



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 04:19 PM EST

PDB ID : 6WMP
EMDB ID : EMD-21850
Title : F. tularensis RNAPs70-iglA DNA complex
Authors : Travis, B.A.; Brennan, R.G.; Schumacher, M.A.
Deposited on : 2020-04-21
Resolution : 2.98 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

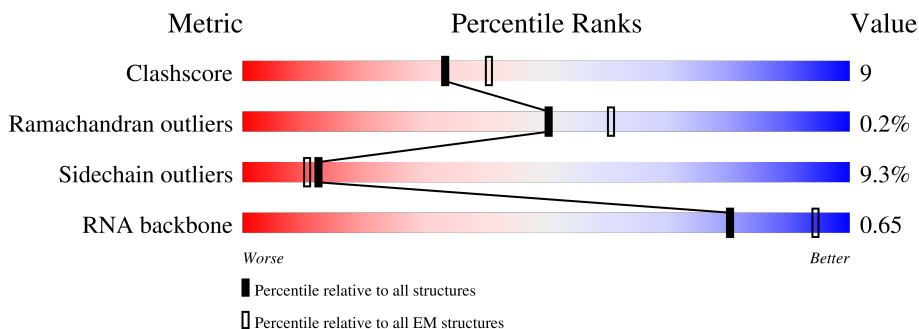
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	323	
2	B	317	
3	C	1358	
4	D	1604	
5	E	72	
6	F	13	
7	G	24	

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Mol	Chain	Length	Quality of chain
8	R	10	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>10%60%40%</div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 22296 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 DNA-directed RNA polymerase subunit alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	0	0
			1694	1078	282	332	2		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit alpha 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	230	Total	C	N	O	S	0	0
			1765	1114	289	356	6		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1196	Total	C	N	O	S	0	0
			8711	5480	1541	1653	37		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1159	Total	C	N	O	S	0	0
			8637	5443	1530	1623	41		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	69	Total	C	N	O	S	0	0
			515	321	92	99	3		

- Molecule 6 is a DNA chain called DNA NT-strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	13	Total	C	N	O	P	0	0
			265	125	52	75	13		

- Molecule 7 is a DNA chain called DNA T-strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	24	Total	C	N	O	P	0	0
			483	232	80	148	23		

- Molecule 8 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	10	Total	C	N	O	P	0	0
			223	99	47	67	10		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total	Mg	0
			1	1	

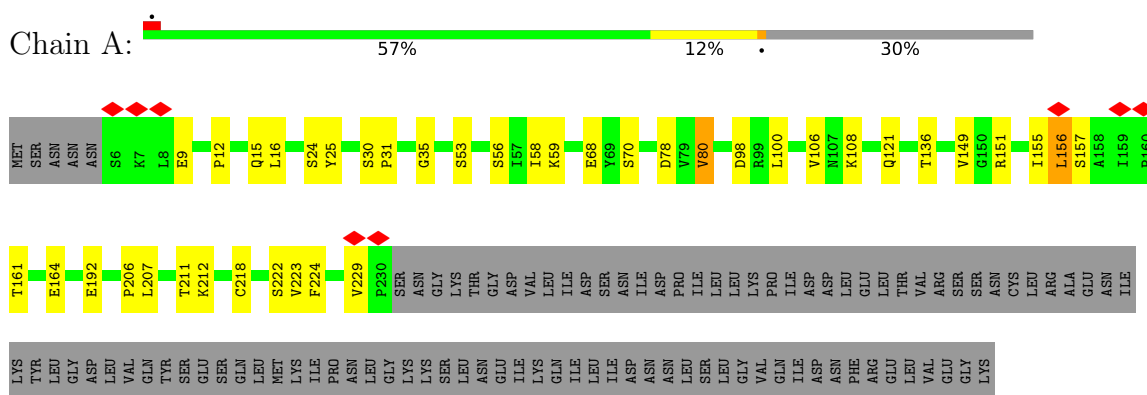
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

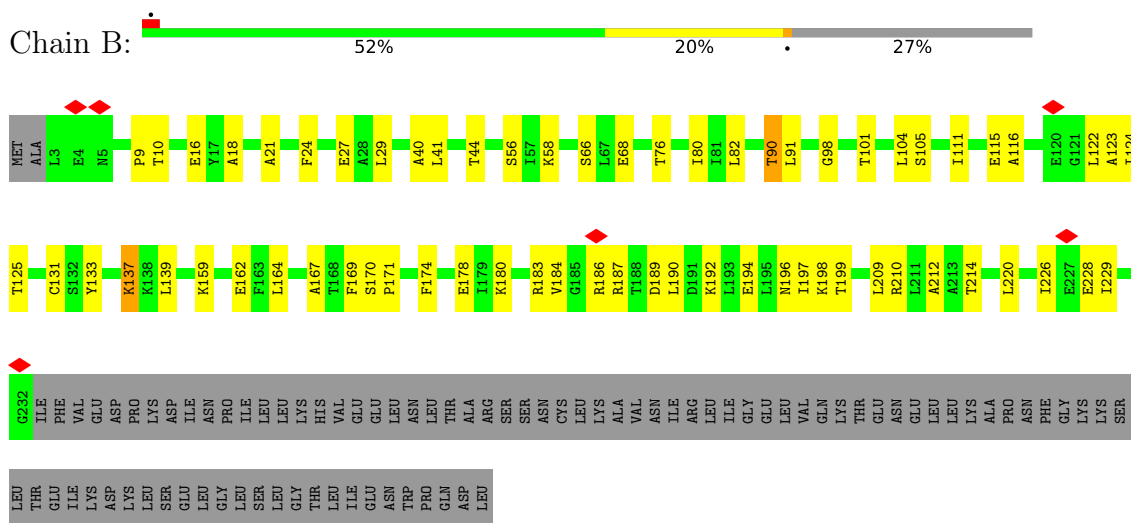
3 Residue-property plots

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.

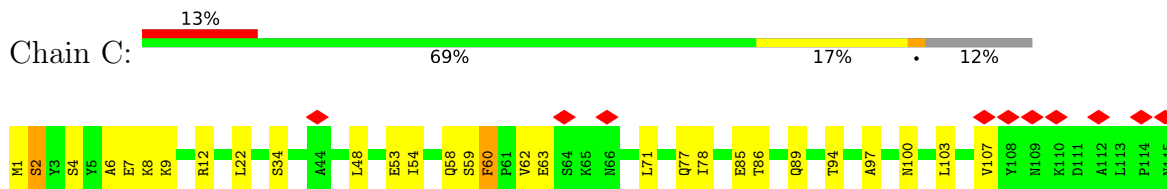
- Molecule 1: DNA-directed RNA polymerase subunit alpha 1



- Molecule 2: DNA-directed RNA polymerase subunit alpha 2



- Molecule 3: DNA-directed RNA polymerase subunit beta



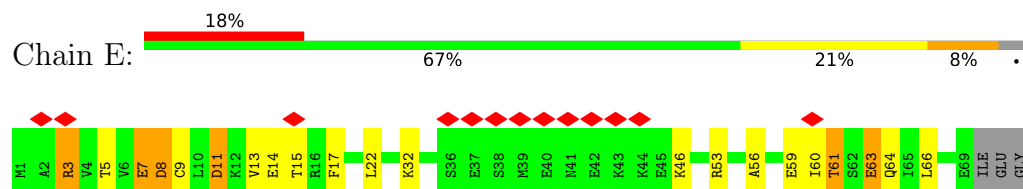


MET	ASN	ASN	GLY	ILE	LEU	HIS	GLN	ASP	TYR	ASN		S12	K13	R14	F15		K19	V27	S30	V36	K37	K38	P39	E40	T41	I42	N43	Y44	R45	L46	F47		R51	C56	A57	K58	I59	P60	G61		V66	E67	C68		K72	Y73	K74	R75	L76	K77	H78		C83	E84	R85	
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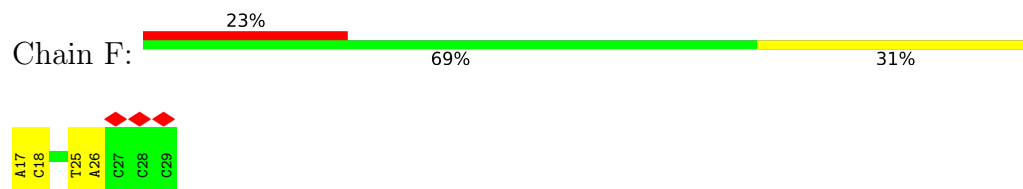


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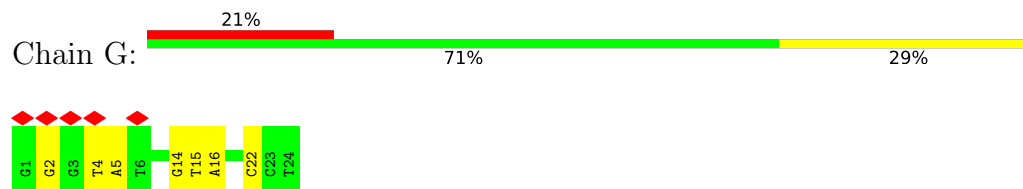
- Molecule 5: DNA-directed RNA polymerase subunit omega



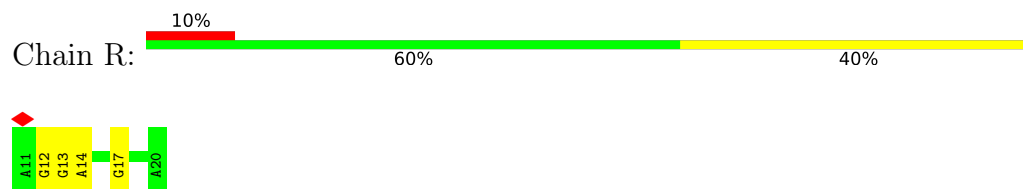
- Molecule 6: DNA NT-strand



- Molecule 7: DNA T-strand



- Molecule 8: RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	137682	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	376.64, 376.64, 376.64	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.54	0/1714	0.55	0/2327
2	B	0.50	0/1785	0.59	0/2409
3	C	0.55	0/8843	0.56	1/11982 (0.0%)
4	D	0.50	0/8755	0.55	0/11848
5	E	0.39	0/516	0.55	0/695
6	F	0.70	0/297	0.82	0/455
7	G	1.01	0/538	0.98	0/828
8	R	0.83	0/251	1.03	0/391
All	All	0.55	0/22699	0.59	1/30935 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	1
4	D	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	578	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	170	SER	Peptide
3	C	198	ILE	Peptide
4	D	1286	LYS	Peptide

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	A	1694	0	1718	18	0
2	B	1765	0	1763	42	0
3	C	8711	0	8162	135	0
4	D	8637	0	8502	204	0
5	E	515	0	513	15	0
6	F	265	0	145	2	0
7	G	483	0	274	7	0
8	R	223	0	110	2	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	22296	0	21187	396	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 9.

All (396) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:208:SER:HA	4:D:212:LYS:HB3	1.59	0.83
2:B:133:TYR:OH	2:B:137:LYS:O	1.97	0.82
3:C:809:TRP:O	3:C:810:ASN:ND2	2.11	0.82
4:D:195:GLU:O	4:D:199:LEU:HB2	1.80	0.82
3:C:1234:ASP:OD1	3:C:1234:ASP:N	2.10	0.81
3:C:531:ARG:NH2	3:C:579:ALA:O	2.16	0.78
3:C:1321:VAL:O	4:D:384:ARG:NH1	2.17	0.78
3:C:1:MET:N	3:C:1171:VAL:O	2.18	0.77
3:C:520:GLN:O	3:C:522:ASN:N	2.18	0.76
4:D:813:THR:OG1	4:D:815:ASP:OD1	2.03	0.76
3:C:809:TRP:O	4:D:631:THR:OG1	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:SER:HB2	3:C:8:LYS:HE2	1.69	0.73
4:D:277:LEU:HD12	4:D:293:GLU:HB3	1.70	0.73
3:C:1281:ARG:NH1	7:G:16:DA:OP1	2.22	0.73
2:B:111:ILE:HD11	2:B:133:TYR:HB2	1.70	0.72
4:D:477:GLU:HG3	4:D:481:LEU:HD12	1.72	0.71
1:A:16:LEU:HD12	1:A:207:LEU:HG	1.73	0.71
3:C:1141:LYS:NZ	3:C:1161:GLU:OE2	2.19	0.71
4:D:143:ILE:HG21	4:D:186:LEU:HD11	1.71	0.70
4:D:799:ASP:OD1	4:D:1336:LYS:NZ	2.23	0.70
3:C:211:LYS:HD2	3:C:214:GLY:HA2	1.73	0.69
3:C:815:GLU:HB2	4:D:459:PHE:HD2	1.57	0.69
3:C:708:GLU:HB3	3:C:796:LEU:H	1.56	0.69
3:C:891:PRO:HA	3:C:915:VAL:HA	1.75	0.69
1:A:207:LEU:O	1:A:211:THR:HG23	1.93	0.69
2:B:123:ALA:O	2:B:125:THR:OG1	2.08	0.69
4:D:61:GLY:O	4:D:96:ARG:NH1	2.25	0.69
4:D:899:LEU:HD11	4:D:1237:ASN:HD22	1.58	0.68
4:D:306:ASP:HB3	4:D:326:ALA:HB3	1.75	0.68
4:D:815:ASP:OD1	4:D:815:ASP:N	2.26	0.68
3:C:123:ARG:HD3	3:C:489:LYS:HE3	1.74	0.68
3:C:176:ILE:HD11	3:C:431:VAL:HG21	1.76	0.68
4:D:1297:ILE:O	4:D:1301:SER:OG	2.12	0.67
3:C:349:ILE:O	3:C:353:LEU:N	2.21	0.67
3:C:1044:GLU:O	3:C:1048:LYS:N	2.26	0.67
4:D:770:PHE:O	4:D:773:THR:OG1	2.12	0.67
2:B:98:GLY:HA3	2:B:122:LEU:HD11	1.77	0.67
4:D:248:ARG:HH11	4:D:264:ASN:HD21	1.43	0.67
4:D:810:ASP:OD1	4:D:879:ARG:NH2	2.22	0.67
4:D:1277:ASN:O	4:D:1281:ARG:N	2.19	0.65
3:C:153:GLN:NE2	3:C:536:LEU:O	2.29	0.65
3:C:4:SER:HB2	3:C:7:GLU:HB3	1.79	0.64
4:D:159:THR:HG22	4:D:161:GLU:H	1.63	0.64
4:D:159:THR:O	4:D:163:TYR:N	2.31	0.64
4:D:51:ARG:HH22	4:D:58:LYS:HD3	1.63	0.64
3:C:553:VAL:HG23	4:D:777:ARG:HD2	1.79	0.64
3:C:403:GLY:O	3:C:407:LEU:HB2	1.98	0.64
3:C:198:ILE:HG22	3:C:199:ASP:H	1.62	0.63
1:A:229:VAL:HG13	2:B:10:THR:HA	1.81	0.63
3:C:1219:ASN:HD22	3:C:1221:GLN:HB2	1.62	0.63
3:C:843:ARG:HA	3:C:1060:VAL:HA	1.80	0.63
4:D:131:LYS:H	4:D:131:LYS:HD2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:833:VAL:HG12	4:D:865:VAL:HB	1.80	0.62
4:D:166:ALA:O	4:D:170:TYR:N	2.28	0.62
1:A:121:GLN:O	1:A:121:GLN:NE2	2.32	0.62
4:D:110:VAL:HG12	4:D:298:GLN:HE22	1.65	0.61
4:D:1262:PHE:O	4:D:1264:LYS:N	2.33	0.61
4:D:111:HIS:HD2	4:D:113:TRP:H	1.46	0.61
3:C:1259:SER:O	4:D:346:ASP:HB3	2.00	0.61
5:E:14:GLU:HB3	5:E:15:THR:HG23	1.82	0.61
3:C:1266:VAL:O	4:D:97:ARG:NH2	2.26	0.61
4:D:56:CYS:SG	4:D:57:ALA:N	2.74	0.61
3:C:760:ARG:HG3	3:C:835:ILE:HB	1.83	0.60
3:C:520:GLN:HG3	3:C:762:ASN:HB2	1.82	0.59
4:D:243:LEU:HD12	4:D:244:PRO:HD2	1.83	0.59
2:B:192:LYS:NZ	2:B:194:GLU:OE2	2.36	0.59
4:D:504:ILE:HD13	4:D:623:MET:HG3	1.84	0.59
3:C:440:ASP:O	3:C:442:LYS:NZ	2.33	0.59
4:D:823:VAL:HG12	4:D:828:VAL:HA	1.83	0.59
4:D:845:VAL:HG22	4:D:873:ILE:HD13	1.85	0.59
3:C:222:GLU:O	3:C:223:ASN:OD1	2.20	0.59
3:C:12:ARG:NH2	3:C:701:PRO:O	2.27	0.59
4:D:219:LEU:O	4:D:223:GLU:HG3	2.03	0.59
4:D:273:ARG:HD3	4:D:296:MET:HB3	1.85	0.58
3:C:890:THR:O	3:C:916:VAL:N	2.27	0.58
2:B:66:SER:HB3	2:B:68:GLU:HG2	1.85	0.58
3:C:107:VAL:O	3:C:119:VAL:N	2.36	0.58
4:D:306:ASP:OD1	4:D:306:ASP:N	2.33	0.58
3:C:694:PRO:HB3	3:C:790:ALA:HB2	1.86	0.58
4:D:423:ARG:HG2	4:D:424:ALA:H	1.68	0.58
5:E:3:ARG:HE	5:E:3:ARG:HA	1.68	0.58
4:D:910:SER:O	4:D:910:SER:OG	2.20	0.57
4:D:571:THR:HG22	4:D:573:GLY:H	1.69	0.57
2:B:111:ILE:HD13	2:B:131:CYS:HB3	1.86	0.57
1:A:68:GLU:HG2	1:A:80:VAL:HG23	1.87	0.57
3:C:1308:ASP:OD1	4:D:343:LYS:NZ	2.38	0.57
4:D:1286:LYS:HE3	4:D:1286:LYS:HA	1.85	0.57
3:C:510:THR:HG23	7:G:22:DC:H5"	1.87	0.56
3:C:717:ASN:O	3:C:769:GLN:NE2	2.35	0.56
3:C:882:GLY:O	3:C:921:ARG:NH1	2.38	0.56
3:C:806:PHE:O	4:D:636:SER:OG	2.10	0.56
4:D:674:ASN:HA	4:D:677:TYR:O	2.05	0.56
4:D:207:LYS:O	4:D:209:THR:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1273:GLY:H	3:C:1278:GLY:HA2	1.69	0.56
3:C:195:TRP:CD2	3:C:203:LYS:HD2	2.41	0.56
3:C:935:VAL:HG13	3:C:1064:VAL:HG12	1.87	0.56
4:D:1317:THR:O	4:D:1321:THR:HG23	2.05	0.56
4:D:1296:GLY:O	4:D:1300:SER:OG	2.13	0.56
2:B:90:THR:HG23	2:B:123:ALA:HB3	1.88	0.56
3:C:474:VAL:HG23	3:C:500:PRO:HG2	1.86	0.56
3:C:809:TRP:CH2	3:C:1094:LEU:HD11	2.41	0.56
1:A:30:SER:HB2	1:A:31:PRO:HD3	1.88	0.55
3:C:447:ASP:O	3:C:453:ASN:ND2	2.38	0.55
3:C:475:GLU:HA	3:C:478:ILE:HG22	1.89	0.55
4:D:578:LEU:HD13	4:D:587:PHE:CD1	2.41	0.55
5:E:13:VAL:HG12	5:E:14:GLU:H	1.70	0.55
3:C:71:LEU:HD12	3:C:478:ILE:HD11	1.88	0.55
2:B:44:THR:HG23	2:B:212:ALA:HB1	1.88	0.55
2:B:178:GLU:OE1	2:B:180:LYS:NZ	2.34	0.55
3:C:97:ALA:HB2	3:C:134:LEU:HD11	1.88	0.55
3:C:4:SER:HB2	3:C:7:GLU:CB	2.37	0.55
4:D:428:HIS:CE1	4:D:430:LEU:HB2	2.41	0.55
4:D:86:CYS:HB3	4:D:88:VAL:HG23	1.87	0.54
4:D:1306:SER:HB3	4:D:1309:SER:HB3	1.88	0.54
3:C:520:GLN:O	3:C:525:SER:HB2	2.07	0.54
3:C:627:ASP:O	3:C:629:ASN:N	2.39	0.54
5:E:8:ASP:HB3	5:E:56:ALA:HB1	1.89	0.54
4:D:913:VAL:O	4:D:917:GLN:HG2	2.07	0.54
4:D:1327:SER:O	4:D:1327:SER:OG	2.24	0.54
3:C:414:ASP:OD1	3:C:414:ASP:N	2.41	0.54
3:C:885:LEU:HD11	3:C:922:MET:HG2	1.89	0.54
4:D:332:LYS:NZ	7:G:14:DG:OP1	2.36	0.54
4:D:267:TYR:O	4:D:271:ILE:HG13	2.08	0.54
3:C:614:GLU:HA	3:C:617:TYR:HD2	1.71	0.53
4:D:206:SER:HA	4:D:212:LYS:NZ	2.23	0.53
4:D:504:ILE:HG21	4:D:623:MET:HA	1.90	0.53
4:D:673:GLU:OE1	4:D:678:ASN:ND2	2.41	0.53
1:A:25:TYR:CD2	1:A:206:PRO:HG3	2.44	0.53
3:C:548:PHE:CE1	4:D:785:LEU:HD22	2.44	0.53
4:D:798:VAL:O	4:D:802:GLN:HB2	2.08	0.53
4:D:831:PRO:HD2	4:D:834:GLU:OE1	2.09	0.53
3:C:156:ARG:HH21	3:C:448:ILE:HD11	1.74	0.53
3:C:533:ILE:HD11	3:C:578:LEU:HG	1.91	0.53
3:C:1120:ARG:O	3:C:1122:ASN:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:846:VAL:HB	4:D:852:VAL:HG12	1.91	0.52
4:D:847:THR:HG22	4:D:851:VAL:O	2.08	0.52
5:E:59:GLU:O	5:E:61:THR:N	2.43	0.52
3:C:578:LEU:HD22	3:C:582:ALA:HB3	1.91	0.52
3:C:1143:GLU:HB2	3:C:1189:LYS:HG2	1.90	0.52
4:D:192:ILE:HG23	4:D:222:LEU:HD23	1.90	0.52
4:D:428:HIS:CD2	4:D:921:GLU:HG3	2.44	0.52
3:C:440:ASP:HB3	3:C:442:LYS:HZ1	1.74	0.52
2:B:174:PHE:HE2	2:B:196:ASN:HD22	1.56	0.52
2:B:210:ARG:O	2:B:214:THR:HG23	2.09	0.51
3:C:433:GLU:O	3:C:436:ILE:HG13	2.10	0.51
4:D:659:ILE:HD12	4:D:680:ILE:HG12	1.92	0.51
3:C:478:ILE:HD12	3:C:496:VAL:HG12	1.92	0.51
1:A:59:LYS:NZ	1:A:164:GLU:OE2	2.44	0.51
2:B:167:ALA:HB1	2:B:169:PHE:CZ	2.44	0.51
3:C:1221:GLN:HA	3:C:1237:VAL:O	2.10	0.51
4:D:142:TYR:HB2	4:D:158:LEU:O	2.10	0.51
2:B:115:GLU:CG	2:B:116:ALA:H	2.24	0.51
3:C:77:GLN:NE2	3:C:100:ASN:HD22	2.08	0.51
4:D:66:TYR:CZ	4:D:76:LEU:HD13	2.46	0.51
4:D:27:VAL:O	4:D:30:SER:OG	2.21	0.51
3:C:71:LEU:HD22	3:C:103:LEU:HB3	1.93	0.51
3:C:216:THR:HG23	3:C:353:LEU:HD22	1.92	0.51
4:D:1243:THR:O	4:D:1243:THR:OG1	2.22	0.51
4:D:391:THR:H	4:D:394:GLN:HE21	1.57	0.51
4:D:89:GLU:OE1	4:D:89:GLU:N	2.43	0.50
7:G:15:DT:H2'	7:G:16:DA:C8	2.46	0.50
4:D:67:GLU:HB2	4:D:74:LYS:HG2	1.94	0.50
4:D:121:ARG:HH21	4:D:1322:GLU:HG2	1.76	0.50
2:B:40:ALA:O	2:B:44:THR:HG22	2.11	0.50
4:D:346:ASP:OD1	4:D:346:ASP:N	2.44	0.50
4:D:854:LEU:HD21	4:D:864:LEU:HD22	1.93	0.50
3:C:1268:GLN:HG3	3:C:1310:ILE:HD11	1.93	0.50
4:D:1269:GLU:O	4:D:1273:ILE:HG12	2.12	0.50
3:C:207:THR:HA	3:C:210:LEU:HB2	1.94	0.49
3:C:659:SER:OG	3:C:660:ALA:N	2.44	0.49
3:C:1310:ILE:HG13	3:C:1333:GLU:HG3	1.93	0.49
4:D:391:THR:H	4:D:394:GLN:NE2	2.09	0.49
3:C:814:PHE:HB3	4:D:355:VAL:HG21	1.94	0.49
4:D:824:GLU:OE2	4:D:826:GLY:N	2.45	0.49
4:D:846:VAL:HA	4:D:852:VAL:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:PHE:O	3:C:62:VAL:HG13	2.11	0.49
1:A:156:LEU:HG	1:A:157:SER:H	1.78	0.49
3:C:731:ASP:OD1	3:C:731:ASP:N	2.46	0.49
2:B:101:THR:O	2:B:116:ALA:HA	2.13	0.49
4:D:39:PRO:HG3	4:D:272:ASN:OD1	2.12	0.49
3:C:748:ASN:N	3:C:748:ASN:OD1	2.46	0.49
4:D:655:ALA:O	4:D:659:ILE:HG12	2.13	0.49
4:D:897:ARG:O	4:D:1239:LYS:NZ	2.45	0.49
1:A:35:GLY:N	1:A:192:GLU:OE2	2.44	0.48
1:A:218:CYS:SG	2:B:220:LEU:HD12	2.53	0.48
4:D:510:TYR:O	4:D:543:HIS:HE1	1.96	0.48
2:B:189:ASP:OD1	2:B:189:ASP:N	2.41	0.48
3:C:22:LEU:HD13	3:C:606:ILE:HG13	1.96	0.48
3:C:824:ILE:HG23	3:C:829:LYS:HB2	1.95	0.48
4:D:416:GLU:H	5:E:46:LYS:NZ	2.10	0.48
4:D:131:LYS:H	4:D:131:LYS:CD	2.25	0.48
2:B:137:LYS:H	2:B:137:LYS:HD2	1.79	0.48
4:D:209:THR:CB	7:G:2:DG:H3'	2.44	0.48
4:D:577:LEU:O	4:D:580:ILE:HG12	2.13	0.48
3:C:627:ASP:C	3:C:629:ASN:H	2.17	0.48
1:A:106:VAL:HB	1:A:108:LYS:HG2	1.94	0.48
3:C:1351:PHE:HB3	4:D:15:PHE:HB3	1.95	0.48
4:D:262:ASP:OD1	4:D:262:ASP:N	2.45	0.48
4:D:462:ASP:OD1	4:D:462:ASP:N	2.45	0.48
4:D:1362:LYS:HB3	4:D:1362:LYS:HE3	1.64	0.48
4:D:582:PRO:HD2	4:D:585:LEU:HD12	1.94	0.48
2:B:18:ALA:HB3	2:B:21:ALA:HB3	1.96	0.48
3:C:197:ARG:HG2	3:C:198:ILE:O	2.14	0.48
4:D:408:ASP:OD1	4:D:409:ILE:N	2.47	0.48
3:C:187:GLU:OE2	3:C:197:ARG:NH2	2.47	0.47
4:D:382:LYS:HA	4:D:382:LYS:HD3	1.53	0.47
4:D:598:GLU:O	4:D:602:ILE:HG13	2.14	0.47
3:C:834:HIS:ND1	3:C:1072:LYS:HD2	2.30	0.47
4:D:177:SER:OG	4:D:178:MET:N	2.46	0.47
2:B:104:LEU:HD12	2:B:111:ILE:HG12	1.96	0.47
4:D:108:PRO:HG2	4:D:181:GLU:HG2	1.96	0.47
2:B:184:VAL:HG23	2:B:190:LEU:HD12	1.97	0.47
3:C:813:ASN:OD1	3:C:813:ASN:N	2.45	0.47
3:C:852:ILE:HA	3:C:888:LYS:HA	1.96	0.47
4:D:58:LYS:HG3	4:D:87:GLY:O	2.15	0.47
4:D:414:ILE:HD12	4:D:437:PRO:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1361:GLU:HA	4:D:1364:ARG:HG2	1.96	0.47
3:C:718:CYS:SG	3:C:791:THR:HG21	2.54	0.47
4:D:368:LYS:HB2	4:D:368:LYS:HE3	1.68	0.47
4:D:833:VAL:O	4:D:834:GLU:HB3	2.14	0.47
5:E:9:CYS:SG	5:E:56:ALA:HB2	2.55	0.47
3:C:627:ASP:HB3	3:C:633:VAL:HG12	1.97	0.47
4:D:613:LYS:HA	4:D:616:VAL:HG22	1.96	0.47
4:D:394:GLN:O	4:D:398:MET:HG2	2.15	0.47
3:C:800:HIS:NE2	3:C:829:LYS:O	2.48	0.46
4:D:398:MET:HB2	4:D:403:GLU:HG3	1.97	0.46
2:B:82:LEU:HD21	4:D:524:LEU:HG	1.97	0.46
3:C:614:GLU:HA	3:C:617:TYR:CD2	2.49	0.46
3:C:478:ILE:HG23	3:C:479:ARG:H	1.81	0.46
3:C:601:LYS:HB2	3:C:631:HIS:CE1	2.50	0.46
3:C:1322:ASP:HA	4:D:384:ARG:HH12	1.80	0.46
4:D:126:LEU:HD21	4:D:187:LEU:HD23	1.97	0.46
2:B:115:GLU:HG2	2:B:116:ALA:H	1.80	0.46
3:C:186:PHE:CE1	3:C:432:ILE:HD11	2.51	0.46
3:C:476:LYS:HB3	3:C:476:LYS:HE3	1.63	0.46
4:D:397:ARG:O	4:D:400:GLU:HG3	2.15	0.46
3:C:369:TYR:O	3:C:373:ARG:HG2	2.16	0.46
4:D:41:THR:OG1	4:D:42:ILE:N	2.48	0.46
4:D:762:GLU:H	4:D:762:GLU:HG3	1.45	0.46
4:D:1278:ASP:HB2	4:D:1287:GLU:OE1	2.16	0.46
8:R:12:G:H2'	8:R:13:G:C8	2.51	0.46
3:C:62:VAL:HG23	3:C:63:GLU:H	1.80	0.46
8:R:12:G:H2'	8:R:13:G:H8	1.80	0.46
3:C:1039:ILE:O	3:C:1043:PHE:CB	2.64	0.46
4:D:1219:ASP:O	4:D:1223:ILE:HG23	2.15	0.46
2:B:16:GLU:N	2:B:16:GLU:OE2	2.47	0.46
3:C:1258:ARG:NH2	3:C:1261:GLY:H	2.14	0.46
4:D:652:ILE:HD13	4:D:757:THR:HB	1.98	0.46
4:D:834:GLU:HG2	4:D:834:GLU:O	2.16	0.45
4:D:124:LEU:HD23	4:D:221:LEU:HD22	1.97	0.45
2:B:123:ALA:O	2:B:125:THR:N	2.49	0.45
3:C:205:CYS:SG	3:C:206:ALA:N	2.90	0.45
3:C:351:ASP:O	3:C:355:TYR:HB2	2.16	0.45
4:D:166:ALA:O	4:D:169:ASN:N	2.34	0.45
4:D:390:THR:OG1	4:D:391:THR:N	2.49	0.45
4:D:1268:ILE:HG23	4:D:1272:ARG:HG3	1.99	0.45
3:C:1164:ASN:OD1	3:C:1170:LYS:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1307:SER:OG	3:C:1308:ASP:N	2.50	0.45
4:D:648:LYS:HZ2	4:D:759:ASN:HD22	1.64	0.45
3:C:705:THR:HG22	3:C:1196:THR:O	2.16	0.45
3:C:1351:PHE:HB3	4:D:15:PHE:CB	2.46	0.45
4:D:111:HIS:CD2	4:D:113:TRP:HB2	2.52	0.45
4:D:306:ASP:HA	4:D:324:SER:CB	2.46	0.45
4:D:1357:SER:HA	4:D:1360:ILE:HD12	1.97	0.45
2:B:198:LYS:HE3	2:B:198:LYS:HB2	1.72	0.45
3:C:844:ASP:N	3:C:1059:GLY:O	2.45	0.45
3:C:963:ASP:O	3:C:967:ALA:N	2.39	0.45
6:F:25:DT:H2"	6:F:26:DA:C8	2.52	0.45
4:D:589:LEU:O	4:D:592:LYS:HE2	2.16	0.45
4:D:746:LYS:HE3	4:D:752:ILE:HG12	1.99	0.45
2:B:105:SER:HA	2:B:133:TYR:CE2	2.52	0.45
3:C:536:LEU:HD21	3:C:574:LEU:HD13	1.99	0.44
4:D:265:ASP:O	4:D:269:ARG:HG3	2.17	0.44
4:D:313:ALA:O	4:D:314:VAL:C	2.55	0.44
4:D:674:ASN:OD1	4:D:674:ASN:N	2.38	0.44
4:D:809:GLU:O	4:D:893:LYS:HG3	2.17	0.44
4:D:1147:ASP:HA	4:D:1192:VAL:O	2.16	0.44
2:B:186:ARG:O	2:B:186:ARG:NH2	2.50	0.44
3:C:6:ALA:HA	3:C:9:LYS:HD2	1.98	0.44
3:C:59:SER:OG	3:C:475:GLU:OE2	2.29	0.44
3:C:203:LYS:HB3	3:C:203:LYS:HE2	1.78	0.44
5:E:15:THR:C	5:E:17:PHE:H	2.21	0.44
3:C:657:ASP:OD1	3:C:657:ASP:N	2.48	0.44
4:D:1212:LYS:HB3	4:D:1216:GLU:OE2	2.17	0.44
4:D:51:ARG:NH2	4:D:58:LYS:HD3	2.31	0.44
4:D:73:TYR:HD2	4:D:83:CYS:SG	2.40	0.44
4:D:121:ARG:HG3	4:D:1325:ILE:HD12	2.00	0.44
4:D:1289:GLU:N	4:D:1289:GLU:OE1	2.51	0.44
1:A:12:PRO:HA	1:A:31:PRO:HD2	1.99	0.44
3:C:566:THR:OG1	4:D:777:ARG:NH2	2.47	0.44
4:D:138:TYR:CE1	4:D:298:GLN:HG2	2.51	0.44
4:D:500:PRO:HB3	4:D:504:ILE:HB	2.00	0.44
5:E:64:GLN:CD	5:E:64:GLN:H	2.21	0.44
4:D:895:TYR:HD2	4:D:905:VAL:HG21	1.82	0.43
4:D:926:LEU:HB3	4:D:1232:GLN:HG3	1.99	0.43
3:C:140:THR:HG22	3:C:530:LYS:HE2	2.00	0.43
3:C:675:GLU:OE1	3:C:675:GLU:N	2.42	0.43
4:D:56:CYS:SG	4:D:58:LYS:N	2.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:502:GLN:O	4:D:727:ALA:HB1	2.18	0.43
2:B:80:ILE:HD11	2:B:131:CYS:SG	2.58	0.43
3:C:815:GLU:HB2	4:D:459:PHE:CD2	2.46	0.43
3:C:428:ILE:O	3:C:432:ILE:HG12	2.19	0.43
4:D:121:ARG:NH2	4:D:1322:GLU:HG2	2.32	0.43
4:D:1351:LEU:HD23	4:D:1351:LEU:HA	1.87	0.43
4:D:206:SER:HA	4:D:212:LYS:HZ2	1.81	0.43
4:D:279:LYS:O	4:D:283:LEU:HD13	2.18	0.43
4:D:803:ASP:OD1	4:D:803:ASP:N	2.34	0.43
4:D:835:ARG:NH1	4:D:1238:ASP:OD2	2.52	0.43
4:D:747:PRO:HB3	4:D:778:LYS:HD3	2.00	0.43
4:D:1239:LYS:O	4:D:1243:THR:HG22	2.19	0.43
2:B:91:LEU:HD12	2:B:91:LEU:HA	1.80	0.43
4:D:1148:GLY:O	4:D:1191:GLN:HA	2.19	0.43
4:D:555:PHE:N	4:D:555:PHE:CD1	2.86	0.43
4:D:767:LEU:HD23	4:D:767:LEU:HA	1.81	0.43
6:F:17:DA:H1'	6:F:18:DC:H5'	2.00	0.43
2:B:226:ILE:HA	2:B:229:ILE:HB	1.99	0.43
4:D:1359:LYS:O	4:D:1363:MET:HG3	2.19	0.43
4:D:393:LYS:HB2	4:D:393:LYS:HE2	1.56	0.42
3:C:564:ILE:HD11	4:D:769:TYR:HE2	1.84	0.42
3:C:1217:ALA:C	3:C:1219:ASN:H	2.23	0.42
3:C:1219:ASN:C	3:C:1221:GLN:H	2.22	0.42
4:D:678:ASN:H	4:D:681:ILE:HG23	1.85	0.42
3:C:528:THR:HG21	3:C:690:ARG:HD2	2.01	0.42
4:D:195:GLU:O	4:D:199:LEU:CB	2.61	0.42
3:C:58:GLN:HE21	3:C:58:GLN:HB3	1.55	0.42
1:A:15:GLN:HG2	1:A:16:LEU:H	1.84	0.42
1:A:212:LYS:HD2	1:A:212:LYS:HA	1.68	0.42
3:C:1346:GLY:H	4:D:111:HIS:HE1	1.67	0.42
4:D:824:GLU:O	4:D:824:GLU:HG2	2.20	0.42
2:B:9:PRO:O	2:B:10:THR:HB	2.18	0.42
3:C:54:ILE:O	3:C:58:GLN:HG3	2.19	0.42
4:D:115:LEU:O	4:D:120:SER:HB3	2.19	0.42
4:D:489:LEU:HD11	4:D:607:PHE:CE2	2.55	0.42
4:D:1274:LEU:C	4:D:1276:GLU:H	2.23	0.42
5:E:11:ASP:OD1	5:E:11:ASP:N	2.51	0.42
7:G:4:DT:H2''	7:G:5:DA:C8	2.54	0.42
2:B:137:LYS:H	2:B:137:LYS:CD	2.32	0.42
2:B:104:LEU:CD1	2:B:111:ILE:HG12	2.49	0.42
4:D:416:GLU:HB2	5:E:46:LYS:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:804:LEU:HD12	4:D:804:LEU:HA	1.79	0.42
4:D:38:LYS:HB2	4:D:40:GLU:HG2	2.02	0.42
4:D:395:ALA:O	4:D:399:VAL:HG23	2.19	0.42
3:C:89:GLN:H	3:C:89:GLN:HG2	1.62	0.42
4:D:368:LYS:HE2	4:D:441:GLU:HG2	2.02	0.42
4:D:424:ALA:HB3	4:D:425:PRO:HD3	2.01	0.42
3:C:596:LYS:HE3	3:C:596:LYS:HB3	1.80	0.41
4:D:448:HIS:CE1	4:D:450:LEU:HB2	2.55	0.41
1:A:224:PHE:CE2	2:B:41:LEU:HD11	2.56	0.41
2:B:9:PRO:HG3	2:B:29:LEU:HD21	2.02	0.41
3:C:726:GLU:HB3	3:C:778:LYS:HD3	2.02	0.41
3:C:728:ALA:C	3:C:729:GLU:HG3	2.40	0.41
4:D:142:TYR:O	4:D:157:LEU:HA	2.19	0.41
4:D:871:ASN:N	4:D:871:ASN:HD22	2.18	0.41
2:B:159:LYS:HB2	2:B:164:LEU:HD11	2.02	0.41
3:C:1352:ASP:OD1	4:D:19:LYS:HD3	2.20	0.41
4:D:659:ILE:O	4:D:663:THR:HG23	2.20	0.41
5:E:5:THR:HG22	5:E:7:GLU:H	1.85	0.41
3:C:197:ARG:HE	3:C:197:ARG:HB2	1.60	0.41
4:D:427:LEU:HD23	4:D:427:LEU:HA	1.80	0.41
1:A:155:ILE:HD13	1:A:155:ILE:HA	1.93	0.41
2:B:104:LEU:CD2	2:B:139:LEU:HB3	2.50	0.41
4:D:368:LYS:HB3	4:D:407:TRP:CZ3	2.55	0.41
4:D:746:LYS:H	4:D:746:LYS:HG2	1.61	0.41
4:D:906:ASN:ND2	5:E:15:THR:HA	2.34	0.41
5:E:63:GLU:HA	5:E:66:LEU:HD12	2.02	0.41
2:B:24:PHE:CE2	2:B:197:ILE:HD12	2.56	0.41
4:D:677:TYR:C	4:D:679:ASN:H	2.23	0.41
4:D:861:ASP:O	4:D:865:VAL:HG22	2.21	0.41
4:D:1241:ILE:O	4:D:1245:VAL:HG23	2.21	0.41
5:E:22:LEU:HB3	5:E:66:LEU:HD13	2.02	0.41
1:A:58:ILE:O	1:A:161:THR:HG21	2.20	0.41
2:B:174:PHE:HE2	2:B:196:ASN:ND2	2.19	0.41
3:C:744:SER:OG	3:C:745:GLN:N	2.54	0.41
3:C:1094:LEU:HD23	3:C:1094:LEU:HA	1.94	0.41
4:D:641:ASP:OD1	4:D:641:ASP:N	2.53	0.41
4:D:666:TYR:HB2	4:D:675:GLU:CB	2.51	0.41
4:D:759:ASN:ND2	4:D:762:GLU:OE2	2.54	0.41
4:D:827:GLU:N	4:D:827:GLU:OE1	2.54	0.41
4:D:866:GLU:HG2	4:D:867:LEU:HD12	2.02	0.41
4:D:1326:ASN:N	4:D:1326:ASN:OD1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:478:ILE:HG23	3:C:479:ARG:N	2.36	0.41
3:C:493:LYS:HE3	3:C:493:LYS:HB2	1.64	0.41
4:D:679:ASN:O	4:D:683:ILE:HG12	2.21	0.41
4:D:897:ARG:HA	4:D:903:ARG:O	2.21	0.41
7:G:15:DT:H2'	7:G:16:DA:H8	1.85	0.41
3:C:1241:TYR:HD1	3:C:1241:TYR:HA	1.75	0.40
4:D:544:ALA:O	4:D:572:VAL:HG23	2.21	0.40
4:D:908:GLY:HA2	4:D:1351:LEU:HD12	2.02	0.40
4:D:601:LYS:HB2	4:D:601:LYS:HE2	1.87	0.40
4:D:1222:LEU:HD21	4:D:1242:GLU:HG3	2.03	0.40
3:C:554:HIS:ND1	3:C:556:THR:OG1	2.51	0.40
4:D:73:TYR:HD1	4:D:78:HIS:CE1	2.40	0.40
4:D:659:ILE:HD12	4:D:680:ILE:HG23	2.04	0.40
4:D:36:VAL:HG12	4:D:59:ILE:HD13	2.03	0.40
4:D:335:ARG:HD3	4:D:335:ARG:HA	1.90	0.40
4:D:1341:ILE:HD11	4:D:1343:ARG:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	223/323 (69%)	194 (87%)	29 (13%)	0	100	100
2	B	228/317 (72%)	186 (82%)	40 (18%)	2 (1%)	17	53
3	C	1190/1358 (88%)	1022 (86%)	167 (14%)	1 (0%)	51	83
4	D	1155/1604 (72%)	1016 (88%)	137 (12%)	2 (0%)	47	80
5	E	67/72 (93%)	49 (73%)	17 (25%)	1 (2%)	10	39
All	All	2863/3674 (78%)	2467 (86%)	390 (14%)	6 (0%)	50	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	521	ASP
4	D	1263	VAL
4	D	1287	GLU
5	E	60	ILE
2	B	171	PRO
2	B	124	ILE

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	187/287 (65%)	172 (92%)	15 (8%)	12	38
2	B	193/276 (70%)	181 (94%)	12 (6%)	18	50
3	C	824/1169 (70%)	739 (90%)	85 (10%)	7	26
4	D	869/1374 (63%)	792 (91%)	77 (9%)	9	33
5	E	51/64 (80%)	43 (84%)	8 (16%)	2	11
All	All	2124/3170 (67%)	1927 (91%)	197 (9%)	12	31

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	24	SER
1	A	53	SER
1	A	56	SER
1	A	70	SER
1	A	78	ASP
1	A	80	VAL
1	A	98	ASP
1	A	100	LEU
1	A	136	THR
1	A	149	VAL
1	A	151	ARG
1	A	156	LEU
1	A	222	SER

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Mol	Chain	Res	Type
1	A	223	VAL
2	B	27	GLU
2	B	56	SER
2	B	58	LYS
2	B	76	THR
2	B	90	THR
2	B	137	LYS
2	B	162	GLU
2	B	183	ARG
2	B	187	ARG
2	B	199	THR
2	B	209	LEU
2	B	228	GLU
3	C	2	SER
3	C	34	SER
3	C	48	LEU
3	C	53	GLU
3	C	60	PHE
3	C	78	ILE
3	C	85	GLU
3	C	86	THR
3	C	94	THR
3	C	124	GLU
3	C	137	THR
3	C	140	THR
3	C	157	SER
3	C	175	ARG
3	C	188	PHE
3	C	193	ILE
3	C	199	ASP
3	C	207	THR
3	C	355	TYR
3	C	390	LEU
3	C	398	SER
3	C	417	SER
3	C	424	GLU
3	C	434	GLU
3	C	442	LYS
3	C	446	ASP
3	C	479	ARG
3	C	480	GLU
3	C	481	SER

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Mol	Chain	Res	Type
3	C	515	SER
3	C	517	PHE
3	C	521	ASP
3	C	528	THR
3	C	543	ARG
3	C	550	VAL
3	C	566	THR
3	C	578	LEU
3	C	580	SER
3	C	586	ASP
3	C	613	ASP
3	C	623	SER
3	C	625	LYS
3	C	649	GLU
3	C	650	SER
3	C	651	SER
3	C	677	ASP
3	C	684	MET
3	C	696	LEU
3	C	700	LYS
3	C	722	ARG
3	C	726	GLU
3	C	734	ARG
3	C	740	ASP
3	C	741	THR
3	C	748	ASN
3	C	749	LEU
3	C	789	PHE
3	C	813	ASN
3	C	823	ARG
3	C	832	SER
3	C	873	VAL
3	C	926	THR
3	C	1094	LEU
3	C	1104	ASP
3	C	1108	VAL
3	C	1113	ASN
3	C	1133	LEU
3	C	1135	SER
3	C	1173	LEU
3	C	1182	LEU
3	C	1186	ASP

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Mol	Chain	Res	Type
3	C	1219	ASN
3	C	1234	ASP
3	C	1241	TYR
3	C	1242	MET
3	C	1245	LEU
3	C	1260	THR
3	C	1262	SER
3	C	1277	PHE
3	C	1281	ARG
3	C	1305	VAL
3	C	1322	ASP
3	C	1342	VAL
3	C	1343	ARG
3	C	1352	ASP
4	D	19	LYS
4	D	27	VAL
4	D	51	ARG
4	D	67	GLU
4	D	68	CYS
4	D	85	ARG
4	D	100	MET
4	D	104	ASP
4	D	110	VAL
4	D	117	SER
4	D	118	LEU
4	D	144	VAL
4	D	146	ASP
4	D	174	PHE
4	D	191	ASP
4	D	193	GLU
4	D	204	GLU
4	D	258	PHE
4	D	262	ASP
4	D	269	ARG
4	D	279	LYS
4	D	282	ASP
4	D	292	ASN
4	D	302	ASP
4	D	307	ASN
4	D	312	ARG
4	D	315	THR
4	D	317	SER

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Mol	Chain	Res	Type
4	D	346	ASP
4	D	358	SER
4	D	391	THR
4	D	393	LYS
4	D	397	ARG
4	D	412	THR
4	D	420	LEU
4	D	462	ASP
4	D	501	THR
4	D	530	ASP
4	D	561	THR
4	D	570	THR
4	D	581	LEU
4	D	636	SER
4	D	639	VAL
4	D	646	ASP
4	D	664	GLU
4	D	673	GLU
4	D	681	ILE
4	D	728	ARG
4	D	748	ASP
4	D	750	THR
4	D	751	MET
4	D	761	ARG
4	D	762	GLU
4	D	815	ASP
4	D	824	GLU
4	D	833	VAL
4	D	834	GLU
4	D	840	THR
4	D	846	VAL
4	D	859	LEU
4	D	862	GLU
4	D	865	VAL
4	D	897	ARG
4	D	904	GLN
4	D	905	VAL
4	D	910	SER
4	D	926	LEU
4	D	1127	ARG
4	D	1227	SER
4	D	1243	THR

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Mol	Chain	Res	Type
4	D	1267	SER
4	D	1270	LEU
4	D	1301	SER
4	D	1304	THR
4	D	1306	SER
4	D	1309	SER
4	D	1331	ASN
5	E	3	ARG
5	E	7	GLU
5	E	8	ASP
5	E	11	ASP
5	E	32	LYS
5	E	53	ARG
5	E	61	THR
5	E	63	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	107	ASN
1	A	121	GLN
2	B	11	ASN
2	B	219	GLN
3	C	20	HIS
3	C	31	GLN
3	C	49	HIS
3	C	58	GLN
3	C	77	GLN
3	C	219	GLN
3	C	425	ASN
3	C	520	GLN
3	C	522	ASN
3	C	810	ASN
3	C	874	HIS
3	C	1219	ASN
3	C	1268	GLN
3	C	1336	ASN
4	D	102	HIS
4	D	111	HIS
4	D	156	GLN
4	D	264	ASN

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Mol	Chain	Res	Type
4	D	292	ASN
4	D	362	HIS
4	D	394	GLN
4	D	422	ASN
4	D	543	HIS
4	D	665	GLN
4	D	759	ASN
4	D	774	HIS
4	D	871	ASN
4	D	1232	GLN
4	D	1237	ASN
5	E	64	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	R	9/10 (90%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	R	14	A
8	R	17	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

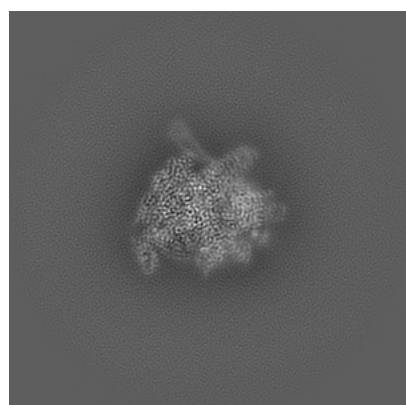
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21850. These allow visual inspection of the internal detail of the map and identification of artifacts.

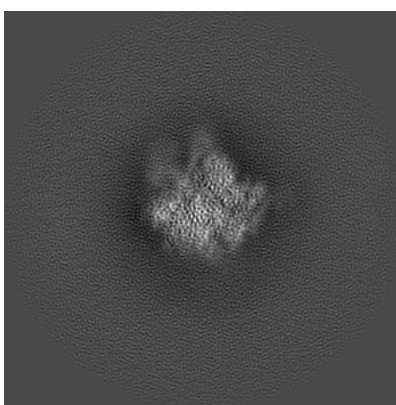
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

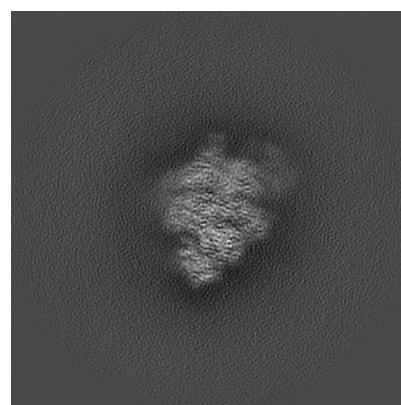
6.1.1 Primary map



X



Y

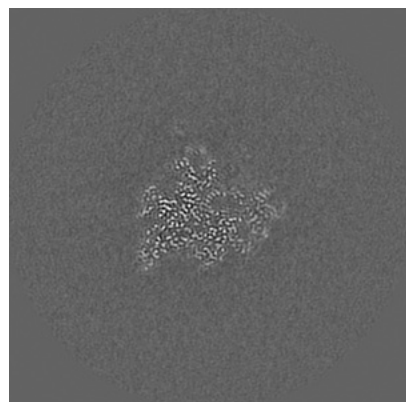


Z

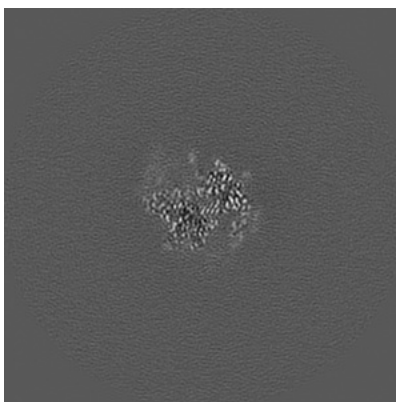
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

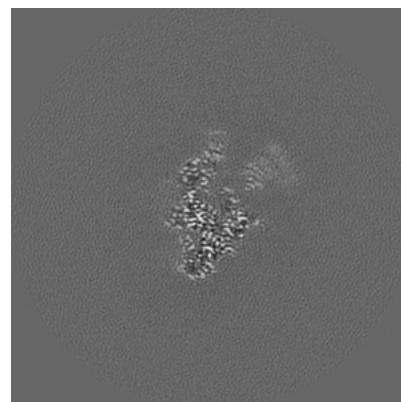
6.2.1 Primary map



X Index: 176



Y Index: 176

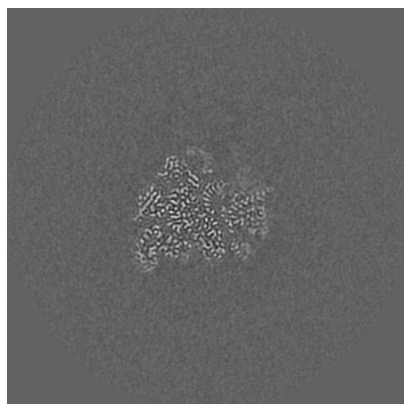


Z Index: 176

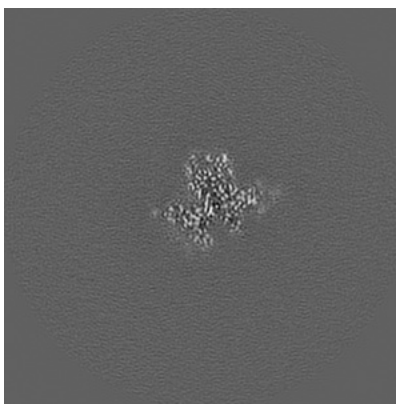
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

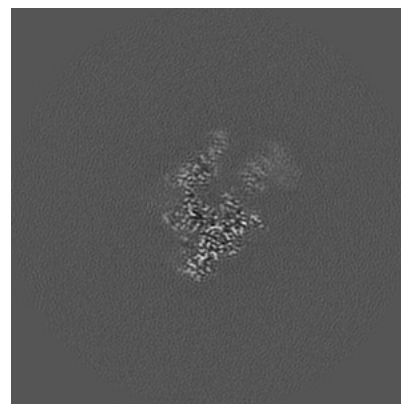
6.3.1 Primary map



X Index: 172



Y Index: 159

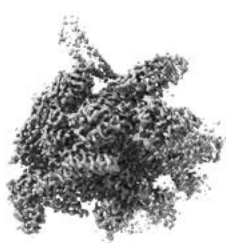


Z Index: 178

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

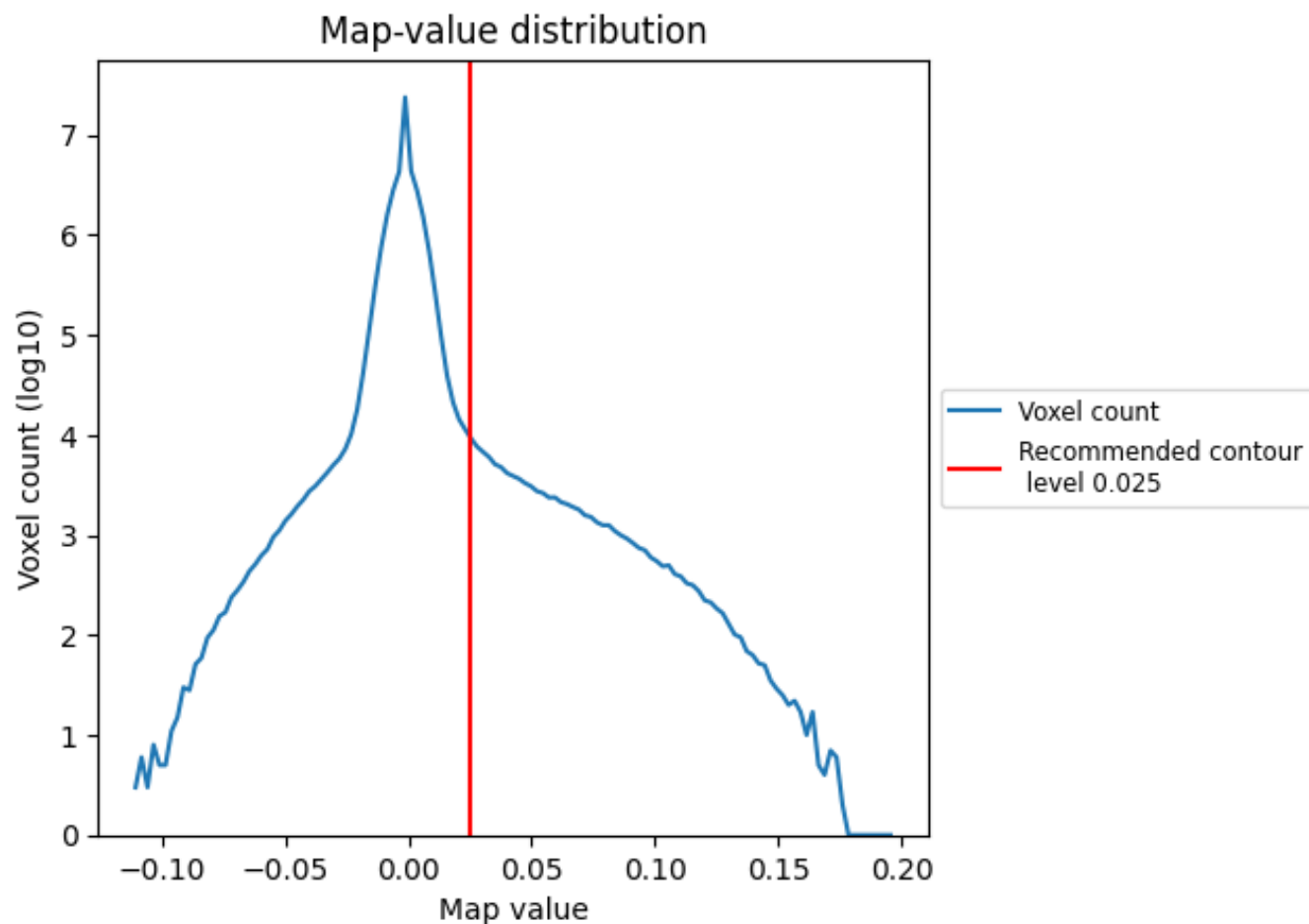
6.5 Mask visualisation

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

7 Map analysis [i](#)

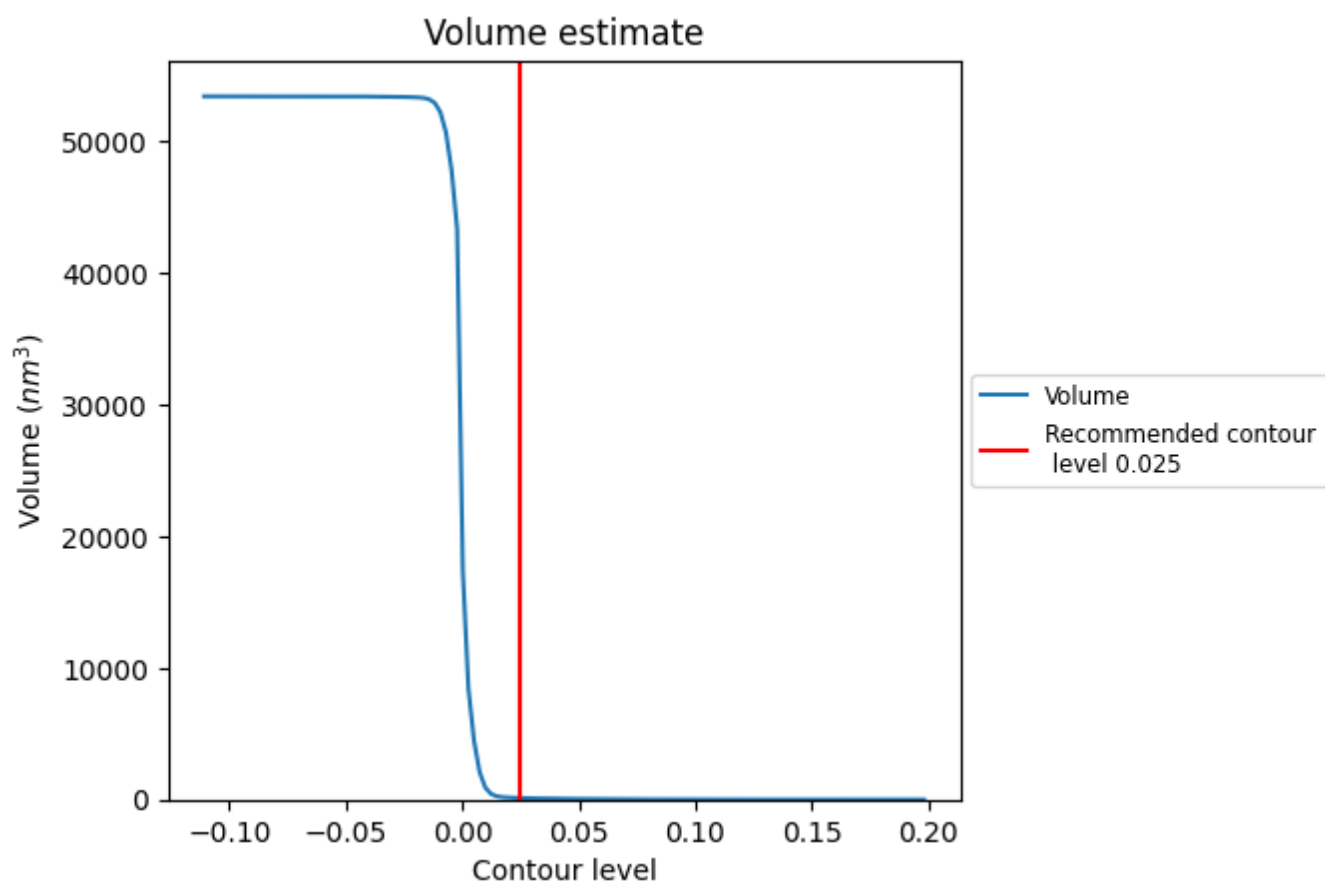
This section contains the results of statistical analysis of the map.

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.

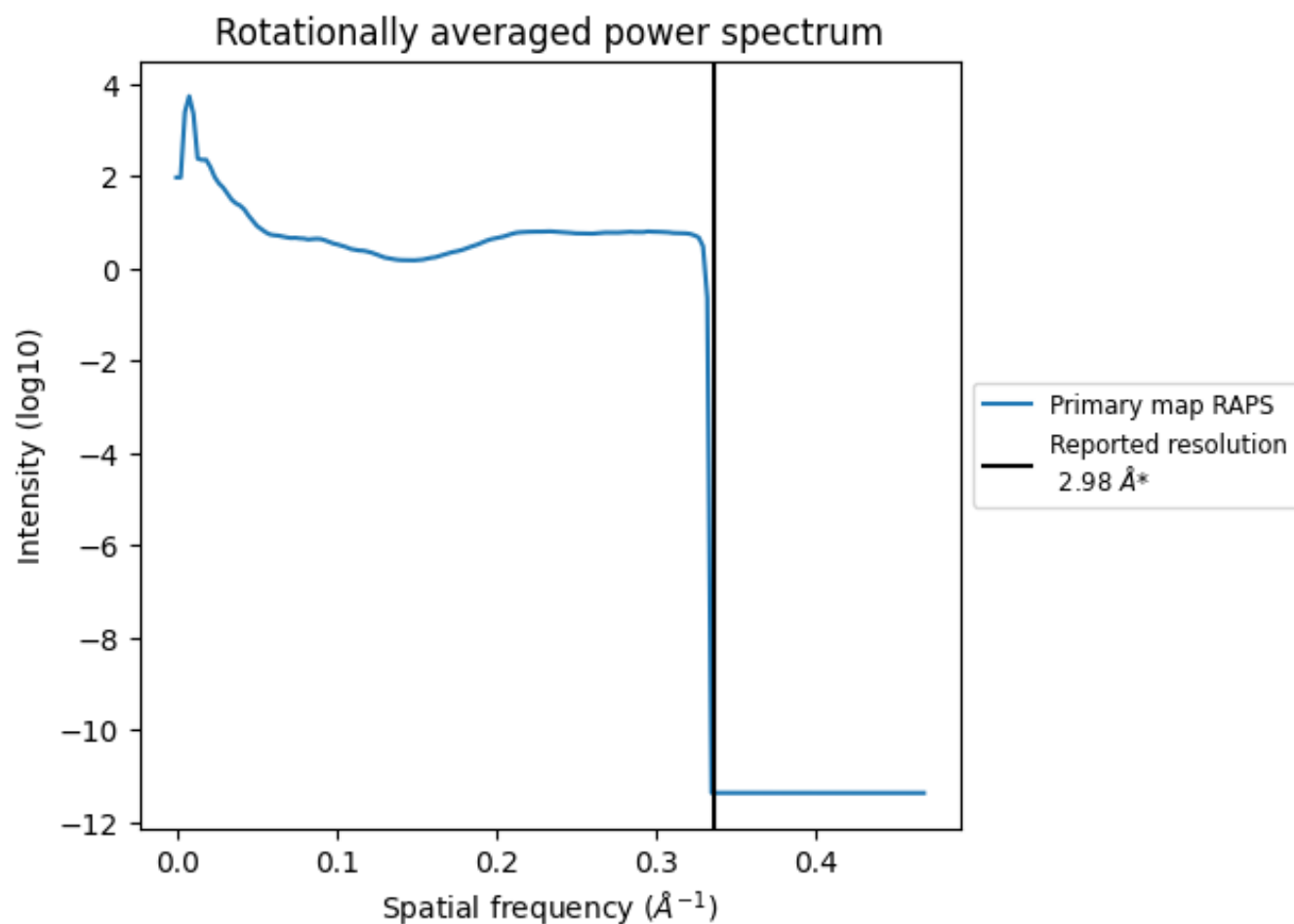
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm³; this corresponds to an approximate mass of 105 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 ⓘ

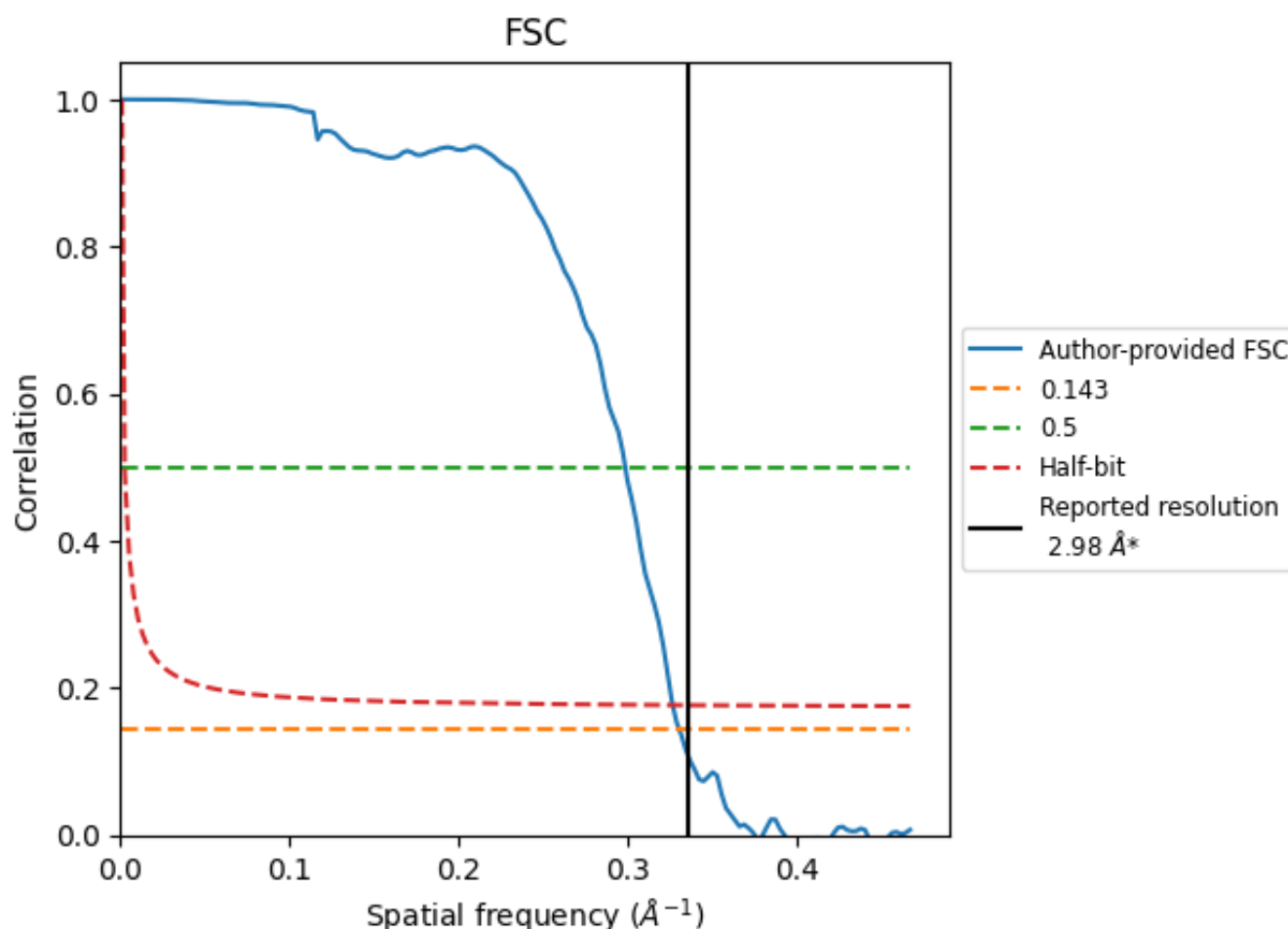


*Reported resolution corresponds to spatial frequency of 0.336 Å⁻¹

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 0.336 Å⁻¹

8.2 Resolution estimates [i](#)

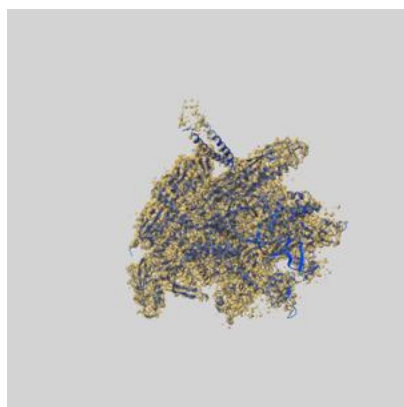
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	3.02	3.35	3.06
Unmasked-calculated*	-	-	-

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

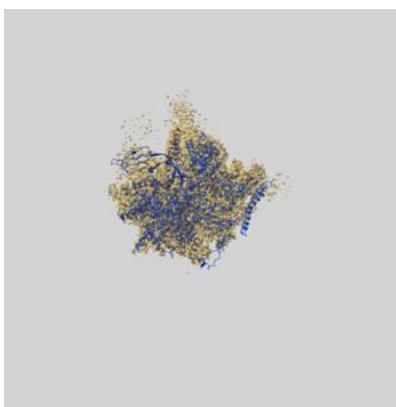
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21850 and PDB model 6WMP. Per-residue inclusion information can be found in section 3 on page 6.

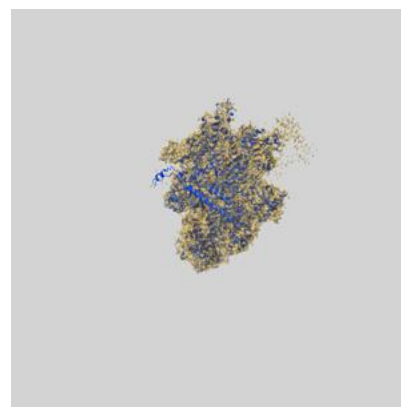
9.1 Map-model overlay [i](#)



X



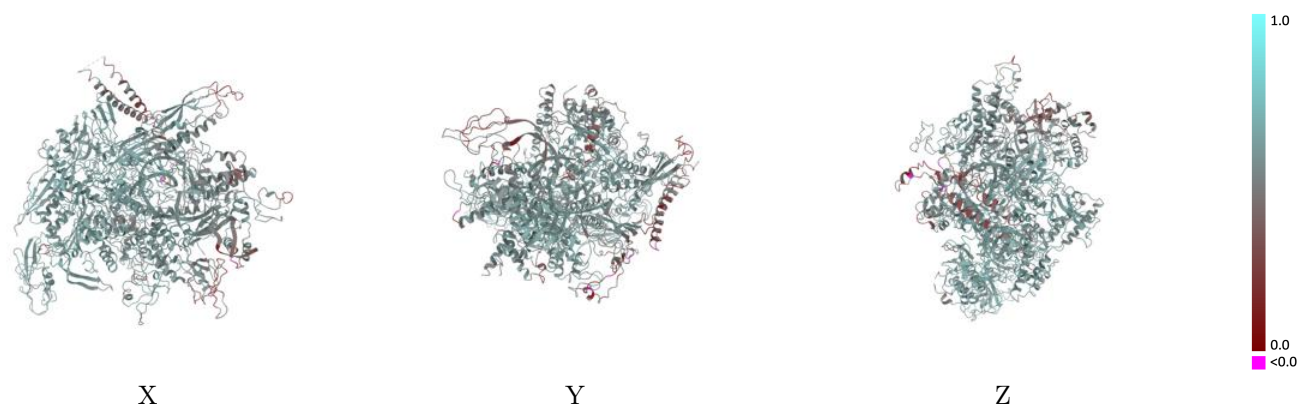
Y



Z

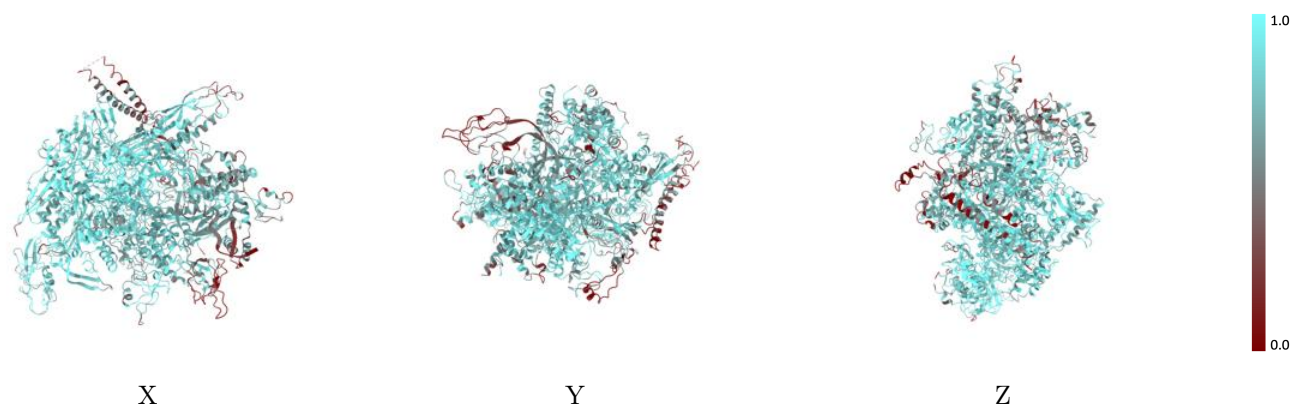
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



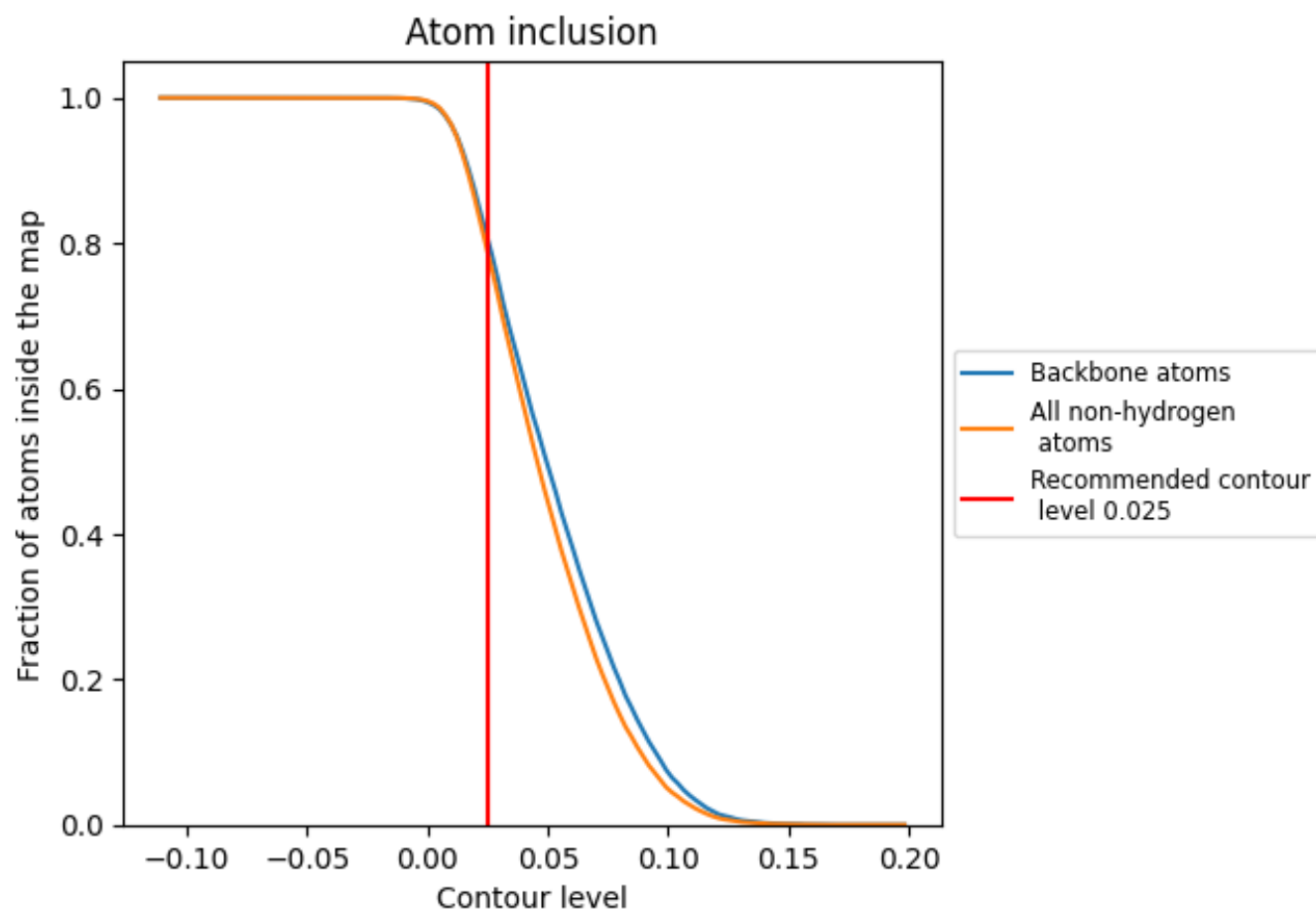
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 79% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7880	<div></div> 0.5690
A	<div></div> 0.8605	<div></div> 0.5950
B	<div></div> 0.8300	<div></div> 0.5880
C	<div></div> 0.7906	<div></div> 0.5650
D	<div></div> 0.7857	<div></div> 0.5720
E	<div></div> 0.6329	<div></div> 0.5260
F	<div></div> 0.5132	<div></div> 0.4860
G	<div></div> 0.6770	<div></div> 0.5270
R	<div></div> 0.8251	<div></div> 0.5740

1.0

0.0

<0.0