



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:56 PM UTC

PDB ID : 7XHO / pdb_00007xho
EMDB ID : EMD-33197
Title : Structure of human inner kinetochore CCAN complex
Authors : Tian, T.; Wang, C.L.; Yang, Z.S.; Sun, L.F.; Zang, J.Y.
Deposited on : 2022-04-09
Resolution : 3.29 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

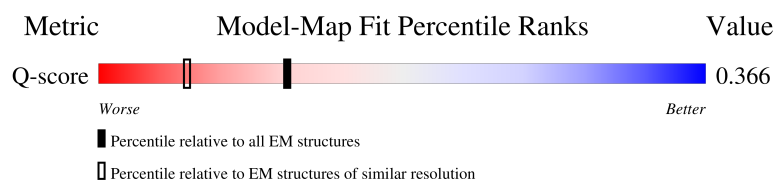
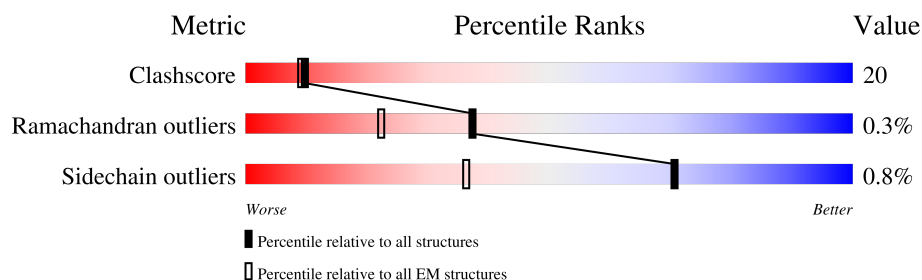
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

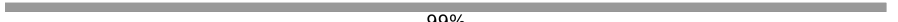
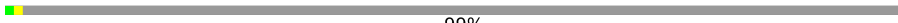
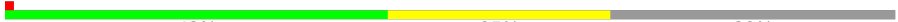
The reported resolution of this entry is 3.29 Å.

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



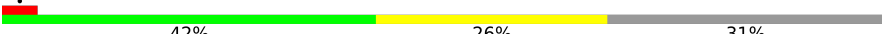
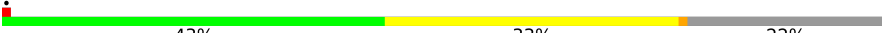
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14466 (2.79 - 3.79)

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 $\leq 5\%$. 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	C	943	 99%
1	c	943	 99%
2	H	247	 52% 27% 21%
3	I	756	 43% 25% 32%

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Mol	Chain	Length	Quality of chain
4	K	269	
5	L	344	
6	M	180	
7	N	339	
8	O	300	
9	P	288	
10	Q	268	
11	S	138	
12	T	561	
13	W	88	
14	X	81	
15	R	177	
16	U	418	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 22243 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Centromere protein C.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	C	5	Total	C	N	O	0	0
			40	28	5	7		
1	c	13	Total	C	N	O	0	0
			105	69	17	19		

- Molecule 2 is a protein called Centromere protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	195	Total	C	N	O	S	0	0
			1560	980	273	299	8		

- Molecule 3 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	517	Total	C	N	O	S	0	0
			4111	2700	661	724	26		

- Molecule 4 is a protein called Centromere protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	230	Total	C	N	O	S	0	0
			1869	1183	312	364	10		

- Molecule 5 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	302	Total	C	N	O	S	0	0
			2422	1576	395	437	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	116	ASP	ASN	engineered mutation	UNP Q8N0S6

- Molecule 6 is a protein called Centromere protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	168	Total	C	N	O	S	0	0
			1298	825	232	234	7		

- Molecule 7 is a protein called Centromere protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	305	Total	C	N	O	S	0	0
			2492	1600	434	448	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	84	ASP	GLU	variant	UNP Q96H22

- Molecule 8 is a protein called Centromere protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	206	Total	C	N	O	S	0	0
			1588	1017	269	294	8		

- Molecule 9 is a protein called Centromere protein P.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	224	Total	C	N	O	S	0	0
			1808	1144	311	344	9		

- Molecule 10 is a protein called Centromere protein Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	164	Total	C	N	O	S	0	0
			1175	718	207	242	8		

- Molecule 11 is a protein called Centromere protein S.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	97	Total	C	N	O	S	0	0
			790	494	141	150	5		

- Molecule 12 is a protein called Centromere protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	99	Total	C	N	O	S	0	0
			804	516	139	142	7		

- Molecule 13 is a protein called CENP-W.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	75	Total	C	N	O	S	0	0
			584	367	119	95	3		

- Molecule 14 is a protein called Centromere protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	74	Total	C	N	O	S	0	0
			590	378	104	107	1		

- Molecule 15 is a protein called Centromere protein R.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	R	62	Total	C	N	O	0	0
			308	184	62	62		

- Molecule 16 is a protein called Centromere protein U.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	U	140	Total	C	N	O	0	0
			699	419	140	140		

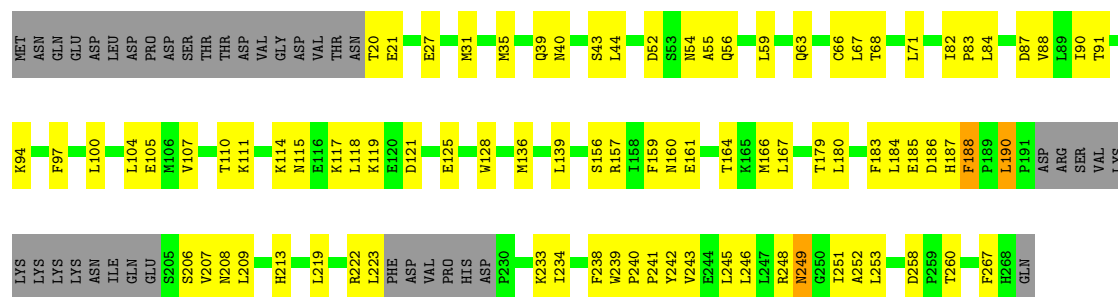
Response	Percentage
Best for the country	52%
Not the best for the country	27%
Don't know	21%



Frequency	Percentage
Daily	43%
Weekly	25%
Monthly	32%

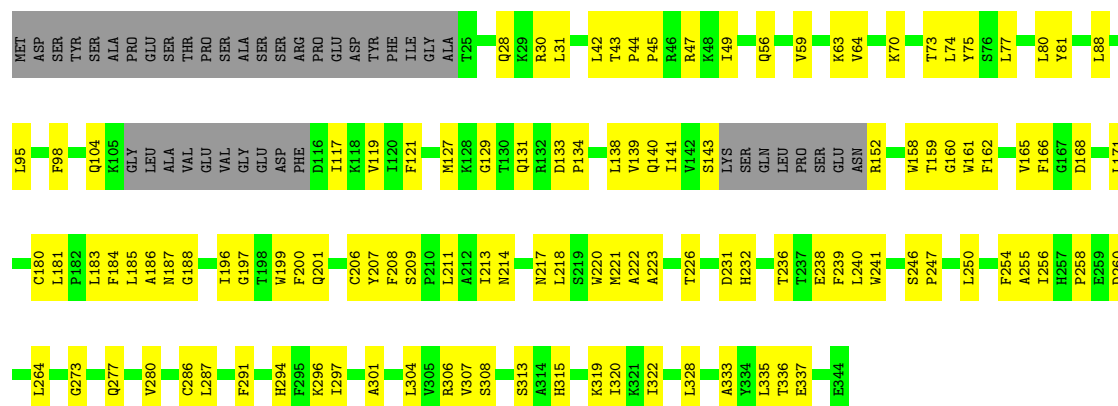


Category	Percentage
Very bad	53%
Bad	31%
Good	1%
Very good	14%



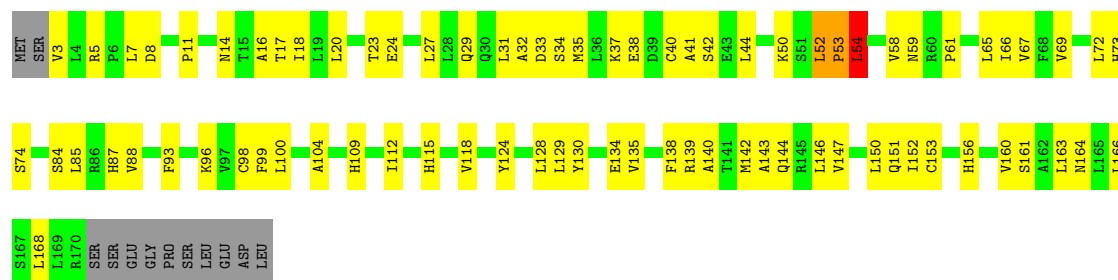
• Molecule 5: Centromere protein L

Chain L: 55% 33% 12%



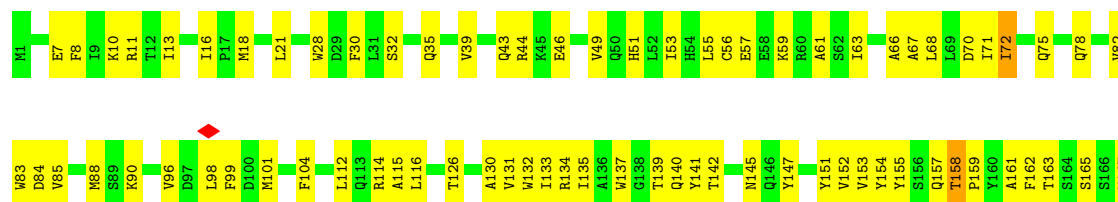
• Molecule 6: Centromere protein M

Chain M: 50% 42% 7%



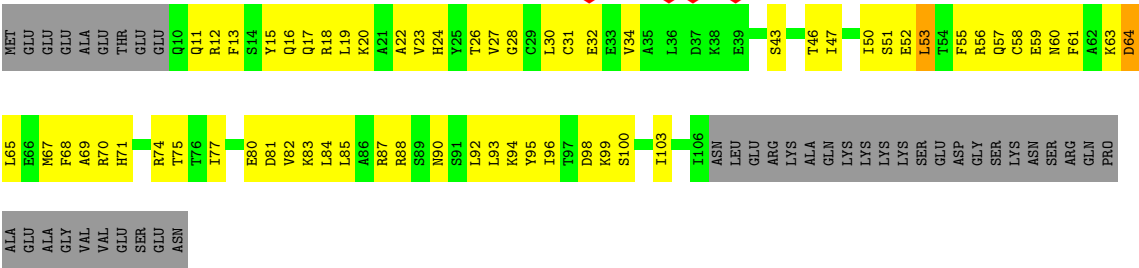
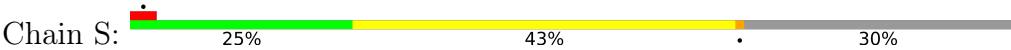
• Molecule 7: Centromere protein N

Chain N: 51% 39% 10%

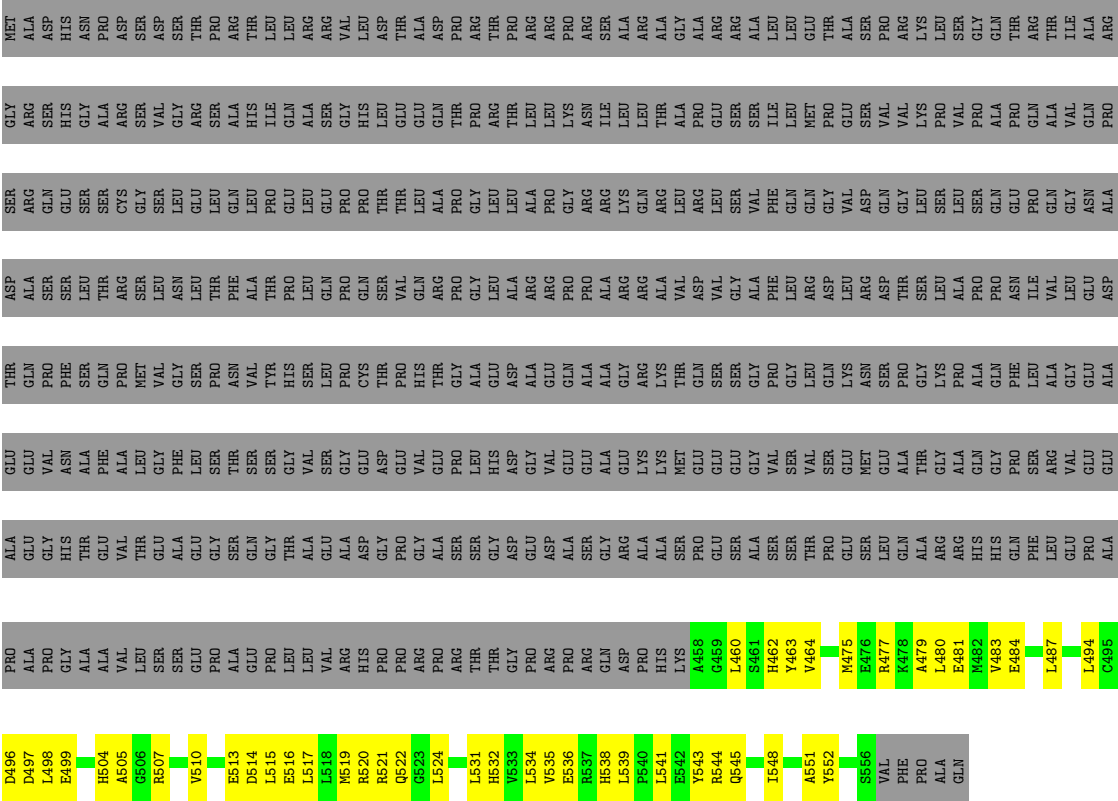




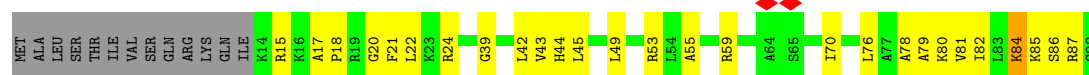
• Molecule 11: Centromere protein S



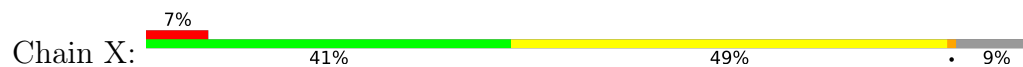
• Molecule 12: Centromere protein T



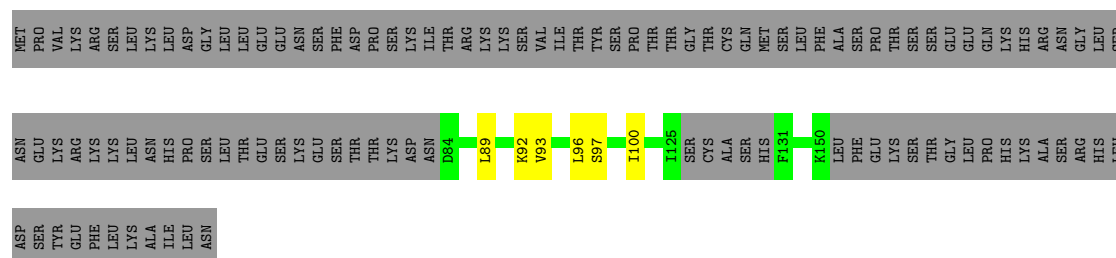
- Molecule 13: CENP-W



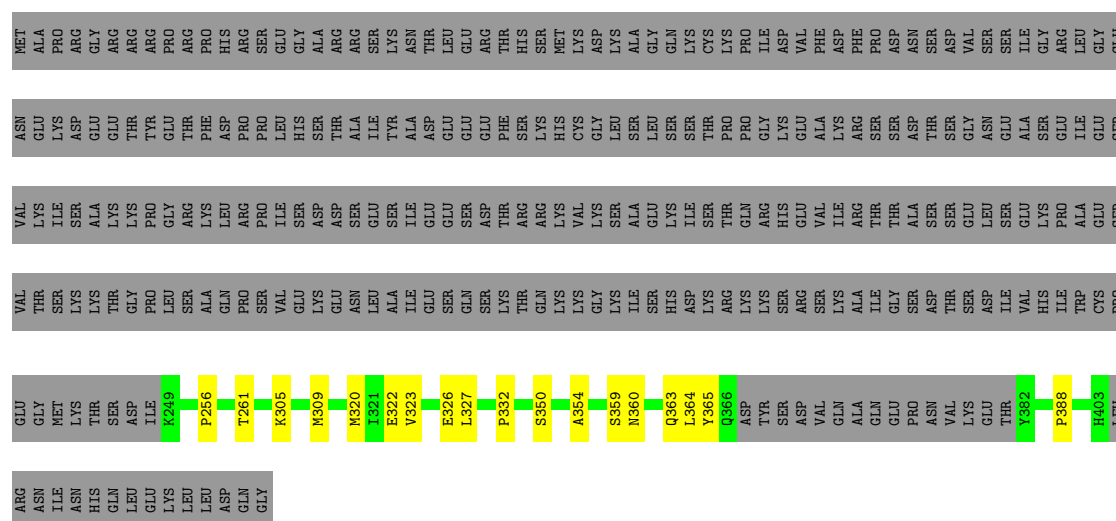
- Molecule 14: Centromere protein X



- Molecule 15: Centromere protein R



- Molecule 16: Centromere protein U



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	200560	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	5.448	Depositor
Minimum map value	-2.649	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	380.64, 380.64, 380.64	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.22, 1.22, 1.22	Depositor

5 Model quality

5.1 Standard geometry

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	C	0.31	0/40	0.75	0/53
1	c	0.25	0/106	0.73	0/141
2	H	0.15	0/1566	0.48	1/2093 (0.0%)
3	I	0.16	0/4210	0.51	3/5704 (0.1%)
4	K	0.19	0/1897	0.54	1/2558 (0.0%)
5	L	0.16	0/2487	0.46	0/3379
6	M	0.19	0/1320	0.42	0/1791
7	N	0.20	0/2546	0.53	1/3439 (0.0%)
8	O	0.23	0/1624	0.54	1/2208 (0.0%)
9	P	0.25	0/1839	0.64	8/2474 (0.3%)
10	Q	0.25	0/1175	0.76	2/1580 (0.1%)
11	S	0.19	0/799	0.57	0/1070
12	T	0.21	0/821	0.63	0/1105
13	W	0.18	0/590	0.53	0/785
14	X	0.19	0/596	0.55	0/801
15	R	0.22	0/306	0.50	0/424
16	U	0.21	0/697	0.67	3/972 (0.3%)
All	All	0.20	0/22619	0.55	20/30577 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
9	P	166	PHE	N-CA-C	-7.29	104.19	113.23
3	I	156	CYS	N-CA-C	-6.95	95.99	110.80
9	P	195	VAL	N-CA-C	6.77	117.59	107.51
3	I	599	ILE	N-CA-C	-6.56	106.40	112.96
10	Q	222	PRO	N-CA-CB	6.46	110.03	103.25
16	U	256	PRO	N-CA-CB	6.29	110.25	103.33
16	U	388	PRO	N-CA-CB	6.28	110.24	103.33
16	U	332	PRO	N-CA-CB	6.21	110.16	103.33
9	P	194	ALA	CA-C-N	-6.10	114.94	122.93
9	P	194	ALA	C-N-CA	-6.10	114.94	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	272	GLU	N-CA-C	-6.02	97.98	110.80
10	Q	100	ILE	N-CA-CB	-6.01	98.15	111.50
9	P	192	PRO	CB-CA-C	-5.67	102.21	111.56
9	P	195	VAL	N-CA-CB	-5.56	104.46	111.41
4	K	234	ILE	N-CA-CB	-5.46	104.74	112.12
3	I	157	SER	N-CA-C	-5.29	103.91	110.41
9	P	192	PRO	N-CA-CB	-5.28	97.71	103.25
9	P	194	ALA	N-CA-C	-5.27	105.94	112.38
2	H	123	SER	N-CA-C	5.12	118.30	111.75
8	O	120	ARG	CA-CB-CG	5.05	124.20	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	C	40	0	36	6	0
1	c	105	0	106	5	0
2	H	1560	0	1633	80	0
3	I	4111	0	4032	165	0
4	K	1869	0	1857	76	0
5	L	2422	0	2396	104	0
6	M	1298	0	1349	73	0
7	N	2492	0	2509	117	0
8	O	1588	0	1540	72	0
9	P	1808	0	1810	75	0
10	Q	1175	0	1058	49	0
11	S	790	0	798	76	0
12	T	804	0	814	47	0
13	W	584	0	631	29	0
14	X	590	0	620	43	0
15	R	308	0	127	4	0
16	U	699	0	303	10	0
All	All	22243	0	21619	865	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 20.

All (865) 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)
3:I:155:LYS:O	3:I:156:CYS:O	1.86	0.92
12:T:515:LEU:HD13	13:W:42:LEU:HB3	1.53	0.90
2:H:101:LEU:HD21	3:I:586:GLY:HA2	1.57	0.85
9:P:111:CYS:SG	9:P:112:HIS:N	2.49	0.84
7:N:269:TYR:HB2	7:N:295:ILE:HB	1.58	0.84
7:N:271:LEU:HD22	7:N:273:THR:HB	1.58	0.83
9:P:208:ILE:HG23	9:P:283:CYS:HB3	1.61	0.81
2:H:145:GLN:HE21	3:I:729:GLN:HB2	1.45	0.80
12:T:498:LEU:HG	12:T:510:VAL:HG21	1.61	0.80
9:P:165:MET:SD	9:P:168:ARG:NH2	2.54	0.79
5:L:47:ARG:NH1	5:L:337:GLU:OE2	2.15	0.79
7:N:271:LEU:HB2	7:N:293:CYS:H	1.47	0.79
5:L:238:GLU:HA	5:L:255:ALA:HA	1.68	0.76
8:O:100:ASN:HD22	9:P:63:LEU:HD13	1.52	0.75
4:K:104:LEU:HA	4:K:107:VAL:HG12	1.69	0.75
3:I:394:GLN:NE2	5:L:209:SER:OG	2.20	0.74
7:N:68:LEU:HA	7:N:71:ILE:HD12	1.69	0.74
5:L:218:LEU:HD23	5:L:304:LEU:HB3	1.69	0.74
9:P:196:TYR:O	9:P:207:GLY:N	2.19	0.74
11:S:87:ARG:O	11:S:87:ARG:NH1	2.19	0.74
5:L:313:SER:HB3	5:L:322:ILE:HB	1.69	0.74
2:H:141:MET:HE1	3:I:728:LEU:HD22	1.69	0.74
5:L:95:LEU:HD11	5:L:196:ILE:HG12	1.70	0.74
3:I:67:GLN:NE2	3:I:68:MET:SD	2.61	0.73
5:L:256:ILE:HA	7:N:293:CYS:HB3	1.70	0.73
8:O:145:GLN:HG2	8:O:147:PRO:HD2	1.70	0.73
7:N:248:VAL:HG22	7:N:317:ALA:HB2	1.70	0.72
3:I:611:ARG:HG2	3:I:640:PHE:HZ	1.55	0.72
3:I:480:GLN:NE2	6:M:128:LEU:O	2.23	0.71
7:N:56:CYS:HB2	7:N:61:ALA:HB2	1.72	0.71
10:Q:113:LEU:HA	10:Q:116:ARG:HG2	1.70	0.71
2:H:93:LYS:O	2:H:97:GLU:HB2	1.91	0.70
4:K:240:PRO:HA	4:K:243:VAL:HG12	1.73	0.70
9:P:194:ALA:HB1	9:P:283:CYS:HB2	1.73	0.70
7:N:82:VAL:O	7:N:165:SER:OG	2.09	0.70
5:L:183:LEU:HD11	5:L:335:LEU:HB3	1.73	0.70
9:P:93:MET:HE1	9:P:100:LYS:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:72:LEU:HA	6:M:112:ILE:HD12	1.74	0.70
8:O:111:THR:HA	9:P:167:PHE:HD2	1.57	0.70
11:S:11:GLN:OE1	11:S:12:ARG:NH1	2.25	0.70
2:H:211:VAL:HG22	4:K:267:PHE:HB2	1.73	0.70
3:I:412:LYS:O	3:I:416:ASN:ND2	2.24	0.69
6:M:18:ILE:HG13	6:M:65:LEU:HB3	1.74	0.69
7:N:16:ILE:HD11	7:N:21:LEU:HD13	1.74	0.69
9:P:114:VAL:HG13	9:P:143:GLU:HG3	1.75	0.69
8:O:170:GLN:CD	8:O:170:GLN:H	2.01	0.68
7:N:98:LEU:HA	8:O:217:LEU:HD22	1.74	0.68
3:I:389:TYR:HD1	3:I:434:SER:HB2	1.58	0.68
2:H:57:TYR:HE1	6:M:7:LEU:HB3	1.58	0.68
3:I:456:LEU:HB3	3:I:496:SER:HB2	1.74	0.68
3:I:550:LEU:HD23	6:M:160:VAL:HG21	1.76	0.68
3:I:569:CYS:O	3:I:613:ASN:ND2	2.26	0.68
10:Q:85:GLN:HA	10:Q:88:MET:SD	2.33	0.68
11:S:65:LEU:HD21	11:S:85:LEU:HD22	1.75	0.68
8:O:159:ILE:HA	8:O:213:PRO:HB3	1.75	0.68
1:C:306:ASP:HA	7:N:334:PHE:O	1.94	0.67
2:H:161:ARG:NH1	3:I:427:PHE:O	2.24	0.67
7:N:115:ALA:O	7:N:140:GLN:NE2	2.27	0.67
7:N:177:GLN:NE2	16:U:320:MET:O	2.27	0.67
10:Q:181:ASN:HA	10:Q:184:GLN:HG3	1.75	0.67
7:N:78:GLN:NE2	7:N:199:ASP:OD2	2.27	0.67
2:H:49:GLN:HG2	6:M:156:HIS:HA	1.77	0.67
7:N:204:ILE:HG12	7:N:261:GLN:HE21	1.58	0.67
10:Q:132:GLU:OE1	10:Q:132:GLU:N	2.26	0.67
11:S:16:GLN:O	11:S:20:LYS:HG3	1.95	0.67
7:N:56:CYS:HA	7:N:59:LYS:HB2	1.76	0.66
2:H:52:GLN:HE22	6:M:161:SER:HA	1.60	0.66
6:M:129:LEU:HB2	6:M:142:MET:HE1	1.78	0.66
4:K:136:MET:HA	4:K:136:MET:HE2	1.76	0.66
10:Q:91:VAL:O	10:Q:95:ILE:HG12	1.94	0.66
7:N:116:LEU:HD23	7:N:174:LEU:HD23	1.76	0.66
11:S:55:PHE:HE1	14:X:22:HIS:HE2	1.44	0.66
5:L:133:ASP:HA	5:L:171:LEU:HD11	1.78	0.66
5:L:168:ASP:HA	5:L:171:LEU:HB2	1.77	0.66
8:O:194:ALA:HB1	8:O:215:CYS:HB2	1.78	0.66
9:P:169:SER:O	9:P:173:PHE:N	2.29	0.66
2:H:121:ARG:HD3	2:H:122:GLN:H	1.61	0.65
8:O:151:HIS:O	8:O:152:HIS:ND1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:27:VAL:HG13	11:S:47:ILE:HD11	1.78	0.65
3:I:182:ASN:ND2	3:I:208:LEU:O	2.30	0.65
6:M:140:ALA:O	6:M:144:GLN:NE2	2.28	0.65
9:P:122:ILE:HG22	9:P:135:VAL:HG12	1.79	0.65
2:H:141:MET:SD	3:I:601:ASN:ND2	2.69	0.65
3:I:595:LEU:HB3	4:K:100:LEU:HD11	1.78	0.65
14:X:48:GLU:HA	14:X:51:VAL:HG12	1.79	0.65
14:X:71:GLU:HA	14:X:74:LEU:HG	1.78	0.65
3:I:120:LYS:HB3	3:I:123:ASN:HB3	1.78	0.65
11:S:64:ASP:OD1	12:T:521:ARG:NH1	2.30	0.65
12:T:534:LEU:HD22	13:W:49:LEU:HD11	1.78	0.65
1:c:262:PHE:HA	1:c:266:PHE:HB2	1.79	0.65
2:H:136:LEU:HD11	4:K:105:GLU:HG3	1.78	0.64
12:T:516:GLU:HB3	12:T:531:LEU:HD22	1.79	0.64
8:O:168:TYR:O	8:O:171:THR:OG1	2.13	0.64
3:I:128:ARG:HH21	3:I:164:PHE:HA	1.62	0.64
9:P:77:ASN:ND2	9:P:110:ASN:O	2.29	0.64
10:Q:183:ILE:HA	10:Q:186:LEU:HB2	1.79	0.64
11:S:77:ILE:HD12	14:X:30:VAL:HG22	1.79	0.64
11:S:17:GLN:HA	11:S:20:LYS:HZ1	1.62	0.64
13:W:82:ILE:O	13:W:86:SER:OG	2.16	0.64
3:I:139:ILE:HD11	3:I:177:ARG:HB2	1.80	0.64
5:L:236:THR:HA	5:L:258:PRO:HD3	1.80	0.64
11:S:53:LEU:HD11	14:X:74:LEU:HD22	1.80	0.64
7:N:99:PHE:HB3	8:O:212:ASN:HD21	1.62	0.64
3:I:96:GLU:HA	3:I:100:TRP:HA	1.80	0.63
3:I:530:MET:HE1	3:I:579:LEU:HB2	1.79	0.63
1:C:302:GLU:HA	7:N:271:LEU:HD23	1.80	0.63
11:S:67:MET:HG3	12:T:517:LEU:HD11	1.79	0.63
5:L:74:LEU:HB3	5:L:211:LEU:HB3	1.79	0.63
10:Q:89:GLU:HA	10:Q:92:ILE:HD12	1.78	0.63
11:S:24:HIS:HA	11:S:27:VAL:HG12	1.79	0.63
9:P:91:THR:HG22	9:P:95:GLU:HG2	1.81	0.63
2:H:77:GLN:O	2:H:81:LYS:N	2.30	0.63
5:L:127:MET:HE1	5:L:328:LEU:HD11	1.80	0.63
8:O:170:GLN:HB3	8:O:174:GLN:HB3	1.80	0.63
11:S:69:ALA:HA	11:S:74:ARG:HH21	1.63	0.62
3:I:509:SER:HB2	3:I:510:MET:HE2	1.81	0.62
5:L:77:LEU:HD22	5:L:162:PHE:HD2	1.63	0.62
8:O:254:CYS:HB3	8:O:257:VAL:HG12	1.82	0.62
2:H:148:TRP:NE1	3:I:566:GLU:OE1	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:174:LEU:HD12	7:N:177:GLN:HB3	1.82	0.62
9:P:105:HIS:HB3	9:P:120:PHE:HD2	1.63	0.62
9:P:278:LEU:O	9:P:282:LEU:HB2	2.00	0.62
7:N:43:GLN:HG3	7:N:44:ARG:HG2	1.81	0.62
3:I:138:VAL:HG12	3:I:141:GLU:HG3	1.81	0.62
3:I:207:LEU:HD21	3:I:262:PHE:HE1	1.65	0.62
3:I:686:PRO:HA	3:I:689:LEU:HB3	1.81	0.61
6:M:58:VAL:O	6:M:59:ASN:ND2	2.33	0.61
7:N:207:LYS:HE2	7:N:330:ARG:HD3	1.83	0.61
16:U:305:LYS:O	16:U:309:MET:N	2.33	0.61
6:M:5:ARG:NH1	6:M:8:ASP:OD1	2.34	0.61
8:O:153:HIS:HB2	8:O:155:VAL:HG23	1.82	0.61
3:I:597:THR:HG23	3:I:687:SER:HB2	1.81	0.61
8:O:212:ASN:HB2	8:O:217:LEU:H	1.65	0.61
11:S:87:ARG:NH2	12:T:497:ASP:OD1	2.33	0.61
5:L:88:LEU:HD12	5:L:121:PHE:HB3	1.82	0.61
2:H:130:MET:SD	4:K:94:LYS:NZ	2.72	0.60
2:H:164:LEU:HD22	4:K:136:MET:HG2	1.82	0.60
3:I:113:LEU:HA	3:I:117:LEU:HD11	1.83	0.60
5:L:74:LEU:HB2	5:L:320:ILE:HD12	1.82	0.60
14:X:15:VAL:HG13	14:X:35:LEU:HD22	1.82	0.60
5:L:301:ALA:HA	6:M:74:SER:HB2	1.83	0.60
10:Q:82:ASP:O	10:Q:85:GLN:HG3	2.01	0.60
10:Q:145:ARG:HA	10:Q:148:ASP:HB3	1.82	0.60
7:N:68:LEU:HD23	7:N:72:ILE:HD11	1.82	0.60
2:H:188:SER:O	2:H:191:ASN:ND2	2.34	0.60
14:X:44:VAL:O	14:X:48:GLU:HG2	2.01	0.60
7:N:157:GLN:HB2	8:O:160:PRO:HD2	1.84	0.60
3:I:596:ASP:OD1	3:I:596:ASP:N	2.34	0.60
9:P:87:ASP:HA	9:P:101:VAL:HG23	1.82	0.60
10:Q:93:MET:HE1	11:S:20:LYS:C	2.27	0.60
11:S:88:ARG:O	13:W:87:ARG:NH1	2.35	0.60
3:I:74:GLU:HG2	3:I:117:LEU:HD13	1.83	0.60
10:Q:78:LYS:O	10:Q:81:ARG:HG3	2.02	0.60
7:N:114:ARG:HG3	10:Q:158:LEU:HD13	1.83	0.59
2:H:97:GLU:O	2:H:101:LEU:HG	2.02	0.59
7:N:7:GLU:OE1	7:N:11:ARG:NH2	2.35	0.59
7:N:153:VAL:HG21	7:N:198:LEU:HD21	1.84	0.59
10:Q:101:LYS:HD3	10:Q:101:LYS:N	2.18	0.59
7:N:193:LEU:HG	7:N:331:MET:HA	1.84	0.59
8:O:164:ILE:O	8:O:168:TYR:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:30:LEU:O	11:S:34:VAL:HG12	2.02	0.59
11:S:95:TYR:O	11:S:99:LYS:HG2	2.02	0.59
12:T:543:TYR:OH	13:W:17:ALA:O	2.13	0.59
9:P:127:ASN:OD1	9:P:128:LYS:N	2.34	0.59
14:X:35:LEU:O	14:X:39:VAL:HG23	2.02	0.59
2:H:57:TYR:CE1	6:M:7:LEU:HB3	2.38	0.59
3:I:155:LYS:O	3:I:156:CYS:C	2.45	0.59
11:S:19:LEU:HD11	14:X:17:ARG:HG2	1.84	0.59
4:K:245:LEU:O	4:K:249:ASN:ND2	2.36	0.59
3:I:150:TRP:CE2	3:I:152:CYS:HB2	2.38	0.59
3:I:526:LEU:HG	3:I:530:MET:HG2	1.85	0.59
9:P:126:GLN:HA	9:P:131:LEU:HA	1.85	0.59
10:Q:85:GLN:HB3	10:Q:117:LEU:HD21	1.83	0.59
6:M:14:ASN:ND2	6:M:41:ALA:O	2.36	0.59
6:M:32:ALA:HB1	7:N:237:ILE:HG12	1.84	0.59
6:M:72:LEU:HD12	6:M:104:ALA:HB2	1.85	0.59
12:T:513:GLU:OE2	12:T:513:GLU:N	2.33	0.59
7:N:84:ASP:N	7:N:163:THR:O	2.29	0.58
2:H:146:GLU:OE1	4:K:115:ASN:ND2	2.36	0.58
3:I:391:TRP:CD1	5:L:207:TYR:HH	2.21	0.58
7:N:126:THR:OG1	7:N:130:ALA:O	2.22	0.58
3:I:146:LYS:HE2	3:I:184:LEU:HD11	1.86	0.58
8:O:111:THR:HG23	9:P:167:PHE:CD2	2.38	0.58
7:N:171:ASN:O	7:N:175:LEU:N	2.34	0.58
10:Q:117:LEU:HA	10:Q:120:GLN:NE2	2.18	0.58
4:K:258:ASP:OD1	4:K:260:THR:OG1	2.19	0.58
5:L:220:TRP:NE1	5:L:277:GLN:OE1	2.36	0.58
5:L:231:ASP:O	5:L:232:HIS:ND1	2.36	0.58
6:M:147:VAL:HG12	6:M:151:GLN:HE21	1.69	0.58
11:S:23:VAL:O	11:S:27:VAL:HG12	2.04	0.58
3:I:600:LEU:HD22	3:I:685:HIS:CE1	2.38	0.58
14:X:41:LEU:HA	14:X:44:VAL:HG12	1.86	0.58
11:S:52:GLU:O	11:S:56:ARG:HG2	2.03	0.58
9:P:188:LYS:HD2	9:P:197:LEU:HD23	1.85	0.58
10:Q:186:LEU:O	10:Q:190:VAL:HG23	2.04	0.58
6:M:17:THR:HG21	6:M:61:PRO:HB2	1.85	0.57
6:M:27:LEU:HD21	6:M:134:GLU:HG3	1.86	0.57
7:N:67:ALA:HB1	7:N:134:ARG:HD3	1.86	0.57
8:O:161:LEU:HD23	8:O:164:ILE:HD12	1.86	0.57
2:H:215:VAL:HG11	4:K:213:HIS:NE2	2.20	0.57
3:I:270:LYS:O	3:I:274:LEU:N	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:16:ALA:HB1	6:M:150:LEU:HG	1.86	0.57
11:S:20:LYS:HG2	11:S:55:PHE:CE2	2.40	0.57
13:W:84:LYS:HB3	14:X:79:LEU:HD21	1.86	0.57
7:N:46:GLU:HA	7:N:49:VAL:HG22	1.85	0.57
9:P:217:GLU:H	9:P:242:VAL:HG23	1.69	0.57
6:M:69:VAL:HG13	6:M:100:LEU:HD22	1.87	0.57
13:W:81:VAL:O	13:W:85:LYS:HG2	2.05	0.57
2:H:121:ARG:HD3	2:H:122:GLN:N	2.19	0.57
3:I:391:TRP:HD1	5:L:207:TYR:CE2	2.23	0.57
14:X:76:GLN:HA	14:X:79:LEU:HB3	1.85	0.57
16:U:350:SER:O	16:U:354:ALA:N	2.23	0.57
4:K:66:CYS:HB3	6:M:163:LEU:HD22	1.87	0.57
1:C:305:ILE:HG12	7:N:337:ARG:HA	1.87	0.57
8:O:223:LYS:HD3	8:O:232:PRO:HB3	1.87	0.57
3:I:637:TYR:O	3:I:641:ASN:ND2	2.38	0.56
4:K:245:LEU:HD12	12:T:551:ALA:HB3	1.86	0.56
7:N:301:HIS:CE1	7:N:304:GLU:HB2	2.40	0.56
3:I:631:ASN:ND2	3:I:633:SER:OG	2.38	0.56
5:L:70:LYS:HB3	5:L:187:ASN:ND2	2.20	0.56
9:P:115:THR:O	9:P:142:MET:HE3	2.06	0.56
7:N:271:LEU:N	7:N:293:CYS:O	2.33	0.56
11:S:71:HIS:HE1	12:T:514:ASP:HA	1.69	0.56
14:X:79:LEU:HD23	14:X:80:ASP:HB3	1.85	0.56
2:H:126:LEU:HD12	4:K:94:LYS:HD2	1.88	0.56
5:L:143:SER:O	5:L:152:ARG:N	2.37	0.56
9:P:121:GLN:HB3	9:P:137:ASP:HB2	1.88	0.56
12:T:519:MET:HA	12:T:522:GLN:OE1	2.05	0.56
3:I:266:GLU:O	3:I:270:LYS:N	2.38	0.56
11:S:82:VAL:HB	14:X:37:LEU:HD22	1.88	0.56
3:I:588:PHE:HD1	3:I:603:LEU:HD11	1.70	0.56
6:M:52:LEU:HD23	6:M:88:VAL:HG22	1.86	0.56
7:N:271:LEU:HD12	7:N:293:CYS:SG	2.45	0.56
12:T:507:ARG:NH1	12:T:514:ASP:OD2	2.35	0.56
14:X:44:VAL:HA	14:X:47:VAL:HB	1.86	0.56
1:C:302:GLU:HA	7:N:271:LEU:CD2	2.35	0.56
3:I:101:LYS:H	3:I:134:ILE:HG13	1.69	0.56
7:N:82:VAL:HA	7:N:196:ARG:HA	1.88	0.56
13:W:21:PHE:HA	13:W:24:ARG:HD3	1.88	0.56
11:S:26:THR:O	11:S:30:LEU:HG	2.05	0.56
4:K:107:VAL:HA	4:K:110:THR:HG22	1.88	0.56
4:K:187:HIS:CE1	4:K:245:LEU:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:206:SER:HA	4:K:238:PHE:HB2	1.87	0.56
9:P:204:CYS:HB3	9:P:222:TRP:HB3	1.88	0.56
2:H:172:LEU:HD13	4:K:139:LEU:HD11	1.88	0.56
7:N:90:LYS:NZ	7:N:184:LYS:O	2.30	0.56
10:Q:103:LYS:HE2	11:S:18:ARG:HB3	1.87	0.56
3:I:102:ASN:OD1	3:I:103:GLY:N	2.39	0.55
14:X:11:ARG:H	14:X:14:LEU:HD12	1.71	0.55
2:H:137:ASN:O	2:H:141:MET:HG3	2.05	0.55
3:I:508:LEU:HB3	3:I:577:LEU:HD11	1.89	0.55
8:O:120:ARG:HD2	8:O:120:ARG:O	2.07	0.55
4:K:208:ASN:OD1	4:K:209:LEU:N	2.38	0.55
5:L:238:GLU:O	5:L:308:SER:N	2.40	0.55
9:P:217:GLU:HB3	9:P:243:PRO:HD3	1.87	0.55
5:L:42:LEU:HA	6:M:115:HIS:NE2	2.21	0.55
8:O:223:LYS:HG2	8:O:297:SER:HB3	1.89	0.55
5:L:214:ASN:OD1	5:L:217:ASN:ND2	2.35	0.55
3:I:142:ASP:HA	3:I:145:VAL:HG22	1.88	0.55
3:I:689:LEU:O	3:I:693:VAL:HG23	2.06	0.55
6:M:40:CYS:SG	6:M:151:GLN:NE2	2.80	0.55
4:K:240:PRO:HD2	4:K:241:PRO:HD2	1.89	0.55
5:L:222:ALA:HB1	5:L:239:PHE:HE1	1.72	0.55
9:P:221:VAL:HG12	9:P:223:ARG:HG2	1.89	0.55
1:c:270:VAL:HA	1:c:272:ARG:NH1	2.22	0.55
5:L:297:ILE:HA	7:N:315:ALA:HA	1.89	0.54
6:M:52:LEU:HB2	6:M:84:SER:HB2	1.89	0.54
6:M:52:LEU:O	6:M:53:PRO:C	2.50	0.54
3:I:482:PHE:HE1	3:I:547:ALA:HB2	1.73	0.54
8:O:111:THR:HA	9:P:167:PHE:CD2	2.41	0.54
11:S:13:PHE:HA	11:S:16:GLN:HE21	1.71	0.54
12:T:539:LEU:HD11	13:W:45:LEU:HB2	1.89	0.54
5:L:139:VAL:O	5:L:160:GLY:N	2.41	0.54
10:Q:92:ILE:HD11	10:Q:113:LEU:HD13	1.88	0.54
11:S:22:ALA:HB1	14:X:14:LEU:HD22	1.89	0.54
2:H:218:ASN:ND2	4:K:249:ASN:O	2.41	0.54
10:Q:146:ALA:HA	10:Q:149:LYS:HE2	1.89	0.54
6:M:3:VAL:HG22	6:M:87:HIS:HA	1.89	0.54
2:H:118:LYS:HD2	4:K:94:LYS:HE3	1.88	0.54
8:O:149:ARG:NH1	8:O:150:ILE:O	2.40	0.54
8:O:162:GLU:O	8:O:166:ALA:N	2.41	0.54
5:L:140:GLN:HA	5:L:159:THR:HA	1.89	0.54
5:L:238:GLU:HB3	5:L:308:SER:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:29:GLN:NE2	6:M:33:ASP:OD1	2.40	0.54
6:M:69:VAL:HA	6:M:100:LEU:HB3	1.90	0.54
7:N:251:ILE:HG21	7:N:318:PRO:HA	1.90	0.54
2:H:211:VAL:O	2:H:215:VAL:HG23	2.08	0.54
4:K:166:MET:HE2	4:K:166:MET:HA	1.90	0.54
11:S:19:LEU:O	11:S:23:VAL:HG12	2.08	0.54
11:S:103:ILE:HD12	14:X:36:GLN:HB3	1.90	0.54
7:N:158:THR:HG21	7:N:206:PHE:CE1	2.42	0.53
8:O:210:GLN:OE1	8:O:219:SER:OG	2.23	0.53
9:P:179:TYR:O	9:P:183:THR:OG1	2.22	0.53
10:Q:187:ALA:O	10:Q:191:GLU:HG3	2.08	0.53
8:O:117:LEU:HD22	9:P:65:SER:HB2	1.89	0.53
12:T:475:MET:N	12:T:475:MET:HE3	2.22	0.53
3:I:446:TRP:HZ2	3:I:452:ARG:HA	1.73	0.53
10:Q:87:MET:O	10:Q:90:SER:OG	2.23	0.53
3:I:125:VAL:HG23	3:I:160:THR:HG22	1.91	0.53
9:P:170:LEU:O	9:P:174:VAL:HG22	2.08	0.53
6:M:18:ILE:HB	6:M:150:LEU:HD22	1.88	0.53
6:M:38:GLU:OE2	6:M:38:GLU:N	2.40	0.53
7:N:10:LYS:HB2	7:N:53:ILE:HD12	1.91	0.53
8:O:238:LEU:HB3	8:O:249:ASP:HB3	1.91	0.53
9:P:170:LEU:HA	9:P:173:PHE:HB3	1.91	0.53
11:S:99:LYS:O	11:S:103:ILE:HG12	2.09	0.53
3:I:592:LEU:O	3:I:685:HIS:NE2	2.32	0.53
14:X:19:LEU:HD23	14:X:30:VAL:HG21	1.90	0.53
7:N:192:ASP:HB2	7:N:331:MET:HE2	1.90	0.52
7:N:331:MET:HE1	7:N:334:PHE:HA	1.91	0.52
10:Q:109:HIS:NE2	10:Q:113:LEU:HD11	2.24	0.52
3:I:475:PHE:HB3	3:I:539:TYR:CZ	2.44	0.52
5:L:138:LEU:HD13	5:L:140:GLN:HE21	1.73	0.52
7:N:320:SER:OG	7:N:322:LEU:HB2	2.09	0.52
8:O:159:ILE:HG22	8:O:213:PRO:HA	1.91	0.52
12:T:513:GLU:H	12:T:513:GLU:CD	2.17	0.52
7:N:68:LEU:O	7:N:72:ILE:HD12	2.10	0.52
7:N:28:TRP:CE2	7:N:30:PHE:HB2	2.45	0.52
3:I:198:CYS:SG	13:W:15:ARG:NH1	2.82	0.52
3:I:542:TRP:HZ2	6:M:168:LEU:HA	1.74	0.52
8:O:224:LEU:HD23	8:O:226:PRO:HD3	1.91	0.52
9:P:119:GLU:HB2	9:P:139:ASN:HB3	1.91	0.52
10:Q:182:LYS:HA	10:Q:185:ILE:HD12	1.90	0.52
12:T:477:ARG:HA	12:T:480:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:481:GLU:HA	12:T:484:GLU:HG2	1.92	0.52
2:H:51:LYS:HG2	4:K:31:MET:HE1	1.92	0.52
3:I:66:LEU:HD23	3:I:92:LEU:HG	1.92	0.52
11:S:84:LEU:HD11	12:T:504:HIS:ND1	2.25	0.52
16:U:359:SER:O	16:U:363:GLN:N	2.36	0.52
2:H:168:SER:OG	3:I:378:CYS:SG	2.60	0.52
4:K:40:ASN:HA	4:K:43:SER:HB2	1.91	0.52
4:K:88:VAL:HG13	4:K:90:ILE:HG12	1.91	0.52
5:L:75:TYR:HA	5:L:211:LEU:H	1.75	0.52
6:M:67:VAL:HG21	6:M:146:LEU:HD22	1.91	0.51
8:O:209:LEU:HD23	8:O:211:ARG:HB3	1.91	0.51
12:T:479:ALA:O	12:T:483:VAL:HG23	2.10	0.51
2:H:138:LYS:HD2	3:I:726:GLN:HE22	1.75	0.51
2:H:215:VAL:HG13	4:K:251:ILE:HG12	1.92	0.51
3:I:566:GLU:OE2	3:I:602:GLN:NE2	2.43	0.51
7:N:8:PHE:HA	7:N:11:ARG:HE	1.75	0.51
7:N:99:PHE:HB3	8:O:212:ASN:ND2	2.25	0.51
2:H:112:LEU:HB2	3:I:686:PRO:HG3	1.93	0.51
2:H:161:ARG:NH2	3:I:426:CYS:O	2.38	0.51
5:L:117:ILE:HG23	5:L:141:ILE:HG23	1.93	0.51
12:T:496:ASP:HA	12:T:499:GLU:HG2	1.92	0.51
8:O:166:ALA:HA	8:O:170:GLN:HE22	1.74	0.51
5:L:260:ASP:HB3	7:N:291:LEU:HG	1.92	0.51
6:M:44:LEU:HD21	6:M:147:VAL:HG13	1.92	0.51
7:N:210:ASN:HB2	8:O:152:HIS:CD2	2.46	0.51
2:H:54:LEU:HD22	4:K:31:MET:HB2	1.93	0.51
2:H:150:LEU:HD11	4:K:119:LYS:HE3	1.93	0.51
4:K:188:PHE:CE2	4:K:190:LEU:HG	2.46	0.51
5:L:74:LEU:HD12	5:L:211:LEU:HD13	1.92	0.51
5:L:74:LEU:HD23	5:L:320:ILE:HB	1.93	0.51
11:S:27:VAL:HG11	11:S:51:SER:HB3	1.92	0.51
14:X:31:SER:O	14:X:35:LEU:N	2.35	0.51
2:H:96:PHE:HA	2:H:99:LYS:HB3	1.92	0.51
5:L:75:TYR:HB2	5:L:184:PHE:HB3	1.93	0.51
8:O:193:GLN:NE2	8:O:245:THR:O	2.44	0.51
12:T:536:GLU:O	12:T:544:ARG:NH2	2.44	0.51
15:R:92:LYS:O	15:R:96:LEU:N	2.37	0.51
4:K:82:ILE:HG13	4:K:83:PRO:HD3	1.91	0.50
9:P:270:GLY:O	9:P:274:ALA:N	2.34	0.50
6:M:118:VAL:HA	6:M:128:LEU:HD22	1.93	0.50
7:N:159:PRO:HD3	8:O:164:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:54:LEU:HG	2:H:58:LYS:HE2	1.92	0.50
3:I:107:GLU:HG2	3:I:141:GLU:HA	1.94	0.50
5:L:77:LEU:HD22	5:L:162:PHE:CD2	2.44	0.50
8:O:133:ASN:OD1	8:O:133:ASN:N	2.45	0.50
2:H:141:MET:HB3	3:I:601:ASN:HD21	1.76	0.50
3:I:73:PHE:HE2	3:I:88:LEU:HD22	1.77	0.50
3:I:128:ARG:HH11	3:I:128:ARG:HG2	1.77	0.50
3:I:193:GLN:HB3	12:T:541:LEU:HB2	1.93	0.50
15:R:89:LEU:O	15:R:93:VAL:N	2.37	0.50
3:I:459:VAL:HG21	3:I:478:LEU:HD11	1.93	0.50
10:Q:163:ASP:HA	10:Q:166:VAL:HG12	1.94	0.50
12:T:534:LEU:O	12:T:538:HIS:ND1	2.43	0.50
1:c:263:SER:OG	1:c:264:THR:N	2.43	0.50
3:I:430:GLU:HB3	3:I:507:TRP:CZ2	2.46	0.50
14:X:48:GLU:HA	14:X:51:VAL:CG1	2.42	0.50
5:L:241:TRP:CZ3	5:L:304:LEU:HG	2.47	0.49
5:L:260:ASP:OD2	7:N:292:ARG:NE	2.35	0.49
3:I:428:LEU:HD22	3:I:430:GLU:HG2	1.94	0.49
7:N:85:VAL:HG22	7:N:162:PHE:HD1	1.76	0.49
3:I:134:ILE:HB	3:I:135:PRO:HD3	1.94	0.49
3:I:427:PHE:HB2	4:K:128:TRP:CE2	2.47	0.49
3:I:570:ASP:HA	3:I:613:ASN:HD21	1.77	0.49
14:X:53:GLY:HA2	14:X:56:GLN:HE21	1.77	0.49
15:R:96:LEU:O	15:R:100:ILE:N	2.43	0.49
3:I:510:MET:HA	3:I:513:HIS:HB3	1.94	0.49
5:L:239:PHE:HB3	5:L:304:LEU:HD21	1.95	0.49
7:N:157:GLN:HG3	8:O:213:PRO:HB2	1.94	0.49
11:S:20:LYS:HA	11:S:23:VAL:HG12	1.93	0.49
1:c:270:VAL:HG23	1:c:270:VAL:O	2.11	0.49
2:H:223:SER:HA	12:T:552:TYR:CD1	2.48	0.49
8:O:197:LEU:HD23	8:O:280:LEU:HG	1.94	0.49
10:Q:90:SER:O	10:Q:93:MET:HB2	2.12	0.49
10:Q:146:ALA:HA	10:Q:149:LYS:CE	2.43	0.49
11:S:24:HIS:HA	11:S:27:VAL:CG1	2.43	0.49
12:T:532:HIS:CD2	12:T:548:ILE:HG22	2.48	0.49
5:L:171:LEU:HD23	5:L:180:CYS:SG	2.53	0.49
5:L:213:ILE:HG13	5:L:320:ILE:HD13	1.93	0.49
8:O:190:ARG:HH12	8:O:214:LEU:HB3	1.78	0.49
12:T:543:TYR:CZ	13:W:17:ALA:HB3	2.48	0.49
2:H:144:GLN:HE21	4:K:111:LYS:HE3	1.78	0.49
3:I:471:LYS:HA	3:I:475:PHE:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:131:GLN:H	5:L:131:GLN:CD	2.19	0.49
6:M:52:LEU:HD21	6:M:66:ILE:HD13	1.94	0.49
7:N:101:MET:H	8:O:210:GLN:NE2	2.10	0.49
11:S:43:SER:O	11:S:47:ILE:HG22	2.13	0.49
13:W:55:ALA:O	13:W:59:ARG:HG2	2.13	0.49
3:I:145:VAL:HA	3:I:148:VAL:HG23	1.93	0.49
5:L:223:ALA:HB3	5:L:280:VAL:HG22	1.94	0.49
7:N:96:VAL:HG22	7:N:184:LYS:HB2	1.94	0.49
11:S:80:GLU:HA	11:S:83:LYS:HB2	1.94	0.49
3:I:219:VAL:HG13	3:I:249:LEU:HD23	1.94	0.48
4:K:97:PHE:HD1	4:K:100:LEU:HD12	1.78	0.48
8:O:115:GLY:HA2	8:O:124:VAL:HA	1.95	0.48
5:L:264:LEU:HD11	5:L:286:CYS:HB3	1.96	0.48
2:H:206:ILE:O	2:H:210:THR:N	2.43	0.48
7:N:247:ARG:O	7:N:251:ILE:HG12	2.13	0.48
9:P:212:SER:N	9:P:286:GLU:OE1	2.45	0.48
12:T:460:LEU:O	12:T:464:VAL:HG22	2.13	0.48
12:T:541:LEU:O	12:T:545:GLN:HG3	2.13	0.48
6:M:23:THR:HA	6:M:50:LYS:HG3	1.96	0.48
6:M:143:ALA:O	6:M:147:VAL:HG23	2.13	0.48
2:H:172:LEU:HD23	3:I:379:VAL:HG13	1.95	0.48
2:H:215:VAL:O	2:H:219:LEU:HB2	2.12	0.48
3:I:467:PHE:HA	3:I:470:VAL:HG12	1.95	0.48
11:S:61:PHE:CD2	11:S:85:LEU:HD21	2.48	0.48
12:T:522:GLN:HB3	13:W:53:ARG:NH1	2.28	0.48
13:W:21:PHE:HA	13:W:24:ARG:HH11	1.78	0.48
14:X:73:VAL:O	14:X:77:LEU:N	2.37	0.48
2:H:161:ARG:NE	4:K:125:GLU:OE1	2.44	0.48
3:I:243:LYS:HD2	3:I:251:SER:H	1.79	0.48
6:M:20:LEU:HD21	6:M:35:MET:HE1	1.94	0.48
7:N:167:MET:HB3	7:N:169:ARG:HH11	1.79	0.48
2:H:108:LEU:HD11	3:I:595:LEU:HG	1.96	0.48
6:M:16:ALA:HB2	6:M:156:HIS:CE1	2.49	0.48
8:O:148:LEU:HD13	8:O:174:GLN:OE1	2.14	0.48
9:P:204:CYS:O	9:P:221:VAL:HA	2.14	0.48
2:H:78:ILE:HD11	4:K:56:GLN:HE21	1.79	0.48
2:H:89:ILE:O	2:H:93:LYS:HB2	2.14	0.48
2:H:238:LEU:HD12	3:I:183:LEU:HB3	1.95	0.48
3:I:444:PRO:O	6:M:130:TYR:HB2	2.14	0.48
5:L:44:PRO:HB3	5:L:277:GLN:HB3	1.95	0.48
7:N:154:TYR:HD1	7:N:161:ALA:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:268:GLN:HG2	7:N:296:LYS:HG2	1.95	0.48
11:S:28:GLY:O	11:S:32:GLU:HG2	2.14	0.48
13:W:81:VAL:HA	14:X:79:LEU:HD11	1.96	0.48
2:H:194:ARG:HH22	4:K:156:SER:HA	1.79	0.47
7:N:90:LYS:HG3	7:N:185:HIS:ND1	2.29	0.47
9:P:153:PHE:CZ	9:P:165:MET:HB2	2.49	0.47
9:P:188:LYS:HD2	9:P:197:LEU:HB3	1.96	0.47
14:X:57:ALA:O	14:X:61:ASP:N	2.47	0.47
2:H:50:THR:HG23	4:K:31:MET:SD	2.55	0.47
9:P:102:LEU:HB3	9:P:121:GLN:HE21	1.78	0.47
9:P:188:LYS:O	9:P:192:PRO:HB3	2.14	0.47
11:S:83:LYS:HA	11:S:83:LYS:HD3	1.62	0.47
14:X:52:ARG:O	14:X:56:GLN:HG2	2.13	0.47
3:I:192:LEU:HD11	3:I:202:CYS:SG	2.54	0.47
3:I:483:PHE:CE2	6:M:168:LEU:HB3	2.49	0.47
5:L:129:GLY:N	5:L:165:VAL:HG23	2.30	0.47
3:I:558:LEU:HA	3:I:561:ILE:HD12	1.97	0.47
5:L:165:VAL:H	5:L:336:THR:HG21	1.79	0.47
5:L:240:LEU:HB3	5:L:306:ARG:HB3	1.97	0.47
8:O:133:ASN:HD22	8:O:196:ARG:NH2	2.13	0.47
8:O:223:LYS:HZ1	8:O:231:PHE:H	1.62	0.47
3:I:192:LEU:HD12	3:I:198:CYS:HA	1.97	0.47
3:I:110:ASP:O	3:I:114:ASN:ND2	2.48	0.47
3:I:138:VAL:HG22	3:I:139:ILE:H	1.80	0.47
4:K:20:THR:OG1	4:K:21:GLU:N	2.47	0.47
9:P:194:ALA:CB	9:P:283:CYS:HB2	2.44	0.47
11:S:20:LYS:HA	11:S:23:VAL:CG1	2.44	0.47
13:W:39:GLY:O	13:W:43:VAL:HG13	2.14	0.47
2:H:146:GLU:HB2	4:K:115:ASN:HD21	1.80	0.47
3:I:64:ASP:O	3:I:67:GLN:HG3	2.14	0.47
3:I:147:ALA:O	3:I:150:TRP:HB3	2.15	0.47
3:I:588:PHE:HE1	3:I:647:MET:HE3	1.79	0.47
5:L:95:LEU:HD23	5:L:119:VAL:HG11	1.96	0.47
5:L:213:ILE:HD12	5:L:320:ILE:HG21	1.96	0.47
6:M:72:LEU:HD22	6:M:112:ILE:HB	1.96	0.47
7:N:112:LEU:HD11	7:N:137:TRP:HH2	1.79	0.47
8:O:129:ALA:HB2	8:O:134:LEU:HB3	1.97	0.47
10:Q:88:MET:C	10:Q:88:MET:HE2	2.39	0.47
11:S:20:LYS:HG2	11:S:55:PHE:CD2	2.49	0.47
2:H:101:LEU:HD22	3:I:589:TYR:HB2	1.96	0.47
3:I:389:TYR:HE2	5:L:30:ARG:HH11	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:581:VAL:O	3:I:610:TYR:OH	2.24	0.47
9:P:127:ASN:N	9:P:130:ARG:O	2.48	0.47
11:S:55:PHE:HE1	14:X:22:HIS:NE2	2.10	0.47
11:S:92:LEU:HA	11:S:95:TYR:HB2	1.96	0.47
4:K:27:GLU:O	4:K:31:MET:HG2	2.15	0.47
8:O:221:THR:O	8:O:221:THR:OG1	2.32	0.47
9:P:218:LEU:HD12	9:P:219:VAL:H	1.79	0.47
12:T:463:TYR:OH	13:W:22:LEU:HD21	2.14	0.47
16:U:360:ASN:O	16:U:364:LEU:N	2.45	0.47
3:I:100:TRP:HD1	3:I:130:LEU:HG	1.80	0.47
4:K:252:ALA:O	4:K:253:LEU:HD23	2.15	0.47
11:S:27:VAL:HG23	14:X:46:VAL:HG11	1.97	0.47
11:S:67:MET:SD	12:T:520:ARG:HG2	2.55	0.47
3:I:107:GLU:O	3:I:111:ILE:HG23	2.15	0.46
3:I:222:LEU:HD11	3:I:238:LEU:HG	1.96	0.46
3:I:482:PHE:CE1	3:I:547:ALA:HB2	2.50	0.46
2:H:151:GLU:HG2	3:I:567:LYS:HE3	1.98	0.46
3:I:471:LYS:HA	3:I:475:PHE:HD2	1.80	0.46
5:L:250:LEU:HA	7:N:299:SER:HB2	1.96	0.46
8:O:182:GLU:HG3	9:P:168:ARG:HG2	1.96	0.46
2:H:234:LYS:HA	2:H:237:VAL:HG12	1.97	0.46
6:M:73:HIS:CE1	6:M:109:HIS:HB2	2.50	0.46
7:N:63:ILE:HA	7:N:66:ALA:HB3	1.97	0.46
9:P:84:GLN:HE22	9:P:106:ARG:HE	1.63	0.46
9:P:151:SER:O	9:P:154:VAL:HG22	2.15	0.46
9:P:198:SER:HB3	9:P:205:SER:HB3	1.97	0.46
13:W:79:ALA:HB3	13:W:80:LYS:NZ	2.31	0.46
2:H:223:SER:O	2:H:225:VAL:HG13	2.16	0.46
3:I:534:SER:N	3:I:579:LEU:HD21	2.31	0.46
3:I:595:LEU:HD23	3:I:686:PRO:HB2	1.97	0.46
12:T:462:HIS:CE1	13:W:18:PRO:HD3	2.51	0.46
3:I:380:ARG:HA	3:I:385:LEU:HD11	1.98	0.46
5:L:232:HIS:CG	5:L:232:HIS:O	2.69	0.46
9:P:263:ARG:NH1	10:Q:222:PRO:O	2.48	0.46
5:L:134:PRO:HD3	5:L:171:LEU:HD21	1.98	0.46
5:L:294:HIS:C	7:N:322:LEU:HD12	2.41	0.46
7:N:53:ILE:O	7:N:57:GLU:HG2	2.15	0.46
7:N:271:LEU:CD2	7:N:273:THR:HB	2.39	0.46
8:O:131:GLU:OE1	8:O:282:GLN:NE2	2.39	0.46
8:O:205:LEU:HA	8:O:222:TYR:HA	1.96	0.46
9:P:176:TRP:CZ3	9:P:224:ILE:HB	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:420:THR:HG22	3:I:423:ARG:HH22	1.80	0.46
10:Q:87:MET:HE2	10:Q:87:MET:HB2	1.90	0.46
3:I:243:LYS:HE2	3:I:250:ILE:HG23	1.97	0.46
7:N:130:ALA:HA	7:N:155:TYR:HA	1.97	0.46
10:Q:95:ILE:O	10:Q:99:SER:N	2.47	0.46
11:S:53:LEU:HD22	11:S:56:ARG:HD3	1.98	0.46
11:S:60:ASN:O	11:S:64:ASP:HB2	2.16	0.46
5:L:70:LYS:HB3	5:L:187:ASN:HD22	1.80	0.46
6:M:67:VAL:HG22	6:M:98:CYS:HB2	1.97	0.46
11:S:59:GLU:OE1	11:S:59:GLU:HA	2.15	0.46
11:S:98:ASP:OD1	11:S:99:LYS:N	2.49	0.46
2:H:93:LYS:HD2	2:H:96:PHE:CE1	2.51	0.45
3:I:611:ARG:HG2	3:I:640:PHE:CZ	2.43	0.45
5:L:28:GLN:CD	5:L:28:GLN:H	2.24	0.45
6:M:24:GLU:HG3	6:M:27:LEU:HD12	1.97	0.45
7:N:195:SER:HB3	7:N:201:LEU:HD21	1.96	0.45
10:Q:162:ILE:O	10:Q:166:VAL:HG12	2.16	0.45
7:N:259:TYR:O	7:N:259:TYR:CG	2.70	0.45
1:C:304:ILE:HB	7:N:322:LEU:HD22	1.97	0.45
2:H:215:VAL:HG11	4:K:213:HIS:CE1	2.51	0.45
3:I:483:PHE:CD2	6:M:168:LEU:HB3	2.52	0.45
4:K:114:LYS:O	4:K:118:LEU:HB2	2.16	0.45
5:L:131:GLN:OE1	5:L:131:GLN:N	2.38	0.45
10:Q:83:HIS:O	10:Q:87:MET:HG3	2.16	0.45
11:S:71:HIS:CE1	12:T:514:ASP:HA	2.50	0.45
13:W:18:PRO:HD2	13:W:44:HIS:CD2	2.51	0.45
5:L:73:THR:HA	5:L:319:LYS:HA	1.99	0.45
6:M:52:LEU:O	6:M:54:LEU:HB2	2.16	0.45
9:P:197:LEU:HD13	9:P:206:MET:HG3	1.98	0.45
10:Q:180:LYS:HA	10:Q:180:LYS:HD3	1.79	0.45
11:S:56:ARG:O	11:S:59:GLU:HB2	2.17	0.45
12:T:460:LEU:HD22	12:T:487:LEU:HB3	1.99	0.45
3:I:464:PHE:HE2	3:I:533:VAL:HG23	1.81	0.45
5:L:222:ALA:HB2	5:L:307:VAL:HG11	1.98	0.45
7:N:13:ILE:HG22	7:N:49:VAL:HG12	1.99	0.45
11:S:90:ASN:HA	11:S:93:LEU:HB2	1.98	0.45
13:W:42:LEU:HD23	13:W:42:LEU:HA	1.86	0.45
2:H:92:VAL:O	2:H:96:PHE:HD1	1.99	0.45
3:I:128:ARG:HA	3:I:131:LYS:HB3	1.98	0.45
3:I:145:VAL:HB	3:I:164:PHE:HZ	1.82	0.45
3:I:387:ARG:HD2	5:L:81:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:572:TYR:HD2	3:I:578:PRO:HA	1.82	0.45
2:H:184:ILE:HA	2:H:187:ASP:OD2	2.17	0.45
2:H:192:SER:O	2:H:196:LYS:NZ	2.43	0.45
3:I:108:GLU:O	3:I:112:LEU:HD22	2.17	0.45
7:N:269:TYR:N	7:N:295:ILE:O	2.50	0.45
7:N:294:LEU:O	7:N:296:LYS:HG3	2.16	0.45
9:P:142:MET:HB3	9:P:143:GLU:H	1.56	0.45
10:Q:102:GLU:HB3	10:Q:105:GLU:HB2	1.97	0.45
3:I:120:LYS:O	3:I:124:ALA:N	2.28	0.45
3:I:534:SER:HB3	3:I:579:LEU:HD11	1.98	0.45
3:I:546:THR:O	3:I:550:LEU:HG	2.17	0.45
4:K:248:ARG:HE	12:T:544:ARG:HH11	1.65	0.45
6:M:96:LYS:HG2	6:M:153:CYS:HB3	1.98	0.45
9:P:216:PHE:HE2	16:U:364:LEU:O	2.00	0.45
3:I:491:CYS:SG	3:I:557:LEU:HA	2.57	0.45
4:K:160:ASN:O	4:K:164:THR:HG23	2.17	0.45
5:L:70:LYS:HB3	5:L:70:LYS:HE3	1.83	0.45
7:N:8:PHE:HA	7:N:11:ARG:NE	2.32	0.45
7:N:157:GLN:NE2	8:O:212:ASN:HD22	2.14	0.45
8:O:230:SER:HB2	8:O:297:SER:HB2	1.99	0.45
11:S:74:ARG:NH2	11:S:81:ASP:OD1	2.50	0.45
1:C:305:ILE:HA	7:N:336:ILE:O	2.17	0.45
3:I:71:GLY:HA2	3:I:74:GLU:CD	2.42	0.45
3:I:110:ASP:HB3	3:I:145:VAL:HG11	1.99	0.45
9:P:88:LEU:HB3	9:P:100:LYS:HE3	1.98	0.45
12:T:524:LEU:HD23	12:T:524:LEU:HA	1.74	0.45
2:H:237:VAL:HG21	3:I:146:LYS:HZ3	1.80	0.44
3:I:100:TRP:CD1	3:I:130:LEU:HG	2.53	0.44
4:K:180:LEU:O	4:K:184:LEU:HB2	2.17	0.44
5:L:246:SER:OG	5:L:247:PRO:HD3	2.17	0.44
6:M:52:LEU:N	6:M:53:PRO:HD2	2.32	0.44
7:N:39:VAL:HG22	7:N:51:HIS:ND1	2.31	0.44
9:P:154:VAL:HG12	9:P:166:PHE:CE2	2.53	0.44
9:P:223:ARG:HA	9:P:223:ARG:HD3	1.77	0.44
3:I:64:ASP:O	3:I:68:MET:HG2	2.17	0.44
3:I:391:TRP:HD1	5:L:207:TYR:CZ	2.35	0.44
4:K:35:MET:HE1	6:M:11:PRO:HG2	1.99	0.44
6:M:164:ASN:O	6:M:168:LEU:HG	2.16	0.44
9:P:125:ILE:O	9:P:132:SER:N	2.50	0.44
13:W:59:ARG:HH22	13:W:70:ILE:HD13	1.83	0.44
3:I:427:PHE:HB2	4:K:128:TRP:CZ2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:52:LEU:HD12	6:M:54:LEU:HD13	1.99	0.44
7:N:70:ASP:OD2	7:N:151:TYR:OH	2.35	0.44
16:U:323:VAL:O	16:U:327:LEU:N	2.39	0.44
2:H:176:GLN:HE22	3:I:379:VAL:HG11	1.82	0.44
4:K:246:LEU:HA	4:K:251:ILE:HD12	1.99	0.44
5:L:159:THR:O	5:L:159:THR:OG1	2.35	0.44
5:L:296:LYS:HG2	7:N:320:SER:HB3	1.98	0.44
7:N:88:MET:HB3	7:N:185:HIS:CG	2.52	0.44
9:P:105:HIS:HB3	9:P:120:PHE:CD2	2.50	0.44
11:S:68:PHE:CD2	11:S:84:LEU:HD12	2.53	0.44
3:I:375:TYR:O	3:I:379:VAL:HG22	2.18	0.44
4:K:87:ASP:OD2	4:K:91:THR:OG1	2.35	0.44
7:N:71:ILE:HG23	7:N:132:TRP:CD1	2.53	0.44
10:Q:139:SER:O	10:Q:143:MET:SD	2.76	0.44
2:H:93:LYS:HZ1	3:I:545:THR:HG23	1.83	0.44
5:L:161:TRP:O	5:L:185:LEU:N	2.44	0.44
7:N:200:SER:OG	7:N:262:PRO:HD2	2.17	0.44
8:O:222:TYR:OH	8:O:271:HIS:ND1	2.46	0.44
3:I:155:LYS:C	3:I:156:CYS:O	2.53	0.44
3:I:222:LEU:HD23	3:I:222:LEU:HA	1.81	0.44
6:M:99:PHE:O	6:M:128:LEU:HD12	2.18	0.44
2:H:206:ILE:HG13	2:H:210:THR:HG23	2.00	0.44
4:K:117:LYS:O	4:K:121:ASP:HB2	2.18	0.44
5:L:59:VAL:HB	5:L:64:VAL:HG21	1.99	0.44
5:L:200:PHE:HB3	5:L:206:CYS:SG	2.57	0.44
7:N:173:PRO:O	7:N:177:GLN:HB2	2.18	0.44
14:X:56:GLN:O	14:X:60:GLU:HG2	2.16	0.44
3:I:222:LEU:HB3	3:I:239:LEU:HD21	2.00	0.44
3:I:426:CYS:HA	3:I:461:TRP:CZ2	2.53	0.44
5:L:63:LYS:HD3	5:L:63:LYS:HA	1.67	0.44
5:L:80:LEU:HD11	5:L:181:LEU:HD12	1.99	0.44
5:L:197:GLY:O	5:L:201:GLN:HG3	2.17	0.44
6:M:115:HIS:O	6:M:118:VAL:HG12	2.18	0.44
7:N:145:ASN:HD21	7:N:147:TYR:HB2	1.83	0.44
10:Q:93:MET:HE1	11:S:20:LYS:O	2.17	0.44
11:S:19:LEU:HG	14:X:21:LEU:HD22	1.99	0.44
5:L:168:ASP:OD1	5:L:168:ASP:N	2.45	0.43
5:L:184:PHE:CZ	5:L:186:ALA:HB2	2.52	0.43
8:O:127:SER:HA	8:O:137:SER:HA	2.00	0.43
8:O:296:MET:HE3	8:O:296:MET:HA	1.99	0.43
14:X:45:PHE:O	14:X:81:PHE:HZ	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:239:PHE:CE2	5:L:287:LEU:HD21	2.53	0.43
8:O:190:ARG:HD3	8:O:190:ARG:C	2.44	0.43
8:O:237:LEU:HD21	8:O:275:PHE:HD2	1.83	0.43
2:H:158:ARG:NH2	3:I:426:CYS:SG	2.86	0.43
3:I:582:LEU:HD11	3:I:636:THR:O	2.18	0.43
3:I:723:LEU:O	3:I:728:LEU:HB2	2.18	0.43
8:O:133:ASN:HD22	8:O:196:ARG:HH21	1.65	0.43
10:Q:84:LEU:HG	10:Q:131:MET:SD	2.58	0.43
4:K:185:GLU:O	4:K:188:PHE:HB3	2.18	0.43
5:L:239:PHE:HD1	5:L:307:VAL:HG12	1.83	0.43
6:M:115:HIS:HA	6:M:118:VAL:HG12	2.00	0.43
10:Q:182:LYS:C	10:Q:182:LYS:HD2	2.44	0.43
15:R:93:VAL:O	15:R:97:SER:N	2.48	0.43
7:N:261:GLN:HG2	7:N:303:LEU:HD12	2.00	0.43
2:H:225:VAL:HG23	2:H:227:TRP:N	2.33	0.43
9:P:246:ALA:HA	9:P:249:LEU:HD13	2.00	0.43
2:H:221:LEU:HB2	3:I:187:PHE:CE1	2.52	0.43
3:I:478:LEU:O	3:I:482:PHE:HB2	2.19	0.43
4:K:164:THR:O	4:K:167:LEU:HG	2.19	0.43
3:I:550:LEU:HD22	6:M:152:ILE:HD11	2.00	0.43
7:N:82:VAL:HG23	7:N:195:SER:C	2.44	0.43
7:N:140:GLN:HB3	10:Q:151:ASN:CG	2.43	0.43
7:N:202:LYS:HG2	7:N:206:PHE:CE2	2.54	0.43
8:O:217:LEU:HD12	8:O:217:LEU:HA	1.88	0.43
10:Q:100:ILE:HG22	10:Q:101:LYS:HD3	2.01	0.43
13:W:20:GLY:O	13:W:24:ARG:HG3	2.18	0.43
3:I:71:GLY:O	3:I:75:LYS:HG2	2.18	0.43
3:I:471:LYS:HB3	3:I:472:PRO:HD3	2.00	0.43
4:K:39:GLN:NE2	4:K:43:SER:OG	2.52	0.43
5:L:166:PHE:HD2	5:L:333:ALA:HB2	1.84	0.43
6:M:135:VAL:HG13	6:M:138:PHE:HB2	2.01	0.43
7:N:297:PHE:CZ	7:N:323:LEU:HD11	2.54	0.43
9:P:251:LYS:HD2	9:P:251:LYS:HA	1.79	0.43
11:S:15:TYR:O	11:S:19:LEU:HD22	2.19	0.43
3:I:579:LEU:HD12	3:I:579:LEU:HA	1.82	0.43
5:L:214:ASN:OD1	5:L:214:ASN:N	2.50	0.43
3:I:547:ALA:HB1	3:I:557:LEU:HD21	2.00	0.42
4:K:157:ARG:O	4:K:161:GLU:HG2	2.18	0.42
4:K:222:ARG:NH1	4:K:223:LEU:O	2.52	0.42
5:L:43:THR:O	5:L:45:PRO:HD3	2.19	0.42
7:N:133:ILE:N	7:N:152:VAL:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:19:LEU:CD1	14:X:17:ARG:HG2	2.49	0.42
11:S:47:ILE:HA	11:S:50:ILE:HG22	2.00	0.42
11:S:71:HIS:HB2	12:T:517:LEU:HD13	2.01	0.42
5:L:201:GLN:HG2	5:L:206:CYS:O	2.18	0.42
6:M:52:LEU:H	6:M:84:SER:HB2	1.84	0.42
7:N:256:PHE:CZ	7:N:324:THR:HG22	2.54	0.42
9:P:147:CYS:O	9:P:151:SER:N	2.53	0.42
11:S:59:GLU:O	11:S:63:LYS:HG2	2.18	0.42
11:S:61:PHE:O	11:S:65:LEU:HD23	2.19	0.42
11:S:75:THR:HG23	14:X:28:THR:HG22	2.01	0.42
14:X:35:LEU:HA	14:X:38:MET:HG2	2.01	0.42
2:H:194:ARG:HG3	4:K:159:PHE:CE1	2.54	0.42
6:M:29:GLN:HE22	7:N:237:ILE:HD13	1.84	0.42
6:M:100:LEU:HD12	6:M:142:MET:HE2	2.01	0.42
7:N:115:ALA:HB3	7:N:174:LEU:HD21	2.01	0.42
7:N:155:TYR:OH	7:N:202:LYS:HG3	2.17	0.42
8:O:146:LYS:HA	8:O:146:LYS:HD3	1.67	0.42
14:X:38:MET:SD	14:X:38:MET:N	2.92	0.42
3:I:78:ILE:HD13	3:I:85:ASP:HB2	2.01	0.42
13:W:18:PRO:HD2	13:W:44:HIS:HD2	1.83	0.42
13:W:79:ALA:HB3	13:W:80:LYS:HZ2	1.85	0.42
2:H:223:SER:HA	12:T:552:TYR:HD1	1.84	0.42
3:I:493:VAL:HA	3:I:496:SER:HB3	2.02	0.42
4:K:40:ASN:O	4:K:44:LEU:HG	2.19	0.42
7:N:157:GLN:HB3	8:O:161:LEU:HD21	2.02	0.42
8:O:113:LEU:HD23	8:O:126:ILE:HG12	2.01	0.42
10:Q:96:LEU:HG	10:Q:106:ILE:HG21	2.00	0.42
12:T:535:VAL:HA	12:T:539:LEU:HD13	2.01	0.42
12:T:535:VAL:HG13	12:T:544:ARG:HG3	2.00	0.42
3:I:150:TRP:CZ2	3:I:152:CYS:HB2	2.54	0.42
4:K:68:THR:O	4:K:71:LEU:HG	2.19	0.42
4:K:183:PHE:O	4:K:186:ASP:HB3	2.19	0.42
7:N:32:SER:OG	7:N:35:GLN:OE1	2.38	0.42
7:N:71:ILE:O	7:N:75:GLN:HG3	2.19	0.42
7:N:85:VAL:HG11	7:N:205:VAL:HG21	2.02	0.42
8:O:182:GLU:HB2	9:P:171:HIS:CE1	2.55	0.42
9:P:168:ARG:HA	9:P:171:HIS:HB3	2.02	0.42
10:Q:245:LEU:O	10:Q:249:SER:N	2.52	0.42
11:S:94:LYS:HA	11:S:94:LYS:HD3	1.93	0.42
14:X:47:VAL:O	14:X:51:VAL:HG12	2.20	0.42
5:L:45:PRO:HD2	5:L:220:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:315:HIS:O	5:L:320:ILE:HG12	2.19	0.42
10:Q:147:ARG:HD2	10:Q:151:ASN:OD1	2.19	0.42
3:I:165:TYR:CE2	3:I:197:LEU:HD13	2.54	0.42
9:P:135:VAL:HG11	9:P:163:LEU:HD22	2.01	0.42
11:S:58:CYS:HA	11:S:61:PHE:HB2	2.02	0.42
7:N:18:MET:O	7:N:21:LEU:HD23	2.19	0.42
9:P:284:ALA:O	9:P:288:ASN:N	2.44	0.42
10:Q:133:ASP:O	10:Q:137:VAL:HG13	2.20	0.42
13:W:59:ARG:NH2	13:W:70:ILE:HB	2.34	0.42
1:c:270:VAL:HA	1:c:272:ARG:HH11	1.85	0.42
5:L:77:LEU:HD13	5:L:208:PHE:CE2	2.55	0.42
5:L:158:TRP:CZ2	5:L:184:PHE:HZ	2.37	0.42
7:N:104:PHE:HE2	7:N:131:VAL:HG11	1.85	0.41
7:N:112:LEU:HD12	7:N:112:LEU:HA	1.85	0.41
11:S:96:ILE:O	11:S:100:SER:OG	2.37	0.41
14:X:10:PHE:CB	14:X:39:VAL:HG13	2.50	0.41
4:K:59:LEU:HD21	6:M:93:PHE:HB2	2.00	0.41
5:L:45:PRO:HG2	5:L:47:ARG:NE	2.35	0.41
9:P:76:ILE:HD12	9:P:111:CYS:HB2	2.01	0.41
11:S:68:PHE:HE2	11:S:84:LEU:HB2	1.85	0.41
11:S:70:ARG:CZ	11:S:70:ARG:HA	2.51	0.41
12:T:507:ARG:NH2	12:T:514:ASP:OD1	2.38	0.41
3:I:120:LYS:HD3	3:I:121:PHE:H	1.83	0.41
3:I:395:THR:O	3:I:399:GLU:HB2	2.20	0.41
9:P:85:THR:HA	9:P:103:GLN:HA	2.01	0.41
9:P:117:GLN:HE22	9:P:119:GLU:HG2	1.85	0.41
10:Q:173:THR:O	10:Q:177:GLN:HG2	2.21	0.41
16:U:322:GLU:O	16:U:326:GLU:N	2.46	0.41
2:H:178:GLU:O	2:H:182:GLN:HG2	2.20	0.41
3:I:128:ARG:HG2	3:I:128:ARG:NH1	2.35	0.41
9:P:94:THR:HG1	9:P:97:SER:HG	1.66	0.41
11:S:71:HIS:NE2	12:T:505:ALA:HB2	2.34	0.41
2:H:52:GLN:NE2	6:M:161:SER:HA	2.33	0.41
3:I:107:GLU:HG3	3:I:140:SER:OG	2.21	0.41
3:I:148:VAL:O	3:I:161:LYS:NZ	2.53	0.41
3:I:443:LEU:HD23	3:I:443:LEU:HA	1.85	0.41
4:K:219:LEU:HG	4:K:233:LYS:HA	2.02	0.41
4:K:242:TYR:O	4:K:245:LEU:HB3	2.21	0.41
5:L:43:THR:N	5:L:44:PRO:HD3	2.35	0.41
5:L:217:ASN:O	5:L:221:MET:HG2	2.20	0.41
8:O:222:TYR:HH	8:O:271:HIS:HD1	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:11:ARG:HB2	14:X:14:LEU:HG	2.02	0.41
2:H:217:GLN:OE1	3:I:218:ARG:NH2	2.53	0.41
4:K:59:LEU:HD13	6:M:124:TYR:O	2.21	0.41
4:K:67:LEU:HG	6:M:163:LEU:HD11	2.02	0.41
6:M:37:LYS:HE3	6:M:37:LYS:HB2	1.91	0.41
8:O:170:GLN:HG3	8:O:180:LEU:HD11	2.02	0.41
8:O:229:GLN:CD	8:O:229:GLN:H	2.28	0.41
14:X:72:LYS:O	14:X:75:PRO:HD2	2.20	0.41
2:H:108:LEU:HD12	3:I:686:PRO:HG2	2.03	0.41
3:I:189:PHE:HA	3:I:205:LEU:HD11	2.02	0.41
3:I:233:PRO:HB3	3:I:260:ILE:HD13	2.03	0.41
5:L:49:ILE:HG12	5:L:273:GLY:O	2.21	0.41
5:L:315:HIS:H	5:L:320:ILE:HA	1.85	0.41
7:N:139:THR:HG23	7:N:141:TYR:H	1.85	0.41
9:P:81:HIS:HA	9:P:106:ARG:O	2.20	0.41
9:P:150:LEU:O	9:P:154:VAL:HG13	2.21	0.41
10:Q:116:ARG:NH1	16:U:261:THR:O	2.37	0.41
10:Q:142:ASN:O	10:Q:145:ARG:HG2	2.20	0.41
10:Q:179:LEU:HD23	10:Q:180:LYS:HE2	2.02	0.41
11:S:71:HIS:CG	12:T:517:LEU:HD22	2.55	0.41
12:T:543:TYR:CE2	13:W:17:ALA:HB3	2.55	0.41
2:H:238:LEU:HG	3:I:183:LEU:HD23	2.02	0.41
3:I:106:SER:OG	3:I:141:GLU:OE2	2.28	0.41
4:K:55:ALA:O	4:K:59:LEU:HB2	2.21	0.41
5:L:222:ALA:O	5:L:226:THR:HG23	2.21	0.41
5:L:294:HIS:O	7:N:322:LEU:HD12	2.20	0.41
6:M:31:LEU:HD11	6:M:146:LEU:HD12	2.01	0.41
7:N:139:THR:HG22	7:N:142:THR:HG22	2.03	0.41
7:N:207:LYS:HB3	8:O:152:HIS:HA	2.03	0.41
8:O:287:PHE:HD1	8:O:287:PHE:HA	1.77	0.41
11:S:31:CYS:SG	11:S:47:ILE:HD13	2.61	0.41
14:X:38:MET:HA	14:X:41:LEU:HG	2.03	0.41
14:X:69:GLN:O	14:X:73:VAL:HG22	2.20	0.41
2:H:179:LYS:O	2:H:183:LYS:HG2	2.21	0.41
2:H:194:ARG:HG3	4:K:159:PHE:CZ	2.55	0.41
2:H:216:PHE:CE2	4:K:179:THR:HB	2.56	0.41
3:I:217:PHE:HD2	3:I:221:LYS:HE2	1.86	0.41
3:I:446:TRP:CZ2	3:I:452:ARG:HA	2.54	0.41
4:K:52:ASP:OD1	4:K:52:ASP:N	2.43	0.41
4:K:239:TRP:HE1	4:K:241:PRO:HB2	1.86	0.41
5:L:43:THR:H	6:M:115:HIS:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:240:LEU:N	5:L:306:ARG:O	2.43	0.41
5:L:254:PHE:CD2	5:L:291:PHE:HD2	2.39	0.41
7:N:35:GLN:HG2	7:N:55:LEU:HD22	2.02	0.41
8:O:252:VAL:HG11	8:O:271:HIS:HB3	2.03	0.41
11:S:46:THR:OG1	14:X:65:VAL:O	2.39	0.41
12:T:515:LEU:O	12:T:515:LEU:HD23	2.20	0.41
13:W:78:ALA:O	13:W:82:ILE:HG12	2.21	0.41
14:X:10:PHE:HB2	14:X:39:VAL:HG13	2.01	0.41
4:K:63:GLN:CD	6:M:166:LEU:HD11	2.45	0.41
6:M:34:SER:OG	6:M:139:ARG:NH1	2.52	0.41
3:I:138:VAL:H	3:I:141:GLU:HG3	1.86	0.40
3:I:231:MET:HE1	5:L:104:GLN:HE21	1.86	0.40
5:L:31:LEU:HD23	5:L:31:LEU:HA	1.89	0.40
6:M:85:LEU:HD13	6:M:124:TYR:CE1	2.56	0.40
7:N:83:TRP:CE2	7:N:198:LEU:HD22	2.56	0.40
8:O:293:LYS:HB2	8:O:293:LYS:HE2	1.97	0.40
9:P:108:SER:HA	9:P:117:GLN:HA	2.03	0.40
10:Q:106:ILE:HA	10:Q:109:HIS:HB3	2.03	0.40
11:S:61:PHE:HD2	11:S:85:LEU:HD21	1.85	0.40
3:I:570:ASP:O	3:I:574:ASN:HB2	2.20	0.40
5:L:158:TRP:HA	5:L:188:GLY:HA3	2.02	0.40
11:S:67:MET:HA	11:S:70:ARG:HB2	2.03	0.40
2:H:136:LEU:HD13	4:K:104:LEU:HB2	2.02	0.40
2:H:172:LEU:HB2	4:K:139:LEU:HD21	2.03	0.40
3:I:464:PHE:CZ	3:I:532:SER:HB3	2.57	0.40
5:L:56:GLN:H	5:L:56:GLN:CD	2.29	0.40
5:L:161:TRP:HB3	5:L:185:LEU:HB2	2.03	0.40
6:M:42:SER:OG	6:M:156:HIS:ND1	2.42	0.40
7:N:202:LYS:HG2	7:N:206:PHE:CD2	2.57	0.40
8:O:170:GLN:HG3	8:O:180:LEU:CD1	2.52	0.40
9:P:85:THR:HG23	9:P:103:GLN:HG2	2.04	0.40
9:P:155:SER:O	9:P:159:GLU:N	2.55	0.40
3:I:112:LEU:HD23	3:I:113:LEU:N	2.36	0.40
7:N:247:ARG:CZ	7:N:317:ALA:HB3	2.52	0.40
8:O:220:PHE:HD1	8:O:222:TYR:HD2	1.69	0.40
9:P:216:PHE:CD2	16:U:365:TYR:HA	2.57	0.40
12:T:494:LEU:O	12:T:498:LEU:HB2	2.21	0.40
3:I:400:CYS:O	3:I:403:TYR:HB2	2.20	0.40
4:K:54:ASN:OD1	4:K:54:ASN:C	2.64	0.40
5:L:98:PHE:CD2	5:L:199:TRP:HB2	2.56	0.40
5:L:306:ARG:HB2	5:L:315:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:112:LEU:HD11	7:N:137:TRP:CH2	2.56	0.40
7:N:135:ILE:HD13	7:N:175:LEU:HD11	2.04	0.40
7:N:154:TYR:CD1	7:N:161:ALA:HB2	2.55	0.40
8:O:278:LYS:HG3	8:O:279:PRO:HD2	2.02	0.40
9:P:94:THR:OG1	9:P:97:SER:OG	2.35	0.40
9:P:206:MET:O	9:P:219:VAL:HA	2.22	0.40
11:S:57:GLN:O	11:S:61:PHE:HD1	2.04	0.40
13:W:76:LEU:HD23	13:W:76:LEU:HA	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	C	3/943 (0%)	2 (67%)	1 (33%)	0	100	100
1	c	11/943 (1%)	9 (82%)	2 (18%)	0	100	100
2	H	191/247 (77%)	181 (95%)	10 (5%)	0	100	100
3	I	503/756 (66%)	470 (93%)	31 (6%)	2 (0%)	30	60
4	K	224/269 (83%)	204 (91%)	17 (8%)	3 (1%)	9	35
5	L	296/344 (86%)	272 (92%)	24 (8%)	0	100	100
6	M	166/180 (92%)	148 (89%)	17 (10%)	1 (1%)	21	52
7	N	299/339 (88%)	271 (91%)	28 (9%)	0	100	100
8	O	204/300 (68%)	183 (90%)	21 (10%)	0	100	100
9	P	220/288 (76%)	196 (89%)	21 (10%)	3 (1%)	9	33
10	Q	156/268 (58%)	153 (98%)	3 (2%)	0	100	100
11	S	95/138 (69%)	93 (98%)	2 (2%)	0	100	100
12	T	97/561 (17%)	95 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	W	73/88 (83%)	72 (99%)	1 (1%)	0	100	100
14	X	72/81 (89%)	72 (100%)	0	0	100	100
15	R	58/177 (33%)	55 (95%)	3 (5%)	0	100	100
16	U	136/418 (32%)	132 (97%)	4 (3%)	0	100	100
All	All	2804/6340 (44%)	2608 (93%)	187 (7%)	9 (0%)	37	65

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	156	CYS
9	P	76	ILE
9	P	192	PRO
4	K	190	LEU
4	K	207	VAL
9	P	144	PRO
4	K	188	PHE
6	M	54	LEU
3	I	135	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	4/875 (0%)	4 (100%)	0	100	100
1	c	12/875 (1%)	12 (100%)	0	100	100
2	H	174/224 (78%)	173 (99%)	1 (1%)	78	81
3	I	440/691 (64%)	437 (99%)	3 (1%)	76	80
4	K	211/260 (81%)	209 (99%)	2 (1%)	70	78
5	L	268/306 (88%)	268 (100%)	0	100	100
6	M	147/158 (93%)	144 (98%)	3 (2%)	48	68
7	N	273/311 (88%)	271 (99%)	2 (1%)	76	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	O	170/263 (65%)	169 (99%)	1 (1%)	78	81
9	P	204/259 (79%)	203 (100%)	1 (0%)	81	83
10	Q	109/248 (44%)	108 (99%)	1 (1%)	70	78
11	S	86/121 (71%)	84 (98%)	2 (2%)	44	66
12	T	88/461 (19%)	88 (100%)	0	100	100
13	W	61/77 (79%)	60 (98%)	1 (2%)	55	72
14	X	65/67 (97%)	64 (98%)	1 (2%)	57	72
All	All	2312/5196 (44%)	2294 (99%)	18 (1%)	70	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	122	GLN
3	I	112	LEU
3	I	150	TRP
3	I	418	LEU
4	K	84	LEU
4	K	249	ASN
6	M	52	LEU
6	M	53	PRO
6	M	54	LEU
7	N	72	ILE
7	N	158	THR
8	O	204	LEU
9	P	167	PHE
10	Q	100	ILE
11	S	53	LEU
11	S	64	ASP
13	W	84	LYS
14	X	79	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	52	GLN
2	H	145	GLN
2	H	176	GLN
2	H	182	GLN

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Mol	Chain	Res	Type
2	H	201	ASN
3	I	67	GLN
3	I	114	ASN
3	I	123	ASN
3	I	394	GLN
3	I	406	ASN
3	I	407	ASN
3	I	613	ASN
3	I	631	ASN
3	I	641	ASN
3	I	642	HIS
3	I	726	GLN
4	K	39	GLN
4	K	56	GLN
4	K	115	ASN
4	K	126	GLN
4	K	187	HIS
5	L	37	GLN
5	L	140	GLN
5	L	187	ASN
5	L	290	HIS
5	L	325	HIS
6	M	29	GLN
6	M	113	HIS
6	M	122	HIS
6	M	144	GLN
6	M	151	GLN
7	N	54	HIS
7	N	103	GLN
7	N	106	ASN
7	N	145	ASN
7	N	208	GLN
8	O	100	ASN
8	O	145	GLN
8	O	151	HIS
8	O	153	HIS
8	O	170	GLN
8	O	175	HIS
8	O	185	ASN
8	O	212	ASN
8	O	229	GLN
8	O	267	GLN

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Mol	Chain	Res	Type
8	O	281	HIS
9	P	288	ASN
10	Q	83	HIS
10	Q	107	GLN
10	Q	175	ASN
11	S	16	GLN
11	S	105	GLN
12	T	493	HIS
12	T	532	HIS
13	W	71	ASN
14	X	36	GLN
14	X	69	GLN

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 oligosaccharides 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](#)

There are no chain breaks in this entry.

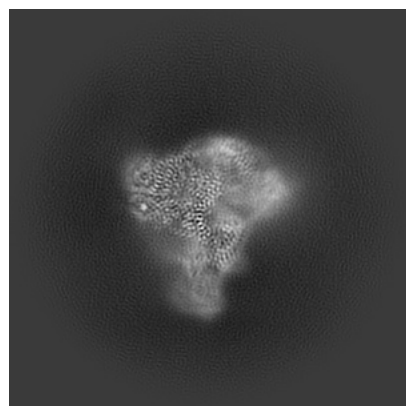
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33197. These allow visual inspection of the internal detail of the map and identification of artifacts.

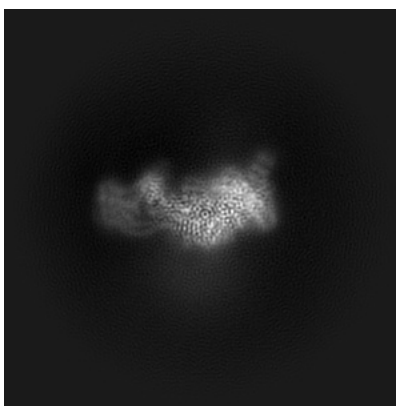
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

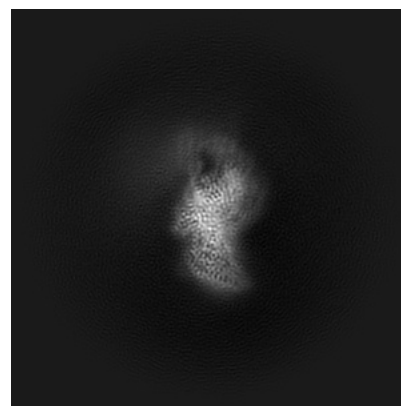
6.1.1 Primary map



X

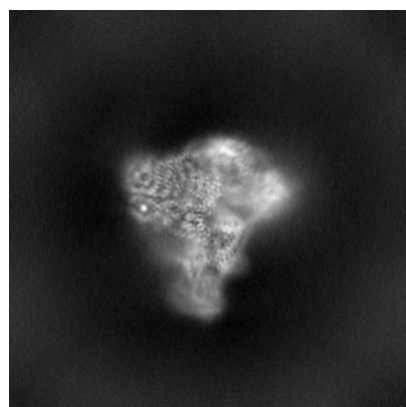


Y

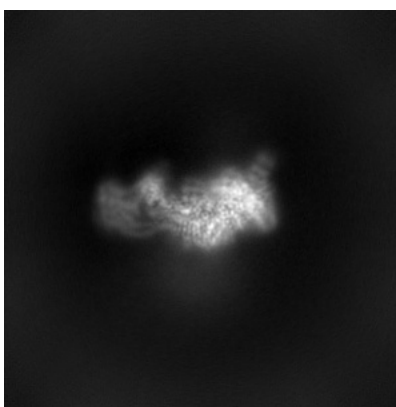


Z

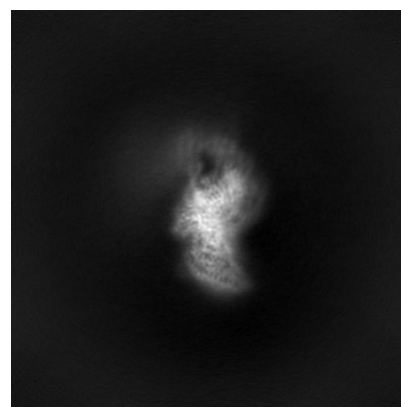
6.1.2 Raw map



X



Y

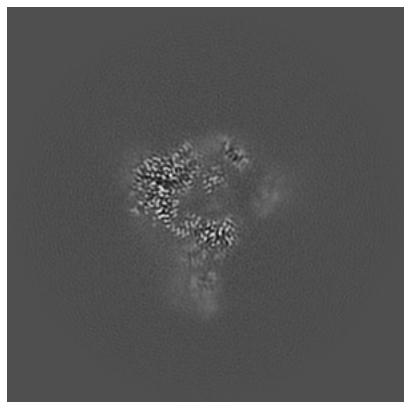


Z

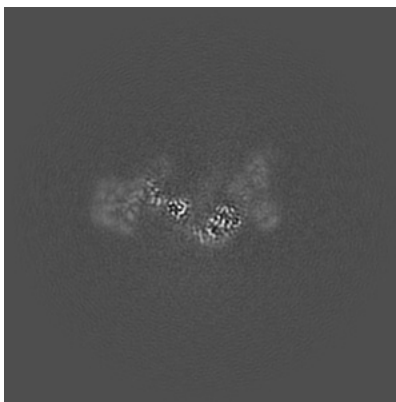
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

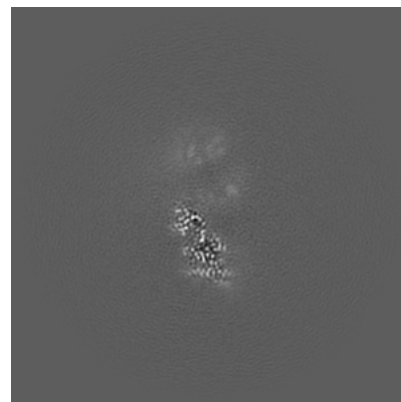
6.2.1 Primary map



X Index: 156

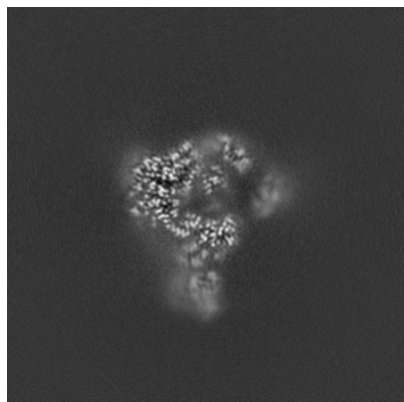


Y Index: 156

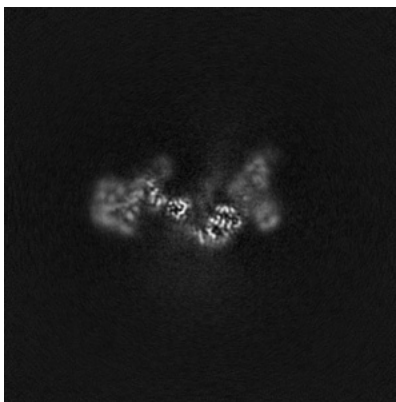


Z Index: 156

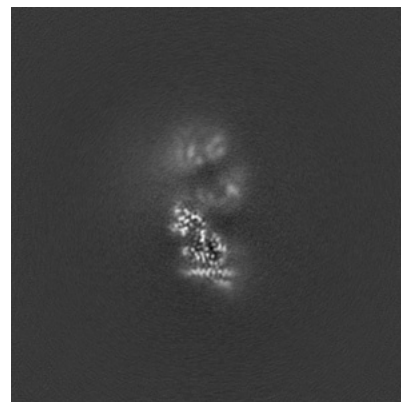
6.2.2 Raw map



X Index: 156



Y Index: 156

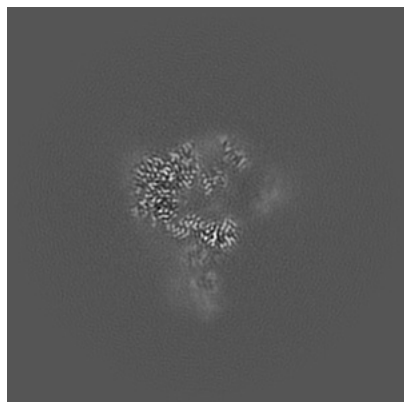


Z Index: 156

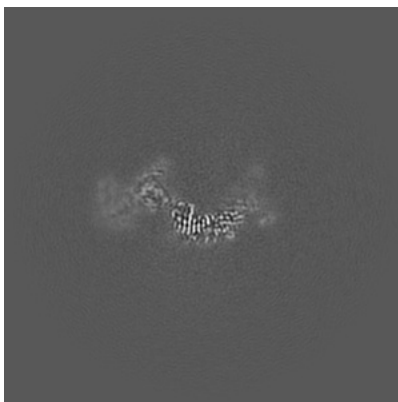
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

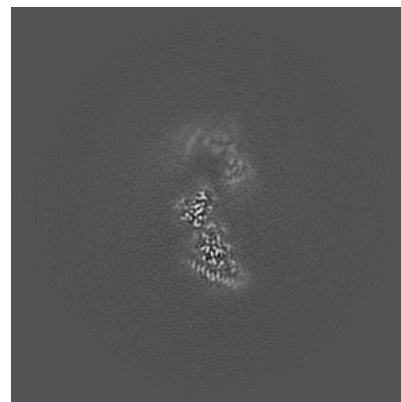
6.3.1 Primary map



X Index: 155

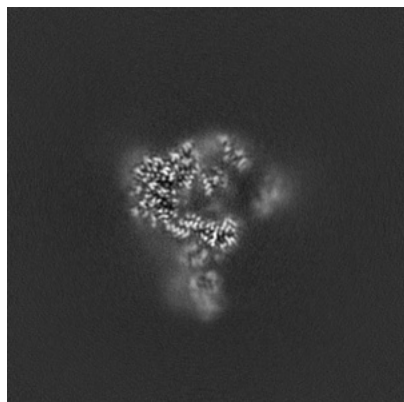


Y Index: 149

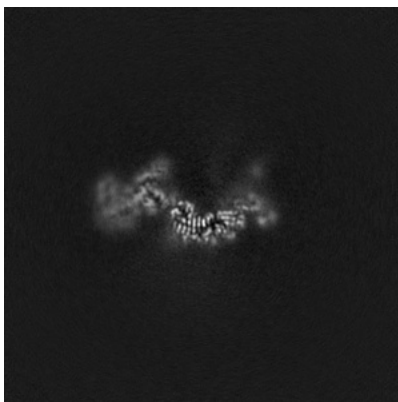


Z Index: 171

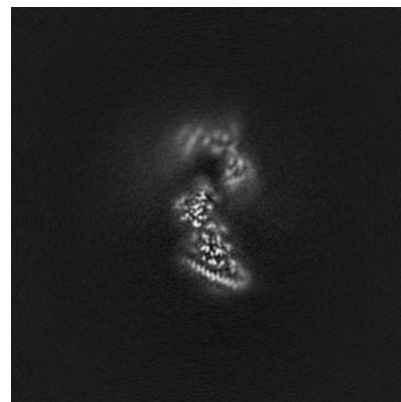
6.3.2 Raw map



X Index: 155



Y Index: 148

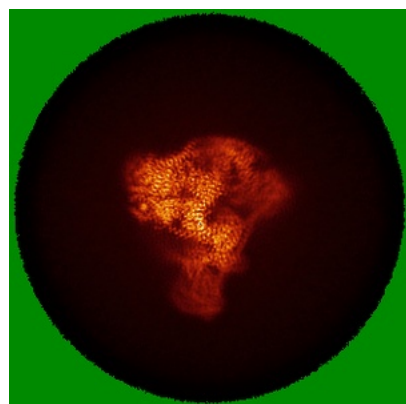


Z Index: 171

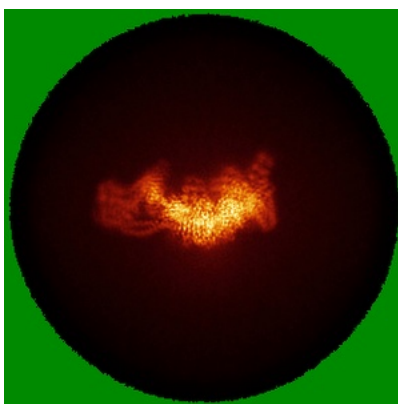
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

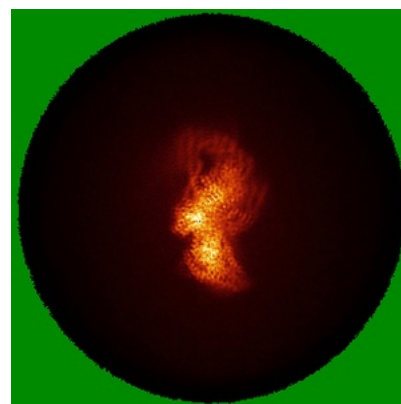
6.4.1 Primary map



X

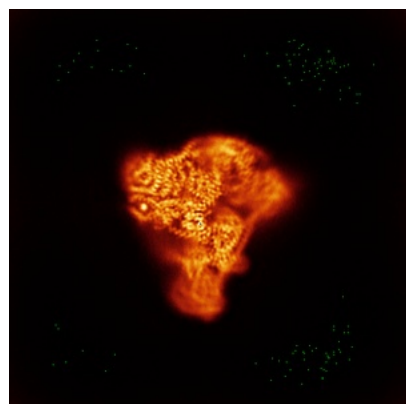


Y

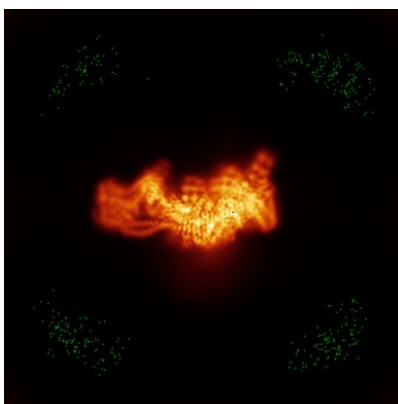


Z

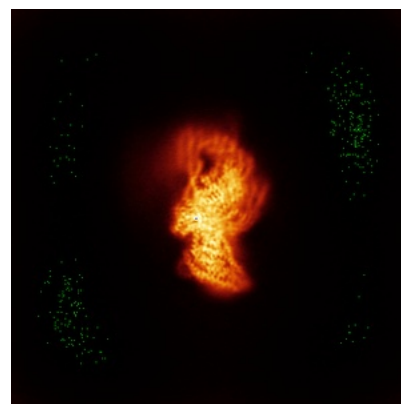
6.4.2 Raw map



X



Y

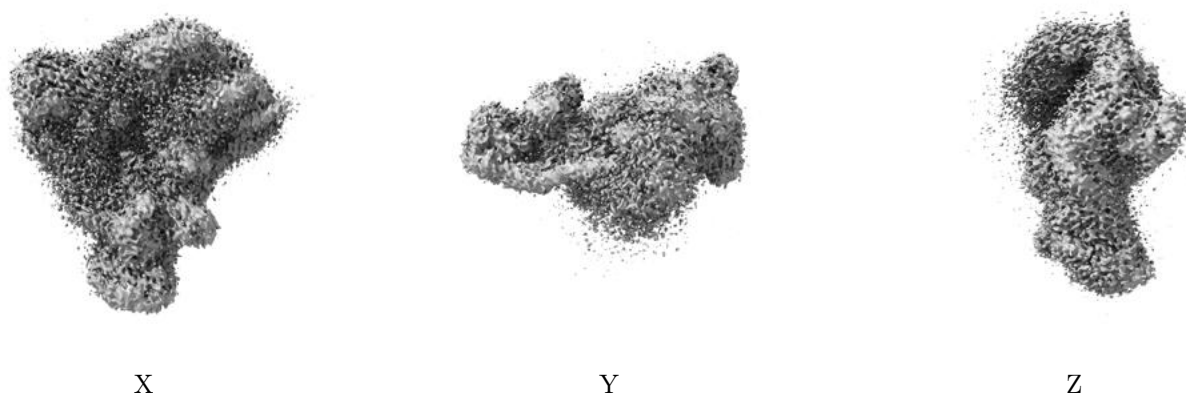


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

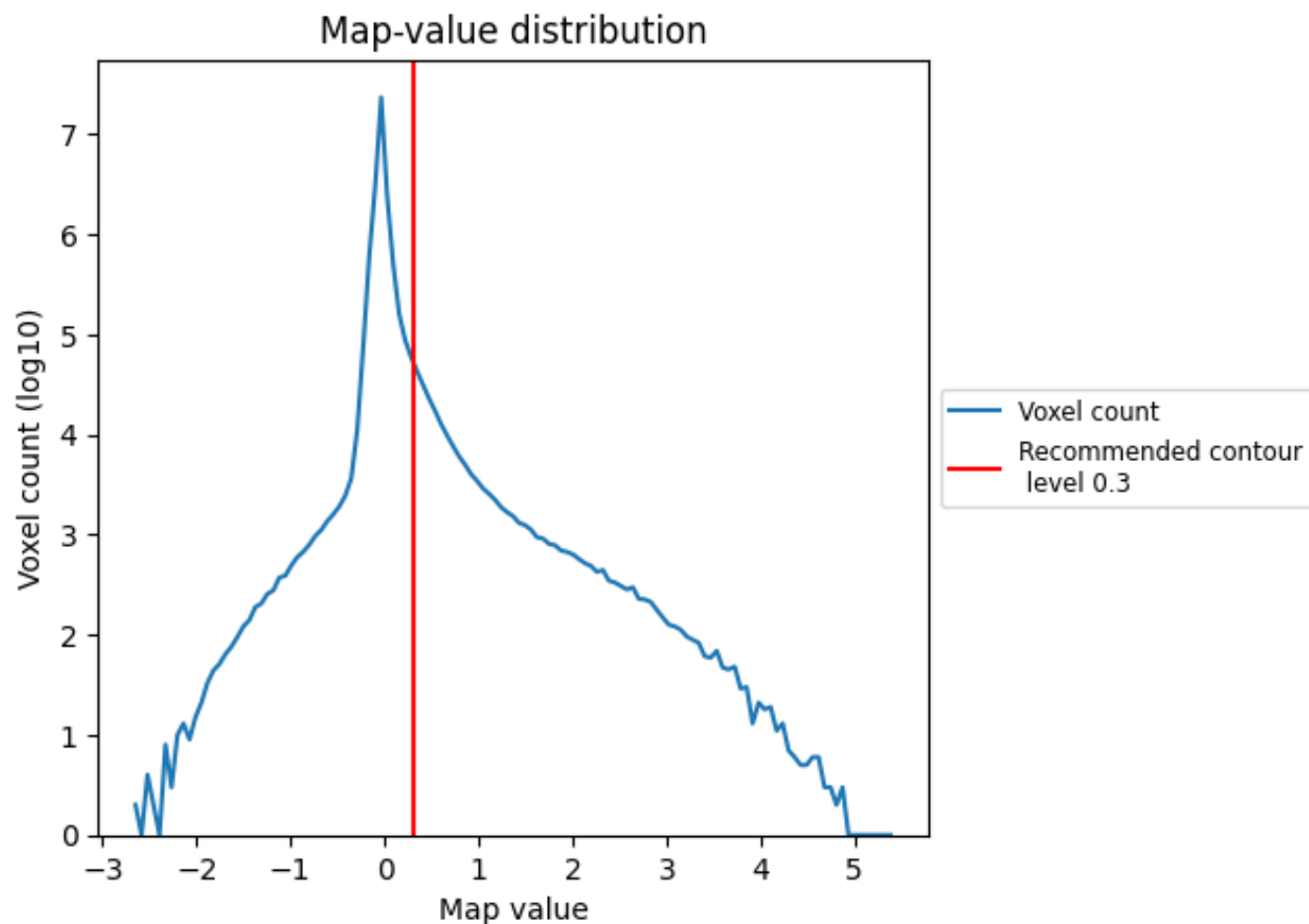
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

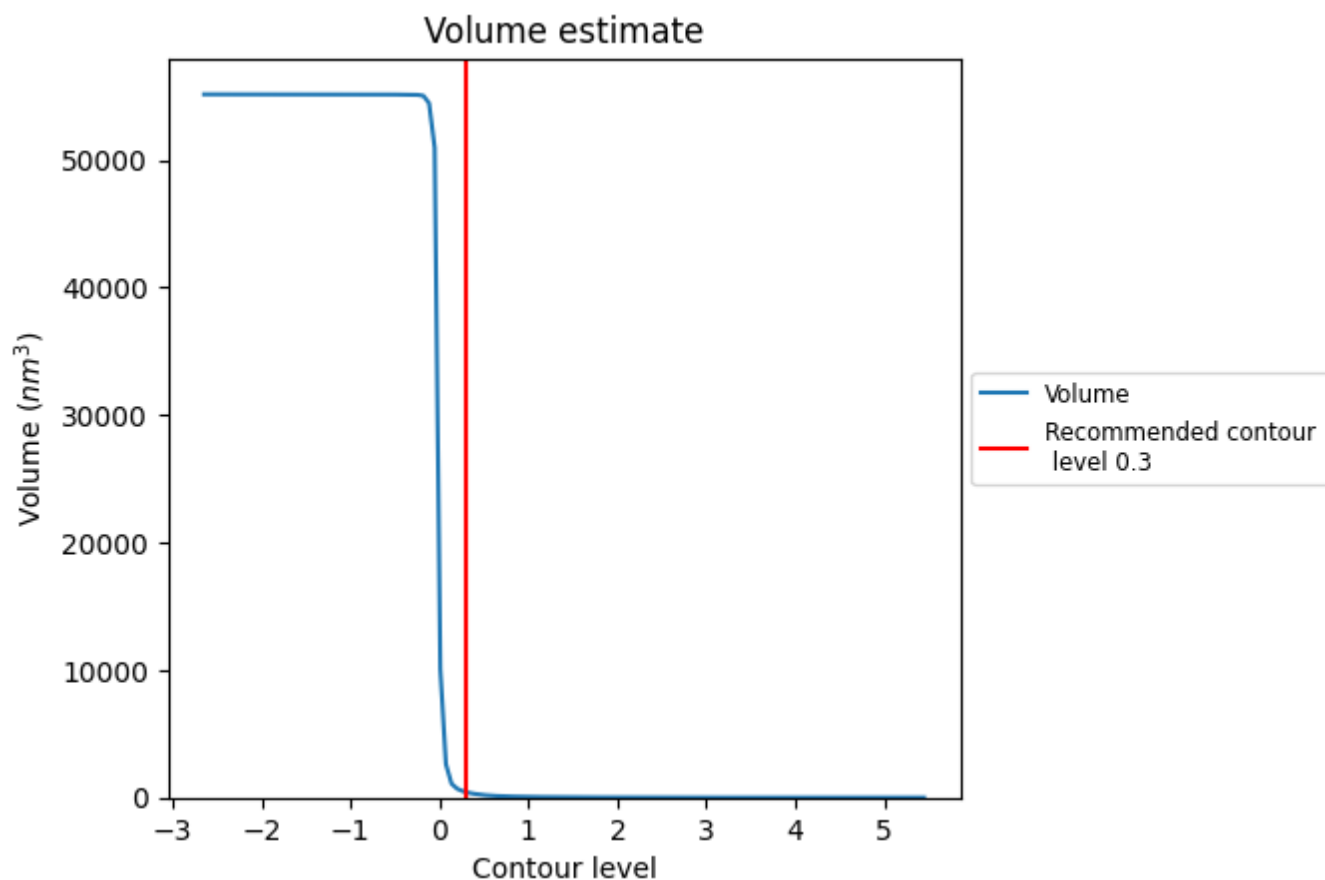
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

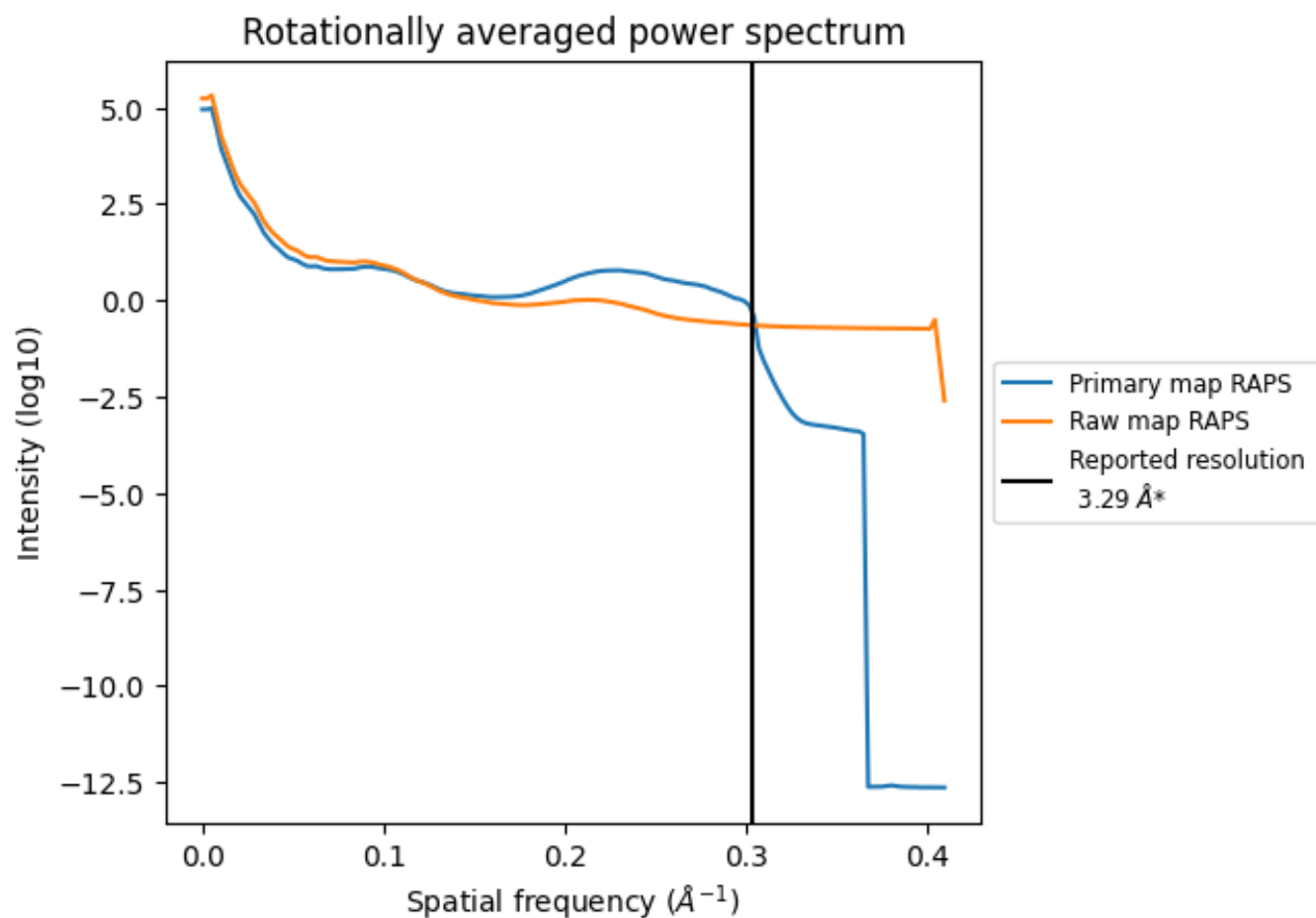
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 427 nm³; this corresponds to an approximate mass of 385 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 ⓘ

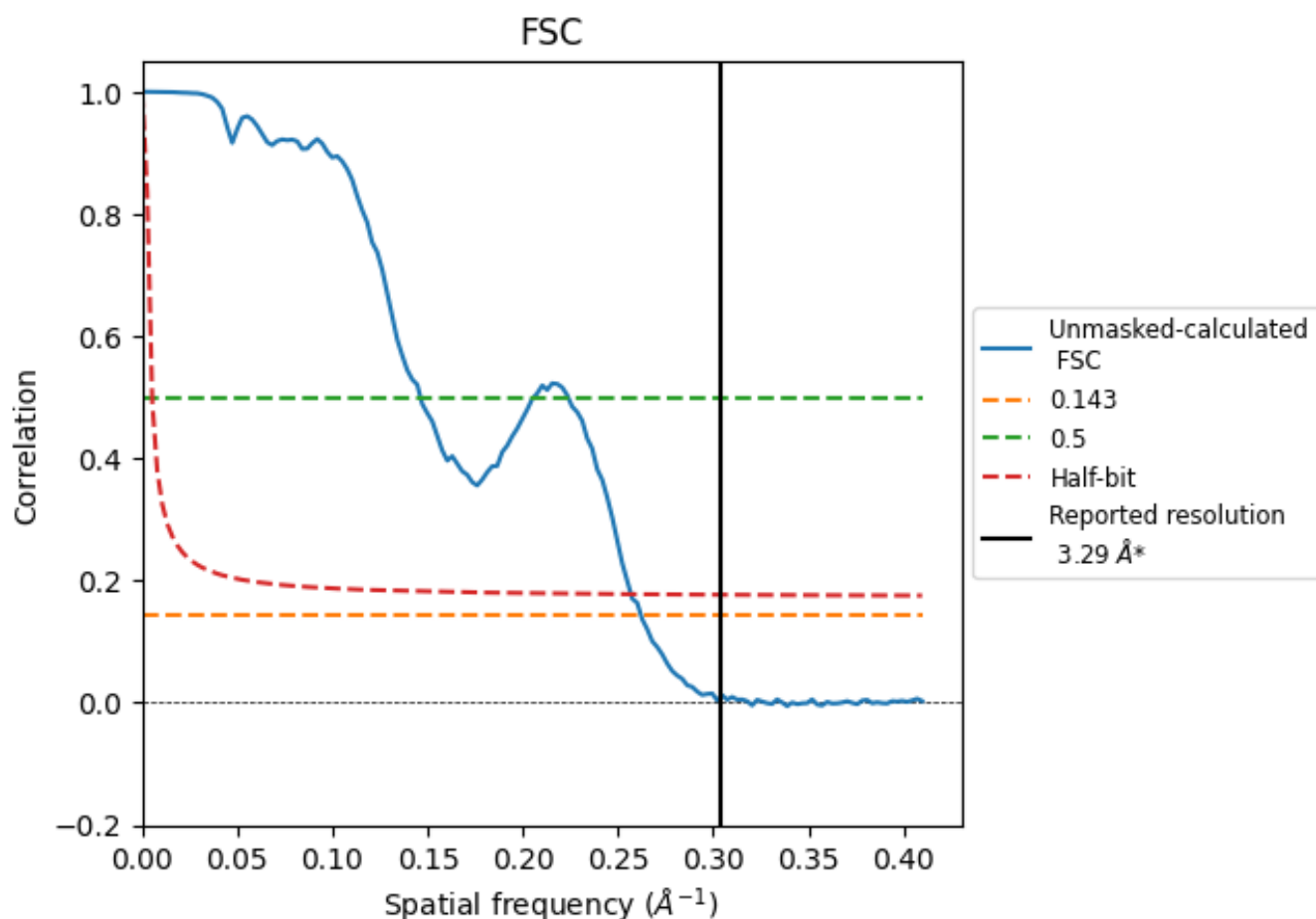


*Reported resolution corresponds to spatial frequency of 0.304 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of $0.304 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

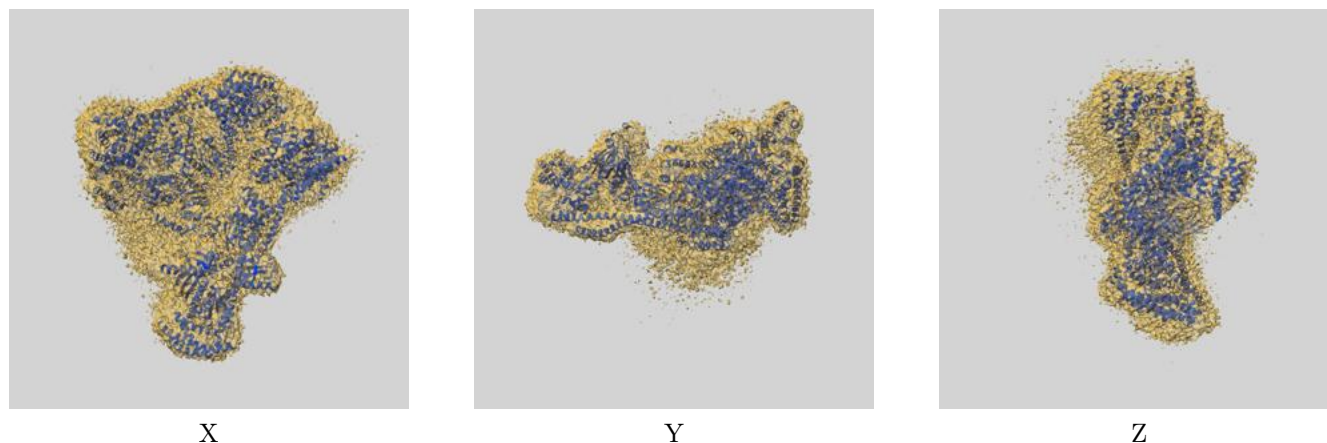
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	6.84	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.29 by more than 10 %

9 Map-model fit [i](#)

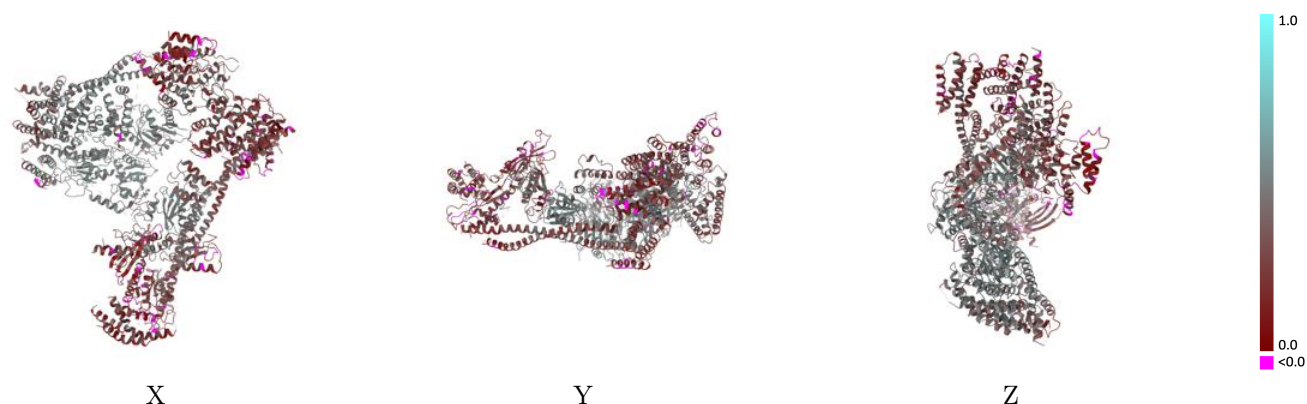
This section contains information regarding the fit between EMDB map EMD-33197 and PDB model 7XHO. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.3 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 Q-score mapped to coordinate model [i](#)

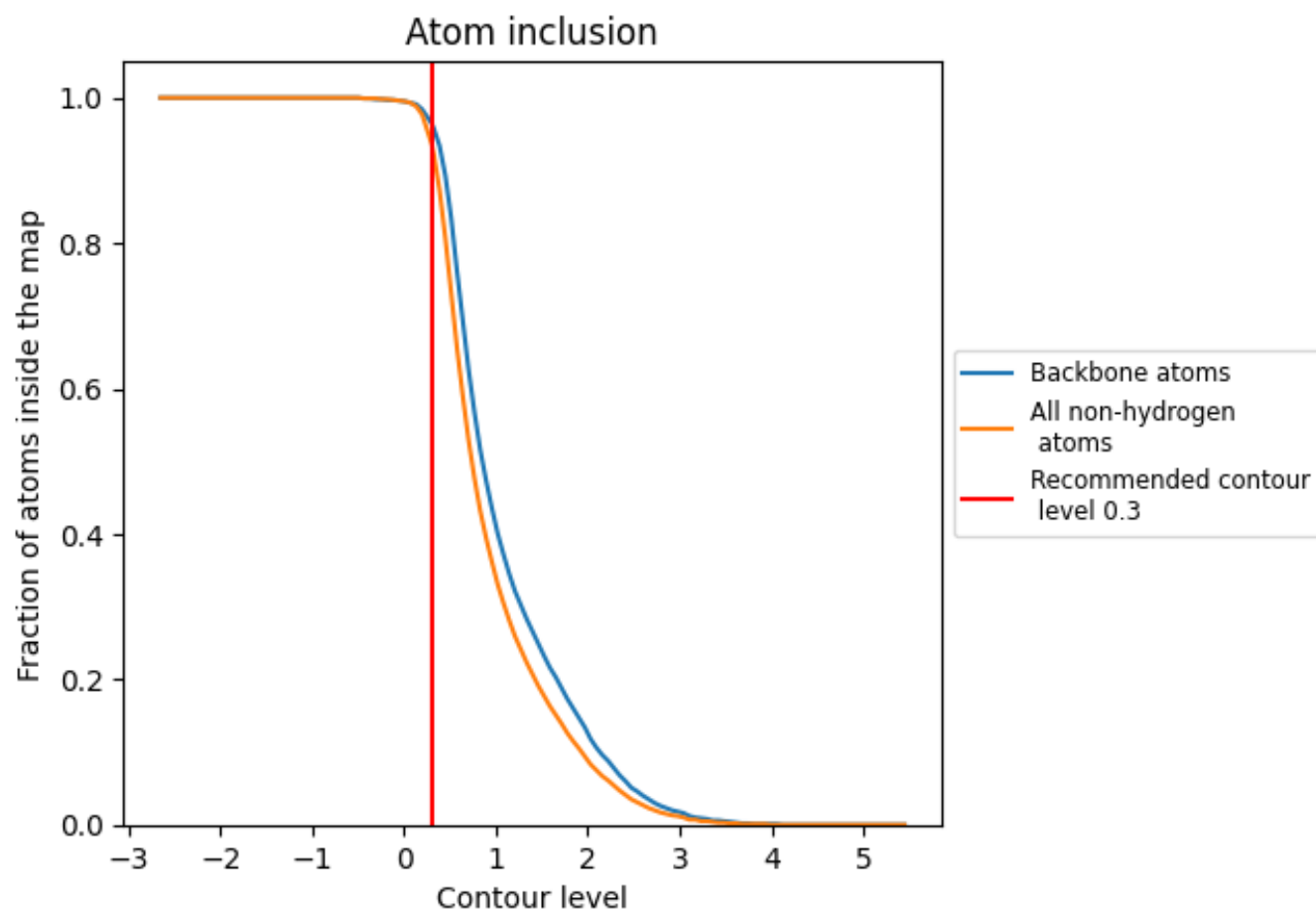


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9370	 0.3660
C	 0.6250	 0.1220
H	 0.9550	 0.4220
I	 0.9310	 0.3890
K	 0.9590	 0.4110
L	 0.9590	 0.4880
M	 0.9660	 0.5110
N	 0.9500	 0.4450
O	 0.8870	 0.3260
P	 0.9220	 0.1920
Q	 0.9420	 0.2480
R	 0.9680	 0.2460
S	 0.9080	 0.2200
T	 0.9530	 0.3360
U	 0.9910	 0.2830
W	 0.9240	 0.2730
X	 0.8210	 0.1640
c	 0.8740	 0.3170

