



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:46 PM UTC

PDB ID : 7F66 / pdb_00007f66
EMDB ID : EMD-31474
Title : eIF2B-SFSV NSs-1-eIF2
Authors : Kashiwagi, K.; Ito, T.
Deposited on : 2021-06-24
Resolution : 2.76 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:

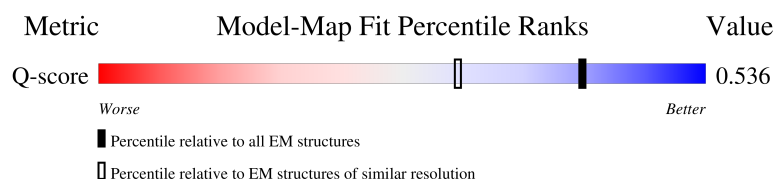
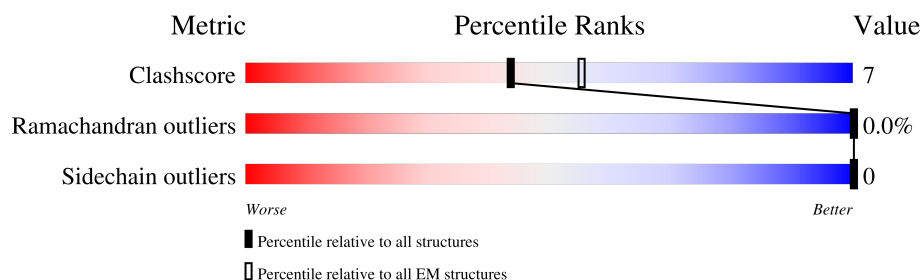
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.76 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.



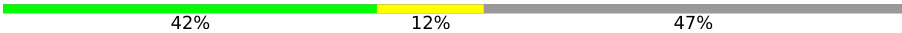
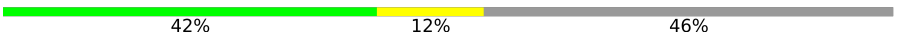
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10642 (2.26 - 3.26)

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	A	307	
1	B	307	
2	C	351	
2	D	351	

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Mol	Chain	Length	Quality of chain
3	E	452	
3	F	452	
4	G	523	
4	H	523	
5	I	721	
5	J	721	
6	K	261	
6	L	261	
7	N	315	
8	O	14	
9	S	472	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 33739 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	293	Total	C	N	O	S	0	0
			2275	1462	377	424	12		
1	B	293	Total	C	N	O	S	0	0
			2275	1462	377	424	12		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q14232
A	0	PRO	-	expression tag	UNP Q14232
B	-1	GLY	-	expression tag	UNP Q14232
B	0	PRO	-	expression tag	UNP Q14232

- Molecule 2 is a protein called Translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	335	Total	C	N	O	S	0	0
			2631	1662	463	491	15		
2	D	331	Total	C	N	O	S	0	0
			2596	1644	453	484	15		

- Molecule 3 is a protein called Translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	241	Total	C	N	O	S	0	0
			1798	1160	301	328	9		
3	F	246	Total	C	N	O	S	0	0
			1869	1207	310	339	13		

- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	356	Total	C	N	O	S	0	0
			2769	1752	492	511	14		
4	H	355	Total	C	N	O	S	0	0
			2765	1749	493	509	14		

- Molecule 5 is a protein called Translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	427	Total	C	N	O	S	0	0
			3336	2104	591	626	15		
5	J	591	Total	C	N	O	S	0	0
			4149	2590	755	789	15		

- Molecule 6 is a protein called Non-structural protein NS-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	197	Total	C	N	O	S	0	0
			1589	1011	274	290	14		
6	L	197	Total	C	N	O	S	0	0
			1589	1011	274	290	14		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	275	Total	C	N	O	S	0	0
			1818	1145	335	331	7		

- Molecule 8 is a protein called eIF2beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	14	Total	C	N	O	0	0
			70	42	14	14		

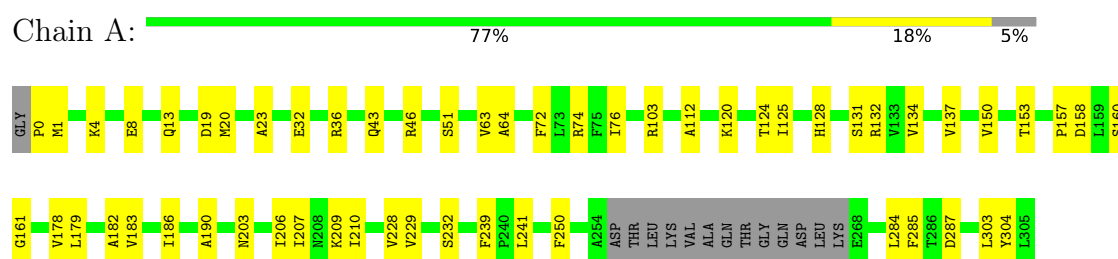
- Molecule 9 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	410	Total	C	N	O	S	0	0
			2210	1338	444	424	4		

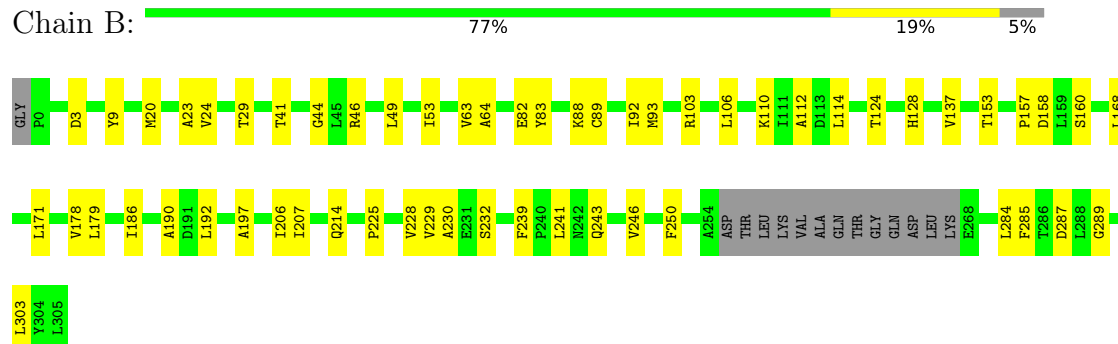
3 Residue-property plots [i](#)

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.

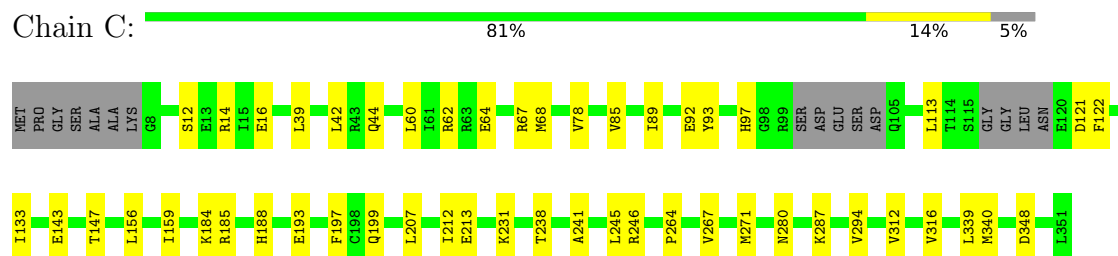
- Molecule 1: Translation initiation factor eIF-2B subunit alpha



- Molecule 1: Translation initiation factor eIF-2B subunit alpha



- Molecule 2: Translation initiation factor eIF-2B subunit beta



- Molecule 2: Translation initiation factor eIF-2B subunit beta



SER
LEU
PRO
THR
THR
PRO
ILE
HIS
SER
HIS
VAL
ASP
GLU
ASN
ASP
GLU
SER
SER
SER
SER
ASP
ASP
PHE

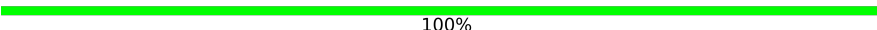
- Molecule 7: Eukaryotic translation initiation factor 2 subunit 1

Chain N:  75% 12% 13%

MET PRO GLY L3 F7 Y8 Q9 V19 M20 V21 V22 V23 I26 V33 V34 L35 L36 E37 I41 M44 S48 R53 R54 I55 R56 S57 I58 N59 K60 E68 C69 V70 E78 K79 G80 Y81 L84 S85 K86 R87 E93 A94 I95 K96 F101 V107

I110 L118 E119 Y120 Q125 L129 R132 W135 V277 THR ASP THR ASP GLU THR LEU ALA ARG ARG MET GLU ARG LEU GLU ARG ASN ALA VAL ASP GLY ASP ASP ASP ALA GLU MET GLU LYS ALA ASP

- Molecule 8: eIF2beta

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Eukaryotic translation initiation factor 2 subunit 3

Chain S:  84% 13%

MET ALA GLY GLY GLY ALA VAL THR LEU GLN PRO HIS LEU SER ARG GLN ASP L20 G45 L91 ASP ASP PRO SER CYS PRO ARG PRO GLU CYS TYR ARG SER CYS GLY SER SER THR PRO ASP GLU PHE PRO THR ASP ILE PRO GLY THR LYS GLY M123 A154 I179

MET LYS LEU LYS H184 F223 ILE SER ALA GLN L228 G276 G280 E295 G338 P345 T346 L347 G359 G362 A363 L364 E387 G388 E402 R445 K449 H450 I454 T468 VAL ASP ASP ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114377	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	38.958	Depositor
Minimum map value	-17.508	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size ($\text{\AA}$)	373.05, 373.05, 373.05	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.829, 0.829, 0.829	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.12	0/2312	0.29	0/3121
1	B	0.17	0/2312	0.39	2/3122 (0.1%)
2	C	0.11	0/2680	0.27	0/3621
2	D	0.11	0/2645	0.25	0/3575
3	E	0.11	0/1825	0.33	0/2477
3	F	0.13	0/1899	0.32	1/2569 (0.0%)
4	G	0.12	0/2821	0.28	0/3833
4	H	0.11	0/2817	0.25	0/3828
5	I	0.10	0/3405	0.28	0/4635
5	J	0.10	0/4216	0.27	0/5764
6	K	0.11	0/1627	0.31	0/2196
6	L	0.12	0/1627	0.34	0/2196
7	N	0.12	0/1840	0.30	0/2503
9	S	0.08	0/2219	0.28	0/3057
All	All	0.12	0/34245	0.29	3/46497 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	GLU	N-CA-C	8.59	120.72	111.36
1	B	83	TYR	N-CA-C	5.96	120.60	112.68
3	F	79	PRO	CA-N-CD	-5.28	104.61	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2275	0	2350	39	0
1	B	2275	0	2347	33	0
2	C	2631	0	2637	31	0
2	D	2596	0	2603	38	0
3	E	1798	0	1753	44	0
3	F	1869	0	1850	40	0
4	G	2769	0	2830	24	0
4	H	2765	0	2829	30	0
5	I	3336	0	3306	39	0
5	J	4149	0	3666	50	0
6	K	1589	0	1554	34	0
6	L	1589	0	1554	28	0
7	N	1818	0	1462	28	0
8	O	70	0	18	0	0
9	S	2210	0	1294	8	0
All	All	33739	0	32053	428	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 7.

All (428) 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:F:91:ARG:HA	3:F:216:MET:HE1	1.51	0.92
2:D:166:MET:HE3	2:D:229:VAL:HG21	1.65	0.76
7:N:19:VAL:HG21	7:N:35:LEU:HD23	1.66	0.76
3:F:110:THR:OG1	3:F:268:LYS:NZ	2.21	0.73
6:L:61:LEU:HA	6:L:64:PHE:HD2	1.53	0.73
3:E:158:ILE:HD11	3:E:199:LEU:HD12	1.71	0.72
3:F:167:LEU:HD23	3:F:265:SER:HB3	1.72	0.71
3:E:167:LEU:HD23	3:E:265:SER:HB2	1.72	0.70
5:J:432:THR:HG22	5:J:433:SER:H	1.56	0.70
6:L:15:ASP:H	6:L:23:SER:HB2	1.57	0.70
1:A:112:ALA:HA	1:A:137:VAL:HG12	1.74	0.69
5:I:139:ASP:HB2	5:I:257:ALA:HB1	1.75	0.69
1:A:232:SER:OG	1:A:287:ASP:OD1	2.09	0.69
3:E:194:ARG:NH1	3:E:195:PHE:O	2.26	0.68
2:C:159:ILE:O	2:C:185:ARG:NH1	2.26	0.68
3:E:118:VAL:HG21	4:G:198:ILE:HD12	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:172:ARG:NH2	5:I:177:ASN:OD1	2.27	0.67
7:N:48:SER:O	7:N:87:ARG:NH2	2.28	0.66
3:F:72:LYS:HB2	3:F:75:ILE:HD11	1.76	0.66
3:F:173:GLU:HA	3:F:176:LEU:HB2	1.77	0.66
4:H:247:GLU:OE2	4:H:250:ARG:NH1	2.28	0.65
3:F:115:HIS:HA	3:F:118:VAL:HG22	1.79	0.65
4:H:393:TYR:O	5:J:339:ARG:NH2	2.29	0.65
6:L:85:PRO:HB3	6:L:187:TYR:CZ	2.31	0.65
2:C:188:HIS:ND1	2:C:213:GLU:OE1	2.29	0.65
7:N:68:GLU:OE2	7:N:86:LYS:NZ	2.24	0.65
2:D:189:VAL:HB	2:D:214:THR:HG22	1.79	0.64
3:E:8:MET:HE2	3:E:86:THR:HG22	1.79	0.64
2:C:156:LEU:O	2:C:185:ARG:NH1	2.30	0.64
4:G:223:ASN:OD1	4:G:441:TYR:OH	2.17	0.63
9:S:346:THR:HG23	9:S:347:LEU:HD12	1.81	0.63
3:E:133:ARG:NH1	3:E:134:LYS:O	2.31	0.63
1:A:128:HIS:O	1:A:153:THR:OG1	2.17	0.62
1:A:229:VAL:HG12	1:A:285:PHE:HB2	1.80	0.62
2:D:14:ARG:NH1	2:D:44:GLN:OE1	2.30	0.61
6:K:6:MET:HG3	6:K:34:HIS:HB2	1.82	0.61
1:A:1:MET:HE2	1:A:36:ARG:HE	1.64	0.61
3:E:128:LEU:HD11	3:E:229:ILE:HD12	1.82	0.61
2:C:193:GLU:OE2	4:H:364:ARG:NH1	2.33	0.61
6:L:120:PRO:HG2	6:L:193:ILE:HD11	1.83	0.61
3:F:94:TYR:CD1	3:F:216:MET:HE3	2.35	0.61
4:G:275:ASN:ND2	4:G:441:TYR:O	2.34	0.60
4:H:292:ARG:NH2	4:H:295:GLU:OE2	2.34	0.60
5:J:208:THR:HG23	5:J:209:THR:HG23	1.84	0.60
6:K:23:SER:C	6:K:152:ARG:HH12	2.10	0.60
5:I:66:VAL:HG12	5:I:76:ILE:HB	1.83	0.60
2:C:93:TYR:O	2:C:97:HIS:HB3	2.02	0.60
2:D:147:THR:HG22	2:D:327:ASN:HD22	1.66	0.60
5:I:271:ASP:OD1	5:I:274:ARG:NH2	2.32	0.59
2:C:89:ILE:HG12	2:C:133:ILE:HD13	1.83	0.58
1:A:13:GLN:HE21	1:A:20:MET:HE1	1.68	0.58
1:B:206:ILE:HG21	1:B:228:VAL:HG11	1.86	0.58
1:B:239:PHE:HE2	1:B:241:LEU:HD23	1.67	0.58
3:E:158:ILE:HG22	3:E:170:MET:HG3	1.85	0.58
5:J:449:ILE:HG22	5:J:458:GLU:HB2	1.84	0.58
6:K:85:PRO:HB3	6:K:187:TYR:CE1	2.39	0.58
5:I:172:ARG:NH2	5:I:255:GLN:OE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:178:VAL:HG12	5:J:286:GLN:HG2	1.86	0.58
7:N:7:PHE:HB2	7:N:37:GLU:HB2	1.85	0.58
6:K:111:PRO:HD2	6:K:114:LEU:HD23	1.86	0.57
1:B:168:LEU:HD12	1:B:171:LEU:HD12	1.86	0.57
5:J:282:ILE:HG13	5:J:283:LEU:HD23	1.86	0.57
5:J:138:VAL:HG13	5:J:143:LEU:HB2	1.87	0.57
1:A:1:MET:HE1	1:A:32:GLU:HG3	1.87	0.57
1:A:120:LYS:NZ	2:C:280:ASN:O	2.34	0.57
6:L:190:PHE:HA	6:L:193:ILE:HG22	1.87	0.57
9:S:280:GLY:HA2	9:S:338:GLY:HA2	1.86	0.57
3:E:191:PRO:HB2	5:I:243:ASP:HB3	1.87	0.57
4:H:275:ASN:ND2	4:H:441:TYR:O	2.36	0.57
1:B:41:THR:HG22	1:B:44:GLY:H	1.70	0.56
3:E:230:PRO:O	3:E:234:ARG:HG3	2.05	0.56
3:F:191:PRO:HB2	5:J:243:ASP:HB3	1.86	0.56
1:A:178:VAL:HG21	1:A:186:ILE:HG13	1.86	0.56
2:D:193:GLU:OE1	2:D:201:HIS:NE2	2.32	0.56
3:E:212:VAL:O	3:E:216:MET:HG2	2.06	0.56
5:I:183:MET:SD	5:I:269:ARG:NH1	2.79	0.56
4:H:493:PRO:HD2	4:H:496:LEU:HD12	1.87	0.56
1:B:303:LEU:HD11	2:D:113:LEU:HD12	1.86	0.56
5:I:58:PRO:HB3	5:I:455:ASP:HB3	1.86	0.56
1:A:239:PHE:CE2	4:G:499:LEU:HG	2.40	0.55
3:F:128:LEU:HB3	3:F:263:ILE:HG12	1.88	0.55
5:J:211:ARG:NH2	5:J:280:GLU:OE2	2.35	0.55
1:A:19:ASP:OD1	1:A:132:ARG:NE	2.36	0.55
4:G:448:GLN:NE2	4:G:450:ASP:O	2.38	0.55
7:N:26:ILE:HG21	7:N:58:ILE:HG21	1.89	0.55
1:A:303:LEU:HD11	2:C:113:LEU:HD12	1.89	0.55
4:G:435:LEU:HD23	4:G:501:ILE:HD11	1.88	0.55
9:S:45:GLY:N	9:S:154:ALA:O	2.37	0.55
1:A:63:VAL:HG21	1:A:207:ILE:HG21	1.89	0.55
5:J:147:ASP:HA	5:J:252:CYS:O	2.06	0.55
1:A:183:VAL:HB	1:B:214:GLN:NE2	2.22	0.54
4:H:354:ARG:O	4:H:355:ARG:NH1	2.40	0.54
3:E:134:LYS:HA	3:E:199:LEU:HD22	1.89	0.54
3:F:115:HIS:NE2	3:F:116:GLU:OE2	2.40	0.54
1:B:23:ALA:HB2	1:B:64:ALA:HB1	1.89	0.54
1:B:63:VAL:HG21	1:B:207:ILE:HG21	1.90	0.54
5:I:318:VAL:HG12	5:I:321:LEU:HB2	1.88	0.54
6:L:98:SER:OG	6:L:135:ARG:NH1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:463:LEU:HD21	4:H:486:ASN:HB3	1.90	0.54
5:J:139:ASP:HB2	5:J:257:ALA:HB1	1.89	0.54
1:A:23:ALA:HB2	1:A:64:ALA:HB1	1.88	0.54
3:E:122:ARG:NH2	4:G:198:ILE:O	2.41	0.53
3:F:212:VAL:O	3:F:216:MET:HG2	2.08	0.53
6:L:119:TRP:CE2	6:L:173:GLU:HG3	2.44	0.53
5:J:47:LEU:HD23	5:J:93:VAL:HG12	1.89	0.53
2:D:318:PRO:HA	2:D:321:ILE:HD12	1.89	0.53
6:K:119:TRP:HZ2	6:K:169:LYS:HG2	1.73	0.53
5:J:72:ASN:O	5:J:333:GLN:NE2	2.41	0.53
1:A:228:VAL:HB	1:A:284:LEU:HD23	1.90	0.53
9:S:449:LYS:O	9:S:450:HIS:ND1	2.42	0.53
5:I:65:ARG:HA	5:I:68:LEU:HG	1.91	0.53
6:K:117:LEU:HB3	6:K:201:LEU:HD21	1.91	0.53
1:B:49:LEU:O	1:B:53:ILE:HG12	2.08	0.53
1:A:46:ARG:NH1	6:K:5:TYR:O	2.41	0.53
5:I:205:VAL:HG12	5:I:212:VAL:HA	1.91	0.53
5:J:207:SER:HB3	5:J:239:GLU:HG3	1.90	0.53
6:L:62:ALA:HA	6:L:65:TYR:CZ	2.44	0.53
1:B:229:VAL:HG12	1:B:285:PHE:HB2	1.91	0.52
5:J:66:VAL:HG12	5:J:76:ILE:HB	1.90	0.52
6:K:116:ALA:O	6:K:200:ARG:NE	2.43	0.52
4:H:435:LEU:HD23	4:H:501:ILE:HD11	1.90	0.52
6:K:21:LEU:O	6:K:152:ARG:NH2	2.43	0.52
2:D:152:ALA:O	2:D:180:GLU:HG2	2.10	0.52
2:D:245:LEU:HB2	2:D:316:VAL:HB	1.92	0.52
2:D:62:ARG:NH2	2:D:348:ASP:OD1	2.43	0.52
5:I:47:LEU:HD11	5:I:153:GLY:HA2	1.92	0.52
3:F:183:LYS:HA	5:J:223:ARG:HG3	1.90	0.52
4:H:327:ILE:O	4:H:354:ARG:NH1	2.39	0.52
5:J:92:PHE:HD1	5:J:121:ARG:HB2	1.75	0.52
5:J:236:ASP:OD1	5:J:236:ASP:N	2.41	0.52
6:K:60:SER:HA	6:K:185:ASN:HB2	1.92	0.52
2:D:295:LEU:HD12	2:D:296:PRO:HD2	1.92	0.52
3:E:89:SER:O	3:E:93:ILE:HG12	2.09	0.52
5:I:113:ARG:NH1	5:I:329:ASP:OD2	2.32	0.52
9:S:445:ARG:HB3	9:S:454:ILE:HG13	1.91	0.52
5:J:656:HIS:O	5:J:660:GLY:N	2.43	0.51
2:D:159:ILE:O	2:D:185:ARG:NH1	2.41	0.51
1:B:88:LYS:HE3	1:B:92:ILE:HD11	1.93	0.51
2:C:121:ASP:OD1	2:C:122:PHE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:319:ILE:HG22	4:G:345:ILE:HD11	1.93	0.51
5:J:195:ARG:NH2	5:J:242:TYR:O	2.40	0.51
5:J:205:VAL:HG11	5:J:289:MET:SD	2.51	0.51
7:N:23:VAL:HA	7:N:33:VAL:HG12	1.92	0.51
1:B:112:ALA:HA	1:B:137:VAL:HG22	1.93	0.51
5:J:62:ASP:OD1	5:J:62:ASP:N	2.43	0.50
1:A:206:ILE:HG21	1:A:228:VAL:HG11	1.93	0.50
2:D:180:GLU:OE1	2:D:183:ARG:NH1	2.45	0.50
3:E:194:ARG:HH12	5:I:237:GLY:HA2	1.76	0.50
5:J:156:ILE:HG13	5:J:309:VAL:HG11	1.93	0.50
3:F:41:ASN:O	3:F:45:ARG:HG3	2.12	0.50
3:F:118:VAL:HG21	4:H:198:ILE:HD12	1.93	0.50
6:K:6:MET:HG2	6:K:38:VAL:HG21	1.93	0.50
6:K:23:SER:O	6:K:152:ARG:NH1	2.33	0.50
6:K:59:ASN:HB3	6:K:84:LYS:HG3	1.94	0.50
3:F:122:ARG:NH2	4:H:198:ILE:O	2.44	0.50
4:G:473:LEU:HD13	4:G:484:LEU:HD21	1.94	0.50
4:H:319:ILE:HG22	4:H:345:ILE:HD11	1.94	0.50
1:A:125:ILE:HB	1:A:150:VAL:HG22	1.92	0.50
1:A:131:SER:HB3	1:A:134:VAL:HG22	1.94	0.50
1:B:89:CYS:O	1:B:93:MET:HG3	2.12	0.50
4:H:409:LEU:HD12	4:H:413:SER:HB2	1.94	0.50
9:S:276:GLY:HA3	9:S:345:PRO:HG3	1.94	0.50
6:L:119:TRP:CD1	6:L:120:PRO:HA	2.47	0.49
7:N:70:VAL:HG11	7:N:84:LEU:HB3	1.93	0.49
2:D:208:SER:OG	2:D:214:THR:OG1	2.28	0.49
6:K:101:ASP:OD1	6:K:102:LEU:N	2.43	0.49
2:D:217:MET:HB3	4:G:485:LEU:HD21	1.95	0.49
3:E:115:HIS:O	3:E:119:ASP:HB2	2.13	0.49
4:G:311:LYS:HD2	4:G:441:TYR:HB3	1.93	0.49
5:I:415:ASP:OD1	5:I:415:ASP:N	2.45	0.49
5:I:90:GLU:OE2	5:I:121:ARG:NE	2.42	0.49
2:D:274:LEU:HD23	2:D:343:LEU:HD12	1.95	0.49
6:L:59:ASN:HB3	6:L:84:LYS:HB2	1.94	0.48
6:L:88:TYR:HB2	6:L:91:GLN:HE22	1.78	0.48
2:D:245:LEU:HD11	2:D:267:VAL:HG21	1.94	0.48
4:G:493:PRO:HD2	4:G:496:LEU:HD12	1.96	0.48
5:J:70:LEU:HD21	5:J:310:CYS:HA	1.94	0.48
6:K:148:SER:O	6:K:152:ARG:HD2	2.13	0.48
1:A:134:VAL:HA	1:A:137:VAL:HG22	1.96	0.48
3:E:94:TYR:CD1	3:E:216:MET:HE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:318:VAL:HG12	5:I:318:VAL:O	2.13	0.48
5:I:422:ARG:HH21	5:I:440:ASN:HD21	1.62	0.48
6:K:12:ILE:HG12	6:K:25:VAL:HG22	1.95	0.48
4:H:247:GLU:N	4:H:247:GLU:OE1	2.47	0.48
6:L:55:PHE:O	6:L:58:ARG:NH2	2.46	0.48
6:L:166:ALA:O	6:L:170:ILE:HG12	2.14	0.48
3:E:132:MET:HG2	3:E:201:ASP:HA	1.94	0.48
6:K:175:ARG:HH12	6:K:181:ASP:CG	2.21	0.48
6:L:119:TRP:CZ2	6:L:173:GLU:HG3	2.49	0.48
5:J:77:ASP:HB3	5:J:328:THR:HG21	1.96	0.48
5:J:128:TYR:OH	5:J:137:ASP:OD2	2.24	0.48
1:B:9:TYR:HD2	1:B:29:THR:HG23	1.79	0.48
5:J:171:ARG:HD3	5:J:288:HIS:CE1	2.49	0.48
7:N:55:ILE:HG13	7:N:60:LYS:HD3	1.96	0.48
5:I:422:ARG:NE	5:I:440:ASN:OD1	2.37	0.47
1:B:46:ARG:HE	6:L:7:PHE:HE2	1.63	0.47
3:E:46:VAL:HB	4:G:198:ILE:HG12	1.97	0.47
4:H:466:LYS:NZ	4:H:468:GLY:O	2.47	0.47
5:I:156:ILE:HG13	5:I:309:VAL:HG11	1.95	0.47
5:J:432:THR:HG22	5:J:433:SER:N	2.26	0.47
6:K:119:TRP:CG	6:K:120:PRO:HA	2.50	0.47
1:A:72:PHE:O	1:A:76:ILE:HG12	2.14	0.47
3:E:262:ASP:HB3	3:E:264:TYR:HE1	1.79	0.47
3:F:37:TRP:HD1	3:F:70:LYS:HD2	1.79	0.47
3:E:160:VAL:HA	3:E:167:LEU:HA	1.97	0.47
3:F:229:ILE:O	3:F:233:VAL:HG23	2.15	0.47
5:I:205:VAL:HG11	5:I:289:MET:SD	2.54	0.47
5:I:324:GLU:HG2	5:I:337:HIS:HB2	1.96	0.47
1:B:3:ASP:HB2	6:L:80:PHE:HE1	1.79	0.47
7:N:35:LEU:HD13	7:N:41:ILE:HG13	1.96	0.47
6:L:22:LEU:O	6:L:23:SER:HB3	2.14	0.47
9:S:402:GLU:OE2	9:S:445:ARG:NE	2.47	0.47
1:A:4:LYS:HG2	1:A:8:GLU:OE1	2.14	0.46
4:H:203:ILE:HA	4:H:259:TYR:HE1	1.80	0.46
7:N:20:MET:HG3	7:N:101:PHE:CG	2.49	0.46
7:N:93:GLU:OE1	7:N:93:GLU:N	2.46	0.46
2:D:317:PRO:HD2	2:D:320:LEU:HD12	1.97	0.46
3:E:268:LYS:HE3	3:E:270:ALA:HB3	1.96	0.46
3:F:232:LEU:HB3	3:F:263:ILE:HD11	1.97	0.46
6:K:88:TYR:OH	6:K:185:ASN:OD1	2.30	0.46
7:N:93:GLU:HA	7:N:96:LYS:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:125:GLN:O	7:N:129:LEU:HG	2.16	0.46
4:G:246:GLU:OE2	7:N:81:TYR:OH	2.27	0.46
6:K:134:ASP:OD1	6:K:134:ASP:N	2.47	0.46
6:L:128:ILE:HD11	6:L:193:ILE:HG23	1.96	0.46
2:C:213:GLU:HA	4:H:481:SER:HB2	1.98	0.46
3:E:224:ILE:HG12	3:E:228:LEU:HD23	1.98	0.46
3:F:129:ALA:HB3	3:F:206:CYS:HB2	1.97	0.46
6:L:97:LEU:HA	6:L:100:PHE:HD2	1.81	0.46
2:D:170:PHE:CD1	2:D:203:MET:HB2	2.51	0.46
3:F:88:ASP:OD1	3:F:91:ARG:NH1	2.49	0.46
3:F:156:ASP:OD1	3:F:156:ASP:N	2.46	0.46
5:I:303:LEU:HB3	5:I:428:ARG:HH12	1.80	0.46
9:S:295:GLU:O	9:S:359:GLY:N	2.48	0.46
3:F:131:LEU:HD11	3:F:268:LYS:HD2	1.97	0.45
4:G:467:ARG:HA	4:G:467:ARG:HD3	1.73	0.45
6:L:150:ILE:HG21	6:L:163:ILE:HD13	1.97	0.45
6:L:198:CYS:O	6:L:202:ILE:HG12	2.16	0.45
4:G:247:GLU:HB2	7:N:81:TYR:HE2	1.82	0.45
4:H:320:SER:HA	4:H:345:ILE:HG12	1.98	0.45
1:A:13:GLN:NE2	1:A:20:MET:HE1	2.28	0.45
1:A:103:ARG:NH1	1:A:287:ASP:OD2	2.49	0.45
2:C:207:LEU:HD22	2:C:212:ILE:HD12	1.98	0.45
4:G:250:ARG:HH12	7:N:44:MET:HG3	1.82	0.45
1:A:124:THR:HB	1:A:190:ALA:HA	1.98	0.45
1:A:157:PRO:HD3	1:B:179:LEU:HD13	1.98	0.45
1:B:158:ASP:O	1:B:160:SER:N	2.47	0.45
1:B:239:PHE:CE2	4:H:499:LEU:HG	2.52	0.45
2:C:62:ARG:NH2	2:C:348:ASP:OD1	2.50	0.45
4:H:411:ASN:ND2	4:H:413:SER:OG	2.43	0.45
5:J:134:VAL:O	5:J:138:VAL:HG23	2.17	0.45
3:F:215:LEU:HD13	3:F:228:LEU:HD13	1.97	0.45
4:H:423:LEU:HD23	4:H:423:LEU:HA	1.84	0.45
3:F:261:LEU:H	3:F:261:LEU:HD23	1.82	0.45
6:L:131:ILE:HG21	6:L:190:PHE:CD2	2.52	0.45
2:C:92:GLU:CD	7:N:53:ARG:HH21	2.25	0.45
5:J:450:SER:OG	5:J:456:ALA:HB2	2.17	0.45
1:A:153:THR:O	1:A:161:GLY:HA3	2.17	0.44
4:H:394:VAL:O	4:H:397:GLU:HG2	2.17	0.44
1:A:179:LEU:HD13	1:B:157:PRO:HD3	1.99	0.44
2:D:346:PRO:HA	2:D:349:HIS:CE1	2.52	0.44
4:H:205:PRO:HA	4:H:208:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:238:THR:HB	2:C:246:ARG:HB3	1.99	0.44
3:E:91:ARG:HA	3:E:216:MET:HE1	1.99	0.44
3:E:94:TYR:HB2	3:E:216:MET:CE	2.47	0.44
3:F:89:SER:O	3:F:93:ILE:HG23	2.17	0.44
3:F:194:ARG:NH1	3:F:195:PHE:O	2.50	0.44
5:J:65:ARG:HA	5:J:68:LEU:HG	1.99	0.44
2:C:16:GLU:OE1	2:C:67:ARG:NH2	2.50	0.44
5:I:47:LEU:HD23	5:I:93:VAL:HG22	1.98	0.44
6:K:160:ASP:N	6:K:160:ASP:OD1	2.49	0.44
2:C:143:GLU:O	2:C:147:THR:OG1	2.31	0.44
3:E:203:HIS:HA	3:E:205:TYR:HE1	1.82	0.44
3:F:175:ASP:OD1	3:F:175:ASP:N	2.50	0.44
4:H:515:VAL:HA	4:H:518:VAL:HG22	2.00	0.44
1:B:128:HIS:O	1:B:153:THR:OG1	2.31	0.44
2:D:132:ASN:O	2:D:135:GLU:HG3	2.16	0.44
3:E:196:HIS:HB3	3:E:199:LEU:HG	1.99	0.44
3:F:132:MET:O	3:F:268:LYS:HG2	2.18	0.44
5:I:154:ASP:N	5:I:154:ASP:OD1	2.51	0.44
1:B:20:MET:HE2	1:B:24:VAL:HG12	2.00	0.43
1:B:232:SER:HB2	1:B:287:ASP:OD1	2.18	0.43
4:G:403:LEU:HD13	4:G:420:THR:HG23	1.98	0.43
6:L:58:ARG:HG2	6:L:64:PHE:CZ	2.53	0.43
1:A:158:ASP:O	1:A:160:SER:N	2.51	0.43
2:C:287:LYS:HB3	2:C:312:VAL:HG22	1.99	0.43
3:F:134:LYS:HB3	3:F:269:GLU:HA	2.00	0.43
5:I:414:CYS:HB2	5:I:433:SER:H	1.83	0.43
5:J:92:PHE:CE2	5:J:143:LEU:HB3	2.54	0.43
7:N:21:VAL:HB	7:N:33:VAL:HB	2.00	0.43
4:G:233:LEU:HD21	4:G:280:LEU:HD22	2.01	0.43
3:F:44:GLU:HG2	3:F:73:PRO:HD2	1.99	0.43
5:I:450:SER:OG	5:I:451:LEU:N	2.51	0.43
3:E:203:HIS:HA	3:E:205:TYR:CE1	2.54	0.43
5:I:201:VAL:HG21	5:I:215:PHE:CE2	2.54	0.43
5:I:283:LEU:O	5:I:283:LEU:HD12	2.17	0.43
3:E:90:LEU:O	3:E:216:MET:HE1	2.18	0.43
3:F:8:MET:HE2	3:F:86:THR:HA	2.00	0.43
4:G:177:VAL:HG12	4:G:179:LEU:H	1.84	0.43
4:G:422:GLN:O	4:G:426:VAL:HG23	2.18	0.43
5:I:416:ASN:HB2	5:I:434:GLN:HG2	2.01	0.43
2:C:231:LYS:HG3	2:C:264:PRO:HG2	2.00	0.43
7:N:69:CYS:SG	7:N:94:ALA:HA	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:VAL:HG22	1:A:182:ALA:HB3	2.00	0.43
1:B:178:VAL:HG11	1:B:186:ILE:HG13	2.00	0.43
2:C:245:LEU:HD11	2:C:267:VAL:HG21	2.00	0.43
5:J:179:SER:HA	5:J:286:GLN:O	2.19	0.43
6:L:112:ASN:O	6:L:115:LYS:HG3	2.19	0.43
1:B:243:GLN:O	1:B:246:VAL:HG12	2.19	0.43
3:E:235:LYS:HD3	3:E:235:LYS:HA	1.83	0.43
5:J:113:ARG:NH2	5:J:329:ASP:OD1	2.47	0.43
2:C:42:LEU:HD13	2:C:85:VAL:HG21	2.01	0.43
3:E:115:HIS:NE2	3:E:116:GLU:OE2	2.52	0.43
3:E:122:ARG:HB3	4:G:209:ARG:HG2	2.00	0.43
3:F:160:VAL:HA	3:F:167:LEU:HA	2.00	0.43
5:J:150:LEU:HB3	5:J:250:SER:OG	2.19	0.43
7:N:78:GLU:HG2	7:N:79:LYS:HG3	2.01	0.43
1:A:43:GLN:NE2	6:K:8:ASP:OD2	2.52	0.42
2:D:240:LEU:HD12	2:D:244:ALA:HB3	2.00	0.42
5:J:55:ARG:HH21	5:J:302:ASN:HD22	1.65	0.42
6:K:170:ILE:HD11	6:K:193:ILE:HG12	2.01	0.42
1:A:74:ARG:HD3	1:A:304:TYR:CE1	2.53	0.42
1:A:239:PHE:HE2	1:A:241:LEU:HD23	1.84	0.42
1:B:106:LEU:O	1:B:110:LYS:HG3	2.19	0.42
2:C:60:LEU:O	2:C:64:GLU:HG2	2.19	0.42
2:C:241:ALA:HA	2:C:340:MET:SD	2.59	0.42
2:D:276:PRO:HB2	2:D:349:HIS:CD2	2.54	0.42
3:E:232:LEU:HB3	3:E:263:ILE:HD11	2.02	0.42
4:H:173:TYR:CG	4:H:187:SER:HB3	2.54	0.42
7:N:70:VAL:CG1	7:N:84:LEU:HB3	2.49	0.42
7:N:129:LEU:HD23	7:N:132:ARG:CZ	2.50	0.42
2:D:166:MET:HE2	2:D:217:MET:HE1	2.01	0.42
2:D:207:LEU:HB2	2:D:214:THR:HG21	2.00	0.42
3:E:115:HIS:HA	3:E:118:VAL:HG22	2.01	0.42
5:J:316:ARG:HH12	5:J:324:GLU:CD	2.26	0.42
5:J:186:LYS:NZ	5:J:295:GLU:O	2.46	0.42
5:J:201:VAL:HG21	5:J:215:PHE:CE2	2.53	0.42
6:L:12:ILE:HG12	6:L:25:VAL:HG22	2.00	0.42
2:C:197:PHE:O	2:C:199:GLN:N	2.51	0.42
4:G:250:ARG:NH1	7:N:44:MET:HG3	2.34	0.42
4:H:196:MET:HE1	4:H:203:ILE:HD11	2.00	0.42
5:J:418:GLU:HB3	5:J:436:VAL:HG22	2.01	0.42
1:B:124:THR:HB	1:B:190:ALA:HA	2.01	0.42
2:D:226:MET:HE2	2:D:226:MET:HB2	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:194:ARG:NH1	5:J:237:GLY:HA2	2.35	0.42
3:F:203:HIS:HA	3:F:205:TYR:CZ	2.54	0.42
5:J:138:VAL:HA	5:J:143:LEU:HD23	1.99	0.42
6:K:60:SER:OG	6:K:63:ASP:OD2	2.37	0.42
1:A:209:LYS:HG3	1:A:210:ILE:H	1.85	0.42
1:B:103:ARG:NH2	2:D:115:SER:O	2.53	0.42
1:B:114:LEU:HD13	1:B:289:GLY:HA2	2.01	0.42
2:D:129:LEU:O	2:D:133:ILE:HG12	2.19	0.42
3:E:221:ILE:HG23	3:E:227:GLU:HG2	2.00	0.42
5:I:265:ASP:N	5:I:265:ASP:OD1	2.49	0.42
1:A:203:ASN:OD1	1:A:203:ASN:N	2.49	0.42
2:D:56:GLU:HA	2:D:59:GLU:HG2	2.01	0.42
5:J:103:LYS:HD2	5:J:122:ILE:HD13	2.01	0.42
5:J:214:HIS:HB2	5:J:230:LEU:HD21	2.02	0.42
5:J:246:ASP:OD2	5:J:269:ARG:NH2	2.47	0.42
1:B:197:ALA:HB3	1:B:230:ALA:HB2	2.02	0.41
2:C:68:MET:HB3	2:C:78:VAL:HG11	2.02	0.41
3:F:94:TYR:CG	3:F:216:MET:HE3	2.55	0.41
3:E:224:ILE:O	3:E:229:ILE:HG12	2.19	0.41
5:I:168:HIS:NE2	5:I:172:ARG:HD2	2.35	0.41
5:J:44:GLN:NE2	5:J:90:GLU:OE1	2.52	0.41
2:C:14:ARG:HH12	2:C:44:GLN:HG3	1.85	0.41
2:D:246:ARG:HB2	2:D:285:PHE:CZ	2.55	0.41
3:F:176:LEU:HD23	3:F:176:LEU:HA	1.93	0.41
3:F:179:GLU:HG3	5:J:225:ALA:HB1	2.03	0.41
5:I:316:ARG:HH21	5:I:337:HIS:CG	2.38	0.41
6:L:57:ARG:HH12	6:L:80:PHE:HB3	1.85	0.41
2:C:12:SER:O	2:C:16:GLU:HG2	2.20	0.41
4:H:413:SER:HB3	4:H:491:VAL:HG13	2.01	0.41
5:I:432:THR:O	5:I:435:VAL:HG23	2.19	0.41
6:K:98:SER:HA	6:K:129:PHE:HB3	2.02	0.41
6:L:74:TRP:HB2	6:L:83:VAL:HG23	2.02	0.41
3:F:64:CYS:HA	3:F:67:PHE:HB2	2.03	0.41
5:I:230:LEU:HD13	5:I:238:VAL:HG21	2.03	0.41
7:N:118:LEU:HB3	7:N:120:TYR:CE2	2.56	0.41
2:C:39:LEU:HD23	2:C:39:LEU:HA	1.95	0.41
3:E:128:LEU:HB3	3:E:263:ILE:HD13	2.02	0.41
3:E:170:MET:HE3	3:E:230:PRO:HG3	2.01	0.41
4:H:422:GLN:O	4:H:426:VAL:HG23	2.20	0.41
6:L:83:VAL:HG12	6:L:83:VAL:O	2.21	0.41
2:D:68:MET:HB3	2:D:78:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:62:ALA:HA	6:K:65:TYR:CE2	2.55	0.41
2:D:193:GLU:HG2	2:D:218:THR:HA	2.02	0.41
2:D:249:THR:HA	2:D:314:ASP:HB2	2.03	0.41
3:E:208:LYS:HG2	3:E:210:TYR:CE2	2.56	0.41
4:G:287:VAL:HG13	4:G:291:LYS:HD3	2.01	0.41
1:A:51:SER:HB3	6:K:80:PHE:HB2	2.01	0.41
1:B:192:LEU:HB3	1:B:225:PRO:HG2	2.03	0.41
1:B:228:VAL:HB	1:B:284:LEU:HD13	2.02	0.41
2:D:33:GLU:OE2	2:D:36:ARG:NH1	2.54	0.41
2:D:337:TYR:O	2:D:340:MET:HB2	2.21	0.41
3:F:88:ASP:HA	3:F:91:ARG:HG2	2.02	0.41
5:I:281:GLU:HG2	5:I:282:ILE:N	2.35	0.41
5:J:125:SER:HB3	5:J:128:TYR:CE2	2.55	0.41
6:K:120:PRO:HG3	6:K:153:MET:HE2	2.03	0.41
2:D:52:SER:N	2:D:56:GLU:OE2	2.42	0.41
3:E:27:LEU:HD13	3:E:56:THR:HG21	2.03	0.41
7:N:19:VAL:HG23	7:N:37:GLU:OE2	2.21	0.41
1:A:0:PRO:HG3	6:K:79:TYR:CZ	2.55	0.40
1:A:63:VAL:HG22	1:A:250:PHE:CG	2.56	0.40
1:B:63:VAL:HG22	1:B:250:PHE:CG	2.56	0.40
3:F:128:LEU:HD21	3:F:229:ILE:HG23	2.03	0.40
7:N:9:GLN:HA	7:N:135:TRP:CE2	2.56	0.40
7:N:44:MET:O	7:N:84:LEU:HB2	2.21	0.40
7:N:107:VAL:O	7:N:110:ILE:HG12	2.21	0.40
2:C:156:LEU:HD11	2:C:184:LYS:HD3	2.04	0.40
2:C:245:LEU:HB2	2:C:316:VAL:HB	2.03	0.40
2:C:271:MET:HE1	2:C:339:LEU:HD13	2.03	0.40
3:E:8:MET:HE2	3:E:86:THR:HA	2.03	0.40
5:I:106:LEU:HD23	5:I:106:LEU:HA	1.90	0.40
6:K:57:ARG:HH12	6:K:80:PHE:HB3	1.86	0.40
6:K:60:SER:OG	6:K:60:SER:O	2.39	0.40
6:K:62:ALA:HA	6:K:65:TYR:CZ	2.57	0.40
2:D:87:LYS:HD3	2:D:343:LEU:C	2.46	0.40
3:E:107:ASP:OD1	3:E:107:ASP:N	2.53	0.40
3:E:187:LEU:HD12	5:I:224:PHE:HD2	1.85	0.40
5:I:276:LEU:HD21	5:I:285:ASN:O	2.21	0.40
6:K:171:LEU:HD23	6:K:171:LEU:HA	1.90	0.40
2:D:39:LEU:HD23	2:D:39:LEU:HA	1.94	0.40
2:C:294:VAL:HG13	4:H:387:LEU:HG	2.03	0.40
3:E:229:ILE:O	3:E:233:VAL:HG23	2.21	0.40
5:J:61:LYS:HD3	5:J:452:HIS:ND1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:282:ILE:O	5:J:283:LEU:HD23	2.20	0.40
6:K:119:TRP:CD1	6:K:120:PRO:HA	2.56	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	289/307 (94%)	284 (98%)	5 (2%)	0	100	100
1	B	289/307 (94%)	281 (97%)	8 (3%)	0	100	100
2	C	329/351 (94%)	318 (97%)	11 (3%)	0	100	100
2	D	325/351 (93%)	314 (97%)	11 (3%)	0	100	100
3	E	233/452 (52%)	219 (94%)	14 (6%)	0	100	100
3	F	238/452 (53%)	226 (95%)	12 (5%)	0	100	100
4	G	354/523 (68%)	348 (98%)	6 (2%)	0	100	100
4	H	353/523 (68%)	349 (99%)	4 (1%)	0	100	100
5	I	425/721 (59%)	407 (96%)	18 (4%)	0	100	100
5	J	585/721 (81%)	553 (94%)	32 (6%)	0	100	100
6	K	193/261 (74%)	177 (92%)	15 (8%)	1 (0%)	24	43
6	L	193/261 (74%)	177 (92%)	15 (8%)	1 (0%)	24	43
7	N	273/315 (87%)	260 (95%)	13 (5%)	0	100	100
9	S	402/472 (85%)	362 (90%)	40 (10%)	0	100	100
All	All	4481/6017 (74%)	4275 (95%)	204 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	K	61	LEU
6	L	23	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	250/261 (96%)	250 (100%)	0	100	100
1	B	249/261 (95%)	249 (100%)	0	100	100
2	C	287/298 (96%)	287 (100%)	0	100	100
2	D	284/298 (95%)	284 (100%)	0	100	100
3	E	179/398 (45%)	179 (100%)	0	100	100
3	F	192/398 (48%)	192 (100%)	0	100	100
4	G	312/444 (70%)	312 (100%)	0	100	100
4	H	311/444 (70%)	311 (100%)	0	100	100
5	I	375/626 (60%)	375 (100%)	0	100	100
5	J	374/626 (60%)	374 (100%)	0	100	100
6	K	176/233 (76%)	176 (100%)	0	100	100
6	L	176/233 (76%)	176 (100%)	0	100	100
7	N	124/280 (44%)	124 (100%)	0	100	100
9	S	52/397 (13%)	52 (100%)	0	100	100
All	All	3341/5197 (64%)	3341 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	128	HIS
1	A	214	GLN
1	A	244	GLN

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Mol	Chain	Res	Type
1	B	214	GLN
1	B	244	GLN
2	C	53	ASN
2	C	110	HIS
2	C	199	GLN
2	C	277	GLN
2	D	132	ASN
2	D	138	ASN
2	D	260	HIS
2	D	277	GLN
2	D	349	HIS
3	E	190	HIS
4	G	185	GLN
4	G	329	ASN
4	G	371	HIS
4	G	431	ASN
4	H	185	GLN
4	H	213	GLN
4	H	411	ASN
4	H	448	GLN
4	H	470	HIS
5	I	118	ASN
5	I	341	ASN
5	I	359	ASN
5	I	376	ASN
5	I	388	ASN
5	I	407	GLN
5	J	341	ASN
5	J	359	ASN
5	J	376	ASN
5	J	388	ASN
5	J	407	GLN
6	K	112	ASN
6	L	31	ASN
9	S	76	ASN
9	S	458	GLN

5.3.3 RNA ⓘ

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.

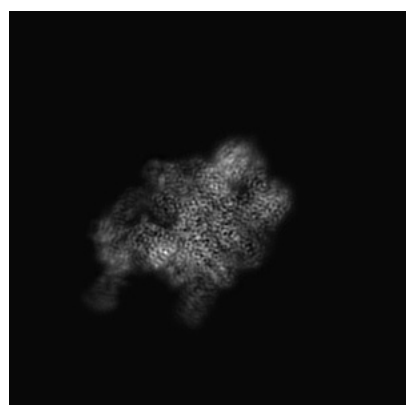
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31474. These allow visual inspection of the internal detail of the map and identification of artifacts.

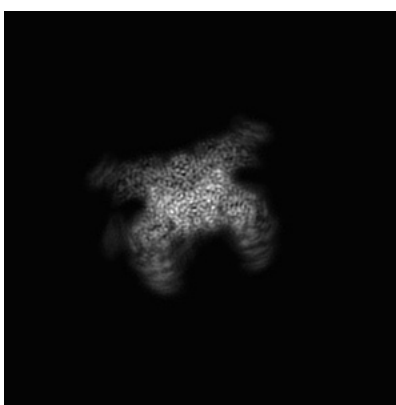
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

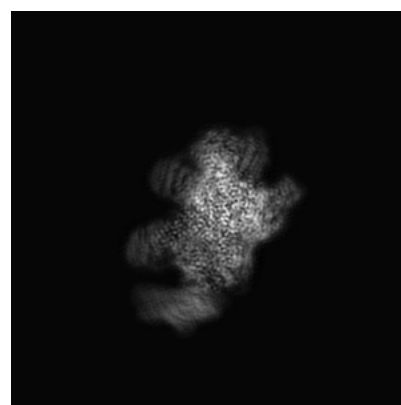
6.1.1 Primary map



X



Y

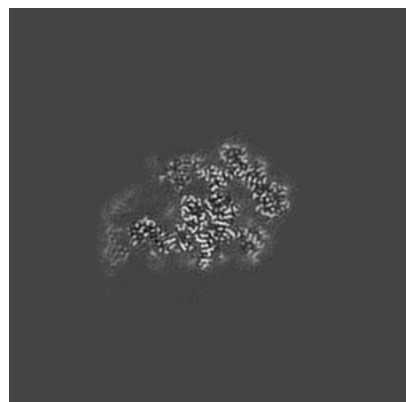


Z

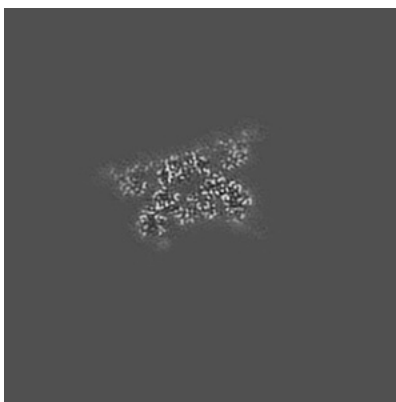
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

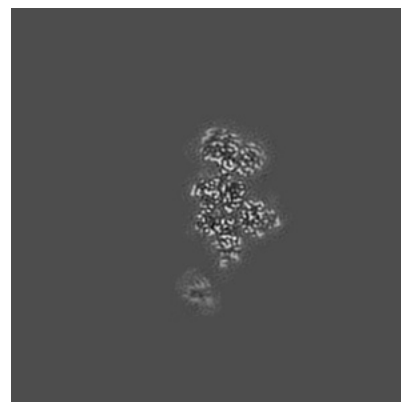
6.2.1 Primary map



X Index: 225



Y Index: 225

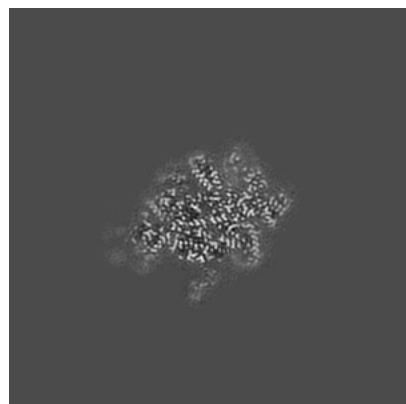


Z Index: 225

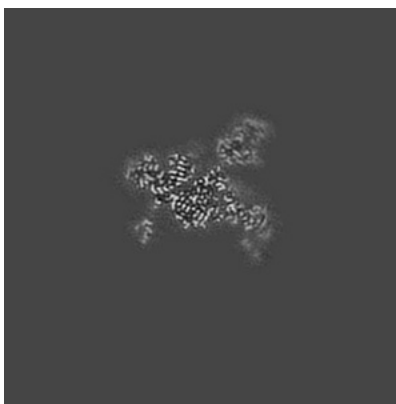
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

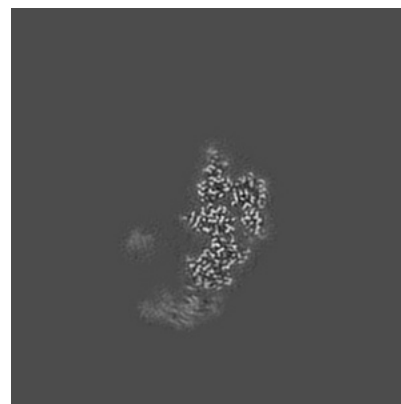
6.3.1 Primary map



X Index: 238



Y Index: 239

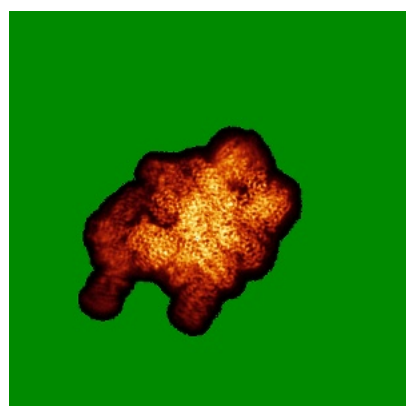


Z Index: 194

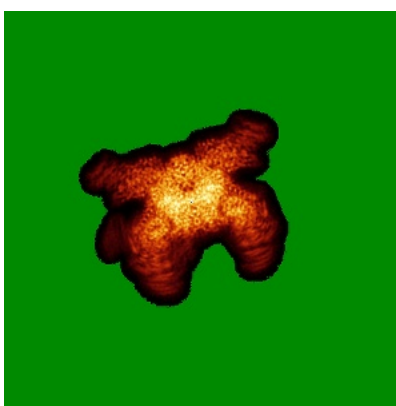
The images above show the largest variance slices of the map in three orthogonal directions.

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

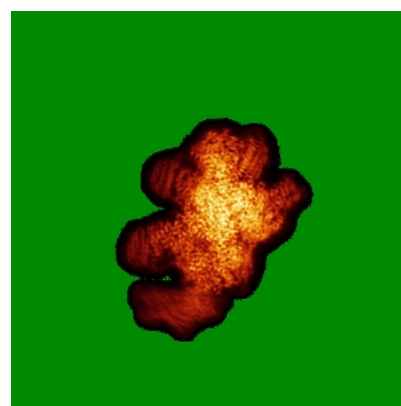
6.4.1 Primary map



X



Y

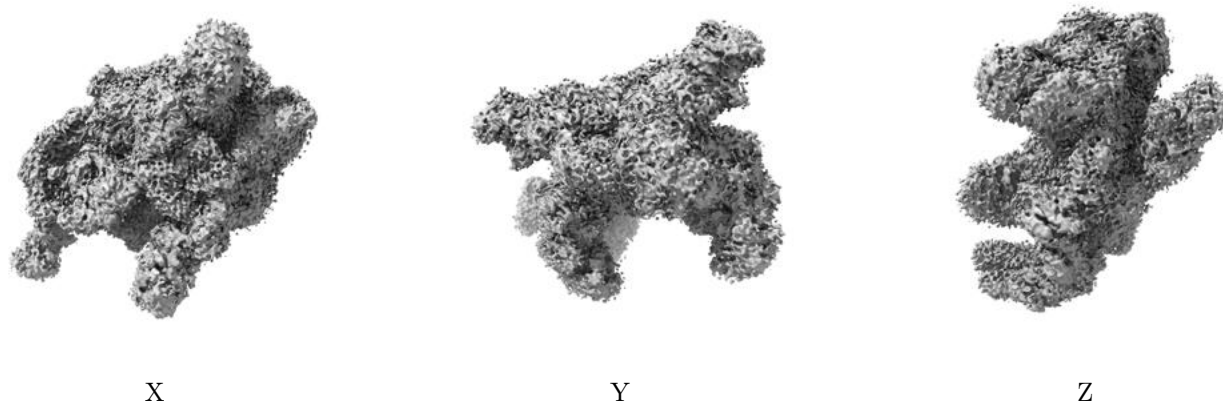


Z

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 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

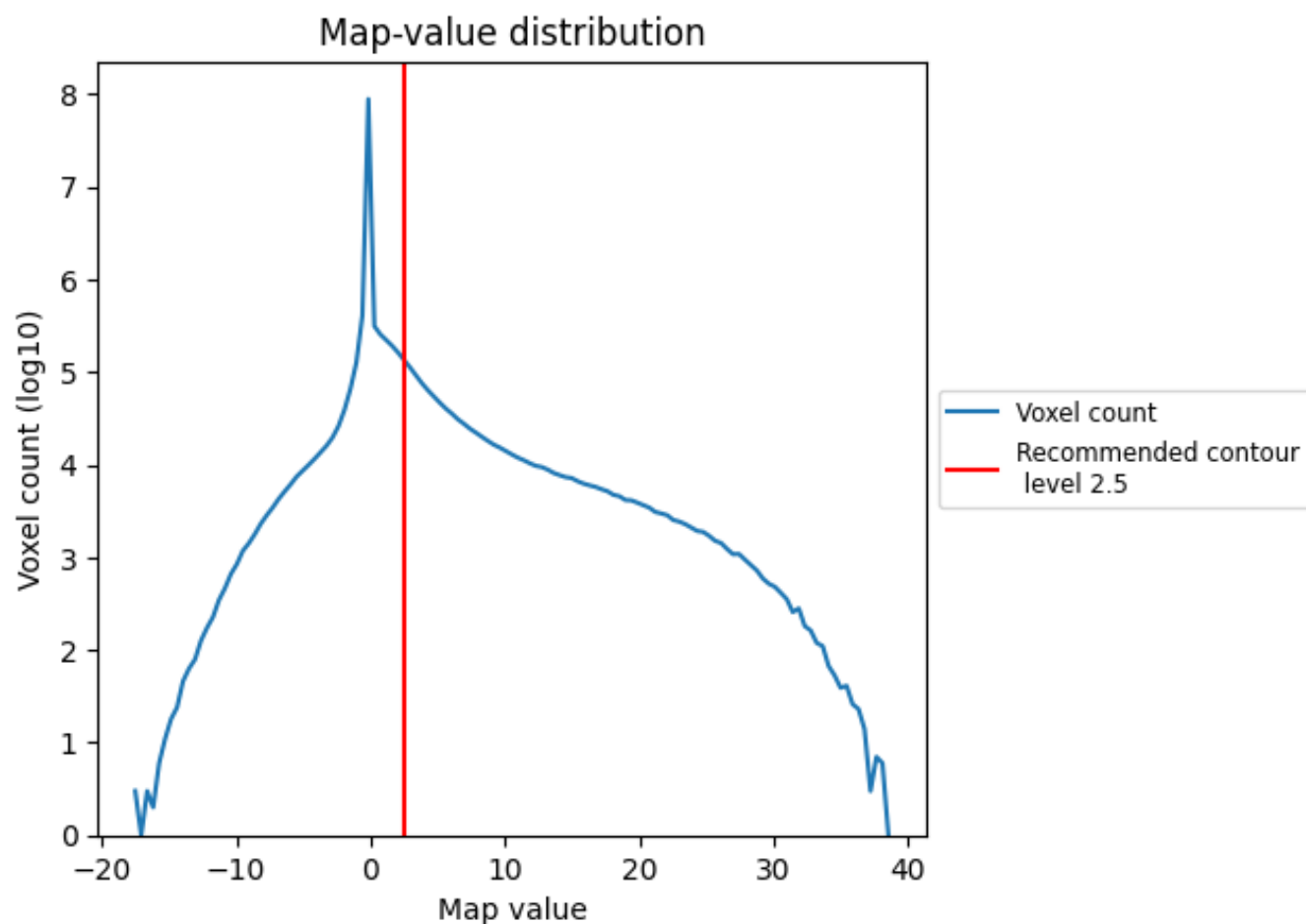
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

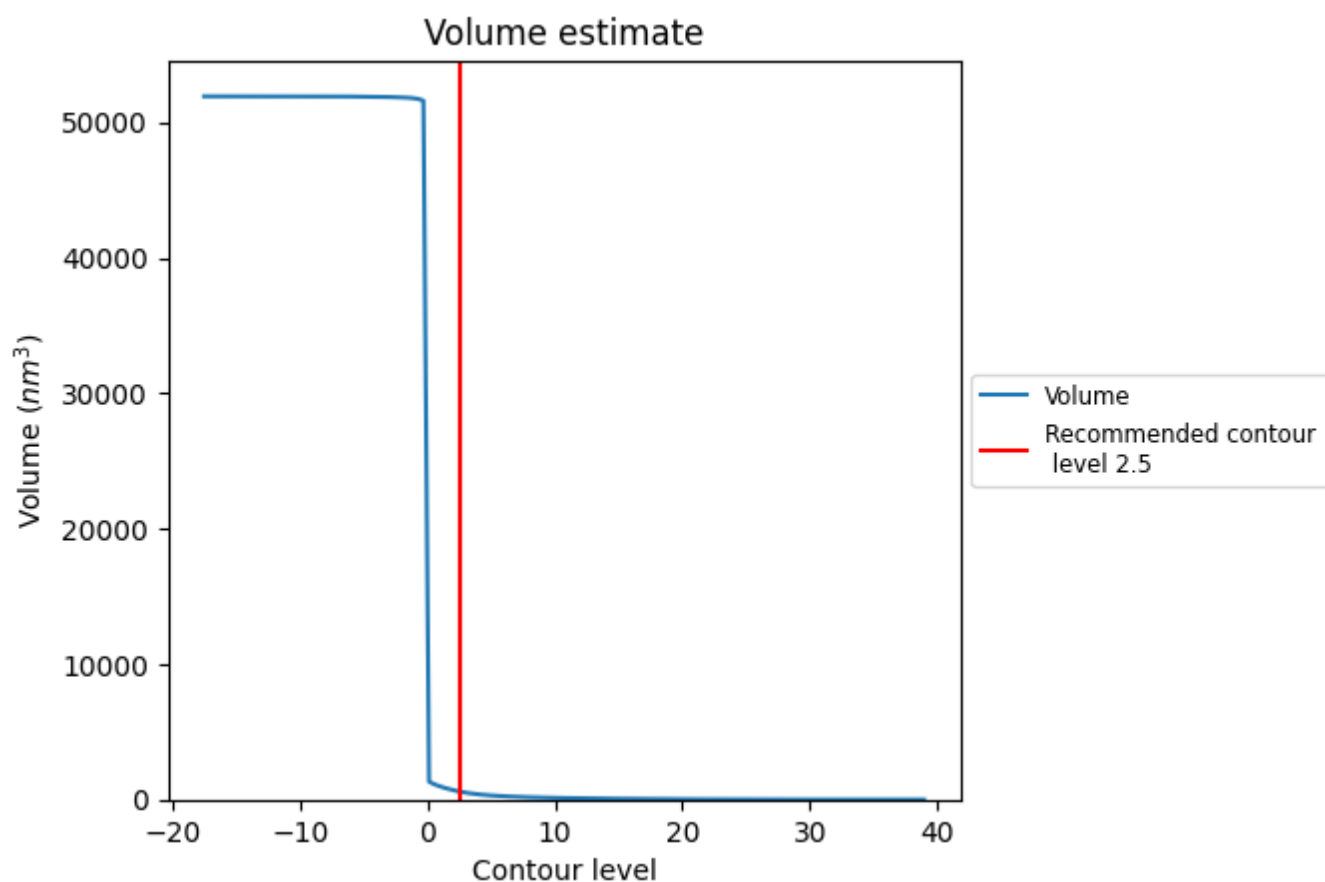
This section contains the results of statistical analysis of the map.

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.

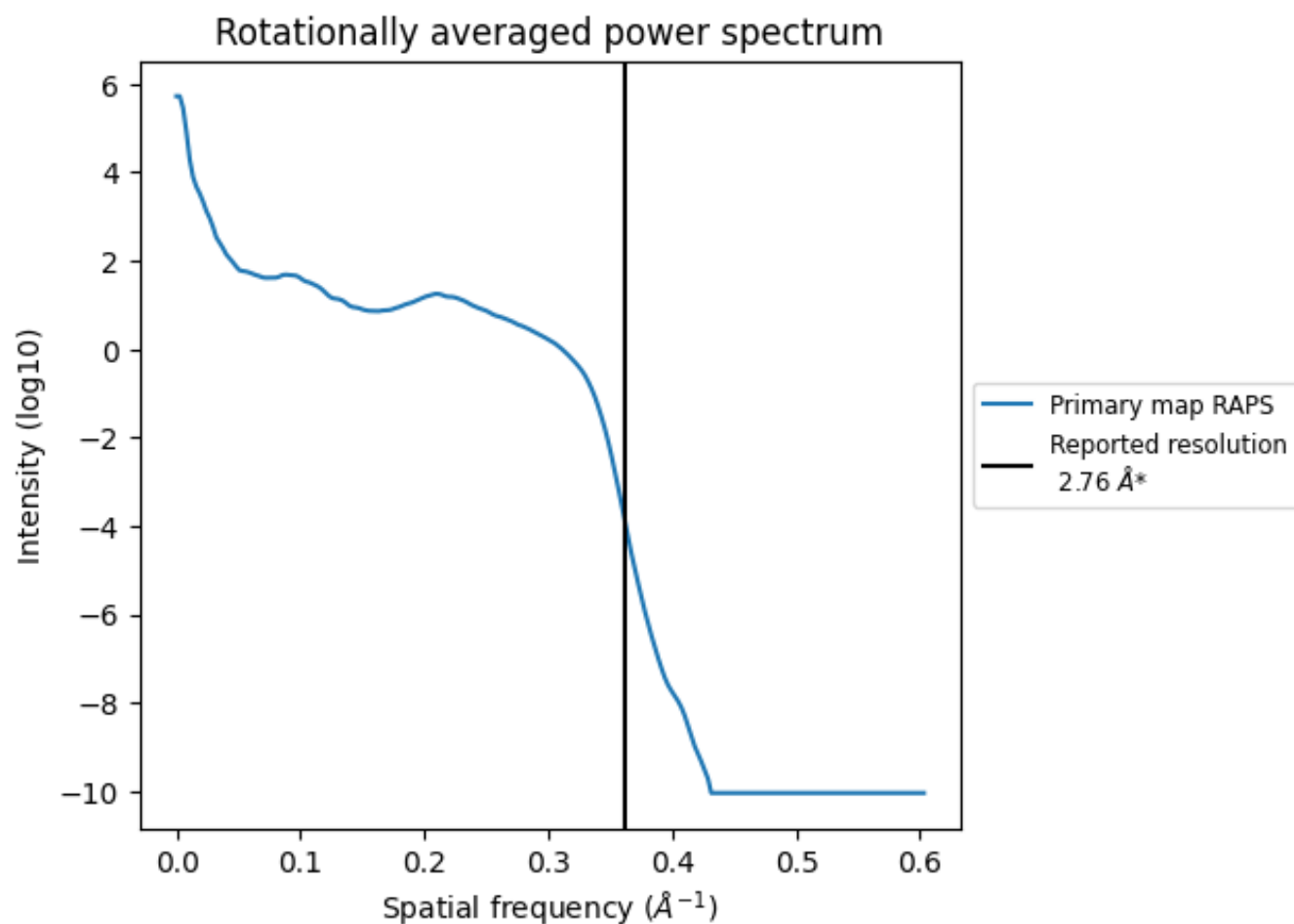
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 596 nm^3 ; this corresponds to an approximate mass of 538 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 0.362 Å⁻¹

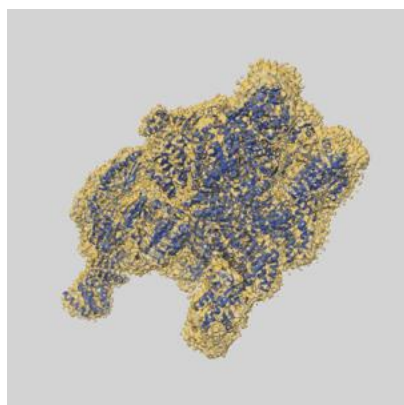
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

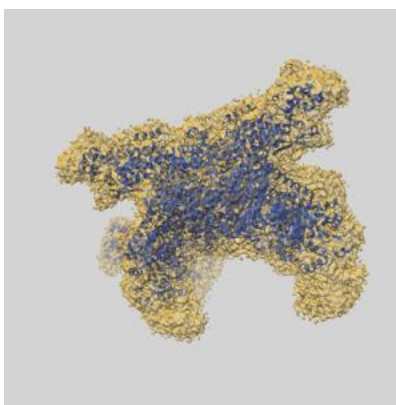
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31474 and PDB model 7F66. Per-residue inclusion information can be found in section 3 on page 6.

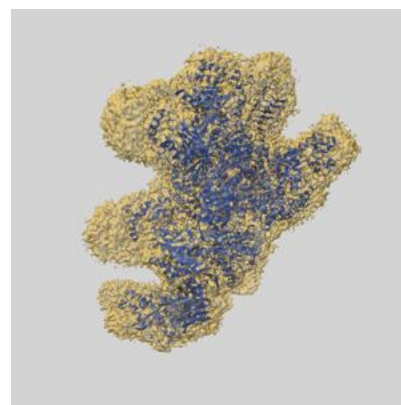
9.1 Map-model overlay [i](#)



X



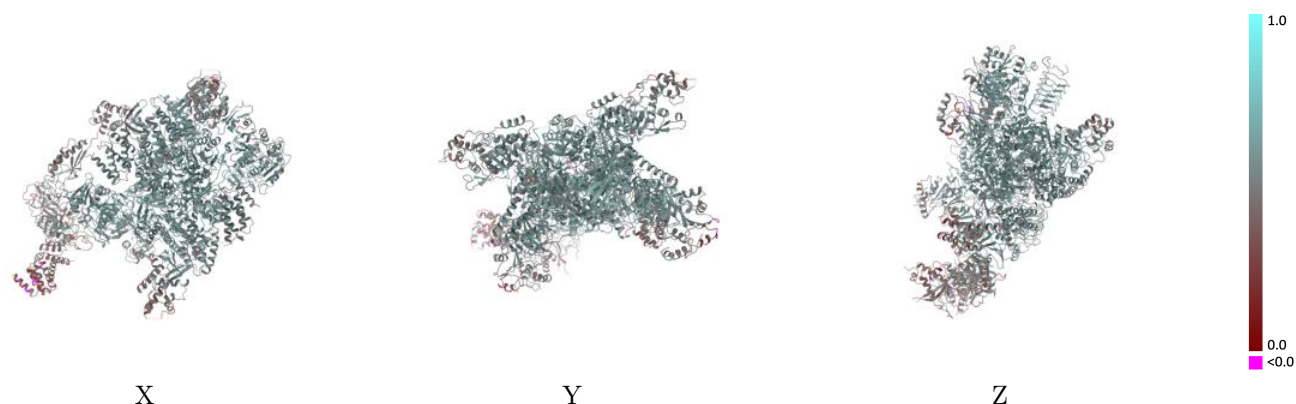
Y



Z

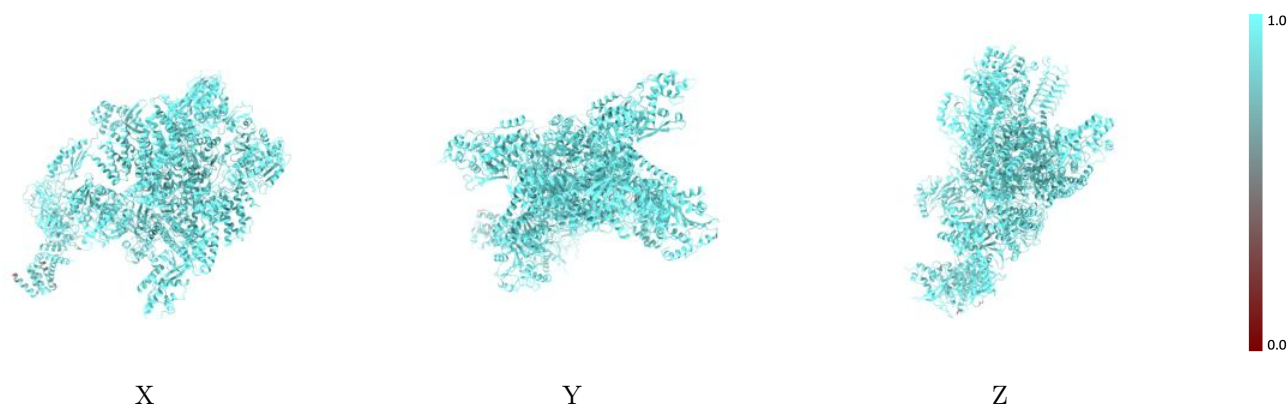
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



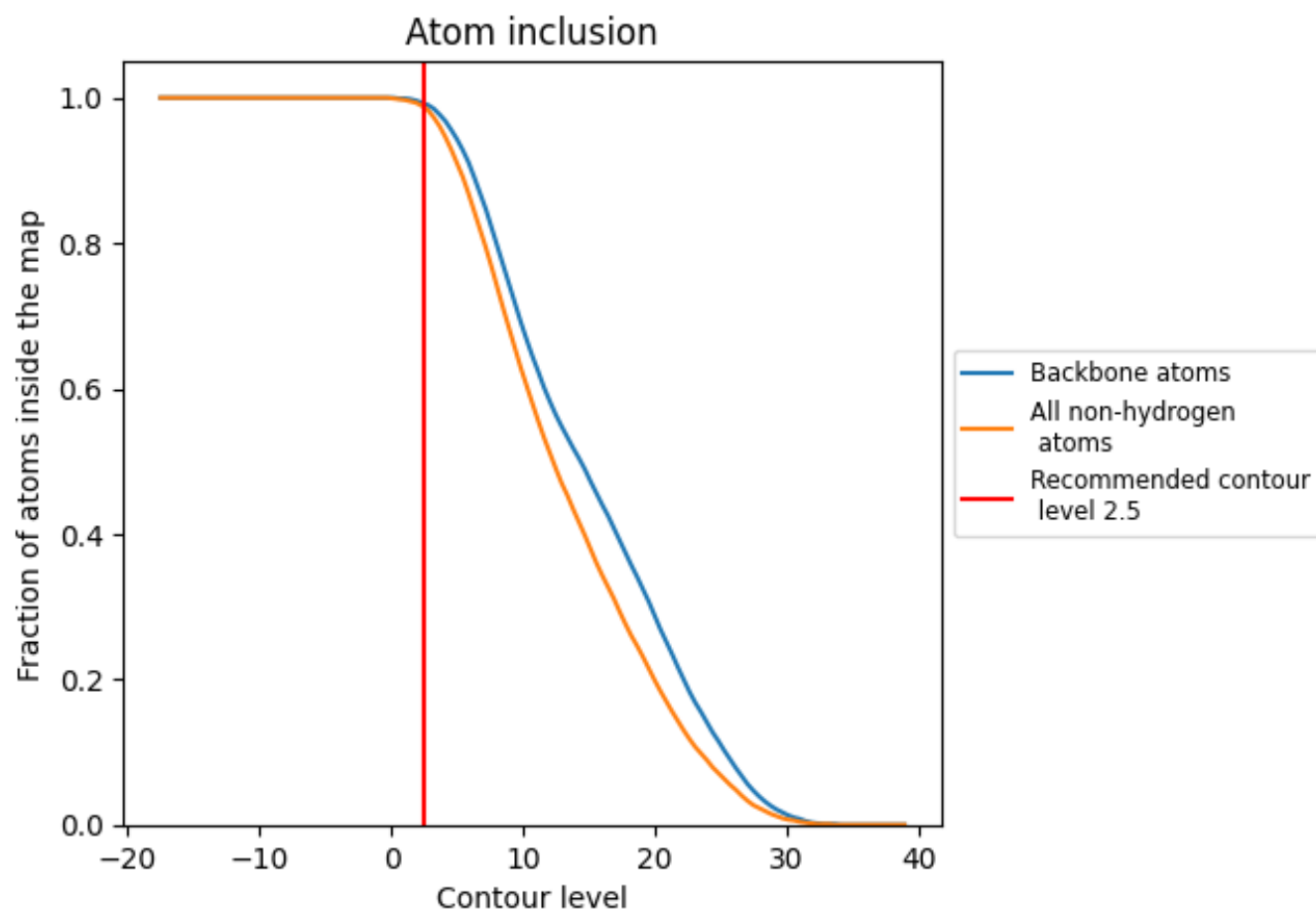
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 99% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9870	 0.5360
A	 0.9950	 0.5700
B	 0.9940	 0.5650
C	 0.9940	 0.5710
D	 0.9940	 0.5680
E	 0.9890	 0.5050
F	 0.9830	 0.5070
G	 0.9950	 0.5910
H	 0.9970	 0.5920
I	 0.9980	 0.5590
J	 0.9760	 0.5100
K	 0.9920	 0.5180
L	 0.9720	 0.4900
N	 0.9650	 0.4550
O	 1.0000	 0.3130
S	 0.9670	 0.4370

