



Full wwPDB EM Validation Report ⓘ

Nov 19, 2024 – 12:35 PM JST

PDB ID : 8ZB1
EMDB ID : EMD-39894
Title : Cryo-EM structure of the C26-FB1-bound Lac1-Lip1 complex
Authors : Xie, T.; Zhang, Z.; Fang, Q.; Gong, X.
Deposited on : 2024-04-25
Resolution : 2.86 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.39

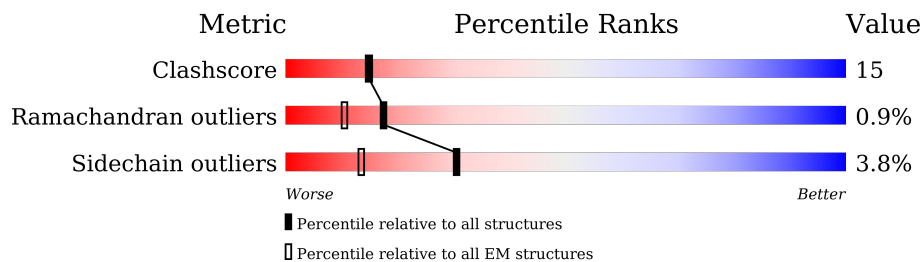
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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	428	
1	C	428	
2	B	150	
2	D	150	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7756 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 Ceramide synthase LAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	315	2636	1783	417	423	13	0	0
1	C	315	2636	1783	417	423	13	0	0

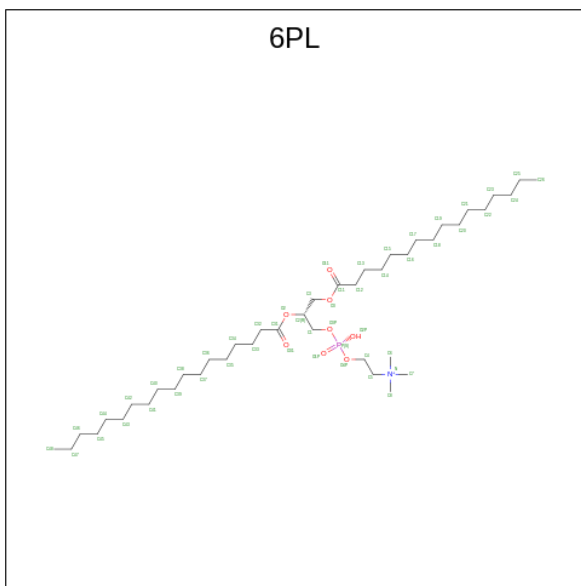
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	LEU	-	expression tag	UNP P28496
A	420	GLU	-	expression tag	UNP P28496
A	421	ASP	-	expression tag	UNP P28496
A	422	TYR	-	expression tag	UNP P28496
A	423	LYS	-	expression tag	UNP P28496
A	424	ASP	-	expression tag	UNP P28496
A	425	ASP	-	expression tag	UNP P28496
A	426	ASP	-	expression tag	UNP P28496
A	427	ASP	-	expression tag	UNP P28496
A	428	LYS	-	expression tag	UNP P28496
C	419	LEU	-	expression tag	UNP P28496
C	420	GLU	-	expression tag	UNP P28496
C	421	ASP	-	expression tag	UNP P28496
C	422	TYR	-	expression tag	UNP P28496
C	423	LYS	-	expression tag	UNP P28496
C	424	ASP	-	expression tag	UNP P28496
C	425	ASP	-	expression tag	UNP P28496
C	426	ASP	-	expression tag	UNP P28496
C	427	ASP	-	expression tag	UNP P28496
C	428	LYS	-	expression tag	UNP P28496

- Molecule 2 is a protein called Ceramide synthase subunit LIP1.

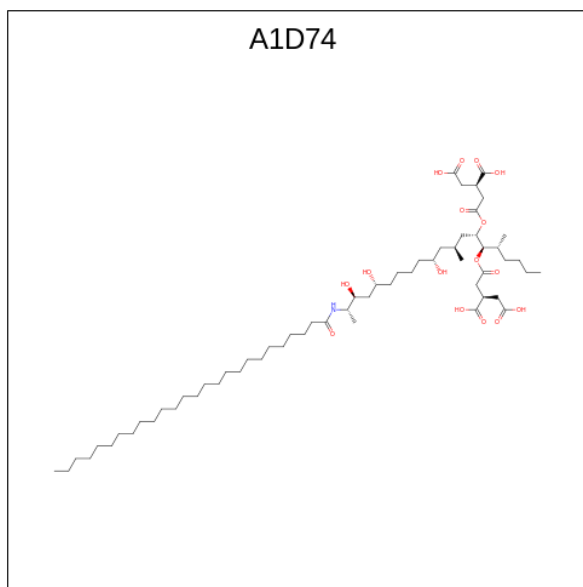
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	133	Total	C	N	O	S	0	0
			1089	703	178	202	6		
2	D	133	Total	C	N	O	S	0	0
			1089	703	178	202	6		

- Molecule 3 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: 6PL) (formula: C₄₂H₈₅NO₈P).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C			0
			18	18			
3	A	1	Total	C			0
			18	18			
3	B	1	Total	C	O	P	0
			40	31	8	1	
3	C	1	Total	C			0
			18	18			
3	C	1	Total	C			0
			18	18			
3	D	1	Total	C	O	P	0
			40	31	8	1	


- Molecule 4 is (2 {R})-2-[2-[(5 {R},6 {R},7 {S},9 {S},11 {R},16 {R},18 {S},19 {S})-6-[(3 {R})-3-carboxy-5-oxidanyl-5-oxidanylidene-pentanoyl]oxy-19-(hexacosanoylamino)-5,9-dimethyl-11,16,18-tris(oxidanyl)icosan-7-yl]oxy-2-oxidanylidene-ethyl]butanedioic acid (three-letter code: A1D74) (formula: C₆₀H₁₀₉NO₁₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
4	A	1	77	60	1	16	0
4	C	1	77	60	1	16	0


GLY
ILE
LEU
LYS
ASP
ARG
SER
ASP
SER
GLU
SER
ASP
GLU
GLU
SER
ASP
GLU
SER
SER
THR
THR
THR
PRO
THR
ASP
SER
THR
PRO
THR
LYS
LYS
ASP
ILE
LEU
GLU
ASP
TYR
LYS
LYS
ASP
ASP
ASP
LYS

- Molecule 2: Ceramide synthase subunit LIP1

Chain B:  75% 13% 11%

MET
SER
GLN
PRO
THR
PRO
ILE
ILE
THR
THR
LYS
SER
ALA
ALA
LYS
PRO
LYS
P18
I29
I34
E38
Y39
F40
Q60
V64
D76
E80
I88
E93
P94
N95
L99
S100
F101
Y114
K120
V129
G130
L137
L141
M150

- Molecule 2: Ceramide synthase subunit LIP1

Chain D:  77% 12% 11%

MET
SER
GLN
PRO
THR
PRO
ILE
ILE
THR
THR
LYS
SER
ALA
ALA
LYS
PRO
LYS
P18
I29
I34
E38
Y39
F40
Q60
V64
D76
I88
E93
P94
N95
L99
D107
Y114
K120
V129
G130
L137
L141
M150

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	275501	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.303	Depositor
Minimum map value	-3.033	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	274.432, 274.432, 274.432	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.072, 1.072, 1.072	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: 6PL, A1D74

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	0.61	13/2726 (0.5%)	0.57	4/3710 (0.1%)
1	C	0.61	13/2726 (0.5%)	0.57	4/3710 (0.1%)
2	B	0.34	0/1122	0.46	0/1523
2	D	0.34	0/1122	0.46	0/1523
All	All	0.55	26/7696 (0.3%)	0.54	8/10466 (0.1%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	PHE	CA-C	-7.88	1.32	1.52
1	C	201	PHE	CA-C	-7.87	1.32	1.52
1	C	200	TRP	CG-CD1	-7.16	1.26	1.36
1	A	200	TRP	CG-CD1	-7.16	1.26	1.36
1	A	200	TRP	CD2-CE2	-7.06	1.32	1.41
1	C	200	TRP	CD2-CE2	-7.00	1.32	1.41
1	C	200	TRP	CZ3-CH2	-6.71	1.29	1.40
1	A	200	TRP	CZ3-CH2	-6.67	1.29	1.40
1	A	200	TRP	C-O	-6.62	1.10	1.23
1	C	200	TRP	C-O	-6.61	1.10	1.23
1	A	201	PHE	CA-CB	-6.45	1.39	1.53
1	C	201	PHE	C-O	-6.41	1.11	1.23
1	C	201	PHE	CA-CB	-6.39	1.39	1.53
1	A	201	PHE	C-O	-6.38	1.11	1.23
1	A	202	PHE	CG-CD2	-5.77	1.30	1.38
1	C	202	PHE	CG-CD1	-5.70	1.30	1.38
1	A	202	PHE	CG-CD1	-5.68	1.30	1.38
1	C	202	PHE	CG-CD2	-5.68	1.30	1.38
1	C	201	PHE	CB-CG	-5.63	1.41	1.51
1	A	201	PHE	CB-CG	-5.61	1.41	1.51
1	A	200	TRP	CA-C	-5.56	1.38	1.52
1	C	200	TRP	CA-C	-5.51	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	202	PHE	C-O	-5.48	1.12	1.23
1	A	202	PHE	C-O	-5.46	1.12	1.23
1	C	202	PHE	N-CA	-5.06	1.36	1.46
1	A	202	PHE	N-CA	-5.01	1.36	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	TRP	C-N-CA	7.42	140.24	121.70
1	A	200	TRP	C-N-CA	7.42	140.24	121.70
1	C	201	PHE	N-CA-CB	6.59	122.47	110.60
1	A	201	PHE	N-CA-CB	6.57	122.42	110.60
1	A	302	LEU	CA-CB-CG	5.50	127.95	115.30
1	C	302	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	201	PHE	O-C-N	5.21	131.03	122.70
1	C	201	PHE	O-C-N	5.17	130.97	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2636	0	2623	93	0
1	C	2636	0	2623	97	0
2	B	1089	0	1045	17	0
2	D	1089	0	1045	15	0
3	A	36	0	70	5	0
3	B	40	0	56	4	0
3	C	36	0	70	6	0
3	D	40	0	56	4	0
4	A	77	0	0	7	0
4	C	77	0	0	7	0
All	All	7756	0	7588	229	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 15.

All (229) 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:C:279:TYR:CE1	4:C:503:A1D74:C19	2.31	1.14
1:A:279:TYR:CE1	4:A:503:A1D74:C19	2.31	1.14
2:B:40:PHE:HB2	3:B:201:6PL:H182	1.07	1.03
2:D:40:PHE:HB2	3:D:201:6PL:H182	1.07	1.03
1:C:382:ILE:HG23	1:C:383:LEU:HD22	1.46	0.96
1:A:382:ILE:HG23	1:A:383:LEU:HD22	1.46	0.95
1:C:279:TYR:HE1	4:C:503:A1D74:C19	1.80	0.95
2:D:40:PHE:CB	3:D:201:6PL:H182	1.97	0.95
1:A:279:TYR:HE1	4:A:503:A1D74:C19	1.80	0.93
2:B:40:PHE:CB	3:B:201:6PL:H182	1.97	0.92
1:C:129:GLY:O	3:C:501:6PL:H351	1.77	0.85
1:A:129:GLY:O	3:A:501:6PL:H351	1.77	0.85
2:D:40:PHE:HB2	3:D:201:6PL:C18	2.02	0.82
1:A:156:ARG:HB2	1:A:157:PRO:HD3	1.62	0.81
1:C:156:ARG:HB2	1:C:157:PRO:HD3	1.62	0.80
2:B:40:PHE:HB2	3:B:201:6PL:C18	2.02	0.78
1:C:246:ARG:O	1:C:247:LYS:C	2.22	0.78
1:A:246:ARG:O	1:A:247:LYS:C	2.22	0.77
1:A:163:HIS:CD2	1:A:163:HIS:H	2.02	0.77
1:A:323:LEU:HD12	1:A:365:GLN:HE21	1.49	0.75
1:C:323:LEU:HD12	1:C:365:GLN:HE21	1.49	0.75
1:A:264:TRP:HB2	3:A:501:6PL:H431	1.70	0.74
1:C:163:HIS:H	1:C:163:HIS:CD2	2.02	0.74
1:C:264:TRP:HB2	3:C:501:6PL:H431	1.70	0.74
1:C:382:ILE:CG2	1:C:383:LEU:HD22	2.19	0.72
1:A:382:ILE:CG2	1:A:383:LEU:HD22	2.19	0.71
2:D:88:ILE:HG12	2:D:129:VAL:HG21	1.71	0.71
2:B:88:ILE:HG12	2:B:129:VAL:HG21	1.71	0.71
1:A:284:VAL:HG21	1:A:317:LEU:HD13	1.76	0.67
1:C:379:LEU:O	1:C:382:ILE:HG22	1.94	0.67
1:C:284:VAL:HG21	1:C:317:LEU:HD13	1.76	0.67
1:A:379:LEU:O	1:A:382:ILE:HG22	1.94	0.67
1:A:246:ARG:O	1:A:246:ARG:HG2	1.95	0.66
1:C:246:ARG:O	1:C:246:ARG:HG2	1.95	0.66
1:A:87:PRO:HB2	1:A:145:PHE:HB2	1.78	0.66
1:C:166:SER:HB3	1:C:169:ARG:HB2	1.76	0.66
1:C:286:ASP:OD1	4:C:503:A1D74:C30	2.45	0.66
1:A:329:VAL:O	1:A:333:PHE:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:PRO:HB2	1:C:145:PHE:HB2	1.78	0.65
1:A:166:SER:HB3	1:A:169:ARG:HB2	1.76	0.65
1:C:382:ILE:CG2	1:C:383:LEU:CD2	2.75	0.65
1:C:382:ILE:HG23	1:C:383:LEU:CD2	2.26	0.65
1:C:329:VAL:O	1:C:333:PHE:HB2	1.96	0.64
1:A:156:ARG:HB2	1:A:157:PRO:CD	2.27	0.64
1:A:286:ASP:OD1	4:A:503:A1D74:C30	2.44	0.64
1:A:382:ILE:CG2	1:A:383:LEU:CD2	2.75	0.64
1:C:156:ARG:HB2	1:C:157:PRO:CD	2.27	0.64
1:C:156:ARG:CB	1:C:157:PRO:HD3	2.28	0.63
1:A:304:PHE:CE2	1:A:382:ILE:HD12	2.34	0.63
1:C:304:PHE:CE2	1:C:382:ILE:HD12	2.34	0.62
1:A:156:ARG:CB	1:A:157:PRO:HD3	2.28	0.61
1:A:151:MET:HA	1:A:155:ILE:HD12	1.82	0.61
2:B:137:LEU:O	2:B:141:LEU:HB2	2.01	0.61
1:A:323:LEU:HD12	1:A:365:GLN:NE2	2.17	0.60
1:C:172:ARG:HB3	1:C:297:TYR:CZ	2.37	0.60
1:A:377:ARG:HG2	1:A:377:ARG:HH21	1.67	0.59
1:C:377:ARG:HG2	1:C:377:ARG:HH21	1.67	0.59
2:D:137:LEU:O	2:D:141:LEU:HB2	2.01	0.59
1:A:172:ARG:HB3	1:A:297:TYR:CZ	2.37	0.59
1:C:151:MET:HA	1:C:155:ILE:HD12	1.82	0.58
1:C:172:ARG:HB3	1:C:297:TYR:OH	2.03	0.58
1:C:98:TYR:OH	1:C:104:THR:O	2.19	0.58
1:A:172:ARG:HB3	1:A:297:TYR:OH	2.03	0.58
1:C:84:TRP:HB3	1:C:148:GLU:HB2	1.86	0.57
1:A:304:PHE:CE2	1:A:382:ILE:CD1	2.88	0.57
1:A:84:TRP:HB3	1:A:148:GLU:HB2	1.86	0.57
1:C:207:MET:HE3	1:C:274:MET:HG3	1.86	0.57
2:D:64:VAL:HG12	2:D:130:GLY:HA3	1.88	0.56
1:C:91:LEU:HD11	1:C:142:PHE:HA	1.88	0.56
1:C:280:ILE:O	1:C:284:VAL:HG22	2.06	0.56
1:A:189:PHE:CE2	1:A:223:PHE:HB2	2.41	0.56
2:B:64:VAL:HG12	2:B:130:GLY:HA3	1.88	0.56
1:A:246:ARG:O	1:A:247:LYS:O	2.23	0.56
1:C:304:PHE:CE2	1:C:382:ILE:CD1	2.88	0.56
1:A:91:LEU:HD11	1:A:142:PHE:HA	1.88	0.56
1:C:246:ARG:O	1:C:247:LYS:O	2.23	0.55
1:C:323:LEU:HD12	1:C:365:GLN:NE2	2.17	0.55
1:C:156:ARG:CB	1:C:157:PRO:CD	2.85	0.55
1:A:207:MET:HG3	1:A:274:MET:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:HD1	1:A:220:PHE:O	1.90	0.55
1:C:189:PHE:CE2	1:C:223:PHE:HB2	2.41	0.55
1:A:280:ILE:O	1:A:284:VAL:HG22	2.06	0.55
1:A:98:TYR:OH	1:A:104:THR:O	2.19	0.54
2:B:114:TYR:CD1	2:B:120:LYS:HB3	2.43	0.54
1:C:207:MET:HG3	1:C:274:MET:HA	1.89	0.54
1:A:382:ILE:HG23	1:A:383:LEU:CD2	2.26	0.54
2:D:114:TYR:CD1	2:D:120:LYS:HB3	2.43	0.54
1:A:189:PHE:CD2	1:A:223:PHE:HD1	2.26	0.54
3:A:501:6PL:H332	2:B:38:GLU:OE1	2.07	0.53
1:C:220:PHE:HD1	1:C:220:PHE:O	1.90	0.53
1:A:260:LEU:HD12	3:A:501:6PL:H441	1.90	0.53
1:A:156:ARG:CB	1:A:157:PRO:CD	2.85	0.53
3:C:501:6PL:H332	2:D:38:GLU:OE1	2.07	0.53
1:C:284:VAL:CG2	1:C:317:LEU:HD13	2.39	0.53
1:C:260:LEU:HD12	3:C:501:6PL:H441	1.90	0.53
1:A:289:LEU:HB2	1:A:310:PHE:CE1	2.44	0.52
1:A:128:LYS:NZ	1:A:267:TYR:O	2.39	0.52
1:A:354:LEU:HB3	1:A:355:PRO:HD3	1.92	0.52
1:A:377:ARG:HG2	1:A:377:ARG:NH2	2.23	0.52
1:C:189:PHE:CD2	1:C:223:PHE:HD1	2.26	0.52
1:C:377:ARG:HG2	1:C:377:ARG:NH2	2.23	0.52
1:C:289:LEU:HB2	1:C:310:PHE:CE1	2.44	0.52
1:C:128:LYS:NZ	1:C:267:TYR:O	2.39	0.51
1:A:199:LEU:HD11	1:A:273:LYS:HG2	1.93	0.51
1:A:284:VAL:CG2	1:A:317:LEU:HD13	2.39	0.51
1:C:354:LEU:HB3	1:C:355:PRO:HD3	1.92	0.51
1:A:165:THR:O	1:A:165:THR:HG22	2.09	0.51
1:C:168:HIS:O	1:C:172:ARG:HD3	2.11	0.51
1:A:316:TYR:HD2	1:A:317:LEU:HG	1.76	0.51
1:C:165:THR:O	1:C:165:THR:HG22	2.09	0.51
2:D:99:LEU:HD23	2:D:99:LEU:H	1.76	0.51
1:A:168:HIS:O	1:A:172:ARG:HD3	2.11	0.50
2:B:99:LEU:H	2:B:99:LEU:HD23	1.75	0.50
1:C:199:LEU:HD11	1:C:273:LYS:HG2	1.93	0.50
2:D:60:GLN:HB2	2:D:64:VAL:HG23	1.94	0.50
1:A:158:PHE:CD1	1:A:177:MET:CE	2.94	0.50
1:C:158:PHE:CD1	1:C:177:MET:CE	2.94	0.50
1:C:163:HIS:CD2	1:C:163:HIS:N	2.78	0.50
1:A:158:PHE:CD1	1:A:177:MET:HE1	2.47	0.49
2:B:60:GLN:HB2	2:B:64:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:HIS:CD2	1:A:163:HIS:N	2.78	0.49
1:C:316:TYR:HD2	1:C:317:LEU:HG	1.76	0.49
1:C:347:GLN:HE22	1:C:349:LYS:HB3	1.77	0.49
2:D:93:GLU:OE1	2:D:95:ASN:ND2	2.38	0.49
2:B:76:ASP:OD1	2:B:76:ASP:N	2.46	0.49
1:A:181:PHE:O	1:A:185:VAL:HG23	2.13	0.49
1:C:181:PHE:O	1:C:185:VAL:HG23	2.13	0.49
1:A:304:PHE:HE2	1:A:382:ILE:HD12	1.77	0.48
1:A:347:GLN:HE22	1:A:349:LYS:HB3	1.77	0.48
1:C:304:PHE:HE2	1:C:382:ILE:HD12	1.77	0.48
1:C:147:ARG:HH21	1:C:147:ARG:HG2	1.79	0.48
1:C:158:PHE:CE1	1:C:177:MET:HE3	2.49	0.48
1:C:86:ALA:HB3	1:C:87:PRO:HD3	1.96	0.48
1:A:147:ARG:HG2	1:A:147:ARG:HH21	1.79	0.47
1:A:244:LYS:HA	1:A:244:LYS:HD3	1.56	0.47
3:C:502:6PL:H321	3:C:502:6PL:H352	1.32	0.47
1:A:86:ALA:HB3	1:A:87:PRO:HD3	1.96	0.47
1:C:158:PHE:CD1	1:C:177:MET:HE3	2.49	0.47
1:C:244:LYS:HD3	1:C:244:LYS:HA	1.56	0.47
1:A:304:PHE:CD2	1:A:382:ILE:CD1	2.98	0.47
1:A:302:LEU:HD23	1:A:302:LEU:O	2.14	0.47
1:A:304:PHE:CD2	1:A:382:ILE:HD12	2.50	0.47
1:C:302:LEU:HD23	1:C:302:LEU:O	2.14	0.47
1:A:186:SER:CB	3:A:502:6PL:H481	2.45	0.47
1:C:151:MET:SD	1:C:174:MET:HG2	2.55	0.47
1:C:304:PHE:CD2	1:C:382:ILE:HD12	2.50	0.47
1:C:304:PHE:CD2	1:C:382:ILE:CD1	2.98	0.47
4:C:503:A1D74:C67	4:C:503:A1D74:C61	2.93	0.47
1:A:156:ARG:HD2	1:A:156:ARG:HA	1.51	0.46
2:D:76:ASP:OD1	2:D:76:ASP:N	2.46	0.46
1:C:120:ILE:O	1:C:123:THR:HG22	2.15	0.46
1:A:167:LYS:HB3	1:A:167:LYS:HE3	1.42	0.46
1:C:186:SER:CB	3:C:502:6PL:H481	2.45	0.46
1:A:126:TYR:N	1:A:126:TYR:CD2	2.83	0.46
1:C:334:ARG:HG2	1:C:339:TYR:CZ	2.51	0.46
1:A:151:MET:SD	1:A:174:MET:HG2	2.55	0.46
1:A:120:ILE:O	1:A:123:THR:HG22	2.15	0.46
1:A:334:ARG:HG2	1:A:339:TYR:CZ	2.51	0.46
1:C:347:GLN:NE2	1:C:349:LYS:O	2.49	0.46
1:A:207:MET:HE3	1:A:274:MET:HG3	1.97	0.46
1:A:279:TYR:CD1	4:A:503:A1D74:C19	2.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:GLN:NE2	1:A:349:LYS:O	2.49	0.46
1:A:172:ARG:CB	1:A:297:TYR:OH	2.64	0.45
1:C:180:ILE:HG13	1:C:290:SER:HB3	1.98	0.45
4:A:503:A1D74:C61	4:A:503:A1D74:C67	2.94	0.45
1:A:180:ILE:HG13	1:A:290:SER:HB3	1.98	0.45
1:C:126:TYR:N	1:C:126:TYR:CD2	2.83	0.45
1:C:172:ARG:CB	1:C:297:TYR:OH	2.64	0.45
1:A:246:ARG:C	1:A:247:LYS:O	2.54	0.45
2:B:93:GLU:OE1	2:B:95:ASN:ND2	2.38	0.45
1:A:78:ILE:HG22	1:A:85:ILE:HG21	1.99	0.45
1:C:250:ASN:C	1:C:252:LEU:N	2.71	0.44
1:C:246:ARG:C	1:C:247:LYS:O	2.54	0.44
1:C:238:LEU:HD23	1:C:238:LEU:HA	1.81	0.44
1:C:255:HIS:NE2	4:C:503:A1D74:N28	2.65	0.44
1:C:207:MET:CE	1:C:274:MET:HG3	2.47	0.44
3:D:201:6PL:H332	3:D:201:6PL:H361	1.61	0.44
1:A:243:GLU:OE1	1:A:244:LYS:O	2.36	0.44
1:A:255:HIS:NE2	4:A:503:A1D74:N28	2.65	0.44
1:C:156:ARG:HA	1:C:156:ARG:HD2	1.51	0.44
2:B:34:ILE:O	2:B:38:GLU:HG2	2.18	0.44
1:A:180:ILE:HD11	1:A:291:PHE:HA	2.00	0.44
1:A:207:MET:CE	1:A:274:MET:HG3	2.47	0.44
1:C:78:ILE:HG22	1:C:85:ILE:HG21	1.99	0.44
1:A:158:PHE:CE1	1:A:177:MET:HE3	2.53	0.44
1:A:172:ARG:CB	1:A:297:TYR:CZ	3.01	0.43
1:A:250:ASN:C	1:A:252:LEU:N	2.71	0.43
1:C:243:GLU:OE1	1:C:244:LYS:O	2.35	0.43
3:B:201:6PL:H361	3:B:201:6PL:H332	1.61	0.43
1:C:250:ASN:C	1:C:252:LEU:H	2.22	0.43
1:C:220:PHE:O	1:C:220:PHE:CD1	2.70	0.43
1:A:101:SER:OG	1:A:102:GLY:N	2.50	0.42
1:A:333:PHE:O	1:A:349:LYS:NZ	2.46	0.42
1:C:167:LYS:HE3	1:C:167:LYS:HB3	1.42	0.42
1:C:180:ILE:HD11	1:C:291:PHE:HA	2.00	0.42
1:C:333:PHE:O	1:C:349:LYS:NZ	2.46	0.42
2:D:34:ILE:O	2:D:38:GLU:HG2	2.18	0.42
1:A:157:PRO:O	1:A:161:ARG:HD3	2.20	0.42
1:A:250:ASN:C	1:A:252:LEU:H	2.22	0.42
1:A:219:LEU:HA	1:A:222:VAL:HG22	2.01	0.42
1:C:101:SER:OG	1:C:102:GLY:N	2.50	0.42
1:C:219:LEU:HA	1:C:222:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:PRO:O	1:C:161:ARG:HD3	2.20	0.42
1:A:223:PHE:CE2	1:A:279:TYR:HD2	2.38	0.42
1:A:233:GLN:HA	1:A:236:CYS:SG	2.60	0.42
2:B:101:PHE:HE1	2:B:150:MET:HE3	1.85	0.42
4:A:503:A1D74:C61	4:A:503:A1D74:C69	2.98	0.41
2:B:64:VAL:HA	2:B:129:VAL:O	2.20	0.41
1:C:172:ARG:CB	1:C:297:TYR:CZ	3.01	0.41
2:D:64:VAL:HA	2:D:129:VAL:O	2.20	0.41
1:A:147:ARG:HG3	1:A:178:TYR:CE2	2.56	0.41
4:C:503:A1D74:C61	4:C:503:A1D74:C69	2.98	0.41
1:C:279:TYR:CD1	4:C:503:A1D74:C19	2.95	0.41
1:C:223:PHE:CE2	1:C:279:TYR:HD2	2.38	0.41
1:C:233:GLN:HA	1:C:236:CYS:SG	2.60	0.41
1:C:285:SER:CB	1:C:318:ARG:HE	2.34	0.41
1:A:204:THR:O	1:A:207:MET:HB3	2.21	0.41
1:A:363:ALA:O	1:A:367:VAL:HG23	2.20	0.41
1:C:158:PHE:CD1	1:C:177:MET:HE1	2.55	0.41
1:C:382:ILE:HG22	1:C:383:LEU:HD23	2.03	0.41
1:A:78:ILE:O	1:A:82:HIS:N	2.52	0.41
2:D:107:ASP:N	2:D:107:ASP:OD1	2.50	0.41
1:C:250:ASN:O	1:C:252:LEU:N	2.54	0.40
2:B:76:ASP:O	2:B:80:GLU:HG3	2.21	0.40
2:B:114:TYR:HD1	2:B:120:LYS:HB3	1.85	0.40
1:C:194:MET:HE3	1:C:201:PHE:H	1.86	0.40
1:A:220:PHE:O	1:A:220:PHE:CD1	2.70	0.40
1:C:204:THR:O	1:C:207:MET:HB3	2.21	0.40
1:C:220:PHE:CD1	1:C:220:PHE:C	2.94	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	313/428 (73%)	289 (92%)	20 (6%)	4 (1%)	10	22
1	C	313/428 (73%)	288 (92%)	21 (7%)	4 (1%)	10	22
2	B	131/150 (87%)	125 (95%)	6 (5%)	0	100	100
2	D	131/150 (87%)	125 (95%)	6 (5%)	0	100	100
All	All	888/1156 (77%)	827 (93%)	53 (6%)	8 (1%)	17	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	HIS
1	A	202	PHE
1	A	246	ARG
1	C	163	HIS
1	C	202	PHE
1	C	246	ARG
1	A	247	LYS
1	C	247	LYS

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	279/391 (71%)	265 (95%)	14 (5%)	20	40
1	C	279/391 (71%)	265 (95%)	14 (5%)	20	40
2	B	120/135 (89%)	119 (99%)	1 (1%)	79	90
2	D	120/135 (89%)	119 (99%)	1 (1%)	79	90
All	All	798/1052 (76%)	768 (96%)	30 (4%)	30	54

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	LYS
1	A	126	TYR
1	A	156	ARG

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Mol	Chain	Res	Type
1	A	163	HIS
1	A	175	GLU
1	A	201	PHE
1	A	220	PHE
1	A	238	LEU
1	A	244	LYS
1	A	246	ARG
1	A	299	ASP
1	A	377	ARG
1	A	381	ARG
1	A	382	ILE
2	B	29	ILE
1	C	106	LYS
1	C	126	TYR
1	C	156	ARG
1	C	163	HIS
1	C	175	GLU
1	C	201	PHE
1	C	220	PHE
1	C	238	LEU
1	C	244	LYS
1	C	246	ARG
1	C	299	ASP
1	C	377	ARG
1	C	381	ARG
1	C	382	ILE
2	D	29	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	HIS
1	A	347	GLN
1	A	365	GLN
1	C	163	HIS
1	C	347	GLN
1	C	365	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	6PL	C	501	-	17,17,51	0.22	0	16,16,59	0.63	0
3	6PL	C	502	-	17,17,51	0.22	0	16,16,59	0.62	0
3	6PL	B	201	-	39,39,51	1.07	2 (5%)	43,44,59	1.14	4 (9%)
3	6PL	D	201	-	39,39,51	1.07	2 (5%)	43,44,59	1.14	4 (9%)
4	A1D74	A	503	-	76,76,76	1.12	6 (7%)	89,92,92	1.33	12 (13%)
3	6PL	A	502	-	17,17,51	0.22	0	16,16,59	0.62	0
4	A1D74	C	503	-	76,76,76	1.12	6 (7%)	89,92,92	1.33	12 (13%)
3	6PL	A	501	-	17,17,51	0.22	0	16,16,59	0.63	0

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	6PL	C	501	-	-	10/15/15/55	-
3	6PL	C	502	-	-	11/15/15/55	-
3	6PL	B	201	-	-	15/41/41/55	-
3	6PL	D	201	-	-	15/41/41/55	-
4	A1D74	A	503	-	-	41/96/96/96	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6PL	A	502	-	-	11/15/15/55	-
4	A1D74	C	503	-	-	41/96/96/96	-
3	6PL	A	501	-	-	10/15/15/55	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	A1D74	C26-N28	5.43	1.45	1.34
4	C	503	A1D74	C26-N28	5.43	1.45	1.34
3	B	201	6PL	O3-C11	4.28	1.45	1.33
3	D	201	6PL	O3-C11	4.28	1.45	1.33
3	B	201	6PL	O2-C31	4.13	1.45	1.34
3	D	201	6PL	O2-C31	4.13	1.45	1.34
4	A	503	A1D74	O47-C46	-3.32	1.40	1.46
4	C	503	A1D74	O47-C46	-3.32	1.40	1.46
4	A	503	A1D74	O66-C59	-2.97	1.40	1.44
4	C	503	A1D74	O66-C59	-2.97	1.40	1.44
4	A	503	A1D74	O47-C48	2.21	1.40	1.34
4	C	503	A1D74	O47-C48	2.21	1.40	1.34
4	C	503	A1D74	O66-C67	2.18	1.40	1.34
4	A	503	A1D74	O66-C67	2.17	1.40	1.34
4	A	503	A1D74	O27-C26	-2.11	1.19	1.23
4	C	503	A1D74	O27-C26	-2.11	1.19	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	A1D74	O47-C48-C49	4.65	120.01	111.46
4	C	503	A1D74	O47-C48-C49	4.65	120.01	111.46
4	C	503	A1D74	O66-C67-C69	4.63	119.97	111.46
4	A	503	A1D74	O66-C67-C69	4.61	119.93	111.46
3	B	201	6PL	O2-C31-C32	3.92	119.94	111.50
3	D	201	6PL	O2-C31-C32	3.92	119.94	111.50
4	A	503	A1D74	C30-C29-C31	-2.78	109.49	112.12
4	C	503	A1D74	C30-C29-C31	-2.75	109.52	112.12
4	A	503	A1D74	C60-C59-C46	-2.70	109.39	115.36
4	C	503	A1D74	C60-C59-C46	-2.70	109.39	115.36
3	B	201	6PL	O3-C11-C12	2.62	120.14	111.91
3	D	201	6PL	O3-C11-C12	2.62	120.14	111.91
4	A	503	A1D74	C25-C26-N28	2.43	120.05	115.83
4	C	503	A1D74	C25-C26-N28	2.43	120.05	115.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	6PL	O2P-P-O1P	2.36	119.92	110.68
3	B	201	6PL	O2P-P-O1P	2.36	119.91	110.68
4	A	503	A1D74	O73-C71-C70	2.22	120.03	114.21
4	C	503	A1D74	O73-C71-C70	2.22	120.03	114.21
4	A	503	A1D74	O52-C51-C50	2.20	119.97	114.21
4	C	503	A1D74	O52-C51-C50	2.19	119.94	114.21
4	C	503	A1D74	O58-C48-C49	-2.16	119.95	124.73
4	A	503	A1D74	O68-C67-C69	-2.16	119.97	124.73
4	C	503	A1D74	O68-C67-C69	-2.16	119.97	124.73
4	A	503	A1D74	O58-C48-C49	-2.14	120.00	124.73
4	C	503	A1D74	C59-O66-C67	-2.13	113.98	117.53
4	A	503	A1D74	C59-O66-C67	-2.13	113.98	117.53
4	A	503	A1D74	C45-C46-C59	-2.11	109.30	113.34
4	C	503	A1D74	C45-C46-C59	-2.11	109.30	113.34
4	C	503	A1D74	C43-C42-C40	-2.04	112.08	115.59
4	A	503	A1D74	C43-C42-C40	-2.03	112.10	115.59
3	B	201	6PL	C2-O2-C31	-2.02	112.81	117.79
3	D	201	6PL	C2-O2-C31	-2.02	112.81	117.79

There are no chirality outliers.

All (154) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	A1D74	C43-C45-C46-O47
4	A	503	A1D74	C59-C46-O47-C48
4	A	503	A1D74	C31-C33-C34-C36
4	A	503	A1D74	C31-C33-C34-O35
4	A	503	A1D74	C49-C48-O47-C46
4	A	503	A1D74	O58-C48-O47-C46
4	A	503	A1D74	C69-C67-O66-C59
4	A	503	A1D74	C29-C31-C33-C34
4	A	503	A1D74	O32-C31-C33-C34
4	A	503	A1D74	C67-C69-C70-C71
4	A	503	A1D74	C49-C50-C54-C55
4	A	503	A1D74	C51-C50-C54-C55
4	A	503	A1D74	C54-C50-C51-O52
4	A	503	A1D74	C54-C50-C51-O53
4	A	503	A1D74	C30-C29-N28-C26
4	C	503	A1D74	C43-C45-C46-O47
4	C	503	A1D74	C59-C46-O47-C48
4	C	503	A1D74	C31-C33-C34-C36
4	C	503	A1D74	C31-C33-C34-O35

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Mol	Chain	Res	Type	Atoms
4	C	503	A1D74	C49-C48-O47-C46
4	C	503	A1D74	O58-C48-O47-C46
4	C	503	A1D74	C69-C67-O66-C59
4	C	503	A1D74	C29-C31-C33-C34
4	C	503	A1D74	O32-C31-C33-C34
4	C	503	A1D74	C67-C69-C70-C71
4	C	503	A1D74	C49-C50-C54-C55
4	C	503	A1D74	C51-C50-C54-C55
4	C	503	A1D74	C54-C50-C51-O52
4	C	503	A1D74	C54-C50-C51-O53
4	C	503	A1D74	C30-C29-N28-C26
4	A	503	A1D74	O68-C67-O66-C59
4	C	503	A1D74	O68-C67-O66-C59
3	B	201	6PL	C12-C11-O3-C3
3	D	201	6PL	C12-C11-O3-C3
3	B	201	6PL	O11-C11-O3-C3
3	D	201	6PL	O11-C11-O3-C3
3	A	502	6PL	C32-C33-C34-C35
3	C	502	6PL	C32-C33-C34-C35
4	A	503	A1D74	C17-C18-C19-C20
4	C	503	A1D74	C17-C18-C19-C20
3	A	502	6PL	C34-C35-C36-C37
3	A	502	6PL	C43-C44-C45-C46
3	C	502	6PL	C34-C35-C36-C37
3	C	502	6PL	C43-C44-C45-C46
4	A	503	A1D74	C08-C09-C10-C11
4	C	503	A1D74	C08-C09-C10-C11
3	A	502	6PL	C44-C45-C46-C47
3	C	502	6PL	C44-C45-C46-C47
3	A	502	6PL	C41-C42-C43-C44
3	C	502	6PL	C41-C42-C43-C44
3	A	502	6PL	C42-C43-C44-C45
3	B	201	6PL	C21-C22-C23-C24
3	C	502	6PL	C42-C43-C44-C45
3	D	201	6PL	C21-C22-C23-C24
3	A	501	6PL	C34-C35-C36-C37
3	B	201	6PL	C33-C34-C35-C36
3	C	501	6PL	C34-C35-C36-C37
3	D	201	6PL	C33-C34-C35-C36
4	A	503	A1D74	C13-C14-C15-C16
4	C	503	A1D74	C13-C14-C15-C16
3	A	501	6PL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
3	C	501	6PL	C33-C34-C35-C36
3	A	502	6PL	C38-C39-C40-C41
3	C	502	6PL	C38-C39-C40-C41
3	A	501	6PL	C43-C44-C45-C46
3	C	501	6PL	C43-C44-C45-C46
4	A	503	A1D74	C06-C07-C08-C09
3	A	502	6PL	C33-C34-C35-C36
3	C	502	6PL	C33-C34-C35-C36
4	C	503	A1D74	C06-C07-C08-C09
3	A	501	6PL	C32-C33-C34-C35
3	C	501	6PL	C32-C33-C34-C35
3	B	201	6PL	C15-C16-C17-C18
3	D	201	6PL	C15-C16-C17-C18
4	C	503	A1D74	C19-C20-C21-C22
4	A	503	A1D74	C19-C20-C21-C22
4	A	503	A1D74	C23-C24-C25-C26
4	C	503	A1D74	C23-C24-C25-C26
3	B	201	6PL	C39-C40-C41-C42
3	D	201	6PL	C39-C40-C41-C42
3	B	201	6PL	C36-C37-C38-C39
3	D	201	6PL	C36-C37-C38-C39
4	A	503	A1D74	C02-C03-C04-C05
4	C	503	A1D74	C02-C03-C04-C05
4	A	503	A1D74	C18-C19-C20-C21
4	C	503	A1D74	C18-C19-C20-C21
3	A	501	6PL	C40-C41-C42-C43
3	A	501	6PL	C41-C42-C43-C44
3	C	501	6PL	C41-C42-C43-C44
3	C	501	6PL	C40-C41-C42-C43
3	A	502	6PL	C35-C36-C37-C38
3	C	502	6PL	C35-C36-C37-C38
3	B	201	6PL	C1-O3P-P-O1P
3	D	201	6PL	C1-O3P-P-O1P
3	A	502	6PL	C39-C40-C41-C42
3	C	502	6PL	C39-C40-C41-C42
4	A	503	A1D74	C09-C10-C11-C12
4	C	503	A1D74	C09-C10-C11-C12
4	C	503	A1D74	C60-C61-C62-C63
3	A	502	6PL	C31-C32-C33-C34
3	C	502	6PL	C31-C32-C33-C34
4	A	503	A1D74	C60-C61-C62-C63
4	C	503	A1D74	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
4	A	503	A1D74	C22-C23-C24-C25
3	A	501	6PL	C39-C40-C41-C42
3	C	501	6PL	C39-C40-C41-C42
4	A	503	A1D74	C38-C39-C40-O41
4	C	503	A1D74	C38-C39-C40-O41
4	A	503	A1D74	C07-C08-C09-C10
4	C	503	A1D74	C07-C08-C09-C10
4	A	503	A1D74	C01-C02-C03-C04
4	C	503	A1D74	C01-C02-C03-C04
4	A	503	A1D74	C60-C59-O66-C67
4	C	503	A1D74	C60-C59-O66-C67
4	A	503	A1D74	C21-C22-C23-C24
4	C	503	A1D74	C21-C22-C23-C24
3	B	201	6PL	C11-C12-C13-C14
3	D	201	6PL	C11-C12-C13-C14
4	A	503	A1D74	C67-C69-C70-C74
4	C	503	A1D74	C67-C69-C70-C74
4	A	503	A1D74	C50-C54-C55-O56
4	C	503	A1D74	C50-C54-C55-O56
3	B	201	6PL	C12-C13-C14-C15
3	D	201	6PL	C12-C13-C14-C15
4	A	503	A1D74	C04-C05-C06-C07
4	C	503	A1D74	C04-C05-C06-C07
3	B	201	6PL	C1-C2-C3-O3
3	D	201	6PL	C1-C2-C3-O3
3	B	201	6PL	O2-C2-C3-O3
3	D	201	6PL	O2-C2-C3-O3
4	A	503	A1D74	O66-C59-C60-C65
4	C	503	A1D74	O66-C59-C60-C65
4	A	503	A1D74	C50-C54-C55-O57
4	C	503	A1D74	C50-C54-C55-O57
4	A	503	A1D74	O47-C46-C59-C60
4	C	503	A1D74	O47-C46-C59-C60
4	A	503	A1D74	C46-C59-O66-C67
4	C	503	A1D74	C46-C59-O66-C67
3	A	501	6PL	C45-C46-C47-C48
3	C	501	6PL	C45-C46-C47-C48
4	A	503	A1D74	O47-C46-C59-O66
4	C	503	A1D74	O47-C46-C59-O66
3	C	501	6PL	C37-C38-C39-C40
4	A	503	A1D74	C31-C29-N28-C26
4	C	503	A1D74	C31-C29-N28-C26

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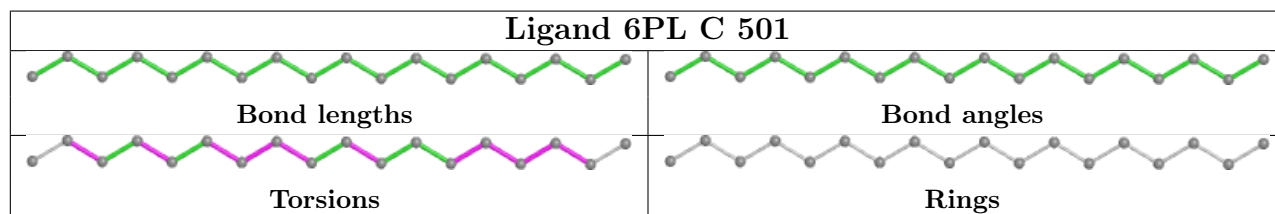
Mol	Chain	Res	Type	Atoms
3	A	501	6PL	C37-C38-C39-C40
3	B	201	6PL	O2-C31-C32-C33
3	D	201	6PL	O2-C31-C32-C33
3	B	201	6PL	C19-C20-C21-C22
3	D	201	6PL	C19-C20-C21-C22
3	A	501	6PL	C31-C32-C33-C34
3	C	501	6PL	C31-C32-C33-C34
3	B	201	6PL	O31-C31-C32-C33
3	D	201	6PL	O31-C31-C32-C33

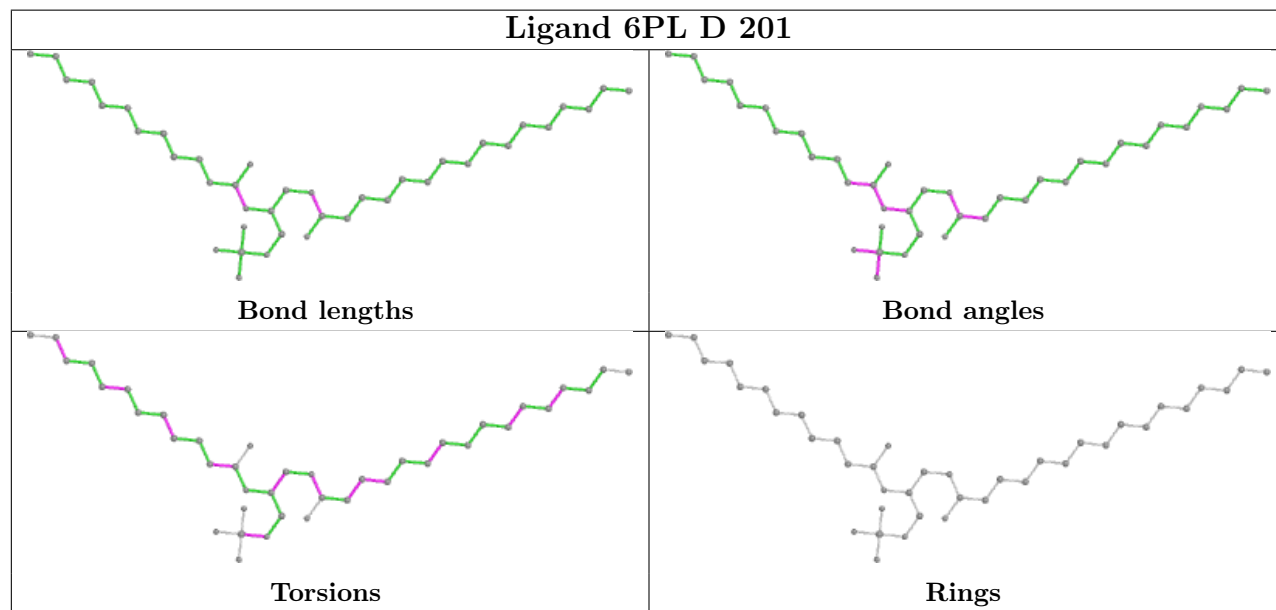
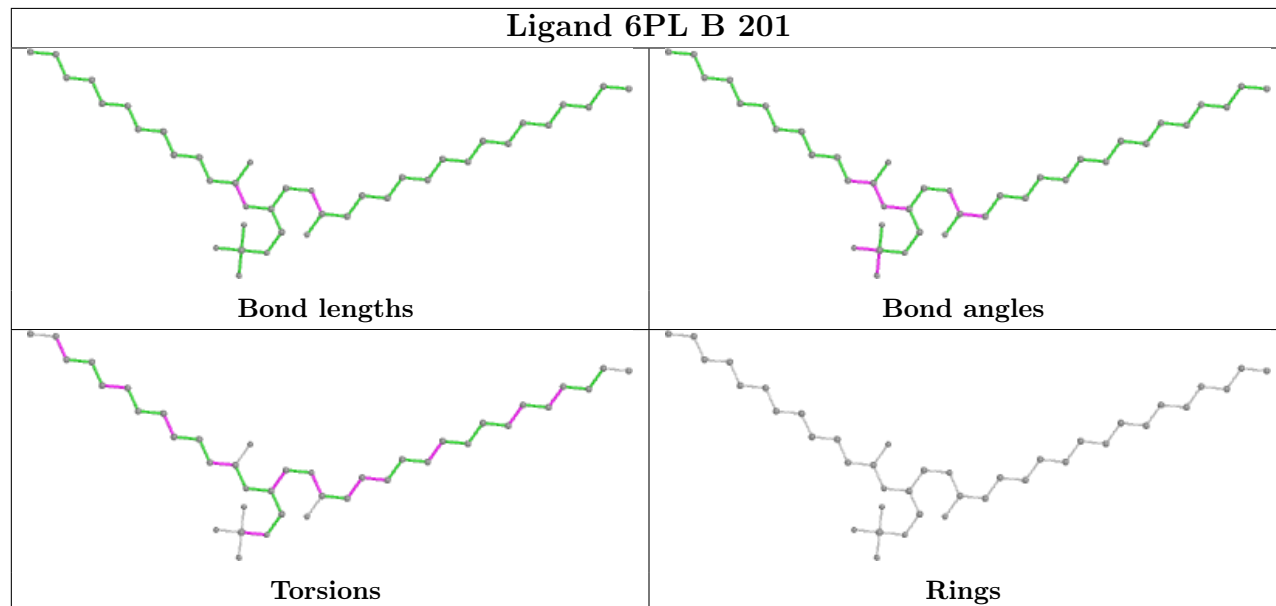
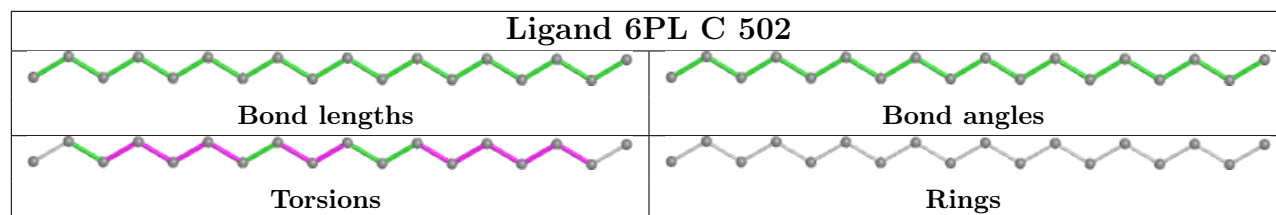
There are no ring outliers.

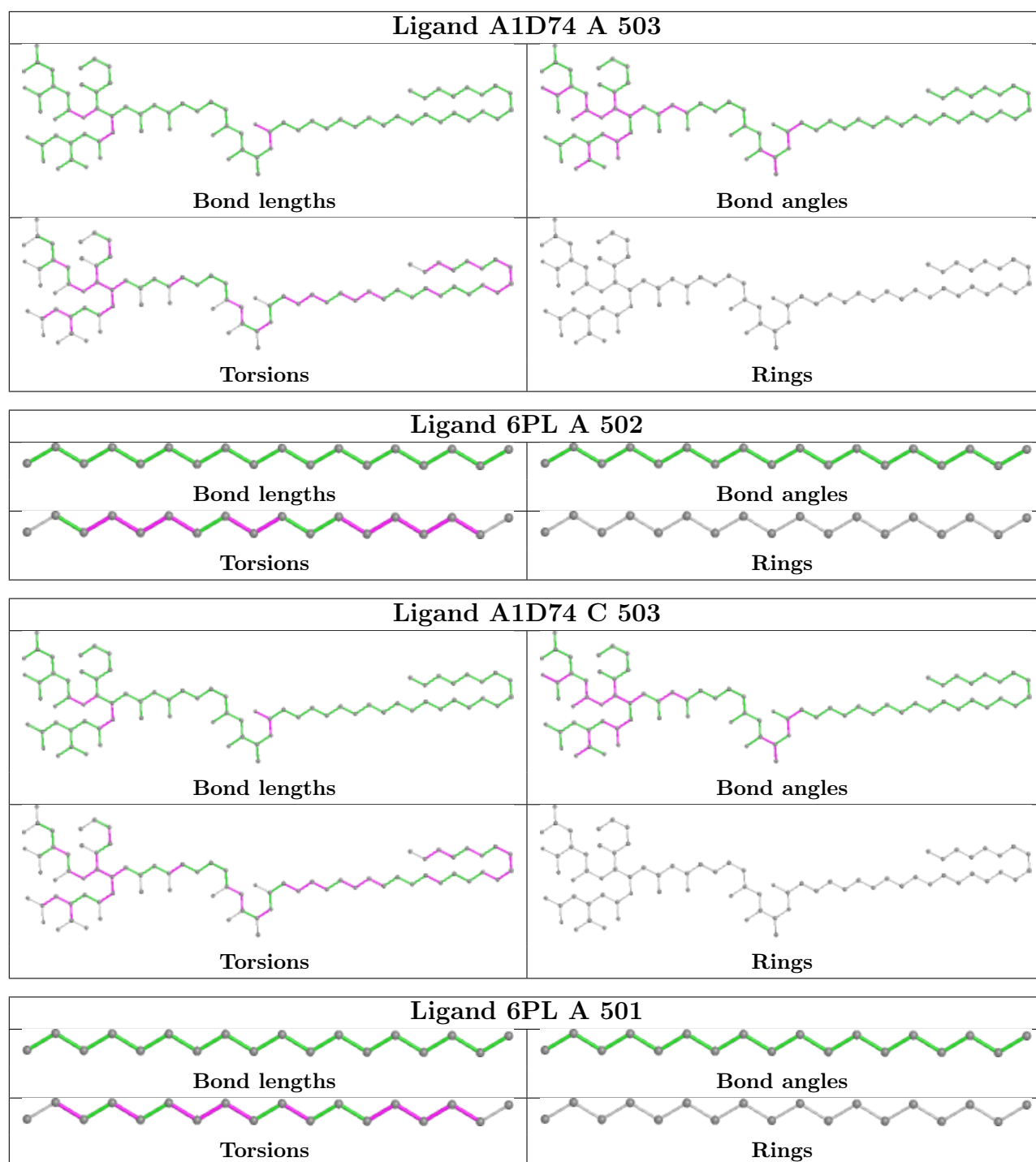
8 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	6PL	4	0
3	C	502	6PL	2	0
3	B	201	6PL	4	0
3	D	201	6PL	4	0
4	A	503	A1D74	7	0
3	A	502	6PL	1	0
4	C	503	A1D74	7	0
3	A	501	6PL	4	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.

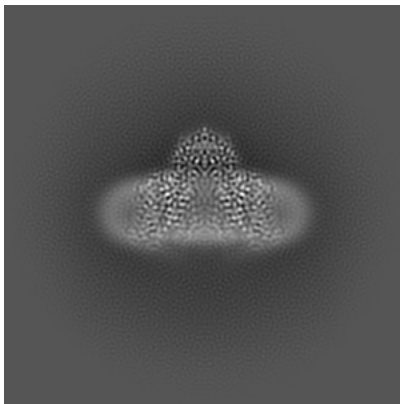
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39894. These allow visual inspection of the internal detail of the map and identification of artifacts.

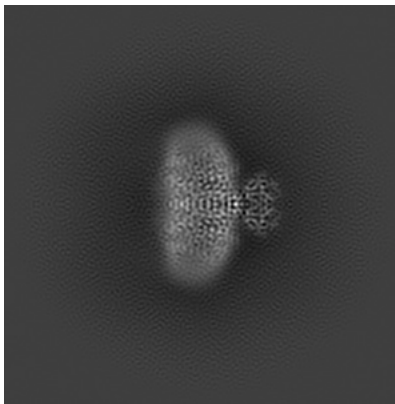
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

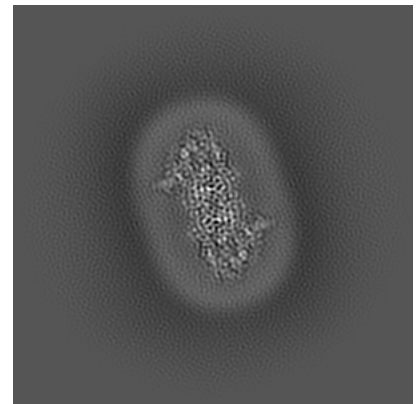
6.1.1 Primary map



X

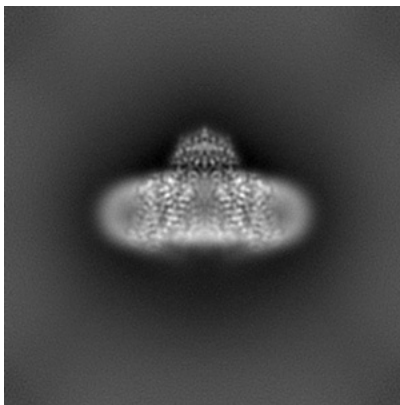


Y

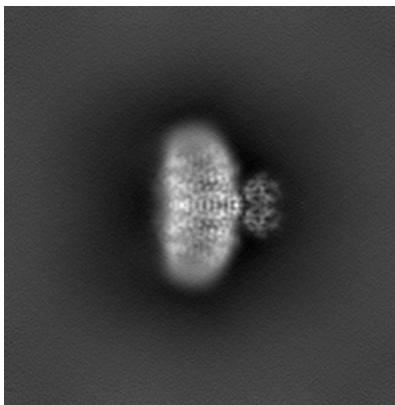


Z

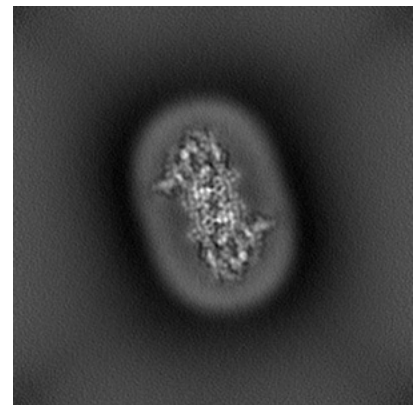
6.1.2 Raw map



X



Y

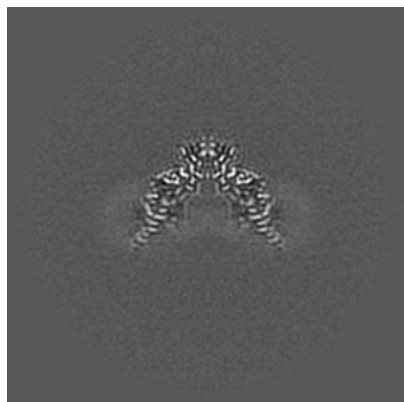


Z

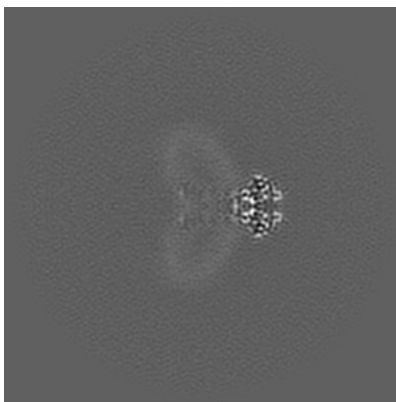
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

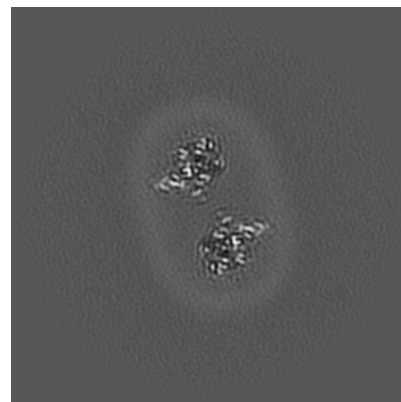
6.2.1 Primary map



X Index: 128

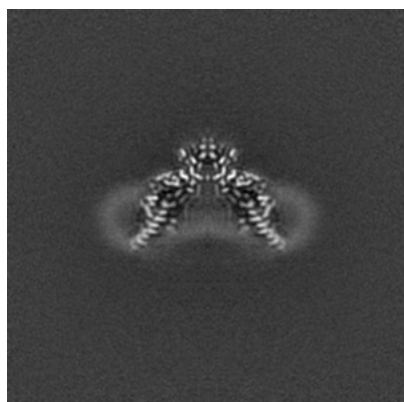


Y Index: 128

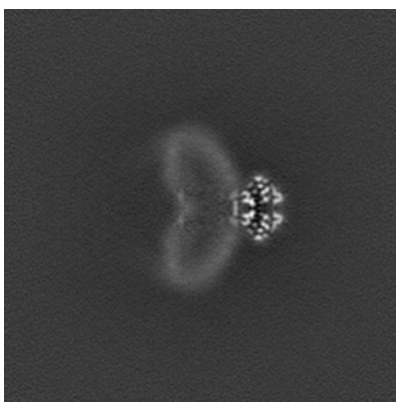


Z Index: 128

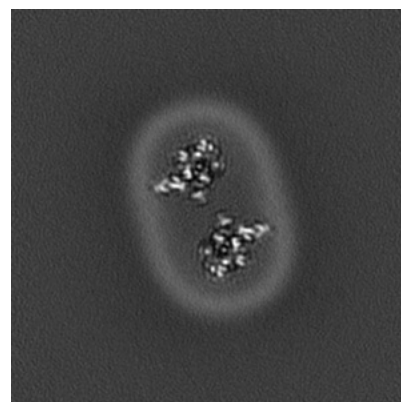
6.2.2 Raw map



X Index: 128



Y Index: 128

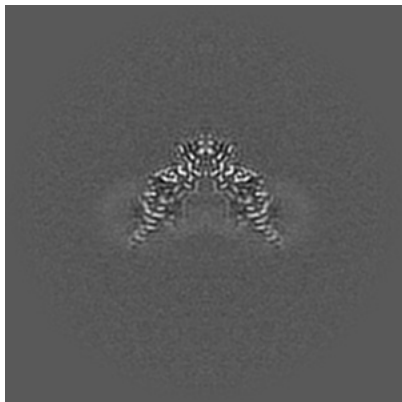


Z Index: 128

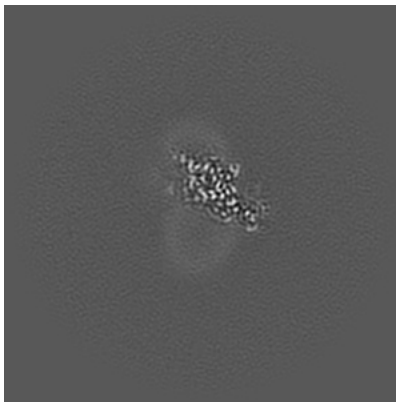
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

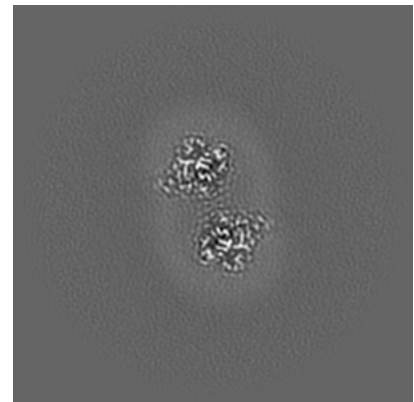
6.3.1 Primary map



X Index: 128

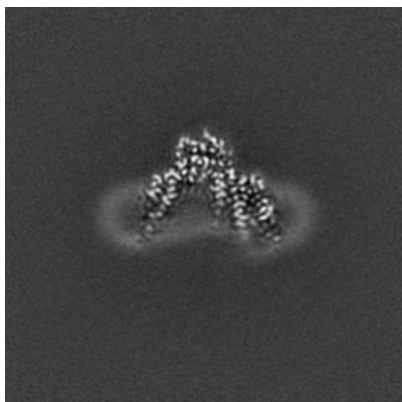


Y Index: 109

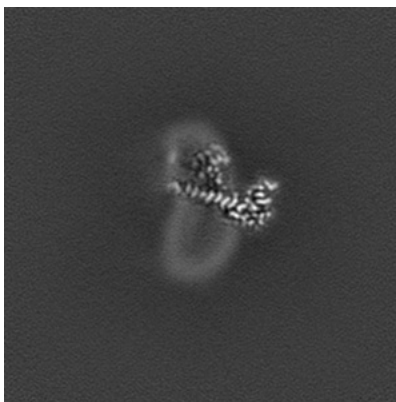


Z Index: 138

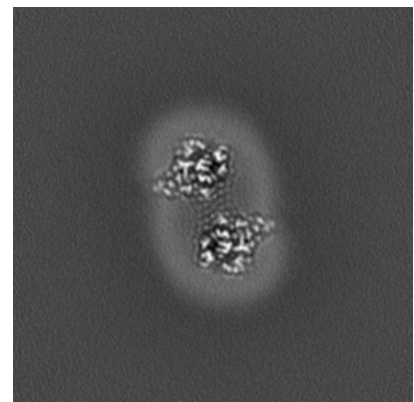
6.3.2 Raw map



X Index: 124



Y Index: 118

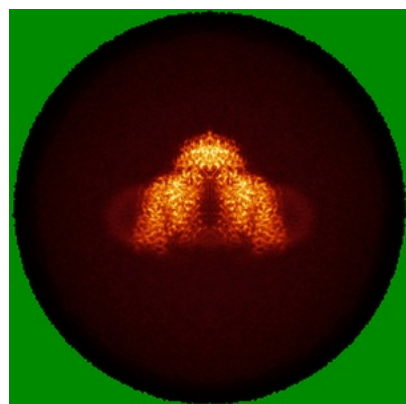


Z Index: 138

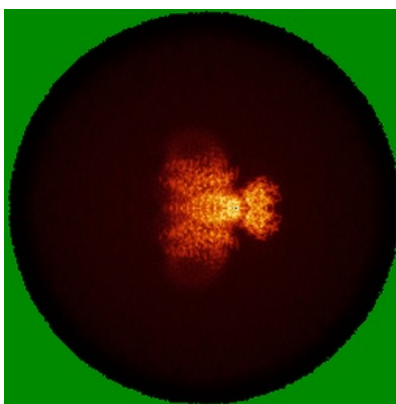
The images above show the largest variance slices of the map in three orthogonal directions.

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

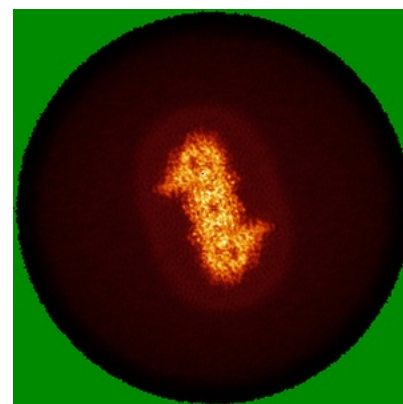
6.4.1 Primary map



X

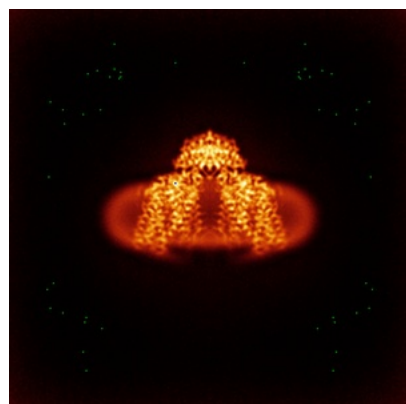


Y

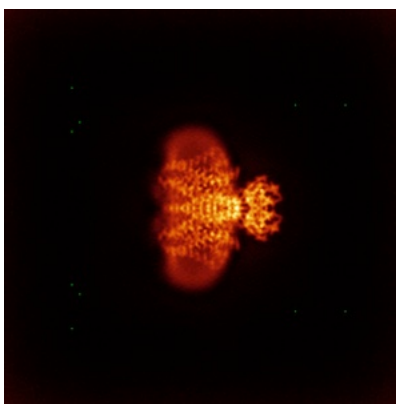


Z

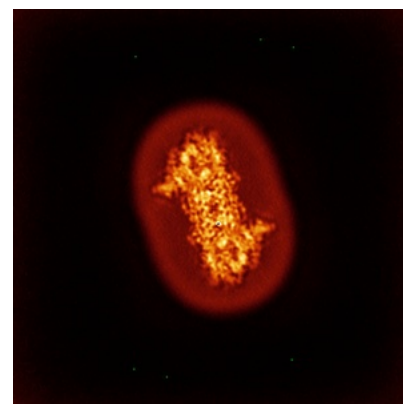
6.4.2 Raw map



X



Y

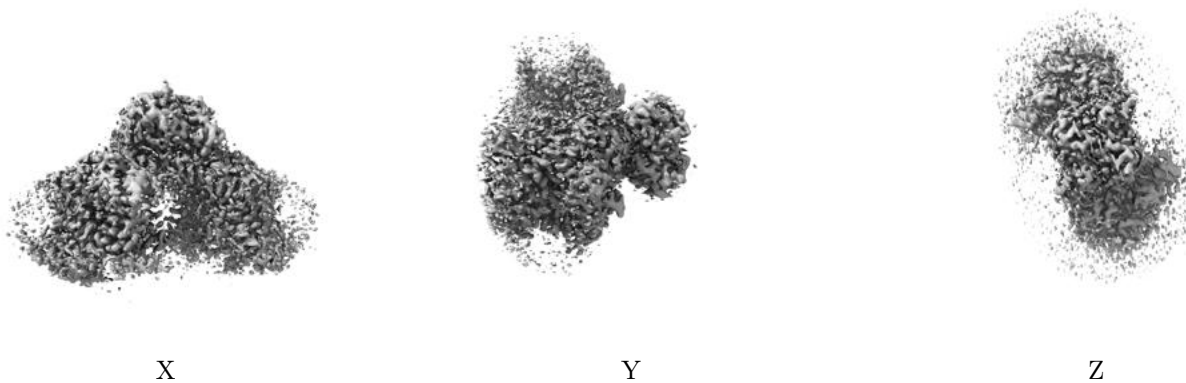


Z

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

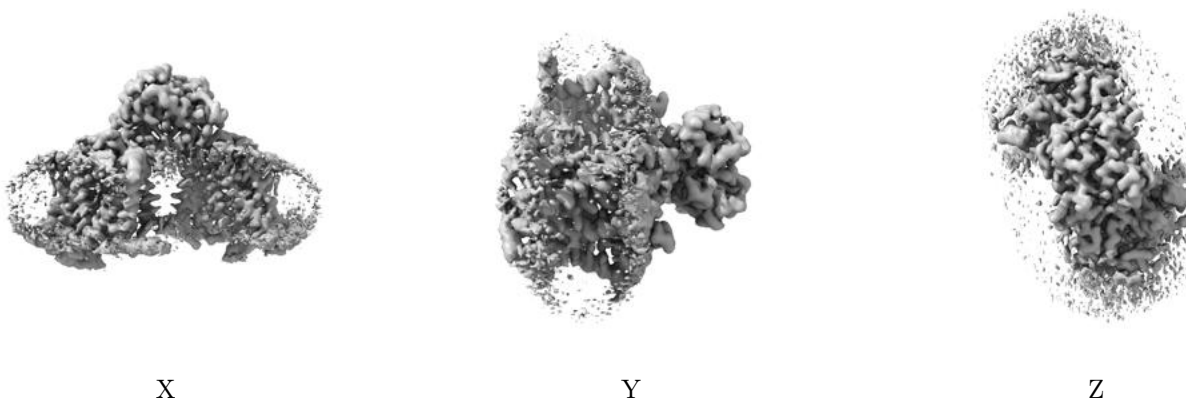
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

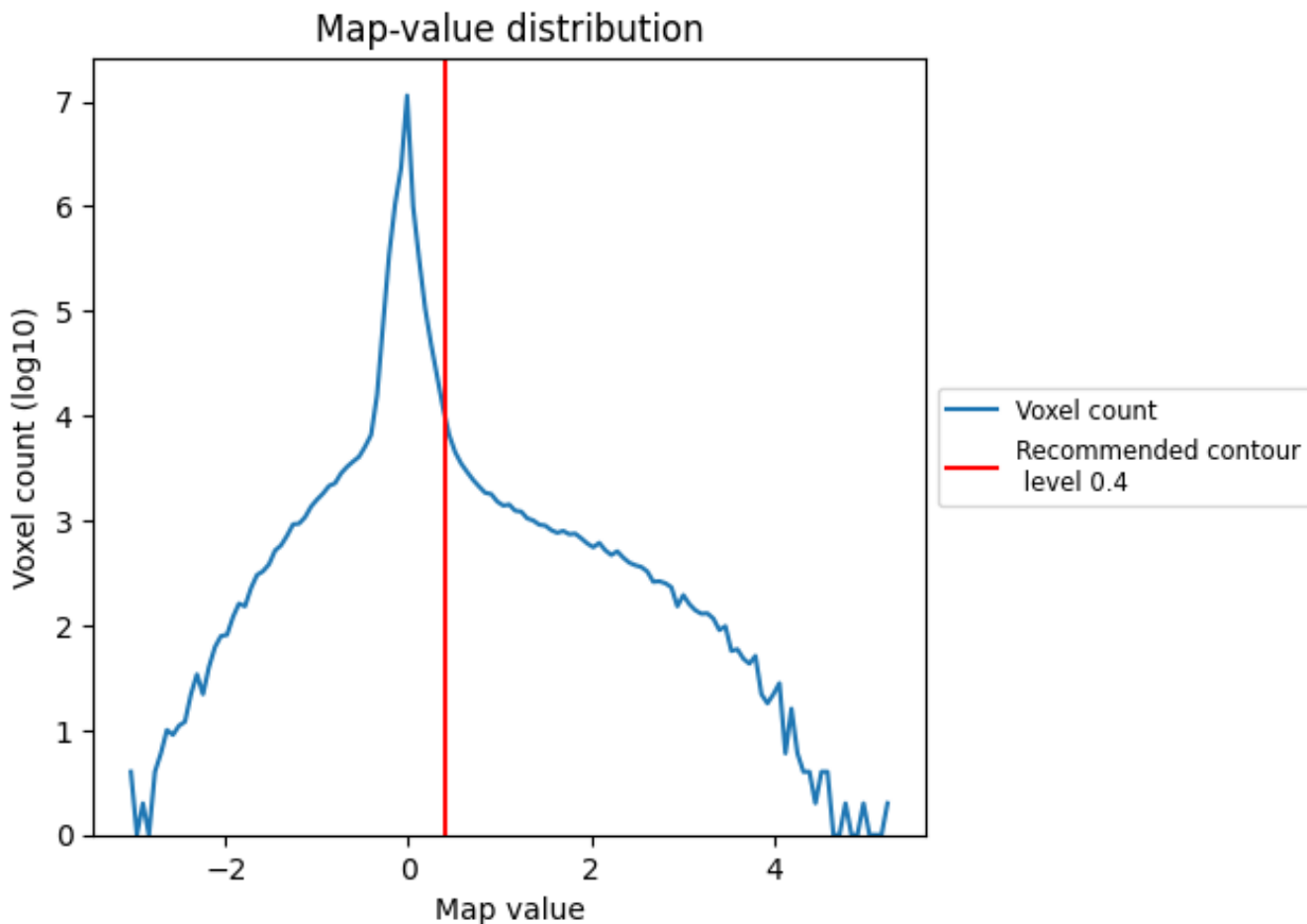
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

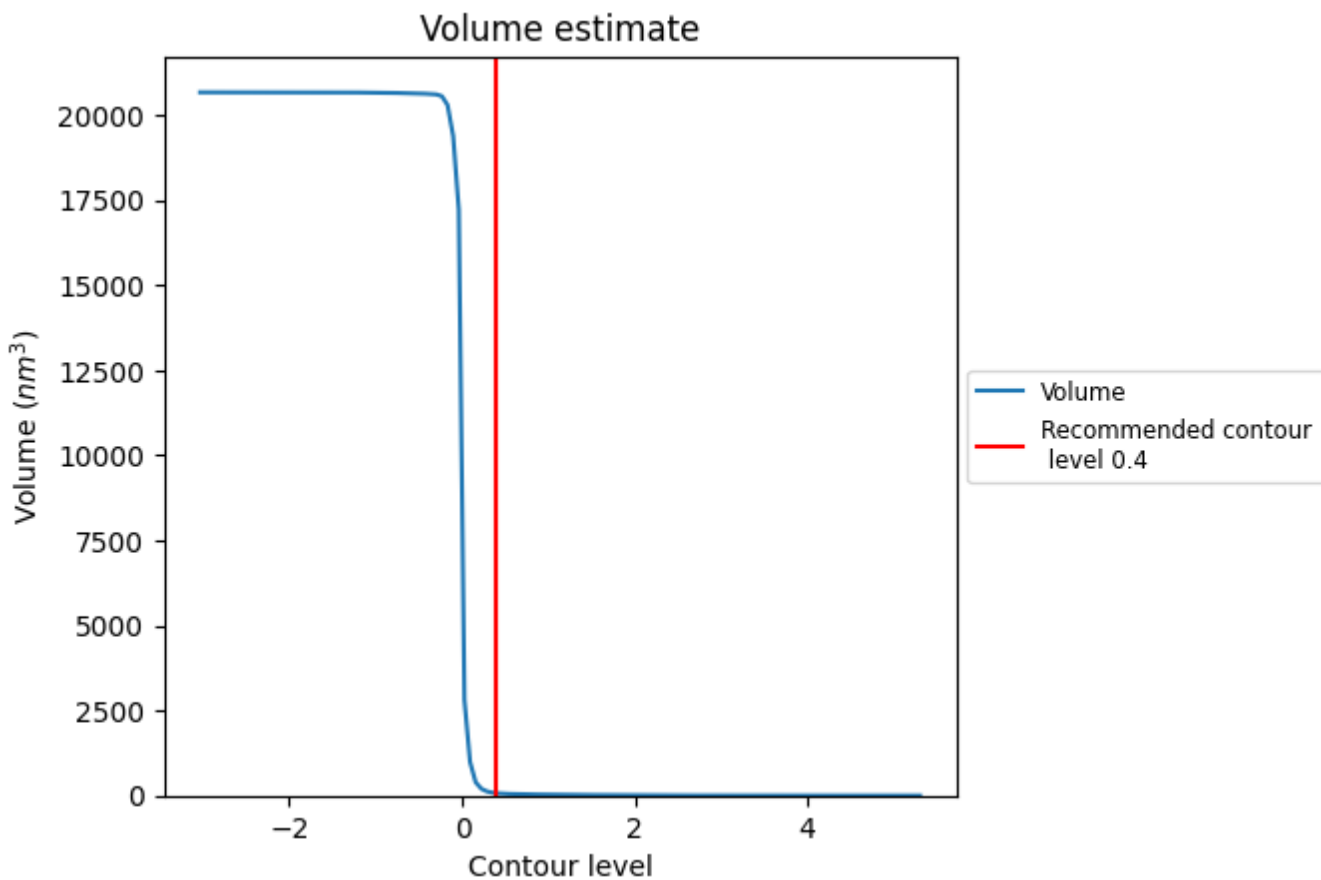
This section contains the results of statistical analysis of the map.

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.

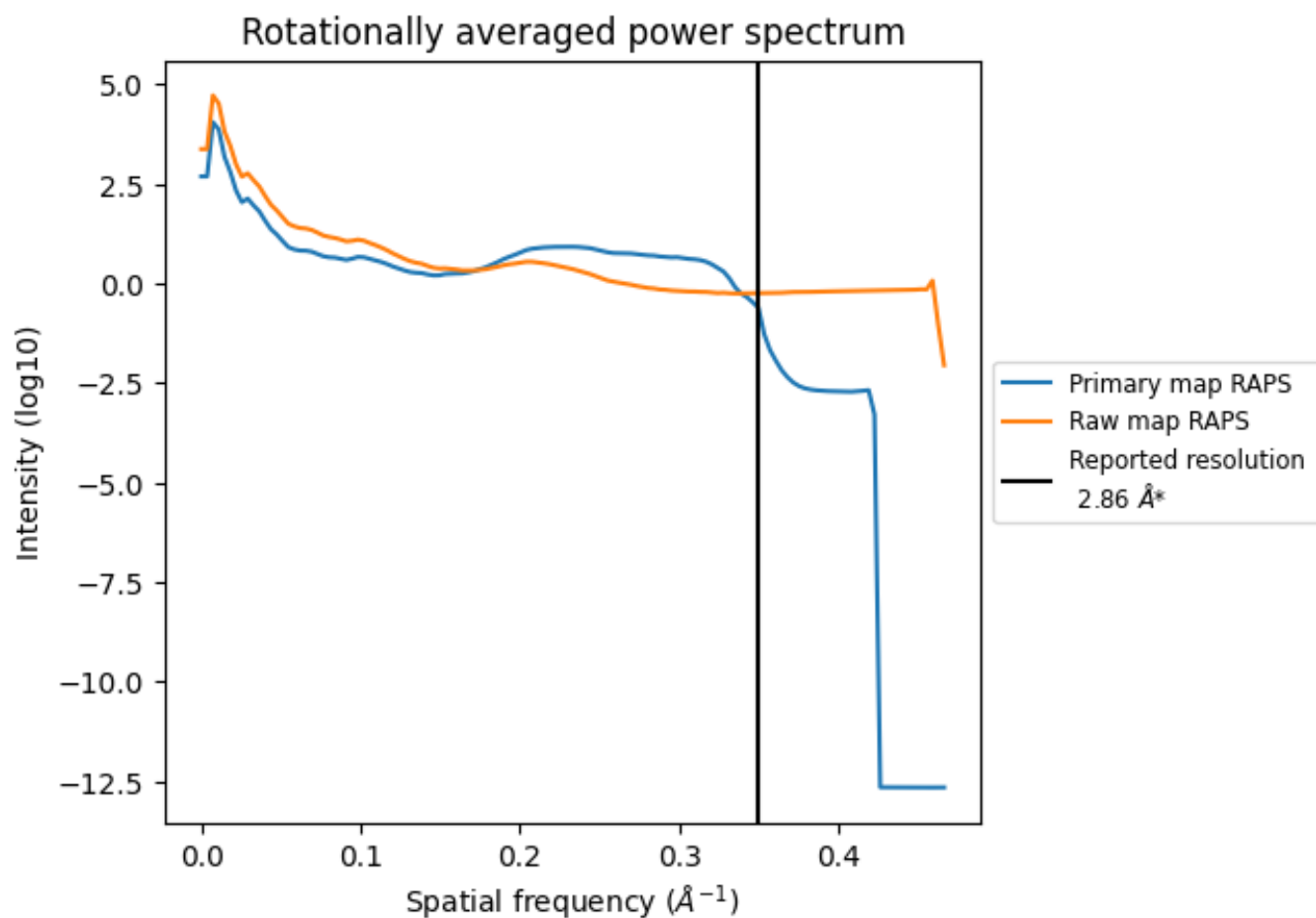
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm³; this corresponds to an approximate mass of 63 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

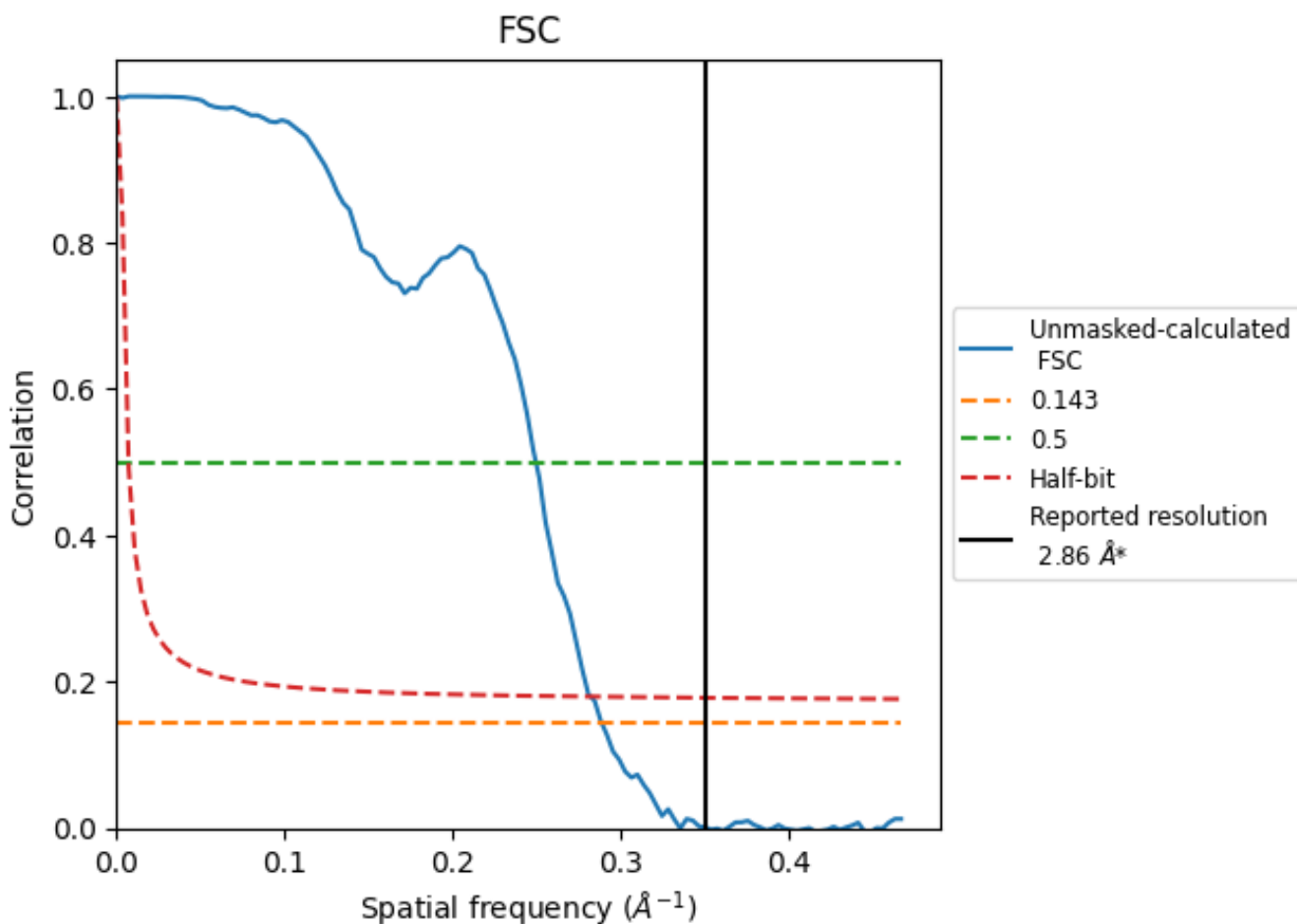


*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

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 0.350 Å⁻¹

8.2 Resolution estimates [i](#)

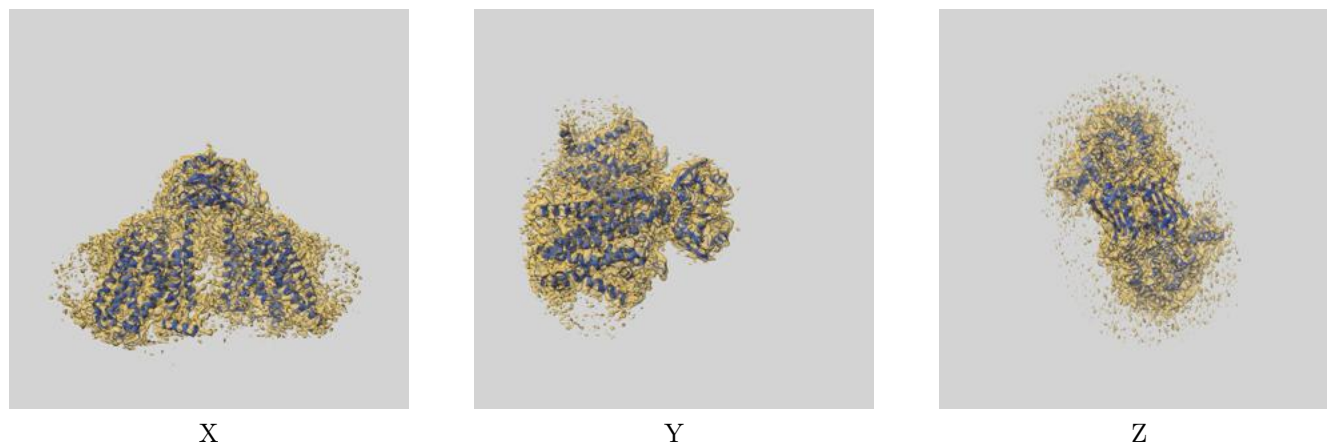
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.47	4.01	3.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.47 differs from the reported value 2.86 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39894 and PDB model 8ZB1. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



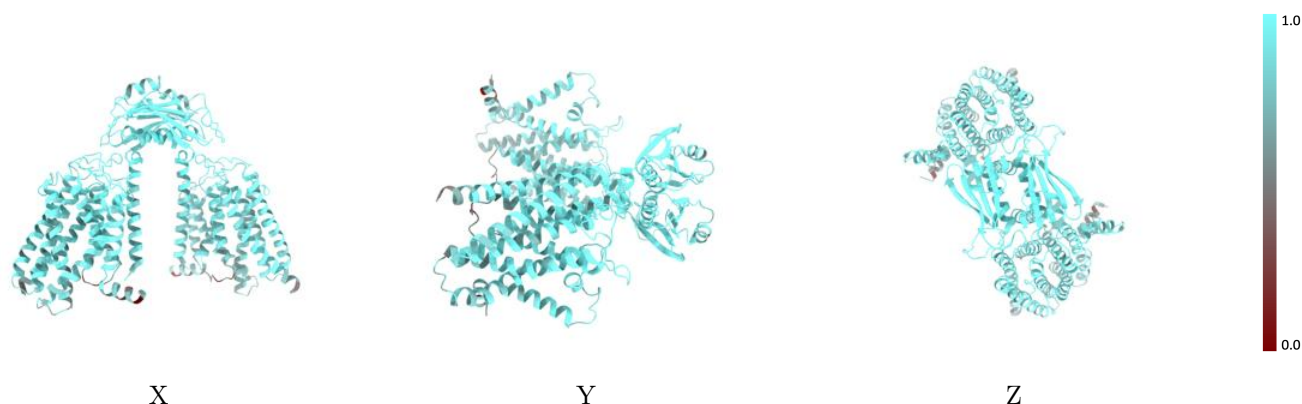
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



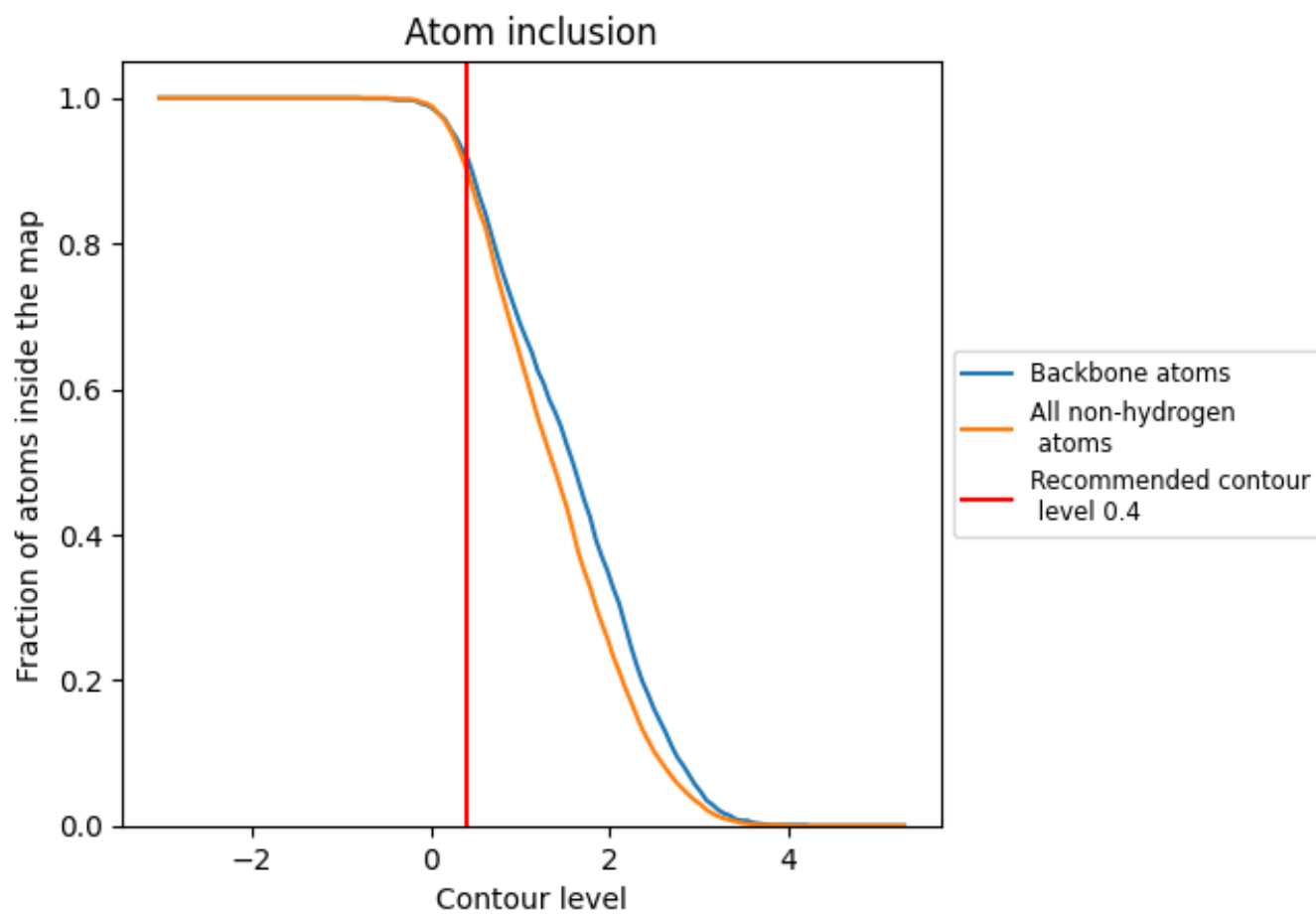
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).









9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9030	 0.5560
A	 0.8870	 0.5410
B	 0.9440	 0.5940
C	 0.8860	 0.5410
D	 0.9430	 0.5940

