



## Full wwPDB EM Validation Report ⓘ

Sep 30, 2023 – 07:29 am BST

PDB ID : 8P3Q  
EMDB ID : EMD-17392  
Title : Homomeric GluA2 flip R/G-unedited Q/R-edited F231A mutant in tandem with TARP gamma-2, desensitized conformation 3  
Authors : Zhang, D.; Krieger, J.M.; Yamashita, K.; Greger, I.  
Deposited on : 2023-05-18  
Resolution : 2.95 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.dev50  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

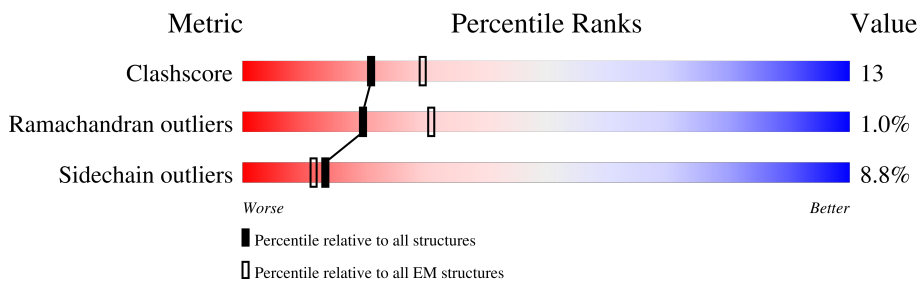
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	883	 9% 31% 13% 55%
1	B	883	 11% 28% 16% 55%
1	C	883	 11% 30% 13% 55%
1	D	883	 11% 32% 12% 55%
2	E	323	 40% 11% 45%
2	F	323	 42% 10% 45%
2	G	323	 44% 9% 45%
2	H	323	 43% 9% 45%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18047 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	399	Total 3059	C 1992	N 492	O 554	S 21	0	0
1	B	398	Total 3037	C 1981	N 487	O 549	S 20	0	0
1	C	396	Total 3024	C 1972	N 483	O 549	S 20	0	0
1	D	397	Total 3025	C 1972	N 485	O 548	S 20	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	ALA	PHE	engineered mutation	UNP P19491
A	586	ARG	GLN	variant	UNP P19491
A	743	ARG	GLY	conflict	UNP P19491
B	231	ALA	PHE	engineered mutation	UNP P19491
B	586	ARG	GLN	variant	UNP P19491
B	743	ARG	GLY	conflict	UNP P19491
C	231	ALA	PHE	engineered mutation	UNP P19491
C	586	ARG	GLN	variant	UNP P19491
C	743	ARG	GLY	conflict	UNP P19491
D	231	ALA	PHE	engineered mutation	UNP P19491
D	586	ARG	GLN	variant	UNP P19491
D	743	ARG	GLY	conflict	UNP P19491

- Molecule 2 is a protein called Voltage-dependent calcium channel gamma-2 subunit.

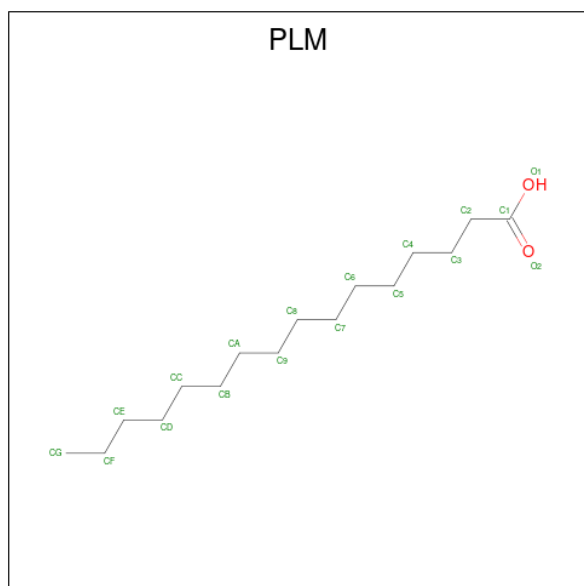
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	177	Total 1364	C 895	N 221	O 237	S 11	0	0
2	F	178	Total 1373	C 901	N 223	O 238	S 11	0	0
2	G	177	Total 1368	C 897	N 222	O 238	S 11	0	0

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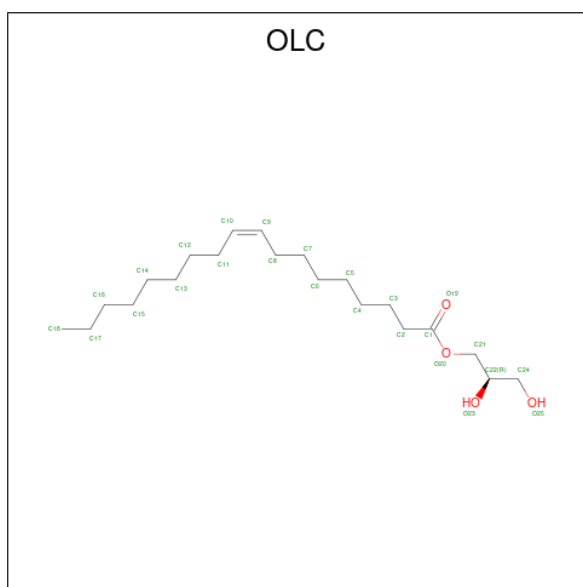
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	177	1369	899	223	236	11	0	0

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



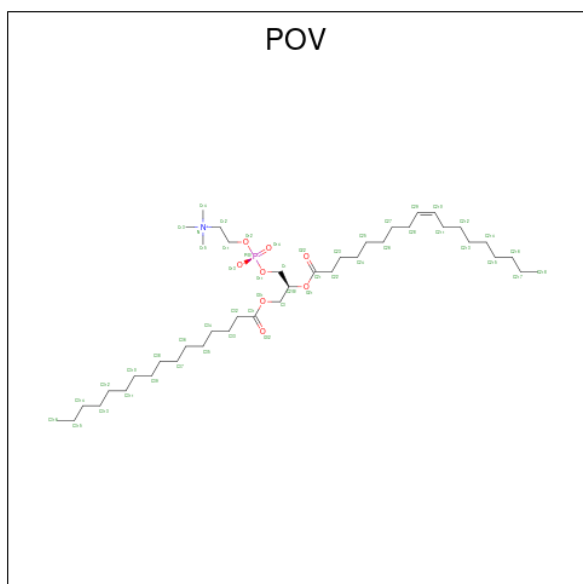
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	A	1	18	16	2	0
3	B	1	18	16	2	0
3	C	1	18	16	2	0
3	D	1	18	16	2	0
3	F	1	18	16	2	0
3	F	1	16	14	2	0
3	G	1	18	16	2	0

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			25	21	4	
4	B	1	Total	C	O	0
			25	21	4	
4	C	1	Total	C	O	0
			25	21	4	
4	D	1	Total	C	O	0
			25	21	4	

- Molecule 5 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
5	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
5	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
5	D	1	Total	C	N	O	P	0
			40	30	1	8	1	
5	G	1	Total	C	O	P		0
			34	25	8	1		
5	G	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 6 is water.

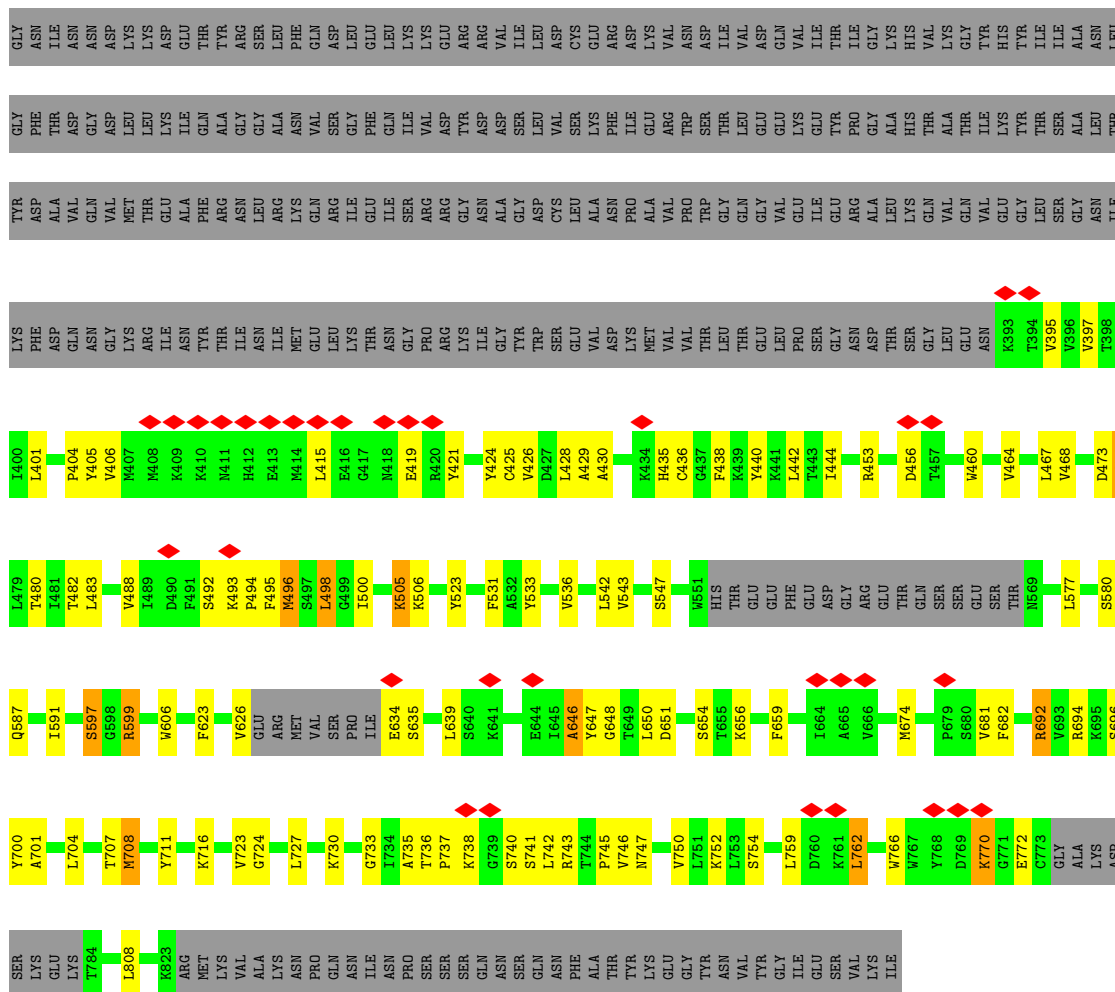
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	O	0
			1	1	
6	C	1	Total	O	0
			1	1	
6	D	3	Total	O	0
			3	3	
6	F	1	Total	O	0
			1	1	
6	G	1	Total	O	0
			1	1	



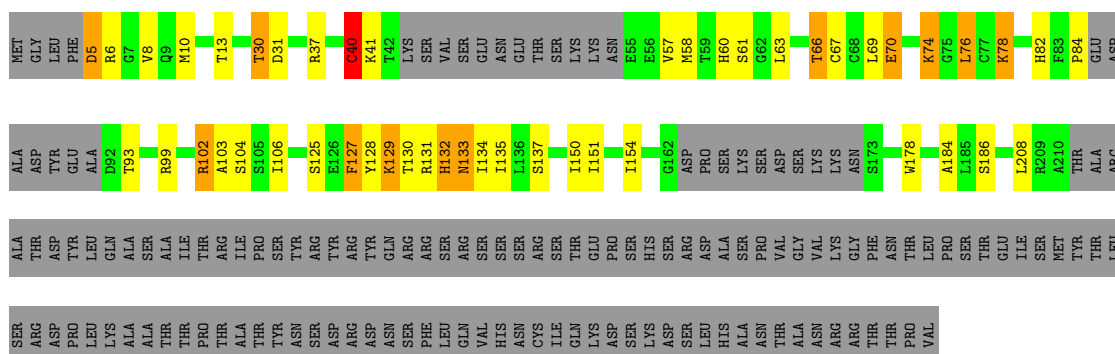




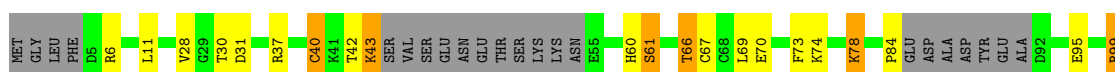




● Molecule 2: Voltage-dependent calcium channel gamma-2 subunit



● Molecule 2: Voltage-dependent calcium channel gamma-2 subunit





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62156	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.871	Depositor
Minimum map value	-0.843	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.2	Depositor
Map size ( $\text{\AA}$ )	370.048, 370.048, 370.048	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.4455, 1.4455, 1.4455	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: POV, OLC, 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	0.44	0/3127	0.63	0/4229
1	B	0.43	0/3105	0.63	1/4202 (0.0%)
1	C	0.43	0/3092	0.61	0/4184
1	D	0.45	0/3093	0.65	1/4187 (0.0%)
2	E	0.46	0/1395	0.63	0/1885
2	F	0.46	0/1404	0.63	0/1896
2	G	0.45	0/1399	0.61	0/1890
2	H	0.46	0/1400	0.62	0/1890
All	All	0.45	0/18015	0.63	2/24363 (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	484	VAL	O-C-N	5.48	131.47	122.70
1	D	599	ARG	NE-CZ-NH2	-5.21	117.69	120.30

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	3059	0	3020	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3037	0	2999	124	0
1	C	3024	0	2976	101	0
1	D	3025	0	2977	96	0
2	E	1364	0	1346	24	0
2	F	1373	0	1359	16	0
2	G	1368	0	1352	16	0
2	H	1369	0	1361	22	0
3	A	18	0	31	1	0
3	B	18	0	31	0	0
3	C	18	0	31	0	0
3	D	18	0	31	1	0
3	F	34	0	55	1	0
3	G	18	0	31	0	0
4	A	25	0	40	1	0
4	B	25	0	40	1	0
4	C	25	0	40	0	0
4	D	25	0	40	0	0
5	A	39	0	50	2	0
5	B	42	0	56	1	0
5	D	40	0	52	0	0
5	G	76	0	96	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	D	3	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
All	All	18047	0	18014	475	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 13.

All (475) 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:485:ARG:HB3	1:B:491:PHE:HE2	1.22	1.02
1:A:498:LEU:HD22	1:A:730:LYS:HB2	1.53	0.90
1:D:405:TYR:HB3	1:D:425:CYS:HB2	1.60	0.84
1:B:647:TYR:HB3	1:B:701:ALA:HB3	1.60	0.83
1:B:713:GLU:HA	1:B:720:THR:HB	1.60	0.83
1:C:633:ILE:HD12	1:C:638:ASP:HB3	1.62	0.80
1:C:640:SER:HB3	1:C:670:MET:HG3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:635:SER:HA	1:D:724:GLY:CA	2.12	0.80
1:A:496:MET:HB3	1:A:732:TYR:HB2	1.64	0.79
1:D:635:SER:HA	1:D:724:GLY:HA3	1.64	0.79
1:D:494:PRO:HA	1:D:733:GLY:HA2	1.64	0.79
1:B:408:MET:HB3	1:B:412:HIS:CG	2.17	0.78
1:B:485:ARG:HD2	1:B:491:PHE:CZ	2.17	0.78
1:A:683:VAL:HB	1:A:688:GLU:HB3	1.66	0.78
1:A:714:GLN:HB3	1:A:771:GLY:HA2	1.67	0.77
1:C:395:VAL:HG13	1:C:473:ASP:HB2	1.66	0.76
1:B:485:ARG:HB3	1:B:491:PHE:CE2	2.14	0.76
1:B:485:ARG:HD2	1:B:491:PHE:HZ	1.50	0.76
1:A:586:ARG:HH21	1:B:586:ARG:HB2	1.51	0.75
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.68	0.75
1:A:480:THR:HG21	1:A:730:LYS:HD2	1.70	0.73
1:A:696:SER:HB3	1:A:699:LYS:HB2	1.70	0.73
1:A:498:LEU:HB3	1:A:707:THR:HG23	1.70	0.71
1:A:545:ARG:HH21	1:A:570:GLU:HB3	1.56	0.70
1:C:495:PHE:HB2	1:C:759:LEU:HD22	1.71	0.70
1:B:397:VAL:HG13	1:B:476:ILE:H	1.56	0.70
1:D:453:ARG:HB3	1:D:460:TRP:CE2	2.27	0.70
1:A:674:MET:HG2	1:A:681:VAL:HG21	1.75	0.69
1:B:449:LYS:HB3	1:B:652:SER:HB3	1.75	0.69
1:A:756:GLN:HG3	1:A:758:VAL:HG23	1.75	0.68
1:A:514:VAL:H	5:A:1003:POV:H13	1.57	0.68
1:C:485:ARG:HB3	1:C:491:PHE:HE2	1.57	0.68
1:C:633:ILE:HD11	1:C:642:GLN:HG2	1.74	0.68
1:A:453:ARG:O	1:A:454:ASP:C	2.31	0.68
1:C:704:LEU:HD12	1:C:708:MET:HB3	1.76	0.68
1:A:755:GLU:HG2	1:D:483:LEU:HG	1.77	0.67
1:C:686:THR:HA	1:C:702:TYR:HE2	1.60	0.67
1:A:498:LEU:HD23	1:A:705:GLU:HB3	1.76	0.66
1:C:692:ARG:HD2	1:C:695:LYS:HE3	1.77	0.66
1:C:702:TYR:CE2	1:C:704:LEU:HB3	2.30	0.66
1:D:401:LEU:HG	1:D:444:ILE:HG13	1.77	0.66
1:C:485:ARG:HB3	1:C:491:PHE:CE2	2.30	0.65
1:C:675:ARG:HH12	1:D:770:LYS:HB3	1.60	0.65
1:D:440:TYR:HE2	1:D:442:LEU:HG	1.62	0.65
1:D:404:PRO:HB3	1:D:711:TYR:CE1	2.32	0.65
1:C:500:ILE:HB	1:C:727:LEU:HB2	1.78	0.64
1:A:740:SER:O	1:A:743:ARG:HB3	1.98	0.64
1:C:696:SER:HB3	1:C:699:LYS:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ARG:HA	1:A:671:TRP:CE2	2.32	0.64
1:C:502:ILE:HG23	1:C:701:ALA:HB1	1.80	0.63
2:F:84:PRO:HD2	2:F:99:ARG:HH11	1.62	0.63
1:C:651:ASP:HA	1:C:682:PHE:HB3	1.79	0.63
1:B:494:PRO:HB3	1:B:731:GLY:HA3	1.81	0.63
1:C:514:VAL:H	5:G:1103:POV:H15A	1.64	0.63
1:A:494:PRO:HA	1:A:733:GLY:HA2	1.80	0.62
1:A:651:ASP:HA	1:A:682:PHE:HB3	1.81	0.62
1:C:499:GLY:HA3	1:C:726:ASN:HB3	1.81	0.62
1:D:500:ILE:HB	1:D:727:LEU:HB2	1.82	0.62
1:D:634:GLU:HA	1:D:723:VAL:HB	1.82	0.62
1:A:604:VAL:HG12	1:B:799:LEU:HD12	1.82	0.61
1:D:475:ALA:HB3	1:D:735:ALA:HB3	1.82	0.61
2:H:61:SER:HA	2:H:66:THR:HA	1.81	0.61
1:B:405:TYR:HA	1:B:424:TYR:HB3	1.82	0.61
1:A:501:SER:O	1:A:703:LEU:HA	2.01	0.61
1:A:692:ARG:HB3	1:A:700:TYR:CD2	2.36	0.61
1:B:672:THR:HA	1:B:675:ARG:HE	1.66	0.61
1:D:424:TYR:CD1	1:D:762:LEU:HB3	2.36	0.60
1:C:404:PRO:HB2	1:C:766:TRP:HB3	1.83	0.60
1:B:692:ARG:HB3	1:B:700:TYR:CD2	2.36	0.60
1:C:424:TYR:CD2	1:C:762:LEU:HB3	2.37	0.60
1:D:429:ALA:HA	1:D:476:ILE:HD13	1.84	0.60
1:C:492:SER:HB2	1:C:747:ASN:HA	1.84	0.59
1:A:764:ASN:HA	1:A:768:TYR:HD2	1.67	0.59
1:D:425:CYS:HA	1:D:428:LEU:HB3	1.82	0.59
2:G:67:CYS:HA	2:G:77:CYS:HA	1.84	0.59
2:H:30:THR:HG21	2:H:178:TRP:HH2	1.66	0.59
1:D:395:VAL:HG13	1:D:473:ASP:HB2	1.84	0.59
1:B:400:ILE:HG22	1:B:477:ALA:HB1	1.84	0.59
1:B:464:VAL:CG2	1:B:485:ARG:HD3	2.33	0.59
1:A:490:ASP:HB3	1:A:743:ARG:NE	2.18	0.59
1:B:480:THR:HA	1:B:732:TYR:HA	1.84	0.59
1:C:686:THR:HA	1:C:702:TYR:CE2	2.38	0.59
1:D:646:ALA:HB1	1:D:681:VAL:HG12	1.85	0.59
1:A:500:ILE:HG12	1:A:655:THR:HG23	1.85	0.59
1:A:417:GLY:HA2	1:A:420:ARG:HH21	1.68	0.58
1:A:644:GLU:O	1:A:699:LYS:HA	2.02	0.58
1:B:450:TYR:HE1	1:B:650:LEU:HD23	1.68	0.58
1:C:503:MET:HG2	1:C:693:VAL:HG11	1.86	0.58
1:D:421:TYR:CE1	1:D:444:ILE:HG12	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:741:SER:O	1:D:745:PRO:HD2	2.04	0.57
1:B:752:LYS:O	1:B:756:GLN:HG2	2.04	0.57
2:E:63:LEU:O	2:E:102:ARG:NH2	2.36	0.57
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.86	0.57
1:C:633:ILE:HA	1:C:638:ASP:HB3	1.87	0.57
2:H:34:LEU:HD11	2:H:174:TYR:HB2	1.86	0.57
1:D:674:MET:HG2	1:D:681:VAL:HG21	1.87	0.57
1:C:647:TYR:O	1:C:674:MET:HG2	2.05	0.57
1:B:394:THR:HG22	1:B:441:LYS:HB2	1.87	0.57
1:C:692:ARG:HB3	1:C:700:TYR:CD2	2.40	0.57
1:A:490:ASP:HB3	1:A:743:ARG:HE	1.69	0.57
1:A:545:ARG:NH2	1:A:570:GLU:HB3	2.19	0.57
1:D:523:TYR:HB2	3:D:1001:PLM:H21	1.86	0.57
2:H:41:LYS:HG3	2:H:76:LEU:HD22	1.87	0.57
1:B:543:VAL:HG22	1:C:810:ALA:HB2	1.87	0.57
1:B:495:PHE:O	1:B:759:LEU:HB3	2.05	0.56
1:D:440:TYR:CE2	1:D:442:LEU:HG	2.40	0.56
1:D:460:TRP:NE1	1:D:488:VAL:HG11	2.20	0.56
1:A:498:LEU:CD2	1:A:730:LYS:HB2	2.30	0.56
1:C:675:ARG:HA	1:C:682:PHE:CE2	2.40	0.56
1:D:424:TYR:HH	1:D:495:PHE:HD1	1.52	0.56
1:D:404:PRO:HB2	1:D:766:TRP:HB3	1.88	0.56
1:B:398:THR:HG21	1:B:466:GLU:HB2	1.88	0.55
1:B:433:ALA:HB1	1:B:438:PHE:O	2.06	0.55
1:D:543:VAL:CG1	1:D:597:SER:HB2	2.36	0.55
1:A:460:TRP:CE2	1:A:488:VAL:HG21	2.41	0.55
1:A:666:VAL:HA	1:A:669:LYS:HD3	1.88	0.55
1:B:498:LEU:HB3	1:B:707:THR:HG23	1.88	0.55
1:B:429:ALA:HA	1:B:476:ILE:HD13	1.87	0.55
1:B:490:ASP:HB2	1:B:736:THR:OG1	2.05	0.55
2:E:37:ARG:HH21	2:E:58:MET:HG2	1.71	0.55
2:F:30:THR:HG21	2:F:178:TRP:CH2	2.42	0.55
1:A:498:LEU:HD11	1:A:732:TYR:CD1	2.41	0.55
1:D:696:SER:HB3	1:D:699:LYS:HB2	1.89	0.55
1:B:648:GLY:HA3	1:B:681:VAL:O	2.07	0.55
1:D:424:TYR:HD1	1:D:762:LEU:HB3	1.71	0.55
1:A:628:ARG:HH11	1:A:785:SER:HB3	1.72	0.54
1:D:399:THR:HG23	1:D:444:ILE:HD13	1.89	0.54
1:D:453:ARG:HB3	1:D:460:TRP:CD2	2.42	0.54
1:D:464:VAL:O	1:D:468:VAL:HG23	2.08	0.54
1:D:496:MET:HG2	1:D:707:THR:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:696:SER:HB3	1:D:699:LYS:H	1.71	0.54
1:B:659:PHE:CZ	1:B:703:LEU:HD13	2.42	0.54
1:B:503:MET:HB3	1:B:702:TYR:HB3	1.89	0.54
1:C:474:ILE:HB	1:C:742:LEU:HD12	1.90	0.54
1:D:421:TYR:HE1	1:D:444:ILE:HG12	1.72	0.54
2:G:60:HIS:CE1	2:G:67:CYS:HB3	2.43	0.54
1:D:405:TYR:HA	1:D:425:CYS:H	1.71	0.54
2:F:110:LEU:HA	2:F:113:ILE:HD12	1.91	0.54
1:D:406:VAL:HG22	1:D:426:VAL:HG23	1.91	0.53
2:F:192:MET:HG2	3:F:1302:PLM:HC1	1.90	0.53
1:B:633:ILE:HD12	1:B:639:LEU:HD23	1.90	0.53
1:C:429:ALA:HA	1:C:476:ILE:HD13	1.90	0.53
1:A:662:SER:OG	1:A:667:PHE:HB2	2.08	0.53
1:C:432:ILE:HG23	1:C:436:CYS:SG	2.49	0.53
2:G:34:LEU:HD12	2:G:175:SER:O	2.08	0.53
1:D:704:LEU:HD12	1:D:708:MET:HB3	1.90	0.52
1:C:502:ILE:CG2	1:C:701:ALA:HB1	2.39	0.52
1:B:502:ILE:HB	1:B:723:VAL:HG23	1.90	0.52
1:B:395:VAL:HG13	1:B:473:ASP:HB2	1.91	0.52
2:F:61:SER:HA	2:F:66:THR:HA	1.92	0.52
1:A:482:THR:HG21	1:A:654:SER:CB	2.40	0.52
1:C:480:THR:HG21	1:C:730:LYS:HD2	1.92	0.52
2:H:30:THR:HG21	2:H:178:TRP:CH2	2.44	0.52
1:B:464:VAL:HG21	1:B:485:ARG:HD3	1.92	0.52
1:A:651:ASP:HB2	1:A:683:VAL:C	2.30	0.52
1:B:453:ARG:HB2	1:B:460:TRP:CE2	2.45	0.52
1:C:436:CYS:SG	1:C:746:VAL:HA	2.49	0.52
1:C:671:TRP:HA	1:C:674:MET:HE2	1.91	0.52
1:B:402:GLU:HG2	1:B:478:PRO:HG3	1.92	0.52
1:C:633:ILE:HG12	1:C:645:ILE:HD12	1.92	0.52
2:G:30:THR:HG21	2:G:178:TRP:HH2	1.75	0.52
1:B:702:TYR:CD2	1:B:704:LEU:HD13	2.45	0.51
1:A:480:THR:HG22	1:A:482:THR:CG2	2.40	0.51
1:C:702:TYR:CD2	1:C:704:LEU:HB3	2.44	0.51
1:A:477:ALA:HB1	1:A:478:PRO:HD2	1.92	0.51
2:G:6:ARG:O	2:G:8:VAL:N	2.36	0.51
1:A:574:PHE:O	1:A:575:ASN:HB2	2.10	0.51
1:D:505:LYS:HE2	1:D:694:ARG:HA	1.92	0.51
2:G:39:VAL:HG12	2:G:55:GLU:O	2.11	0.51
2:H:34:LEU:HD22	2:H:160:ASN:ND2	2.26	0.51
1:B:500:ILE:HB	1:B:727:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:66:THR:HG23	2:E:78:LYS:HD2	1.92	0.51
1:A:492:SER:HB2	1:A:747:ASN:HA	1.93	0.51
1:B:411:ASN:O	1:B:415:LEU:HG	2.11	0.51
1:C:505:LYS:HB3	1:C:698:GLY:N	2.26	0.51
1:D:635:SER:HA	1:D:724:GLY:HA2	1.90	0.51
2:E:82:HIS:O	2:E:84:PRO:HD3	2.11	0.51
2:E:129:LYS:HG2	2:E:130:THR:H	1.75	0.51
2:H:200:MET:O	2:H:204:ARG:HG2	2.11	0.50
1:B:404:PRO:HB3	1:B:711:TYR:CE1	2.46	0.50
2:E:131:ARG:O	2:E:133:ASN:N	2.44	0.50
1:B:503:MET:HG2	1:B:693:VAL:HG11	1.92	0.50
1:B:505:LYS:HD3	1:B:694:ARG:HA	1.92	0.50
2:E:30:THR:HG21	2:E:178:TRP:CZ2	2.46	0.50
1:A:481:ILE:HD12	1:A:494:PRO:HG3	1.94	0.50
1:C:649:THR:HB	1:C:655:THR:HG22	1.91	0.50
1:C:399:THR:HG21	1:C:406:VAL:HG21	1.94	0.50
1:A:480:THR:HG22	1:A:482:THR:HG23	1.93	0.50
1:B:477:ALA:HB1	1:B:478:PRO:HD2	1.92	0.50
1:C:792:VAL:O	1:C:795:VAL:HG12	2.12	0.50
2:G:121:CYS:HB2	2:G:138:ALA:HB2	1.94	0.50
1:A:575:ASN:ND2	1:D:599:ARG:HH22	2.09	0.50
1:A:649:THR:HG21	1:A:655:THR:HG22	1.92	0.50
1:C:690:VAL:O	1:C:693:VAL:HB	2.12	0.50
1:D:766:TRP:CE3	1:D:770:LYS:HE3	2.46	0.50
1:C:651:ASP:O	1:C:656:LYS:HD3	2.11	0.49
2:G:125:SER:HA	2:G:134:ILE:HD11	1.93	0.49
1:A:587:GLN:HG3	1:D:606:TRP:CG	2.47	0.49
1:D:543:VAL:HG13	1:D:597:SER:HB2	1.94	0.49
1:D:692:ARG:HG2	1:D:700:TYR:CG	2.47	0.49
1:B:399:THR:OG1	1:B:406:VAL:HG21	2.12	0.49
1:C:494:PRO:HA	1:C:732:TYR:O	2.12	0.49
1:C:742:LEU:O	1:C:746:VAL:HG13	2.12	0.49
2:G:127:PHE:O	2:G:128:TYR:C	2.50	0.49
2:G:135:ILE:HG23	2:G:201:PHE:HB2	1.95	0.49
1:B:425:CYS:HA	1:B:428:LEU:HB3	1.93	0.49
1:B:450:TYR:CE1	1:B:650:LEU:HD23	2.48	0.49
1:C:675:ARG:HH22	1:D:770:LYS:HA	1.77	0.49
1:C:689:GLY:O	1:C:693:VAL:HG23	2.13	0.49
2:E:84:PRO:HD2	2:E:99:ARG:HD3	1.93	0.49
1:B:640:SER:HB2	1:B:669:LYS:HD3	1.94	0.49
1:B:748:LEU:HD23	1:B:751:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:TYR:HA	1:C:424:TYR:HB3	1.95	0.49
1:D:650:LEU:O	1:D:656:LYS:HB2	2.12	0.49
1:A:482:THR:HG21	1:A:654:SER:HB2	1.94	0.49
5:B:1003:POV:H35A	5:B:1003:POV:H25	1.95	0.49
1:C:409:LYS:HG2	1:C:422:GLU:HB3	1.95	0.49
1:C:753:LEU:HB3	1:C:758:VAL:HB	1.95	0.49
1:D:480:THR:HG21	1:D:730:LYS:HD2	1.94	0.49
1:A:480:THR:CG2	1:A:730:LYS:HB3	2.43	0.49
1:A:628:ARG:NH1	1:A:785:SER:HB3	2.28	0.49
1:C:409:LYS:HA	1:C:422:GLU:HG2	1.95	0.49
1:A:435:HIS:ND1	1:A:752:LYS:HD3	2.27	0.48
1:A:506:LYS:HB2	1:A:719:ASP:HA	1.94	0.48
1:C:489:ILE:HD11	1:C:491:PHE:CZ	2.48	0.48
1:D:436:CYS:SG	1:D:746:VAL:HA	2.53	0.48
1:D:492:SER:HB2	1:D:747:ASN:HB2	1.96	0.48
2:F:40:CYS:O	2:F:78:LYS:HG2	2.14	0.48
1:C:753:LEU:HD22	1:C:758:VAL:HG21	1.94	0.48
1:D:692:ARG:HB3	1:D:700:TYR:CD2	2.47	0.48
1:A:412:HIS:HB2	1:A:420:ARG:HG2	1.96	0.48
1:D:743:ARG:O	1:D:747:ASN:N	2.43	0.48
1:B:640:SER:HB3	1:B:670:MET:HG3	1.95	0.48
1:B:633:ILE:HD13	1:B:638:ASP:HB3	1.96	0.48
2:F:104:SER:O	2:F:106:ILE:N	2.46	0.48
2:H:40:CYS:O	2:H:78:LYS:HG2	2.14	0.48
1:A:765:LYS:O	1:A:770:LYS:HG2	2.14	0.48
1:B:445:VAL:HG21	1:B:462:GLY:HA2	1.96	0.48
1:B:488:VAL:O	1:B:738:LYS:HB2	2.14	0.48
1:B:396:VAL:HA	1:B:441:LYS:HB3	1.96	0.48
1:C:502:ILE:HG12	1:C:639:LEU:CD1	2.44	0.48
1:A:498:LEU:HD13	1:A:730:LYS:O	2.13	0.47
1:C:675:ARG:HA	1:C:682:PHE:CZ	2.50	0.47
2:F:129:LYS:HB2	2:F:129:LYS:HE3	1.65	0.47
1:B:395:VAL:HG12	1:B:474:ILE:HG22	1.96	0.47
1:B:796:PHE:HB3	2:F:154:ILE:HD13	1.96	0.47
1:B:800:VAL:HG11	2:F:151:ILE:HD11	1.95	0.47
2:H:67:CYS:HA	2:H:77:CYS:HA	1.96	0.47
2:G:30:THR:HG21	2:G:178:TRP:CH2	2.49	0.47
1:B:424:TYR:CE2	1:B:762:LEU:HB3	2.49	0.47
1:B:445:VAL:HG21	1:B:462:GLY:C	2.34	0.47
1:D:435:HIS:ND1	1:D:752:LYS:HG2	2.30	0.47
1:D:453:ARG:HA	1:D:460:TRP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:TYR:HB3	1:A:425:CYS:HB2	1.96	0.47
1:A:467:LEU:HD22	1:A:737:PRO:HD3	1.95	0.47
1:A:499:GLY:HA2	1:A:730:LYS:HG2	1.97	0.47
1:B:754:SER:HA	1:B:759:LEU:HD11	1.96	0.47
1:D:406:VAL:HA	1:D:426:VAL:HG23	1.97	0.47
2:E:41:LYS:HB2	2:E:76:LEU:HB3	1.97	0.47
2:H:31:ASP:HA	2:H:62:GLY:HA3	1.97	0.47
1:A:503:MET:HG2	1:A:693:VAL:HG11	1.97	0.47
1:B:693:VAL:CG2	1:B:702:TYR:HB2	2.45	0.47
1:D:415:LEU:HB3	1:D:419:GLU:CB	2.44	0.47
1:D:467:LEU:HD22	1:D:737:PRO:HD3	1.96	0.47
1:D:742:LEU:O	1:D:746:VAL:HG13	2.14	0.47
2:H:110:LEU:HA	2:H:113:ILE:HD12	1.97	0.47
1:A:604:VAL:CG1	1:B:799:LEU:HA	2.44	0.47
1:A:646:ALA:HB3	1:A:700:TYR:HA	1.96	0.47
1:D:430:ALA:HA	1:D:440:TYR:CE1	2.50	0.46
2:E:70:GLU:HA	2:E:74:LYS:HE3	1.96	0.46
2:E:127:PHE:O	2:E:128:TYR:C	2.51	0.46
2:E:150:ILE:O	2:E:154:ILE:HG12	2.15	0.46
1:B:693:VAL:HG22	1:B:700:TYR:O	2.15	0.46
1:D:480:THR:CG2	1:D:730:LYS:HD2	2.46	0.46
2:H:73:PHE:HB2	2:H:76:LEU:HB2	1.95	0.46
1:B:449:LYS:HB3	1:B:652:SER:CB	2.45	0.46
1:B:714:GLN:HG3	1:B:768:TYR:HD1	1.80	0.46
1:C:649:THR:O	1:C:682:PHE:HA	2.14	0.46
1:B:493:LYS:O	1:B:750:VAL:HG11	2.16	0.46
1:B:498:LEU:HD22	1:B:730:LYS:HG3	1.97	0.46
1:B:397:VAL:CG2	1:B:440:TYR:HB2	2.46	0.46
1:B:397:VAL:HG13	1:B:476:ILE:N	2.26	0.46
1:B:496:MET:HG2	1:B:707:THR:HG21	1.98	0.46
1:C:505:LYS:HG2	1:C:697:LYS:HA	1.98	0.46
1:C:707:THR:HG22	1:C:763:LYS:HZ2	1.80	0.46
2:G:104:SER:O	2:G:106:ILE:N	2.48	0.46
1:B:447:ASP:HB2	1:B:449:LYS:HE3	1.97	0.46
1:B:485:ARG:HD2	1:B:491:PHE:CE2	2.50	0.46
1:B:639:LEU:HD13	1:B:647:TYR:CG	2.50	0.46
1:B:418:ASN:HB3	1:B:442:LEU:HD12	1.98	0.46
1:C:672:THR:HA	1:C:675:ARG:HH21	1.81	0.46
1:D:397:VAL:HG22	1:D:474:ILE:CG2	2.46	0.46
2:E:5:ASP:HB2	2:E:8:VAL:CG1	2.46	0.46
2:H:31:ASP:OD2	2:H:65:ARG:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:ILE:HG23	1:B:639:LEU:HD11	1.97	0.45
1:A:405:TYR:CZ	1:A:478:PRO:HB3	2.52	0.45
1:A:412:HIS:HA	1:A:415:LEU:HB2	1.97	0.45
1:A:545:ARG:HG2	1:A:551:TRP:CZ2	2.50	0.45
1:A:765:LYS:O	1:A:769:ASP:HB2	2.16	0.45
1:B:645:ILE:HG12	1:B:699:LYS:HA	1.98	0.45
1:B:647:TYR:HA	1:B:701:ALA:O	2.16	0.45
2:E:125:SER:O	2:E:129:LYS:HG3	2.17	0.45
2:H:5:ASP:HB2	2:H:8:VAL:HG13	1.98	0.45
1:A:742:LEU:HB3	1:A:746:VAL:HG13	1.98	0.45
1:B:686:THR:HA	1:B:702:TYR:OH	2.15	0.45
1:D:436:CYS:HB3	1:D:745:PRO:CB	2.46	0.45
1:D:531:PHE:HZ	2:E:184:ALA:HB1	1.81	0.45
2:F:6:ARG:HH12	2:F:204:ARG:HD2	1.81	0.45
1:B:500:ILE:HG12	1:B:655:THR:HG23	1.99	0.45
1:C:503:MET:SD	1:C:690:VAL:HG22	2.56	0.45
1:C:677:ALA:HB3	1:C:681:VAL:HG22	1.97	0.45
1:C:690:VAL:O	1:C:694:ARG:HG3	2.17	0.45
1:A:515:PHE:HZ	5:A:1003:POV:H23	1.82	0.45
3:A:1001:PLM:H31	4:A:1002:OLC:H24	1.99	0.45
1:C:503:MET:HB2	1:C:503:MET:HE3	1.82	0.45
1:D:477:ALA:HB1	1:D:478:PRO:HD2	1.98	0.45
2:F:60:HIS:HB2	2:F:67:CYS:HB2	1.99	0.45
2:F:113:ILE:O	2:F:117:MET:HG2	2.16	0.45
1:B:467:LEU:HB2	1:B:489:ILE:HG21	1.98	0.45
1:C:658:PHE:O	1:C:662:SER:N	2.50	0.45
1:D:482:THR:HG21	1:D:654:SER:HB2	1.97	0.45
1:B:500:ILE:HD11	1:B:658:PHE:HB3	1.98	0.45
1:B:686:THR:HG23	1:B:702:TYR:HE2	1.81	0.45
1:A:583:ALA:O	1:A:609:THR:HG21	2.16	0.45
1:C:438:PHE:CE1	1:C:440:TYR:HB3	2.51	0.45
1:C:490:ASP:HB2	1:C:736:THR:OG1	2.17	0.44
1:B:683:VAL:HG11	1:B:689:GLY:HA2	1.99	0.44
1:C:503:MET:O	1:C:701:ALA:HA	2.17	0.44
1:D:453:ARG:O	1:D:453:ARG:HG3	2.17	0.44
1:A:800:VAL:HB	2:E:151:ILE:HD11	1.98	0.44
1:B:450:TYR:HB2	1:B:653:GLY:HA2	2.00	0.44
1:D:424:TYR:HA	1:D:766:TRP:CD1	2.52	0.44
1:D:473:ASP:HB3	1:D:742:LEU:HD12	1.98	0.44
2:E:30:THR:HG21	2:E:178:TRP:CH2	2.52	0.44
1:B:481:ILE:HG12	1:B:491:PHE:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:543:VAL:HG11	1:D:597:SER:HB2	1.98	0.44
1:A:416:GLU:C	1:A:420:ARG:HB2	2.38	0.44
1:B:505:LYS:HB3	1:B:698:GLY:N	2.33	0.44
1:C:501:SER:O	1:C:703:LEU:HA	2.17	0.44
1:D:533:TYR:CE1	1:D:580:SER:HB2	2.53	0.44
1:D:647:TYR:HB3	1:D:701:ALA:HB3	1.99	0.44
2:H:159:ALA:O	2:H:160:ASN:C	2.56	0.44
1:B:424:TYR:CD2	1:B:762:LEU:HB3	2.52	0.44
1:B:505:LYS:HB3	1:B:697:LYS:C	2.38	0.44
1:D:505:LYS:CE	1:D:694:ARG:HA	2.47	0.44
2:G:71:GLY:H	2:G:74:LYS:HB3	1.83	0.44
1:D:460:TRP:CE2	1:D:488:VAL:HG21	2.52	0.43
1:D:647:TYR:HA	1:D:701:ALA:O	2.18	0.43
2:H:41:LYS:HG2	2:H:78:LYS:HB3	1.99	0.43
1:A:763:LYS:O	1:A:764:ASN:C	2.55	0.43
1:A:670:MET:O	1:A:674:MET:HG3	2.18	0.43
1:A:764:ASN:HA	1:A:768:TYR:CD2	2.49	0.43
1:B:692:ARG:HB3	1:B:700:TYR:CE2	2.53	0.43
1:C:477:ALA:HB1	1:C:478:PRO:HD2	2.01	0.43
1:C:749:ALA:O	1:C:753:LEU:HG	2.18	0.43
1:B:397:VAL:HG12	1:B:399:THR:HB	1.99	0.43
1:D:716:LYS:HG3	1:D:772:GLU:HB3	1.99	0.43
1:A:671:TRP:HZ3	1:A:682:PHE:CZ	2.36	0.43
1:B:492:SER:OG	1:B:750:VAL:HG21	2.19	0.43
1:C:397:VAL:HG23	1:C:440:TYR:HB2	2.00	0.43
1:D:533:TYR:HE1	1:D:580:SER:HB2	1.84	0.43
2:G:57:VAL:O	2:G:59:THR:HG23	2.18	0.43
1:A:803:LEU:HD21	1:D:536:VAL:HG22	2.01	0.43
1:B:450:TYR:OH	1:B:478:PRO:HG2	2.19	0.43
1:C:690:VAL:HG11	1:C:712:ILE:HG21	1.99	0.43
1:C:502:ILE:HD12	1:C:724:GLY:HA3	2.01	0.43
1:C:648:GLY:HA3	1:C:681:VAL:HB	2.01	0.43
1:C:690:VAL:CG1	1:C:712:ILE:HG21	2.49	0.43
2:E:129:LYS:C	2:E:131:ARG:H	2.22	0.43
1:A:590:ASP:OD1	1:A:590:ASP:N	2.50	0.43
1:C:606:TRP:CG	1:D:587:GLN:HG3	2.53	0.43
1:D:467:LEU:HD11	1:D:475:ALA:HB2	2.01	0.43
2:E:10:MET:HA	2:E:13:THR:HG22	2.01	0.43
1:A:460:TRP:NE1	1:A:488:VAL:HG11	2.33	0.43
1:B:463:MET:SD	1:B:477:ALA:HB3	2.59	0.43
1:C:482:THR:OG1	1:C:485:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:147:LEU:O	2:F:150:ILE:HG22	2.18	0.43
1:B:713:GLU:HG3	1:B:720:THR:O	2.19	0.42
1:C:450:TYR:HE2	1:C:478:PRO:HG2	1.84	0.42
1:C:656:LYS:HE2	1:C:660:ARG:HH22	1.84	0.42
1:A:664:ILE:HG22	1:A:666:VAL:HB	2.00	0.42
1:B:397:VAL:HG21	1:B:440:TYR:HB2	2.01	0.42
1:B:479:LEU:HG	1:B:491:PHE:CZ	2.55	0.42
1:C:492:SER:HB3	1:C:746:VAL:HG23	2.00	0.42
1:A:407:MET:O	1:A:408:MET:C	2.57	0.42
1:B:505:LYS:H	1:B:698:GLY:HA2	1.84	0.42
2:E:61:SER:HA	2:E:66:THR:HA	2.02	0.42
2:H:40:CYS:HB3	2:H:68:CYS:HB2	1.28	0.42
1:C:453:ARG:O	1:C:454:ASP:C	2.58	0.42
1:C:675:ARG:HA	1:C:682:PHE:HE2	1.84	0.42
2:E:40:CYS:HB2	2:E:41:LYS:H	1.67	0.42
2:F:127:PHE:O	2:F:128:TYR:C	2.58	0.42
2:H:6:ARG:HH12	2:H:10:MET:HB2	1.85	0.42
1:B:418:ASN:HA	1:B:421:TYR:HD2	1.85	0.42
1:B:765:LYS:HA	1:B:769:ASP:HB2	2.01	0.42
1:C:490:ASP:O	1:C:735:ALA:HA	2.20	0.42
1:D:651:ASP:CB	1:D:682:PHE:HB3	2.50	0.42
1:B:696:SER:HB3	1:B:699:LYS:HB2	2.01	0.42
1:B:763:LYS:O	1:B:764:ASN:C	2.57	0.42
1:C:706:SER:HB3	1:C:726:ASN:OD1	2.19	0.42
1:C:763:LYS:O	1:C:767:TRP:HB2	2.19	0.42
1:D:696:SER:HB3	1:D:699:LYS:CB	2.50	0.42
1:D:659:PHE:CG	1:D:674:MET:HE1	2.55	0.42
2:F:42:THR:O	2:F:43:LYS:C	2.57	0.42
2:H:41:LYS:HB3	2:H:76:LEU:HD13	2.01	0.42
1:A:659:PHE:CD1	1:A:667:PHE:HB3	2.55	0.42
1:A:409:LYS:HG3	1:A:419:GLU:O	2.20	0.41
1:B:500:ILE:HD11	1:B:655:THR:HA	2.01	0.41
1:C:690:VAL:HG21	1:C:712:ILE:HG13	2.02	0.41
1:A:418:ASN:HA	1:A:442:LEU:HD12	2.02	0.41
1:A:647:TYR:CE1	1:A:670:MET:HG2	2.54	0.41
1:B:395:VAL:HG12	1:B:474:ILE:CG2	2.50	0.41
1:B:409:LYS:N	1:B:412:HIS:HB3	2.35	0.41
1:B:475:ALA:N	1:B:735:ALA:O	2.53	0.41
1:C:425:CYS:HA	1:C:428:LEU:HB3	2.03	0.41
1:D:404:PRO:HB3	1:D:711:TYR:CZ	2.54	0.41
1:B:515:PHE:CG	4:B:1002:OLC:H21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:LEU:HD23	1:B:742:LEU:HA	1.81	0.41
1:B:766:TRP:HA	1:B:770:LYS:HB2	2.01	0.41
2:E:131:ARG:O	2:E:132:HIS:C	2.58	0.41
1:B:633:ILE:HD13	1:B:633:ILE:HA	1.87	0.41
1:B:693:VAL:HG23	1:B:702:TYR:HB2	2.00	0.41
1:C:763:LYS:HA	1:C:767:TRP:CE3	2.55	0.41
2:G:207:GLN:O	2:G:210:ALA:HB3	2.21	0.41
1:A:475:ALA:HB3	1:A:735:ALA:HB3	2.02	0.41
1:B:690:VAL:HG13	1:B:712:ILE:HG21	2.02	0.41
1:C:438:PHE:CD2	1:C:742:LEU:HD11	2.55	0.41
1:C:699:LYS:HA	1:C:699:LYS:HD3	1.73	0.41
1:A:408:MET:H	1:A:408:MET:HG2	1.65	0.41
1:B:646:ALA:O	1:B:701:ALA:N	2.46	0.41
1:C:485:ARG:HB2	1:C:485:ARG:HE	1.77	0.41
1:C:674:MET:SD	1:C:703:LEU:HD12	2.61	0.41
1:C:678:GLU:HA	1:C:679:PRO:C	2.40	0.41
1:C:743:ARG:O	1:C:746:VAL:HG22	2.20	0.41
1:D:498:LEU:HB3	1:D:707:THR:HG23	2.02	0.41
1:D:639:LEU:HD23	1:D:639:LEU:HA	1.84	0.41
1:C:460:TRP:NE1	1:C:488:VAL:HG11	2.34	0.41
1:C:618:ALA:O	1:C:619:ASN:C	2.59	0.41
1:D:651:ASP:CA	1:D:682:PHE:HB3	2.51	0.41
2:H:70:GLU:H	2:H:74:LYS:HG3	1.85	0.41
1:D:505:LYS:HD2	1:D:505:LYS:HA	1.66	0.41
1:D:533:TYR:OH	1:D:577:LEU:HB3	2.20	0.41
1:A:672:THR:HA	1:A:675:ARG:HE	1.86	0.41
1:A:744:THR:HB	1:A:745:PRO:HD3	2.03	0.41
1:B:463:MET:HE3	1:B:479:LEU:HD13	2.03	0.41
1:B:486:GLU:OE2	1:B:491:PHE:HB2	2.20	0.41
1:D:648:GLY:HA3	1:D:681:VAL:O	2.21	0.41
1:D:736:THR:HB	1:D:740:SER:HB3	2.03	0.41
1:D:740:SER:OG	1:D:742:LEU:HB2	2.20	0.41
1:B:639:LEU:HD22	1:B:647:TYR:CD1	2.55	0.41
1:C:635:SER:HA	1:C:724:GLY:HA2	2.02	0.41
1:D:746:VAL:O	1:D:750:VAL:HG23	2.21	0.41
1:A:623:PHE:HA	1:B:784:THR:HG21	2.02	0.40
1:A:736:THR:HB	1:A:740:SER:CB	2.51	0.40
1:B:397:VAL:HG23	1:B:441:LYS:H	1.86	0.40
1:B:463:MET:CE	1:B:479:LEU:HD13	2.52	0.40
1:C:502:ILE:HG12	1:C:639:LEU:HD12	2.02	0.40
1:D:415:LEU:HB3	1:D:419:GLU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:12:LEU:HD12	2:G:12:LEU:HA	1.93	0.40
2:H:41:LYS:CB	2:H:76:LEU:HD13	2.51	0.40
2:H:129:LYS:O	2:H:130:THR:HG22	2.21	0.40
1:B:489:ILE:HD12	1:B:735:ALA:HB1	2.03	0.40
1:B:404:PRO:HB2	1:B:766:TRP:HB3	2.04	0.40
1:B:433:ALA:O	1:B:437:GLY:N	2.54	0.40
1:C:714:GLN:HG3	1:C:768:TYR:HD1	1.86	0.40
2:E:104:SER:O	2:E:106:ILE:N	2.53	0.40
1:A:574:PHE:O	1:A:575:ASN:CB	2.70	0.40
1:A:606:TRP:CG	1:B:587:GLN:HG3	2.56	0.40
1:B:445:VAL:HG13	1:B:448:GLY:HA2	2.03	0.40
1:A:494:PRO:HA	1:A:733:GLY:CA	2.49	0.40
1:C:520:PRO:HB3	1:C:619:ASN:HB3	2.04	0.40
1:D:424:TYR:HB2	1:D:766:TRP:HB2	2.02	0.40
1:D:493:LYS:HD3	1:D:493:LYS:HA	1.83	0.40
1:D:639:LEU:HD13	1:D:647:TYR:CD2	2.57	0.40
2:E:60:HIS:NE2	2:E:67:CYS:HB3	2.37	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	391/883 (44%)	359 (92%)	26 (7%)	6 (2%)	10 38
1	B	390/883 (44%)	370 (95%)	18 (5%)	2 (0%)	29 64
1	C	388/883 (44%)	369 (95%)	16 (4%)	3 (1%)	19 53
1	D	389/883 (44%)	358 (92%)	29 (8%)	2 (0%)	29 64
2	E	169/323 (52%)	156 (92%)	10 (6%)	3 (2%)	8 33
2	F	170/323 (53%)	157 (92%)	12 (7%)	1 (1%)	25 60
2	G	169/323 (52%)	160 (95%)	6 (4%)	3 (2%)	8 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	169/323 (52%)	153 (90%)	14 (8%)	2 (1%)	13	43
All	All	2235/4824 (46%)	2082 (93%)	131 (6%)	22 (1%)	20	48

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	ASP
1	B	456	ASP
1	C	456	ASP
1	D	456	ASP
1	D	646	ALA
2	E	132	HIS
2	E	103	ALA
1	A	453	ARG
1	A	455	ALA
1	A	575	ASN
1	C	507	PRO
2	H	61	SER
1	A	417	GLY
1	A	574	PHE
1	C	405	TYR
2	G	132	HIS
2	E	40	CYS
2	F	105	SER
2	G	40	CYS
2	G	128	TYR
2	H	70	GLU
1	B	474	ILE

### 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	316/757 (42%)	294 (93%)	22 (7%)	15	43
1	B	313/757 (41%)	295 (94%)	18 (6%)	20	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	311/757 (41%)	284 (91%)	27 (9%)	10	33
1	D	311/757 (41%)	291 (94%)	20 (6%)	17	47
2	E	141/275 (51%)	119 (84%)	22 (16%)	2	11
2	F	142/275 (52%)	118 (83%)	24 (17%)	2	9
2	G	142/275 (52%)	131 (92%)	11 (8%)	13	39
2	H	142/275 (52%)	126 (89%)	16 (11%)	6	21
All	All	1818/4128 (44%)	1658 (91%)	160 (9%)	13	33

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	414	MET
1	A	420	ARG
1	A	453	ARG
1	A	498	LEU
1	A	594	ARG
1	A	627	GLU
1	A	669	LYS
1	A	673	TYR
1	A	692	ARG
1	A	699	LYS
1	A	708	MET
1	A	728	ASP
1	A	752	LYS
1	A	756	GLN
1	A	759	LEU
1	A	760	ASP
1	A	761	LYS
1	A	762	LEU
1	A	764	ASN
1	A	787	LEU
1	A	819	ARG
1	A	821	GLU
1	B	409	LYS
1	B	414	MET
1	B	480	THR
1	B	498	LEU
1	B	543	VAL
1	B	589	CYS
1	B	590	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	650	LEU
1	B	654	SER
1	B	699	LYS
1	B	708	MET
1	B	743	ARG
1	B	759	LEU
1	B	760	ASP
1	B	762	LEU
1	B	770	LYS
1	B	787	LEU
1	B	795	VAL
1	C	407	MET
1	C	414	MET
1	C	432	ILE
1	C	474	ILE
1	C	485	ARG
1	C	489	ILE
1	C	498	LEU
1	C	595	SER
1	C	623	PHE
1	C	633	ILE
1	C	641	LYS
1	C	675	ARG
1	C	676	SER
1	C	686	THR
1	C	699	LYS
1	C	708	MET
1	C	728	ASP
1	C	742	LEU
1	C	743	ARG
1	C	759	LEU
1	C	761	LYS
1	C	762	LEU
1	C	763	LYS
1	C	768	TYR
1	C	770	LYS
1	C	787	LEU
1	C	816	TYR
1	D	438	PHE
1	D	474	ILE
1	D	496	MET
1	D	498	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	505	LYS
1	D	506	LYS
1	D	542	LEU
1	D	547	SER
1	D	591	ILE
1	D	597	SER
1	D	623	PHE
1	D	626	VAL
1	D	692	ARG
1	D	708	MET
1	D	738	LYS
1	D	754	SER
1	D	759	LEU
1	D	762	LEU
1	D	770	LYS
1	D	808	LEU
2	E	5	ASP
2	E	6	ARG
2	E	30	THR
2	E	31	ASP
2	E	40	CYS
2	E	57	VAL
2	E	66	THR
2	E	69	LEU
2	E	70	GLU
2	E	74	LYS
2	E	76	LEU
2	E	78	LYS
2	E	93	THR
2	E	102	ARG
2	E	127	PHE
2	E	129	LYS
2	E	133	ASN
2	E	134	ILE
2	E	135	ILE
2	E	137	SER
2	E	186	SER
2	E	208	LEU
2	F	11	LEU
2	F	28	VAL
2	F	31	ASP
2	F	37	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	40	CYS
2	F	43	LYS
2	F	61	SER
2	F	66	THR
2	F	69	LEU
2	F	70	GLU
2	F	73	PHE
2	F	74	LYS
2	F	78	LYS
2	F	95	GLU
2	F	99	ARG
2	F	125	SER
2	F	127	PHE
2	F	128	TYR
2	F	129	LYS
2	F	130	THR
2	F	134	ILE
2	F	150	ILE
2	F	200	MET
2	F	208	LEU
2	G	6	ARG
2	G	12	LEU
2	G	40	CYS
2	G	55	GLU
2	G	60	HIS
2	G	65	ARG
2	G	76	LEU
2	G	129	LYS
2	G	131	ARG
2	G	134	ILE
2	G	208	LEU
2	H	6	ARG
2	H	8	VAL
2	H	37	ARG
2	H	40	CYS
2	H	41	LYS
2	H	42	THR
2	H	43	LYS
2	H	65	ARG
2	H	69	LEU
2	H	70	GLU
2	H	73	PHE

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Mol	Chain	Res	Type
2	H	74	LYS
2	H	76	LEU
2	H	96	TYR
2	H	127	PHE
2	H	134	ILE

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

Mol	Chain	Res	Type
1	A	575	ASN
1	A	756	GLN
1	C	435	HIS
1	D	756	GLN
1	D	791	ASN
2	E	133	ASN
2	F	82	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 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
5	POV	D	1003	-	39,39,51	0.36	0	45,47,59	0.45	0
4	OLC	C	1001	-	24,24,24	0.41	0	25,25,25	0.24	0
3	PLM	C	1002	-	17,17,17	0.50	0	17,17,17	0.60	0
3	PLM	F	1301	-	17,17,17	0.50	0	17,17,17	0.52	0
4	OLC	A	1002	-	24,24,24	0.28	0	25,25,25	0.25	0
5	POV	G	1103	-	41,41,51	0.33	0	47,49,59	0.48	0
3	PLM	F	1302	-	15,15,17	0.66	0	15,15,17	0.50	0
5	POV	B	1003	-	41,41,51	0.38	0	47,49,59	0.47	0
4	OLC	B	1002	-	24,24,24	0.32	0	25,25,25	0.27	0
5	POV	A	1003	-	38,38,51	0.37	0	44,46,59	0.51	0
3	PLM	B	1001	-	17,17,17	0.52	0	17,17,17	0.55	0
5	POV	G	1102	-	33,33,51	0.49	0	37,38,59	0.78	1 (2%)
4	OLC	D	1002	-	24,24,24	0.23	0	25,25,25	0.32	0
3	PLM	G	1101	-	17,17,17	0.62	0	17,17,17	0.39	0
3	PLM	D	1001	-	17,17,17	0.53	0	17,17,17	0.55	0
3	PLM	A	1001	-	17,17,17	0.57	0	17,17,17	0.46	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
5	POV	D	1003	-	-	22/43/43/55	-
4	OLC	C	1001	-	-	12/24/24/24	-
3	PLM	C	1002	-	-	5/15/15/15	-
3	PLM	F	1301	-	-	8/15/15/15	-
4	OLC	A	1002	-	-	9/24/24/24	-
5	POV	G	1103	-	-	26/45/45/55	-
3	PLM	F	1302	-	-	7/13/13/15	-
5	POV	B	1003	-	-	16/45/45/55	-
4	OLC	B	1002	-	-	12/24/24/24	-
5	POV	A	1003	-	-	19/42/42/55	-
3	PLM	B	1001	-	-	11/15/15/15	-
5	POV	G	1102	-	-	15/35/35/55	-
4	OLC	D	1002	-	-	15/24/24/24	-
3	PLM	G	1101	-	-	9/15/15/15	-
3	PLM	D	1001	-	-	9/15/15/15	-
3	PLM	A	1001	-	-	9/15/15/15	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	G	1102	POV	O13-P-O14	2.25	119.48	110.68

There are no chirality outliers.

All (204) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1002	OLC	C21-C22-C24-O25
5	A	1003	POV	C1-O11-P-O14
5	A	1003	POV	O12-C11-C12-N
5	D	1003	POV	C1-O11-P-O14
5	G	1102	POV	C1-O11-P-O14
5	G	1102	POV	C22-C21-O21-C2
5	G	1103	POV	C1-O11-P-O14
5	G	1103	POV	O12-C11-C12-N
5	A	1003	POV	O32-C31-O31-C3
5	G	1102	POV	O32-C31-O31-C3
5	G	1102	POV	O22-C21-O21-C2
5	A	1003	POV	C32-C31-O31-C3
5	G	1102	POV	C32-C31-O31-C3
3	D	1001	PLM	C5-C6-C7-C8
5	G	1103	POV	C32-C31-O31-C3
4	B	1002	OLC	C2-C1-O20-C21
4	D	1002	OLC	C2-C1-O20-C21
3	F	1302	PLM	C3-C4-C5-C6
4	D	1002	OLC	O19-C1-O20-C21
3	F	1302	PLM	C1-C2-C3-C4
3	G	1101	PLM	C1-C2-C3-C4
5	D	1003	POV	C31-C32-C33-C34
4	B	1002	OLC	O19-C1-O20-C21
5	G	1102	POV	C311-C310-C39-C38
4	D	1002	OLC	O23-C22-C24-O25
4	C	1001	OLC	C1-C2-C3-C4
5	A	1003	POV	C31-C32-C33-C34
5	D	1003	POV	C21-C22-C23-C24
3	F	1302	PLM	C9-CA-CB-CC
5	G	1102	POV	C21-C22-C23-C24
5	G	1103	POV	O32-C31-O31-C3
5	A	1003	POV	C1-O11-P-O12
5	G	1103	POV	C1-O11-P-O12
4	B	1002	OLC	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	B	1003	POV	C25-C26-C27-C28
4	D	1002	OLC	C11-C12-C13-C14
5	G	1102	POV	C24-C25-C26-C27
5	B	1003	POV	O22-C21-O21-C2
3	D	1001	PLM	CA-CB-CC-CD
5	G	1103	POV	C2-C1-O11-P
3	G	1101	PLM	CC-CD-CE-CF
5	G	1102	POV	C25-C26-C27-C28
3	D	1001	PLM	C1-C2-C3-C4
5	G	1102	POV	C37-C38-C39-C310
4	A	1002	OLC	C11-C12-C13-C14
5	G	1103	POV	C34-C35-C36-C37
4	A	1002	OLC	C21-C22-C24-O25
4	D	1002	OLC	O20-C21-C22-O23
5	G	1103	POV	C23-C24-C25-C26
3	B	1001	PLM	C1-C2-C3-C4
4	A	1002	OLC	C1-C2-C3-C4
5	G	1103	POV	C31-C32-C33-C34
3	C	1002	PLM	C9-CA-CB-CC
3	F	1301	PLM	C8-C9-CA-CB
4	C	1001	OLC	C11-C12-C13-C14
3	A	1001	PLM	C5-C6-C7-C8
3	B	1001	PLM	C3-C4-C5-C6
3	D	1001	PLM	C3-C4-C5-C6
5	D	1003	POV	C23-C24-C25-C26
5	A	1003	POV	C1-C2-C3-O31
5	B	1003	POV	C22-C21-O21-C2
4	A	1002	OLC	O23-C22-C24-O25
3	B	1001	PLM	CB-CC-CD-CE
3	D	1001	PLM	C7-C8-C9-CA
4	C	1001	OLC	C2-C3-C4-C5
5	D	1003	POV	C33-C34-C35-C36
3	A	1001	PLM	C2-C3-C4-C5
5	D	1003	POV	C22-C23-C24-C25
3	B	1001	PLM	C5-C6-C7-C8
3	F	1302	PLM	CB-CC-CD-CE
5	D	1003	POV	C32-C33-C34-C35
5	D	1003	POV	C34-C35-C36-C37
3	B	1001	PLM	C8-C9-CA-CB
5	B	1003	POV	C21-C22-C23-C24
4	C	1001	OLC	O20-C21-C22-C24
3	F	1302	PLM	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	B	1001	PLM	CA-CB-CC-CD
3	A	1001	PLM	C3-C4-C5-C6
5	B	1003	POV	O21-C2-C3-O31
5	G	1102	POV	C33-C34-C35-C36
4	C	1001	OLC	C12-C13-C14-C15
5	B	1003	POV	C32-C33-C34-C35
4	B	1002	OLC	C10-C11-C12-C13
3	F	1301	PLM	C2-C3-C4-C5
4	A	1002	OLC	C7-C8-C9-C10
4	D	1002	OLC	C5-C6-C7-C8
5	G	1103	POV	C33-C34-C35-C36
3	G	1101	PLM	CD-CE-CF-CG
3	A	1001	PLM	CC-CD-CE-CF
5	B	1003	POV	C22-C23-C24-C25
4	D	1002	OLC	C6-C7-C8-C9
5	G	1103	POV	C26-C27-C28-C29
3	A	1001	PLM	CD-CE-CF-CG
4	C	1001	OLC	C2-C1-O20-C21
5	D	1003	POV	C22-C21-O21-C2
3	F	1302	PLM	CA-CB-CC-CD
4	C	1001	OLC	O19-C1-O20-C21
3	D	1001	PLM	C6-C7-C8-C9
5	G	1103	POV	C11-C12-N-C15
5	A	1003	POV	O11-C1-C2-C3
5	G	1103	POV	C21-C22-C23-C24
5	G	1102	POV	C2-C1-O11-P
4	D	1002	OLC	C14-C15-C16-C17
4	D	1002	OLC	C15-C16-C17-C18
5	G	1103	POV	C37-C38-C39-C310
5	B	1003	POV	C1-C2-C3-O31
5	A	1003	POV	O22-C21-O21-C2
4	C	1001	OLC	O20-C21-C22-O23
3	B	1001	PLM	C6-C7-C8-C9
5	A	1003	POV	O11-C1-C2-O21
5	G	1102	POV	O11-C1-C2-O21
5	D	1003	POV	O22-C21-O21-C2
5	A	1003	POV	C211-C212-C213-C214
5	B	1003	POV	C211-C212-C213-C214
3	F	1301	PLM	C5-C6-C7-C8
3	D	1001	PLM	C9-CA-CB-CC
5	G	1103	POV	C11-C12-N-C14
4	D	1002	OLC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	B	1001	PLM	C7-C8-C9-CA
4	A	1002	OLC	C4-C5-C6-C7
4	A	1002	OLC	O20-C21-C22-C24
5	D	1003	POV	C3-C2-O21-C21
5	D	1003	POV	C2-C1-O11-P
5	A	1003	POV	C22-C21-O21-C2
3	G	1101	PLM	C2-C3-C4-C5
4	B	1002	OLC	C13-C14-C15-C16
4	B	1002	OLC	C14-C15-C16-C17
5	D	1003	POV	C26-C27-C28-C29
4	A	1002	OLC	C15-C16-C17-C18
3	D	1001	PLM	CB-CC-CD-CE
5	A	1003	POV	C11-O12-P-O11
5	B	1003	POV	C11-O12-P-O11
5	A	1003	POV	C1-O11-P-O13
5	G	1103	POV	C1-O11-P-O13
3	A	1001	PLM	CA-CB-CC-CD
4	D	1002	OLC	O20-C21-C22-C24
5	G	1103	POV	C12-C11-O12-P
3	F	1302	PLM	C7-C8-C9-CA
3	G	1101	PLM	C6-C7-C8-C9
3	G	1101	PLM	C3-C4-C5-C6
5	A	1003	POV	O21-C2-C3-O31
5	G	1103	POV	C11-C12-N-C13
3	F	1301	PLM	C6-C7-C8-C9
5	G	1102	POV	C1-C2-O21-C21
3	F	1301	PLM	C3-C4-C5-C6
5	D	1003	POV	C1-O11-P-O12
3	C	1002	PLM	CA-CB-CC-CD
4	C	1001	OLC	C7-C8-C9-C10
5	B	1003	POV	C2-C1-O11-P
5	A	1003	POV	C27-C28-C29-C210
5	D	1003	POV	C210-C211-C212-C213
5	G	1103	POV	C211-C210-C29-C28
4	D	1002	OLC	C3-C4-C5-C6
5	A	1003	POV	C25-C26-C27-C28
3	A	1001	PLM	CB-CC-CD-CE
5	B	1003	POV	C26-C27-C28-C29
5	G	1103	POV	C210-C211-C212-C213
5	A	1003	POV	C33-C34-C35-C36
4	D	1002	OLC	C7-C8-C9-C10
4	A	1002	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	F	1301	PLM	O2-C1-C2-C3
5	G	1103	POV	C32-C33-C34-C35
4	B	1002	OLC	C11-C12-C13-C14
4	D	1002	OLC	C1-C2-C3-C4
5	G	1103	POV	C22-C23-C24-C25
5	G	1102	POV	O11-C1-C2-C3
3	G	1101	PLM	O1-C1-C2-C3
3	G	1101	PLM	O2-C1-C2-C3
3	B	1001	PLM	O2-C1-C2-C3
3	B	1001	PLM	CC-CD-CE-CF
3	F	1301	PLM	O1-C1-C2-C3
3	D	1001	PLM	C8-C9-CA-CB
3	F	1301	PLM	CA-CB-CC-CD
4	B	1002	OLC	C7-C8-C9-C10
4	C	1001	OLC	C5-C6-C7-C8
5	D	1003	POV	C11-C12-N-C14
4	B	1002	OLC	C4-C5-C6-C7
5	G	1103	POV	O31-C31-C32-C33
4	C	1001	OLC	C9-C10-C11-C12
4	B	1002	OLC	C6-C7-C8-C9
4	C	1001	OLC	C4-C5-C6-C7
3	B	1001	PLM	O1-C1-C2-C3
5	B	1003	POV	C29-C210-C211-C212
5	A	1003	POV	C23-C24-C25-C26
5	B	1003	POV	C23-C24-C25-C26
5	D	1003	POV	O21-C2-C3-O31
5	G	1103	POV	C311-C310-C39-C38
3	G	1101	PLM	CA-CB-CC-CD
5	D	1003	POV	O31-C31-C32-C33
5	G	1103	POV	C29-C210-C211-C212
4	B	1002	OLC	C5-C6-C7-C8
3	C	1002	PLM	O2-C1-C2-C3
5	G	1103	POV	O32-C31-C32-C33
5	B	1003	POV	C27-C28-C29-C210
5	D	1003	POV	C1-O11-P-O13
5	B	1003	POV	C3-C2-O21-C21
3	A	1001	PLM	O1-C1-C2-C3
3	C	1002	PLM	O1-C1-C2-C3
3	C	1002	PLM	CC-CD-CE-CF
5	D	1003	POV	O32-C31-C32-C33
5	D	1003	POV	C27-C28-C29-C210
4	B	1002	OLC	C15-C16-C17-C18

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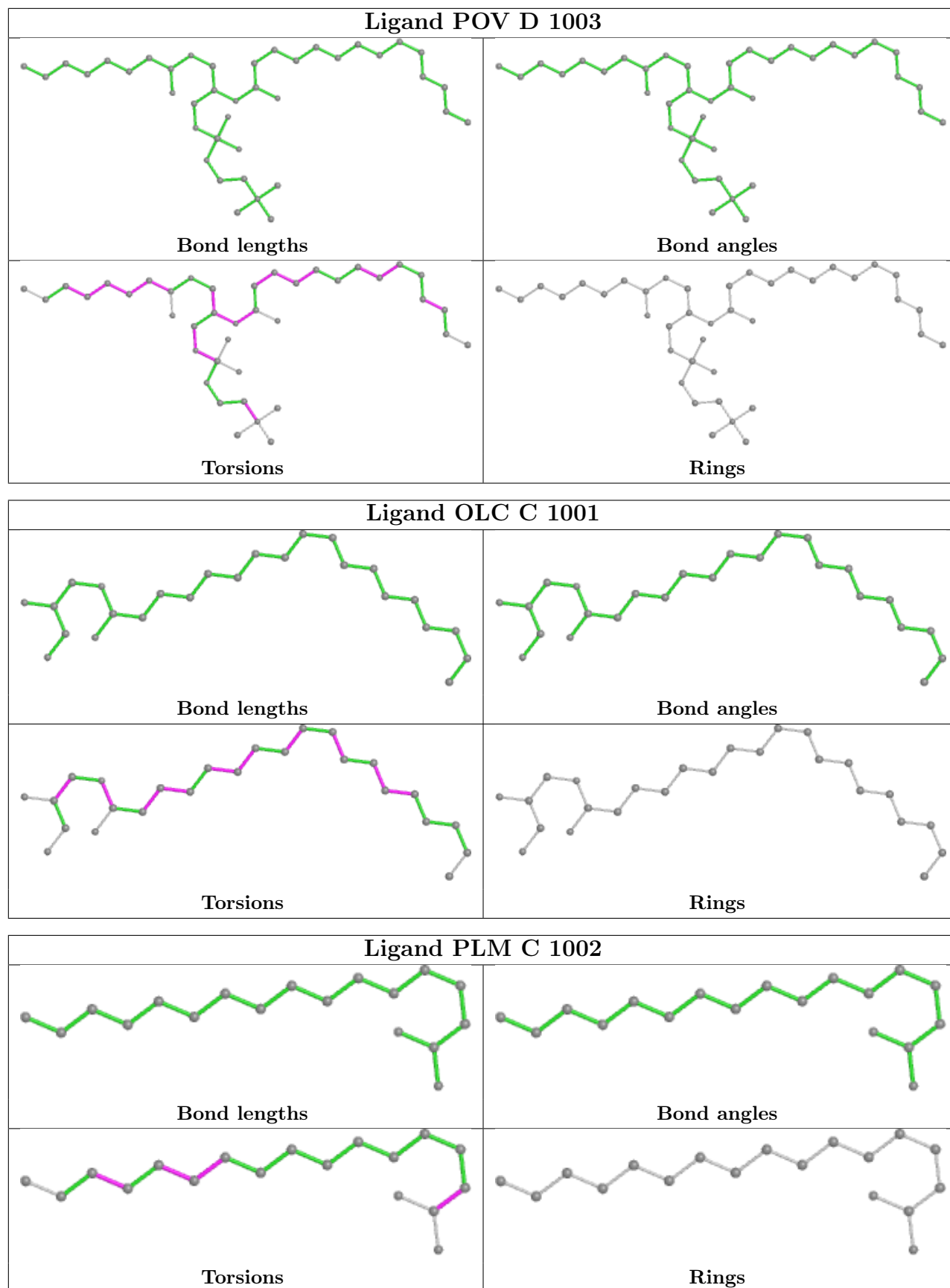
Mol	Chain	Res	Type	Atoms
5	D	1003	POV	C11-C12-N-C13
3	A	1001	PLM	O2-C1-C2-C3

There are no ring outliers.

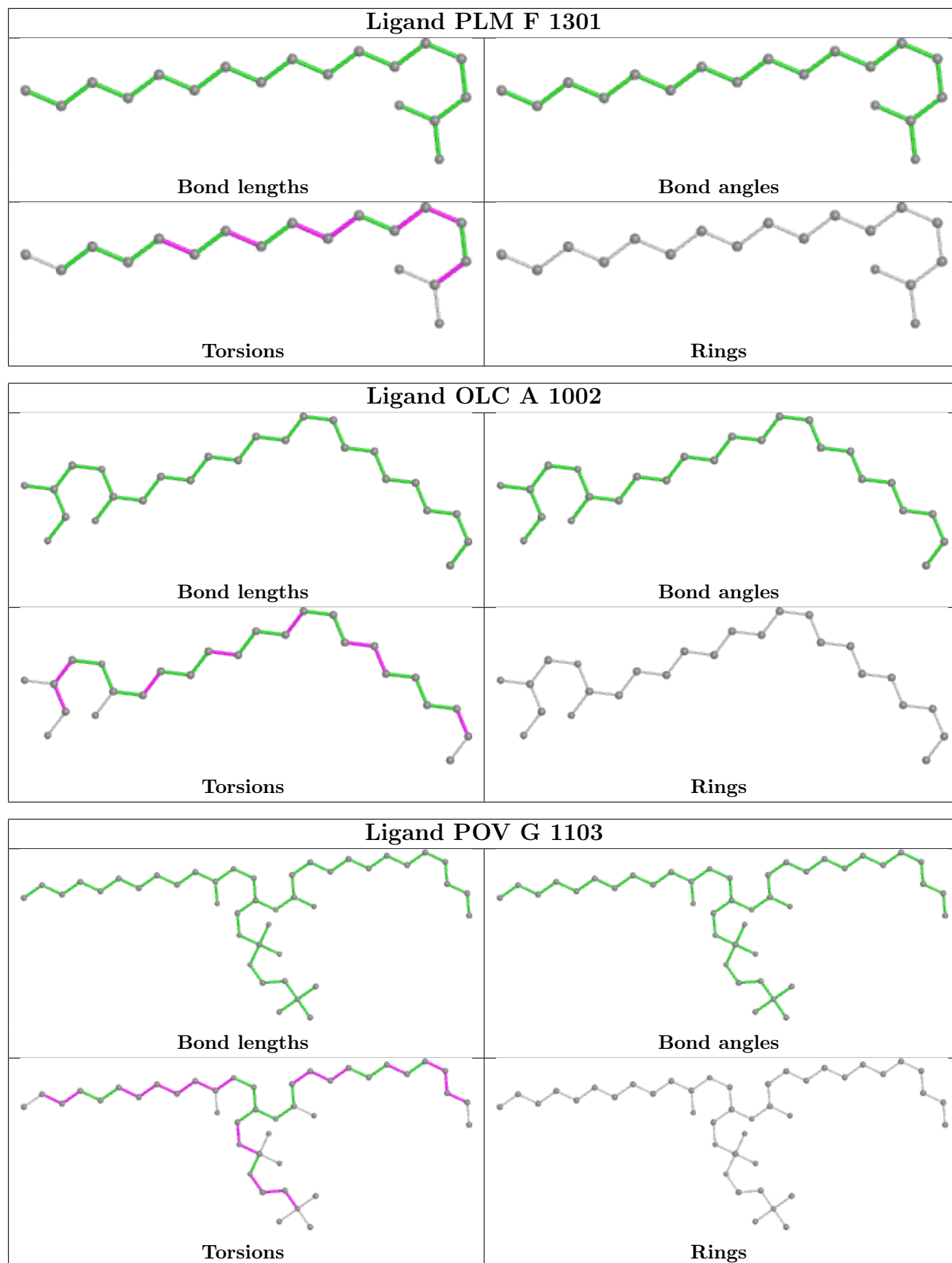
8 monomers are involved in 8 short contacts:

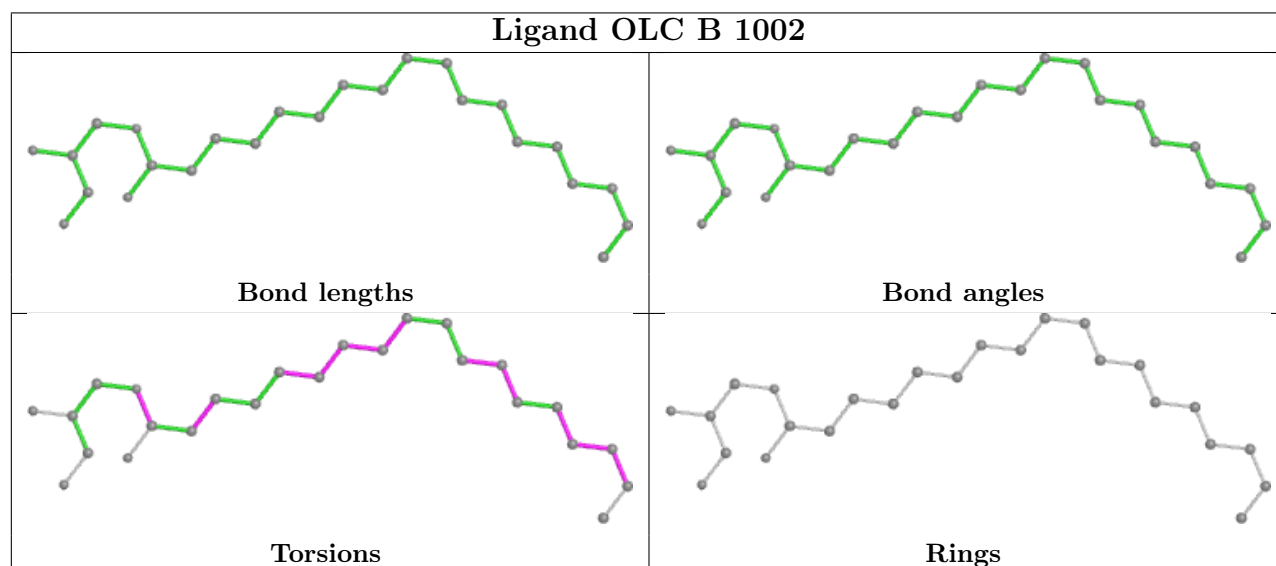
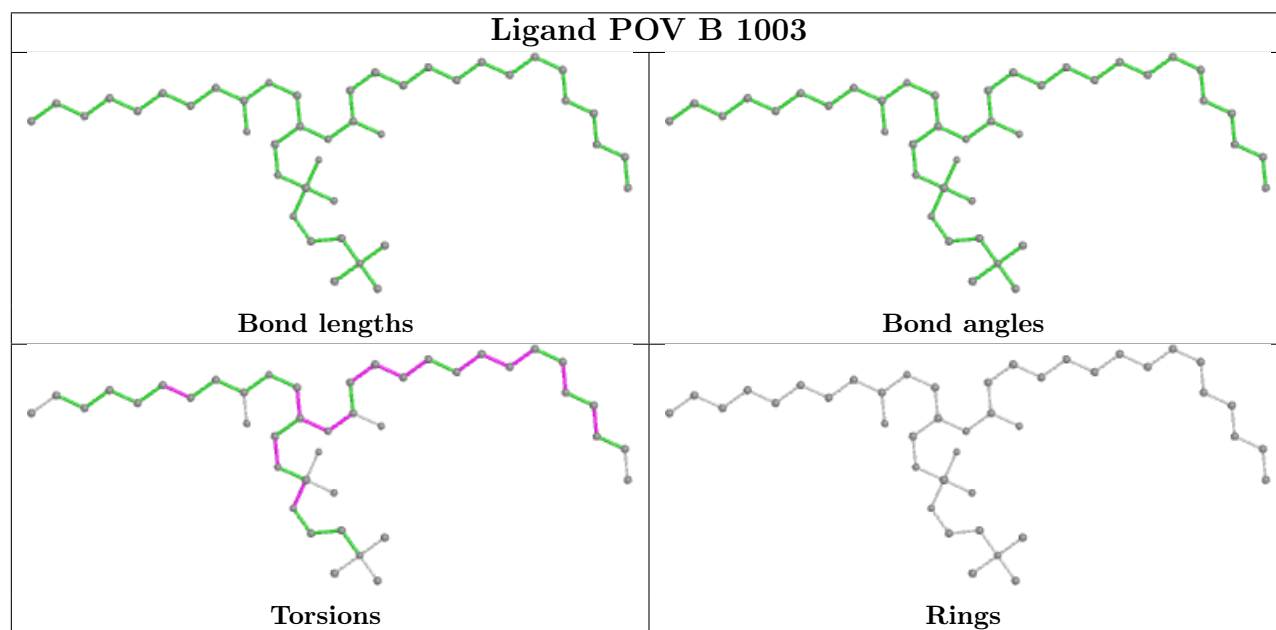
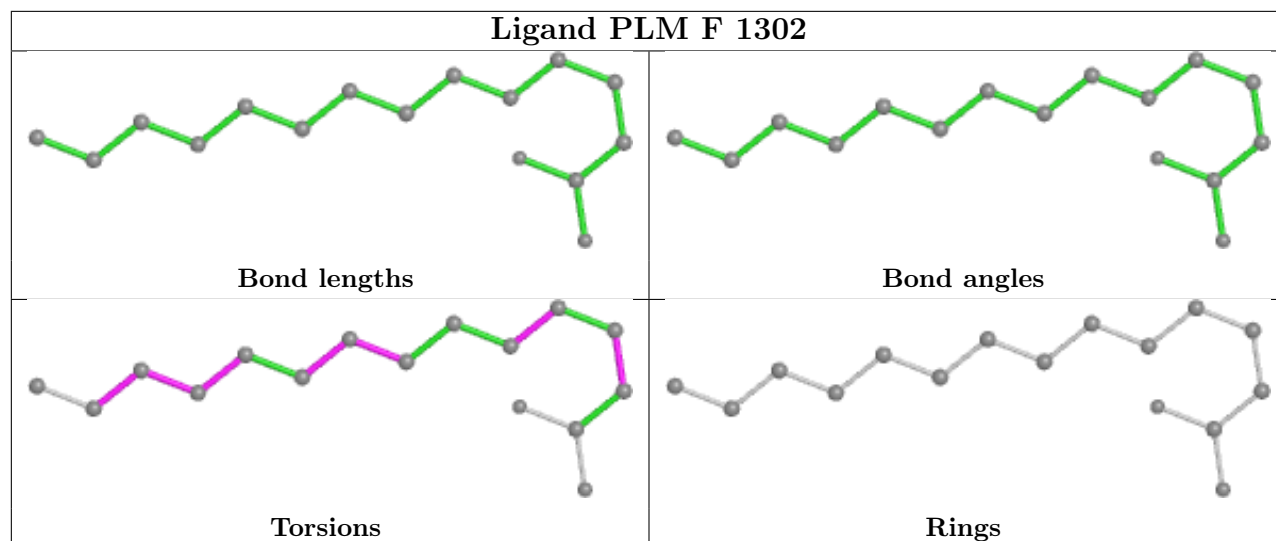
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	OLC	1	0
5	G	1103	POV	1	0
3	F	1302	PLM	1	0
5	B	1003	POV	1	0
4	B	1002	OLC	1	0
5	A	1003	POV	2	0
3	D	1001	PLM	1	0
3	A	1001	PLM	1	0

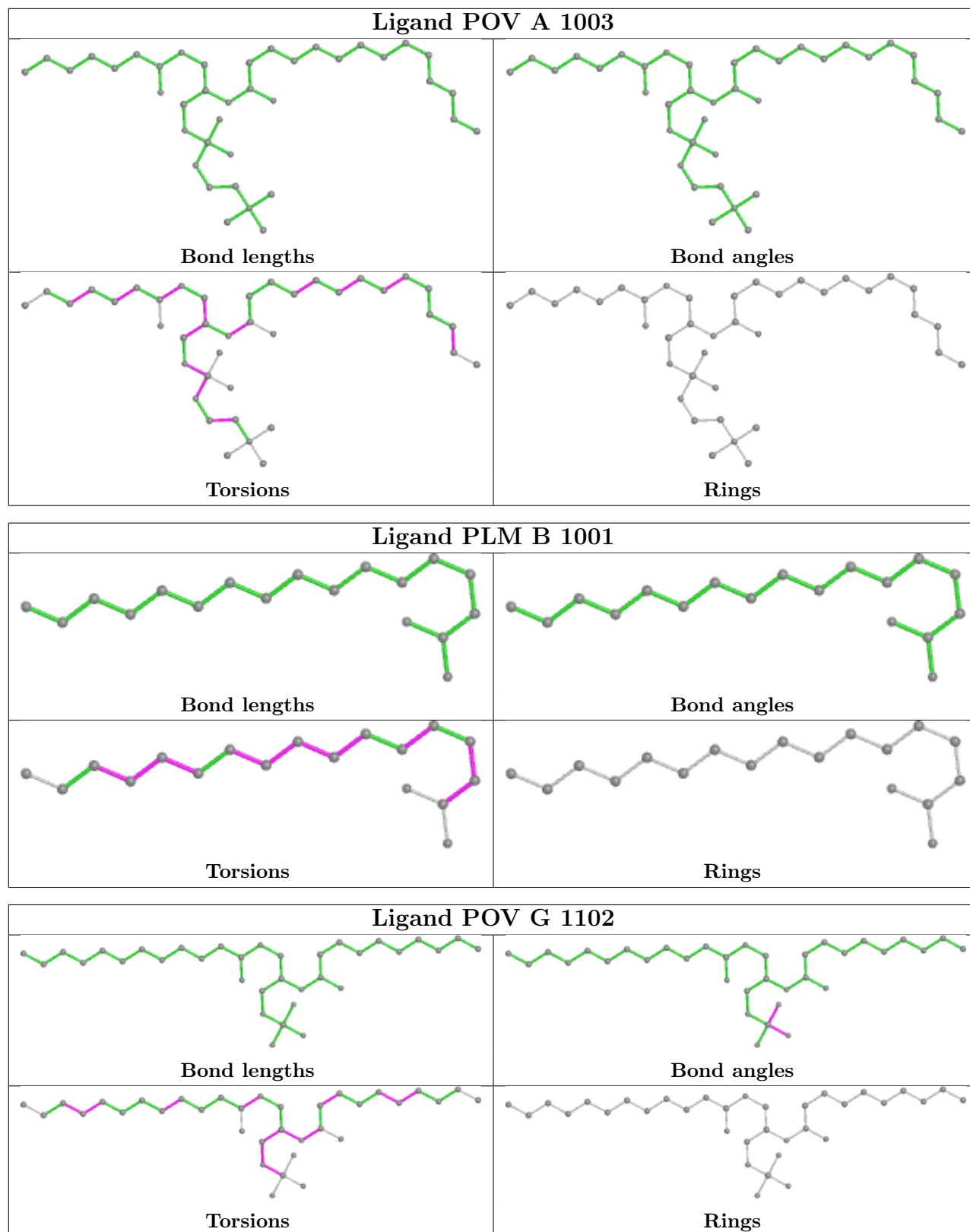
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

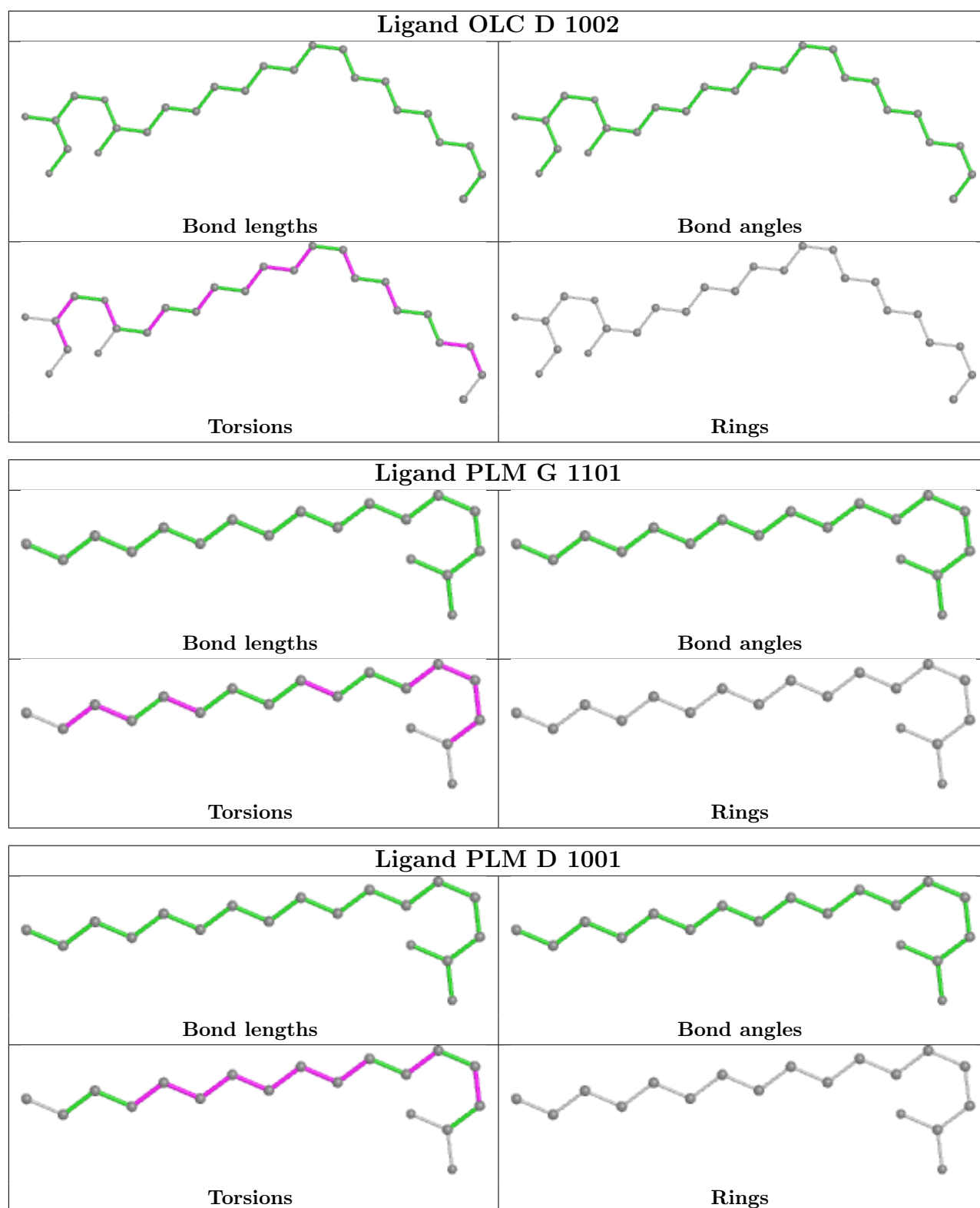


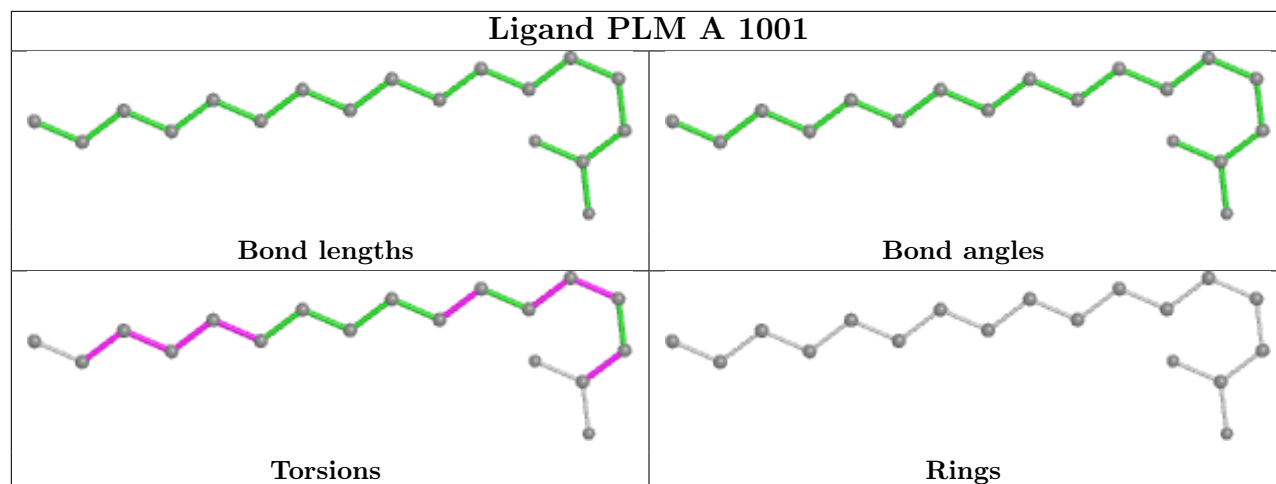












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

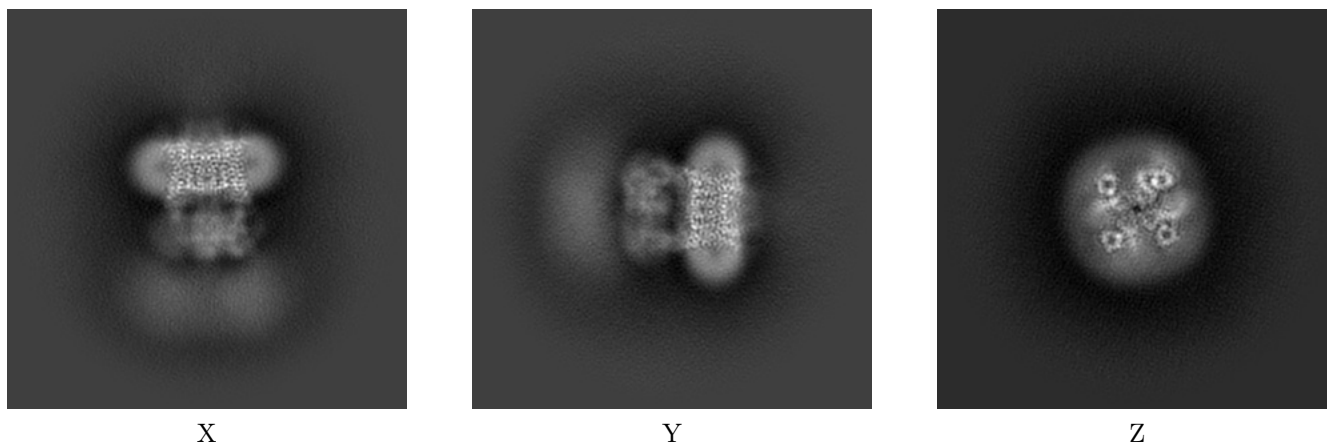
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17392. These allow visual inspection of the internal detail of the map and identification of artifacts.

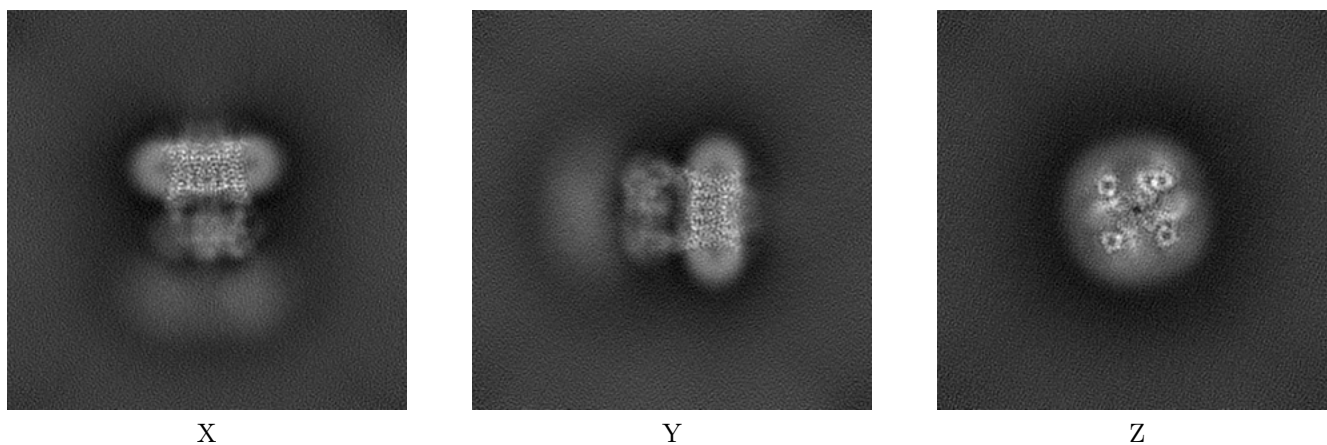
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



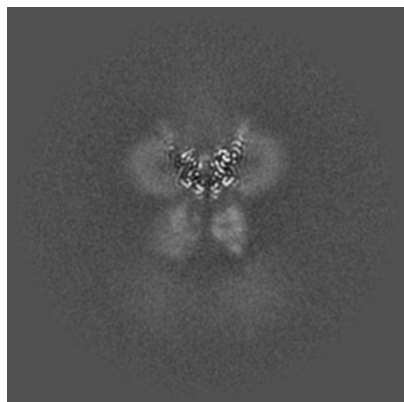
#### 6.1.2 Raw map



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

## 6.2 Central slices [i](#)

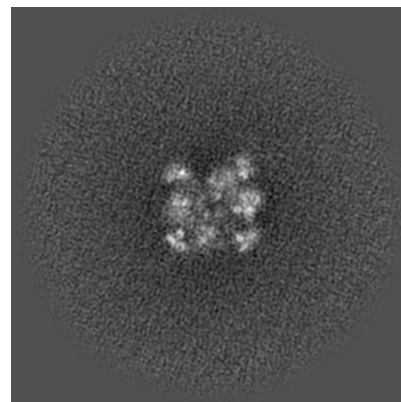
### 6.2.1 Primary map



X Index: 128

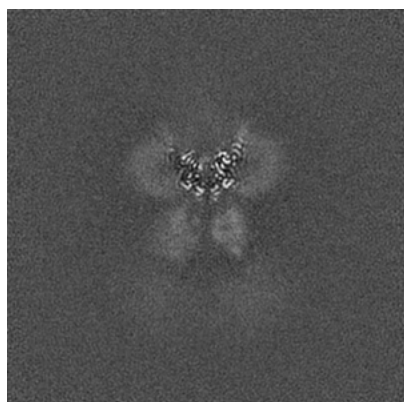


Y Index: 128

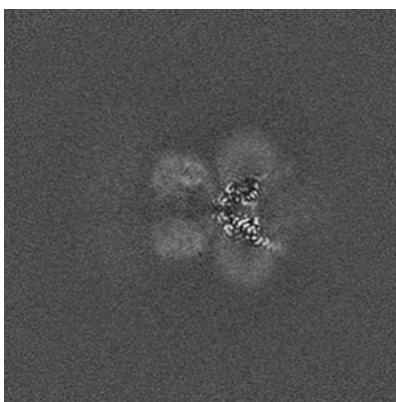


Z Index: 128

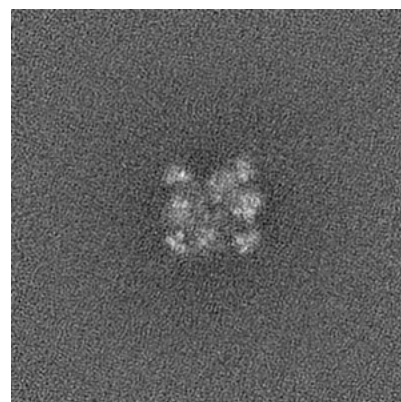
### 6.2.2 Raw map



X Index: 128



Y Index: 128

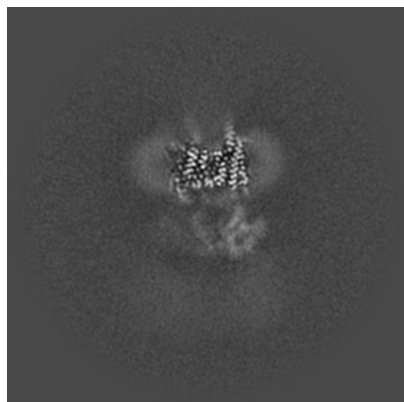


Z Index: 128

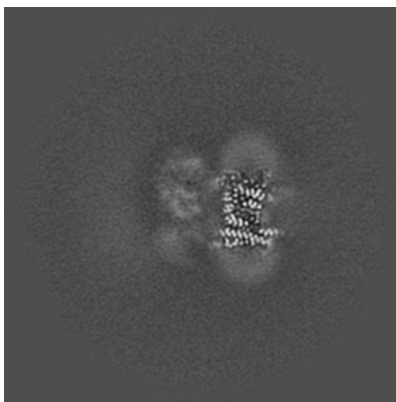
The images above show central slices of the map in three orthogonal directions.

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

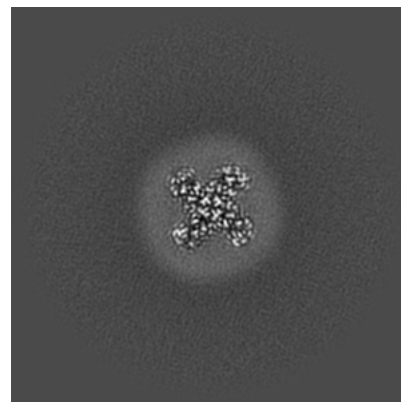
### 6.3.1 Primary map



X Index: 139

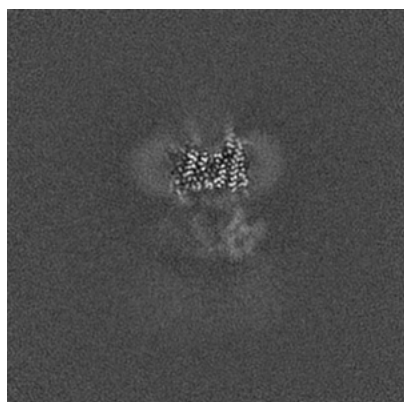


Y Index: 139

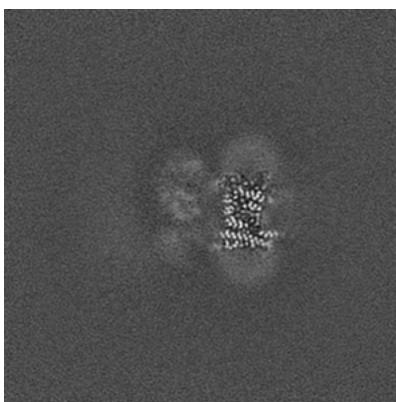


Z Index: 144

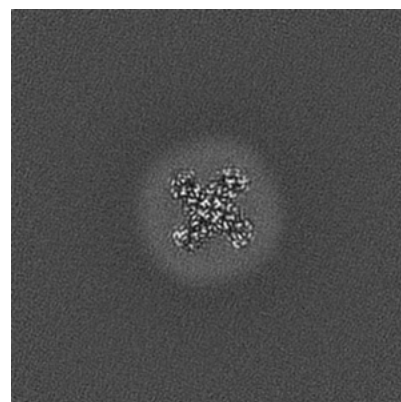
### 6.3.2 Raw map



X Index: 139



Y Index: 139



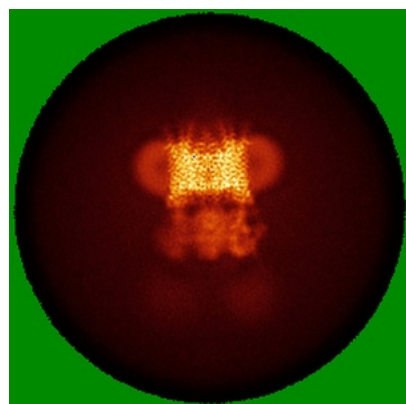
Z Index: 144

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

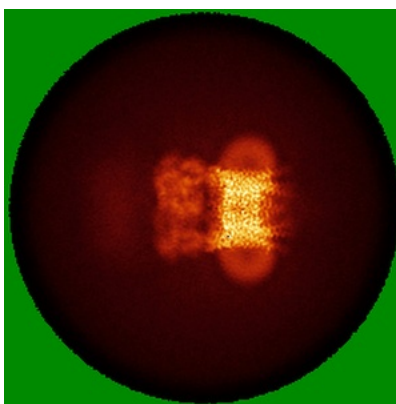


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

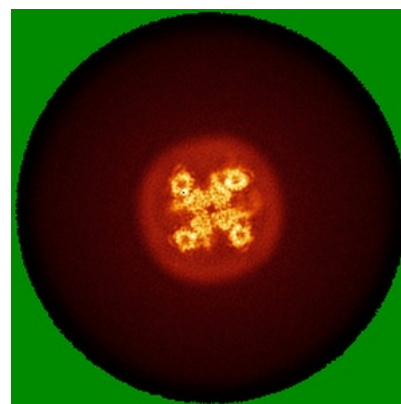
### 6.4.1 Primary map



X

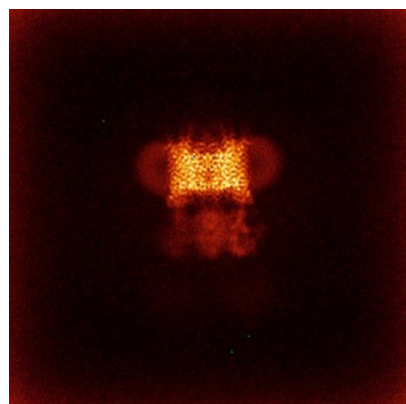


Y

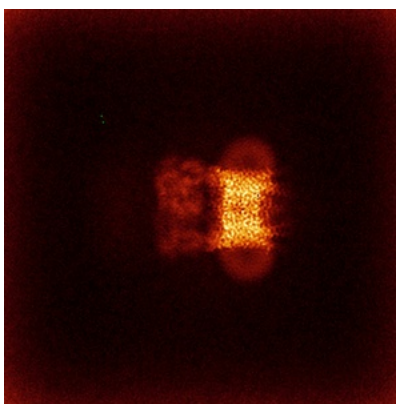


Z

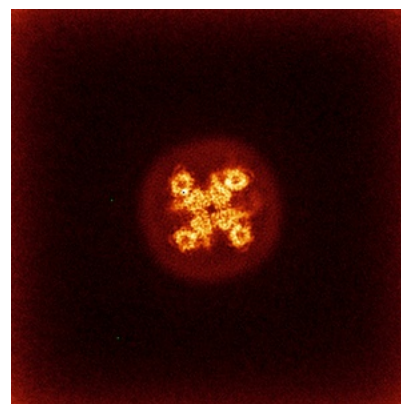
### 6.4.2 Raw map



X



Y

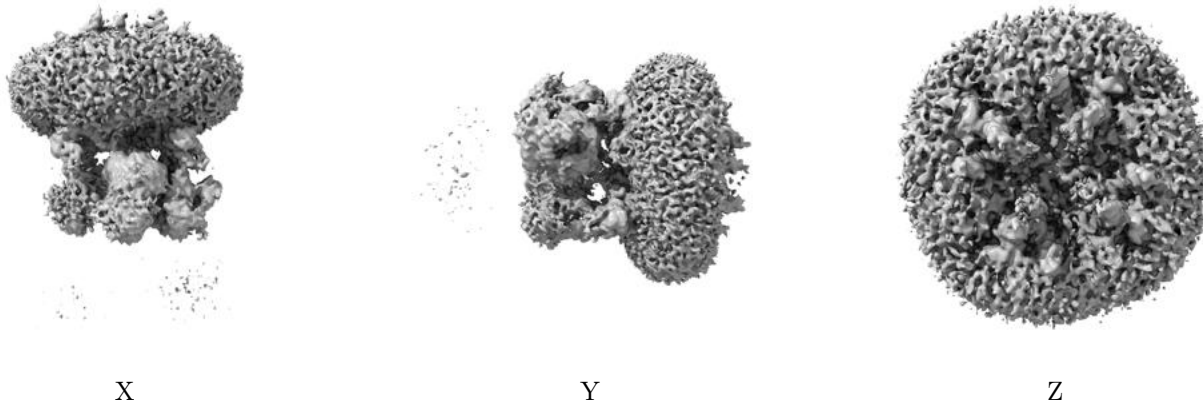


Z

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.

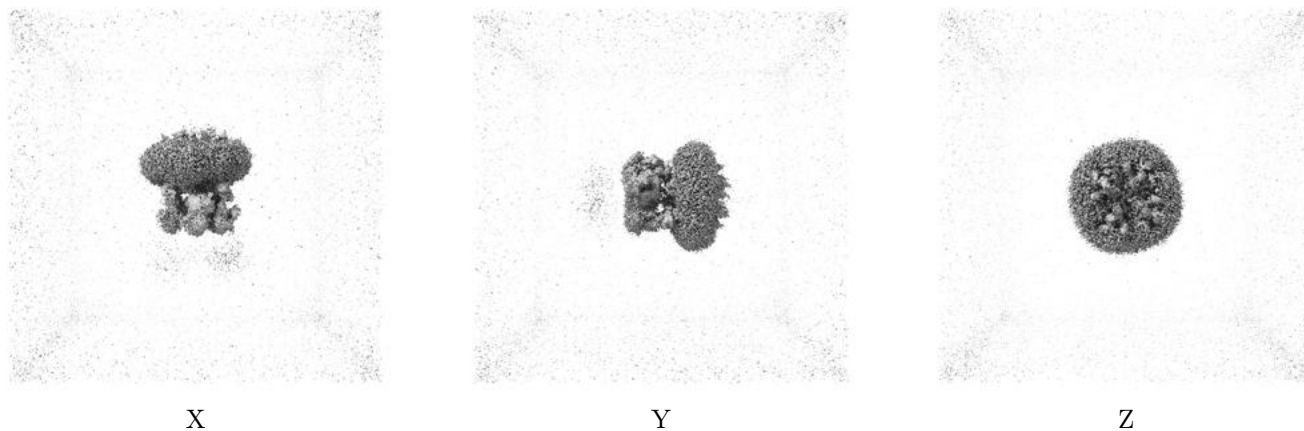
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

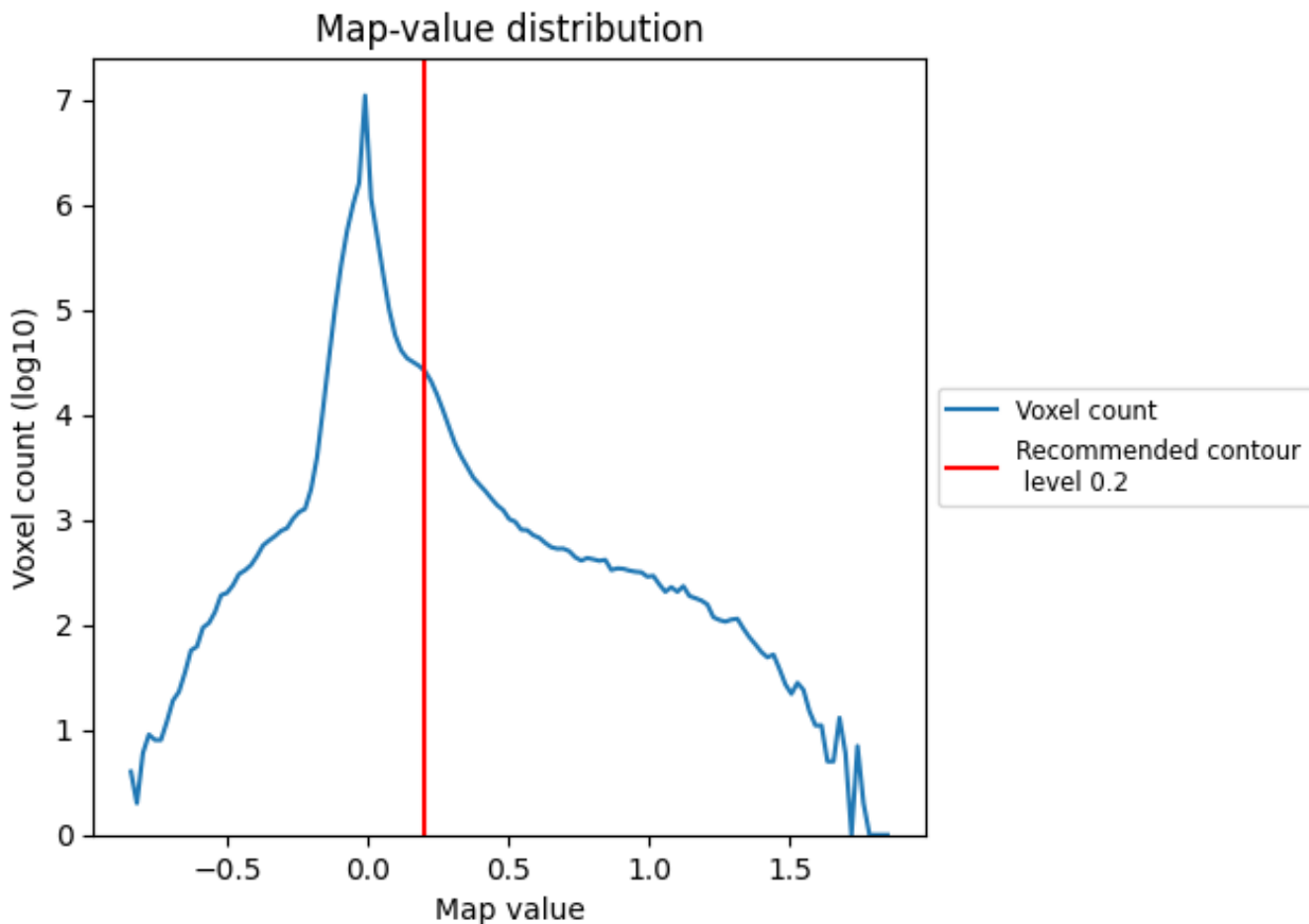
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

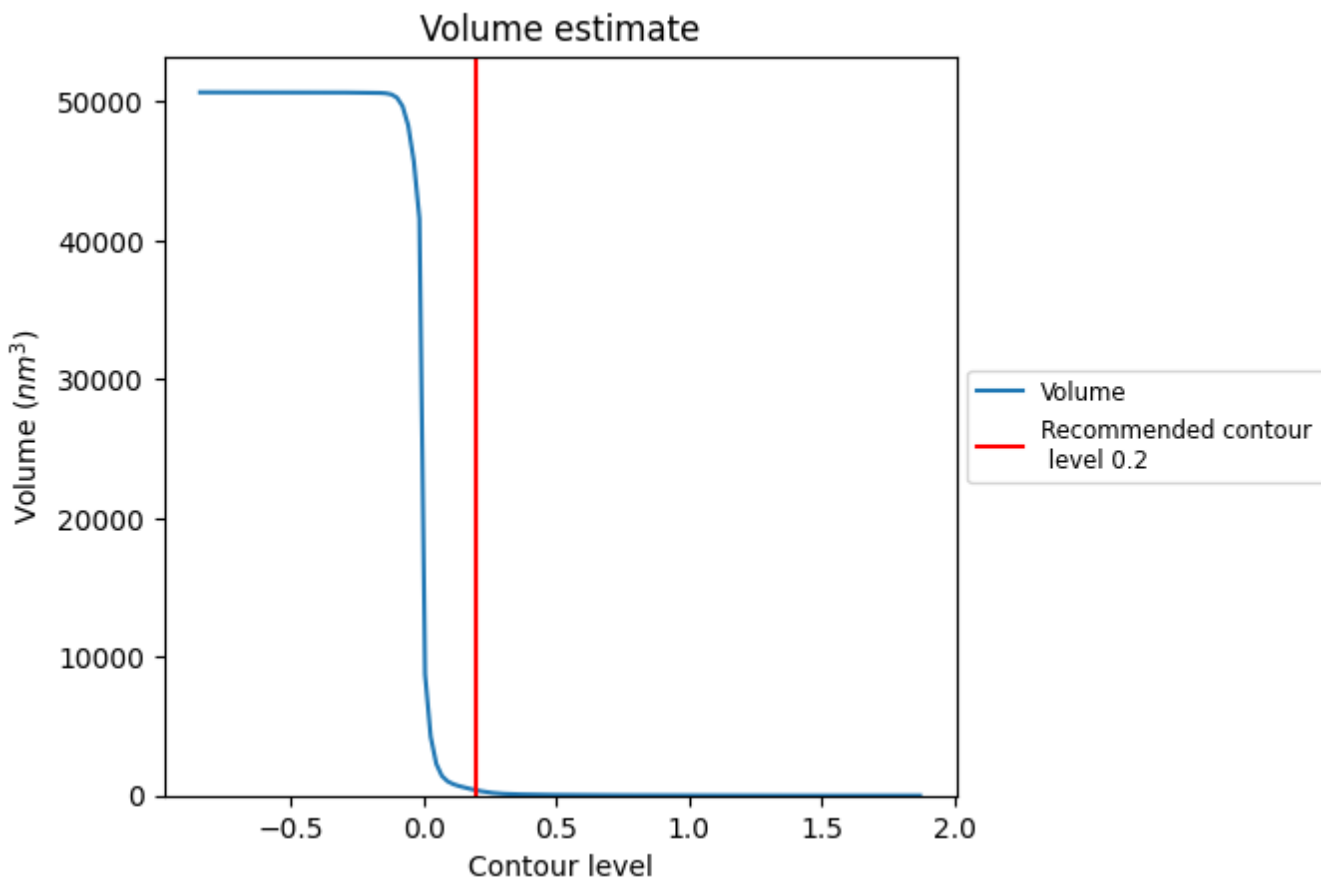
This section contains the results of statistical analysis of the map.

### 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.

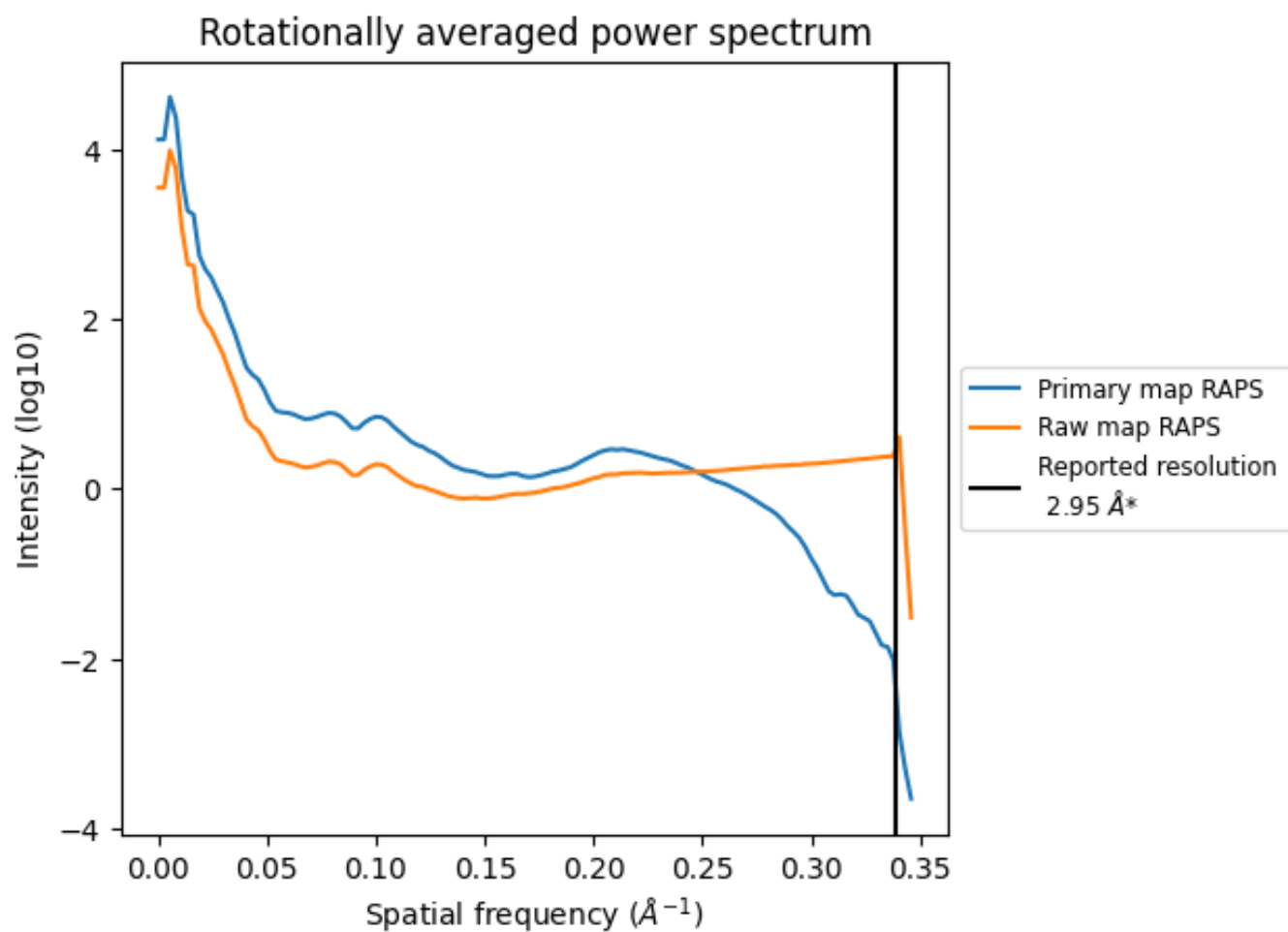
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 377 nm<sup>3</sup>; this corresponds to an approximate mass of 341 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

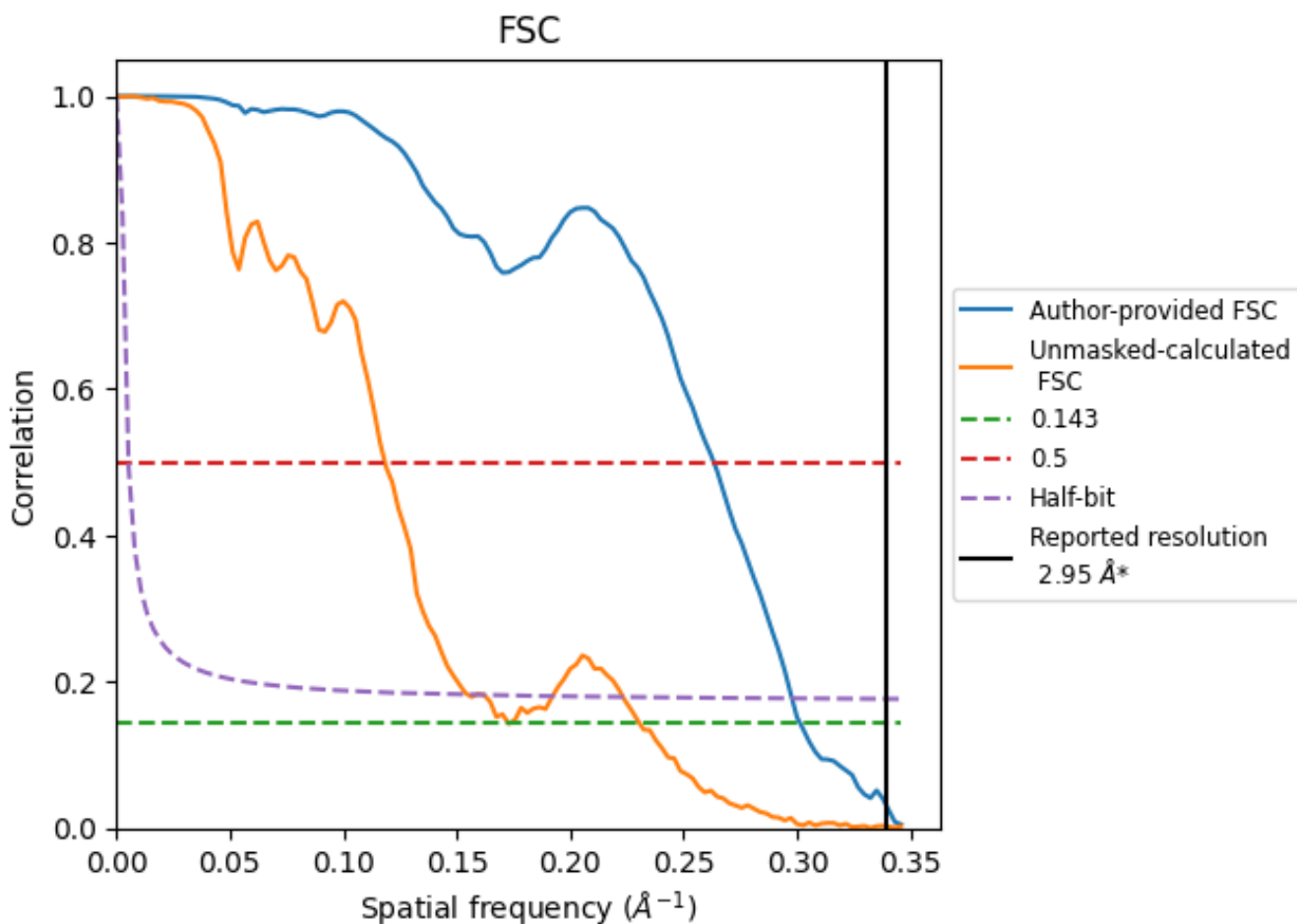


\*Reported resolution corresponds to spatial frequency of  $0.339 \text{ \AA}^{-1}$

## 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 0.339 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	3.32	3.80	3.36
Unmasked-calculated*	5.79	8.45	6.45

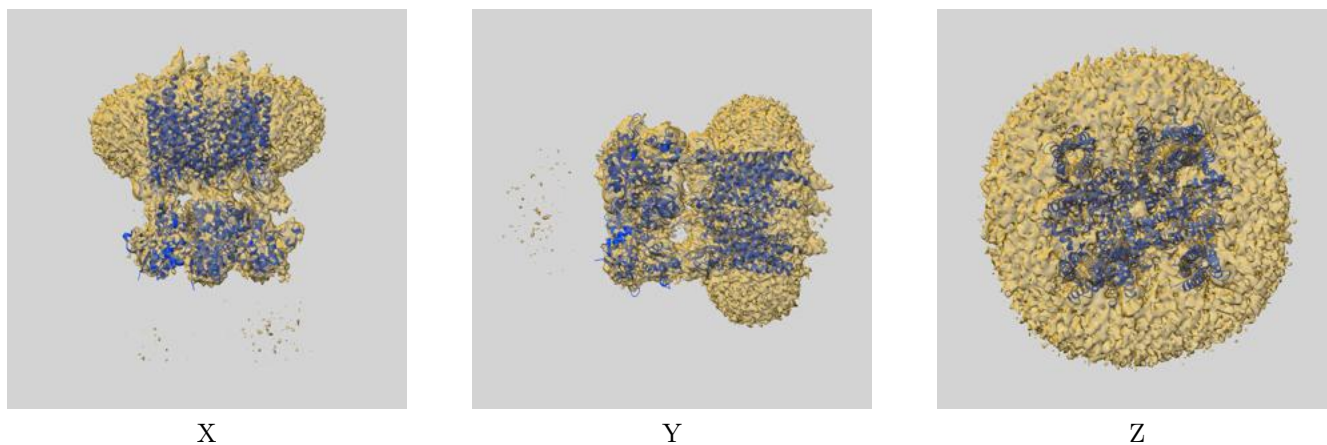
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.32 differs from the reported value 2.95 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.79 differs from the reported value 2.95 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-17392 and PDB model 8P3Q. Per-residue inclusion information can be found in section 3 on page 7.

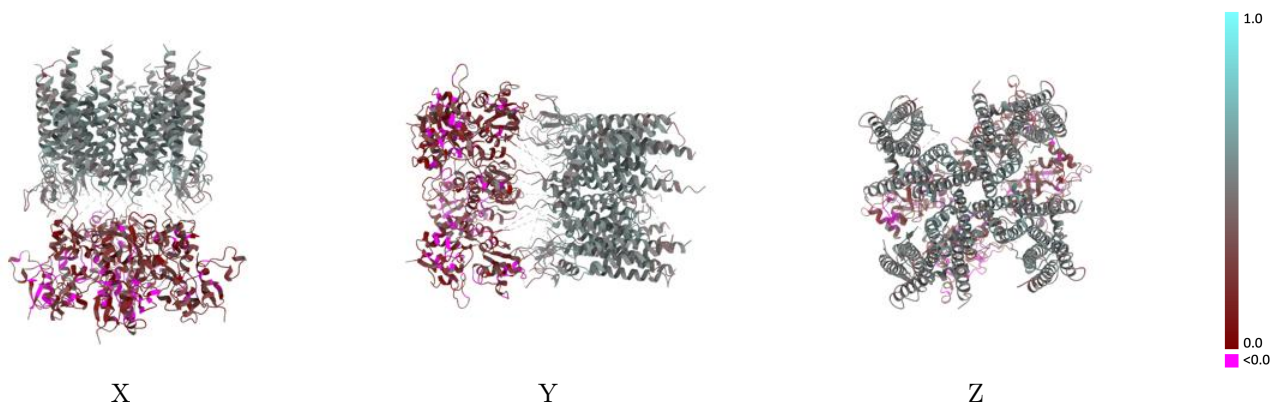
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

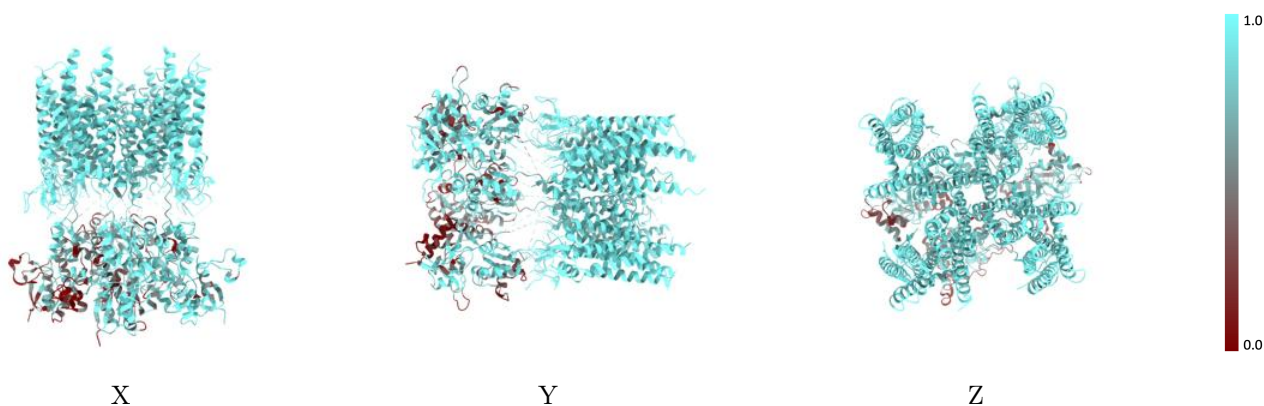


## 9.2 Q-score mapped to coordinate model [i](#)



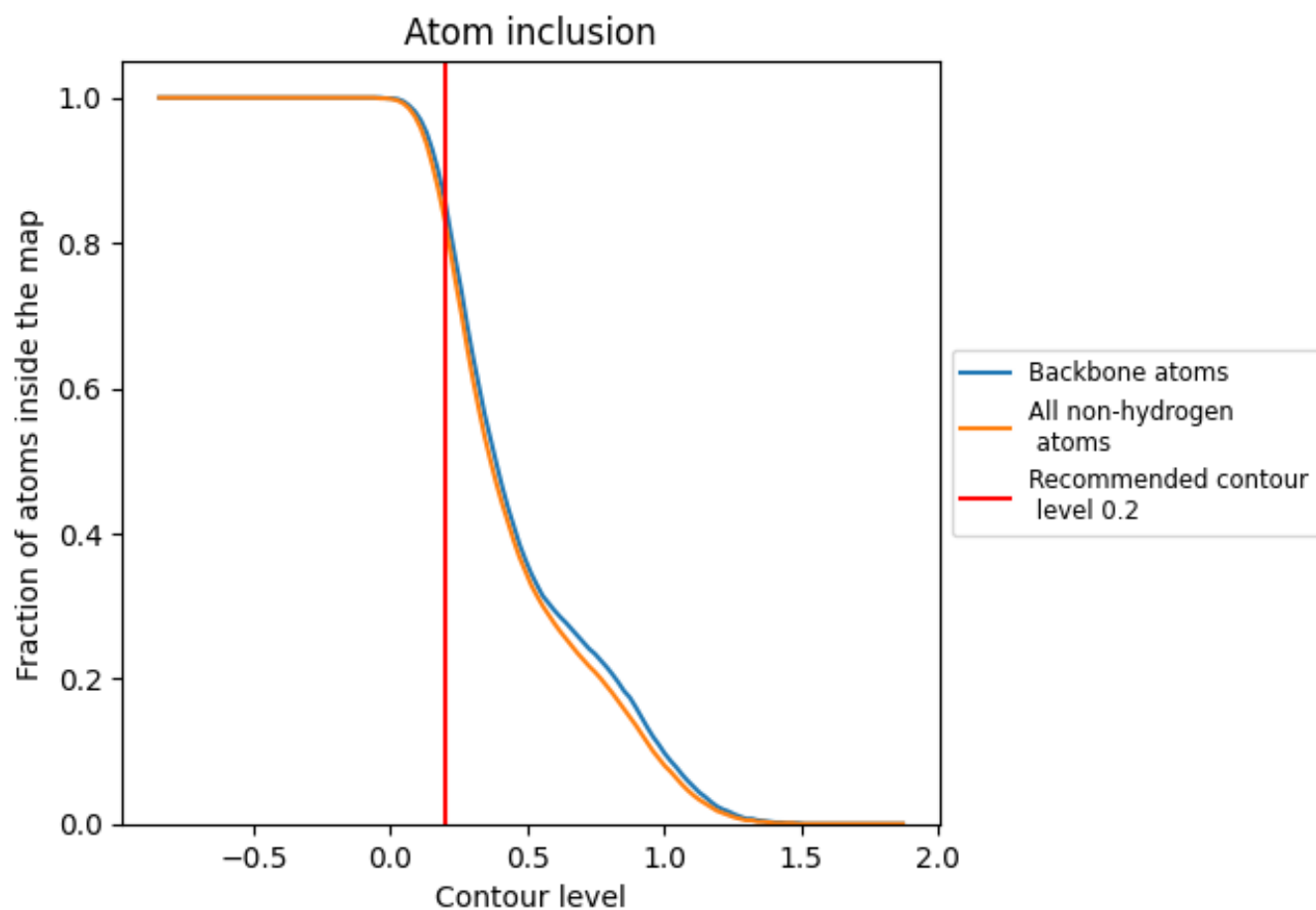
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 83% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8290	 0.3570
A	 0.8920	 0.3270
B	 0.7460	 0.2870
C	 0.6820	 0.2820
D	 0.8180	 0.2960
E	 0.9380	 0.4870
F	 0.9490	 0.4880
G	 0.9310	 0.4860
H	 0.9430	 0.4850

