Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 02:48 PM EST

PDB ID	:	6E1M
EMDB ID	:	EMD-8957
Title	:	Structure of AtTPC1(DDE) reconstituted in saposin A
Authors	:	Kintzer, A.F.; Green, E.M.; Cheng, Y.; Stroud, R.M.
Deposited on	:	2018-07-10
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

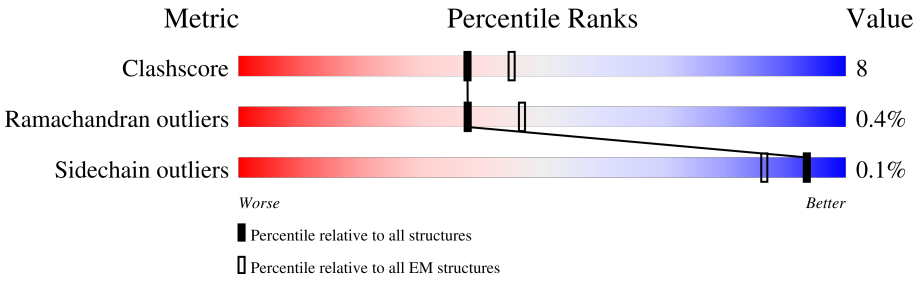
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 <=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	727	20% 60% 13% · 26%
1	B	727	20% 61% 12% · 26%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLM	A	807	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8913 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 Two pore calcium channel protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	536	Total	C	N	O	P	S	0	0
			4278	2815	663	777	3	20		
1	B	536	Total	C	N	O	P	S	0	0
			4278	2815	663	777	3	20		

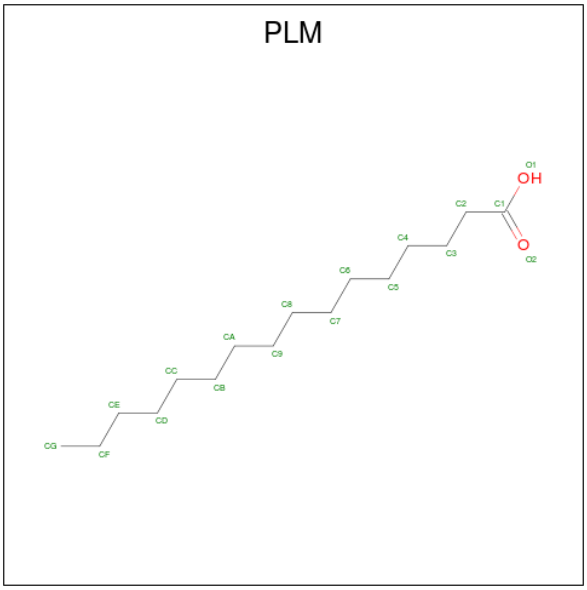
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	initiating methionine	UNP Q94KI8
A	240	ASN	ASP	engineered mutation	UNP Q94KI8
A	454	ASN	ASP	engineered mutation	UNP Q94KI8
A	528	GLN	GLU	engineered mutation	UNP Q94KI8
A	734	LEU	-	expression tag	UNP Q94KI8
A	735	VAL	-	expression tag	UNP Q94KI8
A	736	PRO	-	expression tag	UNP Q94KI8
A	737	ARG	-	expression tag	UNP Q94KI8
B	11	MET	-	initiating methionine	UNP Q94KI8
B	240	ASN	ASP	engineered mutation	UNP Q94KI8
B	454	ASN	ASP	engineered mutation	UNP Q94KI8
B	528	GLN	GLU	engineered mutation	UNP Q94KI8
B	734	LEU	-	expression tag	UNP Q94KI8
B	735	VAL	-	expression tag	UNP Q94KI8
B	736	PRO	-	expression tag	UNP Q94KI8
B	737	ARG	-	expression tag	UNP Q94KI8

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
2	A	5	Total	Ca	0
			5	5	
2	B	2	Total	Ca	0
			2	2	

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			126	112	14	
3	A	1	Total	C	O	0
			126	112	14	
3	A	1	Total	C	O	0
			126	112	14	
3	A	1	Total	C	O	0
			126	112	14	
3	A	1	Total	C	O	0
			126	112	14	
3	A	1	Total	C	O	0
			126	112	14	
3	A	1	Total	C	O	0
			126	112	14	
3	B	1	Total	C	O	0
			126	112	14	
3	B	1	Total	C	O	0
			126	112	14	
3	B	1	Total	C	O	0
			126	112	14	
3	B	1	Total	C	O	0
			126	112	14	
3	B	1	Total	C	O	0
			126	112	14	
3	B	1	Total	C	O	0
			126	112	14	

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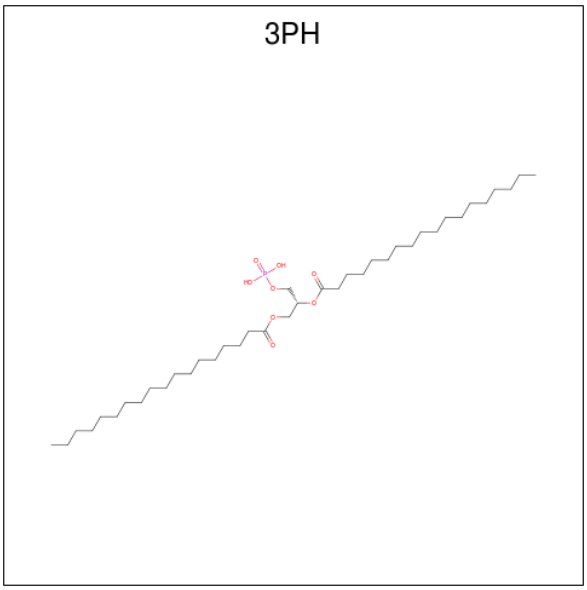
Mol	Chain	Residues	Atoms			AltConf
3	B	1	Total 126	C 112	O 14	0

- Molecule 4 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 48	C 39	O 8	P 1	0
4	B	1	Total 48	C 39	O 8	P 1	0

- Molecule 5 is water.

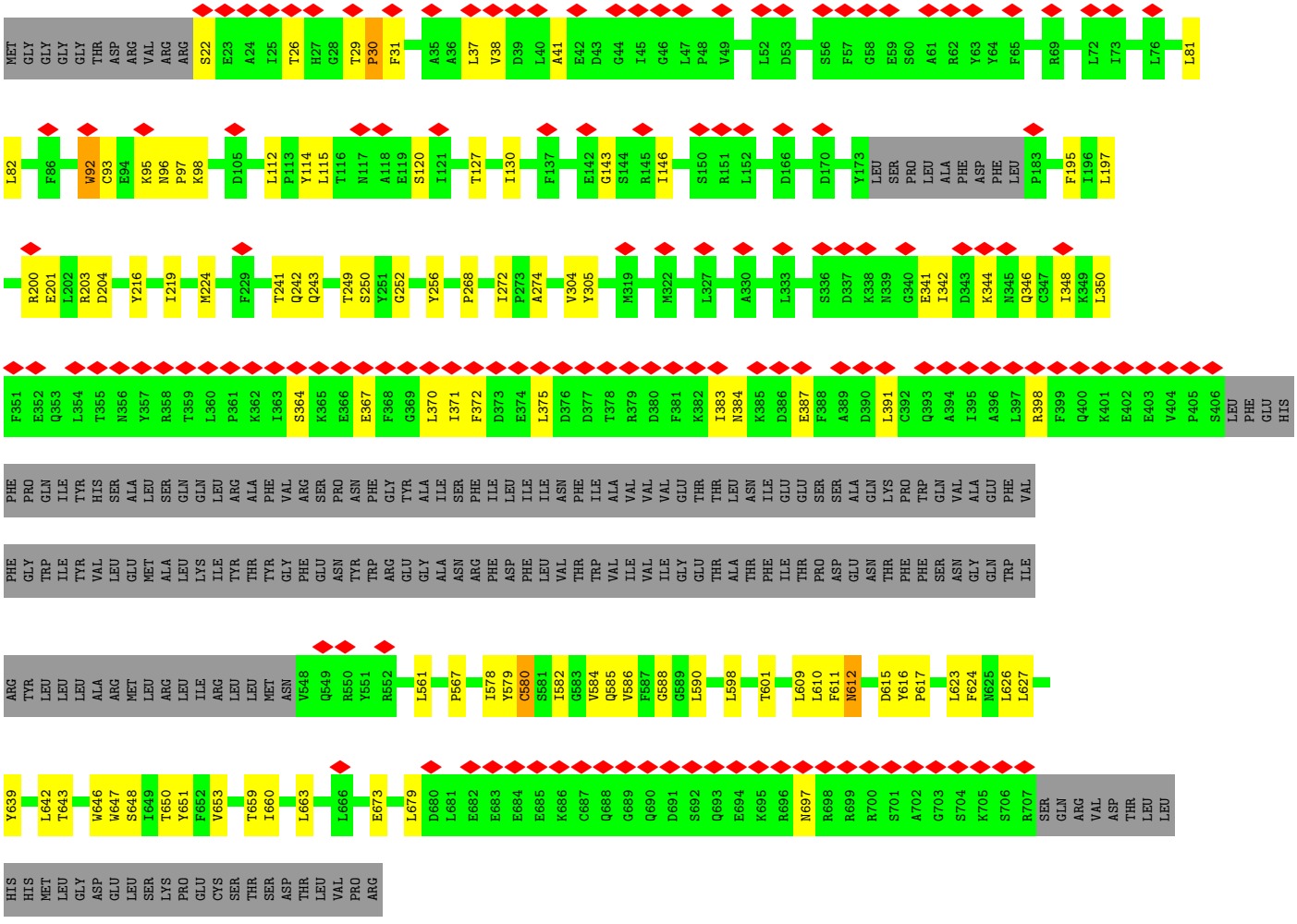
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	O 1	0
5	B	1	Total 1	O 1	0

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.

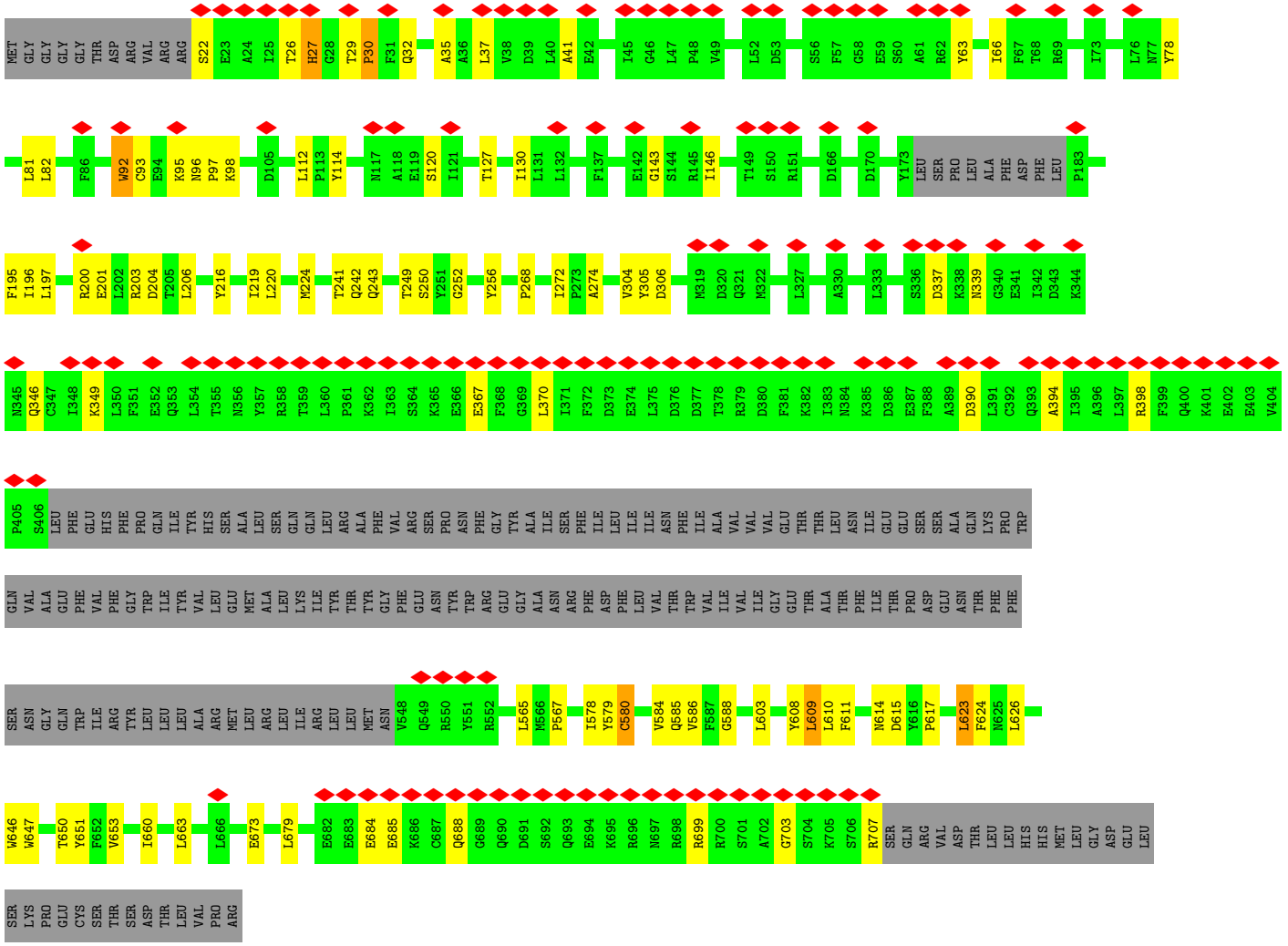
• Molecule 1: Two pore calcium channel protein 1

Chain A:



• Molecule 1: Two pore calcium channel protein 1

Chain B:


MET GLY GLY GLY GLY THR ASP ARG VAL ARG ARG S22 E23 A24 I25 T26 H27 G28 T29 P30 F31 Q32 A35 A36 L37 V38 D39 L40 A41 E42 I45 G46 L47 P48 V49 L52 D53 S56 F57 G58 E59 S60 A61 R62 Y63 I66 F67 T68 R69 I73 L76 N77 Y78
L81 L82 F86 W92 C93 E94 K95 N96 P97 K98 D105 L112 P113 Y114 N117 A118 E119 S120 I121 T127 I130 L131 L132 F137 E142 G143 S144 R145 I146 T149 S150 R151 D166 D170 Y173 LEU SER PRO LEU ALA PHE ASP PHE LEU P183
F195 I196 L197 R200 E201 L202 R203 D204 T205 L206 Y216 I219 L220 M224 T241 Q242 Q243 T249 S250 Y251 G252 Y256 P268 I272 P273 A274 V304 Y305 D306 M319 D320 Q321 M322 L327 A330 L333 S336 D337 K338 N339 G340 E341 I342 D343 K344
N345 Q346 C347 I348 K349 L350 F351 E352 Q353 L354 T355 N356 Y357 R358 T359 L360 P361 K362 I363 S364 K365 E366 E367 F368 G369 L370 I371 F372 D373 E374 L375 D376 D377 T378 R379 D380 F381 K382 I383 N384 K385 D386 E387 F388 A389 D390 L391 C392 Q393 A394 I395 A396 L397 R398 F399 Q400 K401 E402 E403 V404
P405 S406 LEU PHE GLU HIS PHE PRO GLN ILE TYR HIS SER ALA LEU SER GLN GLN LEU ARG ALA PHE VAL ARG SER PRO ASN PHE GLY TYR ALA ILE SER PHE ILE LEU ILE ILE ASN PHE ILE ALA VAL VAL VAL GLU THR THR LEU ASN ILE GLU GLU SER SER ALA GLN LYS PRO TRP
GLN VAL ALA GLU PHE VAL PHE GLY TRP ILE TYR VAL LEU GLU MET ALA LEU LYS ILE TYR THR TYR GLY PHE GLU ASN TYR TRP ARG GLU GLY ALA ASN ARG PHE ASP PHE LEU VAL THR TRP VAL ILE VAL ILE GLY GLU THR ALA THR PHE ILE THR PRO ASP GLU ASN THR PHE PHE
SER ASN GLY GLN TRP ILE ARG TYR LEU LEU LEU ALA ARG MET LEU ARG LEU ILE ARG LEU LEU MET ASN V548 Q549 R550 Y551 R552 L565 M566 P567 I578 Y579 C580 V584 Q585 V586 F587 G588 L603 Y608 L609 L610 F611 N614 D615 Y616 P617 L623 F624 N625 L626
W646 W647 T650 Y651 F652 V653 I660 L663 L666 E673 L679 E682 E683 E684 E685 K686 C687 Q688 G689 Q690 D691 S692 Q693 E694 K695 R696 N697 R698 R699 R700 S701 A702 G703 S704 K705 S706 R707 SER GLN ARG VAL ASP THR LEU LEU HIS HIS MET LEU GLY ASP GLU LEU
SER LYS PRO GLU CYS SER THR SER ASP THR LEU VAL PRO ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	224577	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	41132	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	62.522	Depositor
Minimum map value	-50.330	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	8.0	Depositor
Map size (Å)	311.1936, 311.1936, 311.1936	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2156, 1.2156, 1.2156	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PLM, TPO, SEP, 3PH

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	0.84	2/4349 (0.0%)	0.80	6/5912 (0.1%)
1	B	0.84	2/4349 (0.0%)	0.78	4/5912 (0.1%)
All	All	0.84	4/8698 (0.0%)	0.79	10/11824 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	580	CYS	CB-SG	-7.64	1.69	1.82
1	A	580	CYS	CB-SG	-7.61	1.69	1.82
1	B	304	VAL	CB-CG1	-6.48	1.39	1.52
1	A	304	VAL	CB-CG1	-5.74	1.40	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	610	LEU	CA-CB-CG	9.68	137.57	115.30
1	A	610	LEU	CB-CG-CD2	-6.71	99.59	111.00
1	A	610	LEU	CB-CG-CD1	-6.47	100.00	111.00
1	B	679	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	610	LEU	N-CA-C	-5.64	95.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	627	LEU	CB-CG-CD1	-5.62	101.44	111.00
1	B	603	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	623	LEU	CB-CG-CD1	-5.15	102.24	111.00
1	A	609	LEU	C-N-CA	5.13	134.53	121.70
1	B	663	LEU	CB-CG-CD1	-5.00	102.50	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	611	PHE	Peptide
1	A	660	ILE	Peptide
1	A	92	TRP	Peptide
1	B	609	LEU	Peptide
1	B	611	PHE	Peptide
1	B	660	ILE	Peptide
1	B	92	TRP	Peptide

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	4278	0	4161	64	0
1	B	4278	0	4161	58	0
2	A	5	0	0	0	0
2	B	2	0	0	0	0
3	A	126	0	216	27	0
3	B	126	0	215	19	0
4	A	48	0	72	3	0
4	B	48	0	69	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	8913	0	8894	145	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 (145) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:806:PLM:H21	3:A:810:PLM:H21	1.57	0.87
1:B:114:TYR:OH	1:B:615:ASP:OD2	1.98	0.81
1:A:114:TYR:OH	1:A:615:ASP:OD2	2.00	0.79
1:A:256:TYR:HB2	3:A:807:PLM:H81	1.75	0.68
1:B:684:GLU:OE2	1:B:707:ARG:NH1	2.28	0.67
1:B:256:TYR:HB2	3:B:804:PLM:H81	1.77	0.66
1:B:197:LEU:O	1:B:203:ARG:NH1	2.28	0.66
1:A:653:VAL:HG21	3:A:807:PLM:HC1	1.78	0.66
1:A:197:LEU:O	1:A:203:ARG:NH1	2.28	0.66
1:B:32:GLN:H	1:B:35:ALA:HB3	1.61	0.65
1:A:579:TYR:O	1:A:651:TYR:OH	2.15	0.65
1:A:201:GLU:HB3	1:A:567:PRO:HB3	1.78	0.64
1:B:92:TRP:HH2	1:B:120:SER:HA	1.62	0.63
1:B:586:VAL:HG11	3:B:806:PLM:H31	1.81	0.62
1:B:653:VAL:HG21	3:B:804:PLM:HC1	1.81	0.62
1:B:305:TYR:OH	1:B:673:GLU:OE2	2.08	0.62
1:A:586:VAL:HG11	3:A:809:PLM:H31	1.81	0.61
1:A:367:GLU:OE1	1:A:398:ARG:NH2	2.34	0.61
1:B:81:LEU:HD21	1:B:127:THR:HA	1.82	0.60
1:A:112:LEU:HD12	1:A:617:PRO:HG3	1.82	0.60
1:A:305:TYR:OH	1:A:673:GLU:OE2	2.04	0.60
1:B:112:LEU:HD12	1:B:617:PRO:HG3	1.82	0.60
1:B:579:TYR:O	1:B:651:TYR:OH	2.16	0.60
1:A:578:ILE:HG21	3:A:809:PLM:HG3	1.85	0.58
1:B:578:ILE:HG21	3:B:806:PLM:HG3	1.85	0.58
1:B:243:GLN:HB2	1:B:274:ALA:HB2	1.84	0.58
1:A:81:LEU:HD21	1:A:127:THR:HA	1.85	0.58
1:B:81:LEU:HG	1:B:130:ILE:HB	1.86	0.57
1:B:684:GLU:O	1:B:688:GLN:N	2.37	0.57
1:B:684:GLU:OE1	1:B:699:ARG:NH1	2.38	0.57
1:B:367:GLU:OE1	1:B:398:ARG:NH2	2.37	0.57
1:A:37:LEU:HD22	1:A:350:LEU:HD22	1.88	0.56
1:B:201:GLU:HB3	1:B:567:PRO:HB3	1.86	0.56
1:B:588:GLY:O	1:B:614:ASN:ND2	2.37	0.56
1:A:224:MET:HG2	3:A:807:PLM:HG1	1.88	0.56
1:B:92:TRP:CH2	1:B:120:SER:HA	2.40	0.55
1:B:252:GLY:HA3	3:B:804:PLM:H51	1.89	0.55
1:A:95:LYS:HD2	1:A:585:GLN:HG2	1.87	0.55
3:A:807:PLM:HC2	3:A:812:PLM:HC1	1.90	0.54
3:A:807:PLM:H62	3:A:812:PLM:H62	1.88	0.54
1:A:588:GLY:O	1:A:590:LEU:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLY:HA3	3:A:807:PLM:H51	1.89	0.54
1:A:375:LEU:HD12	1:A:383:ILE:H	1.72	0.54
1:B:97:PRO:HG2	1:B:98:LYS:HD3	1.90	0.54
1:A:97:PRO:HG2	1:A:98:LYS:HD3	1.89	0.53
1:B:250:SER:OG	3:B:803:PLM:O2	2.27	0.53
1:B:95:LYS:HD2	1:B:585:GLN:HG2	1.90	0.53
1:B:647:TRP:CZ3	3:B:809:PLM:H92	2.44	0.52
1:A:679:LEU:HD22	1:B:306:ASP:OD2	2.08	0.52
1:A:82:LEU:HB3	1:A:195:PHE:HD1	1.75	0.52
1:B:608:TYR:O	1:B:610:LEU:N	2.41	0.52
1:B:346:GLN:HA	1:B:349:LYS:HE2	1.92	0.51
1:A:143:GLY:H	1:A:146:ILE:HD12	1.75	0.51
1:B:143:GLY:H	1:B:146:ILE:HD12	1.76	0.51
1:A:81:LEU:HG	1:A:130:ILE:HB	1.92	0.51
1:B:367:GLU:HA	1:B:370:LEU:HB2	1.93	0.51
3:B:803:PLM:H21	3:B:807:PLM:H21	1.93	0.50
3:A:806:PLM:C2	3:A:810:PLM:H21	2.36	0.50
1:B:82:LEU:HB3	1:B:195:PHE:HD1	1.77	0.49
1:B:685:GLU:HA	1:B:688:GLN:HB2	1.93	0.49
1:A:243:GLN:HB2	1:A:274:ALA:HB2	1.92	0.49
1:B:27:HIS:HA	1:B:30:PRO:HD2	1.95	0.49
1:B:63:TYR:HA	1:B:66:ILE:HD12	1.95	0.48
1:A:384:ASN:HB2	1:A:387:GLU:HG2	1.96	0.48
1:B:200:ARG:HG2	1:B:204:ASP:OD2	2.14	0.48
1:A:241:THR:OG1	1:A:242:GLN:N	2.47	0.48
1:A:372:PHE:HB2	1:A:697:ASN:HD21	1.78	0.48
1:B:390:ASP:O	1:B:394:ALA:N	2.46	0.48
1:A:659:THR:HG22	1:A:663:LEU:HG	1.95	0.48
1:A:92:TRP:CH2	1:A:120:SER:HA	2.48	0.48
1:A:612:ASN:O	1:A:639:TYR:OH	2.30	0.48
1:B:623:LEU:HD23	1:B:626:LEU:HD12	1.96	0.47
1:A:647:TRP:CE3	3:A:812:PLM:H91	2.50	0.47
4:A:813:3PH:H371	4:A:813:3PH:H251	1.96	0.46
4:B:810:3PH:H362	4:B:810:3PH:H331	1.71	0.46
1:A:623:LEU:HD23	1:A:626:LEU:HD12	1.97	0.46
3:B:803:PLM:C1	3:B:807:PLM:H21	2.45	0.46
1:B:216:TYR:HA	1:B:219:ILE:HG22	1.98	0.46
3:B:803:PLM:H21	3:B:807:PLM:C2	2.46	0.46
1:A:586:VAL:HG22	3:A:808:PLM:H41	1.98	0.45
1:A:647:TRP:NE1	3:A:812:PLM:H21	2.31	0.45
1:A:200:ARG:HG2	1:A:204:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LYS:NZ	1:A:364:SER:OG	2.40	0.45
3:B:807:PLM:H52	3:B:807:PLM:H22	1.75	0.45
3:A:809:PLM:H81	3:A:809:PLM:H52	1.27	0.45
1:A:37:LEU:O	1:A:41:ALA:N	2.41	0.44
1:A:646:TRP:CE3	3:A:807:PLM:H61	2.51	0.44
1:B:699:ARG:O	1:B:703:GLY:N	2.50	0.44
1:A:216:TYR:HA	1:A:219:ILE:HG22	1.99	0.44
1:A:249:THR:OG1	1:A:250:SER:N	2.50	0.44
1:A:344:LYS:HE3	1:A:348:ILE:HD11	1.97	0.44
1:B:646:TRP:CE3	3:B:804:PLM:H61	2.53	0.44
3:A:811:PLM:HE2	1:B:624:PHE:CD1	2.53	0.44
1:B:249:THR:OG1	1:B:250:SER:N	2.51	0.44
3:A:808:PLM:HB2	3:A:808:PLM:HE2	1.53	0.44
1:A:590:LEU:HD23	1:A:642:LEU:HB3	2.00	0.44
3:B:809:PLM:HB2	3:B:809:PLM:H82	1.53	0.44
3:B:805:PLM:HA1	3:B:805:PLM:H72	1.40	0.43
1:A:38:VAL:HA	1:A:41:ALA:HB3	1.99	0.43
1:A:650:THR:HG23	3:A:812:PLM:HF2	1.99	0.43
3:B:805:PLM:HE2	3:B:805:PLM:HB2	1.53	0.43
1:B:241:THR:OG1	1:B:242:GLN:N	2.50	0.43
1:A:341:GLU:HB2	1:A:383:ILE:HB	2.00	0.43
1:A:598:LEU:O	1:A:601:THR:OG1	2.33	0.43
1:A:93:CYS:SG	1:A:97:PRO:HG3	2.59	0.43
1:A:580:CYS:O	1:A:584:VAL:N	2.43	0.43
3:A:810:PLM:H22	3:A:810:PLM:H52	1.64	0.43
3:A:812:PLM:H52	3:A:812:PLM:H82	1.52	0.42
1:B:241:THR:HG23	1:B:243:GLN:H	1.83	0.42
4:A:813:3PH:H362	4:A:813:3PH:H322	2.01	0.42
1:A:624:PHE:CD1	3:B:808:PLM:HE2	2.54	0.42
1:B:565:LEU:HD23	1:B:565:LEU:HA	1.90	0.42
1:B:78:TYR:O	1:B:82:LEU:HG	2.20	0.42
1:A:92:TRP:NE1	1:A:115:LEU:HD12	2.34	0.42
1:B:650:THR:HG23	3:B:809:PLM:HD1	2.02	0.42
3:B:803:PLM:O2	3:B:807:PLM:H21	2.20	0.42
1:A:561:LEU:HA	1:A:561:LEU:HD23	1.87	0.41
1:B:580:CYS:O	1:B:584:VAL:N	2.42	0.41
1:A:96:ASN:OD1	1:A:96:ASN:N	2.52	0.41
1:A:367:GLU:HA	1:A:370:LEU:HB2	2.02	0.41
3:A:806:PLM:H81	3:A:806:PLM:HB2	1.13	0.41
3:A:807:PLM:H71	3:A:812:PLM:H62	2.01	0.41
1:B:93:CYS:SG	1:B:97:PRO:HG3	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ILE:HD12	1:A:219:ILE:HA	1.90	0.41
1:B:37:LEU:O	1:B:41:ALA:N	2.47	0.41
1:B:337:ASP:OD2	1:B:339:ASN:ND2	2.53	0.41
1:A:582:ILE:HD11	3:A:808:PLM:HB1	2.02	0.41
1:A:371:ILE:HD11	1:A:391:LEU:HD13	2.02	0.41
1:B:196:ILE:HG21	1:B:206:LEU:HD22	2.03	0.41
1:B:220:LEU:HA	1:B:220:LEU:HD12	1.87	0.41
1:A:586:VAL:HG21	3:A:809:PLM:H62	2.03	0.41
1:A:615:ASP:HB3	1:A:616:TYR:H	1.78	0.41
3:A:806:PLM:HD1	3:A:806:PLM:HA1	1.77	0.41
1:B:96:ASN:N	1:B:96:ASN:OD1	2.52	0.41
4:B:810:3PH:H362	4:B:810:3PH:H252	2.03	0.41
1:A:30:PRO:HB2	1:A:31:PHE:H	1.63	0.40
1:A:252:GLY:CA	3:A:807:PLM:H51	2.51	0.40
1:A:643:THR:OG1	1:A:648:SER:OG	2.34	0.40
1:B:268:PRO:O	1:B:272:ILE:HG13	2.20	0.40
4:A:813:3PH:H251	4:A:813:3PH:H351	2.03	0.40
1:B:224:MET:SD	3:B:804:PLM:HF1	2.61	0.40
1:A:268:PRO:O	1:A:272:ILE:HG13	2.21	0.40
1:A:342:ILE:HG23	1:A:346:GLN:HB3	2.02	0.40
1:B:37:LEU:HD12	1:B:37:LEU:HA	1.90	0.40
1:A:647:TRP:CZ3	3:A:812:PLM:H91	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	528/727 (73%)	478 (90%)	49 (9%)	1 (0%)	47	77
1	B	528/727 (73%)	483 (92%)	42 (8%)	3 (1%)	25	57
All	All	1056/1454 (73%)	961 (91%)	91 (9%)	4 (0%)	38	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	B	30	PRO
1	B	27	HIS
1	B	609	LEU

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	448/648 (69%)	447 (100%)	1 (0%)	93 97
1	B	448/648 (69%)	448 (100%)	0	100 100
All	All	896/1296 (69%)	895 (100%)	1 (0%)	93 97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	612	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	242	GLN
1	B	618	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)

6 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TPO	B	26	1	8,10,11	1.59	1 (12%)	10,14,16	1.86	1 (10%)
1	SEP	B	22	1	8,9,10	1.55	1 (12%)	8,12,14	1.97	2 (25%)
1	TPO	A	26	1	8,10,11	1.11	0	10,14,16	1.93	2 (20%)
1	TPO	B	29	1	8,10,11	1.06	0	10,14,16	1.82	3 (30%)
1	SEP	A	22	1	8,9,10	1.55	1 (12%)	8,12,14	2.03	2 (25%)
1	TPO	A	29	1	8,10,11	1.56	1 (12%)	10,14,16	2.04	2 (20%)

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
1	TPO	B	26	1	-	2/9/11/13	-
1	SEP	B	22	1	-	2/5/8/10	-
1	TPO	A	26	1	-	1/9/11/13	-
1	TPO	B	29	1	-	4/9/11/13	-
1	SEP	A	22	1	-	4/5/8/10	-
1	TPO	A	29	1	-	4/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	SEP	P-O1P	3.38	1.61	1.50
1	A	29	TPO	P-O1P	3.37	1.61	1.50
1	B	26	TPO	P-O1P	3.36	1.61	1.50
1	B	22	SEP	P-O1P	3.35	1.61	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	TPO	P-OG1-CB	-5.62	106.24	123.21
1	B	26	TPO	P-OG1-CB	-5.27	107.29	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	26	TPO	P-OG1-CB	-4.95	108.26	123.21
1	B	29	TPO	P-OG1-CB	-4.71	108.99	123.21
1	A	22	SEP	OG-CB-CA	4.06	112.10	108.14
1	B	22	SEP	P-OG-CB	-3.79	107.85	118.30
1	B	22	SEP	OG-CB-CA	3.60	111.65	108.14
1	A	22	SEP	P-OG-CB	-3.52	108.60	118.30
1	A	26	TPO	CG2-CB-CA	-2.79	107.67	113.16
1	A	29	TPO	O-C-CA	-2.33	118.66	124.78
1	B	29	TPO	O-C-CA	-2.22	118.97	124.78
1	B	29	TPO	CG2-CB-CA	-2.05	109.12	113.16

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	22	SEP	N-CA-CB-OG
1	A	22	SEP	CB-OG-P-O1P
1	A	22	SEP	CB-OG-P-O2P
1	A	22	SEP	CB-OG-P-O3P
1	A	29	TPO	N-CA-CB-OG1
1	A	29	TPO	O-C-CA-CB
1	A	29	TPO	CB-OG1-P-O3P
1	B	22	SEP	N-CA-CB-OG
1	B	26	TPO	CB-OG1-P-O1P
1	B	29	TPO	N-CA-CB-CG2
1	B	29	TPO	N-CA-CB-OG1
1	B	29	TPO	C-CA-CB-CG2
1	B	29	TPO	O-C-CA-CB
1	A	29	TPO	CB-OG1-P-O1P
1	A	26	TPO	CB-OG1-P-O3P
1	B	26	TPO	CB-OG1-P-O2P
1	B	22	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 7 are monoatomic - leaving 16 for Mogul analysis.

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	PLM	B	804	-	17,17,17	0.53	0	17,17,17	0.86	0
3	PLM	B	808	-	17,17,17	0.60	0	17,17,17	0.93	2 (11%)
3	PLM	B	807	-	17,17,17	0.62	0	17,17,17	0.70	0
3	PLM	A	810	-	17,17,17	0.62	0	17,17,17	0.69	0
3	PLM	A	812	1	17,17,17	0.56	0	17,17,17	0.75	0
3	PLM	A	811	1	17,17,17	0.59	0	17,17,17	0.74	0
3	PLM	B	803	-	17,17,17	0.54	0	17,17,17	0.84	0
3	PLM	A	808	-	17,17,17	0.52	0	17,17,17	0.77	0
4	3PH	B	810	1	47,47,47	0.93	2 (4%)	51,52,52	0.96	2 (3%)
3	PLM	A	809	-	17,17,17	0.52	0	17,17,17	0.92	0
3	PLM	A	806	-	17,17,17	0.54	0	17,17,17	0.89	1 (5%)
3	PLM	B	809	1	17,17,17	0.52	0	17,17,17	0.69	0
4	3PH	A	813	1	47,47,47	0.94	2 (4%)	51,52,52	1.10	3 (5%)
3	PLM	B	806	-	17,17,17	0.52	0	17,17,17	0.91	0
3	PLM	B	805	-	17,17,17	0.52	0	17,17,17	0.77	0
3	PLM	A	807	-	17,17,17	0.53	0	17,17,17	0.82	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	PLM	B	804	-	-	9/15/15/15	-
3	PLM	B	808	-	-	7/15/15/15	-
3	PLM	B	807	-	-	14/15/15/15	-
3	PLM	A	810	-	-	13/15/15/15	-
3	PLM	A	812	1	-	11/15/15/15	-
3	PLM	A	811	1	-	7/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLM	B	803	-	-	10/15/15/15	-
3	PLM	A	808	-	-	9/15/15/15	-
4	3PH	B	810	1	-	28/49/49/49	-
3	PLM	A	809	-	-	11/15/15/15	-
3	PLM	A	806	-	-	12/15/15/15	-
3	PLM	B	809	1	-	10/15/15/15	-
4	3PH	A	813	1	-	27/49/49/49	-
3	PLM	B	806	-	-	11/15/15/15	-
3	PLM	B	805	-	-	9/15/15/15	-
3	PLM	A	807	-	-	9/15/15/15	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	813	3PH	O31-C31	2.60	1.40	1.33
4	B	810	3PH	O31-C31	2.49	1.40	1.33
4	A	813	3PH	O21-C21	2.30	1.40	1.34
4	B	810	3PH	O21-C21	2.27	1.40	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	810	3PH	O21-C21-C22	4.35	120.87	111.50
4	A	813	3PH	O21-C21-C22	4.04	120.21	111.50
4	A	813	3PH	O31-C31-C32	2.86	120.89	111.91
4	B	810	3PH	O31-C31-C32	2.84	120.81	111.91
4	A	813	3PH	C36-C35-C34	2.52	127.22	114.42
3	B	808	PLM	O1-C1-C2	2.23	121.19	114.03
3	B	808	PLM	O1-C1-O2	-2.22	117.77	123.30
3	A	806	PLM	O1-C1-C2	2.08	120.71	114.03

There are no chirality outliers.

All (197) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	813	3PH	C1-O11-P-O13
4	A	813	3PH	C1-O11-P-O14
4	A	813	3PH	C22-C21-O21-C2
4	B	810	3PH	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
4	B	810	3PH	C1-O11-P-O14
4	B	810	3PH	C1-O11-P-O12
4	B	810	3PH	C22-C21-O21-C2
4	A	813	3PH	O22-C21-O21-C2
4	B	810	3PH	O22-C21-O21-C2
3	B	805	PLM	C7-C8-C9-CA
3	A	808	PLM	C7-C8-C9-CA
3	B	804	PLM	CB-CC-CD-CE
3	A	807	PLM	CB-CC-CD-CE
3	A	808	PLM	CB-CC-CD-CE
3	B	805	PLM	CB-CC-CD-CE
4	A	813	3PH	C22-C23-C24-C25
3	A	808	PLM	C5-C6-C7-C8
3	B	803	PLM	C8-C9-CA-CB
3	B	803	PLM	CA-CB-CC-CD
3	B	805	PLM	C5-C6-C7-C8
3	B	809	PLM	C8-C9-CA-CB
3	A	806	PLM	CA-CB-CC-CD
3	A	809	PLM	C7-C8-C9-CA
3	A	812	PLM	C5-C6-C7-C8
3	B	806	PLM	C7-C8-C9-CA
3	A	806	PLM	C8-C9-CA-CB
4	A	813	3PH	C32-C31-O31-C3
3	A	810	PLM	C2-C3-C4-C5
4	A	813	3PH	C37-C38-C39-C3A
4	B	810	3PH	C31-C32-C33-C34
3	A	809	PLM	C5-C6-C7-C8
3	B	806	PLM	C5-C6-C7-C8
4	B	810	3PH	C24-C25-C26-C27
4	A	813	3PH	O32-C31-O31-C3
3	B	807	PLM	C2-C3-C4-C5
4	A	813	3PH	C24-C25-C26-C27
3	A	807	PLM	C3-C4-C5-C6
3	A	807	PLM	C7-C8-C9-CA
3	B	803	PLM	C5-C6-C7-C8
3	B	804	PLM	C7-C8-C9-CA
4	B	810	3PH	C27-C28-C29-C2A
4	B	810	3PH	C34-C35-C36-C37
3	A	810	PLM	C8-C9-CA-CB
3	B	804	PLM	C3-C4-C5-C6
3	B	804	PLM	CD-CE-CF-CG
4	A	813	3PH	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
3	B	804	PLM	CA-CB-CC-CD
4	A	813	3PH	C2C-C2D-C2E-C2F
3	A	806	PLM	C5-C6-C7-C8
4	B	810	3PH	C2C-C2D-C2E-C2F
3	A	812	PLM	CC-CD-CE-CF
3	B	807	PLM	C8-C9-CA-CB
3	A	807	PLM	CA-CB-CC-CD
3	A	809	PLM	C8-C9-CA-CB
3	A	809	PLM	CA-CB-CC-CD
3	B	806	PLM	C8-C9-CA-CB
3	B	806	PLM	CA-CB-CC-CD
3	B	809	PLM	CC-CD-CE-CF
4	A	813	3PH	C27-C28-C29-C2A
4	A	813	3PH	C29-C2A-C2B-C2C
4	B	810	3PH	C2D-C2E-C2F-C2G
3	A	807	PLM	C5-C6-C7-C8
4	A	813	3PH	C25-C26-C27-C28
3	B	807	PLM	C4-C5-C6-C7
3	A	809	PLM	CC-CD-CE-CF
3	B	804	PLM	C5-C6-C7-C8
3	B	804	PLM	C8-C9-CA-CB
3	B	806	PLM	CC-CD-CE-CF
4	A	813	3PH	C2D-C2E-C2F-C2G
4	B	810	3PH	C29-C2A-C2B-C2C
3	A	808	PLM	C8-C9-CA-CB
3	B	805	PLM	C3-C4-C5-C6
3	B	805	PLM	C8-C9-CA-CB
3	A	807	PLM	C8-C9-CA-CB
3	A	808	PLM	C3-C4-C5-C6
4	B	810	3PH	C23-C24-C25-C26
3	A	810	PLM	C9-CA-CB-CC
3	A	812	PLM	CA-CB-CC-CD
3	B	807	PLM	C9-CA-CB-CC
3	A	810	PLM	C5-C6-C7-C8
4	B	810	3PH	C37-C38-C39-C3A
3	B	803	PLM	C6-C7-C8-C9
3	A	806	PLM	C2-C3-C4-C5
3	B	808	PLM	CA-CB-CC-CD
3	A	806	PLM	C6-C7-C8-C9
3	A	806	PLM	C7-C8-C9-CA
3	A	811	PLM	CA-CB-CC-CD
3	A	812	PLM	C7-C8-C9-CA

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Mol	Chain	Res	Type	Atoms
3	A	809	PLM	C9-CA-CB-CC
3	B	806	PLM	C9-CA-CB-CC
4	A	813	3PH	C3C-C3D-C3E-C3F
4	B	810	3PH	C3A-C3B-C3C-C3D
3	B	809	PLM	C4-C5-C6-C7
3	B	807	PLM	C1-C2-C3-C4
3	A	810	PLM	C4-C5-C6-C7
3	B	809	PLM	C3-C4-C5-C6
3	B	809	PLM	C1-C2-C3-C4
3	A	807	PLM	CD-CE-CF-CG
3	B	803	PLM	C7-C8-C9-CA
3	A	812	PLM	C4-C5-C6-C7
3	B	809	PLM	C2-C3-C4-C5
3	A	808	PLM	CA-CB-CC-CD
3	B	803	PLM	C9-CA-CB-CC
3	B	807	PLM	C3-C4-C5-C6
3	A	812	PLM	C1-C2-C3-C4
3	A	806	PLM	C9-CA-CB-CC
3	A	812	PLM	C2-C3-C4-C5
3	B	805	PLM	CA-CB-CC-CD
4	B	810	3PH	C33-C34-C35-C36
3	A	809	PLM	CB-CC-CD-CE
3	B	806	PLM	CB-CC-CD-CE
4	A	813	3PH	C33-C34-C35-C36
3	A	807	PLM	C2-C3-C4-C5
3	A	812	PLM	C3-C4-C5-C6
3	A	812	PLM	C8-C9-CA-CB
4	B	810	3PH	C26-C27-C28-C29
3	A	811	PLM	C3-C4-C5-C6
3	A	810	PLM	C3-C4-C5-C6
4	A	813	3PH	C28-C29-C2A-C2B
3	B	803	PLM	C2-C3-C4-C5
3	A	812	PLM	C6-C7-C8-C9
3	B	808	PLM	C7-C8-C9-CA
3	A	810	PLM	CB-CC-CD-CE
3	B	809	PLM	CA-CB-CC-CD
3	B	807	PLM	C6-C7-C8-C9
4	A	813	3PH	C3E-C3F-C3G-C3H
4	B	810	3PH	C28-C29-C2A-C2B
3	A	811	PLM	C7-C8-C9-CA
4	B	810	3PH	C25-C26-C27-C28
3	A	806	PLM	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	B	807	PLM	CB-CC-CD-CE
4	B	810	3PH	C39-C3A-C3B-C3C
3	B	809	PLM	C7-C8-C9-CA
3	B	805	PLM	CD-CE-CF-CG
4	B	810	3PH	C2-C1-O11-P
3	B	804	PLM	C2-C3-C4-C5
3	A	810	PLM	CA-CB-CC-CD
3	A	808	PLM	CD-CE-CF-CG
3	B	808	PLM	C6-C7-C8-C9
3	B	807	PLM	CD-CE-CF-CG
3	A	808	PLM	C4-C5-C6-C7
3	B	806	PLM	C4-C5-C6-C7
3	A	806	PLM	C4-C5-C6-C7
3	A	809	PLM	C4-C5-C6-C7
3	A	810	PLM	CD-CE-CF-CG
3	B	803	PLM	C4-C5-C6-C7
3	A	806	PLM	CD-CE-CF-CG
3	B	808	PLM	C2-C3-C4-C5
4	A	813	3PH	C38-C39-C3A-C3B
3	B	803	PLM	CD-CE-CF-CG
3	B	807	PLM	CA-CB-CC-CD
3	A	811	PLM	C6-C7-C8-C9
3	A	807	PLM	C4-C5-C6-C7
4	A	813	3PH	C2-C1-O11-P
4	B	810	3PH	C38-C39-C3A-C3B
4	B	810	3PH	C3C-C3D-C3E-C3F
3	A	808	PLM	C6-C7-C8-C9
3	B	805	PLM	C4-C5-C6-C7
3	B	809	PLM	CD-CE-CF-CG
3	A	810	PLM	C6-C7-C8-C9
3	A	812	PLM	CD-CE-CF-CG
4	B	810	3PH	C2F-C2G-C2H-C2I
3	B	809	PLM	C6-C7-C8-C9
4	A	813	3PH	C2F-C2G-C2H-C2I
4	A	813	3PH	C1-O11-P-O12
3	B	804	PLM	C4-C5-C6-C7
4	A	813	3PH	C2A-C2B-C2C-C2D
3	B	808	PLM	O2-C1-C2-C3
3	B	803	PLM	C3-C4-C5-C6
4	A	813	3PH	C3A-C3B-C3C-C3D
3	B	805	PLM	C6-C7-C8-C9
3	B	806	PLM	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	809	PLM	O2-C1-C2-C3
3	B	807	PLM	O2-C1-C2-C3
4	B	810	3PH	C2A-C2B-C2C-C2D
3	B	808	PLM	O1-C1-C2-C3
3	A	809	PLM	O1-C1-C2-C3
4	B	810	3PH	O32-C31-O31-C3
3	B	807	PLM	O1-C1-C2-C3
3	B	806	PLM	O1-C1-C2-C3
4	B	810	3PH	C35-C36-C37-C38
3	A	809	PLM	CD-CE-CF-CG
4	B	810	3PH	C32-C31-O31-C3
3	B	806	PLM	CD-CE-CF-CG
3	B	807	PLM	C7-C8-C9-CA
3	B	808	PLM	C9-CA-CB-CC
3	A	806	PLM	O1-C1-C2-C3
3	A	806	PLM	O2-C1-C2-C3
4	A	813	3PH	O31-C31-C32-C33
3	A	810	PLM	O1-C1-C2-C3
3	A	810	PLM	O2-C1-C2-C3
3	A	810	PLM	CC-CD-CE-CF
4	A	813	3PH	O32-C31-C32-C33
3	B	807	PLM	CC-CD-CE-CF
3	A	811	PLM	O1-C1-C2-C3
3	A	811	PLM	C9-CA-CB-CC
3	A	811	PLM	O2-C1-C2-C3

There are no ring outliers.

16 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	804	PLM	5	0
3	B	808	PLM	1	0
3	B	807	PLM	5	0
3	A	810	PLM	3	0
3	A	812	PLM	8	0
3	A	811	PLM	1	0
3	B	803	PLM	5	0
3	A	808	PLM	3	0
4	B	810	3PH	2	0
3	A	809	PLM	4	0
3	A	806	PLM	4	0
3	B	809	PLM	3	0

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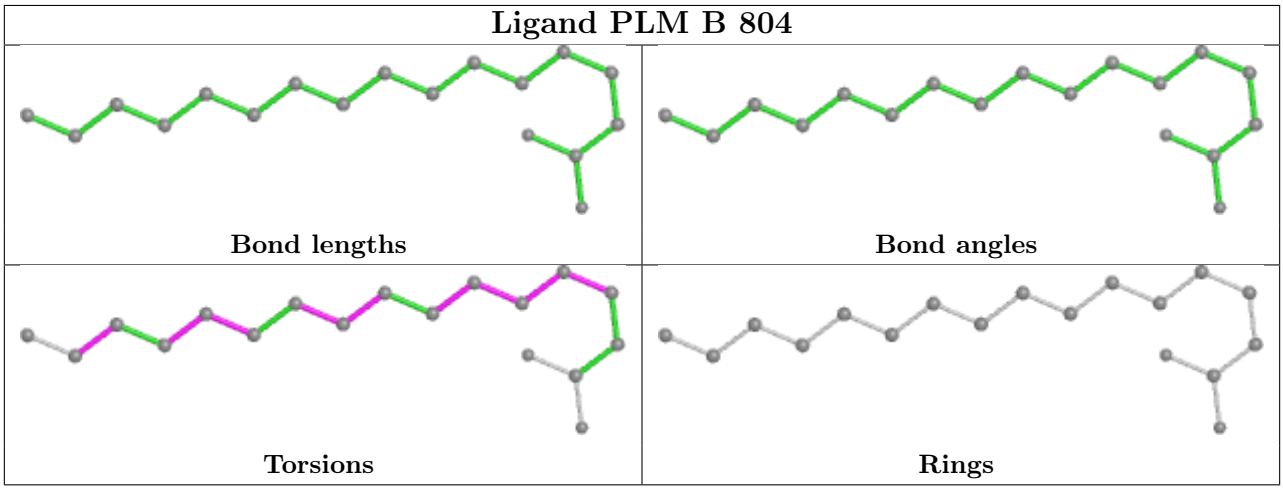
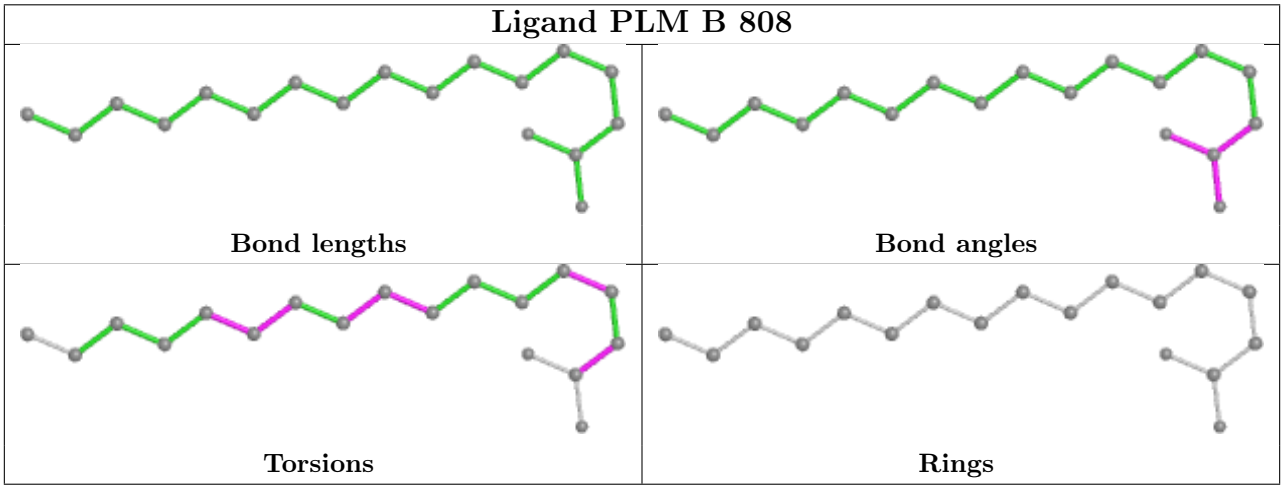
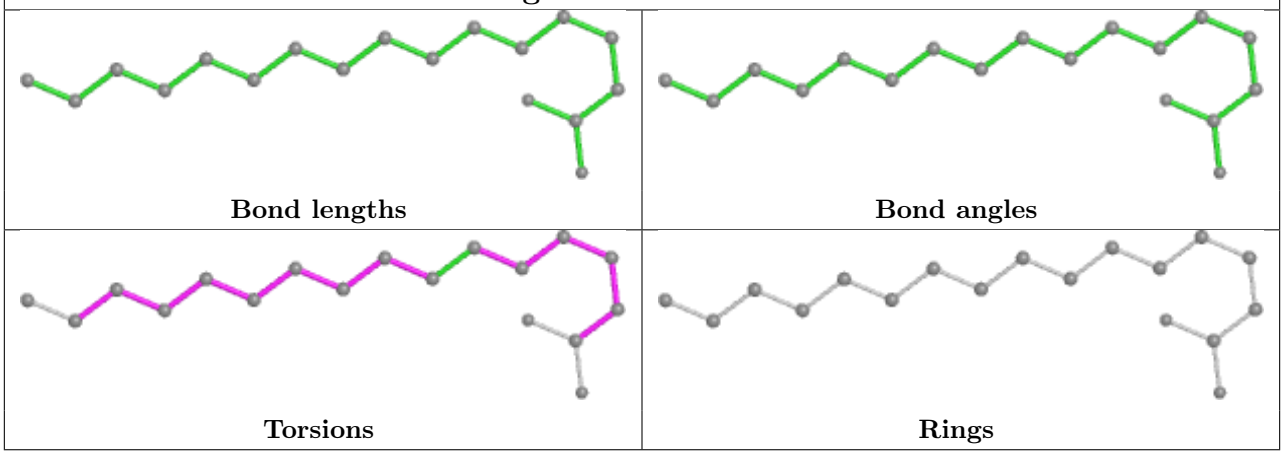
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	813	3PH	3	0
3	B	806	PLM	2	0
3	B	805	PLM	2	0
3	A	807	PLM	9	0

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 then 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.

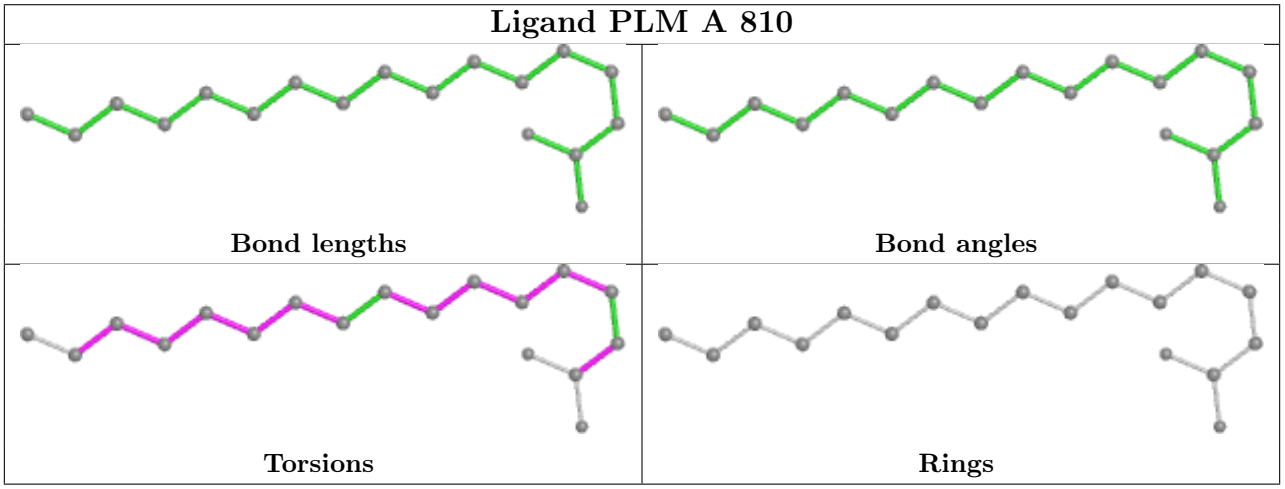




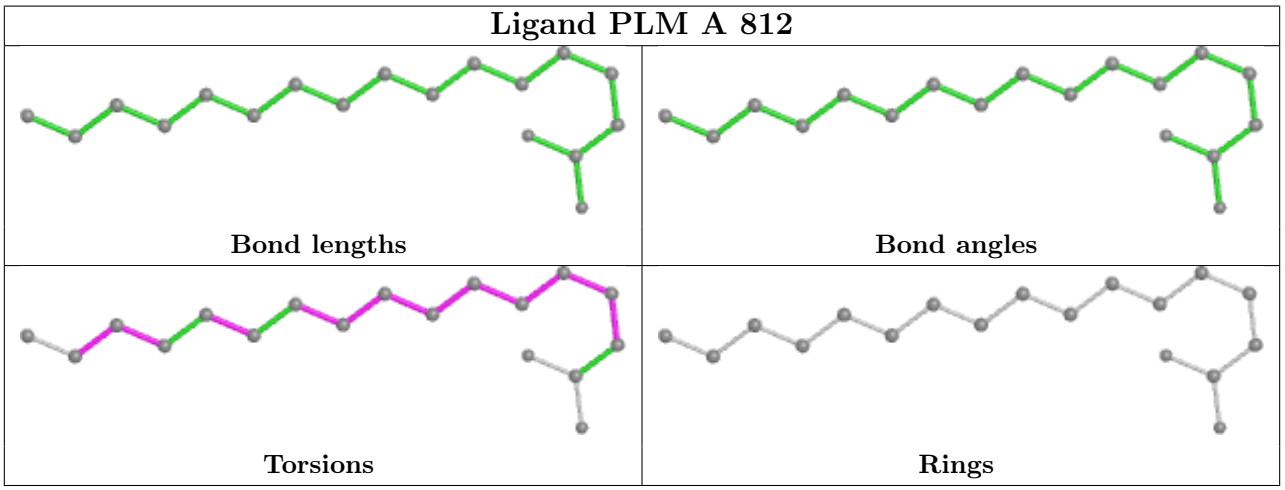
Ligand PLM B 807



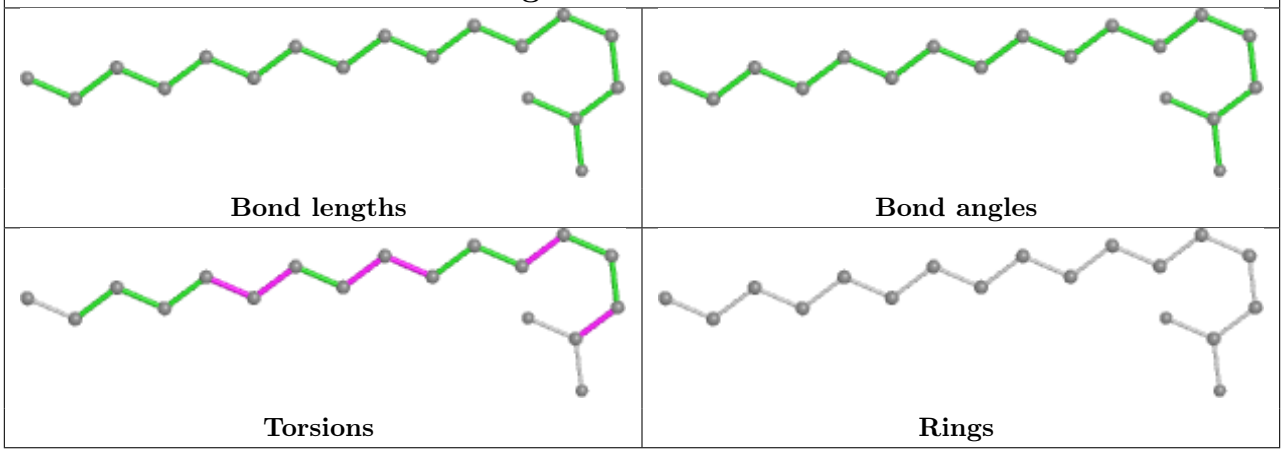
Ligand PLM A 810



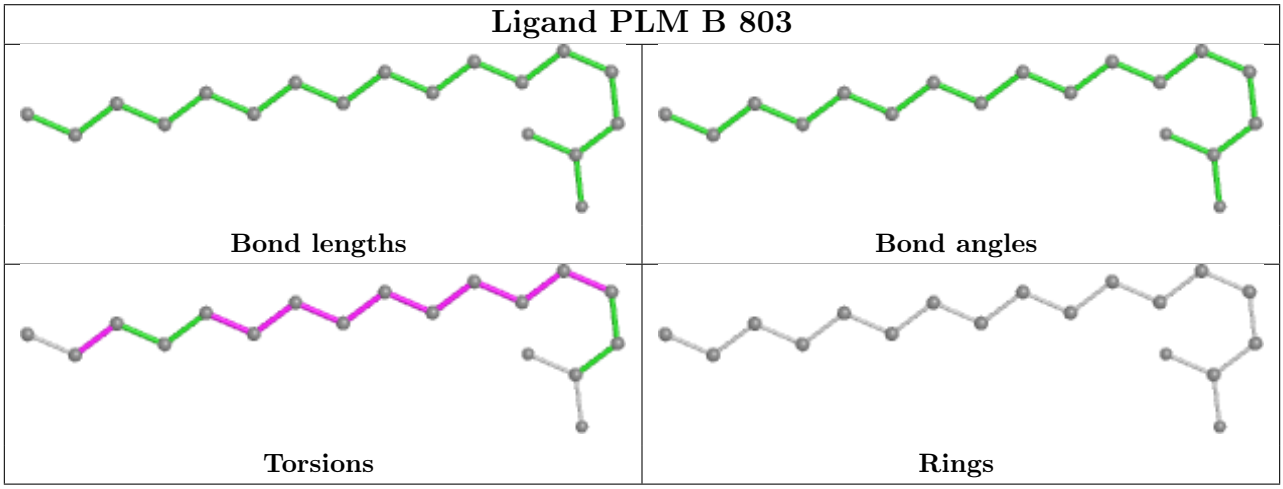
Ligand PLM A 812



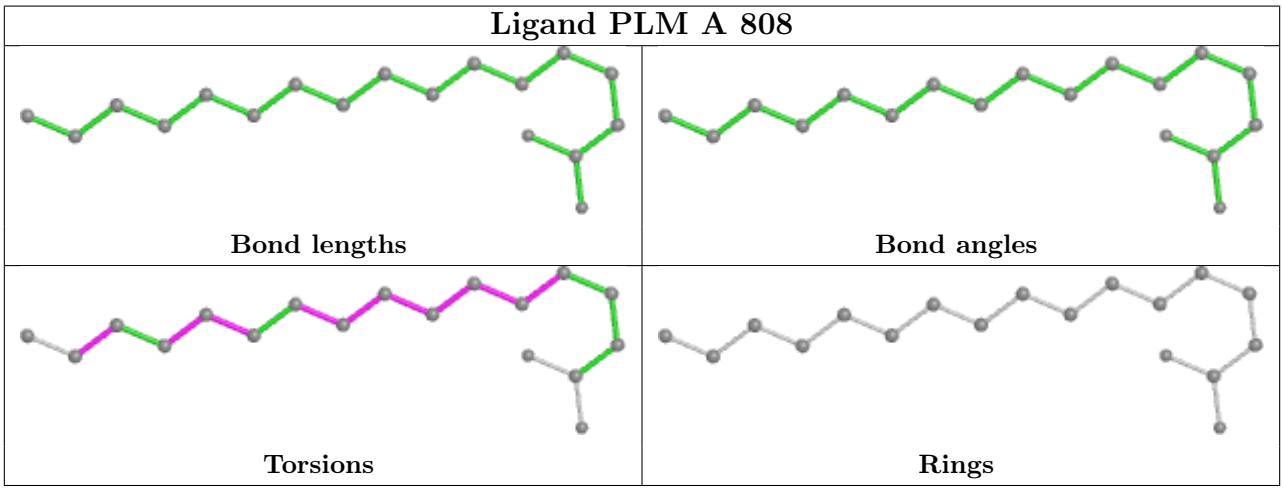
Ligand PLM A 811



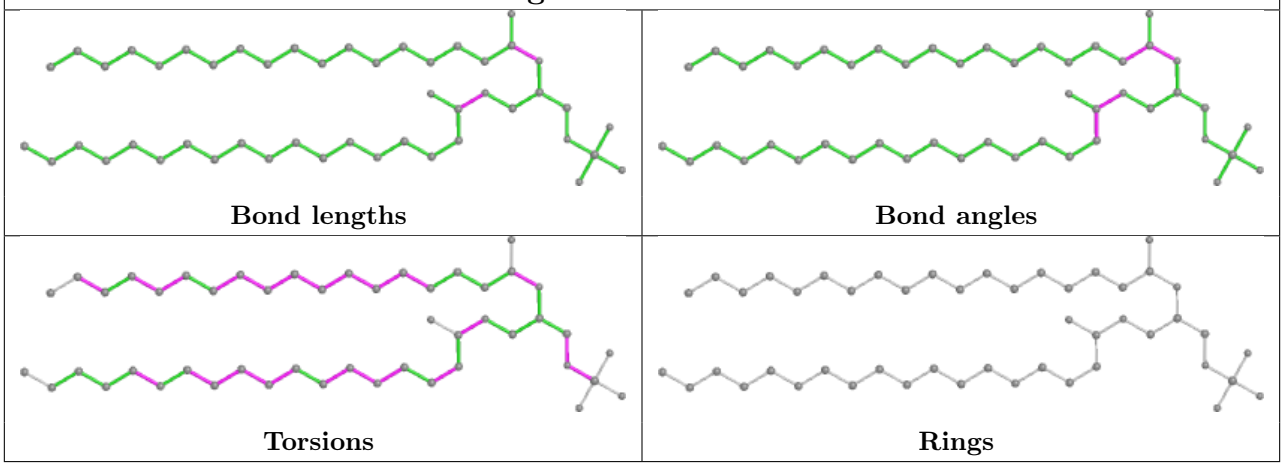
Ligand PLM B 803



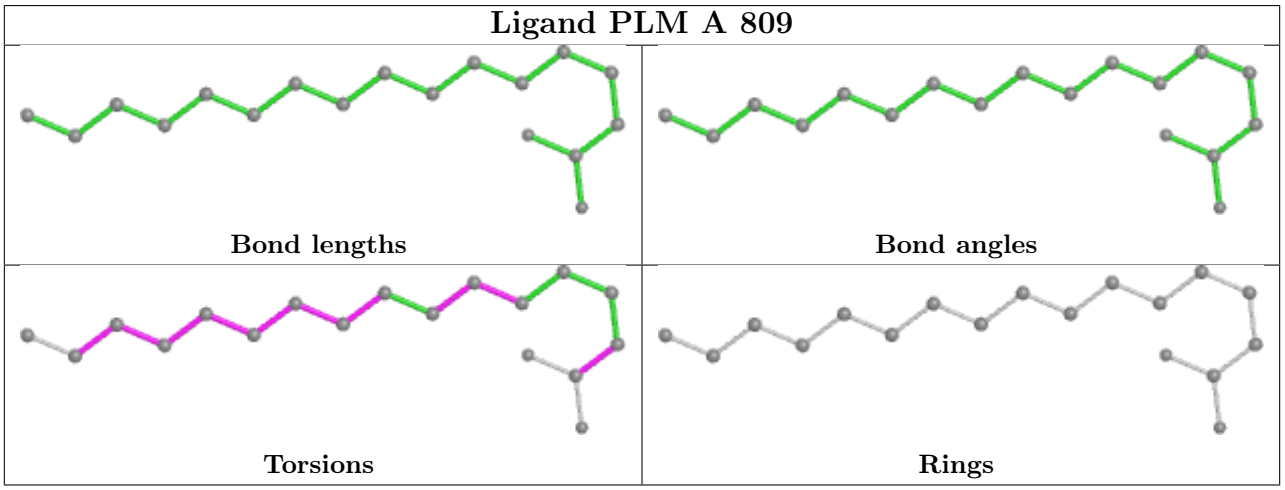
Ligand PLM A 808



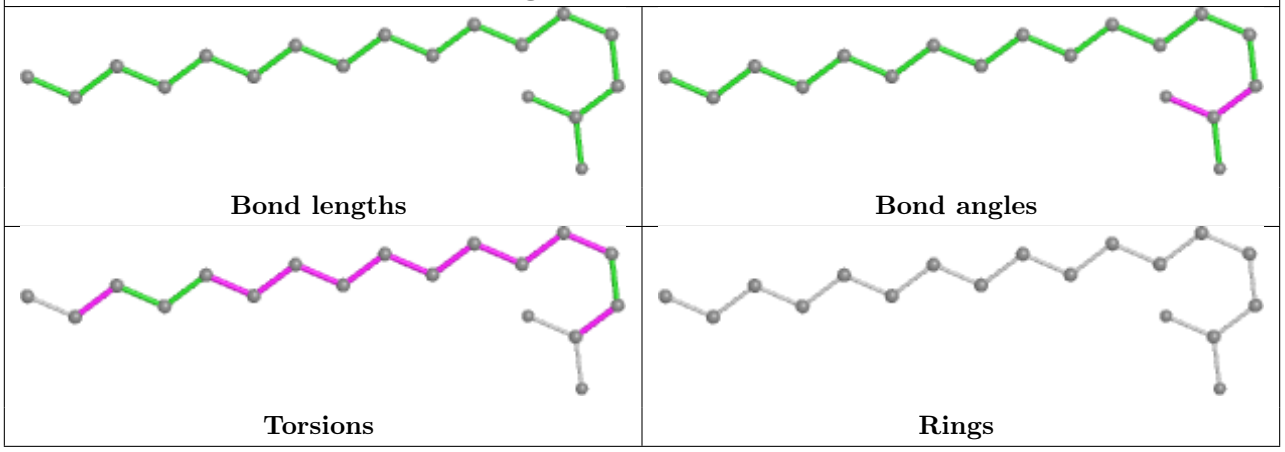
Ligand 3PH B 810



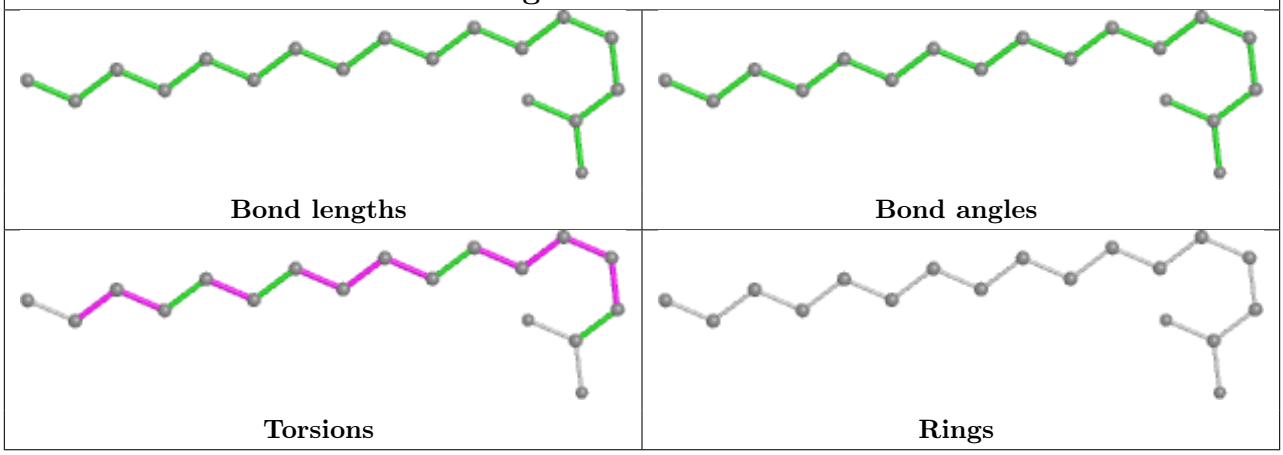
Ligand PLM A 809



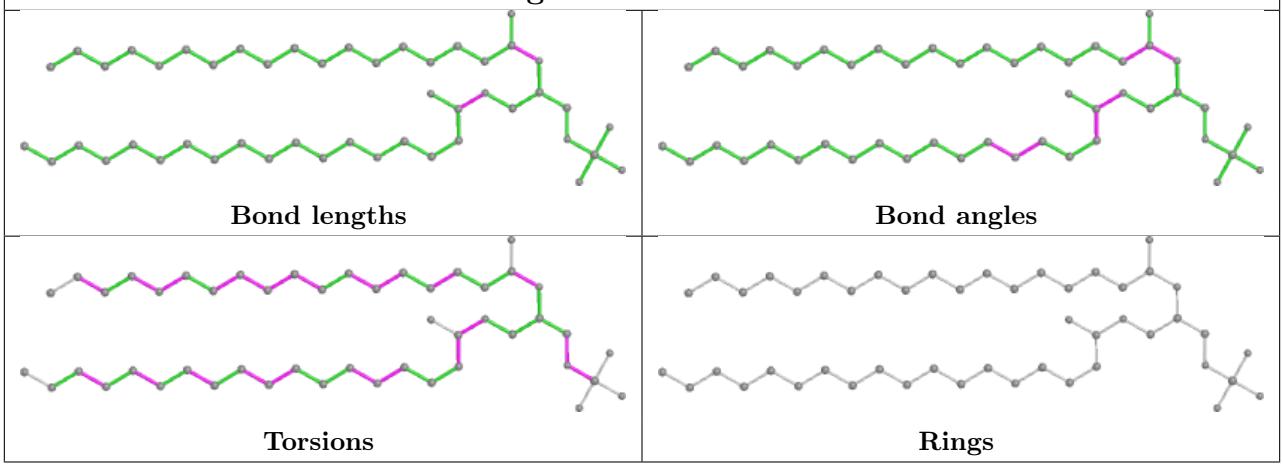
Ligand PLM A 806



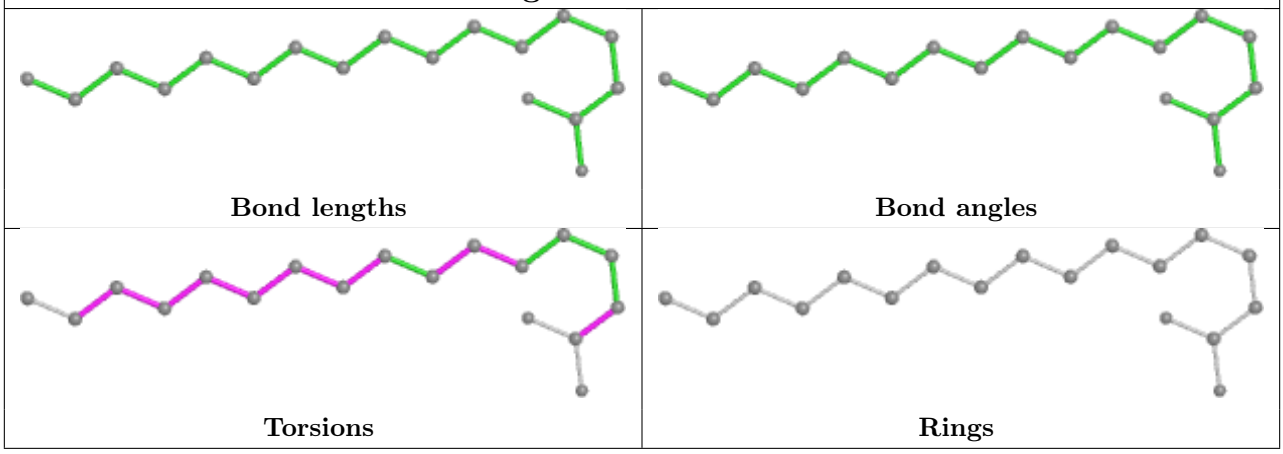
Ligand PLM B 809

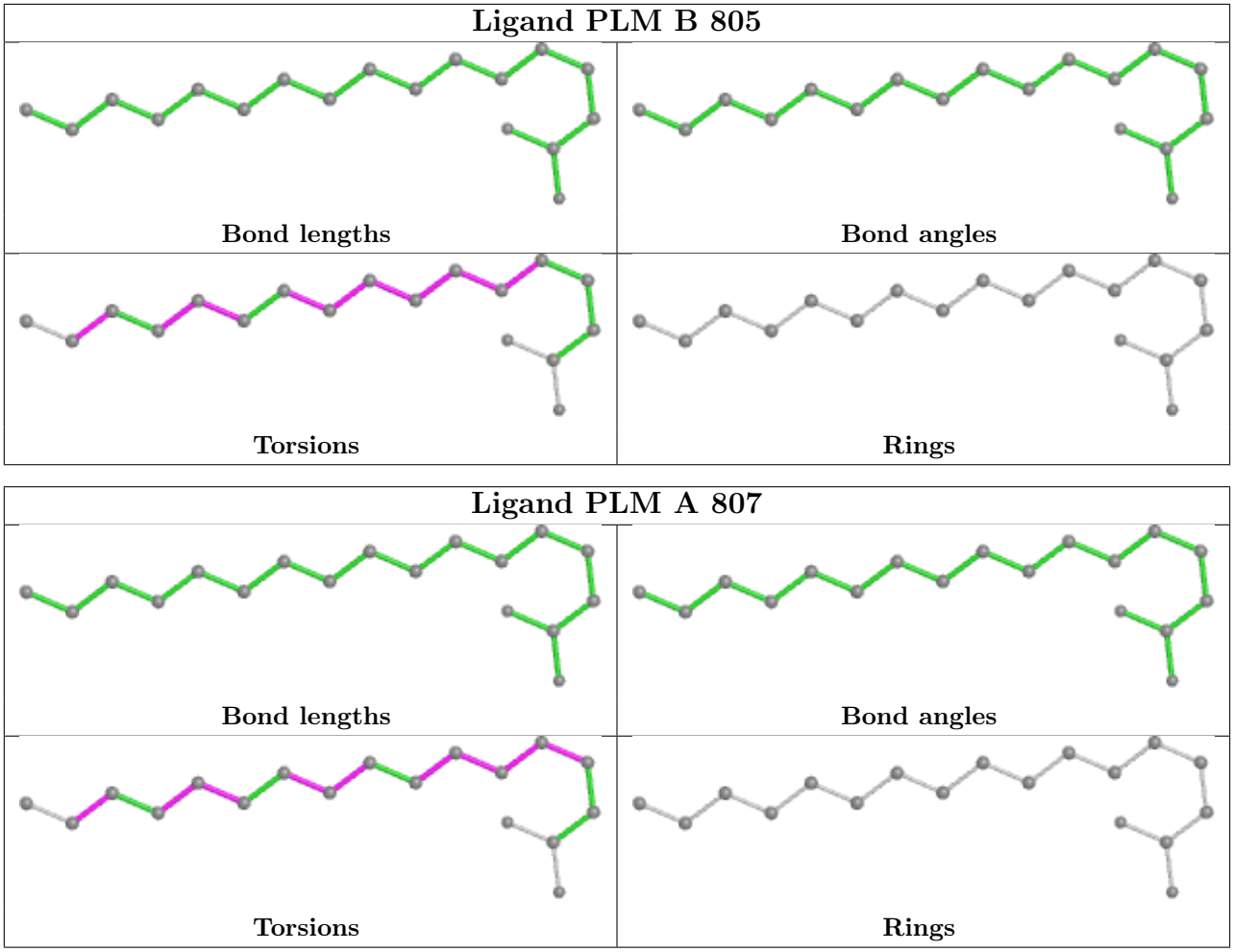


Ligand 3PH A 813



Ligand PLM B 806





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.

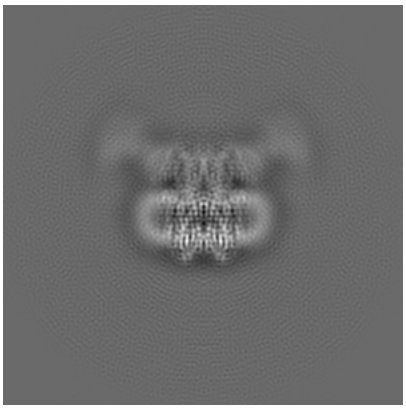
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8957. These allow visual inspection of the internal detail of the map and identification of artifacts.

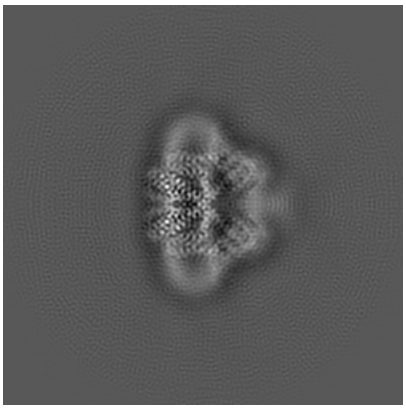
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

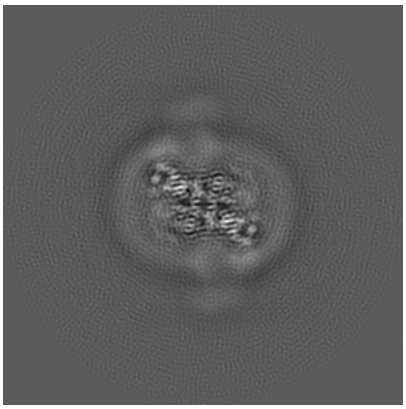
6.1.1 Primary map



X

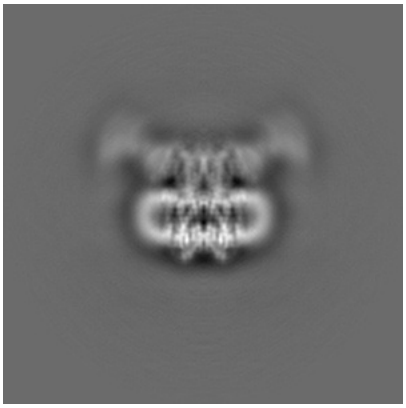


Y

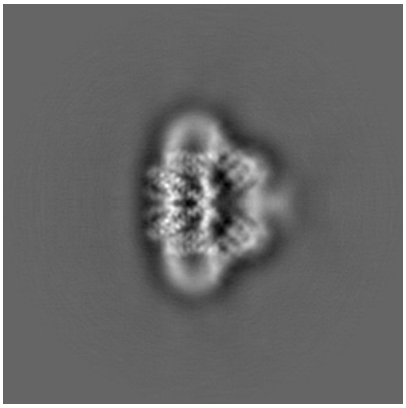


Z

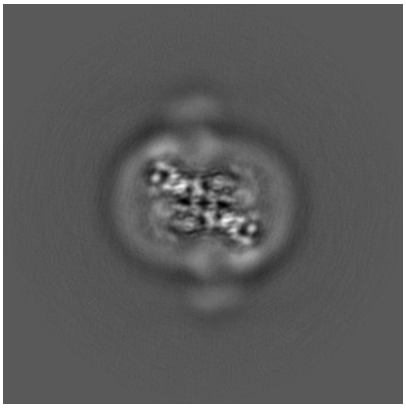
6.1.2 Raw map



X



Y

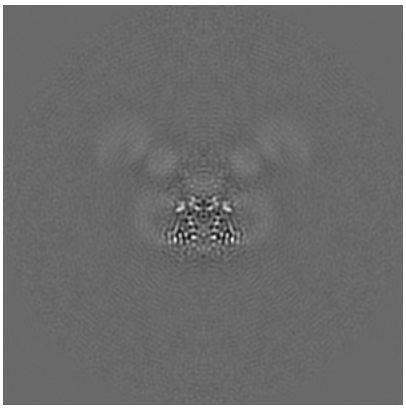


Z

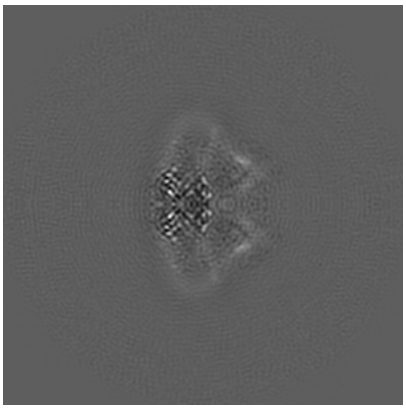
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

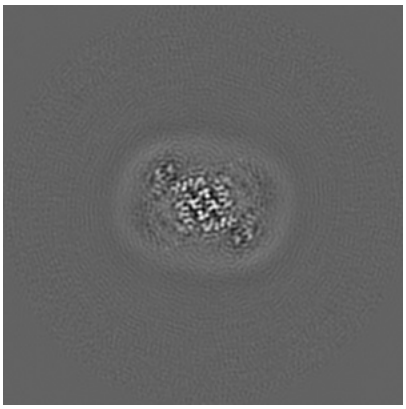
6.2.1 Primary map



X Index: 128

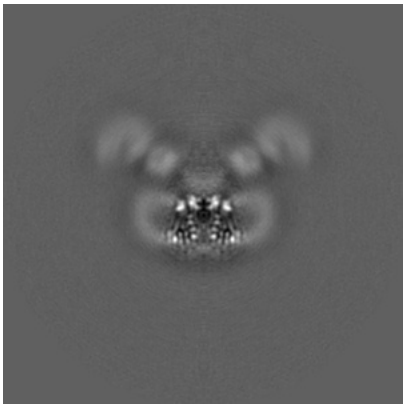


Y Index: 128

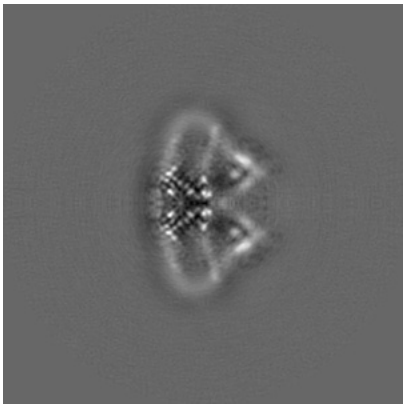


Z Index: 128

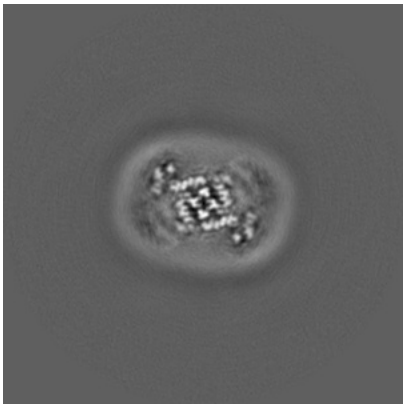
6.2.2 Raw map



X Index: 128



Y Index: 128

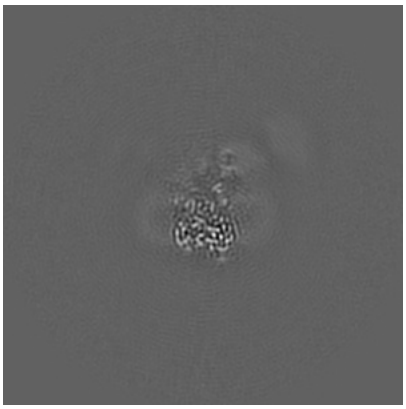


Z Index: 128

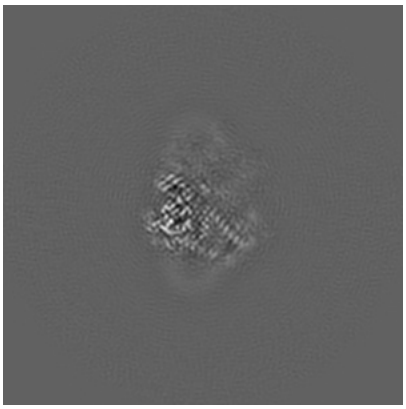
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

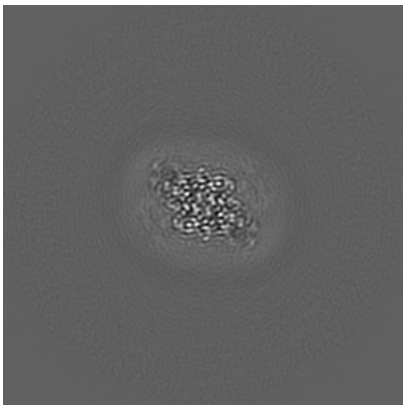
6.3.1 Primary map



X Index: 117

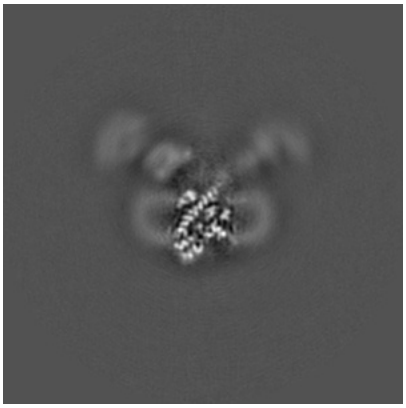


Y Index: 139

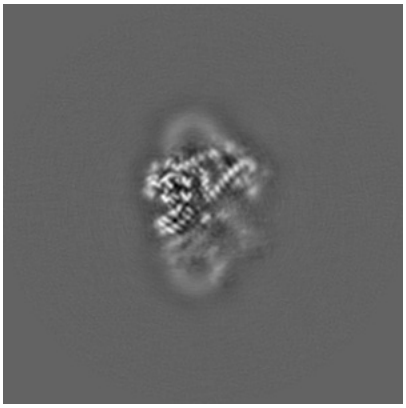


Z Index: 108

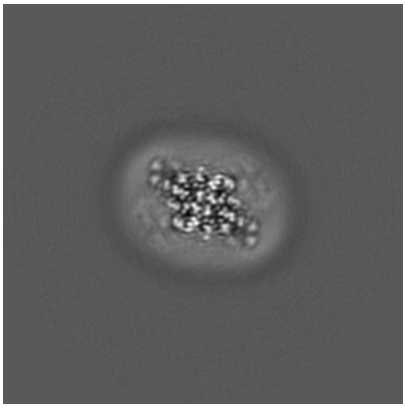
6.3.2 Raw map



X Index: 133



Y Index: 117

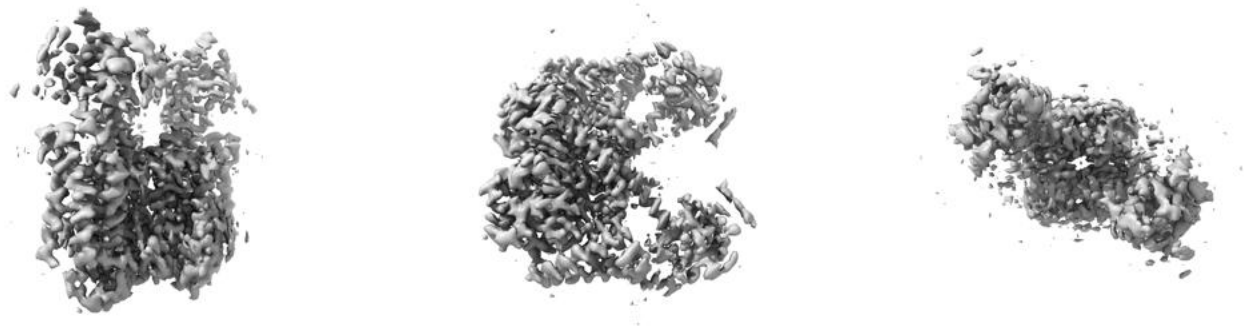


Z Index: 108

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

6.4 Orthogonal surface views (i)

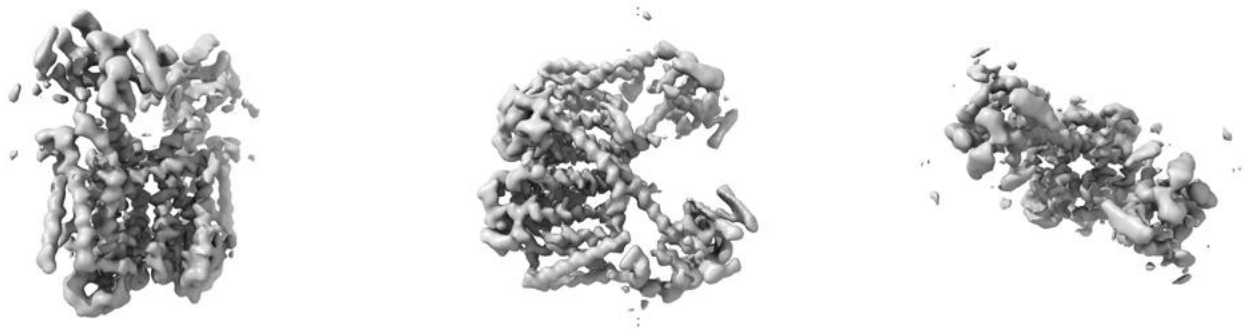
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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.

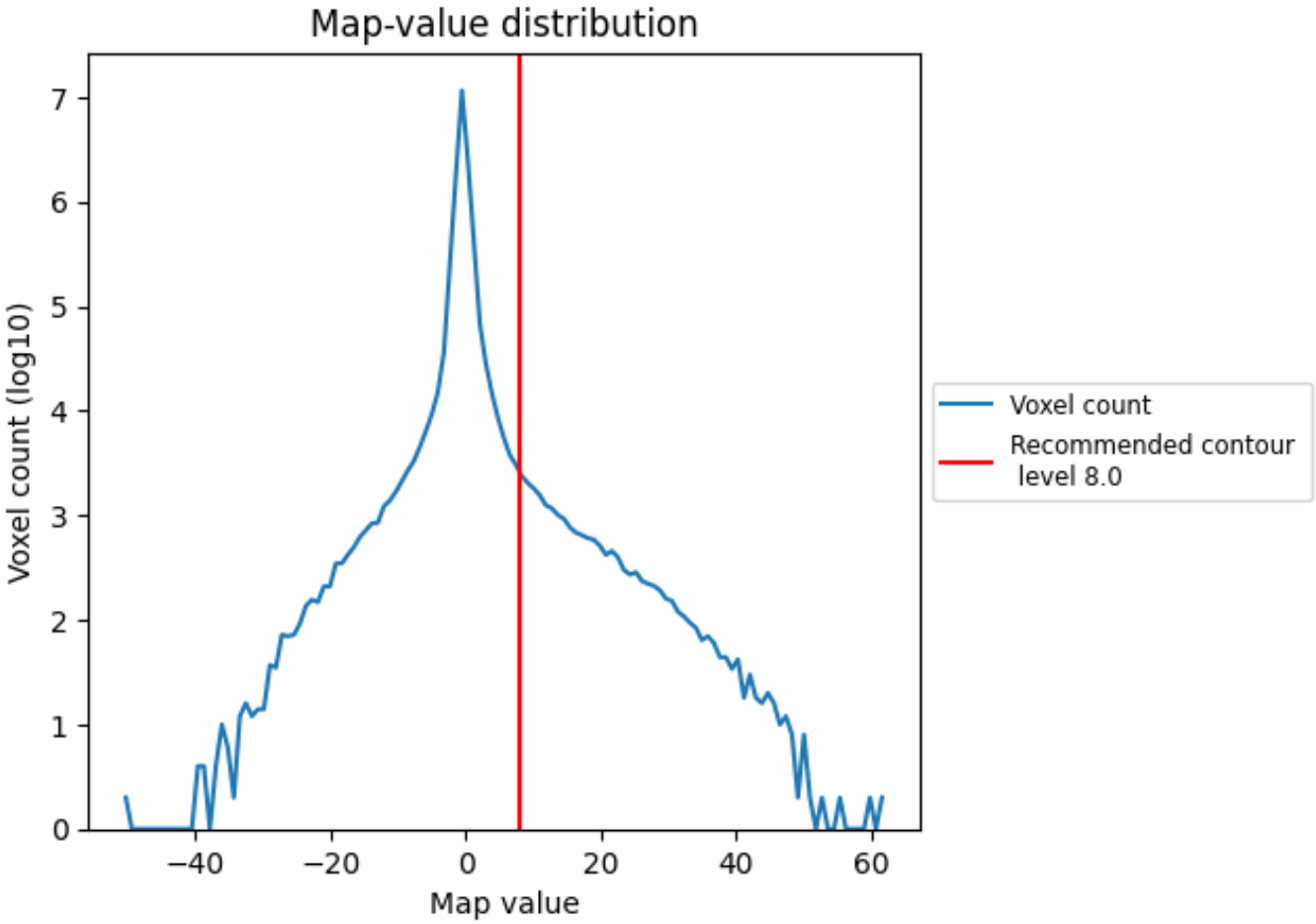
6.5 Mask visualisation (i)

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

7 Map analysis

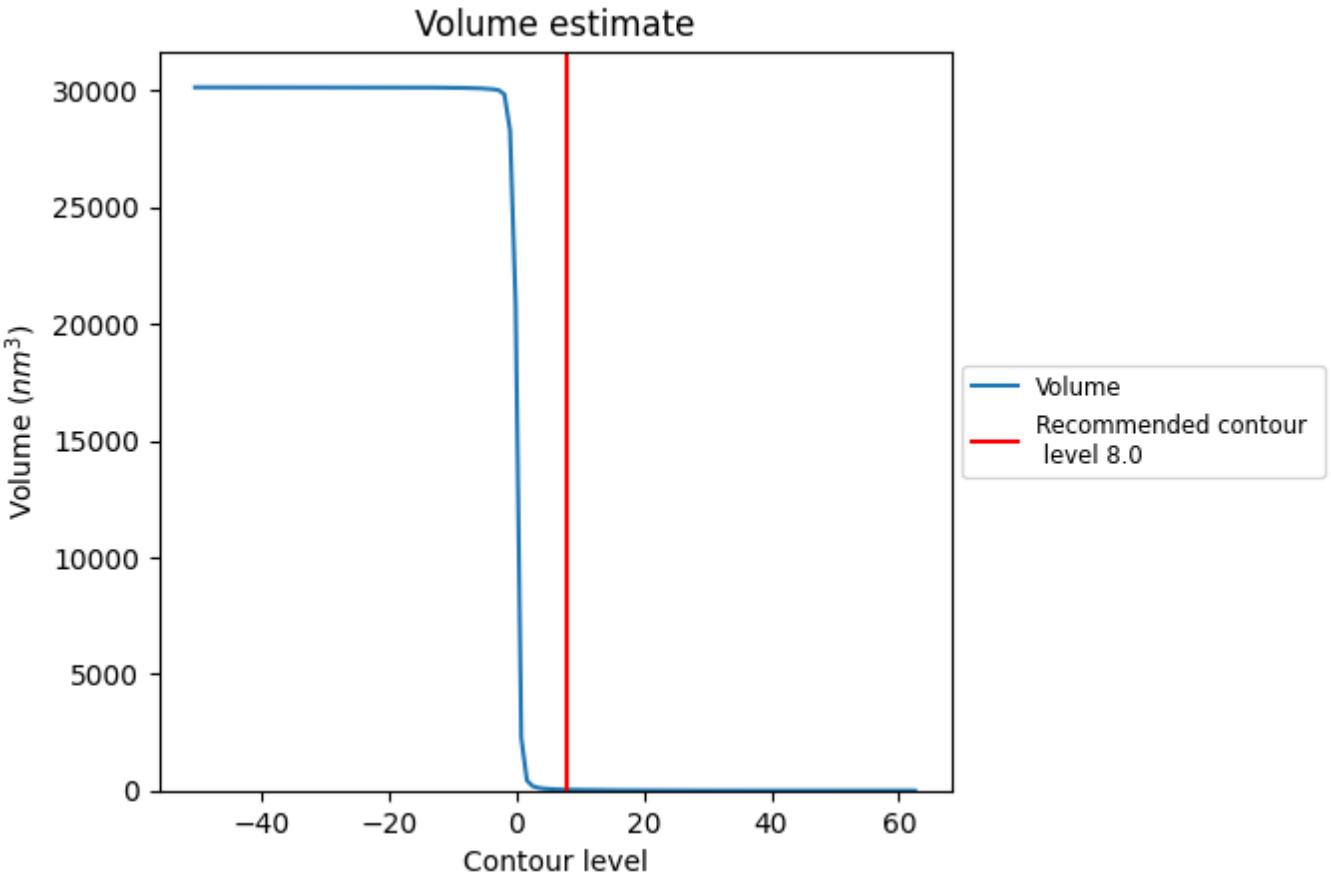
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

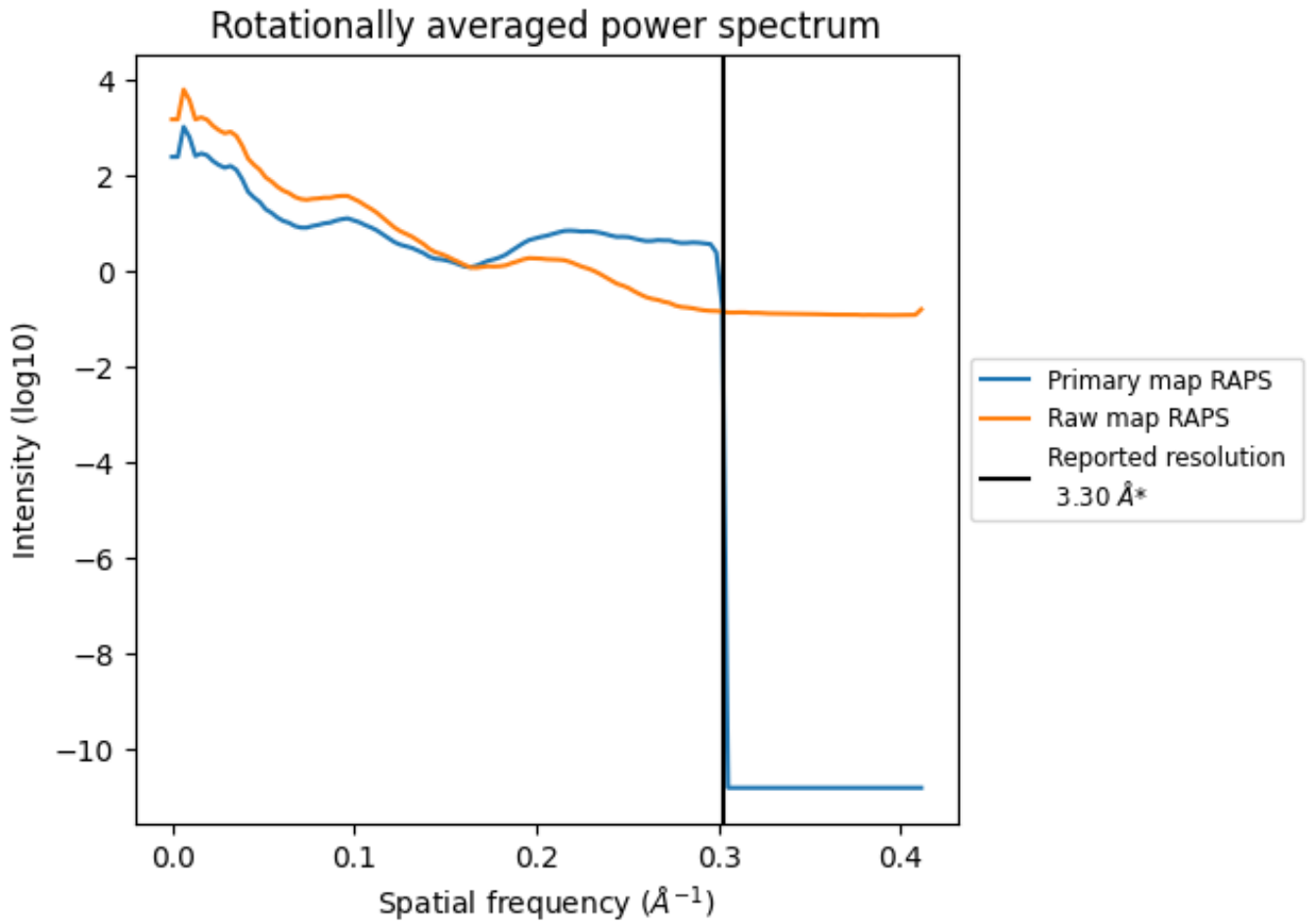
7.2 Volume estimate



The volume at the recommended contour level is 38 nm^3; this corresponds to an approximate mass of 34 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)

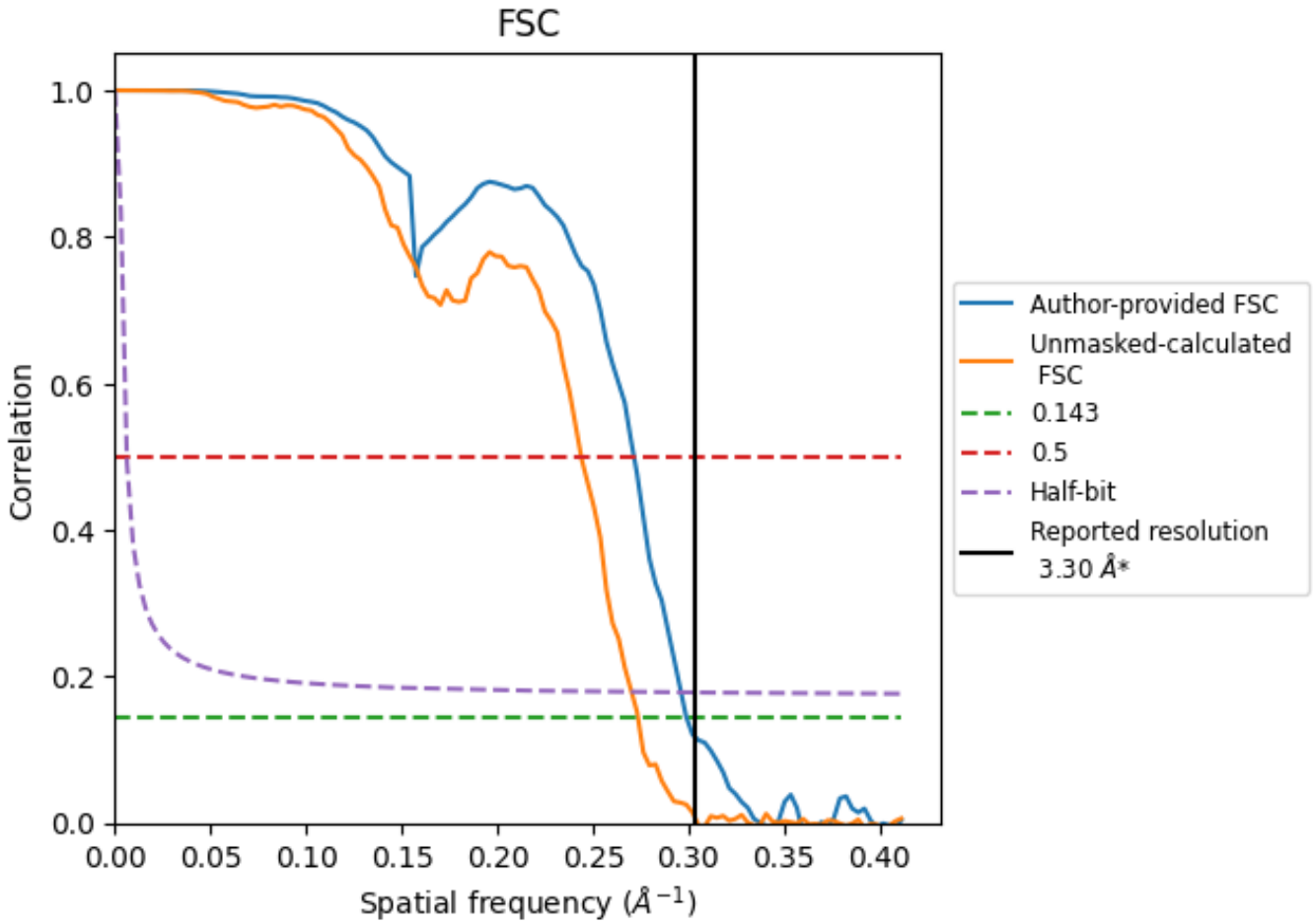


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

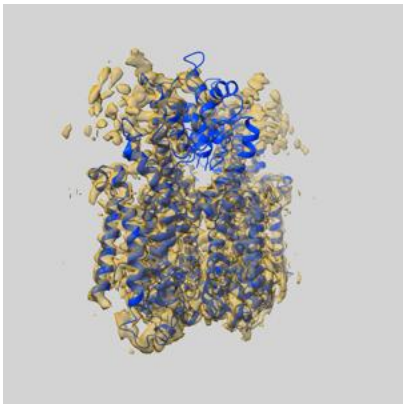
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.34	3.68	3.37
Unmasked-calculated*	3.65	4.10	3.70

*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 3.65 differs from the reported value 3.3 by more than 10 %

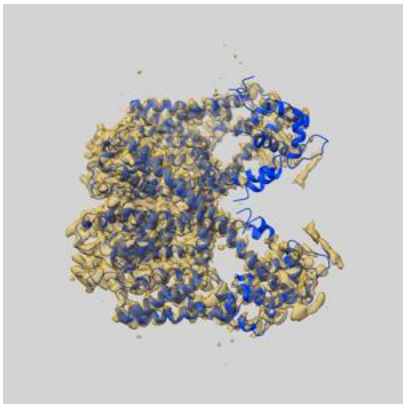
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8957 and PDB model 6E1M. Per-residue inclusion information can be found in section 3 on page 6.

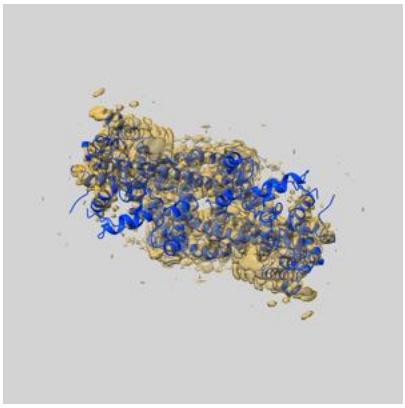
9.1 Map-model overlay



X



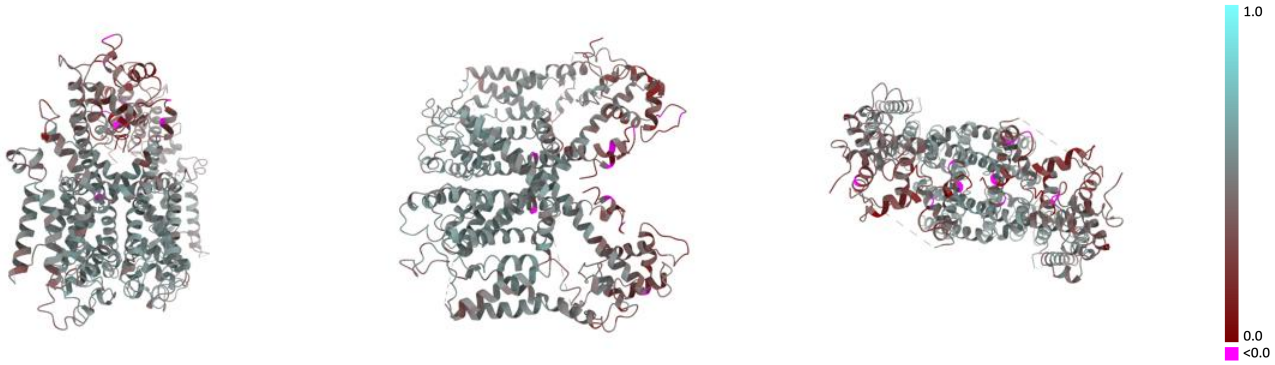
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0 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.

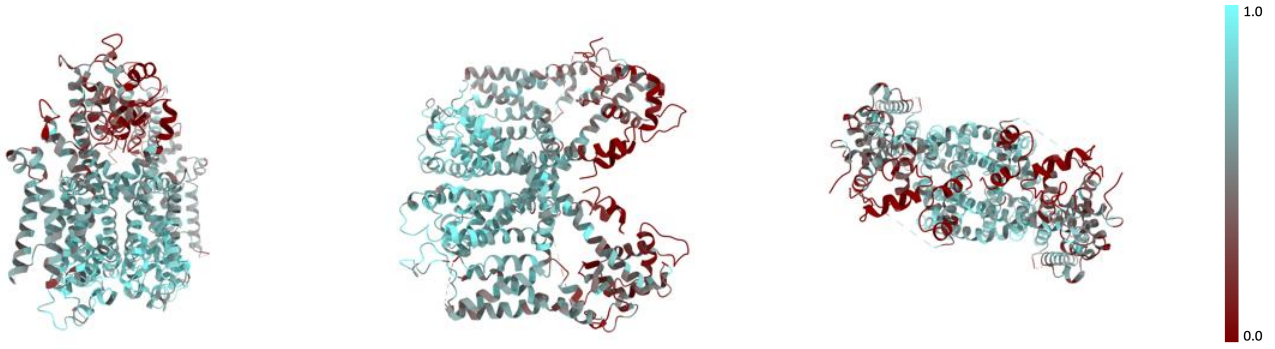
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

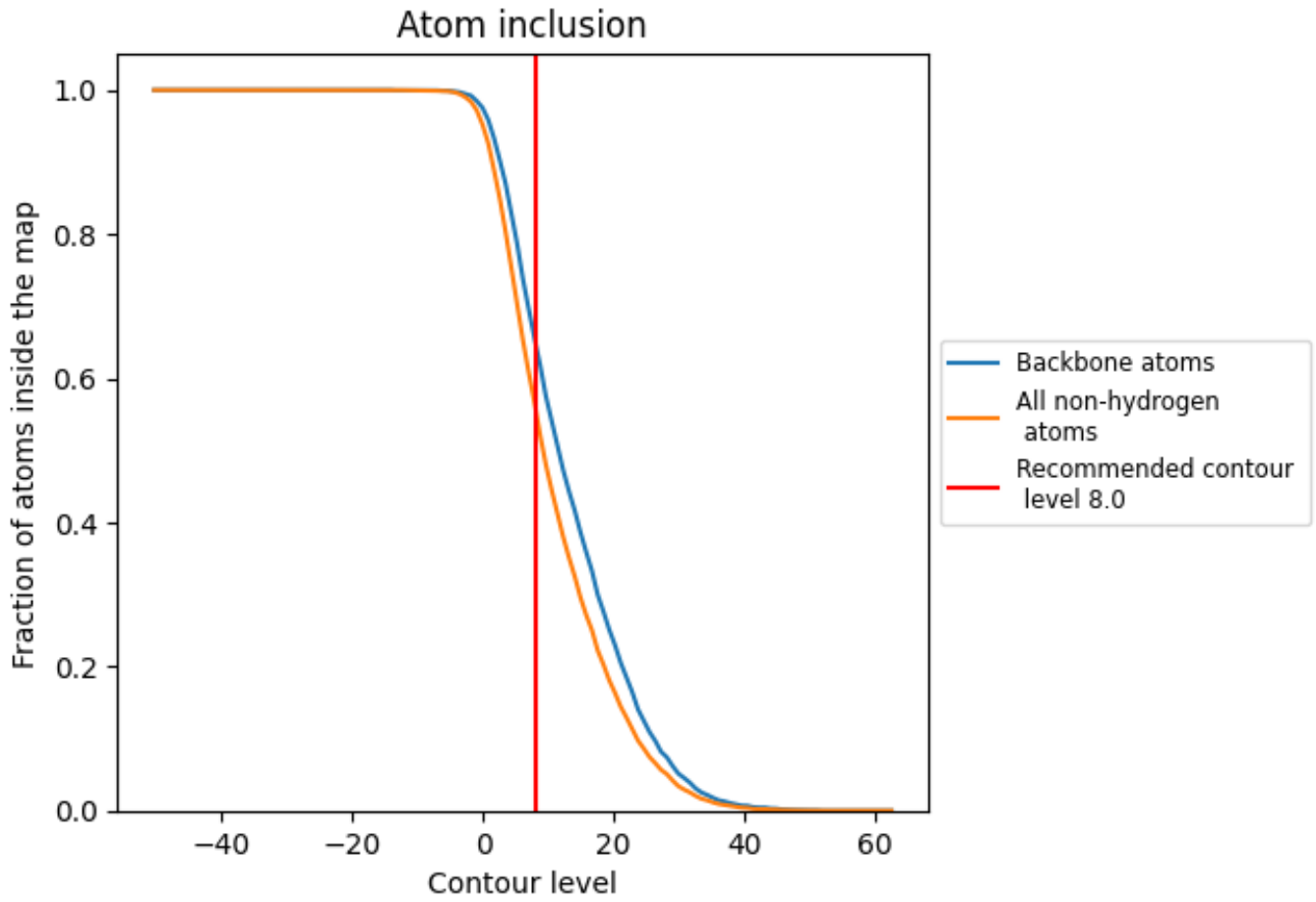
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (8.0).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 56% 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 (8.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5603	0.4620
A	0.5645	0.4630
B	0.5633	0.4610