



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 03:44 AM EST

PDB ID : 8FHD
EMDB ID : EMD-29082
Title : Cryo-EM structure of human voltage-gated sodium channel Nav1.6
Authors : Fan, X.; Huang, J.; Yan, N.
Deposited on : 2022-12-14
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.39

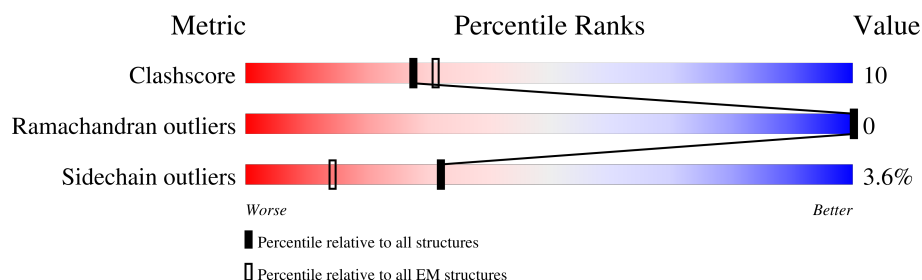
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1980	
2	C	218	
3	D	9	
4	F	2	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 12686 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.

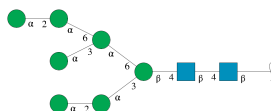
- Molecule 1 is a protein called Sodium channel protein type 8 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1294	Total	C	N	O	S	0	0
			10442	6912	1642	1805	83		

- Molecule 2 is a protein called Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	173	Total	C	N	O	S	0	0
			1416	902	232	272	10		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



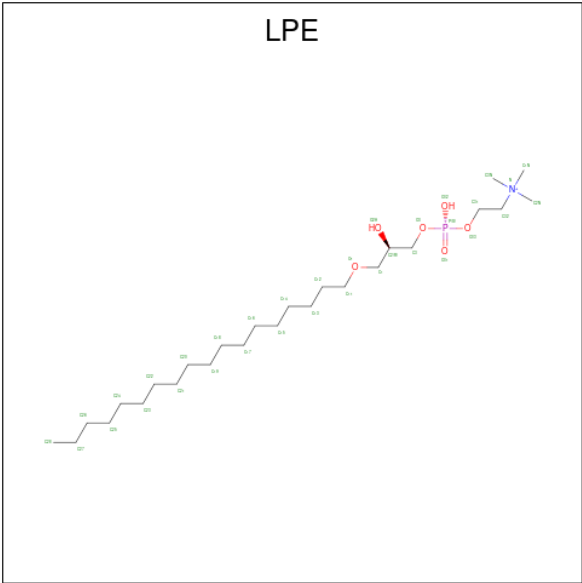
Mol	Chain	Residues	Atoms			AltCon
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $\text{C}_{27}\text{H}_{46}\text{O}$).



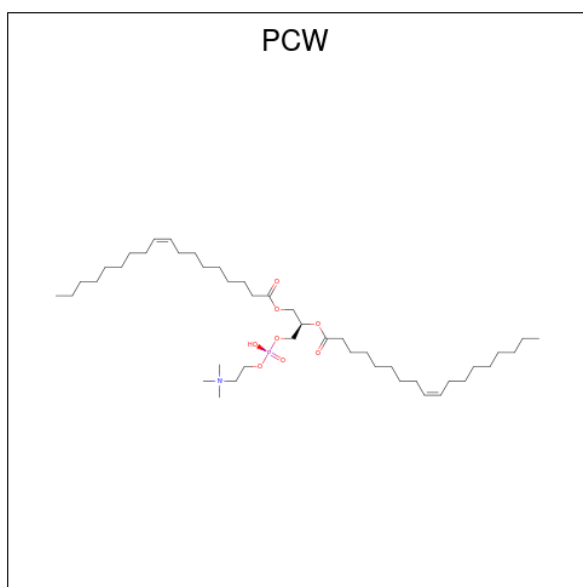
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			28	27	1	

- Molecule 8 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: $C_{26}H_{57}NO_6P$).



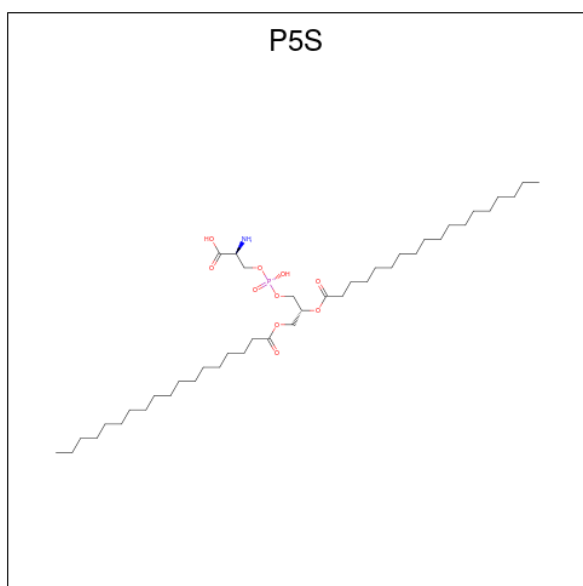
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
8	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
8	A	1	Total	C	N	O	P	0
			25	17	1	6	1	

- Molecule 9 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



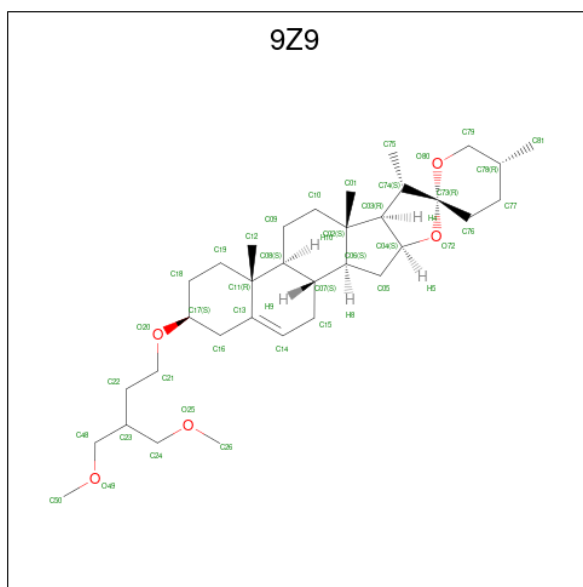
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			53	43	1	8	1	
9	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
9	A	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 10 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: C₄₂H₈₂NO₁₀P).



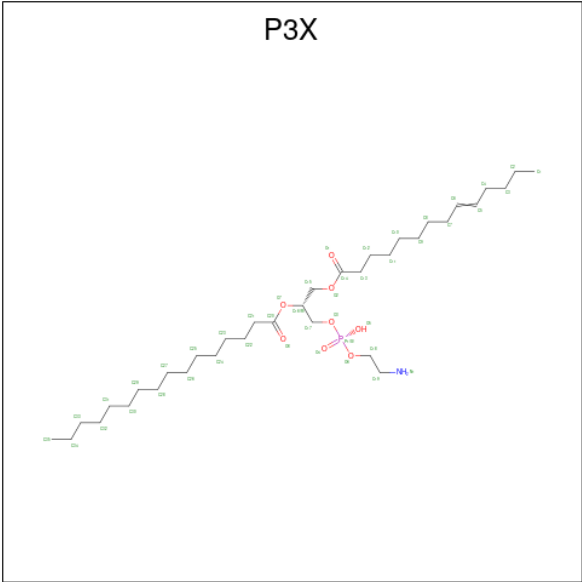
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
10	A	1	Total	C	N	O	P	0
			35	24	1	9	1	

- Molecule 11 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula: C₃₄H₅₆O₅).



Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total	C	O	0
			39	34	5	

- Molecule 12 is (5E,17R,20S)-23-amino-20-hydroxy-14,20-dioxo-15,19,21-trioxa-20lambda 5 -phosphatricos-5-en-17-yl hexadecanoate (three-letter code: P3X) (formula: C₃₅H₆₈NO₈P).

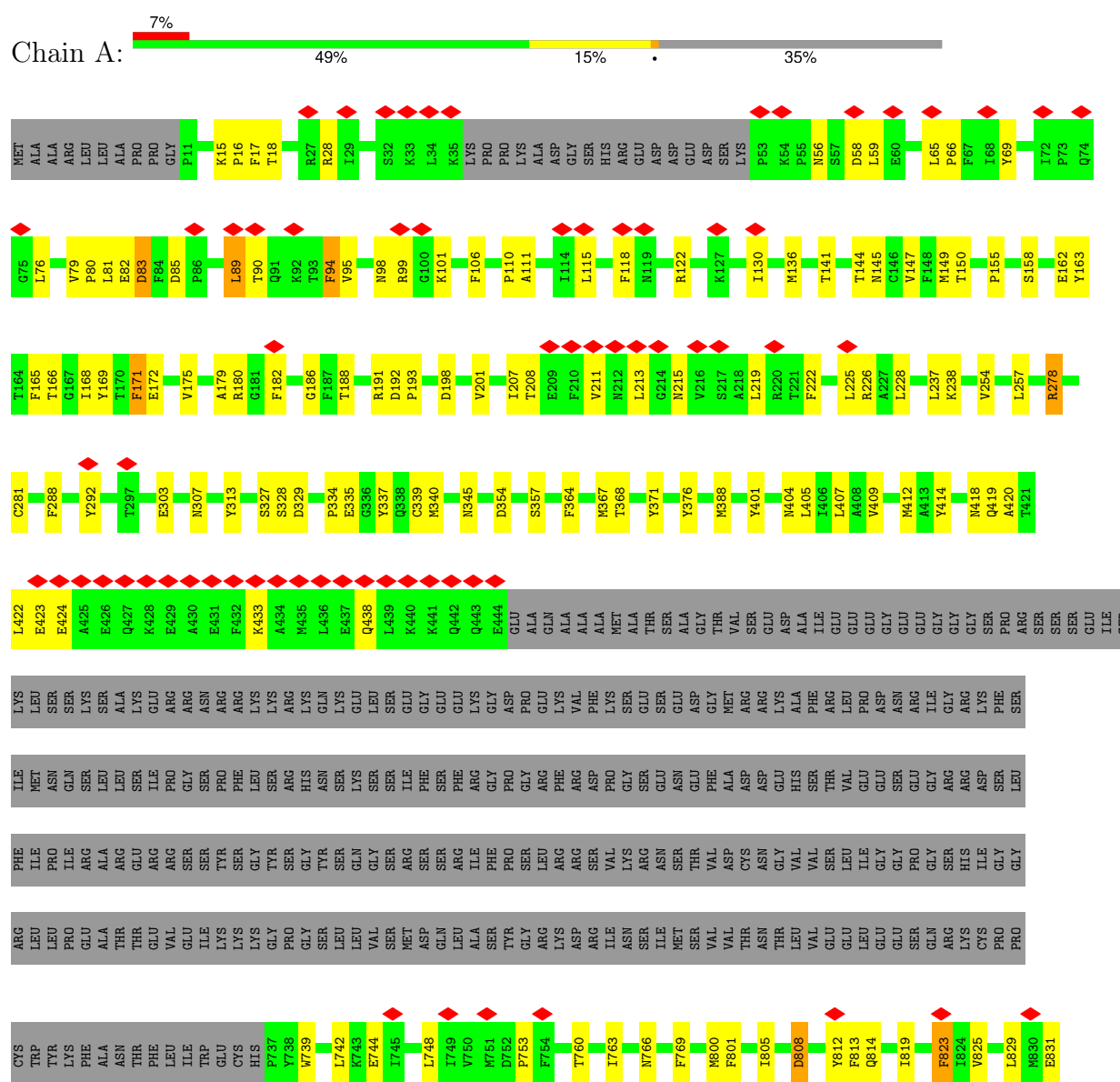


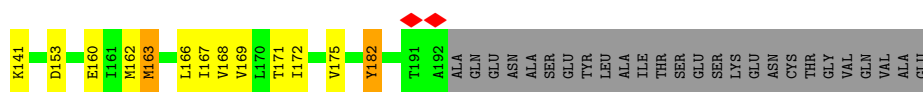
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	N	O	P	0
			45	35	1	8	1	

3 Residue-property plots [i](#)

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

- Molecule 1: Sodium channel protein type 8 subunit alpha





- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 22% 56% 22%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74103	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.039	Depositor
Minimum map value	-2.070	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	356.47998, 356.47998, 356.47998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P3X, NAG, MAN, CLR, LPE, P5S, Y01, 9Z9, PCW, BMA

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	0.26	0/10700	0.46	0/14490
2	C	0.25	0/1442	0.49	0/1949
All	All	0.26	0/12142	0.47	0/16439

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	10442	0	10604	212	0
2	C	1416	0	1380	23	0
3	D	105	0	88	7	0
4	F	28	0	25	1	0
5	A	56	0	52	2	0
5	C	42	0	39	1	0
6	A	140	0	196	5	0
7	A	28	0	46	0	0
8	A	125	0	175	6	0
9	A	144	0	203	8	0
10	A	76	0	96	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	39	0	0	0	0
12	A	45	0	0	0	0
All	All	12686	0	12904	243	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 10.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LYS:HD2	1:A:16:PRO:HD2	1.58	0.84
1:A:110:PRO:HA	1:A:122:ARG:HH22	1.47	0.80
1:A:65:LEU:HD12	1:A:66:PRO:HD2	1.64	0.79
1:A:357:SER:HB3	9:A:2012:PCW:H332	1.66	0.76
1:A:1593:VAL:O	1:A:1597:ILE:HD12	1.86	0.75
1:A:168:ILE:O	1:A:171:PHE:HB3	1.86	0.75
1:A:288:PHE:HB3	3:D:6:MAN:H62	1.68	0.75
1:A:1330:VAL:HG21	1:A:1462:VAL:HG21	1.70	0.73
1:A:1403:TYR:HB3	9:A:2009:PCW:H181	1.71	0.73
1:A:65:LEU:HD11	1:A:69:TYR:HD2	1.55	0.71
3:D:4:MAN:H4	3:D:5:MAN:H5	1.73	0.70
1:A:814:GLN:OE1	1:A:814:GLN:N	2.25	0.70
1:A:303:GLU:O	1:A:307:ASN:ND2	2.27	0.68
1:A:1616:PHE:HA	1:A:1619:ILE:HD12	1.77	0.66
1:A:254:VAL:HG21	1:A:409:VAL:HG21	1.78	0.65
1:A:1365:PHE:O	1:A:1431:GLN:NE2	2.30	0.65
1:A:1190:THR:HG21	2:C:182:TYR:HA	1.79	0.65
1:A:1262:ASN:ND2	1:A:1265:CYS:SG	2.69	0.64
1:A:339:CYS:O	3:D:1:NAG:H3	1.97	0.63
1:A:906:CYS:HB3	1:A:912:CYS:HA	1.81	0.63
1:A:405:LEU:HD21	1:A:1640:LEU:HD13	1.81	0.63
1:A:760:THR:HA	1:A:763:ILE:HD12	1.81	0.62
1:A:257:LEU:HD13	1:A:1637:ILE:HD12	1.82	0.62
1:A:1182:LYS:O	1:A:1186:ILE:HG12	2.00	0.61
2:C:168:VAL:O	2:C:172:ILE:HG23	2.00	0.61
1:A:180:ARG:HD2	1:A:188:THR:HA	1.82	0.61
2:C:129:PHE:HB2	2:C:132:TYR:HB3	1.83	0.60
1:A:1372:ASN:HA	1:A:1430:GLU:HA	1.83	0.60
1:A:59:LEU:HD23	1:A:85:ASP:HB3	1.83	0.59
1:A:80:PRO:HB3	1:A:94:PHE:HE1	1.68	0.59
1:A:1638:ARG:NH1	10:A:2013:P5S:O15	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1701:ILE:HD11	1:A:1710:LEU:HD12	1.85	0.58
1:A:1611:VAL:HG13	1:A:1612:SER:H	1.69	0.57
1:A:1634:ALA:HB1	1:A:1637:ILE:HG12	1.87	0.57
1:A:1535:ASN:OD1	1:A:1626:ARG:NH1	2.38	0.57
1:A:825:VAL:O	1:A:829:LEU:HG	2.04	0.56
1:A:79:VAL:O	1:A:81:LEU:HD22	2.05	0.56
1:A:419:GLN:O	1:A:423:GLU:HG2	2.06	0.56
1:A:1496:GLY:O	10:A:2013:P5S:N	2.39	0.56
2:C:75:ASN:OD1	2:C:99:LYS:NZ	2.33	0.56
1:A:1536:MET:HB2	1:A:1627:ILE:HD12	1.89	0.55
1:A:115:LEU:O	1:A:122:ARG:NH2	2.40	0.55
1:A:1591:VAL:HG11	9:A:2014:PCW:H20	1.88	0.55
6:A:2017:Y01:HBD	6:A:2018:Y01:HAD2	1.87	0.55
1:A:111:ALA:H	1:A:122:ARG:HH12	1.53	0.55
1:A:1415:TRP:O	1:A:1419:MET:HG3	2.07	0.55
1:A:145:ASN:O	1:A:149:MET:HG3	2.07	0.55
1:A:1684:ASP:OD2	2:C:46:ARG:NH1	2.40	0.54
2:C:71:LEU:HD13	2:C:78:LEU:HD11	1.88	0.54
10:A:2013:P5S:H28	10:A:2013:P5S:H43	1.88	0.54
1:A:201:VAL:HG21	1:A:226:ARG:HG2	1.88	0.54
1:A:65:LEU:HB3	1:A:101:LYS:HD2	1.89	0.54
1:A:840:LEU:HA	1:A:843:LEU:HB2	1.89	0.54
1:A:15:LYS:NZ	1:A:18:THR:OG1	2.40	0.54
1:A:1744:PHE:HD1	9:A:2009:PCW:H40	1.70	0.54
1:A:1409:VAL:HA	1:A:1415:TRP:HB3	1.89	0.54
1:A:840:LEU:O	1:A:844:ARG:HG3	2.07	0.54
1:A:910:GLN:OE1	1:A:910:GLN:N	2.40	0.54
1:A:15:LYS:HD2	1:A:16:PRO:CD	2.35	0.53
1:A:1248:LEU:O	1:A:1252:THR:HG23	2.08	0.53
1:A:1352:LYS:HB3	1:A:1425:SER:HB2	1.91	0.53
1:A:1503:PRO:O	1:A:1579:TYR:OH	2.25	0.53
1:A:845:SER:HB3	1:A:1344:MET:HG3	1.90	0.52
1:A:1219:ASP:N	1:A:1219:ASP:OD1	2.42	0.52
1:A:155:PRO:HD2	1:A:158:SER:HB3	1.90	0.52
1:A:211:VAL:HG12	1:A:213:LEU:H	1.75	0.52
10:A:2013:P5S:H3A	9:A:2014:PCW:H52	1.91	0.52
1:A:1714:ILE:HG21	1:A:1742:GLY:HA3	1.91	0.52
1:A:1223:GLU:OE1	1:A:1229:ARG:NH1	2.43	0.52
1:A:192:ASP:OD1	1:A:193:PRO:HD2	2.10	0.52
1:A:1590:PHE:O	1:A:1594:ILE:HG12	2.10	0.51
1:A:889:PHE:CG	1:A:960:VAL:HG22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1569:CYS:HA	1:A:1572:LYS:HE3	1.92	0.51
1:A:89:LEU:H	1:A:89:LEU:HD12	1.75	0.51
1:A:801:PHE:CE1	1:A:805:ILE:HD11	2.46	0.51
1:A:98:ASN:HB3	1:A:130:ILE:HB	1.92	0.51
1:A:329:ASP:OD1	1:A:329:ASP:N	2.38	0.51
1:A:367:MET:HE3	1:A:368:THR:HG23	1.92	0.51
1:A:1241:TYR:HH	2:C:171:THR:HG1	1.48	0.51
1:A:169:TYR:O	1:A:172:GLU:HG2	2.10	0.51
1:A:1276:LEU:O	1:A:1280:ILE:HG23	2.12	0.51
1:A:1697:CYS:O	1:A:1701:ILE:HG12	2.11	0.51
3:D:5:MAN:H2	3:D:6:MAN:H5	1.93	0.50
1:A:1717:ARG:HB3	1:A:1719:PRO:HD2	1.93	0.50
1:A:1606:ILE:HG22	1:A:1610:PHE:HB3	1.93	0.50
1:A:17:PHE:HB2	1:A:80:PRO:HB2	1.93	0.50
1:A:1615:LEU:HG	1:A:1619:ILE:HD11	1.93	0.50
1:A:1427:LYS:HB2	1:A:1430:GLU:CD	2.33	0.49
1:A:921:ASP:N	1:A:921:ASP:OD1	2.45	0.49
1:A:364:PHE:CE1	1:A:961:MET:HE1	2.48	0.49
1:A:1299:ARG:HG2	1:A:1302:ARG:HD3	1.95	0.49
1:A:753:PRO:HG3	1:A:996:ASN:HB3	1.95	0.49
2:C:93:ASN:OD1	5:C:301:NAG:N2	2.46	0.49
1:A:1506:ARG:HB3	1:A:1508:LEU:HD22	1.94	0.48
1:A:1264:TRP:HE1	8:A:2011:LPE:H322	1.78	0.48
1:A:186:GLY:O	1:A:191:ARG:NH1	2.47	0.48
2:C:166:LEU:HA	2:C:169:VAL:HG12	1.96	0.48
1:A:1191:CYS:SG	1:A:1252:THR:OG1	2.71	0.48
1:A:327:SER:OG	1:A:329:ASP:OD1	2.31	0.47
1:A:80:PRO:HB3	1:A:94:PHE:CE1	2.48	0.47
1:A:182:PHE:O	1:A:182:PHE:CD1	2.68	0.47
1:A:1324:ILE:HG22	1:A:1325:PRO:HD3	1.95	0.47
1:A:1372:ASN:N	1:A:1372:ASN:OD1	2.47	0.47
1:A:141:THR:HA	1:A:144:THR:HG22	1.97	0.47
2:C:153:ASP:N	2:C:153:ASP:OD1	2.46	0.47
1:A:906:CYS:HB3	1:A:912:CYS:CA	2.45	0.47
1:A:405:LEU:HD12	1:A:1768:ASN:ND2	2.29	0.47
1:A:1332:LEU:O	1:A:1336:ILE:HG22	2.15	0.47
1:A:162:GLU:O	1:A:165:PHE:HB2	2.15	0.47
1:A:1651:LEU:HD22	1:A:1760:MET:HG2	1.97	0.47
1:A:1435:GLU:HG2	1:A:1438:ILE:HD13	1.96	0.46
6:A:2017:Y01:HAP1	6:A:2017:Y01:HAO2	1.45	0.46
1:A:404:ASN:HD22	1:A:1764:ILE:HG21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:HD13	1:A:79:VAL:HG21	1.96	0.46
1:A:175:VAL:O	1:A:179:ALA:N	2.44	0.46
1:A:1498:LYS:HB2	1:A:1498:LYS:HE2	1.75	0.46
1:A:739:TRP:CD1	1:A:742:LEU:HD11	2.49	0.46
1:A:237:LEU:HD22	1:A:881:VAL:HG23	1.97	0.46
1:A:420:ALA:O	1:A:424:GLU:HG2	2.14	0.46
1:A:1391:ASN:HD21	1:A:1395:ASN:HD21	1.63	0.46
1:A:1626:ARG:H	1:A:1626:ARG:HG3	1.53	0.46
3:D:8:MAN:O3	3:D:9:MAN:H5	2.16	0.46
1:A:215:ASN:O	1:A:219:LEU:HG	2.15	0.46
1:A:831:GLU:HG3	1:A:840:LEU:HD11	1.97	0.46
1:A:1185:TRP:CD1	1:A:1189:LYS:HD2	2.51	0.46
1:A:1427:LYS:O	1:A:1430:GLU:HG2	2.16	0.46
1:A:1648:LEU:HD23	1:A:1648:LEU:HA	1.82	0.45
1:A:1217:PHE:HE1	8:A:2016:LPE:H3N3	1.81	0.45
1:A:354:ASP:HB3	1:A:1544:ASP:HB3	1.97	0.45
1:A:207:ILE:HG22	1:A:208:THR:HG23	1.99	0.45
1:A:1365:PHE:CZ	5:A:2003:NAG:H83	2.52	0.45
6:A:2018:Y01:HBC	6:A:2018:Y01:HAM2	1.61	0.45
1:A:364:PHE:HE1	1:A:961:MET:HE1	1.80	0.45
1:A:278:ARG:HD2	1:A:345:ASN:HD21	1.82	0.45
1:A:1585:TRP:CE2	10:A:2013:P5S:H21A	2.52	0.45
1:A:823:PHE:HD1	1:A:823:PHE:O	2.00	0.45
2:C:93:ASN:HB2	2:C:107:PHE:HB2	1.98	0.45
1:A:281:CYS:HB3	1:A:337:TYR:HB3	2.00	0.44
1:A:1586:ASN:N	1:A:1586:ASN:OD1	2.49	0.44
1:A:1666:SER:O	1:A:1670:MET:HG3	2.18	0.44
1:A:847:ARG:H	1:A:847:ARG:HG2	1.55	0.44
1:A:198:ASP:HA	1:A:201:VAL:HG12	1.97	0.44
1:A:999:ILE:HD12	1:A:999:ILE:HA	1.85	0.44
10:A:2013:P5S:H26A	9:A:2014:PCW:H382	2.00	0.44
1:A:180:ARG:HB3	1:A:188:THR:HB	2.00	0.44
1:A:1767:GLU:OE1	1:A:1767:GLU:HA	2.18	0.44
2:C:172:ILE:HA	2:C:175:VAL:HG22	1.99	0.44
1:A:744:GLU:O	1:A:748:LEU:HG	2.17	0.44
1:A:376:TYR:OH	1:A:1696:ILE:HG23	2.18	0.44
1:A:1238:VAL:HG22	2:C:167:ILE:HG13	2.00	0.44
1:A:1698:LEU:HG	1:A:1749:TYR:CE2	2.53	0.44
1:A:1597:ILE:HD12	1:A:1597:ILE:H	1.83	0.44
1:A:1626:ARG:HA	1:A:1629:ARG:HE	1.83	0.44
1:A:313:TYR:HB2	1:A:337:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1579:TYR:O	1:A:1586:ASN:ND2	2.49	0.43
1:A:1580:TYR:HA	1:A:1586:ASN:ND2	2.32	0.43
2:C:141:LYS:HB3	2:C:141:LYS:HE3	1.68	0.43
1:A:837:VAL:HG13	1:A:838:GLU:H	1.82	0.43
1:A:1365:PHE:CE1	5:A:2003:NAG:H83	2.53	0.43
1:A:1643:ALA:HB2	1:A:1771:VAL:HG11	2.00	0.43
1:A:1349:PHE:HA	1:A:1352:LYS:HD3	2.00	0.43
1:A:198:ASP:O	1:A:201:VAL:HG12	2.18	0.43
1:A:1531:LEU:HD23	1:A:1531:LEU:HA	1.82	0.43
1:A:1741:VAL:HG13	8:A:2010:LPE:H2N1	2.00	0.43
1:A:17:PHE:CD2	1:A:82:GLU:HG3	2.54	0.43
1:A:1602:LEU:O	1:A:1605:ILE:N	2.48	0.43
2:C:74:GLU:O	2:C:77:VAL:HG22	2.19	0.43
1:A:819:ILE:HD12	1:A:819:ILE:H	1.84	0.43
1:A:1506:ARG:HD2	1:A:1506:ARG:HA	1.87	0.43
1:A:1663:PHE:CE2	8:A:2016:LPE:H121	2.54	0.43
1:A:334:PRO:HD3	2:C:46:ARG:HD3	2.01	0.42
1:A:1665:PHE:HD1	1:A:1745:PHE:CE2	2.37	0.42
1:A:1595:LEU:HA	1:A:1598:VAL:HG12	2.01	0.42
1:A:1717:ARG:HE	1:A:1717:ARG:HA	1.83	0.42
10:A:2013:P5S:H44	10:A:2013:P5S:H40A	2.00	0.42
2:C:58:THR:HB	2:C:67:PHE:HB3	2.00	0.42
4:F:1:NAG:H4	4:F:2:NAG:H2	1.56	0.42
1:A:17:PHE:O	1:A:118:PHE:HZ	2.03	0.42
1:A:1663:PHE:HE2	8:A:2016:LPE:H121	1.84	0.42
1:A:83:ASP:HA	1:A:95:VAL:HG21	2.02	0.42
1:A:808:ASP:HB2	1:A:812:TYR:HD2	1.85	0.42
1:A:1293:LYS:HB2	1:A:1293:LYS:HE3	1.75	0.42
1:A:1683:ASP:OD1	1:A:1683:ASP:N	2.52	0.42
9:A:2009:PCW:H341	6:A:2018:Y01:HAK2	2.00	0.42
1:A:980:PHE:O	1:A:982:ALA:N	2.53	0.42
1:A:1194:ILE:HD13	1:A:1194:ILE:HA	1.84	0.42
1:A:1467:PHE:HD2	1:A:1762:ILE:HG21	1.85	0.42
2:C:74:GLU:HG2	2:C:75:ASN:OD1	2.20	0.42
1:A:163:TYR:O	1:A:166:THR:OG1	2.25	0.42
1:A:238:LYS:HB2	1:A:238:LYS:HE3	1.72	0.42
1:A:1576:LEU:HD11	1:A:1579:TYR:HD2	1.85	0.42
1:A:1595:LEU:HA	1:A:1595:LEU:HD23	1.81	0.42
1:A:288:PHE:HB3	3:D:6:MAN:C6	2.44	0.42
1:A:409:VAL:HA	1:A:412:MET:HE3	2.02	0.42
1:A:1271:ILE:O	1:A:1274:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1595:LEU:HD13	1:A:1622:ALA:HB2	2.02	0.42
1:A:1687:ASN:ND2	1:A:1689:GLU:OE2	2.53	0.42
6:A:2018:Y01:HAO2	6:A:2018:Y01:HAA1	2.02	0.42
1:A:94:PHE:CD2	1:A:106:PHE:HB2	2.55	0.42
1:A:28:ARG:HB3	1:A:90:THR:HG22	2.02	0.41
1:A:335:GLU:OE2	1:A:335:GLU:N	2.46	0.41
1:A:1238:VAL:HG23	2:C:163:MET:HG3	2.02	0.41
1:A:1602:LEU:HG	1:A:1606:ILE:HD11	2.00	0.41
1:A:1678:HIS:HE1	1:A:1687:ASN:HD22	1.68	0.41
1:A:800:MET:HE2	1:A:825:VAL:HG21	2.03	0.41
1:A:933:LEU:HD21	1:A:964:GLY:HA3	2.00	0.41
1:A:388:MET:HE1	8:A:2015:LPE:H121	2.02	0.41
1:A:1244:ILE:HD11	1:A:1276:LEU:HG	2.02	0.41
1:A:1490:ASN:O	1:A:1494:LYS:HG2	2.21	0.41
1:A:1250:LYS:HE2	1:A:1250:LYS:HB2	1.84	0.41
2:C:78:LEU:HD22	2:C:92:TRP:HB2	2.02	0.41
1:A:766:ASN:OD1	1:A:850:ARG:NH2	2.54	0.41
1:A:1594:ILE:O	1:A:1598:VAL:HG12	2.20	0.41
1:A:813:PHE:N	1:A:814:GLN:OE1	2.51	0.41
1:A:1426:ARG:HB2	1:A:1430:GLU:OE2	2.20	0.41
1:A:56:ASN:HD21	1:A:58:ASP:HB3	1.85	0.41
1:A:147:VAL:O	1:A:150:THR:HB	2.21	0.41
9:A:2014:PCW:H321	9:A:2014:PCW:H2	1.84	0.41
3:D:8:MAN:H4	3:D:9:MAN:O6	2.21	0.41
1:A:278:ARG:H	1:A:278:ARG:HG2	1.72	0.41
1:A:327:SER:OG	1:A:328:SER:N	2.54	0.41
1:A:1178:GLU:HG2	1:A:1181:GLY:H	1.86	0.41
1:A:1467:PHE:CD2	1:A:1762:ILE:HG21	2.56	0.41
1:A:1585:TRP:CD1	1:A:1632:LYS:HE2	2.56	0.41
1:A:1611:VAL:HG13	1:A:1612:SER:N	2.33	0.41
1:A:1638:ARG:HG2	10:A:2013:P5S:O15	2.21	0.41
2:C:58:THR:OG1	2:C:120:GLU:HB2	2.21	0.41
1:A:836:ASP:OD1	1:A:836:ASP:N	2.54	0.41
1:A:1318:ASN:OD1	1:A:1319:ALA:N	2.54	0.41
2:C:44:LYS:H	2:C:44:LYS:HG2	1.53	0.41
1:A:418:ASN:O	1:A:422:LEU:HG	2.21	0.40
1:A:1234:TYR:CE1	2:C:160:GLU:HG3	2.56	0.40
1:A:191:ARG:HA	1:A:191:ARG:HD2	1.88	0.40
1:A:225:LEU:HA	1:A:228:LEU:HD23	2.04	0.40
1:A:401:TYR:HD1	1:A:1764:ILE:HD11	1.85	0.40
1:A:407:LEU:HD23	1:A:969:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:PRO:HB2	1:A:1000:SER:HB3	2.02	0.40
1:A:976:LEU:HD11	1:A:1460:ILE:HG21	2.03	0.40
1:A:1182:LYS:HE2	1:A:1182:LYS:HB2	1.81	0.40
1:A:65:LEU:HD11	1:A:69:TYR:CD2	2.45	0.40
1:A:94:PHE:CE2	1:A:106:PHE:HD2	2.40	0.40
1:A:433:LYS:HD3	1:A:433:LYS:HA	1.82	0.40
1:A:983:ASP:OD1	1:A:984:ASN:N	2.55	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	1286/1980 (65%)	1220 (95%)	66 (5%)	0	100	100
2	C	171/218 (78%)	169 (99%)	2 (1%)	0	100	100
All	All	1457/2198 (66%)	1389 (95%)	68 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	1146/1746 (66%)	1106 (96%)	40 (4%)	31	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	157/190 (83%)	150 (96%)	7 (4%)	23	53
All	All	1303/1936 (67%)	1256 (96%)	47 (4%)	32	60

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
1	A	89	LEU
1	A	94	PHE
1	A	99	ARG
1	A	136	MET
1	A	171	PHE
1	A	222	PHE
1	A	278	ARG
1	A	292	TYR
1	A	340	MET
1	A	371	TYR
1	A	414	TYR
1	A	438	GLN
1	A	769	PHE
1	A	808	ASP
1	A	823	PHE
1	A	833	SER
1	A	944	CYS
1	A	979	SER
1	A	980	PHE
1	A	994	MET
1	A	1196	GLU
1	A	1206	PHE
1	A	1286	TYR
1	A	1334	CYS
1	A	1337	PHE
1	A	1415	TRP
1	A	1466	ASN
1	A	1478	ASP
1	A	1518	PHE
1	A	1540	MET
1	A	1548	LYS
1	A	1577	ARG
1	A	1607	GLU
1	A	1610	PHE
1	A	1616	PHE

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Mol	Chain	Res	Type
1	A	1656	LEU
1	A	1695	MET
1	A	1732	PHE
1	A	1738	ASN
2	C	21	CYS
2	C	25	ASP
2	C	75	ASN
2	C	83	ASP
2	C	162	MET
2	C	163	MET
2	C	182	TYR

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

Mol	Chain	Res	Type
1	A	119	ASN
1	A	1678	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

11 monosaccharides 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	$\# Z > 2$
3	NAG	D	1	3,1	14,14,15	0.55	0	17,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	2	3	14,14,15	0.38	0	17,19,21	0.89	1 (5%)
3	BMA	D	3	3	11,11,12	0.63	0	15,15,17	0.81	0
3	MAN	D	4	3	11,11,12	0.69	0	15,15,17	0.61	0
3	MAN	D	5	3	11,11,12	0.77	0	15,15,17	0.69	0
3	MAN	D	6	3	11,11,12	0.35	0	15,15,17	1.06	2 (13%)
3	MAN	D	7	3	11,11,12	0.39	0	15,15,17	0.46	0
3	MAN	D	8	3	11,11,12	0.90	1 (9%)	15,15,17	1.59	2 (13%)
3	MAN	D	9	3	11,11,12	0.20	0	15,15,17	0.57	0
4	NAG	F	1	4,2	14,14,15	0.38	0	17,19,21	0.78	0
4	NAG	F	2	4	14,14,15	0.40	0	17,19,21	0.75	1 (5%)

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	NAG	D	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	5/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1
3	MAN	D	7	3	-	0/2/19/22	1/1/1/1
3	MAN	D	8	3	-	0/2/19/22	0/1/1/1
3	MAN	D	9	3	-	2/2/19/22	0/1/1/1
4	NAG	F	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	8	MAN	C2-C3	2.33	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	8	MAN	C1-C2-C3	4.03	115.51	109.64
3	D	2	NAG	O5-C1-C2	-3.24	106.28	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	8	MAN	O2-C2-C3	2.72	115.79	110.15
4	F	2	NAG	O5-C1-C2	-2.44	107.52	111.29
3	D	6	MAN	O5-C1-C2	2.10	115.81	110.79
3	D	6	MAN	C1-C2-C3	2.10	112.70	109.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C3-C2-N2-C7
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
4	F	2	NAG	C3-C2-N2-C7
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
3	D	3	BMA	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
4	F	1	NAG	C8-C7-N2-C2
3	D	6	MAN	O5-C5-C6-O6
4	F	1	NAG	O7-C7-N2-C2
3	D	9	MAN	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	D	9	MAN	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	7	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 8 short contacts:

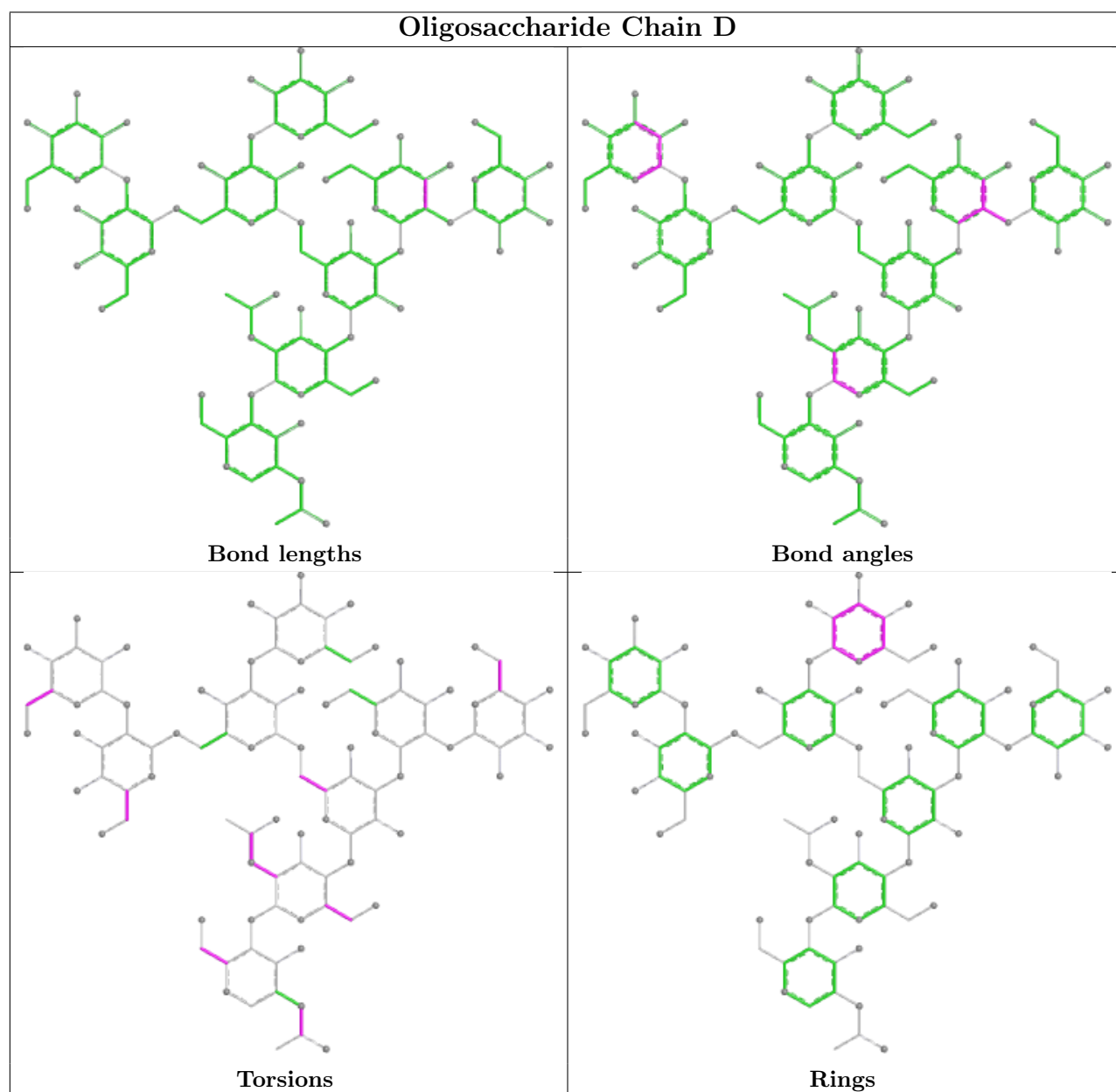
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	8	MAN	2	0

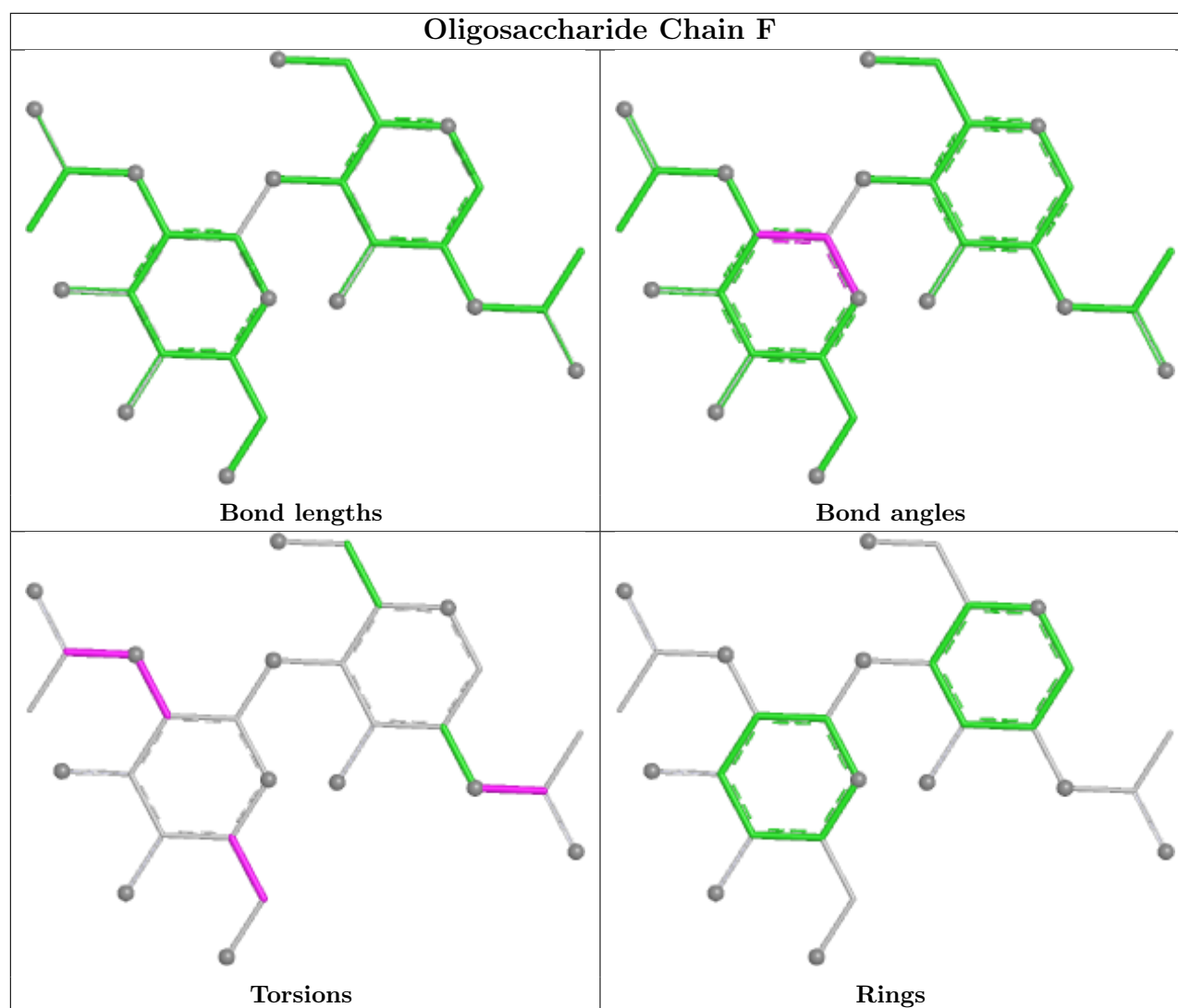
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	6	MAN	3	0
4	F	1	NAG	1	0
3	D	4	MAN	1	0
4	F	2	NAG	1	0
3	D	5	MAN	2	0
3	D	1	NAG	1	0
3	D	9	MAN	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
6	Y01	A	2007	-	38,38,38	0.45	0	57,57,57	0.52	0
8	LPE	A	2016	-	24,24,33	0.28	0	28,30,39	0.39	0
8	LPE	A	2011	-	27,27,33	0.27	0	31,33,39	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	302	2	14,14,15	0.27	0	17,19,21	0.61	0
5	NAG	A	2003	1	14,14,15	0.66	0	17,19,21	1.55	1 (5%)
5	NAG	A	2002	1	14,14,15	0.29	0	17,19,21	0.82	1 (5%)
8	LPE	A	2010	-	21,21,33	0.31	0	25,27,39	0.40	0
12	P3X	A	2021	-	44,44,44	1.09	5 (11%)	47,49,49	0.97	2 (4%)
10	P5S	A	2019	-	33,34,53	0.46	0	34,40,60	0.45	0
5	NAG	A	2001	1	14,14,15	0.30	0	17,19,21	0.65	0
6	Y01	A	2005	-	38,38,38	0.46	0	57,57,57	0.49	0
9	PCW	A	2012	-	46,46,53	0.31	0	52,54,61	0.35	0
9	PCW	A	2009	-	52,52,53	0.31	0	58,60,61	0.44	1 (1%)
5	NAG	A	2004	1	14,14,15	0.32	0	17,19,21	0.56	0
5	NAG	C	303	2	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
7	CLR	A	2006	-	31,31,31	0.39	0	48,48,48	0.61	0
8	LPE	A	2008	-	24,24,33	0.28	0	28,30,39	0.32	0
5	NAG	C	301	2	14,14,15	0.39	0	17,19,21	0.92	1 (5%)
9	PCW	A	2014	-	43,43,53	0.32	0	49,51,61	0.39	0
6	Y01	A	2017	-	38,38,38	0.47	0	57,57,57	0.57	0
6	Y01	A	2018	-	38,38,38	0.45	0	57,57,57	0.54	0
8	LPE	A	2015	-	24,24,33	0.28	0	28,30,39	0.38	0
10	P5S	A	2013	-	40,40,53	0.31	0	43,45,60	0.42	0
11	9Z9	A	2020	-	44,44,44	0.26	0	64,68,68	0.49	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
6	Y01	A	2007	-	-	2/19/77/77	0/4/4/4
8	LPE	A	2016	-	-	3/25/25/34	-
8	LPE	A	2011	-	-	3/28/28/34	-
5	NAG	C	302	2	-	2/6/23/26	0/1/1/1
5	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
8	LPE	A	2010	-	-	3/22/22/34	-
12	P3X	A	2021	-	-	31/48/48/48	-
10	P5S	A	2019	-	-	4/39/39/59	-
5	NAG	A	2001	1	-	3/6/23/26	0/1/1/1
6	Y01	A	2005	-	-	9/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PCW	A	2012	-	-	6/50/50/57	-
9	PCW	A	2009	-	-	9/56/56/57	-
5	NAG	A	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	C	303	2	-	4/6/23/26	0/1/1/1
7	CLR	A	2006	-	-	0/10/68/68	0/4/4/4
8	LPE	A	2008	-	-	1/25/25/34	-
5	NAG	C	301	2	-	1/6/23/26	0/1/1/1
9	PCW	A	2014	-	-	13/47/47/57	-
6	Y01	A	2017	-	-	7/19/77/77	0/4/4/4
6	Y01	A	2018	-	-	5/19/77/77	0/4/4/4
8	LPE	A	2015	-	-	6/25/25/34	-
10	P5S	A	2013	-	-	9/44/44/59	-
11	9Z9	A	2020	-	-	2/12/100/100	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	2021	P3X	C6-C5	3.79	1.53	1.31
12	A	2021	P3X	O7-C16	-2.61	1.40	1.46
12	A	2021	P3X	O2-C14	2.35	1.40	1.33
12	A	2021	P3X	O2-C15	-2.21	1.40	1.45
12	A	2021	P3X	O7-C20	2.18	1.40	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2003	NAG	C2-N2-C7	-4.10	117.41	122.90
12	A	2021	P3X	O7-C20-C21	4.07	120.28	111.48
5	C	301	NAG	C1-O5-C5	3.16	116.42	112.19
12	A	2021	P3X	O2-C14-C13	2.65	119.91	111.83
5	C	303	NAG	C1-O5-C5	2.62	115.70	112.19
5	A	2002	NAG	O5-C1-C2	-2.35	107.65	111.29
9	A	2009	PCW	O2-C31-C32	2.12	116.07	111.48

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2001	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	A	2001	NAG	O7-C7-N2-C2
5	A	2003	NAG	C8-C7-N2-C2
5	A	2003	NAG	O7-C7-N2-C2
5	C	302	NAG	C8-C7-N2-C2
5	C	302	NAG	O7-C7-N2-C2
6	A	2018	Y01	OAG-CAY-OAW-CBC
6	A	2018	Y01	CAM-CAY-OAW-CBC
8	A	2016	LPE	C2-C3-O3-P
8	A	2016	LPE	C3-O3-P-O32
8	A	2016	LPE	C3-O3-P-O33
9	A	2009	PCW	C32-C31-O2-C2
9	A	2009	PCW	O31-C31-O2-C2
9	A	2012	PCW	C1-O3P-P-O2P
9	A	2012	PCW	C4-O4P-P-O2P
9	A	2014	PCW	C2-C1-O3P-P
9	A	2014	PCW	C5-C4-O4P-P
9	A	2014	PCW	C32-C31-O2-C2
9	A	2014	PCW	O31-C31-O2-C2
10	A	2013	P5S	C3-O16-P12-O15
10	A	2019	P5S	N-CA-CB-OG
12	A	2021	P3X	C21-C20-O7-C16
12	A	2021	P3X	C18-O6-P1-O3
12	A	2021	P3X	C18-O6-P1-O5
12	A	2021	P3X	O8-C20-O7-C16
5	A	2002	NAG	O7-C7-N2-C2
5	C	303	NAG	C8-C7-N2-C2
5	C	303	NAG	O7-C7-N2-C2
9	A	2009	PCW	C2-C1-O3P-P
5	A	2002	NAG	C8-C7-N2-C2
12	A	2021	P3X	C13-C14-O2-C15
12	A	2021	P3X	C24-C25-C26-C27
6	A	2005	Y01	CAJ-CAO-CBB-CBE
6	A	2017	Y01	CAC-CBB-CBE-CAP
6	A	2017	Y01	CAC-CBB-CBE-CBI
6	A	2017	Y01	CAO-CBB-CBE-CBI
6	A	2005	Y01	CAO-CAJ-CAN-CBA
6	A	2005	Y01	CAJ-CAO-CBB-CAC
12	A	2021	P3X	O1-C14-O2-C15
10	A	2019	P5S	OXT-C-CA-N
6	A	2017	Y01	CAO-CBB-CBE-CAP
12	A	2021	P3X	C4-C5-C6-C7
12	A	2021	P3X	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
12	A	2021	P3X	C26-C27-C28-C29
12	A	2021	P3X	C11-C12-C13-C14
12	A	2021	P3X	C31-C32-C33-C34
12	A	2021	P3X	C28-C29-C30-C31
10	A	2013	P5S	C2-C3-O16-P12
12	A	2021	P3X	C11-C10-C9-C8
12	A	2021	P3X	C20-C21-C22-C23
12	A	2021	P3X	C25-C26-C27-C28
12	A	2021	P3X	C6-C7-C8-C9
5	A	2001	NAG	O5-C5-C6-O6
9	A	2014	PCW	C12-C11-O3-C3
6	A	2005	Y01	CAC-CBB-CBE-CAP
5	C	301	NAG	O5-C5-C6-O6
5	C	303	NAG	O5-C5-C6-O6
12	A	2021	P3X	C21-C22-C23-C24
6	A	2005	Y01	CAO-CBB-CBE-CBI
12	A	2021	P3X	C22-C23-C24-C25
6	A	2017	Y01	CAJ-CAO-CBB-CAC
6	A	2005	Y01	CAC-CBB-CBE-CBI
9	A	2014	PCW	C23-C24-C25-C26
9	A	2014	PCW	O3-C11-C12-C13
8	A	2015	LPE	C2-C1-O1-C11
9	A	2014	PCW	O11-C11-O3-C3
12	A	2021	P3X	O2-C15-C16-C17
9	A	2009	PCW	O3P-C1-C2-O2
6	A	2005	Y01	CAO-CBB-CBE-CAP
6	A	2018	Y01	CAO-CAJ-CAN-CBA
12	A	2021	P3X	C10-C11-C12-C13
8	A	2010	LPE	C32-C31-O33-P
8	A	2011	LPE	C32-C31-O33-P
8	A	2008	LPE	O33-C31-C32-N
8	A	2010	LPE	O33-C31-C32-N
8	A	2011	LPE	O33-C31-C32-N
8	A	2015	LPE	O33-C31-C32-N
9	A	2009	PCW	O4P-C4-C5-N
9	A	2014	PCW	O4P-C4-C5-N
12	A	2021	P3X	C9-C10-C11-C12
9	A	2014	PCW	O3P-C1-C2-C3
10	A	2013	P5S	C40-C41-C42-C43
12	A	2021	P3X	C27-C28-C29-C30
9	A	2014	PCW	O3P-C1-C2-O2
12	A	2021	P3X	C32-C33-C34-C35

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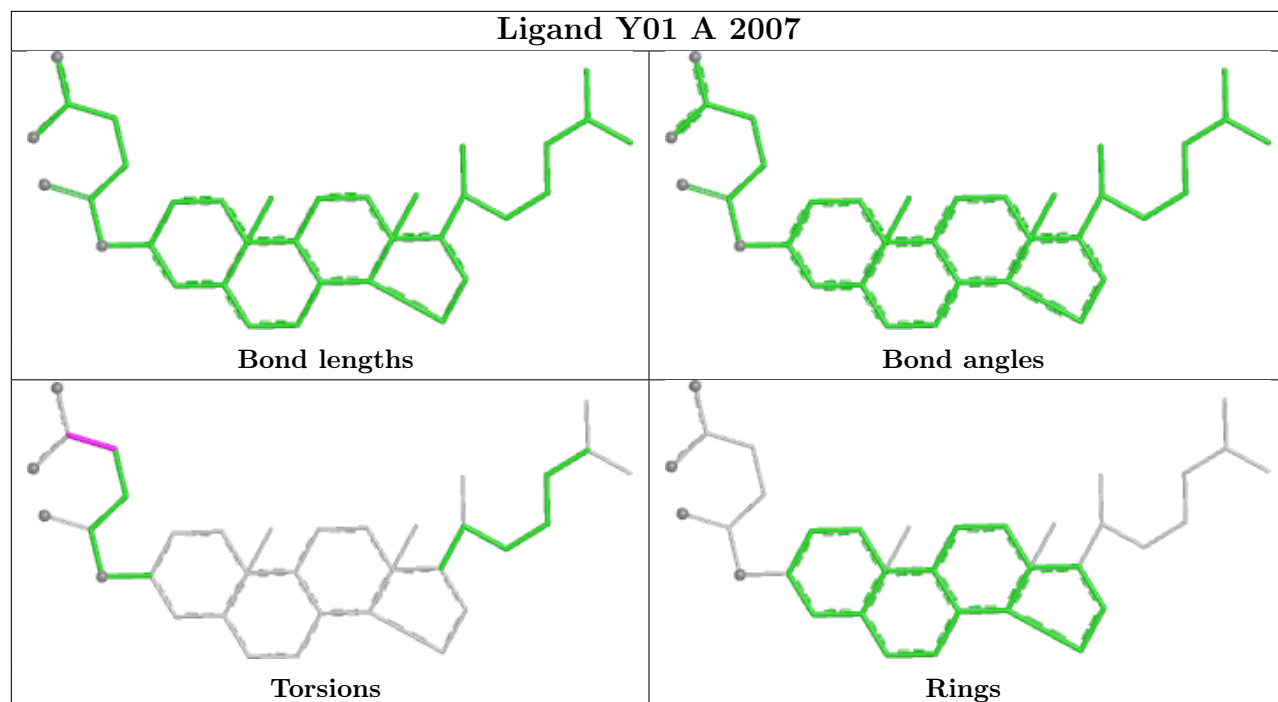
Mol	Chain	Res	Type	Atoms
12	A	2021	P3X	C30-C31-C32-C33
12	A	2021	P3X	O2-C15-C16-O7
9	A	2009	PCW	C19-C20-C21-C22
9	A	2012	PCW	C19-C20-C21-C22
8	A	2010	LPE	C31-O33-P-O31
8	A	2011	LPE	C31-O33-P-O31
8	A	2015	LPE	C3-O3-P-O31
8	A	2015	LPE	C31-O33-P-O31
9	A	2009	PCW	C4-O4P-P-O2P
10	A	2013	P5S	C3-O16-P12-OG
10	A	2013	P5S	C3-O16-P12-O13
12	A	2021	P3X	C18-O6-P1-O4
9	A	2009	PCW	O3P-C1-C2-C3
9	A	2012	PCW	C39-C40-C41-C42
9	A	2014	PCW	C11-C12-C13-C14
9	A	2014	PCW	O11-C11-C12-C13
11	A	2020	9Z9	C21-C22-C23-C24
6	A	2007	Y01	CAM-CAL-CAX-OAH
12	A	2021	P3X	C16-C17-O3-P1
10	A	2013	P5S	O19-C1-C2-O37
6	A	2007	Y01	CAM-CAL-CAX-OAF
5	C	303	NAG	C1-C2-N2-C7
6	A	2018	Y01	CAM-CAL-CAX-OAH
8	A	2015	LPE	C12-C11-O1-C1
12	A	2021	P3X	C29-C30-C31-C32
6	A	2005	Y01	CAM-CAL-CAX-OAH
6	A	2017	Y01	CAM-CAL-CAX-OAH
6	A	2018	Y01	CAM-CAL-CAX-OAF
6	A	2005	Y01	CAM-CAL-CAX-OAF
6	A	2017	Y01	CAM-CAL-CAX-OAF
8	A	2015	LPE	O1-C11-C12-C13
10	A	2019	P5S	C43-C44-C45-C46
10	A	2013	P5S	C23-C24-C25-C26
9	A	2012	PCW	C34-C35-C36-C37
9	A	2009	PCW	O2-C2-C3-O3
12	A	2021	P3X	C15-C16-O7-C20
12	A	2021	P3X	C17-C16-O7-C20
11	A	2020	9Z9	C21-C22-C23-C48
10	A	2013	P5S	C28-C29-C30-C31
10	A	2019	P5S	O-C-CA-N
9	A	2012	PCW	O2-C31-C32-C33
10	A	2013	P5S	O37-C38-C39-C40

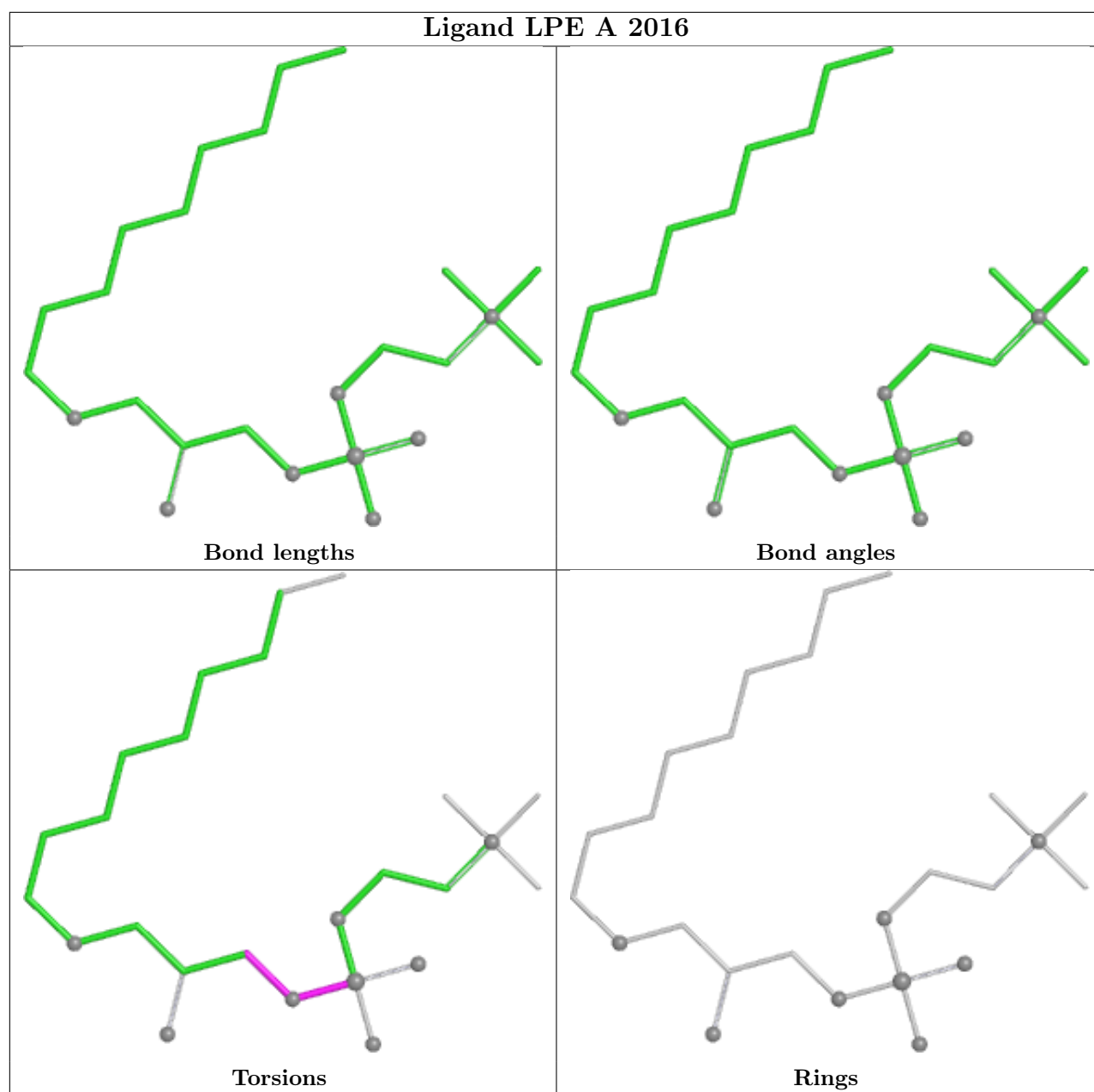
There are no ring outliers.

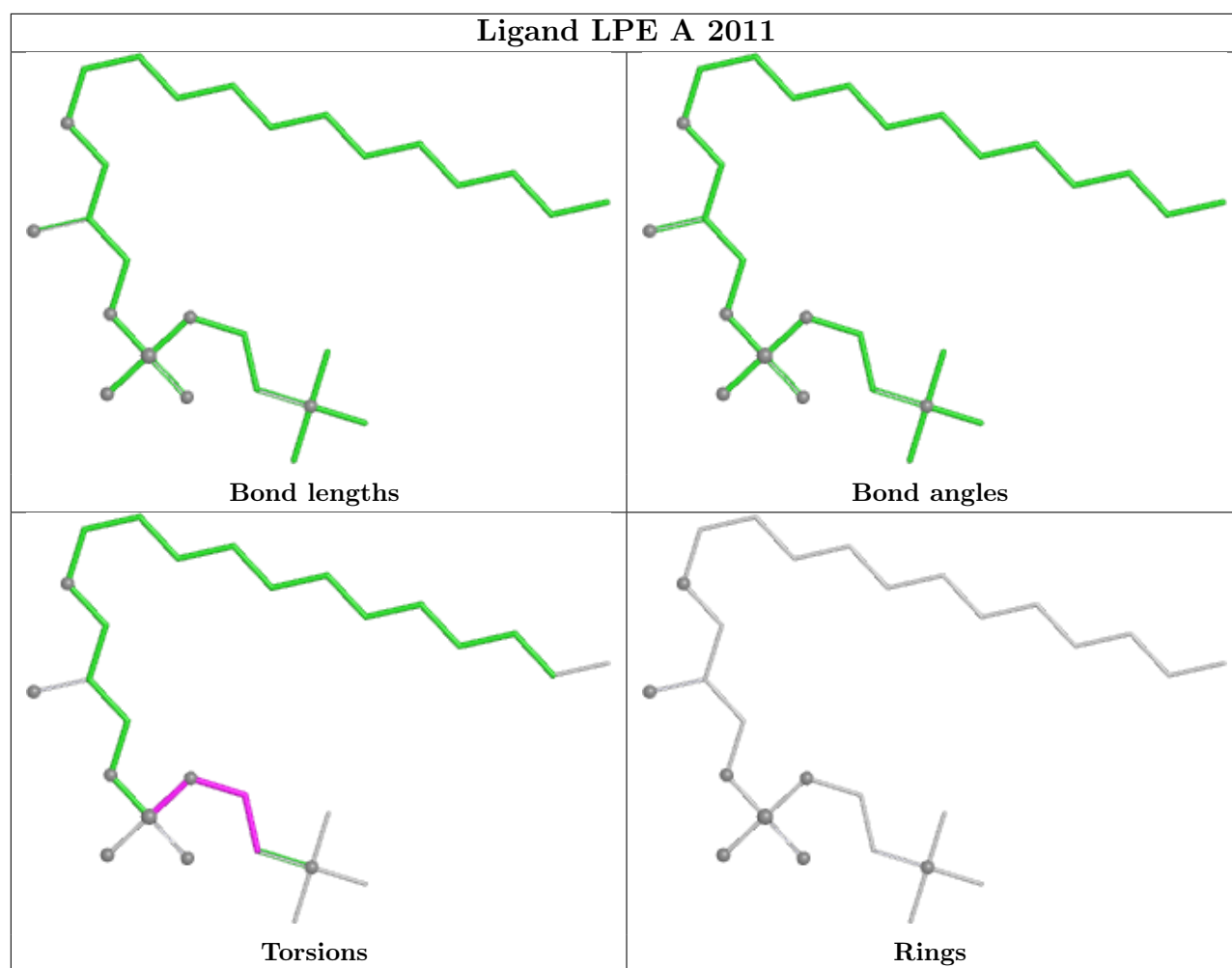
12 monomers are involved in 27 short contacts:

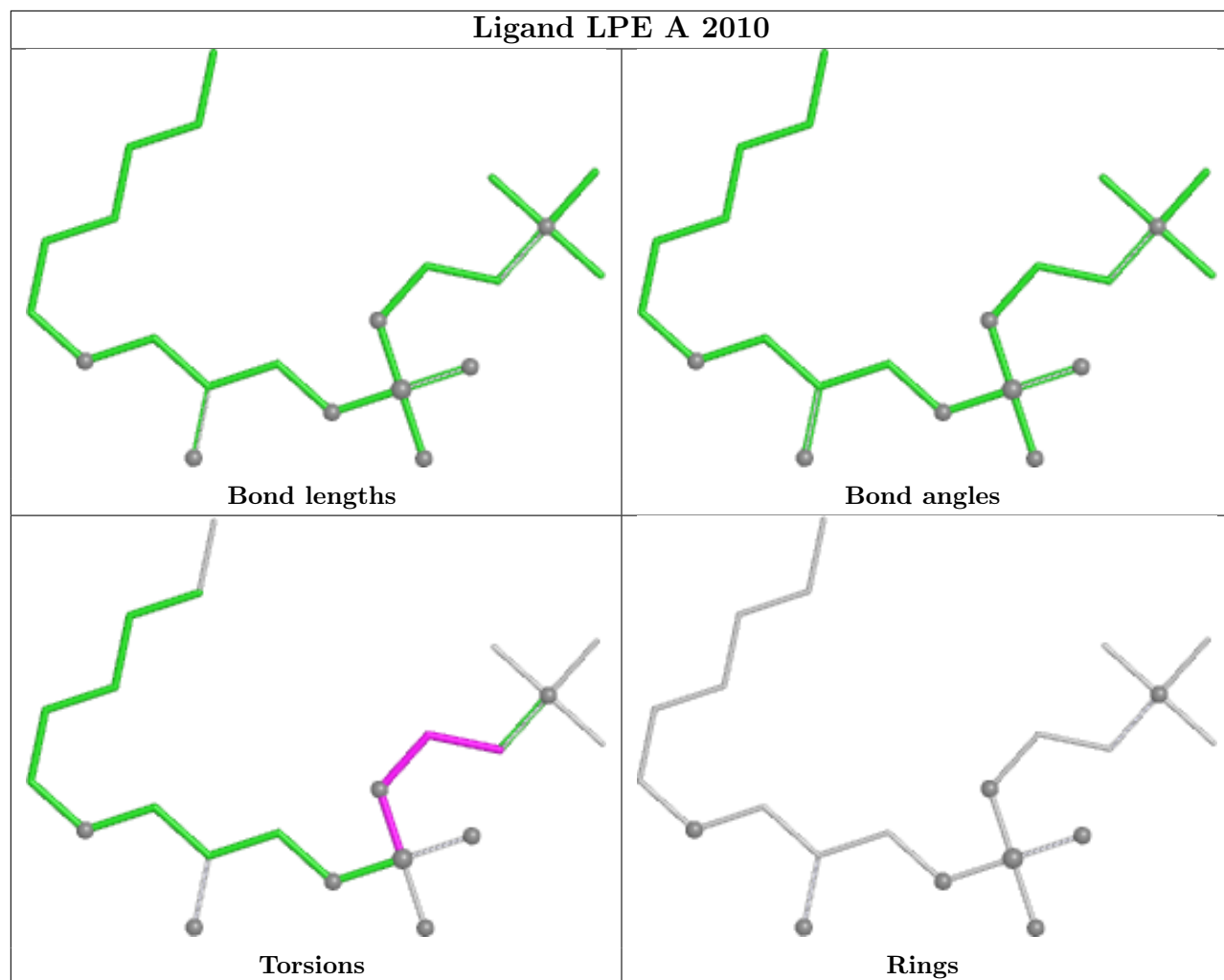
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2016	LPE	3	0
8	A	2011	LPE	1	0
5	A	2003	NAG	2	0
8	A	2010	LPE	1	0
9	A	2012	PCW	1	0
9	A	2009	PCW	3	0
5	C	301	NAG	1	0
9	A	2014	PCW	4	0
6	A	2017	Y01	2	0
6	A	2018	Y01	4	0
8	A	2015	LPE	1	0
10	A	2013	P5S	8	0

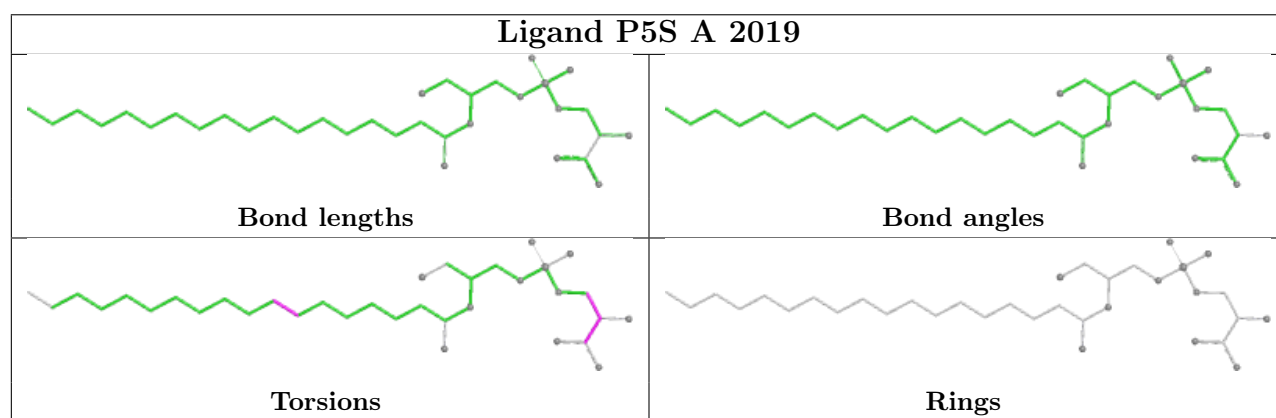
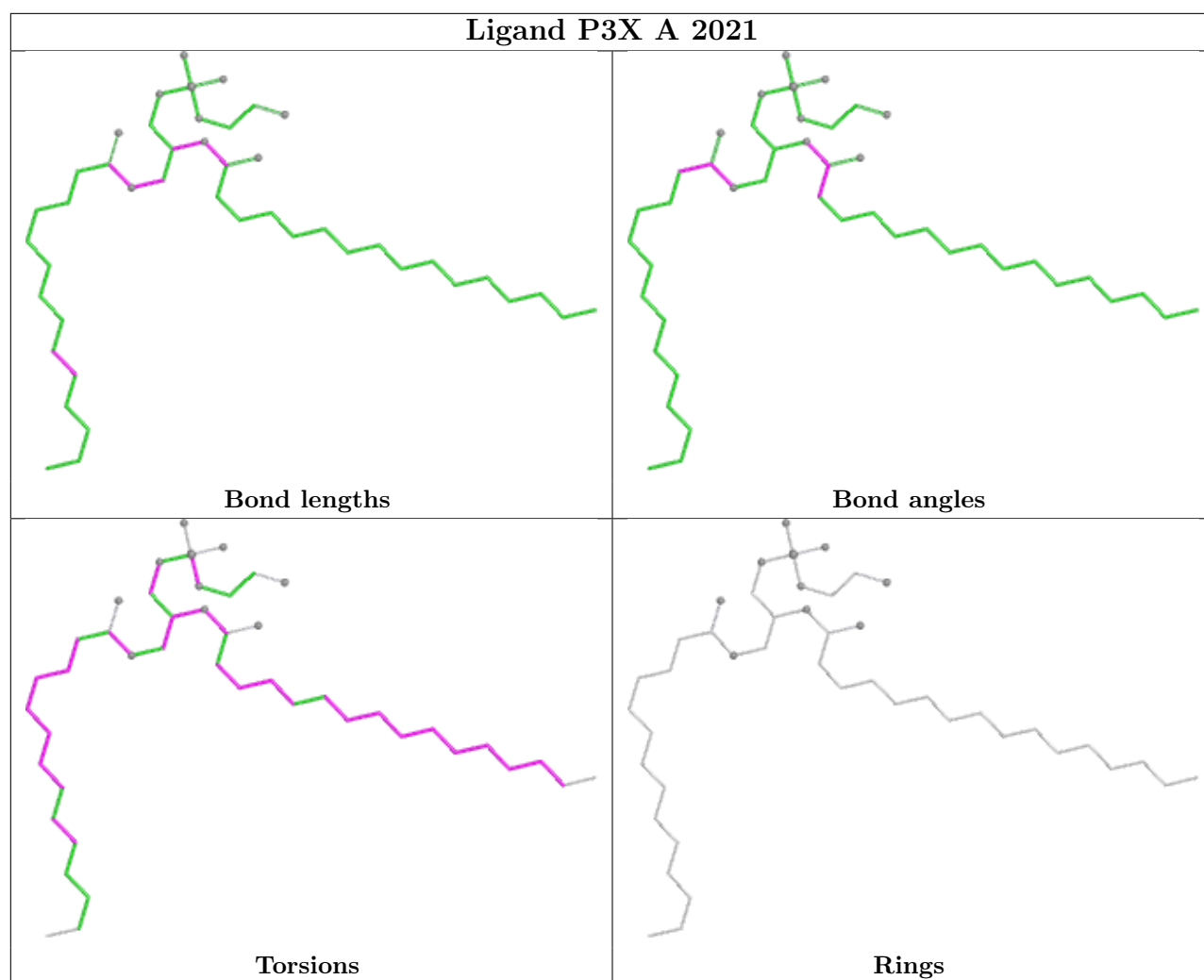
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

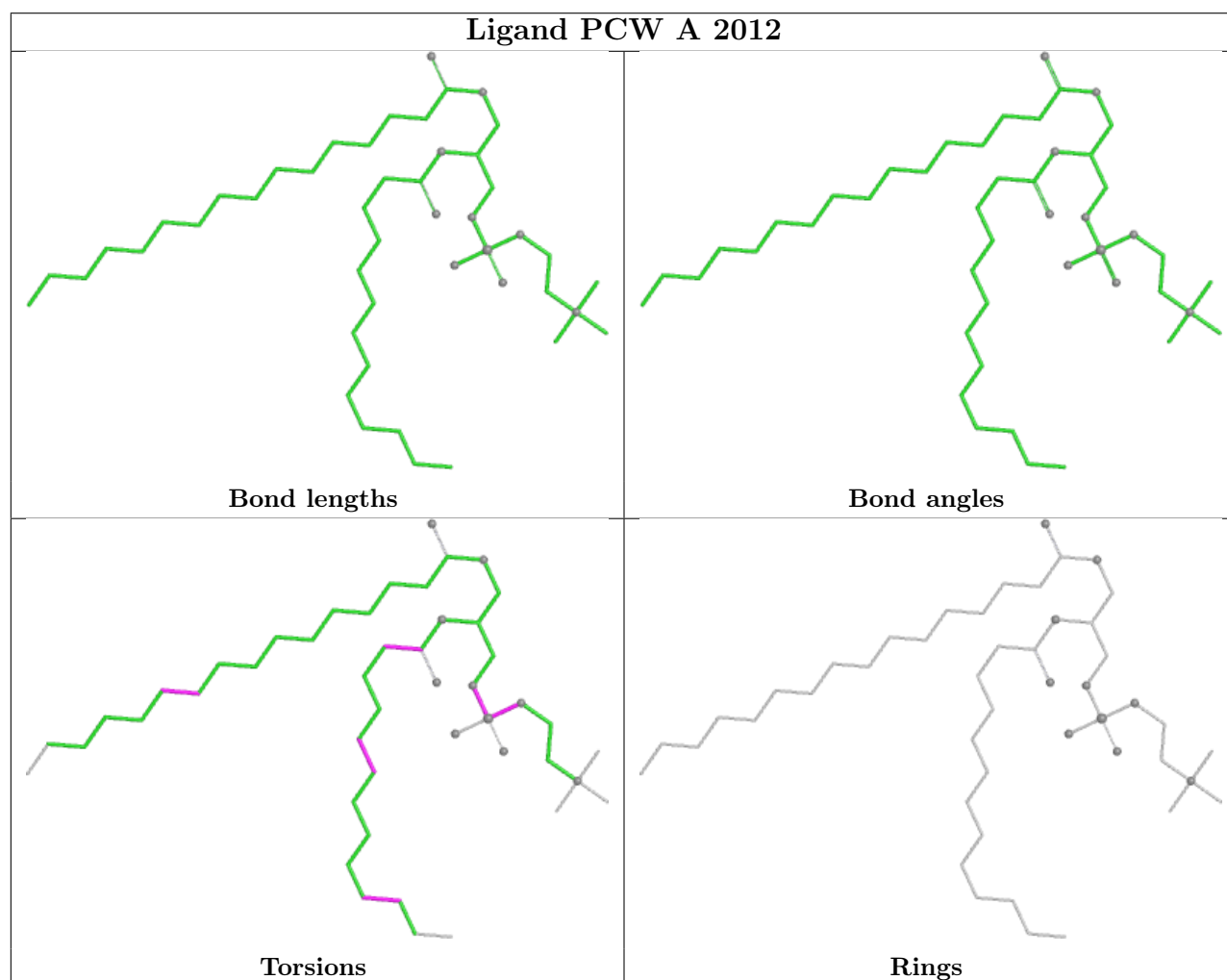
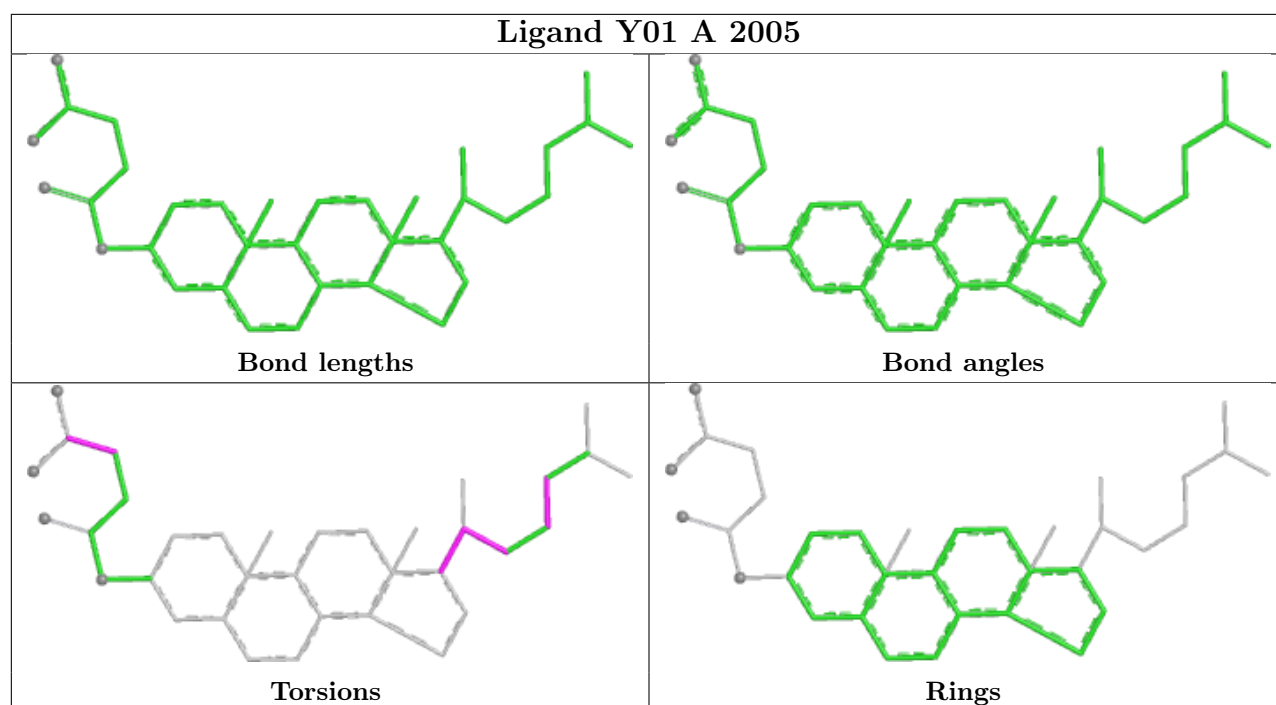


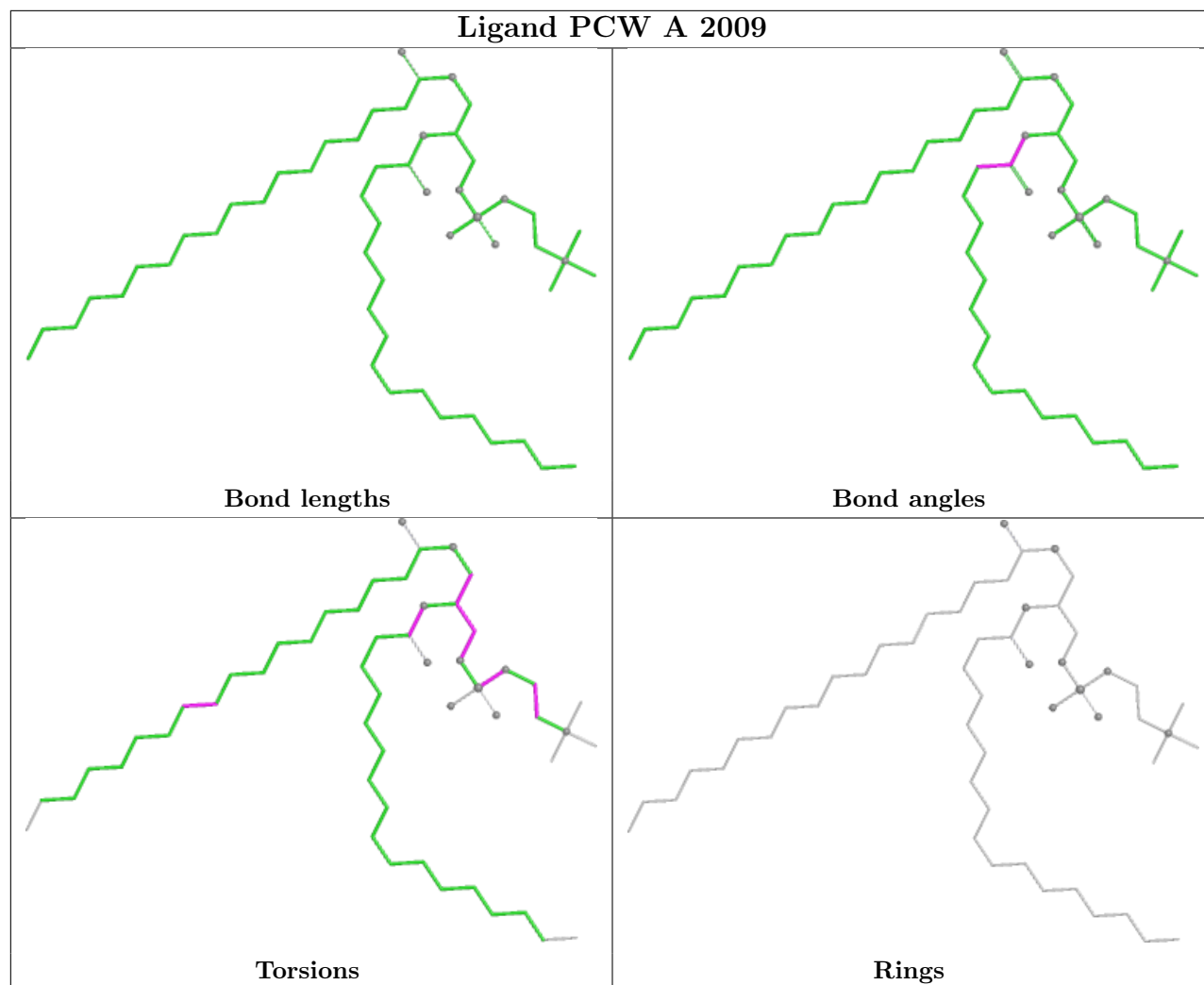


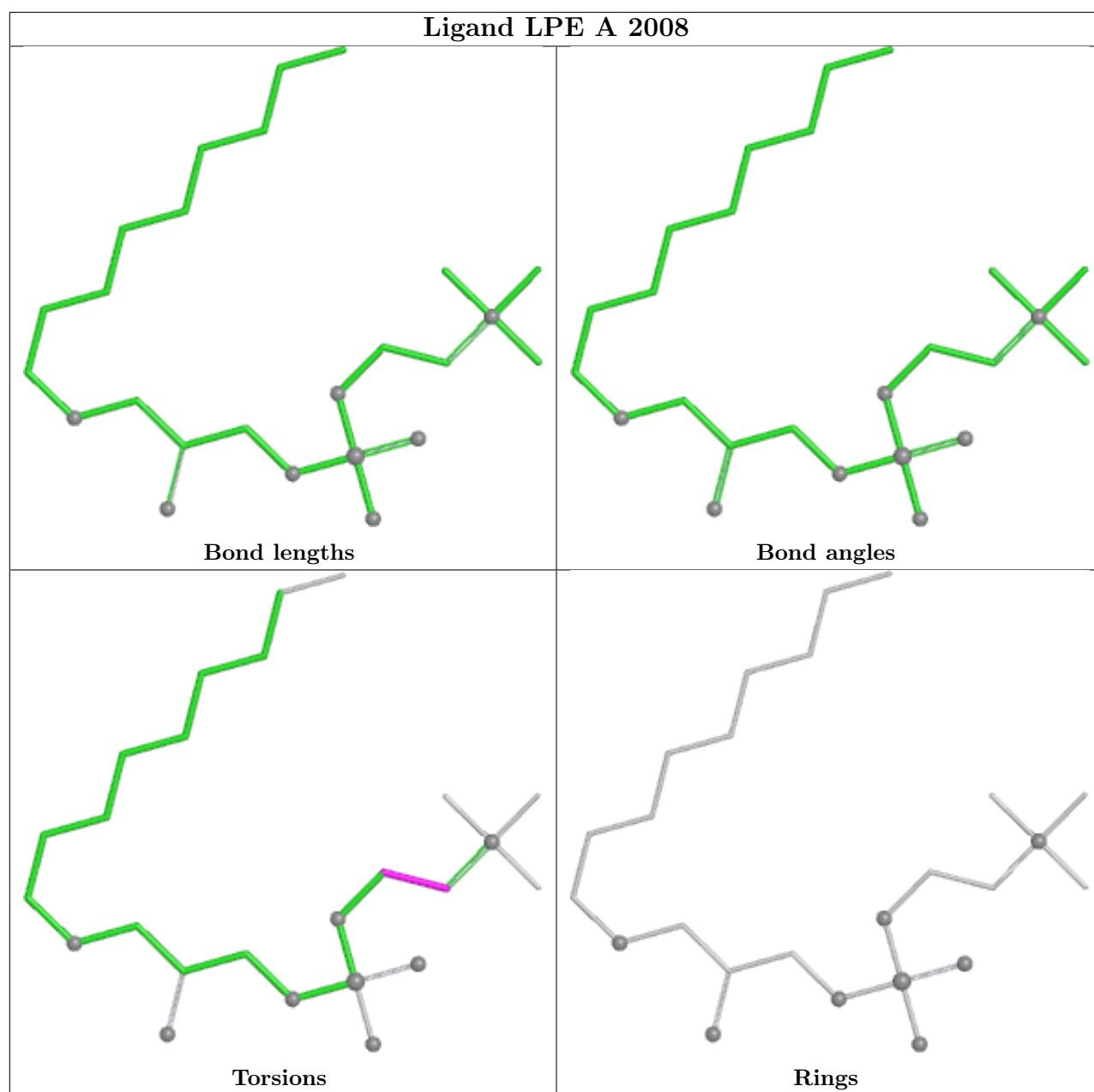


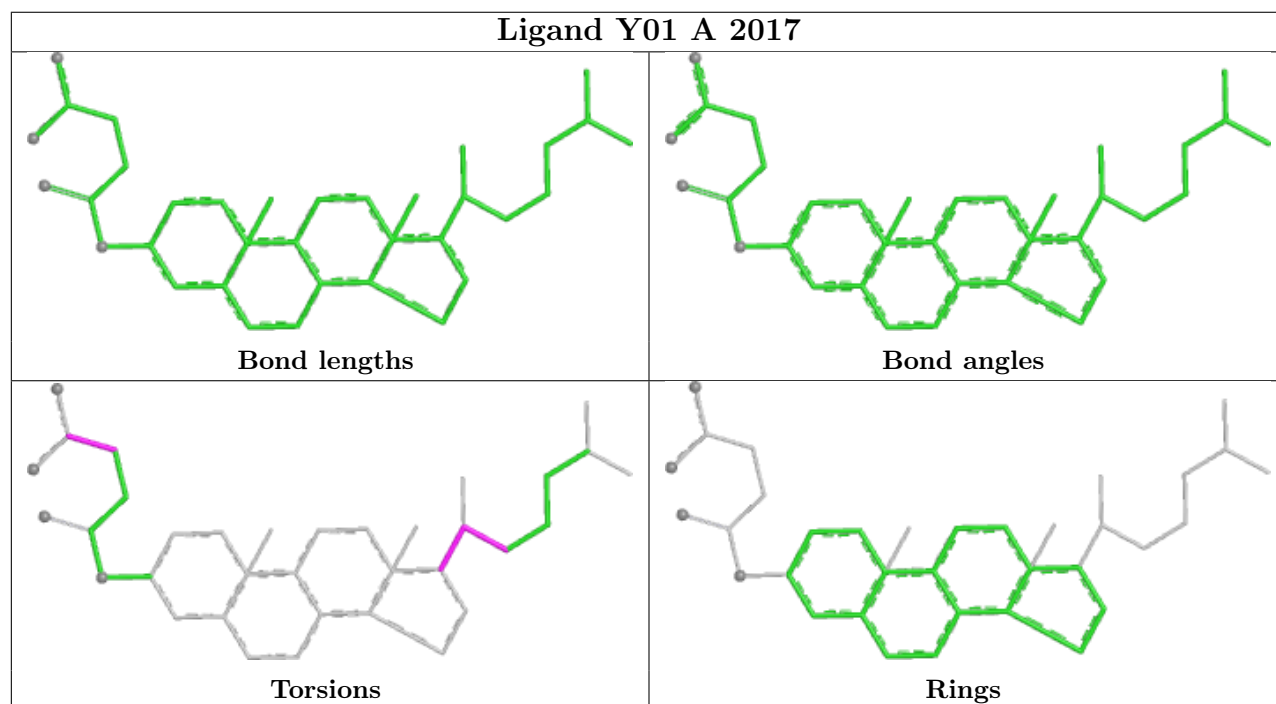
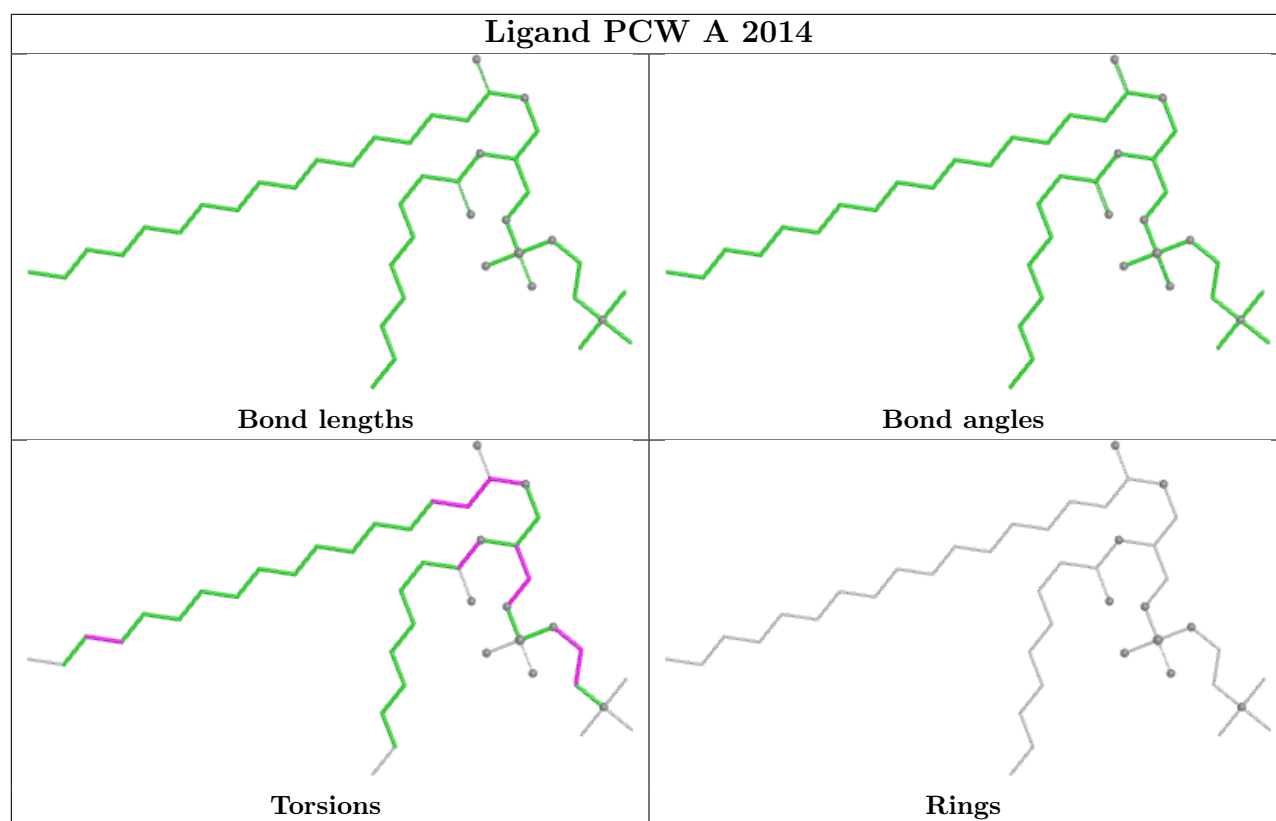


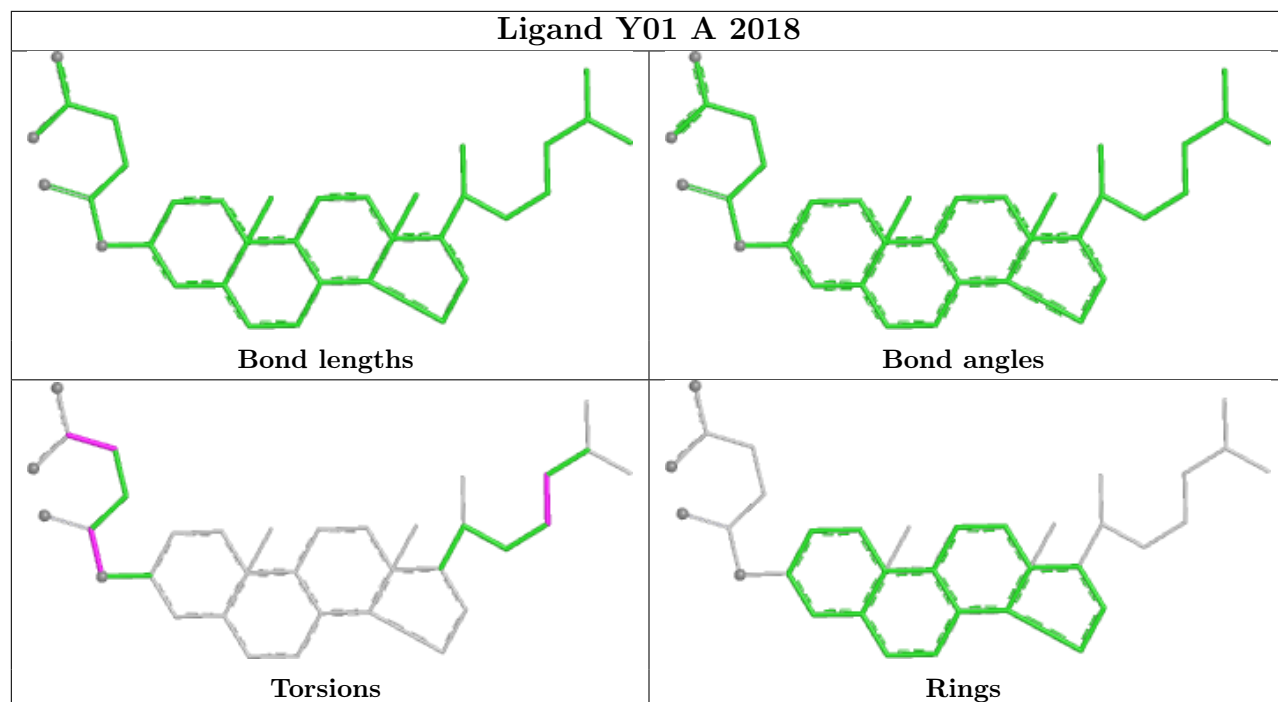


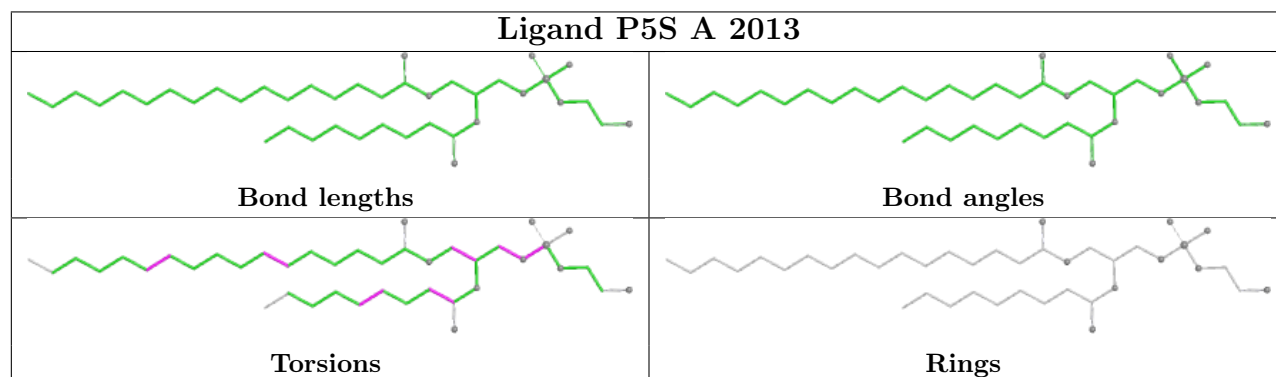
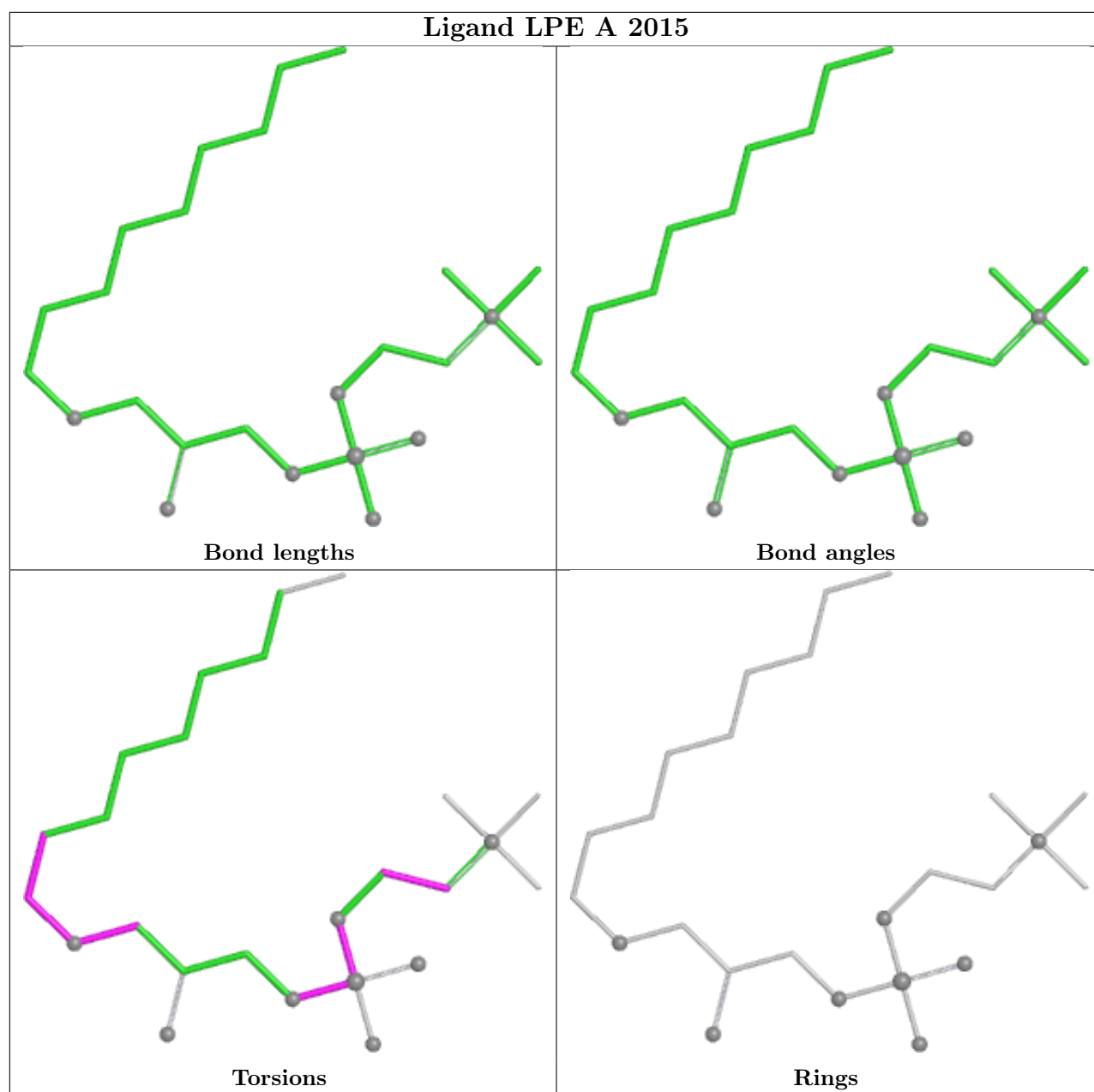


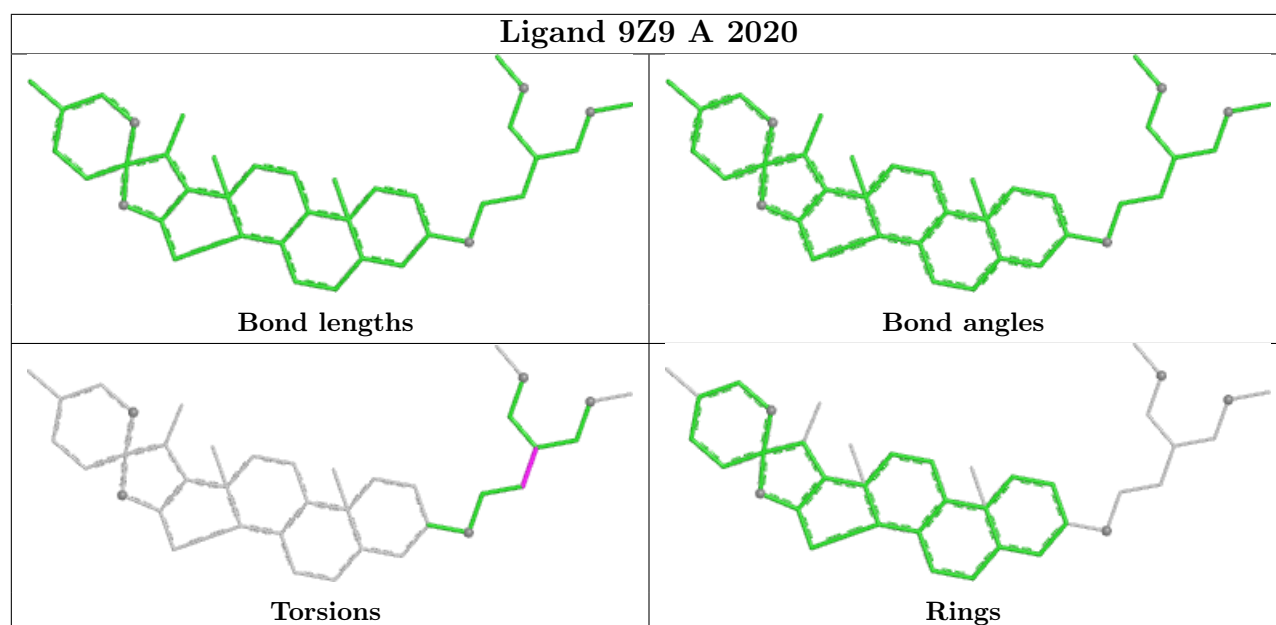












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

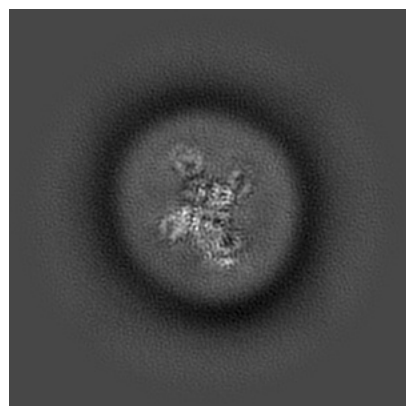
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29082. These allow visual inspection of the internal detail of the map and identification of artifacts.

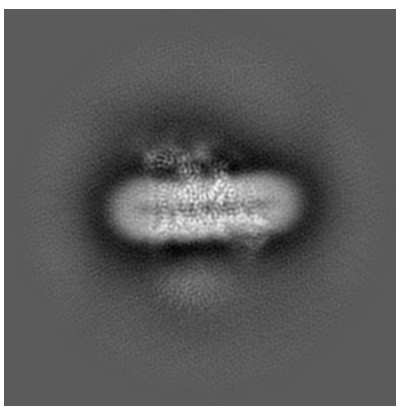
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

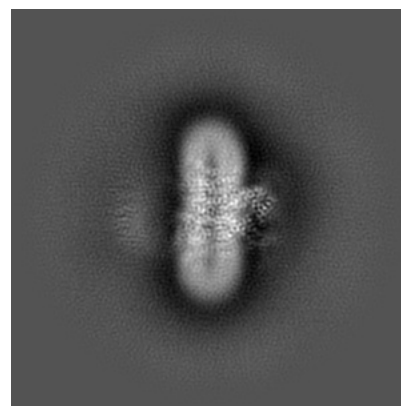
6.1.1 Primary map



X

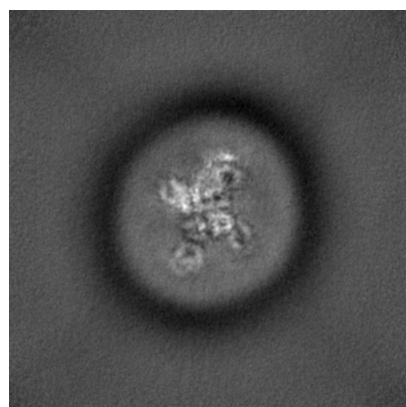


Y

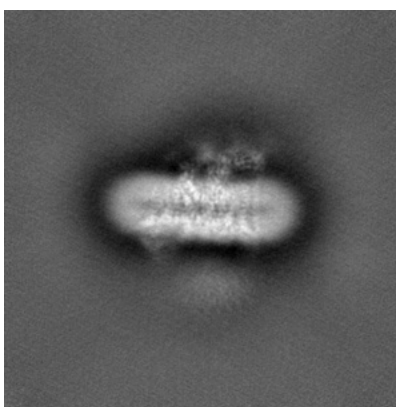


Z

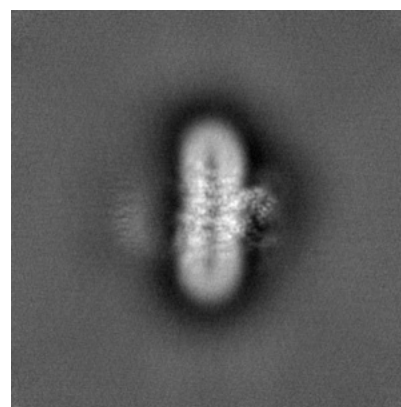
6.1.2 Raw map



X



Y

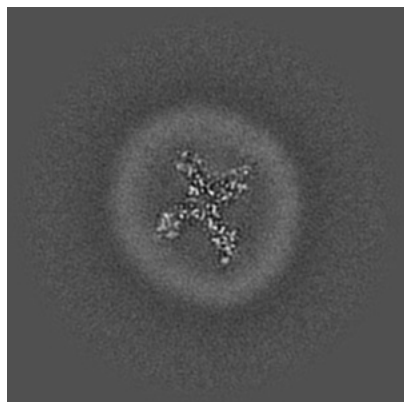


Z

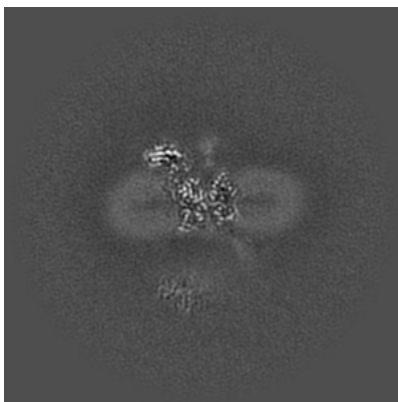
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

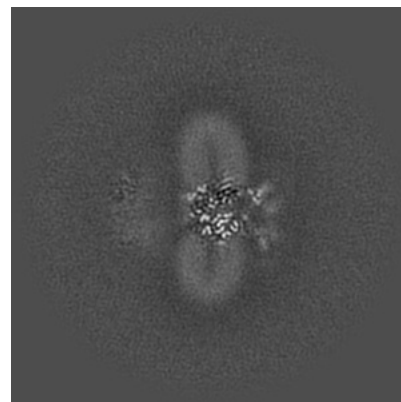
6.2.1 Primary map



X Index: 160

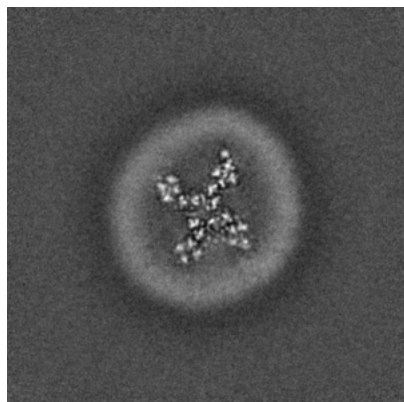


Y Index: 160

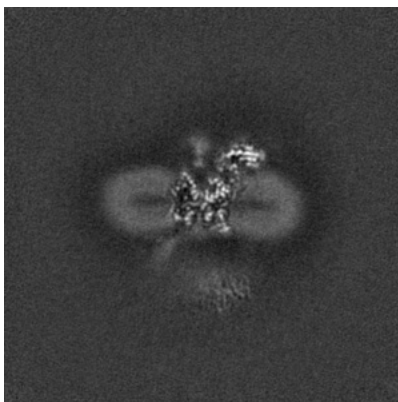


Z Index: 160

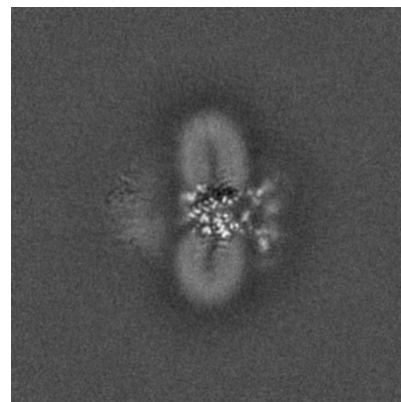
6.2.2 Raw map



X Index: 160



Y Index: 160

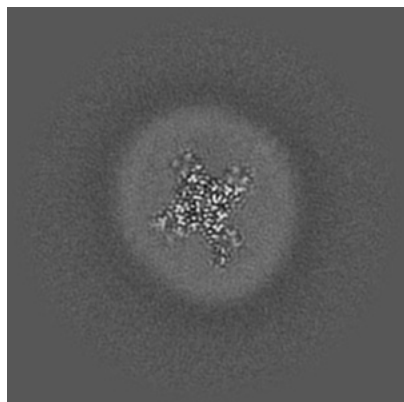


Z Index: 160

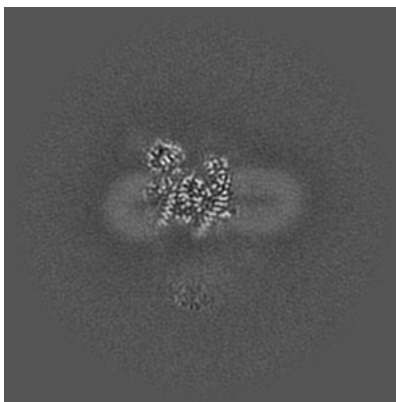
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

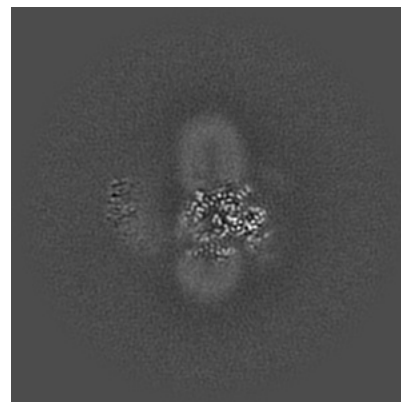
6.3.1 Primary map



X Index: 170

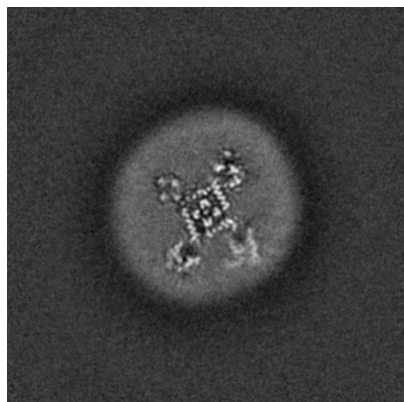


Y Index: 167

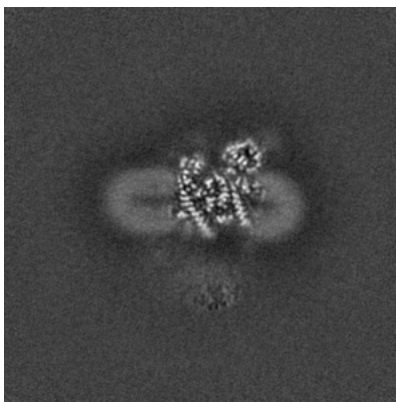


Z Index: 148

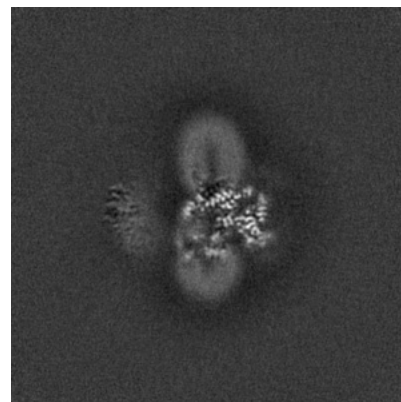
6.3.2 Raw map



X Index: 150



Y Index: 167

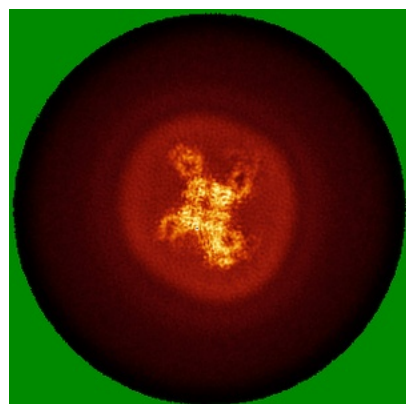


Z Index: 175

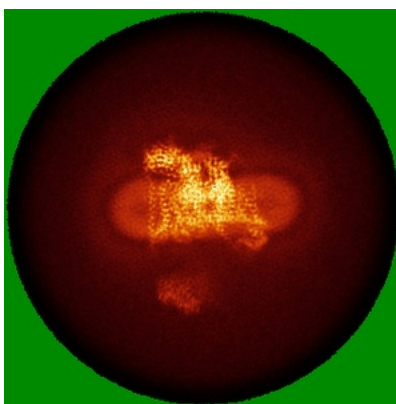
The images above show the largest variance slices of the map in three orthogonal directions.

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

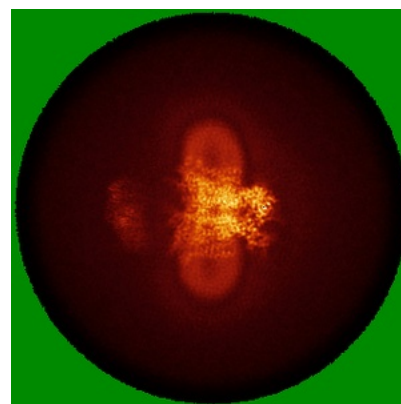
6.4.1 Primary map



X

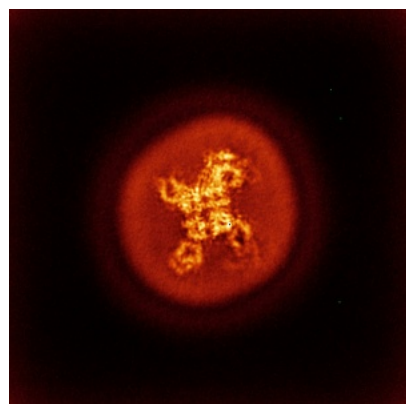


Y

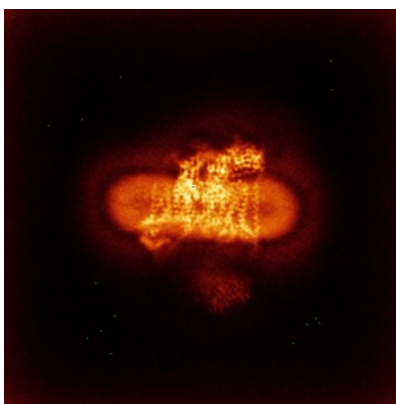


Z

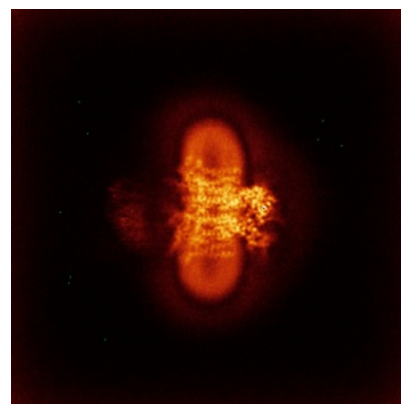
6.4.2 Raw map



X



Y

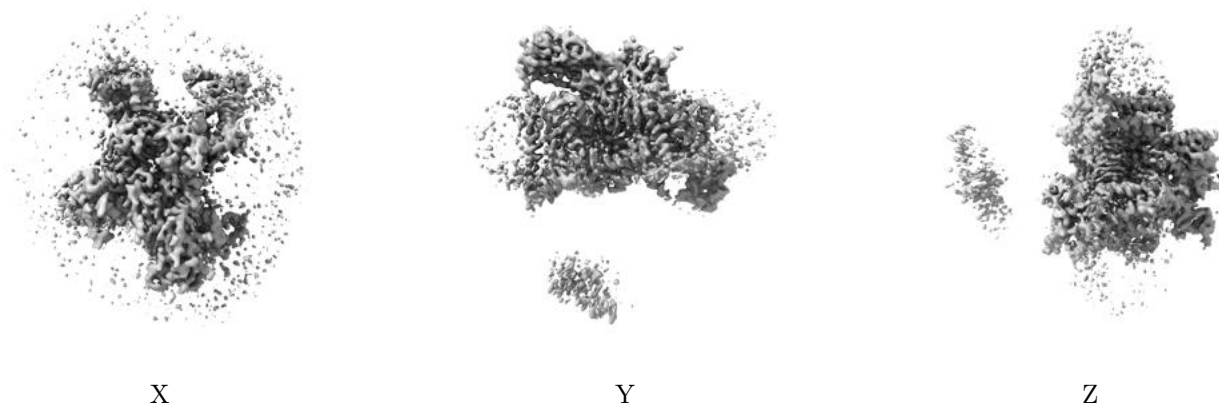


Z

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 0.6. 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.

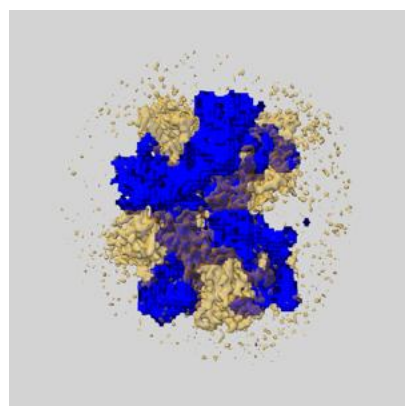
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

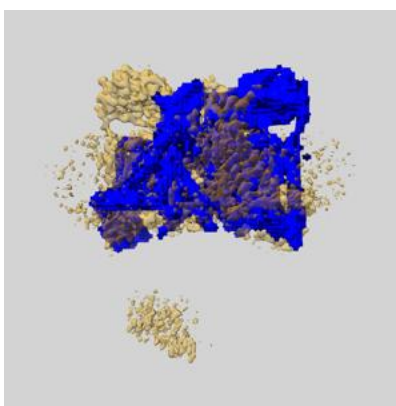
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

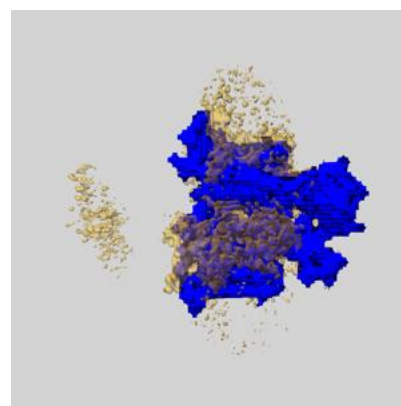
6.6.1 emd_29082_msk_1.map [i](#)



X



Y

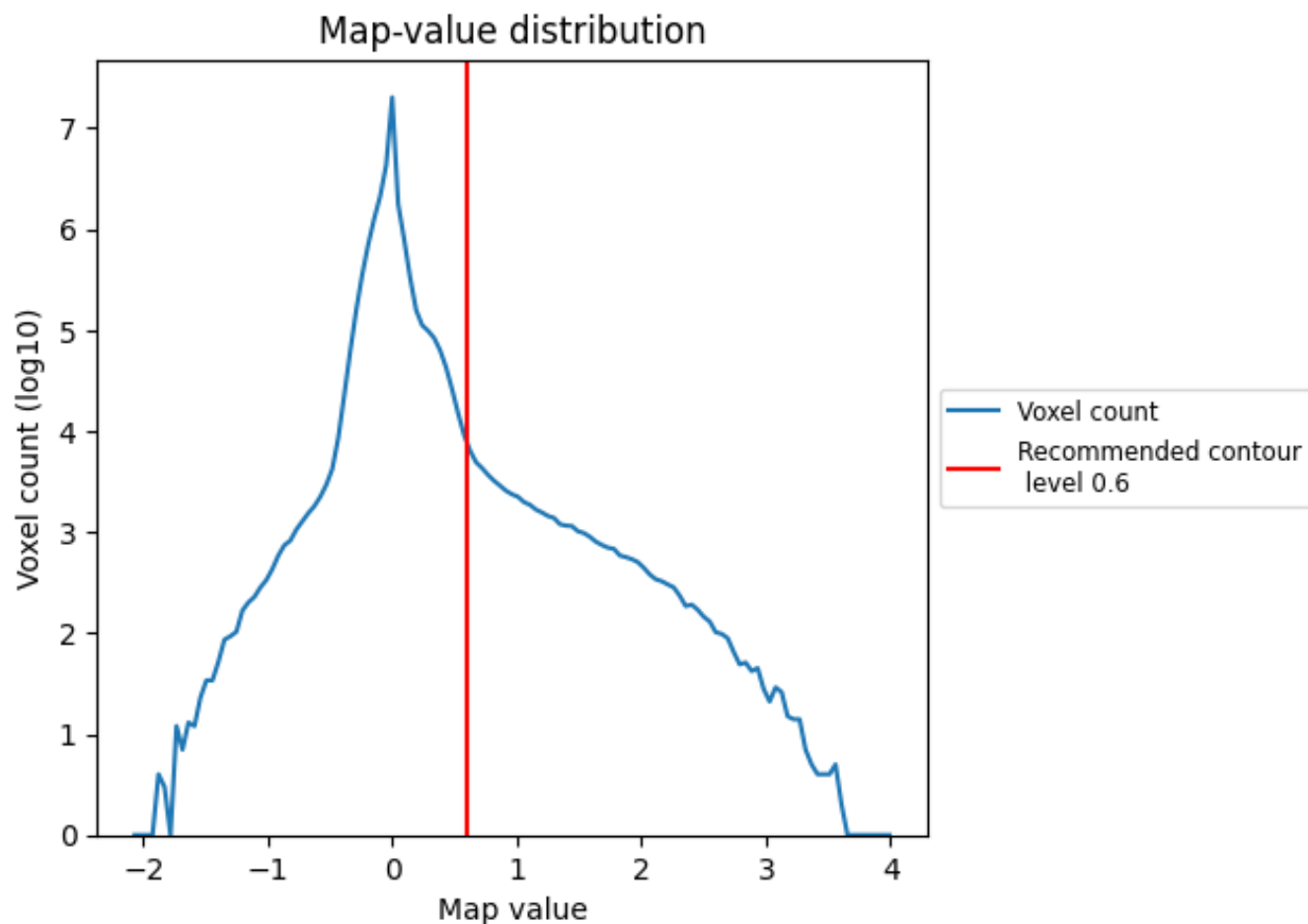


Z

7 Map analysis [i](#)

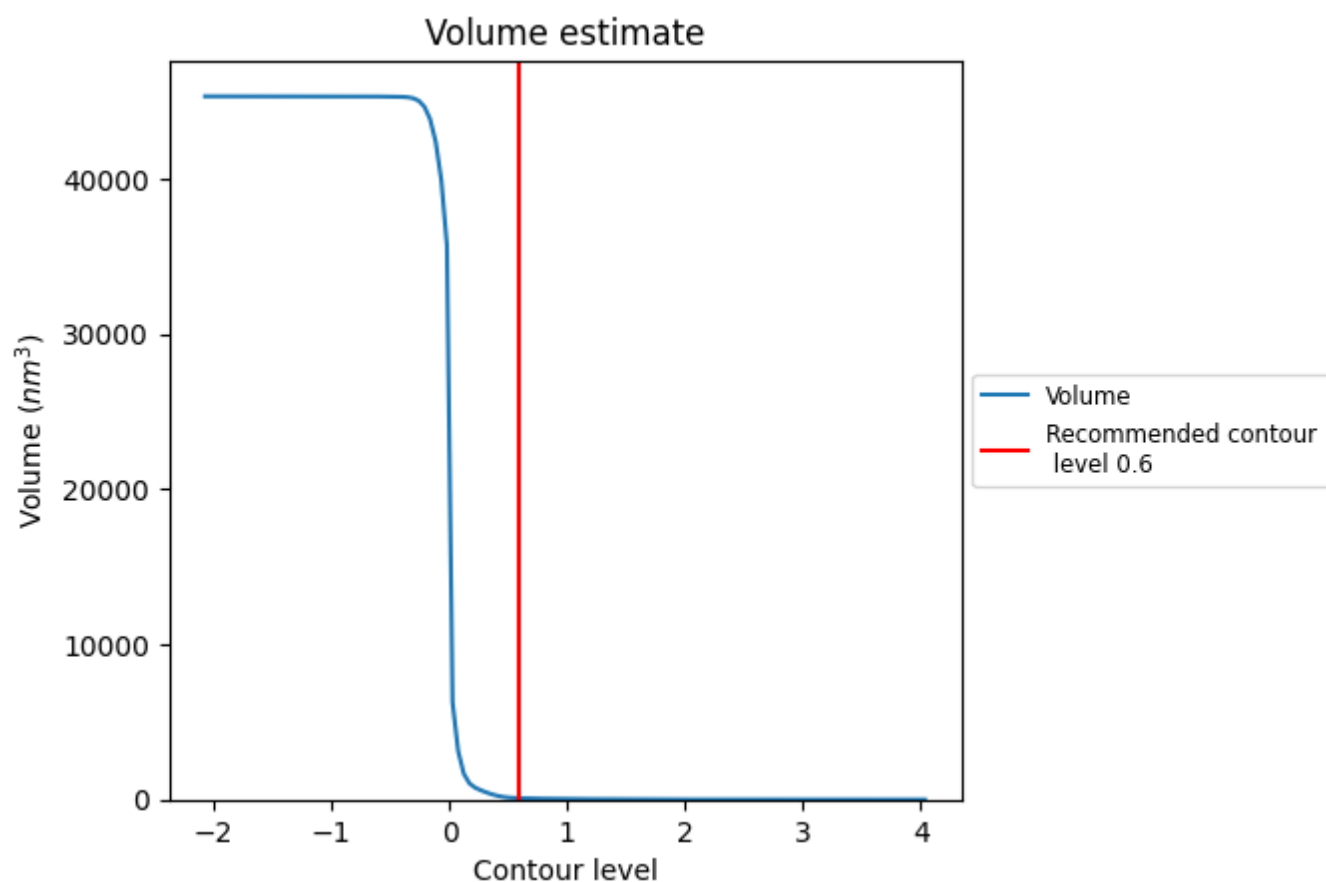
This section contains the results of statistical analysis of the map.

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.

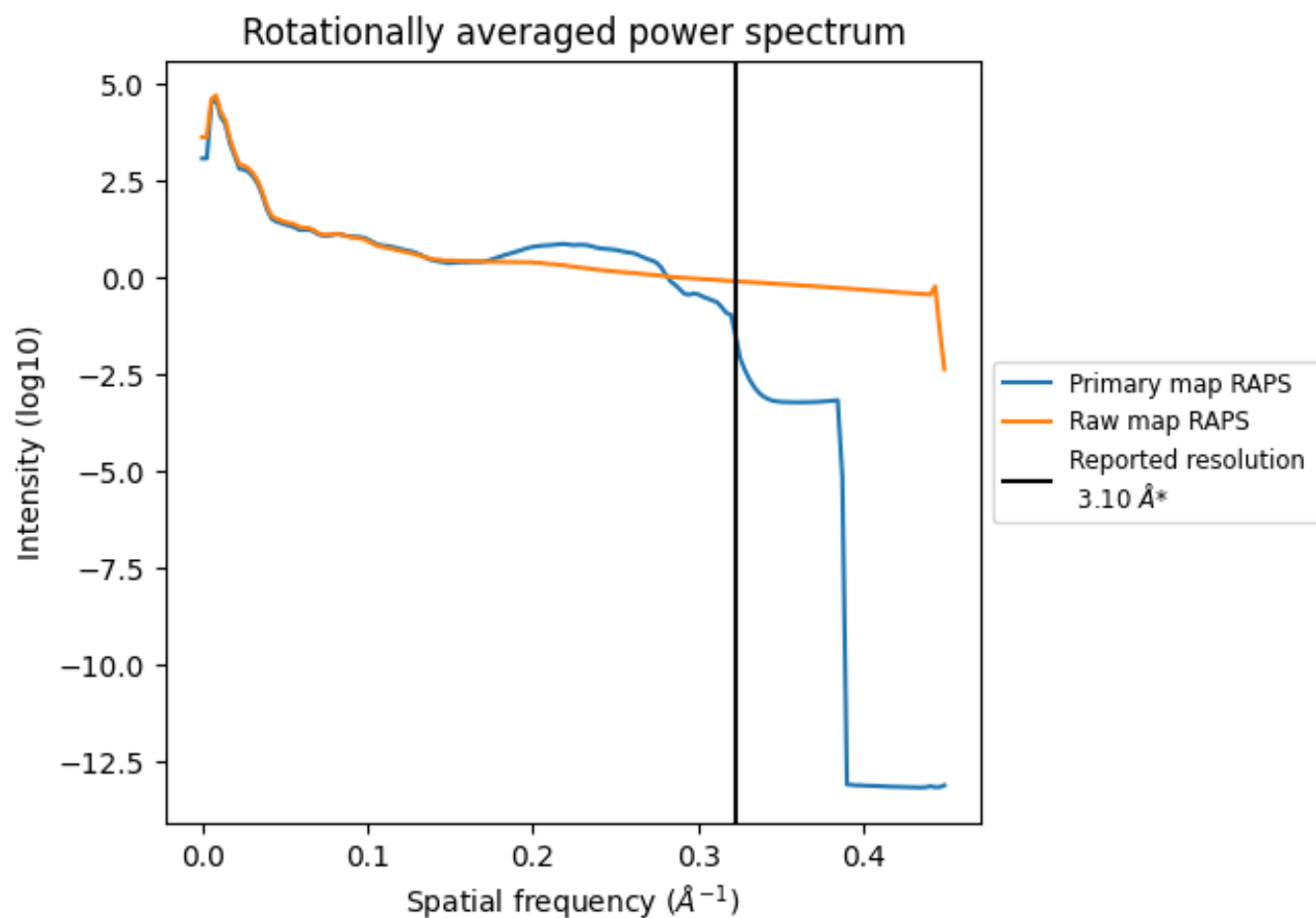
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm³; this corresponds to an approximate mass of 77 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

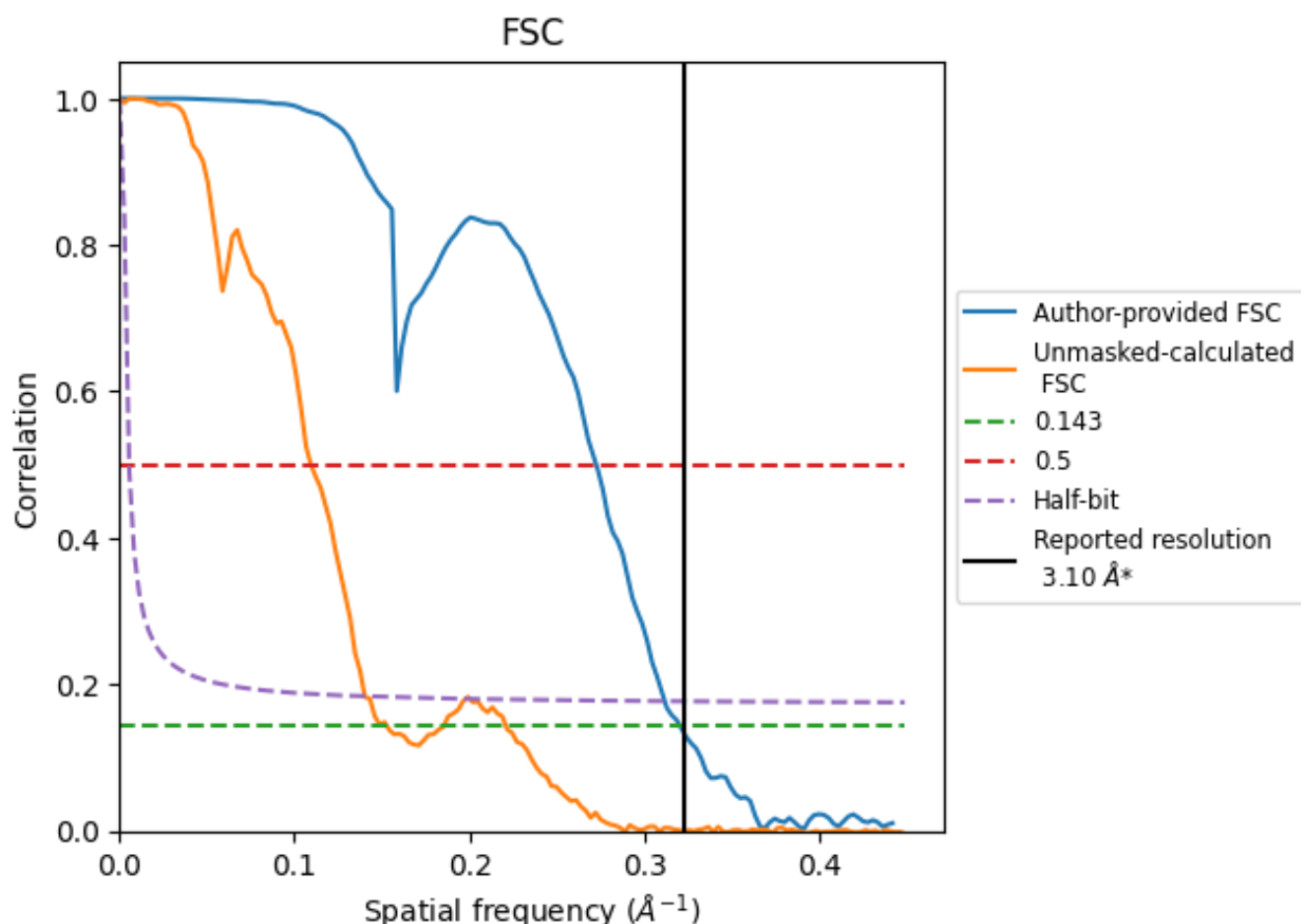


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

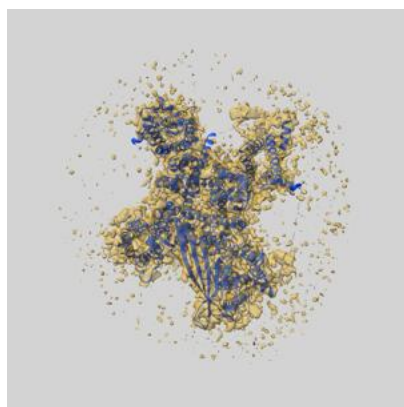
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.67	3.21
Unmasked-calculated*	6.54	9.14	7.13

*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 6.54 differs from the reported value 3.1 by more than 10 %

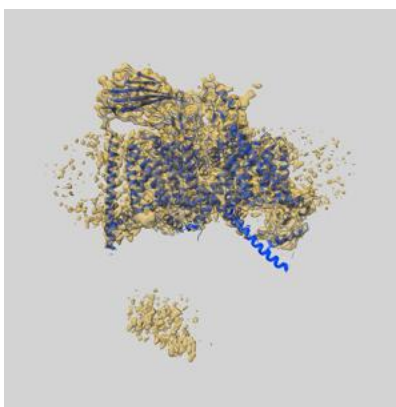
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29082 and PDB model 8FHD. Per-residue inclusion information can be found in section 3 on page 10.

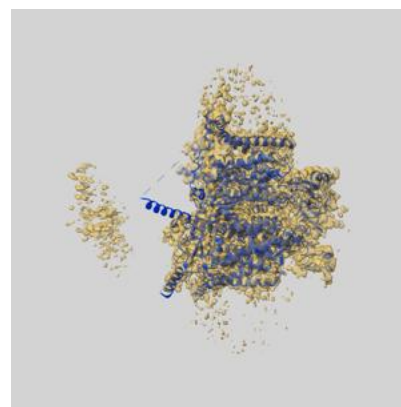
9.1 Map-model overlay [i](#)



X



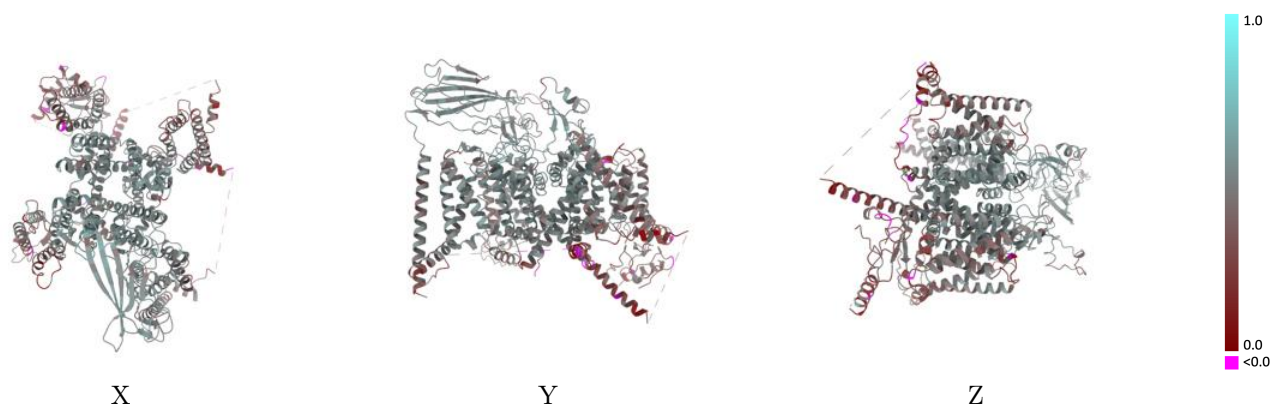
Y



Z

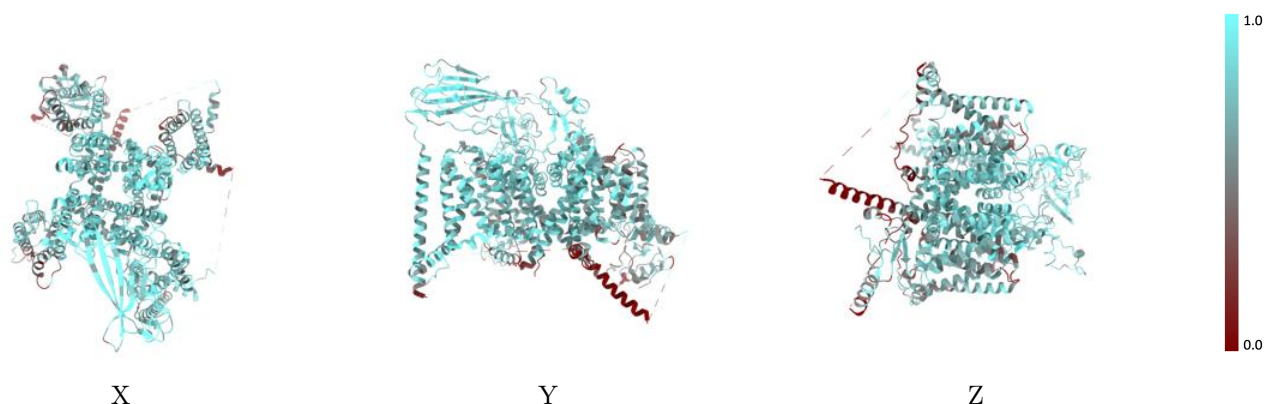
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



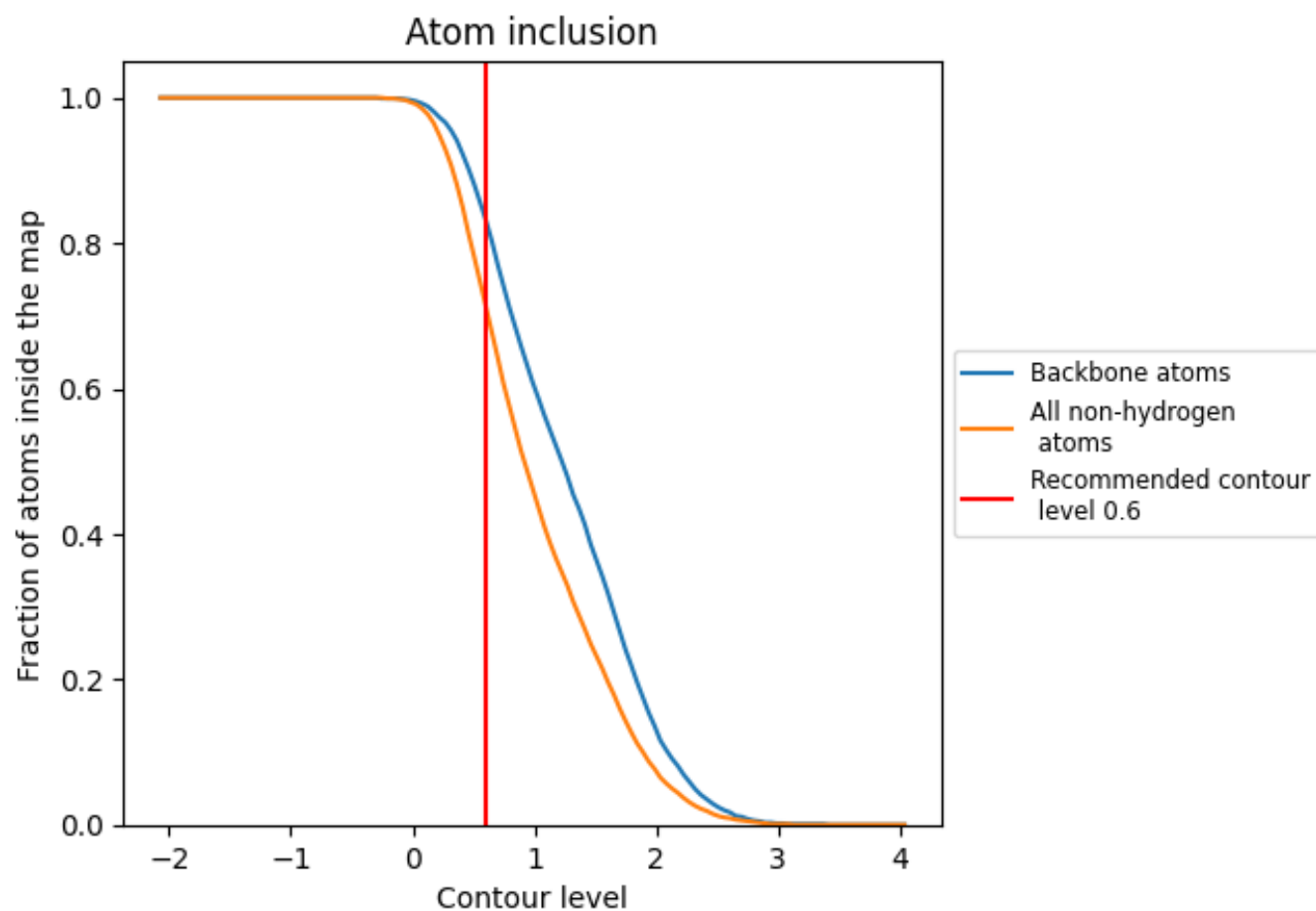
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 71% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7130	<div></div> 0.4590
A	<div></div> 0.7000	<div></div> 0.4540
C	<div></div> 0.8000	<div></div> 0.5000
D	<div></div> 0.8570	<div></div> 0.4930
F	<div></div> 0.8210	<div></div> 0.4180

