Preliminary Full wwPDB EM Validation Report ⓘ

Aug 12, 2022 – 05:40 PM JST

Deposition ID : D_1300031558

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:

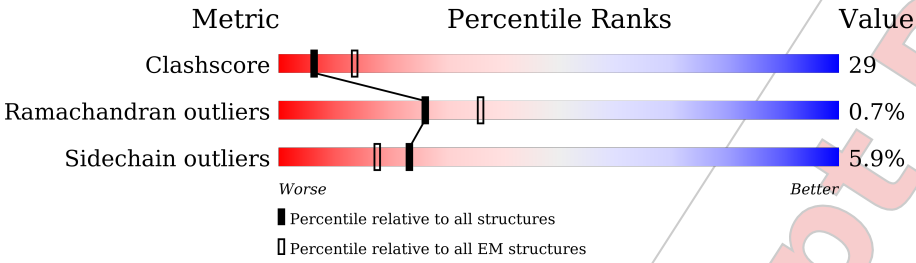
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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	231	23% 72% 27% .
2	B	229	21% 62% 31% 7%
3	C	226	22% 66% 32% .
3	K	226	26% 58% 37% .
4	D	225	19% 76% 23% .
4	E	225	18% 68% 28% .
4	F	225	20% 65% 32% .
4	G	225	20% 68% 27% 5%

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Mol	Chain	Length	Quality of chain
4	H	225	19% 72% 23%
5	L	229	39% 56% 37% 7%
6	J	104	5% 49% 43% 6%
7	R	107	13% 39% 45% 16%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19328 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	231	1794	1128	303	355	8	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	226	1762	1111	298	345	8	0	0
3	K	226	1763	1111	298	346	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	225	1757	1108	297	344	8	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	229	Total	C	N	O	S	0	0
			1787	1124	300	354	9		

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	104	Total	C	N	O	S	0	0
			839	521	147	164	7		

- Molecule 7 is a protein.

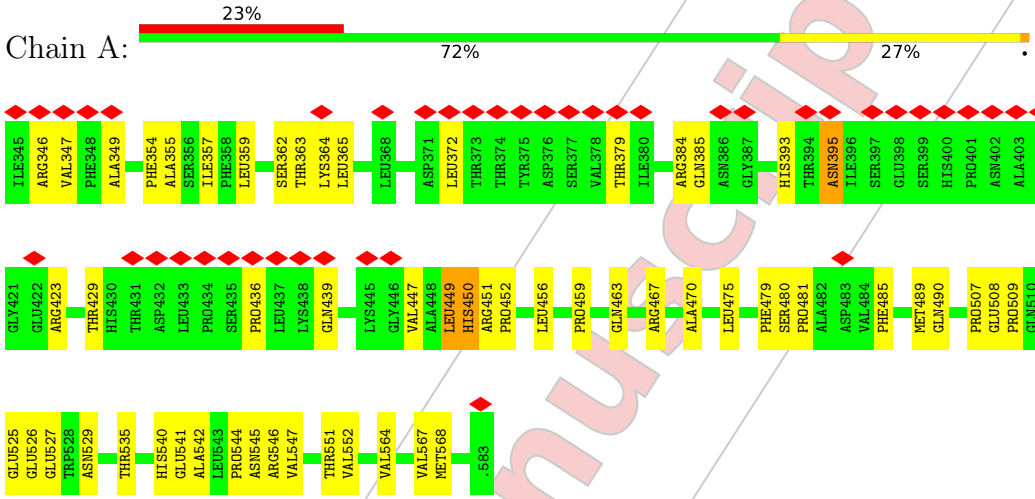
Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	107	Total	C	N	O	S	0	0
			816	510	144	155	7		

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.

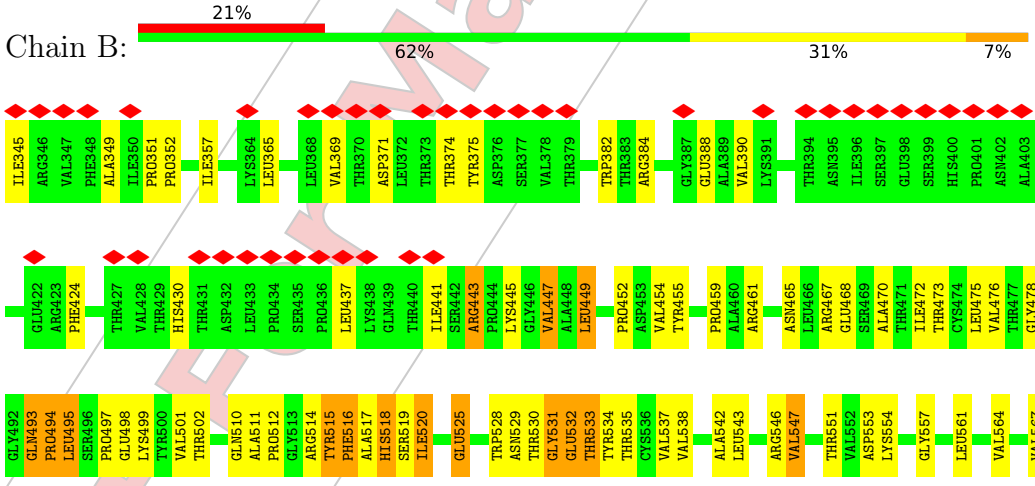
- Molecule 1:

Chain A:



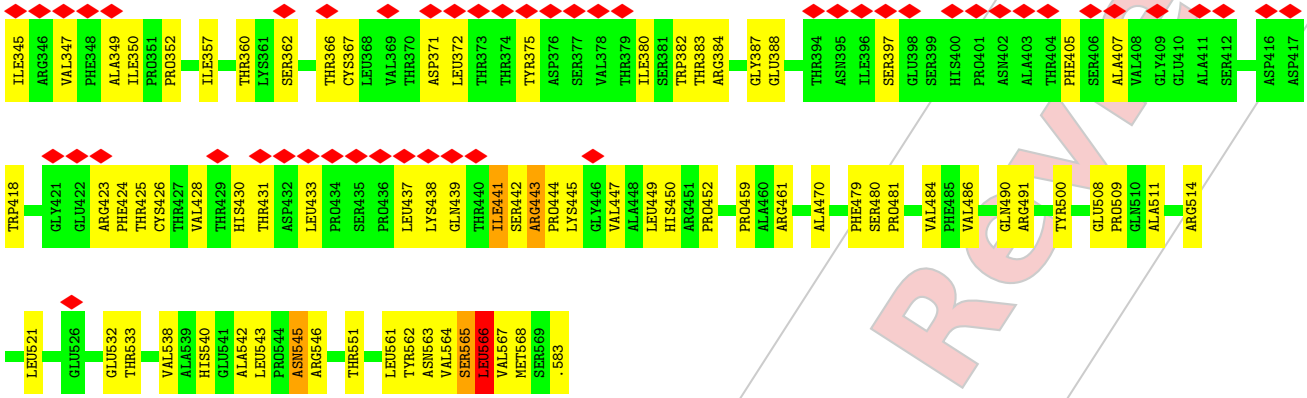
- Molecule 2:

Chain B:



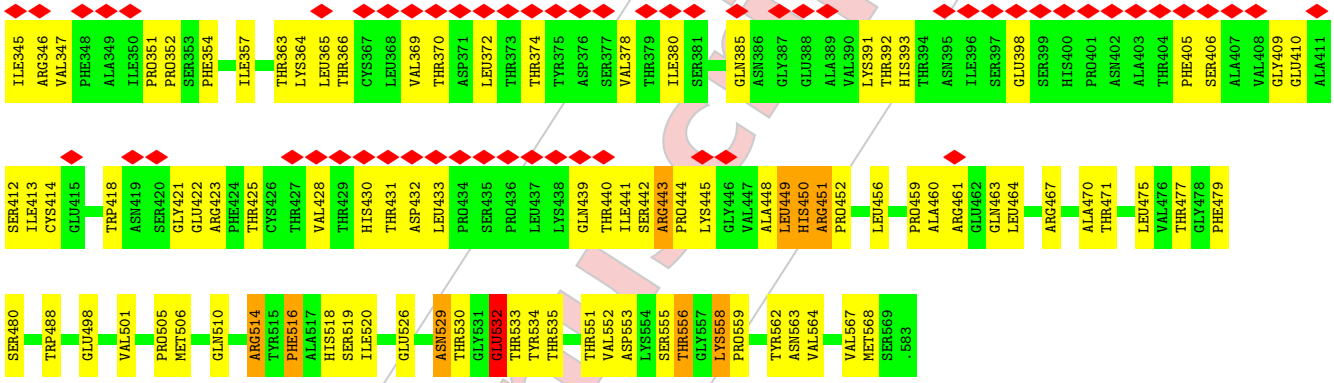
- Molecule 3:

Chain C:



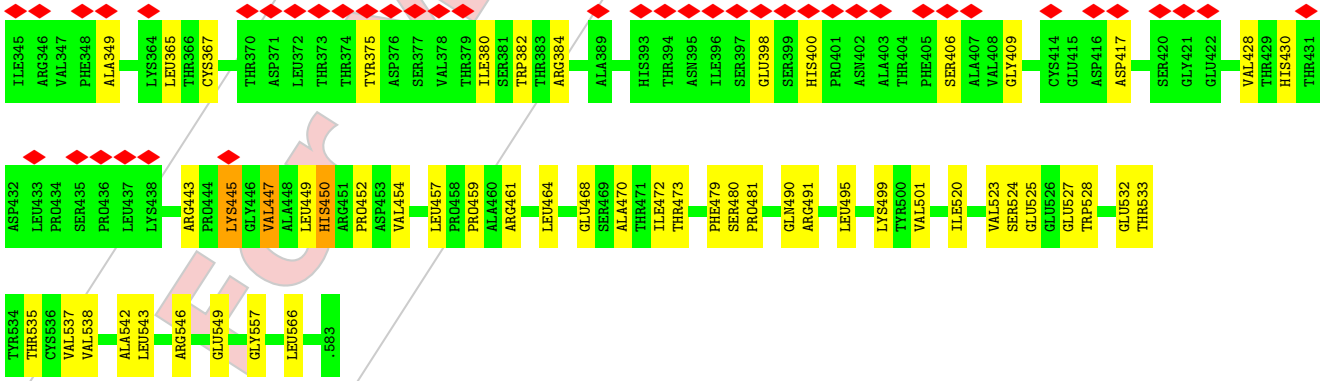
• Molecule 3:

Chain K:



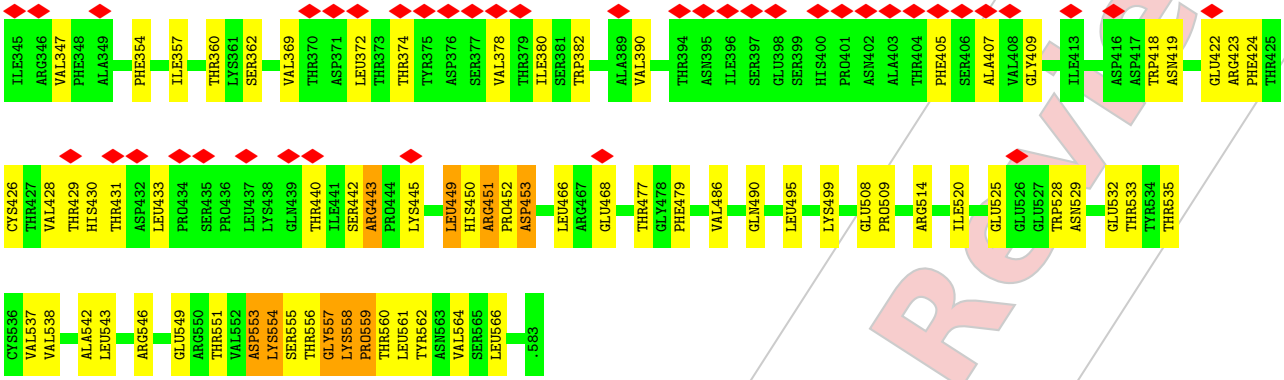
• Molecule 4:

Chain D:



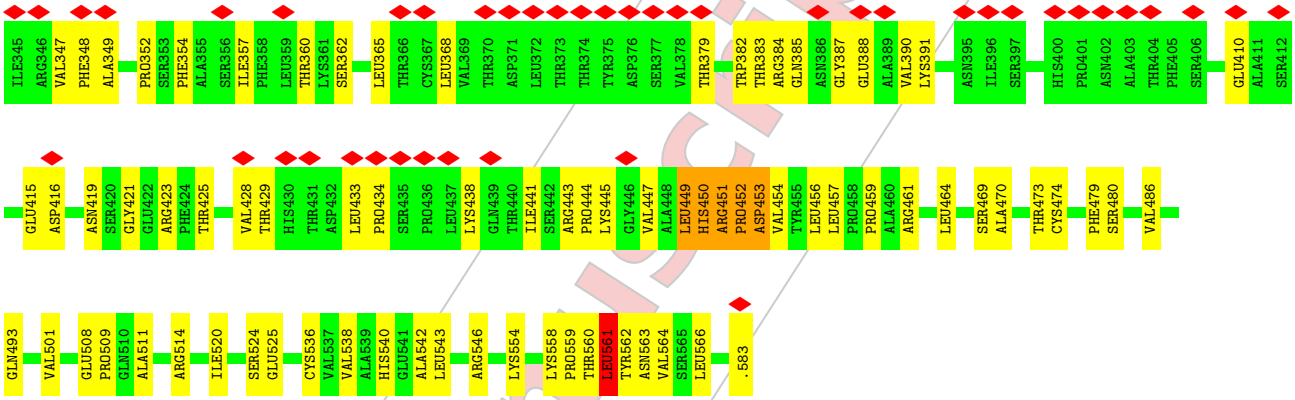
• Molecule 4:

Chain E:



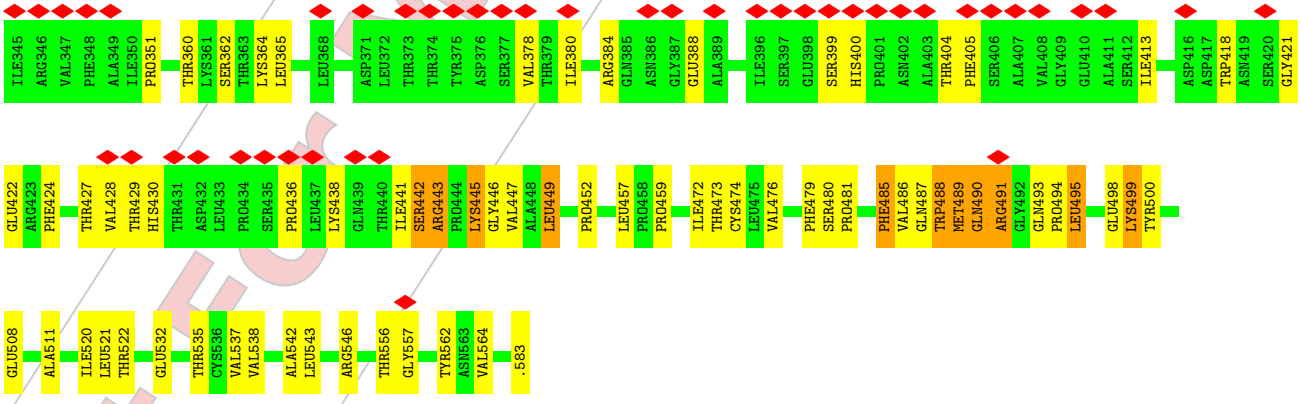
• Molecule 4:

Chain F:



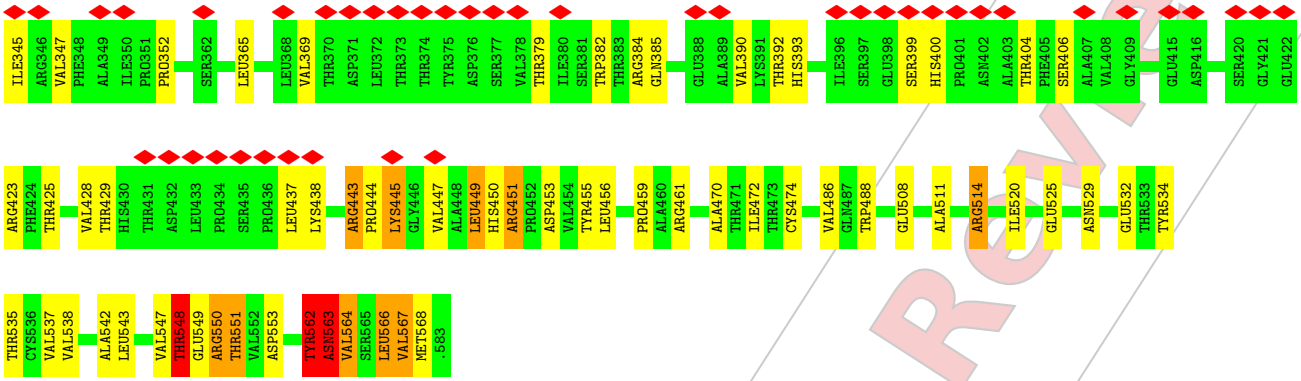
• Molecule 4:

Chain G:



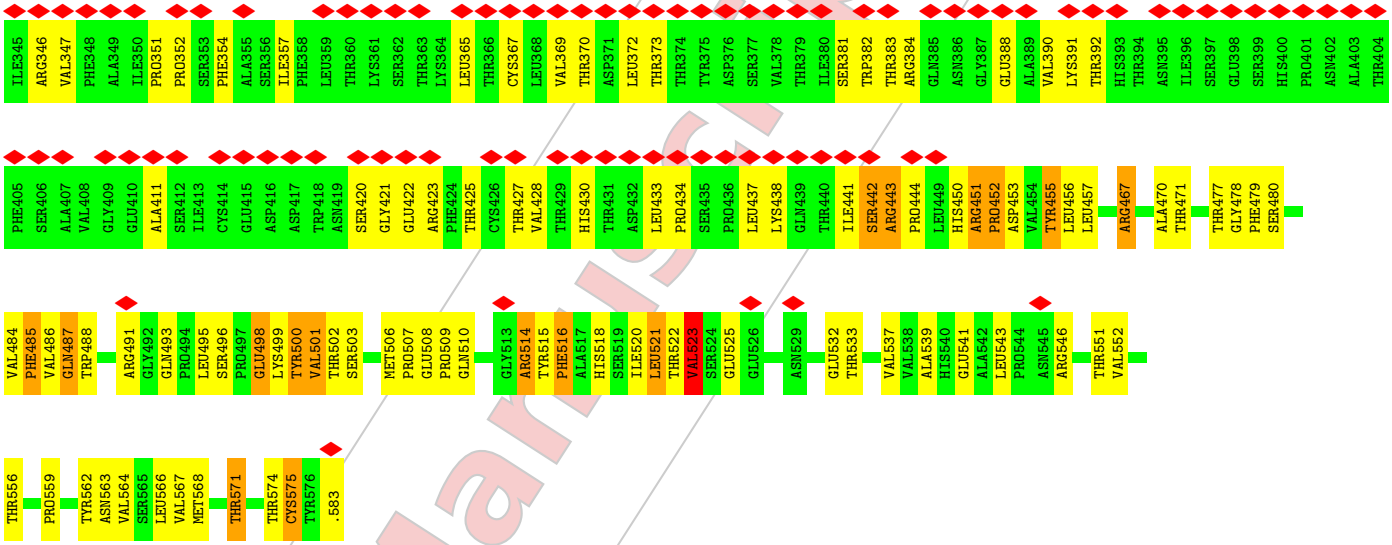
• Molecule 4:

Chain H:



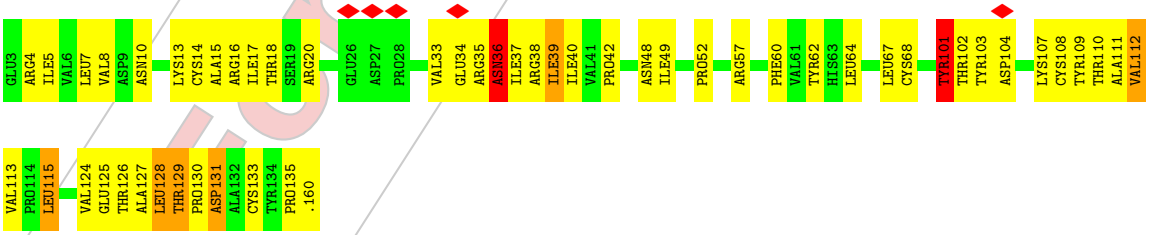
• Molecule 5:

Chain L:



• Molecule 6:

Chain J:



• Molecule 7:

Chain R:

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	2.272	Depositor
Minimum map value	-1.543	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.19	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	0.27	0/1825	0.52	0/2500
2	B	0.82	6/1814 (0.3%)	0.81	4/2485 (0.2%)
3	C	0.41	0/1793	0.59	1/2455 (0.0%)
3	K	0.54	1/1794 (0.1%)	0.67	1/2457 (0.0%)
4	D	0.35	0/1788	0.57	0/2449
4	E	0.40	0/1788	0.74	1/2449 (0.0%)
4	F	0.49	2/1788 (0.1%)	0.66	3/2449 (0.1%)
4	G	0.67	4/1787 (0.2%)	0.65	2/2447 (0.1%)
4	H	0.58	6/1788 (0.3%)	0.69	4/2449 (0.2%)
5	L	0.48	0/1818	0.74	1/2490 (0.0%)
6	J	0.80	2/838 (0.2%)	0.88	1/1139 (0.1%)
7	R	0.49	0/827	0.83	2/1115 (0.2%)
All	All	0.54	21/19648 (0.1%)	0.69	20/26884 (0.1%)

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	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	101	TYR	CE1-CZ	-8.97	1.26	1.38
2	B	534	TYR	CB-CG	-8.32	1.39	1.51
4	H	562	TYR	CG-CD2	-6.76	1.30	1.39
4	F	453	ASP	CB-CG	-6.70	1.37	1.51
4	G	488	TRP	CZ3-CH2	-6.68	1.29	1.40
4	G	488	TRP	CD2-CE2	-6.41	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	563	ASN	C-O	-6.22	1.11	1.23
2	B	534	TYR	CG-CD1	-6.09	1.31	1.39
2	B	520	ILE	C-O	-5.66	1.12	1.23
4	G	488	TRP	CE2-CZ2	-5.48	1.30	1.39
3	K	534	TYR	CB-CG	-5.46	1.43	1.51
4	G	488	TRP	CE3-CZ3	-5.40	1.29	1.38
2	B	534	TYR	CE1-CZ	-5.38	1.31	1.38
4	H	562	TYR	CB-CG	-5.35	1.43	1.51
4	H	563	ASN	CA-C	-5.22	1.39	1.52
4	H	562	TYR	CE1-CZ	-5.17	1.31	1.38
6	J	101	TYR	CG-CD1	-5.16	1.32	1.39
2	B	517	ALA	C-O	-5.16	1.13	1.23
4	H	548	THR	C-O	-5.13	1.13	1.23
2	B	515	TYR	CE1-CZ	-5.12	1.31	1.38
4	F	452	PRO	CA-C	-5.01	1.42	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	558	LYS	C-N-CD	-20.25	76.05	120.60
2	B	533	THR	N-CA-C	8.24	133.25	111.00
4	G	480	SER	C-N-CD	-7.83	103.37	120.60
4	F	453	ASP	CB-CG-OD1	-7.06	111.94	118.30
6	J	115	LEU	CB-CG-CD2	-7.03	99.04	111.00
4	F	561	LEU	N-CA-C	-6.94	92.25	111.00
2	B	531	GLY	N-CA-C	-6.40	97.10	113.10
2	B	520	ILE	CB-CA-C	-6.20	99.20	111.60
3	K	533	THR	N-CA-C	6.00	127.21	111.00
4	H	564	VAL	CG1-CB-CG2	-5.86	101.52	110.90
4	H	568	MET	CB-CG-SD	-5.56	95.71	112.40
7	R	104	CYS	CA-CB-SG	-5.55	104.01	114.00
3	C	566	LEU	CB-CG-CD1	-5.49	101.67	111.00
4	F	561	LEU	CA-CB-CG	-5.41	102.85	115.30
4	H	562	TYR	N-CA-C	5.36	125.48	111.00
4	H	549	GLU	CB-CA-C	-5.28	99.83	110.40
2	B	495	LEU	CA-CB-CG	-5.04	103.70	115.30
4	G	480	SER	C-N-CA	5.04	143.18	122.00
7	R	120	LEU	CA-CB-CG	-5.02	103.75	115.30
5	L	442	SER	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	562	TYR	Mainchain

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	1794	0	1752	59	0
2	B	1783	0	1739	91	0
3	C	1762	0	1718	86	0
3	K	1763	0	1725	125	0
4	D	1757	0	1720	47	0
4	E	1757	0	1717	118	0
4	F	1757	0	1720	85	0
4	G	1756	0	1718	78	0
4	H	1757	0	1719	84	0
5	L	1787	0	1732	188	0
6	J	839	0	833	102	0
7	R	816	0	835	136	0
All	All	19328	0	18928	1095	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 (1095) 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)
6:J:49:ILE:HG13	6:J:103:TYR:CE1	1.34	1.62
4:E:418:TRP:CD2	4:E:443:ARG:CD	1.81	1.61
4:E:418:TRP:CD2	4:E:443:ARG:HD2	1.09	1.60
4:E:418:TRP:CE2	4:E:443:ARG:HD2	1.18	1.59
4:E:418:TRP:CE2	4:E:443:ARG:CD	1.86	1.54
5:L:488:TRP:CD2	5:L:521:LEU:CD2	1.90	1.54
5:L:452:PRO:CG	5:L:479:PHE:CA	1.81	1.54
3:C:564:VAL:HG21	4:H:566:LEU:CD2	1.34	1.53
5:L:452:PRO:HG3	5:L:479:PHE:CA	1.09	1.53
4:E:418:TRP:CZ2	4:E:443:ARG:CG	1.87	1.52
3:C:563:ASN:ND2	3:C:583:NAG:C1	1.68	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:452:PRO:HG2	5:L:479:PHE:CB	1.38	1.50
4:E:529:ASN:HA	4:E:554:LYS:CE	1.13	1.47
2:B:419:ASN:CA	2:B:443:ARG:HH12	1.21	1.47
4:E:418:TRP:CH2	4:E:443:ARG:HG2	1.47	1.47
6:J:49:ILE:CG1	6:J:103:TYR:HE1	1.24	1.47
4:E:418:TRP:CZ2	4:E:443:ARG:HG2	0.94	1.45
4:E:529:ASN:CA	4:E:554:LYS:HE2	1.18	1.44
4:F:450:HIS:ND1	4:F:514:ARG:NE	1.66	1.43
7:R:96:GLU:HG2	7:R:122:VAL:CG2	1.48	1.42
3:C:564:VAL:CG2	4:H:566:LEU:HD21	1.50	1.42
7:R:35:ILE:O	7:R:88:LEU:CD1	1.68	1.41
4:E:529:ASN:C	4:E:554:LYS:HE2	1.37	1.40
3:K:516:PHE:CE2	5:L:520:ILE:HD11	1.55	1.39
7:R:35:ILE:O	7:R:88:LEU:CD2	1.68	1.37
4:F:450:HIS:ND1	4:F:514:ARG:CZ	1.87	1.36
3:C:418:TRP:CZ2	3:C:443:ARG:HB3	1.43	1.33
5:L:452:PRO:CG	5:L:479:PHE:CB	2.01	1.32
4:E:418:TRP:CG	4:E:443:ARG:HD2	1.64	1.32
3:K:516:PHE:CE2	5:L:520:ILE:CD1	2.12	1.32
4:E:418:TRP:CH2	4:E:443:ARG:CG	2.08	1.31
4:F:450:HIS:CE1	4:F:514:ARG:CD	2.14	1.31
5:L:452:PRO:HB3	5:L:478:GLY:C	1.50	1.31
3:C:423:ARG:HA	3:C:442:SER:OG	1.14	1.29
4:F:450:HIS:CE1	4:F:514:ARG:HD3	1.68	1.29
4:F:450:HIS:CE1	4:F:514:ARG:NE	1.99	1.29
6:J:49:ILE:CG1	6:J:103:TYR:CE1	2.03	1.28
5:L:443:ARG:HD3	5:L:444:PRO:CD	1.63	1.28
3:K:422:GLU:O	3:K:443:ARG:NH1	1.64	1.28
7:R:75:ARG:O	7:R:92:THR:HG22	1.34	1.25
4:E:418:TRP:CE2	4:E:443:ARG:HG2	1.69	1.25
4:E:423:ARG:HG3	4:E:442:SER:OG	1.36	1.25
5:L:452:PRO:CG	5:L:479:PHE:HA	1.54	1.25
3:K:516:PHE:HE2	5:L:520:ILE:CD1	1.49	1.23
3:K:526:GLU:C	3:K:529:ASN:OD1	1.77	1.22
5:L:488:TRP:CE3	5:L:521:LEU:HD23	1.75	1.21
3:C:418:TRP:CZ2	3:C:443:ARG:CB	2.15	1.21
5:L:488:TRP:CG	5:L:521:LEU:HD21	1.76	1.21
5:L:488:TRP:CE2	5:L:521:LEU:HD22	1.76	1.20
7:R:34:THR:OG1	7:R:88:LEU:HD12	1.35	1.20
4:E:418:TRP:CE2	4:E:443:ARG:CG	2.13	1.20
3:K:526:GLU:O	3:K:529:ASN:OD1	1.56	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:535:THR:HG22	2:B:551:THR:OG1	1.42	1.19
2:B:418:TRP:NE1	2:B:443:ARG:CG	2.01	1.18
4:F:450:HIS:CE1	4:F:514:ARG:CZ	2.25	1.18
4:G:490:GLN:OE1	4:G:532:GLU:HG3	1.42	1.17
3:C:418:TRP:CE2	3:C:443:ARG:HB3	1.79	1.17
5:L:452:PRO:CG	5:L:479:PHE:HB3	1.69	1.16
5:L:452:PRO:HB2	5:L:477:THR:O	1.44	1.16
5:L:488:TRP:O	5:L:495:LEU:HB2	1.41	1.16
2:B:490:GLN:O	2:B:493:GLN:OE1	1.63	1.15
4:E:423:ARG:CG	4:E:442:SER:OG	1.94	1.15
7:R:35:ILE:O	7:R:88:LEU:CG	1.94	1.14
7:R:35:ILE:O	7:R:88:LEU:HD22	1.41	1.14
7:R:96:GLU:CG	7:R:122:VAL:CG2	2.24	1.14
5:L:452:PRO:CG	5:L:479:PHE:N	2.09	1.14
5:L:452:PRO:HG3	5:L:479:PHE:N	1.63	1.14
3:C:449:LEU:HD23	3:C:481:PRO:HD3	1.29	1.13
6:J:39:ILE:HD13	6:J:62:TYR:CE1	1.83	1.13
7:R:35:ILE:O	7:R:88:LEU:HD13	1.41	1.13
3:K:526:GLU:CA	3:K:529:ASN:OD1	1.97	1.12
7:R:36:LYS:HB3	7:R:86:LEU:CD1	1.79	1.12
2:B:419:ASN:HA	2:B:443:ARG:NH1	1.39	1.11
4:E:529:ASN:CA	4:E:554:LYS:CE	1.79	1.11
5:L:488:TRP:CG	5:L:521:LEU:CD2	2.29	1.11
7:R:96:GLU:CG	7:R:122:VAL:HG21	1.80	1.11
4:D:450:HIS:CE1	4:D:480:SER:OG	2.04	1.11
6:J:39:ILE:CD1	6:J:62:TYR:CD1	2.32	1.11
2:B:418:TRP:NE1	2:B:443:ARG:HG2	1.54	1.11
3:C:423:ARG:CA	3:C:442:SER:OG	1.99	1.11
6:J:49:ILE:CD1	6:J:103:TYR:CE1	2.33	1.10
5:L:478:GLY:HA2	5:L:514:ARG:HG3	1.11	1.09
5:L:491:ARG:HB3	5:L:493:GLN:NE2	1.68	1.09
5:L:452:PRO:CB	5:L:478:GLY:C	2.19	1.09
6:J:39:ILE:HD11	6:J:62:TYR:CD1	1.88	1.09
3:K:535:THR:HG22	3:K:551:THR:HB	1.35	1.08
3:K:526:GLU:HA	3:K:529:ASN:OD1	1.52	1.08
5:L:491:ARG:CB	5:L:493:GLN:HE22	1.64	1.08
5:L:488:TRP:CD2	5:L:521:LEU:HD22	1.79	1.07
5:L:443:ARG:CD	5:L:444:PRO:HD3	1.84	1.07
4:G:421:GLY:HA2	4:G:443:ARG:HD2	1.10	1.07
4:E:418:TRP:NE1	4:E:443:ARG:HD2	1.70	1.07
5:L:491:ARG:HB3	5:L:493:GLN:HE22	0.91	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:34:THR:OG1	7:R:88:LEU:CD1	2.03	1.06
4:E:418:TRP:CD1	4:E:443:ARG:HD2	1.90	1.05
7:R:36:LYS:CB	7:R:86:LEU:HD11	1.85	1.05
4:H:443:ARG:HE	4:H:443:ARG:HA	1.20	1.04
4:H:535:THR:HG22	4:H:551:THR:OG1	1.58	1.04
4:H:543:LEU:HD13	4:H:548:THR:HG22	1.38	1.04
6:J:39:ILE:HD11	6:J:62:TYR:CG	1.92	1.03
2:B:418:TRP:HE1	2:B:443:ARG:CG	1.67	1.03
4:G:418:TRP:O	4:G:443:ARG:NE	1.92	1.02
7:R:26:GLU:HB3	7:R:124:SER:HA	1.39	1.02
5:L:443:ARG:CD	5:L:444:PRO:CD	2.36	1.02
4:E:529:ASN:HA	4:E:554:LYS:HE3	1.04	1.01
7:R:27:GLY:HA3	7:R:94:LEU:CD2	1.90	1.01
5:L:443:ARG:CG	5:L:444:PRO:HD2	1.91	1.01
3:C:349:ALA:HB1	3:C:441:ILE:HG21	1.40	1.00
4:E:418:TRP:CD2	4:E:443:ARG:HD3	1.96	1.00
5:L:488:TRP:CD2	5:L:521:LEU:HD21	1.86	1.00
7:R:26:GLU:HB3	7:R:124:SER:CA	1.92	1.00
4:E:418:TRP:CH2	4:E:443:ARG:HG3	1.94	0.99
4:D:449:LEU:HD21	4:D:481:PRO:HD3	1.43	0.99
3:K:535:THR:HG22	3:K:551:THR:CB	1.91	0.99
7:R:22:GLU:HA	7:R:118:VAL:HG23	1.41	0.99
7:R:96:GLU:HG2	7:R:122:VAL:HG23	1.45	0.99
3:K:516:PHE:CE2	5:L:520:ILE:HD13	1.95	0.98
3:K:463:GLN:CG	5:L:455:TYR:CE2	2.47	0.98
6:J:39:ILE:CD1	6:J:62:TYR:CG	2.45	0.98
2:B:418:TRP:CE2	2:B:443:ARG:HG2	1.99	0.98
3:K:422:GLU:O	3:K:443:ARG:CZ	2.11	0.97
5:L:508:GLU:HG2	5:L:509:PRO:HD2	1.45	0.97
7:R:27:GLY:HA3	7:R:94:LEU:HD22	1.44	0.96
5:L:488:TRP:CE3	5:L:521:LEU:CD2	2.40	0.95
4:G:421:GLY:CA	4:G:443:ARG:HD2	1.96	0.95
5:L:452:PRO:HB3	5:L:478:GLY:O	1.65	0.95
4:E:418:TRP:CE3	4:E:443:ARG:CD	2.49	0.94
4:E:529:ASN:C	4:E:554:LYS:CE	2.22	0.94
4:G:421:GLY:HA2	4:G:443:ARG:CD	1.96	0.94
5:L:488:TRP:CE2	5:L:521:LEU:CD2	2.42	0.94
1:A:449:LEU:HD13	1:A:542:ALA:HB2	1.50	0.94
2:B:418:TRP:HE1	2:B:443:ARG:HG3	1.32	0.94
3:K:514:ARG:HG3	3:K:514:ARG:HH11	1.30	0.94
4:D:450:HIS:ND1	4:D:480:SER:OG	1.96	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:488:TRP:CD2	5:L:521:LEU:HD23	1.82	0.93
1:A:450:HIS:ND1	1:A:480:SER:HB3	1.83	0.93
4:E:418:TRP:CZ3	4:E:443:ARG:HG3	2.04	0.92
5:L:478:GLY:CA	5:L:514:ARG:HG3	2.00	0.92
5:L:506:MET:O	5:L:515:TYR:HB3	1.69	0.91
7:R:45:ARG:HD3	7:R:107:GLY:O	1.70	0.91
5:L:508:GLU:CG	5:L:509:PRO:HD2	1.99	0.91
4:E:418:TRP:CZ3	4:E:443:ARG:CG	2.53	0.91
4:D:443:ARG:NH2	4:D:445:LYS:HD3	1.85	0.91
7:R:39:LEU:H	7:R:39:LEU:HD12	1.36	0.91
5:L:443:ARG:HD3	5:L:444:PRO:HD3	0.92	0.91
3:C:564:VAL:CG2	4:H:566:LEU:CD2	2.25	0.91
7:R:22:GLU:HA	7:R:118:VAL:CG2	2.01	0.90
7:R:96:GLU:HG2	7:R:122:VAL:HG22	1.52	0.90
4:D:449:LEU:CD2	4:D:481:PRO:HD3	2.01	0.90
3:C:418:TRP:CZ3	3:C:442:SER:HA	2.06	0.90
3:K:516:PHE:HZ	5:L:501:VAL:HG11	1.36	0.90
5:L:443:ARG:CB	5:L:444:PRO:HD2	2.00	0.90
7:R:96:GLU:CB	7:R:122:VAL:HG21	2.01	0.90
6:J:34:GLU:HG3	6:J:36:ASN:OD1	1.71	0.89
4:H:443:ARG:HA	4:H:443:ARG:NE	1.81	0.89
6:J:49:ILE:HD11	6:J:103:TYR:CE1	2.07	0.89
5:L:500:TYR:HB2	5:L:521:LEU:HD13	1.54	0.89
4:E:450:HIS:NE2	4:E:514:ARG:NH1	2.21	0.88
4:E:443:ARG:HB2	4:E:443:ARG:CZ	2.02	0.88
1:A:450:HIS:CE1	1:A:480:SER:HB3	2.10	0.87
4:F:452:PRO:HB3	4:F:479:PHE:HB3	1.57	0.87
4:H:449:LEU:HD12	4:H:542:ALA:HB2	1.56	0.87
2:B:419:ASN:HA	2:B:443:ARG:HH12	0.70	0.87
4:E:418:TRP:O	4:E:443:ARG:HD3	1.74	0.86
6:J:39:ILE:HD13	6:J:62:TYR:CD1	2.05	0.86
3:K:501:VAL:HG11	5:L:516:PHE:CZ	2.10	0.86
7:R:75:ARG:O	7:R:92:THR:CG2	2.22	0.86
4:H:543:LEU:HD13	4:H:548:THR:CG2	2.05	0.86
4:H:384:ARG:HD2	4:H:385:GLN:H	1.41	0.86
3:K:463:GLN:CB	5:L:455:TYR:CE2	2.52	0.86
6:J:49:ILE:CG1	6:J:103:TYR:CD1	2.58	0.86
3:C:418:TRP:HZ3	3:C:442:SER:HA	1.37	0.85
4:D:449:LEU:HD21	4:D:481:PRO:CD	2.05	0.85
4:E:423:ARG:CB	4:E:442:SER:OG	2.24	0.85
4:H:543:LEU:CD1	4:H:548:THR:HG22	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:449:LEU:CD2	3:C:481:PRO:HD3	2.06	0.85
4:H:562:TYR:HD1	3:K:562:TYR:HD2	1.25	0.85
2:B:475:LEU:HD13	2:B:518:HIS:CD2	2.12	0.84
2:B:518:HIS:O	2:B:518:HIS:ND1	2.11	0.84
7:R:37:CYS:O	7:R:87:PHE:N	2.09	0.84
3:K:488:TRP:HE1	3:K:519:SER:HG	1.24	0.84
7:R:35:ILE:HD12	7:R:35:ILE:H	1.42	0.83
3:K:422:GLU:O	3:K:443:ARG:NH2	2.10	0.83
3:C:423:ARG:HA	3:C:442:SER:CB	2.09	0.83
4:E:418:TRP:O	4:E:443:ARG:CZ	2.27	0.83
1:A:449:LEU:HD22	1:A:480:SER:O	1.78	0.83
3:K:463:GLN:HG3	5:L:455:TYR:CE2	2.13	0.83
3:K:516:PHE:CZ	5:L:520:ILE:HD11	2.14	0.83
3:K:563:ASN:HB3	5:L:563:ASN:HB3	1.60	0.83
5:L:443:ARG:CD	5:L:444:PRO:HD2	2.07	0.83
7:R:33:VAL:HG13	7:R:91:VAL:CG2	2.09	0.83
6:J:39:ILE:CD1	6:J:62:TYR:CE1	2.58	0.83
4:G:421:GLY:N	4:G:443:ARG:HE	1.77	0.82
4:G:418:TRP:O	4:G:443:ARG:CZ	2.26	0.82
4:D:449:LEU:CD2	4:D:481:PRO:CD	2.57	0.82
3:C:449:LEU:HD23	3:C:481:PRO:CD	2.08	0.82
3:C:418:TRP:CE2	3:C:443:ARG:CB	2.52	0.82
7:R:28:GLU:HA	7:R:28:GLU:OE1	1.79	0.82
7:R:33:VAL:O	7:R:91:VAL:HG22	1.80	0.82
3:C:349:ALA:CB	3:C:441:ILE:HG21	2.10	0.82
5:L:443:ARG:HG2	5:L:443:ARG:HH11	1.45	0.82
7:R:33:VAL:CG1	7:R:91:VAL:CG2	2.58	0.81
7:R:35:ILE:O	7:R:88:LEU:HD11	1.80	0.81
4:F:450:HIS:HE1	4:F:514:ARG:HD3	1.40	0.81
4:H:443:ARG:NE	4:H:444:PRO:HD2	1.96	0.81
7:R:36:LYS:HB3	7:R:86:LEU:HD11	0.90	0.81
5:L:421:GLY:HA2	5:L:443:ARG:NH1	1.97	0.80
6:J:49:ILE:O	6:J:103:TYR:OH	1.99	0.80
3:C:418:TRP:NE1	3:C:443:ARG:HD3	1.94	0.80
4:H:543:LEU:CD1	4:H:548:THR:CG2	2.59	0.80
4:E:418:TRP:CG	4:E:443:ARG:CD	2.40	0.80
2:B:454:VAL:HG21	2:B:538:VAL:HG11	1.65	0.79
7:R:111:ASP:OD1	7:R:111:ASP:N	2.15	0.79
3:K:450:HIS:CB	3:K:514:ARG:HH21	1.95	0.79
7:R:75:ARG:HA	7:R:92:THR:HG21	1.64	0.79
3:K:501:VAL:HG11	5:L:516:PHE:HZ	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:453:ASP:OD2	4:E:477:THR:CG2	2.31	0.79
7:R:27:GLY:CA	7:R:94:LEU:HD22	2.13	0.79
4:E:418:TRP:O	4:E:443:ARG:CD	2.31	0.79
4:H:456:LEU:HD13	4:H:550:ARG:HB3	1.66	0.78
5:L:452:PRO:CB	5:L:477:THR:O	2.30	0.78
5:L:456:LEU:HD22	5:L:552:VAL:HB	1.65	0.78
7:R:33:VAL:CG1	7:R:91:VAL:HG21	2.14	0.78
4:H:563:ASN:OD1	4:H:563:ASN:N	2.09	0.77
4:F:452:PRO:HG3	4:F:540:HIS:CB	2.14	0.77
3:C:418:TRP:HZ3	3:C:442:SER:CA	1.97	0.77
4:E:453:ASP:OD2	4:E:477:THR:HG23	1.84	0.77
3:K:520:ILE:HD12	5:L:516:PHE:CZ	2.20	0.77
4:E:450:HIS:O	4:E:542:ALA:HB3	1.85	0.76
4:F:450:HIS:ND1	4:F:514:ARG:NH2	2.33	0.76
4:E:443:ARG:HB2	4:E:443:ARG:NH1	2.01	0.76
5:L:452:PRO:HB3	5:L:478:GLY:CA	2.14	0.76
4:H:543:LEU:HD22	4:H:548:THR:CG2	2.16	0.76
7:R:75:ARG:C	7:R:92:THR:HG22	2.05	0.76
3:K:535:THR:CG2	3:K:551:THR:HB	2.15	0.76
5:L:452:PRO:HG2	5:L:479:PHE:HB3	0.76	0.76
4:F:384:ARG:HH21	4:F:388:GLU:HG3	1.50	0.75
7:R:41:GLU:OE1	7:R:82:PRO:HB3	1.86	0.75
2:B:475:LEU:HD13	2:B:518:HIS:HD2	1.52	0.75
3:C:352:PRO:HB2	3:C:357:ILE:HD11	1.68	0.75
5:L:443:ARG:HG2	5:L:443:ARG:NH1	2.00	0.75
5:L:452:PRO:CB	5:L:479:PHE:N	2.44	0.75
2:B:465:ASN:HD21	5:L:571:THR:CG2	2.00	0.75
4:E:450:HIS:NE2	4:E:514:ARG:CZ	2.49	0.75
2:B:495:LEU:HD12	2:B:495:LEU:H	1.52	0.75
4:F:450:HIS:CE1	4:F:514:ARG:NH1	2.53	0.75
7:R:26:GLU:HB3	7:R:124:SER:C	2.07	0.75
4:E:537:VAL:HG12	4:E:549:GLU:HG2	1.68	0.74
4:F:454:VAL:HG22	4:F:538:VAL:HG21	1.68	0.74
3:K:451:ARG:NH1	3:K:451:ARG:HB2	2.01	0.74
6:J:113:VAL:CG1	6:J:126:THR:HB	2.17	0.74
5:L:452:PRO:CG	5:L:478:GLY:C	2.51	0.74
3:C:566:LEU:HD12	3:C:566:LEU:O	1.87	0.74
4:H:425:THR:HG21	4:H:438:LYS:HG3	1.68	0.74
4:E:451:ARG:NH1	4:E:451:ARG:HB2	2.02	0.74
2:B:475:LEU:HA	2:B:518:HIS:HB3	1.68	0.74
4:E:423:ARG:HB2	4:E:442:SER:HG	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:418:TRP:O	4:E:443:ARG:NE	2.20	0.74
7:R:35:ILE:C	7:R:88:LEU:CD1	2.56	0.74
6:J:36:ASN:OD1	6:J:36:ASN:N	2.19	0.73
6:J:15:ALA:CB	6:J:67:LEU:HD21	2.19	0.73
4:E:423:ARG:HG2	4:E:440:THR:HG22	1.70	0.73
7:R:35:ILE:HD12	7:R:35:ILE:N	2.01	0.73
7:R:45:ARG:HG3	7:R:45:ARG:HH11	1.52	0.73
4:E:450:HIS:CD2	4:E:514:ARG:CZ	2.72	0.73
3:C:563:ASN:HD22	3:C:583:NAG:C1	1.98	0.73
4:H:562:TYR:CD1	3:K:562:TYR:HD2	2.07	0.73
2:B:502:THR:HA	2:B:519:SER:HB3	1.69	0.73
6:J:39:ILE:HD13	6:J:62:TYR:CZ	2.23	0.73
6:J:113:VAL:HG22	6:J:124:VAL:O	1.89	0.73
7:R:112:ARG:HG3	7:R:112:ARG:HH11	1.54	0.73
4:E:382:TRP:HB2	4:E:390:VAL:HG21	1.69	0.73
4:E:450:HIS:CD2	4:E:514:ARG:NH2	2.57	0.72
7:R:37:CYS:O	7:R:87:PHE:HB3	1.88	0.72
4:F:450:HIS:O	4:F:542:ALA:HB3	1.89	0.72
4:H:543:LEU:CD2	4:H:548:THR:CG2	2.68	0.72
4:F:449:LEU:O	4:F:449:LEU:HD12	1.89	0.72
4:E:450:HIS:O	4:E:542:ALA:CB	2.36	0.72
4:G:490:GLN:HE22	4:G:532:GLU:HA	1.55	0.72
3:K:450:HIS:CG	3:K:514:ARG:HE	2.08	0.72
2:B:502:THR:HA	2:B:519:SER:CB	2.20	0.71
3:C:418:TRP:O	3:C:443:ARG:CD	2.36	0.71
3:K:514:ARG:HG3	3:K:514:ARG:NH1	1.99	0.71
3:C:418:TRP:CE3	3:C:443:ARG:HG2	2.25	0.71
4:E:418:TRP:CD1	4:E:443:ARG:CD	2.68	0.71
4:G:499:LYS:HG2	4:G:521:LEU:HD11	1.73	0.71
3:K:463:GLN:HB2	5:L:455:TYR:CE2	1.92	0.71
3:K:501:VAL:CG1	5:L:516:PHE:HZ	2.04	0.71
5:L:488:TRP:NE1	5:L:521:LEU:HD22	2.06	0.71
4:F:451:ARG:NH1	4:F:451:ARG:HB2	2.06	0.70
3:C:418:TRP:CE2	3:C:443:ARG:CG	2.65	0.70
4:F:453:ASP:OD1	4:F:453:ASP:N	2.22	0.70
5:L:488:TRP:CB	5:L:521:LEU:HD21	2.21	0.70
5:L:488:TRP:CD1	5:L:521:LEU:HD22	2.25	0.70
7:R:33:VAL:HG21	7:R:120:LEU:HD23	1.72	0.70
6:J:52:PRO:HD3	6:J:128:LEU:CD1	2.22	0.70
5:L:452:PRO:HG3	5:L:478:GLY:C	2.10	0.70
4:G:487:GLN:O	4:G:537:VAL:HG22	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:422:GLU:C	3:K:443:ARG:NH1	2.44	0.70
7:R:105:GLY:HA2	7:R:115:THR:HG23	1.71	0.70
4:H:347:VAL:HG22	4:H:369:VAL:HG12	1.73	0.69
6:J:7:LEU:HD23	6:J:8:VAL:HG23	1.72	0.69
4:D:524:SER:OG	4:D:527:GLU:OE1	2.10	0.69
3:K:443:ARG:CD	3:K:443:ARG:H	2.04	0.69
3:K:463:GLN:CG	5:L:455:TYR:HE2	2.00	0.69
5:L:487:GLN:O	5:L:537:VAL:HG12	1.93	0.69
5:L:488:TRP:CG	5:L:521:LEU:HD22	2.14	0.69
2:B:473:THR:HG22	2:B:520:ILE:HG22	1.74	0.69
2:B:452:PRO:HB3	2:B:479:PHE:HB3	1.75	0.69
4:G:443:ARG:O	4:G:443:ARG:HG2	1.93	0.69
4:E:418:TRP:CE3	4:E:443:ARG:HD3	2.23	0.69
4:G:490:GLN:O	4:G:490:GLN:HG3	1.91	0.69
2:B:493:GLN:OE1	2:B:493:GLN:N	2.25	0.69
2:B:520:ILE:HG13	2:B:520:ILE:O	1.92	0.69
6:J:113:VAL:HG11	6:J:126:THR:HB	1.73	0.69
5:L:506:MET:O	5:L:515:TYR:CB	2.40	0.69
7:R:75:ARG:HB2	7:R:92:THR:HG23	1.75	0.69
3:C:486:VAL:HG22	3:C:538:VAL:HG22	1.75	0.68
4:H:384:ARG:HD2	4:H:385:GLN:N	2.07	0.68
6:J:49:ILE:HG13	6:J:103:TYR:HE1	0.53	0.68
7:R:84:LYS:O	7:R:84:LYS:HG2	1.93	0.68
5:L:583:NAG:H5	6:J:20:ARG:HH12	1.59	0.68
1:A:451:ARG:O	1:A:451:ARG:HG3	1.94	0.68
5:L:488:TRP:CZ3	5:L:521:LEU:HD23	2.28	0.68
6:J:39:ILE:HD12	6:J:62:TYR:CD2	2.29	0.68
7:R:22:GLU:CA	7:R:118:VAL:HG23	2.19	0.68
4:E:529:ASN:O	4:E:554:LYS:HE2	1.91	0.68
5:L:443:ARG:CB	5:L:444:PRO:CD	2.71	0.68
3:K:392:THR:HG22	3:K:393:HIS:H	1.59	0.68
5:L:452:PRO:HG3	5:L:479:PHE:HA	0.68	0.68
4:F:360:THR:HG23	4:F:362:SER:H	1.58	0.68
4:F:554:LYS:O	4:F:554:LYS:HG2	1.92	0.68
1:A:544:PRO:O	6:J:135:PRO:HG3	1.94	0.67
2:B:382:TRP:HB2	2:B:390:VAL:HG21	1.77	0.67
4:E:418:TRP:CE3	4:E:443:ARG:CG	2.77	0.67
7:R:33:VAL:HG13	7:R:91:VAL:HG22	1.76	0.67
4:H:543:LEU:HD22	4:H:548:THR:HG22	1.74	0.67
6:J:49:ILE:HD11	6:J:103:TYR:CD1	2.30	0.67
7:R:39:LEU:HD12	7:R:39:LEU:N	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:34:THR:HG1	7:R:88:LEU:HD12	1.55	0.67
5:L:433:LEU:HD12	5:L:434:PRO:HD2	1.77	0.67
5:L:453:ASP:N	5:L:453:ASP:OD1	2.16	0.67
3:K:516:PHE:CZ	5:L:501:VAL:HG11	2.25	0.67
7:R:28:GLU:O	7:R:94:LEU:HB2	1.95	0.67
2:B:475:LEU:HA	2:B:518:HIS:CB	2.25	0.66
6:J:39:ILE:CD1	6:J:62:TYR:CD2	2.77	0.66
3:C:345:ILE:N	3:C:371:ASP:O	2.28	0.66
3:K:451:ARG:HG3	3:K:451:ARG:HH11	1.60	0.66
6:J:42:PRO:HG3	6:J:102:THR:HG22	1.76	0.66
5:L:564:VAL:HG22	6:J:37:ILE:HD12	1.77	0.66
3:C:350:ILE:HB	3:C:366:THR:HB	1.76	0.66
4:H:400:HIS:CE1	4:H:406:SER:HB3	2.29	0.66
2:B:535:THR:CG2	2:B:551:THR:OG1	2.33	0.66
4:E:490:GLN:HE21	4:E:532:GLU:HG2	1.61	0.66
4:F:452:PRO:HG3	4:F:540:HIS:HB3	1.77	0.66
4:F:450:HIS:O	4:F:542:ALA:CB	2.44	0.66
3:K:516:PHE:CD2	5:L:520:ILE:HD13	2.31	0.66
4:G:418:TRP:CH2	4:G:442:SER:O	2.48	0.66
3:K:558:LYS:HD2	3:K:559:PRO:HD2	1.77	0.66
1:A:452:PRO:HB3	1:A:479:PHE:HB3	1.78	0.66
5:L:373:THR:OG1	5:L:430:HIS:NE2	2.28	0.66
4:G:459:PRO:HD3	4:G:472:ILE:HG13	1.77	0.65
4:H:443:ARG:NE	4:H:444:PRO:CD	2.59	0.65
4:H:562:TYR:HD1	3:K:562:TYR:CD2	2.12	0.65
4:D:384:ARG:NH2	4:D:417:ASP:OD2	2.28	0.65
3:K:451:ARG:HH11	3:K:451:ARG:CG	2.09	0.65
2:B:502:THR:HG23	2:B:519:SER:HB3	1.77	0.65
4:F:450:HIS:HE1	4:F:514:ARG:NH1	1.93	0.65
4:F:473:THR:HG22	4:F:520:ILE:HG22	1.77	0.65
6:J:113:VAL:HG13	6:J:126:THR:CG2	2.26	0.65
7:R:33:VAL:HG12	7:R:91:VAL:CG2	2.26	0.65
7:R:41:GLU:OE1	7:R:82:PRO:CB	2.45	0.65
4:E:449:LEU:HD12	4:E:542:ALA:HB2	1.78	0.65
3:C:380:ILE:HG22	3:C:428:VAL:HA	1.77	0.65
3:C:459:PRO:HG3	3:C:470:ALA:HB1	1.78	0.65
1:A:393:HIS:HB3	1:A:410:GLU:H	1.60	0.65
4:F:459:PRO:HG3	4:F:470:ALA:HB1	1.79	0.65
3:K:553:ASP:H	3:K:556:THR:HB	1.62	0.65
6:J:17:ILE:HD11	6:J:64:LEU:HD22	1.78	0.65
4:E:535:THR:HG22	4:E:551:THR:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:574:THR:HG22	6:J:103:TYR:HB2	1.79	0.65
5:L:452:PRO:CD	5:L:479:PHE:HA	2.27	0.64
4:G:418:TRP:CZ2	4:G:443:ARG:HA	2.32	0.64
7:R:75:ARG:CA	7:R:92:THR:CG2	2.75	0.64
6:J:52:PRO:HD3	6:J:128:LEU:HD11	1.79	0.64
4:H:443:ARG:CZ	4:H:444:PRO:CD	2.76	0.64
5:L:351:PRO:HA	5:L:365:LEU:HD13	1.79	0.64
3:K:516:PHE:HE2	5:L:520:ILE:HD13	1.36	0.64
4:G:489:MET:HG2	4:G:535:THR:OG1	1.98	0.64
1:A:346:ARG:NH1	1:A:347:VAL:O	2.31	0.63
3:C:566:LEU:HD11	4:D:566:LEU:HB3	1.80	0.63
3:C:375:TYR:H	3:C:405:PHE:HE2	1.47	0.63
4:E:556:THR:HG22	4:E:556:THR:O	1.98	0.63
4:G:445:LYS:HD2	4:G:446:GLY:H	1.63	0.63
7:R:61:VAL:HG12	7:R:69:LYS:HD3	1.80	0.63
3:K:346:ARG:O	3:K:370:THR:OG1	2.15	0.63
3:K:422:GLU:C	3:K:443:ARG:HH12	1.97	0.63
1:A:551:THR:HG21	6:J:52:PRO:HB2	1.81	0.63
4:G:421:GLY:CA	4:G:443:ARG:CD	2.67	0.63
4:E:380:ILE:HG21	4:E:409:GLY:HA3	1.81	0.63
5:L:506:MET:O	5:L:516:PHE:N	2.31	0.63
2:B:525:GLU:OE2	2:B:525:GLU:HA	1.99	0.62
7:R:91:VAL:HG23	7:R:91:VAL:O	1.99	0.62
4:F:558:LYS:HB3	4:F:559:PRO:HD2	1.81	0.62
7:R:41:GLU:CD	7:R:82:PRO:HB3	2.19	0.62
3:K:451:ARG:HB2	3:K:451:ARG:CZ	2.29	0.62
3:C:418:TRP:CZ3	3:C:442:SER:CA	2.66	0.62
7:R:35:ILE:C	7:R:88:LEU:HD11	2.19	0.62
3:C:449:LEU:CD2	3:C:481:PRO:CD	2.73	0.62
7:R:120:LEU:N	7:R:120:LEU:HD12	2.14	0.62
4:E:451:ARG:HH11	4:E:451:ARG:CG	2.13	0.62
3:K:423:ARG:HD2	3:K:440:THR:HA	1.81	0.62
3:K:450:HIS:CD2	3:K:514:ARG:HE	2.17	0.62
1:A:354:PHE:HA	1:A:357:ILE:HG22	1.82	0.62
7:R:48:LEU:HD11	7:R:102:TYR:HB3	1.82	0.62
7:R:39:LEU:HG	7:R:87:PHE:HB2	1.82	0.62
5:L:433:LEU:HD23	5:L:437:LEU:HD11	1.82	0.61
4:E:451:ARG:HH11	4:E:451:ARG:HG3	1.65	0.61
4:E:418:TRP:NE1	4:E:443:ARG:CD	2.42	0.61
2:B:495:LEU:HD12	2:B:495:LEU:N	2.15	0.61
4:H:451:ARG:NH1	4:H:451:ARG:HG3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:508:GLU:HG2	3:C:511:ALA:HB3	1.82	0.61
3:C:566:LEU:CD2	4:H:564:VAL:HG11	2.30	0.61
4:F:563:ASN:OD1	4:F:583:NAG:N2	2.33	0.61
3:K:365:LEU:HD21	3:K:418:TRP:HZ3	1.66	0.61
3:K:463:GLN:HG3	5:L:455:TYR:HE2	1.62	0.61
5:L:488:TRP:O	5:L:495:LEU:CB	2.33	0.61
7:R:21:PRO:O	7:R:118:VAL:HG23	2.00	0.61
7:R:28:GLU:OE1	7:R:96:GLU:HG3	2.01	0.61
3:C:567:VAL:HG12	3:C:567:VAL:O	1.99	0.61
6:J:34:GLU:CG	6:J:36:ASN:OD1	2.47	0.61
4:E:451:ARG:HB2	4:E:451:ARG:CZ	2.31	0.61
3:K:347:VAL:HG23	3:K:369:VAL:HA	1.83	0.61
3:K:442:SER:HA	3:K:443:ARG:HD2	1.82	0.61
3:K:450:HIS:HB3	3:K:514:ARG:HH21	1.66	0.61
1:A:357:ILE:HG13	1:A:363:THR:HB	1.83	0.60
3:C:347:VAL:O	3:C:439:GLN:NE2	2.33	0.60
4:F:347:VAL:HG21	4:F:428:VAL:HG21	1.82	0.60
5:L:351:PRO:HD3	5:L:441:ILE:HG12	1.83	0.60
5:L:451:ARG:CG	5:L:451:ARG:HH21	2.14	0.60
1:A:545:ASN:ND2	6:J:125:GLU:O	2.35	0.60
4:D:495:LEU:HD23	4:D:499:LYS:HD2	1.81	0.60
4:H:543:LEU:CD2	4:H:548:THR:HG22	2.31	0.60
3:K:556:THR:HG23	3:K:556:THR:O	2.00	0.60
2:B:475:LEU:HD12	2:B:518:HIS:HB3	1.83	0.60
5:L:575:CYS:H	6:J:102:THR:HB	1.66	0.60
6:J:38:ARG:HG2	6:J:38:ARG:O	2.02	0.60
7:R:37:CYS:N	7:R:87:PHE:O	2.33	0.60
1:A:541:GLU:O	1:A:546:ARG:NH1	2.34	0.60
2:B:459:PRO:HG3	2:B:470:ALA:HB1	1.83	0.60
2:B:475:LEU:CD1	2:B:518:HIS:CD2	2.85	0.60
2:B:490:GLN:H	2:B:495:LEU:HD11	1.67	0.60
4:G:499:LYS:HG2	4:G:521:LEU:CD1	2.31	0.60
5:L:369:VAL:HG21	5:L:428:VAL:HG11	1.84	0.60
7:R:21:PRO:O	7:R:118:VAL:CG2	2.49	0.60
4:E:418:TRP:O	4:E:443:ARG:NH1	2.33	0.60
4:F:447:VAL:HG13	4:F:447:VAL:O	2.02	0.60
4:F:454:VAL:CG2	4:F:538:VAL:HG21	2.32	0.60
4:G:421:GLY:N	4:G:443:ARG:NE	2.48	0.60
4:G:418:TRP:HH2	4:G:442:SER:O	1.84	0.59
2:B:547:VAL:HG21	3:C:545:ASN:OD1	2.01	0.59
4:E:557:GLY:HA3	4:F:461:ARG:HH12	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:525:GLU:OE2	4:H:529:ASN:ND2	2.35	0.59
3:C:568:MET:SD	3:K:564:VAL:HG21	2.41	0.59
4:E:354:PHE:HA	4:E:357:ILE:HG12	1.85	0.59
4:G:489:MET:HE2	4:G:494:PRO:HG3	1.84	0.59
6:J:128:LEU:N	6:J:128:LEU:HD23	2.17	0.59
7:R:93:GLN:HE22	7:R:95:THR:HG22	1.67	0.59
7:R:112:ARG:HG3	7:R:112:ARG:NH1	2.18	0.59
4:H:535:THR:CG2	4:H:551:THR:OG1	2.44	0.59
3:C:424:PHE:N	3:C:442:SER:OG	2.35	0.59
4:F:452:PRO:HG3	4:F:540:HIS:HB2	1.85	0.59
5:L:574:THR:HA	6:J:103:TYR:H	1.67	0.59
7:R:34:THR:C	7:R:88:LEU:HD11	2.22	0.59
2:B:375:TYR:HB2	2:B:430:HIS:HE1	1.67	0.59
2:B:461:ARG:NH2	2:B:557:GLY:O	2.35	0.59
5:L:451:ARG:HH21	5:L:451:ARG:HG2	1.65	0.59
5:L:533:THR:O	5:L:551:THR:OG1	2.21	0.58
7:R:19:ILE:HG22	7:R:21:PRO:HD3	1.85	0.58
7:R:71:GLU:O	7:R:75:ARG:NH1	2.36	0.58
2:B:467:ARG:HA	2:B:525:GLU:HG3	1.85	0.58
4:G:443:ARG:NH1	4:G:443:ARG:HG3	2.18	0.58
4:H:443:ARG:CZ	4:H:444:PRO:HD2	2.34	0.58
4:E:452:PRO:HB3	4:E:479:PHE:HB3	1.85	0.58
4:G:443:ARG:HG3	4:G:443:ARG:HH11	1.66	0.58
4:H:385:GLN:OE1	4:H:423:ARG:N	2.37	0.58
4:H:543:LEU:HD22	4:H:548:THR:HG21	1.85	0.58
5:L:452:PRO:CD	5:L:479:PHE:CB	2.77	0.58
7:R:112:ARG:HD2	7:R:112:ARG:O	2.04	0.58
5:L:443:ARG:HG3	5:L:444:PRO:HD2	1.84	0.58
5:L:503:SER:OG	5:L:518:HIS:N	2.34	0.58
2:B:490:GLN:O	2:B:490:GLN:HG2	2.02	0.58
3:K:450:HIS:CG	3:K:514:ARG:HH21	2.22	0.58
2:B:419:ASN:CA	2:B:443:ARG:NH1	2.06	0.58
4:D:447:VAL:O	4:D:447:VAL:HG22	2.03	0.58
4:E:423:ARG:CB	4:E:442:SER:HG	2.11	0.58
3:K:351:PRO:HB3	3:K:418:TRP:CH2	2.39	0.58
7:R:45:ARG:HG3	7:R:45:ARG:NH1	2.19	0.58
2:B:501:VAL:O	2:B:519:SER:HB2	2.04	0.58
4:E:555:SER:HB2	4:E:558:LYS:HG3	1.86	0.58
4:F:452:PRO:CB	4:F:479:PHE:HB3	2.30	0.58
4:H:443:ARG:CZ	4:H:444:PRO:HD3	2.34	0.58
4:H:547:VAL:O	4:H:547:VAL:HG12	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:351:PRO:HB3	3:K:418:TRP:HH2	1.69	0.58
1:A:449:LEU:HD21	1:A:481:PRO:HD3	1.84	0.58
1:A:525:GLU:OE2	1:A:529:ASN:ND2	2.37	0.58
4:G:429:THR:HG22	4:G:436:PRO:HB3	1.86	0.58
7:R:36:LYS:CB	7:R:86:LEU:CD1	2.64	0.58
4:D:473:THR:HG22	4:D:520:ILE:HG22	1.86	0.57
5:L:421:GLY:HA2	5:L:443:ARG:HH12	1.68	0.57
4:E:495:LEU:HD23	4:E:499:LYS:HD3	1.86	0.57
2:B:493:GLN:O	2:B:493:GLN:HG2	2.04	0.57
4:E:423:ARG:HB2	4:E:442:SER:OG	1.99	0.57
5:L:485:PHE:HB3	5:L:539:ALA:HB3	1.86	0.57
4:G:486:VAL:HG22	4:G:538:VAL:HG22	1.87	0.57
6:J:101:TYR:N	6:J:101:TYR:CD1	2.73	0.57
3:C:424:PHE:H	3:C:442:SER:HG	1.51	0.57
4:E:369:VAL:HG11	4:E:428:VAL:HG11	1.86	0.57
3:K:363:THR:OG1	3:K:413:ILE:O	2.22	0.57
7:R:75:ARG:HA	7:R:92:THR:CG2	2.34	0.57
4:F:451:ARG:CB	4:F:451:ARG:CZ	2.83	0.57
4:H:543:LEU:CD1	4:H:548:THR:HG23	2.33	0.57
7:R:75:ARG:HB2	7:R:92:THR:CG2	2.34	0.57
6:J:113:VAL:HG23	6:J:113:VAL:O	2.05	0.57
7:R:50:ARG:NH1	7:R:72:TYR:OH	2.36	0.57
6:J:113:VAL:HG13	6:J:126:THR:HB	1.86	0.57
2:B:512:PRO:O	2:B:514:ARG:N	2.38	0.56
4:D:447:VAL:HG21	4:D:481:PRO:HB3	1.87	0.56
4:F:486:VAL:HG22	4:F:538:VAL:HG22	1.87	0.56
4:H:352:PRO:HD3	4:H:365:LEU:HB3	1.86	0.56
3:K:510:GLN:OE1	5:L:522:THR:HG21	2.05	0.56
5:L:500:TYR:CB	5:L:521:LEU:HD13	2.31	0.56
3:C:418:TRP:CZ3	3:C:443:ARG:HG2	2.41	0.56
4:D:459:PRO:HG3	4:D:470:ALA:HB1	1.87	0.56
4:H:379:THR:HB	4:H:429:THR:HB	1.87	0.56
3:K:449:LEU:HA	3:K:480:SER:O	2.06	0.56
5:L:574:THR:O	5:L:574:THR:OG1	2.19	0.56
1:A:508:GLU:HB3	1:A:511:ALA:HB3	1.86	0.56
3:C:545:ASN:O	3:C:545:ASN:ND2	2.39	0.56
6:J:38:ARG:HH12	6:J:40:ILE:HD11	1.70	0.56
2:B:532:GLU:OE1	2:B:532:GLU:HA	2.05	0.56
4:F:449:LEU:CB	4:F:480:SER:O	2.54	0.56
3:C:372:LEU:HB2	3:C:405:PHE:HB2	1.88	0.56
4:G:473:THR:HG22	4:G:520:ILE:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:450:HIS:CD2	3:K:514:ARG:NE	2.74	0.56
7:R:26:GLU:CB	7:R:124:SER:HA	2.27	0.56
4:D:543:LEU:HB2	4:D:546:ARG:HA	1.88	0.56
2:B:564:VAL:HG23	3:C:564:VAL:HA	1.87	0.55
4:F:383:THR:HG23	4:F:387:GLY:HA2	1.88	0.55
4:F:560:THR:O	4:F:560:THR:HG22	2.04	0.55
3:C:418:TRP:CZ2	3:C:443:ARG:CG	2.89	0.55
4:F:421:GLY:O	4:F:423:ARG:NH1	2.38	0.55
3:K:459:PRO:HB3	3:K:471:THR:H	1.70	0.55
5:L:423:ARG:HG3	5:L:442:SER:OG	2.07	0.55
6:J:49:ILE:HG12	6:J:103:TYR:CD1	2.40	0.55
7:R:29:LEU:O	7:R:93:GLN:HG2	2.05	0.55
1:A:349:ALA:HB2	1:A:439:GLN:HB3	1.88	0.55
3:C:423:ARG:HA	3:C:442:SER:HG	1.61	0.55
4:D:449:LEU:CD2	4:D:481:PRO:HD2	2.33	0.55
4:E:453:ASP:OD2	4:E:477:THR:HG22	2.04	0.55
4:G:380:ILE:HG22	4:G:428:VAL:HG22	1.89	0.55
5:L:365:LEU:HB2	5:L:411:ALA:HB3	1.89	0.55
7:R:96:GLU:OE2	7:R:122:VAL:CG2	2.54	0.55
2:B:465:ASN:HD21	5:L:571:THR:HG22	1.72	0.55
7:R:33:VAL:HG13	7:R:91:VAL:HG21	1.77	0.55
3:C:360:THR:HG22	3:C:362:SER:HB2	1.88	0.55
6:J:104:ASP:HB3	6:J:107:LYS:HB2	1.88	0.55
2:B:490:GLN:N	2:B:495:LEU:HD11	2.21	0.55
4:E:559:PRO:O	4:E:561:LEU:N	2.39	0.55
7:R:29:LEU:C	7:R:29:LEU:HD23	2.26	0.55
4:F:450:HIS:N	4:F:450:HIS:CD2	2.72	0.55
5:L:452:PRO:CB	5:L:478:GLY:O	2.42	0.55
4:E:451:ARG:CZ	4:E:451:ARG:CB	2.85	0.55
5:L:488:TRP:C	5:L:495:LEU:HB2	2.23	0.55
7:R:34:THR:OG1	7:R:88:LEU:HD11	2.01	0.55
2:B:349:ALA:HB1	2:B:441:ILE:HD12	1.89	0.54
4:G:543:LEU:HB2	4:G:546:ARG:HA	1.88	0.54
7:R:28:GLU:OE1	7:R:96:GLU:CG	2.55	0.54
1:A:568:MET:HE1	6:J:37:ILE:HD13	1.88	0.54
5:L:443:ARG:CG	5:L:443:ARG:HH11	2.15	0.54
2:B:418:TRP:NE1	2:B:443:ARG:HG3	1.94	0.54
3:K:391:LYS:HD2	3:K:392:THR:N	2.22	0.54
2:B:489:MET:CE	2:B:537:VAL:HG11	2.37	0.54
3:K:398:GLU:O	3:K:406:SER:OG	2.25	0.54
5:L:566:LEU:HA	6:J:39:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:564:VAL:HG21	4:H:566:LEU:HD21	0.58	0.54
3:K:535:THR:HG22	3:K:551:THR:OG1	2.07	0.54
5:L:506:MET:HB2	5:L:516:PHE:O	2.08	0.54
5:L:425:THR:HB	5:L:438:LYS:HE2	1.90	0.54
6:J:131:ASP:HB2	7:R:44:VAL:HG13	1.90	0.54
3:K:352:PRO:HD3	3:K:365:LEU:HA	1.89	0.54
3:C:484:VAL:HG23	3:C:540:HIS:HB2	1.89	0.54
7:R:96:GLU:HB3	7:R:122:VAL:HG21	1.86	0.54
2:B:384:ARG:HB3	2:B:424:PHE:CE1	2.43	0.53
4:E:553:ASP:N	4:E:553:ASP:OD1	2.40	0.53
4:H:382:TRP:HB2	4:H:390:VAL:HG21	1.90	0.53
4:H:508:GLU:HG2	4:H:511:ALA:H	1.72	0.53
3:K:385:GLN:HB2	3:K:423:ARG:HB3	1.88	0.53
4:D:454:VAL:HG21	4:D:538:VAL:HG11	1.90	0.53
3:K:378:VAL:HG12	3:K:430:HIS:HD2	1.72	0.53
4:D:400:HIS:CD2	4:D:406:SER:HB3	2.43	0.53
4:G:490:GLN:NE2	4:G:532:GLU:HA	2.21	0.53
5:L:384:ARG:HD3	5:L:388:GLU:HB2	1.90	0.53
7:R:96:GLU:CD	7:R:122:VAL:HG21	2.29	0.53
2:B:553:ASP:OD1	2:B:554:LYS:N	2.39	0.53
5:L:498:GLU:OE2	5:L:498:GLU:HA	2.09	0.53
2:B:465:ASN:HD21	5:L:571:THR:HG21	1.71	0.53
3:C:565:SER:O	3:C:565:SER:OG	2.10	0.53
4:F:382:TRP:HB2	4:F:390:VAL:HG21	1.90	0.53
3:K:456:LEU:HD23	3:K:552:VAL:HG13	1.90	0.53
7:R:79:LYS:HE3	7:R:81:TYR:HE2	1.73	0.53
4:D:464:LEU:HD11	4:D:528:TRP:CE3	2.43	0.53
4:H:543:LEU:CD2	4:H:548:THR:HG21	2.38	0.53
1:A:490:GLN:NE2	1:A:527:GLU:OE2	2.41	0.53
3:K:425:THR:HG23	3:K:439:GLN:H	1.73	0.53
5:L:567:VAL:HG22	6:J:40:ILE:HG12	1.91	0.53
2:B:515:TYR:CD1	2:B:515:TYR:N	2.71	0.53
4:H:443:ARG:NH2	4:H:444:PRO:HD3	2.23	0.53
3:K:461:ARG:NH1	3:K:461:ARG:HB2	2.23	0.53
6:J:113:VAL:CG1	6:J:126:THR:CG2	2.86	0.53
6:J:113:VAL:CG1	6:J:126:THR:CB	2.85	0.53
3:C:508:GLU:HG3	3:C:509:PRO:HD2	1.90	0.53
5:L:421:GLY:HA2	5:L:443:ARG:HH11	1.73	0.53
6:J:13:LYS:HZ3	6:J:101:TYR:HE1	1.56	0.53
4:F:564:VAL:HA	4:G:564:VAL:O	2.09	0.52
4:G:400:HIS:ND1	4:G:404:THR:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:96:GLU:CD	7:R:122:VAL:CG2	2.76	0.52
4:D:380:ILE:HG22	4:D:428:VAL:HG22	1.92	0.52
3:K:463:GLN:HG2	5:L:455:TYR:CE2	2.42	0.52
1:A:359:LEU:HD13	6:J:115:LEU:CD1	2.39	0.52
4:D:490:GLN:HG2	4:D:491:ARG:HG3	1.90	0.52
4:G:499:LYS:O	4:G:499:LYS:HG3	2.02	0.52
5:L:451:ARG:HD2	5:L:451:ARG:C	2.30	0.52
1:A:450:HIS:CE1	1:A:480:SER:CB	2.89	0.52
1:A:459:PRO:HG3	1:A:470:ALA:HB1	1.92	0.52
4:D:490:GLN:NE2	4:D:532:GLU:OE1	2.42	0.52
5:L:520:ILE:HG13	5:L:520:ILE:O	2.10	0.52
5:L:382:TRP:HB2	5:L:390:VAL:HG21	1.89	0.52
5:L:488:TRP:CD1	5:L:500:TYR:CD2	2.98	0.52
7:R:75:ARG:CA	7:R:92:THR:HG21	2.33	0.52
1:A:449:LEU:CD2	1:A:481:PRO:HD3	2.40	0.52
1:A:509:PRO:HG3	2:B:501:VAL:HG23	1.91	0.52
4:E:380:ILE:HD11	4:E:407:ALA:HB1	1.91	0.52
4:F:354:PHE:O	4:F:357:ILE:HG22	2.10	0.52
4:F:425:THR:HG21	4:F:438:LYS:HB3	1.92	0.52
4:F:508:GLU:HG3	4:F:509:PRO:HD2	1.92	0.52
4:H:543:LEU:HD11	4:H:548:THR:HG23	1.90	0.52
7:R:120:LEU:N	7:R:120:LEU:CD1	2.73	0.52
4:H:566:LEU:HD23	3:K:568:MET:CE	2.40	0.52
4:E:509:PRO:HB3	4:F:501:VAL:HG13	1.91	0.52
4:H:347:VAL:HG23	4:H:437:LEU:HD22	1.92	0.52
4:H:562:TYR:N	4:H:562:TYR:CD2	2.73	0.52
6:J:49:ILE:CD1	6:J:103:TYR:HE1	1.87	0.52
1:A:449:LEU:HD21	1:A:481:PRO:CD	2.40	0.51
7:R:45:ARG:HH11	7:R:45:ARG:CG	2.18	0.51
1:A:456:LEU:HD23	1:A:552:VAL:HG13	1.92	0.51
4:G:499:LYS:CG	4:G:521:LEU:CD1	2.88	0.51
4:E:564:VAL:HG21	4:F:564:VAL:HG21	1.92	0.51
2:B:529:ASN:HA	2:B:554:LYS:HD3	1.92	0.51
4:E:562:TYR:CE2	4:F:566:LEU:HD21	2.46	0.51
4:G:365:LEU:HG	4:G:424:PHE:HD1	1.75	0.51
6:J:110:THR:HG22	6:J:127:ALA:HA	1.93	0.51
1:A:364:LYS:HD2	1:A:410:GLU:HG3	1.92	0.51
1:A:450:HIS:ND1	1:A:450:HIS:N	2.58	0.51
4:F:543:LEU:HB2	4:F:546:ARG:HA	1.92	0.51
5:L:443:ARG:HB3	5:L:444:PRO:HD2	1.86	0.51
3:C:367:CYS:HB2	3:C:382:TRP:CZ2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:48:LEU:HD13	7:R:104:CYS:SG	2.51	0.51
4:H:443:ARG:CD	4:H:444:PRO:HD2	2.40	0.51
7:R:96:GLU:HA	7:R:122:VAL:HG23	1.93	0.51
4:D:447:VAL:CG2	4:D:481:PRO:HD3	2.41	0.51
4:F:457:LEU:HB2	4:F:473:THR:OG1	2.12	0.51
4:G:413:ILE:HD13	4:G:424:PHE:CE1	2.46	0.51
4:G:479:PHE:CD1	4:G:479:PHE:C	2.83	0.51
3:K:443:ARG:CD	3:K:443:ARG:N	2.72	0.51
4:H:451:ARG:HG3	4:H:451:ARG:HH11	1.75	0.50
5:L:420:SER:OG	5:L:422:GLU:OE1	2.22	0.50
5:L:470:ALA:O	5:L:523:VAL:HG23	2.11	0.50
5:L:516:PHE:C	5:L:516:PHE:CD2	2.84	0.50
6:J:39:ILE:CD1	6:J:62:TYR:CZ	2.90	0.50
4:E:555:SER:OG	4:E:555:SER:O	2.16	0.50
3:K:498:GLU:OE2	5:L:509:PRO:O	2.30	0.50
3:K:567:VAL:HG21	5:L:567:VAL:HG12	1.94	0.50
5:L:471:THR:HA	5:L:521:LEU:O	2.11	0.50
5:L:532:GLU:O	5:L:533:THR:HG22	2.12	0.50
1:A:362:SER:O	1:A:364:LYS:N	2.40	0.50
4:F:416:ASP:N	4:F:416:ASP:OD1	2.44	0.50
7:R:87:PHE:C	7:R:87:PHE:CD1	2.85	0.50
5:L:383:THR:OG1	5:L:438:LYS:NZ	2.44	0.50
2:B:518:HIS:HD1	2:B:518:HIS:H	1.59	0.50
4:G:351:PRO:HG3	4:G:441:ILE:HD11	1.92	0.50
4:H:543:LEU:HD13	4:H:548:THR:N	2.27	0.50
3:K:430:HIS:CD2	3:K:431:THR:H	2.29	0.50
4:E:450:HIS:NE2	4:E:514:ARG:NH2	2.57	0.50
4:G:427:THR:HG22	4:G:438:LYS:HG2	1.94	0.50
3:K:516:PHE:CD2	5:L:520:ILE:CD1	2.83	0.50
7:R:41:GLU:OE1	7:R:82:PRO:HG3	2.11	0.50
7:R:98:ASP:OD1	7:R:98:ASP:N	2.44	0.50
4:D:449:LEU:HD22	4:D:480:SER:O	2.12	0.50
4:H:451:ARG:HH11	4:H:451:ARG:CG	2.24	0.50
4:G:413:ILE:HG21	4:G:424:PHE:CZ	2.47	0.50
4:G:487:GLN:O	4:G:537:VAL:CG2	2.59	0.50
7:R:75:ARG:C	7:R:92:THR:CG2	2.74	0.50
4:G:384:ARG:HG3	4:G:388:GLU:HB3	1.94	0.49
6:J:49:ILE:HD13	6:J:101:TYR:O	2.12	0.49
7:R:45:ARG:NH1	7:R:45:ARG:CG	2.72	0.49
4:H:345:ILE:HG22	4:H:437:LEU:HD21	1.94	0.49
3:K:451:ARG:NH1	3:K:451:ARG:CG	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:5:ILE:O	6:J:18:THR:OG1	2.24	0.49
1:A:384:ARG:HG2	1:A:385:GLN:H	1.78	0.49
3:C:383:THR:HB	3:C:387:GLY:HA2	1.94	0.49
4:D:470:ALA:N	4:D:523:VAL:O	2.45	0.49
3:C:418:TRP:O	3:C:443:ARG:CG	2.61	0.49
3:C:500:TYR:HB3	3:C:521:LEU:HD13	1.93	0.49
3:K:451:ARG:NH1	3:K:451:ARG:CB	2.72	0.49
3:K:506:MET:HB2	3:K:516:PHE:CE1	2.48	0.49
1:A:467:ARG:HA	1:A:525:GLU:HG3	1.94	0.49
4:E:452:PRO:O	4:E:452:PRO:HG2	2.13	0.49
4:G:399:SER:HA	4:G:405:PHE:HA	1.93	0.49
4:H:474:CYS:HB2	4:H:488:TRP:CZ2	2.48	0.49
3:C:418:TRP:HZ2	3:C:443:ARG:HB3	1.50	0.49
4:E:423:ARG:CD	4:E:442:SER:OG	2.60	0.49
4:E:486:VAL:HG22	4:E:538:VAL:HG22	1.94	0.49
4:E:419:ASN:HA	4:E:443:ARG:NH2	2.28	0.49
7:R:27:GLY:HA3	7:R:94:LEU:HD23	1.89	0.49
7:R:35:ILE:H	7:R:35:ILE:CD1	2.21	0.49
4:F:508:GLU:HB3	4:F:511:ALA:HB3	1.94	0.49
3:K:366:THR:HA	3:K:409:GLY:O	2.12	0.49
3:K:443:ARG:H	3:K:443:ARG:HD3	1.75	0.48
3:K:562:TYR:HD1	5:L:562:TYR:HB2	1.77	0.48
2:B:478:GLY:O	2:B:514:ARG:NH2	2.46	0.48
5:L:562:TYR:HA	6:J:35:ARG:HB2	1.96	0.48
4:E:451:ARG:NH1	4:E:451:ARG:CB	2.73	0.48
5:L:486:VAL:O	5:L:500:TYR:OH	2.25	0.48
5:L:506:MET:CB	5:L:507:PRO:HD2	2.42	0.48
5:L:552:VAL:HG13	5:L:556:THR:HG23	1.95	0.48
7:R:37:CYS:C	7:R:87:PHE:HB3	2.32	0.48
3:C:461:ARG:HH11	4:D:557:GLY:HA2	1.78	0.48
3:K:452:PRO:HB3	3:K:479:PHE:HB3	1.95	0.48
6:J:13:LYS:NZ	6:J:101:TYR:HE1	2.12	0.48
6:J:113:VAL:HG11	6:J:126:THR:CB	2.43	0.48
4:E:528:TRP:CH2	4:E:553:ASP:O	2.66	0.48
4:F:562:TYR:HB3	4:G:562:TYR:HB2	1.96	0.48
4:G:490:GLN:OE1	4:G:532:GLU:CG	2.36	0.48
5:L:478:GLY:HA2	5:L:514:ARG:CG	2.07	0.48
4:G:449:LEU:HD12	4:G:449:LEU:HA	1.56	0.48
4:E:559:PRO:C	4:E:561:LEU:H	2.16	0.48
4:H:562:TYR:HB3	3:K:562:TYR:HB2	1.96	0.48
7:R:35:ILE:N	7:R:35:ILE:CD1	2.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:529:ASN:C	4:E:554:LYS:NZ	2.66	0.48
4:F:451:ARG:NH1	4:F:451:ARG:CB	2.77	0.48
2:B:459:PRO:HD3	2:B:472:ILE:HG12	1.96	0.47
2:B:518:HIS:ND1	2:B:518:HIS:N	2.60	0.47
3:C:423:ARG:C	3:C:442:SER:OG	2.50	0.47
3:C:491:ARG:HG3	3:C:491:ARG:HH11	1.79	0.47
3:K:374:THR:HA	3:K:405:PHE:HB2	1.95	0.47
4:F:452:PRO:O	4:F:452:PRO:HG2	2.14	0.47
5:L:506:MET:N	5:L:516:PHE:O	2.46	0.47
6:J:131:ASP:HB2	7:R:44:VAL:CG1	2.44	0.47
7:R:34:THR:HA	7:R:89:VAL:O	2.13	0.47
4:G:422:GLU:HG2	4:G:424:PHE:HE2	1.79	0.47
3:C:452:PRO:HB3	3:C:479:PHE:HB3	1.95	0.47
7:R:42:MET:HG3	7:R:44:VAL:CG2	2.44	0.47
4:D:537:VAL:HG12	4:D:549:GLU:HG2	1.95	0.47
4:E:360:THR:HG23	4:E:362:SER:H	1.79	0.47
4:H:459:PRO:HD3	4:H:472:ILE:HG13	1.96	0.47
6:J:113:VAL:HG13	6:J:126:THR:CB	2.43	0.47
4:D:375:TYR:HD2	4:D:430:HIS:HE1	1.61	0.47
4:D:452:PRO:HB3	4:D:479:PHE:HB3	1.96	0.47
1:A:507:PRO:HA	1:A:515:TYR:HD1	1.79	0.47
4:F:454:VAL:HG13	4:F:474:CYS:SG	2.55	0.47
4:H:543:LEU:HD13	4:H:548:THR:H	1.80	0.47
3:K:443:ARG:HA	3:K:444:PRO:HD2	1.63	0.47
6:J:115:LEU:C	6:J:115:LEU:HD12	2.35	0.47
7:R:33:VAL:HG12	7:R:91:VAL:HG21	1.90	0.47
7:R:86:LEU:CD1	7:R:88:LEU:HD23	2.45	0.47
1:A:475:LEU:HD13	1:A:518:HIS:CE1	2.50	0.47
3:C:397:SER:HB3	3:C:407:ALA:HA	1.96	0.47
4:D:398:GLU:O	4:D:406:SER:OG	2.29	0.47
3:C:384:ARG:HG3	3:C:424:PHE:HE1	1.80	0.47
4:G:489:MET:CG	4:G:535:THR:OG1	2.62	0.47
3:C:490:GLN:NE2	3:C:532:GLU:OE1	2.27	0.47
4:E:347:VAL:HG12	4:E:369:VAL:HG12	1.97	0.47
4:E:374:THR:HA	4:E:405:PHE:HB2	1.96	0.47
4:H:449:LEU:CD1	4:H:542:ALA:HB2	2.38	0.47
5:L:451:ARG:CG	5:L:451:ARG:NH2	2.73	0.47
4:D:449:LEU:HD22	4:D:481:PRO:HD2	1.97	0.46
4:G:489:MET:O	4:G:535:THR:OG1	2.27	0.46
4:H:456:LEU:CD1	4:H:550:ARG:HB3	2.39	0.46
3:K:498:GLU:O	5:L:509:PRO:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:96:GLU:CG	7:R:122:VAL:HG22	2.24	0.46
3:C:450:HIS:CE1	3:C:514:ARG:NE	2.53	0.46
4:E:466:LEU:CD2	4:G:491:ARG:NH1	2.78	0.46
7:R:39:LEU:HD11	7:R:85:ASN:HA	1.97	0.46
2:B:533:THR:O	2:B:533:THR:HG22	2.16	0.46
4:G:479:PHE:CD1	4:G:479:PHE:O	2.68	0.46
6:J:39:ILE:CD1	6:J:62:TYR:CE2	2.99	0.46
6:J:67:LEU:HG	6:J:67:LEU:O	2.15	0.46
7:R:112:ARG:NH1	7:R:112:ARG:CG	2.73	0.46
4:E:418:TRP:CD2	4:E:443:ARG:CG	2.59	0.46
4:E:423:ARG:CG	4:E:442:SER:HG	2.22	0.46
4:F:449:LEU:HA	4:F:480:SER:O	2.16	0.46
4:F:583:NAG:H61	4:G:583:NAG:H4	1.97	0.46
4:G:443:ARG:HH11	4:G:443:ARG:CG	2.29	0.46
4:H:399:SER:OG	4:H:404:THR:O	2.34	0.46
4:H:449:LEU:HD12	4:H:542:ALA:CB	2.37	0.46
7:R:96:GLU:OE2	7:R:122:VAL:HG21	2.14	0.46
7:R:96:GLU:HA	7:R:122:VAL:CG2	2.45	0.46
2:B:516:PHE:CD1	2:B:516:PHE:C	2.89	0.46
5:L:372:LEU:HD23	5:L:430:HIS:CG	2.51	0.46
3:C:533:THR:HB	3:C:551:THR:HG23	1.97	0.46
4:H:567:VAL:HG22	3:K:567:VAL:HG13	1.98	0.46
1:A:395:ASN:HD22	1:A:395:ASN:C	2.17	0.46
1:A:567:VAL:HG12	2:B:567:VAL:HB	1.97	0.46
2:B:369:VAL:HB	2:B:406:SER:HA	1.98	0.46
2:B:516:PHE:O	2:B:516:PHE:CG	2.68	0.46
4:E:449:LEU:HA	4:E:449:LEU:HD13	1.63	0.46
5:L:516:PHE:C	5:L:516:PHE:HD2	2.19	0.46
6:J:39:ILE:HD12	6:J:62:TYR:CE2	2.51	0.46
1:A:355:ALA:HB2	1:A:485:PHE:HB2	1.96	0.46
2:B:449:LEU:HD12	2:B:481:PRO:HD3	1.98	0.46
4:F:379:THR:HB	4:F:429:THR:OG1	2.15	0.46
4:G:485:PHE:CD2	4:G:485:PHE:O	2.68	0.46
4:F:357:ILE:HD11	4:F:415:GLU:HG2	1.97	0.46
4:G:418:TRP:CH2	4:G:442:SER:C	2.89	0.46
4:H:449:LEU:HD13	4:H:449:LEU:HA	1.48	0.46
3:K:351:PRO:HG3	3:K:441:ILE:HG23	1.97	0.46
6:J:52:PRO:CD	6:J:128:LEU:HD11	2.44	0.46
3:C:425:THR:HG21	3:C:438:LYS:HE2	1.98	0.46
3:K:354:PHE:HA	3:K:357:ILE:HG12	1.98	0.46
5:L:491:ARG:HB3	5:L:493:GLN:CD	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:464:LEU:HD22	4:D:525:GLU:HG2	1.97	0.45
4:E:429:THR:HA	4:E:433:LEU:HD21	1.97	0.45
4:E:557:GLY:HA3	4:F:461:ARG:HH22	1.82	0.45
4:G:556:THR:O	4:H:461:ARG:NH2	2.49	0.45
6:J:113:VAL:CG1	6:J:126:THR:HG21	2.46	0.45
1:A:365:LEU:HB3	1:A:418:TRP:CH2	2.51	0.45
3:C:447:VAL:O	3:C:447:VAL:HG13	2.16	0.45
4:D:457:LEU:HB2	4:D:473:THR:OG1	2.16	0.45
4:F:454:VAL:CG2	4:F:538:VAL:CG2	2.94	0.45
6:J:14:CYS:SG	6:J:40:ILE:HB	2.56	0.45
7:R:25:VAL:HG11	7:R:33:VAL:HG23	1.98	0.45
4:F:449:LEU:CA	4:F:480:SER:O	2.64	0.45
4:G:500:TYR:C	4:G:500:TYR:CD2	2.88	0.45
5:L:354:PHE:HA	5:L:357:ILE:HG12	1.99	0.45
2:B:365:LEU:H	2:B:365:LEU:HD23	1.81	0.45
4:E:451:ARG:NH1	4:E:451:ARG:CG	2.72	0.45
5:L:452:PRO:HG3	5:L:478:GLY:O	2.16	0.45
1:A:456:LEU:HD12	1:A:456:LEU:HA	1.81	0.45
1:A:544:PRO:HB2	6:J:135:PRO:CD	2.47	0.45
2:B:482:ALA:HB2	2:B:515:TYR:HE2	1.81	0.45
3:K:448:ALA:HB1	3:K:450:HIS:CE1	2.52	0.45
3:K:475:LEU:HG	3:K:477:THR:HG23	1.98	0.45
6:J:108:CYS:HB2	6:J:133:CYS:HB3	1.62	0.45
3:C:564:VAL:CG2	4:H:566:LEU:HD23	2.39	0.45
1:A:547:VAL:HG11	6:J:113:VAL:HG21	1.99	0.45
1:A:564:VAL:HB	2:B:564:VAL:HA	1.99	0.45
3:C:384:ARG:HG3	3:C:424:PHE:CE1	2.52	0.45
4:D:464:LEU:CD1	4:D:528:TRP:CZ3	2.99	0.45
4:E:520:ILE:HG13	4:E:520:ILE:O	2.16	0.45
6:J:10:ASN:HD22	6:J:67:LEU:CD1	2.30	0.45
6:J:131:ASP:OD2	7:R:107:GLY:HA2	2.17	0.45
7:R:22:GLU:HA	7:R:118:VAL:HG22	1.92	0.45
3:C:349:ALA:HB1	3:C:441:ILE:HD12	1.98	0.45
3:C:382:TRP:CZ2	3:C:426:CYS:HB2	2.52	0.45
3:K:501:VAL:HG11	5:L:516:PHE:CE1	2.50	0.45
1:A:372:LEU:H	1:A:372:LEU:HD23	1.82	0.45
1:A:479:PHE:HB2	1:A:540:HIS:CE1	2.51	0.45
2:B:528:TRP:CE3	2:B:528:TRP:O	2.69	0.45
3:C:430:HIS:CD2	3:C:431:THR:H	2.34	0.45
3:C:433:LEU:HD13	3:C:437:LEU:HG	1.99	0.45
4:G:452:PRO:HB3	4:G:479:PHE:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:48:ASN:HB3	6:J:160:NAG:O5	2.17	0.45
1:A:564:VAL:HG21	5:L:568:MET:HE1	1.99	0.44
2:B:518:HIS:O	2:B:518:HIS:CG	2.70	0.44
4:E:450:HIS:HD2	4:E:514:ARG:NH2	2.13	0.44
4:F:456:LEU:HD11	4:F:536:CYS:SG	2.57	0.44
2:B:417:ASP:OD1	2:B:417:ASP:N	2.50	0.44
4:F:348:PHE:CE1	4:F:368:LEU:HB3	2.52	0.44
4:F:349:ALA:HB3	4:F:441:ILE:HG21	1.99	0.44
4:G:499:LYS:HG3	4:G:521:LEU:HD12	1.98	0.44
3:K:421:GLY:HA2	3:K:443:ARG:HD3	1.98	0.44
2:B:531:GLY:O	2:B:553:ASP:OD1	2.36	0.44
3:K:460:ALA:HB2	5:L:457:LEU:HD23	2.00	0.44
5:L:488:TRP:HD1	5:L:500:TYR:CD2	2.35	0.44
1:A:449:LEU:HD22	1:A:449:LEU:HA	1.70	0.44
4:D:449:LEU:HB3	4:D:542:ALA:HB2	1.98	0.44
4:E:566:LEU:HD11	4:F:562:TYR:HE2	1.83	0.44
4:G:445:LYS:HD2	4:G:446:GLY:N	2.30	0.44
2:B:345:ILE:N	2:B:371:ASP:HB3	2.33	0.44
2:B:374:THR:HG23	2:B:405:PHE:HD2	1.82	0.44
4:D:459:PRO:HD3	4:D:472:ILE:HG12	1.99	0.44
3:K:380:ILE:HG12	3:K:428:VAL:HG12	1.99	0.44
4:D:443:ARG:CZ	4:D:445:LYS:HD3	2.45	0.44
4:D:445:LYS:HD2	4:D:445:LYS:HA	1.45	0.44
4:E:443:ARG:CZ	4:E:443:ARG:CB	2.85	0.44
4:E:553:ASP:H	4:E:556:THR:HG1	1.66	0.44
3:K:459:PRO:HG3	3:K:470:ALA:HB1	1.99	0.44
5:L:559:PRO:HA	6:J:33:VAL:HB	2.00	0.44
1:A:449:LEU:HD13	1:A:542:ALA:CB	2.33	0.44
1:A:568:MET:HE2	6:J:64:LEU:HD11	2.00	0.44
2:B:493:GLN:N	2:B:493:GLN:CD	2.71	0.44
4:F:354:PHE:HA	4:F:357:ILE:HG22	2.00	0.44
4:F:433:LEU:HD12	4:F:434:PRO:HD2	1.99	0.44
4:G:499:LYS:CG	4:G:521:LEU:HD11	2.43	0.44
7:R:21:PRO:C	7:R:118:VAL:HG23	2.37	0.44
3:C:384:ARG:NH2	3:C:388:GLU:HB2	2.33	0.44
4:E:418:TRP:CD1	4:E:443:ARG:NE	2.86	0.44
4:F:391:LYS:NZ	4:F:410:GLU:O	2.45	0.44
5:L:495:LEU:HA	5:L:495:LEU:HD23	1.40	0.44
5:L:347:VAL:HG22	5:L:369:VAL:HG13	1.99	0.43
5:L:347:VAL:HG13	5:L:369:VAL:HG22	2.00	0.43
5:L:559:PRO:HG2	5:L:562:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:PRO:HG2	2:B:357:ILE:HD11	2.00	0.43
4:H:445:LYS:H	4:H:445:LYS:HG2	1.45	0.43
5:L:506:MET:HB3	5:L:507:PRO:HD2	2.00	0.43
6:J:16:ARG:HD3	6:J:16:ARG:O	2.18	0.43
7:R:35:ILE:N	7:R:88:LEU:HD11	2.33	0.43
2:B:449:LEU:HG	2:B:542:ALA:HB2	1.99	0.43
3:C:543:LEU:HB2	3:C:546:ARG:HA	2.00	0.43
4:F:561:LEU:HD23	4:F:561:LEU:HA	1.51	0.43
4:G:508:GLU:HG2	4:G:511:ALA:HB3	2.00	0.43
3:K:464:LEU:O	3:K:467:ARG:NH1	2.49	0.43
3:K:567:VAL:HB	5:L:567:VAL:HA	2.00	0.43
5:L:451:ARG:C	5:L:451:ARG:CD	2.86	0.43
1:A:429:THR:HG23	1:A:436:PRO:HG3	2.01	0.43
1:A:489:MET:HB2	1:A:535:THR:OG1	2.18	0.43
2:B:561:LEU:HB2	3:C:561:LEU:O	2.17	0.43
4:G:474:CYS:HB2	4:G:488:TRP:CZ2	2.53	0.43
3:K:345:ILE:HA	3:K:372:LEU:HG	2.01	0.43
6:J:67:LEU:HA	6:J:67:LEU:HD12	1.85	0.43
5:L:479:PHE:CD1	5:L:515:TYR:O	2.71	0.43
7:R:75:ARG:CB	7:R:92:THR:CG2	2.96	0.43
1:A:379:THR:HB	1:A:429:THR:HB	1.99	0.43
4:D:382:TRP:NE1	4:D:409:GLY:O	2.51	0.43
4:E:419:ASN:HA	4:E:443:ARG:CZ	2.49	0.43
4:H:453:ASP:OD2	4:H:455:TYR:OH	2.31	0.43
3:K:450:HIS:ND1	3:K:450:HIS:N	2.59	0.43
5:L:346:ARG:HB3	5:L:370:THR:O	2.19	0.43
2:B:564:VAL:CG2	3:C:564:VAL:HA	2.48	0.43
4:G:495:LEU:HD12	4:G:495:LEU:HA	1.79	0.43
4:H:392:THR:HG22	4:H:393:HIS:N	2.33	0.43
5:L:391:LYS:NZ	5:L:392:THR:HG22	2.34	0.43
7:R:21:PRO:O	7:R:118:VAL:HG21	2.18	0.43
7:R:41:GLU:OE1	7:R:82:PRO:CG	2.67	0.43
4:G:447:VAL:HG23	4:G:447:VAL:O	2.19	0.43
4:G:489:MET:HE3	4:G:489:MET:HB3	1.86	0.43
4:H:532:GLU:HB3	4:H:534:TYR:CE2	2.53	0.43
7:R:86:LEU:HA	7:R:86:LEU:HD22	1.40	0.43
1:A:463:GLN:HG3	2:B:455:TYR:CZ	2.54	0.43
6:J:20:ARG:HH11	6:J:34:GLU:HG2	1.84	0.43
6:J:109:TYR:H	6:J:129:THR:HG21	1.84	0.43
7:R:45:ARG:O	7:R:106:ALA:HA	2.19	0.43
4:E:378:VAL:HG11	4:E:407:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:382:TRP:CE3	4:E:426:CYS:HB3	2.54	0.42
4:H:392:THR:HG22	4:H:393:HIS:H	1.84	0.42
4:H:486:VAL:HG13	4:H:538:VAL:HG12	2.00	0.42
3:K:501:VAL:CG1	5:L:516:PHE:CZ	2.85	0.42
1:A:564:VAL:HG11	5:L:568:MET:HE1	2.00	0.42
4:D:349:ALA:HA	4:D:367:CYS:HA	2.00	0.42
4:F:558:LYS:HB3	4:F:559:PRO:CD	2.48	0.42
3:K:351:PRO:HG3	3:K:441:ILE:HD12	2.00	0.42
1:A:359:LEU:HD13	6:J:115:LEU:HD13	2.00	0.42
3:C:491:ARG:HG3	3:C:491:ARG:NH1	2.35	0.42
3:C:509:PRO:HB3	4:D:501:VAL:HG23	2.02	0.42
4:F:419:ASN:HA	4:F:443:ARG:HH11	1.85	0.42
4:G:457:LEU:HB2	4:G:473:THR:OG1	2.19	0.42
4:G:557:GLY:HA2	4:H:461:ARG:HH21	1.85	0.42
3:K:514:ARG:NH1	3:K:514:ARG:CG	2.72	0.42
3:K:526:GLU:HA	3:K:529:ASN:CG	2.34	0.42
5:L:367:CYS:HB2	5:L:382:TRP:CZ2	2.55	0.42
6:J:130:PRO:HG2	6:J:130:PRO:O	2.19	0.42
7:R:33:VAL:HG21	7:R:120:LEU:CD2	2.46	0.42
7:R:47:TYR:CE2	7:R:110:THR:HG23	2.55	0.42
2:B:482:ALA:HB2	2:B:515:TYR:CE2	2.54	0.42
3:C:568:MET:HE3	3:C:568:MET:HB3	1.81	0.42
4:E:529:ASN:CA	4:E:554:LYS:HE3	1.93	0.42
4:F:464:LEU:HD22	4:F:525:GLU:HG2	2.01	0.42
7:R:37:CYS:HB2	7:R:87:PHE:CG	2.54	0.42
7:R:112:ARG:HH11	7:R:112:ARG:CG	2.22	0.42
4:F:452:PRO:HD3	4:F:540:HIS:ND1	2.35	0.42
4:G:365:LEU:HG	4:G:424:PHE:CD1	2.53	0.42
3:K:393:HIS:HB2	3:K:410:GLU:H	1.84	0.42
3:K:532:GLU:HA	3:K:532:GLU:OE1	2.19	0.42
5:L:501:VAL:HG12	5:L:520:ILE:HG13	2.01	0.42
1:A:547:VAL:HG21	6:J:124:VAL:HG11	2.02	0.42
2:B:543:LEU:HB2	2:B:546:ARG:HA	2.01	0.42
4:D:365:LEU:H	4:D:365:LEU:HD23	1.85	0.42
4:D:468:GLU:OE1	4:D:468:GLU:HA	2.19	0.42
4:G:499:LYS:HD2	4:G:522:THR:O	2.20	0.42
6:J:101:TYR:N	6:J:101:TYR:HD1	2.15	0.42
7:R:33:VAL:CG2	7:R:120:LEU:HD23	2.46	0.42
1:A:511:ALA:HB1	1:A:514:ARG:HD3	2.01	0.42
2:B:454:VAL:HG22	2:B:476:VAL:HG13	2.02	0.42
4:E:562:TYR:HE2	4:F:566:LEU:HD21	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:454:VAL:HG21	4:F:538:VAL:CG2	2.50	0.42
4:H:520:ILE:O	4:H:520:ILE:HG13	2.19	0.42
4:H:537:VAL:HG23	4:H:548:THR:O	2.20	0.42
3:K:364:LYS:HG2	3:K:412:SER:HA	2.02	0.42
3:K:445:LYS:HB2	3:K:445:LYS:HE2	1.75	0.42
1:A:449:LEU:CD2	1:A:480:SER:O	2.60	0.42
2:B:510:GLN:NE2	2:B:511:ALA:HB2	2.35	0.42
3:C:449:LEU:HA	3:C:480:SER:O	2.20	0.42
4:E:490:GLN:HG3	4:E:532:GLU:HB3	2.00	0.42
5:L:451:ARG:HA	5:L:452:PRO:HD3	1.88	0.42
5:L:510:GLN:OE1	5:L:510:GLN:N	2.39	0.42
6:J:49:ILE:CD1	6:J:103:TYR:CD1	2.86	0.42
6:J:111:ALA:O	6:J:125:GLU:HA	2.20	0.42
4:F:469:SER:HA	4:F:524:SER:HA	2.01	0.42
4:G:378:VAL:HG12	4:G:430:HIS:CD2	2.54	0.42
5:L:500:TYR:HB2	5:L:521:LEU:CD1	2.37	0.42
4:D:449:LEU:HA	4:D:449:LEU:HD23	1.59	0.41
5:L:480:SER:HB3	5:L:514:ARG:HA	2.02	0.41
4:H:450:HIS:CE1	4:H:514:ARG:HE	2.39	0.41
4:H:566:LEU:HD23	3:K:568:MET:HE1	2.01	0.41
7:R:96:GLU:OE2	7:R:122:VAL:HG22	2.19	0.41
2:B:468:GLU:HG2	7:R:67:PHE:CD2	2.55	0.41
4:E:430:HIS:CD2	4:E:431:THR:H	2.38	0.41
6:J:68:CYS:O	6:J:68:CYS:SG	2.79	0.41
4:G:476:VAL:HG12	4:G:479:PHE:HD2	1.84	0.41
5:L:488:TRP:CD1	5:L:521:LEU:CD2	2.87	0.41
7:R:34:THR:CB	7:R:88:LEU:HD12	2.42	0.41
2:B:351:PRO:HB3	2:B:441:ILE:HD11	2.03	0.41
2:B:475:LEU:HA	2:B:518:HIS:HB2	2.01	0.41
4:E:543:LEU:HB2	4:E:546:ARG:HA	2.03	0.41
5:L:381:SER:HB2	5:L:427:THR:HB	2.02	0.41
5:L:575:CYS:H	6:J:102:THR:CB	2.31	0.41
6:J:60:PHE:HB3	6:J:62:TYR:CE2	2.55	0.41
4:F:443:ARG:HA	4:F:444:PRO:HD3	1.94	0.41
4:F:452:PRO:HB3	4:F:479:PHE:CB	2.40	0.41
4:F:493:GLN:OE1	4:F:493:GLN:HA	2.21	0.41
4:H:543:LEU:CG	4:H:548:THR:HG22	2.51	0.41
4:H:562:TYR:CB	3:K:562:TYR:HB2	2.51	0.41
3:K:477:THR:HG22	3:K:516:PHE:HB2	2.03	0.41
3:C:449:LEU:HB3	3:C:542:ALA:HB2	2.01	0.41
4:E:372:LEU:HD21	4:E:430:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:508:GLU:HG3	4:E:509:PRO:HD2	2.01	0.41
4:E:529:ASN:HA	4:E:554:LYS:HE2	0.90	0.41
4:F:385:GLN:OE1	4:F:385:GLN:HA	2.21	0.41
3:K:413:ILE:HG22	3:K:414:CYS:N	2.35	0.41
5:L:506:MET:C	5:L:515:TYR:HB3	2.39	0.41
1:A:524:SER:OG	1:A:526:GLU:OE1	2.39	0.41
2:B:384:ARG:NH1	2:B:388:GLU:HB3	2.36	0.41
4:F:352:PRO:HD3	4:F:365:LEU:HD23	2.03	0.41
4:G:520:ILE:O	4:G:520:ILE:HG13	2.21	0.41
4:D:450:HIS:HE1	4:D:480:SER:OG	1.88	0.41
4:F:449:LEU:HA	4:F:480:SER:OG	2.20	0.41
4:H:532:GLU:HB3	4:H:534:TYR:CD2	2.56	0.41
4:H:553:ASP:OD1	4:H:553:ASP:N	2.54	0.41
3:K:463:GLN:HG2	5:L:455:TYR:HE2	1.79	0.41
3:K:505:PRO:HA	3:K:516:PHE:O	2.20	0.41
5:L:452:PRO:HB2	5:L:477:THR:C	2.29	0.41
5:L:467:ARG:HA	5:L:525:GLU:HG3	2.02	0.41
6:J:109:TYR:H	6:J:129:THR:CG2	2.33	0.41
2:B:465:ASN:ND2	5:L:571:THR:HG21	2.36	0.41
4:F:452:PRO:CA	4:F:479:PHE:HB3	2.51	0.41
3:K:451:ARG:CZ	3:K:451:ARG:CB	2.95	0.41
3:K:461:ARG:HB2	3:K:461:ARG:HH11	1.85	0.41
5:L:470:ALA:O	5:L:523:VAL:CG2	2.69	0.41
6:J:8:VAL:HG12	6:J:10:ASN:H	1.85	0.41
6:J:20:ARG:NH1	6:J:34:GLU:HG2	2.36	0.41
7:R:24:LYS:HD3	7:R:24:LYS:HA	1.95	0.41
4:G:360:THR:HG23	4:G:362:SER:HB3	2.03	0.40
4:H:428:VAL:HB	4:H:437:LEU:HB2	2.03	0.40
5:L:352:PRO:HD3	5:L:365:LEU:HD22	2.03	0.40
5:L:443:ARG:HD3	5:L:443:ARG:HA	1.67	0.40
5:L:488:TRP:O	5:L:495:LEU:N	2.54	0.40
2:B:437:LEU:HD23	2:B:437:LEU:H	1.86	0.40
2:B:502:THR:HA	2:B:519:SER:HB2	1.98	0.40
4:E:532:GLU:O	4:E:533:THR:OG1	2.30	0.40
4:F:451:ARG:HB2	4:F:451:ARG:HH11	1.84	0.40
4:H:459:PRO:HG3	4:H:470:ALA:HB1	2.03	0.40
4:H:535:THR:HA	4:H:551:THR:OG1	2.21	0.40
5:L:543:LEU:HB2	5:L:546:ARG:HA	2.02	0.40
6:J:4:ARG:HG2	6:J:20:ARG:HD2	2.03	0.40
6:J:112:VAL:O	6:J:112:VAL:CG2	2.69	0.40
7:R:35:ILE:N	7:R:88:LEU:CD1	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:533:THR:HB	4:D:535:THR:HG23	2.04	0.40
4:E:468:GLU:N	4:E:525:GLU:OE2	2.54	0.40
4:G:421:GLY:H	4:G:443:ARG:HE	1.61	0.40
4:G:449:LEU:HG	4:G:542:ALA:HB2	2.03	0.40
3:K:432:ASP:OD1	3:K:433:LEU:N	2.53	0.40
1:A:568:MET:CE	6:J:37:ILE:HD13	2.51	0.40
4:E:558:LYS:HB3	4:E:559:PRO:HD3	1.64	0.40
4:G:489:MET:CG	4:G:489:MET:O	2.69	0.40
3:K:506:MET:O	3:K:516:PHE:HD1	2.04	0.40
5:L:506:MET:CB	5:L:507:PRO:CD	2.94	0.40
6:J:133:CYS:O	6:J:133:CYS:SG	2.79	0.40
3:C:423:ARG:CA	3:C:442:SER:HG	2.23	0.40
4:E:422:GLU:HB3	4:E:424:PHE:HE2	1.87	0.40
4:G:364:LYS:HD2	4:G:364:LYS:HA	1.91	0.40
3:K:520:ILE:HD12	5:L:516:PHE:CE1	2.56	0.40
5:L:354:PHE:CZ	5:L:541:GLU:HB3	2.56	0.40
5:L:567:VAL:CG2	6:J:40:ILE:HG12	2.51	0.40
7:R:33:VAL:H	7:R:91:VAL:HG23	1.87	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	228/231 (99%)	213 (93%)	15 (7%)	0	100	100
2	B	226/229 (99%)	191 (84%)	29 (13%)	6 (3%)	5	5
3	C	223/226 (99%)	196 (88%)	26 (12%)	1 (0%)	34	34
3	K	223/226 (99%)	204 (92%)	18 (8%)	1 (0%)	34	34
4	D	222/225 (99%)	207 (93%)	15 (7%)	0	100	100
4	E	222/225 (99%)	200 (90%)	19 (9%)	3 (1%)	11	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	222/225 (99%)	206 (93%)	16 (7%)	0	100	100
4	G	222/225 (99%)	196 (88%)	25 (11%)	1 (0%)	29	29
4	H	222/225 (99%)	202 (91%)	20 (9%)	0	100	100
5	L	224/229 (98%)	205 (92%)	16 (7%)	3 (1%)	12	12
6	J	99/104 (95%)	82 (83%)	16 (16%)	1 (1%)	15	15
7	R	105/107 (98%)	98 (93%)	6 (6%)	1 (1%)	15	15
All	All	2438/2477 (98%)	2200 (90%)	221 (9%)	17 (1%)	26	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	532	GLU
4	E	559	PRO
4	E	560	THR
2	B	494	PRO
2	B	497	PRO
2	B	447	VAL
2	B	449	LEU
2	B	491	ARG
5	L	452	PRO
5	L	575	CYS
4	E	557	GLY
4	G	481	PRO
3	K	532	GLU
6	J	36	ASN
3	C	444	PRO
7	R	113	GLY
5	L	523	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/204 (100%)	199 (98%)	5 (2%)	47	47
2	B	203/203 (100%)	188 (93%)	15 (7%)	13	13
3	C	201/201 (100%)	195 (97%)	6 (3%)	41	41
3	K	201/201 (100%)	188 (94%)	13 (6%)	17	17
4	D	200/200 (100%)	196 (98%)	4 (2%)	55	55
4	E	200/200 (100%)	193 (96%)	7 (4%)	36	36
4	F	200/200 (100%)	195 (98%)	5 (2%)	47	47
4	G	200/200 (100%)	188 (94%)	12 (6%)	19	19
4	H	200/200 (100%)	187 (94%)	13 (6%)	17	17
5	L	204/204 (100%)	185 (91%)	19 (9%)	9	9
6	J	97/97 (100%)	89 (92%)	8 (8%)	11	11
7	R	92/92 (100%)	70 (76%)	22 (24%)	0	0
All	All	2202/2202 (100%)	2073 (94%)	129 (6%)	23	19

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	ASN
1	A	423	ARG
1	A	447	VAL
1	A	449	LEU
1	A	450	HIS
2	B	443	ARG
2	B	445	LYS
2	B	447	VAL
2	B	490	GLN
2	B	491	ARG
2	B	493	GLN
2	B	494	PRO
2	B	498	GLU
2	B	499	LYS
2	B	516	PHE
2	B	518	HIS
2	B	525	GLU
2	B	530	THR
2	B	547	VAL

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Mol	Chain	Res	Type
2	B	571	THR
3	C	441	ILE
3	C	443	ARG
3	C	445	LYS
3	C	545	ASN
3	C	565	SER
3	C	566	LEU
4	D	445	LYS
4	D	447	VAL
4	D	450	HIS
4	D	461	ARG
4	E	443	ARG
4	E	445	LYS
4	E	449	LEU
4	E	451	ARG
4	E	453	ASP
4	E	553	ASP
4	E	554	LYS
4	F	445	LYS
4	F	449	LEU
4	F	450	HIS
4	F	451	ARG
4	F	561	LEU
4	G	442	SER
4	G	443	ARG
4	G	445	LYS
4	G	449	LEU
4	G	485	PHE
4	G	489	MET
4	G	490	GLN
4	G	491	ARG
4	G	493	GLN
4	G	495	LEU
4	G	498	GLU
4	G	499	LYS
4	H	443	ARG
4	H	445	LYS
4	H	447	VAL
4	H	449	LEU
4	H	451	ARG
4	H	514	ARG
4	H	548	THR

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Mol	Chain	Res	Type
4	H	550	ARG
4	H	551	THR
4	H	562	TYR
4	H	563	ASN
4	H	566	LEU
4	H	567	VAL
3	K	443	ARG
3	K	449	LEU
3	K	450	HIS
3	K	451	ARG
3	K	514	ARG
3	K	516	PHE
3	K	518	HIS
3	K	529	ASN
3	K	530	THR
3	K	532	GLU
3	K	555	SER
3	K	556	THR
3	K	558	LYS
5	L	443	ARG
5	L	450	HIS
5	L	451	ARG
5	L	455	TYR
5	L	467	ARG
5	L	484	VAL
5	L	485	PHE
5	L	487	GLN
5	L	496	SER
5	L	498	GLU
5	L	499	LYS
5	L	500	TYR
5	L	501	VAL
5	L	502	THR
5	L	514	ARG
5	L	516	PHE
5	L	521	LEU
5	L	523	VAL
5	L	571	THR
6	J	36	ASN
6	J	39	ILE
6	J	57	ARG
6	J	101	TYR

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Mol	Chain	Res	Type
6	J	112	VAL
6	J	128	LEU
6	J	129	THR
6	J	131	ASP
7	R	26	GLU
7	R	28	GLU
7	R	34	THR
7	R	35	ILE
7	R	39	LEU
7	R	41	GLU
7	R	44	VAL
7	R	86	LEU
7	R	87	PHE
7	R	88	LEU
7	R	90	GLU
7	R	92	THR
7	R	97	SER
7	R	98	ASP
7	R	108	MET
7	R	109	ASN
7	R	111	ASP
7	R	112	ARG
7	R	119	THR
7	R	121	ASN
7	R	123	HIS
7	R	124	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	430	HIS
2	B	465	ASN
2	B	510	GLN
4	D	487	GLN
4	E	490	GLN
4	E	545	ASN
4	F	545	ASN
4	G	430	HIS
4	H	400	HIS
3	K	430	HIS
3	K	518	HIS
5	L	518	HIS

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Mol	Chain	Res	Type
7	R	109	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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
6	J	2
5	L	2
1	A	1
2	B	1
4	G	1
4	H	1
3	K	1
3	C	1
4	F	1
4	E	1
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	574:THR	C	583:NAG	O6	29.11
1	J	135:PRO	C	160:NAG	O3	21.22
1	L	576:TYR	C	583:NAG	O3	19.52
1	B	572:ALA	C	583:NAG	O6	18.96
1	G	568:MET	C	583:NAG	O3	17.32
1	H	568:MET	C	583:NAG	O3	17.31
1	K	569:SER	C	583:NAG	O3	17.26
1	C	569:SER	C	583:NAG	O6	16.94
1	F	568:MET	C	583:NAG	O3	15.73
1	E	568:MET	C	583:NAG	O6	13.64
1	J	68:CYS	C	99:THR	N	13.17
1	D	568:MET	C	583:NAG	O6	13.00
1	L	444:PRO	C	449:LEU	N	9.32

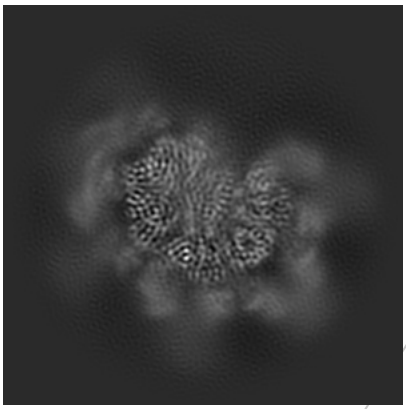
6 Map visualisation

This section contains visualisations of the EMDB entry D_1300031558. These allow visual inspection of the internal detail of the map and identification of artifacts.

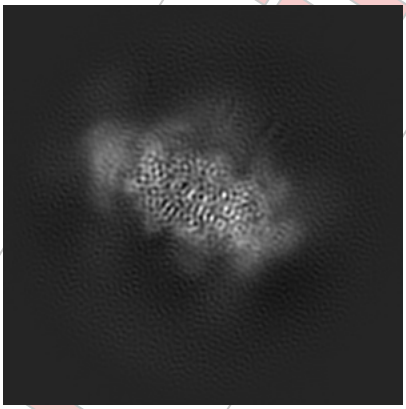
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

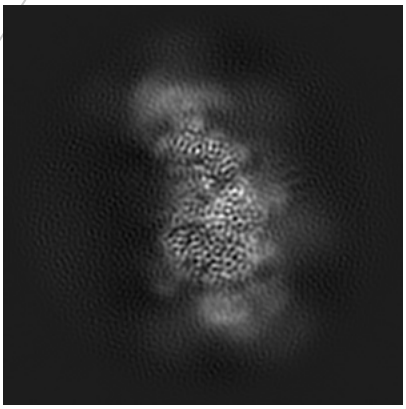
6.1.1 Primary map



X

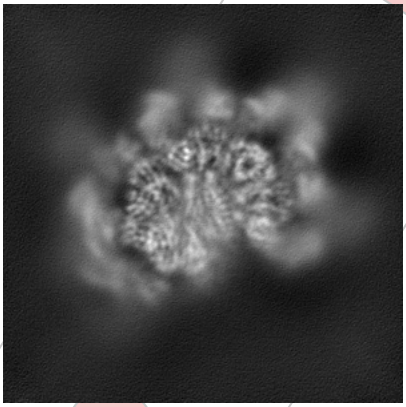


Y

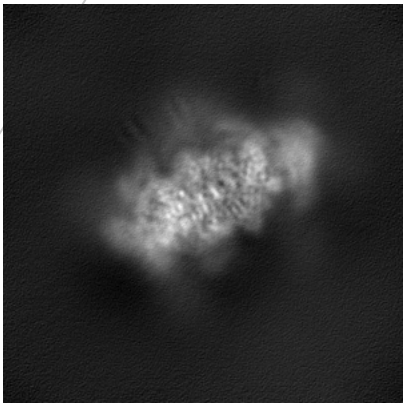


Z

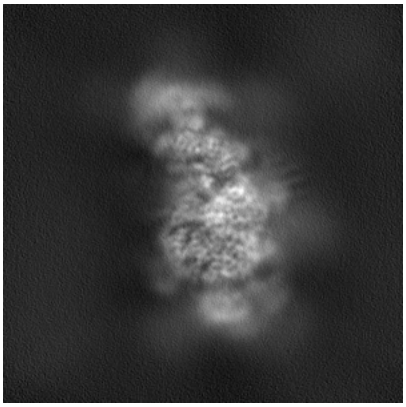
6.1.2 Raw map



X



Y

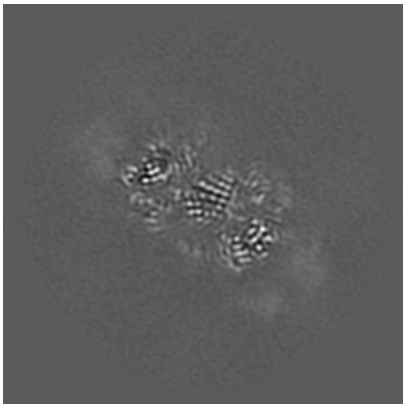


Z

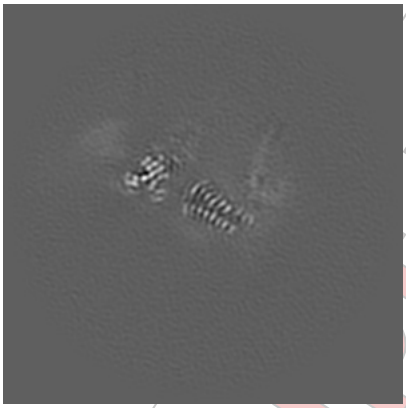
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

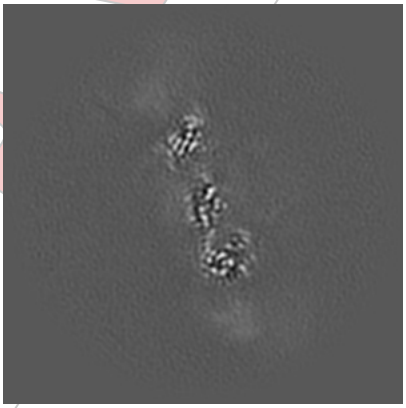
6.2.1 Primary map



X Index: 160

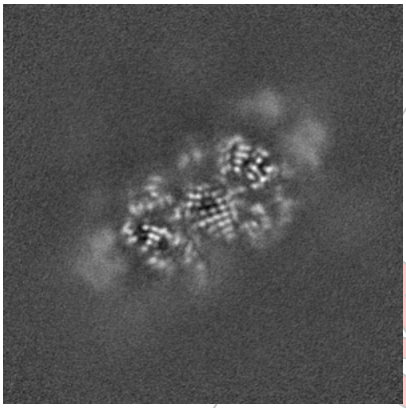


Y Index: 160

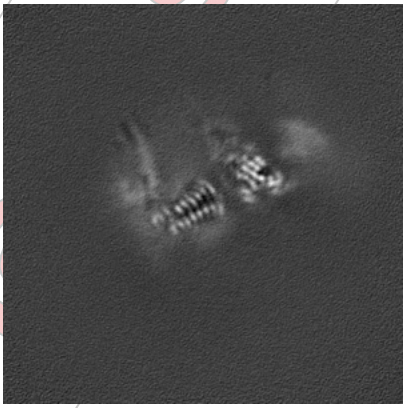


Z Index: 160

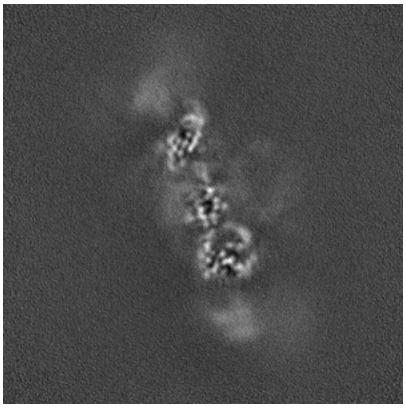
6.2.2 Raw map



X Index: 160



Y Index: 160

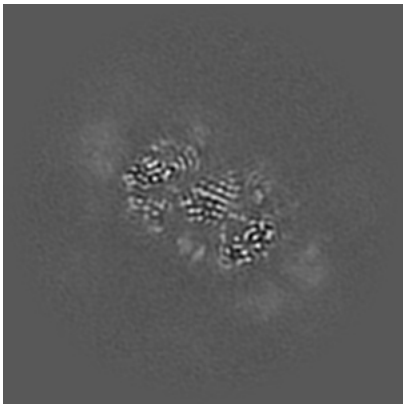


Z Index: 160

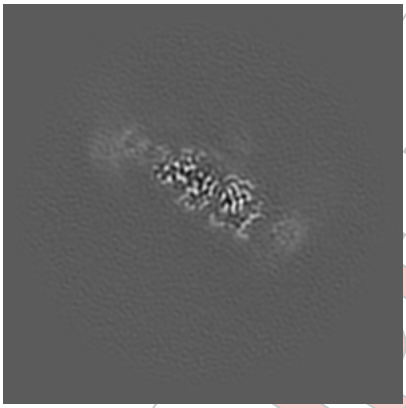
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

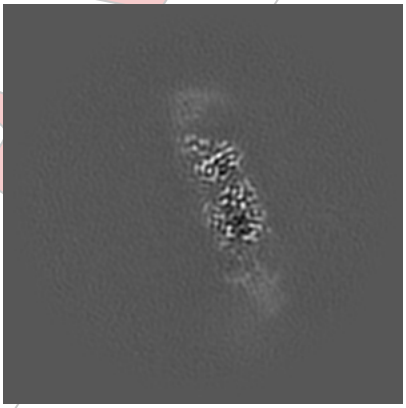
6.3.1 Primary map



X Index: 162

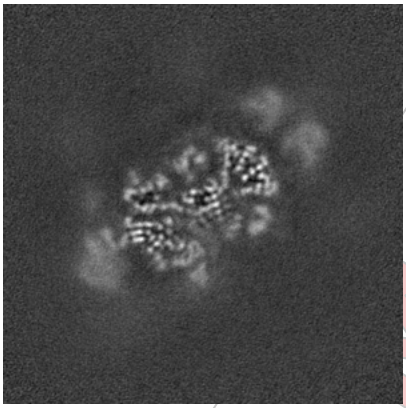


Y Index: 117

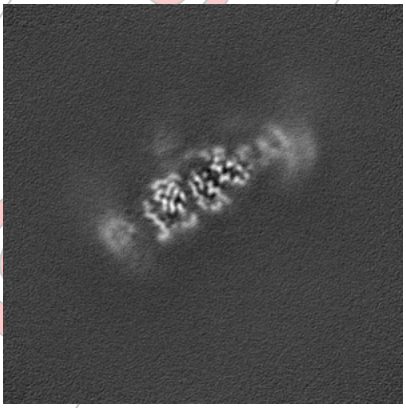


Z Index: 120

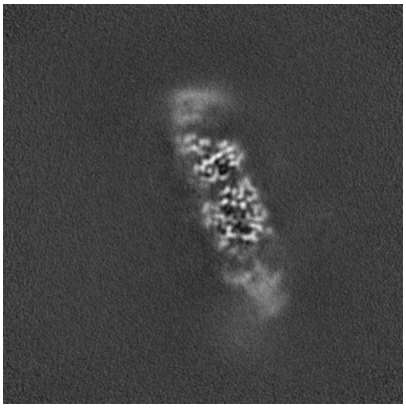
6.3.2 Raw map



X Index: 166



Y Index: 117



Z Index: 199

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

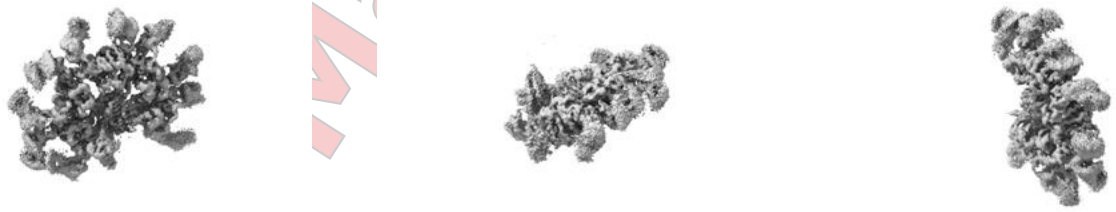
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.19. 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.

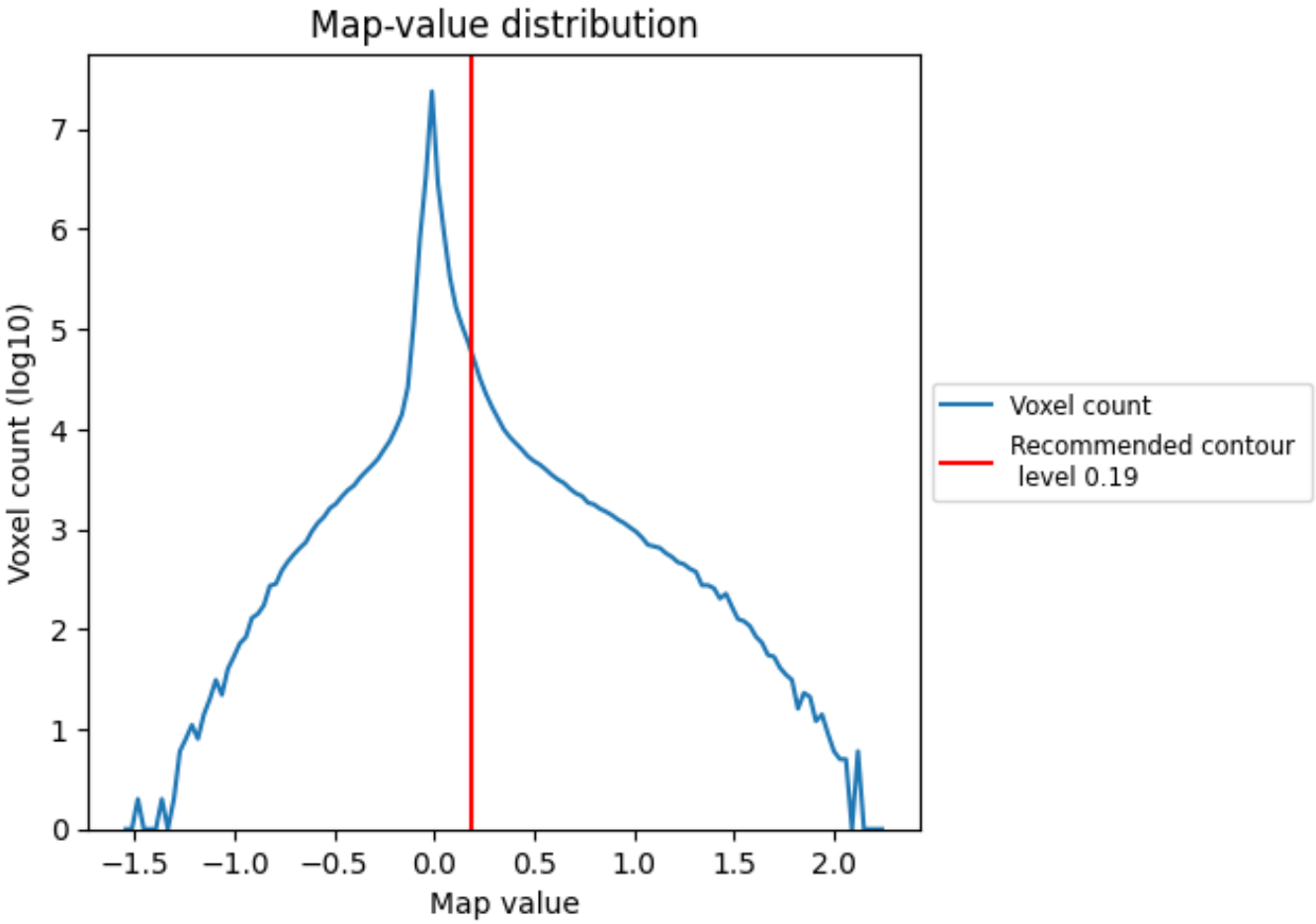
6.5 Mask visualisation (i)

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

7 Map analysis

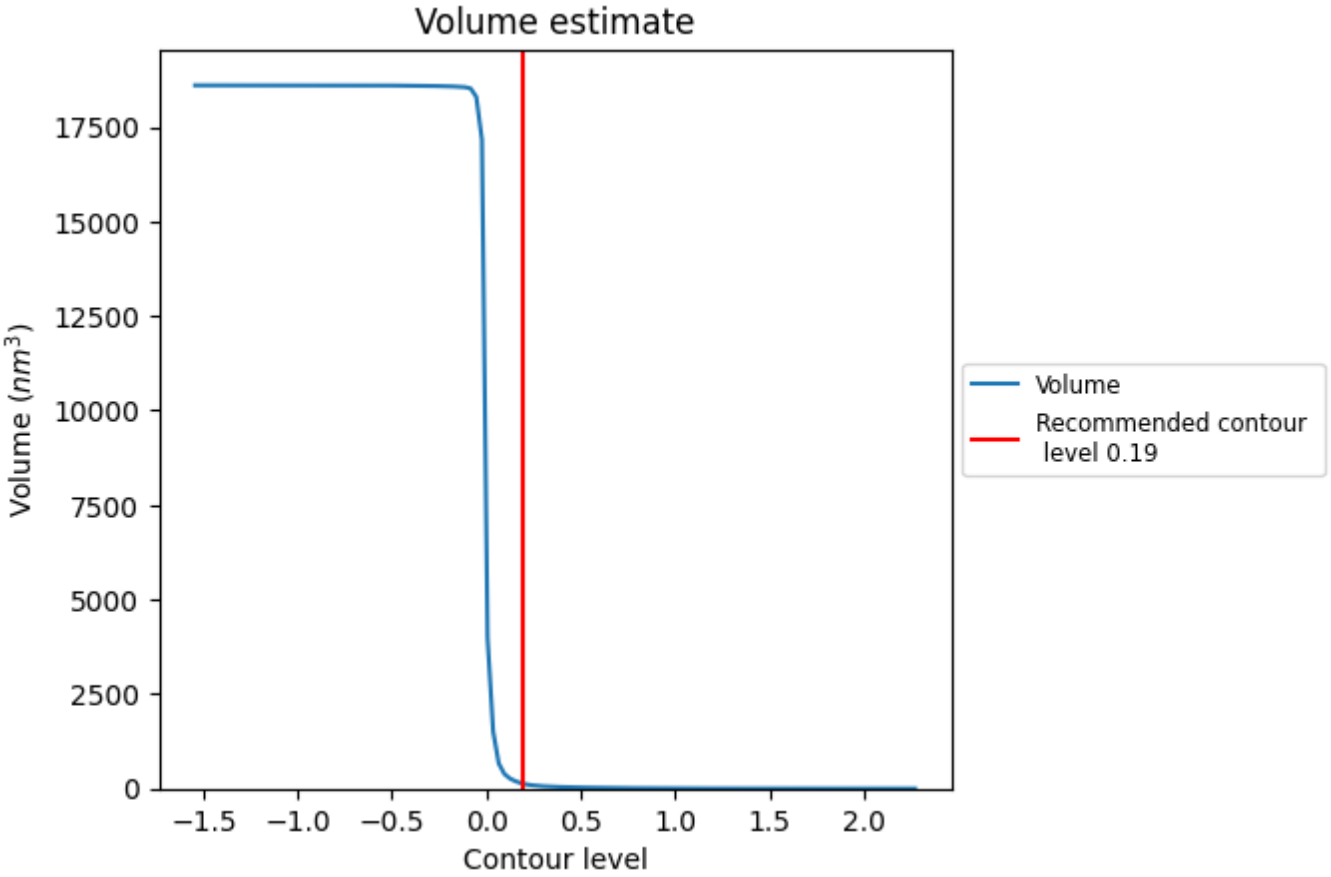
This section contains the results of statistical analysis of the map.

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.

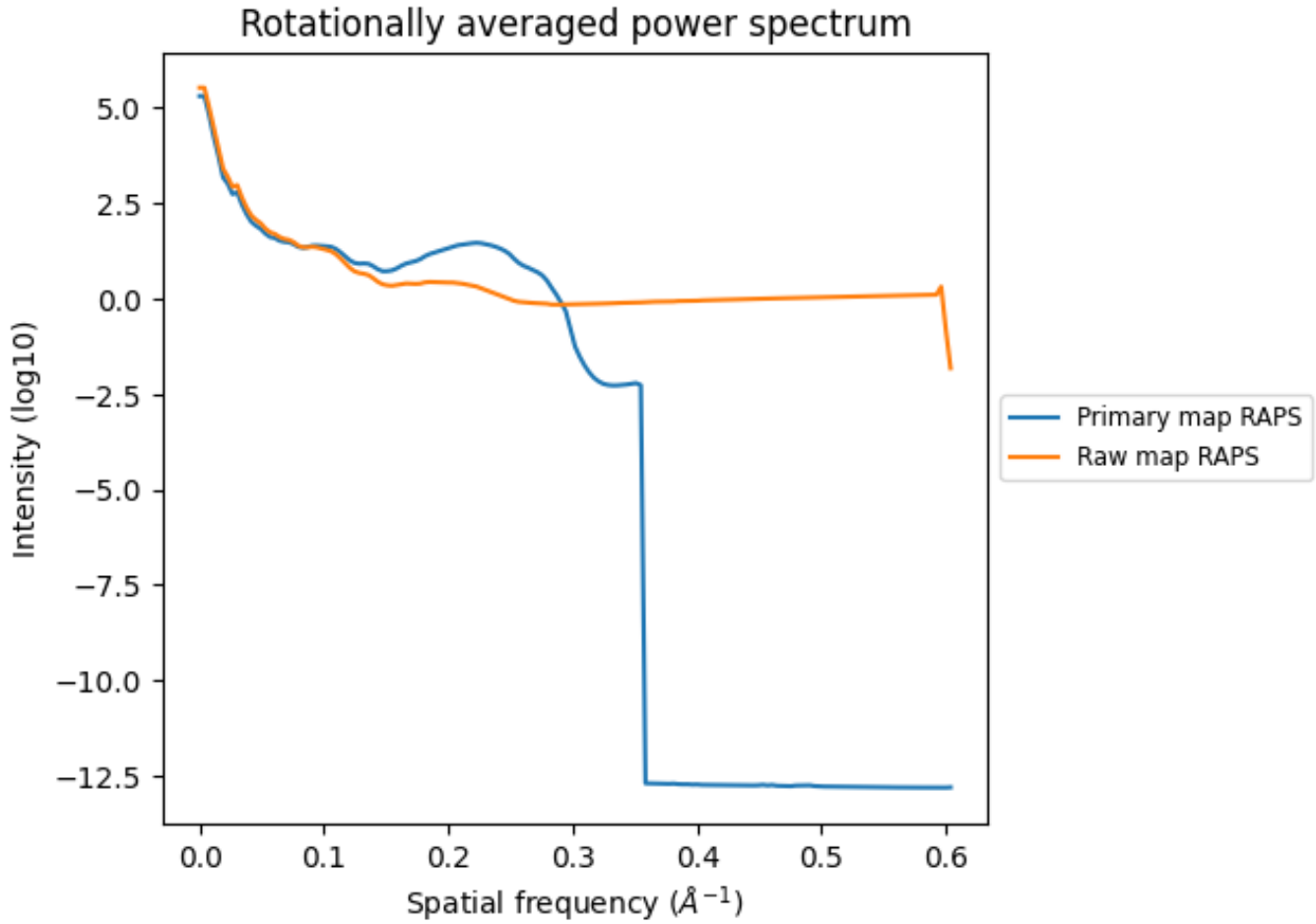
7.2 Volume estimate (i)



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.

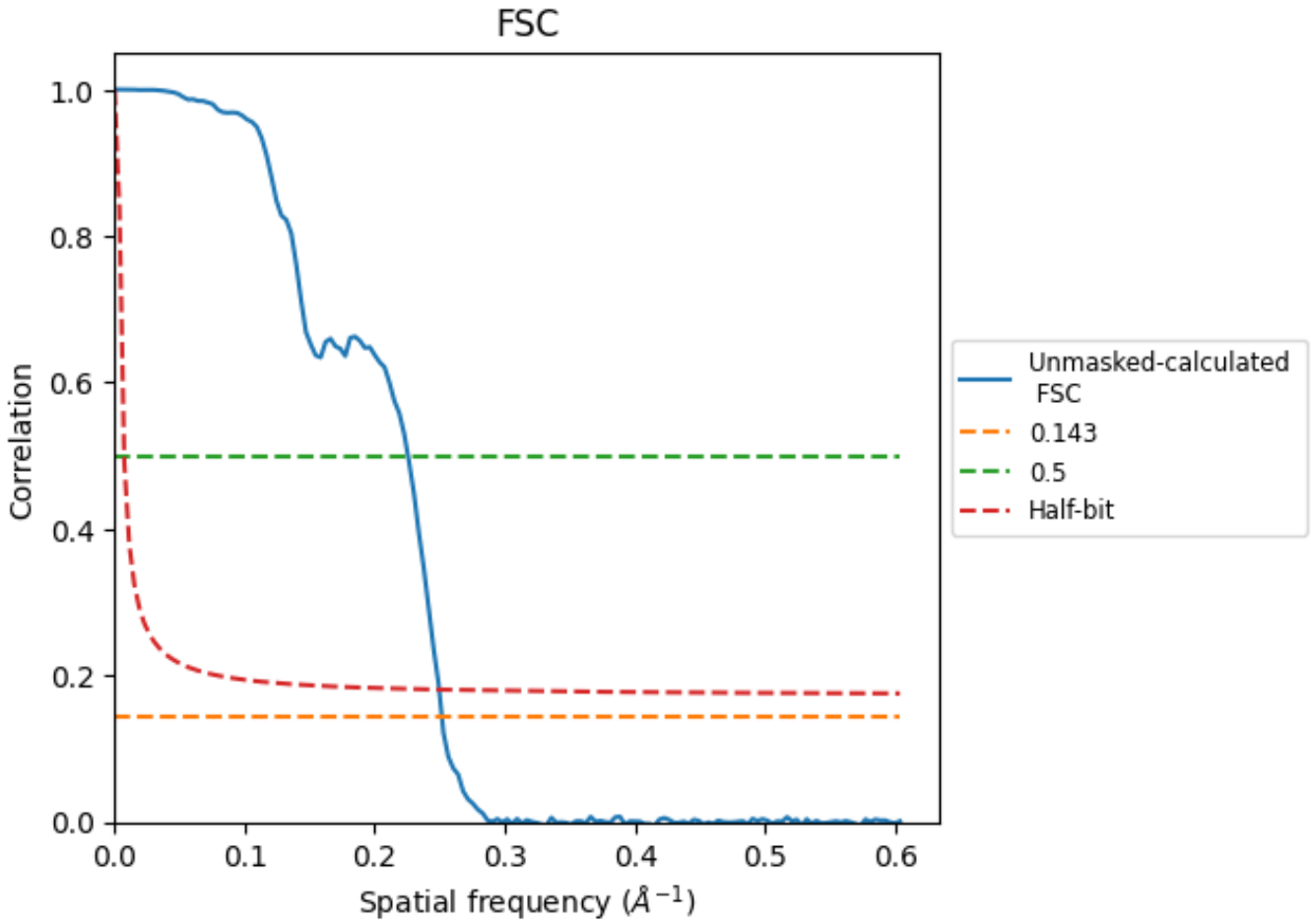
7.3 Rotationally averaged power spectrum (i)



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)

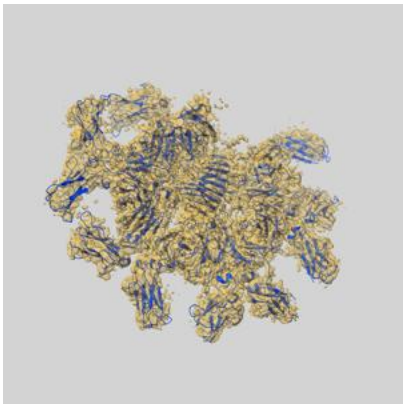
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.97	4.43	4.01

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

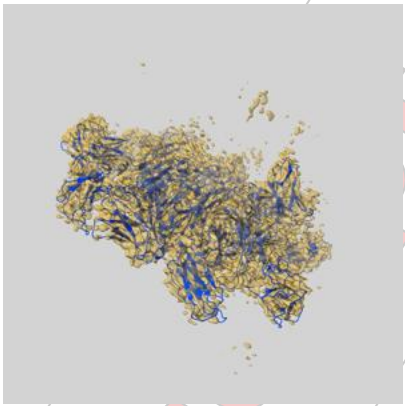
9 Map-model fit

This section contains information regarding the fit between EMDB map D_1300031558 and PDB model D_1300031558. Per-residue inclusion information can be found in section 3 on page 6.

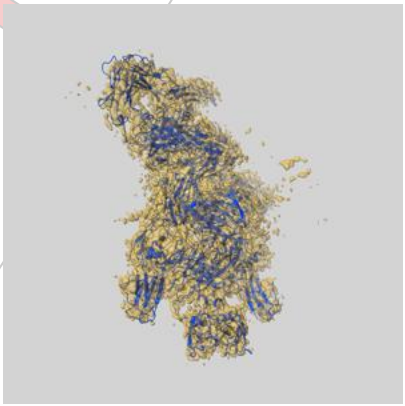
9.1 Map-model overlay



X



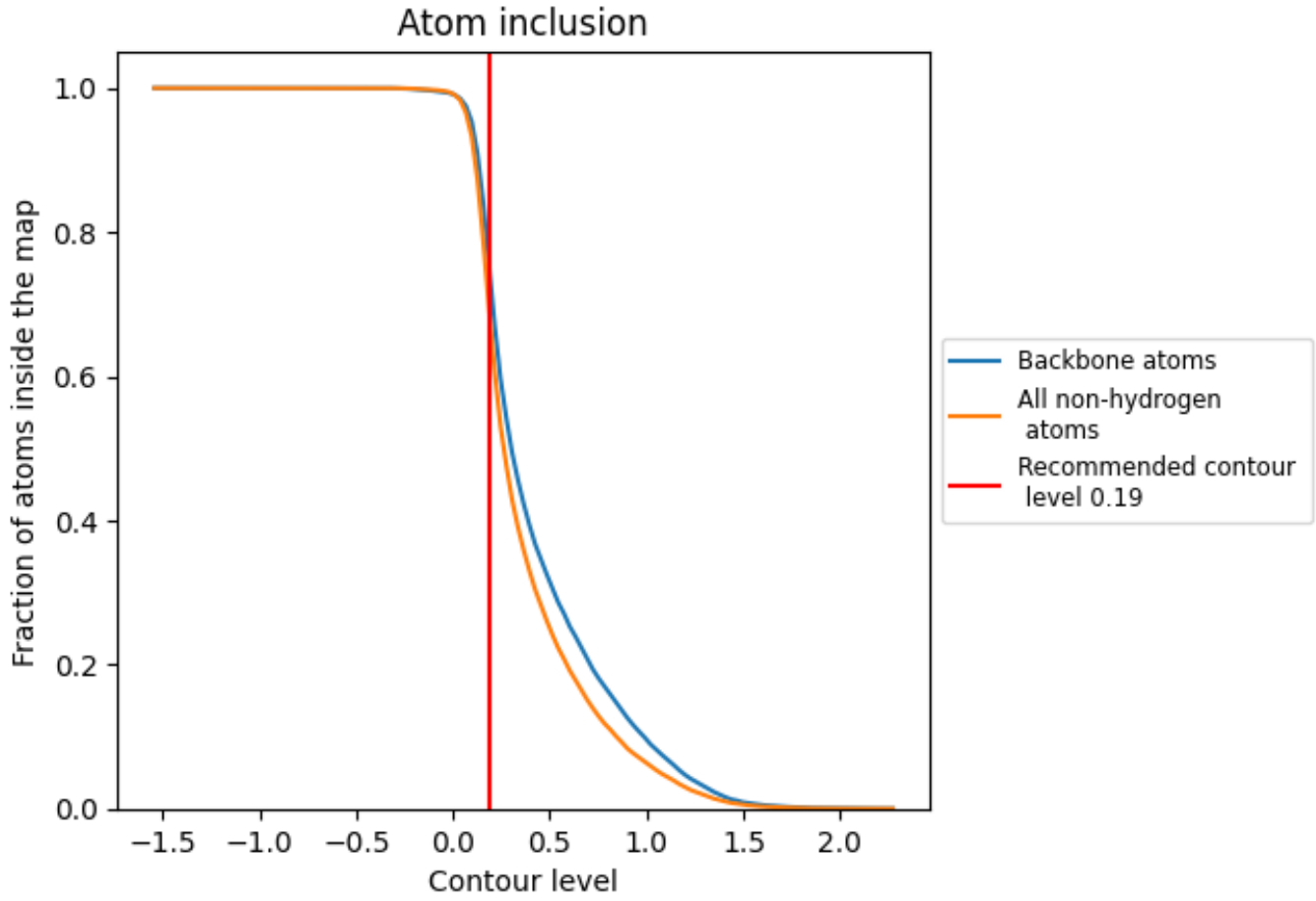
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.19 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, 74% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.