



Full wwPDB EM Validation Report ⓘ

Jan 22, 2024 – 03:03 PM EST

PDB ID : 8GL8
EMDB ID : EMD-40194
Title : The Type 9 Secretion System Extended Translocon - SprA-PorV-PPI-RemZ-SkpA-SprE complex
Authors : Deme, J.C.; Lea, S.M.
Deposited on : 2023-03-21
Resolution : 2.20 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:

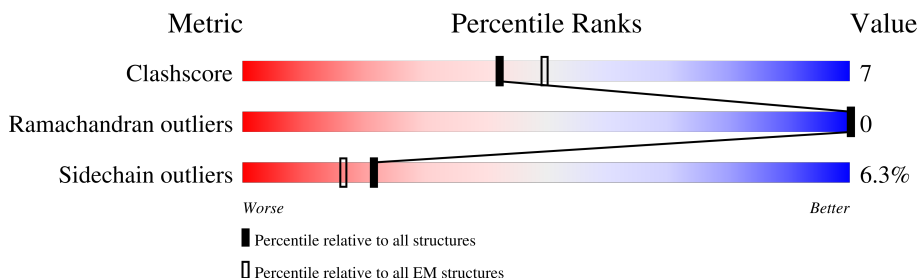
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.20 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

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	2403	
2	B	176	
3	F	402	
4	D	1114	
5	C	341	
5	E	341	
5	G	341	
6	I	870	

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 33279 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 Protein involved in gliding motility SprA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2290	18190	11468	3075	3604	43	0	0

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	128	990	633	160	197	0	0

- Molecule 3 is a protein called Type IX secretion system protein PorV domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	367	2861	1834	462	560	5	0	0

- Molecule 4 is a protein called RemZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	75	748	473	125	149	1	18	0

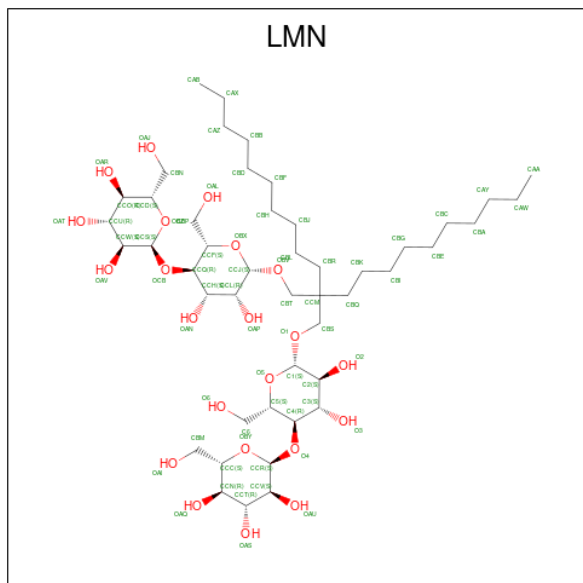
- Molecule 5 is a protein called Periplasmic chaperone for outer membrane proteins Skp.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	173	1435	899	247	285	4	0	0
5	C	172	1414	889	244	276	5	0	0
5	E	152	1251	790	209	248	4	0	0

- Molecule 6 is a protein called SprE.

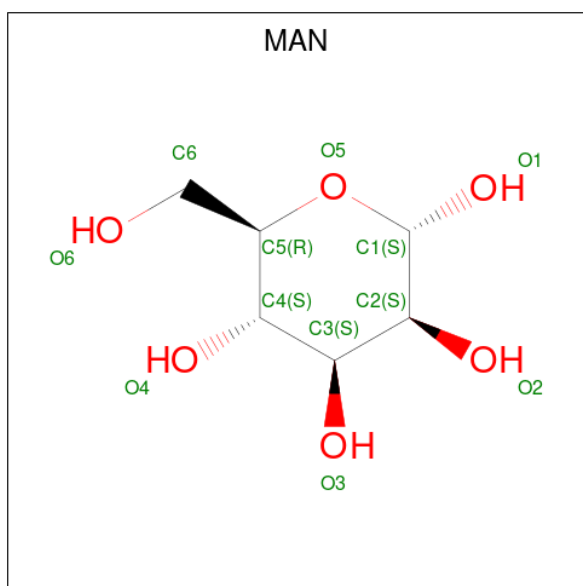
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	624	5168	3297	873	981	17	0	0

- Molecule 7 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: $C_{47}H_{88}O_{22}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	A	1	69	47	22	0

- Molecule 8 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
8	I	1	Total	C	O	0
			11	6	5	
8	I	1	Total	C	O	0
			11	6	5	
8	I	1	Total	C	O	0
			11	6	5	
8	I	1	Total	C	O	0
			11	6	5	
8	I	1	Total	C	O	0
			11	6	5	

- Molecule 9 is water.

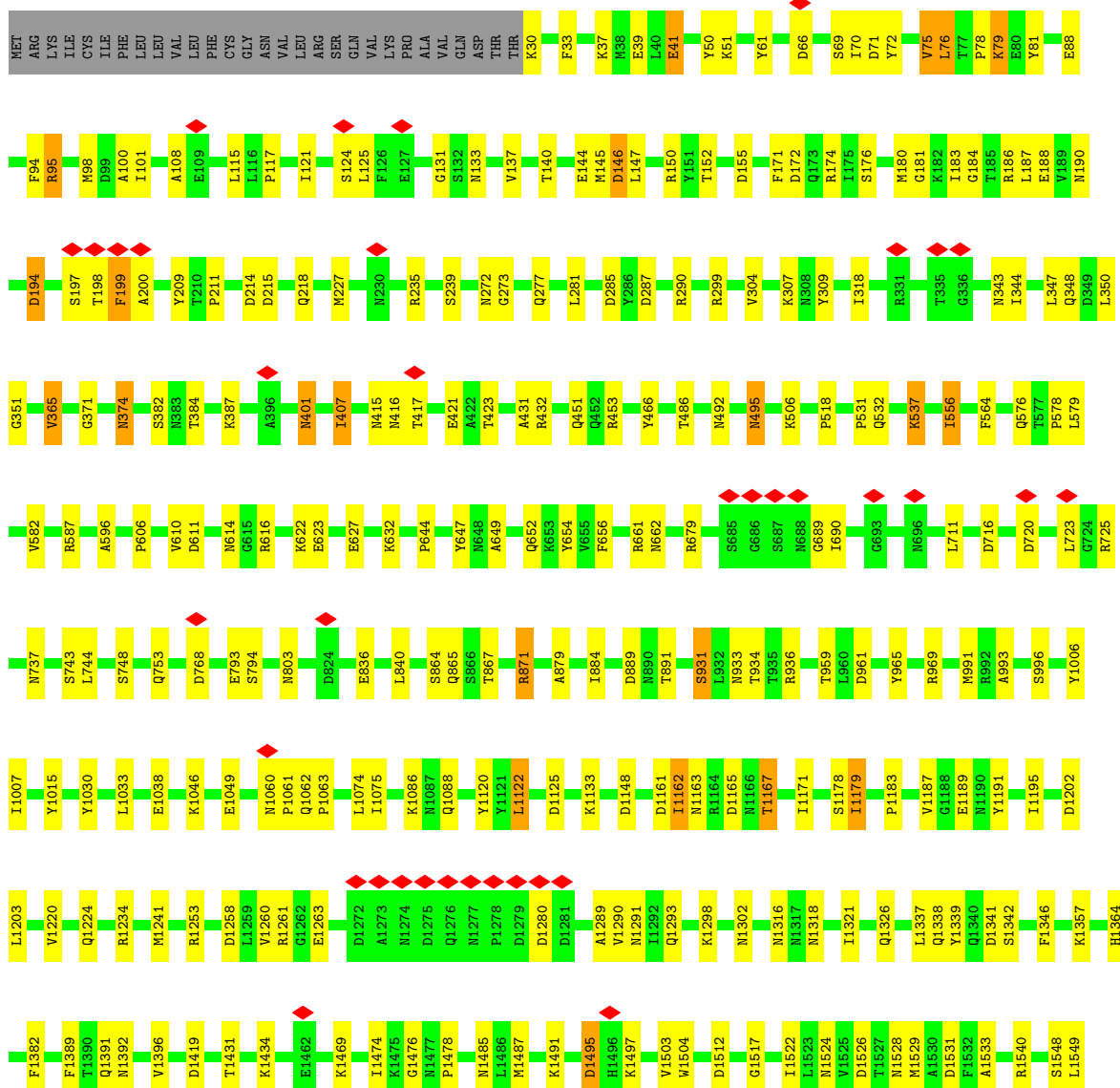
Mol	Chain	Residues	Atoms		AltConf
9	A	767	Total	O	0
			767	767	
9	B	42	Total	O	0
			42	42	
9	F	103	Total	O	0
			103	103	
9	D	23	Total	O	0
			23	23	
9	G	23	Total	O	0
			23	23	
9	C	27	Total	O	0
			27	27	
9	E	15	Total	O	0
			15	15	
9	I	87	Total	O	0
			87	87	

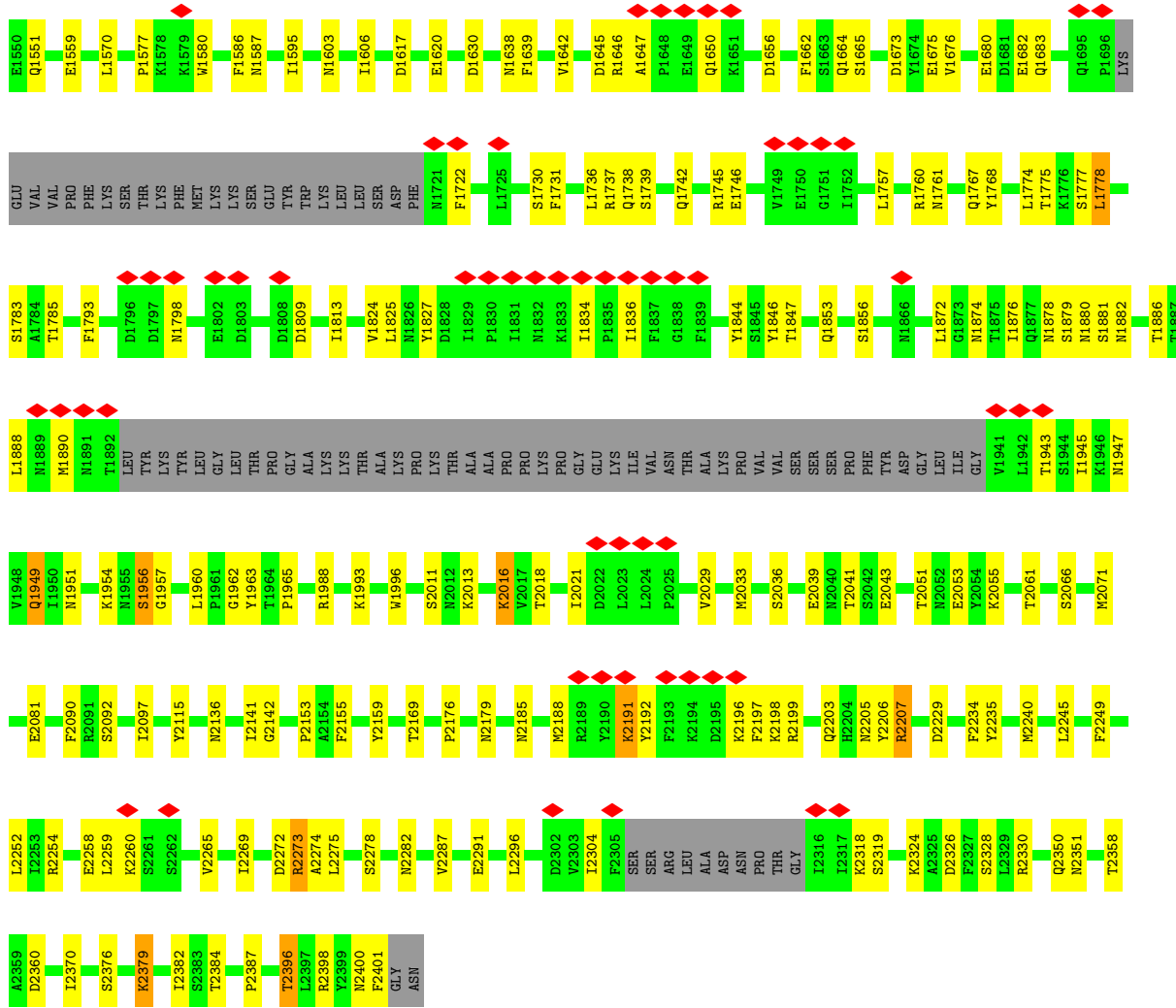
3 Residue-property plots

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.

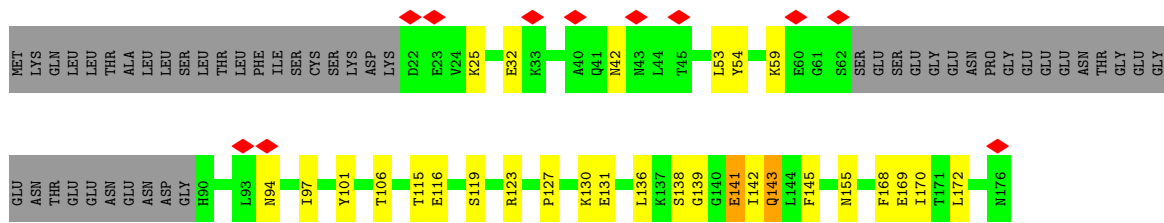
- Molecule 1: Protein involved in gliding motility SprA

Chain A:



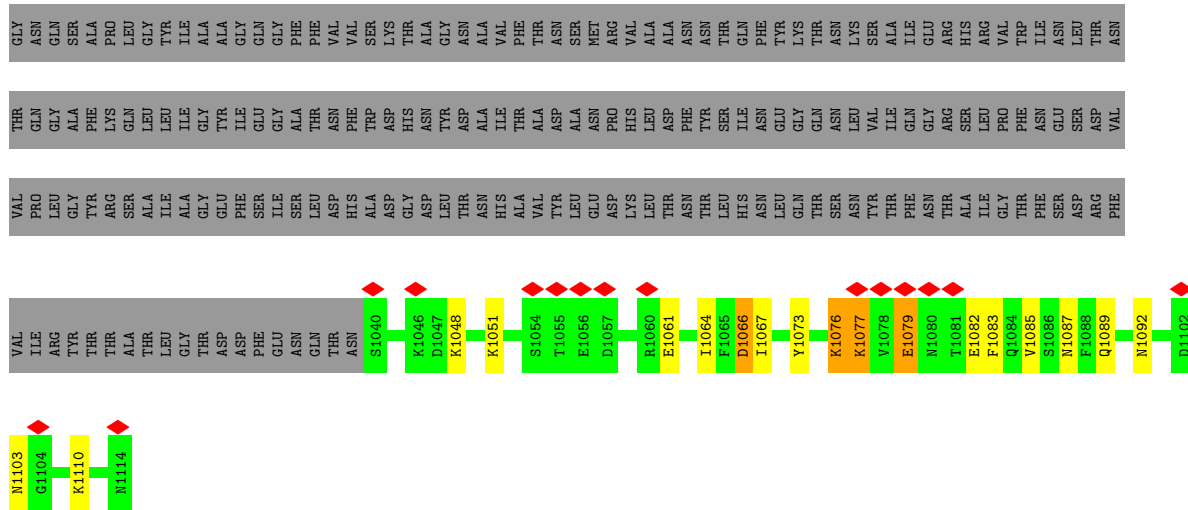


• Molecule 2: Peptidyl-prolyl cis-trans isomerase

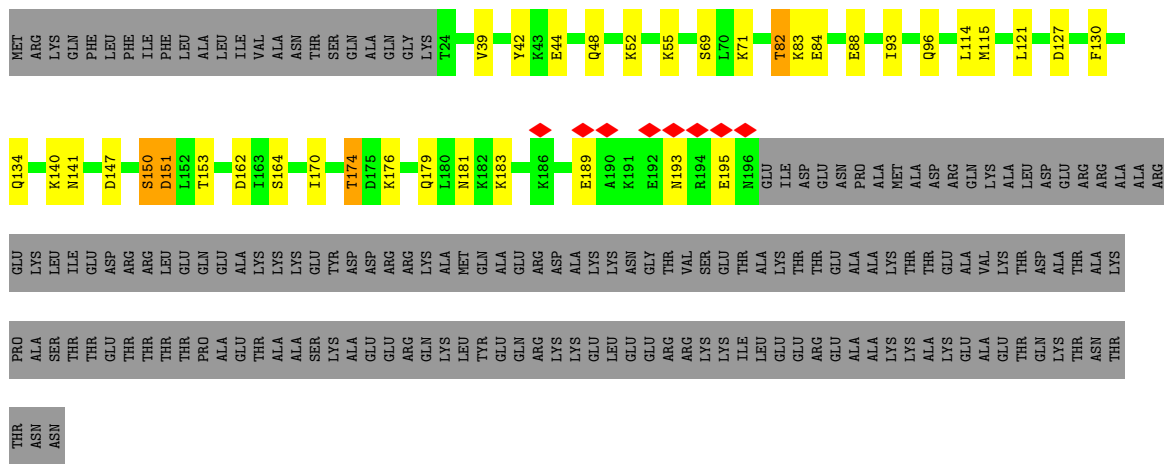


• Molecule 3: Type IX secretion system protein PorV domain-containing protein

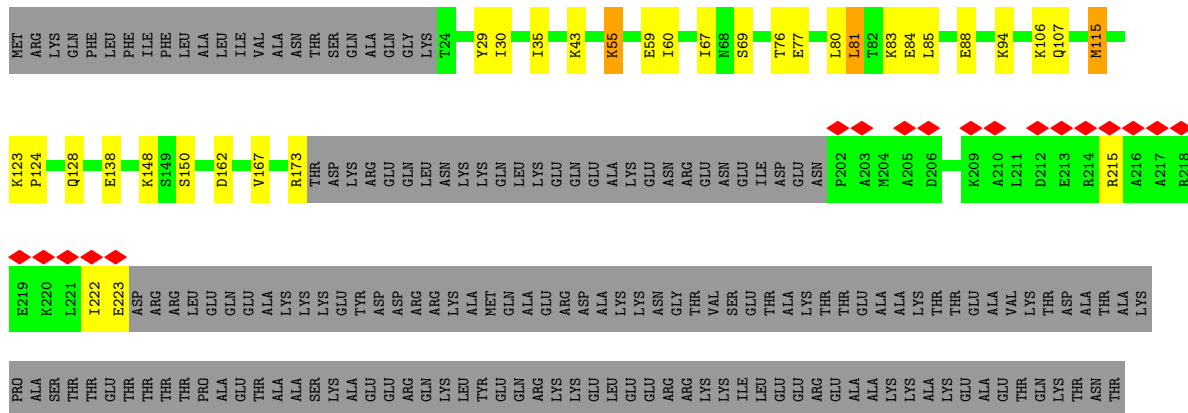
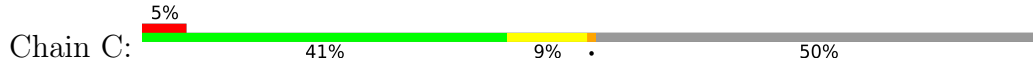


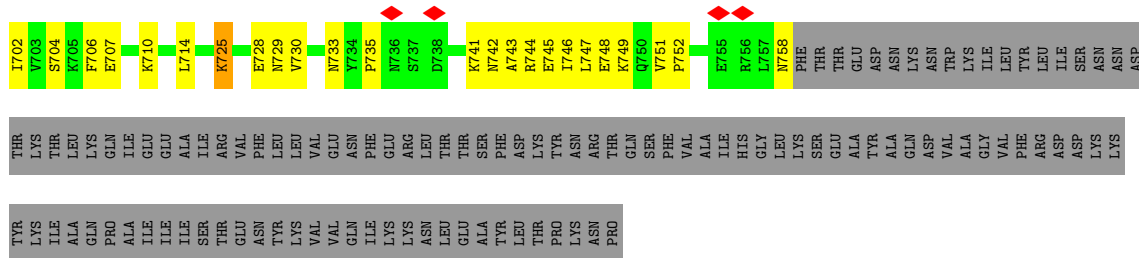


● Molecule 5: Periplasmic chaperone for outer membrane proteins Skp



● Molecule 5: Periplasmic chaperone for outer membrane proteins Skp





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	546490	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 ($e^-/\text{\AA}^2$)	61.2	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	80.750	Depositor
Minimum map value	-40.660	Depositor
Average map value	0.014	Depositor
Map value standard deviation	1.271	Depositor
Recommended contour level	8.54	Depositor
Map size (Å)	372.73602, 372.73602, 372.73602	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8320001, 0.8320001, 0.8320001	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.26	0/18585	0.50	1/25237 (0.0%)
2	B	0.25	0/1009	0.46	0/1370
3	F	0.27	0/2935	0.48	0/3976
4	D	0.26	0/756	0.44	0/1014
5	C	0.26	0/1428	0.46	0/1906
5	E	0.25	0/1265	0.46	0/1693
5	G	0.26	0/1449	0.42	0/1934
6	I	0.27	0/5267	0.46	1/7077 (0.0%)
All	All	0.26	0/32694	0.48	2/44207 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	187	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	1531	ASP	CB-CG-OD1	5.39	123.15	118.30

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	18190	0	17539	244	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	990	0	976	14	0
3	F	2861	0	2715	46	0
4	D	748	0	755	14	0
5	C	1414	0	1437	18	0
5	E	1251	0	1262	22	0
5	G	1435	0	1452	20	0
6	I	5168	0	5148	100	0
7	A	69	0	88	3	0
8	I	66	0	60	0	0
9	A	767	0	0	13	0
9	B	42	0	0	0	0
9	C	27	0	0	1	0
9	D	23	0	0	2	0
9	E	15	0	0	0	0
9	F	103	0	0	0	0
9	G	23	0	0	1	0
9	I	87	0	0	0	0
All	All	33279	0	31432	456	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 (456) 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)
1:A:199:PHE:HD1	1:A:200:ALA:H	1.20	0.89
4:D:1051:LYS:HZ3	4:D:1082[B]:GLU:HB2	1.41	0.84
3:F:157:ALA:HB3	3:F:183:ASP:HB2	1.65	0.79
1:A:1392:ASN:ND2	1:A:1476:GLY:O	2.15	0.75
1:A:1291:ASN:OD1	1:A:1326:GLN:NE2	2.21	0.74
6:I:182:LEU:O	6:I:186:THR:OG1	2.06	0.74
6:I:266:ARG:NH1	6:I:303:ASN:OD1	2.22	0.72
3:F:320:LYS:HE3	3:F:346:SER:HB2	1.73	0.71
6:I:746:ILE:HA	6:I:749:LYS:HB3	1.73	0.71
1:A:199:PHE:HD1	1:A:200:ALA:N	1.89	0.70
5:E:81:LEU:HD12	5:E:85:LEU:HB2	1.72	0.70
1:A:1357:LYS:HB2	1:A:1512:ASP:HB3	1.73	0.70
3:F:381:ASN:HB3	3:F:384:GLU:HG3	1.74	0.70
1:A:1965:PRO:HD3	1:A:1996:TRP:HB2	1.74	0.69
1:A:867:THR:HG22	1:A:1260:VAL:HG22	1.75	0.69
1:A:188:GLU:OE1	1:A:190:ASN:ND2	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1587:ASN:HB3	1:A:1638:ASN:HB2	1.75	0.68
1:A:194:ASP:HB3	1:A:197:SER:HB3	1.75	0.68
1:A:401:ASN:ND2	1:A:415:ASN:OD1	2.21	0.68
1:A:1737:ARG:NH2	1:A:1809:ASP:O	2.29	0.66
1:A:1876:ILE:HD11	1:A:1960:LEU:HD23	1.78	0.65
1:A:1775:THR:HB	1:A:1778:LEU:HB2	1.79	0.64
3:F:122:GLN:N	3:F:122:GLN:OE1	2.31	0.64
1:A:1775:THR:HG22	1:A:1777:SER:H	1.62	0.64
1:A:125:LEU:HD13	6:I:100:LYS:HG3	1.79	0.64
1:A:1165:ASP:OD1	9:A:2601:HOH:O	2.15	0.64
1:A:287:ASP:OD1	1:A:453:ARG:NH2	2.30	0.64
1:A:2274:ALA:HB3	1:A:2287:VAL:HB	1.79	0.63
6:I:700:ASP:HB3	6:I:702:ILE:HG22	1.79	0.63
1:A:556:ILE:HG12	1:A:579:LEU:HD21	1.79	0.63
5:G:84:GLU:O	5:G:88:GLU:HG2	1.97	0.63
6:I:436:GLU:HG3	6:I:439:ARG:HH21	1.60	0.63
2:B:136:LEU:HD21	2:B:142:ILE:HB	1.81	0.63
1:A:1647:ALA:HB3	1:A:1650:GLN:HB2	1.81	0.63
1:A:117:PRO:HB3	6:I:99:THR:HG23	1.79	0.62
6:I:22:SER:O	6:I:30:ASN:ND2	2.32	0.62
1:A:144:GLU:OE1	1:A:2398:ARG:NH1	2.31	0.62
1:A:879:ALA:HA	1:A:991:MET:HG2	1.80	0.62
5:G:170:ILE:O	5:G:174:THR:HG23	1.99	0.62
1:A:374:ASN:ND2	1:A:384:THR:O	2.26	0.62
3:F:123:THR:HG23	3:F:124:GLY:H	1.65	0.62
1:A:1646:ARG:NH1	1:A:1656:ASP:OD2	2.28	0.62
5:E:26:ARG:HH12	5:E:140:LYS:HB3	1.64	0.61
1:A:75:VAL:HG13	5:E:109:GLY:HA2	1.83	0.61
1:A:2196:LYS:O	1:A:2260:LYS:N	2.33	0.61
1:A:215:ASP:O	1:A:218:GLN:NE2	2.33	0.61
1:A:532:GLN:NE2	4:D:1079[B]:GLU:OE2	2.32	0.61
3:F:77:SER:HG	3:F:390:SER:HG	1.48	0.61
1:A:969:ARG:NH1	9:A:2612:HOH:O	2.33	0.61
3:F:59:GLN:O	3:F:209:GLN:NE2	2.33	0.61
3:F:200:GLY:HA2	3:F:238:ASP:O	2.00	0.61
1:A:1167:THR:O	9:A:2601:HOH:O	2.16	0.60
5:C:222:ILE:HD12	5:C:223:GLU:HG3	1.83	0.60
6:I:560:PHE:HA	6:I:563:LYS:HD2	1.83	0.60
1:A:1163:ASN:OD1	9:A:2601:HOH:O	2.16	0.60
6:I:377:ASN:O	6:I:380:THR:OG1	2.19	0.60
3:F:24:ARG:HH11	3:F:263:GLY:HA2	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1061:GLU:HG3	4:D:1076[A]:LYS:HG3	1.84	0.60
1:A:1639:PHE:HB2	1:A:1664:GLN:HB3	1.83	0.59
4:D:1051:LYS:HD3	4:D:1082[A]:GLU:HG2	1.84	0.59
1:A:1738:GLN:HB2	1:A:1761:ASN:HB3	1.84	0.59
1:A:2196:LYS:HB2	1:A:2259:LEU:HD12	1.85	0.59
1:A:1988:ARG:NH1	1:A:2043:GLU:OE2	2.35	0.59
5:C:124:PRO:O	5:C:128:GLN:HG3	2.03	0.59
9:C:402:HOH:O	5:E:160:ARG:NH2	2.36	0.59
1:A:146:ASP:HB2	1:A:172:ASP:HB3	1.85	0.59
1:A:492:ASN:ND2	1:A:495:ASN:OD1	2.36	0.59
6:I:605:GLU:OE2	6:I:628:TYR:OH	2.21	0.59
6:I:380:THR:HA	6:I:381:ARG:NH1	2.18	0.59
1:A:94:PHE:O	1:A:98:MET:HG3	2.02	0.58
3:F:313:GLY:HA3	3:F:317:GLU:HG3	1.85	0.58
1:A:214:ASP:HB3	6:I:42:ILE:HG12	1.85	0.58
1:A:79:LYS:HD3	1:A:79:LYS:O	2.03	0.58
1:A:1825:LEU:HG	1:A:1846:TYR:HB3	1.85	0.58
4:D:1051:LYS:NZ	4:D:1082[B]:GLU:HB2	2.16	0.58
5:G:179:GLN:HG3	6:I:155:ILE:HB	1.86	0.58
1:A:198:THR:HG22	1:A:199:PHE:H	1.69	0.58
1:A:753:GLN:OE1	1:A:794:SER:OG	2.16	0.58
3:F:200:GLY:CA	3:F:238:ASP:O	2.51	0.58
2:B:53:LEU:HD22	2:B:131:GLU:HG3	1.85	0.58
1:A:1258:ASP:OD1	9:A:2602:HOH:O	2.17	0.57
5:E:107:GLN:OE1	5:E:113:ASN:ND2	2.38	0.57
5:C:83:LYS:HE2	5:C:83:LYS:HA	1.86	0.57
3:F:293:LYS:NZ	3:F:297:ASP:OD2	2.33	0.57
1:A:993:ALA:HB2	1:A:1162:ILE:HG22	1.86	0.57
1:A:2097:ILE:HG21	1:A:2153:PRO:HG2	1.87	0.57
6:I:368:TYR:O	6:I:372:THR:HG22	2.05	0.57
1:A:50:TYR:CE1	1:A:61:TYR:HB2	2.40	0.57
4:D:1048:LYS:HB3	4:D:1089[B]:GLN:HG3	1.87	0.57
1:A:1074:LEU:HG	1:A:1075:ILE:HG12	1.86	0.56
6:I:129:ARG:HD3	6:I:137:PRO:HB2	1.87	0.56
1:A:840:LEU:O	1:A:1517:GLY:HA3	2.04	0.56
1:A:2205:ASN:OD1	1:A:2207:ARG:NH2	2.38	0.56
5:G:71:LYS:HG2	5:G:93:ILE:HD13	1.87	0.56
1:A:199:PHE:CZ	1:A:748:SER:HA	2.40	0.56
5:C:76:THR:HA	6:I:749:LYS:HE2	1.88	0.56
1:A:343:ASN:HD22	1:A:407:ILE:HD13	1.70	0.56
1:A:199:PHE:HB2	3:F:84:ASP:HA	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2324:LYS:HB3	1:A:2358:THR:HG22	1.88	0.56
6:I:254:TYR:O	6:I:258:ILE:HG12	2.06	0.56
6:I:350:ARG:NH1	6:I:351:ASN:OD1	2.39	0.56
1:A:1642:VAL:HB	1:A:1662:PHE:HB3	1.88	0.55
6:I:735:PRO:O	6:I:744:ARG:NH2	2.39	0.55
6:I:742:ASN:OD1	6:I:746:ILE:HD13	2.06	0.55
1:A:611:ASP:HB3	1:A:616:ARG:HB2	1.87	0.55
5:E:74:LEU:HD23	5:E:89:ARG:HD2	1.88	0.55
1:A:864:SER:HB3	1:A:1263:GLU:HG2	1.88	0.55
1:A:1683:GLN:HG3	1:A:1738:GLN:HG3	1.88	0.55
1:A:864:SER:O	9:A:2603:HOH:O	2.18	0.55
1:A:931:SER:HB3	1:A:1203:LEU:HB3	1.89	0.55
1:A:1954:LYS:HG3	1:A:2013:LYS:HG2	1.89	0.55
1:A:1993:LYS:NZ	1:A:2051:THR:O	2.32	0.55
3:F:191:GLU:HG3	5:C:215:ARG:HH12	1.70	0.55
1:A:1337:LEU:HD22	1:A:1341:ASP:HB3	1.89	0.55
1:A:70:ILE:HG22	1:A:71:ASP:OD1	2.07	0.55
1:A:2370:ILE:HB	1:A:2396:THR:HG23	1.89	0.54
5:E:163:ILE:HD12	5:E:163:ILE:O	2.06	0.54
6:I:22:SER:H	6:I:30:ASN:HD21	1.54	0.54
1:A:689:GLY:O	1:A:725:ARG:NH1	2.41	0.54
6:I:701:GLU:O	6:I:704:SER:OG	2.25	0.54
1:A:649:ALA:HA	1:A:652:GLN:HB2	1.88	0.54
1:A:281:LEU:HD11	1:A:531:PRO:HD3	1.90	0.54
1:A:348:GLN:NE2	1:A:423:THR:O	2.41	0.54
5:G:48:GLN:NE2	9:G:402:HOH:O	2.40	0.54
1:A:95:ARG:NH2	5:C:150:SER:O	2.41	0.54
1:A:100:ALA:HA	1:A:108:ALA:HB1	1.90	0.54
6:I:641:SER:O	6:I:645:ASN:ND2	2.41	0.54
6:I:675:TYR:HE1	6:I:679:GLN:HE21	1.55	0.54
1:A:137:VAL:HA	1:A:181:GLY:HA3	1.90	0.54
1:A:596:ALA:N	1:A:1798:ASN:O	2.41	0.53
5:E:39:VAL:HG11	5:E:171:LEU:HD12	1.89	0.53
6:I:63:ASP:OD2	6:I:267:LYS:NZ	2.37	0.53
1:A:1577:PRO:HG2	1:A:1580:TRP:NE1	2.23	0.53
1:A:318:ILE:HD13	1:A:466:TYR:HB3	1.90	0.53
1:A:1060:ASN:HB3	1:A:1061:PRO:HD3	1.91	0.53
3:F:87:ASN:O	4:D:1110:LYS:NZ	2.41	0.53
1:A:131:GLY:H	1:A:186:ARG:HG3	1.73	0.53
1:A:1006:TYR:HA	1:A:1220:VAL:HG23	1.90	0.53
5:E:112:GLY:HA2	5:E:116:ARG:HG3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:55:VAL:HG11	3:F:392:THR:HB	1.90	0.53
1:A:576:GLN:NE2	1:A:1746:GLU:OE2	2.32	0.53
1:A:145:MET:O	1:A:2396:THR:HA	2.09	0.53
1:A:183:ILE:HB	1:A:187:LEU:HB3	1.91	0.52
6:I:683:PHE:HA	6:I:686:VAL:HG12	1.91	0.52
3:F:58:GLN:HG2	3:F:109:SER:HB3	1.89	0.52
1:A:1963:TYR:CZ	1:A:1965:PRO:HG2	2.45	0.52
2:B:54:TYR:HB2	2:B:145:PHE:HB2	1.91	0.52
1:A:2071:MET:HE1	1:A:2245:LEU:HB3	1.92	0.52
5:E:148:LYS:NZ	5:E:151:ASP:OD1	2.42	0.52
3:F:304:ILE:O	3:F:307:SER:OG	2.25	0.52
1:A:1293:GLN:NE2	9:A:2630:HOH:O	2.43	0.52
5:E:26:ARG:NH1	5:E:140:LYS:HB3	2.24	0.52
1:A:365:VAL:HG13	1:A:518:PRO:HD2	1.92	0.52
1:A:2252:LEU:N	1:A:2269:ILE:O	2.43	0.52
6:I:142:PHE:HA	6:I:145:ILE:HD12	1.91	0.52
1:A:2304:ILE:HG13	1:A:2318:LYS:HG3	1.92	0.52
4:D:1066:ASP:OD2	4:D:1092[B]:ASN:ND2	2.43	0.52
5:C:30:ILE:HD11	5:C:167:VAL:HG21	1.92	0.52
3:F:309:GLY:N	3:F:318:GLU:OE2	2.37	0.51
1:A:662:ASN:OD1	1:A:1234:ARG:NH2	2.43	0.51
1:A:2033:MET:HE3	1:A:2176:PRO:HG2	1.93	0.51
1:A:2351:ASN:HB3	1:A:2379:LYS:HB3	1.93	0.51
5:G:147:ASP:O	5:G:150:SER:OG	2.28	0.51
1:A:1774:LEU:HD12	1:A:1778:LEU:HD13	1.93	0.51
1:A:146:ASP:OD1	1:A:2396:THR:HB	2.10	0.51
2:B:59:LYS:HG2	2:B:141:GLU:HB2	1.93	0.51
1:A:1298:LYS:O	1:A:1302:ASN:ND2	2.44	0.51
6:I:407:ASP:O	6:I:411:LYS:HD3	2.11	0.51
6:I:568:THR:OG1	6:I:569:GLN:N	2.43	0.51
6:I:710:LYS:HE3	6:I:714:LEU:HD11	1.92	0.51
6:I:396:VAL:HG21	6:I:594:PHE:HE2	1.76	0.51
3:F:57:SER:HB2	3:F:64:LYS:HE3	1.91	0.50
3:F:68:ALA:HB3	3:F:99:LYS:HD2	1.92	0.50
1:A:304:VAL:HA	1:A:307:LYS:HE2	1.93	0.50
1:A:2273:ARG:HD2	1:A:2275:LEU:HD21	1.93	0.50
5:C:115:MET:SD	5:C:115:MET:N	2.85	0.50
1:A:711:LEU:HB3	1:A:716:ASP:HB2	1.94	0.50
6:I:379:LYS:HD2	6:I:379:LYS:O	2.11	0.50
1:A:623:GLU:OE2	1:A:661:ARG:NH2	2.43	0.50
6:I:42:ILE:HD13	6:I:100:LYS:HD3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:ASN:HB2	1:A:1321:ILE:HG13	1.93	0.50
1:A:1834:ILE:HD12	1:A:1836:ILE:HB	1.93	0.50
3:F:357:LEU:HD12	3:F:374:PHE:HE2	1.76	0.50
1:A:865:GLN:HA	1:A:1261:ARG:O	2.12	0.50
6:I:160:ILE:O	6:I:164:LYS:HG2	2.11	0.50
6:I:224:SER:HB3	6:I:230:ARG:HG3	1.93	0.50
1:A:1951:ASN:HB2	1:A:2016:LYS:HB3	1.93	0.50
6:I:621:MET:HB3	6:I:643:ILE:HD11	1.94	0.50
6:I:376:LEU:HD21	6:I:382:GLU:HG2	1.93	0.50
1:A:768:ASP:N	1:A:768:ASP:OD1	2.41	0.50
5:C:76:THR:HG23	5:C:77:GLU:HG3	1.94	0.50
1:A:1202:ASP:OD1	3:F:296:LYS:NZ	2.43	0.49
6:I:38:THR:HG21	6:I:115:ASN:HD21	1.77	0.49
1:A:2081:GLU:CD	1:A:2081:GLU:H	2.16	0.49
2:B:94:ASN:OD1	2:B:123:ARG:NH2	2.31	0.49
5:E:87:GLU:O	5:E:91:THR:HG23	2.13	0.49
1:A:1038:GLU:OE1	9:A:2601:HOH:O	2.19	0.49
2:B:32:GLU:OE2	2:B:54:TYR:OH	2.26	0.49
1:A:140:THR:HB	1:A:180:MET:HE1	1.94	0.49
1:A:209:TYR:CE2	1:A:211:PRO:HG3	2.47	0.49
1:A:2249:PHE:HB3	1:A:2252:LEU:HA	1.95	0.49
6:I:686:VAL:HA	6:I:689:ASN:HB2	1.95	0.49
1:A:309:TYR:O	1:A:587:ARG:NH1	2.44	0.49
6:I:40:TYR:HA	6:I:41:ASN:HA	1.62	0.49
6:I:746:ILE:HG13	6:I:749:LYS:HD3	1.95	0.49
1:A:214:ASP:OD2	6:I:100:LYS:NZ	2.42	0.48
1:A:556:ILE:HG22	1:A:564:PHE:HZ	1.77	0.48
1:A:623:GLU:HB2	1:A:627:GLU:HG2	1.95	0.48
1:A:1187:VAL:HG23	1:A:1195:ILE:HD12	1.95	0.48
1:A:1878:ASN:O	1:A:1957:GLY:HA2	2.14	0.48
5:G:130:PHE:O	5:G:134:GLN:HG2	2.13	0.48
6:I:409:ILE:HG21	6:I:575:ILE:HD13	1.93	0.48
1:A:152:THR:HG21	3:F:131:ARG:HG3	1.95	0.48
1:A:556:ILE:HG22	1:A:564:PHE:CZ	2.48	0.48
1:A:1824:VAL:HG22	1:A:1847:THR:HG23	1.95	0.48
6:I:645:ASN:OD1	6:I:646:ASN:N	2.46	0.48
1:A:865:GLN:HG3	1:A:1289:ALA:HB2	1.95	0.48
6:I:273:TYR:O	6:I:294:TYR:OH	2.21	0.48
1:A:2179:ASN:HB3	1:A:2206:TYR:O	2.12	0.48
4:D:1077[A]:LYS:NZ	9:D:1203:HOH:O	2.46	0.48
5:C:106:LYS:NZ	5:C:107:GLN:OE1	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:102:ILE:O	6:I:106:SER:HB2	2.12	0.48
6:I:743:ALA:O	6:I:747:LEU:HG	2.13	0.48
1:A:199:PHE:CD1	1:A:200:ALA:N	2.73	0.48
1:A:1529:MET:HB3	1:A:1533:ALA:HB3	1.95	0.48
1:A:290:ARG:NH1	1:A:451:GLN:O	2.46	0.48
1:A:803:ASN:HB3	1:A:836:GLU:HG3	1.94	0.48
6:I:428:ILE:HG22	6:I:432:LYS:HE3	1.93	0.48
1:A:1495:ASP:OD1	1:A:1495:ASP:N	2.47	0.48
1:A:2401:PHE:HE1	3:F:366:ILE:HD13	1.78	0.48
1:A:421:GLU:HB3	1:A:1171:ILE:HD11	1.95	0.48
1:A:131:GLY:N	1:A:186:ARG:HG3	2.27	0.48
3:F:216:SER:OG	3:F:220:ASP:O	2.32	0.48
6:I:189:ASN:HB3	6:I:192:THR:HG23	1.95	0.48
1:A:1007:ILE:HD11	1:A:1033:LEU:HD11	1.95	0.47
1:A:1813:ILE:O	1:A:1813:ILE:HG13	2.13	0.47
1:A:1844:TYR:OH	1:A:1882:ASN:OD1	2.32	0.47
1:A:606:PRO:HA	1:A:610:VAL:HG13	1.95	0.47
1:A:2153:PRO:HB3	1:A:2169:THR:HA	1.96	0.47
1:A:1760:ARG:HD2	1:A:1793:PHE:CG	2.49	0.47
1:A:2115:TYR:OH	1:A:2141:ILE:O	2.19	0.47
3:F:95:THR:HG23	3:F:109:SER:HB2	1.96	0.47
1:A:351:GLY:HA2	1:A:382:SER:O	2.15	0.47
1:A:2206:TYR:O	1:A:2207:ARG:NH1	2.47	0.47
5:G:127:ASP:HB3	6:I:140:GLU:HG3	1.94	0.47
6:I:376:LEU:HB3	6:I:383:PHE:HD1	1.79	0.47
6:I:378:PRO:O	6:I:379:LYS:HG3	2.13	0.47
1:A:1364:HIS:HB3	1:A:1504:TRP:HB2	1.95	0.47
3:F:159:ARG:NH1	3:F:183:ASP:OD2	2.47	0.47
6:I:262:ARG:NH2	6:I:302:GLU:OE1	2.34	0.47
1:A:41:GLU:H	1:A:41:GLU:CD	2.17	0.47
3:F:53:SER:HB2	3:F:64:LYS:HB2	1.96	0.47
3:F:80:PRO:HG2	3:F:386:THR:HG23	1.96	0.47
3:F:209:GLN:O	3:F:229:ALA:HA	2.15	0.47
1:A:1179:ILE:HD13	1:A:1179:ILE:HA	1.75	0.47
1:A:371:GLY:O	1:A:387:LYS:NZ	2.48	0.47
1:A:2229:ASP:HB3	1:A:2235:TYR:CE1	2.50	0.47
3:F:329:GLU:HG3	3:F:339:ARG:HG2	1.97	0.47
1:A:235:ARG:HD2	1:A:235:ARG:HA	1.64	0.46
7:A:2501:LMN:HCR	7:A:2501:LMN:H3	1.70	0.46
5:E:116:ARG:HH11	5:E:116:ARG:HB3	1.80	0.46
6:I:95:GLU:HG3	6:I:125:LEU:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:689:ASN:O	6:I:693:LEU:HB2	2.13	0.46
6:I:741:LYS:O	6:I:745:GLU:HG2	2.15	0.46
1:A:2278:SER:O	1:A:2282:ASN:HA	2.15	0.46
1:A:578:PRO:HG2	1:A:1757:LEU:HD11	1.97	0.46
1:A:1434:LYS:NZ	1:A:1478:PRO:O	2.45	0.46
6:I:200:LEU:HB3	6:I:216:LYS:HG3	1.98	0.46
1:A:131:GLY:N	1:A:184:GLY:O	2.49	0.46
1:A:2021:ILE:HB	1:A:2029:VAL:HB	1.98	0.46
1:A:644:PRO:HA	1:A:647:TYR:CE1	2.51	0.46
1:A:1431:THR:HG23	1:A:1606:ILE:HG12	1.97	0.46
6:I:381:ARG:H	6:I:381:ARG:CZ	2.28	0.46
1:A:1680:GLU:OE2	1:A:1682:GLU:HG3	2.15	0.46
5:C:81:LEU:H	5:C:81:LEU:HG	1.56	0.46
1:A:1342:SER:HB3	1:A:1491:LYS:HG3	1.97	0.46
1:A:2382:ILE:HG23	1:A:2384:THR:H	1.81	0.46
6:I:594:PHE:HB3	6:I:596:GLU:HG2	1.98	0.46
6:I:650:SER:O	6:I:654:GLN:NE2	2.48	0.46
1:A:1120:TYR:CE2	1:A:1122:LEU:HB2	2.52	0.45
1:A:1872:LEU:O	1:A:1962:GLY:HA2	2.16	0.45
5:E:83:LYS:HD2	5:E:83:LYS:O	2.16	0.45
6:I:751:VAL:HG23	6:I:752:PRO:HD3	1.97	0.45
1:A:1559:GLU:HG3	1:A:1595:ILE:HG23	1.98	0.45
3:F:137:GLU:HG3	3:F:163:SER:HA	1.98	0.45
4:D:1092[B]:ASN:OD1	9:D:1201:HOH:O	2.21	0.45
6:I:707:GLU:HB3	6:I:730:VAL:HG22	1.98	0.45
1:A:37:LYS:HD3	5:E:151:ASP:HB3	1.98	0.45
1:A:272:ASN:ND2	1:A:737:ASN:OD1	2.32	0.45
3:F:99:LYS:HA	3:F:105:ALA:HA	1.98	0.45
5:G:52:LYS:HB2	5:G:52:LYS:HE3	1.76	0.45
6:I:99:THR:O	6:I:103:GLN:HG2	2.17	0.45
6:I:190:LYS:HG2	6:I:223:PHE:HD2	1.81	0.45
1:A:2401:PHE:CE1	3:F:366:ILE:HD13	2.52	0.45
2:B:25:LYS:HE3	2:B:25:LYS:HB2	1.65	0.45
1:A:2041:THR:HG22	1:A:2061:THR:HG23	1.98	0.45
7:A:2501:LMN:HABA	7:A:2501:LMN:HBB	1.67	0.45
2:B:101:TYR:HA	2:B:169:GLU:O	2.17	0.45
3:F:64:LYS:HB3	3:F:187:PHE:CD2	2.52	0.45
6:I:671:TYR:HB2	6:I:706:PHE:HE1	1.81	0.45
6:I:729:ASN:OD1	6:I:733:ASN:ND2	2.45	0.45
1:A:285:ASP:OD1	9:A:2604:HOH:O	2.21	0.45
1:A:1731:PHE:CD2	1:A:1768:TYR:HB3	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1767:GLN:HB3	1:A:1785:THR:HG23	1.99	0.45
1:A:2199:ARG:NH1	1:A:2258:GLU:OE2	2.47	0.45
1:A:934:THR:HA	1:A:1253:ARG:HD2	1.98	0.44
1:A:2071:MET:HB2	1:A:2159:TYR:O	2.17	0.44
6:I:630:ILE:HG22	6:I:631:THR:CG2	2.47	0.44
1:A:115:LEU:O	6:I:129:ARG:NH2	2.45	0.44
1:A:146:ASP:O	1:A:171:PHE:HA	2.17	0.44
1:A:145:MET:SD	1:A:147:LEU:HD11	2.58	0.44
1:A:933:ASN:OD1	1:A:936:ARG:NE	2.33	0.44
7:A:2501:LMN:H2	7:A:2501:LMN:HBR	1.99	0.44
1:A:347:LEU:HB2	1:A:350:LEU:HB2	1.99	0.44
1:A:537:LYS:HE2	1:A:537:LYS:HB3	1.67	0.44
1:A:1949:GLN:N	1:A:2018:THR:O	2.49	0.44
3:F:100:ILE:HG13	3:F:101:ASN:H	1.82	0.44
1:A:836:GLU:HB3	1:A:1522:ILE:HG22	1.98	0.44
1:A:1993:LYS:HD3	1:A:1993:LYS:HA	1.82	0.44
5:E:101:LEU:HD12	5:E:101:LEU:HA	1.82	0.44
6:I:745:GLU:O	6:I:748:GLU:HG3	2.16	0.44
5:G:162:ASP:OD1	5:G:164:SER:OG	2.25	0.44
6:I:273:TYR:CG	6:I:297:LEU:HD11	2.53	0.44
1:A:959:THR:OG1	1:A:961:ASP:OD1	2.34	0.44
1:A:1030:TYR:O	1:A:1241:MET:HA	2.17	0.44
1:A:1346:PHE:HB2	1:A:1389:PHE:CZ	2.53	0.44
1:A:2188:MET:HE3	1:A:2197:PHE:HB3	1.99	0.44
5:C:55:LYS:HE3	5:C:55:LYS:HB3	1.90	0.44
1:A:33:PHE:HE2	5:C:138:GLU:HG2	1.82	0.44
1:A:1742:GLN:NE2	9:A:2613:HOH:O	2.34	0.44
1:A:2053:GLU:OE2	1:A:2055:LYS:HE2	2.18	0.44
6:I:624:LEU:HD23	6:I:624:LEU:HA	1.87	0.44
1:A:889:ASP:OD1	1:A:891:THR:OG1	2.35	0.44
5:C:30:ILE:HG13	5:C:35:ILE:HD12	1.99	0.44
1:A:647:TYR:HB2	1:A:652:GLN:HG3	2.00	0.43
1:A:720:ASP:OD2	1:A:723:LEU:HB2	2.18	0.43
1:A:2142:GLY:HA3	1:A:2234:PHE:CE2	2.53	0.43
3:F:125:ASP:O	3:F:127:ASN:N	2.51	0.43
1:A:1161:ASP:OD1	9:A:2601:HOH:O	2.21	0.43
1:A:1853:GLN:O	1:A:1874:ASN:HB3	2.18	0.43
6:I:603:LYS:HA	6:I:603:LYS:HD2	1.68	0.43
5:G:189:GLU:O	5:G:193:ASN:HB2	2.18	0.43
6:I:675:TYR:HD1	6:I:675:TYR:O	2.02	0.43
1:A:1338:GLN:HB2	1:A:1341:ASP:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1577:PRO:HG2	1:A:1580:TRP:HE1	1.83	0.43
6:I:421:LYS:HE2	6:I:559:ALA:HB1	1.99	0.43
2:B:127:PRO:O	2:B:131:GLU:HG2	2.17	0.43
5:G:176:LYS:HA	5:G:176:LYS:HD2	1.86	0.43
6:I:609:ARG:HG3	6:I:609:ARG:HH11	1.84	0.43
1:A:2291:GLU:HG3	1:A:2330:ARG:HG2	2.00	0.43
6:I:308:ASP:OD1	6:I:308:ASP:N	2.51	0.43
6:I:654:GLN:H	6:I:654:GLN:HG2	1.60	0.43
1:A:622:LYS:NZ	1:A:627:GLU:OE2	2.50	0.43
5:G:82:THR:OG1	5:G:83:LYS:N	2.51	0.43
6:I:177:LYS:HB3	6:I:177:LYS:HE3	1.75	0.43
1:A:679:ARG:HH22	1:A:1675:GLU:CD	2.21	0.43
1:A:2142:GLY:HA3	1:A:2234:PHE:CD2	2.54	0.43
1:A:2203:GLN:HB3	1:A:2254:ARG:HB3	2.01	0.43
1:A:51:LYS:HE3	1:A:51:LYS:HB3	1.87	0.43
1:A:81:TYR:HE2	5:G:115:MET:HG3	1.82	0.43
1:A:582:VAL:O	1:A:632:LYS:NZ	2.39	0.43
1:A:2370:ILE:HB	1:A:2396:THR:CG2	2.48	0.43
6:I:57:ILE:O	6:I:60:ASN:HB2	2.19	0.43
1:A:78:PRO:O	1:A:79:LYS:HB3	2.18	0.43
1:A:1595:ILE:HB	1:A:1630:ASP:HB3	2.01	0.43
1:A:155:ASP:HB2	1:A:2387:PRO:HD2	2.01	0.42
6:I:748:GLU:HA	6:I:751:VAL:HG22	2.01	0.42
1:A:840:LEU:O	1:A:1517:GLY:CA	2.68	0.42
1:A:1339:TYR:CD1	1:A:1495:ASP:HA	2.54	0.42
1:A:1382:PHE:HA	1:A:1396:VAL:O	2.19	0.42
1:A:2090:PHE:CZ	1:A:2155:PHE:HB2	2.54	0.42
5:G:82:THR:OG1	5:G:84:GLU:OE1	2.37	0.42
6:I:25:ASN:OD1	6:I:25:ASN:N	2.47	0.42
6:I:664:ILE:CG1	6:I:669:LYS:HB2	2.49	0.42
5:C:30:ILE:HD12	5:C:30:ILE:HA	1.82	0.42
5:C:94:LYS:HE2	5:C:94:LYS:HB2	1.78	0.42
3:F:57:SER:O	3:F:57:SER:OG	2.30	0.42
5:C:29:TYR:CZ	5:C:162:ASP:HB2	2.55	0.42
5:E:65:LEU:HD23	5:E:65:LEU:HA	1.91	0.42
6:I:25:ASN:OD1	6:I:30:ASN:ND2	2.52	0.42
6:I:300:ASP:O	6:I:307:TYR:OH	2.30	0.42
6:I:618:LEU:HD23	6:I:652:TYR:CD2	2.54	0.42
5:G:39:VAL:HG12	5:G:42:TYR:H	1.84	0.42
5:E:85:LEU:O	5:E:88:GLU:HG3	2.20	0.42
5:E:94:LYS:HE2	5:E:94:LYS:HB2	1.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:ASN:HB2	3:F:31:PRO:HB2	2.01	0.42
2:B:139:GLY:N	2:B:172:LEU:O	2.41	0.42
1:A:146:ASP:OD2	1:A:174:ARG:NH2	2.52	0.42
1:A:1062:GLN:HA	1:A:1063:PRO:HD3	1.81	0.42
1:A:1965:PRO:CD	1:A:1996:TRP:HB2	2.47	0.42
3:F:44:LEU:HD21	3:F:329:GLU:HB2	2.02	0.42
1:A:556:ILE:HG23	1:A:654:TYR:CZ	2.55	0.42
1:A:1419:ASP:O	1:A:1469:LYS:NZ	2.45	0.42
1:A:2016:LYS:HA	1:A:2016:LYS:HD2	1.60	0.42
5:E:71:LYS:HB2	5:E:71:LYS:HE2	1.80	0.42
1:A:101:ILE:HG12	1:A:115:LEU:HD21	2.02	0.42
1:A:1617:ASP:HB3	1:A:1620:GLU:HB2	2.02	0.42
5:G:195:GLU:OE2	6:I:31:ARG:NH2	2.52	0.42
1:A:1389:PHE:CE1	1:A:1487:MET:HB2	2.54	0.41
1:A:1474:ILE:HD11	1:A:1478:PRO:HD2	2.02	0.41
2:B:142:ILE:HG22	2:B:170:ILE:HB	2.01	0.41
5:G:151:ASP:OD1	5:G:153:THR:OG1	2.32	0.41
5:E:81:LEU:HD13	6:I:675:TYR:CE2	2.55	0.41
1:A:1886:THR:HG22	1:A:1888:LEU:HB2	2.03	0.41
6:I:184:LYS:HD3	6:I:184:LYS:HA	1.88	0.41
1:A:1364:HIS:O	1:A:1503:VAL:HA	2.21	0.41
1:A:1434:LYS:HE2	1:A:1603:ASN:HB3	2.02	0.41
1:A:1524:ASN:ND2	9:A:2632:HOH:O	2.44	0.41
1:A:344:ILE:HD13	1:A:431:ALA:HB3	2.02	0.41
1:A:1049:GLU:HB2	1:A:1088:GLN:O	2.21	0.41
1:A:1391:GLN:O	1:A:1476:GLY:HA3	2.20	0.41
1:A:1673:ASP:OD1	1:A:1676:VAL:HG12	2.21	0.41
6:I:669:LYS:O	6:I:670:GLU:HG2	2.21	0.41
1:A:611:ASP:OD2	1:A:614:ASN:HB2	2.20	0.41
3:F:63:ALA:HA	3:F:155:ALA:HB2	2.02	0.41
3:F:199:ASN:OD1	3:F:199:ASN:N	2.52	0.41
5:G:121:LEU:HD23	5:G:121:LEU:HA	1.92	0.41
5:C:123:LYS:HA	5:C:123:LYS:HD2	1.80	0.41
6:I:663:ASP:N	6:I:663:ASP:OD1	2.54	0.41
1:A:965:TYR:CZ	1:A:1133:LYS:HE3	2.56	0.41
1:A:1191:TYR:HE1	1:A:1224:GLN:HE21	1.68	0.41
6:I:50:LEU:HD12	6:I:50:LEU:HA	1.90	0.41
6:I:725:LYS:O	6:I:728:GLU:HG3	2.20	0.41
1:A:1880:ASN:HB2	1:A:1956:SER:HB2	2.02	0.41
1:A:1015:TYR:CD2	1:A:1183:PRO:HA	2.55	0.41
1:A:1570:LEU:HD12	1:A:1586:PHE:HD2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:82:LEU:HD11	4:D:1067:ILE:O	2.21	0.41
4:D:1083[B]:PHE:CE2	4:D:1085[B]:VAL:HG22	2.56	0.41
6:I:216:LYS:HD3	6:I:216:LYS:HA	1.73	0.41
6:I:630:ILE:HG22	6:I:631:THR:HG23	2.02	0.41
6:I:693:LEU:HB3	6:I:706:PHE:HE2	1.85	0.41
1:A:50:TYR:HE1	1:A:76:LEU:HD11	1.85	0.41
1:A:884:ILE:HA	1:A:884:ILE:HD12	1.80	0.41
1:A:1046:LYS:HD2	1:A:1161:ASP:HB2	2.03	0.41
2:B:143:GLN:HA	2:B:168:PHE:O	2.21	0.41
3:F:208:ILE:HG22	3:F:211:LEU:HD21	2.02	0.41
4:D:1103:ASN:OD1	4:D:1103:ASN:N	2.50	0.41
6:I:626:LYS:HD2	6:I:626:LYS:HA	1.82	0.41
1:A:1548:SER:HB2	1:A:1551:GLN:HG3	2.03	0.41
1:A:1549:LEU:HD23	1:A:1549:LEU:HA	1.85	0.41
5:E:33:GLU:HG2	5:E:149:SER:HB2	2.03	0.41
1:A:1337:LEU:HD23	1:A:1337:LEU:HA	1.90	0.40
5:G:44:GLU:O	5:G:48:GLN:HG2	2.21	0.40
6:I:653:ALA:O	6:I:657:ASN:ND2	2.54	0.40
6:I:725:LYS:HD2	6:I:725:LYS:C	2.41	0.40
1:A:273:GLY:O	1:A:690:ILE:HG12	2.22	0.40
1:A:871:ARG:HD3	9:A:2602:HOH:O	2.20	0.40
4:D:1064:ILE:HD12	4:D:1073:TYR:CD1	2.56	0.40
6:I:615:LYS:HB3	6:I:615:LYS:HE3	1.73	0.40
1:A:1389:PHE:CE1	1:A:1485:ASN:HB3	2.55	0.40
1:A:1876:ILE:HG13	1:A:1960:LEU:HB3	2.03	0.40
1:A:2191:LYS:HE3	1:A:2192:TYR:HE1	1.87	0.40
1:A:2265:VAL:HG22	1:A:2296:LEU:HD23	2.04	0.40
2:B:97:ILE:O	2:B:119:SER:HA	2.21	0.40
3:F:80:PRO:HB2	3:F:83:THR:HG23	2.02	0.40
2:B:127:PRO:HA	2:B:130:LYS:HB2	2.04	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	2282/2403 (95%)	2178 (95%)	104 (5%)	0	100	100
2	B	124/176 (70%)	116 (94%)	8 (6%)	0	100	100
3	F	363/402 (90%)	348 (96%)	15 (4%)	0	100	100
4	D	91/1114 (8%)	85 (93%)	6 (7%)	0	100	100
5	C	168/341 (49%)	164 (98%)	4 (2%)	0	100	100
5	E	150/341 (44%)	139 (93%)	11 (7%)	0	100	100
5	G	171/341 (50%)	169 (99%)	2 (1%)	0	100	100
6	I	618/870 (71%)	587 (95%)	31 (5%)	0	100	100
All	All	3967/5988 (66%)	3786 (95%)	181 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	2016/2114 (95%)	1916 (95%)	100 (5%)	24	30
2	B	109/151 (72%)	101 (93%)	8 (7%)	14	15
3	F	296/325 (91%)	277 (94%)	19 (6%)	17	20
4	D	89/853 (10%)	80 (90%)	9 (10%)	7	7
5	C	152/296 (51%)	138 (91%)	14 (9%)	9	9
5	E	137/296 (46%)	131 (96%)	6 (4%)	28	35
5	G	157/296 (53%)	145 (92%)	12 (8%)	13	14
6	I	553/766 (72%)	498 (90%)	55 (10%)	8	7
All	All	3509/5097 (69%)	3286 (94%)	223 (6%)	21	20

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	39	GLU
1	A	41	GLU
1	A	66	ASP
1	A	69	SER
1	A	72	TYR
1	A	75	VAL
1	A	76	LEU
1	A	79	LYS
1	A	88	GLU
1	A	95	ARG
1	A	121	ILE
1	A	124	SER
1	A	133	ASN
1	A	146	ASP
1	A	150	ARG
1	A	176	SER
1	A	194	ASP
1	A	199	PHE
1	A	227	MET
1	A	239	SER
1	A	277	GLN
1	A	299	ARG
1	A	365	VAL
1	A	374	ASN
1	A	401	ASN
1	A	407	ILE
1	A	416	ASN
1	A	417	THR
1	A	432	ARG
1	A	486	THR
1	A	495	ASN
1	A	506	LYS
1	A	537	LYS
1	A	556	ILE
1	A	656	PHE
1	A	743	SER
1	A	744	LEU
1	A	793	GLU
1	A	871	ARG
1	A	931	SER
1	A	996	SER
1	A	1086	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1122	LEU
1	A	1125	ASP
1	A	1148	ASP
1	A	1162	ILE
1	A	1167	THR
1	A	1178	SER
1	A	1179	ILE
1	A	1189	GLU
1	A	1280	ASP
1	A	1290	VAL
1	A	1495	ASP
1	A	1497	LYS
1	A	1526	ASP
1	A	1528	ASN
1	A	1540	ARG
1	A	1645	ASP
1	A	1665	SER
1	A	1722	PHE
1	A	1730	SER
1	A	1736	LEU
1	A	1739	SER
1	A	1745	ARG
1	A	1778	LEU
1	A	1783	SER
1	A	1827	TYR
1	A	1856	SER
1	A	1879	SER
1	A	1881	SER
1	A	1890	MET
1	A	1943	THR
1	A	1945	ILE
1	A	1947	ASN
1	A	1949	GLN
1	A	1956	SER
1	A	2011	SER
1	A	2016	LYS
1	A	2036	SER
1	A	2039	GLU
1	A	2066	SER
1	A	2092	SER
1	A	2136	ASN
1	A	2185	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2191	LYS
1	A	2198	LYS
1	A	2207	ARG
1	A	2240	MET
1	A	2272	ASP
1	A	2273	ARG
1	A	2319	SER
1	A	2326	ASP
1	A	2328	SER
1	A	2350	GLN
1	A	2360	ASP
1	A	2376	SER
1	A	2379	LYS
1	A	2396	THR
1	A	2400	ASN
2	B	42	ASN
2	B	106	THR
2	B	115	THR
2	B	116	GLU
2	B	138	SER
2	B	141	GLU
2	B	143	GLN
2	B	155	ASN
3	F	58	GLN
3	F	64	LYS
3	F	83	THR
3	F	88	ASP
3	F	101	ASN
3	F	128	GLU
3	F	149	SER
3	F	162	ARG
3	F	173	ASP
3	F	179	SER
3	F	216	SER
3	F	220	ASP
3	F	241	PHE
3	F	250	SER
3	F	254	THR
3	F	302	SER
3	F	349	LYS
3	F	390	SER
3	F	392	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	1066	ASP
4	D	1076[A]	LYS
4	D	1076[B]	LYS
4	D	1077[A]	LYS
4	D	1077[B]	LYS
4	D	1079[A]	GLU
4	D	1079[B]	GLU
4	D	1087[A]	ASN
4	D	1087[B]	ASN
5	G	55	LYS
5	G	69	SER
5	G	82	THR
5	G	96	GLN
5	G	114	LEU
5	G	140	LYS
5	G	141	ASN
5	G	150	SER
5	G	151	ASP
5	G	174	THR
5	G	181	ASN
5	G	183	LYS
5	C	43	LYS
5	C	55	LYS
5	C	59	GLU
5	C	60	ILE
5	C	67	ILE
5	C	69	SER
5	C	80	LEU
5	C	81	LEU
5	C	84	GLU
5	C	85	LEU
5	C	88	GLU
5	C	115	MET
5	C	148	LYS
5	C	173	ARG
5	E	47	SER
5	E	69	SER
5	E	83	LYS
5	E	125	ILE
5	E	126	GLN
5	E	169	ARG
6	I	29	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	I	30	ASN
6	I	33	SER
6	I	54	LEU
6	I	58	LYS
6	I	67	LYS
6	I	127	LYS
6	I	184	LYS
6	I	185	LYS
6	I	188	LEU
6	I	190	LYS
6	I	192	THR
6	I	194	SER
6	I	202	GLU
6	I	225	ARG
6	I	244	VAL
6	I	266	ARG
6	I	269	MET
6	I	292	LYS
6	I	298	VAL
6	I	321	LYS
6	I	337	ARG
6	I	338	LYS
6	I	339	SER
6	I	340	LYS
6	I	371	SER
6	I	372	THR
6	I	376	LEU
6	I	379	LYS
6	I	381	ARG
6	I	408	SER
6	I	426	SER
6	I	438	LYS
6	I	564	GLN
6	I	568	THR
6	I	602	ASP
6	I	603	LYS
6	I	613	GLU
6	I	631	THR
6	I	638	LYS
6	I	639	ILE
6	I	641	SER
6	I	647	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	I	650	SER
6	I	651	ARG
6	I	673	LYS
6	I	674	TRP
6	I	675	TYR
6	I	676	LYS
6	I	680	GLU
6	I	691	ASP
6	I	697	TYR
6	I	698	SER
6	I	725	LYS
6	I	758	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	343	ASN
1	A	1293	GLN
1	A	2332	ASN
4	D	1053	ASN
5	G	48	GLN
5	E	113	ASN
6	I	30	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	I	903	6	11,11,12	0.62	0	15,15,17	1.12	2 (13%)
8	MAN	I	906	6	11,11,12	0.69	0	15,15,17	1.07	2 (13%)
7	LMN	A	2501	-	72,72,72	1.51	8 (11%)	96,98,98	1.10	6 (6%)
8	MAN	I	905	-	11,11,12	0.65	0	15,15,17	1.05	2 (13%)
8	MAN	I	904	6	11,11,12	0.62	0	15,15,17	1.12	2 (13%)
8	MAN	I	901	6	11,11,12	0.66	0	15,15,17	1.13	2 (13%)
8	MAN	I	902	6	11,11,12	0.68	0	15,15,17	1.09	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	I	903	6	-	2/2/19/22	0/1/1/1
8	MAN	I	906	6	-	1/2/19/22	0/1/1/1
7	LMN	A	2501	-	-	32/50/130/130	0/4/4/4
8	MAN	I	905	-	-	0/2/19/22	0/1/1/1
8	MAN	I	904	6	-	1/2/19/22	0/1/1/1
8	MAN	I	901	6	-	2/2/19/22	0/1/1/1
8	MAN	I	902	6	-	2/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2501	LMN	O5-C1	5.46	1.55	1.41
7	A	2501	LMN	O1-C1	-5.40	1.30	1.40
7	A	2501	LMN	CBQ-CCM	3.06	1.59	1.54
7	A	2501	LMN	OBZ-CCS	2.62	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2501	LMN	CBT-CCM	2.44	1.59	1.53
7	A	2501	LMN	OBY-CCR	2.39	1.47	1.41
7	A	2501	LMN	OBX-CCJ	2.24	1.47	1.41
7	A	2501	LMN	CBS-CCM	2.14	1.58	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2501	LMN	CCS-OCB-CCQ	-3.60	109.06	117.96
7	A	2501	LMN	CCR-O4-C4	-3.26	109.89	117.96
8	I	903	MAN	C1-O5-C5	2.94	116.18	112.19
8	I	901	MAN	C1-O5-C5	2.74	115.90	112.19
8	I	904	MAN	C1-O5-C5	2.58	115.69	112.19
7	A	2501	LMN	CCJ-CCL-CCH	2.53	115.27	110.00
7	A	2501	LMN	CCL-CCH-CCQ	2.53	115.45	109.68
8	I	906	MAN	C1-O5-C5	2.52	115.60	112.19
8	I	903	MAN	O2-C2-C3	-2.37	105.39	110.14
8	I	904	MAN	O2-C2-C3	-2.33	105.48	110.14
7	A	2501	LMN	CBL-CBR-CCM	-2.33	109.68	117.16
8	I	902	MAN	C1-O5-C5	2.31	115.32	112.19
8	I	905	MAN	O2-C2-C3	-2.31	105.52	110.14
8	I	906	MAN	O2-C2-C3	-2.26	105.60	110.14
8	I	905	MAN	C1-O5-C5	2.21	115.18	112.19
8	I	901	MAN	O2-C2-C3	-2.18	105.77	110.14
8	I	902	MAN	O2-C2-C3	-2.14	105.86	110.14
7	A	2501	LMN	CBK-CBQ-CCM	-2.08	110.47	117.16

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2501	LMN	C2-C1-O1-CBS
7	A	2501	LMN	O5-C1-O1-CBS
7	A	2501	LMN	CBK-CBQ-CCM-CBR
7	A	2501	LMN	CBK-CBQ-CCM-CBS
7	A	2501	LMN	CBK-CBQ-CCM-CBT
7	A	2501	LMN	CBL-CBR-CCM-CBQ
7	A	2501	LMN	CBL-CBR-CCM-CBS
7	A	2501	LMN	O1-CBS-CCM-CBQ
7	A	2501	LMN	O1-CBS-CCM-CBR
7	A	2501	LMN	OBV-CBT-CCM-CBQ
7	A	2501	LMN	OBV-CBT-CCM-CBR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	2501	LMN	OBX-CCJ-OBV-CBT
7	A	2501	LMN	CCL-CCJ-OBV-CBT
7	A	2501	LMN	OBV-CBT-CCM-CBS
7	A	2501	LMN	O1-CBS-CCM-CBT
8	I	902	MAN	O5-C5-C6-O6
7	A	2501	LMN	C4-C5-C6-O6
7	A	2501	LMN	OBZ-CCS-OCB-CCQ
8	I	902	MAN	C4-C5-C6-O6
8	I	903	MAN	O5-C5-C6-O6
7	A	2501	LMN	OAJ-CBN-CCD-OBZ
7	A	2501	LMN	O5-C5-C6-O6
7	A	2501	LMN	OAJ-CBN-CCD-CCO
8	I	904	MAN	O5-C5-C6-O6
7	A	2501	LMN	CAX-CAZ-CBB-CBD
7	A	2501	LMN	C5-C4-O4-CCR
7	A	2501	LMN	CBC-CBE-CBG-CBI
7	A	2501	LMN	C3-C4-O4-CCR
8	I	903	MAN	C4-C5-C6-O6
7	A	2501	LMN	CBG-CBI-CBK-CBQ
7	A	2501	LMN	CBL-CBR-CCM-CBT
7	A	2501	LMN	CBE-CBG-CBI-CBK
7	A	2501	LMN	CAB-CAX-CAZ-CBB
7	A	2501	LMN	CAZ-CBB-CBD-CBF
7	A	2501	LMN	OAI-CBM-CCC-CCN
7	A	2501	LMN	CBD-CBF-CBH-CBJ
8	I	901	MAN	C4-C5-C6-O6
8	I	901	MAN	O5-C5-C6-O6
7	A	2501	LMN	CBF-CBH-CBJ-CBL
8	I	906	MAN	O5-C5-C6-O6

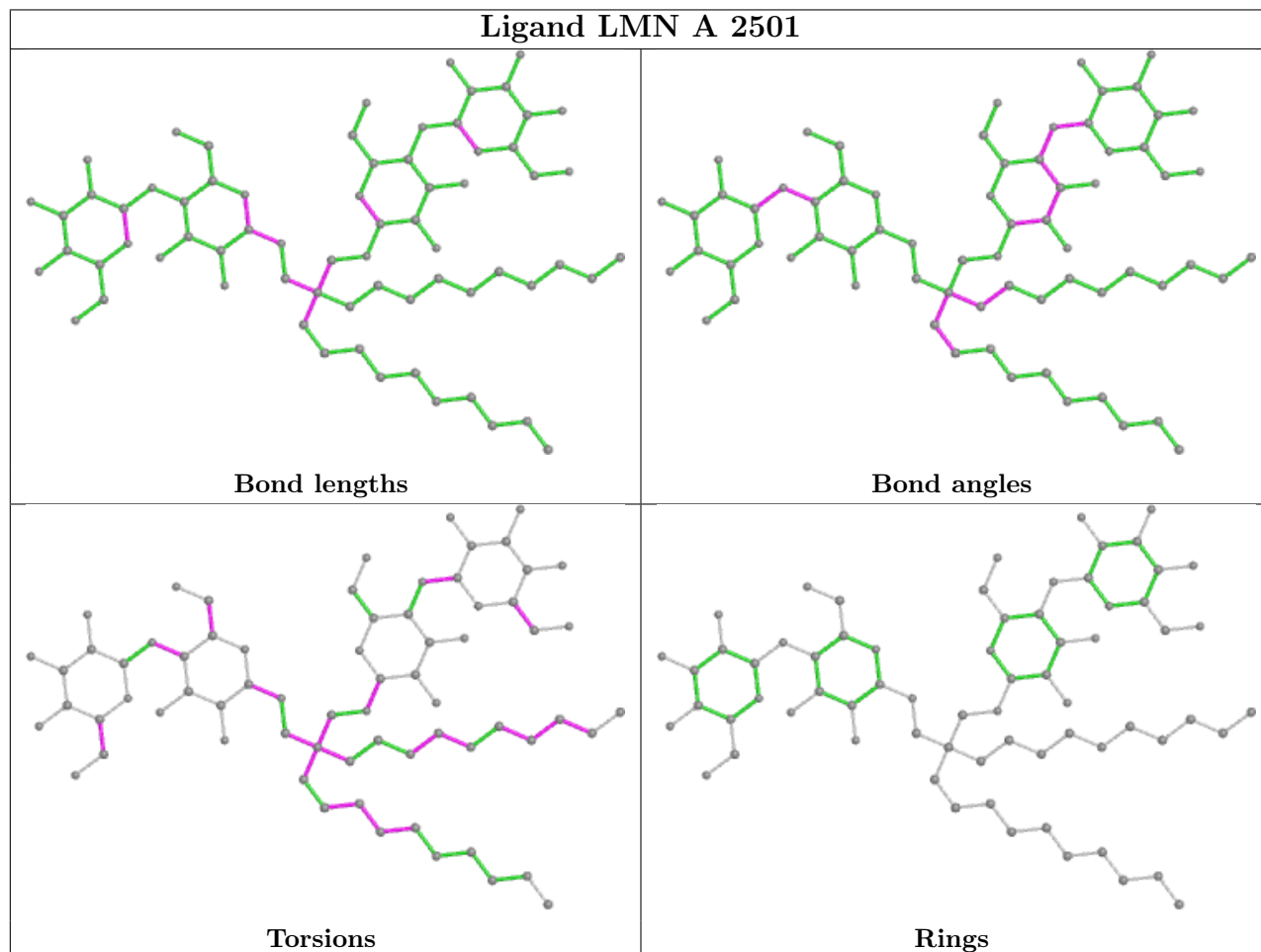
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2501	LMN	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

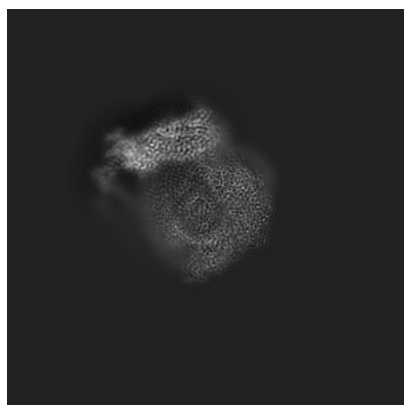
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40194. These allow visual inspection of the internal detail of the map and identification of artifacts.

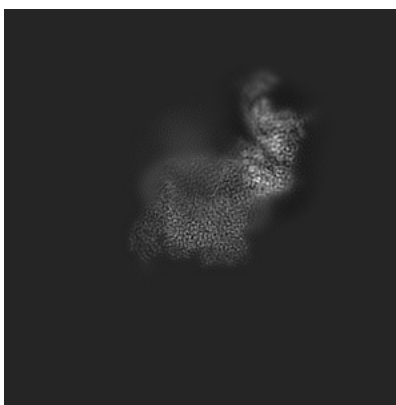
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

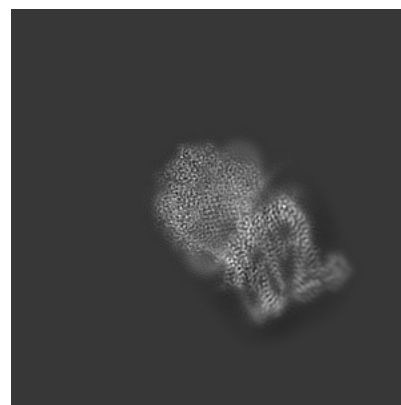
6.1.1 Primary map



X



Y

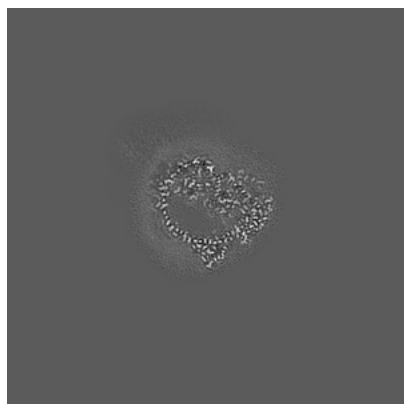


Z

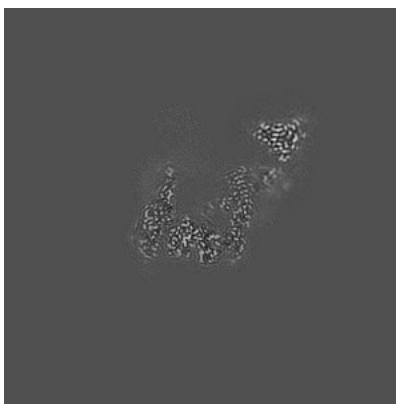
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

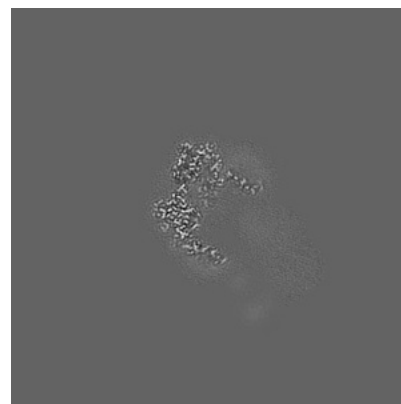
6.2.1 Primary map



X Index: 224



Y Index: 224

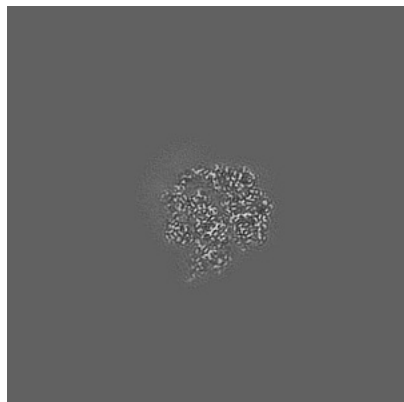


Z Index: 224

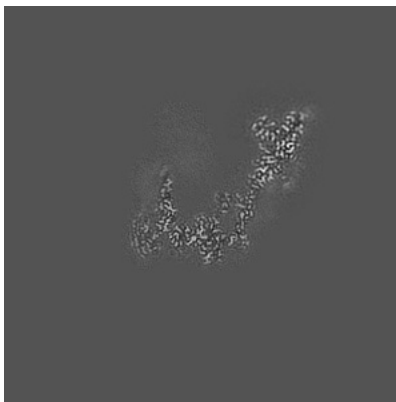
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

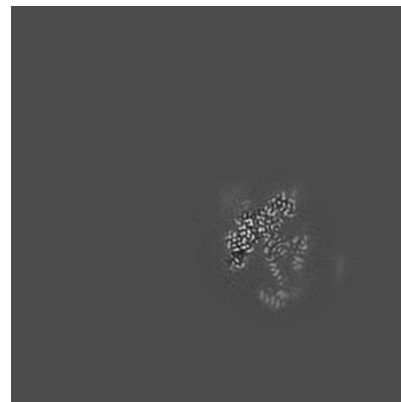
6.3.1 Primary map



X Index: 196



Y Index: 215

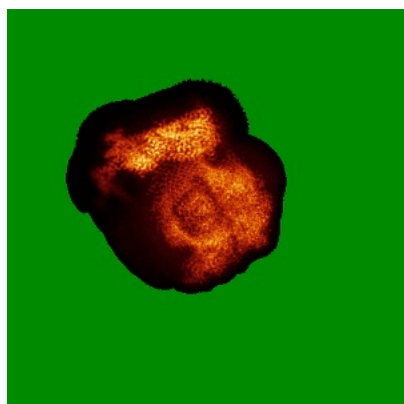


Z Index: 306

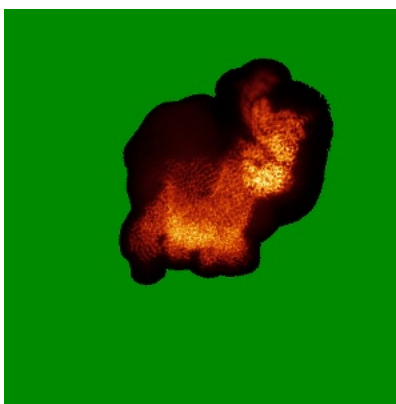
The images above show the largest variance slices of the map in three orthogonal directions.

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

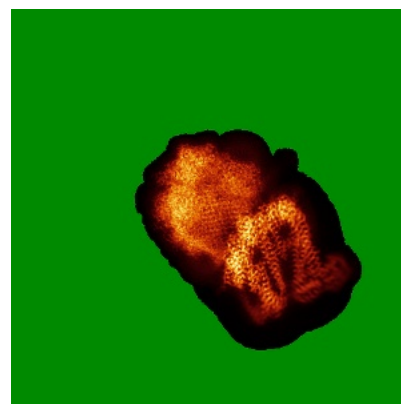
6.4.1 Primary map



X



Y

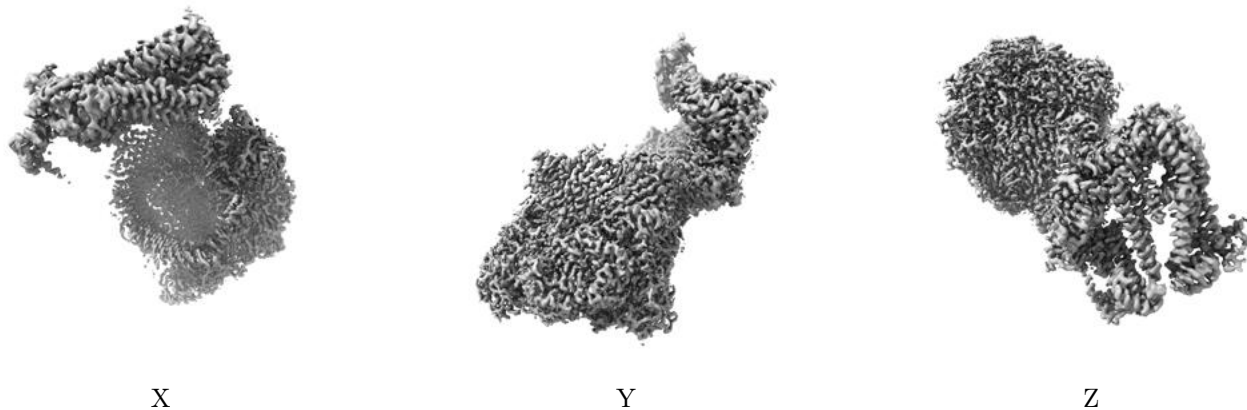


Z

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

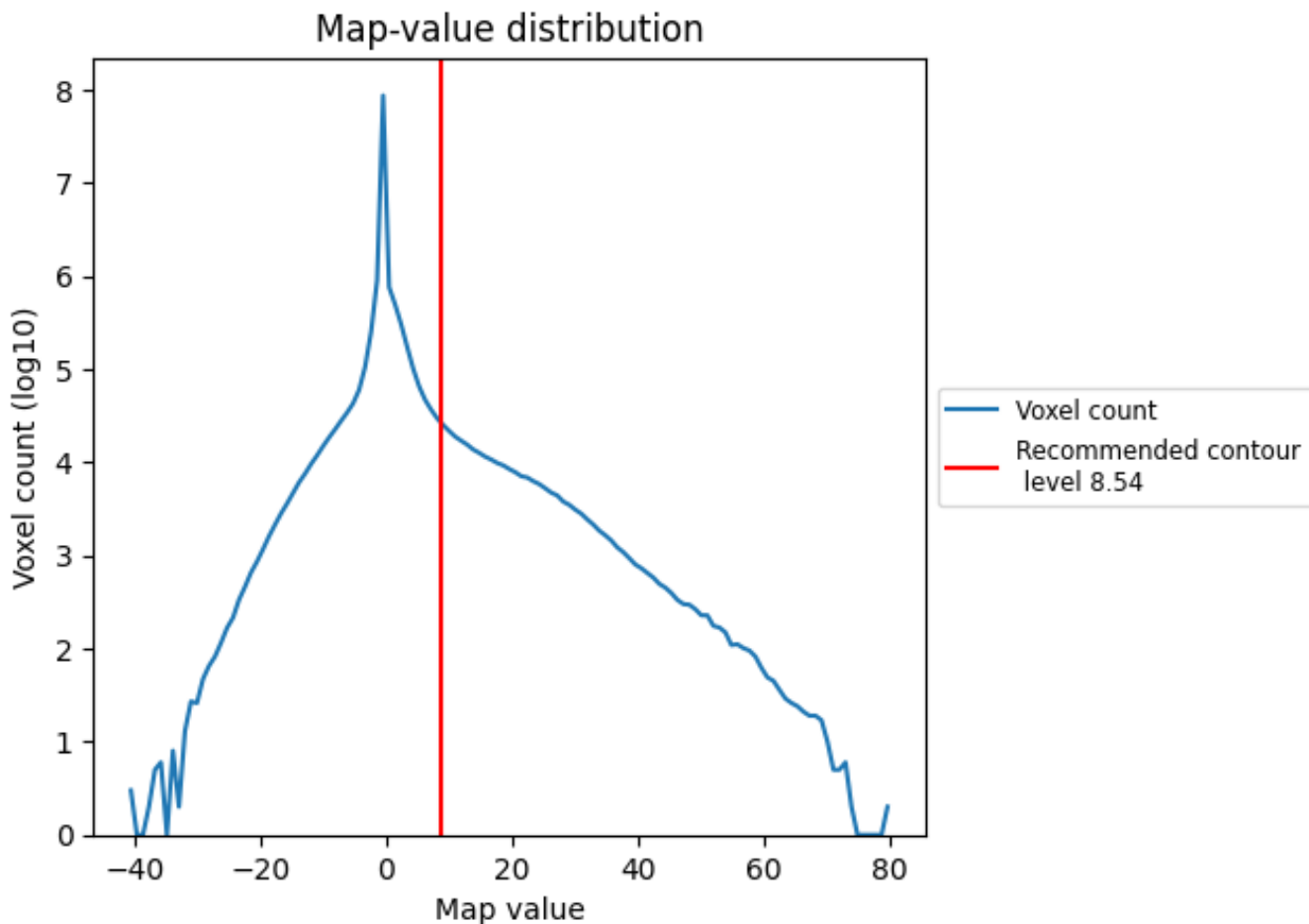
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

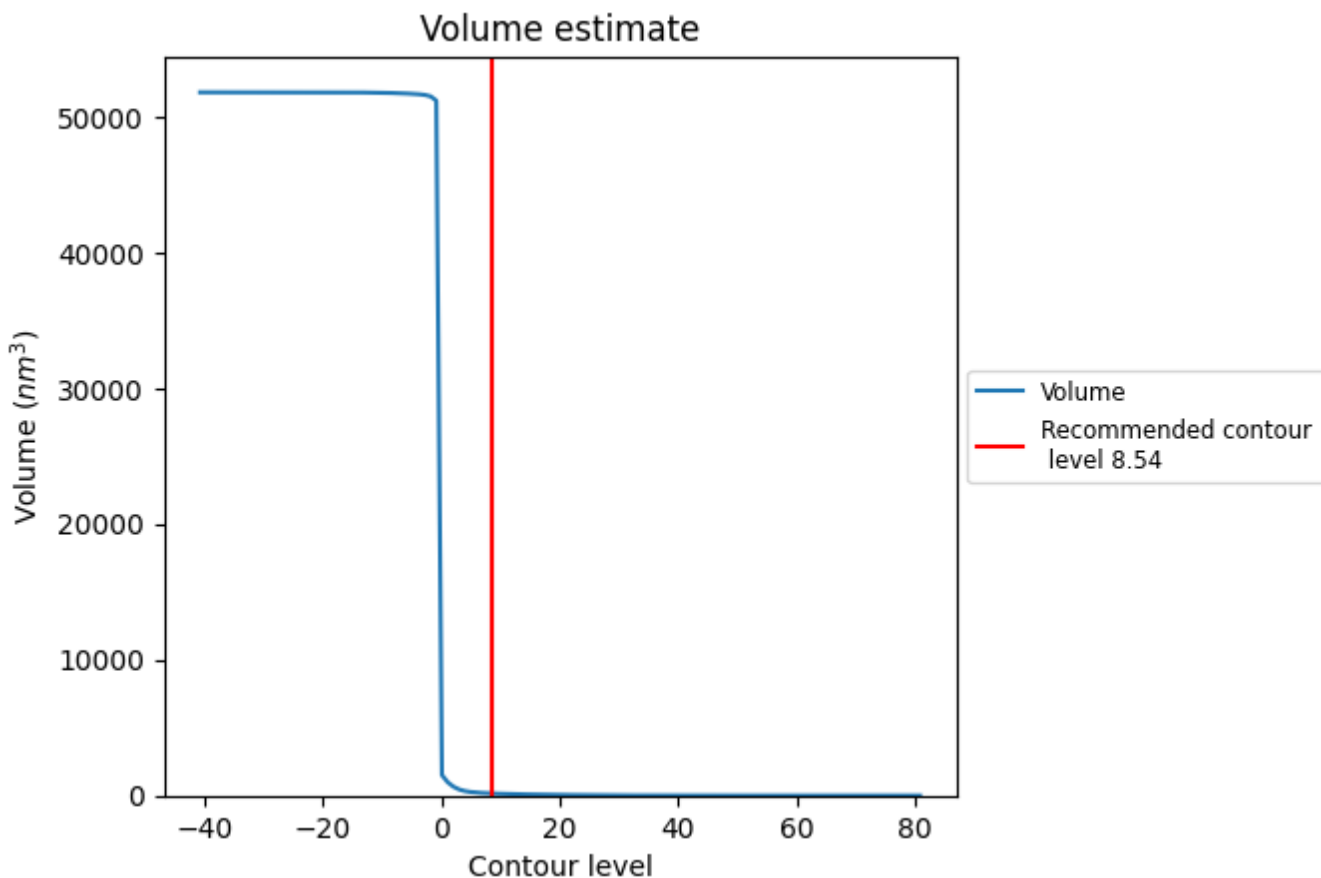
This section contains the results of statistical analysis of the map.

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.

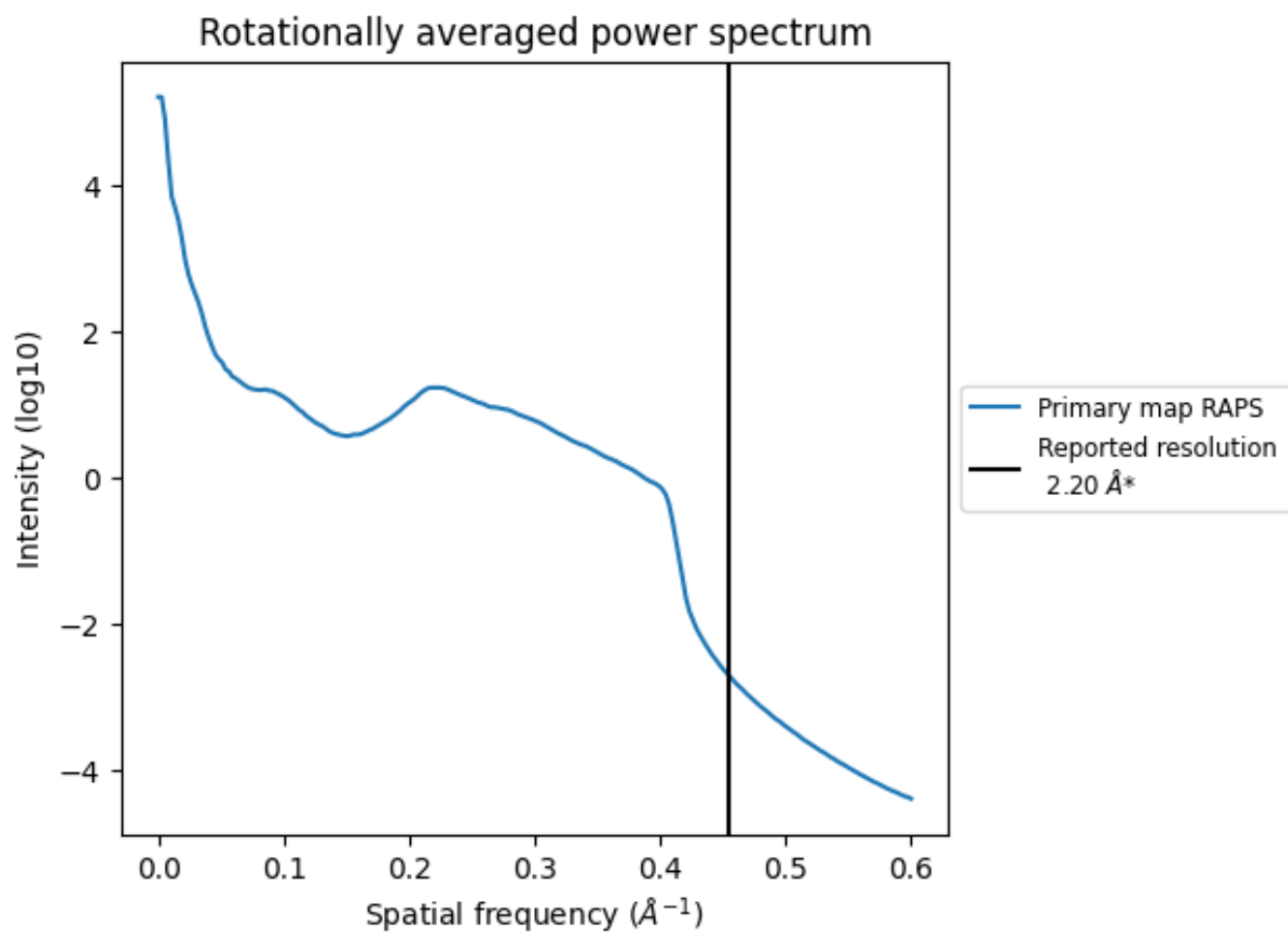
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 156 nm³; this corresponds to an approximate mass of 141 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

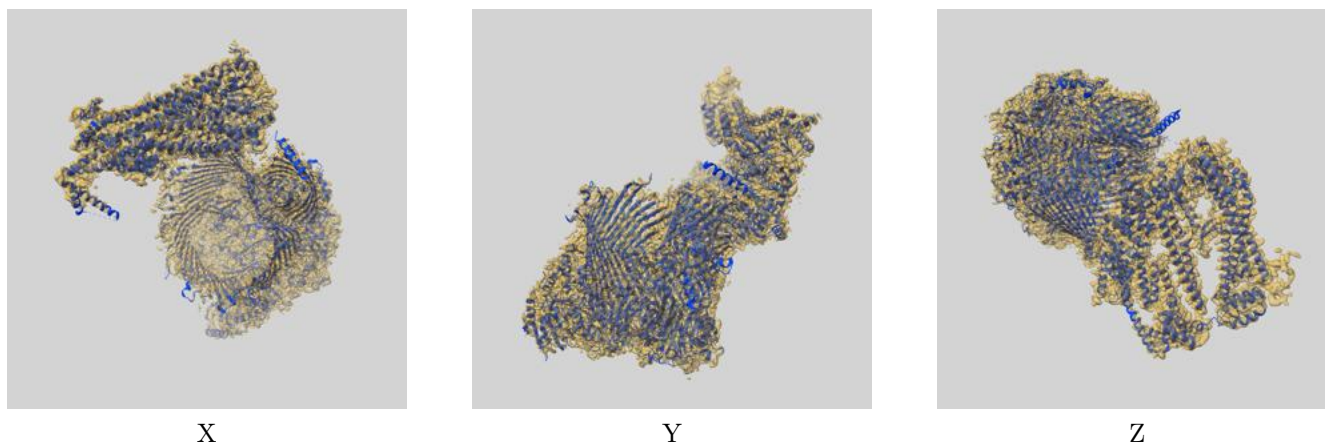
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

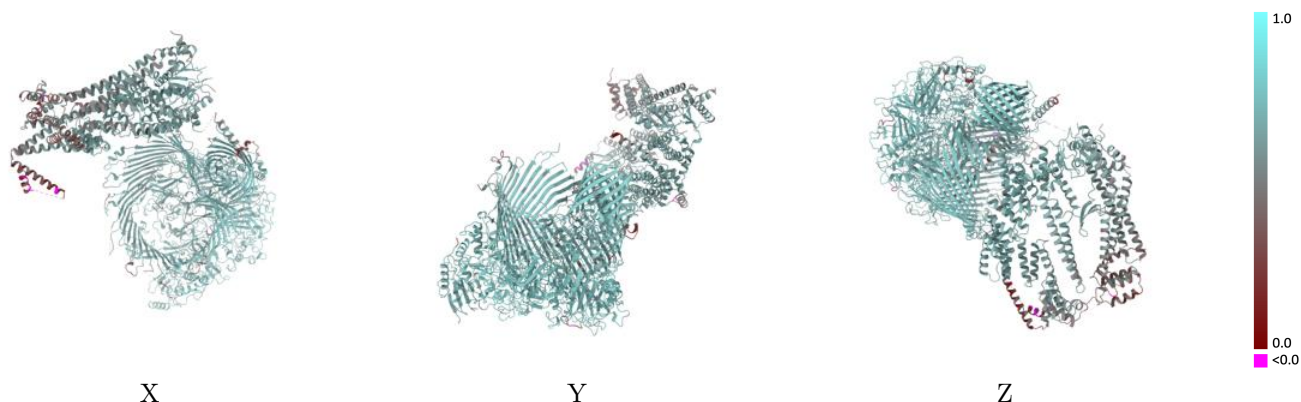
This section contains information regarding the fit between EMDB map EMD-40194 and PDB model 8GL8. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



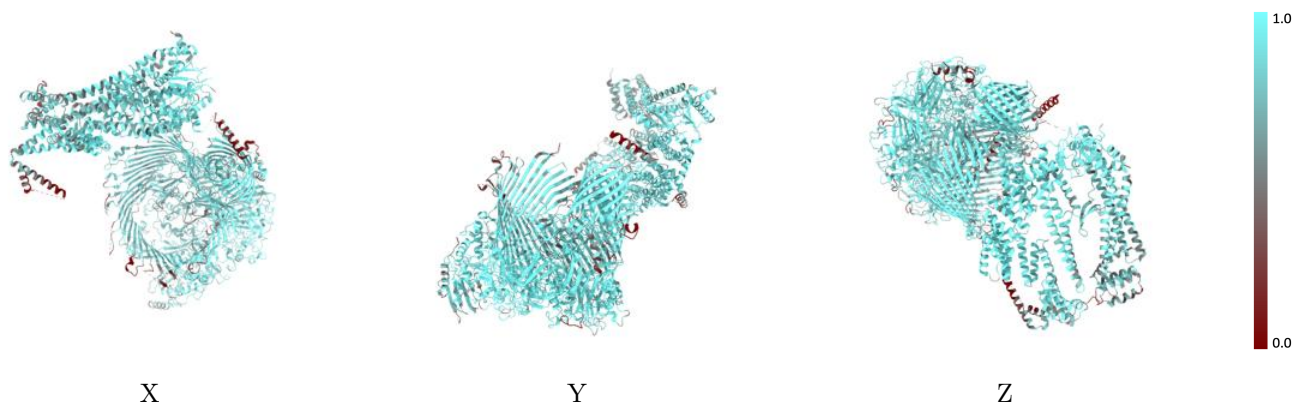
The images above show the 3D surface view of the map at the recommended contour level 8.54 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



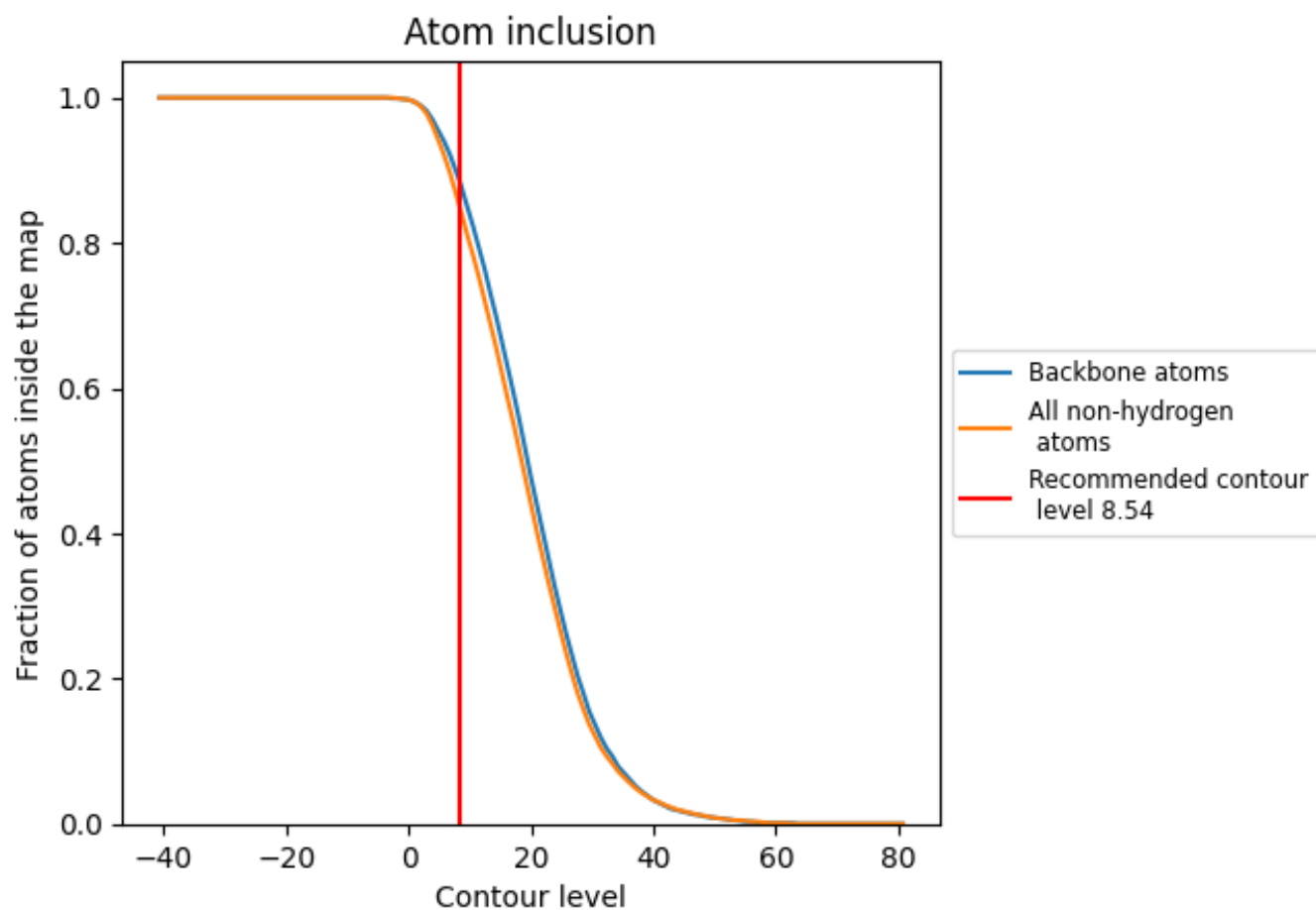
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8.54).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (8.54) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8450	 0.6350
A	 0.8760	 0.6750
B	 0.7490	 0.6420
C	 0.7490	 0.5490
D	 0.6940	 0.6400
E	 0.8230	 0.5450
F	 0.8260	 0.6590
G	 0.8460	 0.5940
I	 0.8240	 0.5390

