466:LEU:O	2.69	0.41
4:E:421:GLY:N	4:E:445:LYS:HE2	2.35	0.41
4:F:449:LEU:CA	4:F:481:PRO:HD3	2.44	0.41
4:F:546:ARG:NH1	4:F:546:ARG:HG2	2.35	0.41
4:G:432:ASP:OD1	4:G:433:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:558:LYS:HA	6:K:559:PRO:HD3	1.87	0.41
7:L:348:PHE:HB3	7:L:368:LEU:HB2	2.02	0.41
7:L:393:HIS:ND1	7:L:396:ILE:HD13	2.36	0.41
8:P:315:LEU:CG	8:P:315:LEU:O	2.69	0.41
8:P:388:LYS:HD2	8:P:388:LYS:HA	1.61	0.41
9:R:48:LEU:HD22	9:R:89:VAL:HG11	2.02	0.41
1:A:490:GLN:HB2	1:A:534:TYR:HE1	1.85	0.41
2:B:385:GLN:HE22	2:B:423:ARG:HB3	1.86	0.41
3:C:397:SER:H	3:C:408:VAL:HG22	1.85	0.41
3:C:509:PRO:HG2	4:D:522:THR:CG2	2.50	0.41
4:D:514:ARG:N	4:D:514:ARG:CD	2.77	0.41
4:D:535:THR:O	4:D:535:THR:OG1	2.33	0.41
4:F:443:ARG:HA	4:F:444:PRO:HD2	1.45	0.41
4:F:484:VAL:O	4:F:484:VAL:HG13	2.18	0.41
4:H:352:PRO:HD2	4:H:418:TRP:HH2	1.84	0.41
4:H:572:ALA:C	4:H:574:THR:H	2.23	0.41
6:K:450:HIS:HB3	6:K:514:ARG:NH2	2.36	0.41
7:L:488:TRP:CE2	7:L:536:CYS:HB2	2.55	0.41
7:L:532:GLU:O	7:L:534:TYR:CE2	2.74	0.41
8:P:131:THR:HG22	8:P:188:VAL:N	2.36	0.41
8:P:295:THR:CG2	8:P:432:ARG:HB2	2.49	0.41
8:P:340:VAL:HG11	8:P:436:GLU:OE1	2.20	0.41
11:U:109:ASN:HD22	11:U:112:ARG:NH2	2.19	0.41
1:A:525:GLU:O	1:A:529:ASN:N	2.54	0.41
2:B:495:LEU:HA	2:B:495:LEU:HD23	1.60	0.41
4:D:449:LEU:H	4:D:449:LEU:HG	1.44	0.41
4:D:539:ALA:HA	4:D:546:ARG:O	2.20	0.41
4:E:450:HIS:HB3	4:E:514:ARG:HH21	1.85	0.41
4:F:545:ASN:ND2	4:F:545:ASN:H	2.19	0.41
4:G:443:ARG:NE	4:G:443:ARG:C	2.73	0.41
4:H:489:MET:SD	4:H:537:VAL:HG11	2.61	0.41
6:K:509:PRO:O	7:L:498:GLU:OE2	2.39	0.41
7:L:362:SER:OG	7:L:363:THR:N	2.53	0.41
7:L:485:PHE:CE2	7:L:487:GLN:HB2	2.56	0.41
8:P:148:TYR:HB3	8:P:155:PRO:CG	2.51	0.41
8:P:245:VAL:CG2	8:P:309:ALA:HB3	2.51	0.41
8:P:466:PHE:CD2	8:P:507:ARG:HG2	2.55	0.41
1:A:548:THR:OG1	1:A:549:GLU:N	2.54	0.41
2:B:545:ASN:HD21	3:C:547:VAL:HG21	1.85	0.41
3:C:400:HIS:ND1	3:C:401:PRO:HD2	2.35	0.41
4:D:367:CYS:SG	4:D:382:TRP:NE1	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:481:PRO:O	4:F:540:HIS:HE1	2.04	0.41
4:G:455:TYR:CZ	4:H:463:GLN:HG3	2.56	0.41
7:L:354:PHE:HD2	7:L:546:ARG:NH2	2.16	0.41
8:P:25:PRO:HA	8:P:26:PRO:HD3	1.89	0.41
1:A:454:VAL:HG21	1:A:538:VAL:HG21	2.02	0.41
1:A:510:GLN:CD	1:A:510:GLN:N	2.73	0.41
1:A:552:VAL:O	1:A:552:VAL:CG1	2.69	0.41
2:B:568:MET:CE	7:L:564:VAL:HG21	2.51	0.41
3:C:484:VAL:O	3:C:484:VAL:CG1	2.69	0.41
3:C:564:VAL:H	3:C:564:VAL:HG23	1.56	0.41
4:D:536:CYS:O	4:D:536:CYS:SG	2.78	0.41
4:G:365:LEU:HD11	4:G:418:TRP:CZ3	2.55	0.41
6:K:463:GLN:HA	7:L:455:TYR:OH	2.21	0.41
6:K:564:VAL:H	6:K:564:VAL:HG23	1.59	0.41
7:L:454:VAL:HG13	7:L:550:ARG:HB2	2.02	0.41
7:L:459:PRO:HD3	7:L:472:ILE:HG12	2.02	0.41
8:P:140:ASN:ND2	8:P:143:LYS:HB2	2.35	0.41
8:P:239:CYS:HB2	8:P:290:PHE:HE1	1.86	0.41
8:P:462:VAL:CG1	8:P:509:VAL:HB	2.51	0.41
8:P:480:TRP:HH2	8:P:482:ASN:HB3	1.82	0.41
9:R:24:LYS:HD3	9:R:119:THR:HG23	2.03	0.41
12:V:22:GLU:HB2	12:V:119:THR:H	1.85	0.41
1:A:573:GLY:O	1:A:574:THR:C	2.59	0.41
2:B:456:LEU:HG	2:B:552:VAL:HB	2.02	0.41
3:C:532:GLU:OE2	3:C:532:GLU:HA	2.21	0.41
4:D:369:VAL:HG13	4:D:405:PHE:CD2	2.56	0.41
4:G:583:NAG:H3	4:G:583:NAG:C8	2.48	0.41
6:K:352:PRO:HG2	6:K:363:THR:HG23	2.02	0.41
6:K:430:HIS:HD2	6:K:433:LEU:H	1.69	0.41
7:L:511:ALA:HB1	7:L:514:ARG:NE	2.36	0.41
8:P:340:VAL:HG12	8:P:436:GLU:CA	2.51	0.41
12:V:69:LYS:O	12:V:73:LYS:HG2	2.21	0.41
12:V:112:ARG:HB2	12:V:112:ARG:HH11	1.85	0.41
1:A:502:THR:CB	1:A:519:SER:HB2	2.33	0.40
3:C:354:PHE:HD1	3:C:357:ILE:HD12	1.85	0.40
3:C:428:VAL:O	3:C:436:PRO:HA	2.21	0.40
4:D:382:TRP:HZ3	4:D:424:PHE:HB3	1.86	0.40
4:D:415:GLU:O	4:D:419:ASN:ND2	2.34	0.40
4:F:423:ARG:HB2	4:F:440:THR:OG1	2.20	0.40
4:F:476:VAL:O	4:F:516:PHE:HA	2.21	0.40
4:F:523:VAL:HG12	4:F:534:TYR:OH	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:508:GLU:HB3	4:H:511:ALA:HB3	2.03	0.40
7:L:367:CYS:O	7:L:369:VAL:HG23	2.21	0.40
8:P:172:ARG:HD2	8:P:190:ASN:O	2.21	0.40
8:P:278:ARG:CA	8:P:422:TRP:HZ2	2.34	0.40
12:V:58:CYS:SG	12:V:110:THR:HG22	2.61	0.40
1:A:441:ILE:HD12	1:A:441:ILE:HA	1.90	0.40
1:A:500:TYR:CD2	1:A:500:TYR:C	2.94	0.40
2:B:456:LEU:HD11	2:B:472:ILE:HG22	2.03	0.40
2:B:510:GLN:OE1	2:B:510:GLN:CA	2.69	0.40
3:C:526:GLU:CD	3:C:526:GLU:N	2.73	0.40
4:F:523:VAL:HG11	4:F:534:TYR:CE2	2.56	0.40
4:H:408:VAL:HG13	4:H:408:VAL:O	2.21	0.40
6:K:506:MET:HB2	6:K:516:PHE:HE1	1.85	0.40
1:A:390:VAL:HG13	1:A:391:LYS:H	1.86	0.40
1:A:452:PRO:HG3	1:A:479:PHE:HB3	2.02	0.40
1:A:489:MET:HE2	1:A:537:VAL:HG21	2.02	0.40
1:A:545:ASN:O	1:A:547:VAL:N	2.52	0.40
2:B:384:ARG:NE	2:B:388:GLU:HB2	2.37	0.40
4:D:493:GLN:N	4:D:493:GLN:CD	2.71	0.40
4:E:543:LEU:HA	4:E:544:PRO:HD3	1.84	0.40
8:P:11:ASN:HA	8:P:108:GLU:O	2.21	0.40
9:R:20:LEU:HD23	9:R:117:LYS:HG2	1.92	0.40
3:C:510:GLN:OE1	3:C:510:GLN:CA	2.70	0.40
4:F:365:LEU:HB3	4:F:382:TRP:CH2	2.56	0.40
4:F:476:VAL:HG12	4:F:479:PHE:CE1	2.56	0.40
4:H:349:ALA:HA	4:H:366:THR:O	2.22	0.40
4:H:567:VAL:HG21	4:H:576:TYR:OH	2.21	0.40
6:K:385:GLN:NE2	6:K:423:ARG:H	2.20	0.40
8:P:354:PRO:HA	8:P:405:THR:HB	2.03	0.40
8:P:471:SER:CB	8:P:475:LYS:HZ3	2.29	0.40
10:S:93:GLN:OE1	10:S:93:GLN:CA	2.70	0.40
13:I:2:NAG:O3	13:I:2:NAG:C7	2.70	0.40
2:B:481:PRO:O	2:B:481:PRO:CG	2.69	0.40
2:B:498:GLU:O	2:B:498:GLU:CG	2.69	0.40
2:B:546:ARG:HE	2:B:546:ARG:HB2	1.47	0.40
3:C:464:LEU:O	3:C:466:LEU:N	2.55	0.40
4:D:365:LEU:HD23	4:D:365:LEU:H	1.86	0.40
4:D:367:CYS:SG	4:D:393:HIS:HE1	2.45	0.40
4:D:499:LYS:HB3	4:D:499:LYS:HE2	1.71	0.40
4:E:364:LYS:HD3	4:E:411:ALA:O	2.21	0.40
4:G:363:THR:OG1	4:G:413:ILE:O	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:363:THR:O	4:H:412:SER:HA	2.22	0.40
4:H:369:VAL:HG12	4:H:372:LEU:HD23	2.02	0.40
8:P:25:PRO:HB3	8:P:329:ASN:ND2	2.36	0.40
8:P:377:CYS:HA	8:P:378:PRO:HD3	1.97	0.40
8:P:447:LYS:H	8:P:465:HIS:CA	2.31	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	229/232 (99%)	195 (85%)	24 (10%)	10 (4%)	2 2
2	B	226/229 (99%)	206 (91%)	17 (8%)	3 (1%)	12 12
3	C	225/228 (99%)	188 (84%)	26 (12%)	11 (5%)	2 2
4	D	222/225 (99%)	204 (92%)	16 (7%)	2 (1%)	17 17
4	E	222/225 (99%)	198 (89%)	19 (9%)	5 (2%)	6 6
4	F	222/225 (99%)	203 (91%)	11 (5%)	8 (4%)	3 3
4	G	222/225 (99%)	206 (93%)	14 (6%)	2 (1%)	17 17
4	H	230/225 (102%)	202 (88%)	19 (8%)	9 (4%)	3 3
5	J	102/106 (96%)	92 (90%)	8 (8%)	2 (2%)	7 7
6	K	230/233 (99%)	202 (88%)	19 (8%)	9 (4%)	3 3
7	L	230/233 (99%)	193 (84%)	29 (13%)	8 (4%)	3 3
8	P	481/495 (97%)	408 (85%)	54 (11%)	19 (4%)	3 3
9	R	99/101 (98%)	80 (81%)	17 (17%)	2 (2%)	7 7
10	S	101/103 (98%)	88 (87%)	11 (11%)	2 (2%)	7 7
11	U	99/103 (96%)	88 (89%)	8 (8%)	3 (3%)	4 4
12	V	104/106 (98%)	97 (93%)	6 (6%)	1 (1%)	15 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3244/3294 (98%)	2850 (88%)	298 (9%)	96 (3%)	7 4

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	546	ARG
1	A	554	LYS
2	B	480	SER
3	C	482	ALA
4	E	494	PRO
4	E	533	THR
4	E	546	ARG
4	F	444	PRO
4	F	480	SER
4	F	546	ARG
4	G	444	PRO
4	H	442	SER
4	H	569	SER
4	H	574	THR
6	K	447	VAL
6	K	492	GLY
6	K	511	ALA
6	K	512	PRO
6	K	541	GLU
7	L	441	ILE
7	L	443	ARG
7	L	481	PRO
8	P	101	LEU
8	P	259	GLU
8	P	261	CYS
8	P	262	ASP
8	P	311	SER
8	P	379	LEU
8	P	399	GLU
8	P	413	LEU
8	P	448	VAL
9	R	66	ASN
10	S	53	ALA
10	S	98	ASP
11	U	96	GLU
1	A	446	GLY
2	B	441	ILE

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Mol	Chain	Res	Type
2	B	497	PRO
3	C	531	GLY
4	E	534	TYR
4	F	449	LEU
4	F	507	PRO
4	F	523	VAL
4	G	478	GLY
4	H	531	GLY
4	H	564	VAL
5	J	64	LEU
7	L	478	GLY
7	L	534	TYR
8	P	310	HIS
8	P	403	ASN
8	P	416	ARG
1	A	491	ARG
1	A	512	PRO
3	C	448	ALA
3	C	509	PRO
3	C	510	GLN
3	C	512	PRO
4	D	497	PRO
4	H	444	PRO
4	H	449	LEU
4	H	559	PRO
5	J	120	GLU
6	K	572	ALA
7	L	444	PRO
7	L	447	VAL
8	P	155	PRO
8	P	378	PRO
8	P	473	TYR
11	U	98	ASP
1	A	497	PRO
1	A	573	GLY
3	C	481	PRO
3	C	523	VAL
3	C	557	GLY
4	D	447	VAL
4	E	509	PRO
4	F	544	PRO
4	H	560	THR

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Mol	Chain	Res	Type
6	K	519	SER
6	K	544	PRO
7	L	483	ASP
8	P	57	SER
8	P	287	ASP
9	R	96	GLU
12	V	113	GLY
3	C	466	LEU
3	C	558	LYS
8	P	157	LEU
1	A	501	VAL
4	F	559	PRO
11	U	42	MET
6	K	444	PRO
1	A	531	GLY
8	P	288	GLY
1	A	481	PRO

5.3.2 Protein sidechains

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	205/203 (101%)	184 (90%)	21 (10%)	7 7
2	B	203/203 (100%)	186 (92%)	17 (8%)	11 11
3	C	203/203 (100%)	182 (90%)	21 (10%)	7 7
4	D	200/200 (100%)	194 (97%)	6 (3%)	41 41
4	E	200/200 (100%)	193 (96%)	7 (4%)	36 36
4	F	200/200 (100%)	182 (91%)	18 (9%)	9 9
4	G	200/200 (100%)	189 (94%)	11 (6%)	21 21
4	H	206/200 (103%)	188 (91%)	18 (9%)	10 10
5	J	100/100 (100%)	94 (94%)	6 (6%)	19 19
6	K	206/201 (102%)	179 (87%)	27 (13%)	4 4
7	L	206/206 (100%)	183 (89%)	23 (11%)	6 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	P	423/423 (100%)	368 (87%)	55 (13%)	4 4
9	R	86/86 (100%)	76 (88%)	10 (12%)	5 5
10	S	88/88 (100%)	74 (84%)	14 (16%)	2 2
11	U	86/88 (98%)	79 (92%)	7 (8%)	11 11
12	V	91/91 (100%)	89 (98%)	2 (2%)	52 52
All	All	2903/2892 (100%)	2640 (91%)	263 (9%)	13 9

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	LYS
1	A	447	VAL
1	A	466	LEU
1	A	467	ARG
1	A	477	THR
1	A	490	GLN
1	A	502	THR
1	A	508	GLU
1	A	510	GLN
1	A	514	ARG
1	A	518	HIS
1	A	519	SER
1	A	532	GLU
1	A	543	LEU
1	A	545	ASN
1	A	550	ARG
1	A	554	LYS
1	A	566	LEU
1	A	568	MET
1	A	571	THR
1	A	574	THR
2	B	423	ARG
2	B	441	ILE
2	B	442	SER
2	B	443	ARG
2	B	445	LYS
2	B	449	LEU
2	B	451	ARG
2	B	454	VAL
2	B	456	LEU

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Mol	Chain	Res	Type
2	B	462	GLU
2	B	480	SER
2	B	526	GLU
2	B	528	TRP
2	B	529	ASN
2	B	530	THR
2	B	532	GLU
2	B	546	ARG
3	C	445	LYS
3	C	450	HIS
3	C	451	ARG
3	C	453	ASP
3	C	456	LEU
3	C	457	LEU
3	C	466	LEU
3	C	467	ARG
3	C	468	GLU
3	C	480	SER
3	C	494	PRO
3	C	508	GLU
3	C	510	GLN
3	C	514	ARG
3	C	525	GLU
3	C	526	GLU
3	C	533	THR
3	C	554	LYS
3	C	565	SER
3	C	566	LEU
3	C	567	VAL
4	D	493	GLN
4	D	495	LEU
4	D	499	LYS
4	D	510	GLN
4	D	514	ARG
4	D	536	CYS
4	E	483	ASP
4	E	493	GLN
4	E	514	ARG
4	E	532	GLU
4	E	535	THR
4	E	538	VAL
4	E	545	ASN

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Mol	Chain	Res	Type
4	F	442	SER
4	F	443	ARG
4	F	445	LYS
4	F	479	PHE
4	F	501	VAL
4	F	502	THR
4	F	506	MET
4	F	520	ILE
4	F	523	VAL
4	F	543	LEU
4	F	544	PRO
4	F	545	ASN
4	F	546	ARG
4	F	548	THR
4	F	550	ARG
4	F	554	LYS
4	F	556	THR
4	F	561	LEU
4	G	443	ARG
4	G	445	LYS
4	G	447	VAL
4	G	449	LEU
4	G	450	HIS
4	G	466	LEU
4	G	473	THR
4	G	475	LEU
4	G	477	THR
4	G	516	PHE
4	G	566	LEU
4	H	442	SER
4	H	443	ARG
4	H	444	PRO
4	H	445	LYS
4	H	449	LEU
4	H	519	SER
4	H	532	GLU
4	H	533	THR
4	H	535	THR
4	H	536	CYS
4	H	556	THR
4	H	561	LEU
4	H	563	ASN

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Mol	Chain	Res	Type
4	H	566	LEU
4	H	568	MET
4	H	574	THR
4	H	575	CYS
4	H	576	TYR
5	J	23	ARG
5	J	26	GLU
5	J	34	GLU
5	J	35	ARG
5	J	107	LYS
5	J	117	TYR
6	K	445	LYS
6	K	449	LEU
6	K	462	GLU
6	K	464	LEU
6	K	474	CYS
6	K	475	LEU
6	K	477	THR
6	K	484	VAL
6	K	489	MET
6	K	490	GLN
6	K	491	ARG
6	K	514	ARG
6	K	516	PHE
6	K	520	ILE
6	K	521	LEU
6	K	524	SER
6	K	526	GLU
6	K	530	THR
6	K	533	THR
6	K	543	LEU
6	K	545	ASN
6	K	556	THR
6	K	558	LYS
6	K	561	LEU
6	K	565	SER
6	K	568	MET
6	K	574	THR
7	L	441	ILE
7	L	443	ARG
7	L	445	LYS
7	L	449	LEU

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Mol	Chain	Res	Type
7	L	450	HIS
7	L	479	PHE
7	L	480	SER
7	L	514	ARG
7	L	534	TYR
7	L	535	THR
7	L	536	CYS
7	L	543	LEU
7	L	545	ASN
7	L	547	VAL
7	L	548	THR
7	L	551	THR
7	L	552	VAL
7	L	556	THR
7	L	558	LYS
7	L	566	LEU
7	L	567	VAL
7	L	574	THR
7	L	575	CYS
8	P	10	VAL
8	P	43	ARG
8	P	60	TYR
8	P	99	ARG
8	P	131	THR
8	P	132	ILE
8	P	151	ILE
8	P	245	VAL
8	P	247	ASN
8	P	257	SER
8	P	259	GLU
8	P	260	ASN
8	P	275	PHE
8	P	287	ASP
8	P	290	PHE
8	P	314	GLN
8	P	315	LEU
8	P	316	GLN
8	P	317	GLU
8	P	340	VAL
8	P	342	LYS
8	P	344	VAL
8	P	349	VAL

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Mol	Chain	Res	Type
8	P	358	LYS
8	P	361	LYS
8	P	377	CYS
8	P	379	LEU
8	P	388	LYS
8	P	392	GLU
8	P	398	LEU
8	P	399	GLU
8	P	400	GLU
8	P	405	THR
8	P	409	ILE
8	P	412	GLN
8	P	413	LEU
8	P	414	THR
8	P	431	TRP
8	P	439	ILE
8	P	446	LEU
8	P	447	LYS
8	P	462	VAL
8	P	464	CYS
8	P	466	PHE
8	P	469	LYS
8	P	470	PHE
8	P	471	SER
8	P	473	TYR
8	P	475	LYS
8	P	478	CYS
8	P	530	GLN
8	P	533	PHE
8	P	537	THR
8	P	540	VAL
8	P	541	TYR
9	R	20	LEU
9	R	24	LYS
9	R	55	SER
9	R	65	THR
9	R	93	GLN
9	R	94	LEU
9	R	95	THR
9	R	96	GLU
9	R	115	THR
9	R	116	GLN

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Mol	Chain	Res	Type
10	S	39	LEU
10	S	42	MET
10	S	50	ARG
10	S	71	GLU
10	S	72	TYR
10	S	73	LYS
10	S	83	ARG
10	S	92	THR
10	S	93	GLN
10	S	94	LEU
10	S	96	GLU
10	S	115	THR
10	S	116	GLN
10	S	117	LYS
11	U	23	VAL
11	U	24	LYS
11	U	25	VAL
11	U	26	GLU
11	U	44	VAL
11	U	83	ARG
11	U	119	THR
12	V	96	GLU
12	V	114	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	GLN
1	A	518	HIS
1	A	540	HIS
2	B	450	HIS
2	B	529	ASN
2	B	545	ASN
3	C	400	HIS
3	C	465	ASN
4	D	393	HIS
4	D	545	ASN
4	E	400	HIS
4	E	487	GLN
4	E	493	GLN
4	F	540	HIS
4	F	545	ASN

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Mol	Chain	Res	Type
6	K	430	HIS
6	K	545	ASN
6	K	563	ASN
7	L	490	GLN
7	L	545	ASN
8	P	310	HIS
8	P	314	GLN
8	P	316	GLN
8	P	403	ASN
8	P	412	GLN
8	P	530	GLN
9	R	93	GLN
9	R	116	GLN
12	V	66	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

2 monosaccharides 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	$\#\|Z\| > 2$
13	NAG	I	1	13,5	14,14,15	3.15	2 (14%)	17,19,21	2.98	7 (41%)
13	NAG	I	2	13	14,14,15	1.09	0	17,19,21	3.30	7 (41%)

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
13	NAG	I	1	13,5	-	4/6/23/26	0/1/1/1
13	NAG	I	2	13	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	I	1	NAG	C1-C2	10.08	1.67	1.52
13	I	1	NAG	O5-C1	-4.51	1.36	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	I	2	NAG	C2-N2-C7	-9.79	108.97	122.90
13	I	1	NAG	O5-C5-C6	-6.42	97.13	107.20
13	I	1	NAG	C1-O5-C5	5.30	119.37	112.19
13	I	2	NAG	C1-O5-C5	5.11	119.11	112.19
13	I	1	NAG	C4-C3-C2	-4.59	104.29	111.02
13	I	2	NAG	C3-C4-C5	-4.37	102.44	110.24
13	I	2	NAG	C4-C3-C2	-4.22	104.84	111.02
13	I	1	NAG	O4-C4-C3	-3.46	102.35	110.35
13	I	1	NAG	O5-C1-C2	-3.22	106.20	111.29
13	I	1	NAG	C1-C2-N2	3.10	115.78	110.49
13	I	1	NAG	O3-C3-C2	-2.80	103.68	109.47
13	I	2	NAG	O3-C3-C2	-2.21	104.88	109.47
13	I	2	NAG	O5-C1-C2	2.17	114.72	111.29
13	I	2	NAG	C1-C2-N2	2.03	113.95	110.49

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	I	1	NAG	C8-C7-N2-C2
13	I	1	NAG	O7-C7-N2-C2
13	I	2	NAG	C8-C7-N2-C2
13	I	2	NAG	O7-C7-N2-C2
13	I	2	NAG	O5-C5-C6-O6
13	I	1	NAG	C3-C2-N2-C7
13	I	1	NAG	C1-C2-N2-C7

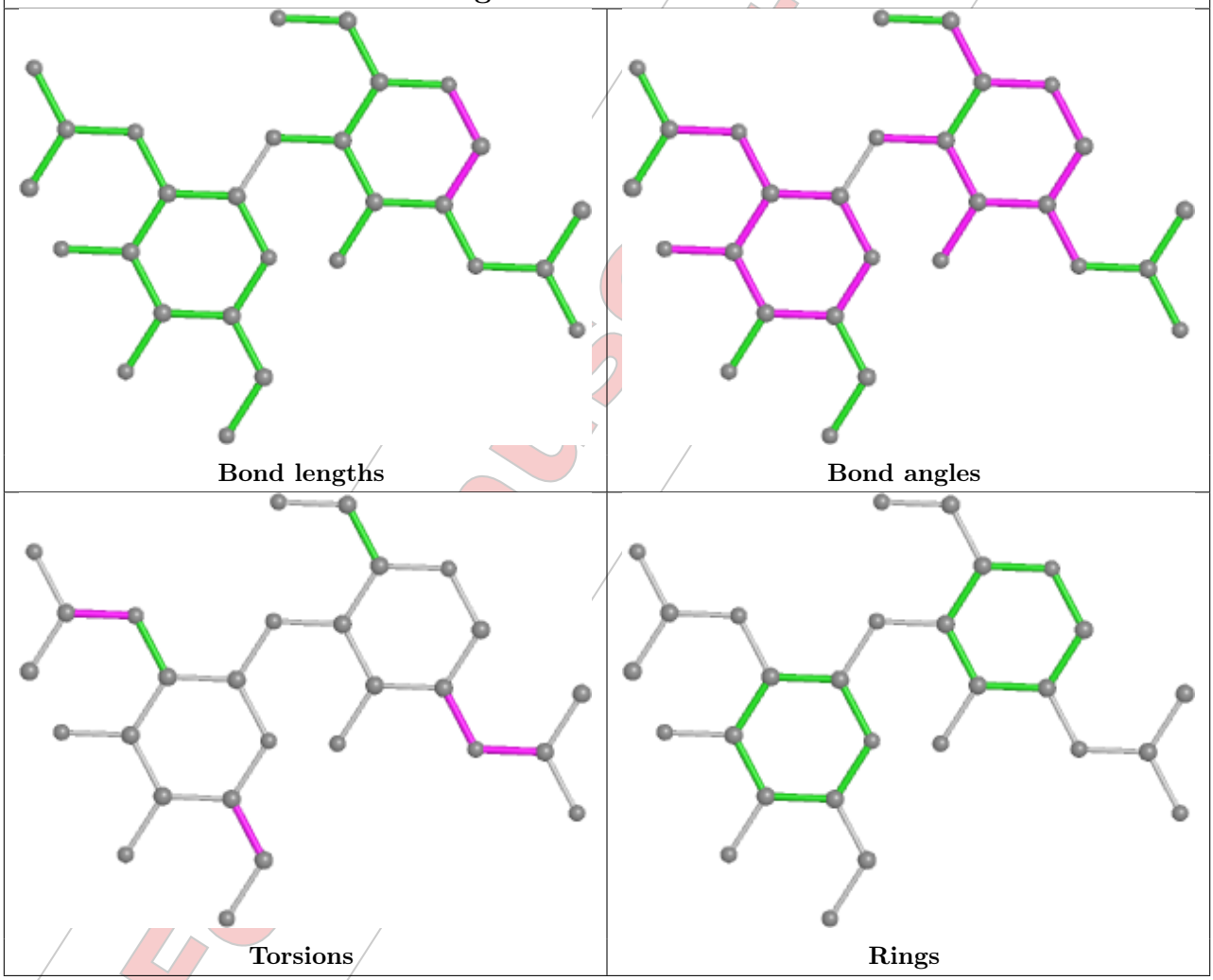
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	I	2	NAG	3	0
13	I	1	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain I



5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	P	6
1	A	1
3	C	1
2	B	1
7	L	1
6	K	1
4	F	1
4	H	1
4	G	1
5	J	1
4	D	1
4	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	575:CYS	C	583:NAG	O6	29.30
1	C	571:THR	C	583:NAG	O6	20.22
1	B	572:ALA	C	583:NAG	O6	19.44
1	L	576:TYR	C	583:NAG	O3	18.65
1	K	576:TYR	C	583:NAG	O3	17.77
1	F	568:MET	C	583:NAG	O3	15.66
1	H	576:TYR	C	583:NAG	O3	15.03
1	G	568:MET	C	583:NAG	O3	14.91
1	P	112:GLY	C	120:LYS	N	14.54
1	P	513:LEU	C	522:GLY	N	14.44
1	J	69:LYS	C	98:GLU	N	14.03
1	D	568:MET	C	583:NAG	O6	12.80
1	E	568:MET	C	583:NAG	O6	12.34
1	P	497:LYS	C	506:SER	N	7.80
1	P	451:ASN	C	462:VAL	N	5.83
1	P	176:ASP	C	185:PHE	N	5.65
1	P	204:ALA	C	210:SER	N	5.10

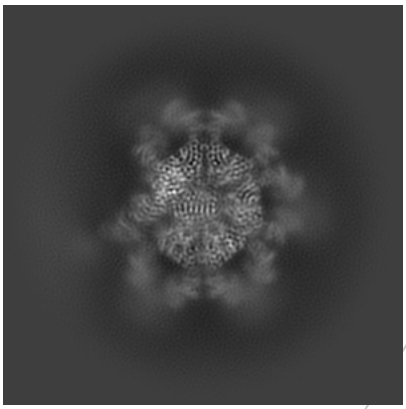
6 Map visualisation

This section contains visualisations of the EMDB entry D_1300031551. These allow visual inspection of the internal detail of the map and identification of artifacts.

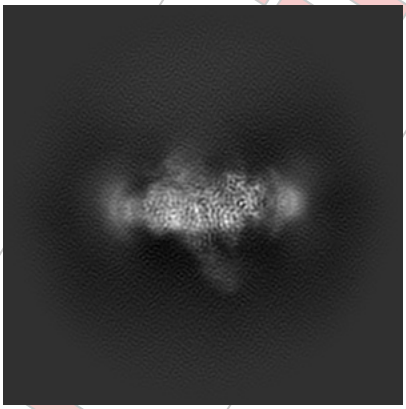
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

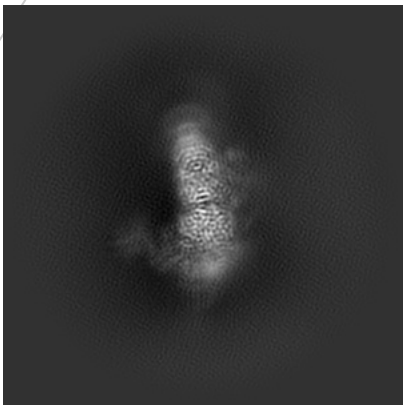
6.1.1 Primary map



X

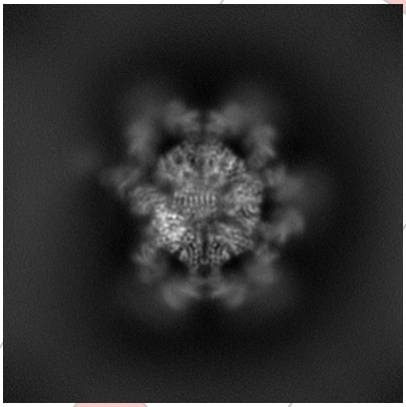


Y

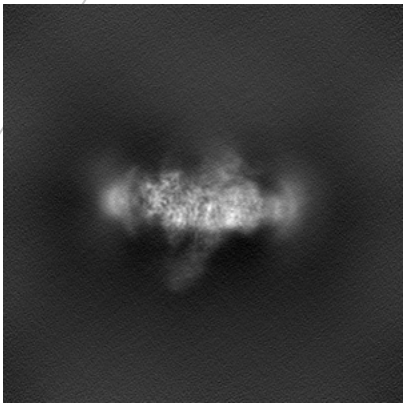


Z

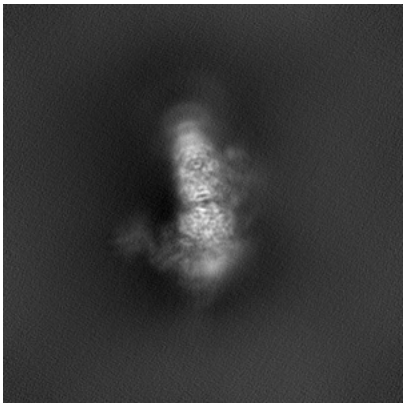
6.1.2 Raw map



X



Y

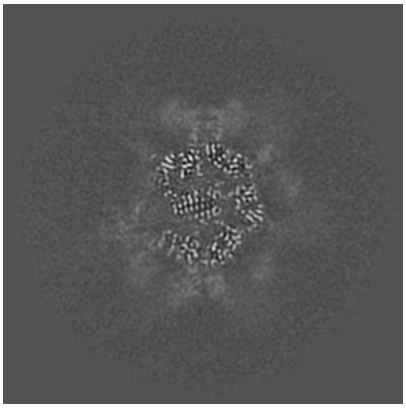


Z

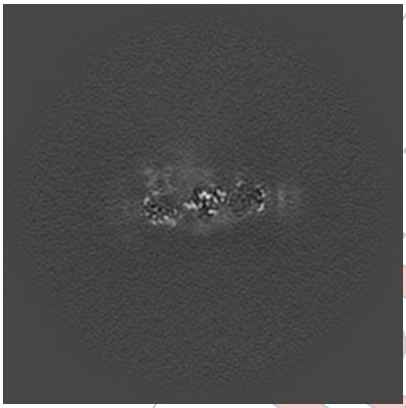
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

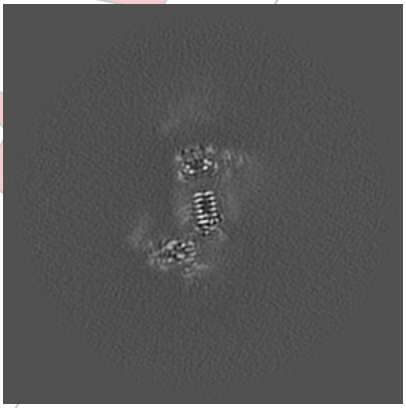
6.2.1 Primary map



X Index: 160

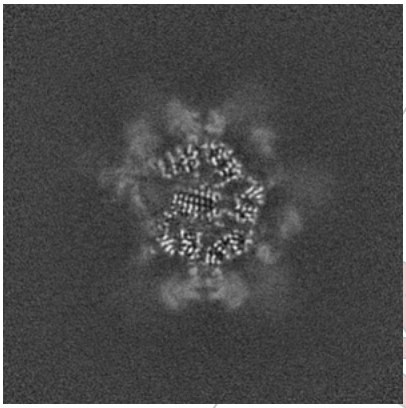


Y Index: 160

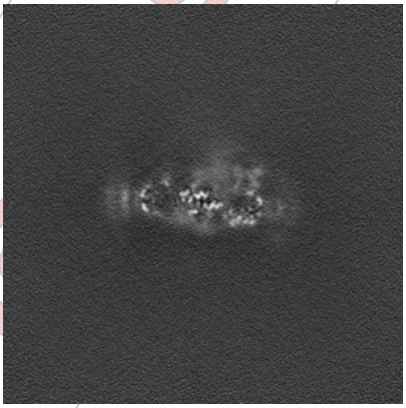


Z Index: 160

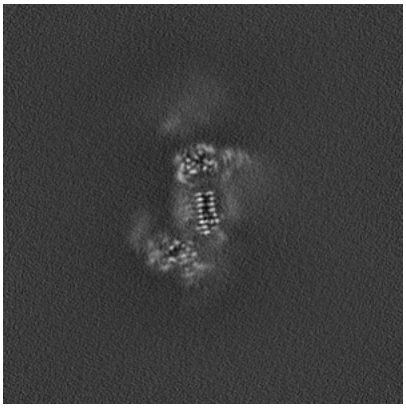
6.2.2 Raw map



X Index: 160



Y Index: 160

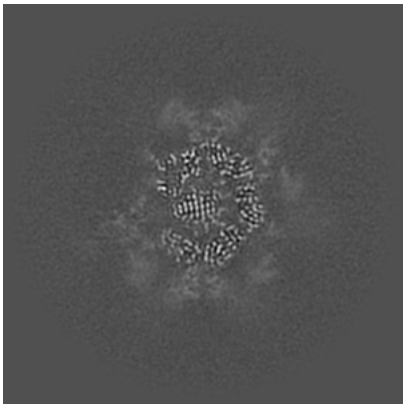


Z Index: 160

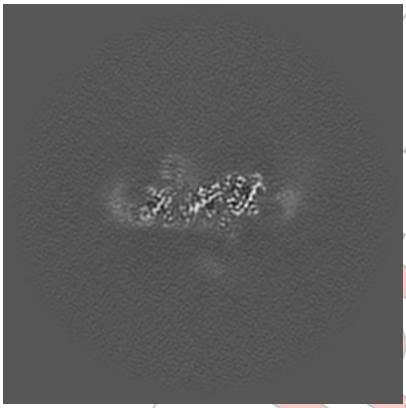
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

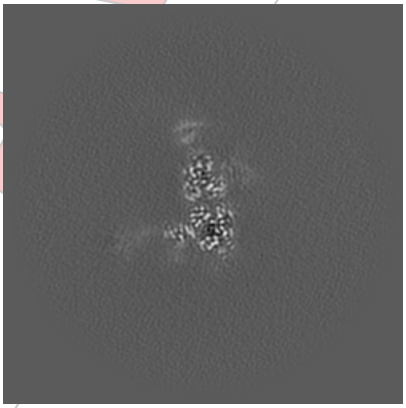
6.3.1 Primary map



X Index: 158

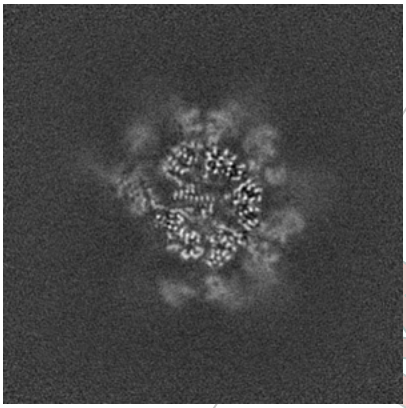


Y Index: 146

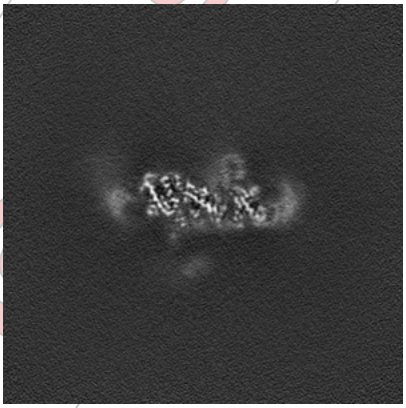


Z Index: 187

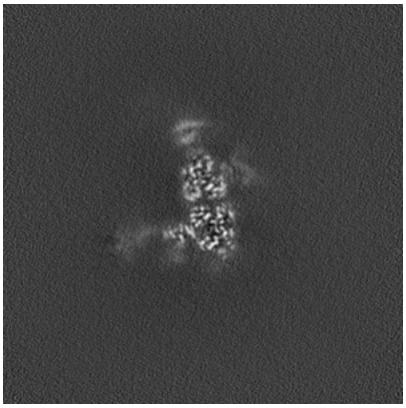
6.3.2 Raw map



X Index: 153



Y Index: 146



Z Index: 132

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.27. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

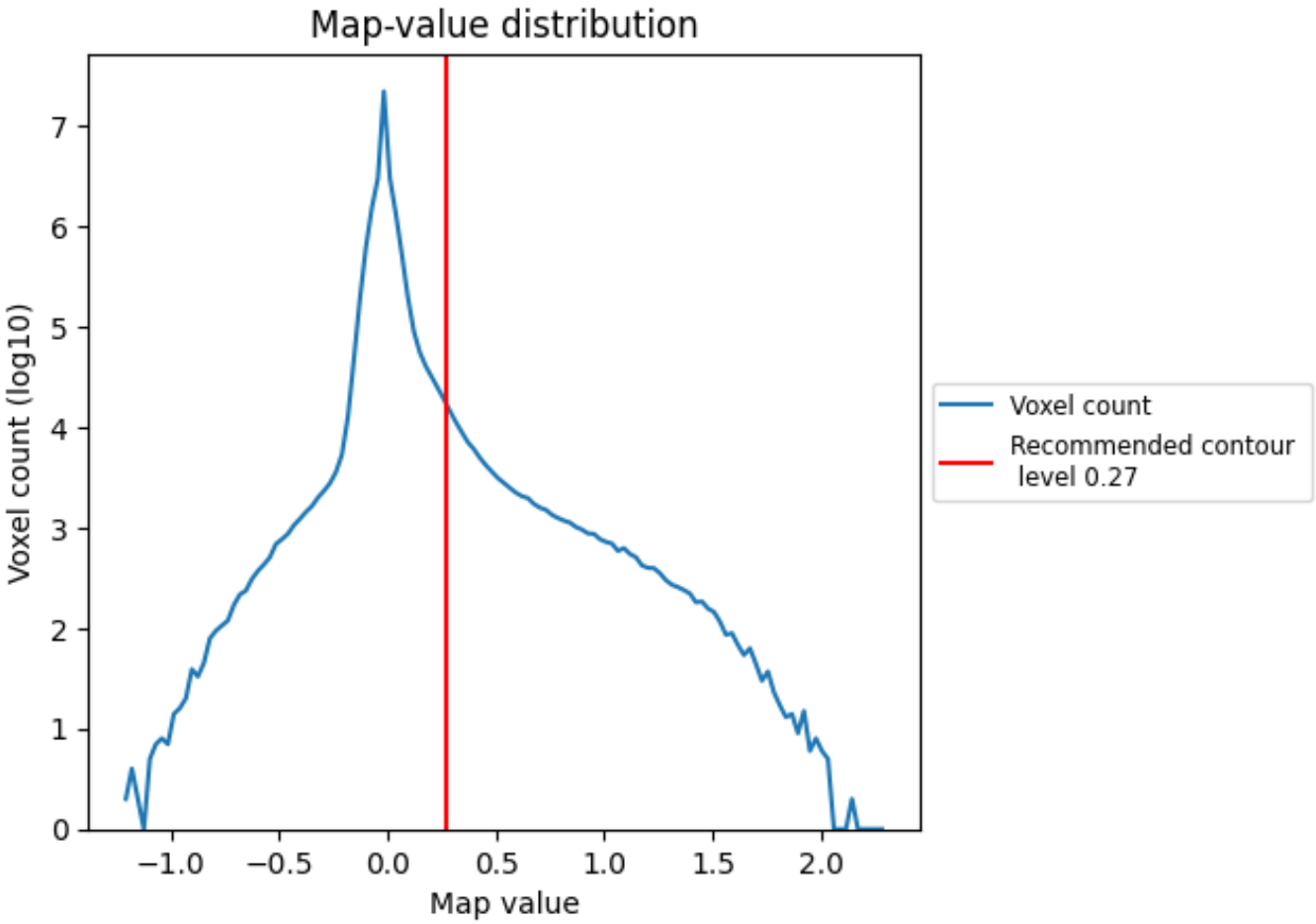
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

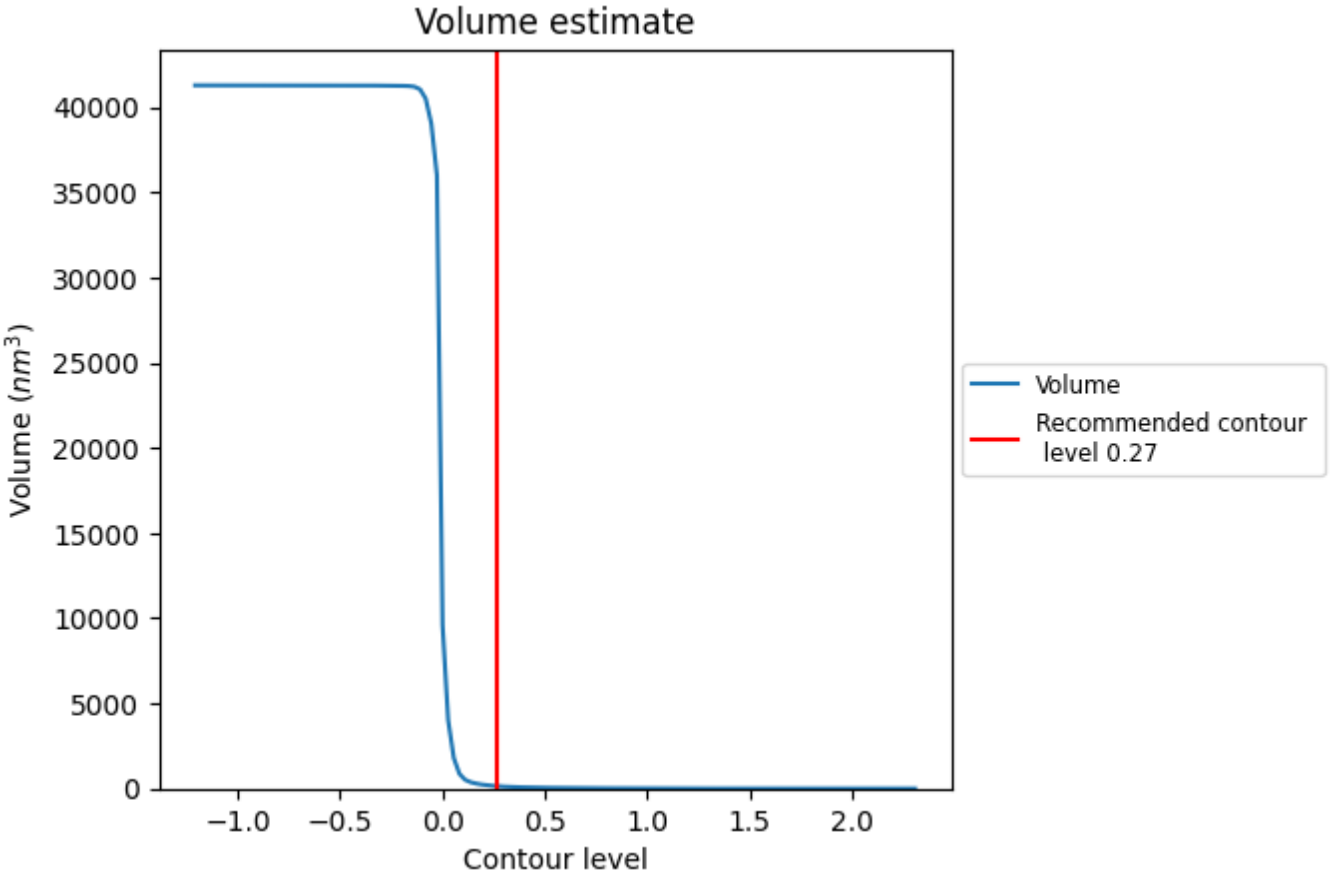
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

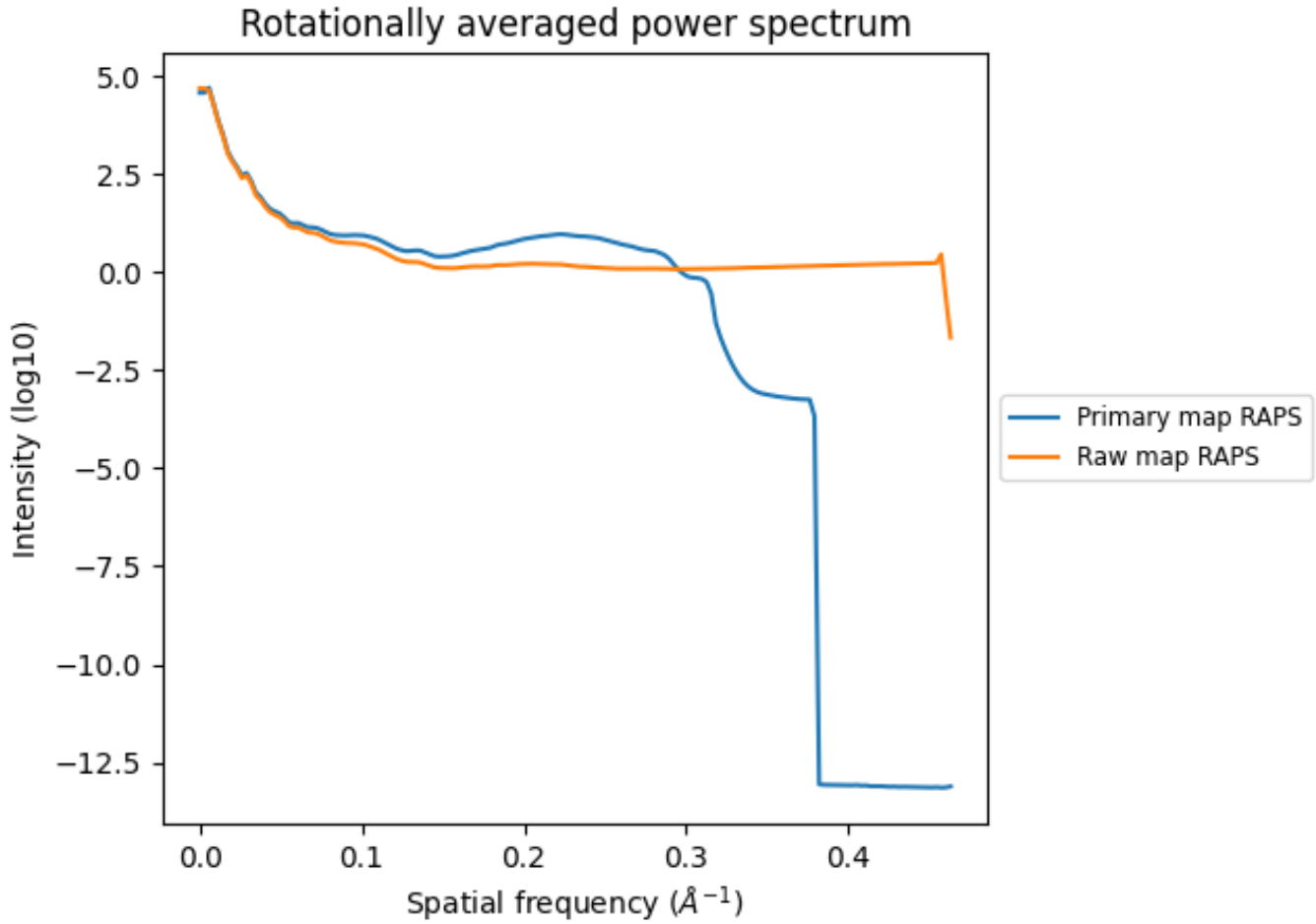
7.2 Volume estimate (i)



The volume at the recommended contour level is 137 nm^3; this corresponds to an approximate mass of 124 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

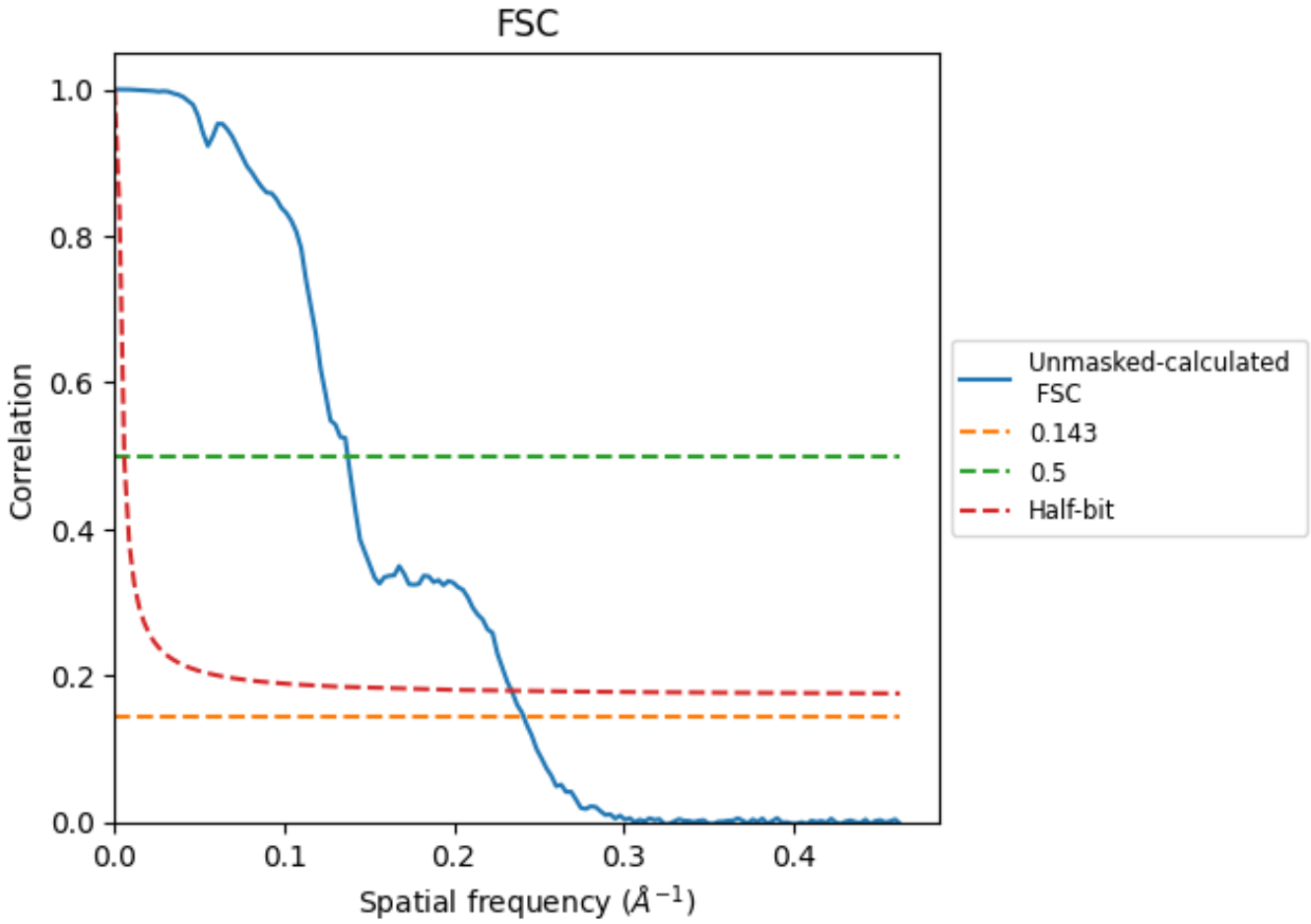
7.3 Rotationally averaged power spectrum (i)



8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



8.2 Resolution estimates (i)

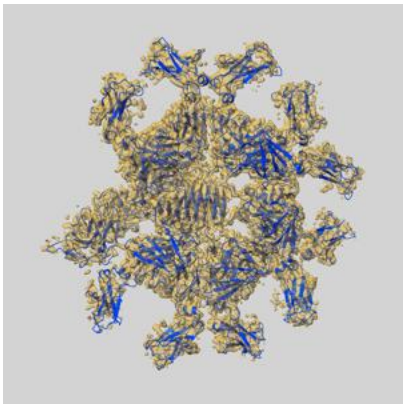
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.15	7.28	4.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

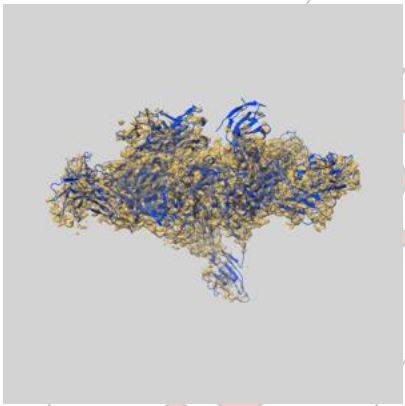
9 Map-model fit

This section contains information regarding the fit between EMDB map D_1300031551 and PDB model D_1300031551. Per-residue inclusion information can be found in section 3 on page 7.

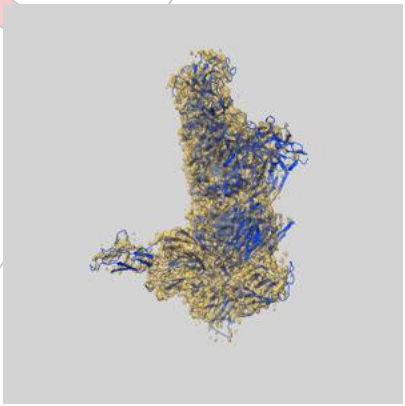
9.1 Map-model overlay



X



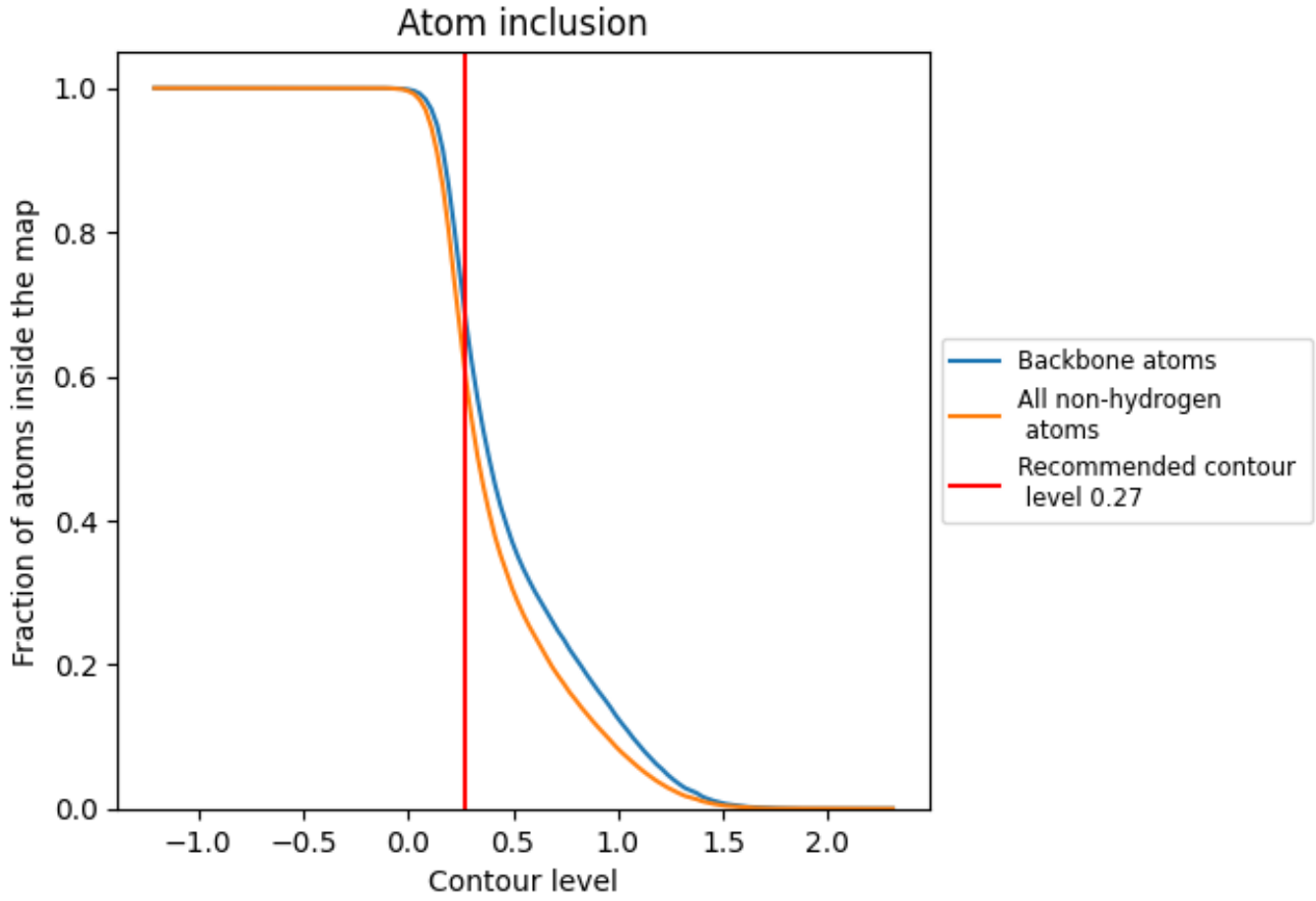
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion



At the recommended contour level, 69% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.