



wwPDB EM Validation Summary Report ⓘ

Aug 31, 2026 – 10:19 AM EDT

PDB ID : 9Y1Q / pdb_00009y1q
EMDB ID : EMD-72403
Title : Alternative NBD1-binding geometry in channel-formed, ATP-bound, VX809-bound, T2a-nanobody-bound wild-type human CFTR (Composite map from PHENIX)
Authors : Hunt, J.F.; Paige, A.S.; Govaerts, C.
Deposited on : 2025-08-30
Resolution : 3.86 Å(reported)

This is a wwPDB EM Validation Summary 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:

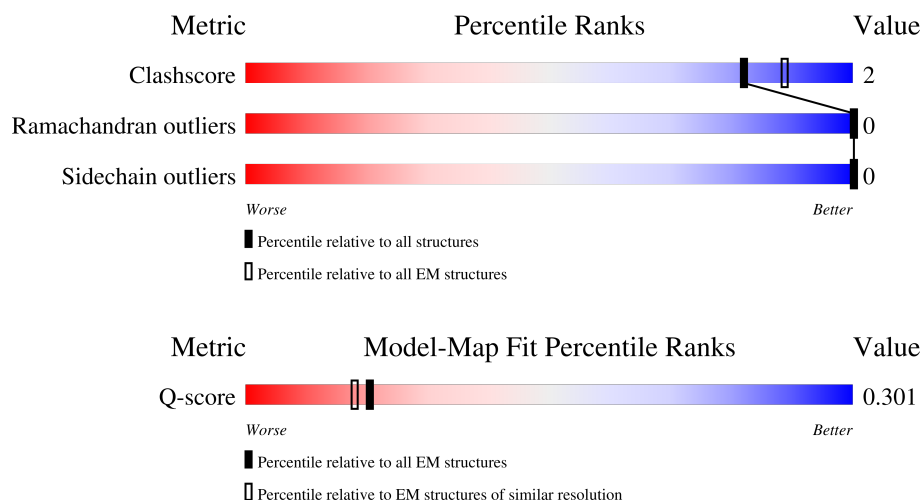
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.86 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8889 (3.36 - 4.35)

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	1523	
2	B	146	
3	C	17	

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
18	VX8	A	4032	-	X	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 20496 atoms, of which 10413 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 Cystic fibrosis transmembrane conductance regulator.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1042	Total	C	H	N	O	S	19	0
			17094	5500	8680	1381	1484	49		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	MET	VAL	variant	UNP P13569
A	1481	LEU	-	expression tag	UNP P13569
A	1482	GLU	-	expression tag	UNP P13569
A	1483	GLU	-	expression tag	UNP P13569
A	1484	ASN	-	expression tag	UNP P13569
A	1485	LEU	-	expression tag	UNP P13569
A	1486	TYR	-	expression tag	UNP P13569
A	1487	PHE	-	expression tag	UNP P13569
A	1488	GLN	-	expression tag	UNP P13569
A	1489	GLY	-	expression tag	UNP P13569
A	1490	GLY	-	expression tag	UNP P13569
A	1491	GLY	-	expression tag	UNP P13569
A	1492	GLY	-	expression tag	UNP P13569
A	1493	SER	-	expression tag	UNP P13569
A	1494	GLY	-	expression tag	UNP P13569
A	1495	GLY	-	expression tag	UNP P13569
A	1496	SER	-	expression tag	UNP P13569
A	1497	TRP	-	expression tag	UNP P13569
A	1498	SER	-	expression tag	UNP P13569
A	1499	HIS	-	expression tag	UNP P13569
A	1500	PRO	-	expression tag	UNP P13569
A	1501	GLN	-	expression tag	UNP P13569
A	1502	PHE	-	expression tag	UNP P13569
A	1503	GLU	-	expression tag	UNP P13569
A	1504	LYS	-	expression tag	UNP P13569
A	1505	ALA	-	expression tag	UNP P13569
A	1506	ALA	-	expression tag	UNP P13569
A	1507	ALA	-	expression tag	UNP P13569

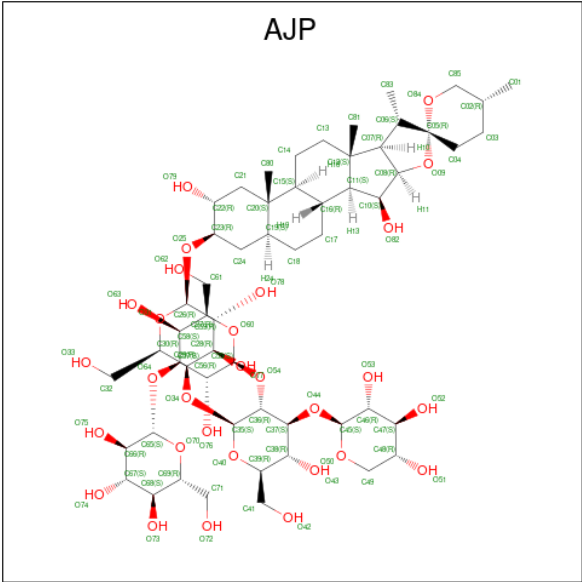
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1508	GLY	-	expression tag	UNP P13569
A	1509	GLY	-	expression tag	UNP P13569
A	1510	GLY	-	expression tag	UNP P13569
A	1511	SER	-	expression tag	UNP P13569
A	1512	GLY	-	expression tag	UNP P13569
A	1513	GLY	-	expression tag	UNP P13569
A	1514	GLY	-	expression tag	UNP P13569
A	1515	SER	-	expression tag	UNP P13569
A	1516	TRP	-	expression tag	UNP P13569
A	1517	SER	-	expression tag	UNP P13569
A	1518	HIS	-	expression tag	UNP P13569
A	1519	PRO	-	expression tag	UNP P13569
A	1520	GLN	-	expression tag	UNP P13569
A	1521	PHE	-	expression tag	UNP P13569
A	1522	GLU	-	expression tag	UNP P13569
A	1523	LYS	-	expression tag	UNP P13569

- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|-------|---|
| 2 | B | 120 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1785 | 562 | 871 | 167 | 181 | 4 | | |

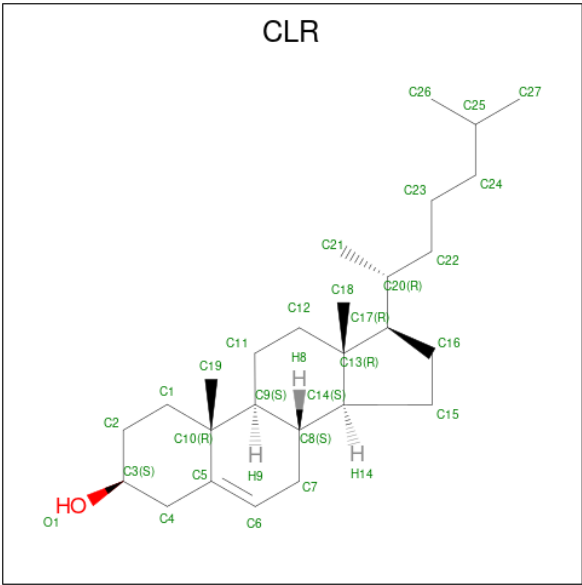
- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|-------|
| 3 | C | 17 | Total | C | H | N | O | 0 | 0 |
| | | | 105 | 51 | 20 | 17 | 17 | | |

- WORLDWIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
4	A	1	90	33	47	10	0

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



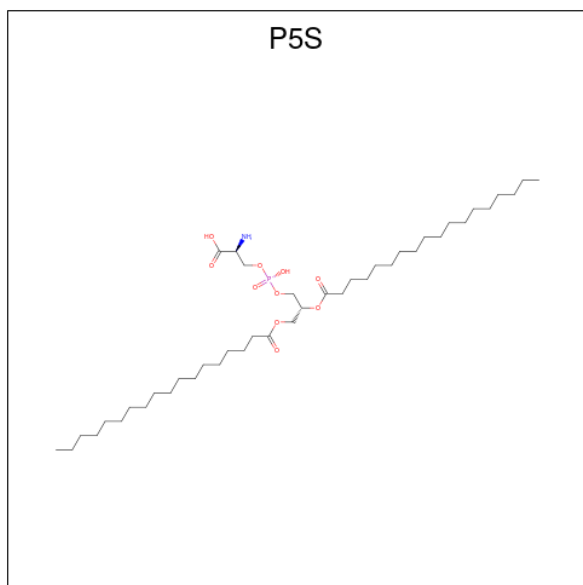
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
5	A	1	74	27	46	1	0
5	A	1	74	27	46	1	0
5	A	1	74	27	46	1	0

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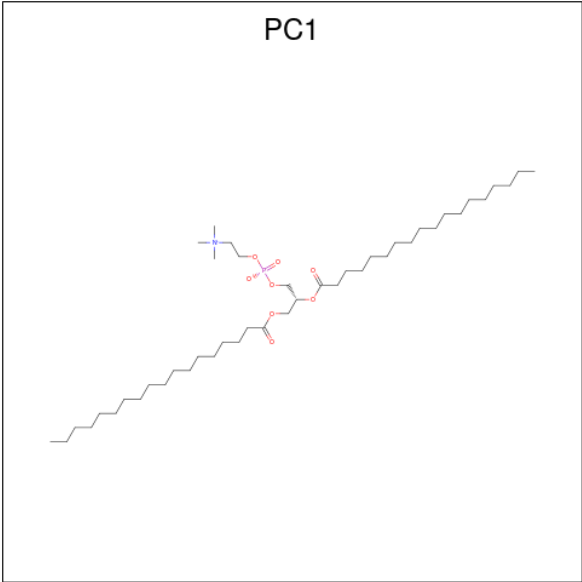
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
5	A	1	74	27	46	1	0

- Molecule 6 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



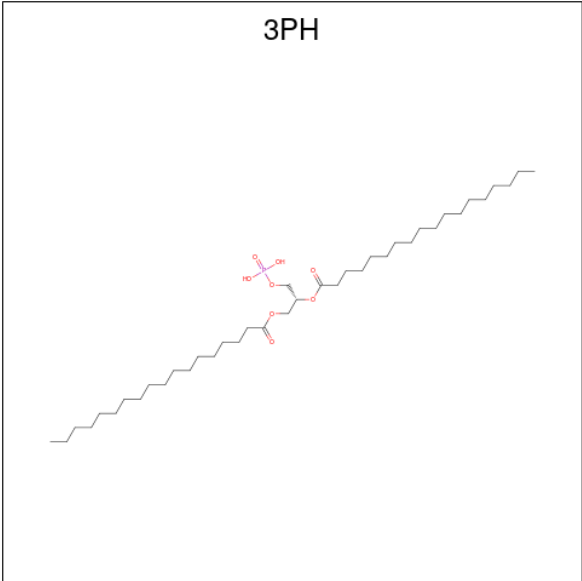
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
6	A	1	32	10	10	1	10	1	0
6	A	1	116	37	67	1	10	1	0

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	H	N	O	P	0
			91	29	52	1	8	1	
7	A	1	Total	C	H	N	O	P	0
			52	16	26	1	8	1	

- Molecule 8 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



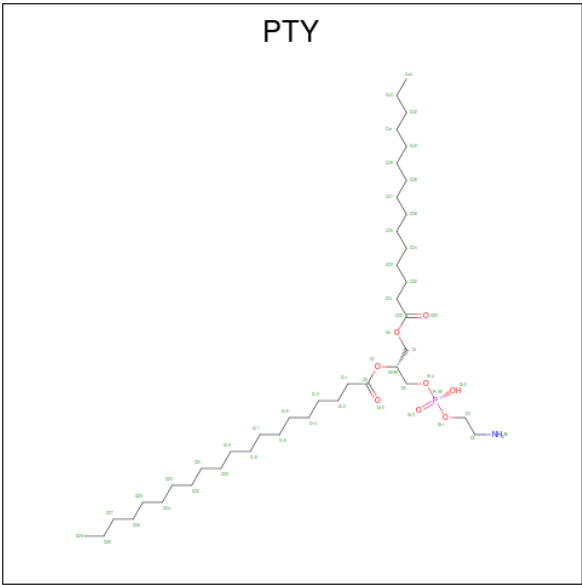
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	H	O	P	0
			45	15	21	8	1	

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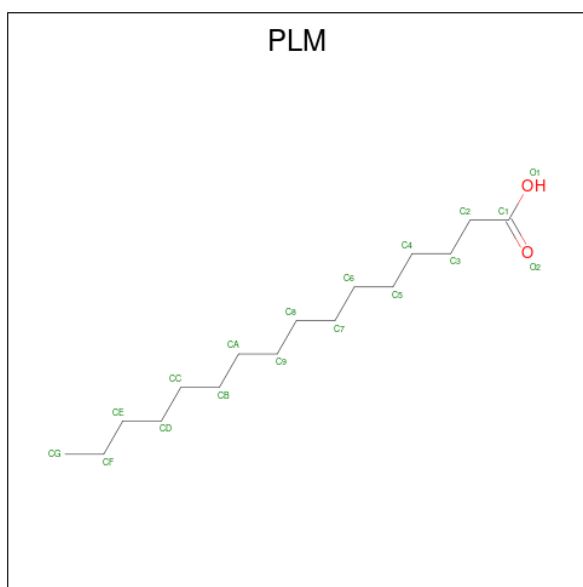
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	H	O	P	0
			36	12	15	8	1	
8	A	1	Total	C	H	O	P	0
			30	10	11	8	1	

- Molecule 9 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



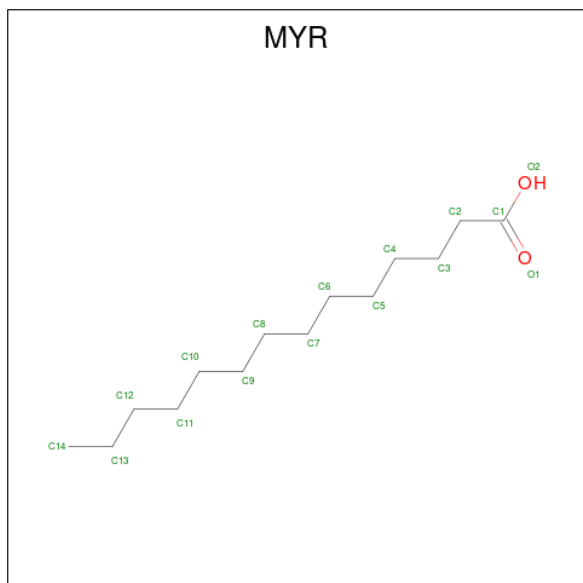
Mol	Chain	Residues	Atoms						AltConf
9	A	1	Total	C	H	N	O	P	0
			63	20	33	1	8	1	
9	A	1	Total	C	H	N	O	P	0
			81	26	45	1	8	1	

- Molecule 10 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



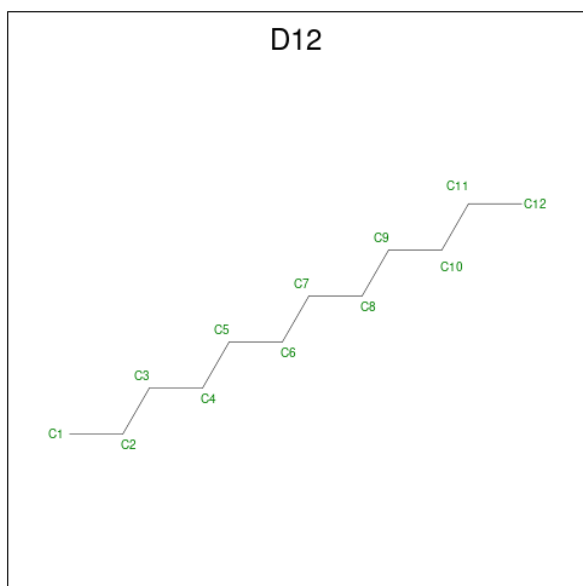
Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	H	O	0
			49	16	31	2	
10	A	1	Total	C	H	O	0
			43	15	26	2	
10	A	1	Total	C	H	O	0
			49	16	31	2	
10	A	1	Total	C	H	O	0
			49	16	31	2	

- Molecule 11 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



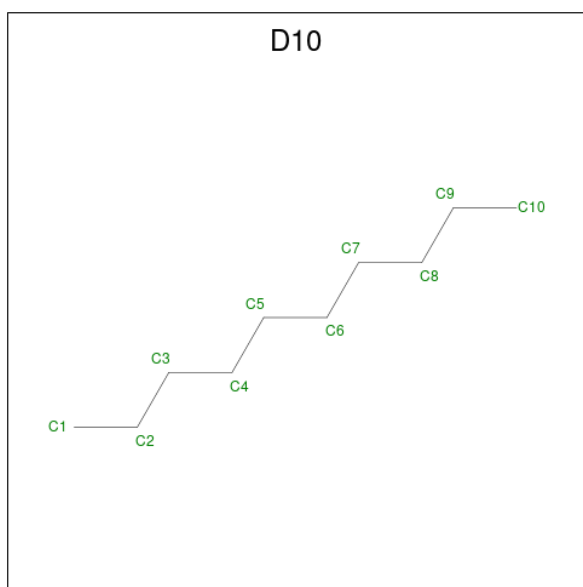
Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total	C	H	0
			38	13	25	

- Molecule 12 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



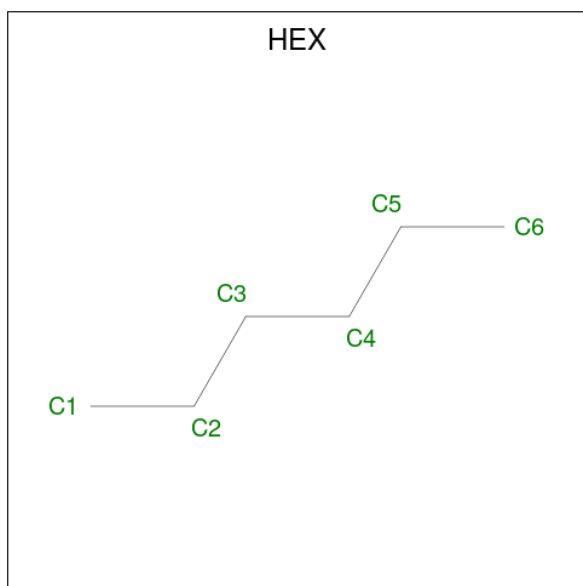
Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	H	0
			29	10	19	
12	A	1	Total	C	H	0
			38	12	26	
12	A	1	Total	C	H	0
			38	12	26	

- Molecule 13 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



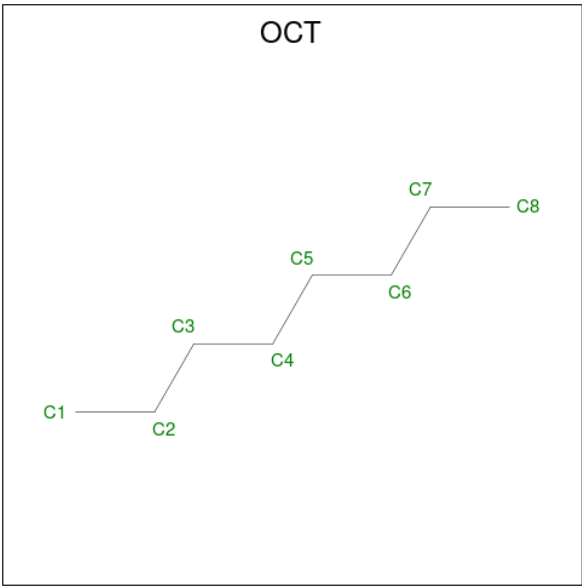
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	H	0
			32	10	22	

- Molecule 14 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).



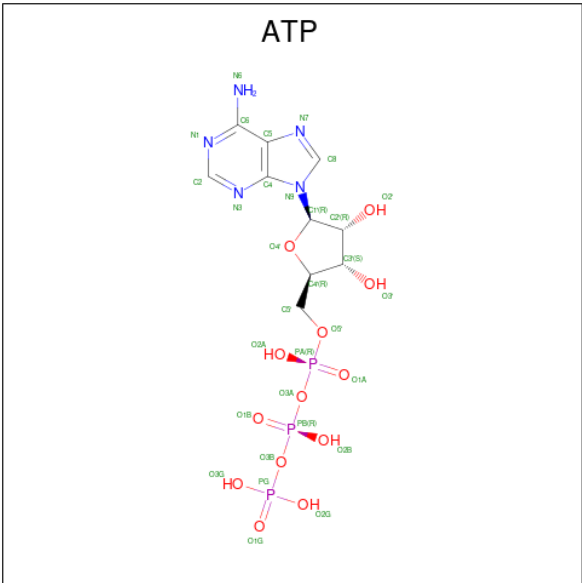
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	H	0
			20	6	14	
14	A	1	Total	C	H	0
			20	6	14	
14	A	1	Total	C	H	0
			11	4	7	

- Molecule 15 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	H	0
			26	8	18	

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

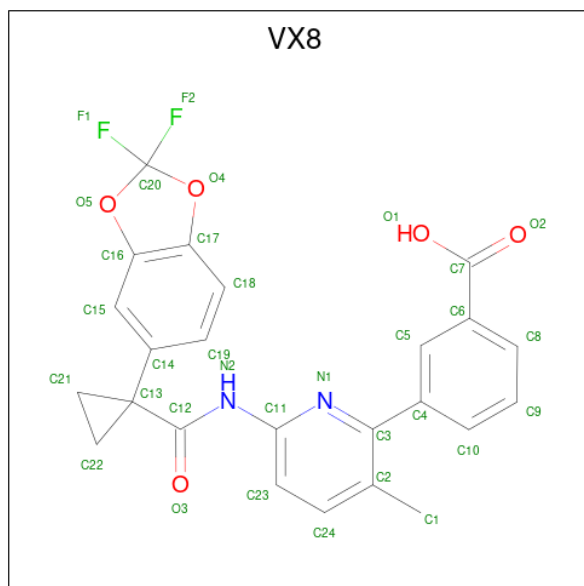


Mol	Chain	Residues	Atoms						AltConf
16	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
16	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Mg	0
			2	2	

- Molecule 18 is Lumacaftor (CCD ID: VX8) (formula: C₂₄H₁₈F₂N₂O₅).

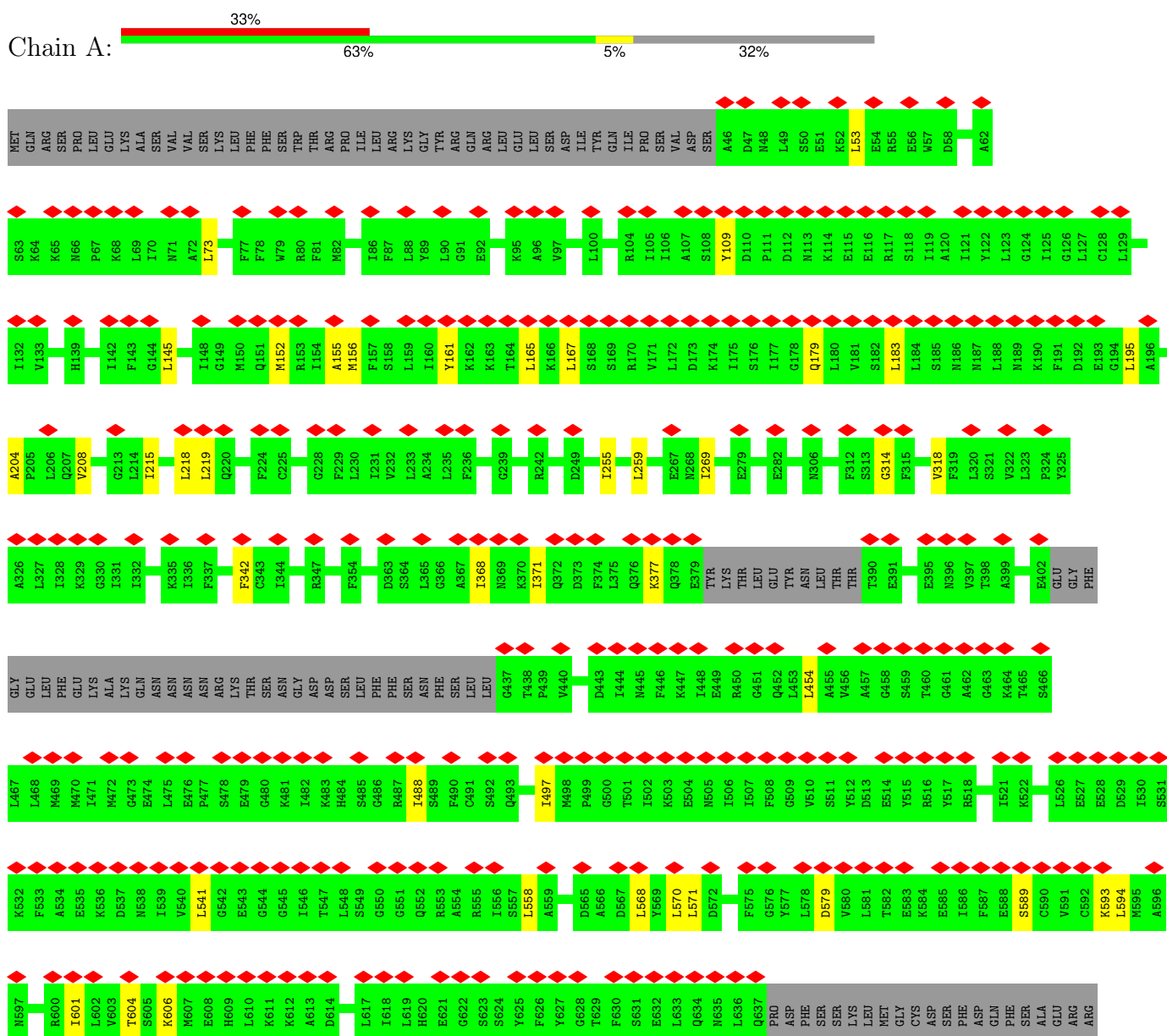


Mol	Chain	Residues	Atoms						AltConf
18	A	1	Total	C	F	H	N	O	0
			50	24	2	17	2	5	

3 Residue-property plots

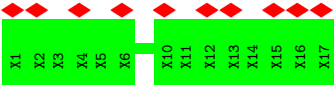
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Cystic fibrosis transmembrane conductance regulator



ALA
ALA
ALA
HIS
HIS
HIS
HIS
HIS
HIS
GLY
ALA
ALA
GLU
GLN
LYS
LEU
ILE
SER
GLU
GLU
ASP
LEU
ASN
GLY
ALA
ALA

● Molecule 3: UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36856	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.0	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	48.351	Depositor
Minimum map value	-27.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.957	Depositor
Recommended contour level	9.5	Depositor
Map size ($\text{\AA}$)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83000004, 0.83000004, 0.83000004	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: HEX, 3PH, P5S, MYR, D10, ATP, AJP, MG, VX8, OCT, PTY, CLR, PC1, D12, PLM

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	0.18	0/8606	0.39	0/11624
2	B	0.13	0/931	0.32	0/1260
All	All	0.18	0/9537	0.38	0/12884

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1030	ARG	Sidechain

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	8414	8680	8655	50	0
2	B	914	871	871	1	0
3	C	85	20	19	0	0
4	A	43	47	0	0	0
5	A	112	184	184	1	0
6	A	71	77	77	0	0
7	A	65	78	78	0	0
8	A	64	47	46	0	0
9	A	66	78	78	0	0
10	A	71	119	119	0	0
11	A	13	25	25	0	0
12	A	34	71	71	0	0
13	A	10	22	21	0	0
14	A	16	35	35	0	0
15	A	8	18	18	0	0
16	A	62	24	24	0	0
17	A	2	0	0	0	0
18	A	33	17	0	0	0
All	All	10083	10413	10321	51	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 2.

The worst 5 of 51 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:HD11	1:A:342:PHE:HB3	1.80	0.63
1:A:73:LEU:HD12	1:A:152:MET:HE3	1.81	0.61
5:A:4002:CLR:H212	5:A:4002:CLR:H183	1.85	0.58
1:A:145:LEU:HD23	1:A:195:LEU:O	2.04	0.57
1:A:919[B]:TYR:CE2	1:A:1007:VAL:HG21	2.42	0.55

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	1043/1523 (68%)	991 (95%)	52 (5%)	0	100	100
2	B	118/146 (81%)	112 (95%)	6 (5%)	0	100	100
All	All	1161/1669 (70%)	1103 (95%)	58 (5%)	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	921/1341 (69%)	921 (100%)	0	100	100
2	B	95/113 (84%)	95 (100%)	0	100	100
All	All	1016/1454 (70%)	1016 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	847	ASN
1	A	1291	GLN
1	A	1348	HIS
1	A	1303	ASN
1	A	376	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](#)

Of 32 ligands modelled in this entry, 2 are monoatomic - leaving 30 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$
7	PC1	A	4018	-	25,25,53	0.69	0	31,33,61	0.65	1 (3%)
5	CLR	A	4021	-	31,31,31	0.45	0	48,48,48	0.90	2 (4%)
12	D12	A	4014	-	9,9,11	0.24	0	8,8,10	0.18	0
14	HEX	A	4025	-	5,5,5	0.26	0	4,4,4	0.16	0
14	HEX	A	4016	-	5,5,5	0.25	0	4,4,4	0.17	0
15	OCT	A	4026	-	7,7,7	0.25	0	6,6,6	0.17	0
7	PC1	A	4007	-	38,38,53	0.58	0	44,46,61	0.53	1 (2%)
8	3PH	A	4024	-	18,18,47	1.00	1 (5%)	21,23,52	0.89	1 (4%)
14	HEX	A	4027	-	3,3,5	0.35	0	2,2,4	0.52	0
9	PTY	A	4009	-	29,29,49	0.57	0	32,34,54	0.57	1 (3%)
5	CLR	A	4002	-	31,31,31	0.40	0	48,48,48	0.97	3 (6%)
11	MYR	A	4013	-	12,12,15	0.25	0	11,11,15	0.16	0
12	D12	A	4020	-	11,11,11	0.24	0	10,10,10	0.16	0
9	PTY	A	4017	-	35,35,49	0.54	0	38,40,54	0.47	0
13	D10	A	4015	-	9,9,9	0.54	0	8,8,8	0.45	0
16	ATP	A	4028	17	32,33,33	0.43	0	48,52,52	0.70	1 (2%)
5	CLR	A	4004	-	31,31,31	0.37	0	48,48,48	0.86	1 (2%)
8	3PH	A	4023	-	20,20,47	0.99	1 (5%)	23,25,52	1.20	3 (13%)
10	PLM	A	4022	-	17,17,17	0.67	0	17,17,17	0.63	0
8	3PH	A	4008	-	23,23,47	0.89	1 (4%)	26,28,52	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	P5S	A	4005	-	20,21,53	0.68	0	22,28,60	1.13	2 (9%)
6	P5S	A	4006	-	47,48,53	0.54	0	49,55,60	0.59	1 (2%)
10	PLM	A	4010	-	17,17,17	0.68	0	17,17,17	0.58	0
10	PLM	A	4012	-	17,17,17	0.66	0	17,17,17	0.61	0
5	CLR	A	4003	-	31,31,31	0.43	0	48,48,48	1.08	3 (6%)
18	VX8	A	4032	-	37,37,37	4.57	22 (59%)	55,57,57	5.84	28 (50%)
4	AJP	A	4001	-	49,49,95	1.13	5 (10%)	75,80,149	1.35	11 (14%)
16	ATP	A	4030	17	32,33,33	0.43	0	48,52,52	0.69	1 (2%)
10	PLM	A	4011	-	16,16,17	0.68	0	16,16,17	0.61	0
12	D12	A	4019	-	11,11,11	0.23	0	10,10,10	0.18	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
7	PC1	A	4018	-	-	15/29/29/57	-
5	CLR	A	4021	-	-	5/10/68/68	0/4/4/4
12	D12	A	4014	-	-	1/7/7/9	-
14	HEX	A	4025	-	-	0/3/3/3	-
14	HEX	A	4016	-	-	0/3/3/3	-
15	OCT	A	4026	-	-	1/5/5/5	-
7	PC1	A	4007	-	-	16/42/42/57	-
8	3PH	A	4024	-	-	5/19/19/49	-
14	HEX	A	4027	-	-	0/1/1/3	-
9	PTY	A	4009	-	-	8/33/33/53	-
5	CLR	A	4002	-	-	6/10/68/68	0/4/4/4
11	MYR	A	4013	-	-	2/10/10/13	-
12	D12	A	4020	-	-	4/9/9/9	-
9	PTY	A	4017	-	-	19/39/39/53	-
13	D10	A	4015	-	-	3/7/7/7	-
16	ATP	A	4028	17	-	8/22/38/38	0/3/3/3
5	CLR	A	4004	-	-	3/10/68/68	0/4/4/4
8	3PH	A	4023	-	-	7/21/21/49	-
10	PLM	A	4022	-	-	5/15/15/15	-
8	3PH	A	4008	-	-	9/25/25/49	-
6	P5S	A	4005	-	-	6/25/25/59	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	P5S	A	4006	-	-	17/54/54/59	-
10	PLM	A	4010	-	-	1/15/15/15	-
10	PLM	A	4012	-	-	1/15/15/15	-
5	CLR	A	4003	-	-	4/10/68/68	0/4/4/4
18	VX8	A	4032	-	-	6/24/38/38	0/5/5/5
4	AJP	A	4001	-	-	2/6/121/220	0/7/7/11
16	ATP	A	4030	17	-	0/22/38/38	0/3/3/3
10	PLM	A	4011	-	-	0/14/14/15	-
12	D12	A	4019	-	-	1/9/9/9	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	4032	VX8	O5-C16	12.37	1.56	1.38
18	A	4032	VX8	C18-C17	10.23	1.60	1.39
18	A	4032	VX8	O4-C17	-8.90	1.24	1.38
18	A	4032	VX8	C15-C16	8.51	1.53	1.38
18	A	4032	VX8	O4-C20	-7.17	1.27	1.38

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	4032	VX8	C20-O4-C17	22.81	126.18	106.09
18	A	4032	VX8	C22-C13-C14	17.19	138.63	118.58
18	A	4032	VX8	O5-C20-O4	-16.36	97.57	110.46
18	A	4032	VX8	O4-C17-C18	9.02	143.45	124.56
18	A	4032	VX8	O4-C17-C16	-9.00	102.84	109.65

There are no chirality outliers.

5 of 155 torsion outliers are listed below:

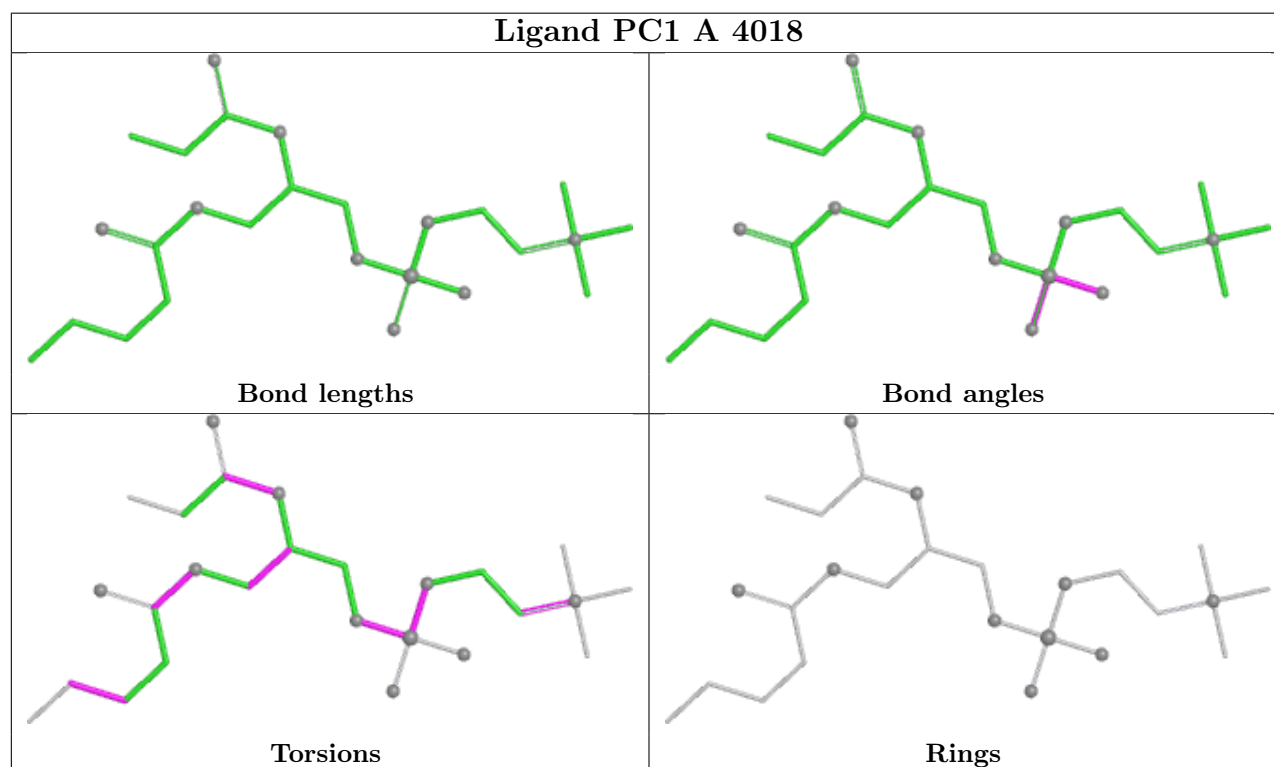
Mol	Chain	Res	Type	Atoms
5	A	4002	CLR	C16-C17-C20-C22
6	A	4006	P5S	CA-CB-OG-P12
7	A	4007	PC1	C11-O13-P-O14
7	A	4007	PC1	O13-C11-C12-N
7	A	4007	PC1	C22-C21-O21-C2

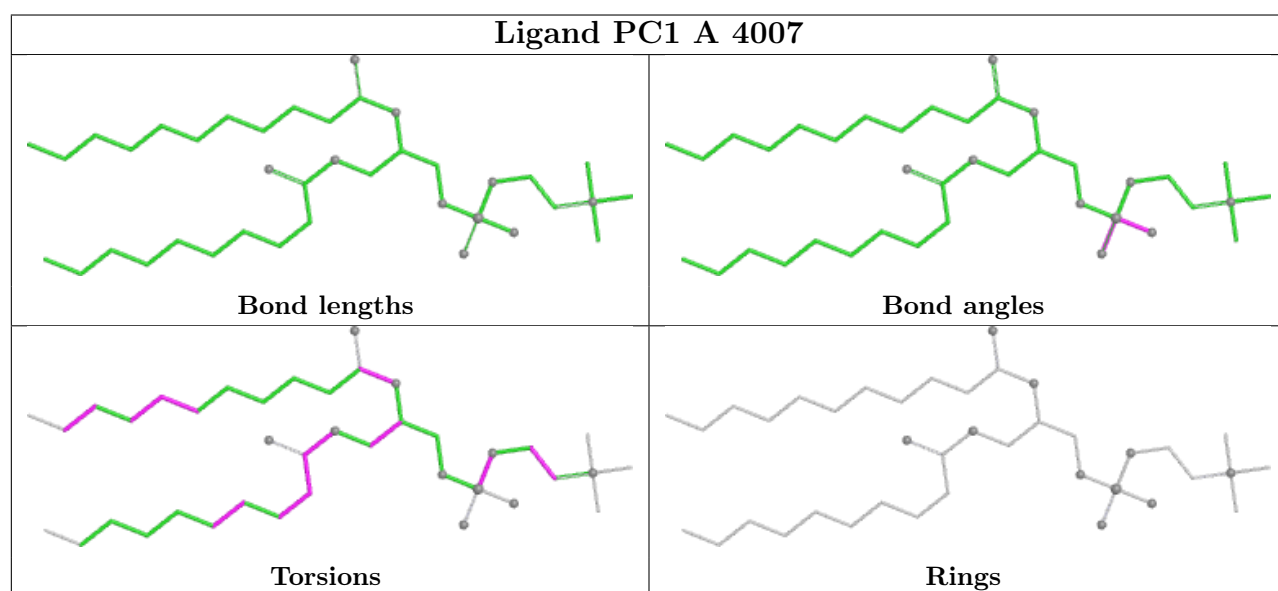
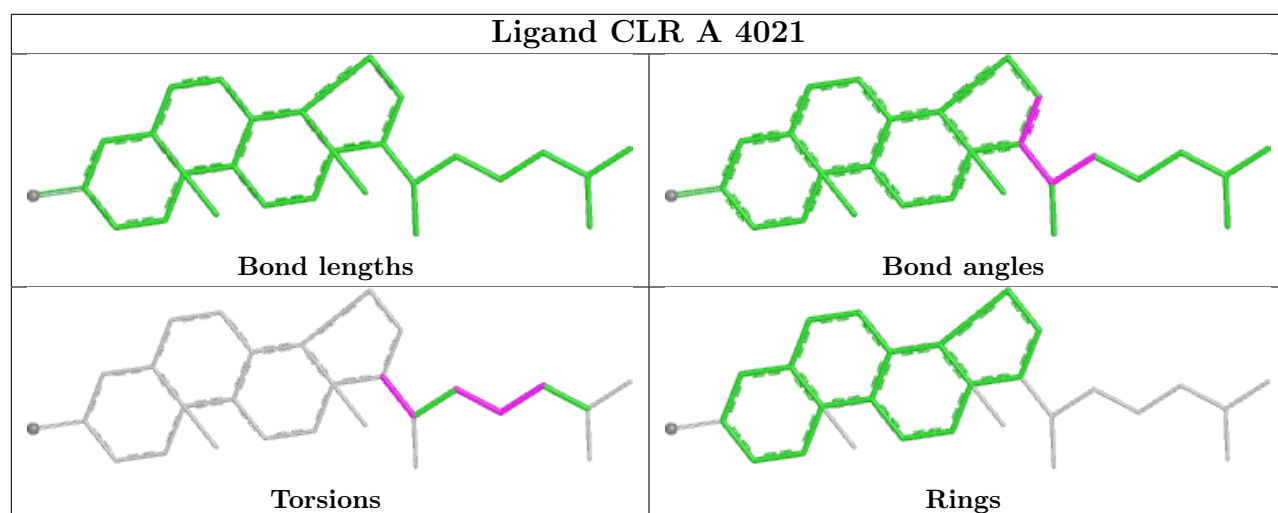
There are no ring outliers.

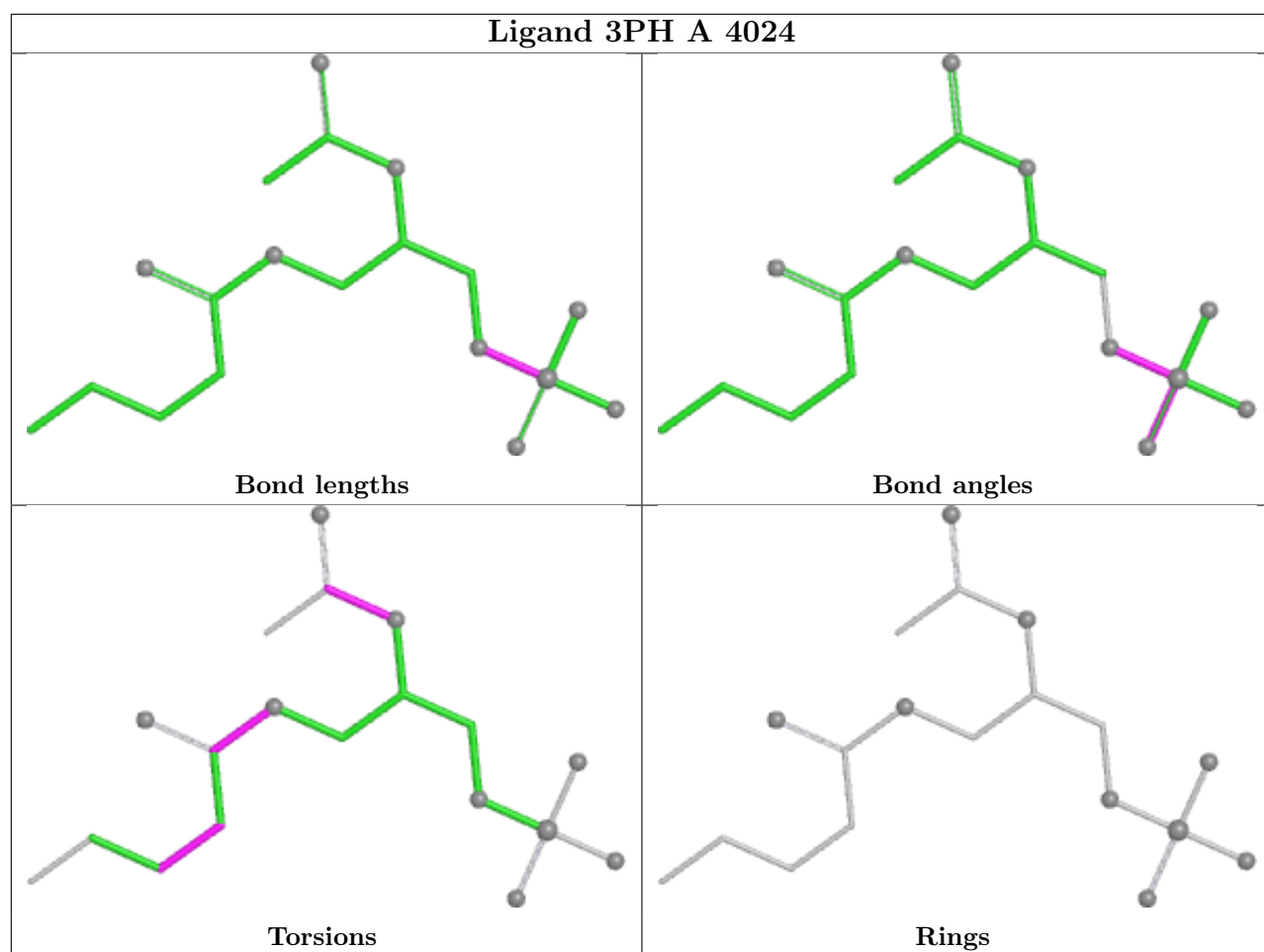
1 monomer is involved in 1 short contact:

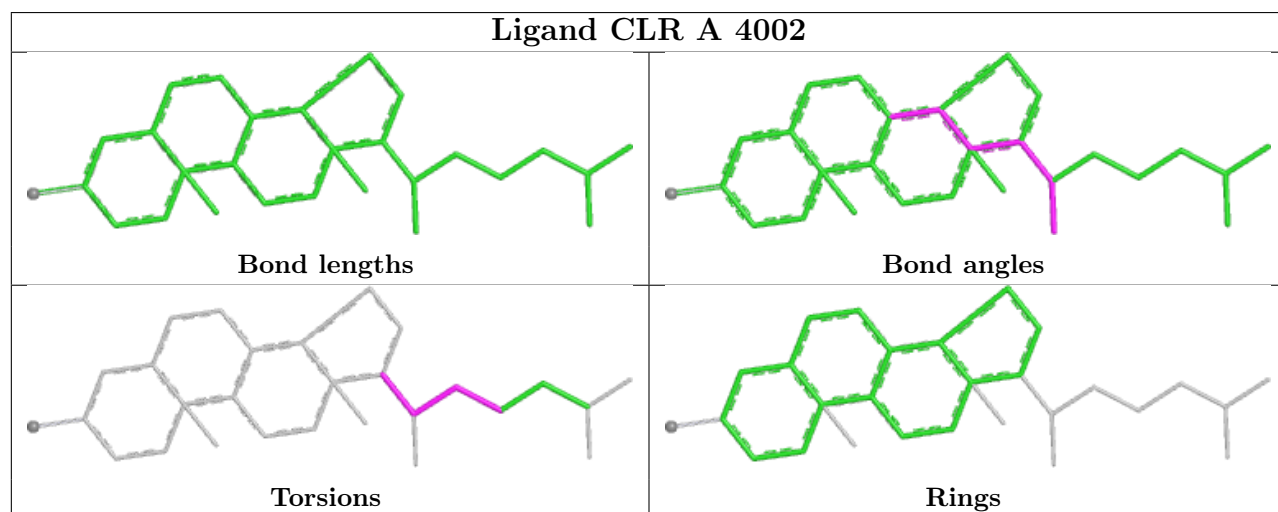
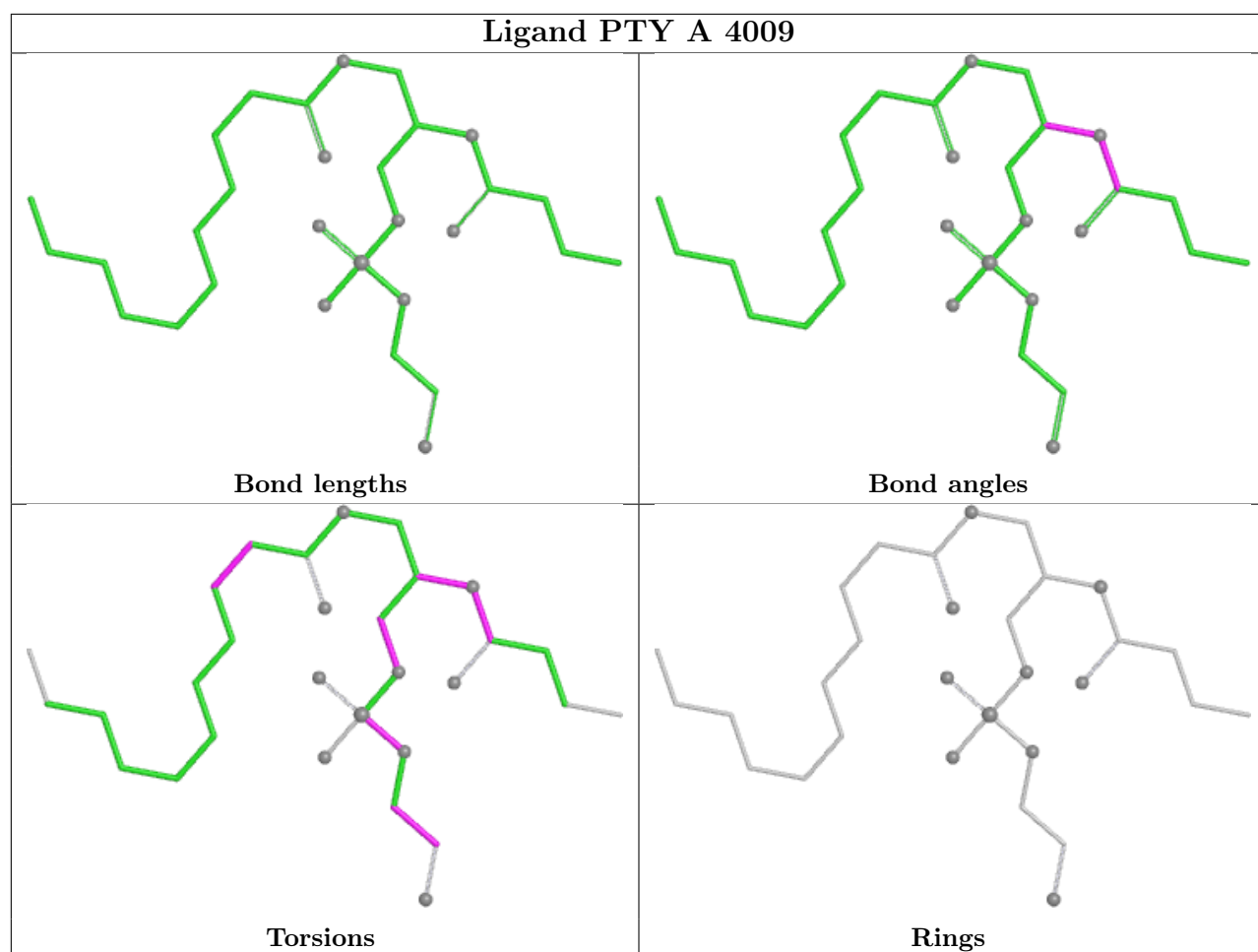
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	4002	CLR	1	0

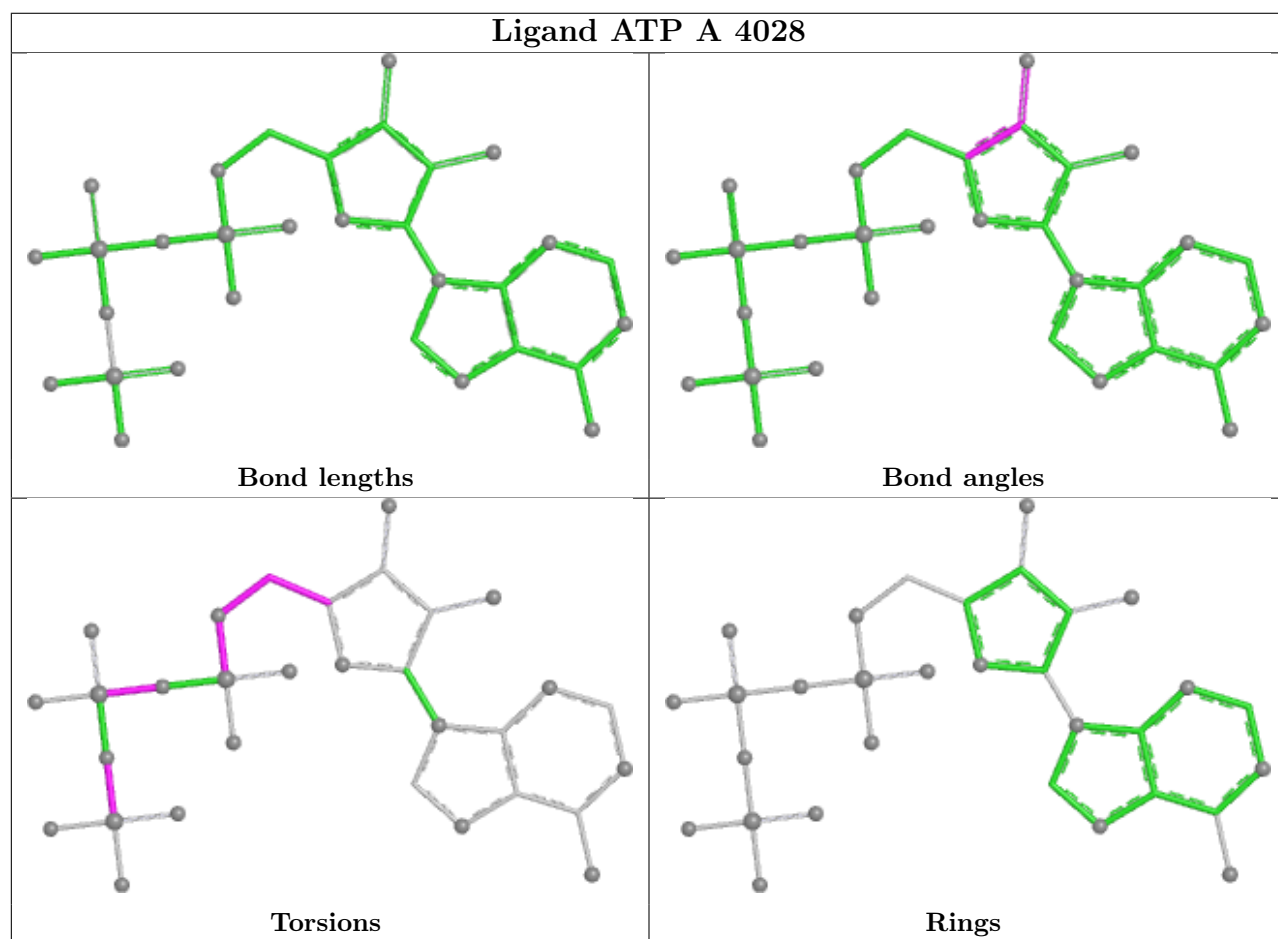
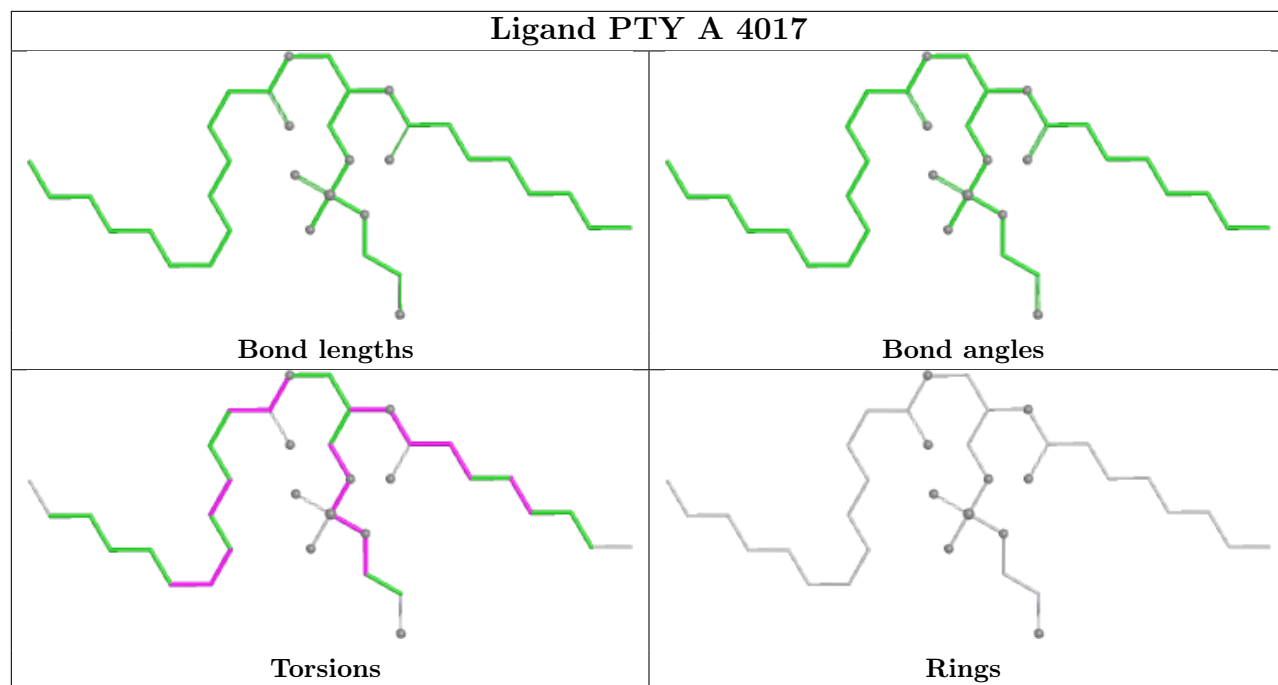
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

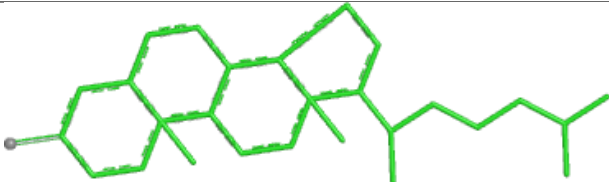
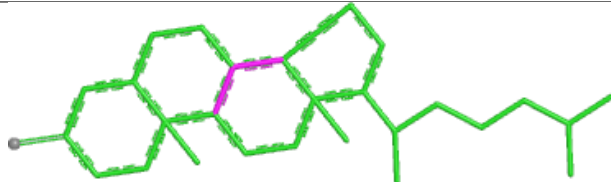
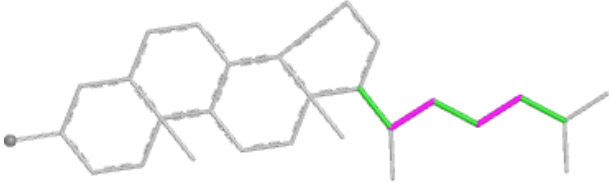
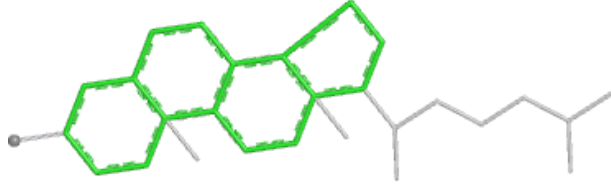


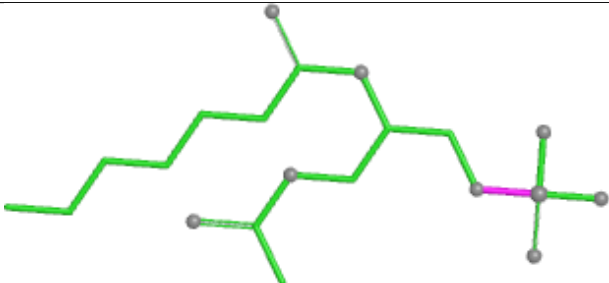
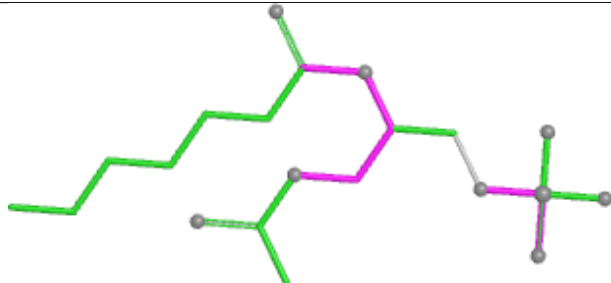
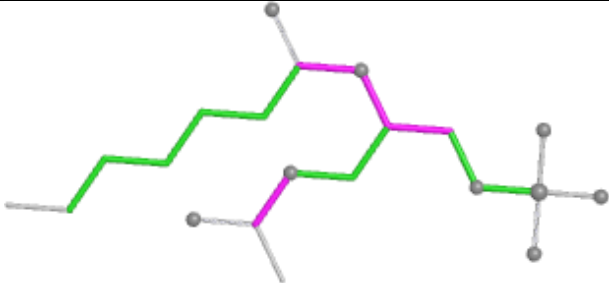
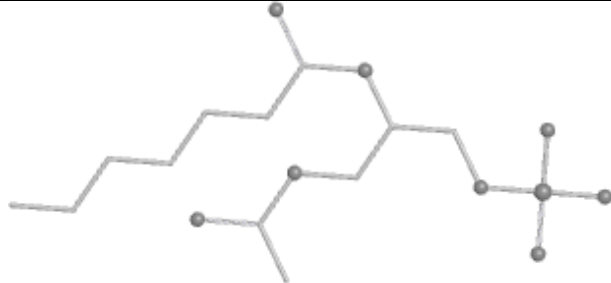


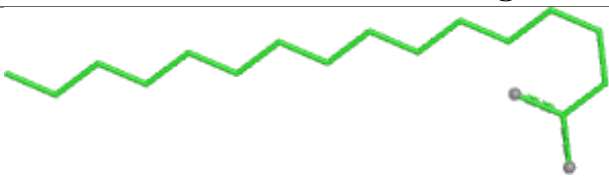
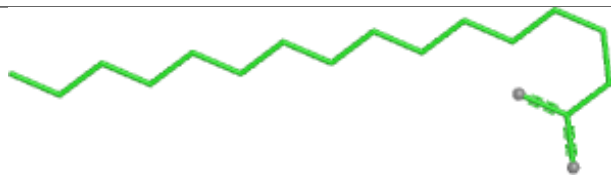
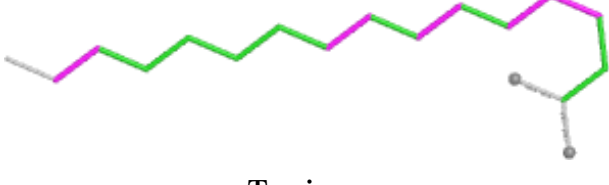
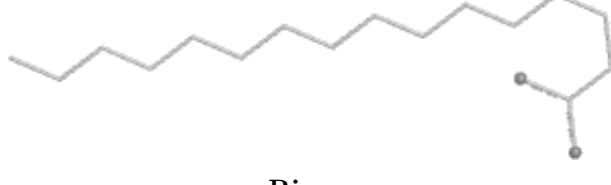


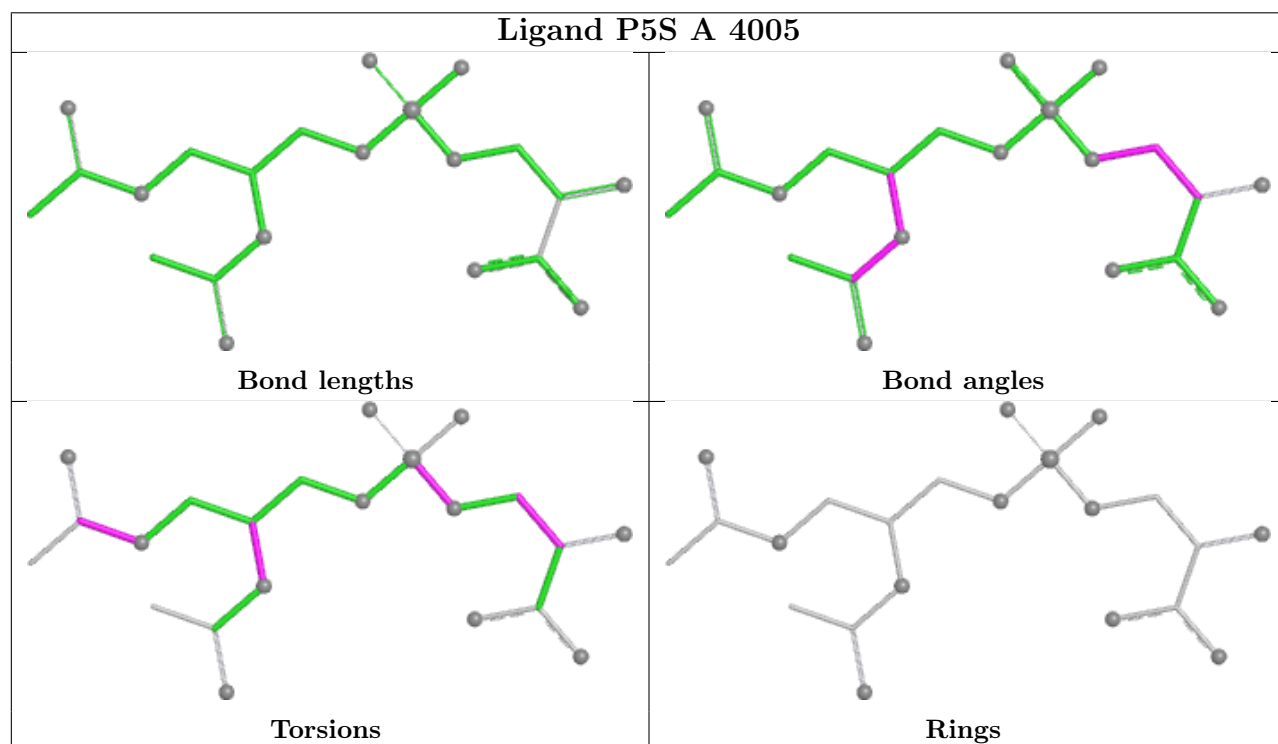
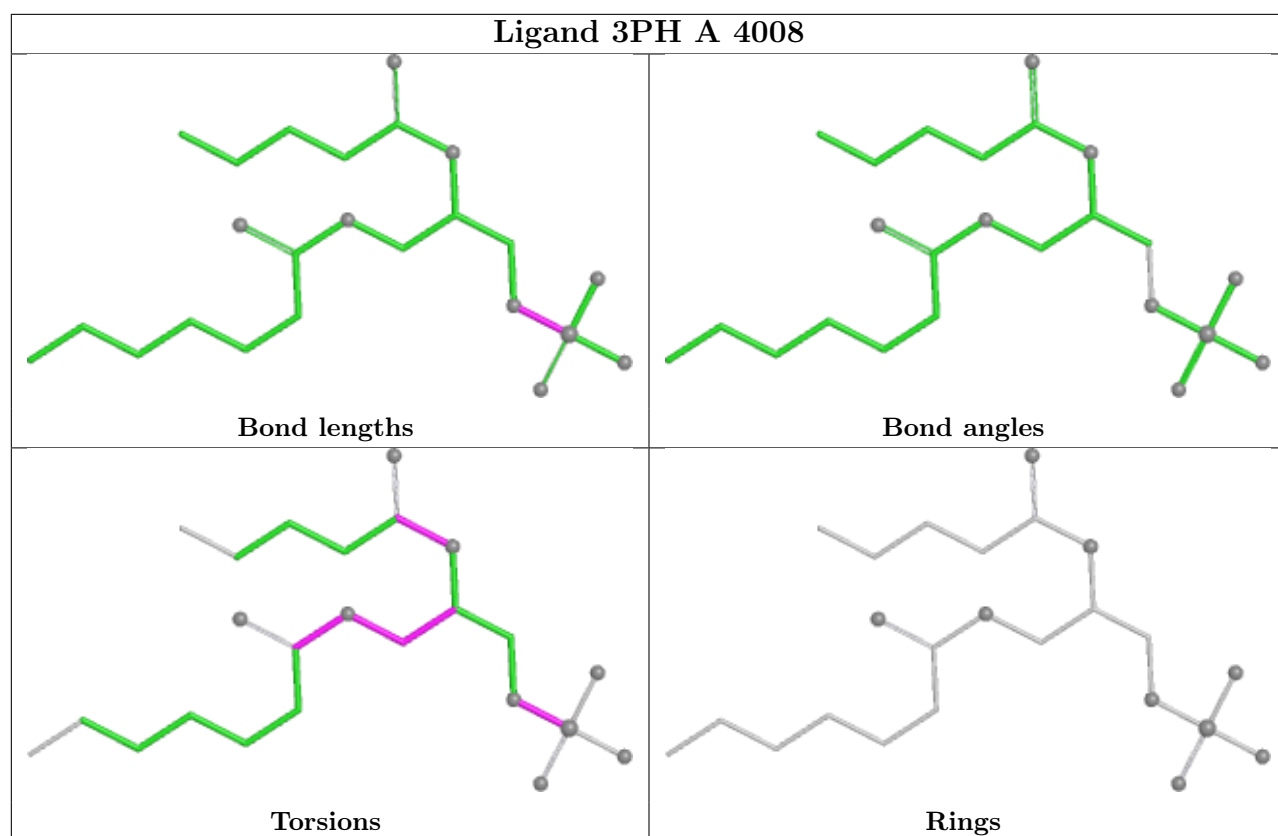


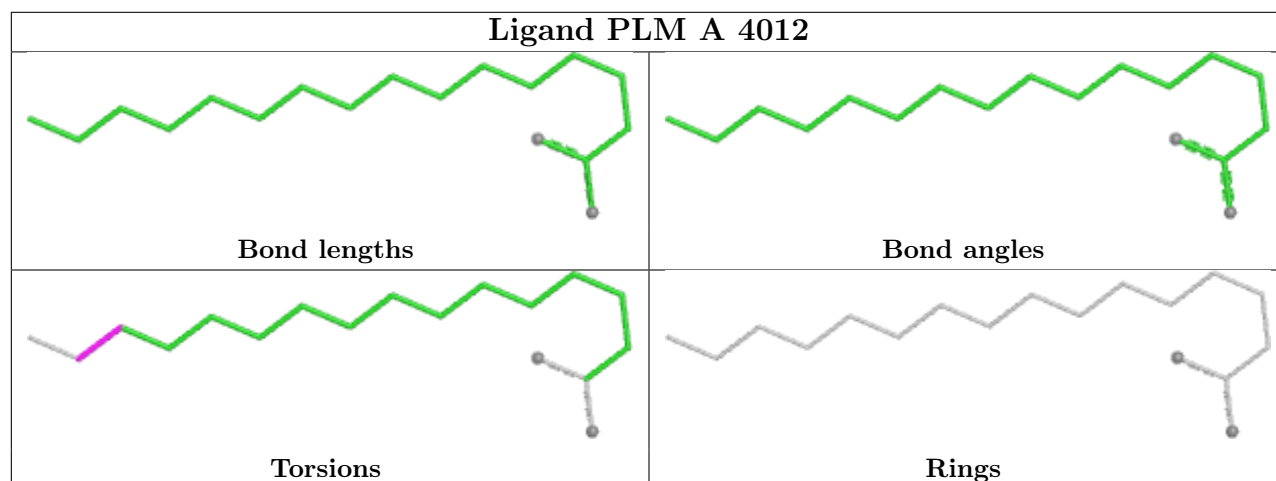
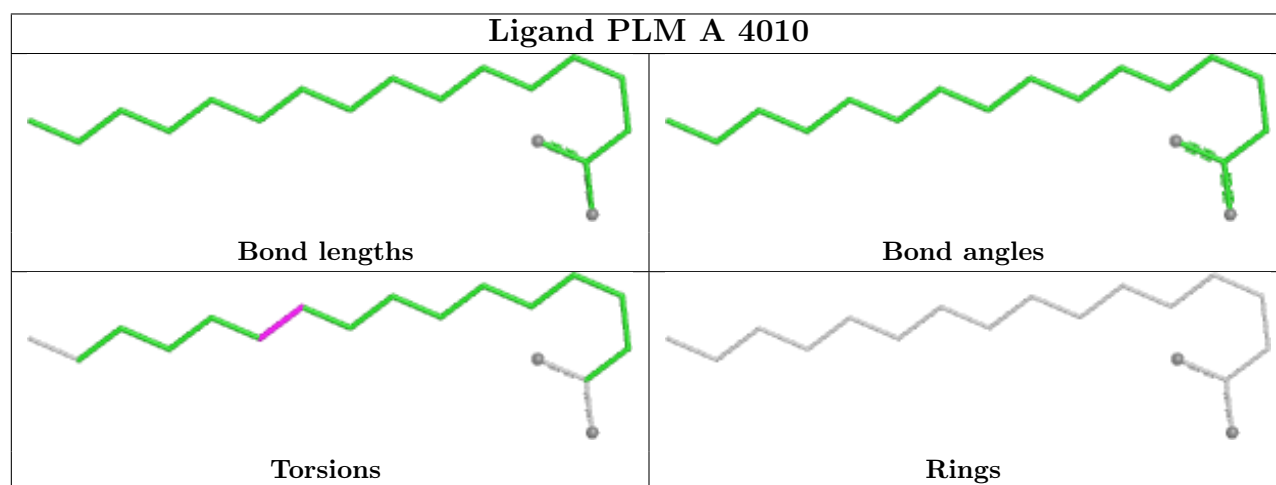
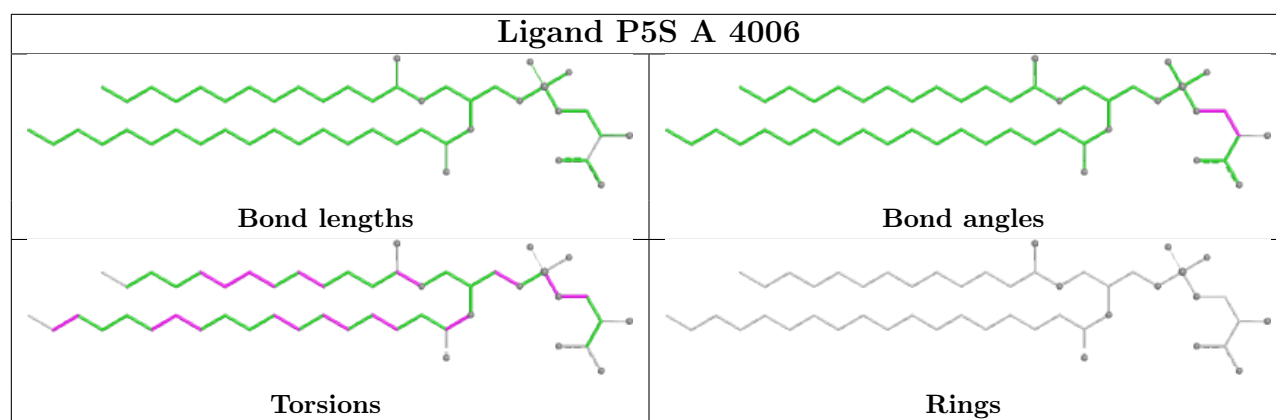


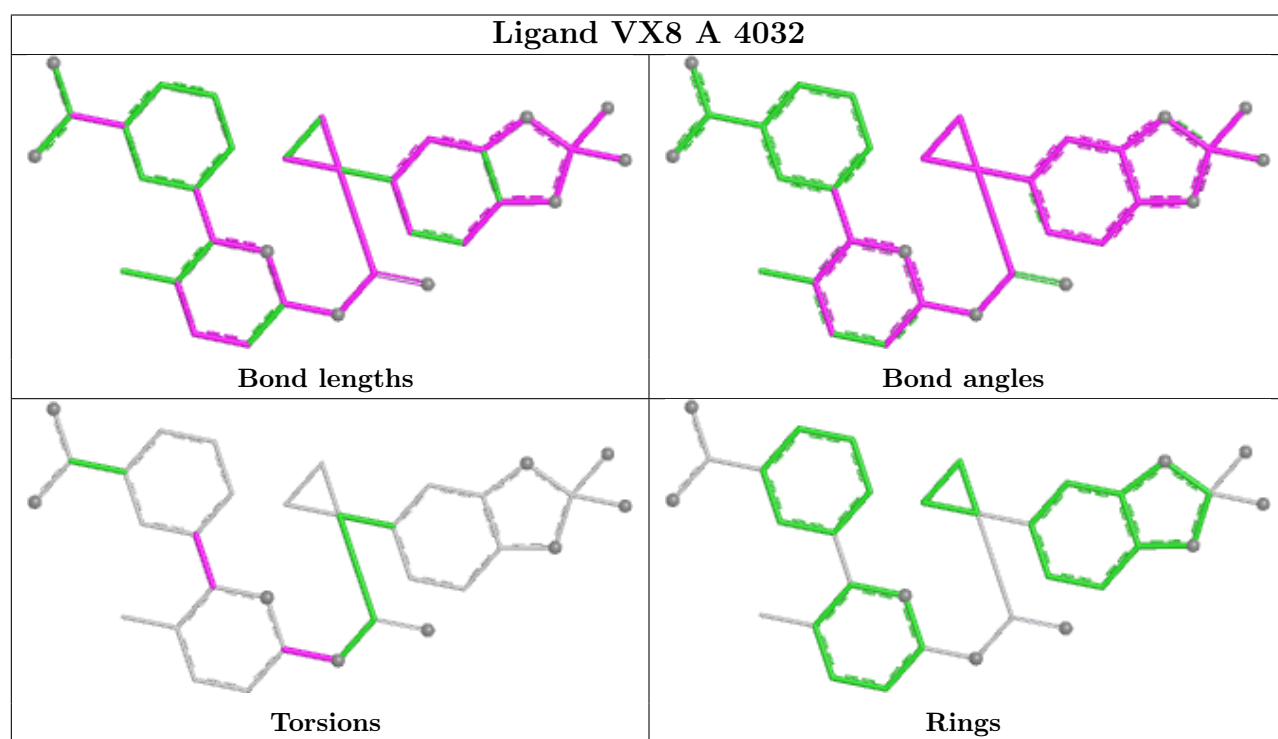
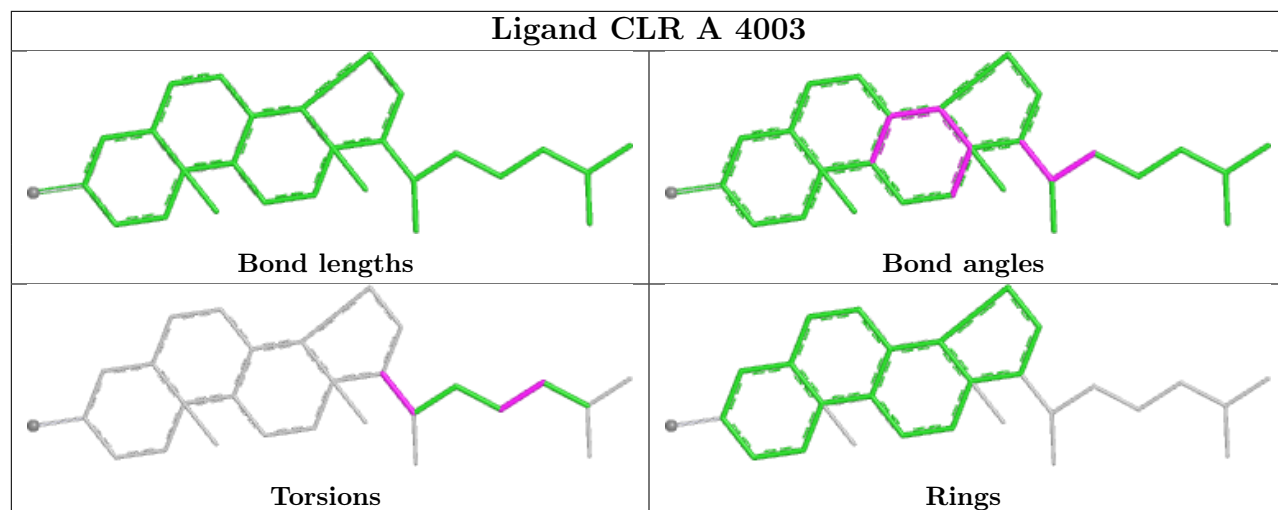
Ligand CLR A 4004	
	
Bond lengths	Bond angles
	
Torsions	Rings

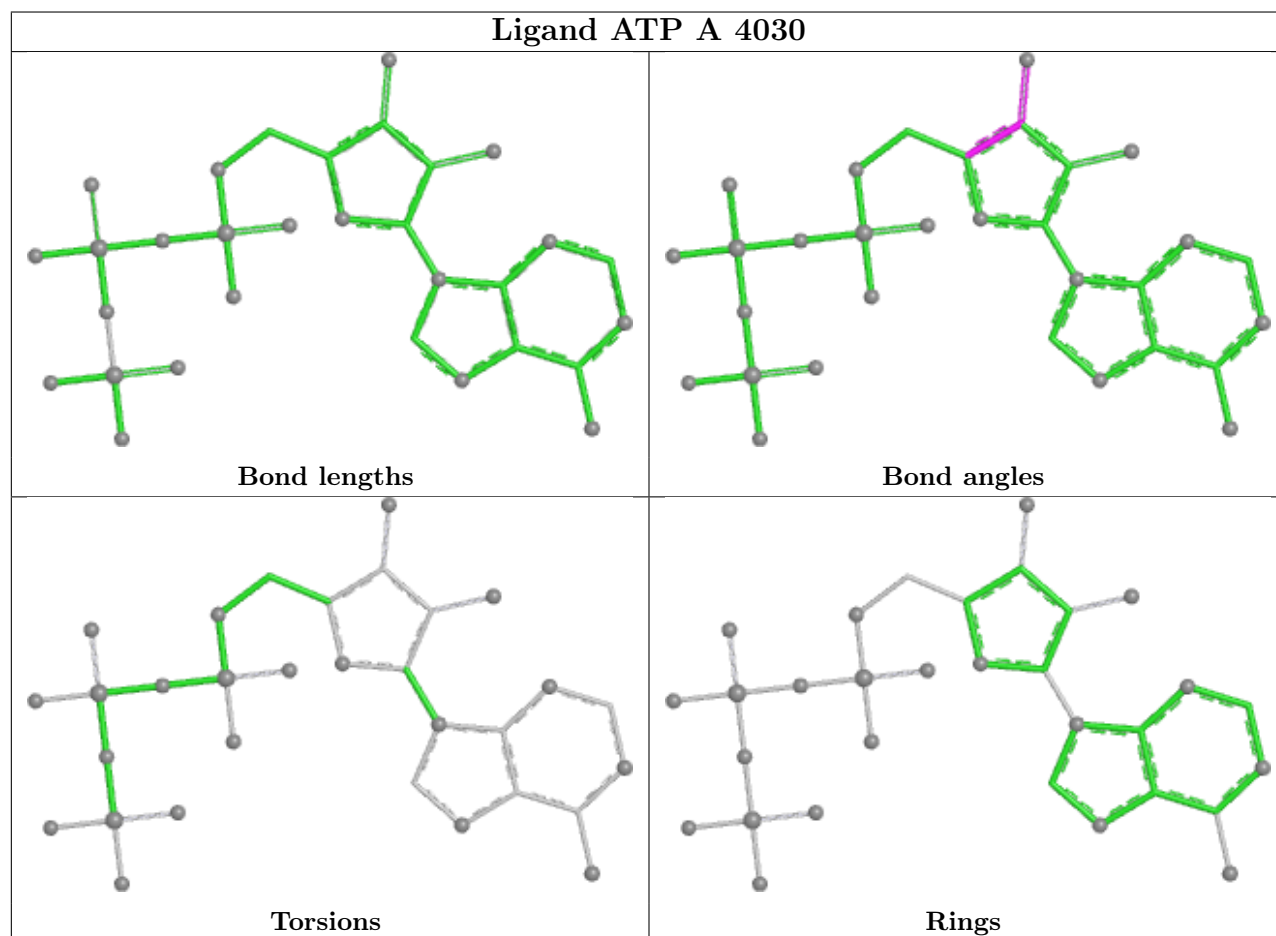
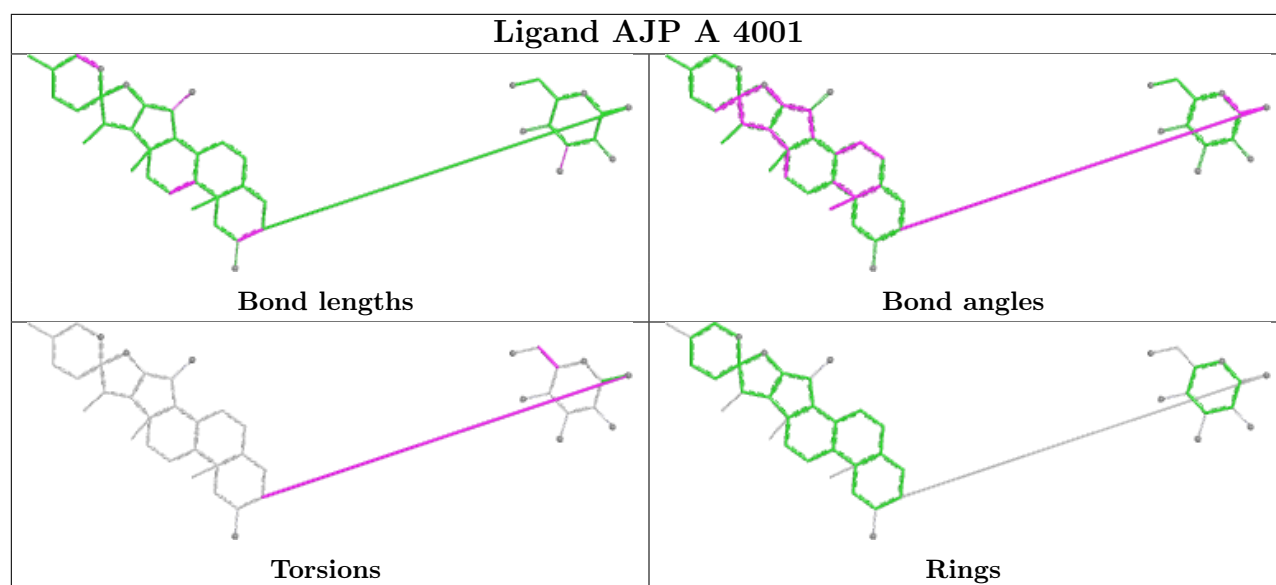
Ligand 3PH A 4023	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLM A 4022	
	
Bond lengths	Bond angles
	
Torsions	Rings









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

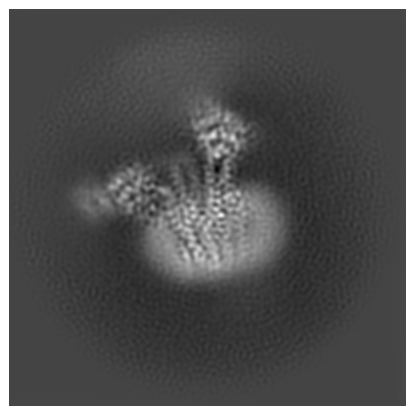
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72403. These allow visual inspection of the internal detail of the map and identification of artifacts.

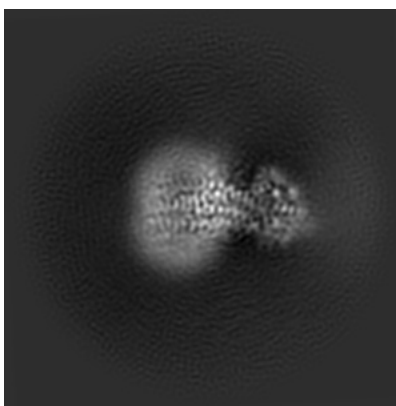
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

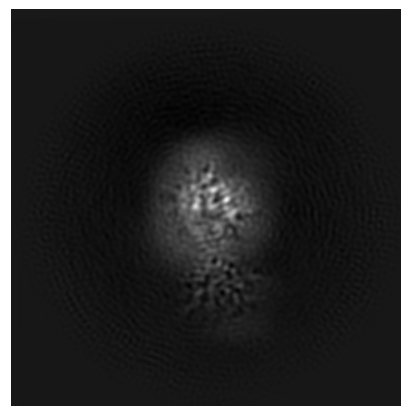
6.1.1 Primary map



X

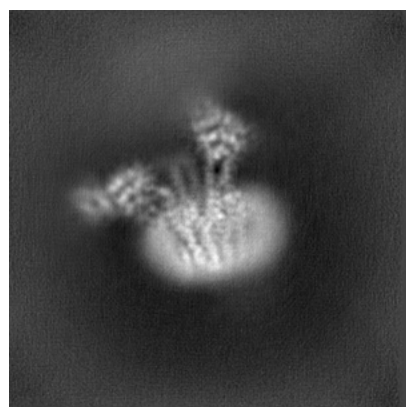


Y

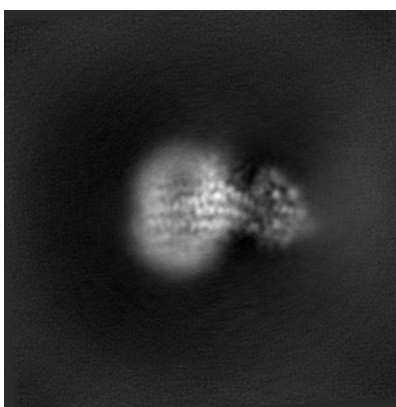


Z

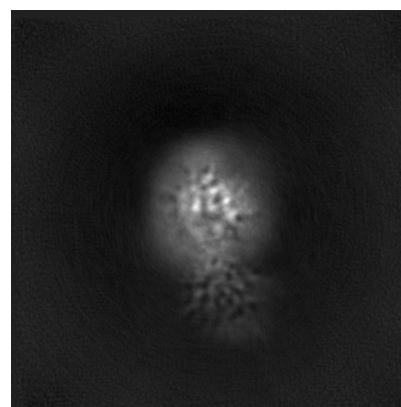
6.1.2 Raw map



X



Y

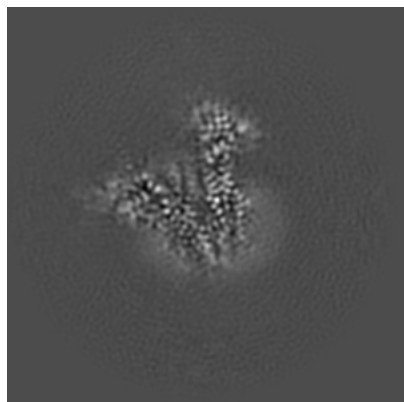


Z

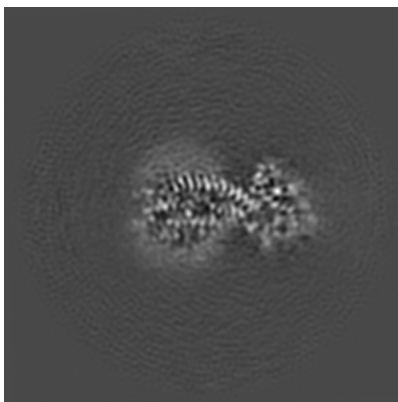
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

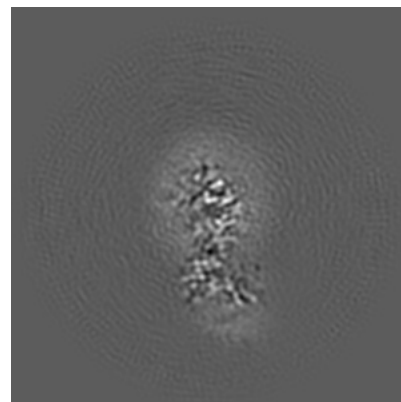
6.2.1 Primary map



X Index: 160

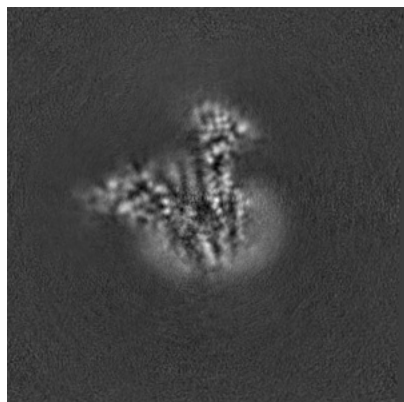


Y Index: 160

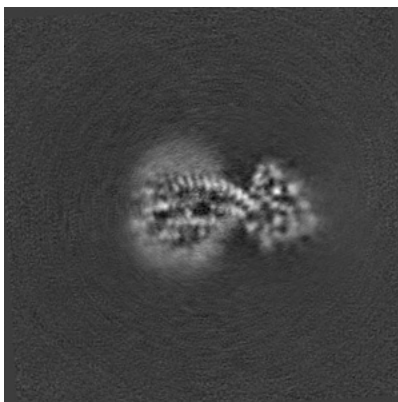


Z Index: 160

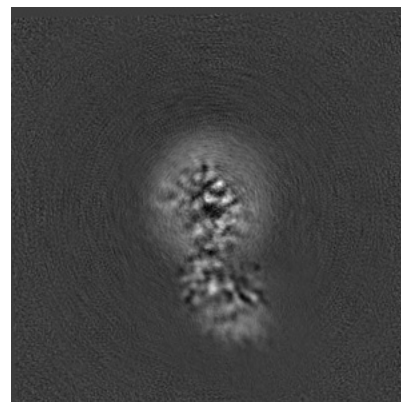
6.2.2 Raw map



X Index: 160



Y Index: 160

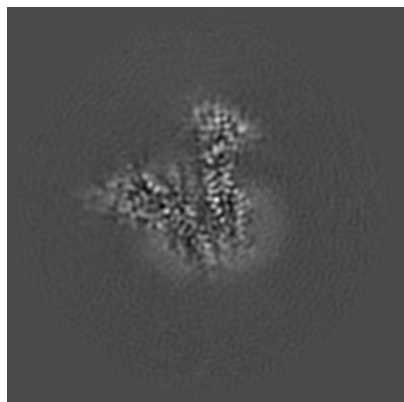


Z Index: 160

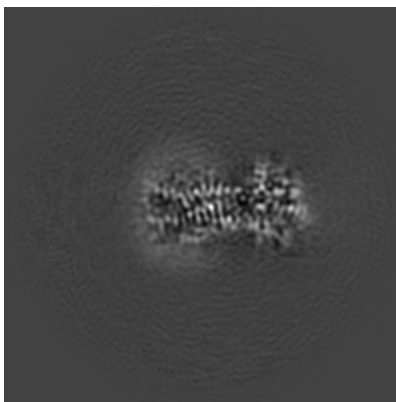
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

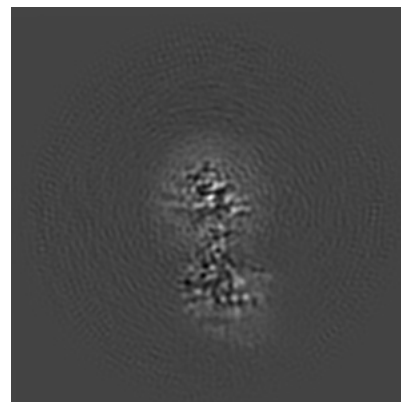
6.3.1 Primary map



X Index: 159

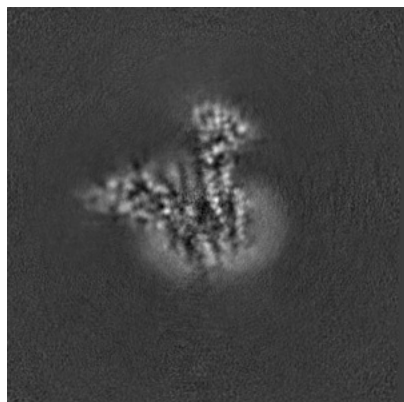


Y Index: 167

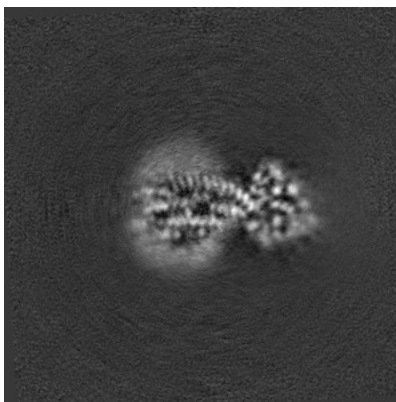


Z Index: 166

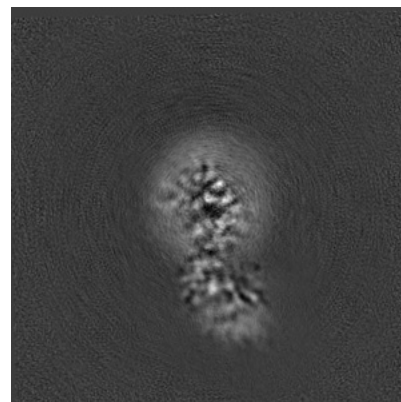
6.3.2 Raw map



X Index: 159



Y Index: 161

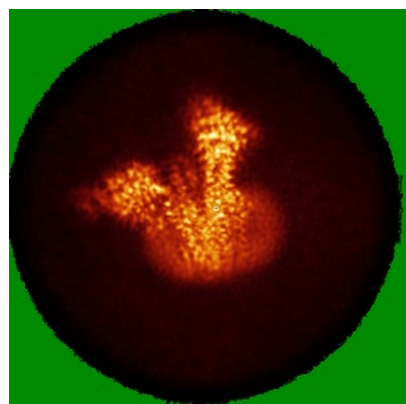


Z Index: 160

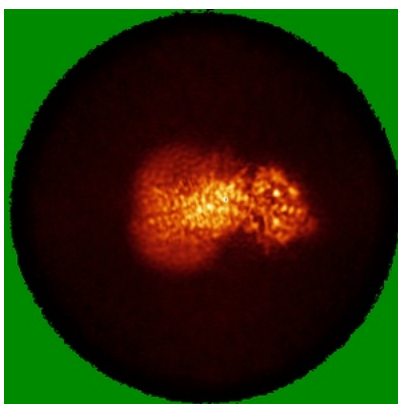
The images above show the largest variance slices of the map in three orthogonal directions.

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

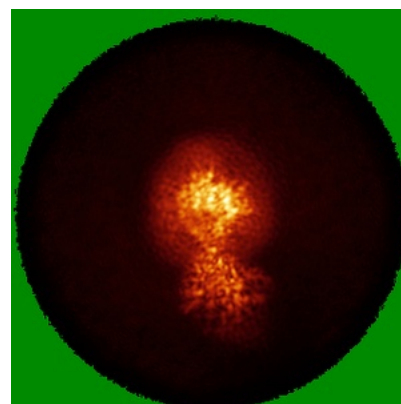
6.4.1 Primary map



X

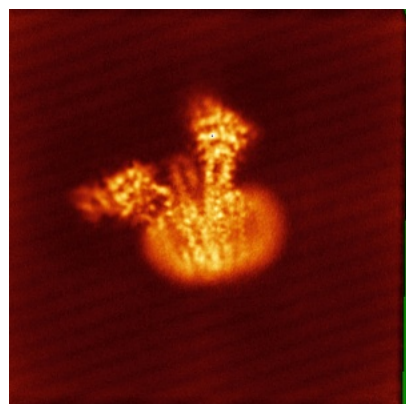


Y

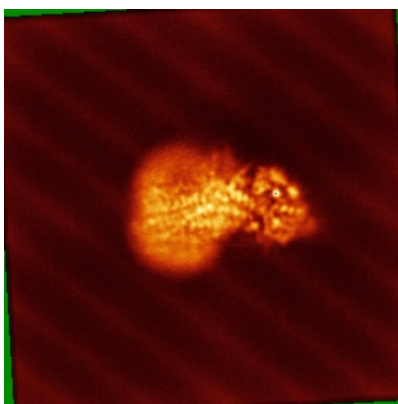


Z

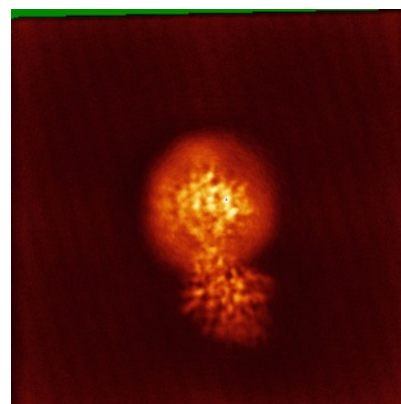
6.4.2 Raw map



X



Y

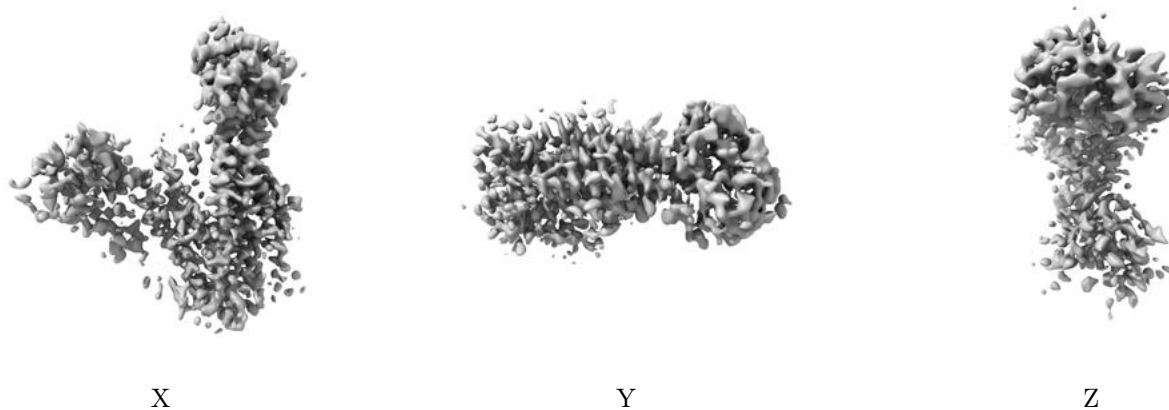


Z

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.

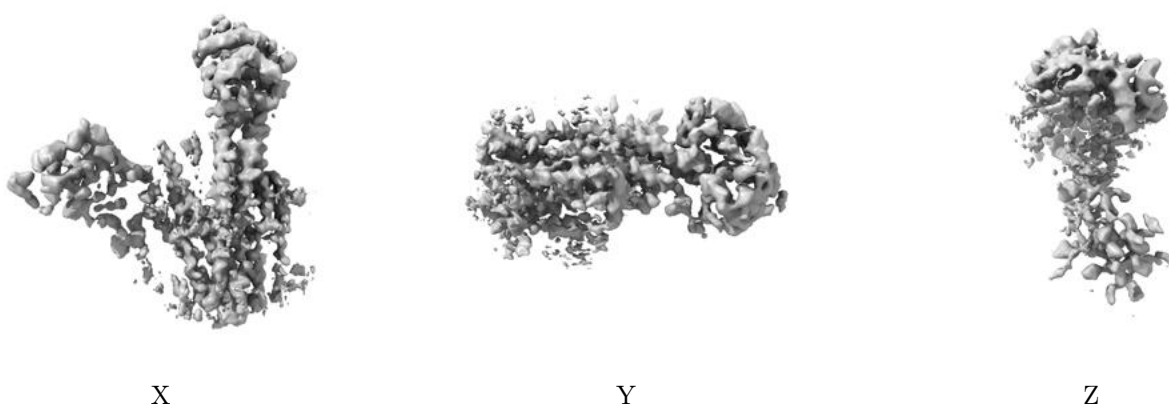
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 9.5. 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.

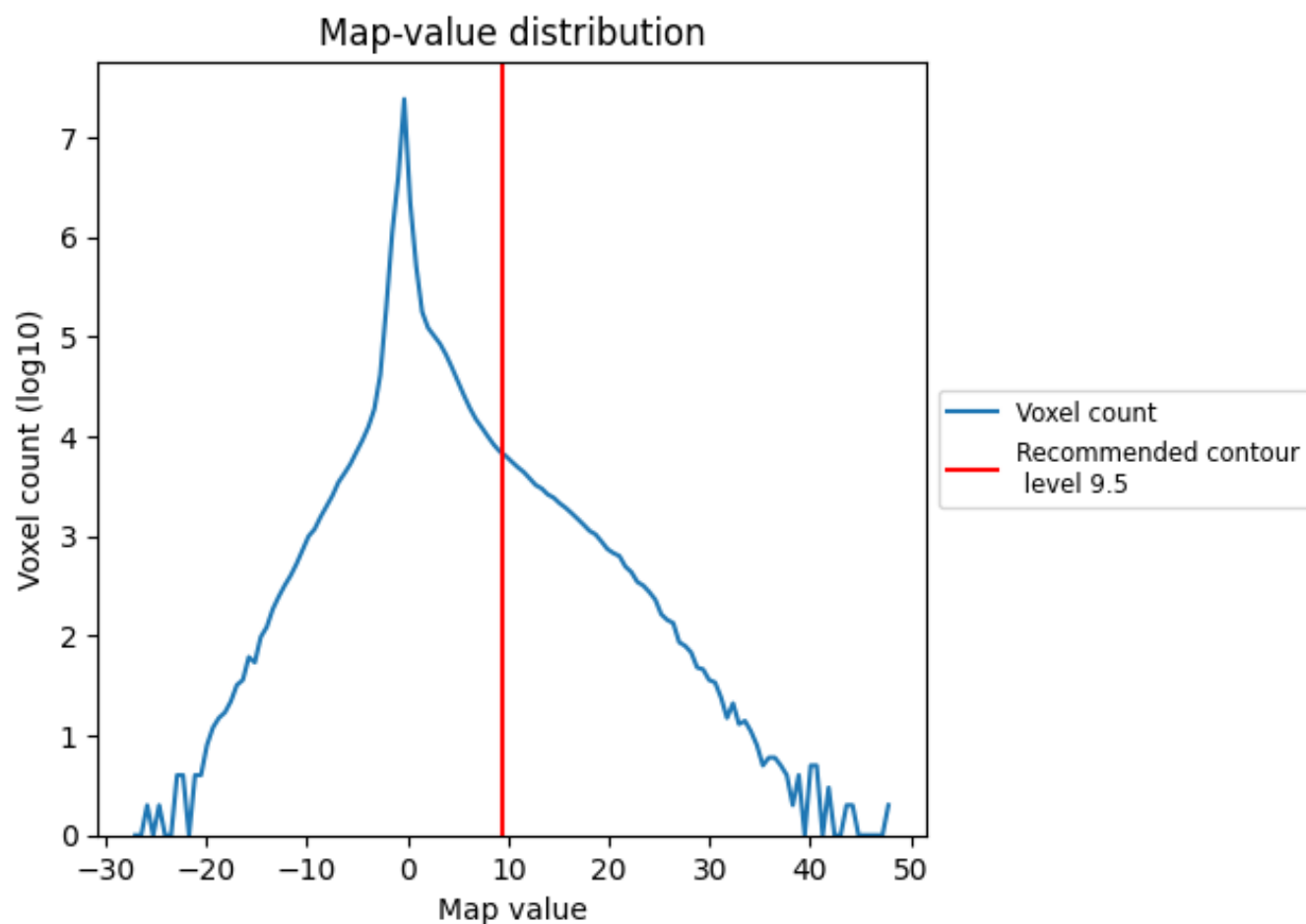
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

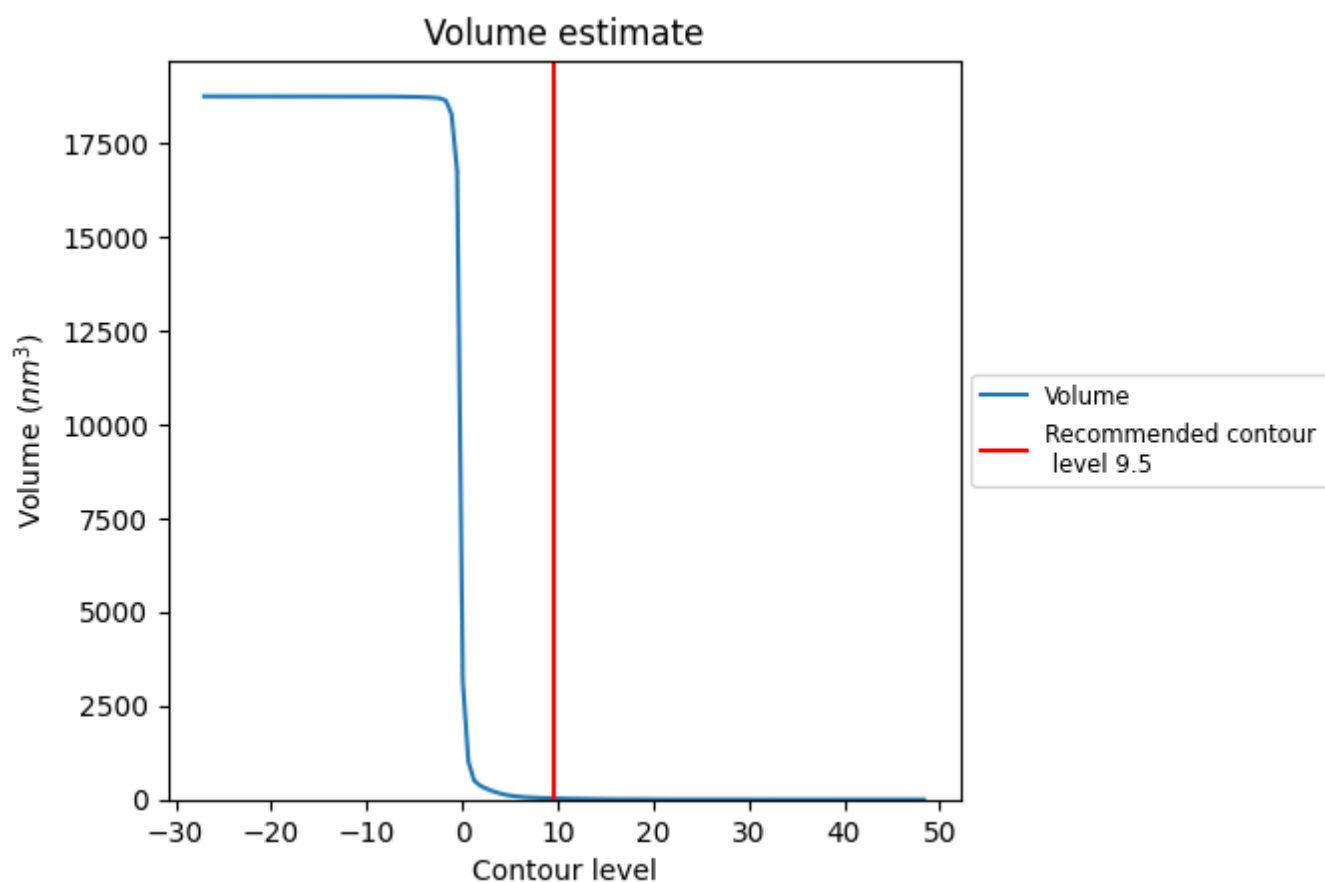
This section contains the results of statistical analysis of the map.

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.

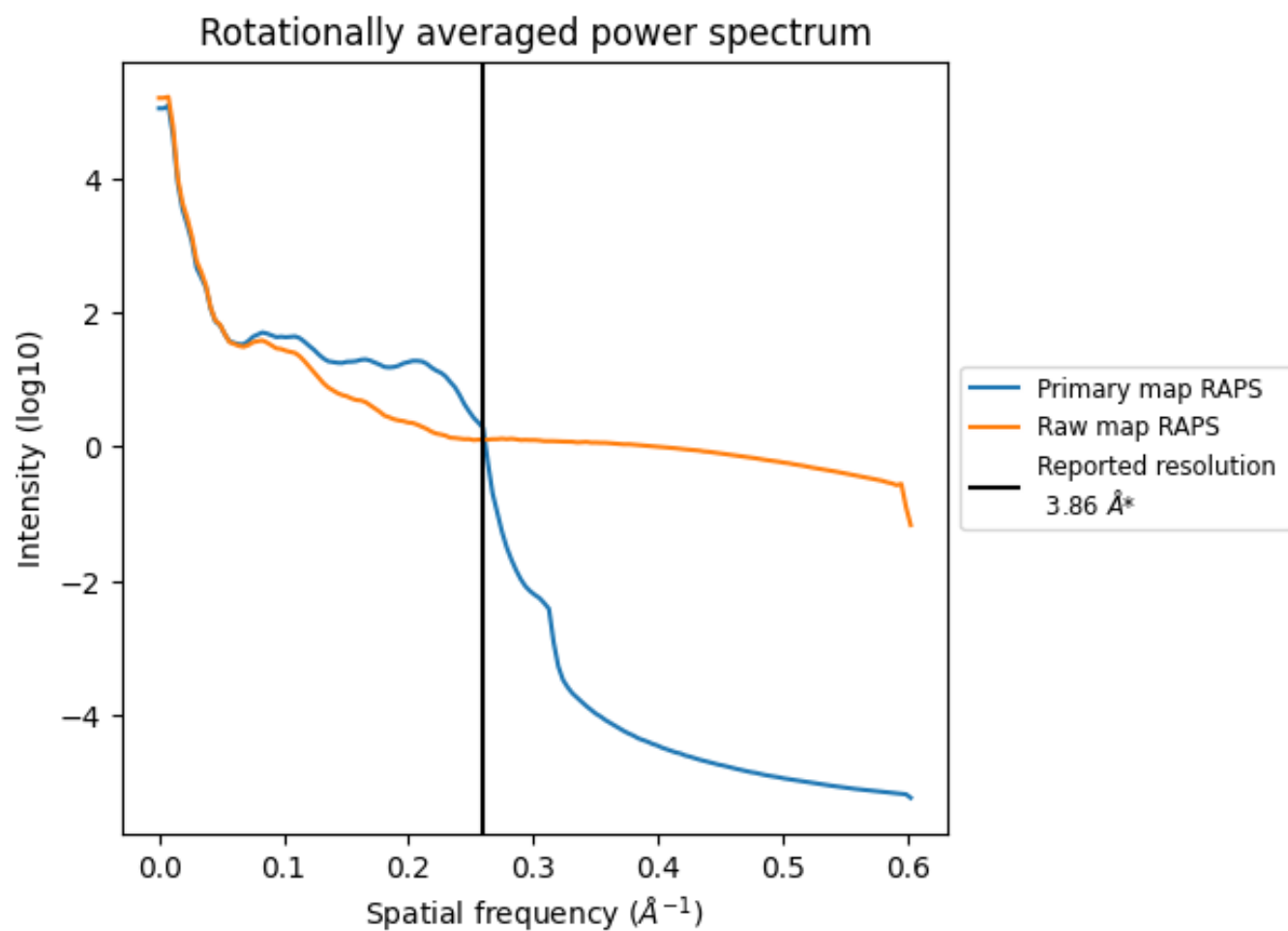
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 32 nm³; this corresponds to an approximate mass of 29 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 ⓘ

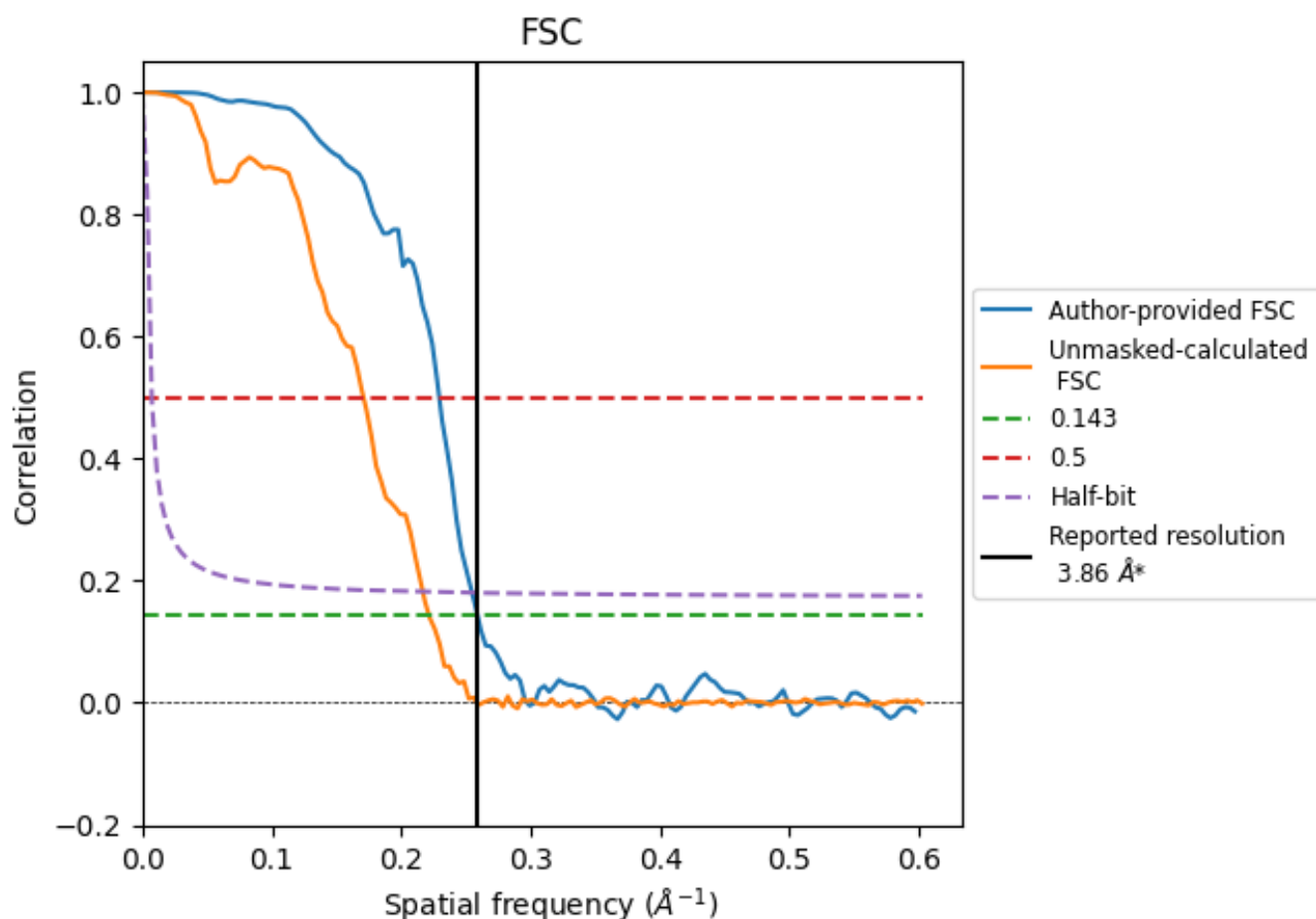


*Reported resolution corresponds to spatial frequency of 0.259 Å⁻¹

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 0.259 Å⁻¹

8.2 Resolution estimates [i](#)

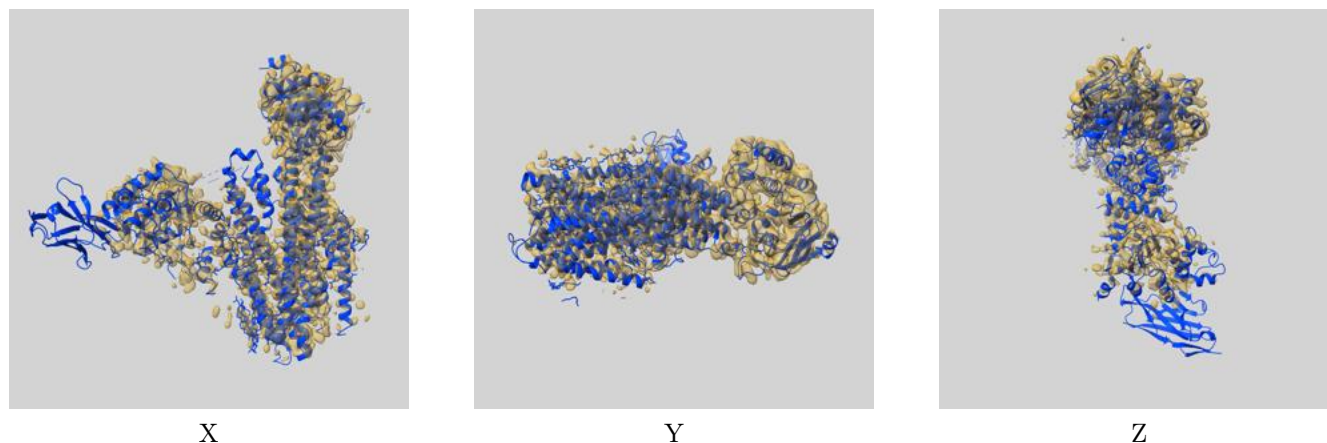
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.86	-	-
Author-provided FSC curve	3.86	4.36	3.93
Unmasked-calculated*	4.51	5.85	4.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 3.86 by more than 10 %

9 Map-model fit [i](#)

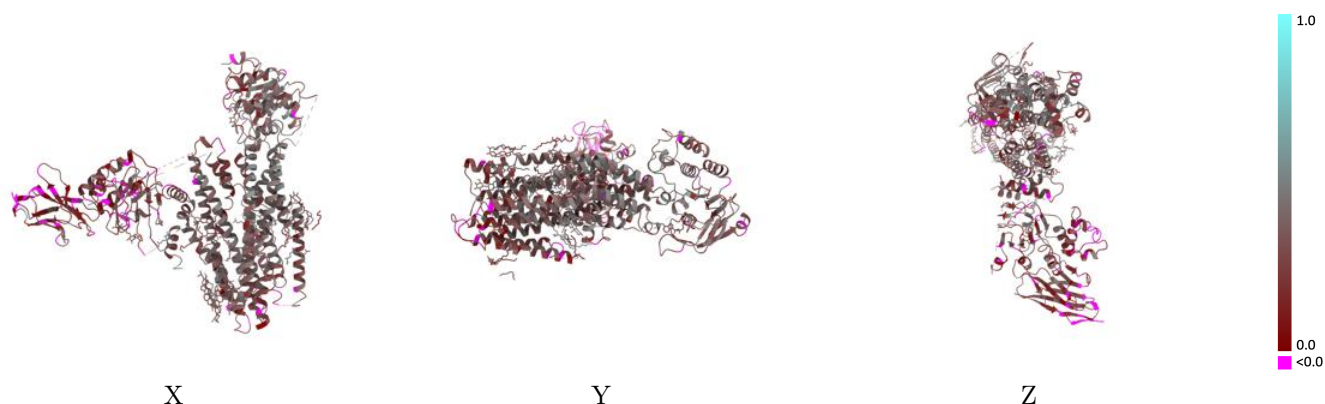
This section contains information regarding the fit between EMDB map EMD-72403 and PDB model 9Y1Q. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



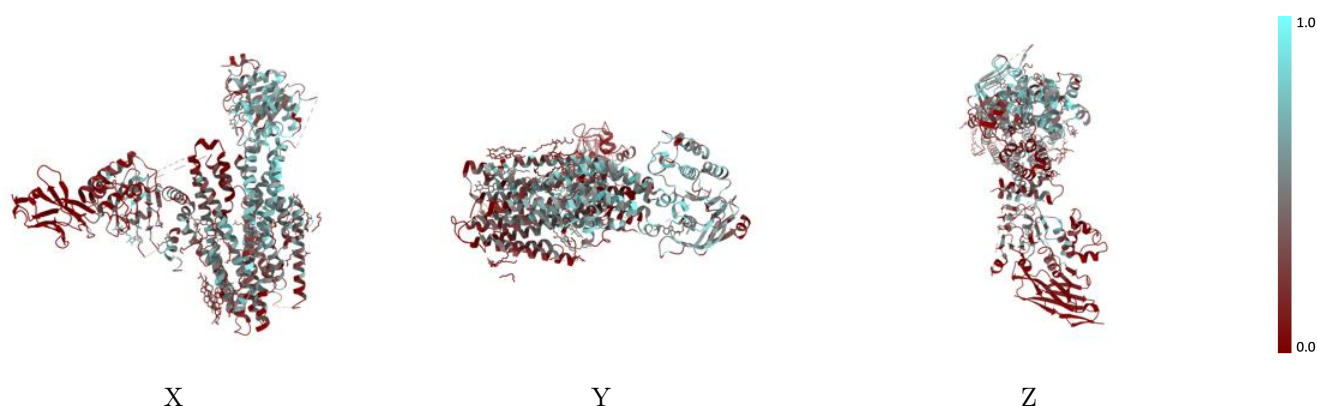
The images above show the 3D surface view of the map at the recommended contour level 9.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



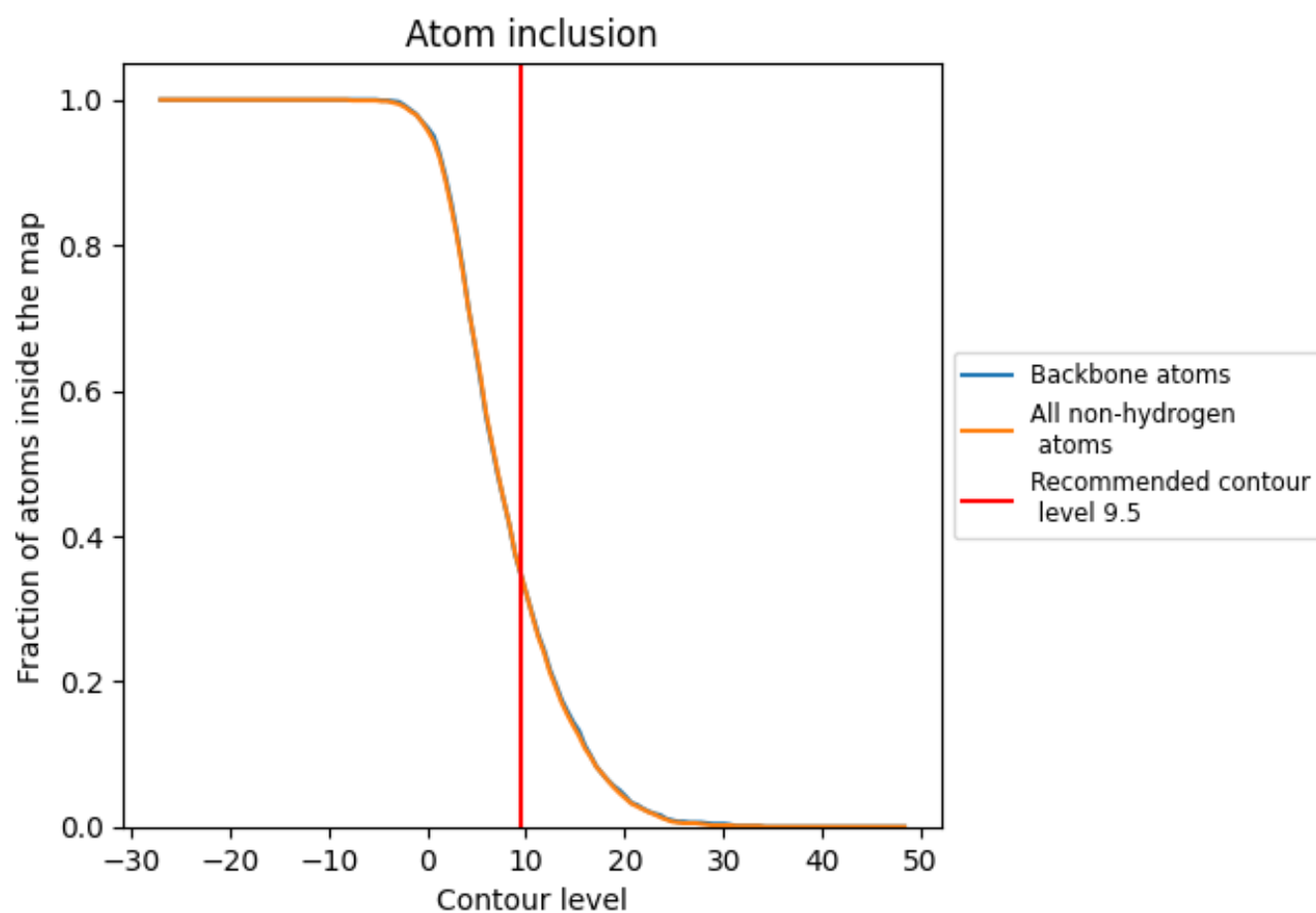
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (9.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 35% of all backbone atoms, 35% 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 (9.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3470	0.3010
A	0.3960	0.3140
B	0.0110	0.1660
C	0.3880	0.3550

