



Full wwPDB EM Validation Report ⓘ

May 13, 2025 – 09:37 AM EDT

PDB ID : 7STO / pdb_00007sto
EMDB ID : EMD-25435
Title : Chitin Synthase 2 from Candida albicans bound to polyoxin D
Authors : Ren, Z.; Chhetri, A.; Lee, S.; Yokoyama, K.
Deposited on : 2021-11-14
Resolution : 3.15 Å(reported)

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

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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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

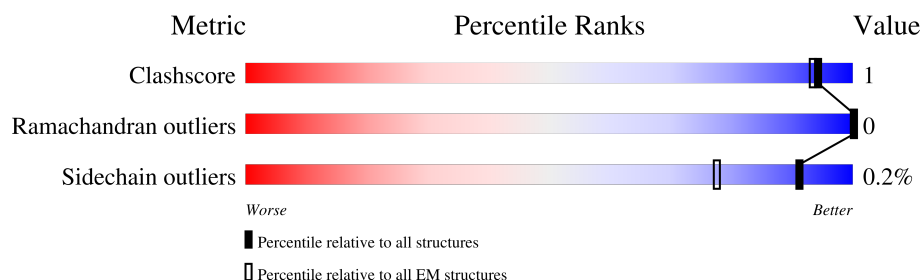
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 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	1039	
1	B	1039	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25662 atoms, of which 12720 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 Chitin synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	790	Total	C	H	N	O	S	0	0
			12410	4102	6134	1024	1122	28		
1	A	790	Total	C	H	N	O	S	0	0
			12410	4102	6134	1024	1122	28		

There are 60 discrepancies between the modelled and reference sequences:

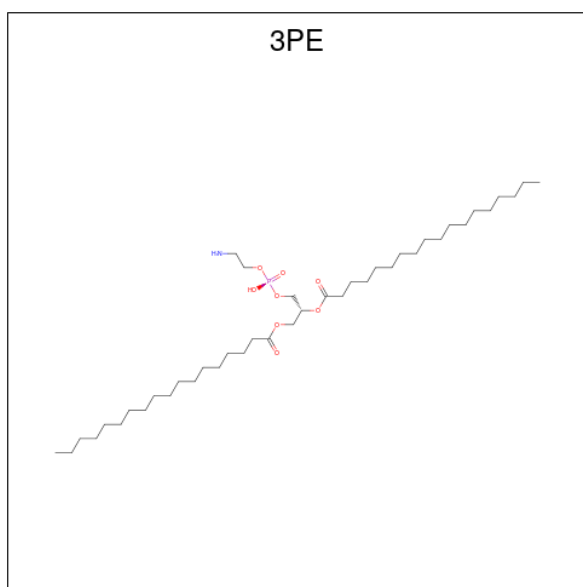
Chain	Residue	Modelled	Actual	Comment	Reference
B	1010	ALA	-	expression tag	UNP A0A1D8PTV3
B	1011	ASN	-	expression tag	UNP A0A1D8PTV3
B	1012	SER	-	expression tag	UNP A0A1D8PTV3
B	1013	LEU	-	expression tag	UNP A0A1D8PTV3
B	1014	GLU	-	expression tag	UNP A0A1D8PTV3
B	1015	VAL	-	expression tag	UNP A0A1D8PTV3
B	1016	LEU	-	expression tag	UNP A0A1D8PTV3
B	1017	PHE	-	expression tag	UNP A0A1D8PTV3
B	1018	GLN	-	expression tag	UNP A0A1D8PTV3
B	1019	GLY	-	expression tag	UNP A0A1D8PTV3
B	1020	PRO	-	expression tag	UNP A0A1D8PTV3
B	1021	ASP	-	expression tag	UNP A0A1D8PTV3
B	1022	TYR	-	expression tag	UNP A0A1D8PTV3
B	1023	LYS	-	expression tag	UNP A0A1D8PTV3
B	1024	ASP	-	expression tag	UNP A0A1D8PTV3
B	1025	ASP	-	expression tag	UNP A0A1D8PTV3
B	1026	ASP	-	expression tag	UNP A0A1D8PTV3
B	1027	ASP	-	expression tag	UNP A0A1D8PTV3
B	1028	LYS	-	expression tag	UNP A0A1D8PTV3
B	1029	ALA	-	expression tag	UNP A0A1D8PTV3
B	1030	HIS	-	expression tag	UNP A0A1D8PTV3
B	1031	HIS	-	expression tag	UNP A0A1D8PTV3
B	1032	HIS	-	expression tag	UNP A0A1D8PTV3
B	1033	HIS	-	expression tag	UNP A0A1D8PTV3
B	1034	HIS	-	expression tag	UNP A0A1D8PTV3
B	1035	HIS	-	expression tag	UNP A0A1D8PTV3

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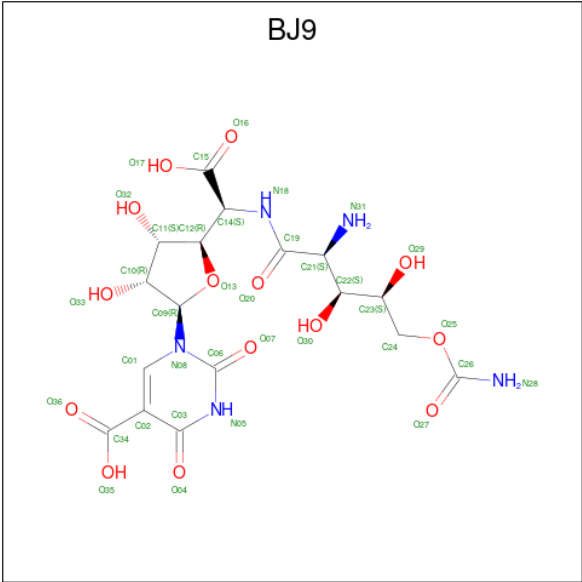
Chain	Residue	Modelled	Actual	Comment	Reference
B	1036	HIS	-	expression tag	UNP A0A1D8PTV3
B	1037	HIS	-	expression tag	UNP A0A1D8PTV3
B	1038	HIS	-	expression tag	UNP A0A1D8PTV3
B	1039	HIS	-	expression tag	UNP A0A1D8PTV3
A	1010	ALA	-	expression tag	UNP A0A1D8PTV3
A	1011	ASN	-	expression tag	UNP A0A1D8PTV3
A	1012	SER	-	expression tag	UNP A0A1D8PTV3
A	1013	LEU	-	expression tag	UNP A0A1D8PTV3
A	1014	GLU	-	expression tag	UNP A0A1D8PTV3
A	1015	VAL	-	expression tag	UNP A0A1D8PTV3
A	1016	LEU	-	expression tag	UNP A0A1D8PTV3
A	1017	PHE	-	expression tag	UNP A0A1D8PTV3
A	1018	GLN	-	expression tag	UNP A0A1D8PTV3
A	1019	GLY	-	expression tag	UNP A0A1D8PTV3
A	1020	PRO	-	expression tag	UNP A0A1D8PTV3
A	1021	ASP	-	expression tag	UNP A0A1D8PTV3
A	1022	TYR	-	expression tag	UNP A0A1D8PTV3
A	1023	LYS	-	expression tag	UNP A0A1D8PTV3
A	1024	ASP	-	expression tag	UNP A0A1D8PTV3
A	1025	ASP	-	expression tag	UNP A0A1D8PTV3
A	1026	ASP	-	expression tag	UNP A0A1D8PTV3
A	1027	ASP	-	expression tag	UNP A0A1D8PTV3
A	1028	LYS	-	expression tag	UNP A0A1D8PTV3
A	1029	ALA	-	expression tag	UNP A0A1D8PTV3
A	1030	HIS	-	expression tag	UNP A0A1D8PTV3
A	1031	HIS	-	expression tag	UNP A0A1D8PTV3
A	1032	HIS	-	expression tag	UNP A0A1D8PTV3
A	1033	HIS	-	expression tag	UNP A0A1D8PTV3
A	1034	HIS	-	expression tag	UNP A0A1D8PTV3
A	1035	HIS	-	expression tag	UNP A0A1D8PTV3
A	1036	HIS	-	expression tag	UNP A0A1D8PTV3
A	1037	HIS	-	expression tag	UNP A0A1D8PTV3
A	1038	HIS	-	expression tag	UNP A0A1D8PTV3
A	1039	HIS	-	expression tag	UNP A0A1D8PTV3

- Molecule 2 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).

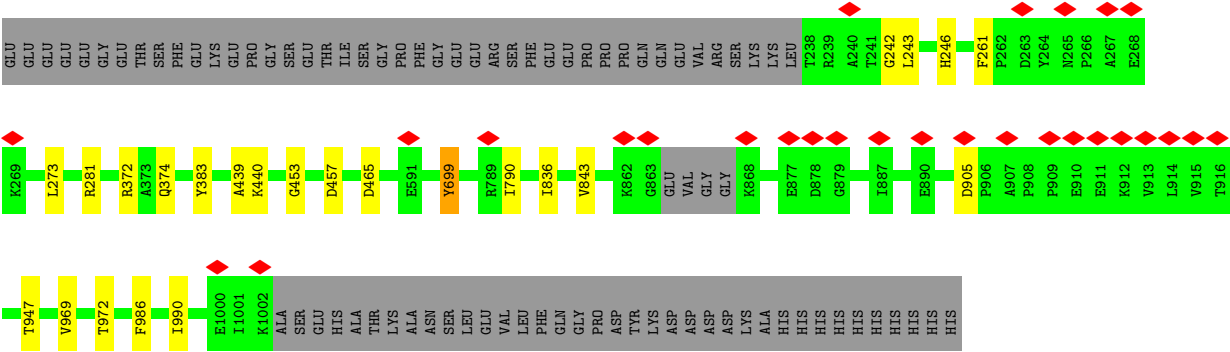


Mol	Chain	Residues	Atoms						AltConf
2	B	1	Total	C	H	N	O	P	0
			95	31	54	1	8	1	
2	B	1	Total	C	H	O	P		0
			88	30	49	8	1		
2	B	1	Total	C	H	N	O	P	0
			98	32	56	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			95	31	54	1	8	1	
2	A	1	Total	C	H	O	P		0
			88	30	49	8	1		
2	A	1	Total	C	H	N	O	P	0
			98	32	56	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			83	27	46	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			83	27	46	1	8	1	

- Molecule 3 is 1-{(2R,3R,4S,5R)-5-[(S)-{[(2S,3S,4S)-2-amino-5-(carbamoyloxy)-3,4-dihydroxypentanoyl]amino}(carboxy)methyl]-3,4-dihydroxyoxolan-2-yl}-2,4-dioxo-1,2,3,4-tetrahydro pyrimidine-5-carboxylic acid (non-preferred name) (CCD ID: BJ9) (formula: C₁₇H₂₃N₅O₁₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	H	N	O	0
			57	17	21	5	14	
3	A	1	Total	C	H	N	O	0
			57	17	21	5	14	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142366	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 ($e^-/\text{\AA}^2$)	60	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	0.226	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.039	Depositor
Map size (\AA)	233.28001, 233.28001, 233.28001	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	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: BJ9, 3PE

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	0.19	0/6433	0.33	1/8724 (0.0%)
1	B	0.19	0/6433	0.33	1/8724 (0.0%)
All	All	0.19	0/12866	0.33	2/17448 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	947	THR	CA-C-O	-5.30	114.36	120.24
1	A	947	THR	CA-C-O	-5.27	114.39	120.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6276	6134	6161	16	0
1	B	6276	6134	6161	15	0
2	A	196	251	259	1	0
2	B	122	159	163	1	0
3	A	36	21	0	1	0
3	B	36	21	0	1	0
All	All	12942	12720	12744	29	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 1.

All (29) 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:B:261:PHE:CD2	1:B:273:LEU:HD21	2.43	0.54
1:A:261:PHE:CD2	1:A:273:LEU:HD21	2.43	0.53
1:B:790:ILE:O	1:B:790:ILE:HG13	2.09	0.51
1:A:790:ILE:O	1:A:790:ILE:HG13	2.09	0.51
1:B:465:ASP:OD2	3:B:1204:BJ9:O20	2.29	0.50
1:A:453:GLY:O	1:A:457:ASP:N	2.42	0.49
1:A:465:ASP:OD2	3:A:1205:BJ9:O20	2.31	0.48
1:A:242:GLY:HA3	1:A:246:HIS:O	2.17	0.45
1:B:242:GLY:HA3	1:B:246:HIS:O	2.17	0.44
1:B:243:LEU:HD22	1:B:281:ARG:NH2	2.32	0.44
1:B:261:PHE:HD2	1:B:273:LEU:HD21	1.83	0.44
1:A:243:LEU:HD22	1:A:281:ARG:NH2	2.32	0.44
1:B:905:ASP:O	1:A:372:ARG:NH2	2.51	0.43
1:B:836:ILE:HD12	2:B:1201:3PE:H371	2.00	0.42
1:A:836:ILE:HD12	2:A:1201:3PE:H371	2.00	0.42
1:B:969:VAL:O	1:B:972:THR:HG22	2.19	0.42
1:A:969:VAL:O	1:A:972:THR:HG22	2.19	0.42
1:A:699:TYR:CE2	1:A:843:VAL:HG21	2.54	0.42
1:B:372:ARG:NH2	1:A:905:ASP:O	2.53	0.42
1:B:699:TYR:CE2	1:B:843:VAL:HG21	2.54	0.42
1:B:453:GLY:O	1:B:457:ASP:N	2.42	0.41
1:B:439:ALA:O	1:B:440:LYS:HB2	2.20	0.41
1:A:261:PHE:HD2	1:A:273:LEU:HD21	1.83	0.41
1:A:439:ALA:O	1:A:440:LYS:HB2	2.20	0.41
1:B:374:GLN:NE2	1:B:383:TYR:CZ	2.89	0.41
1:B:699:TYR:HE2	1:B:843:VAL:HG21	1.86	0.41
1:A:699:TYR:HE2	1:A:843:VAL:HG21	1.86	0.41
1:A:374:GLN:NE2	1:A:383:TYR:CZ	2.89	0.40
1:A:986:PHE:O	1:A:990:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	782/1039 (75%)	764 (98%)	18 (2%)	0	100	100
1	B	782/1039 (75%)	764 (98%)	18 (2%)	0	100	100
All	All	1564/2078 (75%)	1528 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	661/923 (72%)	660 (100%)	1 (0%)	92	96
1	B	661/923 (72%)	660 (100%)	1 (0%)	92	96
All	All	1322/1846 (72%)	1320 (100%)	2 (0%)	91	96

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

Mol	Chain	Res	Type
1	B	699	TYR
1	A	699	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	246	HIS

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Mol	Chain	Res	Type
1	B	429	GLN
1	B	514	ASN
1	B	778	HIS
1	A	429	GLN
1	A	450	GLN
1	A	514	ASN
1	A	554	ASN
1	A	778	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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
2	3PE	B	1202	-	38,38,50	1.02	3 (7%)	41,43,55	1.06	3 (7%)
3	BJ9	A	1205	-	37,37,37	3.40	20 (54%)	52,54,54	1.95	10 (19%)
2	3PE	B	1203	-	41,41,50	0.98	3 (7%)	44,46,55	1.14	2 (4%)
2	3PE	A	1202	-	38,38,50	1.02	3 (7%)	41,43,55	1.06	3 (7%)
2	3PE	A	1203	-	41,41,50	0.98	3 (7%)	44,46,55	1.14	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	3PE	A	1204	-	36,36,50	1.03	3 (8%)	39,41,55	0.99	3 (7%)
2	3PE	A	1206	-	36,36,50	1.03	3 (8%)	39,41,55	1.00	3 (7%)
2	3PE	B	1201	-	40,40,50	0.98	3 (7%)	43,45,55	1.00	2 (4%)
3	BJ9	B	1204	-	37,37,37	3.39	19 (51%)	52,54,54	1.98	10 (19%)
2	3PE	A	1201	-	40,40,50	0.98	3 (7%)	43,45,55	1.00	2 (4%)

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
2	3PE	B	1202	-	-	6/42/42/54	-
3	BJ9	A	1205	-	-	13/37/53/53	0/2/2/2
2	3PE	B	1203	-	-	16/45/45/54	-
2	3PE	A	1202	-	-	6/42/42/54	-
2	3PE	A	1203	-	-	16/45/45/54	-
2	3PE	A	1204	-	-	8/40/40/54	-
2	3PE	A	1206	-	-	8/40/40/54	-
2	3PE	B	1201	-	-	7/44/44/54	-
3	BJ9	B	1204	-	-	11/37/53/53	0/2/2/2
2	3PE	A	1201	-	-	7/44/44/54	-

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1204	BJ9	C06-N08	10.03	1.54	1.38
3	A	1205	BJ9	C06-N08	10.01	1.54	1.38
3	A	1205	BJ9	C06-N05	8.51	1.52	1.38
3	B	1204	BJ9	C06-N05	8.46	1.52	1.38
3	B	1204	BJ9	C19-N18	7.30	1.49	1.34
3	A	1205	BJ9	C19-N18	7.29	1.49	1.34
3	A	1205	BJ9	C26-N28	6.56	1.45	1.33
3	B	1204	BJ9	C26-N28	6.55	1.45	1.33
3	A	1205	BJ9	C01-N08	4.28	1.45	1.38
3	B	1204	BJ9	C01-N08	4.25	1.45	1.38
3	A	1205	BJ9	O04-C03	-4.00	1.16	1.23
3	B	1204	BJ9	O04-C03	-3.97	1.16	1.23
3	A	1205	BJ9	O32-C11	-3.87	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1204	BJ9	O32-C11	-3.86	1.33	1.43
3	B	1204	BJ9	O25-C26	3.28	1.40	1.35
3	A	1205	BJ9	C03-N05	3.21	1.44	1.38
3	B	1204	BJ9	C03-N05	3.20	1.44	1.38
3	A	1205	BJ9	O25-C26	3.17	1.40	1.35
3	B	1204	BJ9	O33-C10	3.10	1.50	1.43
3	A	1205	BJ9	O33-C10	3.08	1.50	1.43
3	A	1205	BJ9	O07-C06	-3.05	1.17	1.23
3	B	1204	BJ9	C01-C02	3.05	1.46	1.38
3	A	1205	BJ9	C01-C02	3.03	1.46	1.38
3	B	1204	BJ9	O07-C06	-2.99	1.17	1.23
2	A	1203	3PE	O21-C2	-2.86	1.39	1.46
2	B	1203	3PE	O21-C2	-2.86	1.39	1.46
3	A	1205	BJ9	C21-C19	-2.83	1.50	1.53
2	B	1201	3PE	O21-C2	-2.70	1.40	1.46
2	A	1201	3PE	O21-C2	-2.70	1.40	1.46
3	B	1204	BJ9	C21-C19	-2.68	1.50	1.53
2	A	1204	3PE	O21-C2	-2.63	1.40	1.46
2	A	1206	3PE	O21-C2	-2.63	1.40	1.46
2	B	1202	3PE	O31-C31	2.62	1.41	1.33
2	A	1202	3PE	O31-C31	2.61	1.41	1.33
3	A	1205	BJ9	O27-C26	-2.60	1.17	1.22
2	B	1202	3PE	O21-C2	-2.60	1.40	1.46
2	A	1202	3PE	O21-C2	-2.60	1.40	1.46
3	B	1204	BJ9	O27-C26	-2.60	1.17	1.22
2	A	1201	3PE	O31-C31	2.51	1.40	1.33
2	B	1201	3PE	O31-C31	2.51	1.40	1.33
2	B	1202	3PE	O21-C21	2.47	1.41	1.34
2	A	1202	3PE	O21-C21	2.47	1.41	1.34
3	A	1205	BJ9	C02-C34	2.44	1.52	1.48
3	A	1205	BJ9	O35-C34	-2.43	1.24	1.30
3	B	1204	BJ9	O35-C34	-2.41	1.24	1.30
3	B	1204	BJ9	C02-C34	2.40	1.52	1.48
2	A	1206	3PE	O31-C31	2.40	1.40	1.33
2	A	1204	3PE	O31-C31	2.40	1.40	1.33
2	B	1203	3PE	O31-C31	2.39	1.40	1.33
2	A	1203	3PE	O31-C31	2.39	1.40	1.33
2	A	1206	3PE	O21-C21	2.35	1.40	1.34
2	A	1204	3PE	O21-C21	2.35	1.40	1.34
3	A	1205	BJ9	O16-C15	2.27	1.28	1.22
3	B	1204	BJ9	O16-C15	2.25	1.28	1.22
2	B	1201	3PE	O21-C21	2.21	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	3PE	O21-C21	2.21	1.40	1.34
3	B	1204	BJ9	O29-C23	-2.09	1.38	1.43
3	A	1205	BJ9	O30-C22	-2.09	1.37	1.43
3	B	1204	BJ9	O30-C22	-2.09	1.37	1.43
3	A	1205	BJ9	O29-C23	-2.08	1.39	1.43
2	B	1203	3PE	O21-C21	2.07	1.40	1.34
2	A	1203	3PE	O21-C21	2.07	1.40	1.34
3	A	1205	BJ9	O17-C15	-2.01	1.24	1.30

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1204	BJ9	O25-C26-N28	7.42	120.34	111.11
3	A	1205	BJ9	O25-C26-N28	7.21	120.08	111.11
3	B	1204	BJ9	C21-C19-N18	4.46	120.11	116.00
3	A	1205	BJ9	C21-C19-N18	4.41	120.07	116.00
3	B	1204	BJ9	C03-N05-C06	-4.25	121.77	127.34
3	A	1205	BJ9	C03-N05-C06	-4.23	121.80	127.34
2	B	1203	3PE	O21-C21-C22	3.96	120.05	111.48
2	A	1203	3PE	O21-C21-C22	3.96	120.04	111.48
3	A	1205	BJ9	C02-C03-N05	3.85	121.19	114.45
3	B	1204	BJ9	C02-C03-N05	3.83	121.15	114.45
3	B	1204	BJ9	O27-C26-N28	-3.69	119.75	125.58
3	A	1205	BJ9	O27-C26-N28	-3.61	119.88	125.58
3	B	1204	BJ9	O25-C26-O27	-3.44	119.91	123.08
2	A	1201	3PE	O21-C21-C22	3.41	118.86	111.48
2	B	1201	3PE	O21-C21-C22	3.41	118.86	111.48
3	A	1205	BJ9	O25-C26-O27	-3.30	120.04	123.08
3	A	1205	BJ9	O04-C03-C02	-3.26	118.80	125.98
3	B	1204	BJ9	O04-C03-C02	-3.26	118.80	125.98
2	B	1203	3PE	O31-C31-C32	3.25	121.75	111.83
2	A	1203	3PE	O31-C31-C32	3.24	121.71	111.83
2	B	1202	3PE	O31-C31-C32	3.12	121.34	111.83
2	A	1202	3PE	O31-C31-C32	3.11	121.31	111.83
2	A	1206	3PE	O31-C31-C32	3.01	121.02	111.83
2	B	1202	3PE	O21-C21-C22	3.01	117.99	111.48
2	A	1202	3PE	O21-C21-C22	3.01	117.99	111.48
2	A	1204	3PE	O31-C31-C32	3.00	121.00	111.83
2	A	1204	3PE	O21-C21-C22	2.92	117.79	111.48
2	A	1206	3PE	O21-C21-C22	2.91	117.78	111.48
3	B	1204	BJ9	C24-C23-C22	-2.45	107.59	112.22
3	A	1205	BJ9	C24-C23-C22	-2.29	107.90	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1205	BJ9	O25-C24-C23	2.23	112.80	108.20
3	B	1204	BJ9	O25-C24-C23	2.22	112.80	108.20
2	A	1201	3PE	O31-C31-C32	2.17	118.46	111.83
2	B	1201	3PE	O31-C31-C32	2.17	118.45	111.83
3	B	1204	BJ9	C11-C12-C14	-2.15	110.89	115.35
3	A	1205	BJ9	C11-C12-C14	-2.14	110.90	115.35
2	A	1202	3PE	C24-C23-C22	-2.10	105.40	113.13
2	B	1202	3PE	C24-C23-C22	-2.09	105.44	113.13
2	A	1206	3PE	C23-C22-C21	-2.09	106.03	113.69
2	A	1204	3PE	C23-C22-C21	-2.08	106.07	113.69

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1201	3PE	O13-C11-C12-N
2	B	1202	3PE	C1-O11-P-O14
2	B	1203	3PE	C1-O11-P-O12
2	B	1203	3PE	C1-O11-P-O13
2	B	1203	3PE	C1-O11-P-O14
2	B	1203	3PE	C2-C1-O11-P
2	B	1203	3PE	O21-C2-C3-O31
2	A	1201	3PE	O13-C11-C12-N
2	A	1202	3PE	C1-O11-P-O14
2	A	1203	3PE	C1-O11-P-O12
2	A	1203	3PE	C1-O11-P-O13
2	A	1203	3PE	C1-O11-P-O14
2	A	1203	3PE	C2-C1-O11-P
2	A	1203	3PE	O21-C2-C3-O31
3	B	1204	BJ9	C19-C21-C22-O30
3	B	1204	BJ9	C22-C23-C24-O25
3	B	1204	BJ9	O29-C23-C24-O25
3	B	1204	BJ9	N28-C26-O25-C24
3	B	1204	BJ9	O27-C26-O25-C24
3	A	1205	BJ9	C19-C21-C22-O30
3	A	1205	BJ9	C22-C23-C24-O25
3	A	1205	BJ9	O29-C23-C24-O25
3	A	1205	BJ9	N28-C26-O25-C24
3	A	1205	BJ9	O27-C26-O25-C24
2	A	1204	3PE	C32-C31-O31-C3
2	A	1206	3PE	C32-C31-O31-C3
2	A	1204	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
2	A	1206	3PE	C21-C22-C23-C24
2	A	1204	3PE	O32-C31-O31-C3
2	A	1206	3PE	O32-C31-O31-C3
2	A	1203	3PE	C22-C21-O21-C2
2	B	1203	3PE	C22-C21-O21-C2
2	B	1203	3PE	C21-C22-C23-C24
2	A	1203	3PE	C21-C22-C23-C24
2	B	1201	3PE	O21-C2-C3-O31
2	A	1201	3PE	O21-C2-C3-O31
2	B	1203	3PE	O22-C21-O21-C2
2	A	1203	3PE	O22-C21-O21-C2
2	B	1203	3PE	C1-C2-C3-O31
2	A	1203	3PE	C1-C2-C3-O31
2	A	1204	3PE	C1-C2-C3-O31
2	A	1206	3PE	C1-C2-C3-O31
3	A	1205	BJ9	C01-C02-C34-O35
3	A	1205	BJ9	C01-C02-C34-O36
2	B	1202	3PE	O21-C2-C3-O31
2	A	1202	3PE	O21-C2-C3-O31
2	B	1202	3PE	C27-C28-C29-C2A
2	A	1202	3PE	C27-C28-C29-C2A
2	B	1202	3PE	C2-C1-O11-P
2	A	1202	3PE	C2-C1-O11-P
2	A	1204	3PE	O21-C2-C3-O31
2	A	1206	3PE	O21-C2-C3-O31
3	B	1204	BJ9	C01-C02-C34-O35
3	A	1205	BJ9	C19-C21-C22-C23
2	B	1202	3PE	C1-C2-C3-O31
2	A	1202	3PE	C1-C2-C3-O31
2	B	1202	3PE	C25-C26-C27-C28
2	A	1202	3PE	C25-C26-C27-C28
2	B	1203	3PE	C2B-C2C-C2D-C2E
2	A	1203	3PE	C2B-C2C-C2D-C2E
2	B	1203	3PE	C32-C33-C34-C35
2	A	1203	3PE	C32-C33-C34-C35
3	B	1204	BJ9	C01-C02-C34-O36
2	B	1201	3PE	C1-C2-C3-O31
2	A	1201	3PE	C1-C2-C3-O31
2	B	1201	3PE	C1-O11-P-O14
2	A	1201	3PE	C1-O11-P-O14
2	B	1203	3PE	C28-C29-C2A-C2B
2	A	1203	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
2	B	1203	3PE	C2A-C2B-C2C-C2D
2	A	1203	3PE	C2A-C2B-C2C-C2D
2	B	1203	3PE	C24-C25-C26-C27
2	A	1203	3PE	C24-C25-C26-C27
3	B	1204	BJ9	C12-C14-N18-C19
2	B	1201	3PE	C3-C2-O21-C21
2	A	1201	3PE	C3-C2-O21-C21
2	A	1204	3PE	C3-C2-O21-C21
2	A	1206	3PE	C3-C2-O21-C21
2	B	1201	3PE	C22-C21-O21-C2
2	A	1201	3PE	C22-C21-O21-C2
3	A	1205	BJ9	C12-C14-N18-C19
3	A	1205	BJ9	O20-C19-C21-N31
2	B	1201	3PE	O22-C21-O21-C2
2	A	1201	3PE	O22-C21-O21-C2
2	B	1203	3PE	C22-C23-C24-C25
2	A	1203	3PE	C22-C23-C24-C25
3	B	1204	BJ9	C19-C21-C22-C23
2	A	1203	3PE	C26-C27-C28-C29
2	B	1203	3PE	C26-C27-C28-C29
3	B	1204	BJ9	O20-C19-C21-N31
3	B	1204	BJ9	N18-C19-C21-N31
3	A	1205	BJ9	N18-C19-C21-N31
3	A	1205	BJ9	C21-C22-C23-O29
3	A	1205	BJ9	N31-C21-C22-O30
2	A	1204	3PE	C22-C23-C24-C25
2	A	1206	3PE	C22-C23-C24-C25
2	A	1204	3PE	O21-C21-C22-C23
2	A	1206	3PE	O21-C21-C22-C23

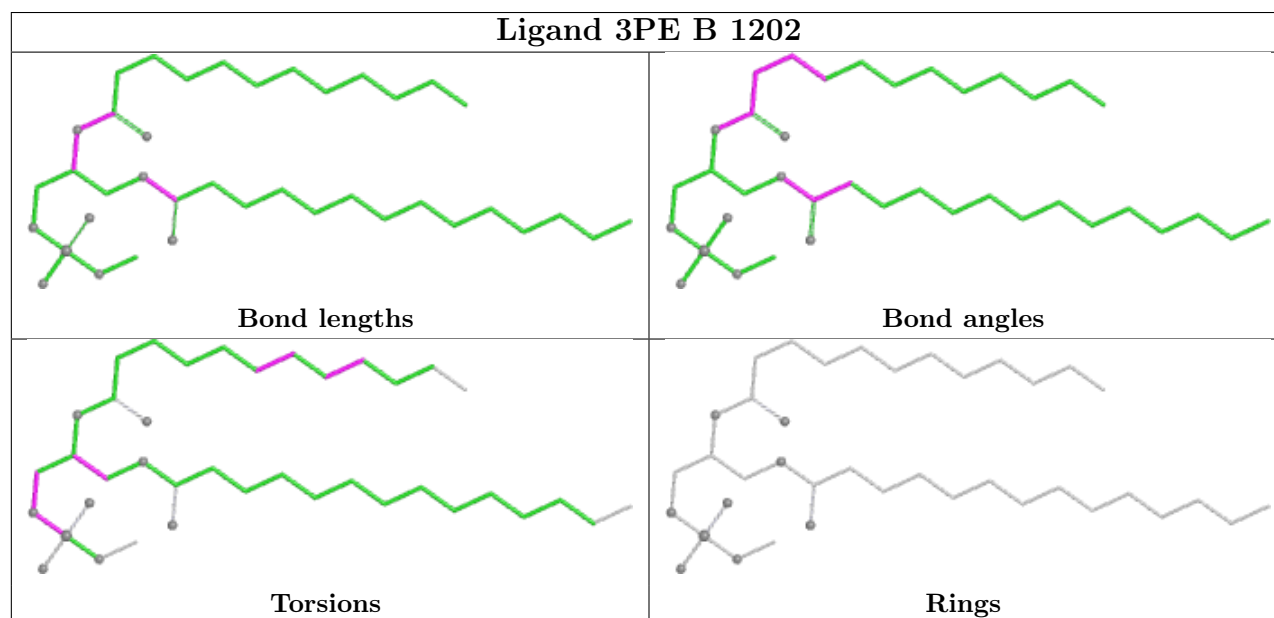
There are no ring outliers.

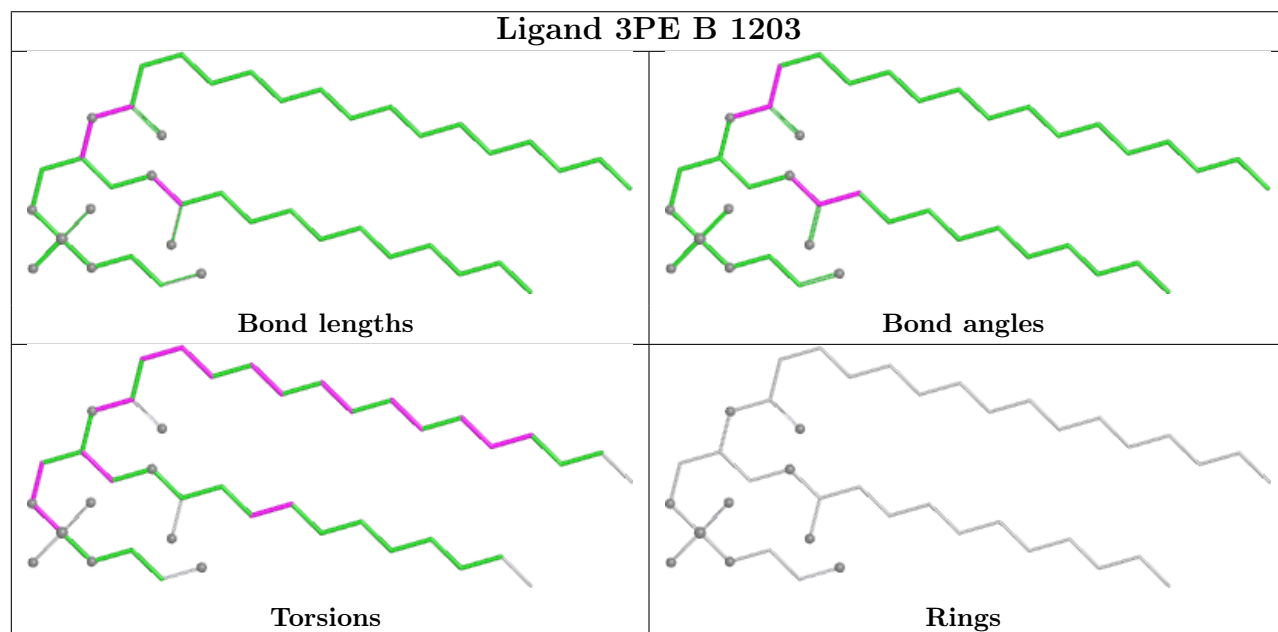
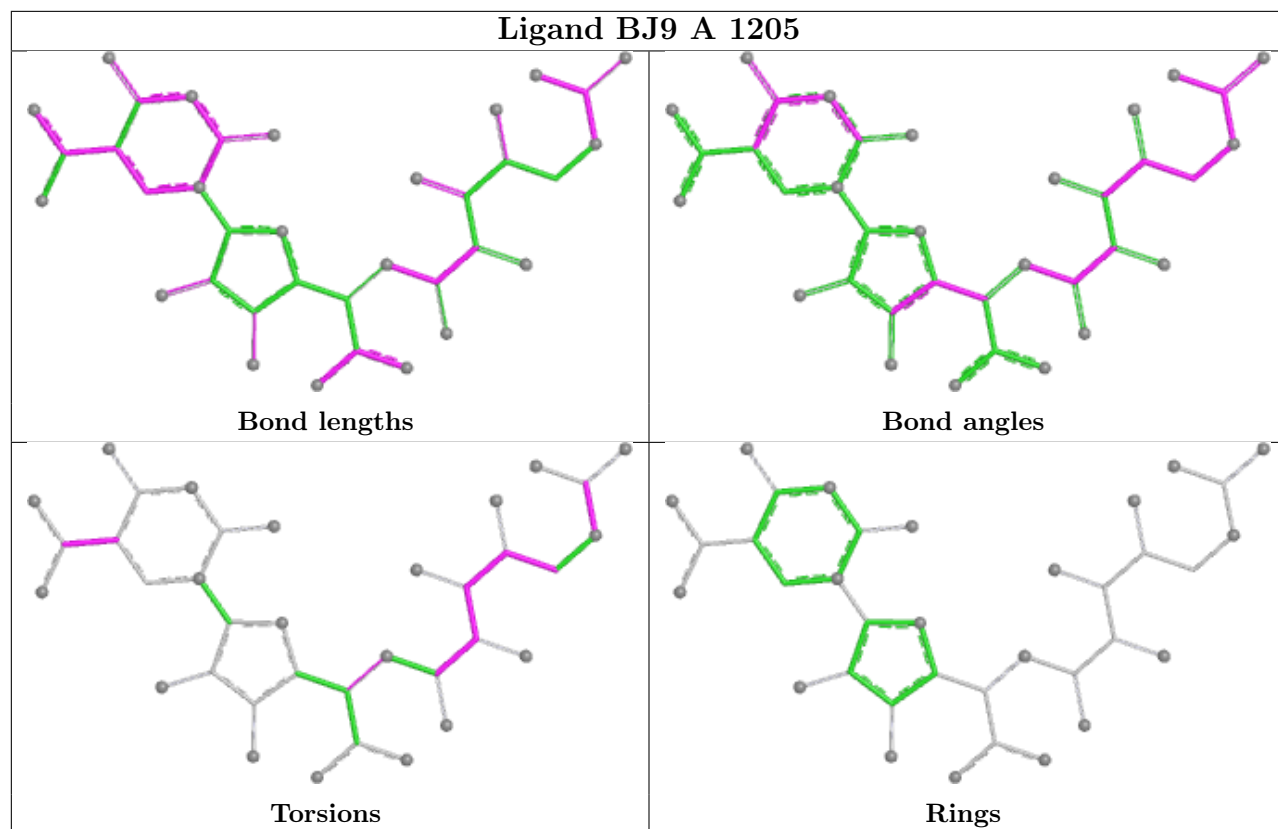
4 monomers are involved in 4 short contacts:

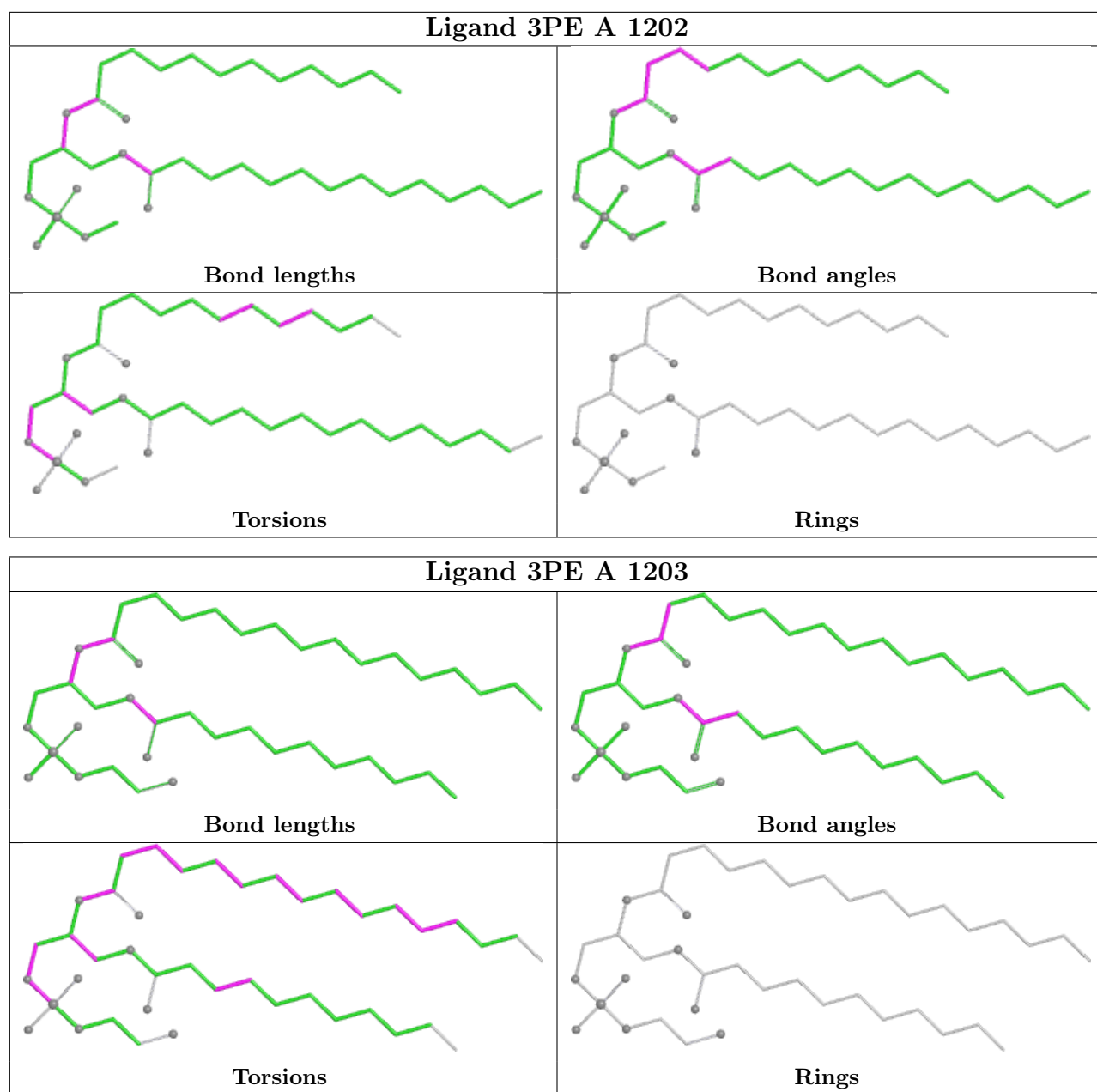
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1205	BJ9	1	0
2	B	1201	3PE	1	0
3	B	1204	BJ9	1	0
2	A	1201	3PE	1	0

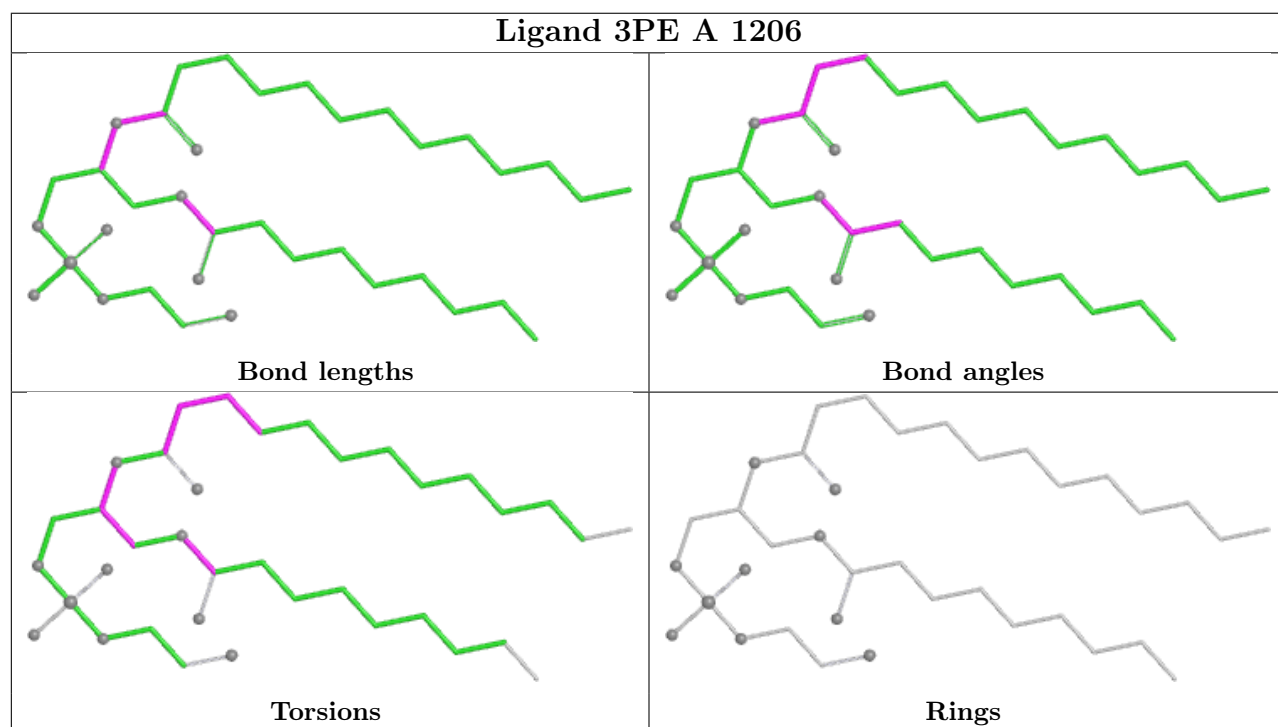
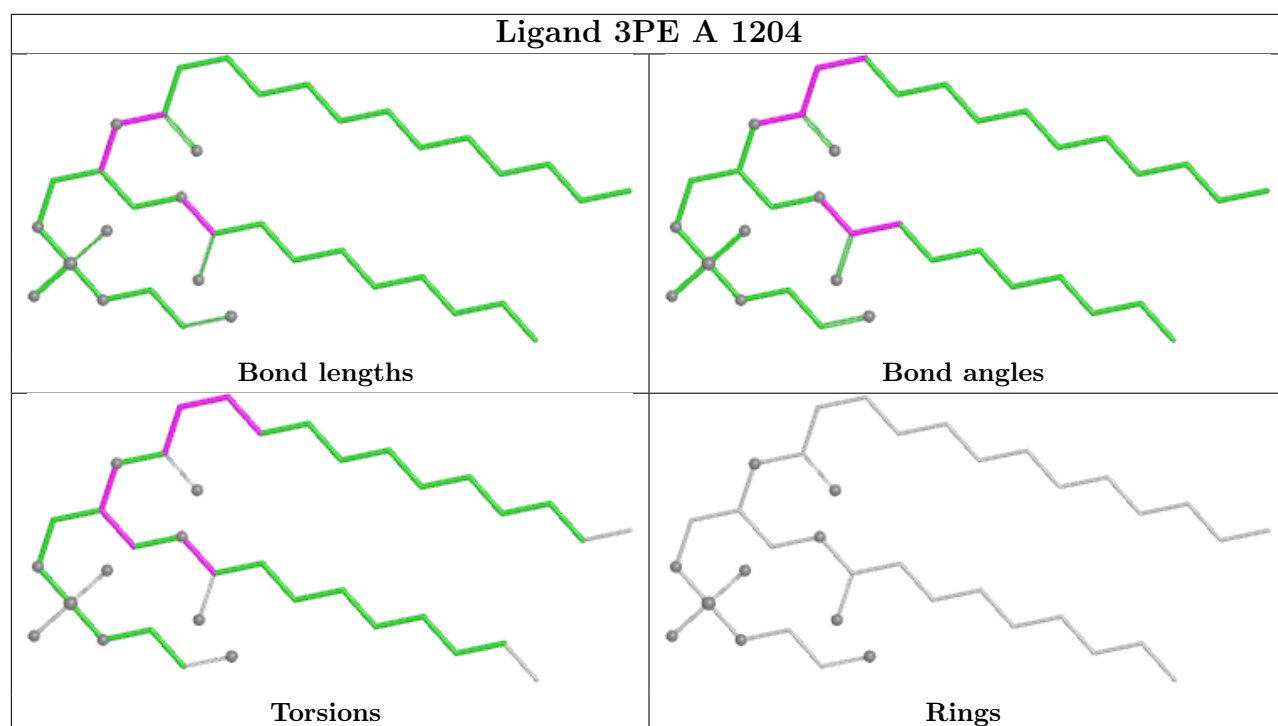
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

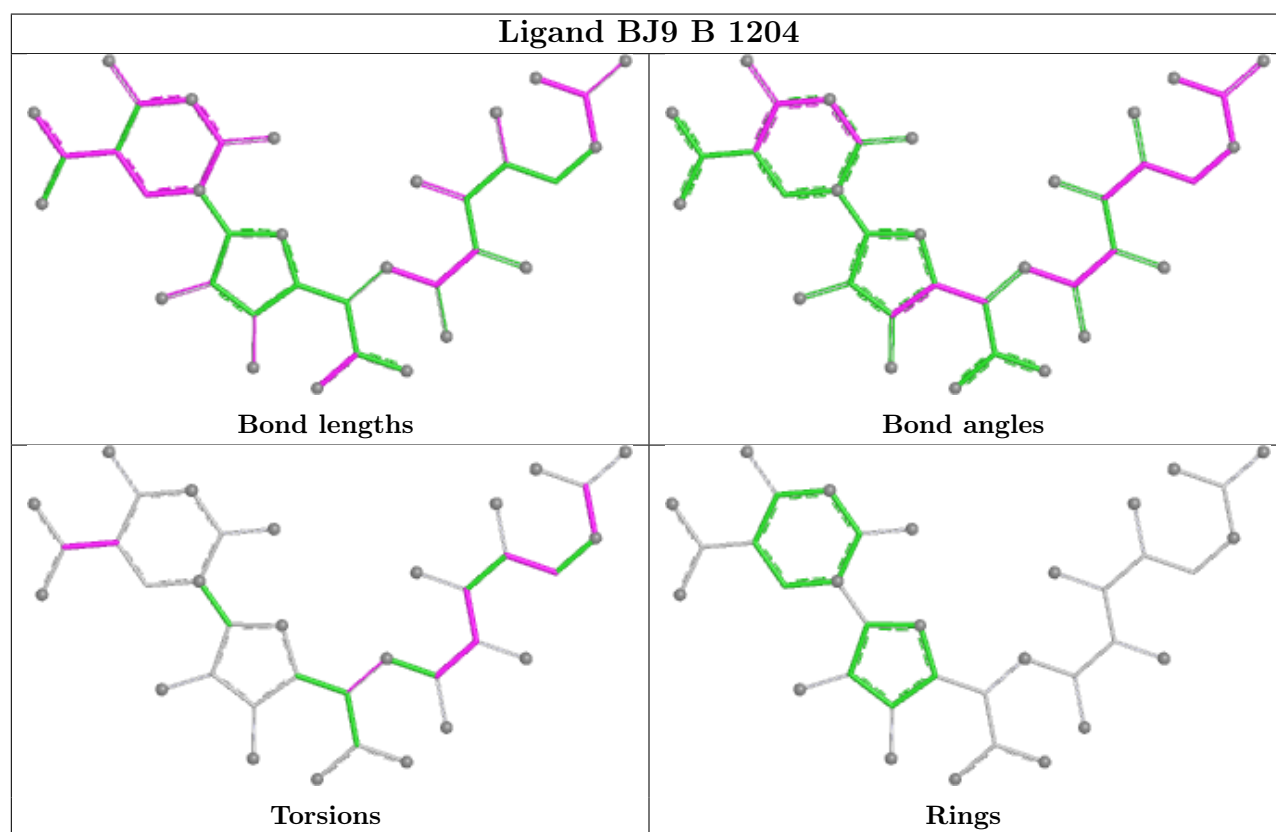
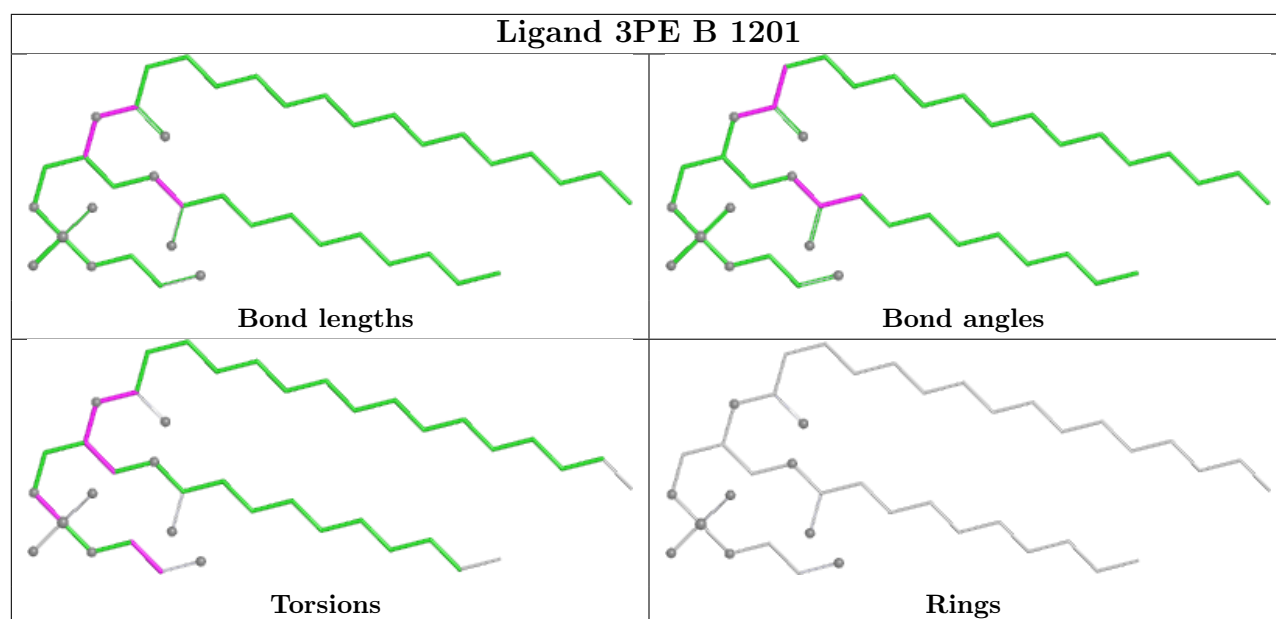
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

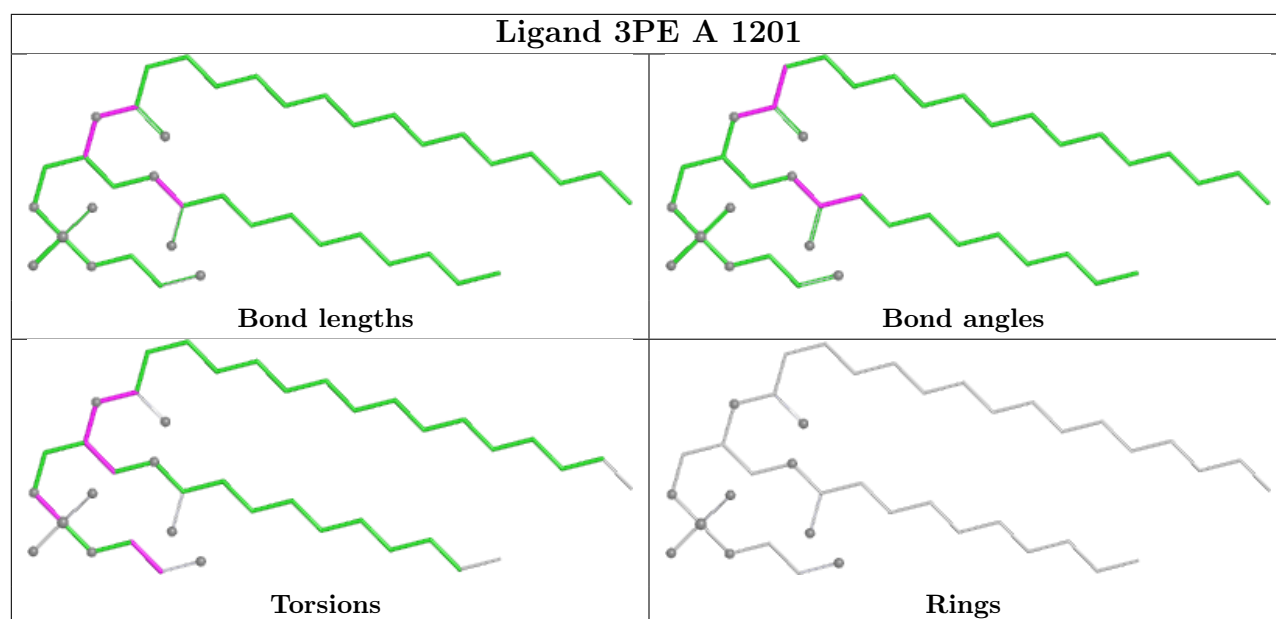












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

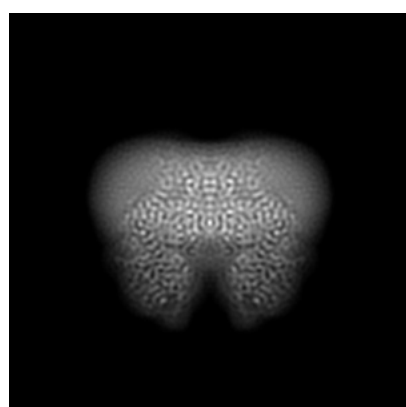
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25435. These allow visual inspection of the internal detail of the map and identification of artifacts.

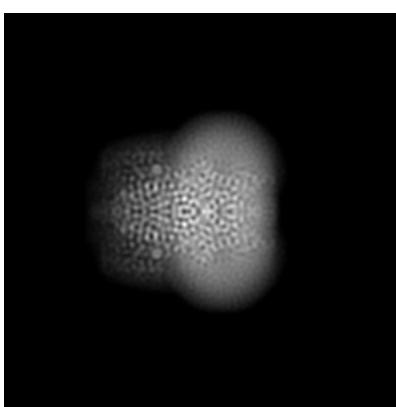
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

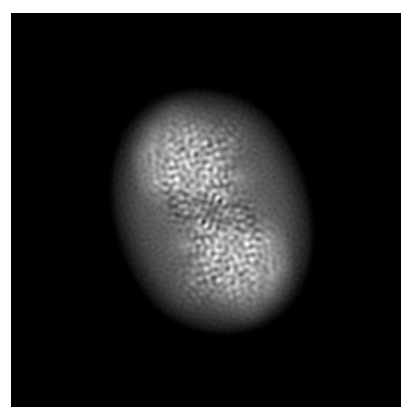
6.1.1 Primary map



X



Y

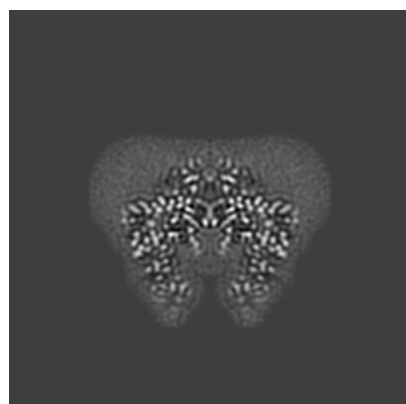


Z

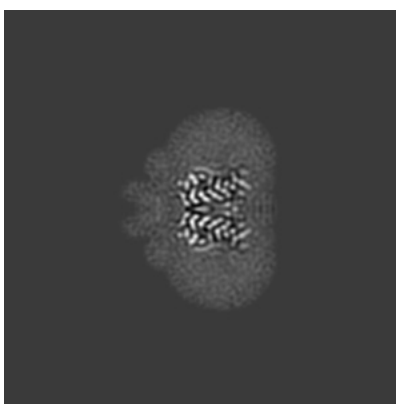
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

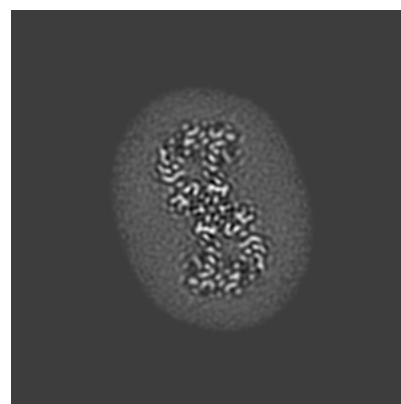
6.2.1 Primary map



X Index: 108



Y Index: 108

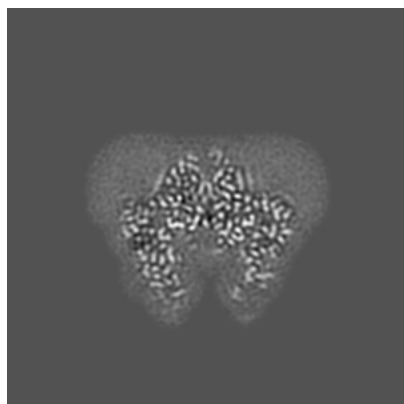


Z Index: 108

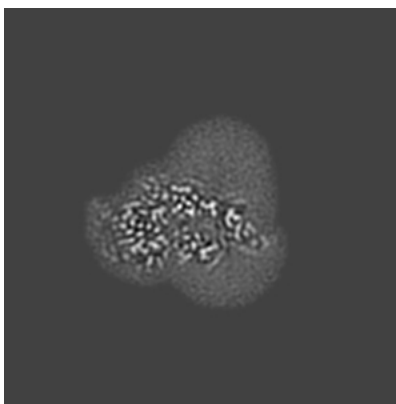
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

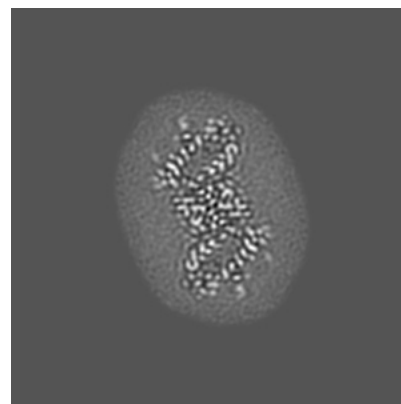
6.3.1 Primary map



X Index: 110



Y Index: 129

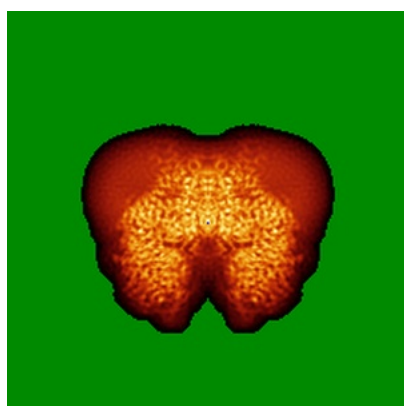


Z Index: 102

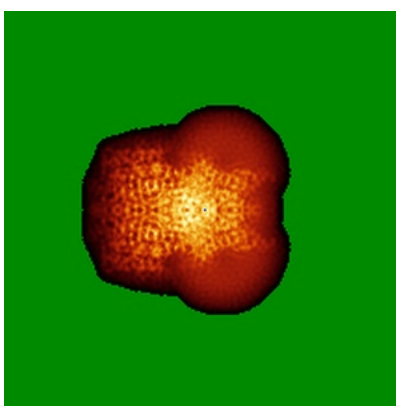
The images above show the largest variance slices of the map in three orthogonal directions.

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

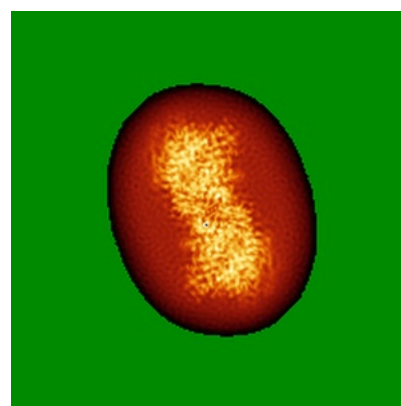
6.4.1 Primary map



X



Y

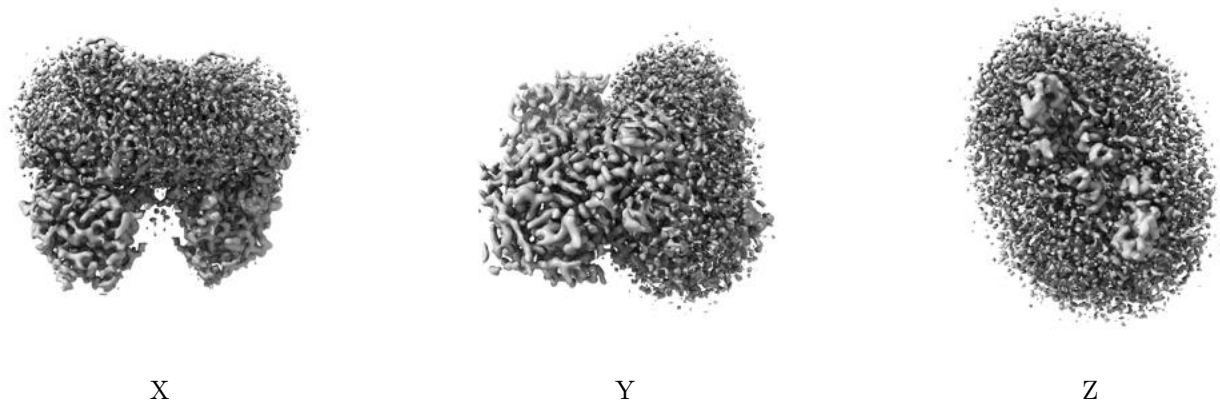


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.039. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

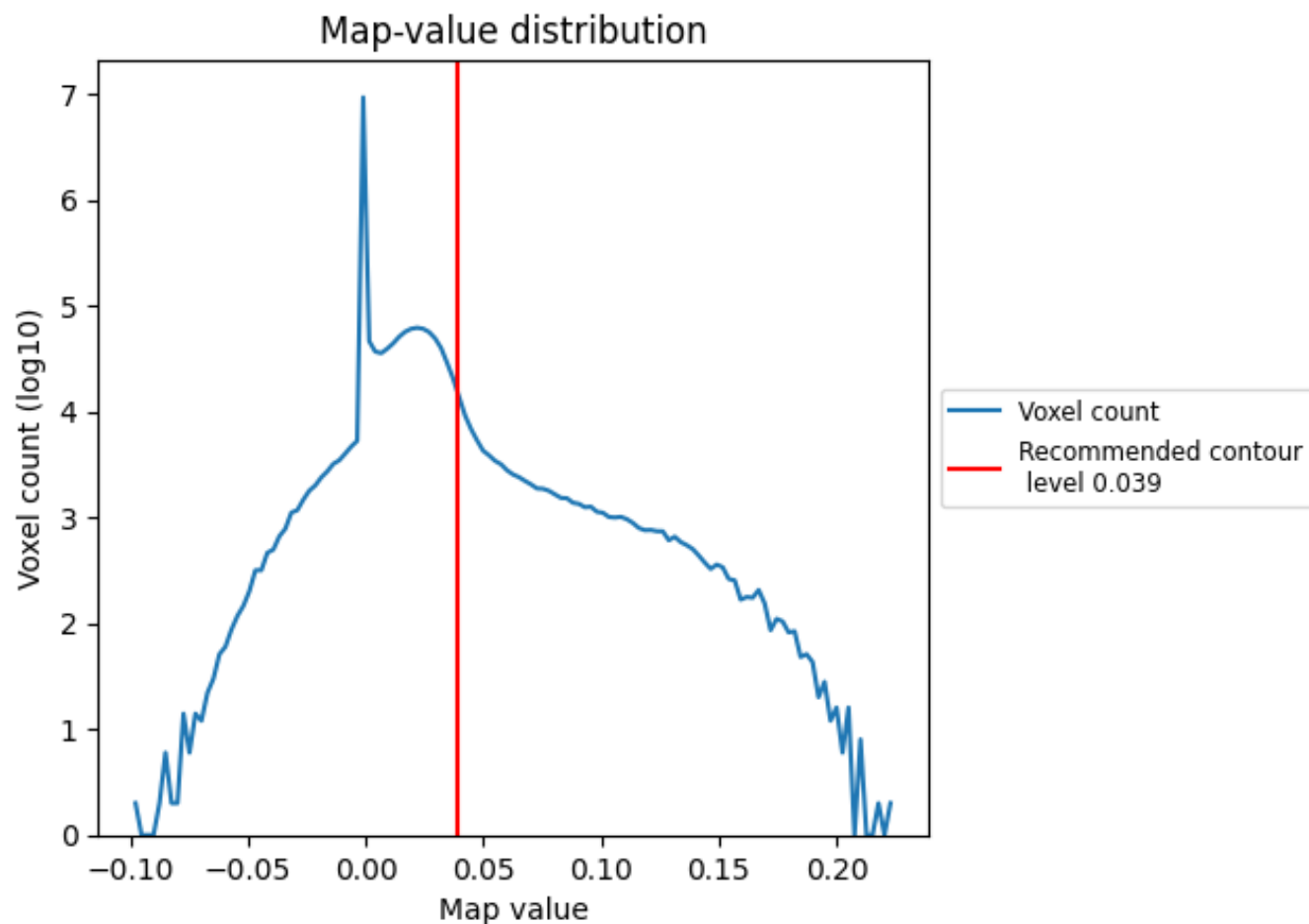
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

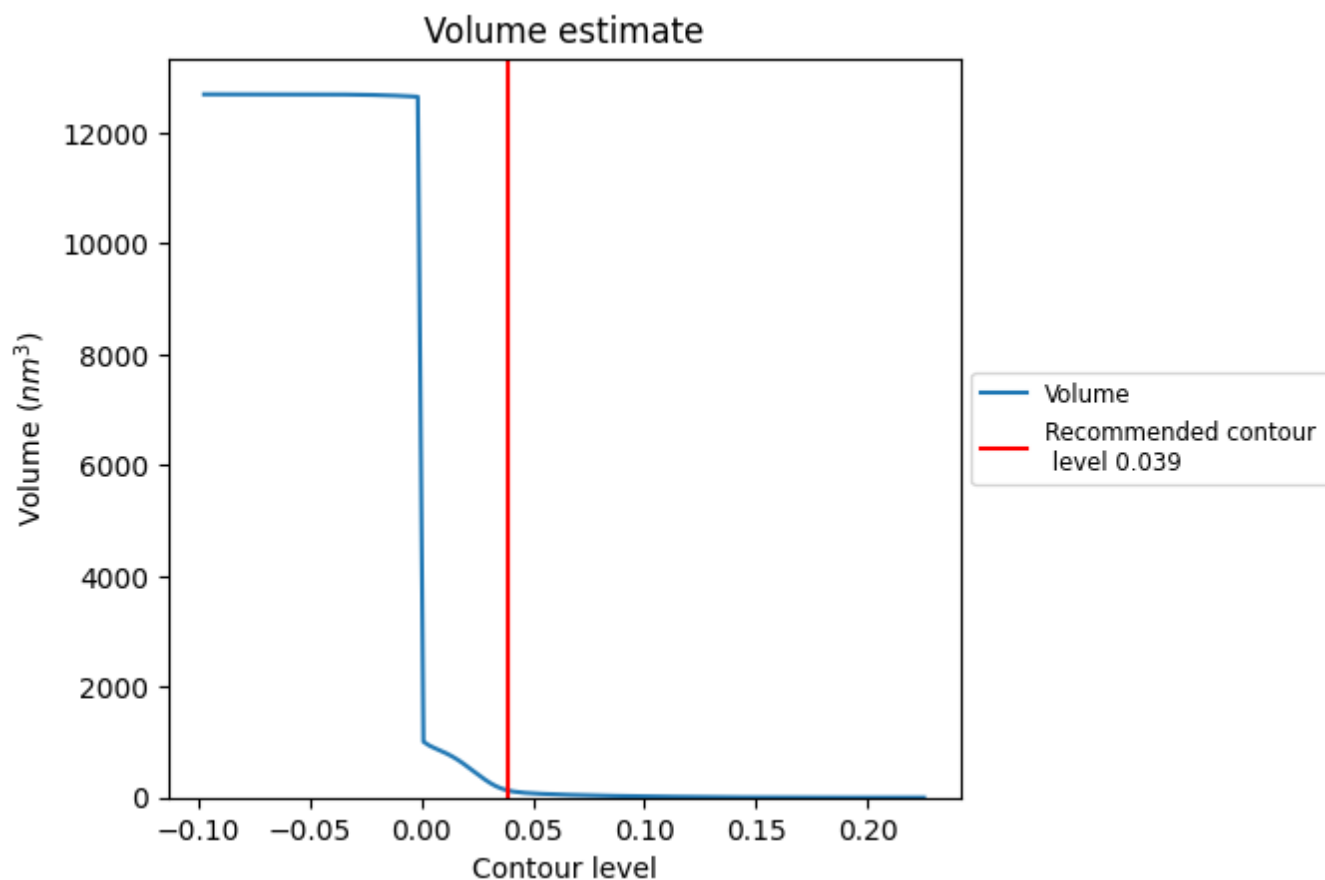
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

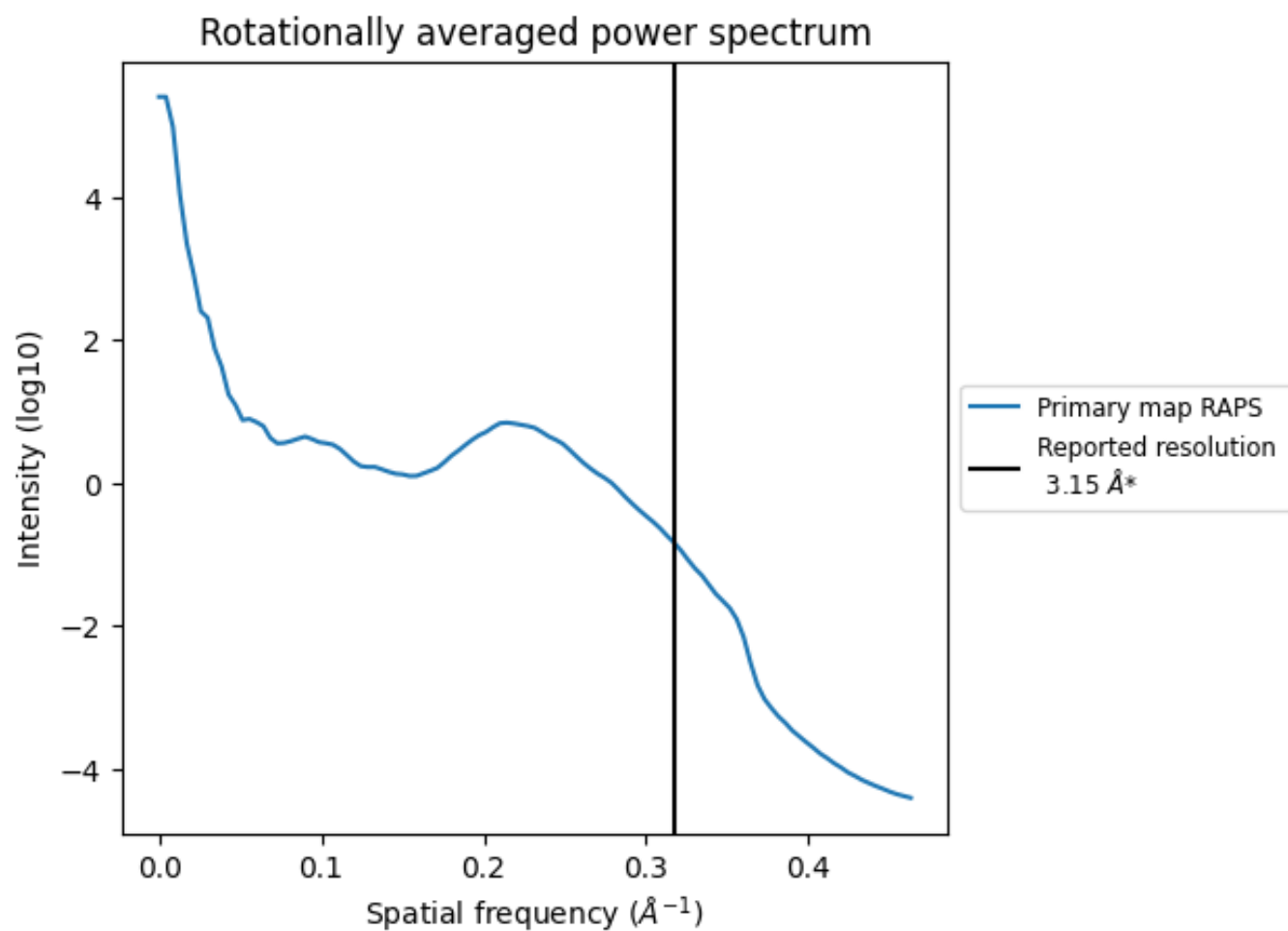
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm³; this corresponds to an approximate mass of 114 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.317 Å⁻¹

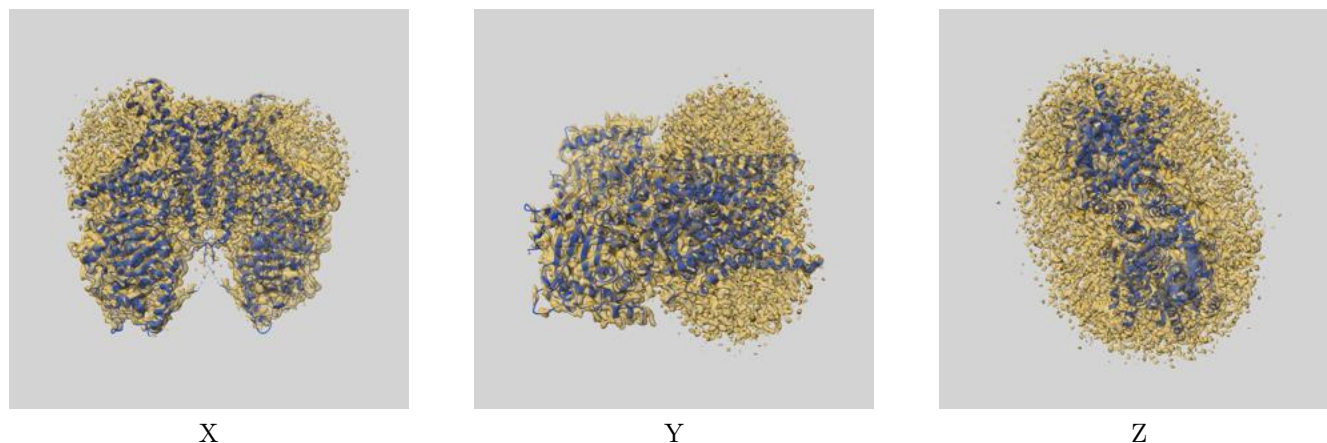
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

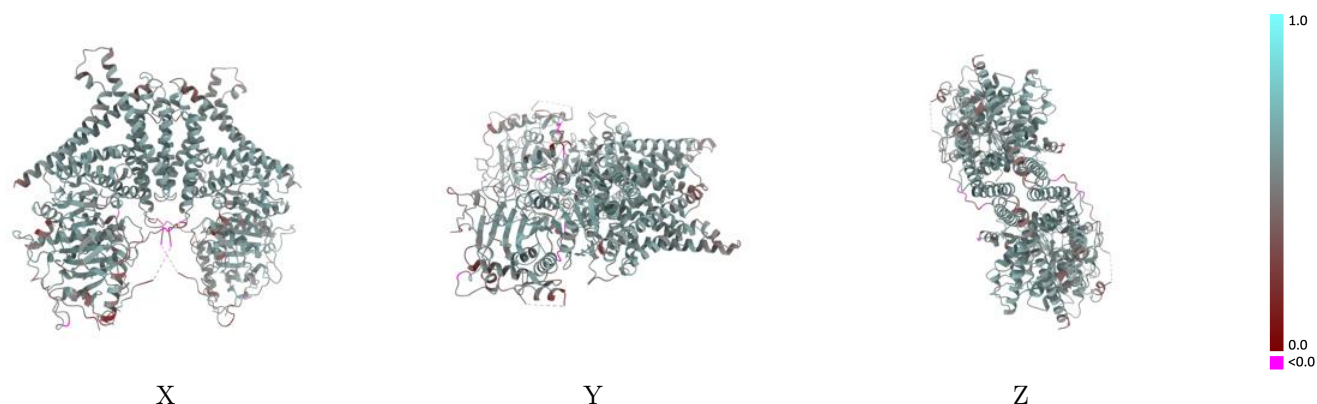
This section contains information regarding the fit between EMDB map EMD-25435 and PDB model 7STO. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



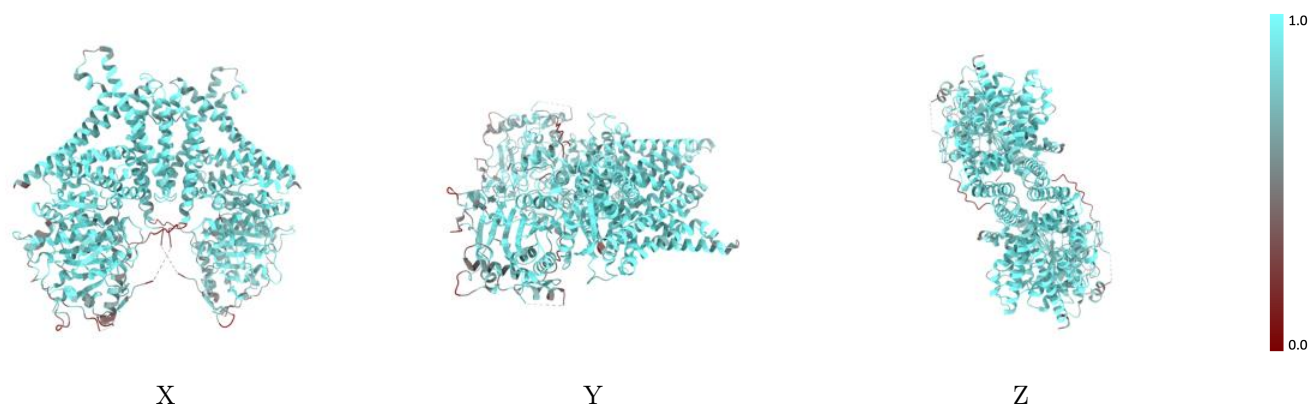
The images above show the 3D surface view of the map at the recommended contour level 0.039 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



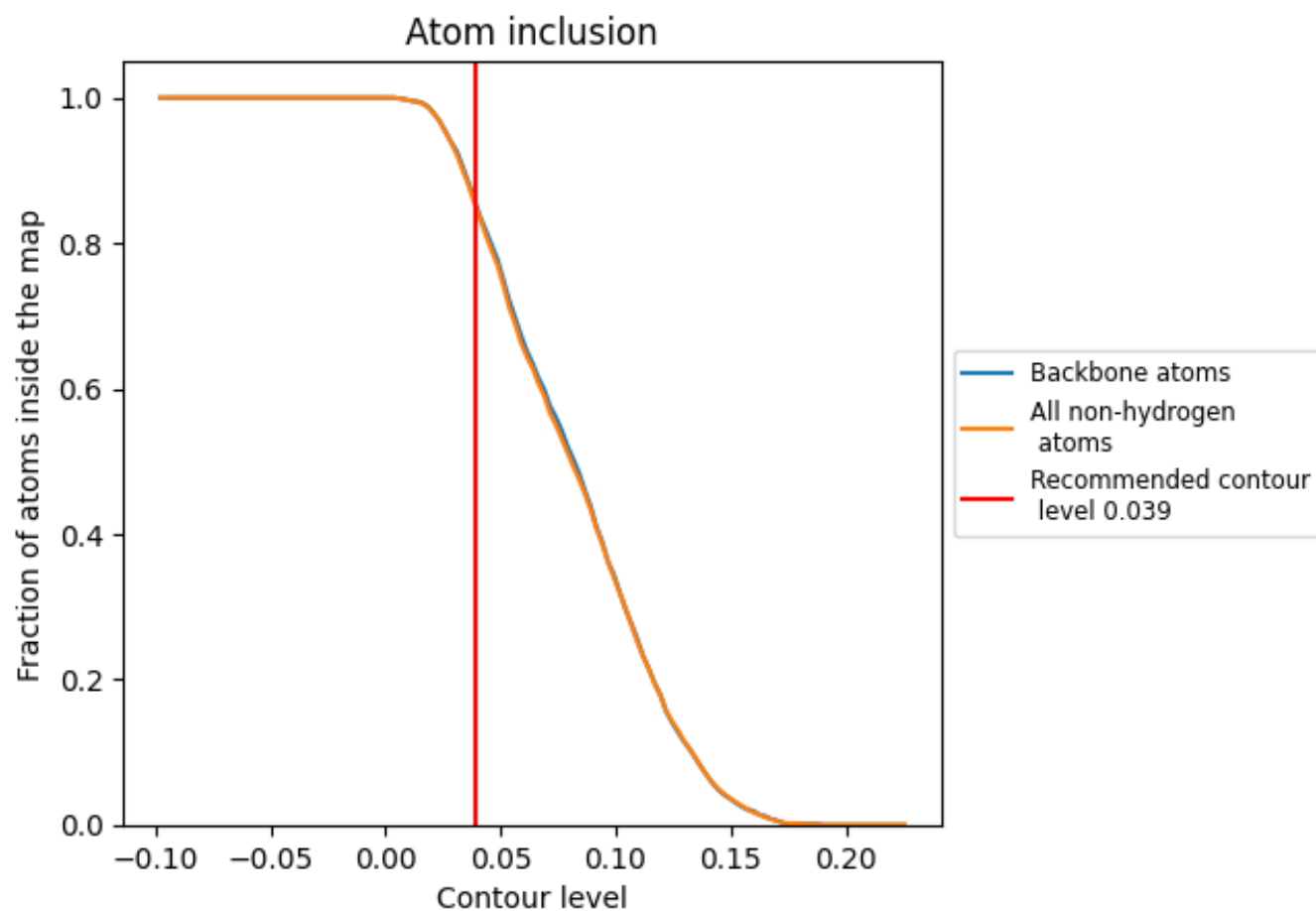
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.039).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.039) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8520	<div><div></div></div> 0.5340
A	<div><div></div></div> 0.8580	<div><div></div></div> 0.5330
B	<div><div></div></div> 0.8560	<div><div></div></div> 0.5350

