



Full wwPDB EM Validation Report ⓘ

Sep 22, 2024 – 12:09 PM EDT

PDB ID : 8VJM
EMDB ID : EMD-43289
Title : SpoIVFB(E44Q variant):pro-sigmaK complex
Authors : Orlando, M.A.; Pouillon, H.J.T.; Mandal, S.; Kroos, L.; Orlando, B.J.
Deposited on : 2024-01-07
Resolution : 4.00 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.dev112
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

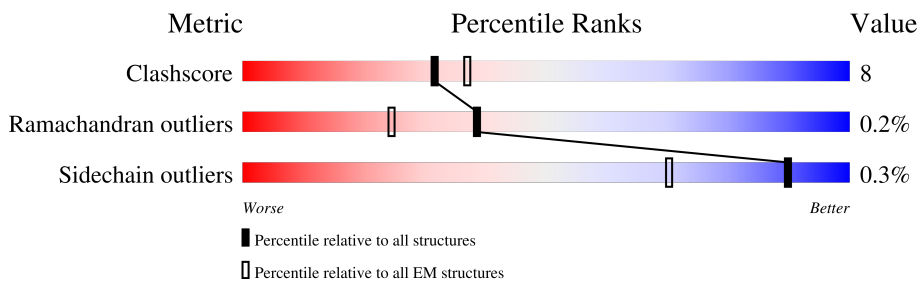
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	314	
1	C	314	
2	B	135	
2	D	135	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6667 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 Stage IV sporulation protein FB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	288	2353	1580	391	372	10	0	0
1	C	288	2353	1580	391	372	10	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLN	GLU	engineered mutation	UNP P26937
A	289	LYS	-	expression tag	UNP P26937
A	290	LEU	-	expression tag	UNP P26937
A	291	ASP	-	expression tag	UNP P26937
A	292	TYR	-	expression tag	UNP P26937
A	293	LYS	-	expression tag	UNP P26937
A	294	ASP	-	expression tag	UNP P26937
A	295	ASP	-	expression tag	UNP P26937
A	296	ASP	-	expression tag	UNP P26937
A	297	ASP	-	expression tag	UNP P26937
A	298	LYS	-	expression tag	UNP P26937
A	299	ASP	-	expression tag	UNP P26937
A	300	TYR	-	expression tag	UNP P26937
A	301	LYS	-	expression tag	UNP P26937
A	302	ASP	-	expression tag	UNP P26937
A	303	ASP	-	expression tag	UNP P26937
A	304	ASP	-	expression tag	UNP P26937
A	305	ASP	-	expression tag	UNP P26937
A	306	LYS	-	expression tag	UNP P26937
A	307	LEU	-	expression tag	UNP P26937
A	308	GLU	-	expression tag	UNP P26937
A	309	HIS	-	expression tag	UNP P26937
A	310	HIS	-	expression tag	UNP P26937
A	311	HIS	-	expression tag	UNP P26937
A	312	HIS	-	expression tag	UNP P26937
A	313	HIS	-	expression tag	UNP P26937

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Chain	Residue	Modelled	Actual	Comment	Reference
A	314	HIS	-	expression tag	UNP P26937
C	44	GLN	GLU	engineered mutation	UNP P26937
C	289	LYS	-	expression tag	UNP P26937
C	290	LEU	-	expression tag	UNP P26937
C	291	ASP	-	expression tag	UNP P26937
C	292	TYR	-	expression tag	UNP P26937
C	293	LYS	-	expression tag	UNP P26937
C	294	ASP	-	expression tag	UNP P26937
C	295	ASP	-	expression tag	UNP P26937
C	296	ASP	-	expression tag	UNP P26937
C	297	ASP	-	expression tag	UNP P26937
C	298	LYS	-	expression tag	UNP P26937
C	299	ASP	-	expression tag	UNP P26937
C	300	TYR	-	expression tag	UNP P26937
C	301	LYS	-	expression tag	UNP P26937
C	302	ASP	-	expression tag	UNP P26937
C	303	ASP	-	expression tag	UNP P26937
C	304	ASP	-	expression tag	UNP P26937
C	305	ASP	-	expression tag	UNP P26937
C	306	LYS	-	expression tag	UNP P26937
C	307	LEU	-	expression tag	UNP P26937
C	308	GLU	-	expression tag	UNP P26937
C	309	HIS	-	expression tag	UNP P26937
C	310	HIS	-	expression tag	UNP P26937
C	311	HIS	-	expression tag	UNP P26937
C	312	HIS	-	expression tag	UNP P26937
C	313	HIS	-	expression tag	UNP P26937
C	314	HIS	-	expression tag	UNP P26937

- Molecule 2 is a protein called RNA polymerase sigma-K factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	116	888	566	150	168	4	0	0
2	D	116	888	566	150	168	4	0	0

There are 40 discrepancies between the modelled and reference sequences:

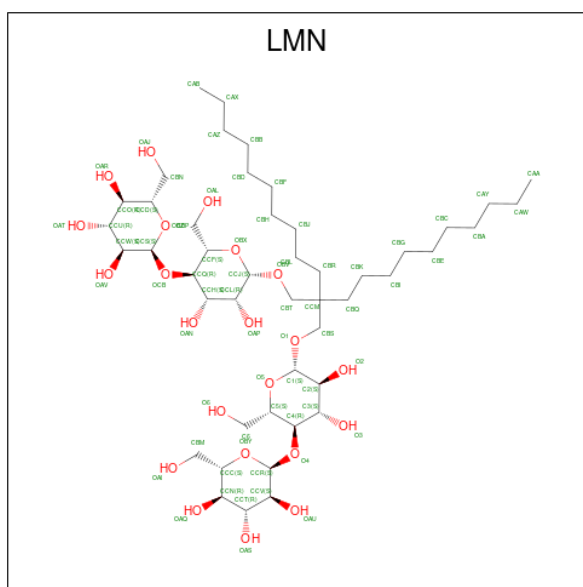
Chain	Residue	Modelled	Actual	Comment	Reference
B	116	LEU	-	expression tag	UNP P12254
B	117	MET	-	expression tag	UNP P12254

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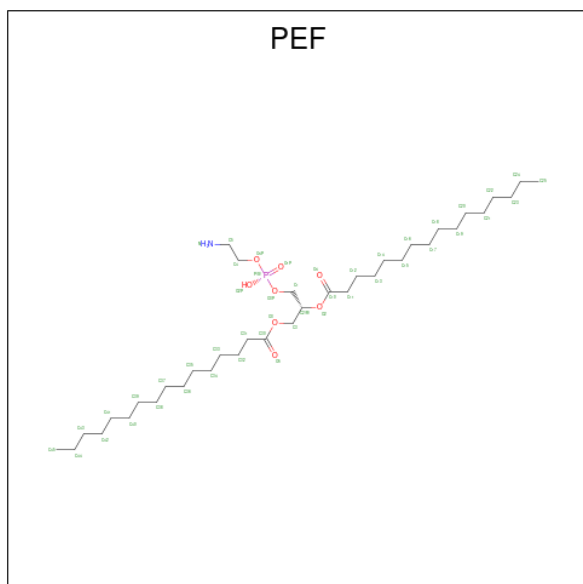
Chain	Residue	Modelled	Actual	Comment	Reference
B	118	HIS	-	expression tag	UNP P12254
B	119	LEU	-	expression tag	UNP P12254
B	120	ARG	-	expression tag	UNP P12254
B	121	ALA	-	expression tag	UNP P12254
B	122	LEU	-	expression tag	UNP P12254
B	123	LYS	-	expression tag	UNP P12254
B	124	LYS	-	expression tag	UNP P12254
B	125	THR	-	expression tag	UNP P12254
B	126	LYS	-	expression tag	UNP P12254
B	127	LYS	-	expression tag	UNP P12254
B	128	GLY	-	expression tag	UNP P12254
B	129	SER	-	expression tag	UNP P12254
B	130	HIS	-	expression tag	UNP P12254
B	131	HIS	-	expression tag	UNP P12254
B	132	HIS	-	expression tag	UNP P12254
B	133	HIS	-	expression tag	UNP P12254
B	134	HIS	-	expression tag	UNP P12254
B	135	HIS	-	expression tag	UNP P12254
D	116	LEU	-	expression tag	UNP P12254
D	117	MET	-	expression tag	UNP P12254
D	118	HIS	-	expression tag	UNP P12254
D	119	LEU	-	expression tag	UNP P12254
D	120	ARG	-	expression tag	UNP P12254
D	121	ALA	-	expression tag	UNP P12254
D	122	LEU	-	expression tag	UNP P12254
D	123	LYS	-	expression tag	UNP P12254
D	124	LYS	-	expression tag	UNP P12254
D	125	THR	-	expression tag	UNP P12254
D	126	LYS	-	expression tag	UNP P12254
D	127	LYS	-	expression tag	UNP P12254
D	128	GLY	-	expression tag	UNP P12254
D	129	SER	-	expression tag	UNP P12254
D	130	HIS	-	expression tag	UNP P12254
D	131	HIS	-	expression tag	UNP P12254
D	132	HIS	-	expression tag	UNP P12254
D	133	HIS	-	expression tag	UNP P12254
D	134	HIS	-	expression tag	UNP P12254
D	135	HIS	-	expression tag	UNP P12254

- Molecule 3 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: C₄₇H₈₈O₂₂).



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

- Molecule 4 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).

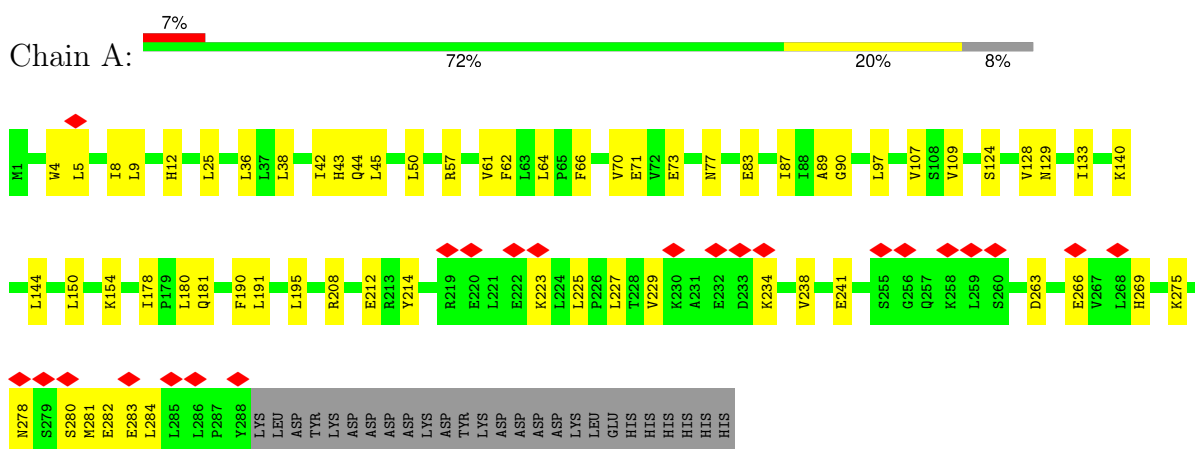


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			47	37	1	8	1	

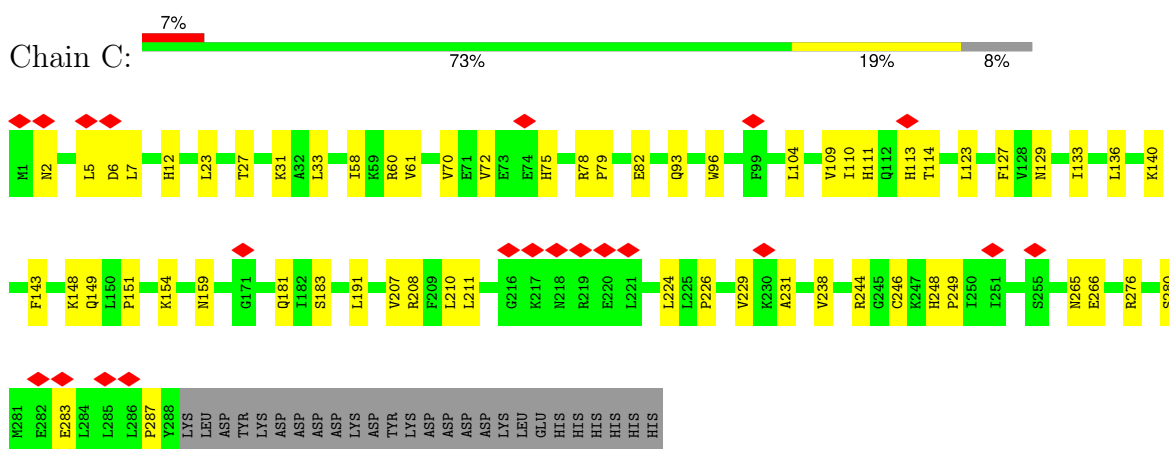
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

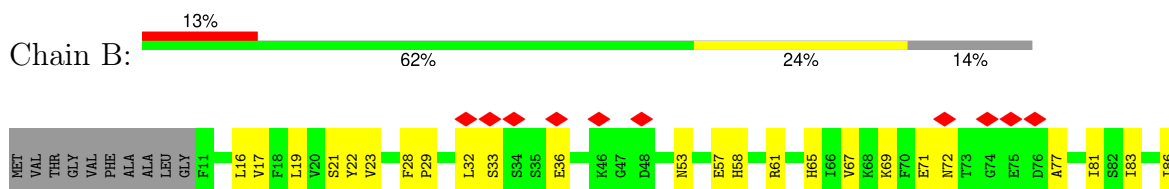
- Molecule 1: Stage IV sporulation protein FB



- Molecule 1: Stage IV sporulation protein FB

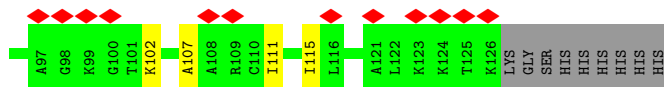
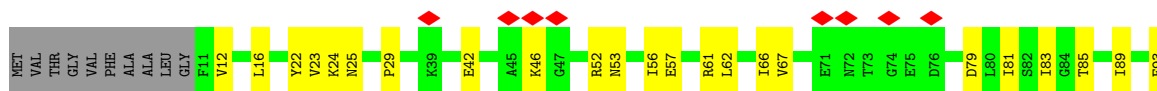


- Molecule 2: RNA polymerase sigma-K factor





• Molecule 2: RNA polymerase sigma-K factor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78352	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.922	Depositor
Minimum map value	-0.597	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	271.58398, 271.58398, 271.58398	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8486999, 0.8486999, 0.8486999	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, PEF

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	0/2424	0.47	0/3293
1	C	0.25	0/2424	0.46	0/3293
2	B	0.25	0/901	0.46	0/1213
2	D	0.24	0/901	0.44	0/1213
All	All	0.25	0/6650	0.46	0/9012

There are no bond length outliers.

There are no bond angle outliers.

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	2353	0	2406	41	0
1	C	2353	0	2406	38	0
2	B	888	0	884	25	0
2	D	888	0	884	18	0
3	A	138	0	176	8	0
4	A	47	0	73	0	0
All	All	6667	0	6829	114	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 8.

All (114) 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:129:ASN:ND2	2:B:21:SER:OG	2.30	0.64
2:B:88:LEU:O	2:B:92:ILE:HG12	1.97	0.63
1:C:110:ILE:HG13	1:C:111:HIS:H	1.63	0.63
1:A:281:MET:HA	1:A:284:LEU:HD13	1.79	0.63
2:D:29:PRO:O	2:D:61:ARG:NH1	2.31	0.63
2:D:79:ASP:O	2:D:83:ILE:HG12	1.98	0.62
1:C:78:ARG:O	1:C:244:ARG:NH2	2.32	0.62
1:C:224:LEU:HD23	1:C:226:PRO:HD3	1.80	0.62
2:B:33:SER:N	2:B:36:GLU:OE2	2.33	0.61
1:A:150:LEU:HD23	1:A:154:LYS:HG2	1.84	0.59
1:A:77:ASN:HB2	1:A:212:GLU:HG2	1.85	0.59
1:C:79:PRO:HD2	1:C:82:GLU:HG3	1.85	0.59
1:C:133:ILE:HG21	1:C:191:LEU:HD13	1.85	0.59
1:C:208:ARG:NH2	2:D:57:GLU:OE1	2.36	0.59
1:C:111:HIS:HE1	1:C:113:HIS:ND1	2.01	0.58
1:C:93:GLN:OE1	1:C:96:TRP:NE1	2.36	0.58
1:C:123:LEU:HD12	1:C:127:PHE:HE2	1.68	0.58
1:A:263:ASP:N	1:A:266:GLU:OE2	2.37	0.58
1:A:223:LYS:HE3	1:A:225:LEU:HD21	1.87	0.56
1:C:104:LEU:HG	1:C:109:VAL:HG11	1.86	0.56
1:A:227:LEU:HD11	1:A:241:GLU:HG3	1.88	0.55
1:C:58:ILE:HG22	1:C:72:VAL:HG12	1.89	0.54
1:A:61:VAL:HG22	1:A:70:VAL:HG22	1.90	0.54
2:D:67:VAL:HG21	2:D:81:ILE:HD13	1.90	0.54
1:C:6:ASP:OD1	1:C:7:LEU:N	2.41	0.53
2:B:65:HIS:O	2:B:69:LYS:HG3	2.07	0.53
1:A:4:TRP:HE1	1:A:45:LEU:HD12	1.74	0.52
2:B:32:LEU:HD12	2:B:36:GLU:HG2	1.89	0.52
2:D:22:TYR:HE2	2:D:24:LYS:HD3	1.74	0.52
1:A:234:LYS:NZ	1:A:278:ASN:OD1	2.39	0.51
2:B:67:VAL:HG21	2:B:81:ILE:HD13	1.92	0.51
1:C:23:LEU:O	1:C:27:THR:HG22	2.10	0.51
1:C:229:VAL:HG11	1:C:238:VAL:HG23	1.93	0.50
1:C:265:ASN:OD1	1:C:266:GLU:N	2.45	0.50
1:C:110:ILE:HG13	1:C:111:HIS:N	2.27	0.50
1:A:5:LEU:HA	1:A:8:ILE:HG22	1.94	0.49
1:C:140:LYS:HE3	2:D:23:VAL:HG12	1.94	0.49
1:A:8:ILE:HG23	1:A:9:LEU:HD12	1.93	0.49
1:A:83:GLU:O	1:A:87:ILE:HG12	2.13	0.49
1:A:208:ARG:NH2	2:B:57:GLU:OE1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ILE:HG21	1:A:191:LEU:HD13	1.95	0.49
2:D:111:ILE:O	2:D:115:ILE:HG13	2.13	0.48
2:D:52:ARG:O	2:D:56:ILE:HG12	2.13	0.48
1:A:36:LEU:HD13	2:B:19:LEU:HD11	1.95	0.48
2:B:32:LEU:H	2:B:32:LEU:HD23	1.79	0.48
2:D:12:VAL:HG22	2:D:16:LEU:HD11	1.94	0.47
2:D:107:ALA:O	2:D:111:ILE:HG22	2.15	0.47
1:C:70:VAL:HG13	1:C:70:VAL:O	2.15	0.47
3:A:403:LMN:HBR	3:A:403:LMN:HBKA	1.71	0.46
2:B:29:PRO:HG2	2:B:58:HIS:HA	1.97	0.46
1:A:107:VAL:HG13	1:A:109:VAL:HG23	1.97	0.46
1:C:75:HIS:HD2	2:D:25:ASN:HB3	1.81	0.46
1:A:25:LEU:HD21	3:A:403:LMN:HBGA	1.97	0.46
1:A:70:VAL:HB	2:B:23:VAL:HG12	1.98	0.46
2:B:71:GLU:HG3	2:B:72:ASN:H	1.81	0.45
2:D:42:GLU:O	2:D:46:LYS:HG3	2.16	0.45
1:A:214:TYR:OH	1:A:269:HIS:ND1	2.50	0.45
1:A:44:GLN:NE2	1:A:70:VAL:HG23	2.32	0.45
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.84	0.45
2:B:83:ILE:HG13	2:B:118:HIS:CD2	2.51	0.45
1:A:181:GLN:NE2	2:B:16:LEU:O	2.50	0.44
1:A:140:LYS:O	1:A:144:LEU:HD13	2.17	0.44
3:A:403:LMN:HBB	1:C:33:LEU:HD12	1.98	0.44
1:C:181:GLN:HE21	1:C:183:SER:HB3	1.82	0.44
1:A:275:LYS:HG2	2:B:86:ILE:HD11	1.99	0.44
1:C:109:VAL:HG13	1:C:110:ILE:HG23	1.98	0.44
1:C:276:ARG:HH12	1:C:283:GLU:HB3	1.83	0.44
1:A:12:HIS:HB2	1:A:62:PHE:HB2	2.00	0.44
1:C:207:VAL:HG21	2:D:85:THR:HG21	2.00	0.44
3:A:401:LMN:HBKA	3:A:401:LMN:HBTA	1.74	0.43
1:A:43:HIS:NE2	1:A:90:GLY:HA3	2.33	0.43
2:B:102:LYS:HD2	2:B:102:LYS:HA	1.73	0.43
2:B:77:ALA:O	2:B:81:ILE:HG12	2.19	0.43
1:A:212:GLU:OE1	2:B:53:ASN:ND2	2.36	0.43
1:C:148:LYS:HB3	1:C:149:GLN:OE1	2.18	0.43
1:C:224:LEU:HD21	1:C:249:PRO:HG2	2.00	0.43
1:A:50:LEU:HD23	1:A:89:ALA:HB2	1.99	0.43
1:A:178:ILE:HG22	1:A:180:LEU:H	1.84	0.42
1:A:229:VAL:HG11	1:A:238:VAL:HG21	2.00	0.42
3:A:403:LMN:H4	3:A:403:LMN:HCV	1.77	0.42
2:B:83:ILE:HG13	2:B:118:HIS:HD2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:PHE:O	2:B:61:ARG:NH2	2.52	0.42
1:C:61:VAL:HG22	1:C:70:VAL:HG23	2.00	0.42
1:C:143:PHE:HB2	1:C:159:ASN:ND2	2.34	0.42
2:D:22:TYR:CE2	2:D:24:LYS:HB2	2.55	0.42
2:D:89:ILE:O	2:D:93:GLU:HB2	2.20	0.42
2:D:102:LYS:HD3	2:D:102:LYS:HA	1.85	0.42
1:C:231:ALA:O	1:C:280:SER:OG	2.37	0.42
1:C:149:GLN:OE1	1:C:149:GLN:N	2.52	0.41
1:C:12:HIS:ND1	1:C:60:ARG:HG2	2.34	0.41
2:B:90:LYS:HD2	2:B:93:GLU:OE2	2.20	0.41
1:C:151:PRO:HB2	1:C:154:LYS:HG2	2.02	0.41
1:C:246:CYS:HB3	1:C:248:HIS:CE1	2.55	0.41
1:A:57:ARG:HB2	1:A:73:GLU:HB3	2.03	0.41
2:B:87:GLY:HA3	2:B:114:GLU:HG3	2.03	0.41
3:A:401:LMN:HBH	3:A:401:LMN:HBB	1.81	0.41
3:A:403:LMN:HBSA	3:A:403:LMN:HBL	1.73	0.41
1:C:211:LEU:HD11	2:D:56:ILE:HD12	2.03	0.41
1:A:42:ILE:HG21	1:A:97:LEU:HD11	2.01	0.41
1:C:31:LYS:HD2	1:C:114:THR:OG1	2.20	0.41
1:A:280:SER:HB2	1:A:282:GLU:OE1	2.20	0.41
1:A:280:SER:OG	1:A:283:GLU:OE1	2.24	0.41
3:A:403:LMN:O4	3:A:403:LMN:O2	2.34	0.41
1:C:2:ASN:HA	1:C:5:LEU:HG	2.02	0.41
1:A:36:LEU:HD11	2:B:17:VAL:HG11	2.03	0.40
1:C:123:LEU:HD12	1:C:127:PHE:CE2	2.53	0.40
1:A:38:LEU:O	1:A:42:ILE:HG12	2.21	0.40
2:B:16:LEU:HD23	2:B:16:LEU:HA	1.98	0.40
1:A:71:GLU:OE2	1:A:71:GLU:HA	2.21	0.40
1:A:124:SER:O	1:A:128:VAL:HG23	2.22	0.40
1:C:210:LEU:HD23	1:C:210:LEU:HA	1.96	0.40
1:A:64:LEU:HD12	1:A:66:PHE:H	1.86	0.40
1:A:190:PHE:HZ	2:B:22:TYR:CZ	2.38	0.40
2:D:62:LEU:O	2:D:66:ILE:HD12	2.22	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	286/314 (91%)	263 (92%)	23 (8%)	0	100	100
1	C	286/314 (91%)	264 (92%)	20 (7%)	2 (1%)	19	55
2	B	114/135 (84%)	112 (98%)	2 (2%)	0	100	100
2	D	114/135 (84%)	111 (97%)	3 (3%)	0	100	100
All	All	800/898 (89%)	750 (94%)	48 (6%)	2 (0%)	38	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	136	LEU
1	C	287	PRO

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	247/283 (87%)	247 (100%)	0	100	100
1	C	247/283 (87%)	246 (100%)	1 (0%)	89	91
2	B	92/113 (81%)	92 (100%)	0	100	100
2	D	92/113 (81%)	91 (99%)	1 (1%)	70	80
All	All	678/792 (86%)	676 (100%)	2 (0%)	90	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	129	ASN
2	D	53	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	129	ASN
1	C	111	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
3	LMN	A	401	-	72,72,72	1.70	15 (20%)	92,98,98	1.10	5 (5%)
4	PEF	A	402	-	46,46,46	0.91	4 (8%)	49,51,51	1.12	2 (4%)
3	LMN	A	403	-	72,72,72	1.68	14 (19%)	92,98,98	1.10	6 (6%)

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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMN	A	401	-	-	26/50/130/130	0/4/4/4
4	PEF	A	402	-	-	17/50/50/50	-
3	LMN	A	403	-	-	33/50/130/130	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	LMN	O5-C1	4.81	1.54	1.41
3	A	403	LMN	O5-C1	4.72	1.54	1.41
3	A	401	LMN	CBS-CCM	4.44	1.63	1.53
3	A	403	LMN	CBS-CCM	4.37	1.63	1.53
3	A	401	LMN	CBT-CCM	4.12	1.62	1.53
3	A	403	LMN	CBT-CCM	4.12	1.62	1.53
3	A	403	LMN	CBR-CCM	3.77	1.61	1.54
3	A	401	LMN	CBR-CCM	3.75	1.61	1.54
3	A	403	LMN	O1-C1	-3.61	1.34	1.40
3	A	401	LMN	O1-C1	-3.42	1.34	1.40
3	A	403	LMN	O4-C4	2.97	1.51	1.43
3	A	403	LMN	OBY-CCR	2.97	1.49	1.41
3	A	401	LMN	OBZ-CCS	2.85	1.49	1.41
3	A	401	LMN	O4-C4	2.82	1.51	1.43
3	A	401	LMN	OBY-CCR	2.81	1.49	1.41
3	A	403	LMN	OBZ-CCS	2.78	1.49	1.41
3	A	401	LMN	OBX-CCF	2.73	1.51	1.44
4	A	402	PEF	O2-C2	-2.67	1.40	1.46
3	A	401	LMN	OBX-CCJ	2.52	1.48	1.41
3	A	403	LMN	C3-C4	-2.50	1.45	1.52
3	A	403	LMN	OBX-CCF	2.43	1.50	1.44
3	A	401	LMN	C3-C4	-2.40	1.45	1.52
4	A	402	PEF	O3-C30	2.39	1.40	1.33
3	A	403	LMN	CBQ-CCM	2.25	1.58	1.54
3	A	403	LMN	O5-C5	2.24	1.49	1.44
3	A	401	LMN	O5-C5	2.23	1.49	1.44
4	A	402	PEF	O2-C10	2.16	1.40	1.34
4	A	402	PEF	O3-C3	-2.15	1.40	1.45
3	A	401	LMN	CBQ-CBK	2.12	1.59	1.52
3	A	403	LMN	CBQ-CBK	2.11	1.59	1.52
3	A	401	LMN	CBQ-CCM	2.07	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	LMN	OCB-CCQ	2.06	1.49	1.43
3	A	403	LMN	OCB-CCQ	2.05	1.49	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	402	PEF	O2-C10-C11	3.93	119.98	111.48
3	A	401	LMN	CCR-O4-C4	-3.63	109.38	117.98
3	A	401	LMN	CCS-OCB-CCQ	-3.44	109.82	117.98
3	A	403	LMN	OBX-CCF-CCQ	3.20	116.34	109.72
3	A	401	LMN	CBK-CBQ-CCM	-2.84	108.58	117.19
4	A	402	PEF	O3-C30-C31	2.72	120.13	111.83
3	A	403	LMN	CBL-CBR-CCM	-2.33	110.11	117.19
3	A	403	LMN	CCR-O4-C4	-2.31	112.50	117.98
3	A	401	LMN	OBX-CCF-CCQ	2.28	114.44	109.72
3	A	401	LMN	CBL-CBR-CCM	-2.24	110.39	117.19
3	A	403	LMN	OBZ-CCD-CCO	2.23	113.71	109.70
3	A	403	LMN	CBK-CBQ-CCM	-2.07	110.89	117.19
3	A	403	LMN	CBN-CCD-CCO	-2.02	108.07	113.02

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	LMN	O5-C1-O1-CBS
3	A	401	LMN	O1-CBS-CCM-CBQ
3	A	401	LMN	O1-CBS-CCM-CBR
3	A	401	LMN	OBV-CBT-CCM-CBQ
3	A	401	LMN	OBV-CBT-CCM-CBR
3	A	401	LMN	OBX-CCJ-OBV-CBT
3	A	403	LMN	C2-C1-O1-CBS
3	A	403	LMN	CCV-CCR-O4-C4
3	A	403	LMN	O1-CBS-CCM-CBQ
3	A	403	LMN	O1-CBS-CCM-CBR
3	A	403	LMN	OBV-CBT-CCM-CBQ
3	A	403	LMN	OBV-CBT-CCM-CBR
3	A	403	LMN	OBX-CCJ-OBV-CBT
3	A	403	LMN	OBZ-CCS-OCB-CCQ
4	A	402	PEF	C1-O3P-P-O2P
4	A	402	PEF	C1-O3P-P-O4P
3	A	403	LMN	OBY-CCR-O4-C4
3	A	401	LMN	OAJ-CBN-CCD-CCO

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Mol	Chain	Res	Type	Atoms
3	A	403	LMN	C4-C5-C6-O6
3	A	401	LMN	O1-CBS-CCM-CBT
3	A	401	LMN	OAJ-CBN-CCD-OBZ
3	A	403	LMN	O5-C5-C6-O6
3	A	403	LMN	OBV-CBT-CCM-CBS
3	A	401	LMN	OAI-CBM-CCC-CCN
3	A	403	LMN	O1-CBS-CCM-CBT
3	A	403	LMN	OAL-CBP-CCF-CCQ
3	A	401	LMN	C2-C1-O1-CBS
3	A	403	LMN	CCL-CCJ-OBV-CBT
3	A	403	LMN	OAL-CBP-CCF-OBX
3	A	401	LMN	OAI-CBM-CCC-OBY
3	A	401	LMN	CBB-CBD-CBF-CBH
3	A	401	LMN	O5-C5-C6-O6
3	A	403	LMN	O5-C1-O1-CBS
3	A	401	LMN	OAL-CBP-CCF-CCQ
3	A	401	LMN	CBI-CBK-CBQ-CCM
3	A	403	LMN	CBI-CBK-CBQ-CCM
4	A	402	PEF	C40-C41-C42-C43
3	A	401	LMN	CBF-CBH-CBJ-CBL
3	A	401	LMN	CBH-CBJ-CBL-CBR
4	A	402	PEF	C12-C13-C14-C15
3	A	403	LMN	CBC-CBE-CBG-CBI
4	A	402	PEF	C35-C36-C37-C38
4	A	402	PEF	C38-C39-C40-C41
3	A	401	LMN	CBC-CBE-CBG-CBI
3	A	403	LMN	CBK-CBQ-CCM-CBT
4	A	402	PEF	C18-C19-C20-C21
3	A	401	LMN	OBV-CBT-CCM-CBS
3	A	403	LMN	CBB-CBD-CBF-CBH
3	A	403	LMN	CAY-CBA-CBC-CBE
4	A	402	PEF	C37-C38-C39-C40
4	A	402	PEF	C10-C11-C12-C13
3	A	401	LMN	CAY-CBA-CBC-CBE
3	A	401	LMN	CAZ-CBB-CBD-CBF
3	A	401	LMN	CBE-CBG-CBI-CBK
3	A	403	LMN	CBK-CBQ-CCM-CBR
3	A	403	LMN	CBE-CBG-CBI-CBK
3	A	403	LMN	CBD-CBF-CBH-CBJ
3	A	403	LMN	C3-C4-O4-CCR
3	A	403	LMN	CBH-CBJ-CBL-CBR
4	A	402	PEF	C11-C10-O2-C2

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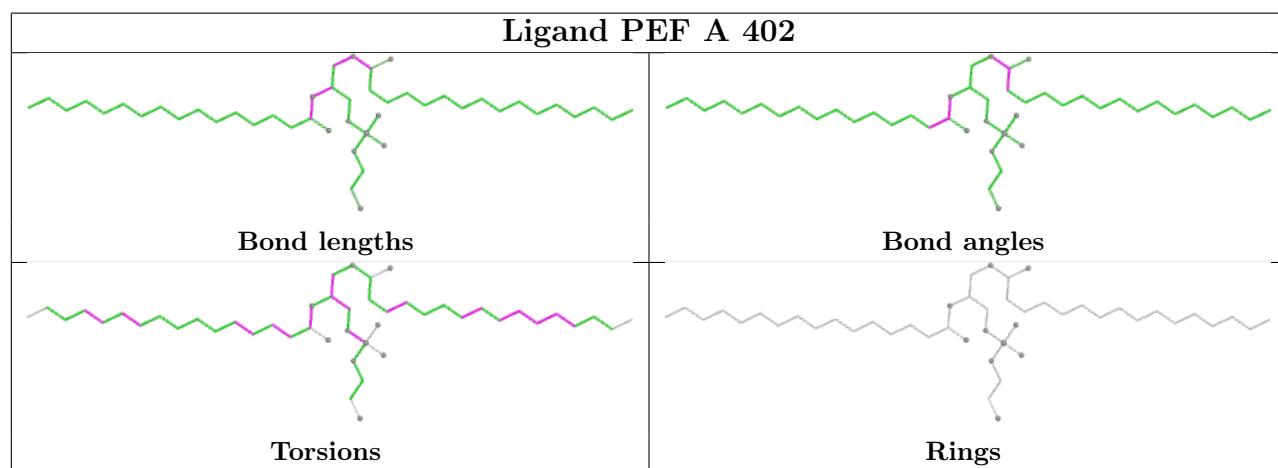
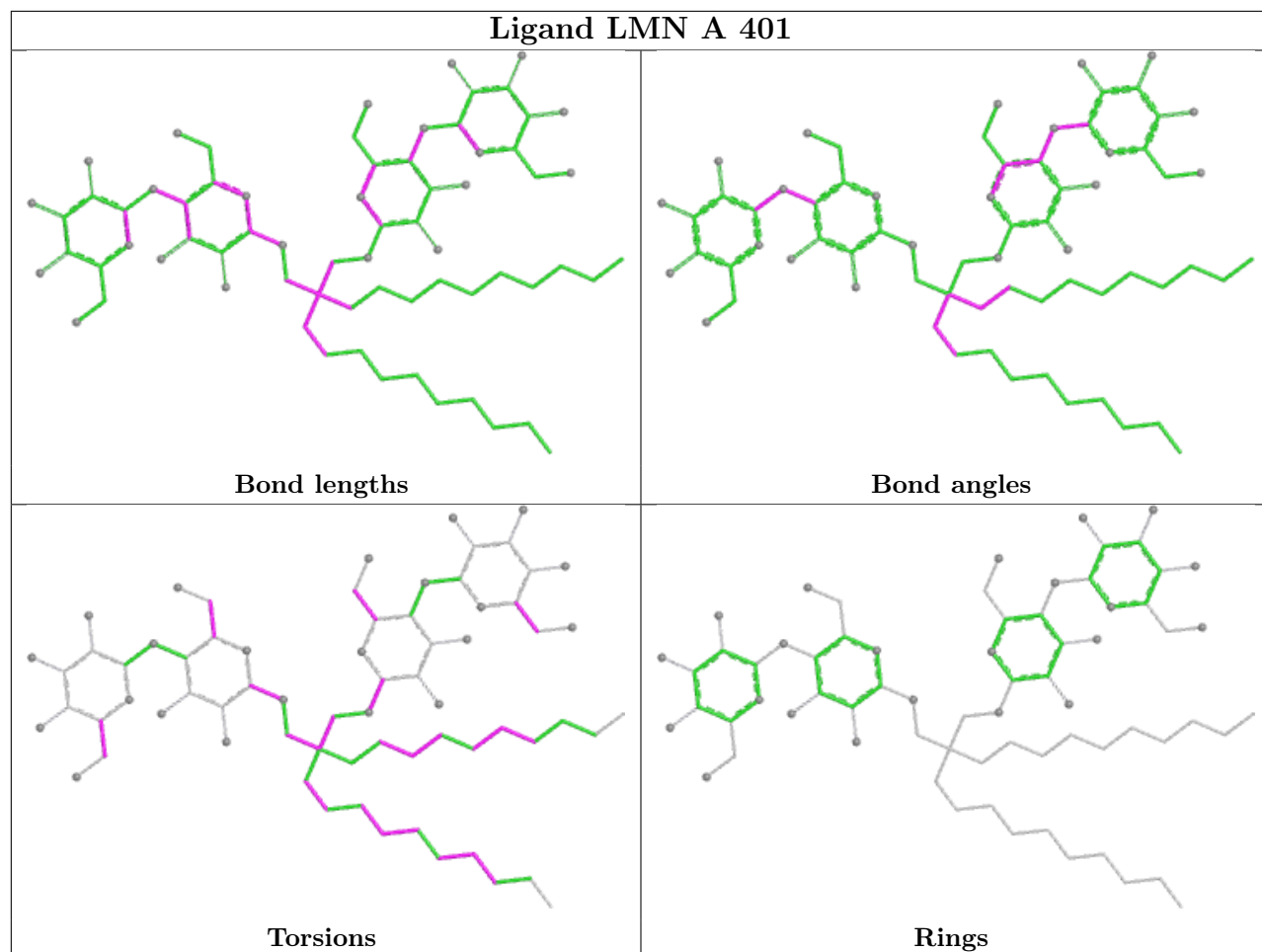
Mol	Chain	Res	Type	Atoms
3	A	403	LMN	CBA-CBC-CBE-CBG
3	A	401	LMN	CCL-CCJ-OBV-CBT
3	A	403	LMN	CBJ-CBL-CBR-CCM
3	A	403	LMN	C5-C4-O4-CCR
4	A	402	PEF	C31-C32-C33-C34
4	A	402	PEF	O3P-C1-C2-C3
4	A	402	PEF	O3P-C1-C2-O2
4	A	402	PEF	O4-C10-O2-C2
3	A	403	LMN	OAI-CBM-CCC-CCN
3	A	401	LMN	CAW-CAY-CBA-CBC
3	A	401	LMN	OAL-CBP-CCF-OBX
4	A	402	PEF	C20-C21-C22-C23
3	A	403	LMN	CBK-CBQ-CCM-CBS
3	A	403	LMN	CAW-CAY-CBA-CBC
4	A	402	PEF	O2-C2-C3-O3
4	A	402	PEF	C39-C40-C41-C42

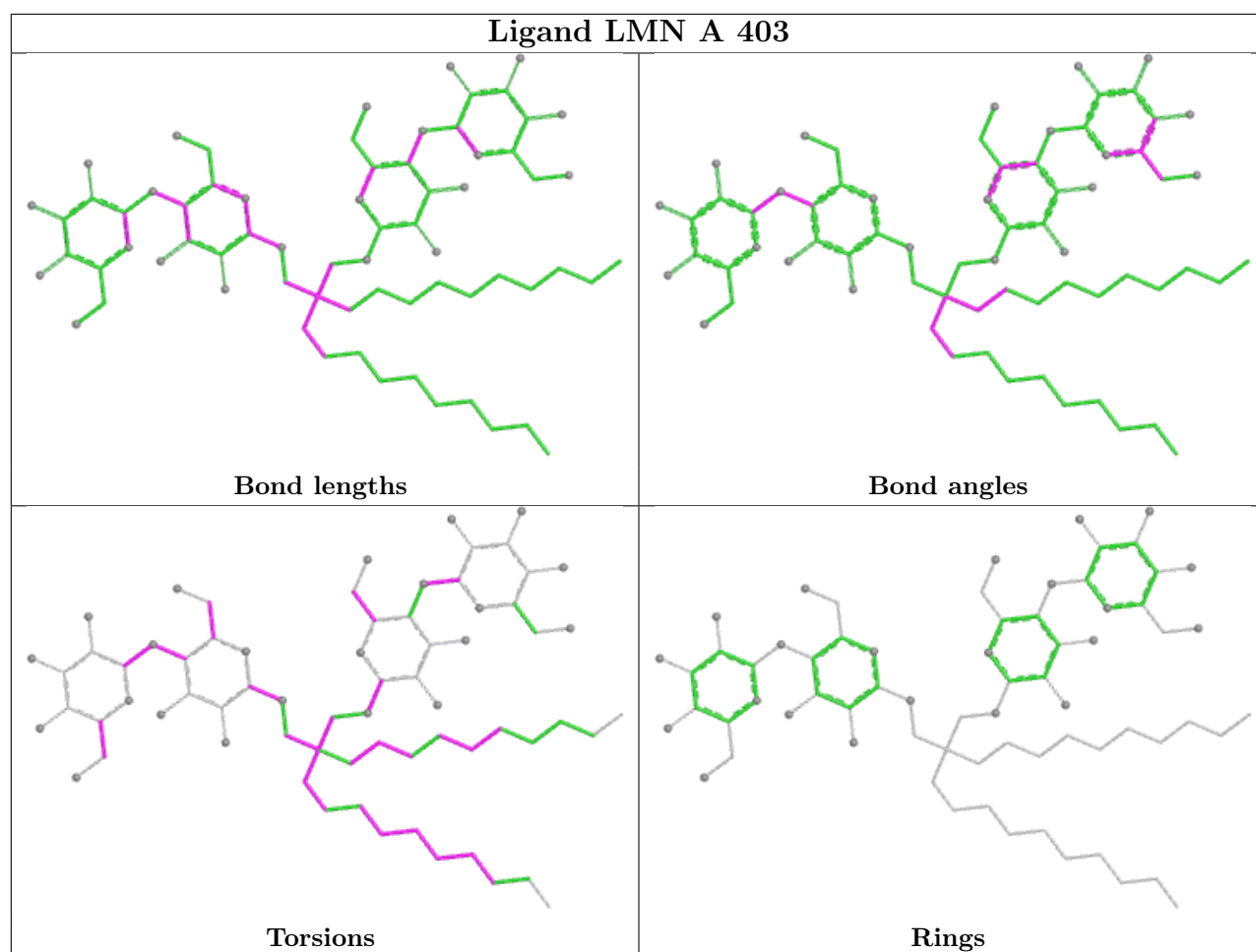
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	LMN	2	0
3	A	403	LMN	6	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.

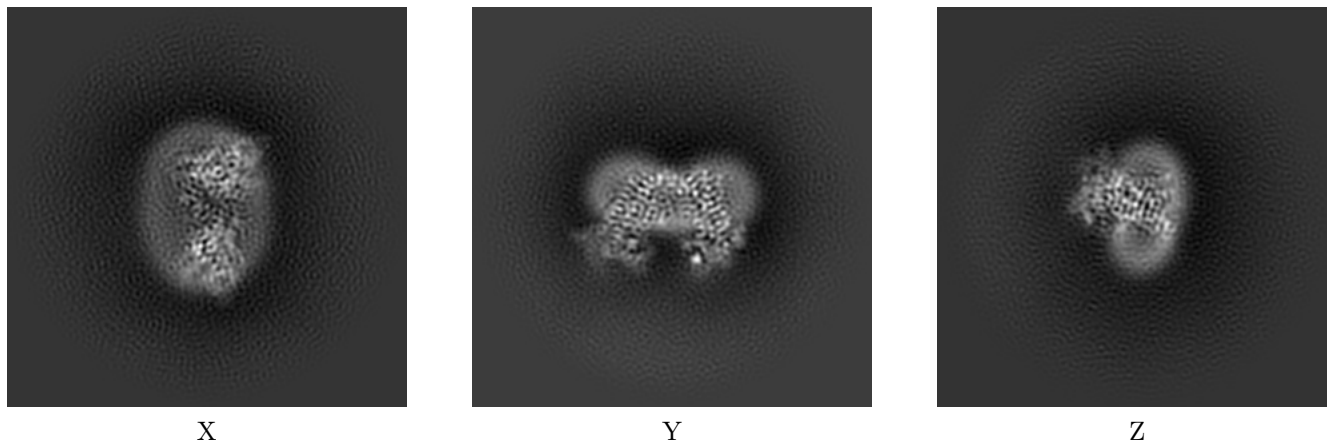
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43289. These allow visual inspection of the internal detail of the map and identification of artifacts.

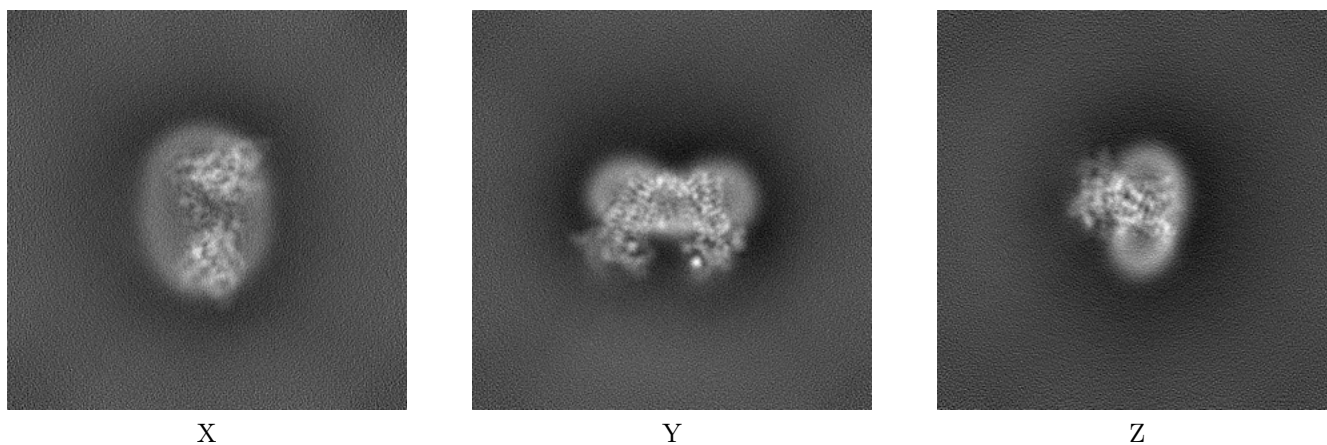
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



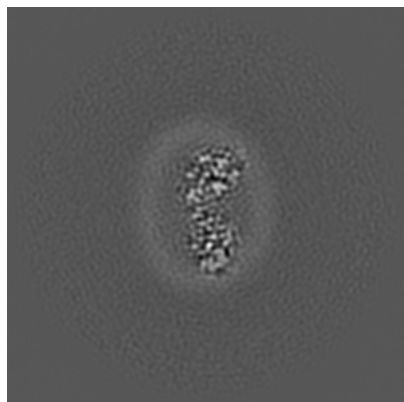
6.1.2 Raw map



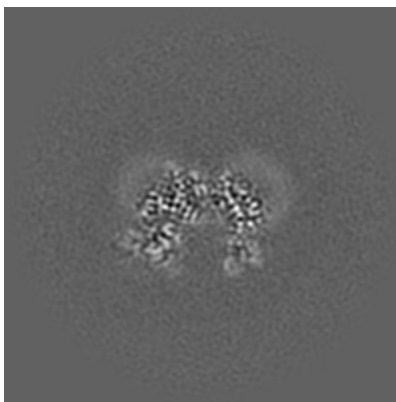
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

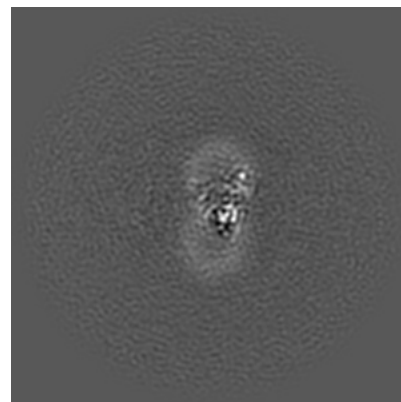
6.2.1 Primary map



X Index: 160

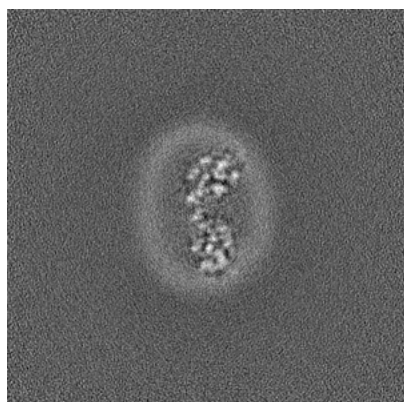


Y Index: 160

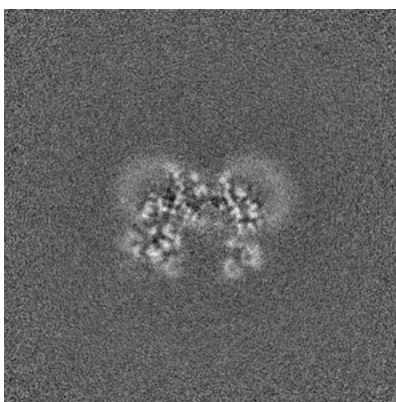


Z Index: 160

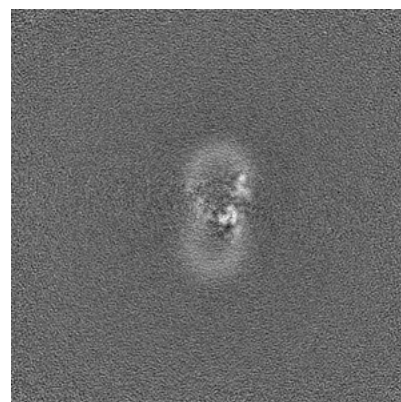
6.2.2 Raw map



X Index: 160



Y Index: 160

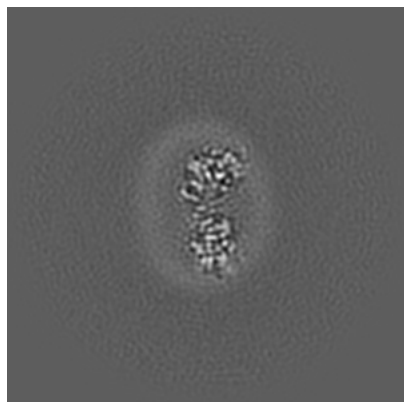


Z Index: 160

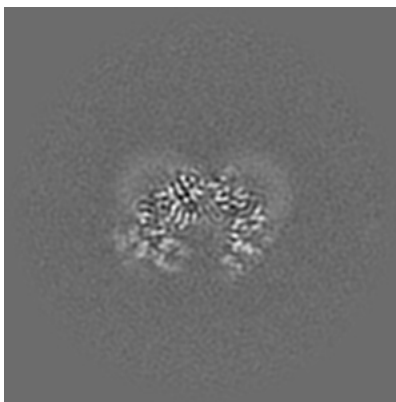
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

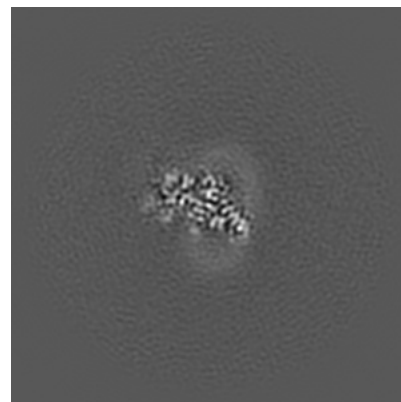
6.3.1 Primary map



X Index: 158

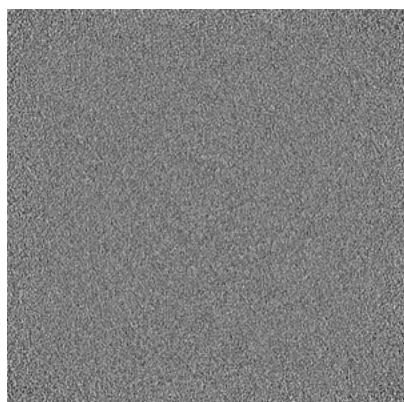


Y Index: 165

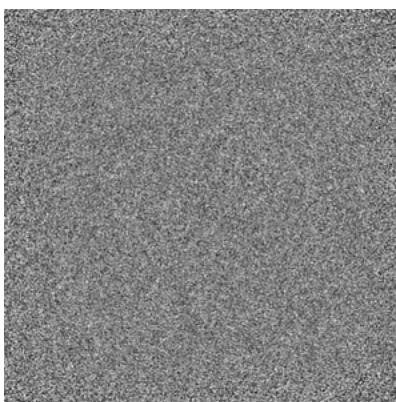


Z Index: 185

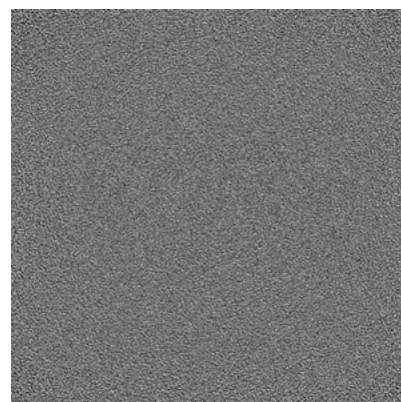
6.3.2 Raw map



X Index: 0



Y Index: 0

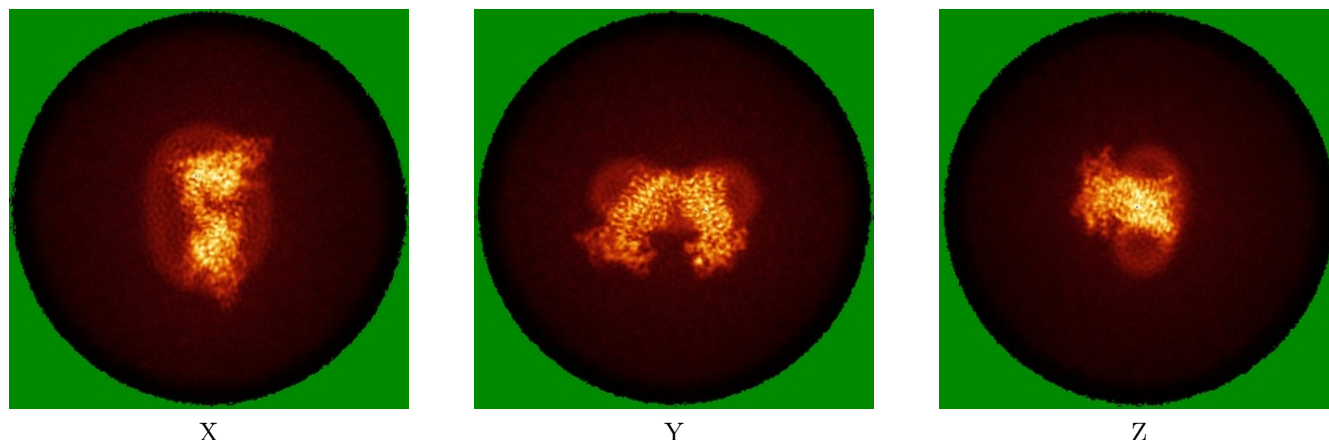


Z Index: 0

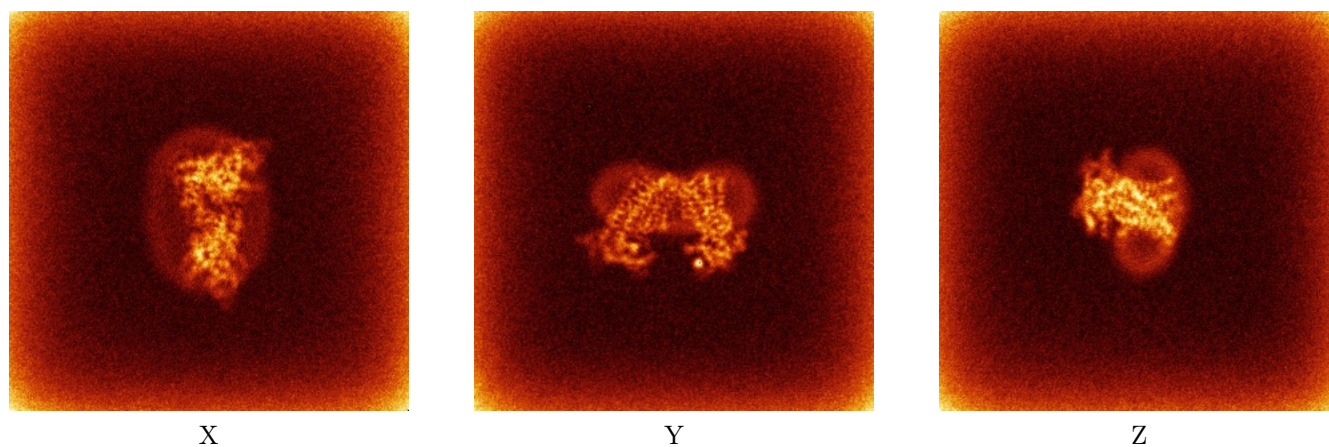
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



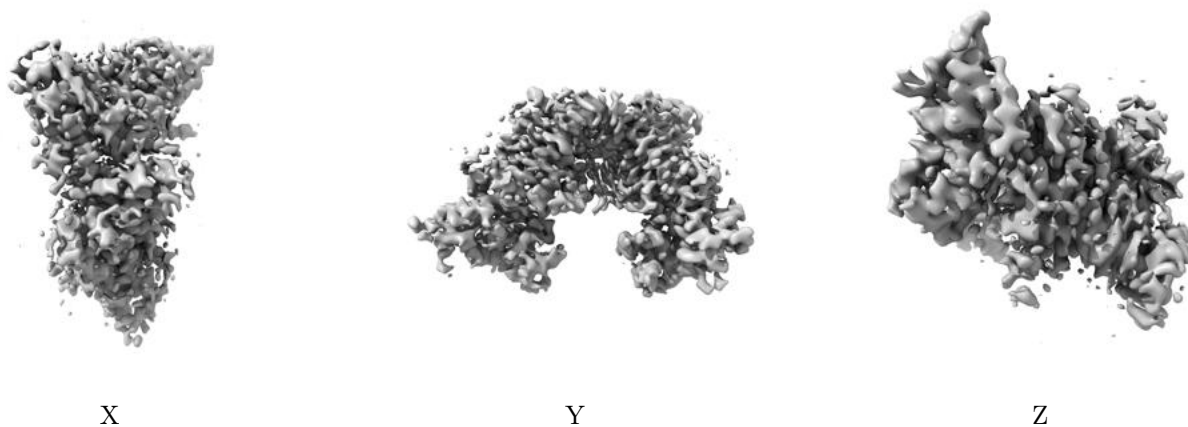
6.4.2 Raw map



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

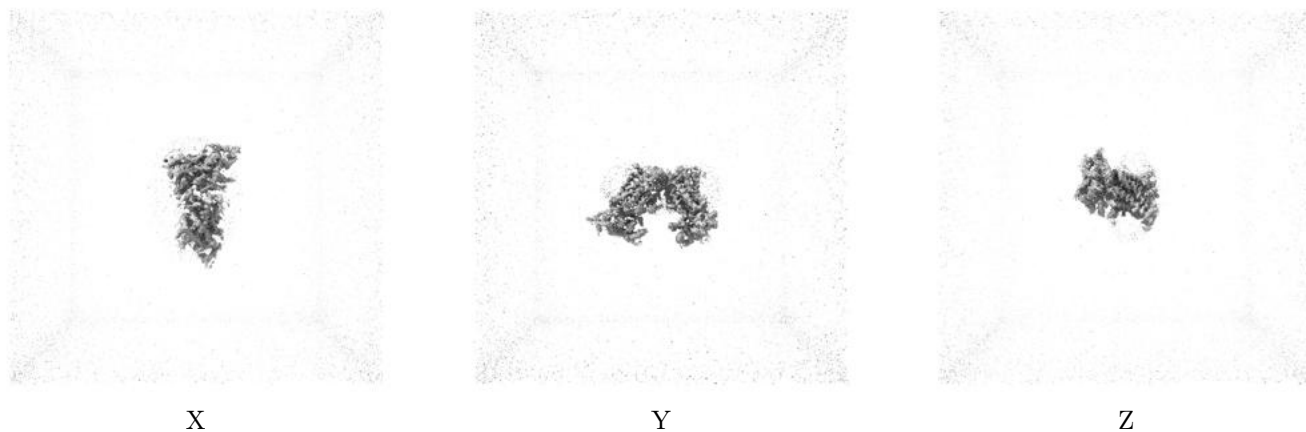
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

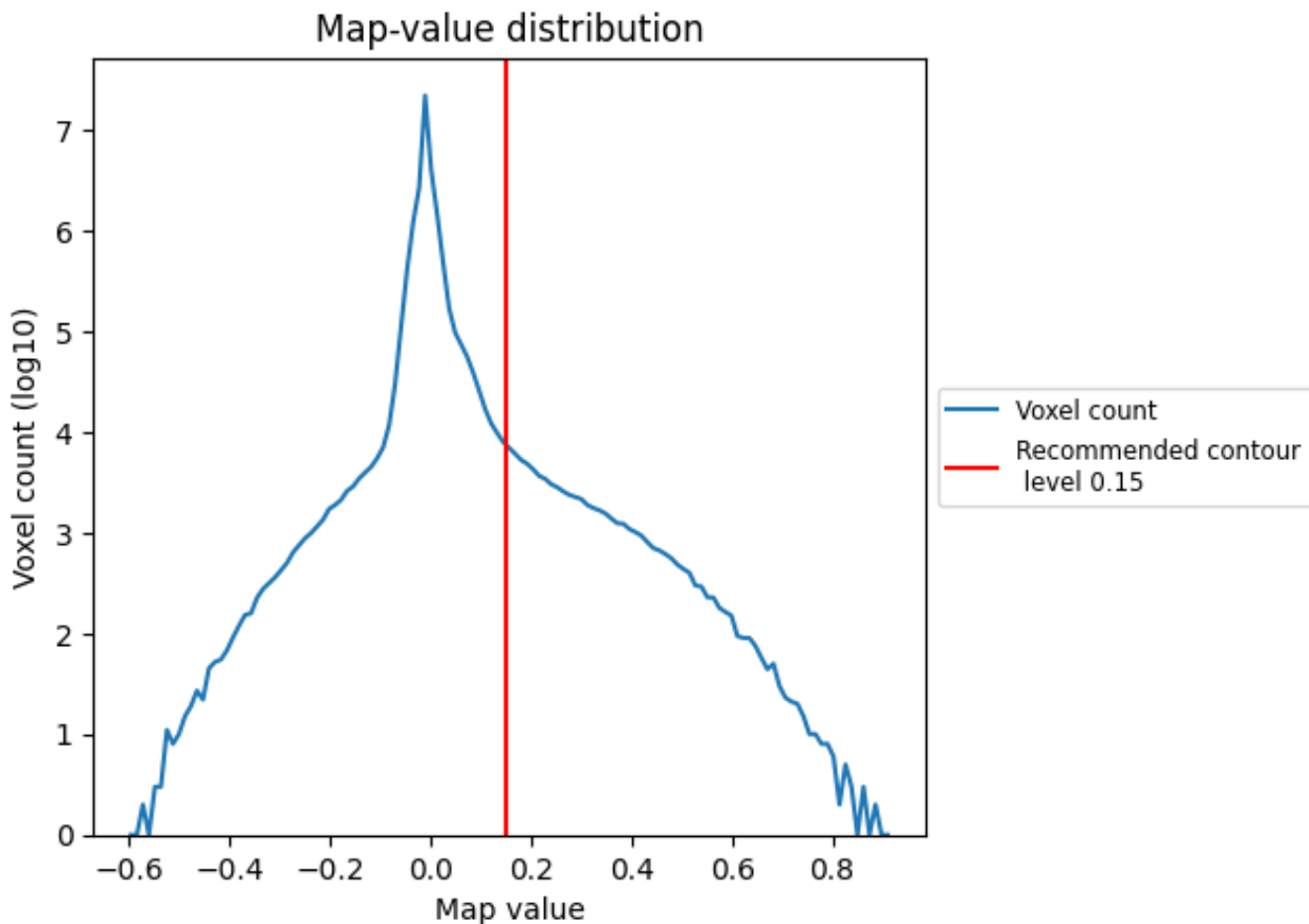
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

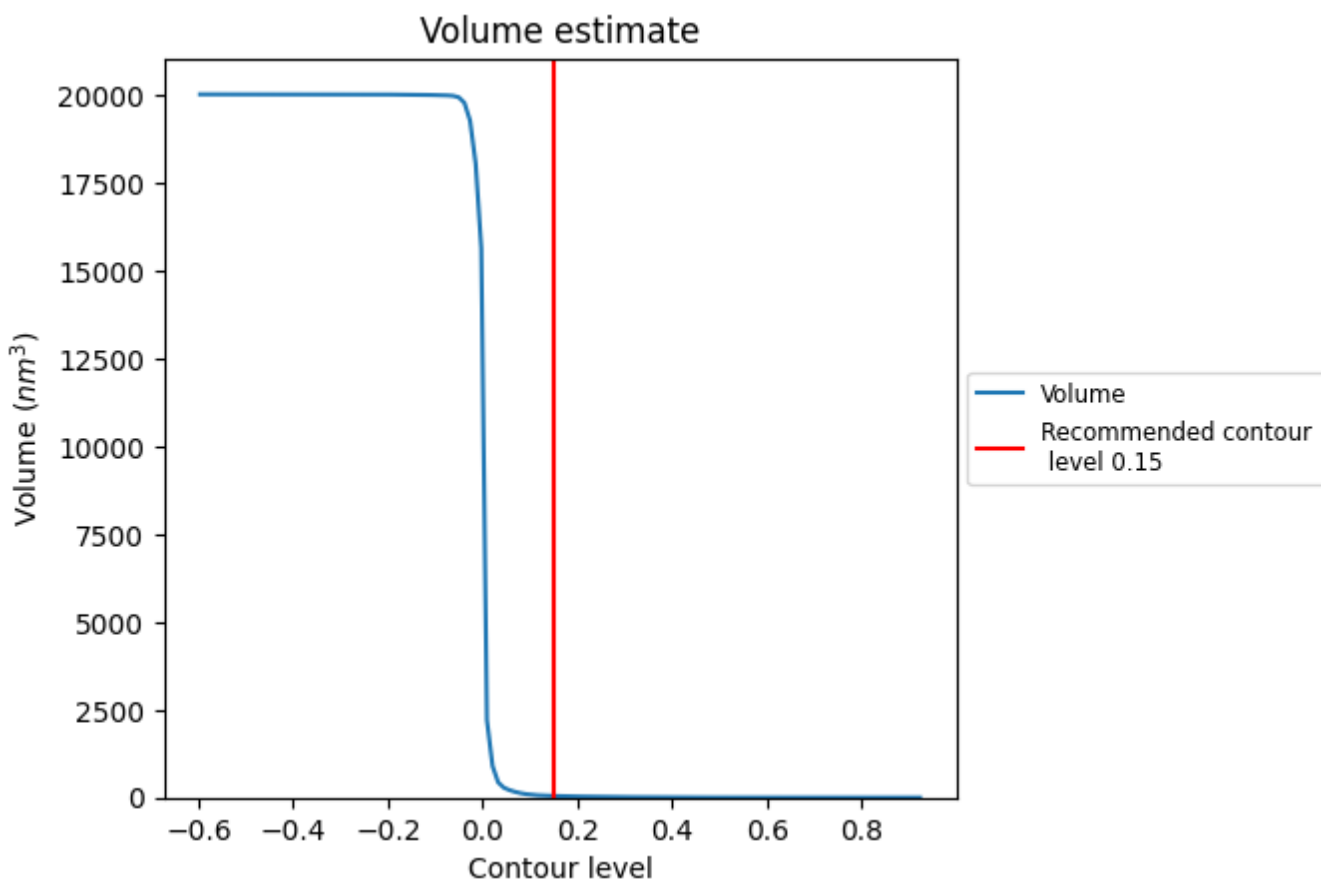
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

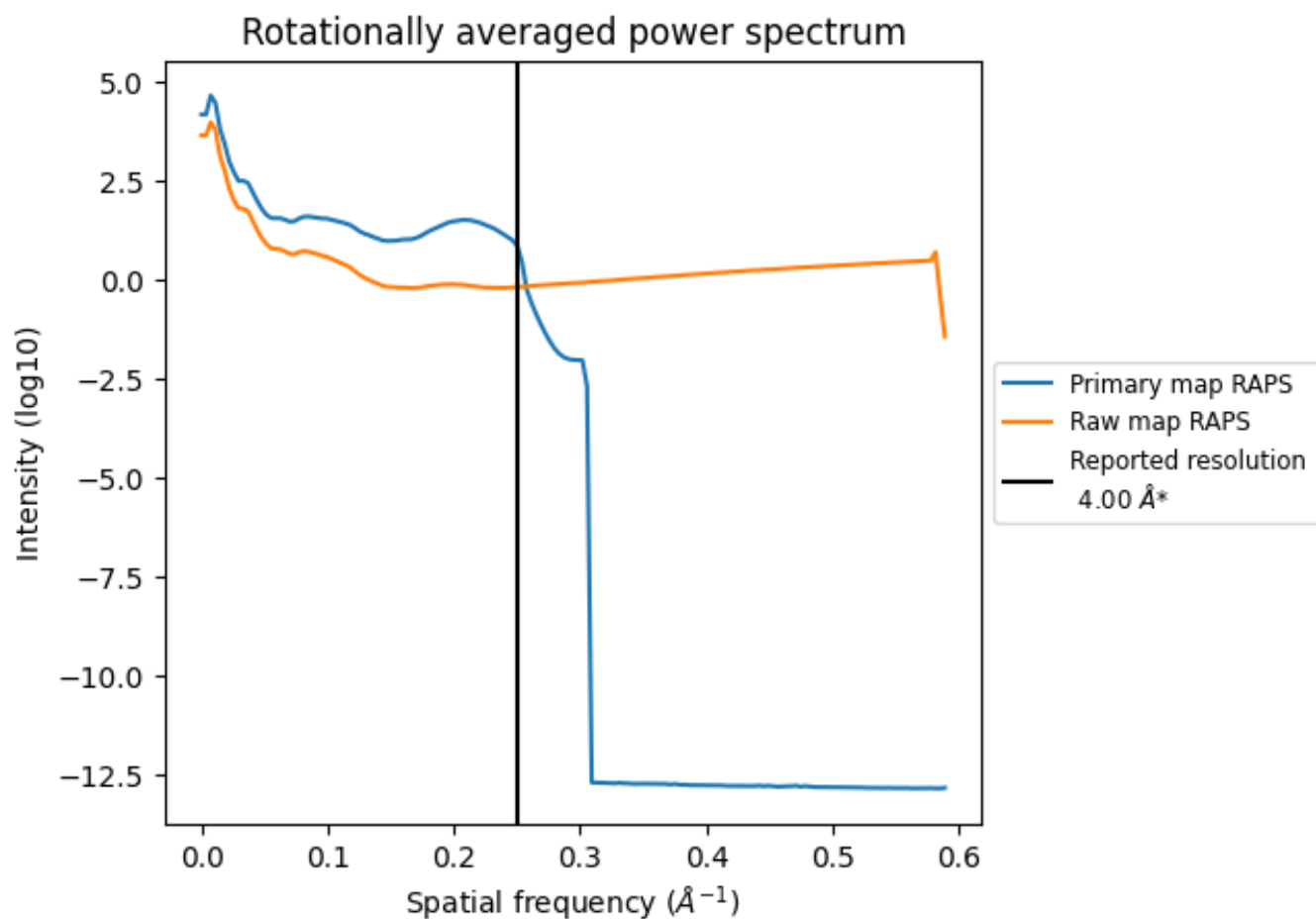
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm³; this corresponds to an approximate mass of 41 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](#)

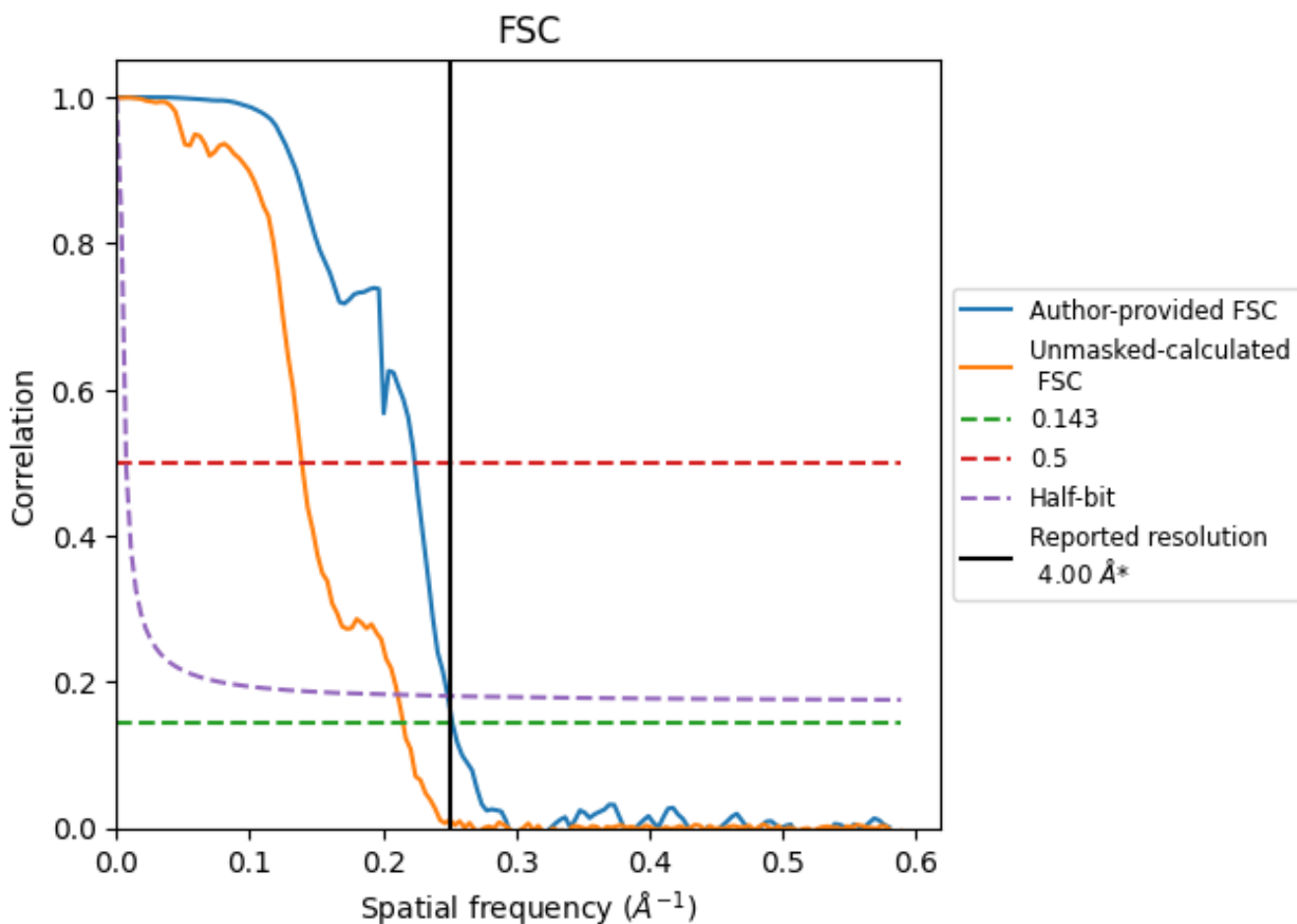


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

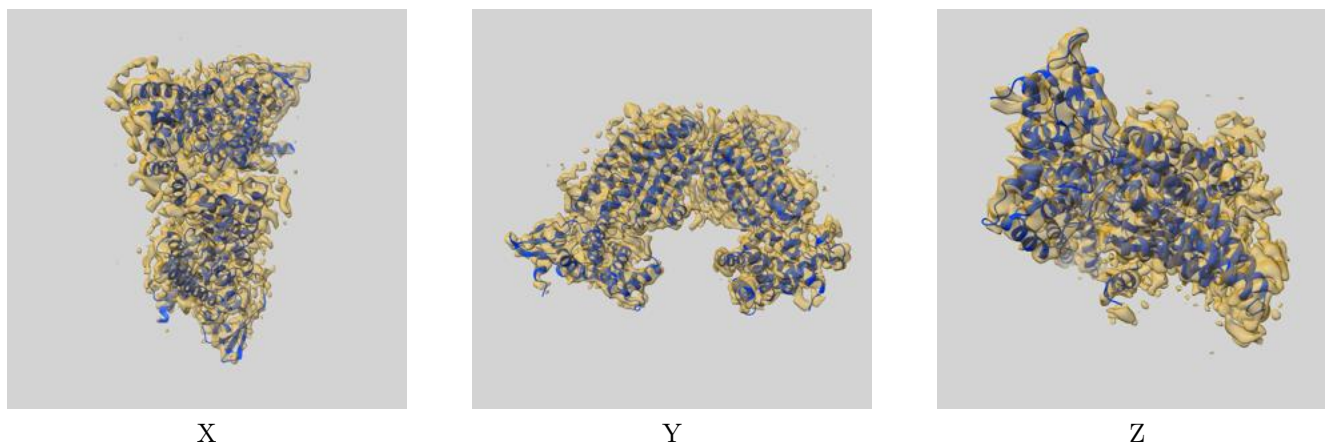
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.96	4.47	4.02
Unmasked-calculated*	4.65	7.18	4.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.65 differs from the reported value 4.0 by more than 10 %

9 Map-model fit [i](#)

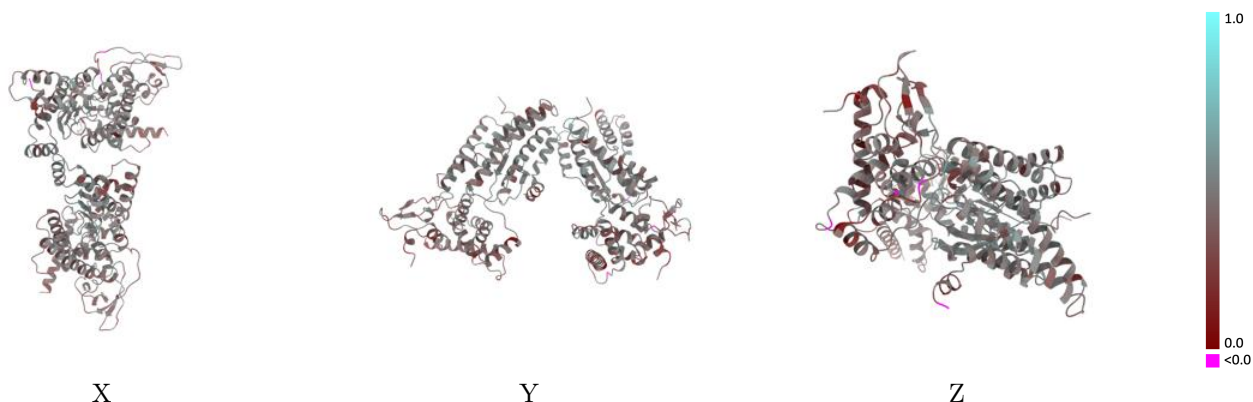
This section contains information regarding the fit between EMDB map EMD-43289 and PDB model 8VJM. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



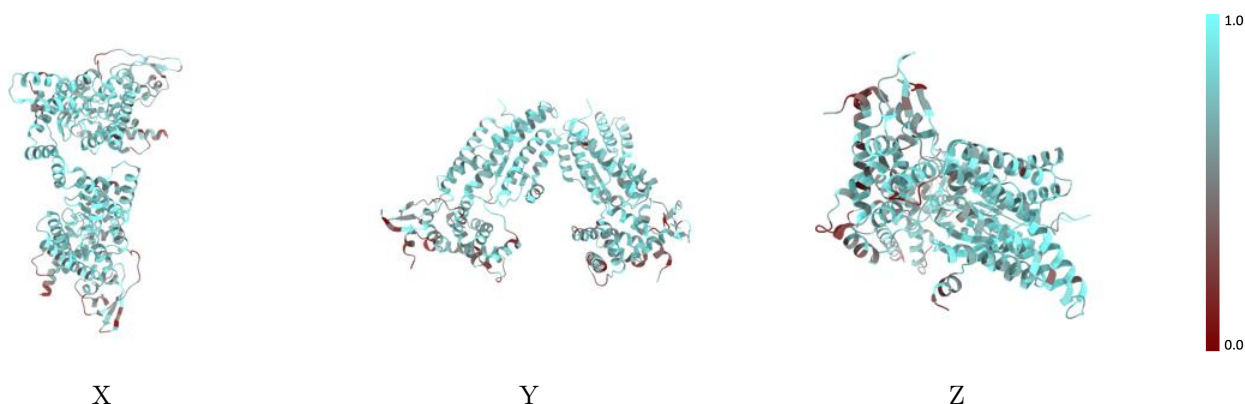
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



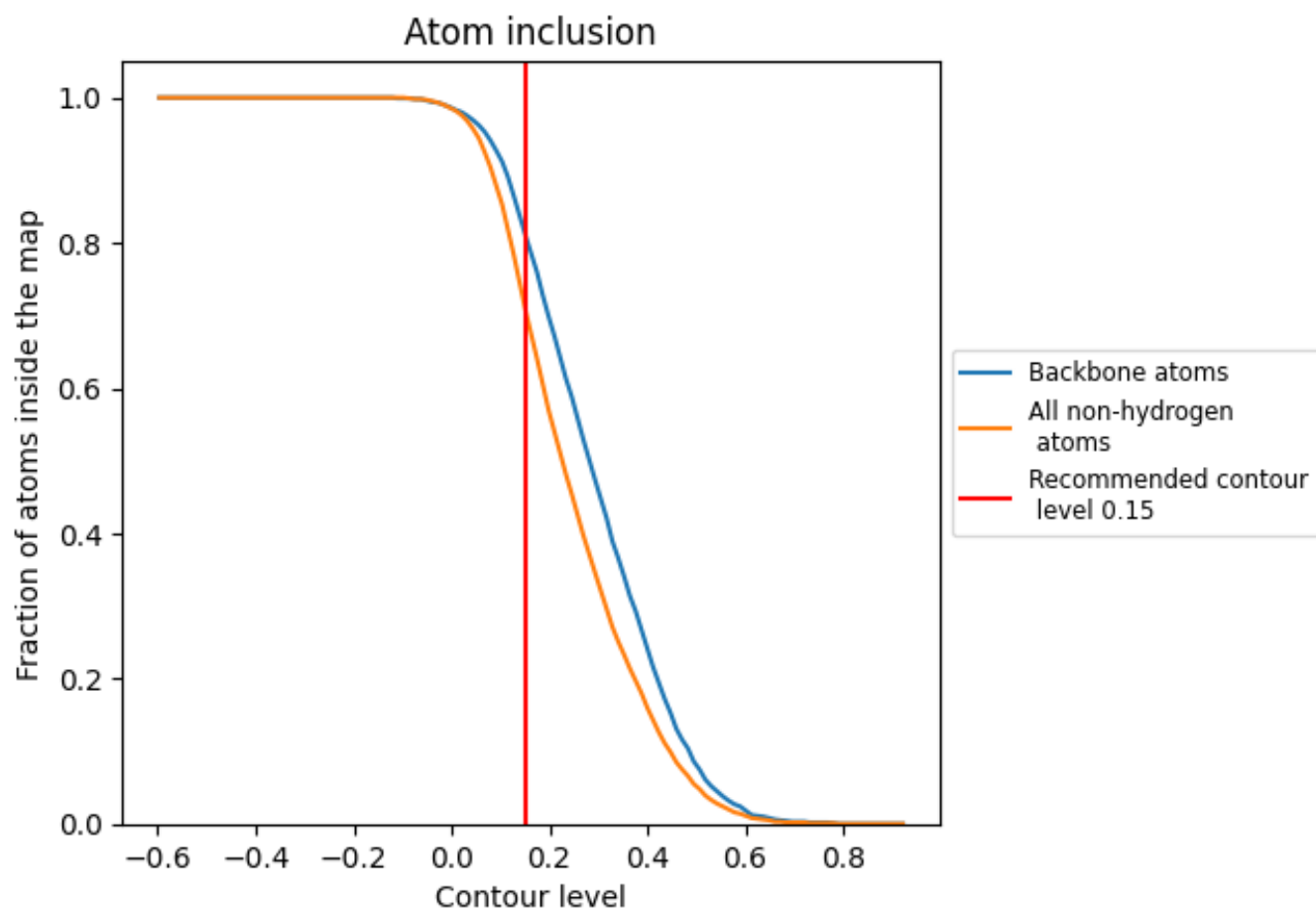
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).











9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7110	 0.4230
A	 0.7180	 0.4330
B	 0.6500	 0.3910
C	 0.7420	 0.4340
D	 0.6720	 0.4010

