



## Full wwPDB EM Validation Report ⓘ

Aug 25, 2024 – 12:26 AM JST

PDB ID : 8X5B  
EMDB ID : EMD-38065  
Title : Cryo-EM structures of human XPR1 in closed states  
Authors : Jiang, D.H.; Yan, R.  
Deposited on : 2023-11-16  
Resolution : 2.84 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev112  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.2

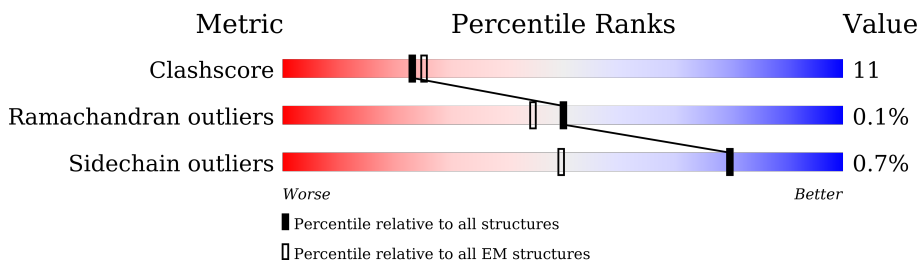
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.84 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  $\geq 3$ , 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	468	
1	F	468	

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
2	PO4	A	703	-	-	X	-
2	PO4	F	703	-	X	X	-
2	PO4	F	704	-	X	X	-

## 2 Entry composition [i](#)

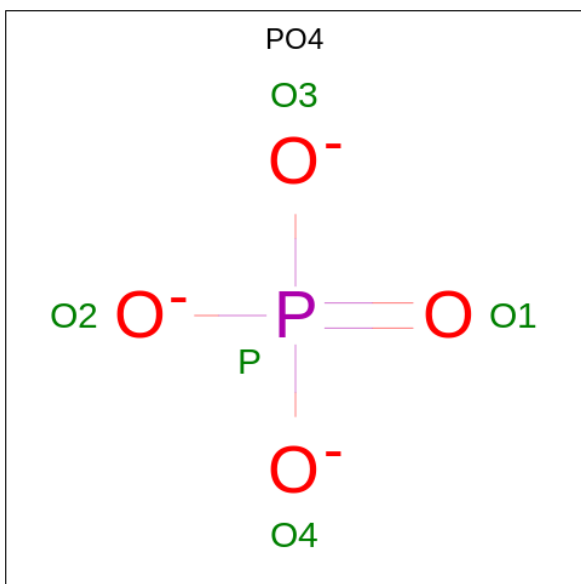
There are 5 unique types of molecules in this entry. The entry contains 6973 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Solute carrier family 53 member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	393	Total 3214	C 2165	N 516	O 517	S 16	0	0
1	A	393	Total 3214	C 2165	N 516	O 517	S 16	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



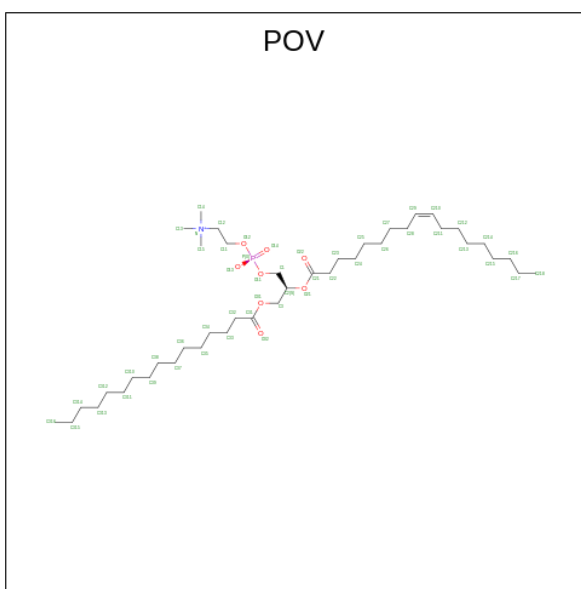
Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
2	F	1	Total 5	O 4	P 1	0
2	F	1	Total 5	O 4	P 1	0
2	F	1	Total 5	O 4	P 1	0
2	F	1	Total 5	O 4	P 1	0
2	A	1	Total 5	O 4	P 1	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
2	A	1	5	4	1	0
2	A	1	5	4	1	0
2	A	1	5	4	1	0

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



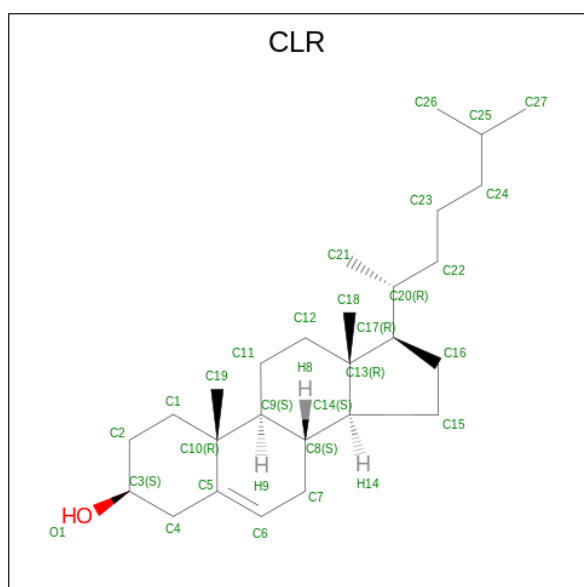
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	F	1	52	42	1	8	1	0
3	F	1	29	19	1	8	1	0
3	F	1	17	14	3			0
3	F	1	18	16	2			0
3	F	1	16	14	2			0
3	F	1	16	14	2			0
3	F	1	14	12	2			0

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Mol	Chain	Residues	Atoms	AltConf
3	F	1	Total C O 18 16 2	0
3	A	1	Total C O P 39 30 8 1	0
3	A	1	Total C O 18 16 2	0
3	A	1	Total C O P 39 30 8 1	0
3	A	1	Total C N O P 52 42 1 8 1	0
3	A	1	Total C N O P 29 19 1 8 1	0
3	A	1	Total C O 17 14 3	0
3	A	1	Total C O 18 16 2	0
3	A	1	Total C O 16 14 2	0
3	A	1	Total C O 16 14 2	0
3	A	1	Total C O 11 9 2	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



Mol	Chain	Residues	Atoms			AltConf
4	F	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	F	7	Total	O	0
			7	7	
5	A	7	Total	O	0
			7	7	



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	253874	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	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 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.798	Depositor
Minimum map value	-4.851	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.140	Depositor
Recommended contour level	0.63	Depositor
Map size ( $\text{\AA}$ )	272.0, 272.0, 272.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.85, 0.85, 0.85	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: PO4, CLR, POV

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	0.42	0/3321	0.63	1/4526 (0.0%)
1	F	0.41	0/3321	0.61	3/4526 (0.1%)
All	All	0.42	0/6642	0.62	4/9052 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	TYR	CB-CA-C	-12.46	85.49	110.40
1	F	585	LEU	CB-CA-C	8.77	126.86	110.20
1	F	619	ASN	N-CA-C	5.76	126.56	111.00
1	F	585	LEU	N-CA-C	-5.07	97.30	111.00

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	3214	0	3185	66	0
1	F	3214	0	3185	61	0
2	A	20	0	0	5	0
2	F	20	0	0	4	0
3	A	255	0	354	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	180	0	256	23	0
4	A	28	0	46	1	0
4	F	28	0	46	1	0
5	A	7	0	0	3	0
5	F	7	0	0	2	0
All	All	6973	0	7072	153	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 11.

All (153) 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:F:705:POV:H36A	3:F:705:POV:H3A	1.52	0.88
3:A:709:POV:O22	3:A:709:POV:H25A	1.74	0.88
3:A:708:POV:H23	3:A:708:POV:H27	1.56	0.87
1:A:497:SER:OG	1:A:582:THR:HG23	1.75	0.86
1:F:573:TRP:CE2	1:F:577:ILE:HD11	2.14	0.81
1:A:270:ARG:HD3	2:A:704:PO4:O2	1.81	0.81
3:A:709:POV:H25A	3:A:709:POV:C21	2.10	0.81
1:A:489:MET:CE	5:A:807:HOH:O	2.35	0.75
1:A:512:TYR:O	1:A:516:VAL:HG23	1.88	0.74
1:A:514:TRP:HZ2	1:A:578:SER:CB	2.03	0.72
1:A:514:TRP:HZ2	1:A:578:SER:OG	1.71	0.72
1:A:512:TYR:O	1:A:515:ILE:HG22	1.91	0.70
1:A:489:MET:SD	1:A:574:THR:HG23	2.31	0.70
1:A:514:TRP:CZ2	1:A:578:SER:CB	2.76	0.69
1:F:512:TYR:O	1:F:516:VAL:HG23	1.94	0.68
1:A:306:ASN:HB2	3:A:708:POV:H14B	1.75	0.67
1:F:306:ASN:HB2	3:F:705:POV:H14B	1.75	0.67
1:A:355:MET:HB3	3:A:708:POV:H21C	1.77	0.67
1:A:489:MET:HE3	5:A:807:HOH:O	1.96	0.66
1:F:441:HIS:H	1:F:441:HIS:CD2	2.14	0.66
1:A:278:LEU:HD21	3:A:708:POV:H21B	1.77	0.65
1:F:373:TRP:CD1	3:F:705:POV:H15	2.33	0.64
1:F:573:TRP:NE1	1:F:577:ILE:HD11	2.11	0.64
1:A:452:GLN:NE2	1:A:581:SER:OG	2.30	0.64
3:A:708:POV:H23	3:A:708:POV:C27	2.27	0.64
1:A:373:TRP:CD1	3:A:708:POV:H15	2.33	0.63
1:A:514:TRP:CZ2	1:A:578:SER:OG	2.50	0.63
3:F:705:POV:H34A	3:F:705:POV:O32	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:GLN:O	1:A:576:GLN:HG2	1.99	0.62
1:A:466:ARG:HD2	2:A:703:PO4:O2	1.99	0.62
1:A:285:LEU:HD21	3:A:708:POV:H35A	1.82	0.62
1:A:306:ASN:O	1:A:310:ASN:ND2	2.30	0.61
1:F:251:LEU:HD21	1:F:331:LEU:HD23	1.82	0.61
1:A:251:LEU:HD21	1:A:331:LEU:HD23	1.82	0.60
1:F:449:ALA:CB	3:F:711:POV:H34A	2.31	0.60
3:A:710:POV:H34A	3:A:710:POV:O32	2.00	0.59
1:F:355:MET:HB3	3:F:705:POV:H21A	1.82	0.59
1:A:420:GLU:HB2	1:A:440:CYS:SG	2.42	0.59
3:F:711:POV:C311	3:F:711:POV:H37	2.31	0.58
1:F:514:TRP:HZ2	1:F:578:SER:CB	2.16	0.58
3:F:711:POV:H37	3:F:711:POV:H31B	1.84	0.58
3:F:706:POV:H26	3:F:706:POV:C22	2.32	0.58
1:A:466:ARG:HD2	2:A:703:PO4:P	2.44	0.58
1:A:573:TRP:O	1:A:577:ILE:HG12	2.04	0.57
3:A:708:POV:O22	3:A:708:POV:H24	2.04	0.57
1:F:489:MET:CE	5:F:807:HOH:O	2.53	0.56
3:F:706:POV:O13	3:F:707:POV:H1A	2.05	0.56
1:A:497:SER:OG	1:A:582:THR:CG2	2.52	0.56
3:A:715:POV:H24	3:A:715:POV:O22	2.07	0.55
1:F:285:LEU:HD21	3:F:705:POV:H38A	1.87	0.55
1:A:499:HIS:CD2	1:A:510:PHE:HE2	2.25	0.54
1:A:373:TRP:CD1	3:A:708:POV:C15	2.91	0.54
1:F:587:HIS:H	1:F:587:HIS:CD2	2.25	0.54
1:A:421:LEU:C	1:A:421:LEU:HD23	2.28	0.54
1:F:273:ARG:NH2	2:F:703:PO4:O2	2.41	0.54
1:F:421:LEU:C	1:F:421:LEU:HD23	2.28	0.54
1:F:449:ALA:HB1	3:F:711:POV:H34A	1.89	0.53
1:A:499:HIS:CD2	1:A:510:PHE:CE2	2.96	0.53
1:F:352:TYR:CE1	3:F:705:POV:H217	2.43	0.53
1:F:585:LEU:HD12	1:F:588:SER:H	1.73	0.53
1:A:466:ARG:CD	2:A:703:PO4:O2	2.55	0.53
1:F:270:ARG:HD3	2:F:703:PO4:O4	2.07	0.53
1:A:445:TYR:O	1:A:447:VAL:HG23	2.09	0.53
1:F:373:TRP:CD1	3:F:705:POV:C15	2.92	0.53
1:A:611:ARG:NH1	2:A:702:PO4:O3	2.42	0.52
1:A:255:ALA:HA	1:A:259:LEU:HD23	1.91	0.52
1:A:489:MET:SD	1:A:574:THR:CG2	2.98	0.52
3:A:708:POV:C27	3:A:708:POV:C23	2.85	0.52
1:F:514:TRP:CZ2	1:F:578:SER:CB	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:ALA:HA	1:F:259:LEU:HD23	1.91	0.52
1:A:466:ARG:O	1:A:470:THR:HG23	2.09	0.52
1:A:518:TYR:CD1	1:A:574:THR:HG22	2.45	0.51
1:F:322:PHE:CE2	3:F:706:POV:H26A	2.46	0.51
1:F:619:ASN:CG	1:F:619:ASN:O	2.49	0.51
1:A:422:LYS:O	1:A:422:LYS:HG3	2.11	0.51
1:F:514:TRP:CZ2	1:F:578:SER:OG	2.61	0.51
1:F:422:LYS:HG3	1:F:422:LYS:O	2.11	0.50
1:F:279:ILE:HG22	3:A:705:POV:H216	1.92	0.50
1:A:518:TYR:CD1	1:A:574:THR:CG2	2.95	0.50
3:F:707:POV:C2	3:F:707:POV:C32	2.86	0.50
1:A:497:SER:CB	1:A:582:THR:HG23	2.40	0.50
1:A:429:LEU:HD12	1:A:429:LEU:O	2.11	0.50
1:F:495:LEU:HD13	1:F:510:PHE:CE1	2.47	0.50
1:A:322:PHE:CE2	3:A:709:POV:H26	2.47	0.49
3:F:706:POV:H26	3:F:706:POV:O22	2.13	0.49
1:F:489:MET:HE2	5:F:807:HOH:O	2.11	0.49
1:A:466:ARG:HH11	1:A:476:HIS:CE1	2.31	0.49
4:A:713:CLR:H212	4:A:713:CLR:H121	1.95	0.49
1:F:395:TRP:O	1:F:399:GLN:HG2	2.13	0.48
1:F:466:ARG:HG3	2:F:704:PO4:O2	2.12	0.48
1:A:489:MET:HE1	5:A:807:HOH:O	2.03	0.48
1:A:395:TRP:O	1:A:399:GLN:HG2	2.13	0.48
1:A:319:ILE:HD13	3:A:709:POV:H23	1.96	0.48
1:F:245:ILE:O	1:F:249:ILE:HG12	2.14	0.48
1:A:245:ILE:O	1:A:249:ILE:HG12	2.14	0.48
1:F:499:HIS:CE1	1:F:502:ARG:NH2	2.82	0.47
1:A:499:HIS:CE1	1:A:502:ARG:NH2	2.83	0.47
1:A:512:TYR:O	1:A:515:ILE:CG2	2.62	0.47
4:F:710:CLR:H121	4:F:710:CLR:H212	1.95	0.47
3:A:714:POV:H34A	3:A:714:POV:O32	2.15	0.47
1:F:623:PHE:HZ	2:F:704:PO4:O3	1.97	0.47
1:F:512:TYR:O	1:F:516:VAL:CG2	2.63	0.46
3:A:710:POV:H37A	3:A:710:POV:H310	1.78	0.46
1:F:338:PRO:HB3	3:F:708:POV:H25A	1.96	0.46
1:F:496:TYR:CE1	1:F:507:THR:CG2	2.99	0.46
1:F:495:LEU:HD23	1:F:495:LEU:HA	1.83	0.45
1:F:619:ASN:O	1:F:619:ASN:OD1	2.33	0.45
1:A:468:ARG:C	1:A:468:ARG:HD2	2.37	0.45
1:F:444:THR:C	1:F:446:GLY:H	2.20	0.45
1:A:499:HIS:NE2	1:A:510:PHE:HE2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:709:POV:C21	3:A:709:POV:C25	2.87	0.45
1:F:466:ARG:NH2	1:F:621:GLY:O	2.42	0.45
1:F:579:ILE:HA	1:F:583:THR:OG1	2.17	0.45
1:F:496:TYR:CE1	1:F:507:THR:HG22	2.52	0.44
1:F:452:GLN:NE2	1:F:577:ILE:O	2.51	0.43
1:A:279:ILE:HG22	3:A:707:POV:H216	1.99	0.43
1:A:536:LEU:HD23	1:A:548:ARG:HD3	2.01	0.43
1:F:441:HIS:CD2	1:F:441:HIS:N	2.83	0.43
1:F:444:THR:C	1:F:446:GLY:N	2.72	0.43
1:F:239:LEU:O	1:F:243:ILE:HG13	2.19	0.42
1:F:241:CYS:HB2	3:A:705:POV:H210	2.01	0.42
3:A:708:POV:H11	3:A:708:POV:H13B	1.76	0.42
1:F:306:ASN:H	3:F:705:POV:H14A	1.85	0.42
1:F:573:TRP:CE2	1:F:577:ILE:CD1	2.95	0.42
1:A:239:LEU:O	1:A:243:ILE:HG13	2.19	0.42
1:F:369:LYS:HB3	1:F:369:LYS:HE3	1.86	0.42
1:F:536:LEU:HD23	1:F:548:ARG:HD3	2.01	0.42
1:A:374:LEU:HD13	3:A:708:POV:H37A	2.01	0.42
3:F:705:POV:H11	3:F:705:POV:H13B	1.79	0.42
1:A:500:LYS:HE3	1:A:500:LYS:HB3	1.89	0.41
1:F:533:ASP:OD1	1:F:611:ARG:NH1	2.53	0.41
1:F:285:LEU:HD21	3:F:705:POV:H35A	2.03	0.41
3:A:712:POV:H33	3:A:712:POV:H36	1.47	0.41
1:F:377:LEU:HD23	1:F:396:LEU:HD22	2.01	0.41
1:A:322:PHE:CD2	3:A:709:POV:H24	2.55	0.41
1:A:533:ASP:OD1	1:A:611:ARG:NH1	2.53	0.41
1:A:412:TYR:CE1	1:A:440:CYS:O	2.74	0.41
1:F:322:PHE:CD2	3:F:706:POV:H26A	2.56	0.41
3:F:706:POV:O22	3:F:706:POV:C26	2.69	0.41
1:A:377:LEU:HD23	1:A:396:LEU:HD22	2.01	0.41
1:F:491:THR:O	1:F:491:THR:HG22	2.21	0.41
1:A:410:LEU:O	1:A:414:ILE:HG13	2.21	0.41
1:A:367:TYR:O	1:A:371:ARG:HG3	2.21	0.41
1:F:474:PHE:HA	1:F:475:PRO:HA	1.90	0.40
1:A:492:PHE:HE2	1:A:517:PHE:CD2	2.39	0.40
1:A:515:ILE:HG23	1:A:516:VAL:N	2.36	0.40
1:A:468:ARG:HD2	1:A:468:ARG:O	2.21	0.40
1:A:518:TYR:OH	1:A:575:ILE:HG23	2.21	0.40
1:F:283:PHE:HE1	3:A:705:POV:H28A	1.85	0.40
3:A:708:POV:H31G	3:A:708:POV:H31D	1.68	0.40
1:F:319:ILE:HD13	1:F:319:ILE:HA	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:429:LEU:O	1:F:429:LEU:HD12	2.21	0.40
1:A:597:ALA:HB3	1:A:598:PRO:HD3	2.04	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	389/468 (83%)	374 (96%)	15 (4%)	0	100	100
1	F	389/468 (83%)	371 (95%)	17 (4%)	1 (0%)	37	55
All	All	778/936 (83%)	745 (96%)	32 (4%)	1 (0%)	50	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	619	ASN

### 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	334/417 (80%)	331 (99%)	3 (1%)	75	88
1	F	334/417 (80%)	332 (99%)	2 (1%)	84	92
All	All	668/834 (80%)	663 (99%)	5 (1%)	80	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	394	PHE
1	F	524	TYR
1	A	394	PHE
1	A	524	TYR
1	A	576	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	441	HIS
1	F	587	HIS
1	A	313	HIS
1	A	452	GLN
1	A	476	HIS
1	A	576	GLN
1	A	587	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](#)

28 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	PO4	A	704	-	4,4,4	1.01	0	6,6,6	0.60	0
3	POV	A	714	-	15,15,51	1.72	2 (13%)	15,15,59	1.23	2 (13%)
3	POV	F	706	-	28,28,51	1.23	2 (7%)	34,36,59	1.55	5 (14%)
4	CLR	F	710	-	31,31,31	1.04	2 (6%)	48,48,48	1.41	9 (18%)
3	POV	F	711	-	15,15,51	0.86	1 (6%)	15,15,59	1.26	1 (6%)
3	POV	A	715	-	10,10,51	1.04	1 (10%)	10,10,59	1.18	1 (10%)
3	POV	F	709	-	15,15,51	1.73	2 (13%)	15,15,59	1.16	0
3	POV	F	708	-	17,17,51	1.15	2 (11%)	17,17,59	1.29	2 (11%)
3	POV	F	712	-	13,13,51	1.83	2 (15%)	13,13,59	1.32	1 (7%)
3	POV	A	706	-	17,17,51	1.17	2 (11%)	17,17,59	1.44	4 (23%)
3	POV	A	712	-	15,15,51	1.72	2 (13%)	15,15,59	1.23	1 (6%)
2	PO4	F	704	-	4,4,4	2.96	4 (100%)	6,6,6	0.42	0
3	POV	F	705	-	51,51,51	0.96	2 (3%)	57,59,59	1.21	6 (10%)
2	PO4	A	702	-	4,4,4	0.79	0	6,6,6	0.48	0
2	PO4	F	702	-	4,4,4	1.04	0	6,6,6	0.36	0
4	CLR	A	713	-	31,31,31	1.04	2 (6%)	48,48,48	1.42	9 (18%)
3	POV	A	710	-	16,16,51	0.88	1 (6%)	16,16,59	1.35	1 (6%)
3	POV	A	705	-	38,38,51	1.00	2 (5%)	42,43,59	1.29	5 (11%)
3	POV	A	711	-	17,17,51	1.18	2 (11%)	17,17,59	1.33	2 (11%)
3	POV	A	708	-	51,51,51	0.92	2 (3%)	57,59,59	1.29	8 (14%)
3	POV	F	707	-	16,16,51	0.87	1 (6%)	16,16,59	1.26	2 (12%)
3	POV	A	707	-	38,38,51	0.99	2 (5%)	42,43,59	1.24	6 (14%)
2	PO4	A	703	-	4,4,4	0.98	0	6,6,6	0.43	0
2	PO4	F	703	-	4,4,4	2.96	4 (100%)	6,6,6	0.42	0
2	PO4	F	701	-	4,4,4	0.96	0	6,6,6	0.47	0
3	POV	A	709	-	28,28,51	1.26	2 (7%)	34,36,59	1.45	4 (11%)
3	POV	F	713	-	17,17,51	1.17	2 (11%)	17,17,59	1.44	4 (23%)
2	PO4	A	701	-	4,4,4	4.49	1 (25%)	6,6,6	0.86	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	POV	A	714	-	-	6/13/13/55	-
3	POV	F	706	-	-	14/32/32/55	-
4	CLR	F	710	-	-	2/10/68/68	0/4/4/4
3	POV	F	711	-	-	6/13/13/55	-
3	POV	A	715	-	-	6/8/8/55	-
3	POV	F	709	-	-	8/13/13/55	-
3	POV	F	708	-	-	8/15/15/55	-
3	POV	F	712	-	-	9/11/11/55	-
3	POV	A	706	-	-	8/15/15/55	-
3	POV	A	712	-	-	8/13/13/55	-
3	POV	F	705	-	-	17/55/55/55	-
4	CLR	A	713	-	-	2/10/68/68	0/4/4/4
3	POV	A	710	-	-	7/15/15/55	-
3	POV	A	705	-	-	13/40/40/55	-
3	POV	A	711	-	-	7/15/15/55	-
3	POV	A	708	-	-	21/55/55/55	-
3	POV	F	707	-	-	12/15/15/55	-
3	POV	A	707	-	-	13/40/40/55	-
3	POV	A	709	-	-	9/32/32/55	-
3	POV	F	713	-	-	8/15/15/55	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PO4	P-O2	-8.81	1.28	1.54
3	A	714	POV	O32-C31	5.46	1.40	1.22
3	F	709	POV	O32-C31	5.45	1.40	1.22
3	F	712	POV	O32-C31	5.45	1.40	1.22
3	A	712	POV	O32-C31	5.33	1.39	1.22
2	F	704	PO4	P-O1	4.52	1.61	1.50
2	F	703	PO4	P-O1	4.49	1.61	1.50
3	F	705	POV	O21-C21	4.01	1.45	1.34
3	A	709	POV	O21-C21	4.00	1.45	1.34
3	A	709	POV	O31-C31	3.99	1.45	1.33
3	F	706	POV	O31-C31	3.96	1.44	1.33
3	F	705	POV	O31-C31	3.94	1.44	1.33
3	A	705	POV	O21-C21	3.92	1.45	1.34
3	A	708	POV	O21-C21	3.91	1.45	1.34
3	A	712	POV	O31-C31	-3.81	1.17	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	706	POV	O21-C21	3.78	1.45	1.34
3	A	707	POV	O31-C31	3.76	1.44	1.33
3	A	705	POV	O31-C31	3.66	1.44	1.33
3	A	707	POV	O21-C21	3.66	1.44	1.34
3	A	711	POV	C29-C210	3.65	1.52	1.31
3	F	708	POV	C29-C210	3.63	1.52	1.31
3	A	706	POV	C29-C210	3.61	1.52	1.31
3	F	713	POV	C29-C210	3.60	1.52	1.31
3	F	709	POV	O31-C31	-3.59	1.18	1.30
3	A	714	POV	O31-C31	-3.53	1.18	1.30
3	A	708	POV	O31-C31	3.51	1.43	1.33
3	F	712	POV	O31-C31	-3.51	1.18	1.30
3	F	711	POV	O31-C31	2.85	1.40	1.30
3	A	715	POV	O21-C21	2.79	1.40	1.30
3	F	713	POV	O21-C21	2.73	1.39	1.30
3	A	706	POV	O21-C21	2.72	1.39	1.30
3	A	711	POV	O21-C21	2.57	1.39	1.30
3	F	708	POV	O21-C21	2.50	1.39	1.30
3	A	710	POV	O31-C31	2.40	1.40	1.33
4	F	710	CLR	C10-C9	-2.31	1.52	1.56
2	F	704	PO4	P-O3	2.30	1.61	1.54
2	F	703	PO4	P-O2	2.30	1.61	1.54
2	F	703	PO4	P-O3	2.30	1.61	1.54
2	F	704	PO4	P-O2	2.27	1.61	1.54
4	A	713	CLR	C10-C9	-2.26	1.52	1.56
3	F	707	POV	O31-C31	2.24	1.39	1.33
4	A	713	CLR	C13-C14	-2.12	1.51	1.55
4	F	710	CLR	C13-C14	-2.09	1.51	1.55
2	F	703	PO4	P-O4	-2.05	1.48	1.54
2	F	704	PO4	P-O4	-2.02	1.48	1.54

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	706	POV	O21-C21-C22	5.42	123.19	111.50
3	A	709	POV	O21-C21-C22	4.75	121.73	111.50
3	F	705	POV	O21-C21-C22	4.29	120.76	111.50
3	A	705	POV	O21-C21-C22	4.25	120.67	111.50
3	A	708	POV	O21-C21-C22	3.90	119.91	111.50
3	A	709	POV	C3-C2-C1	-3.74	102.93	111.79
3	F	706	POV	O31-C31-C32	3.49	120.52	111.38
3	A	709	POV	O31-C31-C32	3.39	120.28	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	705	POV	C3-C2-C1	-3.33	103.92	111.79
4	A	713	CLR	C13-C17-C20	-3.28	114.36	119.49
4	F	710	CLR	C13-C17-C20	-3.27	114.36	119.49
3	A	710	POV	O31-C31-C32	3.20	121.94	111.91
3	F	706	POV	C3-C2-C1	-3.15	104.33	111.79
3	A	708	POV	O31-C31-C32	3.08	121.57	111.91
3	A	707	POV	O21-C21-C22	3.05	118.07	111.50
3	A	707	POV	O31-C31-C32	3.05	121.47	111.91
4	A	713	CLR	C4-C5-C6	-2.92	116.40	120.61
3	A	705	POV	O31-C31-C32	2.90	121.00	111.91
4	F	710	CLR	C4-C5-C6	-2.88	116.45	120.61
3	A	708	POV	O31-C31-O32	-2.81	116.51	123.59
3	F	707	POV	O31-C31-C32	2.76	120.56	111.91
3	A	708	POV	C11-C12-N	-2.75	106.60	115.78
3	A	708	POV	C3-C2-C1	-2.67	105.46	111.79
4	F	710	CLR	C4-C5-C10	2.67	119.97	116.42
4	A	713	CLR	C4-C5-C10	2.66	119.95	116.42
3	F	705	POV	C11-C12-N	-2.66	106.91	115.78
3	F	713	POV	C23-C22-C21	-2.63	107.86	114.47
3	A	706	POV	C23-C22-C21	-2.59	107.95	114.47
3	F	711	POV	C33-C32-C31	-2.58	107.97	114.47
4	F	710	CLR	C11-C12-C13	-2.57	108.38	112.78
4	A	713	CLR	C11-C12-C13	-2.53	108.44	112.78
3	F	706	POV	O21-C21-O22	-2.51	117.65	123.70
3	A	712	POV	C33-C32-C31	-2.47	108.24	114.47
3	A	707	POV	O13-P-O14	2.47	120.34	110.68
3	A	707	POV	O31-C31-O32	-2.45	117.40	123.59
4	F	710	CLR	C2-C3-C4	-2.43	106.97	110.31
4	A	713	CLR	C2-C3-C4	-2.43	106.97	110.31
3	A	705	POV	O31-C31-O32	-2.41	117.50	123.59
4	F	710	CLR	C7-C8-C14	-2.40	107.43	110.91
4	A	713	CLR	C19-C10-C9	-2.40	108.82	111.68
3	A	707	POV	O12-P-O11	-2.39	100.38	106.73
4	A	713	CLR	C7-C8-C14	-2.38	107.45	110.91
3	F	712	POV	C33-C32-C31	-2.35	108.55	114.47
4	F	710	CLR	C19-C10-C9	-2.35	108.88	111.68
3	A	705	POV	O13-P-O14	2.31	119.72	110.68
3	A	706	POV	C211-C210-C29	-2.28	107.25	124.73
3	F	713	POV	C211-C210-C29	-2.27	107.27	124.73
3	A	714	POV	C33-C32-C31	-2.27	108.75	114.47
4	A	713	CLR	C3-C4-C5	-2.26	108.18	112.03
4	F	710	CLR	C3-C4-C5	-2.26	108.19	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	708	POV	C2-O21-C21	-2.22	112.32	117.79
3	F	705	POV	O31-C31-C32	2.17	118.72	111.91
3	F	705	POV	O31-C31-O32	-2.17	118.11	123.59
3	A	705	POV	O21-C21-O22	-2.14	118.54	123.70
3	F	706	POV	O31-C31-O32	-2.14	118.20	123.59
3	F	705	POV	C2-O21-C21	-2.12	112.56	117.79
4	A	713	CLR	C19-C10-C5	2.12	111.77	108.34
3	A	711	POV	C23-C22-C21	-2.11	109.15	114.47
3	A	707	POV	C23-C22-C21	-2.11	105.96	113.62
3	A	706	POV	C28-C29-C210	-2.10	108.65	124.73
3	F	708	POV	C23-C22-C21	-2.09	109.19	114.47
3	A	708	POV	P-O11-C1	-2.09	109.41	121.68
3	F	713	POV	C28-C29-C210	-2.09	108.69	124.73
3	A	709	POV	O31-C31-O32	-2.08	118.33	123.59
3	A	711	POV	C28-C29-C210	-2.07	108.81	124.73
4	F	710	CLR	C19-C10-C5	2.07	111.69	108.34
3	A	708	POV	C24-C23-C22	-2.07	105.75	113.19
3	F	707	POV	C3-C2-C1	-2.05	109.48	113.95
3	A	714	POV	O31-C31-C32	2.05	120.63	114.03
3	F	708	POV	C28-C29-C210	-2.05	108.99	124.73
3	A	706	POV	O21-C21-C22	2.01	120.49	114.03
3	F	713	POV	O21-C21-C22	2.01	120.48	114.03
3	A	715	POV	O21-C21-C22	2.00	120.47	114.03

There are no chirality outliers.

All (184) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	706	POV	O12-C11-C12-N
3	F	707	POV	O11-C1-C2-C3
3	A	705	POV	C1-O11-P-O12
3	A	705	POV	C1-O11-P-O13
3	A	705	POV	C1-O11-P-O14
3	A	707	POV	C1-O11-P-O12
3	A	707	POV	C1-O11-P-O13
3	A	708	POV	C11-O12-P-O11
3	A	708	POV	C11-O12-P-O14
3	A	709	POV	O12-C11-C12-N
3	A	710	POV	O11-C1-C2-C3
3	F	707	POV	O32-C31-O31-C3
3	F	707	POV	C32-C31-O31-C3
3	F	707	POV	C2-C3-O31-C31

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Mol	Chain	Res	Type	Atoms
4	F	710	CLR	C21-C20-C22-C23
4	A	713	CLR	C21-C20-C22-C23
3	F	708	POV	C211-C210-C29-C28
3	A	711	POV	C211-C210-C29-C28
3	F	706	POV	C21-C22-C23-C24
3	F	711	POV	C37-C38-C39-C310
3	A	710	POV	C37-C38-C39-C310
3	A	712	POV	C33-C34-C35-C36
3	F	705	POV	C31-C32-C33-C34
3	A	715	POV	C25-C26-C27-C28
3	F	705	POV	C35-C36-C37-C38
3	F	706	POV	C23-C24-C25-C26
3	A	708	POV	C33-C34-C35-C36
3	A	709	POV	C22-C21-O21-C2
3	A	708	POV	C32-C31-O31-C3
3	A	708	POV	C35-C36-C37-C38
3	A	709	POV	O22-C21-O21-C2
3	F	708	POV	C21-C22-C23-C24
3	A	706	POV	C21-C22-C23-C24
3	F	713	POV	C21-C22-C23-C24
3	A	711	POV	C21-C22-C23-C24
3	A	708	POV	O32-C31-O31-C3
3	F	705	POV	C11-O12-P-O11
3	F	708	POV	C24-C25-C26-C27
3	F	709	POV	C35-C36-C37-C38
3	F	712	POV	C33-C34-C35-C36
3	F	712	POV	C35-C36-C37-C38
3	A	715	POV	C23-C24-C25-C26
3	A	711	POV	C24-C25-C26-C27
3	A	712	POV	C37-C38-C39-C310
3	A	714	POV	C32-C33-C34-C35
3	F	712	POV	C32-C33-C34-C35
3	F	713	POV	C22-C23-C24-C25
3	A	705	POV	O22-C21-O21-C2
3	A	705	POV	C22-C21-O21-C2
3	A	706	POV	C22-C23-C24-C25
3	F	713	POV	C26-C27-C28-C29
3	A	706	POV	C26-C27-C28-C29
3	A	705	POV	C31-C32-C33-C34
3	F	705	POV	C22-C23-C24-C25
3	A	714	POV	C35-C36-C37-C38
3	A	715	POV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
3	F	705	POV	C21-C22-C23-C24
3	F	707	POV	C33-C34-C35-C36
3	F	707	POV	C36-C37-C38-C39
3	F	709	POV	C37-C38-C39-C310
3	F	709	POV	C31-C32-C33-C34
3	A	707	POV	C31-C32-C33-C34
3	F	705	POV	C32-C31-O31-C3
3	F	705	POV	C210-C211-C212-C213
3	A	708	POV	C210-C211-C212-C213
3	F	711	POV	C35-C36-C37-C38
3	F	711	POV	C32-C33-C34-C35
3	A	710	POV	C35-C36-C37-C38
3	A	712	POV	C36-C37-C38-C39
3	F	707	POV	C34-C35-C36-C37
3	A	706	POV	C23-C24-C25-C26
3	F	713	POV	C23-C24-C25-C26
3	A	711	POV	C25-C26-C27-C28
3	A	708	POV	C26-C27-C28-C29
3	F	706	POV	C24-C25-C26-C27
3	F	705	POV	C34-C35-C36-C37
3	F	708	POV	C22-C23-C24-C25
3	F	705	POV	O32-C31-O31-C3
3	F	712	POV	C39-C310-C311-C312
3	A	714	POV	C311-C312-C313-C314
3	A	707	POV	C212-C213-C214-C215
3	F	709	POV	C33-C34-C35-C36
3	F	713	POV	C210-C211-C212-C213
3	F	709	POV	C310-C311-C312-C313
3	A	708	POV	C211-C212-C213-C214
3	F	713	POV	C24-C25-C26-C27
3	A	706	POV	C24-C25-C26-C27
3	A	707	POV	C1-O11-P-O14
3	A	705	POV	C212-C213-C214-C215
3	A	715	POV	C26-C27-C28-C29
3	A	708	POV	C212-C213-C214-C215
3	A	709	POV	C24-C25-C26-C27
3	A	706	POV	C210-C211-C212-C213
3	A	705	POV	O21-C2-C3-O31
3	F	707	POV	C37-C38-C39-C310
3	A	705	POV	C214-C215-C216-C217
3	A	712	POV	C311-C310-C39-C38
3	F	713	POV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
3	A	706	POV	C25-C26-C27-C28
3	A	712	POV	C32-C33-C34-C35
3	A	711	POV	C22-C23-C24-C25
3	F	706	POV	O11-C1-C2-C3
3	A	709	POV	O11-C1-C2-C3
3	F	706	POV	C22-C23-C24-C25
3	A	705	POV	C1-C2-C3-O31
3	A	708	POV	C1-C2-C3-O31
4	F	710	CLR	C17-C20-C22-C23
3	F	713	POV	C211-C210-C29-C28
3	A	706	POV	C211-C210-C29-C28
3	A	708	POV	C312-C313-C314-C315
3	F	706	POV	O11-C1-C2-O21
4	A	713	CLR	C17-C20-C22-C23
3	F	712	POV	C311-C310-C39-C38
3	A	707	POV	O21-C2-C3-O31
3	F	705	POV	C311-C312-C313-C314
3	A	710	POV	C1-C2-C3-O31
3	A	708	POV	C214-C215-C216-C217
3	F	712	POV	C31-C32-C33-C34
3	F	706	POV	C22-C21-O21-C2
3	A	705	POV	C21-C22-C23-C24
3	A	712	POV	C35-C36-C37-C38
3	A	707	POV	C210-C211-C212-C213
3	A	714	POV	C37-C38-C39-C310
3	A	709	POV	O11-C1-C2-O21
3	F	706	POV	O22-C21-O21-C2
3	A	707	POV	O22-C21-O21-C2
3	A	710	POV	C34-C35-C36-C37
3	A	708	POV	O21-C2-C3-O31
3	F	711	POV	C33-C34-C35-C36
3	A	708	POV	C23-C24-C25-C26
3	F	705	POV	C11-O12-P-O14
3	A	707	POV	C22-C21-O21-C2
3	A	708	POV	C313-C314-C315-C316
3	F	709	POV	C34-C35-C36-C37
3	F	708	POV	C27-C28-C29-C210
3	F	705	POV	C1-O11-P-O12
3	F	706	POV	C11-O12-P-O11
3	A	708	POV	C1-O11-P-O12
3	A	709	POV	C11-O12-P-O11
3	F	705	POV	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
3	F	705	POV	C213-C214-C215-C216
3	A	711	POV	C29-C210-C211-C212
3	A	707	POV	C22-C23-C24-C25
3	F	707	POV	C35-C36-C37-C38
3	A	708	POV	C39-C310-C311-C312
3	A	707	POV	O21-C21-C22-C23
3	F	706	POV	C1-C2-C3-O31
3	A	709	POV	O31-C31-C32-C33
3	A	707	POV	C29-C210-C211-C212
3	A	710	POV	O32-C31-O31-C3
3	F	707	POV	C1-C2-C3-O31
3	A	707	POV	C1-C2-C3-O31
3	F	705	POV	C25-C26-C27-C28
3	A	712	POV	C39-C310-C311-C312
3	A	715	POV	O21-C21-C22-C23
3	F	712	POV	C37-C38-C39-C310
3	F	709	POV	O31-C31-C32-C33
3	F	712	POV	O31-C31-C32-C33
3	A	708	POV	C215-C216-C217-C218
3	F	708	POV	C25-C26-C27-C28
3	A	715	POV	O22-C21-C22-C23
3	A	705	POV	C27-C28-C29-C210
3	F	706	POV	O21-C21-C22-C23
3	F	711	POV	O32-C31-C32-C33
3	F	706	POV	O21-C2-C3-O31
3	F	705	POV	C29-C210-C211-C212
3	F	708	POV	O22-C21-C22-C23
3	F	709	POV	O32-C31-C32-C33
3	A	710	POV	C32-C31-O31-C3
3	F	712	POV	O32-C31-C32-C33
3	A	708	POV	C29-C210-C211-C212
3	F	706	POV	O22-C21-C22-C23
3	F	711	POV	O31-C31-C32-C33
3	A	714	POV	O31-C31-C32-C33
3	F	708	POV	O21-C21-C22-C23
3	F	707	POV	O31-C31-C32-C33
3	F	705	POV	C37-C38-C39-C310
3	A	711	POV	C27-C28-C29-C210
3	A	709	POV	O21-C21-C22-C23
3	A	705	POV	C211-C212-C213-C214
3	A	712	POV	O31-C31-C32-C33
3	A	714	POV	O32-C31-C32-C33

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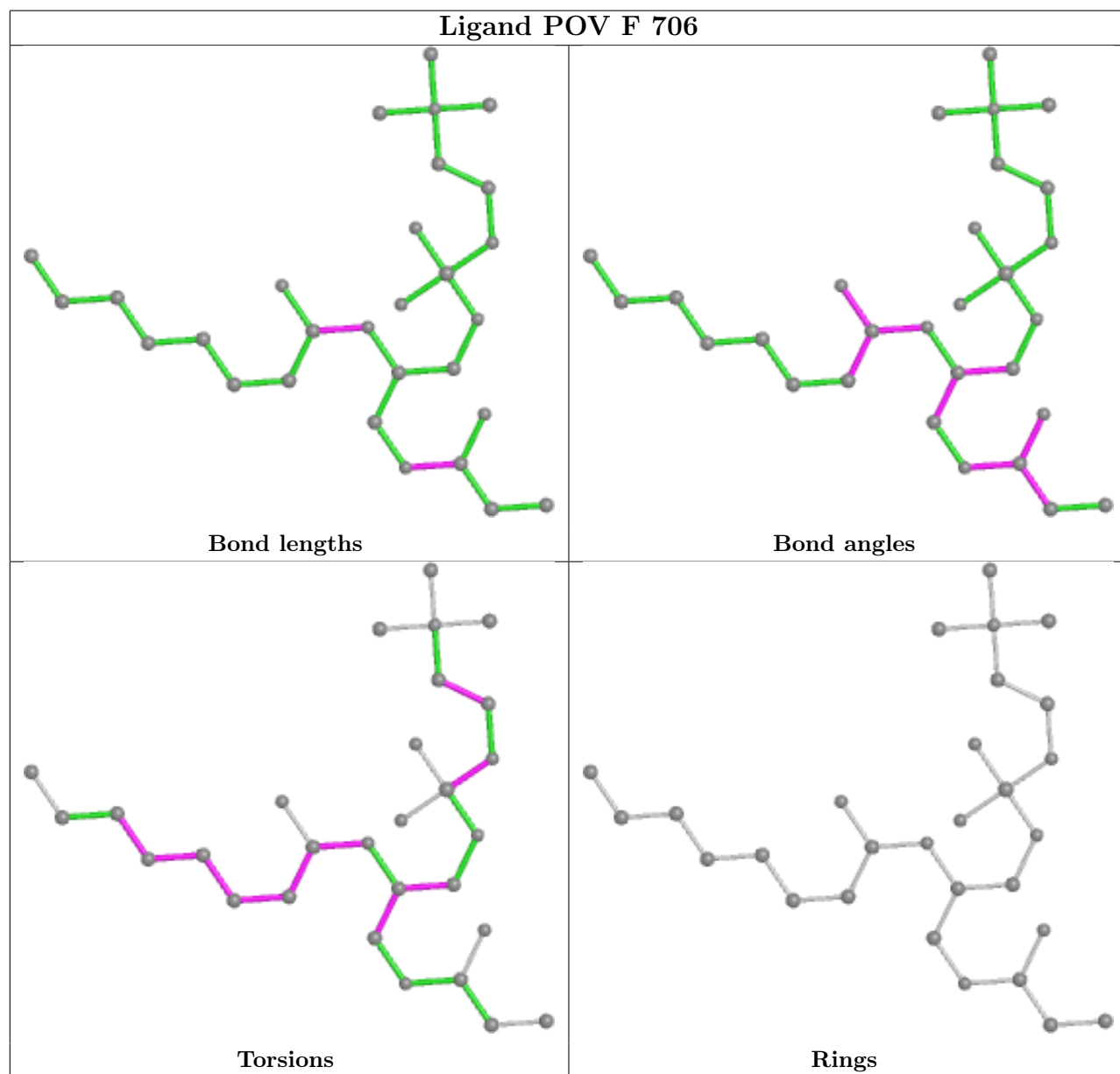
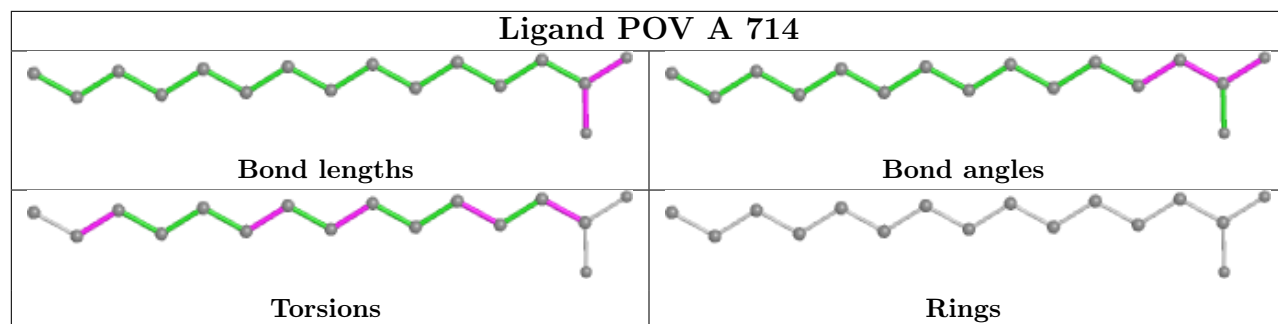
Mol	Chain	Res	Type	Atoms
3	A	708	POV	C27-C28-C29-C210
3	F	707	POV	O32-C31-C32-C33

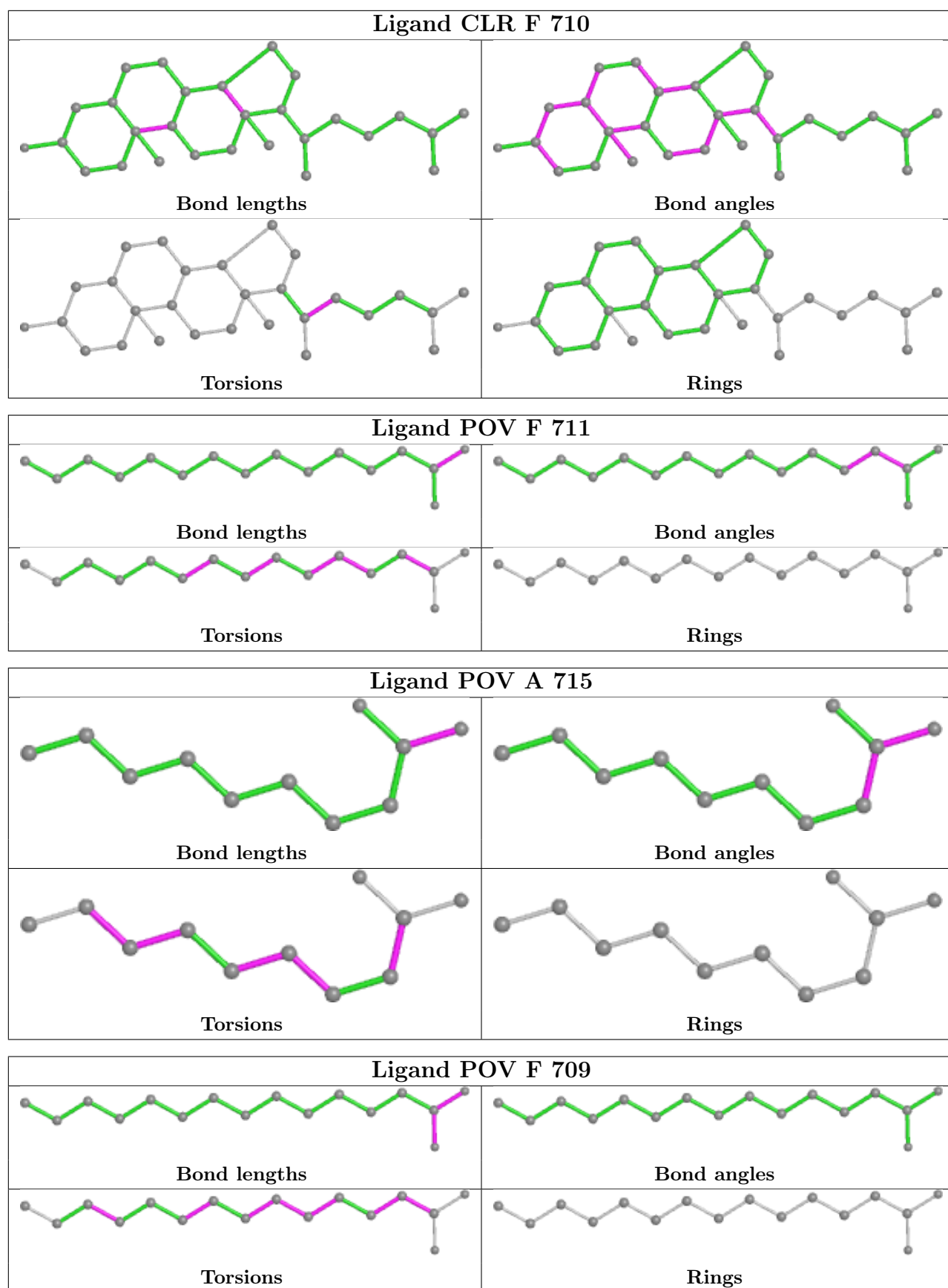
There are no ring outliers.

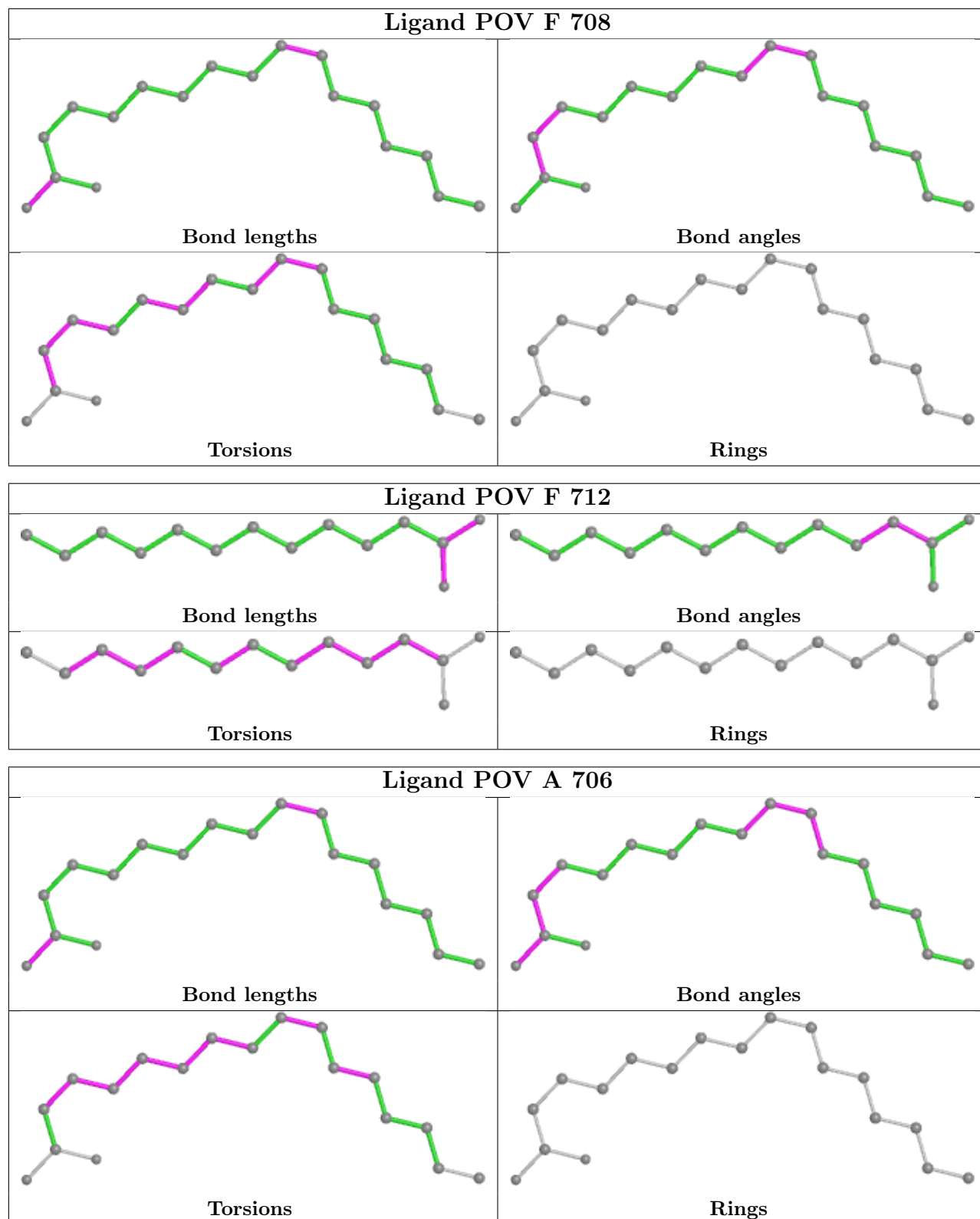
20 monomers are involved in 62 short contacts:

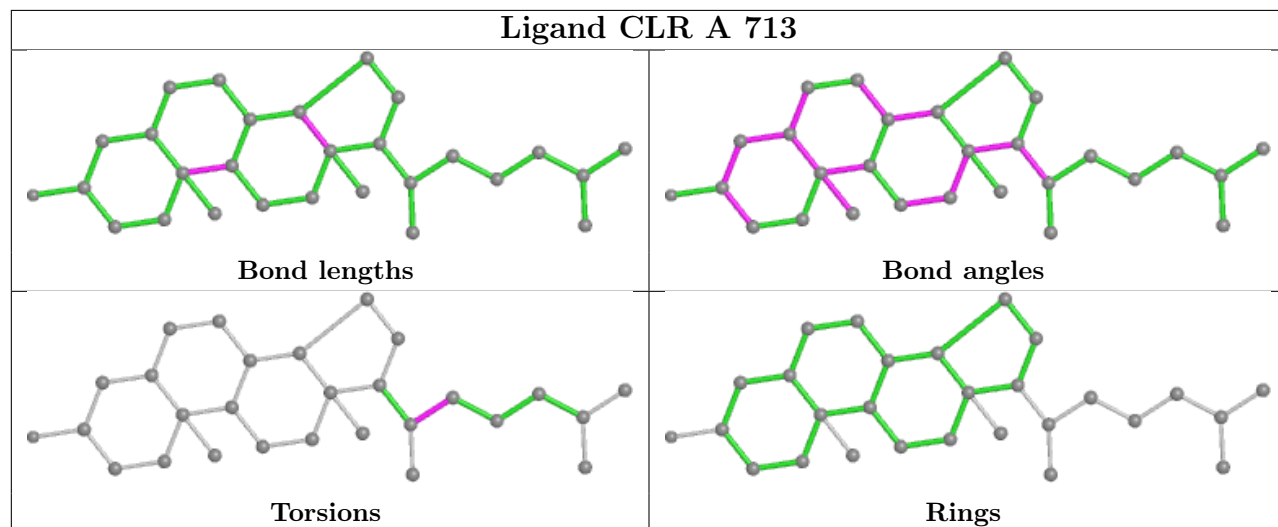
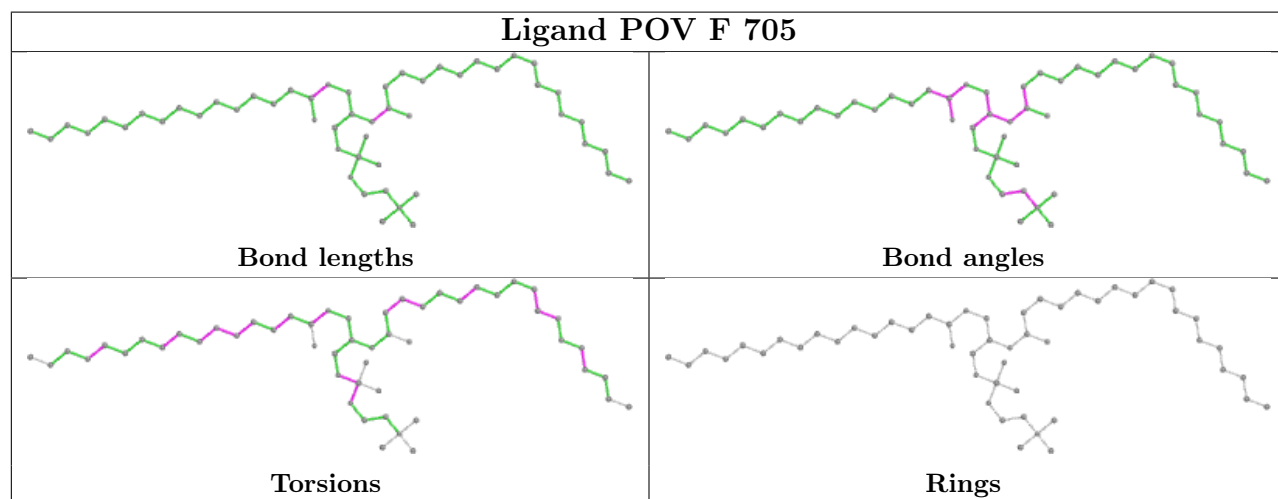
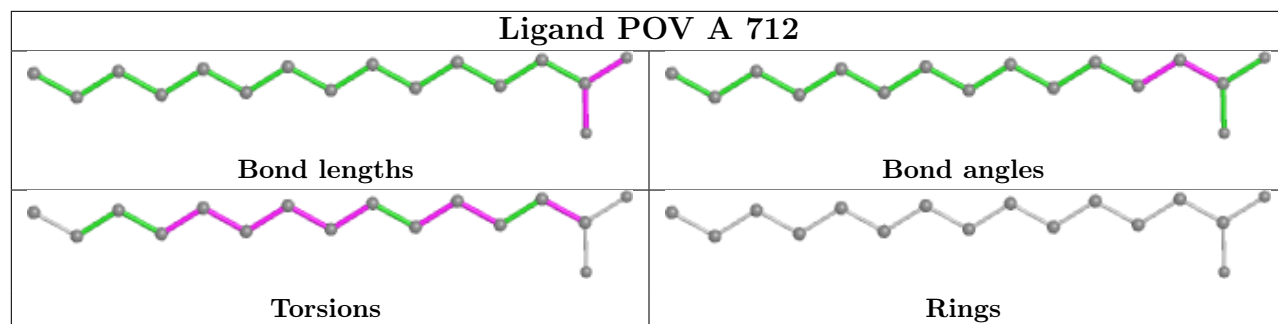
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	704	PO4	1	0
3	A	714	POV	1	0
3	F	706	POV	6	0
4	F	710	CLR	1	0
3	F	711	POV	4	0
3	A	715	POV	1	0
3	F	708	POV	1	0
3	A	712	POV	1	0
2	F	704	PO4	2	0
3	F	705	POV	11	0
2	A	702	PO4	1	0
4	A	713	CLR	1	0
3	A	710	POV	2	0
3	A	705	POV	3	0
3	A	708	POV	13	0
3	F	707	POV	2	0
3	A	707	POV	1	0
2	A	703	PO4	3	0
2	F	703	PO4	2	0
3	A	709	POV	6	0

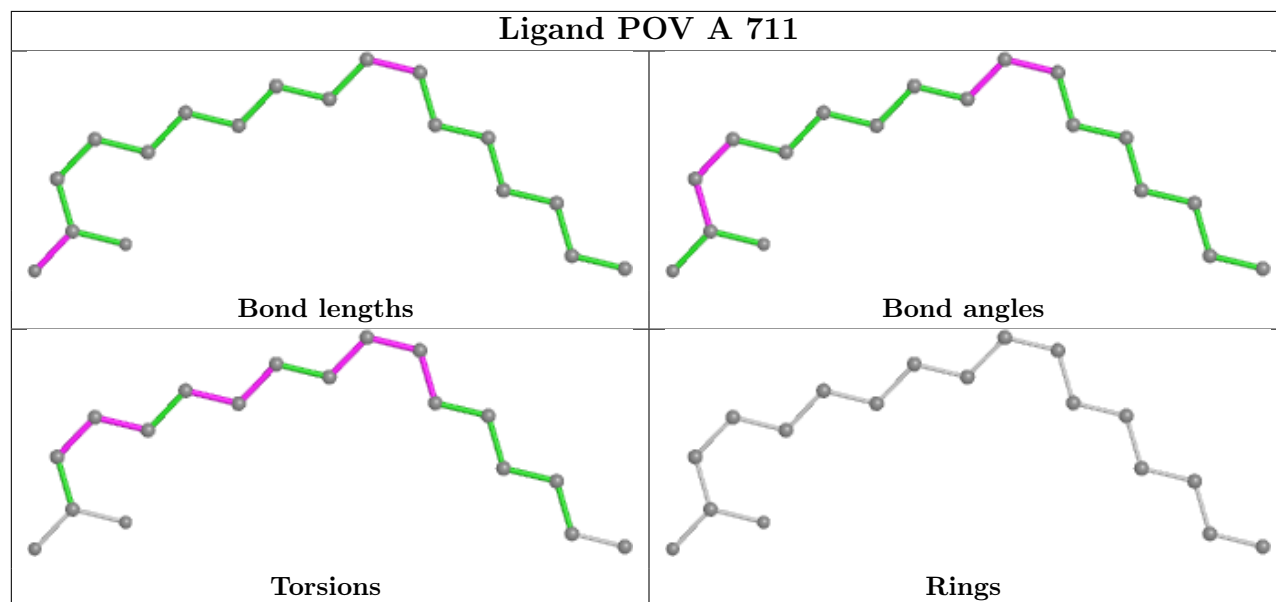
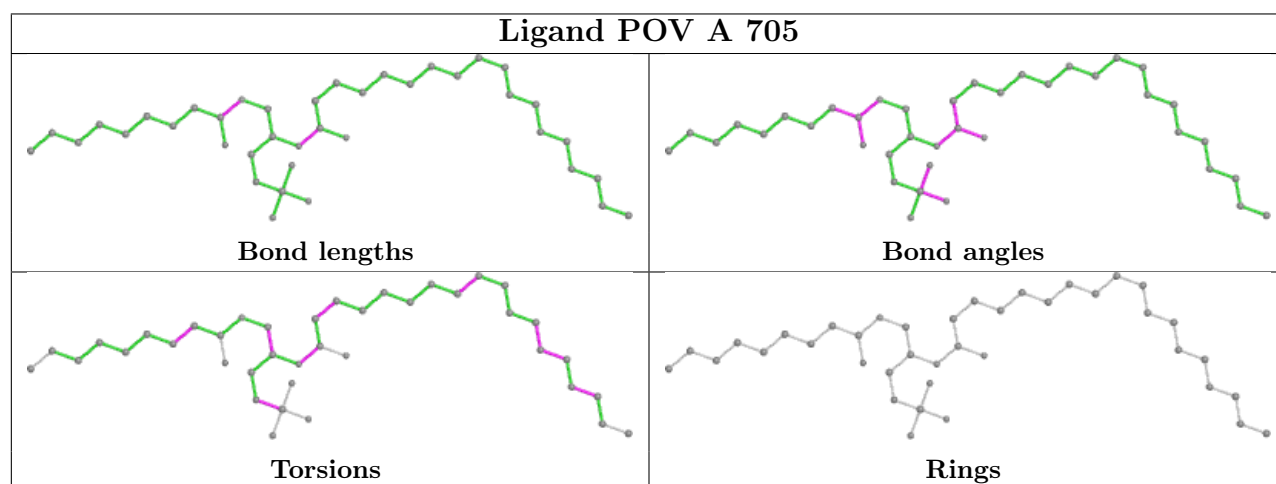
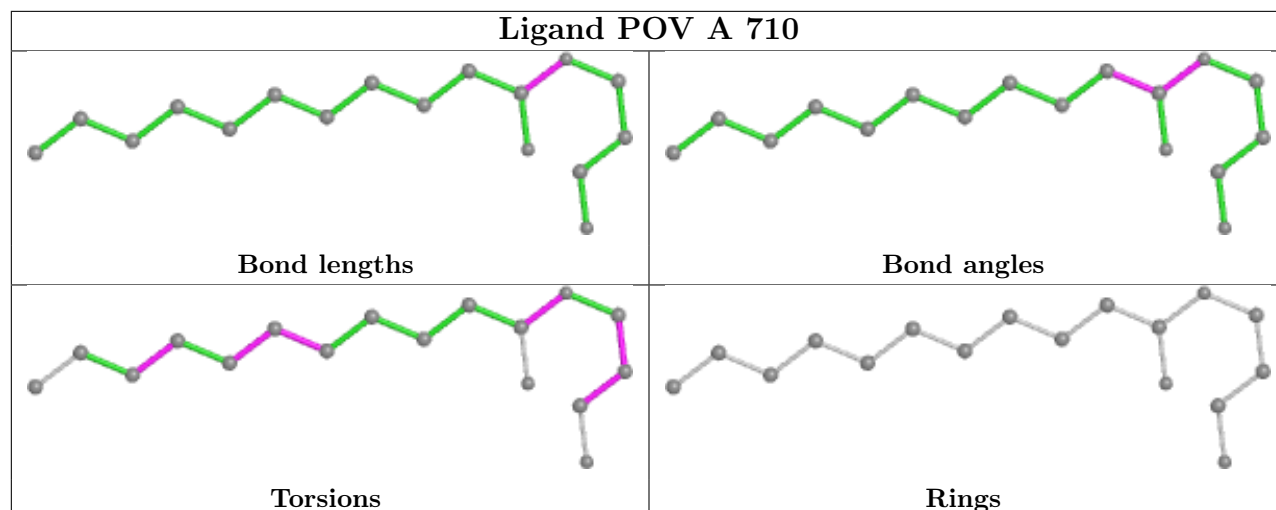
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

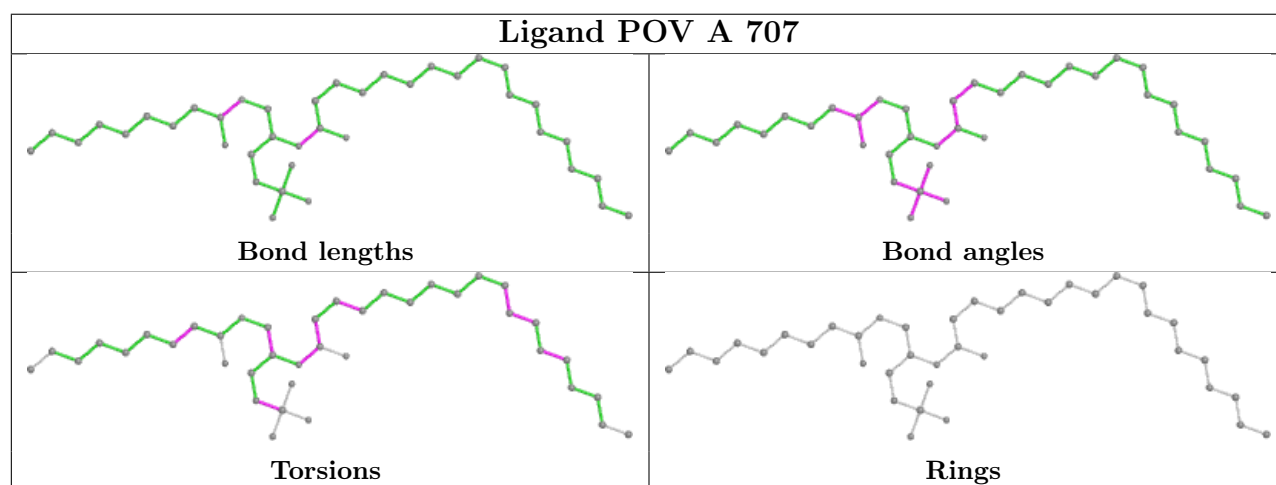
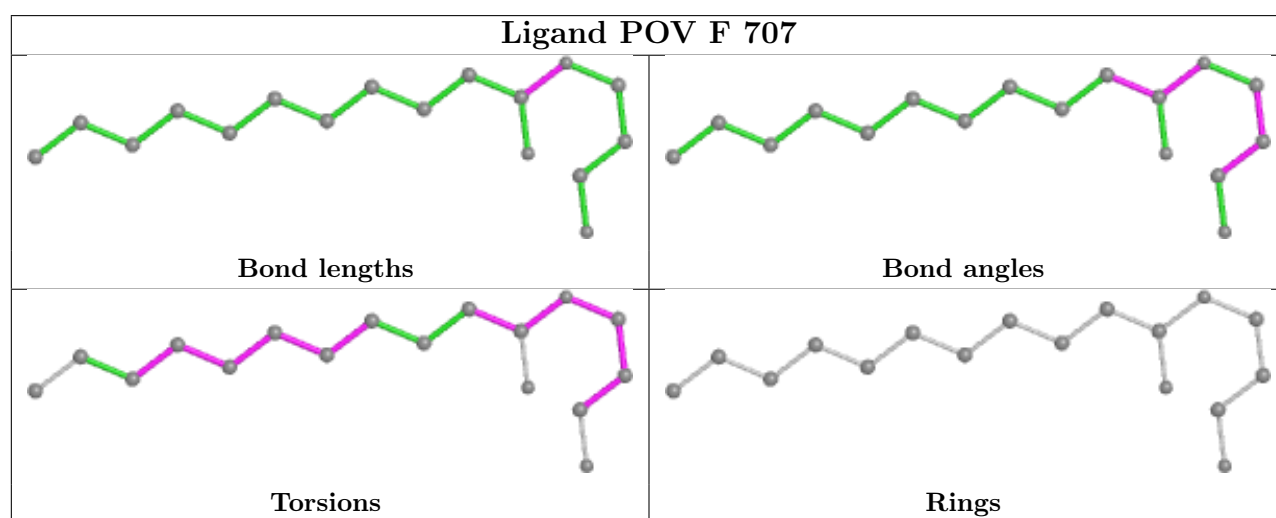
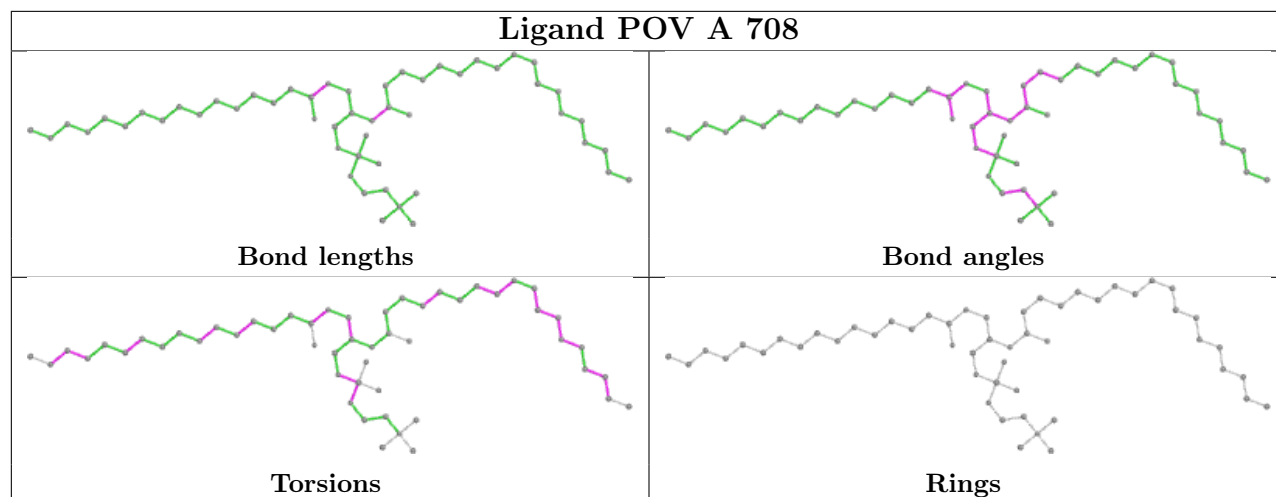


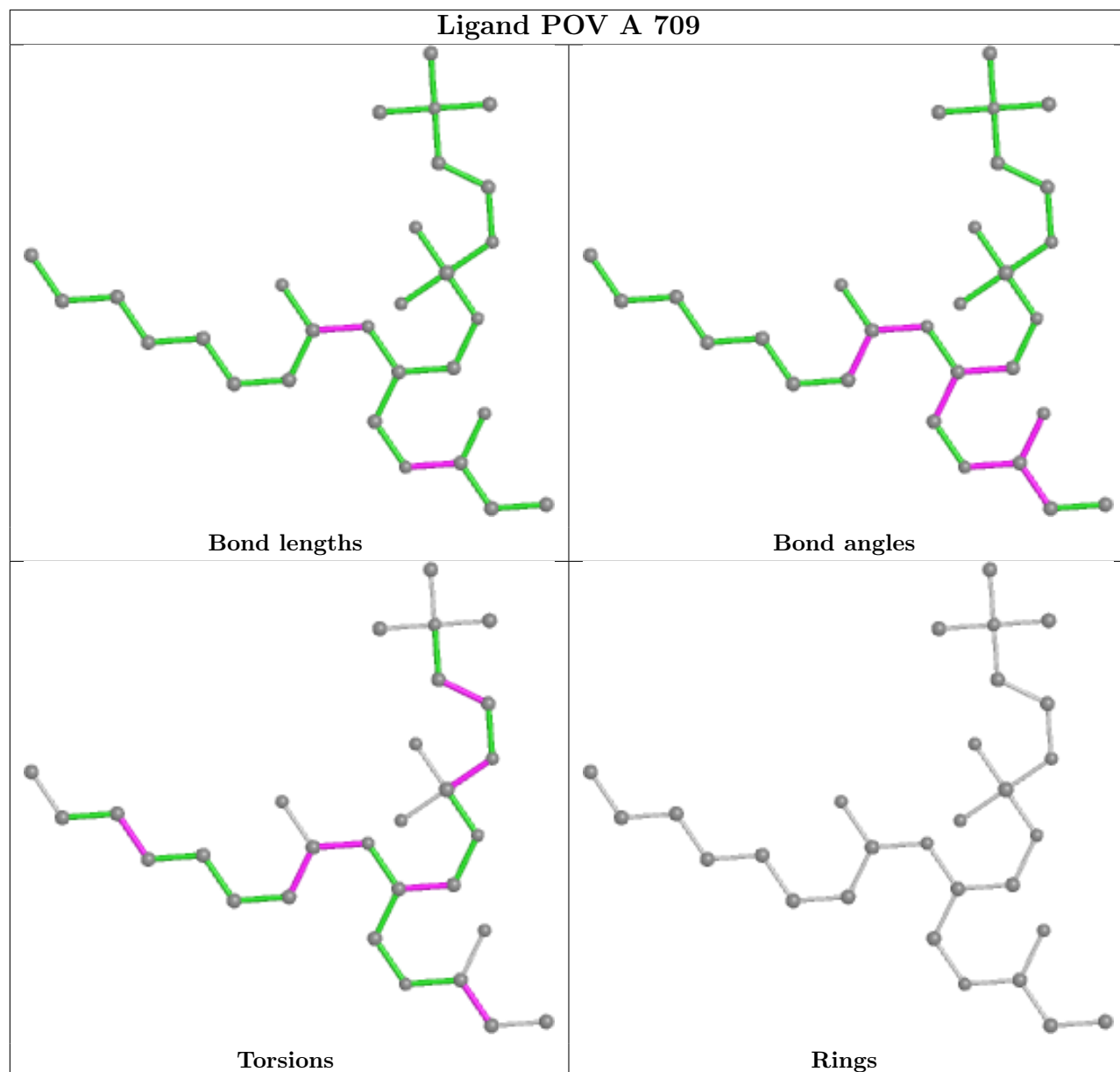




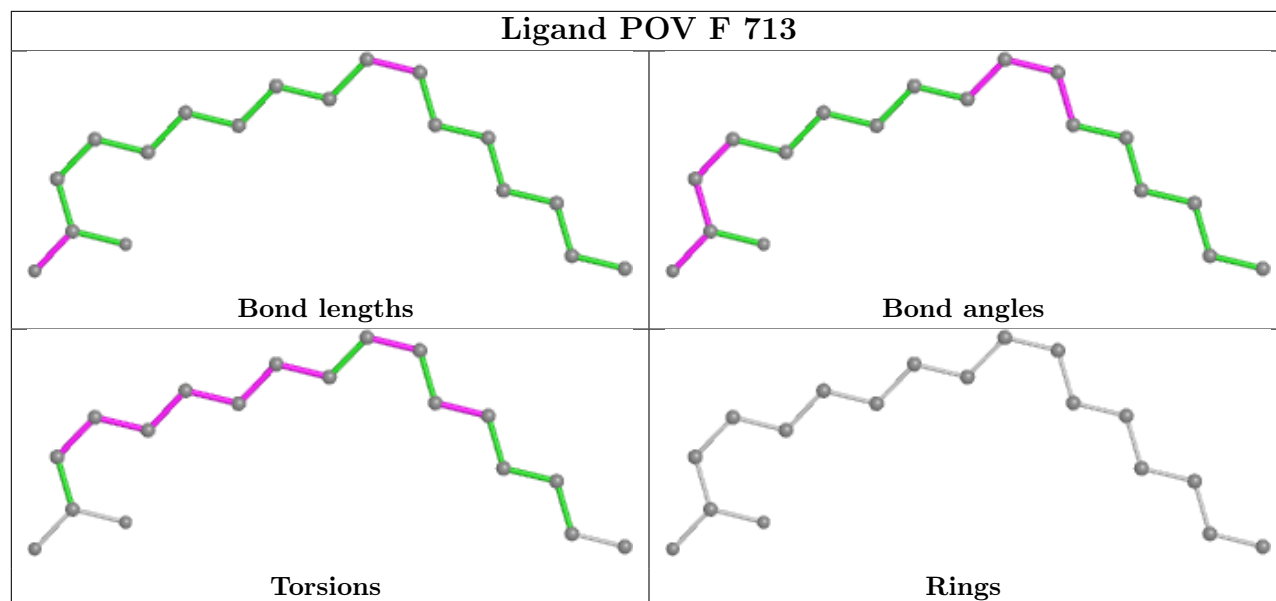












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

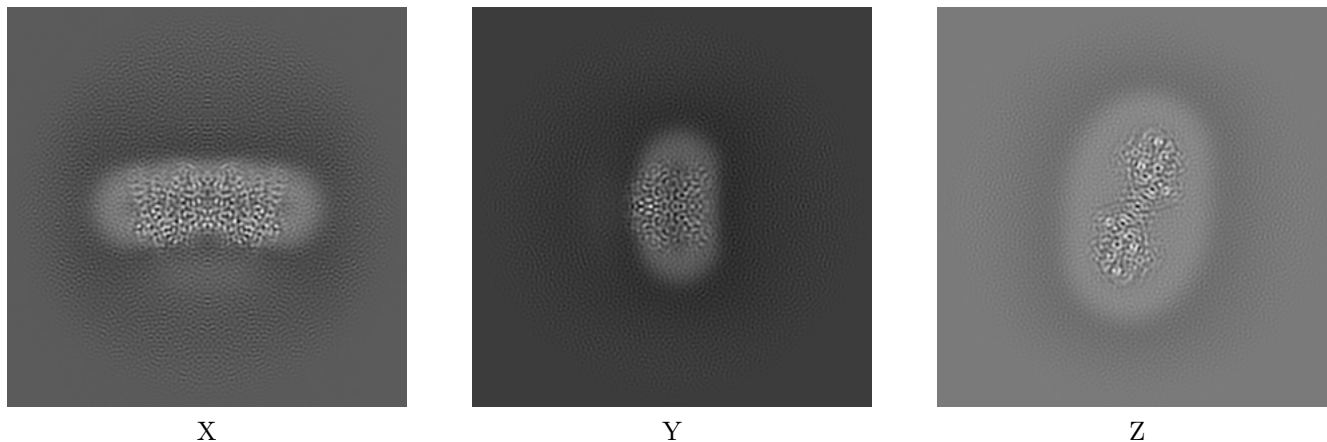
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38065. These allow visual inspection of the internal detail of the map and identification of artifacts.

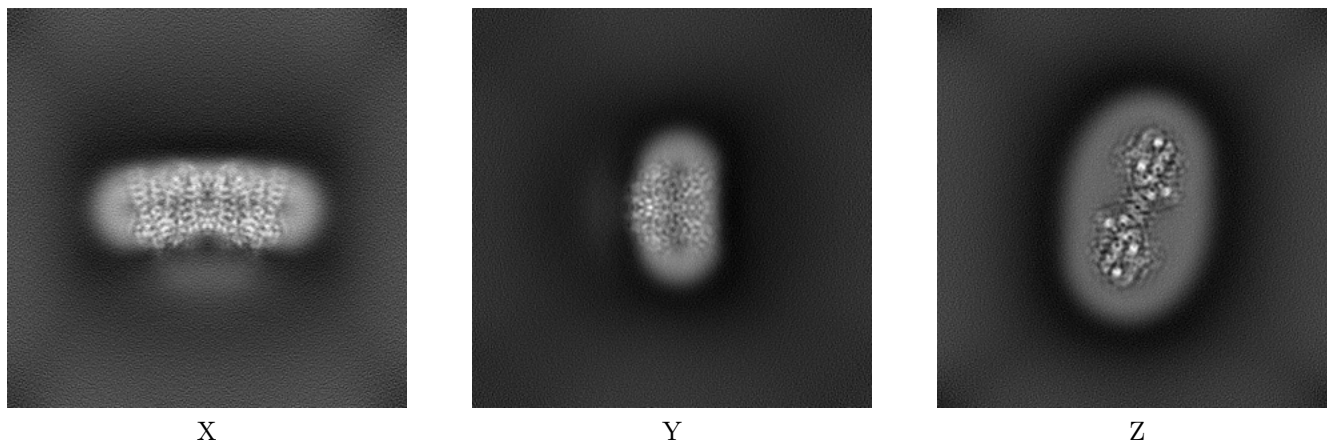
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



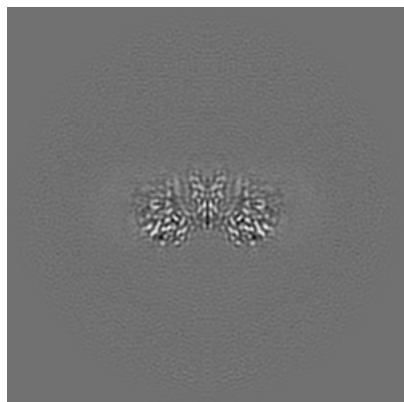
#### 6.1.2 Raw map



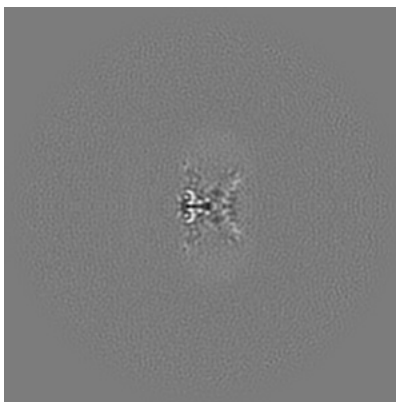
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

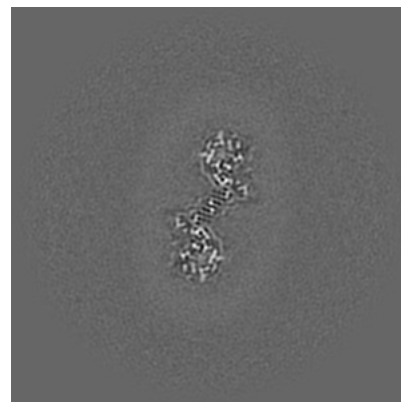
### 6.2.1 Primary map



X Index: 160

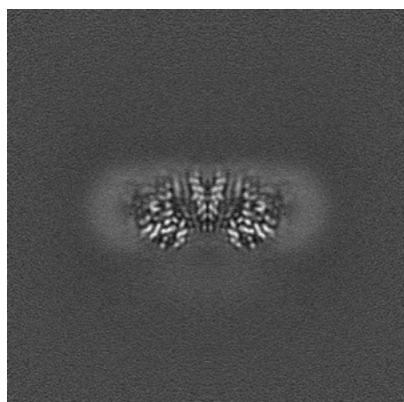


Y Index: 160

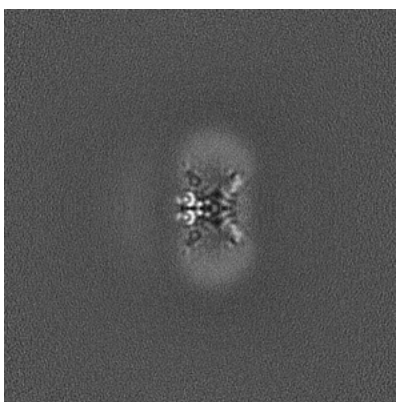


Z Index: 160

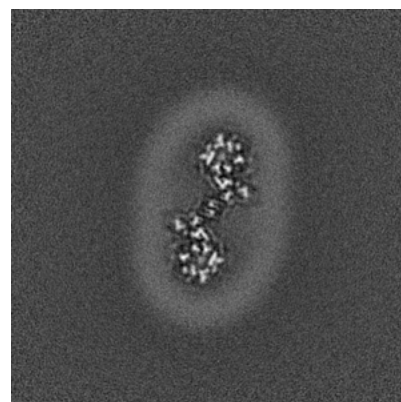
### 6.2.2 Raw map



X Index: 160



Y Index: 160

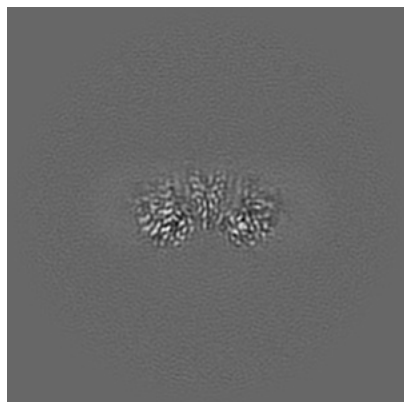


Z Index: 160

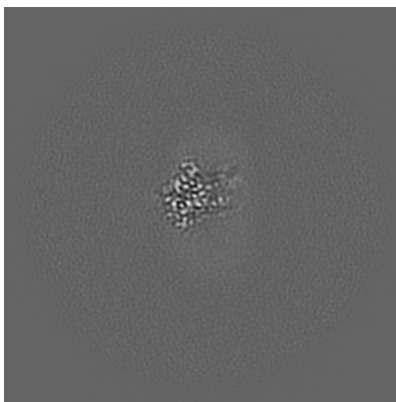
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

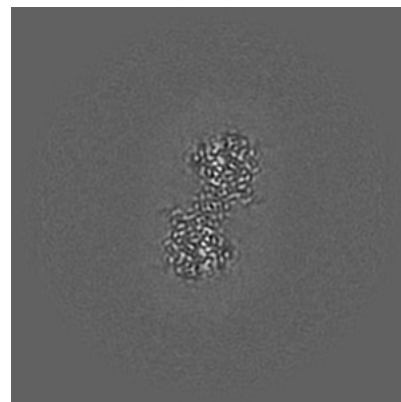
### 6.3.1 Primary map



X Index: 159

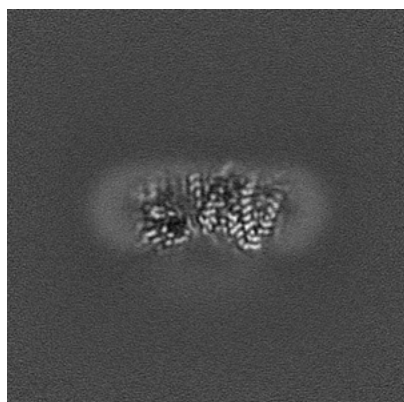


Y Index: 194

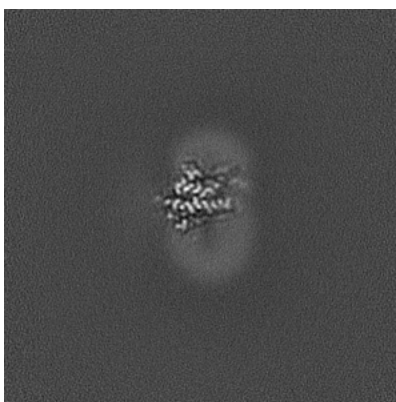


Z Index: 147

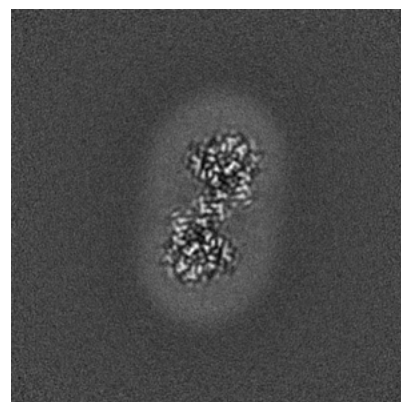
### 6.3.2 Raw map



X Index: 164



Y Index: 193

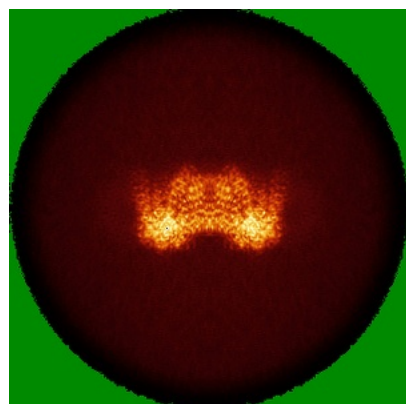


Z Index: 145

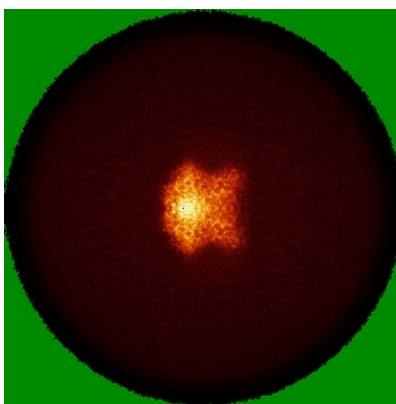
The images above show the largest variance slices of the map in three orthogonal directions.

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

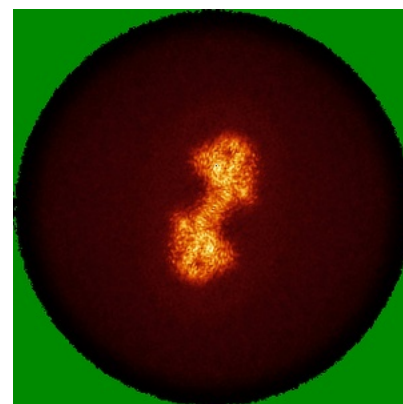
### 6.4.1 Primary map



X

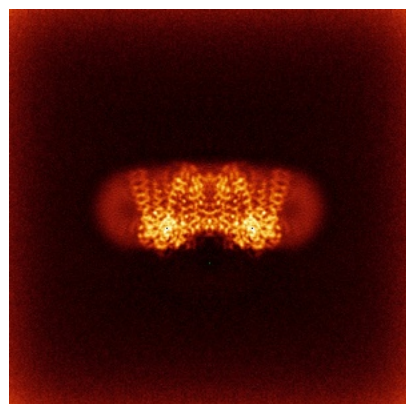


Y

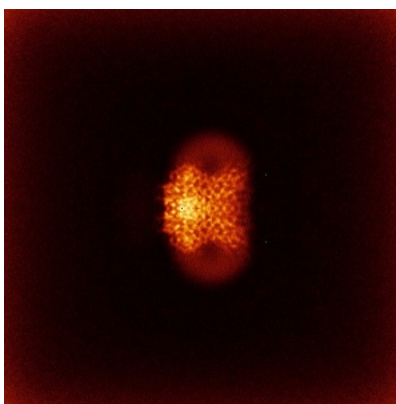


Z

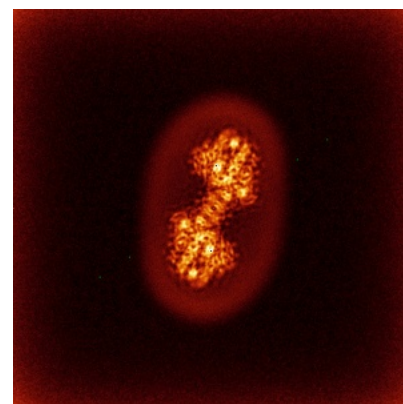
### 6.4.2 Raw map



X



Y

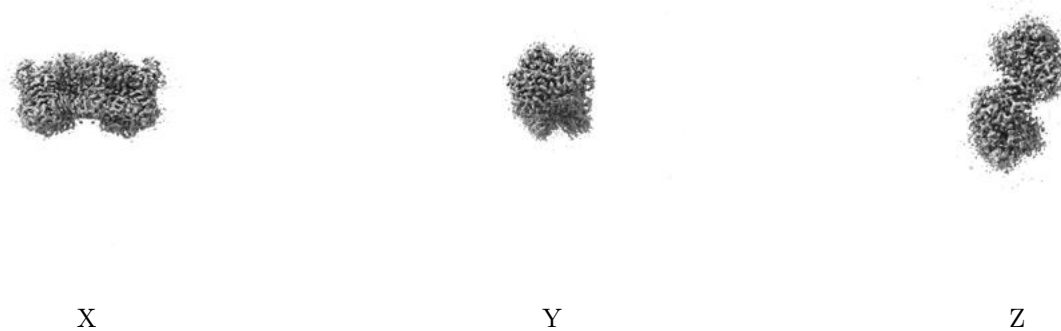


Z

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

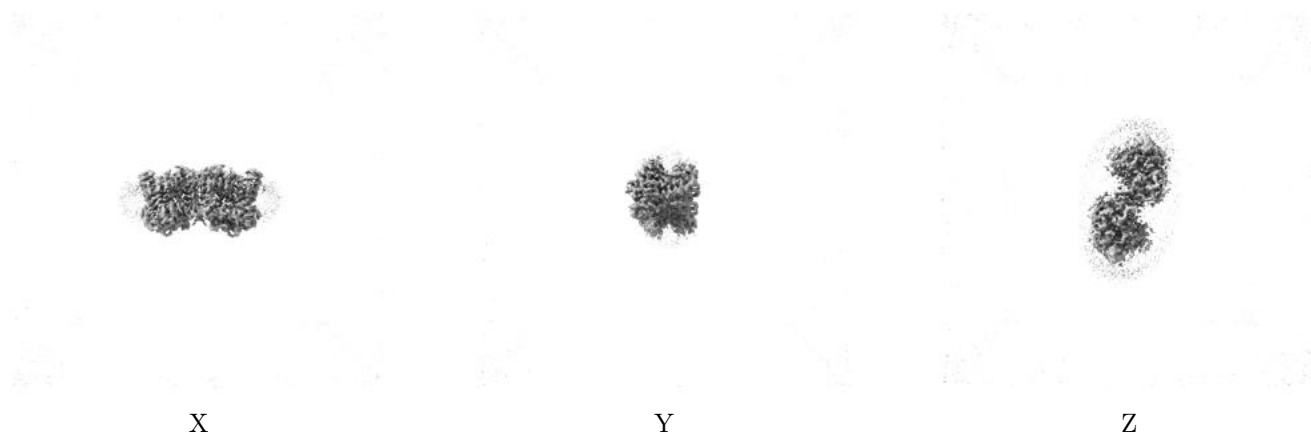
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.63. 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.

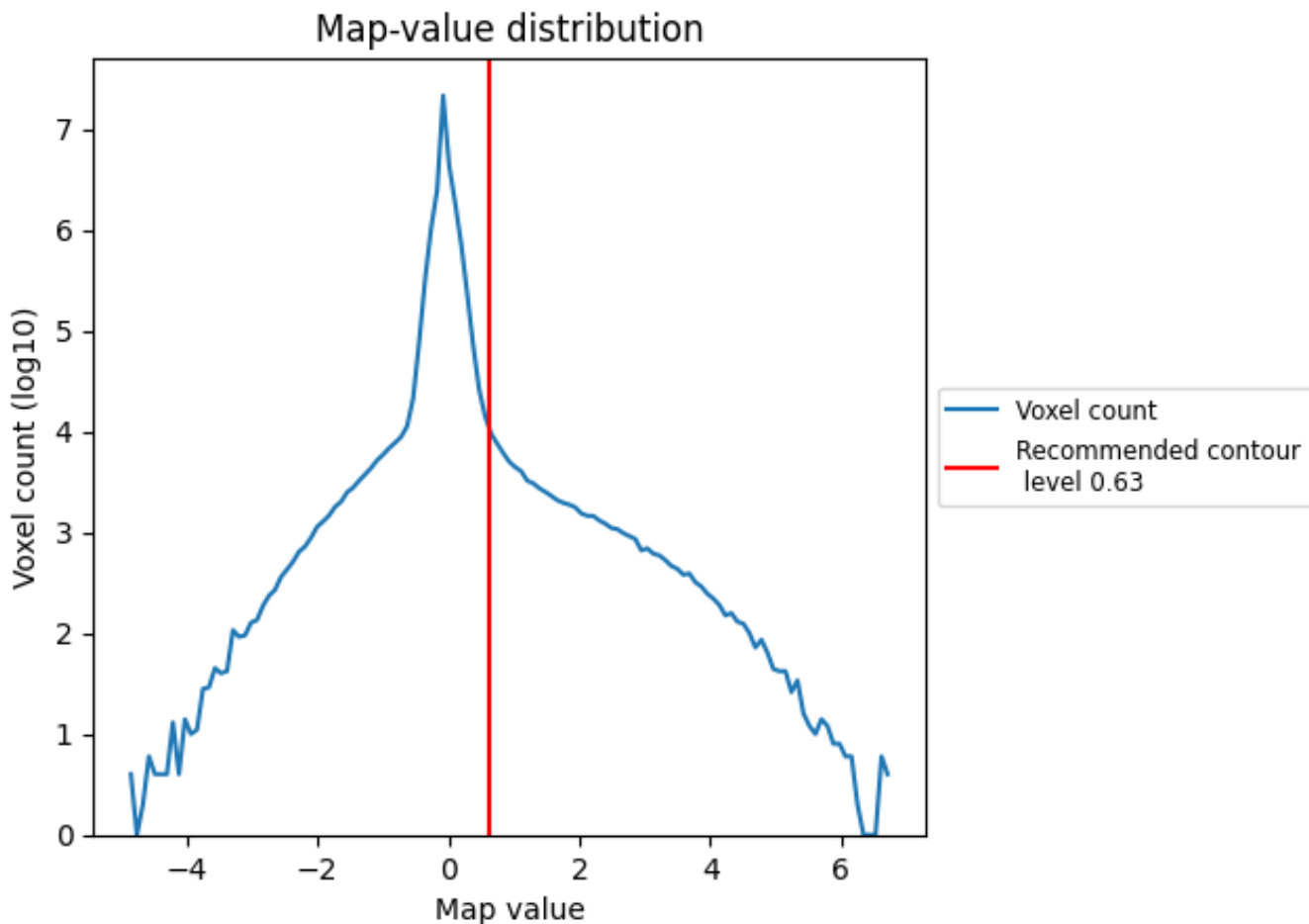
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

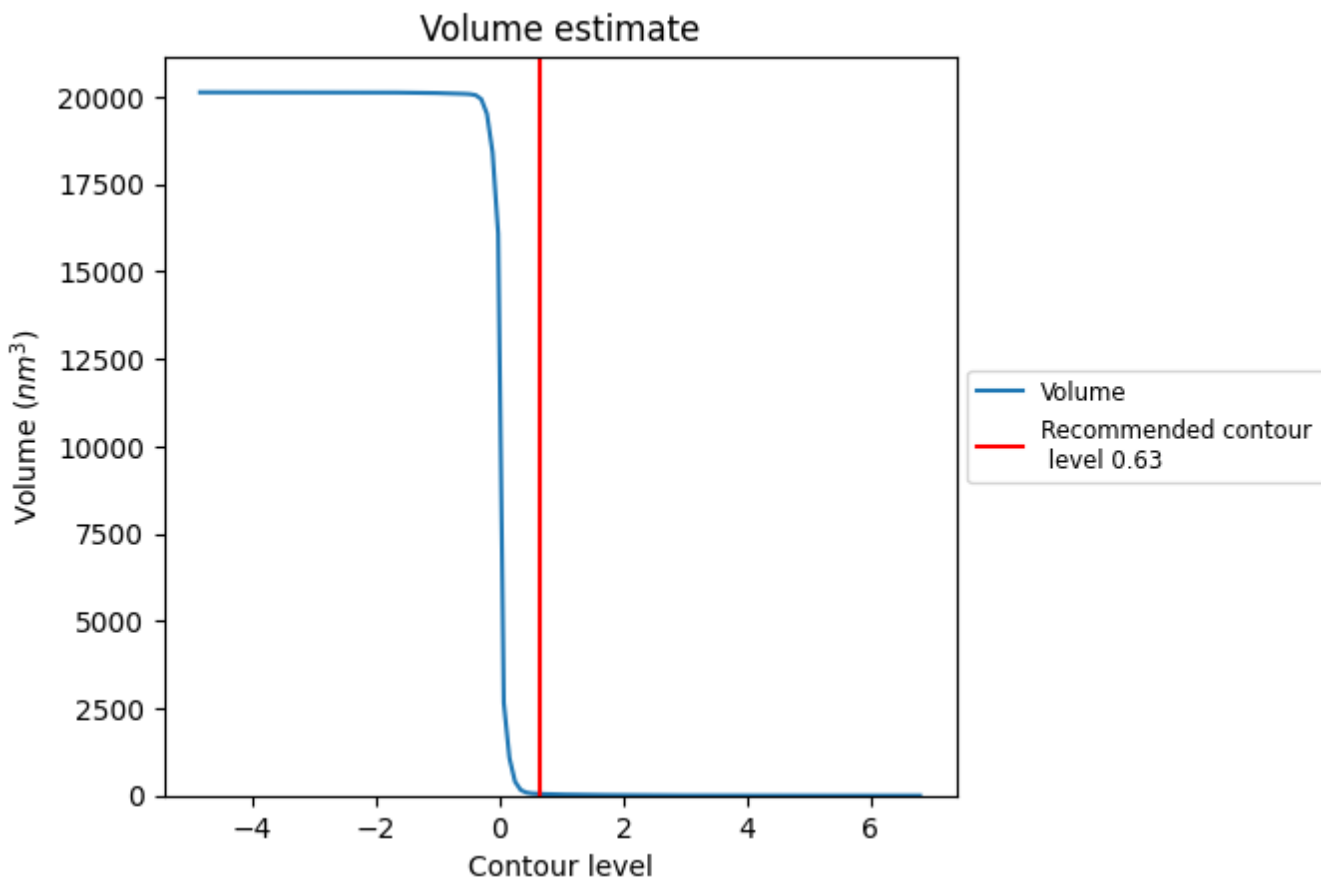
This section contains the results of statistical analysis of the map.

### 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](#)

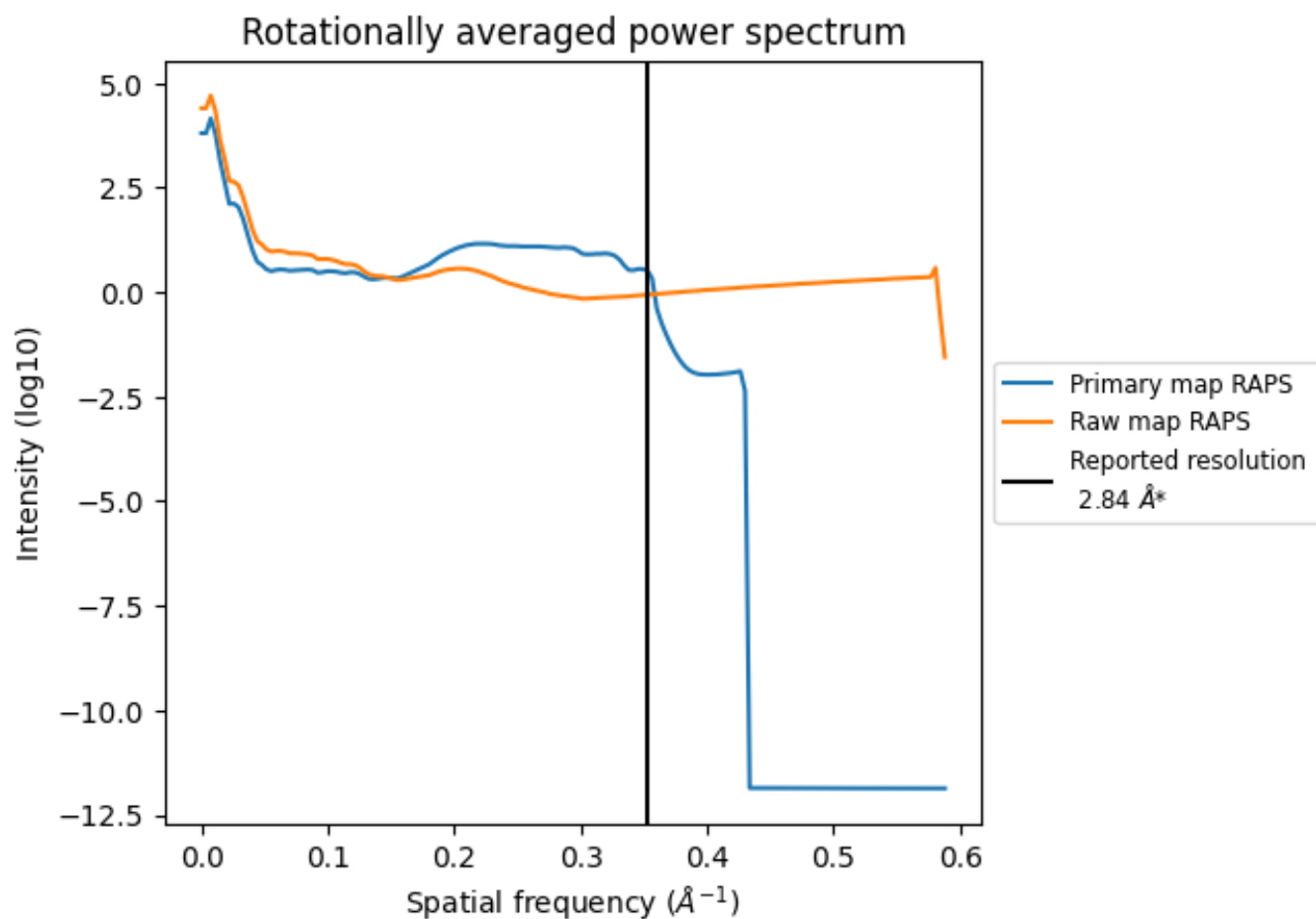


The volume at the recommended contour level is 49 nm<sup>3</sup>; this corresponds to an approximate mass of 45 kDa.

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](#)

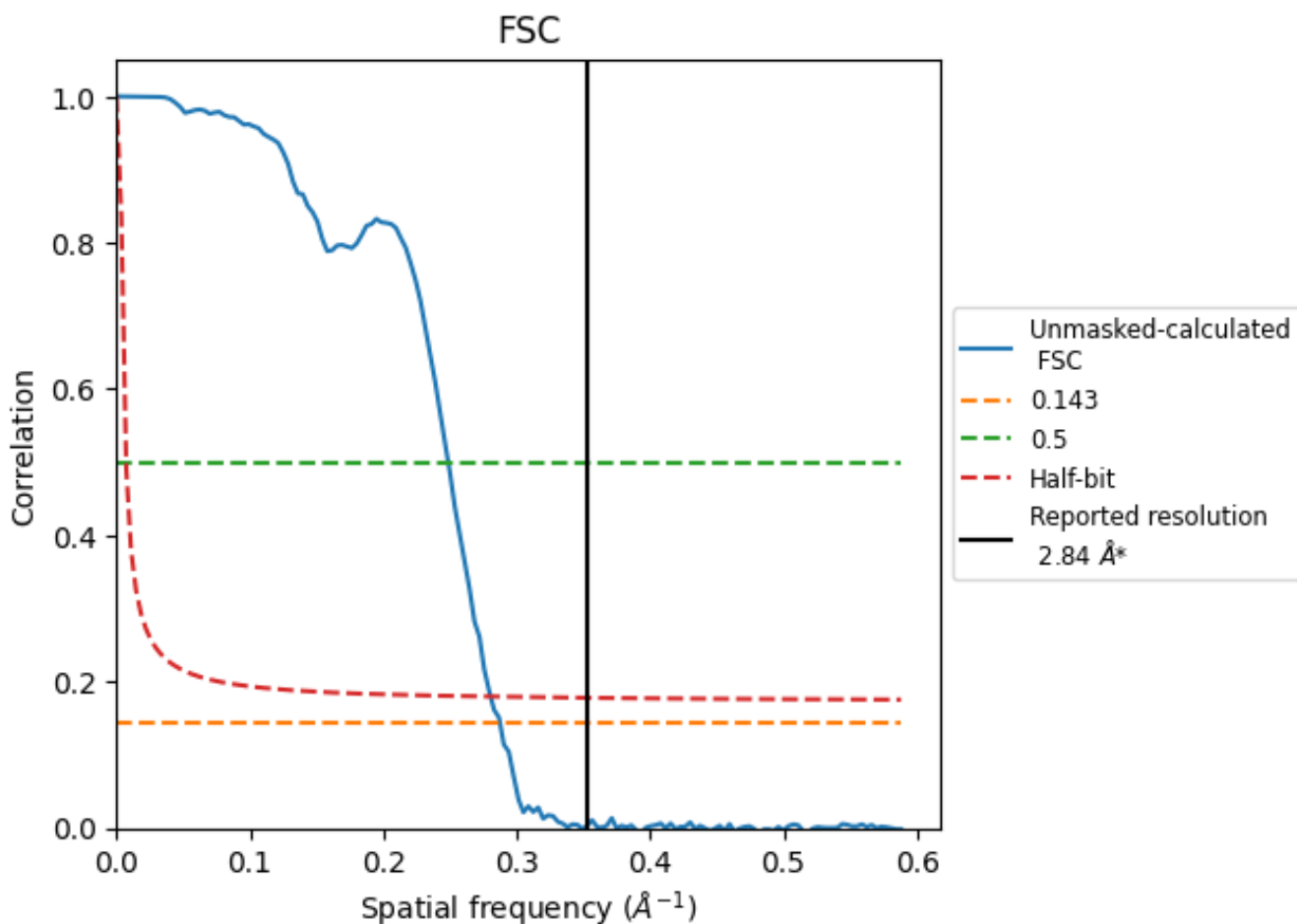


\*Reported resolution corresponds to spatial frequency of 0.352 Å<sup>-1</sup>

## 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 0.352  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

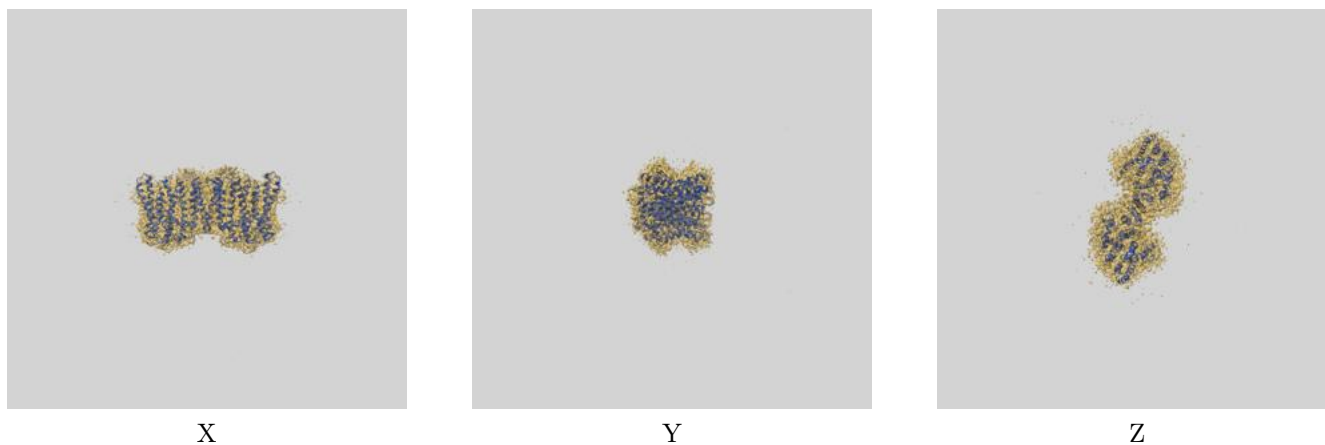
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.48	4.02	3.57

\*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 3.48 differs from the reported value 2.84 by more than 10 %

## 9 Map-model fit [i](#)

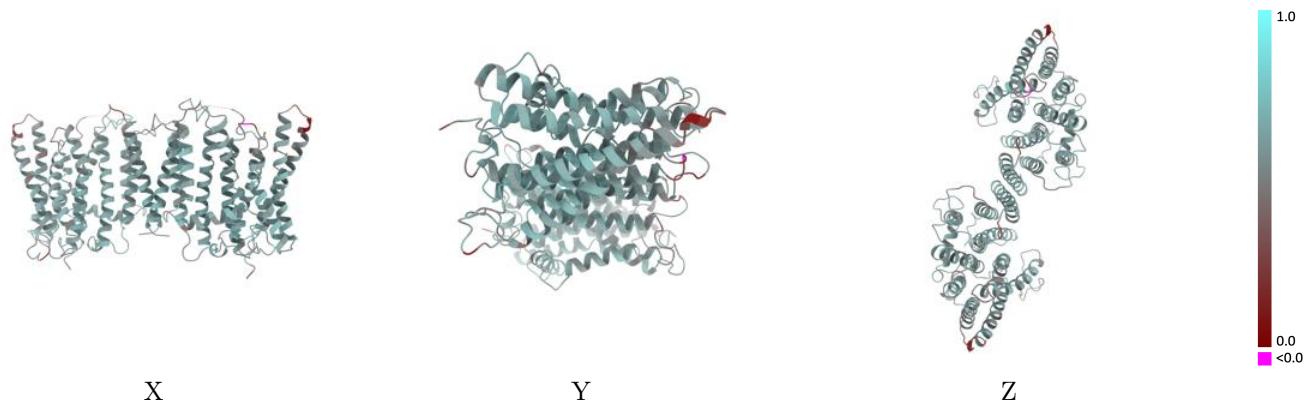
This section contains information regarding the fit between EMDB map EMD-38065 and PDB model 8X5B. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



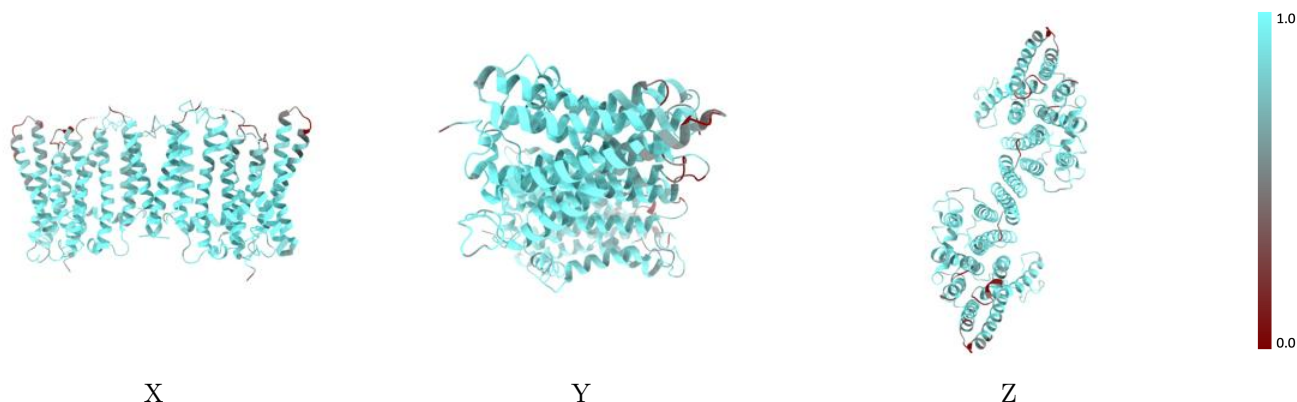
The images above show the 3D surface view of the map at the recommended contour level 0.63 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



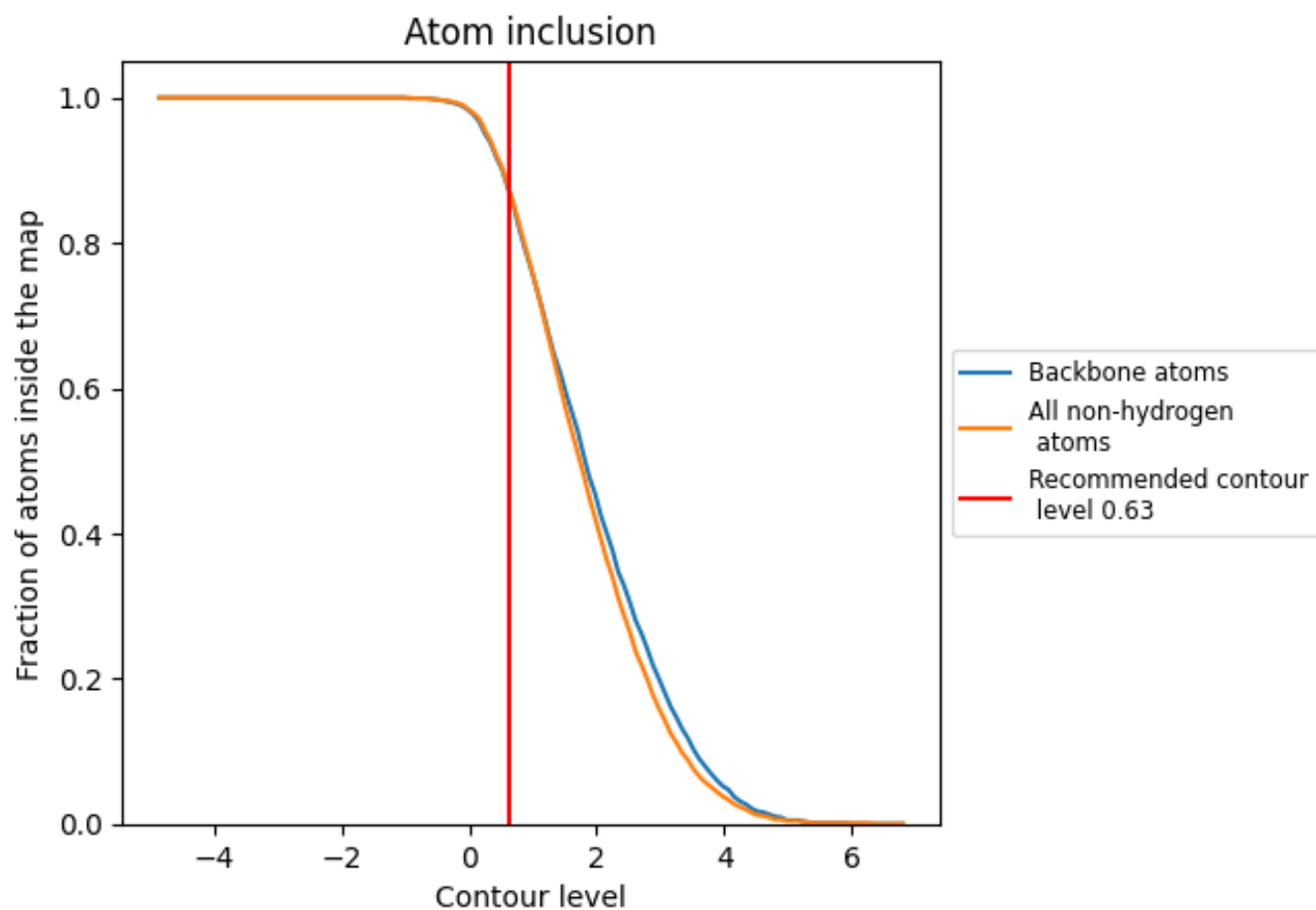
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.63).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

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

The table lists the average atom inclusion at the recommended contour level (0.63) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.5750
A	 0.8740	 0.5760
F	 0.8750	 0.5730

