Preliminary Full wwPDB EM Validation Report ⓘ

Aug 12, 2022 – 09:58 PM JST

Deposition ID : D_1300031559

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:

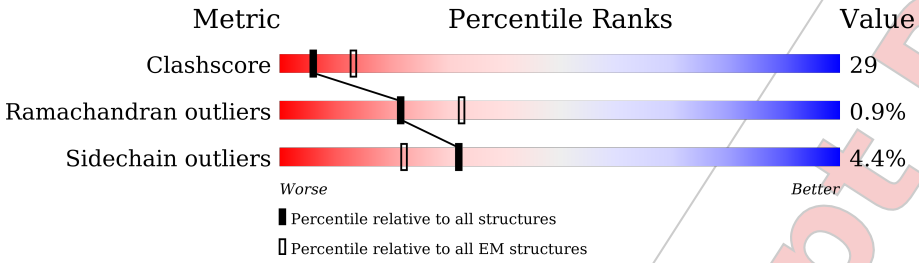
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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	230	27% 62% 35%
2	B	226	14% 69% 28%
2	C	226	7% 70% 27%
3	D	226	5% 61% 37%
3	E	226	6% 66% 30%
3	G	226	6% 62% 37%
4	F	222	8% 60% 39%
5	H	223	5% 62% 37%

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Mol	Chain	Length	Quality of chain
6	J	105	43% 52% 32% 13%
7	K	224	12% 56% 42%
8	L	228	28% 60% 39%
9	R	107	12% 57% 38% 5%
9	S	107	5% 39% 51% 9%
9	U	107	48% 44% 8%
9	V	107	12% 39% 46% 15%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21693 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	230	1787	1124	302	353	8	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	226	1763	1111	298	346	8	0	0
2	C	226	1762	1111	298	345	8	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	226	1763	1111	298	346	8	0	0
3	E	225	1757	1108	297	344	8	0	0
3	G	225	1756	1108	297	343	8	0	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	222	1737	1095	293	341	8	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	223	1744	1100	294	342	8	0	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	104	834	519	148	160	7	0	0

- Molecule 7 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	K	224	1751	1103	296	344	8	0	0

- Molecule 8 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	228	1775	1115	299	352	9	0	0

- Molecule 9 is a protein.

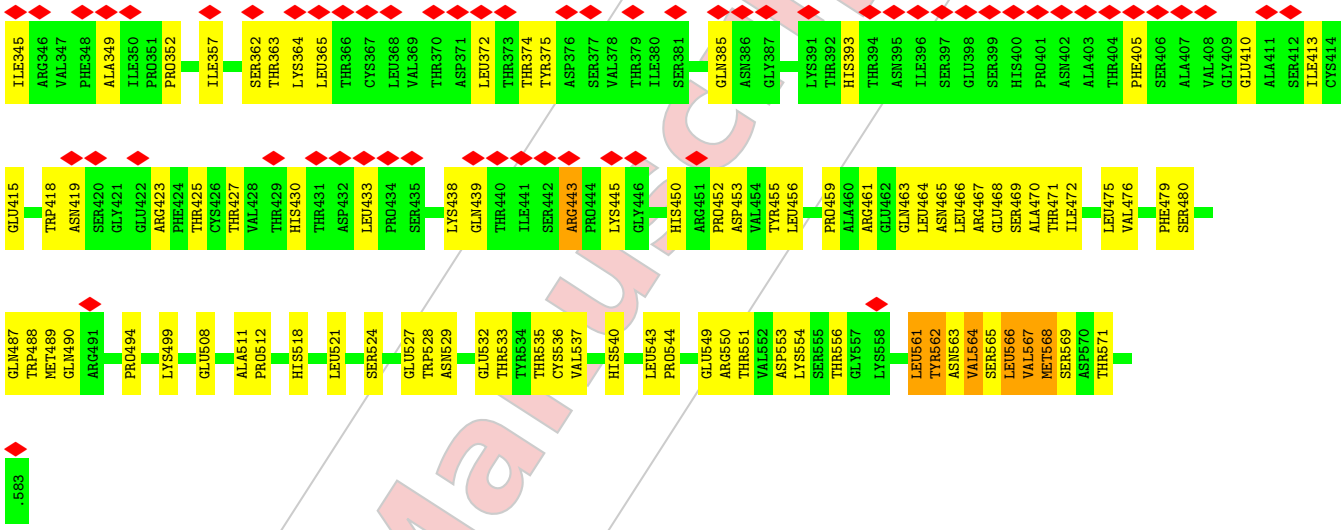
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	R	107	816	510	144	155	7	0	0
9	S	107	816	510	144	155	7	0	0
9	U	107	816	510	144	155	7	0	0
9	V	107	816	510	144	155	7	0	0

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.

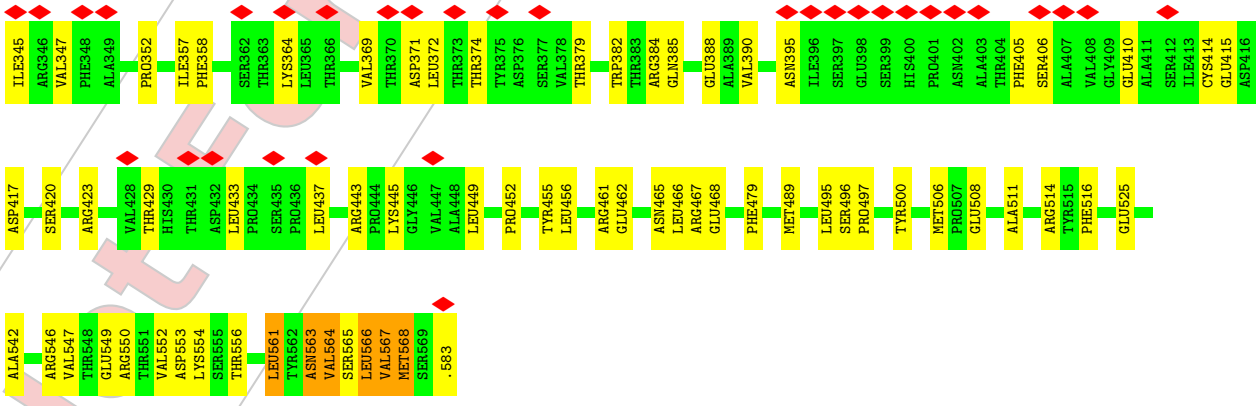
- Molecule 1:

Chain A:



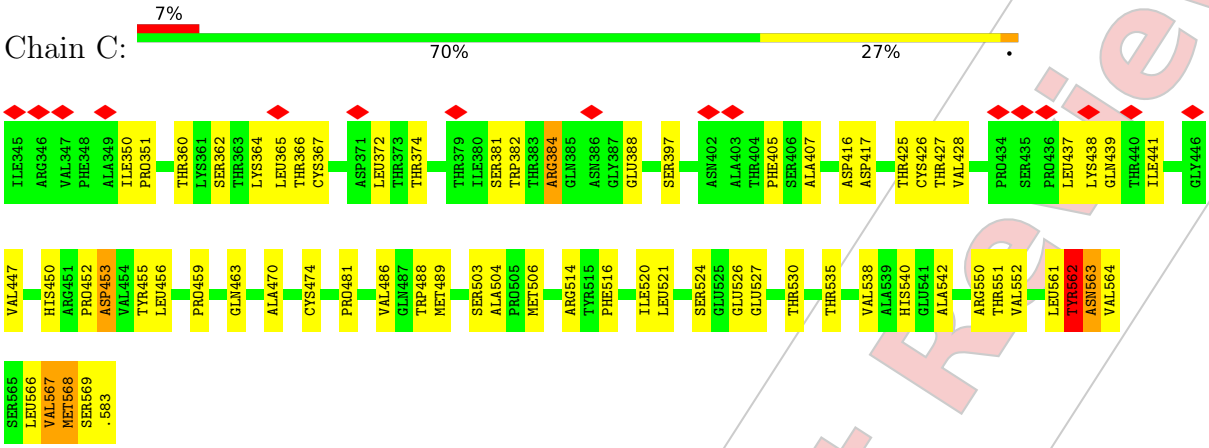
- Molecule 2:

Chain B:



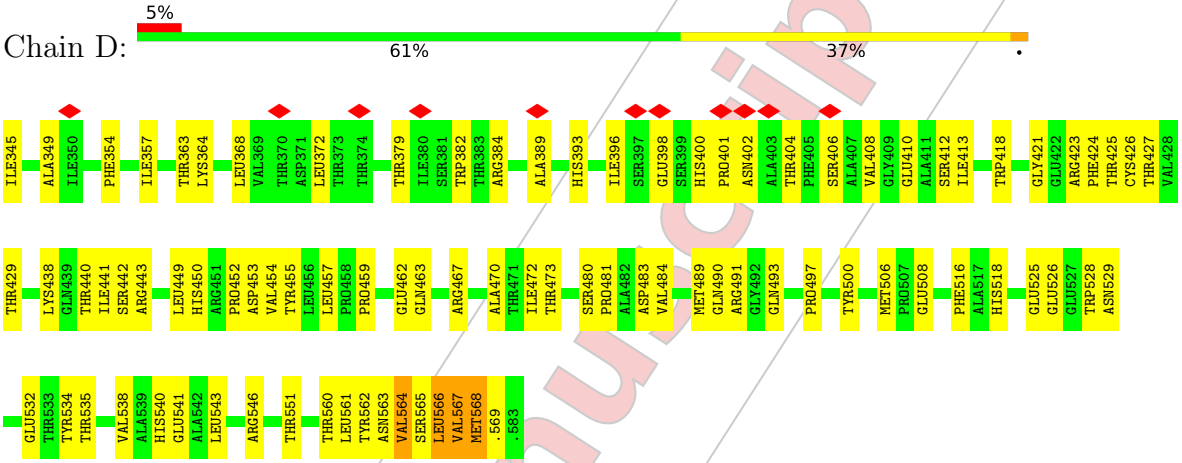
- Molecule 2:

Chain C:



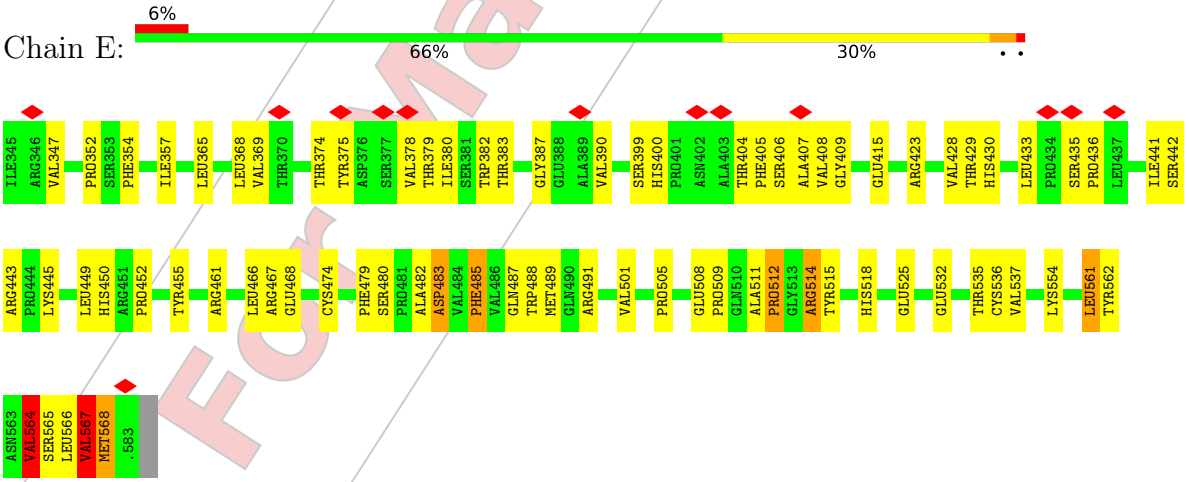
• Molecule 3:

Chain D:



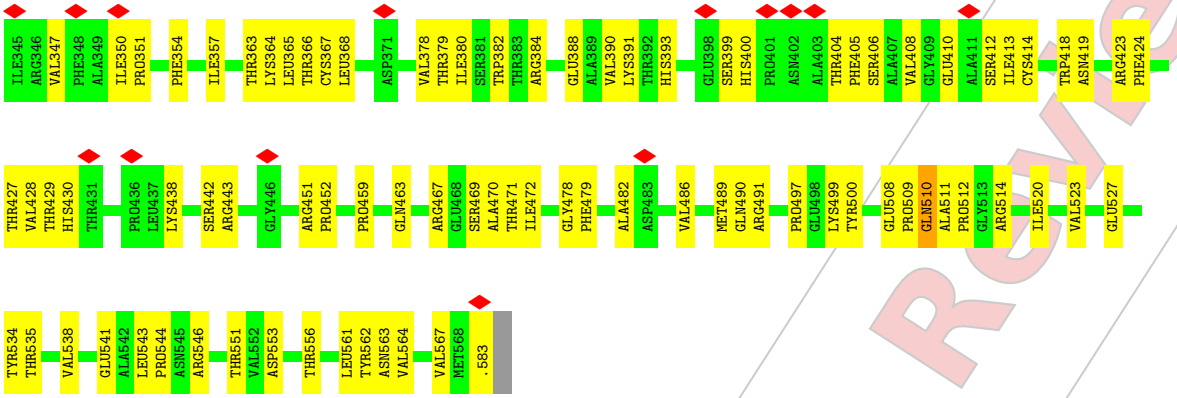
• Molecule 3:

Chain E:

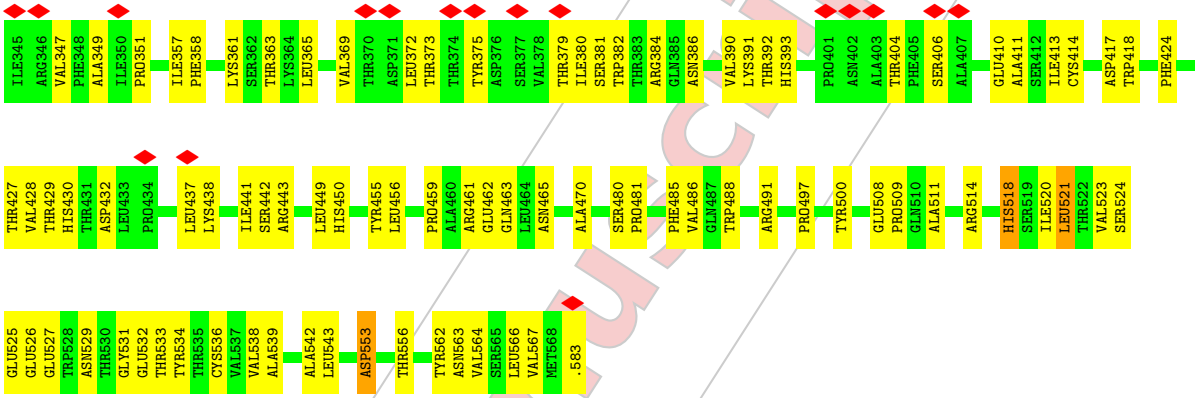


• Molecule 3:

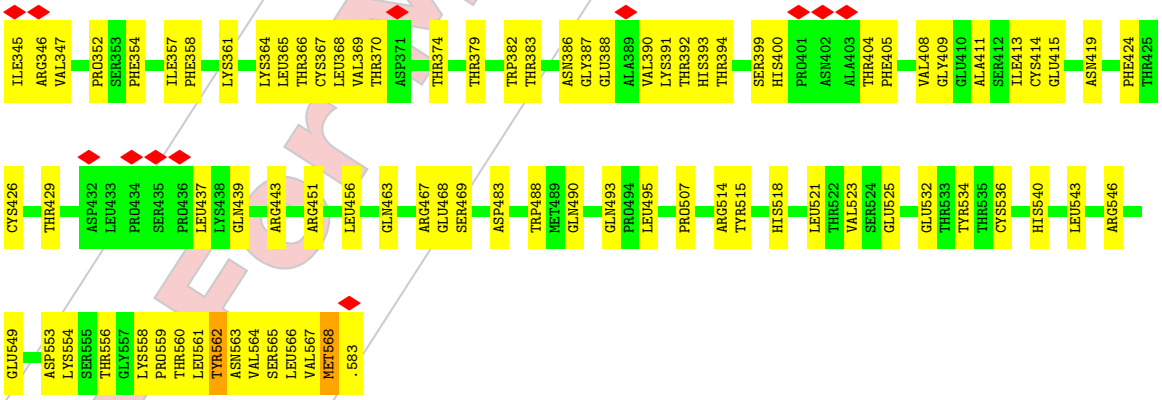
Chain G:



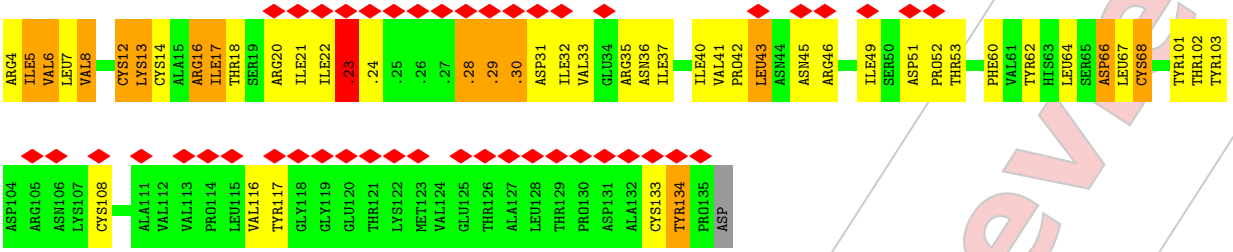
• Molecule 4:



• Molecule 5:

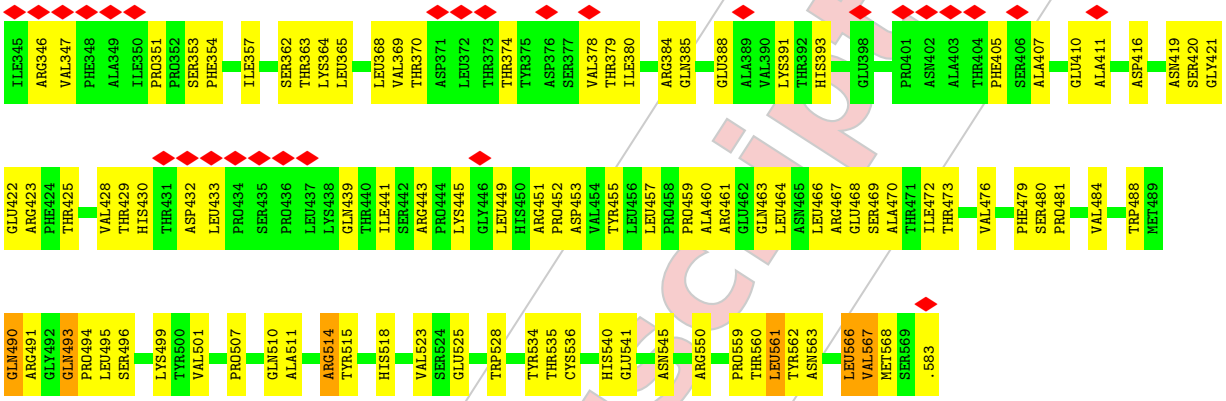


• Molecule 6:



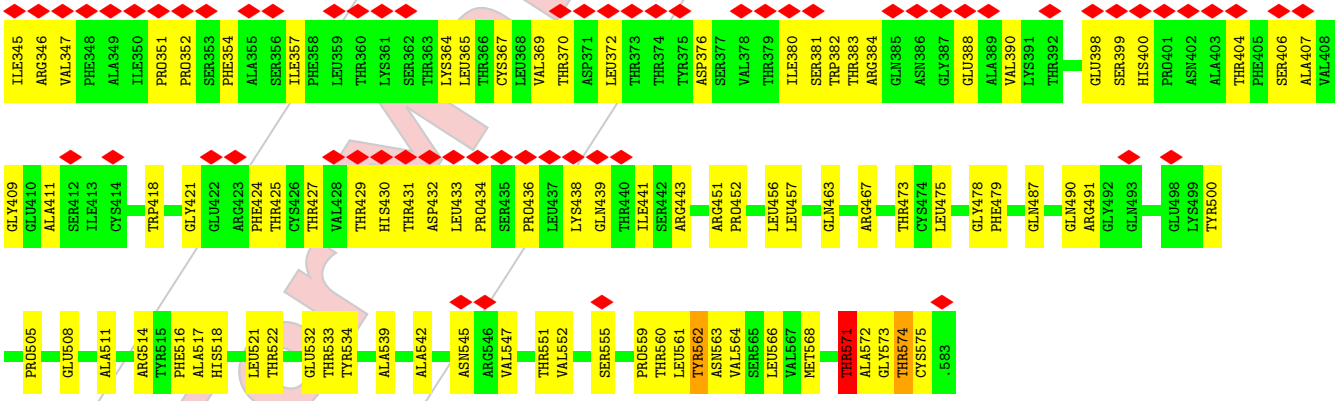
- Molecule 7:

Chain K:



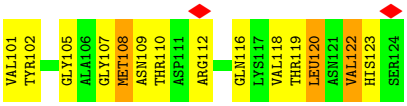
- Molecule 8:

Chain L:



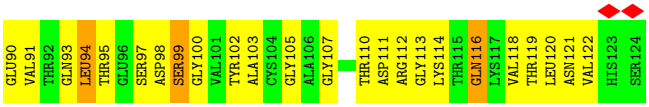
- Molecule 9:

Chain R:



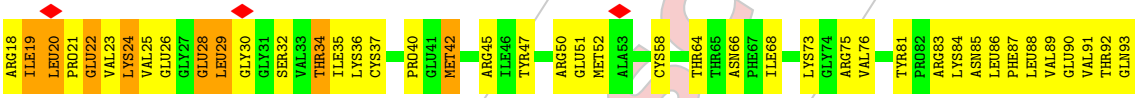
• Molecule 9:

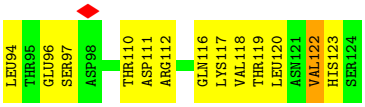
Chain S:



• Molecule 9:

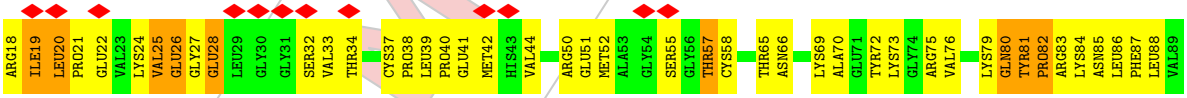
Chain U:

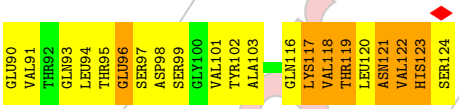




• Molecule 9:

Chain V:





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	0.939	Depositor
Minimum map value	-0.476	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	264.96, 264.96, 264.96	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82799995, 0.82799995, 0.82799995	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	0.28	0/1818	0.60	0/2490
2	B	0.31	0/1794	0.53	0/2457
2	C	0.37	0/1793	0.60	0/2455
3	D	0.26	0/1794	0.54	0/2457
3	E	0.40	0/1788	0.60	0/2449
3	G	0.26	0/1787	0.55	0/2447
4	F	0.31	0/1767	0.58	0/2420
5	H	0.30	0/1774	0.58	0/2430
6	J	0.35	0/847	0.73	0/1150
7	K	0.32	0/1781	0.56	0/2437
8	L	0.28	0/1805	0.57	1/2472 (0.0%)
9	R	0.26	0/827	0.56	0/1115
9	S	0.32	0/827	0.65	0/1115
9	U	0.30	0/827	0.64	1/1115 (0.1%)
9	V	0.44	1/827 (0.1%)	0.76	1/1115 (0.1%)
All	All	0.32	1/22056 (0.0%)	0.59	3/30124 (0.0%)

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
8	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	85	ASN	C-N	9.40	1.55	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	85	ASN	C-N-CA	-8.81	99.67	121.70
8	L	574	THR	C-N-CA	-6.43	105.63	121.70
9	U	42	MET	CA-CB-CG	5.19	122.13	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	L	562	TYR	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	1787	0	1745	111	0
2	B	1763	0	1724	75	0
2	C	1762	0	1723	88	0
3	D	1763	0	1725	102	0
3	E	1757	0	1718	115	0
3	G	1756	0	1720	74	0
4	F	1737	0	1694	103	0
5	H	1744	0	1704	97	0
6	J	834	0	833	127	0
7	K	1751	0	1709	113	0
8	L	1775	0	1724	104	0
9	R	816	0	835	46	0
9	S	816	0	835	67	0
9	U	816	0	835	80	0
9	V	816	0	833	160	0
All	All	21693	0	21357	1268	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 29.

All (1268) 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)
9:V:50:ARG:HG2	9:V:102:TYR:CE1	1.31	1.57
9:R:94:LEU:CD1	9:R:122:VAL:CG1	1.81	1.54
7:K:563:ASN:ND2	7:K:583:NAG:C1	1.71	1.53
3:D:567:VAL:CG2	3:E:567:VAL:CG2	1.84	1.52
2:B:563:ASN:ND2	2:B:583:NAG:C1	1.68	1.52
9:R:94:LEU:HD13	9:R:122:VAL:CG1	1.34	1.51
9:V:81:TYR:CB	9:V:86:LEU:N	1.69	1.51
2:C:563:ASN:ND2	2:C:583:NAG:C1	1.68	1.51
9:V:25:VAL:HG11	9:V:33:VAL:CG2	1.40	1.51
9:R:94:LEU:CD2	9:R:122:VAL:HG11	1.37	1.50
6:J:13:LYS:CG	6:J:67:LEU:HD21	1.43	1.49
2:B:567:VAL:CG2	2:C:567:VAL:HG11	1.44	1.48
9:V:25:VAL:CG1	9:V:33:VAL:HG23	1.00	1.48
9:V:50:ARG:CG	9:V:102:TYR:CE1	1.96	1.48
9:V:81:TYR:HB2	9:V:86:LEU:CA	1.41	1.48
3:D:567:VAL:HG21	3:E:567:VAL:CG2	1.44	1.46
9:U:32:SER:CB	9:U:91:VAL:O	1.64	1.46
1:A:567:VAL:HG23	2:B:567:VAL:CG1	1.48	1.44
3:G:511:ALA:HB2	9:V:66:ASN:ND2	1.34	1.42
9:U:23:VAL:HG13	9:U:120:LEU:CD2	1.47	1.41
2:C:568:MET:HG3	5:H:562:TYR:CE2	1.55	1.40
9:V:81:TYR:CG	9:V:86:LEU:HB2	1.57	1.40
1:A:567:VAL:CG2	2:B:567:VAL:HG12	1.52	1.39
6:J:13:LYS:CD	6:J:67:LEU:HD21	1.51	1.38
9:V:25:VAL:CG1	9:V:33:VAL:CG2	1.90	1.38
9:S:99:SER:CB	9:S:120:LEU:O	1.69	1.37
9:V:81:TYR:CB	9:V:86:LEU:CA	1.99	1.35
3:D:567:VAL:CG2	3:E:567:VAL:HG23	0.89	1.34
5:H:490:GLN:NE2	5:H:532:GLU:CD	1.78	1.34
5:H:532:GLU:CG	5:H:534:TYR:CE1	2.12	1.33
9:U:23:VAL:CG1	9:U:120:LEU:HD23	1.56	1.32
3:G:511:ALA:CB	9:V:66:ASN:ND2	1.95	1.30
5:H:532:GLU:HG2	5:H:534:TYR:CE1	1.66	1.29
6:J:102:THR:HG21	8:L:575:CYS:CB	1.60	1.28
9:S:99:SER:HB3	9:S:120:LEU:O	1.15	1.27
9:V:50:ARG:CG	9:V:102:TYR:HE1	1.35	1.27
3:E:518:HIS:ND1	4:F:518:HIS:CE1	2.03	1.27
9:V:81:TYR:HB3	9:V:86:LEU:N	0.94	1.27
1:A:544:PRO:HB3	6:J:134:TYR:CE1	1.70	1.27
2:B:567:VAL:CG2	2:C:567:VAL:CG1	2.13	1.27
3:G:511:ALA:CB	9:V:66:ASN:HD21	1.46	1.26
9:V:25:VAL:CB	9:V:120:LEU:HD13	1.63	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:567:VAL:HG22	2:C:567:VAL:CG1	1.66	1.26
1:A:566:LEU:HD23	8:L:566:LEU:CD1	1.64	1.25
9:U:34:THR:OG1	9:U:88:LEU:HD12	1.37	1.25
9:V:38:PRO:HD3	9:V:116:GLN:NE2	1.49	1.24
9:V:39:LEU:HD12	9:V:81:TYR:O	1.36	1.23
9:V:81:TYR:HB2	9:V:86:LEU:C	1.40	1.23
9:V:38:PRO:CD	9:V:116:GLN:NE2	2.04	1.21
3:D:569:SER:HA	3:E:568:MET:O	1.39	1.20
6:J:13:LYS:HG2	6:J:67:LEU:CD2	1.71	1.20
1:A:566:LEU:CD2	8:L:566:LEU:CD1	2.19	1.19
3:D:560:THR:OG1	3:E:561:LEU:O	1.62	1.18
5:H:490:GLN:CD	5:H:532:GLU:OE1	1.81	1.17
6:J:6:VAL:HB	6:J:18:THR:HA	1.24	1.16
9:R:94:LEU:CD1	9:R:122:VAL:HG13	1.67	1.16
9:V:24:LYS:CE	9:V:121:ASN:HB2	1.76	1.15
9:V:24:LYS:HA	9:V:120:LEU:CB	1.73	1.15
4:F:531:GLY:C	4:F:553:ASP:OD1	1.86	1.14
9:S:36:LYS:O	9:S:116:GLN:NE2	1.78	1.14
3:E:482:ALA:HB2	3:E:515:TYR:CD1	1.83	1.13
9:V:25:VAL:HB	9:V:120:LEU:CD1	1.77	1.13
9:U:24:LYS:HA	9:U:120:LEU:HB2	1.27	1.13
1:A:564:VAL:HG21	8:L:568:MET:CE	1.77	1.12
6:J:13:LYS:CG	6:J:67:LEU:CD2	2.23	1.12
9:R:94:LEU:HD11	9:R:122:VAL:HG13	1.25	1.12
9:V:81:TYR:CB	9:V:86:LEU:CB	2.28	1.12
2:C:568:MET:CG	5:H:562:TYR:CE2	2.33	1.12
9:V:38:PRO:CD	9:V:116:GLN:HE21	1.58	1.12
2:B:567:VAL:HA	2:C:567:VAL:HG12	1.28	1.11
2:C:568:MET:CG	5:H:562:TYR:HE2	1.62	1.11
2:B:567:VAL:HG22	2:C:567:VAL:HG11	1.13	1.10
9:V:81:TYR:CB	9:V:86:LEU:HB2	1.81	1.10
6:J:102:THR:HG21	8:L:575:CYS:HB2	1.17	1.09
9:V:24:LYS:HA	9:V:120:LEU:HB3	1.09	1.09
9:V:38:PRO:HD2	9:V:116:GLN:HE21	1.08	1.09
6:J:102:THR:HG21	8:L:575:CYS:SG	1.92	1.09
2:B:567:VAL:HG23	2:C:567:VAL:HG11	1.27	1.08
9:R:94:LEU:HD22	9:R:122:VAL:HG11	1.27	1.08
3:D:567:VAL:HG23	3:E:567:VAL:HG23	1.09	1.07
9:R:94:LEU:CD2	9:R:122:VAL:CG1	2.31	1.07
9:R:94:LEU:HD21	9:R:122:VAL:HG11	1.36	1.06
9:V:24:LYS:HE2	9:V:121:ASN:HB2	1.34	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:81:TYR:HB2	9:V:86:LEU:CB	1.84	1.06
4:F:532:GLU:O	4:F:553:ASP:OD2	1.73	1.05
7:K:468:GLU:N	7:K:525:GLU:HG3	1.69	1.05
3:D:567:VAL:HG23	3:E:567:VAL:CG2	1.64	1.05
9:V:25:VAL:H	9:V:120:LEU:HB2	1.19	1.05
4:F:532:GLU:C	4:F:553:ASP:OD2	1.96	1.04
9:V:80:GLN:HE21	9:V:82:PRO:HD3	1.16	1.04
9:R:94:LEU:CG	9:R:122:VAL:HG11	1.88	1.03
6:J:4:ARG:N	6:J:18:THR:HG1	1.54	1.03
1:A:563:ASN:HA	2:B:563:ASN:HB3	1.39	1.03
3:D:560:THR:CB	3:E:561:LEU:O	2.07	1.03
6:J:6:VAL:HB	6:J:18:THR:CA	1.87	1.03
9:U:24:LYS:HA	9:U:120:LEU:CB	1.89	1.02
9:U:32:SER:HB2	9:U:91:VAL:O	0.86	1.02
9:V:50:ARG:HG3	9:V:102:TYR:CE1	1.92	1.02
1:A:566:LEU:HD23	8:L:566:LEU:HD13	1.39	1.02
9:S:31:GLY:O	9:S:94:LEU:CD1	2.08	1.02
9:V:25:VAL:CB	9:V:120:LEU:CD1	2.35	1.01
1:A:566:LEU:CD2	8:L:566:LEU:HD11	1.90	1.01
1:A:564:VAL:HG21	8:L:568:MET:HE1	1.02	1.00
6:J:13:LYS:HD2	6:J:67:LEU:HD21	1.42	1.00
9:V:24:LYS:CA	9:V:120:LEU:HB3	1.90	1.00
9:S:99:SER:OG	9:S:120:LEU:O	1.80	0.99
9:S:41:GLU:HB3	9:S:42:MET:HE2	1.44	0.99
9:U:35:ILE:HD12	9:U:35:ILE:H	1.25	0.98
9:V:25:VAL:HG12	9:V:33:VAL:HG23	0.99	0.98
6:J:103:TYR:HB2	8:L:574:THR:HG22	1.42	0.98
9:V:25:VAL:HG12	9:V:33:VAL:CG2	1.71	0.98
9:V:26:GLU:N	9:V:120:LEU:HD12	1.77	0.98
5:H:490:GLN:HE21	5:H:532:GLU:CD	1.51	0.97
1:A:564:VAL:CG2	8:L:568:MET:HE1	1.94	0.97
9:U:29:LEU:HD12	9:U:29:LEU:H	1.26	0.97
9:V:37:CYS:HA	9:V:116:GLN:HE22	1.28	0.97
3:E:518:HIS:CE1	4:F:518:HIS:CE1	2.52	0.96
1:A:566:LEU:HD21	8:L:566:LEU:HD11	1.44	0.96
9:V:81:TYR:CG	9:V:86:LEU:CB	2.48	0.96
3:E:482:ALA:HB2	3:E:515:TYR:HD1	1.20	0.96
2:C:569:SER:O	3:D:568:MET:O	1.85	0.95
5:H:554:LYS:HE2	5:H:558:LYS:HZ3	1.32	0.94
9:V:24:LYS:HZ3	9:V:121:ASN:HD22	1.14	0.94
3:E:568:MET:HA	3:E:568:MET:CE	1.95	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:81:TYR:CB	9:V:86:LEU:C	2.27	0.94
5:H:560:THR:HB	7:K:560:THR:O	1.68	0.94
6:J:13:LYS:CD	6:J:67:LEU:CD2	2.43	0.94
5:H:532:GLU:HG3	5:H:534:TYR:CE1	2.02	0.93
6:J:102:THR:CG2	8:L:575:CYS:HB2	1.98	0.93
9:V:25:VAL:HG11	9:V:33:VAL:HG22	1.45	0.93
9:U:24:LYS:CA	9:U:120:LEU:HB2	1.95	0.93
9:V:26:GLU:HG2	9:V:121:ASN:O	1.68	0.93
9:V:37:CYS:HA	9:V:116:GLN:NE2	1.83	0.93
3:D:560:THR:HA	3:E:561:LEU:O	1.69	0.92
3:E:518:HIS:ND1	4:F:518:HIS:ND1	2.16	0.92
3:E:568:MET:HA	3:E:568:MET:HE3	1.49	0.92
6:J:17:ILE:HG12	6:J:37:ILE:HG12	1.52	0.91
3:D:569:SER:CA	3:E:568:MET:O	2.19	0.91
3:D:567:VAL:CB	3:E:567:VAL:HG23	1.99	0.91
9:S:41:GLU:HB3	9:S:42:MET:CE	1.99	0.91
9:V:25:VAL:HB	9:V:120:LEU:HD13	0.92	0.91
3:D:560:THR:CA	3:E:561:LEU:O	2.18	0.90
2:B:567:VAL:HG23	2:C:567:VAL:CG1	1.88	0.90
9:R:94:LEU:CD1	9:R:122:VAL:HG12	1.71	0.90
9:V:25:VAL:H	9:V:120:LEU:CB	1.84	0.90
5:H:554:LYS:CE	5:H:558:LYS:HZ3	1.83	0.90
9:V:24:LYS:CA	9:V:120:LEU:CB	2.49	0.90
9:V:26:GLU:HA	9:V:121:ASN:O	1.70	0.90
3:E:518:HIS:CE1	4:F:518:HIS:ND1	2.40	0.90
5:H:532:GLU:CG	5:H:534:TYR:HE1	1.84	0.89
6:J:17:ILE:HB	6:J:37:ILE:HD13	1.54	0.89
9:R:94:LEU:CG	9:R:122:VAL:CG1	2.47	0.89
3:E:518:HIS:ND1	4:F:518:HIS:HE1	1.62	0.89
1:A:544:PRO:HB3	6:J:134:TYR:HE1	1.35	0.89
9:V:25:VAL:CA	9:V:120:LEU:CD1	2.51	0.89
3:E:514:ARG:HD2	3:E:514:ARG:N	1.86	0.89
6:J:4:ARG:NH2	6:J:4:ARG:HB3	1.88	0.89
6:J:17:ILE:CG1	6:J:37:ILE:HG12	2.02	0.88
9:R:120:LEU:H	9:R:120:LEU:HD12	1.37	0.88
9:V:25:VAL:N	9:V:120:LEU:CD1	2.36	0.88
7:K:459:PRO:HG3	7:K:470:ALA:HB1	1.55	0.88
3:G:511:ALA:HB3	9:V:66:ASN:HD21	1.39	0.88
8:L:452:PRO:HB3	8:L:479:PHE:HB3	1.55	0.87
9:U:94:LEU:HD23	9:U:122:VAL:CG1	2.03	0.87
9:U:32:SER:HB2	9:U:91:VAL:C	1.95	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:532:GLU:HG2	5:H:534:TYR:CZ	2.08	0.87
9:V:25:VAL:N	9:V:120:LEU:HB2	1.90	0.87
1:A:567:VAL:CG2	2:B:567:VAL:CG1	2.27	0.87
5:H:532:GLU:HG3	5:H:534:TYR:CD1	2.09	0.87
9:V:26:GLU:CG	9:V:121:ASN:O	2.23	0.86
5:H:532:GLU:CB	5:H:534:TYR:HE1	1.88	0.86
1:A:566:LEU:CD2	8:L:566:LEU:HD13	1.97	0.86
6:J:13:LYS:HG2	6:J:67:LEU:HD21	1.31	0.86
9:V:24:LYS:NZ	9:V:121:ASN:HD22	1.72	0.86
9:V:50:ARG:HG2	9:V:102:TYR:CD1	2.08	0.85
3:G:511:ALA:HB2	9:V:66:ASN:HD22	1.39	0.85
6:J:102:THR:CG2	8:L:575:CYS:SG	2.65	0.85
7:K:468:GLU:H	7:K:525:GLU:HG3	1.36	0.84
9:R:94:LEU:HD22	9:R:122:VAL:CG1	1.97	0.84
9:U:30:GLY:HA2	9:U:93:GLN:HA	1.60	0.84
6:J:17:ILE:HD13	6:J:37:ILE:HD13	1.59	0.84
9:R:94:LEU:HD11	9:R:122:VAL:CG1	1.79	0.84
9:V:25:VAL:CA	9:V:120:LEU:HD13	2.07	0.84
6:J:13:LYS:HD2	6:J:67:LEU:HD11	1.60	0.84
6:J:4:ARG:N	6:J:18:THR:OG1	2.10	0.83
3:E:482:ALA:HB1	3:E:505:PRO:HG3	1.60	0.83
9:R:94:LEU:HD13	9:R:122:VAL:HG12	0.85	0.83
5:H:532:GLU:CB	5:H:534:TYR:CE1	2.61	0.83
9:U:30:GLY:O	9:U:92:THR:O	1.96	0.83
9:S:99:SER:OG	9:S:120:LEU:N	2.12	0.82
9:V:50:ARG:HA	9:V:102:TYR:CD1	2.13	0.82
9:U:22:GLU:HG2	9:U:119:THR:O	1.80	0.82
4:F:523:VAL:HG21	4:F:534:TYR:OH	1.79	0.81
9:V:25:VAL:HG11	9:V:33:VAL:HG23	0.86	0.81
1:A:564:VAL:CG2	8:L:568:MET:CE	2.55	0.81
6:J:103:TYR:H	8:L:574:THR:HA	1.44	0.81
9:V:80:GLN:NE2	9:V:82:PRO:HD3	1.94	0.81
9:V:81:TYR:HB3	9:V:86:LEU:CA	1.83	0.81
1:A:566:LEU:HD11	2:B:566:LEU:HB3	1.62	0.80
3:G:563:ASN:HB2	5:H:563:ASN:HB2	1.60	0.80
6:J:13:LYS:CB	6:J:67:LEU:HD21	2.12	0.80
2:B:567:VAL:CG2	2:C:567:VAL:HG12	2.11	0.80
9:V:80:GLN:NE2	9:V:80:GLN:O	2.14	0.80
3:E:474:CYS:HB2	3:E:488:TRP:CH2	2.17	0.80
1:A:566:LEU:HD21	8:L:566:LEU:CD1	2.01	0.79
7:K:468:GLU:C	7:K:525:GLU:HG2	2.02	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:32:SER:HB3	9:U:91:VAL:O	1.81	0.79
9:V:39:LEU:HD12	9:V:81:TYR:C	2.04	0.79
9:S:50:ARG:HH11	9:S:50:ARG:HG2	1.47	0.78
2:C:568:MET:HG3	5:H:562:TYR:HE2	1.04	0.78
9:U:24:LYS:HA	9:U:120:LEU:CA	2.13	0.78
9:V:25:VAL:N	9:V:120:LEU:CB	2.44	0.78
9:V:26:GLU:H	9:V:120:LEU:HD12	1.46	0.78
5:H:554:LYS:NZ	5:H:558:LYS:HZ3	1.82	0.78
9:V:80:GLN:HA	9:V:87:PHE:HA	1.66	0.78
9:V:101:VAL:HA	9:V:119:THR:HB	1.64	0.78
1:A:561:LEU:HG	2:B:561:LEU:HD21	1.66	0.77
1:A:566:LEU:HD23	8:L:566:LEU:HD12	1.62	0.77
2:C:568:MET:HE1	2:C:568:MET:H	1.49	0.77
3:G:350:ILE:HB	3:G:366:THR:HB	1.65	0.77
6:J:8:VAL:CG2	6:J:68:CYS:HA	2.14	0.77
7:K:560:THR:HG23	8:L:560:THR:O	1.84	0.77
9:S:29:LEU:HA	9:S:94:LEU:O	1.85	0.77
9:U:94:LEU:HD23	9:U:122:VAL:HG13	1.63	0.77
7:K:468:GLU:N	7:K:525:GLU:CG	2.46	0.77
9:U:22:GLU:OE1	9:U:24:LYS:HG2	1.85	0.77
1:A:533:THR:HG23	1:A:553:ASP:HB2	1.67	0.77
9:S:99:SER:OG	9:S:120:LEU:HD23	1.84	0.76
9:V:25:VAL:CA	9:V:120:LEU:HD12	2.15	0.76
2:C:568:MET:CE	3:D:568:MET:HA	2.15	0.76
4:F:531:GLY:CA	4:F:553:ASP:OD1	2.33	0.76
9:V:25:VAL:N	9:V:120:LEU:HD13	1.99	0.76
2:B:563:ASN:HD22	2:B:583:NAG:C1	1.95	0.76
7:K:467:ARG:HH11	7:K:467:ARG:HG3	1.50	0.76
9:S:31:GLY:O	9:S:94:LEU:HD13	1.86	0.76
9:V:50:ARG:HA	9:V:102:TYR:HD1	1.50	0.76
1:A:544:PRO:CB	6:J:134:TYR:CE1	2.62	0.76
7:K:561:LEU:O	7:K:561:LEU:HG	1.86	0.76
8:L:475:LEU:HD13	8:L:518:HIS:HB3	1.68	0.75
9:S:28:GLU:OE1	9:S:28:GLU:HA	1.84	0.75
9:V:25:VAL:H	9:V:120:LEU:CD1	1.99	0.75
3:G:508:GLU:CD	3:G:509:PRO:HD2	2.06	0.75
9:R:120:LEU:HD12	9:R:120:LEU:N	2.01	0.75
9:U:20:LEU:N	9:U:20:LEU:HD22	2.02	0.75
8:L:490:GLN:HE22	8:L:534:TYR:HA	1.51	0.75
1:A:566:LEU:HD11	2:B:566:LEU:CB	2.16	0.75
5:H:560:THR:HG22	7:K:560:THR:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:357:ILE:HD13	4:F:363:THR:HB	1.69	0.74
5:H:379:THR:HB	5:H:429:THR:HB	1.69	0.74
7:K:469:SER:N	7:K:525:GLU:HG2	2.02	0.74
3:G:511:ALA:HB2	9:V:66:ASN:HD21	1.06	0.74
9:U:35:ILE:H	9:U:35:ILE:CD1	2.00	0.74
9:V:33:VAL:HG21	9:V:120:LEU:HD11	1.67	0.74
4:F:500:TYR:CB	4:F:521:LEU:HB3	2.16	0.74
4:F:500:TYR:HB2	4:F:521:LEU:HB3	1.68	0.74
9:U:35:ILE:HD12	9:U:35:ILE:N	2.02	0.74
2:C:524:SER:OG	2:C:527:GLU:OE1	2.06	0.73
2:C:568:MET:SD	2:C:568:MET:N	2.62	0.73
9:S:105:GLY:CA	9:S:113:GLY:O	2.36	0.73
9:V:39:LEU:CD1	9:V:81:TYR:O	2.27	0.73
4:F:486:VAL:HG22	4:F:538:VAL:HG22	1.69	0.73
4:F:532:GLU:O	4:F:553:ASP:CG	2.27	0.73
9:U:29:LEU:HD12	9:U:29:LEU:N	2.02	0.73
9:V:39:LEU:HD11	9:V:81:TYR:N	2.03	0.73
6:J:102:THR:CG2	8:L:575:CYS:CB	2.54	0.73
6:J:13:LYS:HG2	6:J:67:LEU:HD23	1.70	0.73
3:E:514:ARG:HD2	3:E:514:ARG:H	1.54	0.72
7:K:563:ASN:CG	7:K:583:NAG:C1	2.57	0.72
2:C:535:THR:HG22	2:C:551:THR:HG22	1.72	0.72
9:V:50:ARG:HG2	9:V:102:TYR:HE1	0.60	0.72
2:B:567:VAL:CA	2:C:567:VAL:HG12	2.14	0.72
5:H:554:LYS:NZ	5:H:558:LYS:NZ	2.38	0.72
9:U:34:THR:OG1	9:U:88:LEU:CD1	2.30	0.72
9:V:25:VAL:C	9:V:120:LEU:HD12	2.10	0.72
1:A:562:TYR:CD2	6:J:43:LEU:HD11	2.24	0.72
9:V:39:LEU:HD21	9:V:80:GLN:HB2	1.73	0.71
2:B:561:LEU:O	2:B:561:LEU:HD23	1.90	0.71
9:S:105:GLY:HA3	9:S:113:GLY:O	1.90	0.71
7:K:490:GLN:HB2	7:K:495:LEU:HD21	1.70	0.71
9:S:37:CYS:HB2	9:S:87:PHE:HB3	1.73	0.71
5:H:583:NAG:H3	7:K:583:NAG:H4	1.71	0.71
4:F:521:LEU:O	4:F:521:LEU:HD22	1.91	0.71
7:K:425:THR:HG23	7:K:439:GLN:H	1.55	0.71
9:V:24:LYS:NZ	9:V:121:ASN:ND2	2.37	0.71
9:V:38:PRO:HD3	9:V:116:GLN:HE22	1.49	0.71
2:B:414:CYS:SG	2:B:415:GLU:N	2.64	0.70
3:E:374:THR:HA	3:E:405:PHE:HB2	1.71	0.70
7:K:473:THR:HB	7:K:518:HIS:HE2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:568:MET:H	2:C:568:MET:CE	2.03	0.70
5:H:532:GLU:CG	5:H:534:TYR:CD1	2.70	0.70
9:V:24:LYS:HE3	9:V:120:LEU:C	2.12	0.70
6:J:6:VAL:HG11	6:J:18:THR:HB	1.74	0.70
9:U:76:VAL:HG12	9:U:91:VAL:HG22	1.72	0.70
9:V:50:ARG:HG3	9:V:102:TYR:CZ	2.25	0.70
3:D:363:THR:OG1	3:D:413:ILE:O	2.09	0.70
1:A:524:SER:HB2	1:A:527:GLU:HG2	1.74	0.69
4:F:500:TYR:HB3	4:F:521:LEU:CB	2.21	0.69
5:H:374:THR:HA	5:H:405:PHE:HB2	1.74	0.69
8:L:421:GLY:H	8:L:443:ARG:HH12	1.40	0.69
1:A:374:THR:HA	1:A:405:PHE:HB2	1.75	0.69
5:H:347:VAL:HG22	5:H:369:VAL:HG12	1.75	0.69
2:B:563:ASN:ND2	2:B:583:NAG:O5	2.24	0.69
4:F:521:LEU:O	4:F:521:LEU:HD13	1.92	0.69
5:H:382:TRP:HB2	5:H:390:VAL:HG21	1.75	0.69
5:H:463:GLN:NE2	5:H:469:SER:O	2.26	0.69
6:J:4:ARG:HB3	6:J:4:ARG:HH21	1.58	0.69
3:E:423:ARG:HA	3:E:441:ILE:O	1.93	0.68
3:D:567:VAL:HG23	3:E:567:VAL:H	1.56	0.68
7:K:566:LEU:HD22	7:K:566:LEU:O	1.94	0.68
2:B:443:ARG:HH11	2:B:445:LYS:HG2	1.59	0.68
2:C:568:MET:HE2	2:C:568:MET:O	1.94	0.68
3:G:357:ILE:HD13	3:G:363:THR:HB	1.76	0.68
6:J:37:ILE:HB	8:L:564:VAL:HG13	1.74	0.68
9:S:94:LEU:N	9:S:94:LEU:HD12	2.07	0.68
5:H:532:GLU:HB3	5:H:534:TYR:HE1	1.55	0.68
1:A:566:LEU:HD13	1:A:566:LEU:C	2.14	0.68
2:C:568:MET:HE3	3:D:568:MET:HA	1.73	0.68
4:F:461:ARG:HH22	4:F:465:ASN:HD21	1.41	0.67
9:V:81:TYR:CA	9:V:86:LEU:N	2.55	0.67
1:A:363:THR:OG1	1:A:413:ILE:O	2.12	0.67
3:D:402:ASN:OD1	3:D:404:THR:OG1	2.12	0.67
5:H:532:GLU:HB3	5:H:534:TYR:CE1	2.27	0.67
2:C:459:PRO:HG3	2:C:470:ALA:HB1	1.77	0.67
9:V:79:LYS:O	9:V:88:LEU:N	2.21	0.67
9:S:24:LYS:HG2	9:S:120:LEU:HA	1.76	0.67
9:V:22:GLU:HA	9:V:22:GLU:OE1	1.95	0.67
4:F:500:TYR:HB3	4:F:521:LEU:HB2	1.76	0.67
3:D:566:LEU:O	3:E:566:LEU:HB2	1.95	0.66
1:A:393:HIS:HB3	1:A:410:GLU:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:511:ALA:CB	9:V:66:ASN:HD22	1.93	0.66
5:H:490:GLN:NE2	5:H:532:GLU:OE1	0.54	0.66
6:J:13:LYS:CB	6:J:67:LEU:CD2	2.72	0.66
1:A:464:LEU:O	1:A:467:ARG:NH1	2.28	0.66
4:F:449:LEU:HD22	4:F:542:ALA:HB2	1.77	0.66
4:F:583:NAG:H61	3:G:583:NAG:H4	1.75	0.66
7:K:563:ASN:HD22	8:L:563:ASN:HB3	1.61	0.66
9:V:96:GLU:OE1	9:V:96:GLU:HA	1.95	0.66
1:A:566:LEU:HD13	1:A:566:LEU:O	1.96	0.66
9:V:81:TYR:CD1	9:V:86:LEU:HB2	2.27	0.66
6:J:17:ILE:CD1	6:J:37:ILE:CD1	2.68	0.66
3:D:566:LEU:C	3:D:566:LEU:HD12	2.16	0.66
9:V:75:ARG:NH2	9:V:93:GLN:O	2.28	0.66
4:F:500:TYR:CB	4:F:521:LEU:CB	2.74	0.65
6:J:8:VAL:HG23	6:J:68:CYS:HA	1.78	0.65
9:U:23:VAL:CG1	9:U:120:LEU:CD2	2.35	0.65
2:B:384:ARG:HD3	2:B:388:GLU:HB3	1.78	0.65
2:C:568:MET:HG2	5:H:562:TYR:OH	1.96	0.65
2:C:350:ILE:HB	2:C:366:THR:HB	1.78	0.65
8:L:478:GLY:HA2	8:L:514:ARG:HB3	1.79	0.65
4:F:533:THR:HA	4:F:553:ASP:OD2	1.97	0.65
8:L:367:CYS:SG	8:L:439:GLN:NE2	2.70	0.65
9:V:24:LYS:HZ3	9:V:121:ASN:ND2	1.91	0.65
3:G:427:THR:HG22	3:G:438:LYS:HG2	1.79	0.65
7:K:563:ASN:HB3	8:L:563:ASN:HA	1.77	0.65
8:L:418:TRP:O	8:L:443:ARG:NH1	2.29	0.65
9:V:18:ARG:N	9:V:117:LYS:HZ1	1.94	0.65
7:K:493:GLN:OE1	7:K:493:GLN:N	2.29	0.65
9:V:25:VAL:N	9:V:120:LEU:HD12	2.12	0.65
1:A:508:GLU:OE1	1:A:511:ALA:N	2.29	0.65
3:D:567:VAL:HG21	3:E:567:VAL:HG23	0.66	0.65
1:A:566:LEU:O	1:A:566:LEU:HD22	1.97	0.65
3:D:357:ILE:HG12	3:D:363:THR:HG22	1.78	0.65
6:J:13:LYS:HD2	6:J:67:LEU:CD2	2.19	0.65
9:V:27:GLY:HA3	9:V:94:LEU:HD12	1.79	0.65
9:U:19:ILE:C	9:U:19:ILE:HD13	2.17	0.65
9:V:24:LYS:HE3	9:V:121:ASN:HB2	1.76	0.65
4:F:531:GLY:HA2	4:F:553:ASP:OD1	1.97	0.64
8:L:382:TRP:HB2	8:L:390:VAL:HG21	1.79	0.64
1:A:566:LEU:HD12	1:A:566:LEU:H	1.60	0.64
3:G:508:GLU:HG3	3:G:510:GLN:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:PRO:HG2	6:J:116:VAL:HG13	1.79	0.64
2:B:374:THR:HA	2:B:405:PHE:HB2	1.78	0.64
9:V:19:ILE:HG12	9:V:21:PRO:HD3	1.78	0.64
3:D:567:VAL:HG23	3:E:567:VAL:N	2.13	0.64
7:K:566:LEU:HD22	7:K:566:LEU:C	2.17	0.64
3:D:454:VAL:HG21	3:D:538:VAL:HG11	1.79	0.64
9:V:96:GLU:HG3	9:V:123:HIS:NE2	2.07	0.64
6:J:17:ILE:CD1	6:J:37:ILE:HD13	2.27	0.64
3:E:508:GLU:HB2	3:E:514:ARG:O	1.98	0.63
3:E:566:LEU:HD22	4:F:562:TYR:CE2	2.33	0.63
4:F:369:VAL:HB	4:F:406:SER:HA	1.81	0.63
9:S:68:ILE:HD12	9:S:73:LYS:HA	1.79	0.63
2:B:449:LEU:HB3	2:B:542:ALA:HB2	1.80	0.63
6:J:17:ILE:HD13	6:J:37:ILE:CD1	1.90	0.63
9:V:20:LEU:HD13	9:V:20:LEU:O	1.98	0.63
5:H:490:GLN:HE22	5:H:532:GLU:CD	1.63	0.63
6:J:42:PRO:HG3	6:J:101:TYR:HB3	1.79	0.63
8:L:433:LEU:HD12	8:L:434:PRO:HD2	1.80	0.63
9:V:20:LEU:O	9:V:20:LEU:HD22	1.99	0.63
3:E:379:THR:HB	3:E:429:THR:O	1.98	0.63
4:F:393:HIS:HB2	4:F:410:GLU:H	1.64	0.63
6:J:5:ILE:HG22	6:J:5:ILE:O	1.99	0.63
3:E:380:ILE:HD11	3:E:407:ALA:HB1	1.81	0.63
9:R:45:ARG:NH1	9:R:107:GLY:O	2.28	0.63
9:S:37:CYS:HA	9:S:116:GLN:NE2	2.13	0.63
7:K:468:GLU:H	7:K:525:GLU:CG	2.09	0.62
9:R:99:SER:OG	9:R:120:LEU:HD11	1.98	0.62
9:U:75:ARG:NH2	9:U:93:GLN:O	2.32	0.62
9:V:81:TYR:CD2	9:V:86:LEU:HB2	2.26	0.62
9:R:99:SER:OG	9:R:120:LEU:CD1	2.47	0.62
3:E:382:TRP:HB2	3:E:390:VAL:HG21	1.81	0.62
2:B:561:LEU:HD23	2:B:561:LEU:C	2.20	0.62
1:A:566:LEU:CD1	2:B:566:LEU:HA	2.30	0.62
5:H:560:THR:HG22	7:K:559:PRO:HA	1.80	0.62
1:A:563:ASN:HD22	2:B:583:NAG:H2	1.65	0.62
2:C:568:MET:HE2	2:C:568:MET:C	2.20	0.62
3:D:567:VAL:HG23	3:E:567:VAL:HG22	1.75	0.62
5:H:370:THR:HG22	5:H:400:HIS:HE1	1.63	0.61
7:K:563:ASN:ND2	8:L:563:ASN:HB3	2.15	0.61
9:V:39:LEU:CD1	9:V:81:TYR:C	2.67	0.61
3:D:567:VAL:HG23	3:E:567:VAL:CA	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:8:VAL:HG13	6:J:8:VAL:O	1.99	0.61
9:S:50:ARG:HH11	9:S:50:ARG:CG	2.14	0.61
9:V:24:LYS:HA	9:V:120:LEU:CA	2.30	0.61
1:A:362:SER:OG	1:A:364:LYS:NZ	2.32	0.61
3:G:380:ILE:O	3:G:393:HIS:NE2	2.33	0.61
2:B:566:LEU:HD12	2:B:566:LEU:O	2.00	0.61
3:E:564:VAL:HG22	3:E:564:VAL:O	1.99	0.61
6:J:17:ILE:CB	6:J:37:ILE:HD13	2.27	0.61
2:C:351:PRO:HG3	2:C:441:ILE:HD11	1.80	0.61
4:F:384:ARG:HE	4:F:386:ASN:HB2	1.66	0.61
6:J:20:ARG:HH12	6:J:36:ASN:HB2	1.66	0.61
9:U:23:VAL:HG13	9:U:120:LEU:HD22	1.73	0.61
4:F:532:GLU:N	4:F:553:ASP:OD1	2.33	0.61
8:L:384:ARG:HD2	8:L:388:GLU:HB2	1.83	0.61
8:L:487:GLN:NE2	8:L:500:TYR:OH	2.27	0.61
9:U:94:LEU:HD23	9:U:122:VAL:HG12	1.83	0.61
1:A:549:GLU:OE2	1:A:551:THR:OG1	2.18	0.61
4:F:523:VAL:CG2	4:F:534:TYR:OH	2.49	0.61
9:R:83:ARG:HG3	9:R:84:LYS:HG3	1.83	0.61
3:E:368:LEU:HD12	3:E:408:VAL:HB	1.83	0.60
7:K:561:LEU:HD21	8:L:561:LEU:HG	1.81	0.60
9:V:21:PRO:HG2	9:V:118:VAL:HG12	1.83	0.60
9:R:75:ARG:NH2	9:R:93:GLN:O	2.34	0.60
5:H:490:GLN:HE21	5:H:532:GLU:CG	2.14	0.60
6:J:43:LEU:C	6:J:43:LEU:HD23	2.21	0.60
7:K:469:SER:HB2	7:K:523:VAL:O	2.01	0.60
3:D:567:VAL:CG2	3:E:567:VAL:C	2.70	0.60
4:F:413:ILE:HG13	4:F:414:CYS:H	1.65	0.60
4:F:563:ASN:OD1	4:F:583:NAG:N2	2.35	0.60
7:K:346:ARG:O	7:K:370:THR:OG1	2.18	0.60
9:U:23:VAL:HG13	9:U:23:VAL:O	1.99	0.60
1:A:567:VAL:HG13	1:A:567:VAL:O	2.00	0.60
7:K:496:SER:HB2	7:K:499:LYS:HD3	1.83	0.60
9:V:24:LYS:HG2	9:V:120:LEU:HA	1.84	0.60
4:F:533:THR:CA	4:F:553:ASP:OD2	2.50	0.60
2:B:382:TRP:HB2	2:B:390:VAL:HG21	1.83	0.60
2:C:455:TYR:CZ	3:D:463:GLN:OE1	2.54	0.60
2:C:372:LEU:HB2	2:C:405:PHE:HB3	1.85	0.59
7:K:384:ARG:HD2	7:K:388:GLU:HB2	1.84	0.59
2:C:566:LEU:N	2:C:566:LEU:HD12	2.17	0.59
2:B:385:GLN:HG3	2:B:423:ARG:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:352:PRO:HB2	5:H:357:ILE:HD11	1.83	0.59
5:H:532:GLU:OE2	5:H:532:GLU:HA	2.01	0.59
6:J:17:ILE:CG1	6:J:37:ILE:CG1	2.69	0.59
7:K:374:THR:HG23	7:K:405:PHE:HD1	1.65	0.59
7:K:416:ASP:O	7:K:420:SER:OG	2.13	0.59
9:V:25:VAL:H	9:V:120:LEU:HD12	1.65	0.59
9:V:76:VAL:HG12	9:V:91:VAL:HG22	1.83	0.59
1:A:561:LEU:HG	2:B:561:LEU:CD2	2.31	0.59
2:C:381:SER:HG	2:C:427:THR:HG1	1.50	0.59
3:D:567:VAL:CG2	3:E:567:VAL:CB	2.77	0.59
3:G:379:THR:HB	3:G:429:THR:O	2.02	0.59
3:G:486:VAL:HG12	3:G:538:VAL:HG13	1.83	0.59
9:S:76:VAL:HG12	9:S:91:VAL:HG22	1.84	0.59
2:C:568:MET:HE1	3:D:568:MET:HA	1.83	0.59
5:H:468:GLU:OE2	9:V:65:THR:OG1	2.20	0.59
6:J:13:LYS:HD2	6:J:67:LEU:CD1	2.32	0.59
3:G:382:TRP:HB2	3:G:390:VAL:HG21	1.83	0.59
6:J:6:VAL:CG1	6:J:18:THR:HB	2.32	0.59
6:J:13:LYS:HB3	6:J:67:LEU:CD2	2.33	0.59
3:D:562:TYR:HB2	3:E:562:TYR:HB3	1.85	0.59
3:D:564:VAL:HG12	3:D:564:VAL:O	2.03	0.59
9:V:120:LEU:HD23	9:V:120:LEU:N	2.17	0.59
1:A:566:LEU:HD12	1:A:566:LEU:N	2.18	0.59
2:B:467:ARG:HA	2:B:525:GLU:HG3	1.84	0.59
4:F:525:GLU:OE2	4:F:529:ASN:ND2	2.36	0.59
9:R:36:LYS:HE3	9:R:86:LEU:HD13	1.85	0.59
9:U:22:GLU:OE1	9:U:24:LYS:CG	2.51	0.59
9:V:25:VAL:HG21	9:V:34:THR:O	2.02	0.59
3:G:413:ILE:HG22	3:G:414:CYS:H	1.66	0.59
7:K:490:GLN:CB	7:K:495:LEU:HD21	2.32	0.59
9:S:31:GLY:O	9:S:94:LEU:HD11	1.99	0.59
9:S:48:LEU:O	9:S:61:VAL:HG22	2.03	0.59
3:E:514:ARG:HH11	3:E:514:ARG:CG	2.16	0.58
3:G:535:THR:HG22	3:G:551:THR:HG22	1.84	0.58
8:L:427:THR:OG1	8:L:438:LYS:NZ	2.29	0.58
3:G:553:ASP:OD1	3:G:556:THR:OG1	2.17	0.58
3:G:567:VAL:HB	5:H:567:VAL:HA	1.85	0.58
9:S:22:GLU:OE2	9:S:24:LYS:HG3	2.03	0.58
9:U:34:THR:HA	9:U:89:VAL:O	2.03	0.58
2:B:566:LEU:HD12	2:B:568:MET:HG2	1.86	0.58
7:K:467:ARG:C	7:K:525:GLU:HG3	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:541:GLU:N	3:G:541:GLU:OE1	2.36	0.58
7:K:368:LEU:HG	7:K:407:ALA:H	1.68	0.58
9:S:25:VAL:HG12	9:S:120:LEU:HD12	1.85	0.58
1:A:419:ASN:O	1:A:445:LYS:NZ	2.35	0.58
3:D:567:VAL:CB	3:E:567:VAL:CG2	2.69	0.58
8:L:346:ARG:HD2	8:L:370:THR:HG22	1.86	0.58
9:S:48:LEU:HD12	9:S:103:ALA:O	2.04	0.58
3:G:364:LYS:HE3	3:G:410:GLU:HB3	1.85	0.58
1:A:490:GLN:NE2	1:A:532:GLU:OE1	2.36	0.57
1:A:562:TYR:N	1:A:562:TYR:CD1	2.72	0.57
2:C:568:MET:CG	5:H:562:TYR:CZ	2.87	0.57
6:J:6:VAL:HG22	6:J:6:VAL:O	2.04	0.57
9:U:23:VAL:HG13	9:U:120:LEU:HD23	0.67	0.57
4:F:373:THR:HA	4:F:404:THR:HA	1.86	0.57
4:F:520:ILE:HD12	4:F:520:ILE:C	2.24	0.57
7:K:467:ARG:HD2	7:K:467:ARG:N	2.19	0.57
9:U:28:GLU:O	9:U:28:GLU:HG2	2.04	0.57
3:D:459:PRO:HG3	3:D:470:ALA:HB1	1.87	0.57
3:G:463:GLN:HE22	3:G:471:THR:HG23	1.67	0.57
5:H:561:LEU:HD12	5:H:561:LEU:O	2.04	0.57
9:S:24:LYS:HG2	9:S:119:THR:O	2.03	0.57
8:L:351:PRO:HD3	8:L:441:ILE:HG12	1.85	0.57
3:D:525:GLU:OE2	3:D:529:ASN:ND2	2.36	0.57
6:J:22:ILE:O	6:J:24:SER:N	2.38	0.57
8:L:380:ILE:HG21	8:L:409:GLY:HA3	1.85	0.57
2:C:568:MET:SD	5:H:562:TYR:HE2	2.26	0.57
3:E:482:ALA:CB	3:E:515:TYR:HD1	2.07	0.57
8:L:347:VAL:HG22	8:L:369:VAL:HG13	1.87	0.57
8:L:367:CYS:HB2	8:L:382:TRP:CZ2	2.39	0.57
6:J:6:VAL:O	6:J:6:VAL:HG13	2.04	0.57
7:K:563:ASN:O	8:L:563:ASN:HA	2.05	0.57
9:S:28:GLU:O	9:S:94:LEU:O	2.23	0.57
2:B:553:ASP:OD1	2:B:554:LYS:N	2.37	0.57
2:C:562:TYR:CD1	2:C:562:TYR:N	2.72	0.57
3:E:399:SER:HA	3:E:405:PHE:HA	1.86	0.57
6:J:16:ARG:NH2	6:J:16:ARG:HG3	2.18	0.57
7:K:490:GLN:NE2	7:K:534:TYR:CA	2.66	0.57
9:U:20:LEU:HD22	9:U:20:LEU:H	1.69	0.57
5:H:554:LYS:HE2	5:H:558:LYS:NZ	2.16	0.56
7:K:464:LEU:HD12	7:K:525:GLU:OE1	2.05	0.56
9:S:121:ASN:OD1	9:S:122:VAL:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:463:GLN:NE2	3:D:455:TYR:CE2	2.73	0.56
3:E:400:HIS:N	3:E:404:THR:O	2.37	0.56
9:R:69:LYS:HB2	9:R:72:TYR:HB2	1.87	0.56
9:U:32:SER:HB3	9:U:92:THR:HA	1.87	0.56
9:U:81:TYR:O	9:U:85:ASN:N	2.39	0.56
1:A:459:PRO:HG3	1:A:470:ALA:HB1	1.87	0.56
1:A:550:ARG:HH12	2:B:462:GLU:HG2	1.71	0.56
5:H:415:GLU:O	5:H:419:ASN:N	2.30	0.56
9:U:24:LYS:HA	9:U:120:LEU:HA	1.86	0.56
1:A:456:LEU:HD23	1:A:550:ARG:HB2	1.88	0.56
2:C:567:VAL:HG23	3:D:567:VAL:HG12	1.88	0.56
9:V:99:SER:O	9:V:99:SER:OG	2.22	0.56
2:C:561:LEU:CD1	3:D:561:LEU:HA	2.35	0.56
3:D:566:LEU:O	3:E:566:LEU:CB	2.54	0.56
4:F:351:PRO:HB2	4:F:418:TRP:HZ2	1.70	0.56
4:F:521:LEU:HD22	4:F:521:LEU:C	2.25	0.56
6:J:17:ILE:CG1	6:J:37:ILE:CD1	2.84	0.56
2:C:456:LEU:CD2	2:C:552:VAL:HB	2.36	0.56
9:S:69:LYS:HD3	9:S:70:ALA:H	1.70	0.56
3:E:452:PRO:HB3	3:E:479:PHE:HB3	1.86	0.56
3:G:451:ARG:HH12	3:G:544:PRO:HD3	1.71	0.56
9:V:81:TYR:O	9:V:86:LEU:N	2.38	0.56
4:F:459:PRO:HG3	4:F:470:ALA:HB1	1.88	0.56
7:K:472:ILE:HD11	7:K:528:TRP:CZ2	2.39	0.56
1:A:529:ASN:HA	1:A:554:LYS:HE3	1.88	0.56
2:B:546:ARG:HG3	2:B:547:VAL:HG23	1.88	0.56
5:H:426:CYS:SG	5:H:439:GLN:NE2	2.78	0.56
2:C:428:VAL:HB	2:C:437:LEU:HB2	1.88	0.55
3:G:490:GLN:NE2	3:G:491:ARG:HG3	2.21	0.55
9:V:99:SER:HB2	9:V:122:VAL:HG22	1.88	0.55
1:A:488:TRP:HZ3	1:A:521:LEU:HB2	1.71	0.55
1:A:512:PRO:HD2	9:R:66:ASN:HD22	1.72	0.55
3:D:568:MET:HE2	3:D:569:SER:H	1.70	0.55
9:V:25:VAL:CG1	9:V:120:LEU:CD1	2.83	0.55
2:C:425:THR:HA	2:C:439:GLN:O	2.07	0.55
3:E:566:LEU:HD23	3:E:566:LEU:O	2.07	0.55
3:G:490:GLN:HE21	3:G:491:ARG:HG3	1.70	0.55
5:H:562:TYR:N	5:H:562:TYR:CD1	2.72	0.55
1:A:564:VAL:CG2	8:L:568:MET:HE3	2.36	0.55
2:B:345:ILE:HB	2:B:433:LEU:HD11	1.88	0.55
9:U:20:LEU:HB3	9:U:117:LYS:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:GLN:O	1:A:488:TRP:HD1	1.90	0.55
3:D:384:ARG:NH1	3:D:389:ALA:O	2.38	0.55
3:E:565:SER:O	3:E:565:SER:OG	2.15	0.55
3:G:452:PRO:HB3	3:G:479:PHE:HB3	1.89	0.55
7:K:365:LEU:HB2	7:K:411:ALA:HB3	1.87	0.55
2:C:397:SER:HB3	2:C:407:ALA:HA	1.87	0.55
9:R:51:GLU:HA	9:R:58:CYS:HA	1.89	0.55
9:S:83:ARG:HG3	9:S:84:LYS:HG3	1.87	0.55
9:V:34:THR:HG22	9:V:90:GLU:HG3	1.89	0.55
6:J:66:ASP:OD1	6:J:66:ASP:N	2.39	0.55
7:K:467:ARG:HD2	7:K:467:ARG:H	1.72	0.55
6:J:6:VAL:CB	6:J:18:THR:HA	2.17	0.55
9:R:101:VAL:HG12	9:R:119:THR:HB	1.86	0.55
9:S:24:LYS:HE3	9:S:121:ASN:H	1.72	0.55
2:B:466:LEU:HD12	2:B:468:GLU:H	1.72	0.55
9:S:81:TYR:O	9:S:85:ASN:N	2.40	0.55
4:F:450:HIS:CE1	4:F:514:ARG:HH12	2.25	0.54
3:G:400:HIS:HE1	3:G:406:SER:HB2	1.72	0.54
6:J:43:LEU:HA	6:J:60:PHE:CZ	2.42	0.54
7:K:480:SER:HB2	7:K:481:PRO:HD3	1.90	0.54
8:L:351:PRO:HA	8:L:365:LEU:HD13	1.87	0.54
8:L:383:THR:OG1	8:L:425:THR:OG1	2.25	0.54
9:V:27:GLY:C	9:V:94:LEU:HD12	2.26	0.54
2:B:345:ILE:N	2:B:371:ASP:HB3	2.21	0.54
5:H:560:THR:CG2	7:K:559:PRO:HA	2.37	0.54
8:L:354:PHE:HA	8:L:357:ILE:HG12	1.88	0.54
1:A:565:SER:O	1:A:565:SER:OG	2.19	0.54
2:B:358:PHE:HE1	2:B:546:ARG:HD3	1.72	0.54
2:B:417:ASP:O	2:B:420:SER:OG	2.24	0.54
2:C:568:MET:HE3	3:D:568:MET:HB3	1.90	0.54
4:F:413:ILE:HG12	4:F:424:PHE:HZ	1.73	0.54
5:H:567:VAL:HG21	7:K:567:VAL:HG12	1.89	0.54
6:J:22:ILE:HG13	6:J:32:ILE:HB	1.89	0.54
7:K:466:LEU:N	7:K:466:LEU:HD23	2.23	0.54
9:S:40:PRO:HD3	9:S:46:ILE:HD13	1.89	0.54
3:E:482:ALA:CB	3:E:515:TYR:CD1	2.74	0.54
3:G:399:SER:HA	3:G:405:PHE:HA	1.90	0.54
3:G:508:GLU:CG	3:G:509:PRO:HD2	2.38	0.54
1:A:537:VAL:HG12	1:A:549:GLU:HG2	1.89	0.54
3:D:393:HIS:HD2	3:D:396:ILE:HD11	1.73	0.54
3:E:474:CYS:HB2	3:E:488:TRP:HH2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:4:ARG:CZ	6:J:4:ARG:CB	2.85	0.54
7:K:347:VAL:HG23	7:K:369:VAL:HA	1.89	0.54
7:K:490:GLN:NE2	7:K:534:TYR:HA	2.22	0.54
3:E:443:ARG:HE	3:E:445:LYS:HD2	1.73	0.54
3:E:562:TYR:CE2	4:F:566:LEU:HD21	2.43	0.54
3:G:512:PRO:C	3:G:514:ARG:H	2.12	0.54
5:H:392:THR:HG22	5:H:393:HIS:H	1.73	0.54
7:K:385:GLN:HB2	7:K:423:ARG:HB2	1.90	0.54
7:K:457:LEU:HB2	7:K:473:THR:OG1	2.06	0.54
9:V:51:GLU:HA	9:V:58:CYS:HA	1.90	0.54
2:B:565:SER:O	2:B:565:SER:OG	2.21	0.53
3:D:560:THR:OG1	3:E:562:TYR:HA	2.07	0.53
1:A:544:PRO:HB3	6:J:134:TYR:CD1	2.35	0.53
3:E:400:HIS:NE2	3:E:406:SER:HB2	2.24	0.53
4:F:391:LYS:HD2	4:F:392:THR:N	2.23	0.53
5:H:383:THR:HB	5:H:387:GLY:HA2	1.90	0.53
7:K:470:ALA:HB3	7:K:528:TRP:HE1	1.72	0.53
7:K:563:ASN:HB3	8:L:563:ASN:CA	2.38	0.53
3:G:419:ASN:O	3:G:443:ARG:NH2	2.41	0.53
5:H:386:ASN:ND2	5:H:388:GLU:OE2	2.41	0.53
4:F:382:TRP:HB2	4:F:390:VAL:HG21	1.90	0.53
7:K:535:THR:OG1	7:K:550:ARG:O	2.16	0.53
1:A:556:THR:HG23	6:J:46:ARG:HH22	1.73	0.53
3:E:561:LEU:HB3	3:E:562:TYR:CD2	2.43	0.53
9:V:38:PRO:HD2	9:V:116:GLN:NE2	1.85	0.53
9:V:50:ARG:CB	9:V:102:TYR:CE1	2.86	0.53
2:B:452:PRO:HB3	2:B:479:PHE:HB3	1.90	0.53
6:J:4:ARG:HB3	6:J:4:ARG:CZ	2.37	0.53
9:V:95:THR:OG1	9:V:97:SER:OG	2.16	0.53
4:F:485:PHE:HB3	4:F:539:ALA:HB3	1.91	0.53
4:F:500:TYR:HB3	4:F:521:LEU:HB3	1.88	0.53
9:S:99:SER:HG	9:S:120:LEU:HD23	1.73	0.53
2:C:360:THR:HG22	2:C:362:SER:HB2	1.91	0.53
3:E:489:MET:O	3:E:535:THR:OG1	2.25	0.53
5:H:467:ARG:HA	5:H:525:GLU:HG2	1.91	0.53
8:L:367:CYS:HB2	8:L:382:TRP:HZ2	1.74	0.53
8:L:381:SER:HB2	8:L:427:THR:HB	1.90	0.53
1:A:345:ILE:HG21	1:A:433:LEU:HD21	1.90	0.52
3:D:567:VAL:HG23	3:E:567:VAL:C	2.29	0.52
3:E:488:TRP:CZ3	3:E:536:CYS:HB2	2.44	0.52
6:J:43:LEU:HD23	6:J:43:LEU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:443:ARG:HG3	7:K:445:LYS:HD2	1.91	0.52
4:F:527:GLU:OE1	4:F:527:GLU:N	2.38	0.52
7:K:560:THR:HG23	8:L:560:THR:C	2.29	0.52
1:A:363:THR:HG21	1:A:415:GLU:HG3	1.90	0.52
6:J:17:ILE:HG12	6:J:37:ILE:CG1	2.34	0.52
9:V:26:GLU:CA	9:V:121:ASN:O	2.53	0.52
1:A:562:TYR:N	1:A:562:TYR:HD1	2.07	0.52
3:D:453:ASP:OD1	3:D:454:VAL:N	2.43	0.52
3:E:482:ALA:HB1	3:E:505:PRO:CG	2.35	0.52
6:J:16:ARG:HG3	6:J:16:ARG:HH21	1.73	0.52
6:J:103:TYR:CB	8:L:574:THR:HG22	2.30	0.52
9:U:34:THR:HG22	9:U:90:GLU:HB3	1.92	0.52
9:U:97:SER:O	9:U:122:VAL:HG21	2.10	0.52
9:U:111:ASP:OD1	9:U:112:ARG:NH1	2.43	0.52
8:L:384:ARG:HH21	8:L:390:VAL:HG12	1.75	0.52
2:B:372:LEU:O	2:B:405:PHE:N	2.42	0.52
4:F:413:ILE:HG12	4:F:424:PHE:CZ	2.44	0.52
3:G:384:ARG:HD3	3:G:388:GLU:HB3	1.89	0.52
6:J:43:LEU:O	6:J:43:LEU:HG	2.10	0.52
9:R:45:ARG:HD3	9:R:108:MET:HA	1.91	0.52
9:U:23:VAL:HG22	9:U:120:LEU:HD22	1.91	0.52
9:U:34:THR:OG1	9:U:34:THR:O	2.25	0.52
4:F:531:GLY:O	4:F:553:ASP:OD1	2.24	0.52
3:G:499:LYS:HE3	3:G:499:LYS:HA	1.91	0.52
7:K:432:ASP:OD1	7:K:433:LEU:N	2.43	0.52
9:S:75:ARG:NH2	9:S:93:GLN:O	2.38	0.52
3:E:568:MET:HE3	3:E:568:MET:CA	2.32	0.52
7:K:472:ILE:HD11	7:K:528:TRP:CH2	2.45	0.52
2:B:561:LEU:CD2	2:B:561:LEU:N	2.73	0.52
2:C:450:HIS:CE1	2:C:514:ARG:HH21	2.27	0.52
2:C:568:MET:HE3	3:D:568:MET:CA	2.40	0.52
3:G:354:PHE:HA	3:G:357:ILE:HG22	1.92	0.52
7:K:563:ASN:HB3	8:L:563:ASN:CB	2.40	0.52
8:L:533:THR:O	8:L:551:THR:OG1	2.27	0.52
1:A:566:LEU:HD13	2:B:566:LEU:HA	1.92	0.51
3:D:569:SER:O	3:D:569:SER:OG	2.27	0.51
4:F:508:GLU:HB3	4:F:511:ALA:HB3	1.92	0.51
7:K:351:PRO:HA	7:K:365:LEU:HD13	1.90	0.51
2:B:379:THR:HB	2:B:429:THR:H	1.75	0.51
2:C:416:ASP:OD1	2:C:417:ASP:N	2.43	0.51
3:D:345:ILE:HG13	3:D:372:LEU:HD11	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:427:THR:HG23	3:D:438:LYS:HZ1	1.74	0.51
3:E:461:ARG:O	3:E:461:ARG:NH1	2.43	0.51
3:E:501:VAL:HG21	4:F:509:PRO:HD3	1.92	0.51
4:F:523:VAL:HG13	4:F:523:VAL:O	2.11	0.51
8:L:508:GLU:HB2	8:L:511:ALA:O	2.10	0.51
1:A:566:LEU:CD1	1:A:566:LEU:N	2.73	0.51
3:E:383:THR:HB	3:E:387:GLY:HA2	1.92	0.51
3:E:518:HIS:CG	4:F:518:HIS:ND1	2.78	0.51
6:J:49:ILE:HG13	6:J:103:TYR:HE1	1.76	0.51
9:U:34:THR:CB	9:U:88:LEU:HD12	2.38	0.51
8:L:400:HIS:N	8:L:404:THR:O	2.37	0.51
1:A:472:ILE:HD11	1:A:528:TRP:CD1	2.46	0.51
2:C:566:LEU:N	2:C:566:LEU:CD1	2.73	0.51
2:C:568:MET:O	2:C:568:MET:HG2	2.10	0.51
3:G:459:PRO:HG3	3:G:470:ALA:HB1	1.93	0.51
6:J:102:THR:CB	8:L:575:CYS:SG	2.98	0.51
2:C:455:TYR:CE1	3:D:463:GLN:OE1	2.64	0.51
3:D:480:SER:HB3	3:D:481:PRO:HD3	1.93	0.51
3:E:433:LEU:HD22	3:E:436:PRO:HA	1.92	0.51
1:A:466:LEU:HD12	1:A:468:GLU:H	1.75	0.51
1:A:471:THR:HA	1:A:521:LEU:O	2.11	0.51
3:D:421:GLY:N	3:D:443:ARG:HH12	2.09	0.51
3:D:449:LEU:O	3:D:450:HIS:ND1	2.44	0.51
3:D:490:GLN:HG2	3:D:491:ARG:HG3	1.93	0.51
5:H:419:ASN:HA	5:H:443:ARG:HH22	1.75	0.51
9:R:75:ARG:NE	9:R:93:GLN:OE1	2.39	0.51
9:V:24:LYS:HE2	9:V:121:ASN:CB	2.24	0.51
1:A:349:ALA:HB2	1:A:439:GLN:HB3	1.93	0.51
3:D:452:PRO:HG3	3:D:540:HIS:HB3	1.92	0.51
3:E:514:ARG:CG	3:E:514:ARG:NH1	2.73	0.51
4:F:508:GLU:OE1	4:F:511:ALA:N	2.44	0.51
2:C:453:ASP:OD1	2:C:453:ASP:N	2.43	0.51
3:E:482:ALA:HB2	3:E:515:TYR:CE1	2.41	0.51
6:J:17:ILE:HG13	6:J:36:ASN:N	2.26	0.51
8:L:370:THR:OG1	8:L:400:HIS:NE2	2.42	0.51
3:E:474:CYS:HB2	3:E:488:TRP:CZ2	2.44	0.50
6:J:41:VAL:HG22	6:J:62:TYR:OH	2.10	0.50
2:C:486:VAL:HG22	2:C:538:VAL:HG22	1.93	0.50
3:D:567:VAL:HG23	3:E:567:VAL:CB	2.37	0.50
3:G:400:HIS:CE1	3:G:406:SER:HB2	2.46	0.50
9:S:36:LYS:C	9:S:116:GLN:HE22	2.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:47:TYR:OH	9:U:110:THR:O	2.26	0.50
1:A:463:GLN:HG2	2:B:455:TYR:CZ	2.47	0.50
3:G:367:CYS:SG	3:G:382:TRP:NE1	2.84	0.50
9:V:27:GLY:CA	9:V:94:LEU:HD12	2.39	0.50
1:A:450:HIS:H	1:A:480:SER:HB3	1.77	0.50
3:G:459:PRO:HD3	3:G:472:ILE:HG13	1.93	0.50
3:E:566:LEU:HD13	4:F:562:TYR:CE2	2.47	0.50
5:H:553:ASP:OD1	5:H:554:LYS:N	2.44	0.50
9:V:24:LYS:CA	9:V:120:LEU:HB2	2.36	0.50
2:C:384:ARG:NH1	2:C:388:GLU:HB2	2.26	0.50
2:C:568:MET:CE	2:C:568:MET:N	2.73	0.50
4:F:358:PHE:O	4:F:361:LYS:NZ	2.44	0.50
4:F:380:ILE:HD12	4:F:428:VAL:HG12	1.94	0.50
3:G:511:ALA:HB1	9:V:66:ASN:ND2	2.16	0.50
6:J:67:LEU:N	6:J:67:LEU:HD12	2.26	0.50
9:U:75:ARG:NE	9:U:93:GLN:OE1	2.40	0.50
9:V:50:ARG:CG	9:V:102:TYR:CD1	2.80	0.50
6:J:8:VAL:HB	6:J:68:CYS:HA	1.93	0.50
7:K:380:ILE:HG12	7:K:428:VAL:HG12	1.94	0.50
7:K:541:GLU:OE1	7:K:541:GLU:N	2.44	0.50
3:D:379:THR:HB	3:D:429:THR:HG23	1.94	0.50
3:D:467:ARG:HG2	3:D:467:ARG:HH11	1.76	0.50
3:G:423:ARG:HA	3:G:442:SER:OG	2.11	0.50
1:A:357:ILE:HG23	1:A:363:THR:HG22	1.94	0.50
1:A:568:MET:HG3	1:A:571:THR:HG22	1.93	0.50
4:F:379:THR:HB	4:F:429:THR:OG1	2.12	0.50
5:H:358:PHE:HD1	5:H:361:LYS:HZ1	1.60	0.50
7:K:511:ALA:HB1	7:K:514:ARG:HE	1.77	0.50
3:E:357:ILE:HD11	3:E:415:GLU:HG3	1.94	0.49
7:K:493:GLN:HB2	7:K:494:PRO:HD2	1.94	0.49
9:U:29:LEU:H	9:U:29:LEU:CD1	2.10	0.49
9:U:96:GLU:OE2	9:U:123:HIS:HD2	1.95	0.49
2:C:456:LEU:CD2	2:C:552:VAL:CG1	2.90	0.49
4:F:533:THR:N	4:F:553:ASP:OD2	2.43	0.49
3:G:380:ILE:HG22	3:G:428:VAL:HG22	1.94	0.49
3:G:463:GLN:NE2	3:G:469:SER:O	2.40	0.49
5:H:367:CYS:HB2	5:H:382:TRP:CZ2	2.47	0.49
7:K:379:THR:OG1	7:K:429:THR:O	2.29	0.49
3:E:489:MET:HB3	3:E:535:THR:OG1	2.13	0.49
6:J:12:CYS:SG	6:J:13:LYS:N	2.85	0.49
6:J:17:ILE:CG1	6:J:37:ILE:HD13	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:456:LEU:HD23	2:B:552:VAL:HG13	1.93	0.49
3:D:535:THR:HG22	3:D:551:THR:HB	1.94	0.49
6:J:134:TYR:C	6:J:134:TYR:CD2	2.85	0.49
7:K:467:ARG:NE	7:K:467:ARG:HA	2.28	0.49
2:C:540:HIS:CD2	2:C:542:ALA:H	2.30	0.49
4:F:456:LEU:HD11	4:F:536:CYS:SG	2.53	0.49
8:L:382:TRP:CZ3	8:L:424:PHE:HB3	2.48	0.49
9:R:48:LEU:HD11	9:R:102:TYR:HB3	1.94	0.49
9:V:55:SER:OG	9:V:57:THR:OG1	2.17	0.49
2:C:503:SER:OG	2:C:504:ALA:N	2.45	0.49
7:K:467:ARG:NH1	7:K:467:ARG:CG	2.73	0.49
9:R:75:ARG:NH2	9:R:95:THR:HG22	2.27	0.49
9:U:36:LYS:HG2	9:U:86:LEU:HD22	1.94	0.49
9:U:83:ARG:HG3	9:U:84:LYS:HG3	1.94	0.49
3:D:566:LEU:O	3:E:566:LEU:HA	2.13	0.49
5:H:560:THR:CG2	7:K:560:THR:H	2.23	0.49
6:J:17:ILE:HB	6:J:37:ILE:CD1	2.37	0.49
7:K:351:PRO:HB3	7:K:441:ILE:HG21	1.95	0.49
8:L:352:PRO:HD3	8:L:365:LEU:HD22	1.95	0.49
9:S:36:LYS:O	9:S:116:GLN:CD	2.47	0.49
9:U:37:CYS:HB2	9:U:87:PHE:HB3	1.94	0.49
9:V:25:VAL:HG12	9:V:120:LEU:CD1	2.43	0.49
3:D:400:HIS:HD2	3:D:401:PRO:HD2	1.77	0.49
7:K:393:HIS:HB3	7:K:410:GLU:H	1.77	0.49
9:U:24:LYS:CA	9:U:120:LEU:CB	2.64	0.49
4:F:488:TRP:CH2	4:F:521:LEU:HD12	2.48	0.49
5:H:553:ASP:O	5:H:556:THR:OG1	2.29	0.49
1:A:566:LEU:HD11	2:B:566:LEU:CA	2.42	0.48
3:E:433:LEU:HD13	3:E:435:SER:C	2.33	0.48
3:G:350:ILE:HD11	3:G:368:LEU:HD12	1.95	0.48
5:H:352:PRO:HD3	5:H:365:LEU:HB3	1.95	0.48
6:J:42:PRO:HG2	6:J:45:ASN:OD1	2.12	0.48
7:K:507:PRO:HA	7:K:515:TYR:HD1	1.78	0.48
8:L:500:TYR:HB3	8:L:521:LEU:HD13	1.94	0.48
7:K:362:SER:O	7:K:364:LYS:HG2	2.14	0.48
9:S:105:GLY:HA2	9:S:113:GLY:O	2.12	0.48
2:B:347:VAL:HG22	2:B:369:VAL:HG13	1.96	0.48
7:K:419:ASN:HA	7:K:443:ARG:HE	1.78	0.48
9:U:19:ILE:HD13	9:U:21:PRO:HD3	1.93	0.48
1:A:452:PRO:HB3	1:A:479:PHE:HB3	1.95	0.48
2:B:417:ASP:OD1	2:B:417:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:511:ALA:HB1	2:B:514:ARG:HD2	1.96	0.48
6:J:103:TYR:HB2	8:L:574:THR:CG2	2.29	0.48
1:A:352:PRO:HD3	1:A:365:LEU:HA	1.94	0.48
3:G:347:VAL:HG21	3:G:428:VAL:HG21	1.95	0.48
9:S:50:ARG:CG	9:S:50:ARG:NH1	2.73	0.48
1:A:488:TRP:CZ3	1:A:521:LEU:HB2	2.48	0.48
4:F:524:SER:OG	4:F:526:GLU:OE1	2.23	0.48
9:V:24:LYS:C	9:V:120:LEU:HB3	2.34	0.48
3:D:493:GLN:HG2	9:U:42:MET:HE1	1.95	0.48
7:K:467:ARG:HG3	7:K:467:ARG:NH1	2.22	0.48
3:E:354:PHE:HA	3:E:357:ILE:HG22	1.95	0.48
3:E:378:VAL:HA	3:E:430:HIS:HD1	1.77	0.48
3:E:532:GLU:OE1	3:E:532:GLU:N	2.39	0.48
3:G:400:HIS:ND1	3:G:404:THR:HG23	2.29	0.48
6:J:8:VAL:CB	6:J:68:CYS:HA	2.43	0.48
7:K:510:GLN:HB2	8:L:522:THR:HG21	1.96	0.48
8:L:572:ALA:C	8:L:574:THR:H	2.17	0.48
3:D:526:GLU:OE1	3:D:526:GLU:N	2.46	0.48
7:K:461:ARG:NH1	7:K:464:LEU:HD23	2.29	0.48
8:L:457:LEU:HB2	8:L:473:THR:HG23	1.96	0.48
9:U:21:PRO:HB2	9:U:118:VAL:HG12	1.96	0.48
9:U:45:ARG:HG3	9:U:64:THR:HB	1.95	0.48
1:A:352:PRO:HD2	1:A:418:TRP:CZ2	2.49	0.47
2:C:561:LEU:HD11	3:D:560:THR:O	2.14	0.47
3:E:449:LEU:HA	3:E:480:SER:O	2.14	0.47
3:E:455:TYR:HD2	4:F:463:GLN:HE21	1.61	0.47
7:K:455:TYR:CE2	8:L:463:GLN:HB3	2.49	0.47
8:L:532:GLU:HB2	8:L:534:TYR:CZ	2.49	0.47
9:R:76:VAL:HG12	9:R:91:VAL:HG22	1.96	0.47
3:D:543:LEU:HB2	3:D:546:ARG:HA	1.95	0.47
4:F:413:ILE:HG13	4:F:414:CYS:N	2.28	0.47
1:A:494:PRO:HB2	6:J:116:VAL:HG13	1.95	0.47
2:C:550:ARG:NH1	3:D:462:GLU:OE2	2.45	0.47
3:D:453:ASP:OD2	3:D:455:TYR:OH	2.29	0.47
4:F:523:VAL:HG21	4:F:534:TYR:CZ	2.49	0.47
1:A:365:LEU:HD13	1:A:418:TRP:HZ3	1.79	0.47
1:A:564:VAL:HB	6:J:43:LEU:HD12	1.96	0.47
1:A:566:LEU:CD1	2:B:566:LEU:CA	2.93	0.47
9:U:32:SER:HA	9:U:94:LEU:CD1	2.44	0.47
9:V:24:LYS:NZ	9:V:121:ASN:HB2	2.28	0.47
9:V:80:GLN:CD	9:V:80:GLN:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:564:VAL:HG11	7:K:568:MET:SD	2.54	0.47
8:L:429:THR:HG22	8:L:436:PRO:HB3	1.96	0.47
9:U:20:LEU:HB3	9:U:117:LYS:CG	2.44	0.47
2:C:567:VAL:HG23	3:D:567:VAL:O	2.14	0.47
6:J:37:ILE:HD11	6:J:64:LEU:HD21	1.96	0.47
8:L:451:ARG:NE	8:L:542:ALA:O	2.46	0.47
9:S:26:GLU:O	9:S:122:VAL:C	2.53	0.47
1:A:568:MET:HE3	2:B:568:MET:HB2	1.96	0.47
4:F:372:LEU:HD13	4:F:430:HIS:CG	2.49	0.47
7:K:353:SER:O	7:K:357:ILE:HG23	2.14	0.47
8:L:382:TRP:HZ3	8:L:424:PHE:HB3	1.80	0.47
9:S:41:GLU:HB3	9:S:42:MET:HE3	1.89	0.47
2:C:456:LEU:HD23	2:C:552:VAL:HB	1.97	0.47
3:D:483:ASP:OD1	3:D:484:VAL:N	2.48	0.47
3:D:532:GLU:HB2	3:D:534:TYR:CE2	2.50	0.47
5:H:399:SER:OG	5:H:404:THR:O	2.30	0.47
7:K:363:THR:O	7:K:364:LYS:HE2	2.15	0.47
8:L:456:LEU:HD22	8:L:552:VAL:HB	1.96	0.47
4:F:430:HIS:HD2	4:F:432:ASP:H	1.61	0.47
5:H:345:ILE:O	5:H:346:ARG:NH1	2.47	0.47
5:H:414:CYS:SG	5:H:415:GLU:N	2.88	0.47
6:J:6:VAL:HB	6:J:18:THR:CB	2.42	0.47
6:J:14:CYS:SG	6:J:40:ILE:O	2.73	0.47
6:J:32:ILE:HG23	8:L:561:LEU:HD13	1.97	0.47
7:K:449:LEU:HD12	7:K:481:PRO:HG2	1.97	0.47
8:L:432:ASP:OD1	8:L:433:LEU:N	2.48	0.47
9:V:24:LYS:HE3	9:V:121:ASN:N	2.29	0.47
9:V:40:PRO:O	9:V:41:GLU:HG3	2.15	0.47
9:V:101:VAL:HG13	9:V:101:VAL:O	2.15	0.47
4:F:564:VAL:HA	3:G:564:VAL:O	2.15	0.46
5:H:364:LYS:HD3	5:H:411:ALA:O	2.14	0.46
9:R:94:LEU:C	9:R:94:LEU:HD23	2.34	0.46
9:U:51:GLU:HA	9:U:58:CYS:HA	1.95	0.46
2:C:456:LEU:CD2	2:C:552:VAL:HG11	2.45	0.46
6:J:43:LEU:C	6:J:43:LEU:CD2	2.83	0.46
9:U:20:LEU:N	9:U:20:LEU:CD2	2.73	0.46
1:A:385:GLN:HB3	1:A:423:ARG:HB3	1.97	0.46
3:G:543:LEU:HB2	3:G:546:ARG:HA	1.97	0.46
5:H:391:LYS:NZ	5:H:394:THR:OG1	2.49	0.46
5:H:543:LEU:HB2	5:H:546:ARG:HA	1.98	0.46
8:L:345:ILE:HG23	8:L:372:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:372:LEU:HD12	8:L:376:ASP:HA	1.97	0.46
9:S:25:VAL:CG1	9:S:120:LEU:HD12	2.45	0.46
1:A:540:HIS:H	1:A:543:LEU:HD12	1.80	0.46
3:D:425:THR:HG22	3:D:440:THR:HG22	1.97	0.46
4:F:442:SER:OG	4:F:443:ARG:N	2.48	0.46
8:L:352:PRO:HB3	8:L:364:LYS:H	1.80	0.46
9:S:24:LYS:HB3	9:S:24:LYS:HE2	1.33	0.46
9:U:68:ILE:HG21	9:U:73:LYS:HA	1.98	0.46
9:V:24:LYS:C	9:V:120:LEU:CB	2.84	0.46
4:F:497:PRO:HA	4:F:500:TYR:CE1	2.51	0.46
4:F:511:ALA:HB1	4:F:514:ARG:HG3	1.98	0.46
5:H:347:VAL:HG11	5:H:439:GLN:NE2	2.31	0.46
1:A:488:TRP:NE1	1:A:536:CYS:SG	2.89	0.46
3:E:566:LEU:HD23	3:E:566:LEU:N	2.30	0.46
4:F:480:SER:HB3	4:F:481:PRO:HD3	1.98	0.46
6:J:16:ARG:HH21	6:J:16:ARG:CG	2.29	0.46
6:J:41:VAL:HG12	6:J:43:LEU:N	2.31	0.46
7:K:385:GLN:N	7:K:422:GLU:OE2	2.49	0.46
7:K:469:SER:CA	7:K:523:VAL:O	2.64	0.46
8:L:372:LEU:HB3	8:L:430:HIS:CE1	2.51	0.46
9:S:99:SER:OG	9:S:120:LEU:C	2.52	0.46
3:D:423:ARG:HB3	3:D:442:SER:HB2	1.97	0.46
3:E:369:VAL:HG11	3:E:428:VAL:HG11	1.98	0.46
3:E:562:TYR:CD1	3:E:562:TYR:O	2.69	0.46
9:R:29:LEU:HG	9:R:93:GLN:HE21	1.80	0.46
9:S:21:PRO:HD2	9:S:116:GLN:HA	1.97	0.46
9:U:34:THR:HG22	9:U:90:GLU:CB	2.46	0.46
2:B:549:GLU:O	2:B:550:ARG:HD3	2.16	0.46
2:C:520:ILE:HD11	3:D:518:HIS:NE2	2.31	0.46
3:D:418:TRP:O	3:D:443:ARG:NH1	2.49	0.46
9:V:27:GLY:HA3	9:V:94:LEU:CD1	2.44	0.46
6:J:5:ILE:HD13	6:J:5:ILE:N	2.30	0.46
6:J:17:ILE:HA	6:J:36:ASN:O	2.15	0.46
8:L:376:ASP:HB2	8:L:407:ALA:HB3	1.98	0.46
9:U:22:GLU:CG	9:U:119:THR:O	2.60	0.46
9:V:50:ARG:CA	9:V:102:TYR:CD1	2.95	0.46
3:D:567:VAL:CG2	3:E:567:VAL:HG22	2.23	0.46
3:E:485:PHE:O	3:E:485:PHE:CG	2.69	0.46
3:E:566:LEU:HD22	4:F:562:TYR:HE2	1.79	0.46
4:F:461:ARG:O	4:F:461:ARG:NH1	2.49	0.46
4:F:532:GLU:O	4:F:553:ASP:OD1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:505:PRO:HA	8:L:517:ALA:HB2	1.97	0.46
1:A:463:GLN:NE2	1:A:469:SER:O	2.45	0.45
5:H:554:LYS:HZ3	5:H:558:LYS:NZ	2.13	0.45
3:D:457:LEU:HB2	3:D:473:THR:CG2	2.46	0.45
3:G:413:ILE:HG22	3:G:414:CYS:N	2.32	0.45
5:H:354:PHE:HA	5:H:357:ILE:HB	1.98	0.45
9:S:78:LEU:HD12	9:S:87:PHE:CZ	2.51	0.45
2:B:352:PRO:HB2	2:B:357:ILE:HD11	1.98	0.45
2:B:461:ARG:HD2	2:B:461:ARG:HA	1.78	0.45
3:E:485:PHE:O	3:E:485:PHE:CD2	2.70	0.45
3:G:561:LEU:O	5:H:561:LEU:HB2	2.16	0.45
1:A:372:LEU:H	1:A:372:LEU:HD23	1.81	0.45
6:J:6:VAL:HB	6:J:18:THR:N	2.30	0.45
7:K:378:VAL:HG12	7:K:430:HIS:ND1	2.32	0.45
9:S:32:SER:OG	9:S:90:GLU:OE1	2.30	0.45
2:B:369:VAL:HB	2:B:406:SER:HA	1.97	0.45
5:H:507:PRO:HA	5:H:515:TYR:CD1	2.51	0.45
5:H:523:VAL:HG11	5:H:534:TYR:CE2	2.51	0.45
6:J:13:LYS:HB3	6:J:67:LEU:HD23	1.98	0.45
3:D:567:VAL:HB	3:E:567:VAL:CG2	2.46	0.45
4:F:531:GLY:O	4:F:553:ASP:CG	2.55	0.45
1:A:465:ASN:HA	1:A:467:ARG:HH11	1.81	0.45
2:C:474:CYS:HB2	2:C:488:TRP:CZ2	2.52	0.45
6:J:116:VAL:HG23	6:J:117:TYR:N	2.31	0.45
2:C:425:THR:HG21	2:C:438:LYS:HE3	1.99	0.45
3:D:489:MET:HB3	3:D:535:THR:OG1	2.17	0.45
5:H:456:LEU:HD11	5:H:536:CYS:HB3	1.99	0.45
6:J:134:TYR:CD2	6:J:134:TYR:O	2.70	0.45
7:K:459:PRO:HD3	7:K:472:ILE:HD13	1.99	0.45
7:K:523:VAL:HG21	7:K:534:TYR:CE2	2.52	0.45
9:S:100:GLY:O	9:S:119:THR:OG1	2.21	0.45
9:V:102:TYR:O	9:V:117:LYS:HA	2.17	0.45
1:A:567:VAL:HG21	2:B:567:VAL:CG1	2.35	0.45
3:D:354:PHE:CE1	3:D:541:GLU:HB3	2.52	0.45
4:F:462:GLU:OE1	4:F:462:GLU:N	2.46	0.45
9:S:63:SER:OG	9:S:64:THR:N	2.50	0.45
2:C:362:SER:O	2:C:364:LYS:HG3	2.17	0.45
2:C:382:TRP:CE2	2:C:426:CYS:HB2	2.52	0.45
2:C:382:TRP:CZ2	2:C:426:CYS:HB2	2.52	0.45
2:C:405:PHE:HE1	2:C:407:ALA:HB2	1.81	0.45
3:D:382:TRP:CD2	3:D:426:CYS:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:21:ILE:CG1	8:L:555:SER:HA	2.47	0.45
6:J:35:ARG:HD3	6:J:35:ARG:HA	1.84	0.45
8:L:545:ASN:HB3	8:L:547:VAL:HB	1.99	0.45
9:U:30:GLY:C	9:U:92:THR:O	2.54	0.45
9:V:24:LYS:HZ1	9:V:121:ASN:ND2	2.15	0.45
3:G:413:ILE:HG21	3:G:424:PHE:CE2	2.53	0.44
5:H:392:THR:HG22	5:H:393:HIS:N	2.32	0.44
5:H:560:THR:HG22	7:K:560:THR:N	2.28	0.44
5:H:560:THR:O	5:H:560:THR:OG1	2.24	0.44
9:V:37:CYS:HB2	9:V:87:PHE:HB3	1.99	0.44
2:B:508:GLU:OE2	2:B:516:PHE:HB3	2.17	0.44
2:C:568:MET:CE	2:C:568:MET:C	2.85	0.44
3:E:352:PRO:HD3	3:E:365:LEU:HB3	1.98	0.44
3:E:491:ARG:HH21	3:E:532:GLU:HB2	1.82	0.44
3:G:520:ILE:HD11	5:H:518:HIS:NE2	2.32	0.44
3:E:450:HIS:HB2	3:E:480:SER:OG	2.17	0.44
3:E:512:PRO:HD2	9:U:66:ASN:ND2	2.32	0.44
4:F:427:THR:HG23	4:F:438:LYS:HD3	1.99	0.44
3:G:364:LYS:HZ2	3:G:412:SER:HB2	1.82	0.44
3:G:418:TRP:O	3:G:443:ARG:NE	2.50	0.44
5:H:419:ASN:HA	5:H:443:ARG:NH2	2.32	0.44
8:L:572:ALA:C	8:L:574:THR:N	2.70	0.44
9:R:32:SER:HA	9:R:91:VAL:O	2.16	0.44
2:C:561:LEU:HD13	2:C:561:LEU:HA	1.65	0.44
3:D:364:LYS:HD2	3:D:410:GLU:HB2	2.00	0.44
4:F:381:SER:HA	4:F:393:HIS:HE1	1.83	0.44
2:C:526:GLU:O	2:C:530:THR:HG23	2.17	0.44
3:E:415:GLU:OE1	3:E:415:GLU:N	2.50	0.44
4:F:351:PRO:HB3	4:F:441:ILE:HD12	2.00	0.44
6:J:28:PRO:O	6:J:30:GLU:N	2.49	0.44
2:B:462:GLU:HA	2:B:465:ASN:ND2	2.32	0.44
3:D:384:ARG:HA	3:D:424:PHE:HD1	1.82	0.44
3:D:508:GLU:OE2	3:D:516:PHE:HB3	2.17	0.44
9:S:69:LYS:HB3	9:S:72:TYR:HD2	1.83	0.44
1:A:475:LEU:HD13	1:A:518:HIS:CE1	2.53	0.44
4:F:347:VAL:HG22	4:F:369:VAL:HG13	2.00	0.44
4:F:375:TYR:HD2	4:F:430:HIS:HE2	1.66	0.44
4:F:491:ARG:HH11	9:V:42:MET:HG2	1.82	0.44
6:J:21:ILE:HG12	8:L:555:SER:HA	1.99	0.44
9:U:19:ILE:CD1	9:U:21:PRO:HD3	2.48	0.44
1:A:562:TYR:CD2	6:J:43:LEU:CD1	2.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:PRO:HA	2:B:500:TYR:CZ	2.53	0.44
2:C:566:LEU:CD1	2:C:566:LEU:H	2.30	0.44
3:D:481:PRO:HD2	3:D:540:HIS:CE1	2.51	0.44
4:F:349:ALA:HB3	4:F:441:ILE:HG21	2.00	0.44
3:G:423:ARG:HA	3:G:442:SER:HG	1.83	0.44
5:H:567:VAL:CG2	7:K:567:VAL:HG12	2.48	0.44
6:J:14:CYS:HB2	6:J:40:ILE:H	1.83	0.44
9:S:28:GLU:HB3	9:S:29:LEU:H	1.58	0.44
1:A:425:THR:HB	1:A:438:LYS:HE3	2.00	0.44
1:A:488:TRP:HZ3	1:A:521:LEU:CB	2.30	0.44
3:E:430:HIS:H	3:E:433:LEU:CD2	2.30	0.44
3:G:510:GLN:OE1	3:G:510:GLN:HA	2.10	0.44
6:J:13:LYS:HE2	6:J:101:TYR:OH	2.17	0.44
7:K:354:PHE:HA	7:K:357:ILE:HG12	2.00	0.44
9:S:24:LYS:HA	9:S:120:LEU:CB	2.48	0.44
3:E:443:ARG:NE	3:E:445:LYS:HZ2	2.16	0.43
4:F:491:ARG:HD3	9:V:44:VAL:HG11	2.00	0.43
7:K:393:HIS:HA	7:K:410:GLU:HB2	2.00	0.43
7:K:467:ARG:HH11	7:K:467:ARG:CG	2.18	0.43
1:A:443:ARG:HD2	1:A:445:LYS:HZ2	1.82	0.43
1:A:499:LYS:HB3	1:A:521:LEU:HD11	2.00	0.43
1:A:544:PRO:HG3	6:J:134:TYR:HD1	1.83	0.43
1:A:562:TYR:HD2	6:J:43:LEU:HD11	1.76	0.43
1:A:568:MET:HA	6:J:62:TYR:HB2	1.99	0.43
3:D:368:LEU:HB2	3:D:408:VAL:HG12	2.00	0.43
3:D:450:HIS:HB2	3:D:480:SER:H	1.83	0.43
3:D:568:MET:HE1	3:E:568:MET:HE1	1.99	0.43
3:E:487:GLN:O	3:E:537:VAL:HG22	2.18	0.43
3:G:512:PRO:C	3:G:514:ARG:N	2.70	0.43
7:K:452:PRO:HB3	7:K:479:PHE:HB3	2.01	0.43
7:K:490:GLN:NE2	7:K:534:TYR:N	2.66	0.43
7:K:563:ASN:HB3	8:L:563:ASN:HB3	1.99	0.43
8:L:534:TYR:HB2	8:L:552:VAL:O	2.17	0.43
1:A:567:VAL:CG2	2:B:567:VAL:HG11	2.40	0.43
2:B:561:LEU:HD23	2:B:561:LEU:N	2.32	0.43
9:R:95:THR:O	9:R:95:THR:OG1	2.32	0.43
9:U:96:GLU:OE2	9:U:123:HIS:CD2	2.71	0.43
9:V:51:GLU:OE2	9:V:57:THR:O	2.36	0.43
1:A:489:MET:SD	1:A:489:MET:N	2.91	0.43
2:C:506:MET:HB2	2:C:516:PHE:CE1	2.54	0.43
4:F:461:ARG:HH12	4:F:465:ASN:CG	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:378:VAL:HG12	3:G:430:HIS:CD2	2.53	0.43
3:G:489:MET:HE3	3:G:489:MET:HA	2.00	0.43
7:K:467:ARG:HB3	7:K:467:ARG:CZ	2.48	0.43
9:U:22:GLU:CD	9:U:24:LYS:HG2	2.38	0.43
9:U:37:CYS:HA	9:U:116:GLN:NE2	2.33	0.43
2:C:365:LEU:HD23	2:C:365:LEU:H	1.84	0.43
3:G:351:PRO:HA	3:G:365:LEU:HD13	1.99	0.43
2:C:489:MET:O	2:C:535:THR:OG1	2.27	0.43
3:G:366:THR:HG23	3:G:408:VAL:HG13	2.01	0.43
3:G:497:PRO:HA	3:G:500:TYR:CZ	2.53	0.43
6:J:108:CYS:HB2	6:J:133:CYS:HB3	1.70	0.43
8:L:571:THR:C	8:L:573:GLY:H	2.22	0.43
6:J:13:LYS:HE2	6:J:101:TYR:CZ	2.54	0.43
7:K:566:LEU:C	7:K:566:LEU:CD2	2.85	0.43
8:L:451:ARG:HG3	8:L:452:PRO:HD2	2.00	0.43
9:U:24:LYS:H	9:U:24:LYS:HG3	1.53	0.43
7:K:469:SER:HA	7:K:523:VAL:O	2.19	0.43
2:B:564:VAL:O	2:C:564:VAL:HA	2.18	0.43
2:C:568:MET:HG2	5:H:562:TYR:CZ	2.53	0.43
4:F:553:ASP:O	4:F:556:THR:HG23	2.18	0.43
4:F:567:VAL:HG23	3:G:567:VAL:HG13	2.00	0.43
5:H:493:GLN:OE1	7:K:451:ARG:NH1	2.46	0.43
9:U:32:SER:HA	9:U:94:LEU:HD11	2.01	0.43
1:A:427:THR:HB	1:A:438:LYS:NZ	2.33	0.43
3:G:478:GLY:HA2	3:G:514:ARG:HD3	2.01	0.43
5:H:554:LYS:HZ1	5:H:558:LYS:NZ	2.15	0.43
9:U:50:ARG:HH11	9:U:52:MET:HE1	1.84	0.43
7:K:562:TYR:HB3	7:K:563:ASN:H	1.64	0.42
9:R:79:LYS:HB2	9:R:88:LEU:HB2	2.00	0.42
9:S:47:TYR:OH	9:S:110:THR:HA	2.19	0.42
2:C:367:CYS:HB2	2:C:382:TRP:CZ2	2.54	0.42
2:C:456:LEU:HD22	2:C:552:VAL:HB	2.00	0.42
3:G:400:HIS:HD1	3:G:404:THR:HG23	1.84	0.42
5:H:368:LEU:HB3	5:H:408:VAL:HG12	2.00	0.42
5:H:488:TRP:CG	5:H:521:LEU:HD12	2.54	0.42
6:J:5:ILE:HD12	6:J:5:ILE:HA	1.78	0.42
8:L:372:LEU:HD22	8:L:430:HIS:CD2	2.54	0.42
9:R:79:LYS:HA	9:R:79:LYS:HD3	1.82	0.42
3:D:493:GLN:OE1	3:D:493:GLN:N	2.52	0.42
7:K:391:LYS:NZ	7:K:410:GLU:HB3	2.34	0.42
7:K:421:GLY:O	7:K:423:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:566:LEU:HD23	8:L:566:LEU:HG	2.00	0.42
9:S:44:VAL:HG22	9:S:107:GLY:HA2	2.02	0.42
9:V:19:ILE:HD13	9:V:116:GLN:HB3	1.99	0.42
9:V:80:GLN:NE2	9:V:80:GLN:C	2.73	0.42
3:D:566:LEU:O	3:D:566:LEU:HD12	2.20	0.42
3:G:523:VAL:HG21	3:G:534:TYR:OH	2.19	0.42
5:H:451:ARG:HB2	5:H:543:LEU:HD23	2.01	0.42
6:J:103:TYR:N	8:L:574:THR:HA	2.21	0.42
7:K:460:ALA:HB3	7:K:463:GLN:OE1	2.19	0.42
7:K:501:VAL:HG11	8:L:516:PHE:HZ	1.84	0.42
9:R:108:MET:HG2	9:R:109:ASN:N	2.35	0.42
4:F:347:VAL:HG21	4:F:428:VAL:HG21	2.01	0.42
5:H:358:PHE:HZ	7:K:545:ASN:HB3	1.85	0.42
8:L:400:HIS:NE2	8:L:406:SER:HB2	2.34	0.42
9:U:94:LEU:CD2	9:U:122:VAL:HG12	2.49	0.42
1:A:544:PRO:CB	6:J:134:TYR:CD1	2.99	0.42
1:A:544:PRO:HG3	6:J:134:TYR:CD1	2.54	0.42
3:D:349:ALA:HB1	3:D:441:ILE:HD13	2.01	0.42
3:D:567:VAL:CG2	3:E:568:MET:N	2.82	0.42
4:F:379:THR:HB	4:F:429:THR:HG1	1.83	0.42
4:F:488:TRP:CZ2	4:F:521:LEU:HD12	2.55	0.42
9:R:94:LEU:HD23	9:R:95:THR:N	2.34	0.42
9:U:34:THR:O	9:U:88:LEU:CD1	2.67	0.42
3:E:380:ILE:HG21	3:E:409:GLY:HA3	2.02	0.42
4:F:455:TYR:C	4:F:456:LEU:HD12	2.40	0.42
3:G:479:PHE:HE2	3:G:482:ALA:HA	1.84	0.42
9:S:26:GLU:H	9:S:26:GLU:HG2	1.48	0.42
9:V:97:SER:HB2	9:V:98:ASP:H	1.69	0.42
3:E:423:ARG:HE	3:E:442:SER:HB2	1.85	0.42
8:L:491:ARG:NH1	8:L:533:THR:OG1	2.50	0.42
9:S:111:ASP:OD1	9:S:112:ARG:N	2.53	0.42
9:U:40:PRO:HB2	9:U:42:MET:HB3	2.01	0.42
3:D:364:LYS:HZ3	3:D:412:SER:HG	1.63	0.42
6:J:28:PRO:O	6:J:30:GLU:HG2	2.18	0.42
7:K:488:TRP:CZ3	7:K:536:CYS:HB2	2.55	0.42
9:S:48:LEU:HD11	9:S:102:TYR:HB3	2.02	0.42
9:V:57:THR:HB	9:V:58:CYS:H	1.54	0.42
9:V:80:GLN:CD	9:V:80:GLN:N	2.72	0.42
9:V:103:ALA:HA	9:V:116:GLN:O	2.20	0.42
3:E:375:TYR:HB3	3:E:430:HIS:NE2	2.34	0.42
3:E:511:ALA:HB3	3:E:514:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:531:GLY:C	4:F:553:ASP:CG	2.72	0.42
6:J:7:LEU:N	6:J:7:LEU:HD23	2.34	0.42
8:L:365:LEU:HB2	8:L:411:ALA:HB3	2.02	0.42
9:S:24:LYS:HA	9:S:120:LEU:HB3	2.02	0.42
9:S:31:GLY:O	9:S:94:LEU:HD12	2.10	0.42
9:V:25:VAL:HG12	9:V:120:LEU:HD11	2.02	0.42
1:A:489:MET:HG2	1:A:535:THR:HB	2.02	0.41
2:B:395:ASN:ND2	2:B:410:GLU:OE2	2.52	0.41
4:F:461:ARG:NH1	4:F:465:ASN:OD1	2.52	0.41
3:G:567:VAL:N	5:H:566:LEU:O	2.47	0.41
5:H:568:MET:HA	5:H:568:MET:HE2	2.02	0.41
9:S:24:LYS:CG	9:S:120:LEU:HA	2.45	0.41
9:S:99:SER:OG	9:S:120:LEU:CA	2.68	0.41
9:U:25:VAL:HG12	9:U:120:LEU:HD13	2.01	0.41
9:V:70:ALA:HA	9:V:73:LYS:HE3	2.02	0.41
1:A:345:ILE:HG13	1:A:372:LEU:HB3	2.02	0.41
1:A:375:TYR:HD2	1:A:430:HIS:HE1	1.68	0.41
1:A:459:PRO:HB3	1:A:471:THR:H	1.84	0.41
2:B:506:MET:HB2	2:B:516:PHE:CE1	2.55	0.41
3:D:567:VAL:HG22	3:E:568:MET:C	2.40	0.41
3:E:347:VAL:HA	3:E:369:VAL:HG12	2.02	0.41
3:E:466:LEU:HB3	3:E:468:GLU:OE1	2.20	0.41
3:E:508:GLU:OE2	3:E:509:PRO:HD2	2.21	0.41
3:E:515:TYR:N	3:E:515:TYR:CD2	2.86	0.41
6:J:6:VAL:CG1	6:J:18:THR:CB	2.99	0.41
6:J:8:VAL:HG23	6:J:68:CYS:CA	2.48	0.41
6:J:23:ARG:HD3	6:J:23:ARG:HA	1.72	0.41
6:J:29:ASN:O	6:J:31:ASP:N	2.52	0.41
9:U:19:ILE:HD13	9:U:19:ILE:O	2.19	0.41
9:V:52:MET:HG3	9:V:55:SER:H	1.84	0.41
9:V:69:LYS:HB3	9:V:72:TYR:HB2	2.03	0.41
1:A:452:PRO:HG3	1:A:540:HIS:HB3	2.01	0.41
2:B:568:MET:O	2:B:568:MET:SD	2.79	0.41
6:J:102:THR:HB	8:L:575:CYS:SG	2.60	0.41
9:R:47:TYR:CE1	9:R:110:THR:HG23	2.55	0.41
1:A:463:GLN:HE22	1:A:469:SER:C	2.21	0.41
4:F:347:VAL:HG11	4:F:428:VAL:HG11	2.01	0.41
4:F:520:ILE:O	4:F:520:ILE:HG13	2.21	0.41
5:H:483:ASP:O	5:H:540:HIS:HD2	2.03	0.41
5:H:490:GLN:HB2	5:H:495:LEU:HD21	2.02	0.41
9:U:111:ASP:CG	9:U:112:ARG:HH12	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:LYS:HE3	2:B:410:GLU:HB2	2.02	0.41
5:H:549:GLU:N	5:H:549:GLU:OE1	2.54	0.41
6:J:28:PRO:C	6:J:30:GLU:H	2.23	0.41
3:D:427:THR:HA	3:D:438:LYS:HZ2	1.86	0.41
5:H:366:THR:HA	5:H:409:GLY:O	2.21	0.41
6:J:116:VAL:HG23	6:J:117:TYR:H	1.85	0.41
8:L:347:VAL:HG13	8:L:369:VAL:HG22	2.02	0.41
8:L:398:GLU:HG2	8:L:399:SER:H	1.86	0.41
2:C:563:ASN:HB2	3:D:563:ASN:HB3	2.02	0.41
9:R:52:MET:N	9:R:57:THR:O	2.43	0.41
9:V:27:GLY:O	9:V:94:LEU:HD12	2.21	0.41
1:A:476:VAL:HG22	1:A:479:PHE:CD1	2.55	0.41
2:C:452:PRO:HD3	2:C:540:HIS:CD2	2.55	0.41
2:C:562:TYR:N	2:C:562:TYR:HD1	2.16	0.41
3:E:365:LEU:H	3:E:365:LEU:HD23	1.85	0.41
9:V:26:GLU:HG3	9:V:121:ASN:O	2.15	0.41
9:V:99:SER:CB	9:V:122:VAL:HG22	2.50	0.41
2:B:437:LEU:HD23	2:B:437:LEU:H	1.85	0.41
2:C:374:THR:HA	2:C:405:PHE:HD2	1.86	0.41
3:E:514:ARG:NH1	3:E:514:ARG:HG3	2.35	0.41
4:F:365:LEU:HD12	4:F:411:ALA:HB3	2.02	0.41
3:G:365:LEU:HB3	3:G:382:TRP:CZ2	2.56	0.41
5:H:564:VAL:HG12	5:H:565:SER:N	2.36	0.41
6:J:33:VAL:HB	8:L:559:PRO:HA	2.03	0.41
6:J:51:ASP:HA	6:J:52:PRO:HD2	1.94	0.41
7:K:476:VAL:HG23	7:K:479:PHE:HE1	1.85	0.41
7:K:491:ARG:HD2	7:K:491:ARG:O	2.20	0.41
7:K:563:ASN:CB	8:L:562:TYR:O	2.68	0.41
8:L:430:HIS:CG	8:L:431:THR:H	2.38	0.41
9:V:28:GLU:CD	9:V:28:GLU:N	2.73	0.41
1:A:453:ASP:HB3	1:A:455:TYR:CZ	2.56	0.41
3:D:568:MET:HE3	3:E:568:MET:HE3	2.02	0.41
3:E:467:ARG:HE	3:E:525:GLU:HG3	1.86	0.41
7:K:481:PRO:HD2	7:K:540:HIS:CE1	2.56	0.41
8:L:354:PHE:HE2	8:L:539:ALA:HB1	1.85	0.41
9:S:39:LEU:HD23	9:S:39:LEU:HA	1.83	0.41
9:V:32:SER:HA	9:V:91:VAL:O	2.21	0.41
3:G:510:GLN:HB3	3:G:511:ALA:H	1.46	0.40
6:J:41:VAL:HG12	6:J:43:LEU:H	1.85	0.40
9:R:36:LYS:O	9:R:116:GLN:NE2	2.46	0.40
9:R:46:ILE:HD12	9:R:105:GLY:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:24:LYS:CG	9:V:120:LEU:HA	2.50	0.40
9:V:33:VAL:HG12	9:V:91:VAL:HB	2.01	0.40
2:C:456:LEU:HD23	2:C:552:VAL:CB	2.51	0.40
2:C:488:TRP:CG	2:C:521:LEU:HD12	2.56	0.40
4:F:428:VAL:HG23	4:F:437:LEU:HB2	2.03	0.40
4:F:543:LEU:HD23	4:F:543:LEU:HA	1.97	0.40
3:G:527:GLU:OE1	3:G:527:GLU:N	2.53	0.40
5:H:413:ILE:HG21	5:H:424:PHE:CZ	2.55	0.40
9:R:41:GLU:OE2	9:R:82:PRO:HA	2.21	0.40
9:S:33:VAL:CG1	9:S:94:LEU:HD21	2.50	0.40
1:A:345:ILE:HD13	1:A:433:LEU:HD23	2.04	0.40
3:D:497:PRO:HA	3:D:500:TYR:CE2	2.56	0.40
3:E:455:TYR:HD2	4:F:463:GLN:NE2	2.19	0.40
5:H:561:LEU:O	5:H:561:LEU:CG	2.70	0.40
7:K:453:ASP:HB3	7:K:455:TYR:CE1	2.56	0.40
9:R:52:MET:HG3	9:R:55:SER:H	1.87	0.40
9:S:48:LEU:HD12	9:S:48:LEU:HA	1.82	0.40
2:B:567:VAL:HG12	2:B:567:VAL:O	2.20	0.40
3:D:472:ILE:HD11	3:D:528:TRP:CD1	2.56	0.40
4:F:449:LEU:HD23	4:F:449:LEU:HA	1.93	0.40
5:H:347:VAL:HG23	5:H:437:LEU:HD22	2.03	0.40
7:K:369:VAL:H	7:K:407:ALA:HB3	1.85	0.40
7:K:484:VAL:HG12	7:K:540:HIS:CD2	2.57	0.40
8:L:479:PHE:CZ	8:L:505:PRO:HB3	2.57	0.40
9:R:23:VAL:HG12	9:R:118:VAL:HB	2.04	0.40
9:V:39:LEU:CD1	9:V:81:TYR:N	2.78	0.40
1:A:461:ARG:HH22	2:B:556:THR:C	2.25	0.40
2:C:447:VAL:HG11	2:C:481:PRO:HG3	2.03	0.40
3:D:398:GLU:O	3:D:406:SER:OG	2.37	0.40
3:D:506:MET:HB2	3:D:516:PHE:CE1	2.56	0.40
3:D:566:LEU:O	3:D:566:LEU:HG	2.22	0.40
4:F:417:ASP:OD1	4:F:417:ASP:N	2.55	0.40
3:G:561:LEU:HB2	3:G:562:TYR:CE1	2.57	0.40
6:J:6:VAL:HG21	6:J:16:ARG:HG2	2.04	0.40
7:K:467:ARG:CA	7:K:525:GLU:HG3	2.52	0.40
9:S:100:GLY:O	9:S:119:THR:CB	2.69	0.40
9:V:96:GLU:CG	9:V:123:HIS:NE2	2.79	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	227/230 (99%)	212 (93%)	14 (6%)	1 (0%)	34	34
2	B	223/226 (99%)	207 (93%)	15 (7%)	1 (0%)	34	34
2	C	223/226 (99%)	206 (92%)	16 (7%)	1 (0%)	34	34
3	D	223/226 (99%)	208 (93%)	13 (6%)	2 (1%)	17	17
3	E	222/226 (98%)	196 (88%)	22 (10%)	4 (2%)	8	8
3	G	222/226 (98%)	203 (91%)	19 (9%)	0	100	100
4	F	217/222 (98%)	201 (93%)	16 (7%)	0	100	100
5	H	218/223 (98%)	201 (92%)	16 (7%)	1 (0%)	29	29
6	J	100/105 (95%)	75 (75%)	19 (19%)	6 (6%)	1	1
7	K	219/224 (98%)	200 (91%)	19 (9%)	0	100	100
8	L	223/228 (98%)	206 (92%)	16 (7%)	1 (0%)	34	34
9	R	105/107 (98%)	96 (91%)	7 (7%)	2 (2%)	8	8
9	S	105/107 (98%)	90 (86%)	11 (10%)	4 (4%)	3	3
9	U	105/107 (98%)	88 (84%)	17 (16%)	0	100	100
9	V	105/107 (98%)	89 (85%)	15 (14%)	1 (1%)	15	15
All	All	2737/2790 (98%)	2478 (90%)	235 (9%)	24 (1%)	21	17

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	564	VAL
9	S	116	GLN
2	B	563	ASN
3	E	564	VAL
6	J	6	VAL
6	J	23	ARG
9	R	99	SER
9	S	27	GLY

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Mol	Chain	Res	Type
9	S	97	SER
2	C	562	TYR
3	D	565	SER
6	J	29	ASN
6	J	43	LEU
8	L	571	THR
5	H	559	PRO
9	S	41	GLU
1	A	567	VAL
3	E	483	ASP
3	E	567	VAL
6	J	28	PRO
3	E	512	PRO
9	R	123	HIS
9	V	82	PRO
6	J	8	VAL

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	203/203 (100%)	196 (97%)	7 (3%)	37	37
2	B	201/201 (100%)	193 (96%)	8 (4%)	31	31
2	C	201/201 (100%)	195 (97%)	6 (3%)	41	41
3	D	201/200 (100%)	198 (98%)	3 (2%)	65	65
3	E	200/200 (100%)	192 (96%)	8 (4%)	31	31
3	G	200/200 (100%)	197 (98%)	3 (2%)	65	65
4	F	198/198 (100%)	195 (98%)	3 (2%)	65	65
5	H	199/199 (100%)	196 (98%)	3 (2%)	65	65
6	J	98/91 (108%)	87 (89%)	11 (11%)	6	6
7	K	200/200 (100%)	194 (97%)	6 (3%)	41	41
8	L	203/203 (100%)	201 (99%)	2 (1%)	76	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	R	92/92 (100%)	85 (92%)	7 (8%)	13	13
9	S	92/92 (100%)	77 (84%)	15 (16%)	2	2
9	U	92/92 (100%)	82 (89%)	10 (11%)	6	6
9	V	92/92 (100%)	74 (80%)	18 (20%)	1	1
All	All	2472/2464 (100%)	2362 (96%)	110 (4%)	32	28

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	ARG
1	A	561	LEU
1	A	562	TYR
1	A	564	VAL
1	A	566	LEU
1	A	568	MET
1	A	569	SER
2	B	489	MET
2	B	495	LEU
2	B	496	SER
2	B	561	LEU
2	B	564	VAL
2	B	566	LEU
2	B	567	VAL
2	B	568	MET
2	C	384	ARG
2	C	453	ASP
2	C	562	TYR
2	C	563	ASN
2	C	567	VAL
2	C	568	MET
3	D	566	LEU
3	D	567	VAL
3	D	568	MET
3	E	483	ASP
3	E	485	PHE
3	E	514	ARG
3	E	554	LYS
3	E	561	LEU
3	E	564	VAL
3	E	567	VAL
3	E	568	MET

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Mol	Chain	Res	Type
4	F	518	HIS
4	F	521	LEU
4	F	553	ASP
3	G	391	LYS
3	G	467	ARG
3	G	510	GLN
5	H	514	ARG
5	H	562	TYR
5	H	568	MET
6	J	5	ILE
6	J	12	CYS
6	J	13	LYS
6	J	16	ARG
6	J	17	ILE
6	J	23	ARG
6	J	30	GLU
6	J	53	THR
6	J	66	ASP
6	J	68	CYS
6	J	134	TYR
7	K	490	GLN
7	K	493	GLN
7	K	514	ARG
7	K	561	LEU
7	K	566	LEU
7	K	567	VAL
8	L	467	ARG
8	L	571	THR
9	R	95	THR
9	R	96	GLU
9	R	97	SER
9	R	108	MET
9	R	112	ARG
9	R	120	LEU
9	R	122	VAL
9	S	24	LYS
9	S	25	VAL
9	S	26	GLU
9	S	28	GLU
9	S	42	MET
9	S	43	HIS
9	S	45	ARG

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Mol	Chain	Res	Type
9	S	46	ILE
9	S	51	GLU
9	S	94	LEU
9	S	95	THR
9	S	98	ASP
9	S	99	SER
9	S	114	LYS
9	S	118	VAL
9	U	18	ARG
9	U	19	ILE
9	U	20	LEU
9	U	22	GLU
9	U	24	LYS
9	U	26	GLU
9	U	28	GLU
9	U	29	LEU
9	U	34	THR
9	U	122	VAL
9	V	19	ILE
9	V	20	LEU
9	V	25	VAL
9	V	26	GLU
9	V	28	GLU
9	V	57	THR
9	V	80	GLN
9	V	81	TYR
9	V	83	ARG
9	V	84	LYS
9	V	96	GLU
9	V	117	LYS
9	V	118	VAL
9	V	119	THR
9	V	121	ASN
9	V	122	VAL
9	V	123	HIS
9	V	124	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	490	GLN
3	D	400	HIS

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Mol	Chain	Res	Type
3	D	450	HIS
4	F	518	HIS
5	H	400	HIS
5	H	540	HIS
6	J	29	ASN
6	J	63	HIS
9	U	123	HIS
9	V	66	ASN
9	V	80	GLN
9	V	116	GLN
9	V	121	ASN
9	V	123	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	573:GLY	C	583:NAG	O6	25.97
1	L	575:CYS	C	583:NAG	O3	22.17
1	G	568:MET	C	583:NAG	O3	18.65
1	K	569:SER	C	583:NAG	O3	18.65
1	H	568:MET	C	583:NAG	O3	17.41
1	C	569:SER	C	583:NAG	O6	16.47
1	F	568:MET	C	583:NAG	O4	16.36
1	B	569:SER	C	583:NAG	O6	16.23
1	D	569:SER	C	583:NAG	O6	14.46
1	E	568:MET	C	583:NAG	O6	12.47
1	J	69:LYS	C	98:GLU	N	11.20
1	L	444:PRO	C	449:LEU	N	9.82
1	F	444:PRO	C	448:ALA	N	7.68
1	K	446:GLY	C	449:LEU	N	6.69
1	H	444:PRO	C	447:VAL	N	5.02

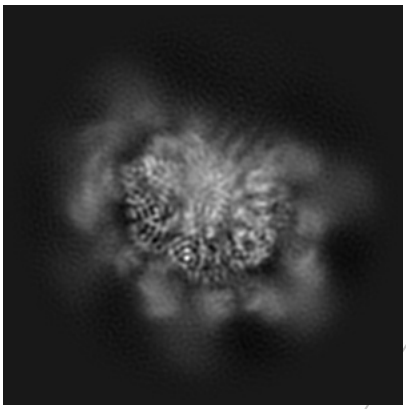
6 Map visualisation

This section contains visualisations of the EMDB entry D_1300031559. These allow visual inspection of the internal detail of the map and identification of artifacts.

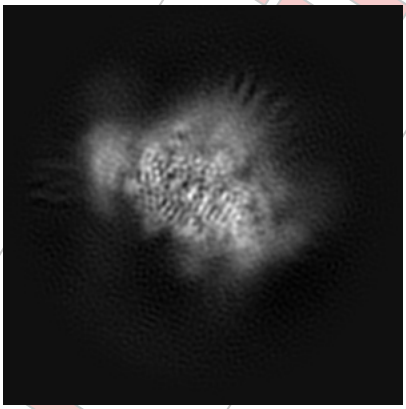
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

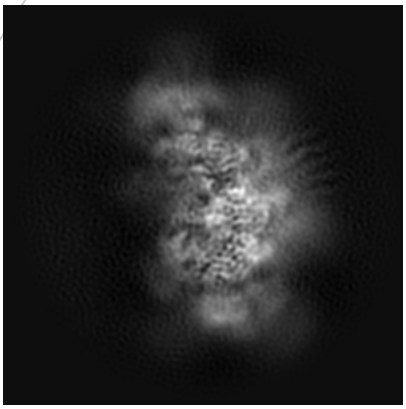
6.1.1 Primary map



X

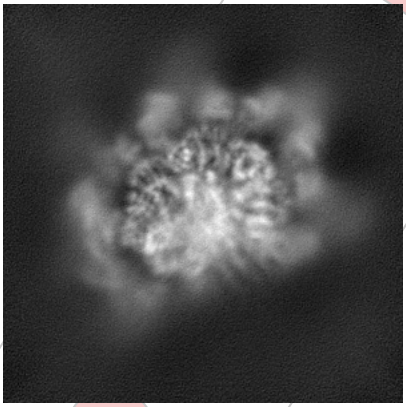


Y

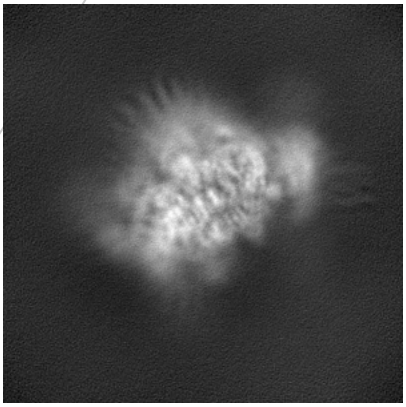


Z

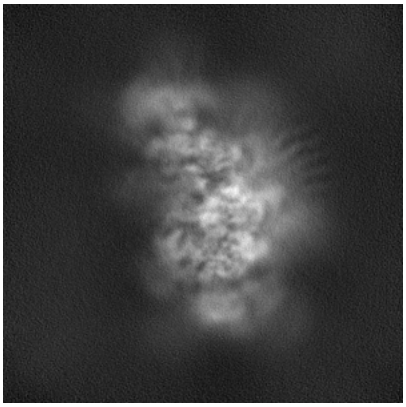
6.1.2 Raw map



X



Y

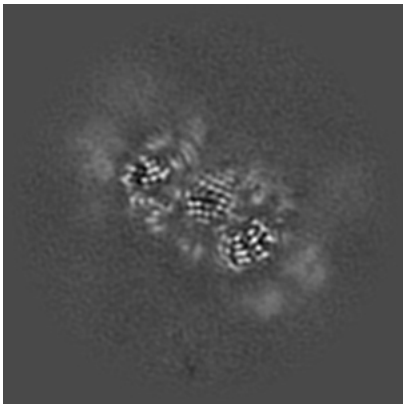


Z

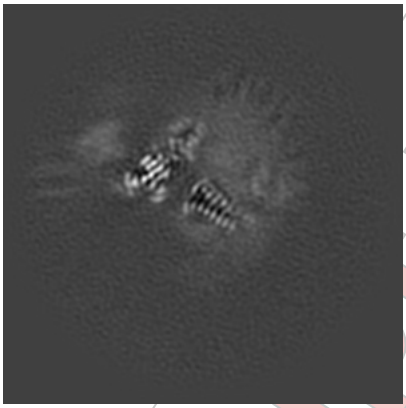
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

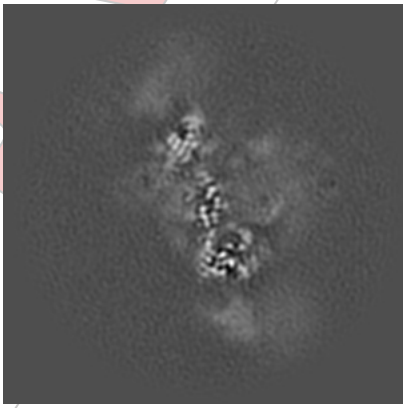
6.2.1 Primary map



X Index: 160

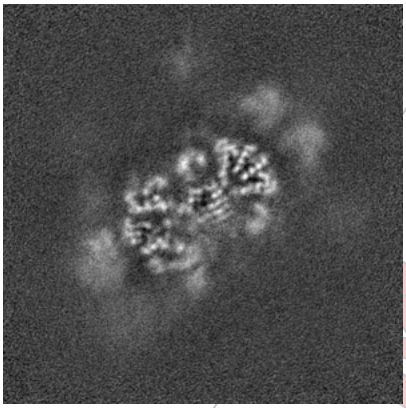


Y Index: 160

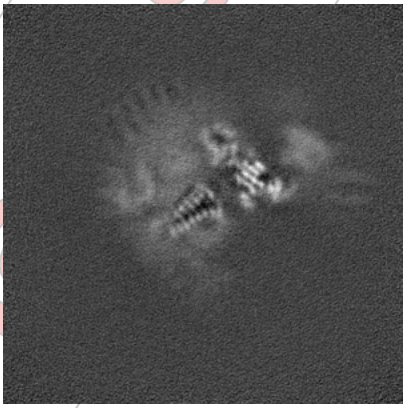


Z Index: 160

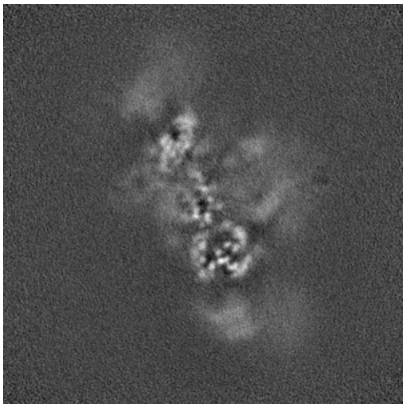
6.2.2 Raw map



X Index: 160



Y Index: 160

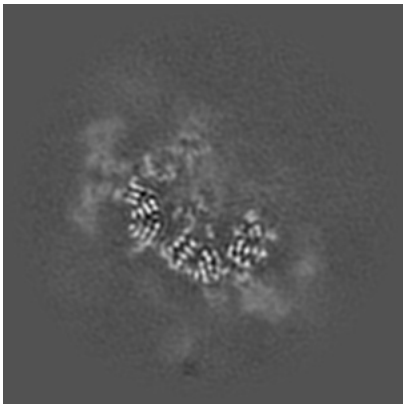


Z Index: 160

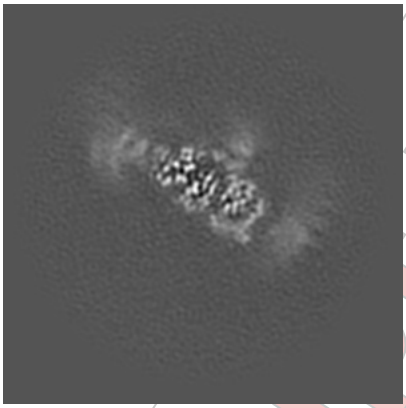
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

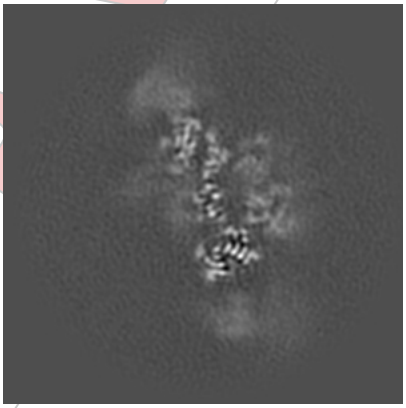
6.3.1 Primary map



X Index: 176

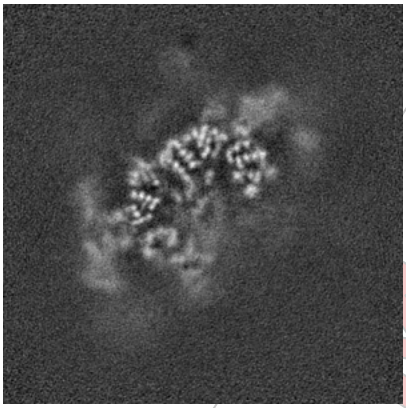


Y Index: 117

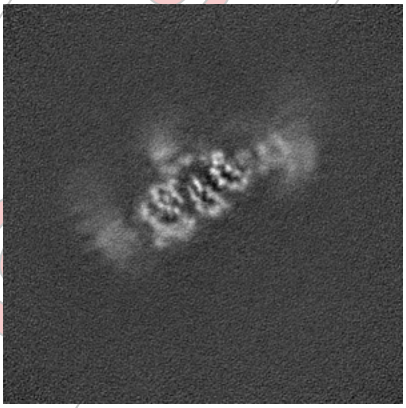


Z Index: 150

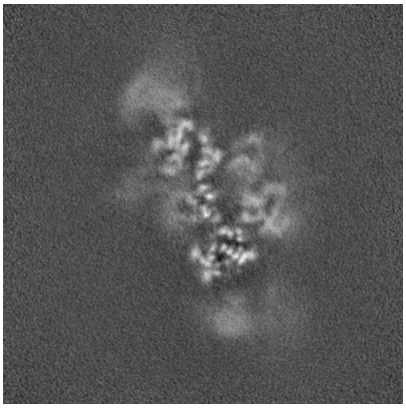
6.3.2 Raw map



X Index: 171



Y Index: 118



Z Index: 169

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

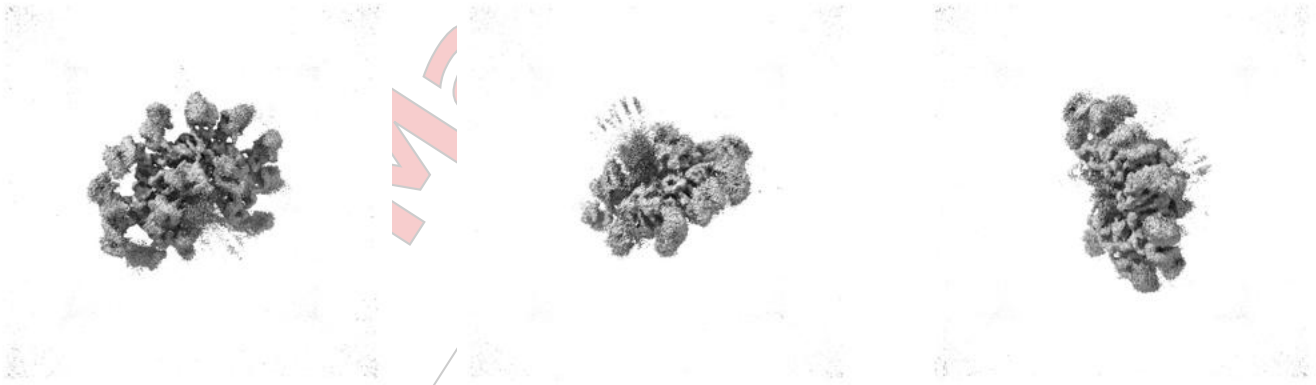
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

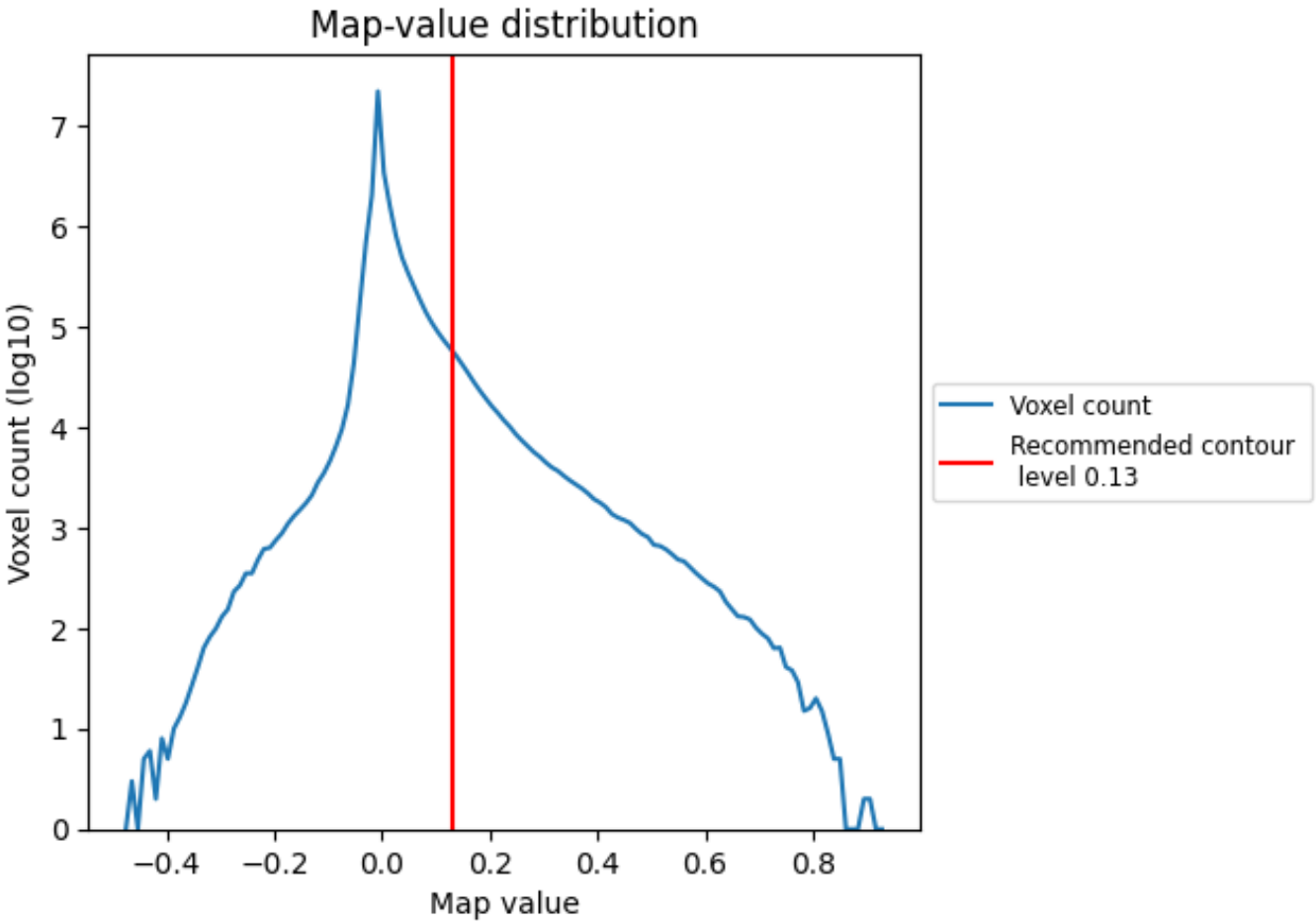
6.5 Mask visualisation (i)

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

7 Map analysis

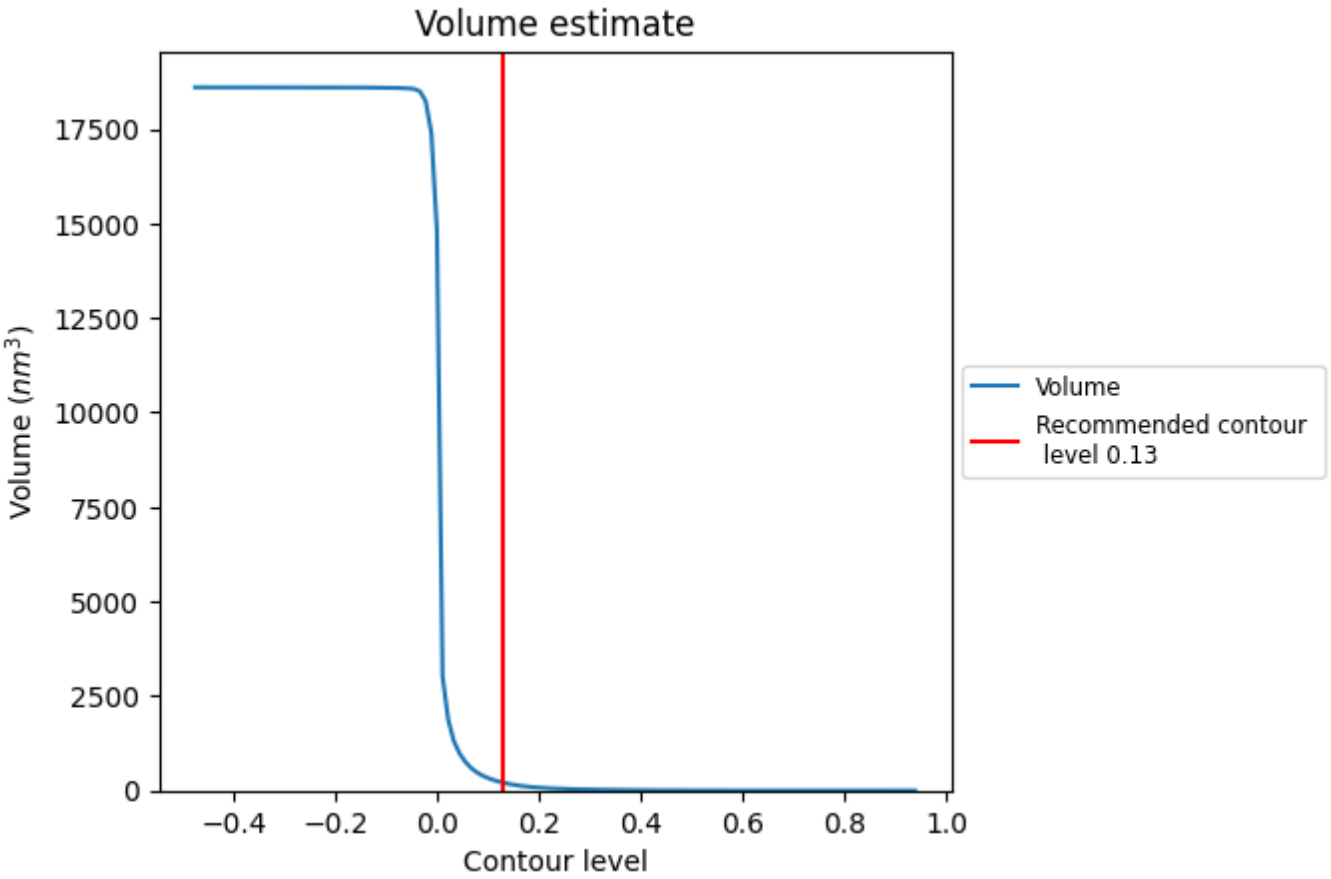
This section contains the results of statistical analysis of the map.

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.

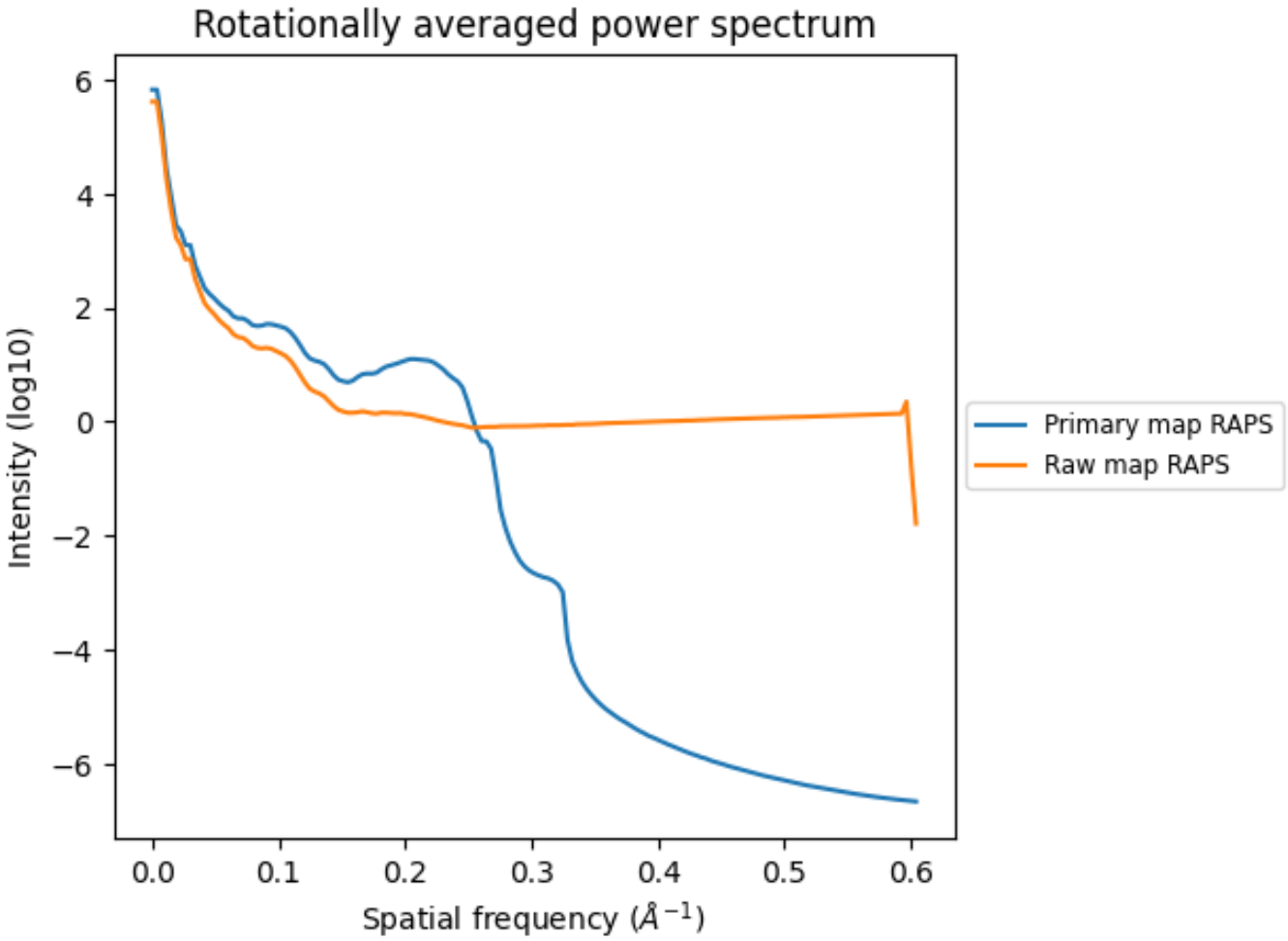
7.2 Volume estimate (i)



The volume at the recommended contour level is 209 nm^3; this corresponds to an approximate mass of 189 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.

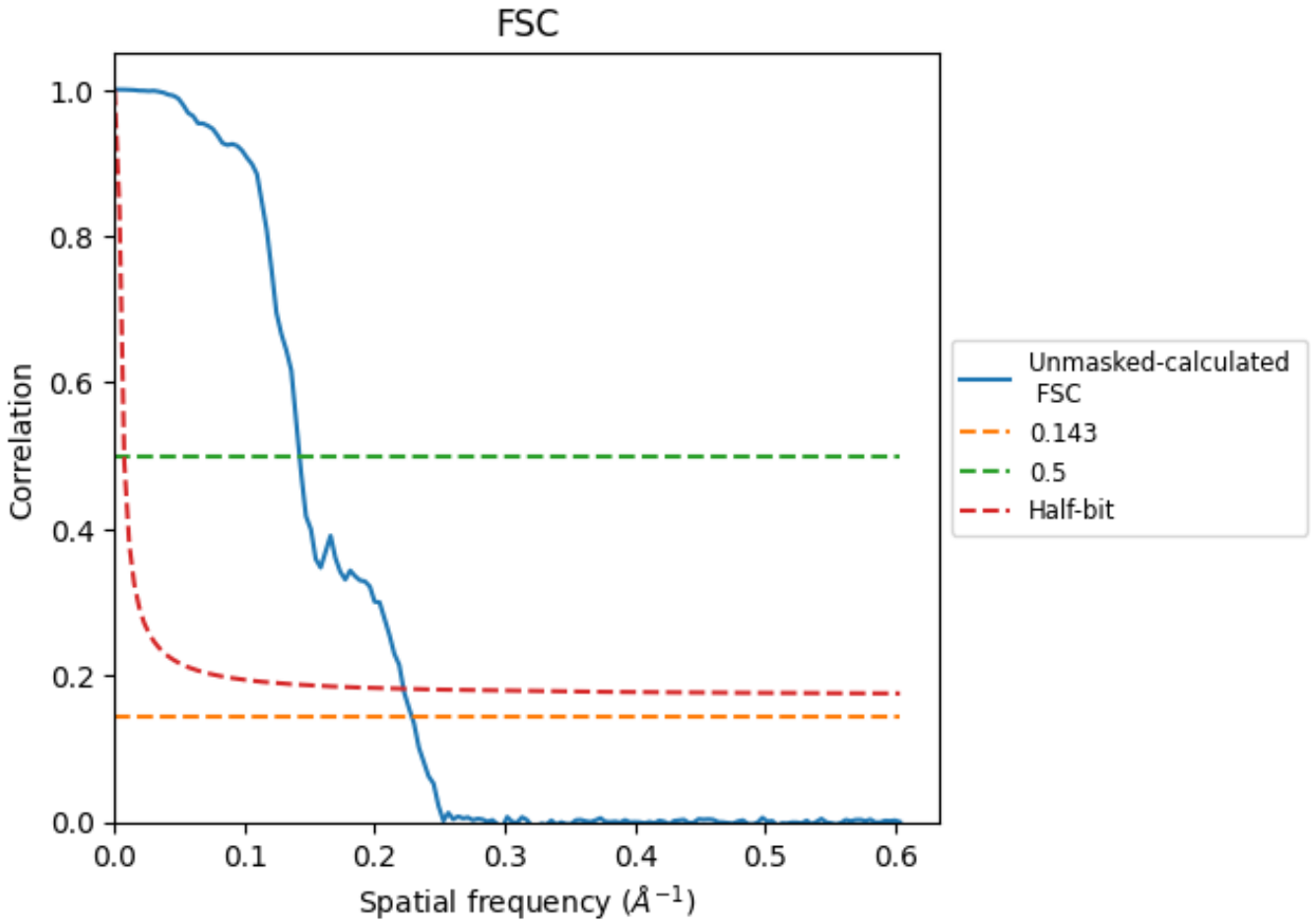
7.3 Rotationally averaged power spectrum (i)



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)

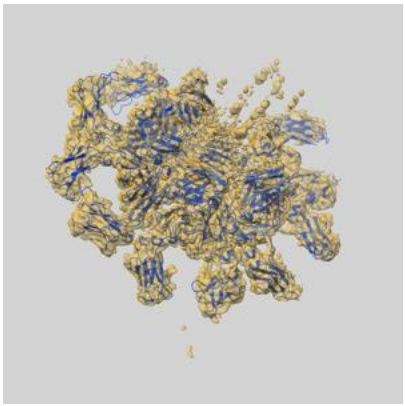
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.37	7.03	4.50

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

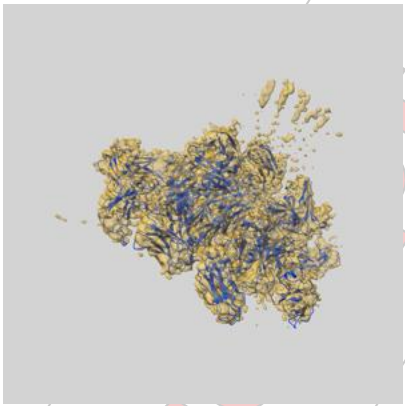
9 Map-model fit

This section contains information regarding the fit between EMDB map D_1300031559 and PDB model D_1300031559. Per-residue inclusion information can be found in section 3 on page 6.

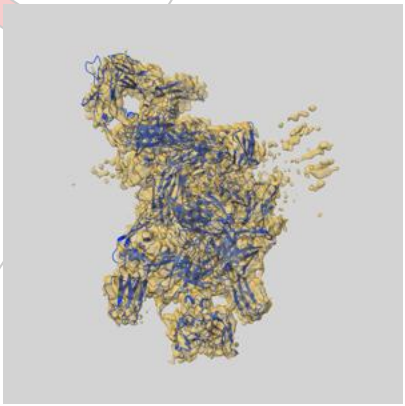
9.1 Map-model overlay



X



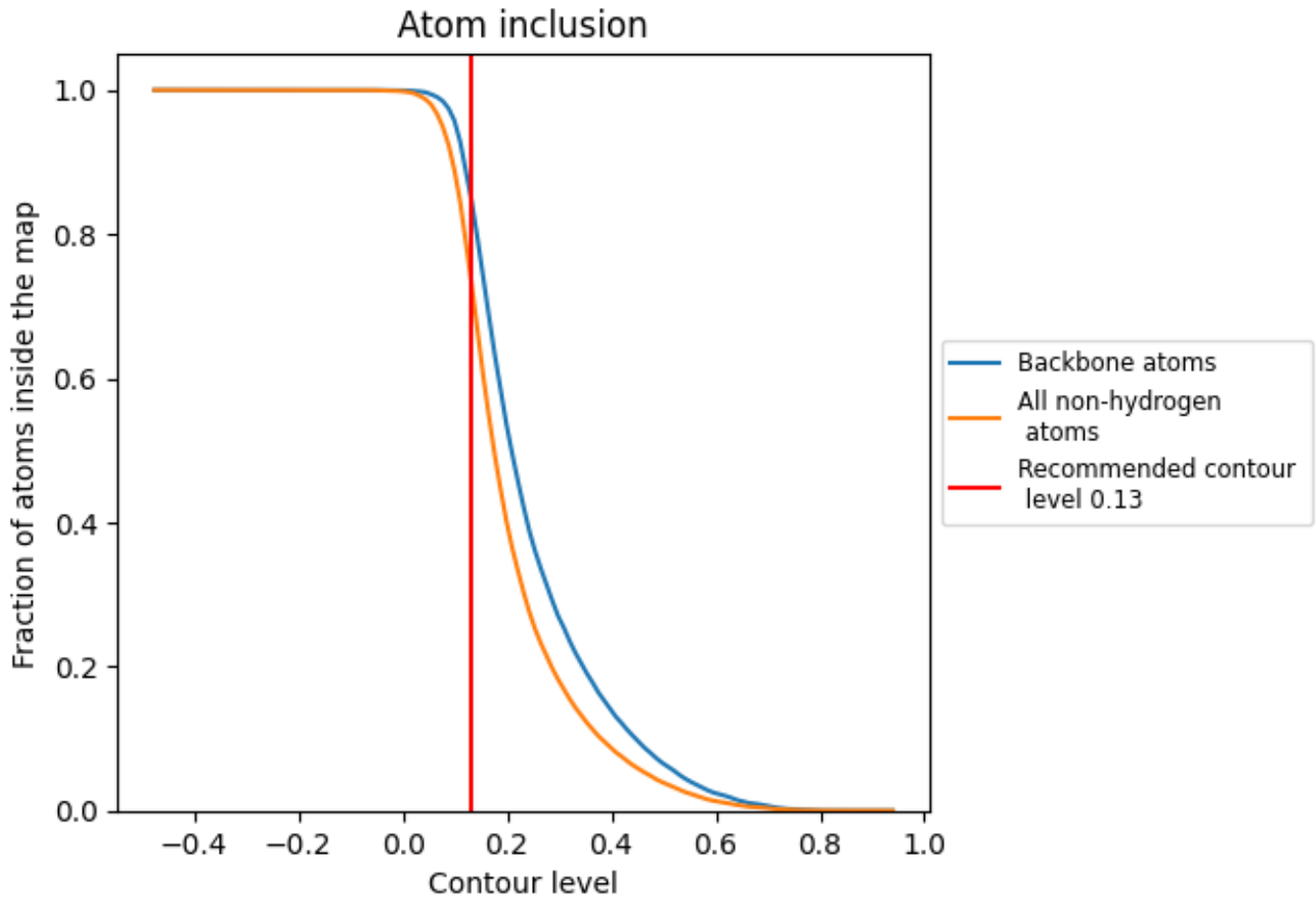
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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 (i)



At the recommended contour level, 86% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.