



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:03 PM UTC

PDB ID : 6UZA / pdb_00006uza
EMDB ID : EMD-20954
Title : Cryo-EM structure of human TRPC6 in complex with antagonist AM-1473
Authors : Bai, Y.; Yu, X.; Huang, X.; Chen, H.
Deposited on : 2019-11-14
Resolution : 3.08 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:

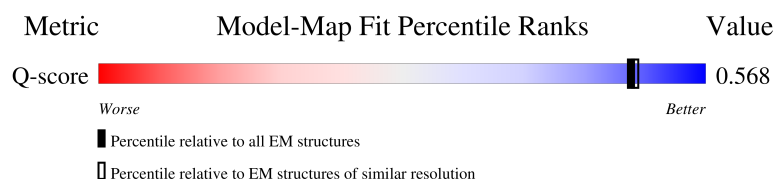
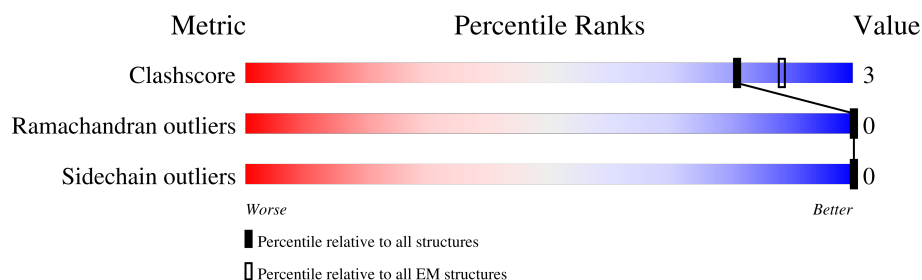
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.08 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14000 (2.58 - 3.58)

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	847	 7% 81% 6% 13%
1	B	847	 7% 81% 6% 13%
1	C	847	 7% 81% 6% 13%
1	D	847	 7% 80% 6% 13%

2 Entry composition [i](#)

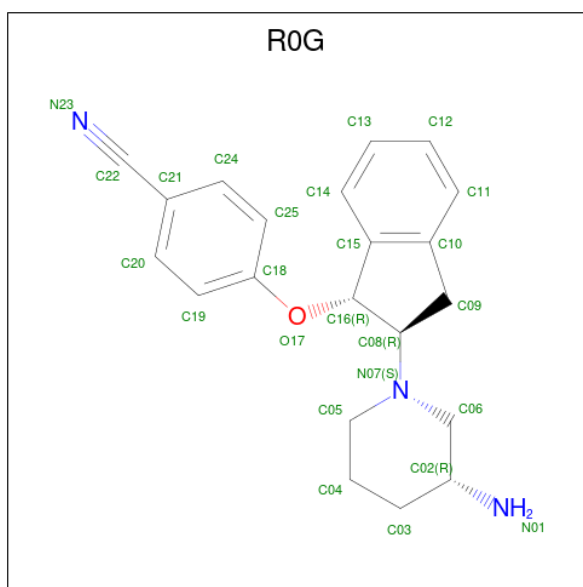
There are 5 unique types of molecules in this entry. The entry contains 23284 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Short transient receptor potential channel 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	734	Total	C	N	O	S	0	0
			5659	3692	947	985	35		
1	B	734	Total	C	N	O	S	0	0
			5659	3692	947	985	35		
1	C	734	Total	C	N	O	S	0	0
			5659	3692	947	985	35		
1	D	734	Total	C	N	O	S	0	0
			5659	3692	947	985	35		

- Molecule 2 is 4-((1R,2R)-2-[(3R)-3-aminopiperidin-1-yl]-2,3-dihydro-1H-inden-1-yl)ox y)benzonitrile (CCD ID: R0G) (formula: C₂₁H₂₃N₃O) (labeled as "Ligand of Interest" by depositor).



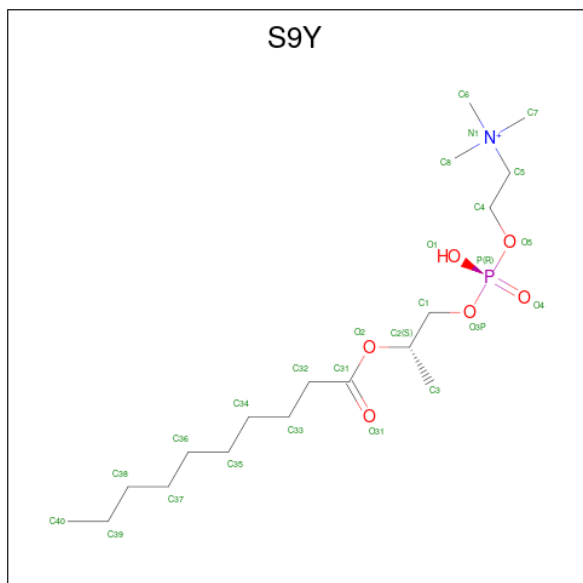
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			25	21	3	1	
2	B	1	Total	C	N	O	0
			25	21	3	1	

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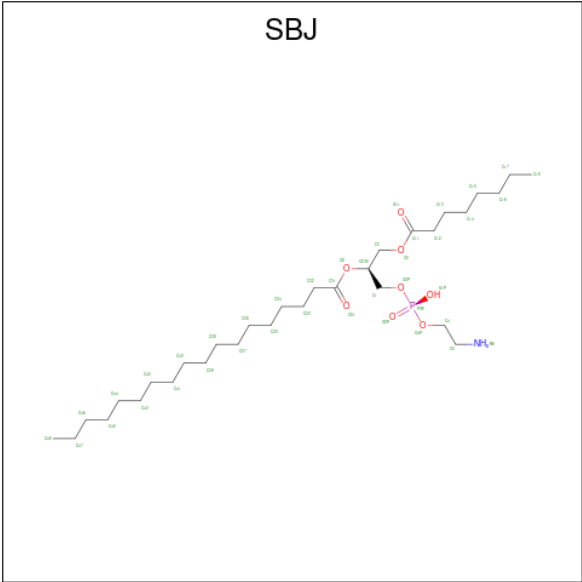
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			25	21	3	1	
2	D	1	Total	C	N	O	0
			25	21	3	1	

- Molecule 3 is 2-[[[(2 {S})-2-decanoyloxypropoxy]-oxidanyl-phosphoryl]oxyethyl-trimethyl-azanium (CCD ID: S9Y) (formula: $C_{18}H_{39}NO_6P$).



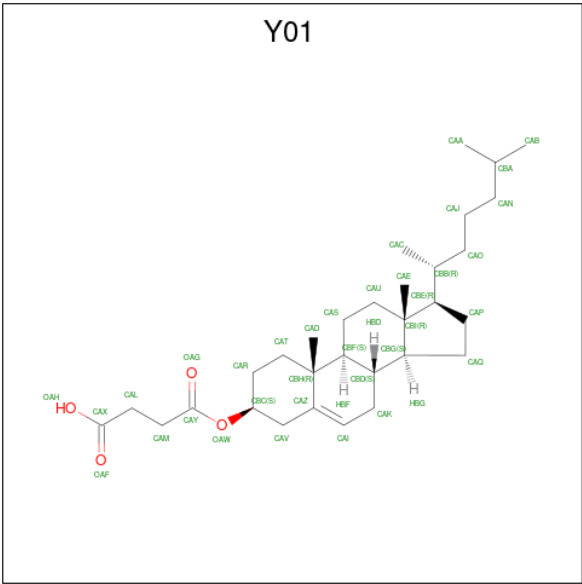
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			26	18	1	6	1	
3	B	1	Total	C	N	O	P	0
			26	18	1	6	1	
3	C	1	Total	C	N	O	P	0
			26	18	1	6	1	
3	D	1	Total	C	N	O	P	0
			26	18	1	6	1	

- Molecule 4 is [(2 {S})-1-[2-azanyloxy(oxidanyl)phosphoryl]oxy-3-octanoyloxy-propan-2-yl] octadecanoate (CCD ID: SBJ) (formula: $C_{31}H_{62}NO_8P$).

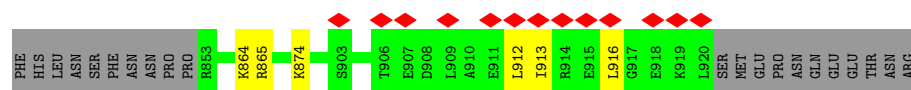


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	C	1	Total	C	N	O	P	0
			41	31	1	8	1	

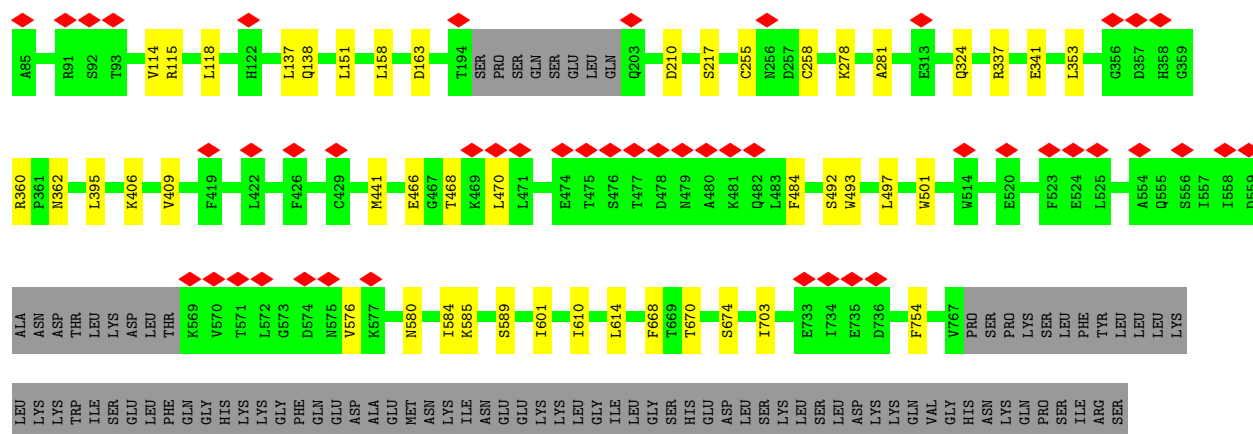
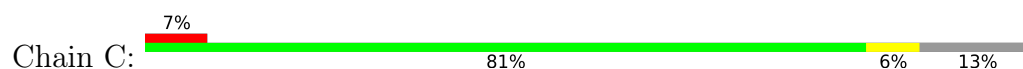
- Molecule 5 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



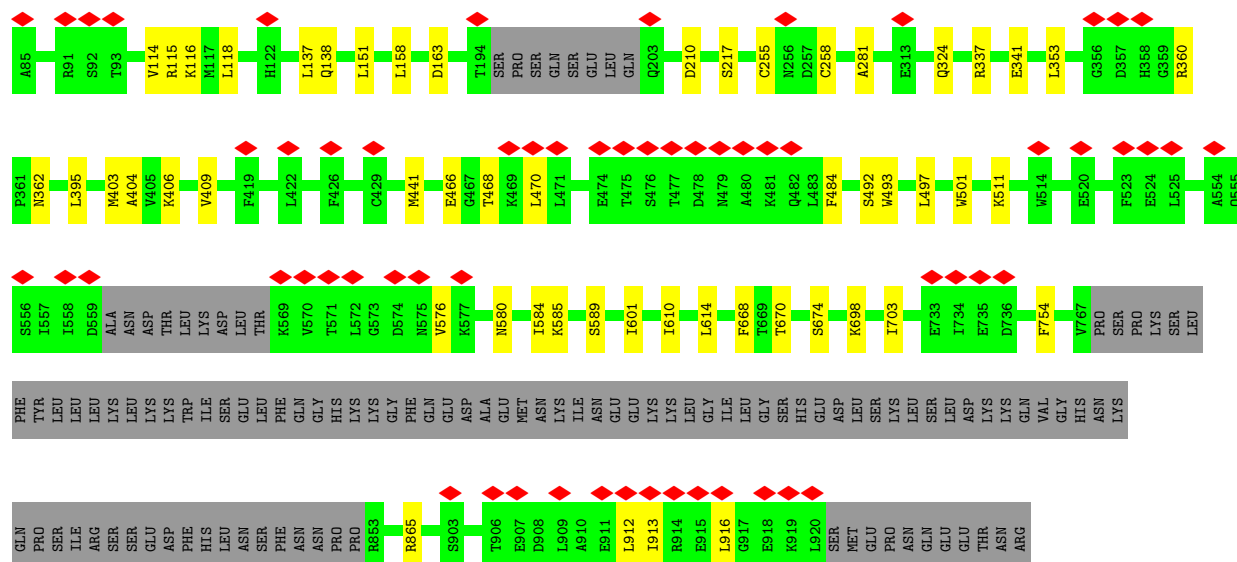
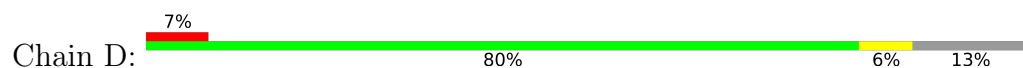
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total 35	C 31	O 4	0
5	A	1	Total 35	C 31	O 4	0
5	B	1	Total 35	C 31	O 4	0
5	B	1	Total 35	C 31	O 4	0
5	C	1	Total 35	C 31	O 4	0
5	C	1	Total 35	C 31	O 4	0
5	D	1	Total 35	C 31	O 4	0
5	D	1	Total 35	C 31	O 4	0



• Molecule 1: Short transient receptor potential channel 6



• Molecule 1: Short transient receptor potential channel 6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90014	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	38.795	Depositor
Minimum map value	-26.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.5	Depositor
Map size ($\text{\AA}$)	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.832, 0.832, 0.832	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: S9Y, SBJ, Y01, R0G

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	0.25	0/5784	0.51	1/7843 (0.0%)
1	B	0.25	0/5784	0.51	1/7843 (0.0%)
1	C	0.25	0/5784	0.51	1/7843 (0.0%)
1	D	0.25	0/5784	0.51	1/7843 (0.0%)
All	All	0.25	0/23136	0.51	4/31372 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	VAL	N-CA-C	-8.96	104.60	113.20
1	B	576	VAL	N-CA-C	-8.96	104.60	113.20
1	C	576	VAL	N-CA-C	-8.96	104.60	113.20
1	D	576	VAL	N-CA-C	-8.96	104.60	113.20

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	5659	0	5525	34	0
1	B	5659	0	5525	34	0
1	C	5659	0	5525	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5659	0	5525	36	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
2	C	25	0	0	0	0
2	D	25	0	0	0	0
3	A	26	0	0	0	0
3	B	26	0	0	0	0
3	C	26	0	0	0	0
3	D	26	0	0	0	0
4	A	82	0	0	0	0
4	B	41	0	0	0	0
4	C	41	0	0	0	0
5	A	70	0	98	1	0
5	B	70	0	98	2	0
5	C	70	0	98	2	0
5	D	70	0	98	0	0
All	All	23284	0	22492	117	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 3.

All (117) 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:916:LEU:HD11	1:C:916:LEU:HD23	1.50	0.94
1:A:916:LEU:HD11	1:B:916:LEU:HD23	1.50	0.94
1:A:916:LEU:HD23	1:D:916:LEU:HD11	1.50	0.93
1:C:916:LEU:HD11	1:D:916:LEU:HD23	1.50	0.93
1:A:916:LEU:CD2	1:D:916:LEU:HD11	2.21	0.71
1:A:916:LEU:HD11	1:B:916:LEU:CD2	2.21	0.70
1:C:916:LEU:HD11	1:D:916:LEU:CD2	2.21	0.70
1:B:916:LEU:HD11	1:C:916:LEU:CD2	2.21	0.69
1:A:255:CYS:SG	1:A:258:CYS:N	2.69	0.66
1:D:255:CYS:SG	1:D:258:CYS:N	2.69	0.65
1:B:255:CYS:SG	1:B:258:CYS:N	2.69	0.64
1:C:255:CYS:SG	1:C:258:CYS:N	2.69	0.63
1:A:703:ILE:HD12	1:D:601:ILE:HD11	1.81	0.62
1:A:601:ILE:HD11	1:B:703:ILE:HD12	1.81	0.61
1:C:601:ILE:HD11	1:D:703:ILE:HD12	1.81	0.61
1:B:601:ILE:HD11	1:C:703:ILE:HD12	1.81	0.60
1:D:584:ILE:HG23	1:D:585:LYS:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ILE:HG23	1:A:585:LYS:HG2	1.86	0.57
1:B:353:LEU:HD13	1:B:362:ASN:HD22	1.69	0.57
1:B:584:ILE:HG23	1:B:585:LYS:HG2	1.86	0.57
1:D:353:LEU:HD13	1:D:362:ASN:HD22	1.69	0.57
1:C:584:ILE:HG23	1:C:585:LYS:HG2	1.86	0.57
1:C:353:LEU:HD13	1:C:362:ASN:HD22	1.69	0.57
1:D:138:GLN:NE2	1:D:163:ASP:OD2	2.38	0.57
1:A:138:GLN:NE2	1:A:163:ASP:OD2	2.38	0.56
1:A:353:LEU:HD13	1:A:362:ASN:HD22	1.69	0.56
1:C:138:GLN:NE2	1:C:163:ASP:OD2	2.38	0.56
1:B:138:GLN:NE2	1:B:163:ASP:OD2	2.38	0.56
1:A:395:LEU:HD11	1:A:441:MET:HG2	1.90	0.54
1:D:395:LEU:HD11	1:D:441:MET:HG2	1.90	0.54
1:B:395:LEU:HD11	1:B:441:MET:HG2	1.90	0.53
1:C:395:LEU:HD11	1:C:441:MET:HG2	1.90	0.53
1:B:137:LEU:HD22	1:B:158:LEU:HD13	1.91	0.53
1:A:137:LEU:HD22	1:A:158:LEU:HD13	1.91	0.52
1:C:137:LEU:HD22	1:C:158:LEU:HD13	1.91	0.52
1:D:137:LEU:HD22	1:D:158:LEU:HD13	1.91	0.51
1:A:484:PHE:HB3	1:A:580:ASN:HA	1.93	0.51
1:D:406:LYS:HA	1:D:409:VAL:HG12	1.93	0.51
1:B:484:PHE:HB3	1:B:580:ASN:HA	1.93	0.51
1:C:497:LEU:HD12	1:C:501:TRP:HZ3	1.76	0.51
1:A:406:LYS:HA	1:A:409:VAL:HG12	1.93	0.51
1:D:497:LEU:HD12	1:D:501:TRP:HZ3	1.76	0.50
1:B:406:LYS:HA	1:B:409:VAL:HG12	1.93	0.50
1:A:497:LEU:HD12	1:A:501:TRP:HZ3	1.76	0.50
1:C:406:LYS:HA	1:C:409:VAL:HG12	1.93	0.50
1:D:484:PHE:HB3	1:D:580:ASN:HA	1.93	0.50
1:C:484:PHE:HB3	1:C:580:ASN:HA	1.93	0.49
1:B:492:SER:OG	1:B:493:TRP:N	2.45	0.49
1:B:497:LEU:HD12	1:B:501:TRP:HZ3	1.76	0.49
1:C:114:VAL:O	1:C:118:LEU:HB2	2.12	0.49
1:A:912:LEU:HB3	1:B:913:ILE:HG21	1.95	0.49
1:A:360:ARG:NH2	1:A:754:PHE:O	2.43	0.49
1:B:912:LEU:HB3	1:C:913:ILE:HG21	1.95	0.49
1:B:114:VAL:O	1:B:118:LEU:HB2	2.12	0.49
1:C:492:SER:OG	1:C:493:TRP:N	2.45	0.49
1:D:492:SER:OG	1:D:493:TRP:N	2.45	0.49
1:A:114:VAL:O	1:A:118:LEU:HB2	2.12	0.48
1:A:492:SER:OG	1:A:493:TRP:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:ILE:O	1:B:614:LEU:HB2	2.13	0.48
1:B:360:ARG:NH2	1:B:754:PHE:O	2.43	0.48
1:C:912:LEU:HB3	1:D:913:ILE:HG21	1.95	0.48
1:D:114:VAL:O	1:D:118:LEU:HB2	2.12	0.48
1:A:610:ILE:O	1:A:614:LEU:HB2	2.13	0.48
1:C:341:GLU:OE1	1:C:865:ARG:NH1	2.40	0.48
1:C:610:ILE:O	1:C:614:LEU:HB2	2.13	0.48
1:B:466:GLU:HA	1:C:670:THR:HG23	1.96	0.48
1:C:466:GLU:HA	1:D:670:THR:HG23	1.96	0.48
1:D:610:ILE:O	1:D:614:LEU:HB2	2.13	0.48
1:A:913:ILE:HG21	1:D:912:LEU:HB3	1.95	0.47
1:A:466:GLU:HA	1:B:670:THR:HG23	1.96	0.47
1:D:341:GLU:OE1	1:D:865:ARG:NH1	2.40	0.47
1:A:670:THR:HG23	1:D:466:GLU:HA	1.96	0.46
1:D:360:ARG:NH2	1:D:754:PHE:O	2.43	0.46
1:C:115:ARG:HG3	1:C:151:LEU:HD21	1.98	0.45
1:C:360:ARG:NH2	1:C:754:PHE:O	2.43	0.45
1:D:115:ARG:HG3	1:D:151:LEU:HD21	1.98	0.45
1:A:341:GLU:OE1	1:A:865:ARG:NH1	2.40	0.45
1:C:281:ALA:O	1:C:324:GLN:NE2	2.39	0.45
1:B:115:ARG:HG3	1:B:151:LEU:HD21	1.98	0.45
1:C:668:PHE:HA	1:C:674:SER:HB2	1.99	0.45
1:B:668:PHE:HA	1:B:674:SER:HB2	1.99	0.45
1:A:116:LYS:HE2	1:A:116:LYS:HB3	1.84	0.44
1:A:864:LYS:NZ	1:B:210:ASP:OD1	2.48	0.44
1:A:115:ARG:HG3	1:A:151:LEU:HD21	1.98	0.44
1:D:698:LYS:HD3	1:D:698:LYS:HA	1.82	0.44
1:D:281:ALA:O	1:D:324:GLN:NE2	2.39	0.44
1:B:116:LYS:HB3	1:B:116:LYS:HE2	1.84	0.44
1:A:468:THR:HG23	1:A:470:LEU:H	1.83	0.43
1:B:864:LYS:NZ	1:C:210:ASP:OD1	2.48	0.43
1:D:668:PHE:HA	1:D:674:SER:HB2	1.99	0.43
5:B:1005:Y01:HAE2	5:B:1005:Y01:HBB	1.84	0.43
5:C:1001:Y01:HAA3	5:C:1001:Y01:HAJ2	1.92	0.43
1:D:468:THR:HG23	1:D:470:LEU:H	1.83	0.43
5:C:1005:Y01:HAE2	5:C:1005:Y01:HBB	1.84	0.43
1:A:668:PHE:HA	1:A:674:SER:HB2	1.99	0.43
1:B:468:THR:HG23	1:B:470:LEU:H	1.83	0.43
1:C:864:LYS:NZ	1:D:210:ASP:OD1	2.48	0.43
1:C:468:THR:HG23	1:C:470:LEU:H	1.83	0.42
1:B:341:GLU:OE1	1:B:865:ARG:NH1	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:874:LYS:HB2	1:B:874:LYS:HE3	1.87	0.42
1:D:511:LYS:HE2	1:D:511:LYS:HB3	1.89	0.42
1:C:913:ILE:HD13	1:C:913:ILE:HA	1.90	0.41
1:C:337:ARG:HD2	1:D:217:SER:HB3	2.02	0.41
5:A:1006:Y01:HAA3	5:A:1006:Y01:HAJ2	1.92	0.41
1:D:116:LYS:HB3	1:D:116:LYS:HE2	1.84	0.41
1:D:589:SER:O	1:D:589:SER:OG	2.34	0.41
1:A:422:LEU:HD23	1:A:422:LEU:HA	1.96	0.41
1:A:217:SER:HB3	1:D:337:ARG:HD2	2.02	0.41
1:A:511:LYS:HB3	1:A:511:LYS:HE2	1.89	0.41
1:B:191:ARG:O	1:B:207:TYR:OH	2.39	0.41
1:C:278:LYS:HB2	1:C:278:LYS:HE3	1.89	0.40
1:A:219:ASP:OD1	1:A:219:ASP:N	2.54	0.40
1:B:337:ARG:HD2	1:C:217:SER:HB3	2.03	0.40
1:A:337:ARG:HD2	1:B:217:SER:HB3	2.03	0.40
1:C:589:SER:O	1:C:589:SER:OG	2.34	0.40
5:B:1001:Y01:HAA3	5:B:1001:Y01:HAJ2	1.92	0.40
1:D:403:MET:HE3	1:D:404:ALA:H	1.87	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	726/847 (86%)	696 (96%)	30 (4%)	0	100	100
1	B	726/847 (86%)	696 (96%)	30 (4%)	0	100	100
1	C	726/847 (86%)	696 (96%)	30 (4%)	0	100	100
1	D	726/847 (86%)	696 (96%)	30 (4%)	0	100	100
All	All	2904/3388 (86%)	2784 (96%)	120 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	564/748 (75%)	564 (100%)	0	100	100
1	B	564/748 (75%)	564 (100%)	0	100	100
1	C	564/748 (75%)	564 (100%)	0	100	100
1	D	564/748 (75%)	564 (100%)	0	100	100
All	All	2256/2992 (75%)	2256 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	145	HIS
1	A	157	ASN
1	A	269	HIS
1	A	347	ASN
1	A	362	ASN
1	A	384	GLN
1	A	889	GLN
1	B	127	ASN
1	B	145	HIS
1	B	157	ASN
1	B	269	HIS
1	B	302	ASN
1	B	347	ASN
1	B	362	ASN
1	B	384	GLN
1	B	889	GLN
1	C	127	ASN
1	C	157	ASN
1	C	269	HIS
1	C	309	ASN
1	C	347	ASN

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Mol	Chain	Res	Type
1	C	358	HIS
1	C	362	ASN
1	C	384	GLN
1	C	889	GLN
1	D	127	ASN
1	D	145	HIS
1	D	157	ASN
1	D	269	HIS
1	D	309	ASN
1	D	316	ASN
1	D	347	ASN
1	D	362	ASN
1	D	384	GLN
1	D	889	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	Y01	D	1001	-	38,38,38	1.98	8 (21%)	57,57,57	2.27	22 (38%)
2	R0G	B	1002	-	27,28,28	2.77	13 (48%)	33,39,39	1.63	6 (18%)
5	Y01	A	1004	-	38,38,38	1.90	8 (21%)	57,57,57	2.30	20 (35%)
4	SBJ	B	1004	-	40,40,40	1.09	2 (5%)	43,45,45	0.85	1 (2%)
4	SBJ	A	1005	-	40,40,40	1.09	2 (5%)	43,45,45	0.85	1 (2%)
3	S9Y	B	1003	-	25,25,25	1.62	4 (16%)	30,32,32	1.20	3 (10%)
5	Y01	B	1001	-	38,38,38	1.98	8 (21%)	57,57,57	2.27	22 (38%)
3	S9Y	A	1002	-	25,25,25	1.62	4 (16%)	30,32,32	1.20	3 (10%)
5	Y01	B	1005	-	38,38,38	1.90	8 (21%)	57,57,57	2.30	20 (35%)
2	R0G	C	1002	-	27,28,28	2.77	13 (48%)	33,39,39	1.63	6 (18%)
4	SBJ	C	1004	-	40,40,40	1.09	2 (5%)	43,45,45	0.85	1 (2%)
3	S9Y	D	1003	-	25,25,25	1.62	4 (16%)	30,32,32	1.20	3 (10%)
4	SBJ	A	1003	-	40,40,40	1.09	2 (5%)	43,45,45	0.85	1 (2%)
2	R0G	D	1002	-	27,28,28	2.77	13 (48%)	33,39,39	1.63	6 (18%)
5	Y01	D	1004	-	38,38,38	1.90	8 (21%)	57,57,57	2.30	20 (35%)
2	R0G	A	1001	-	27,28,28	2.77	13 (48%)	33,39,39	1.63	6 (18%)
5	Y01	A	1006	-	38,38,38	1.98	8 (21%)	57,57,57	2.27	22 (38%)
5	Y01	C	1001	-	38,38,38	1.98	8 (21%)	57,57,57	2.27	22 (38%)
3	S9Y	C	1003	-	25,25,25	1.62	4 (16%)	30,32,32	1.20	3 (10%)
5	Y01	C	1005	-	38,38,38	1.90	8 (21%)	57,57,57	2.30	20 (35%)

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	Y01	D	1001	-	-	11/19/77/77	0/4/4/4
2	R0G	B	1002	-	-	0/10/32/32	0/4/4/4
5	Y01	A	1004	-	-	9/19/77/77	0/4/4/4
4	SBJ	B	1004	-	-	21/44/44/44	-
4	SBJ	A	1005	-	-	21/44/44/44	-
3	S9Y	B	1003	-	-	9/27/27/27	-
5	Y01	B	1001	-	-	11/19/77/77	0/4/4/4
3	S9Y	A	1002	-	-	9/27/27/27	-
5	Y01	B	1005	-	-	9/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	R0G	C	1002	-	-	0/10/32/32	0/4/4/4
4	SBJ	C	1004	-	-	21/44/44/44	-
3	S9Y	D	1003	-	-	9/27/27/27	-
4	SBJ	A	1003	-	-	21/44/44/44	-
2	R0G	D	1002	-	-	0/10/32/32	0/4/4/4
5	Y01	D	1004	-	-	9/19/77/77	0/4/4/4
2	R0G	A	1001	-	-	0/10/32/32	0/4/4/4
5	Y01	A	1006	-	-	11/19/77/77	0/4/4/4
5	Y01	C	1001	-	-	11/19/77/77	0/4/4/4
3	S9Y	C	1003	-	-	9/27/27/27	-
5	Y01	C	1005	-	-	9/19/77/77	0/4/4/4

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	R0G	C15-C16	6.87	1.62	1.51
2	B	1002	R0G	C15-C16	6.87	1.62	1.51
2	C	1002	R0G	C15-C16	6.87	1.62	1.51
2	D	1002	R0G	C15-C16	6.87	1.62	1.51
2	A	1001	R0G	C21-C22	5.42	1.56	1.44
2	B	1002	R0G	C21-C22	5.42	1.56	1.44
2	C	1002	R0G	C21-C22	5.42	1.56	1.44
2	D	1002	R0G	C21-C22	5.42	1.56	1.44
3	A	1002	S9Y	P-O5	5.34	1.80	1.59
3	B	1003	S9Y	P-O5	5.34	1.80	1.59
3	C	1003	S9Y	P-O5	5.34	1.80	1.59
3	D	1003	S9Y	P-O5	5.34	1.80	1.59
2	A	1001	R0G	C10-C15	5.25	1.48	1.39
2	B	1002	R0G	C10-C15	5.25	1.48	1.39
2	C	1002	R0G	C10-C15	5.25	1.48	1.39
2	D	1002	R0G	C10-C15	5.25	1.48	1.39
5	A	1006	Y01	CBH-CBF	4.83	1.63	1.56
5	B	1001	Y01	CBH-CBF	4.83	1.63	1.56
5	C	1001	Y01	CBH-CBF	4.83	1.63	1.56
5	D	1001	Y01	CBH-CBF	4.83	1.63	1.56
5	A	1004	Y01	CBH-CBF	4.57	1.63	1.56
5	B	1005	Y01	CBH-CBF	4.57	1.63	1.56
5	C	1005	Y01	CBH-CBF	4.57	1.63	1.56
5	D	1004	Y01	CBH-CBF	4.57	1.63	1.56
2	A	1001	R0G	C13-C14	4.23	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	R0G	C13-C14	4.23	1.46	1.38
2	C	1002	R0G	C13-C14	4.23	1.46	1.38
2	D	1002	R0G	C13-C14	4.23	1.46	1.38
5	A	1006	Y01	CBI-CBE	4.22	1.62	1.55
5	B	1001	Y01	CBI-CBE	4.22	1.62	1.55
5	C	1001	Y01	CBI-CBE	4.22	1.62	1.55
5	D	1001	Y01	CBI-CBE	4.22	1.62	1.55
5	A	1006	Y01	CAL-CAX	4.10	1.60	1.50
5	B	1001	Y01	CAL-CAX	4.10	1.60	1.50
5	C	1001	Y01	CAL-CAX	4.10	1.60	1.50
5	D	1001	Y01	CAL-CAX	4.10	1.60	1.50
5	A	1004	Y01	CBD-CBG	3.89	1.60	1.53
5	B	1005	Y01	CBD-CBG	3.89	1.60	1.53
5	C	1005	Y01	CBD-CBG	3.89	1.60	1.53
5	D	1004	Y01	CBD-CBG	3.89	1.60	1.53
2	A	1001	R0G	C12-C11	3.88	1.45	1.38
2	B	1002	R0G	C12-C11	3.88	1.45	1.38
2	C	1002	R0G	C12-C11	3.88	1.45	1.38
2	D	1002	R0G	C12-C11	3.88	1.45	1.38
5	A	1006	Y01	CBD-CBG	3.85	1.60	1.53
5	B	1001	Y01	CBD-CBG	3.85	1.60	1.53
5	C	1001	Y01	CBD-CBG	3.85	1.60	1.53
5	D	1001	Y01	CBD-CBG	3.85	1.60	1.53
5	A	1004	Y01	CAL-CAX	3.79	1.59	1.50
5	B	1005	Y01	CAL-CAX	3.79	1.59	1.50
5	C	1005	Y01	CAL-CAX	3.79	1.59	1.50
5	D	1004	Y01	CAL-CAX	3.79	1.59	1.50
5	A	1006	Y01	CAV-CAZ	3.57	1.58	1.51
5	B	1001	Y01	CAV-CAZ	3.57	1.58	1.51
5	C	1001	Y01	CAV-CAZ	3.57	1.58	1.51
5	D	1001	Y01	CAV-CAZ	3.57	1.58	1.51
4	A	1003	SBJ	P-O3P	3.54	1.73	1.59
4	A	1005	SBJ	P-O3P	3.54	1.73	1.59
4	B	1004	SBJ	P-O3P	3.54	1.73	1.59
4	C	1004	SBJ	P-O3P	3.54	1.73	1.59
5	A	1004	Y01	CBI-CBE	3.52	1.61	1.55
5	B	1005	Y01	CBI-CBE	3.52	1.61	1.55
5	C	1005	Y01	CBI-CBE	3.52	1.61	1.55
5	D	1004	Y01	CBI-CBE	3.52	1.61	1.55
5	A	1004	Y01	CAV-CAZ	3.49	1.58	1.51
5	B	1005	Y01	CAV-CAZ	3.49	1.58	1.51
5	C	1005	Y01	CAV-CAZ	3.49	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1004	Y01	CAV-CAZ	3.49	1.58	1.51
5	A	1006	Y01	CAV-CBC	3.36	1.59	1.52
5	B	1001	Y01	CAV-CBC	3.36	1.59	1.52
5	C	1001	Y01	CAV-CBC	3.36	1.59	1.52
5	D	1001	Y01	CAV-CBC	3.36	1.59	1.52
5	A	1004	Y01	CAV-CBC	3.34	1.59	1.52
5	B	1005	Y01	CAV-CBC	3.34	1.59	1.52
5	C	1005	Y01	CAV-CBC	3.34	1.59	1.52
5	D	1004	Y01	CAV-CBC	3.34	1.59	1.52
5	A	1006	Y01	CBB-CBE	3.21	1.59	1.54
5	B	1001	Y01	CBB-CBE	3.21	1.59	1.54
5	C	1001	Y01	CBB-CBE	3.21	1.59	1.54
5	D	1001	Y01	CBB-CBE	3.21	1.59	1.54
2	A	1001	R0G	C25-C24	3.14	1.43	1.38
2	B	1002	R0G	C25-C24	3.14	1.43	1.38
2	C	1002	R0G	C25-C24	3.14	1.43	1.38
2	D	1002	R0G	C25-C24	3.14	1.43	1.38
5	A	1004	Y01	CBB-CBE	2.99	1.59	1.54
5	B	1005	Y01	CBB-CBE	2.99	1.59	1.54
5	C	1005	Y01	CBB-CBE	2.99	1.59	1.54
5	D	1004	Y01	CBB-CBE	2.99	1.59	1.54
2	A	1001	R0G	C14-C15	2.92	1.43	1.39
2	B	1002	R0G	C14-C15	2.92	1.43	1.39
2	C	1002	R0G	C14-C15	2.92	1.43	1.39
2	D	1002	R0G	C14-C15	2.92	1.43	1.39
4	A	1003	SBJ	P-O4P	2.82	1.70	1.59
4	A	1005	SBJ	P-O4P	2.82	1.70	1.59
4	B	1004	SBJ	P-O4P	2.82	1.70	1.59
4	C	1004	SBJ	P-O4P	2.82	1.70	1.59
5	A	1004	Y01	CBD-CBF	2.74	1.58	1.53
5	B	1005	Y01	CBD-CBF	2.74	1.58	1.53
5	C	1005	Y01	CBD-CBF	2.74	1.58	1.53
5	D	1004	Y01	CBD-CBF	2.74	1.58	1.53
5	A	1006	Y01	CBD-CBF	2.74	1.58	1.53
5	B	1001	Y01	CBD-CBF	2.74	1.58	1.53
5	C	1001	Y01	CBD-CBF	2.74	1.58	1.53
5	D	1001	Y01	CBD-CBF	2.74	1.58	1.53
3	A	1002	S9Y	C1-C2	2.67	1.56	1.50
3	B	1003	S9Y	C1-C2	2.67	1.56	1.50
3	C	1003	S9Y	C1-C2	2.67	1.56	1.50
3	D	1003	S9Y	C1-C2	2.67	1.56	1.50
2	A	1001	R0G	C02-N01	2.59	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	R0G	C02-N01	2.59	1.55	1.46
2	C	1002	R0G	C02-N01	2.59	1.55	1.46
2	D	1002	R0G	C02-N01	2.59	1.55	1.46
3	A	1002	S9Y	P-O3P	2.50	1.69	1.59
3	B	1003	S9Y	P-O3P	2.50	1.69	1.59
3	C	1003	S9Y	P-O3P	2.50	1.69	1.59
3	D	1003	S9Y	P-O3P	2.50	1.69	1.59
2	A	1001	R0G	C12-C13	2.40	1.43	1.38
2	B	1002	R0G	C12-C13	2.40	1.43	1.38
2	C	1002	R0G	C12-C13	2.40	1.43	1.38
2	D	1002	R0G	C12-C13	2.40	1.43	1.38
2	A	1001	R0G	C11-C10	2.37	1.43	1.39
2	B	1002	R0G	C11-C10	2.37	1.43	1.39
2	C	1002	R0G	C11-C10	2.37	1.43	1.39
2	D	1002	R0G	C11-C10	2.37	1.43	1.39
2	A	1001	R0G	C19-C18	2.33	1.43	1.38
2	B	1002	R0G	C19-C18	2.33	1.43	1.38
2	C	1002	R0G	C19-C18	2.33	1.43	1.38
2	D	1002	R0G	C19-C18	2.33	1.43	1.38
2	A	1001	R0G	C09-C08	2.16	1.57	1.54
2	B	1002	R0G	C09-C08	2.16	1.57	1.54
2	C	1002	R0G	C09-C08	2.16	1.57	1.54
2	D	1002	R0G	C09-C08	2.16	1.57	1.54
3	A	1002	S9Y	O5-C4	-2.16	1.36	1.44
3	B	1003	S9Y	O5-C4	-2.16	1.36	1.44
3	C	1003	S9Y	O5-C4	-2.16	1.36	1.44
3	D	1003	S9Y	O5-C4	-2.16	1.36	1.44
2	A	1001	R0G	C20-C21	2.08	1.43	1.39
2	B	1002	R0G	C20-C21	2.08	1.43	1.39
2	C	1002	R0G	C20-C21	2.08	1.43	1.39
2	D	1002	R0G	C20-C21	2.08	1.43	1.39

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1006	Y01	OAW-CAY-CAM	6.76	126.10	111.48
5	B	1001	Y01	OAW-CAY-CAM	6.76	126.10	111.48
5	C	1001	Y01	OAW-CAY-CAM	6.76	126.10	111.48
5	D	1001	Y01	OAW-CAY-CAM	6.76	126.10	111.48
5	A	1004	Y01	OAW-CAY-CAM	6.66	125.89	111.48
5	B	1005	Y01	OAW-CAY-CAM	6.66	125.89	111.48
5	C	1005	Y01	OAW-CAY-CAM	6.66	125.89	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1004	Y01	OAW-CAY-CAM	6.66	125.89	111.48
5	A	1006	Y01	CBC-CAV-CAZ	6.05	120.39	111.45
5	B	1001	Y01	CBC-CAV-CAZ	6.05	120.39	111.45
5	C	1001	Y01	CBC-CAV-CAZ	6.05	120.39	111.45
5	D	1001	Y01	CBC-CAV-CAZ	6.05	120.39	111.45
5	A	1004	Y01	CBC-CAV-CAZ	5.90	120.17	111.45
5	B	1005	Y01	CBC-CAV-CAZ	5.90	120.17	111.45
5	C	1005	Y01	CBC-CAV-CAZ	5.90	120.17	111.45
5	D	1004	Y01	CBC-CAV-CAZ	5.90	120.17	111.45
5	A	1004	Y01	CAE-CBI-CAU	-4.98	103.26	110.61
5	B	1005	Y01	CAE-CBI-CAU	-4.98	103.26	110.61
5	C	1005	Y01	CAE-CBI-CAU	-4.98	103.26	110.61
5	D	1004	Y01	CAE-CBI-CAU	-4.98	103.26	110.61
5	A	1006	Y01	CAE-CBI-CAU	-4.89	103.40	110.61
5	B	1001	Y01	CAE-CBI-CAU	-4.89	103.40	110.61
5	C	1001	Y01	CAE-CBI-CAU	-4.89	103.40	110.61
5	D	1001	Y01	CAE-CBI-CAU	-4.89	103.40	110.61
2	A	1001	R0G	C04-C05-N07	4.78	118.94	111.31
2	B	1002	R0G	C04-C05-N07	4.78	118.94	111.31
2	C	1002	R0G	C04-C05-N07	4.78	118.94	111.31
2	D	1002	R0G	C04-C05-N07	4.78	118.94	111.31
5	A	1006	Y01	OAW-CAY-OAG	-4.19	113.91	123.70
5	B	1001	Y01	OAW-CAY-OAG	-4.19	113.91	123.70
5	C	1001	Y01	OAW-CAY-OAG	-4.19	113.91	123.70
5	D	1001	Y01	OAW-CAY-OAG	-4.19	113.91	123.70
5	A	1004	Y01	OAW-CAY-OAG	-4.11	114.09	123.70
5	B	1005	Y01	OAW-CAY-OAG	-4.11	114.09	123.70
5	C	1005	Y01	OAW-CAY-OAG	-4.11	114.09	123.70
5	D	1004	Y01	OAW-CAY-OAG	-4.11	114.09	123.70
5	A	1004	Y01	CAV-CAZ-CAI	3.96	125.94	120.57
5	B	1005	Y01	CAV-CAZ-CAI	3.96	125.94	120.57
5	C	1005	Y01	CAV-CAZ-CAI	3.96	125.94	120.57
5	D	1004	Y01	CAV-CAZ-CAI	3.96	125.94	120.57
5	A	1006	Y01	CAQ-CBG-CBI	-3.73	99.45	103.84
5	B	1001	Y01	CAQ-CBG-CBI	-3.73	99.45	103.84
5	C	1001	Y01	CAQ-CBG-CBI	-3.73	99.45	103.84
5	D	1001	Y01	CAQ-CBG-CBI	-3.73	99.45	103.84
3	A	1002	S9Y	O1-P-O4	3.69	129.59	112.44
3	B	1003	S9Y	O1-P-O4	3.69	129.59	112.44
3	C	1003	S9Y	O1-P-O4	3.69	129.59	112.44
3	D	1003	S9Y	O1-P-O4	3.69	129.59	112.44
5	A	1004	Y01	CAK-CBD-CBG	3.68	116.14	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1005	Y01	CAK-CBD-CBG	3.68	116.14	110.93
5	C	1005	Y01	CAK-CBD-CBG	3.68	116.14	110.93
5	D	1004	Y01	CAK-CBD-CBG	3.68	116.14	110.93
5	A	1006	Y01	CAV-CAZ-CAI	3.57	125.41	120.57
5	B	1001	Y01	CAV-CAZ-CAI	3.57	125.41	120.57
5	C	1001	Y01	CAV-CAZ-CAI	3.57	125.41	120.57
5	D	1001	Y01	CAV-CAZ-CAI	3.57	125.41	120.57
5	A	1004	Y01	CAQ-CBG-CBI	-3.50	99.72	103.84
5	B	1005	Y01	CAQ-CBG-CBI	-3.50	99.72	103.84
5	C	1005	Y01	CAQ-CBG-CBI	-3.50	99.72	103.84
5	D	1004	Y01	CAQ-CBG-CBI	-3.50	99.72	103.84
5	A	1004	Y01	CAD-CBH-CAZ	-3.43	103.15	108.38
5	B	1005	Y01	CAD-CBH-CAZ	-3.43	103.15	108.38
5	C	1005	Y01	CAD-CBH-CAZ	-3.43	103.15	108.38
5	D	1004	Y01	CAD-CBH-CAZ	-3.43	103.15	108.38
5	A	1006	Y01	CAK-CBD-CBG	3.36	115.69	110.93
5	B	1001	Y01	CAK-CBD-CBG	3.36	115.69	110.93
5	C	1001	Y01	CAK-CBD-CBG	3.36	115.69	110.93
5	D	1001	Y01	CAK-CBD-CBG	3.36	115.69	110.93
5	A	1006	Y01	CBF-CBH-CAZ	3.33	114.53	109.65
5	B	1001	Y01	CBF-CBH-CAZ	3.33	114.53	109.65
5	C	1001	Y01	CBF-CBH-CAZ	3.33	114.53	109.65
5	D	1001	Y01	CBF-CBH-CAZ	3.33	114.53	109.65
5	A	1004	Y01	CBF-CBH-CAZ	3.21	114.35	109.65
5	B	1005	Y01	CBF-CBH-CAZ	3.21	114.35	109.65
5	C	1005	Y01	CBF-CBH-CAZ	3.21	114.35	109.65
5	D	1004	Y01	CBF-CBH-CAZ	3.21	114.35	109.65
4	A	1003	SBJ	O1P-P-O2P	3.12	126.95	112.44
4	A	1005	SBJ	O1P-P-O2P	3.12	126.95	112.44
4	B	1004	SBJ	O1P-P-O2P	3.12	126.95	112.44
4	C	1004	SBJ	O1P-P-O2P	3.12	126.95	112.44
2	A	1001	R0G	C20-C21-C22	3.06	124.97	119.97
2	B	1002	R0G	C20-C21-C22	3.06	124.97	119.97
2	C	1002	R0G	C20-C21-C22	3.06	124.97	119.97
2	D	1002	R0G	C20-C21-C22	3.06	124.97	119.97
5	A	1006	Y01	CAD-CBH-CAZ	-3.05	103.73	108.38
5	B	1001	Y01	CAD-CBH-CAZ	-3.05	103.73	108.38
5	C	1001	Y01	CAD-CBH-CAZ	-3.05	103.73	108.38
5	D	1001	Y01	CAD-CBH-CAZ	-3.05	103.73	108.38
5	A	1004	Y01	OAW-CBC-CAV	3.02	114.27	108.04
5	B	1005	Y01	OAW-CBC-CAV	3.02	114.27	108.04
5	C	1005	Y01	OAW-CBC-CAV	3.02	114.27	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1004	Y01	OAW-CBC-CAV	3.02	114.27	108.04
5	A	1006	Y01	CAD-CBH-CAT	-3.01	104.85	109.43
5	B	1001	Y01	CAD-CBH-CAT	-3.01	104.85	109.43
5	C	1001	Y01	CAD-CBH-CAT	-3.01	104.85	109.43
5	D	1001	Y01	CAD-CBH-CAT	-3.01	104.85	109.43
5	A	1006	Y01	OAW-CBC-CAV	2.99	114.20	108.04
5	B	1001	Y01	OAW-CBC-CAV	2.99	114.20	108.04
5	C	1001	Y01	OAW-CBC-CAV	2.99	114.20	108.04
5	D	1001	Y01	OAW-CBC-CAV	2.99	114.20	108.04
5	A	1006	Y01	CAU-CBI-CBE	2.98	120.99	116.60
5	B	1001	Y01	CAU-CBI-CBE	2.98	120.99	116.60
5	C	1001	Y01	CAU-CBI-CBE	2.98	120.99	116.60
5	D	1001	Y01	CAU-CBI-CBE	2.98	120.99	116.60
5	A	1004	Y01	CAU-CBI-CBE	2.94	120.94	116.60
5	B	1005	Y01	CAU-CBI-CBE	2.94	120.94	116.60
5	C	1005	Y01	CAU-CBI-CBE	2.94	120.94	116.60
5	D	1004	Y01	CAU-CBI-CBE	2.94	120.94	116.60
5	A	1004	Y01	CAD-CBH-CAT	-2.82	105.14	109.43
5	B	1005	Y01	CAD-CBH-CAT	-2.82	105.14	109.43
5	C	1005	Y01	CAD-CBH-CAT	-2.82	105.14	109.43
5	D	1004	Y01	CAD-CBH-CAT	-2.82	105.14	109.43
2	A	1001	R0G	C03-C04-C05	2.80	114.44	110.75
2	B	1002	R0G	C03-C04-C05	2.80	114.44	110.75
2	C	1002	R0G	C03-C04-C05	2.80	114.44	110.75
2	D	1002	R0G	C03-C04-C05	2.80	114.44	110.75
5	A	1006	Y01	CAR-CBC-CAV	-2.73	107.18	110.97
5	B	1001	Y01	CAR-CBC-CAV	-2.73	107.18	110.97
5	C	1001	Y01	CAR-CBC-CAV	-2.73	107.18	110.97
5	D	1001	Y01	CAR-CBC-CAV	-2.73	107.18	110.97
3	A	1002	S9Y	O5-P-O4	-2.73	98.13	108.94
3	B	1003	S9Y	O5-P-O4	-2.73	98.13	108.94
3	C	1003	S9Y	O5-P-O4	-2.73	98.13	108.94
3	D	1003	S9Y	O5-P-O4	-2.73	98.13	108.94
5	A	1006	Y01	CAT-CBH-CBF	2.71	112.32	108.74
5	B	1001	Y01	CAT-CBH-CBF	2.71	112.32	108.74
5	C	1001	Y01	CAT-CBH-CBF	2.71	112.32	108.74
5	D	1001	Y01	CAT-CBH-CBF	2.71	112.32	108.74
2	A	1001	R0G	C09-C08-C16	2.67	107.30	103.55
2	B	1002	R0G	C09-C08-C16	2.67	107.30	103.55
2	C	1002	R0G	C09-C08-C16	2.67	107.30	103.55
2	D	1002	R0G	C09-C08-C16	2.67	107.30	103.55
5	A	1004	Y01	CAR-CBC-CAV	-2.64	107.31	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1005	Y01	CAR-CBC-CAV	-2.64	107.31	110.97
5	C	1005	Y01	CAR-CBC-CAV	-2.64	107.31	110.97
5	D	1004	Y01	CAR-CBC-CAV	-2.64	107.31	110.97
2	A	1001	R0G	C19-C20-C21	2.53	123.57	120.35
2	B	1002	R0G	C19-C20-C21	2.53	123.57	120.35
2	C	1002	R0G	C19-C20-C21	2.53	123.57	120.35
2	D	1002	R0G	C19-C20-C21	2.53	123.57	120.35
5	A	1006	Y01	CBD-CAK-CAI	2.49	116.21	112.76
5	B	1001	Y01	CBD-CAK-CAI	2.49	116.21	112.76
5	C	1001	Y01	CBD-CAK-CAI	2.49	116.21	112.76
5	D	1001	Y01	CBD-CAK-CAI	2.49	116.21	112.76
5	A	1004	Y01	CBI-CBE-CBB	-2.39	115.80	119.50
5	B	1005	Y01	CBI-CBE-CBB	-2.39	115.80	119.50
5	C	1005	Y01	CBI-CBE-CBB	-2.39	115.80	119.50
5	D	1004	Y01	CBI-CBE-CBB	-2.39	115.80	119.50
5	A	1004	Y01	CAT-CBH-CBF	2.38	111.88	108.74
5	B	1005	Y01	CAT-CBH-CBF	2.38	111.88	108.74
5	C	1005	Y01	CAT-CBH-CBF	2.38	111.88	108.74
5	D	1004	Y01	CAT-CBH-CBF	2.38	111.88	108.74
5	A	1006	Y01	CBC-OAW-CAY	2.32	123.36	117.80
5	B	1001	Y01	CBC-OAW-CAY	2.32	123.36	117.80
5	C	1001	Y01	CBC-OAW-CAY	2.32	123.36	117.80
5	D	1001	Y01	CBC-OAW-CAY	2.32	123.36	117.80
5	A	1004	Y01	CAR-CAT-CBH	2.32	117.72	112.78
5	B	1005	Y01	CAR-CAT-CBH	2.32	117.72	112.78
5	C	1005	Y01	CAR-CAT-CBH	2.32	117.72	112.78
5	D	1004	Y01	CAR-CAT-CBH	2.32	117.72	112.78
5	A	1004	Y01	CBC-OAW-CAY	2.31	123.33	117.80
5	B	1005	Y01	CBC-OAW-CAY	2.31	123.33	117.80
5	C	1005	Y01	CBC-OAW-CAY	2.31	123.33	117.80
5	D	1004	Y01	CBC-OAW-CAY	2.31	123.33	117.80
5	A	1006	Y01	CAV-CAZ-CBH	-2.30	113.48	116.42
5	B	1001	Y01	CAV-CAZ-CBH	-2.30	113.48	116.42
5	C	1001	Y01	CAV-CAZ-CBH	-2.30	113.48	116.42
5	D	1001	Y01	CAV-CAZ-CBH	-2.30	113.48	116.42
5	A	1006	Y01	CAQ-CBG-CBD	2.22	122.64	119.10
5	B	1001	Y01	CAQ-CBG-CBD	2.22	122.64	119.10
5	C	1001	Y01	CAQ-CBG-CBD	2.22	122.64	119.10
5	D	1001	Y01	CAQ-CBG-CBD	2.22	122.64	119.10
3	A	1002	S9Y	O2-C31-C32	2.22	116.27	111.48
3	B	1003	S9Y	O2-C31-C32	2.22	116.27	111.48
3	C	1003	S9Y	O2-C31-C32	2.22	116.27	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1003	S9Y	O2-C31-C32	2.22	116.27	111.48
5	A	1006	Y01	CAR-CAT-CBH	2.19	117.45	112.78
5	B	1001	Y01	CAR-CAT-CBH	2.19	117.45	112.78
5	C	1001	Y01	CAR-CAT-CBH	2.19	117.45	112.78
5	D	1001	Y01	CAR-CAT-CBH	2.19	117.45	112.78
5	A	1006	Y01	CAD-CBH-CBF	-2.18	109.21	111.66
5	B	1001	Y01	CAD-CBH-CBF	-2.18	109.21	111.66
5	C	1001	Y01	CAD-CBH-CBF	-2.18	109.21	111.66
5	D	1001	Y01	CAD-CBH-CBF	-2.18	109.21	111.66
5	A	1004	Y01	CBG-CBI-CBE	2.17	102.58	100.10
5	B	1005	Y01	CBG-CBI-CBE	2.17	102.58	100.10
5	C	1005	Y01	CBG-CBI-CBE	2.17	102.58	100.10
5	D	1004	Y01	CBG-CBI-CBE	2.17	102.58	100.10
5	A	1006	Y01	CBG-CBI-CBE	2.12	102.53	100.10
5	B	1001	Y01	CBG-CBI-CBE	2.12	102.53	100.10
5	C	1001	Y01	CBG-CBI-CBE	2.12	102.53	100.10
5	D	1001	Y01	CBG-CBI-CBE	2.12	102.53	100.10
2	A	1001	R0G	C24-C21-C20	-2.12	115.33	118.96
2	B	1002	R0G	C24-C21-C20	-2.12	115.33	118.96
2	C	1002	R0G	C24-C21-C20	-2.12	115.33	118.96
2	D	1002	R0G	C24-C21-C20	-2.12	115.33	118.96
5	A	1004	Y01	CAQ-CBG-CBD	2.05	122.37	119.10
5	B	1005	Y01	CAQ-CBG-CBD	2.05	122.37	119.10
5	C	1005	Y01	CAQ-CBG-CBD	2.05	122.37	119.10
5	D	1004	Y01	CAQ-CBG-CBD	2.05	122.37	119.10
5	A	1006	Y01	CBH-CAZ-CAI	-2.05	119.94	122.93
5	B	1001	Y01	CBH-CAZ-CAI	-2.05	119.94	122.93
5	C	1001	Y01	CBH-CAZ-CAI	-2.05	119.94	122.93
5	D	1001	Y01	CBH-CAZ-CAI	-2.05	119.94	122.93
5	A	1004	Y01	CAV-CAZ-CBH	-2.01	113.85	116.42
5	B	1005	Y01	CAV-CAZ-CBH	-2.01	113.85	116.42
5	C	1005	Y01	CAV-CAZ-CBH	-2.01	113.85	116.42
5	D	1004	Y01	CAV-CAZ-CBH	-2.01	113.85	116.42

There are no chirality outliers.

All (200) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	S9Y	C1-O3P-P-O4
3	A	1002	S9Y	O5-C4-C5-N1
3	B	1003	S9Y	C1-O3P-P-O4
3	B	1003	S9Y	O5-C4-C5-N1

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Mol	Chain	Res	Type	Atoms
3	C	1003	S9Y	C1-O3P-P-O4
3	C	1003	S9Y	O5-C4-C5-N1
3	D	1003	S9Y	C1-O3P-P-O4
3	D	1003	S9Y	O5-C4-C5-N1
4	A	1003	SBJ	C32-C31-O2-C2
4	A	1003	SBJ	C1-O3P-P-O1P
4	A	1003	SBJ	C1-O3P-P-O4P
4	A	1003	SBJ	C4-O4P-P-O3P
4	A	1003	SBJ	C4-O4P-P-O1P
4	A	1003	SBJ	O4P-C4-C5-N6
4	A	1005	SBJ	C32-C31-O2-C2
4	A	1005	SBJ	C1-O3P-P-O1P
4	A	1005	SBJ	C1-O3P-P-O4P
4	A	1005	SBJ	C4-O4P-P-O3P
4	A	1005	SBJ	C4-O4P-P-O1P
4	A	1005	SBJ	O4P-C4-C5-N6
4	B	1004	SBJ	C32-C31-O2-C2
4	B	1004	SBJ	C1-O3P-P-O1P
4	B	1004	SBJ	C1-O3P-P-O4P
4	B	1004	SBJ	C4-O4P-P-O3P
4	B	1004	SBJ	C4-O4P-P-O1P
4	B	1004	SBJ	O4P-C4-C5-N6
4	C	1004	SBJ	C32-C31-O2-C2
4	C	1004	SBJ	C1-O3P-P-O1P
4	C	1004	SBJ	C1-O3P-P-O4P
4	C	1004	SBJ	C4-O4P-P-O3P
4	C	1004	SBJ	C4-O4P-P-O1P
4	C	1004	SBJ	O4P-C4-C5-N6
4	A	1003	SBJ	O11-C11-O3-C3
4	A	1005	SBJ	O11-C11-O3-C3
4	B	1004	SBJ	O11-C11-O3-C3
4	C	1004	SBJ	O11-C11-O3-C3
4	A	1003	SBJ	C12-C11-O3-C3
4	A	1005	SBJ	C12-C11-O3-C3
4	B	1004	SBJ	C12-C11-O3-C3
4	C	1004	SBJ	C12-C11-O3-C3
4	A	1003	SBJ	O31-C31-O2-C2
4	A	1005	SBJ	O31-C31-O2-C2
4	B	1004	SBJ	O31-C31-O2-C2
4	C	1004	SBJ	O31-C31-O2-C2
5	A	1004	Y01	CAO-CBB-CBE-CBI
5	B	1005	Y01	CAO-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
5	C	1005	Y01	CAO-CBB-CBE-CBI
5	D	1004	Y01	CAO-CBB-CBE-CBI
5	A	1004	Y01	CAX-CAL-CAM-CAY
5	B	1005	Y01	CAX-CAL-CAM-CAY
5	C	1005	Y01	CAX-CAL-CAM-CAY
5	D	1004	Y01	CAX-CAL-CAM-CAY
5	A	1006	Y01	CAJ-CAO-CBB-CAC
5	B	1001	Y01	CAJ-CAO-CBB-CAC
5	C	1001	Y01	CAJ-CAO-CBB-CAC
5	D	1001	Y01	CAJ-CAO-CBB-CAC
5	A	1006	Y01	CAJ-CAO-CBB-CBE
5	B	1001	Y01	CAJ-CAO-CBB-CBE
5	C	1001	Y01	CAJ-CAO-CBB-CBE
5	D	1001	Y01	CAJ-CAO-CBB-CBE
4	A	1003	SBJ	C32-C33-C34-C35
4	A	1005	SBJ	C32-C33-C34-C35
4	B	1004	SBJ	C32-C33-C34-C35
4	C	1004	SBJ	C32-C33-C34-C35
5	A	1004	Y01	CAJ-CAO-CBB-CAC
5	B	1005	Y01	CAJ-CAO-CBB-CAC
5	C	1005	Y01	CAJ-CAO-CBB-CAC
5	D	1004	Y01	CAJ-CAO-CBB-CAC
5	A	1004	Y01	CAN-CAJ-CAO-CBB
5	B	1005	Y01	CAN-CAJ-CAO-CBB
5	C	1005	Y01	CAN-CAJ-CAO-CBB
5	D	1004	Y01	CAN-CAJ-CAO-CBB
5	A	1006	Y01	CAO-CAJ-CAN-CBA
5	B	1001	Y01	CAO-CAJ-CAN-CBA
5	C	1001	Y01	CAO-CAJ-CAN-CBA
5	D	1001	Y01	CAO-CAJ-CAN-CBA
5	A	1004	Y01	CAC-CBB-CBE-CBI
5	B	1005	Y01	CAC-CBB-CBE-CBI
5	C	1005	Y01	CAC-CBB-CBE-CBI
5	D	1004	Y01	CAC-CBB-CBE-CBI
5	A	1004	Y01	CAO-CBB-CBE-CAP
5	B	1005	Y01	CAO-CBB-CBE-CAP
5	C	1005	Y01	CAO-CBB-CBE-CAP
5	D	1004	Y01	CAO-CBB-CBE-CAP
4	A	1003	SBJ	C33-C34-C35-C36
4	A	1005	SBJ	C33-C34-C35-C36
4	B	1004	SBJ	C33-C34-C35-C36
4	C	1004	SBJ	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
5	A	1004	Y01	CAC-CBB-CBE-CAP
5	B	1005	Y01	CAC-CBB-CBE-CAP
5	C	1005	Y01	CAC-CBB-CBE-CAP
5	D	1004	Y01	CAC-CBB-CBE-CAP
4	A	1003	SBJ	C42-C43-C44-C45
4	A	1005	SBJ	C42-C43-C44-C45
4	B	1004	SBJ	C42-C43-C44-C45
4	C	1004	SBJ	C42-C43-C44-C45
4	A	1003	SBJ	C41-C42-C43-C44
4	A	1005	SBJ	C41-C42-C43-C44
4	B	1004	SBJ	C41-C42-C43-C44
4	C	1004	SBJ	C41-C42-C43-C44
3	A	1002	S9Y	C32-C33-C34-C35
3	B	1003	S9Y	C32-C33-C34-C35
3	C	1003	S9Y	C32-C33-C34-C35
3	D	1003	S9Y	C32-C33-C34-C35
4	A	1003	SBJ	C11-C12-C13-C14
4	A	1005	SBJ	C11-C12-C13-C14
4	B	1004	SBJ	C11-C12-C13-C14
4	C	1004	SBJ	C11-C12-C13-C14
3	A	1002	S9Y	C34-C35-C36-C37
3	B	1003	S9Y	C34-C35-C36-C37
3	C	1003	S9Y	C34-C35-C36-C37
3	D	1003	S9Y	C34-C35-C36-C37
4	A	1003	SBJ	C38-C39-C40-C41
4	A	1005	SBJ	C38-C39-C40-C41
4	B	1004	SBJ	C38-C39-C40-C41
4	C	1004	SBJ	C38-C39-C40-C41
5	A	1006	Y01	CAN-CAJ-CAO-CBB
5	B	1001	Y01	CAN-CAJ-CAO-CBB
5	C	1001	Y01	CAN-CAJ-CAO-CBB
5	D	1001	Y01	CAN-CAJ-CAO-CBB
3	A	1002	S9Y	C36-C37-C38-C39
3	B	1003	S9Y	C36-C37-C38-C39
3	C	1003	S9Y	C36-C37-C38-C39
3	D	1003	S9Y	C36-C37-C38-C39
4	A	1003	SBJ	O3P-C1-C2-O2
4	A	1005	SBJ	O3P-C1-C2-O2
4	B	1004	SBJ	O3P-C1-C2-O2
4	C	1004	SBJ	O3P-C1-C2-O2
3	A	1002	S9Y	C32-C31-O2-C2
3	B	1003	S9Y	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
3	C	1003	S9Y	C32-C31-O2-C2
3	D	1003	S9Y	C32-C31-O2-C2
3	A	1002	S9Y	O31-C31-O2-C2
3	B	1003	S9Y	O31-C31-O2-C2
3	C	1003	S9Y	O31-C31-O2-C2
3	D	1003	S9Y	O31-C31-O2-C2
3	A	1002	S9Y	C35-C36-C37-C38
3	B	1003	S9Y	C35-C36-C37-C38
3	C	1003	S9Y	C35-C36-C37-C38
3	D	1003	S9Y	C35-C36-C37-C38
4	A	1003	SBJ	O3P-C1-C2-C3
4	A	1005	SBJ	O3P-C1-C2-C3
4	B	1004	SBJ	O3P-C1-C2-C3
4	C	1004	SBJ	O3P-C1-C2-C3
4	A	1003	SBJ	C34-C35-C36-C37
4	A	1005	SBJ	C34-C35-C36-C37
4	B	1004	SBJ	C34-C35-C36-C37
4	C	1004	SBJ	C34-C35-C36-C37
4	A	1003	SBJ	C2-C1-O3P-P
4	A	1005	SBJ	C2-C1-O3P-P
4	B	1004	SBJ	C2-C1-O3P-P
4	C	1004	SBJ	C2-C1-O3P-P
3	A	1002	S9Y	C33-C34-C35-C36
3	B	1003	S9Y	C33-C34-C35-C36
3	C	1003	S9Y	C33-C34-C35-C36
3	D	1003	S9Y	C33-C34-C35-C36
5	A	1006	Y01	CAM-CAL-CAX-OAH
5	B	1001	Y01	CAM-CAL-CAX-OAH
5	C	1001	Y01	CAM-CAL-CAX-OAH
5	D	1001	Y01	CAM-CAL-CAX-OAH
4	A	1003	SBJ	C37-C38-C39-C40
4	A	1005	SBJ	C37-C38-C39-C40
4	B	1004	SBJ	C37-C38-C39-C40
4	C	1004	SBJ	C37-C38-C39-C40
5	A	1006	Y01	CAM-CAL-CAX-OAF
5	B	1001	Y01	CAM-CAL-CAX-OAF
5	C	1001	Y01	CAM-CAL-CAX-OAF
5	D	1001	Y01	CAM-CAL-CAX-OAF
5	A	1006	Y01	CAO-CBB-CBE-CBI
5	B	1001	Y01	CAO-CBB-CBE-CBI
5	C	1001	Y01	CAO-CBB-CBE-CBI
5	D	1001	Y01	CAO-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
4	A	1003	SBJ	C36-C37-C38-C39
4	A	1005	SBJ	C36-C37-C38-C39
4	B	1004	SBJ	C36-C37-C38-C39
4	C	1004	SBJ	C36-C37-C38-C39
5	A	1004	Y01	CAM-CAL-CAX-OAH
5	B	1005	Y01	CAM-CAL-CAX-OAH
5	C	1005	Y01	CAM-CAL-CAX-OAH
5	D	1004	Y01	CAM-CAL-CAX-OAH
5	A	1004	Y01	CAM-CAL-CAX-OAF
5	B	1005	Y01	CAM-CAL-CAX-OAF
5	C	1005	Y01	CAM-CAL-CAX-OAF
5	D	1004	Y01	CAM-CAL-CAX-OAF
5	A	1006	Y01	OAG-CAY-OAW-CBC
5	B	1001	Y01	OAG-CAY-OAW-CBC
5	C	1001	Y01	OAG-CAY-OAW-CBC
5	D	1001	Y01	OAG-CAY-OAW-CBC
5	A	1006	Y01	CAC-CBB-CBE-CBI
5	B	1001	Y01	CAC-CBB-CBE-CBI
5	C	1001	Y01	CAC-CBB-CBE-CBI
5	D	1001	Y01	CAC-CBB-CBE-CBI
5	A	1006	Y01	CAJ-CAN-CBA-CAA
5	B	1001	Y01	CAJ-CAN-CBA-CAA
5	C	1001	Y01	CAJ-CAN-CBA-CAA
5	D	1001	Y01	CAJ-CAN-CBA-CAA
5	A	1006	Y01	CAO-CBB-CBE-CAP
5	B	1001	Y01	CAO-CBB-CBE-CAP
5	C	1001	Y01	CAO-CBB-CBE-CAP
5	D	1001	Y01	CAO-CBB-CBE-CAP

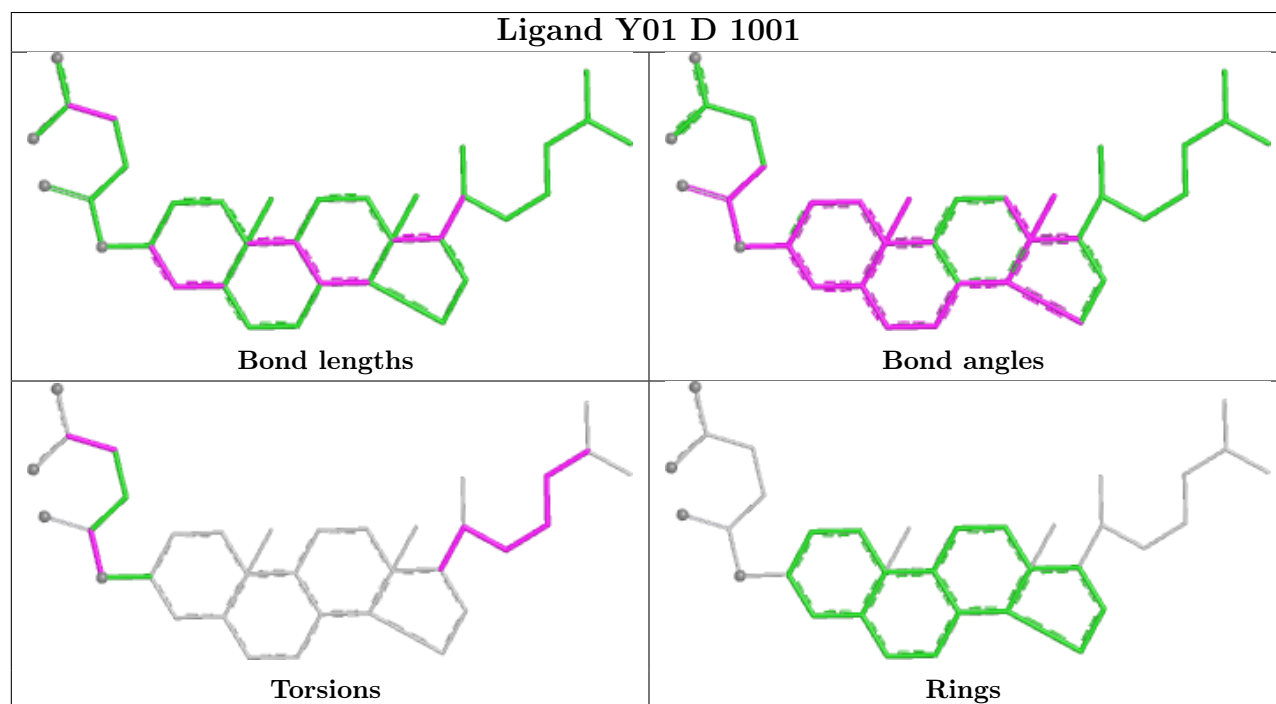
There are no ring outliers.

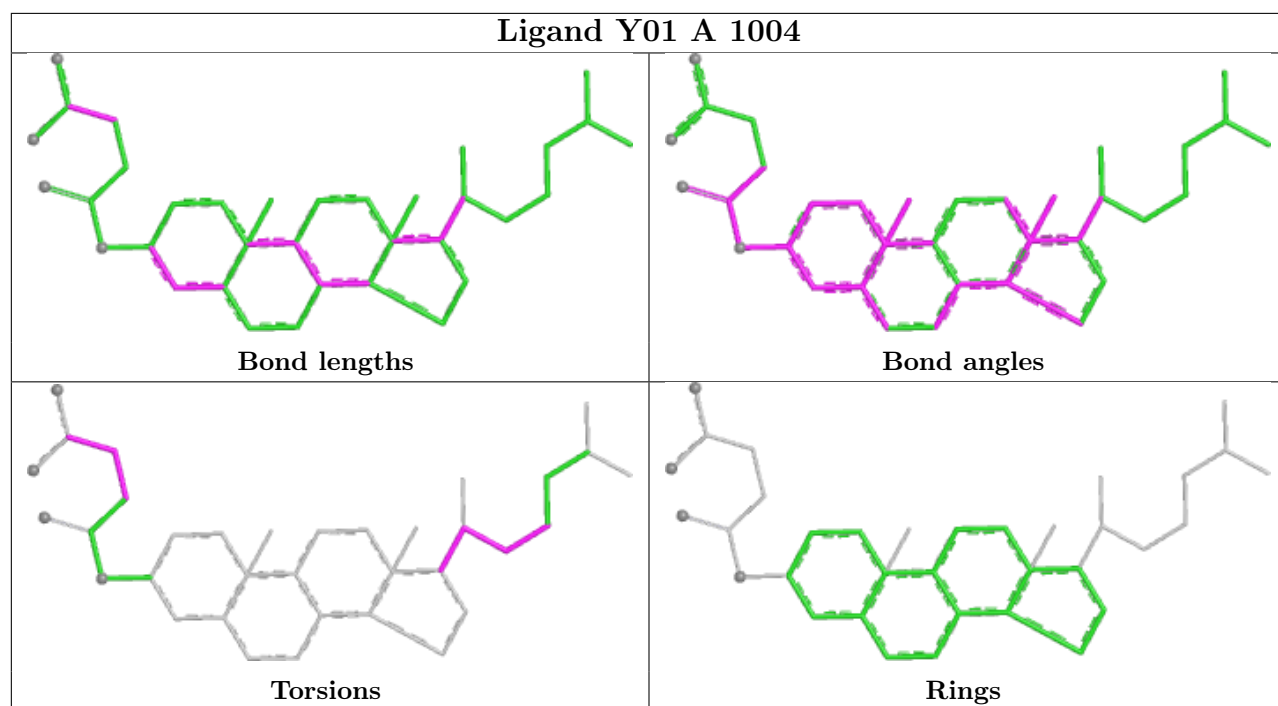
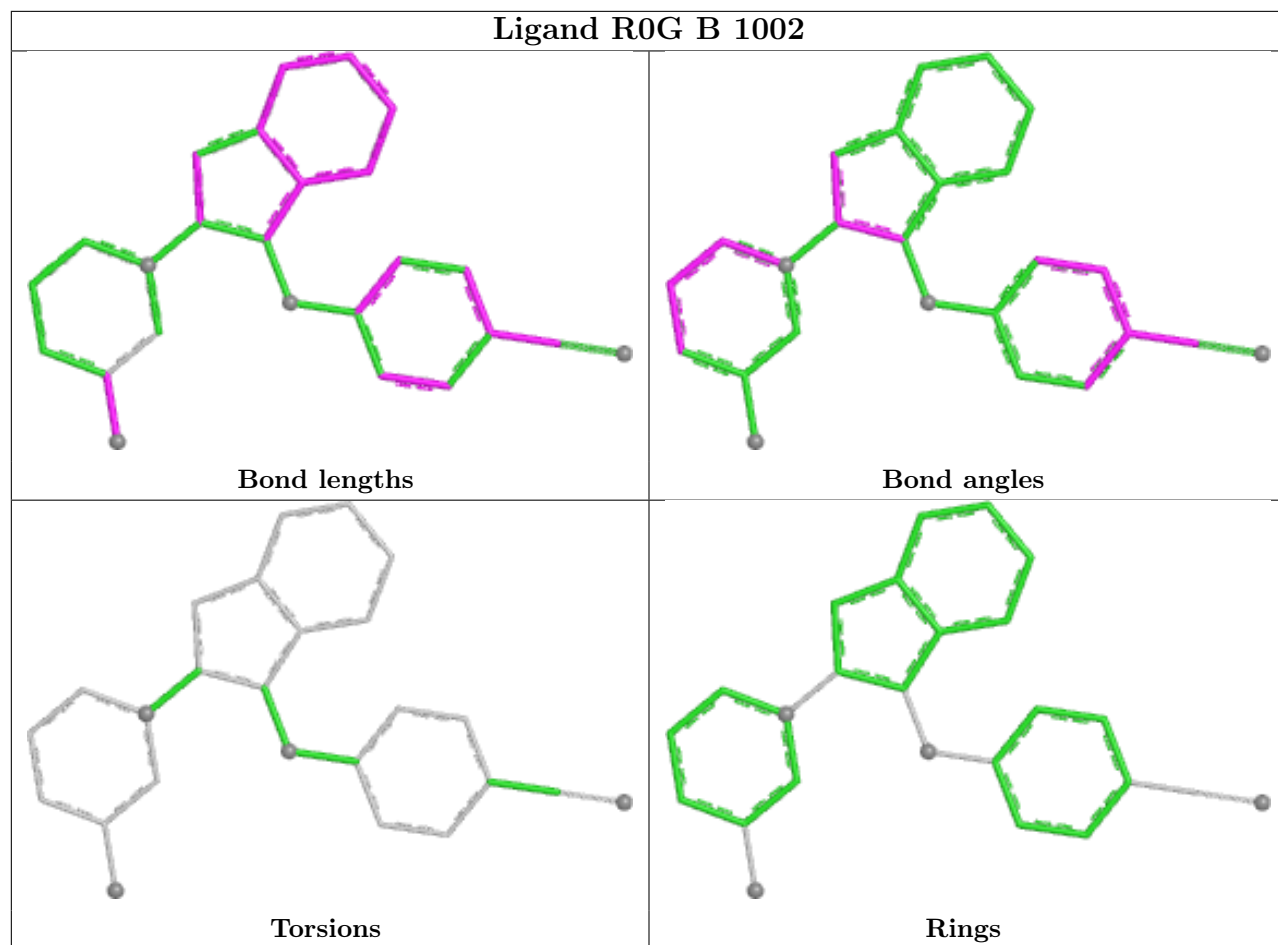
5 monomers are involved in 5 short contacts:

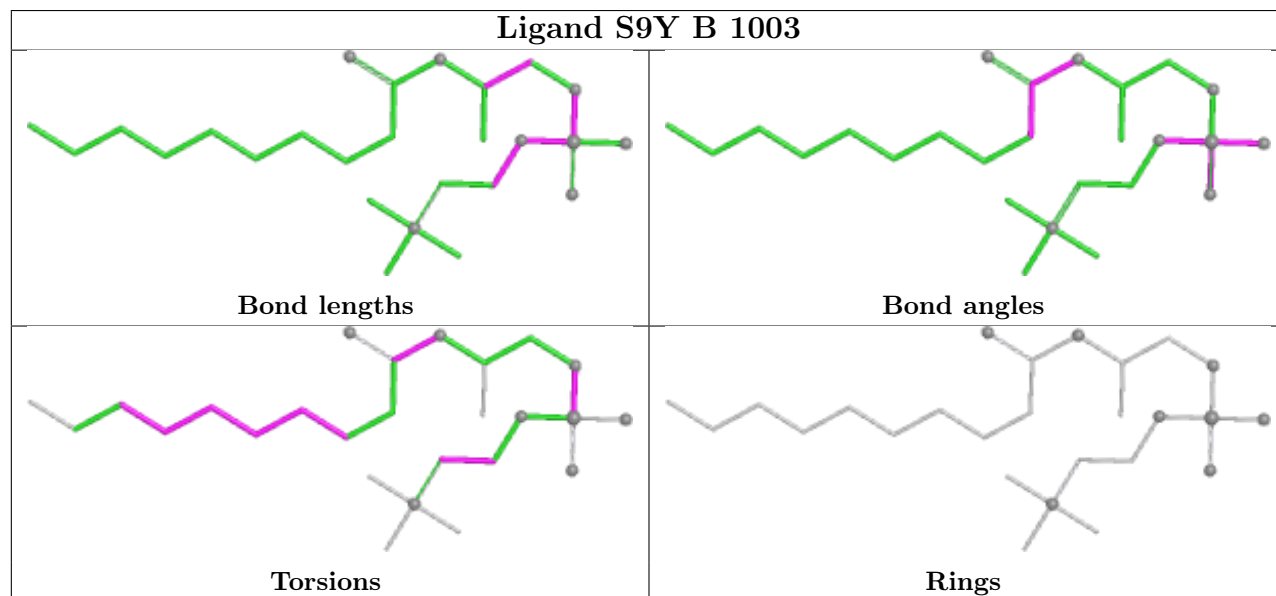
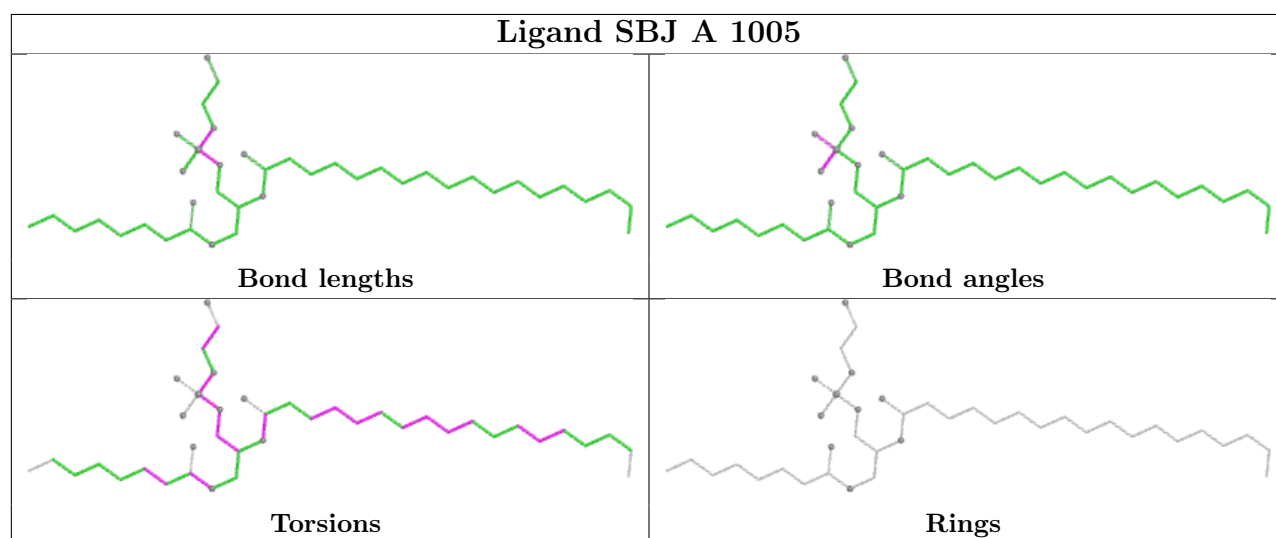
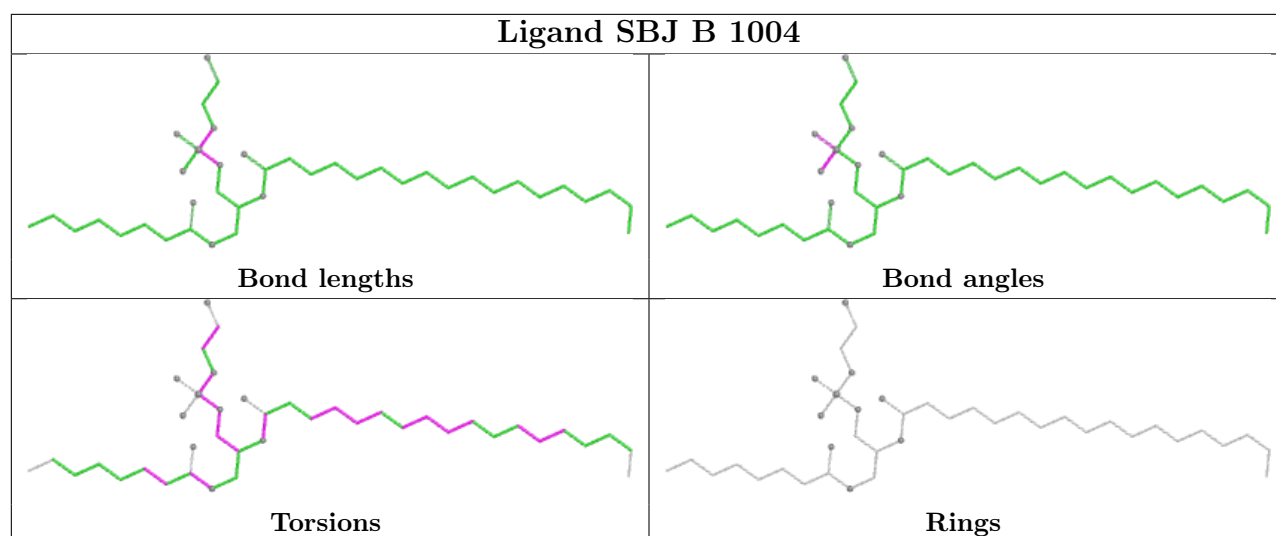
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1001	Y01	1	0
5	B	1005	Y01	1	0
5	A	1006	Y01	1	0
5	C	1001	Y01	1	0
5	C	1005	Y01	1	0

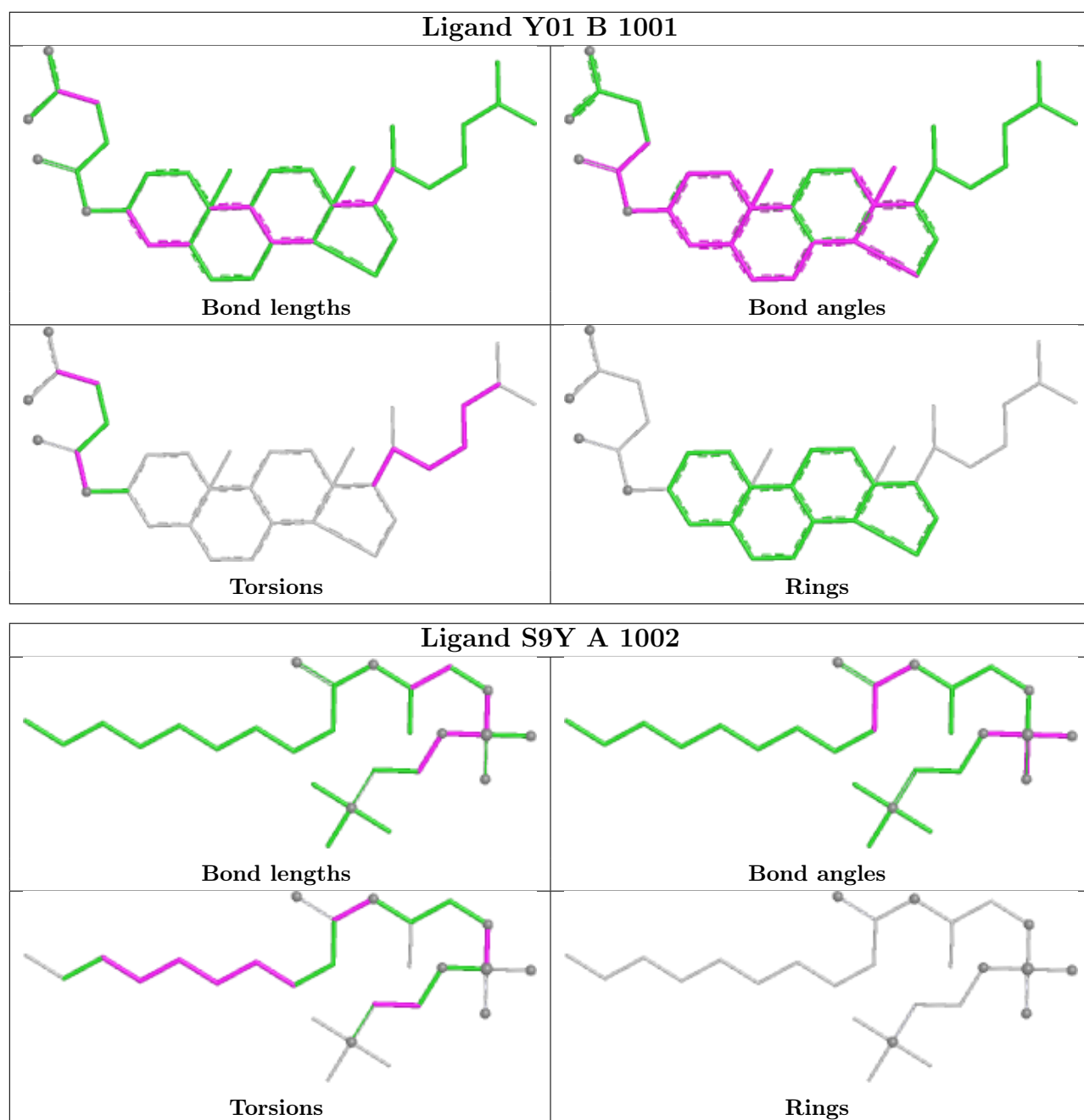
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

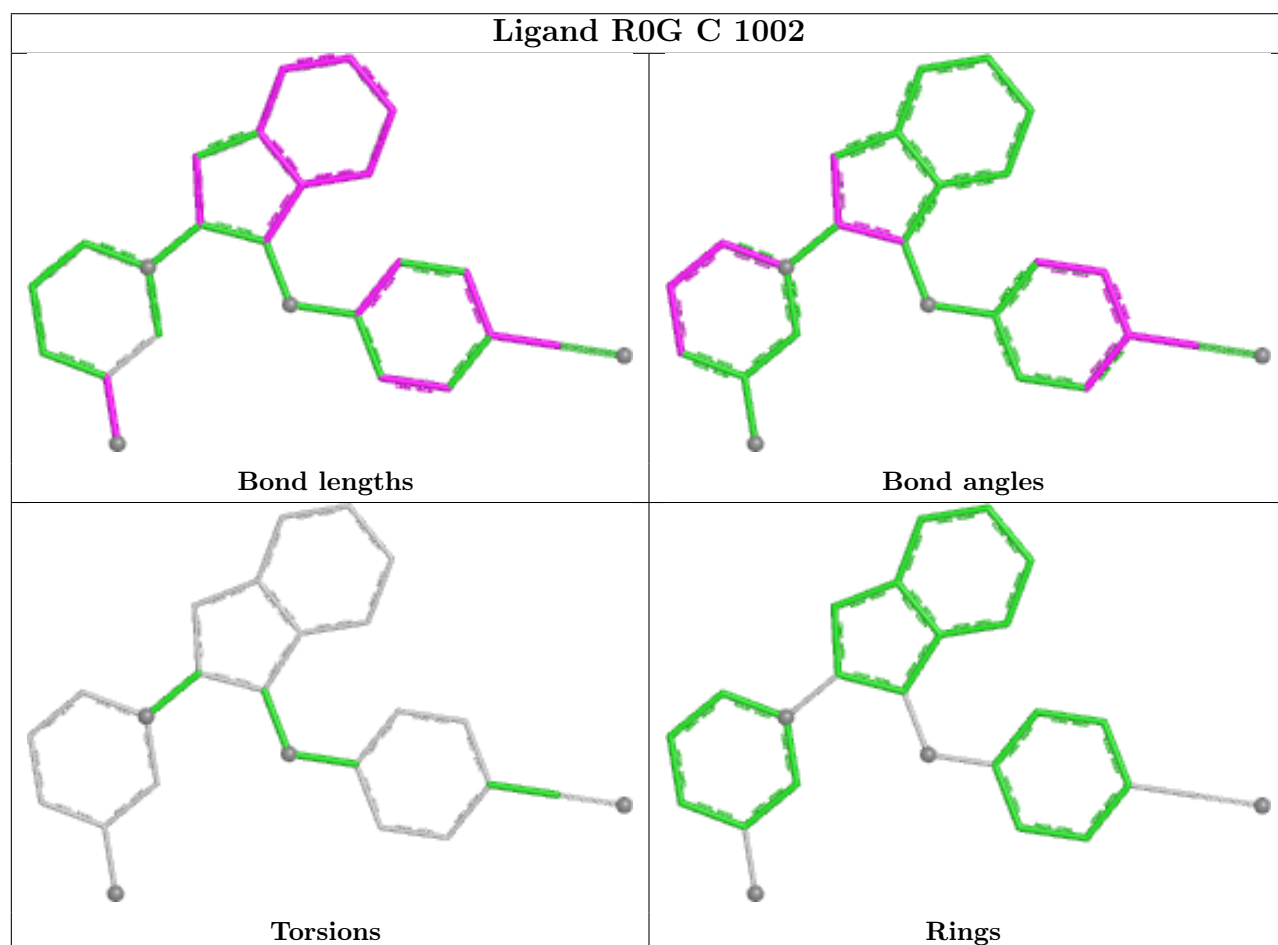
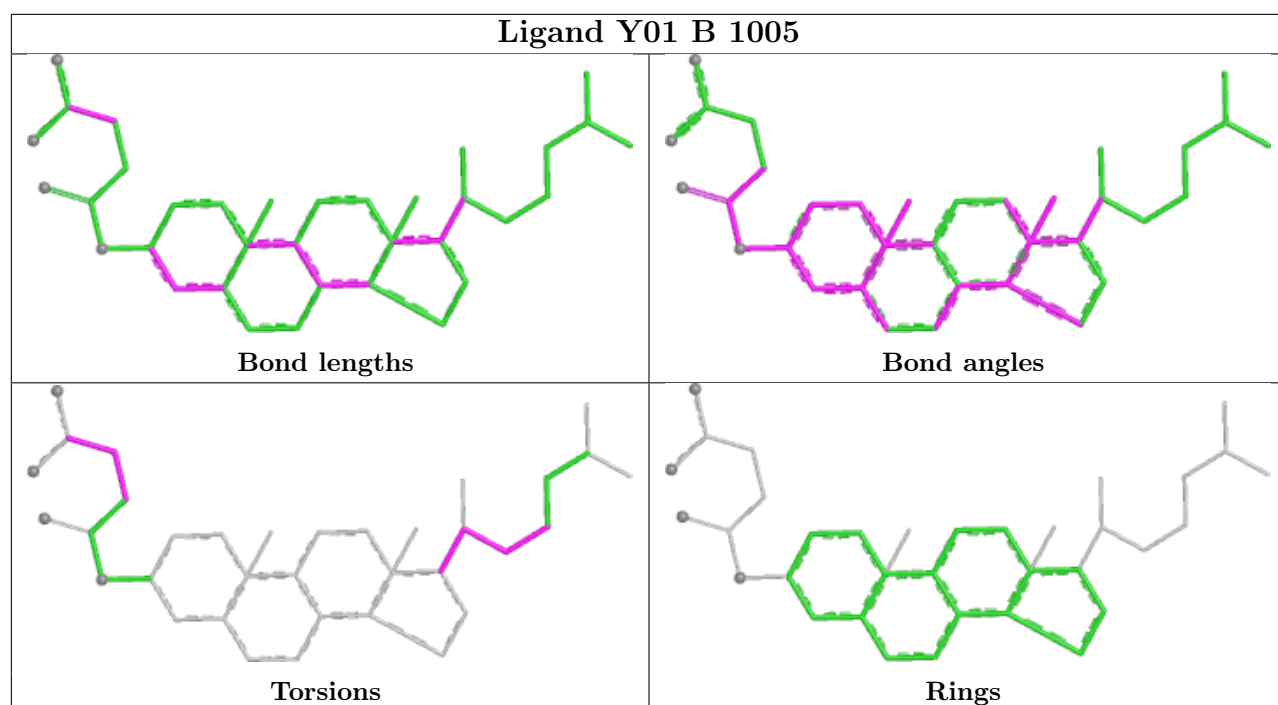
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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

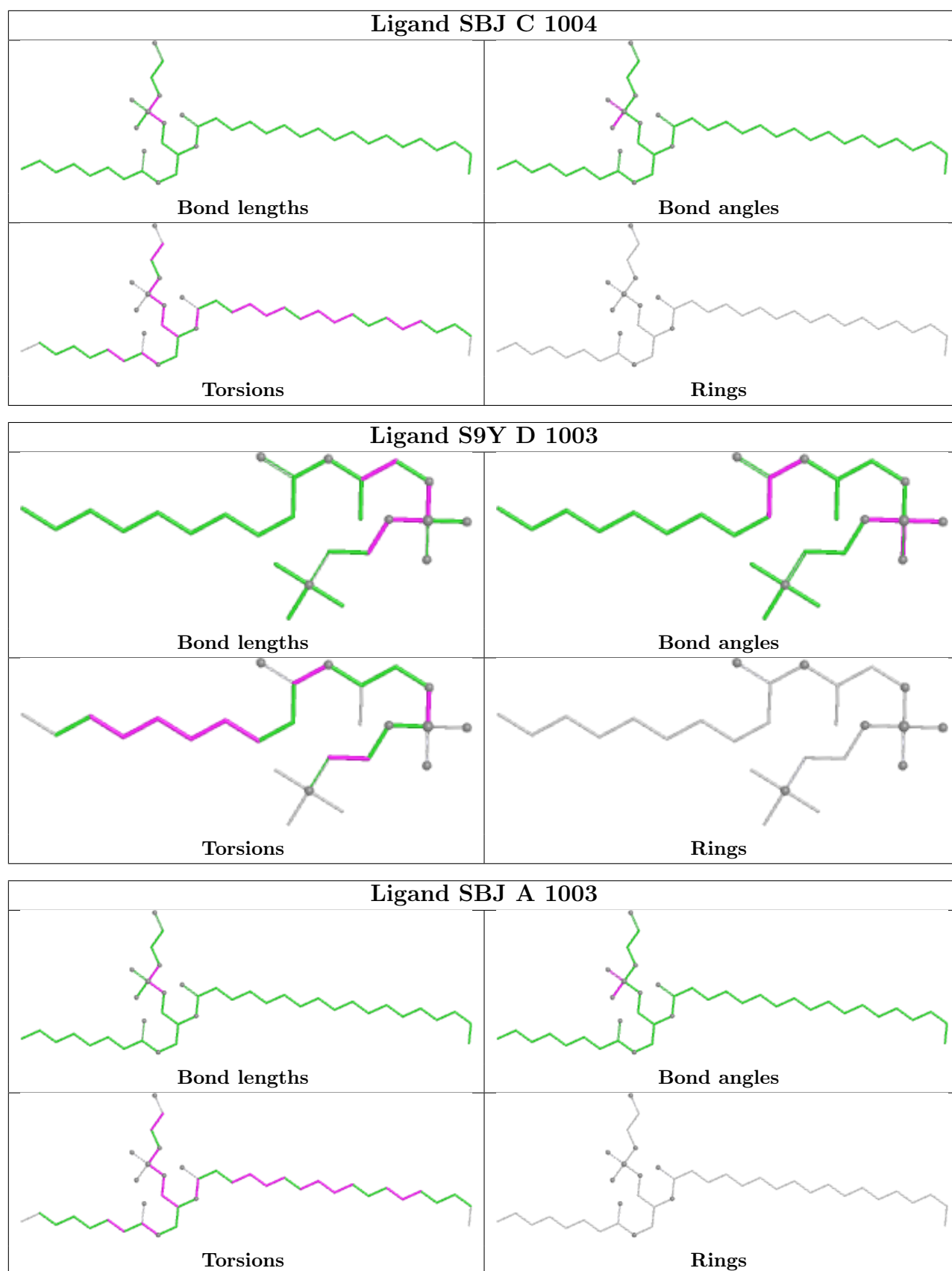


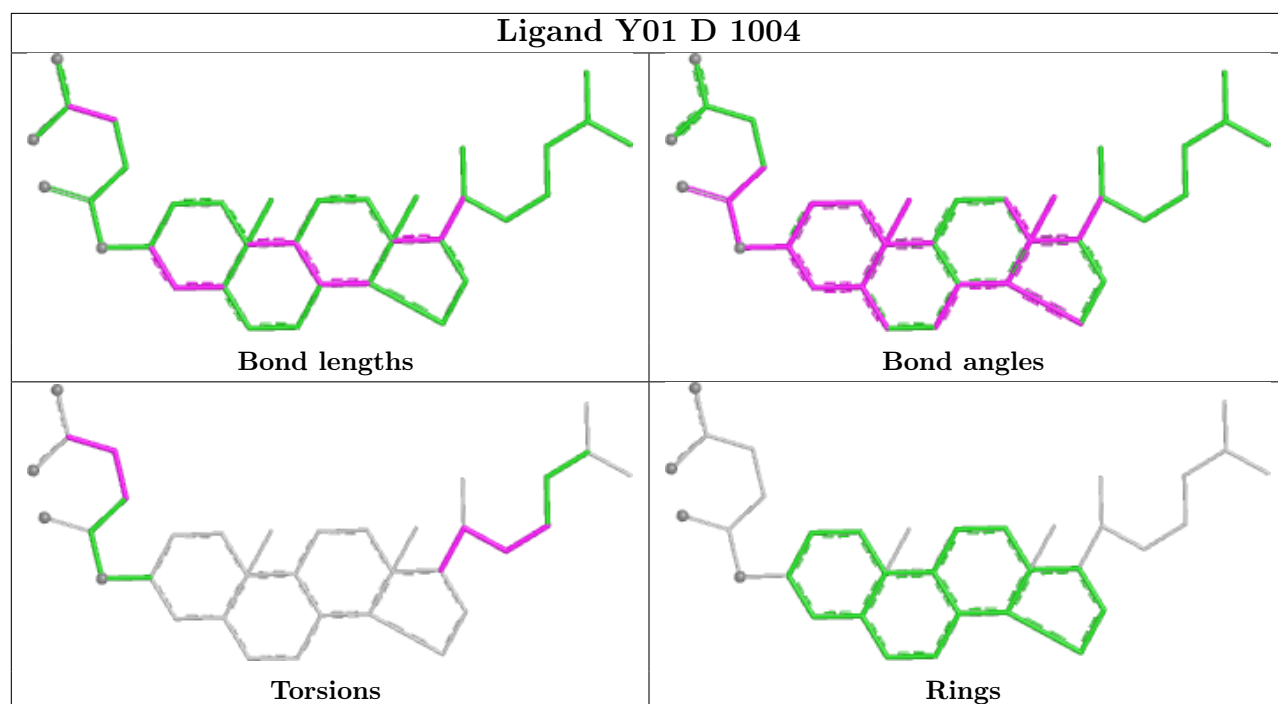
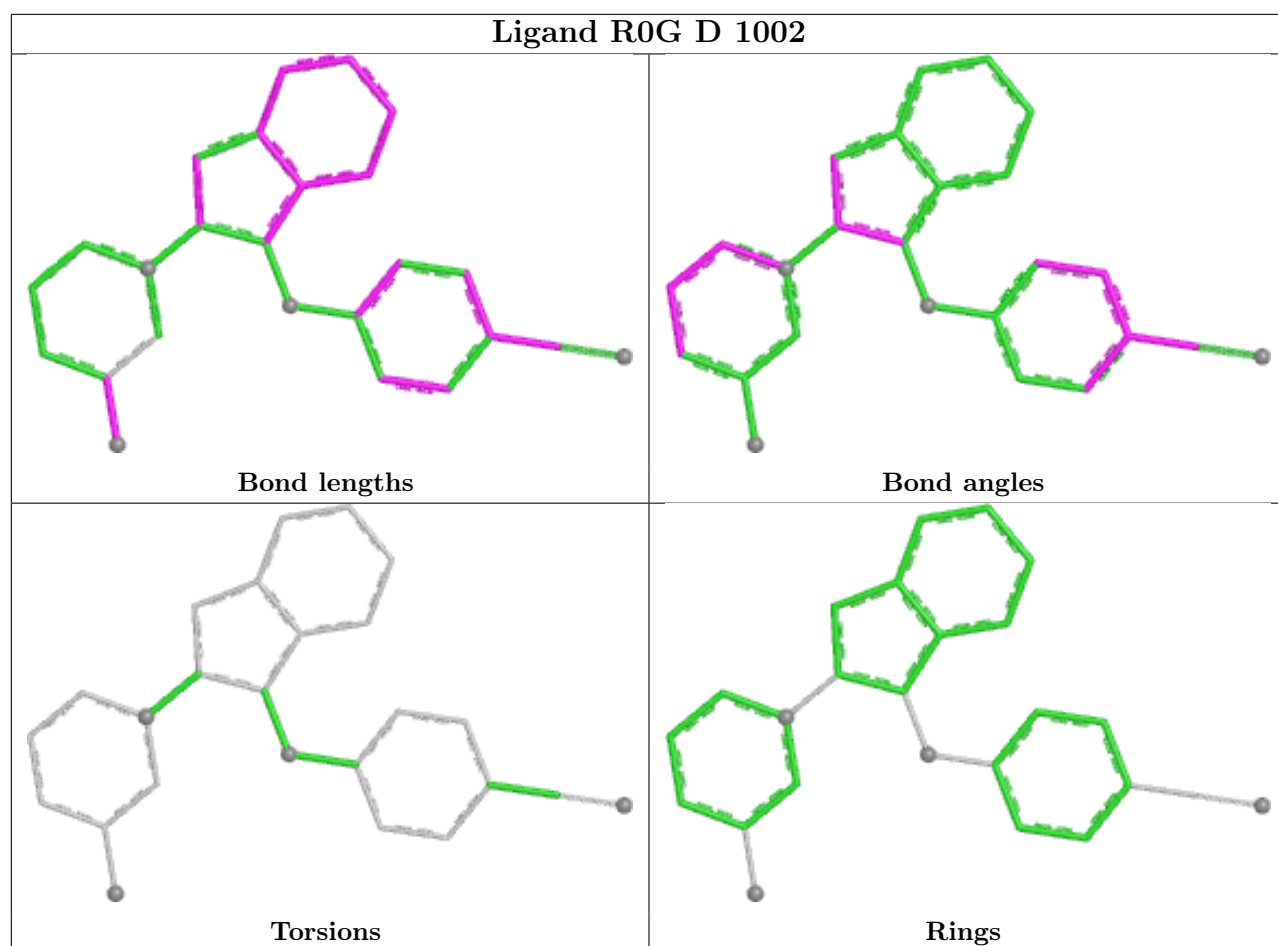


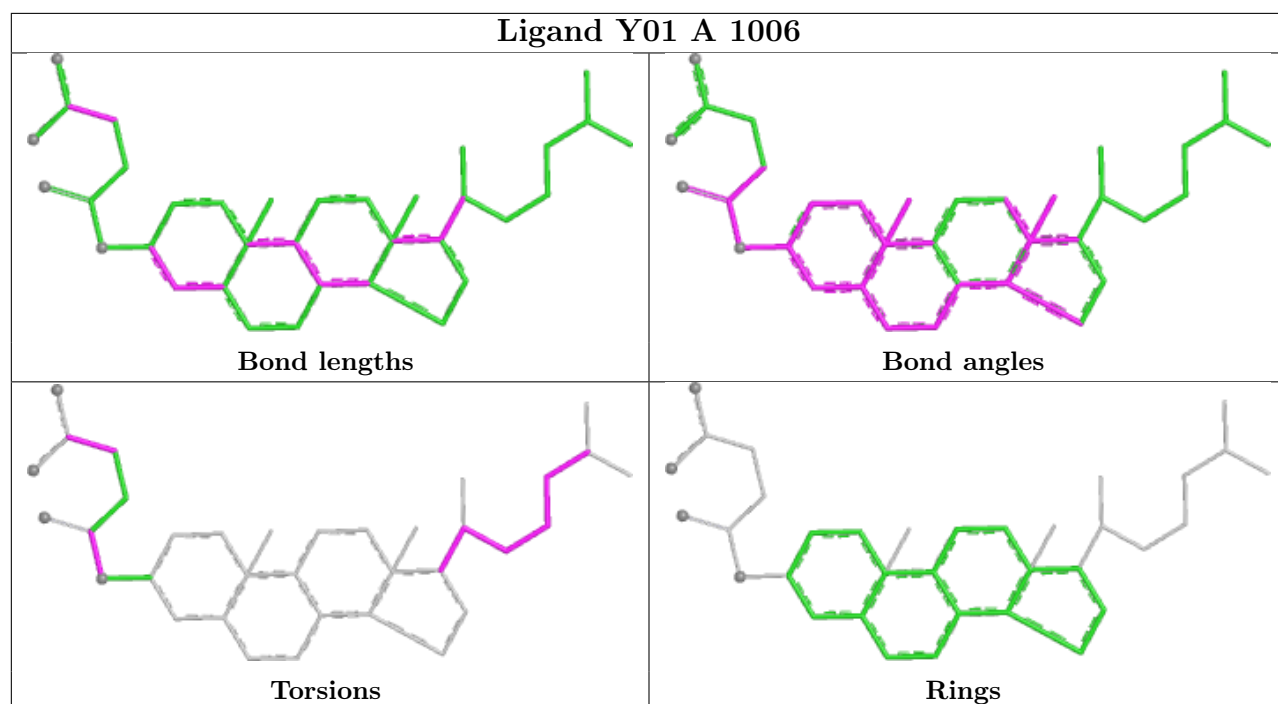
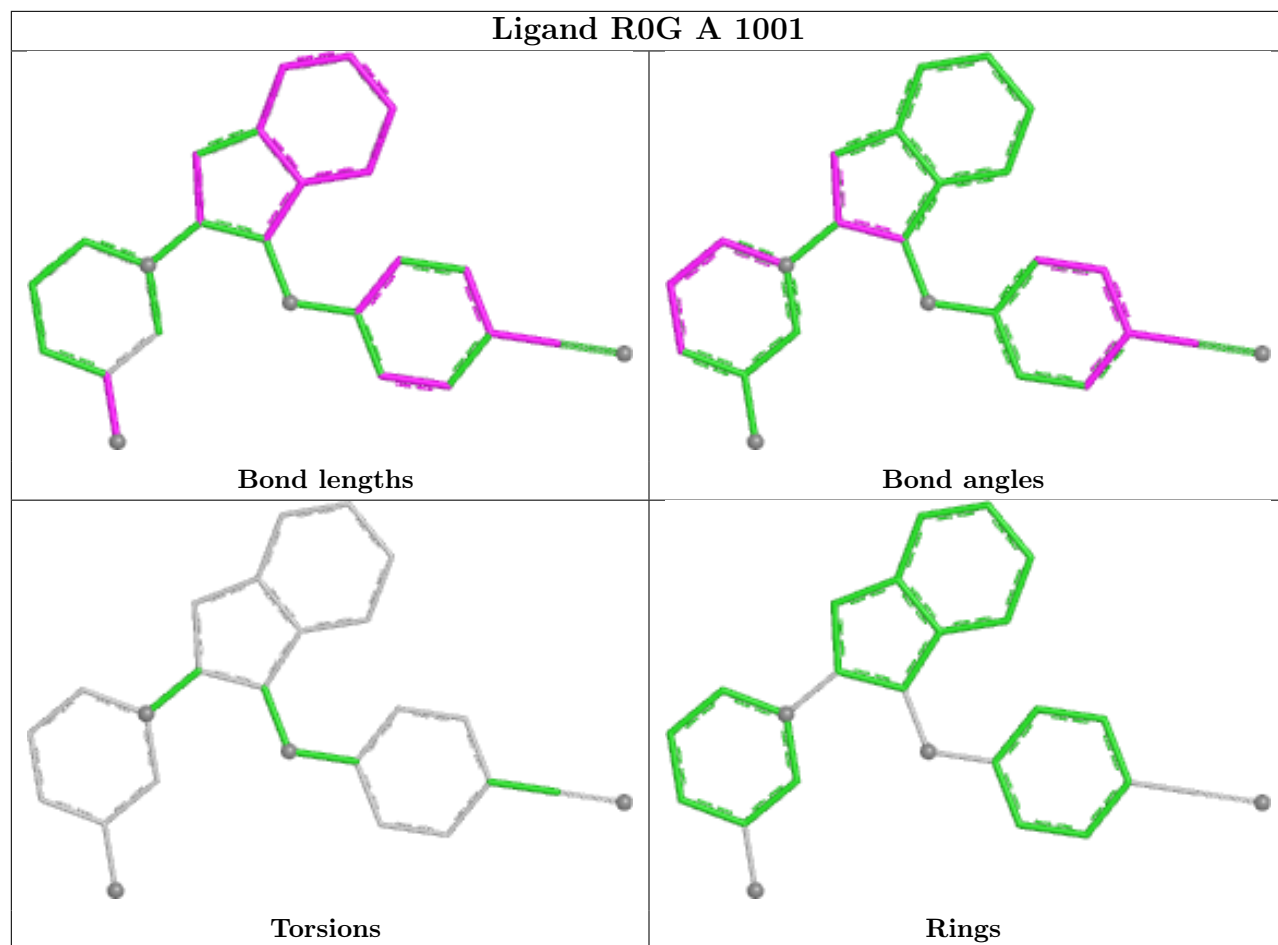


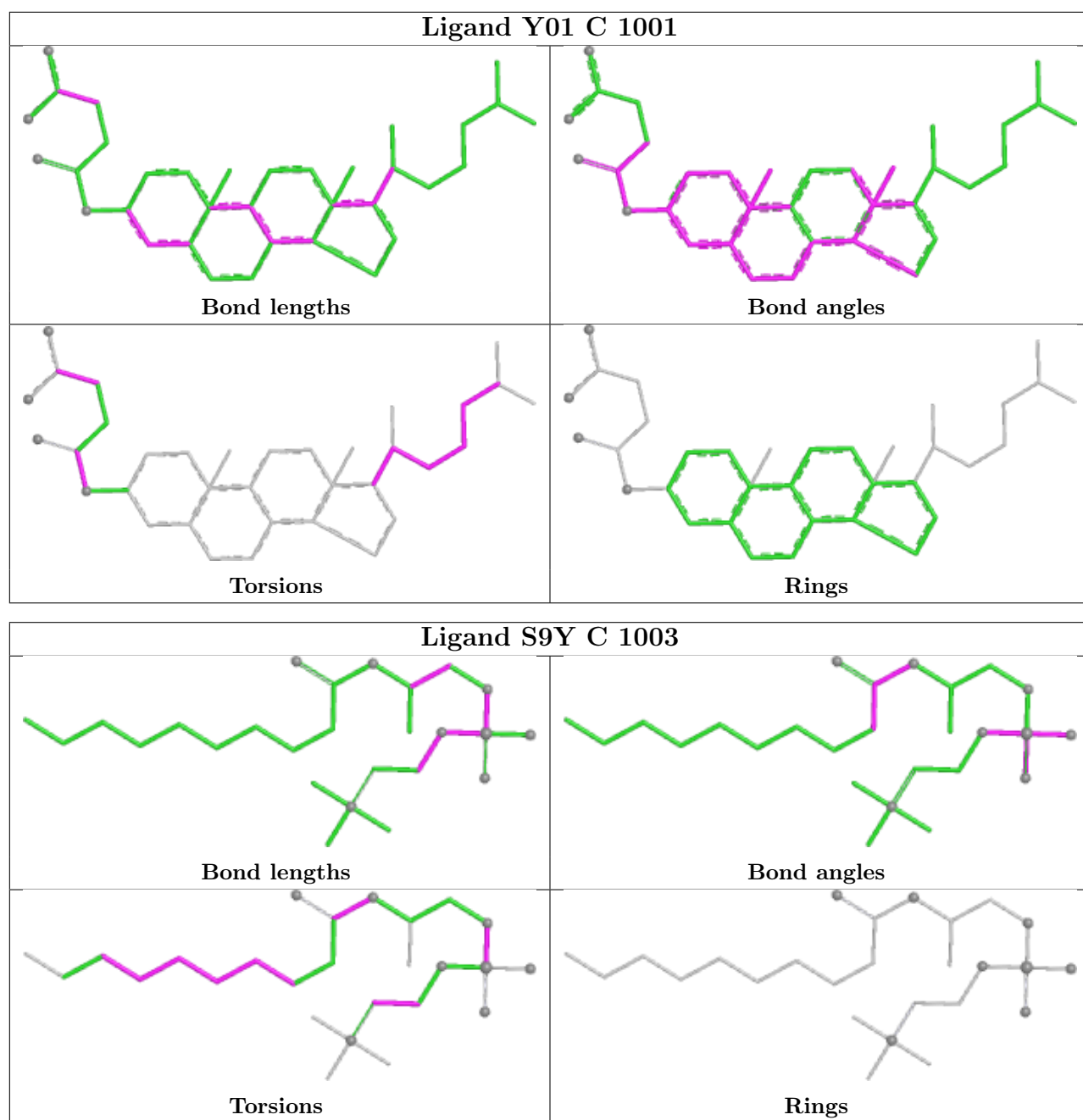


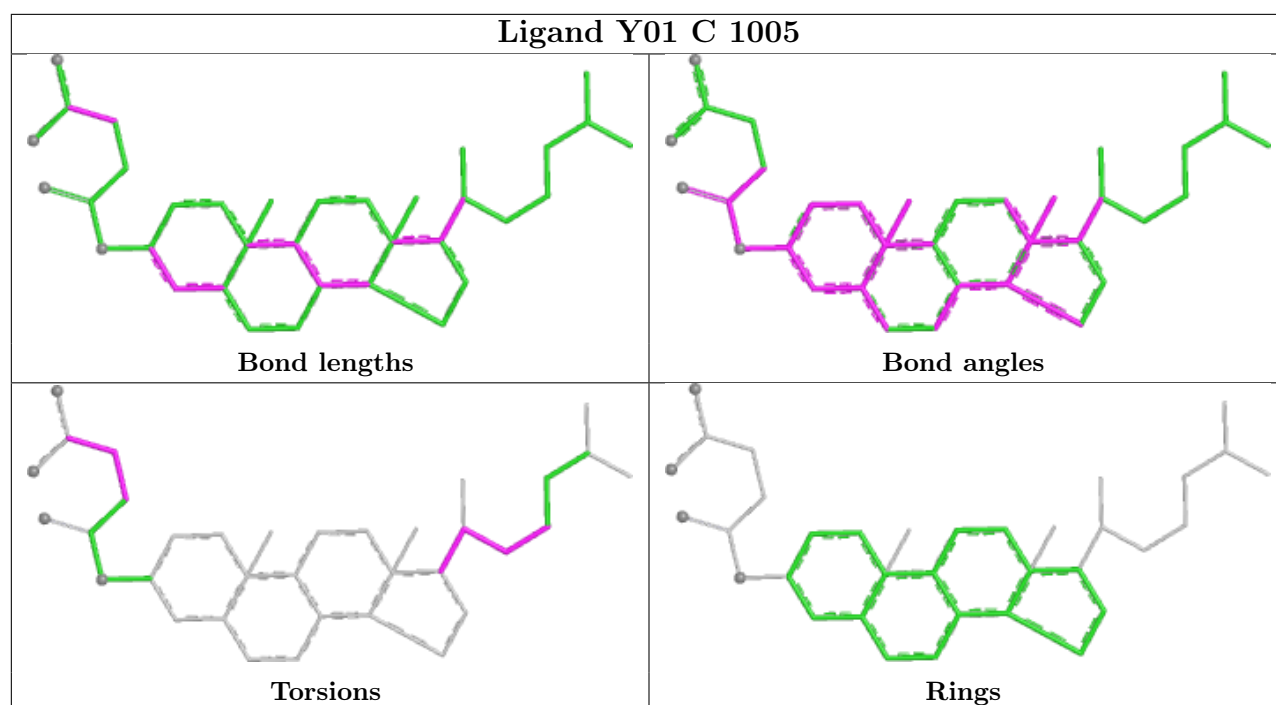












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

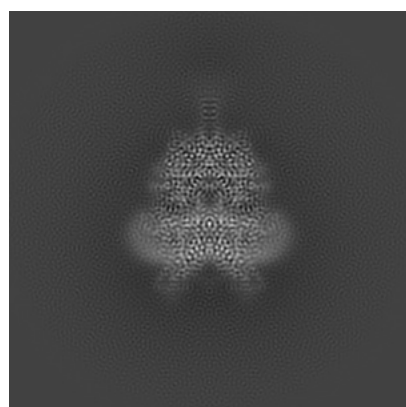
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20954. These allow visual inspection of the internal detail of the map and identification of artifacts.

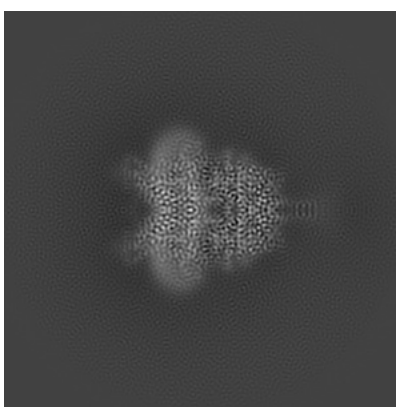
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

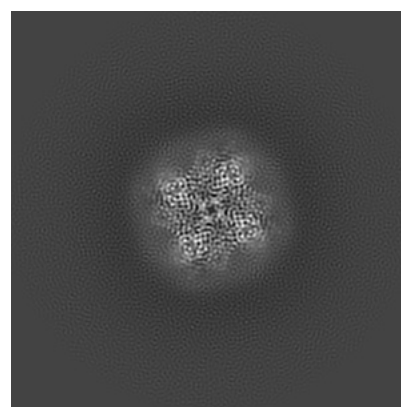
6.1.1 Primary map



X



Y

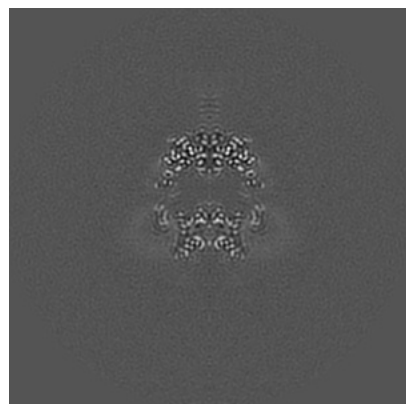


Z

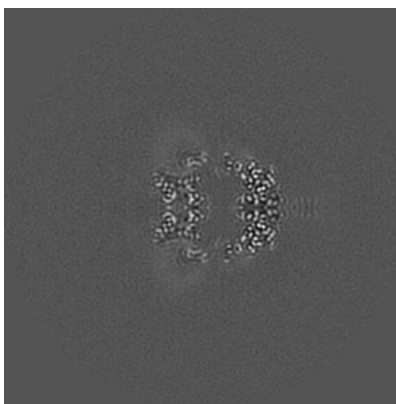
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

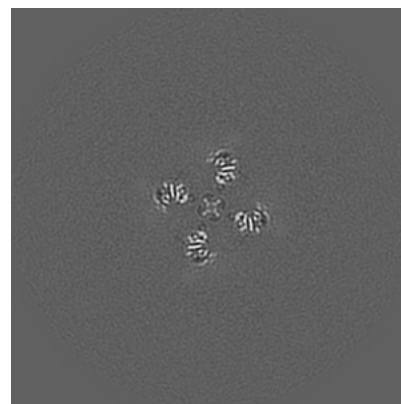
6.2.1 Primary map



X Index: 200



Y Index: 200

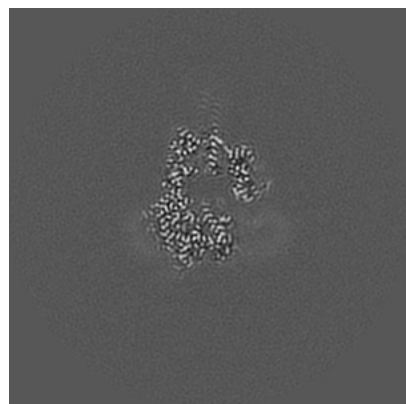


Z Index: 200

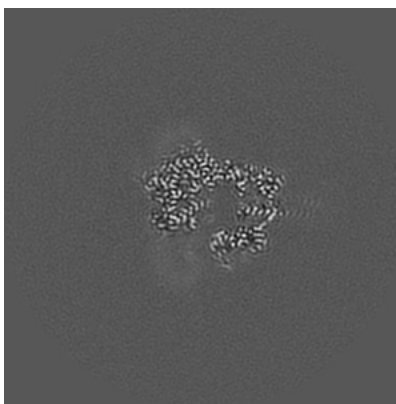
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

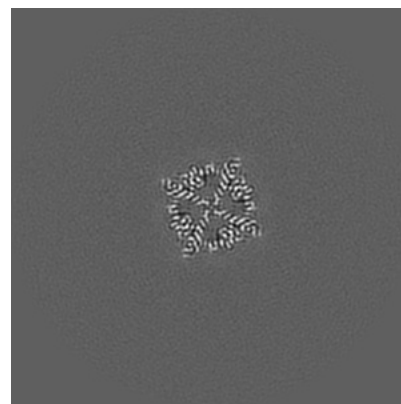
6.3.1 Primary map



X Index: 189



Y Index: 189

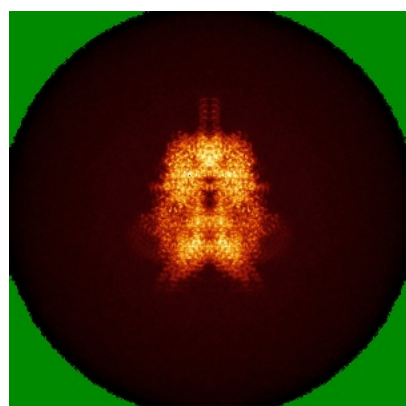


Z Index: 235

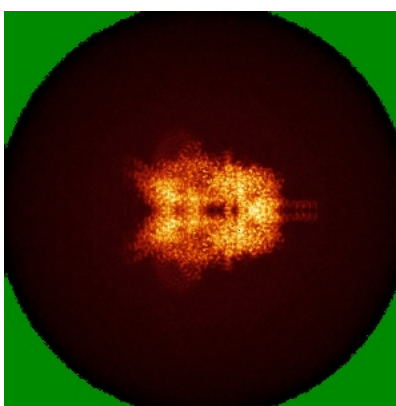
The images above show the largest variance slices of the map in three orthogonal directions.

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

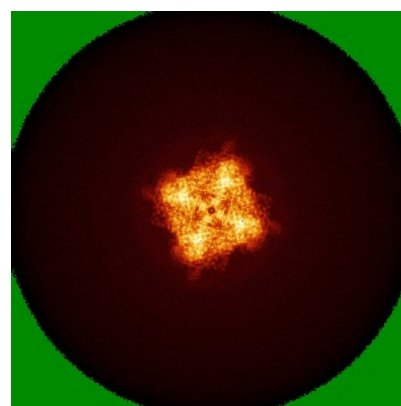
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

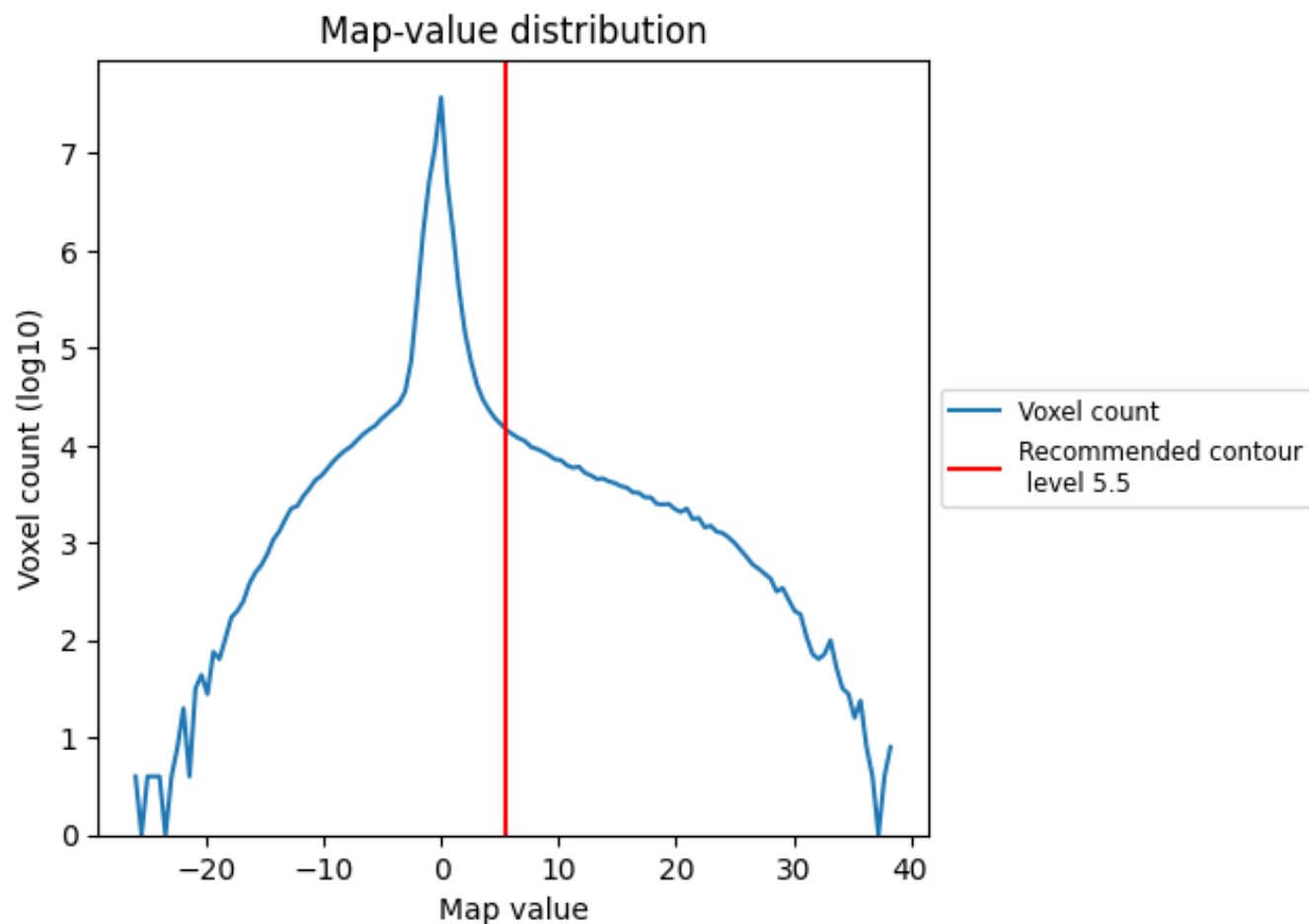
6.6 Mask visualisation

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

7 Map analysis [i](#)

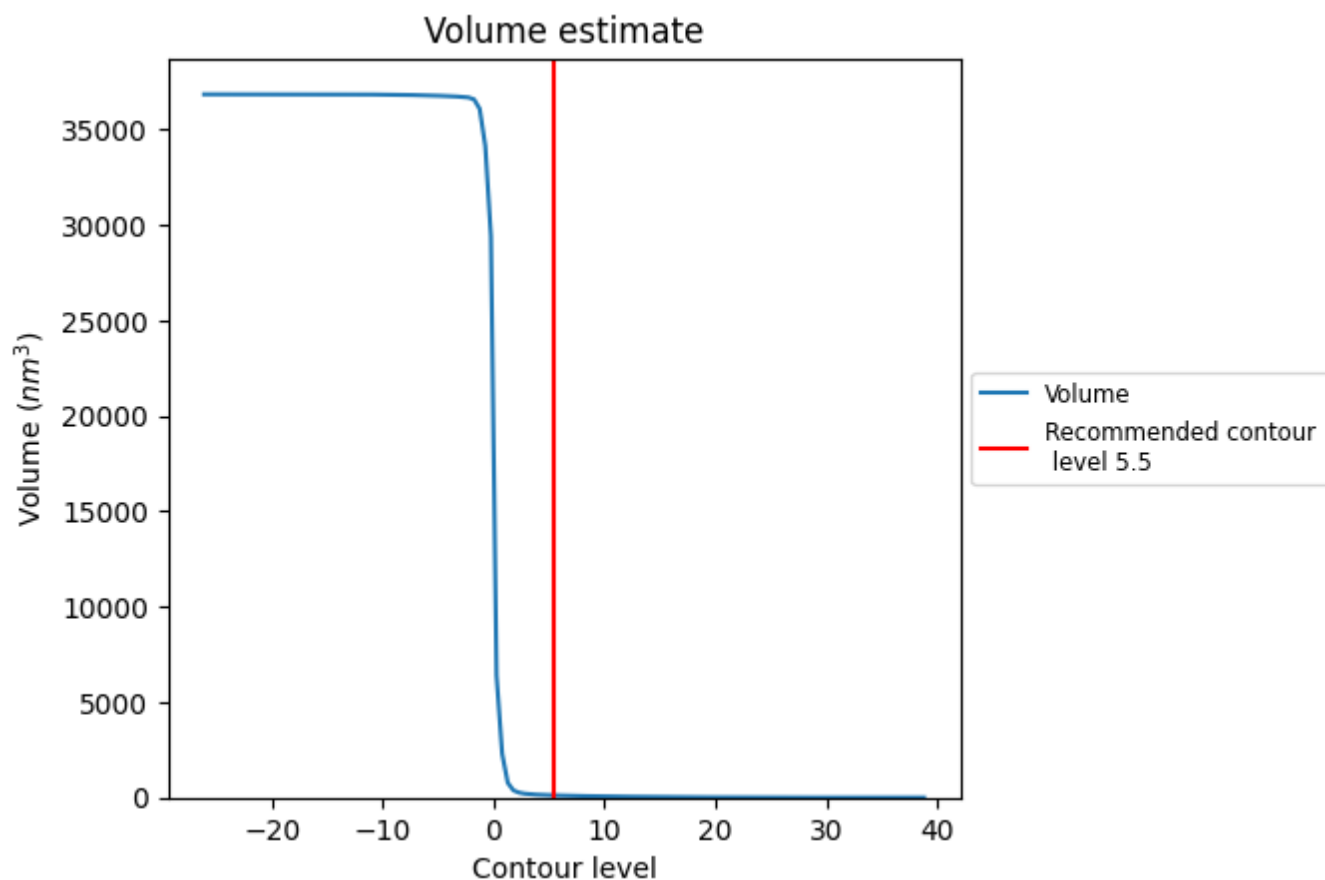
This section contains the results of statistical analysis of the map.

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.

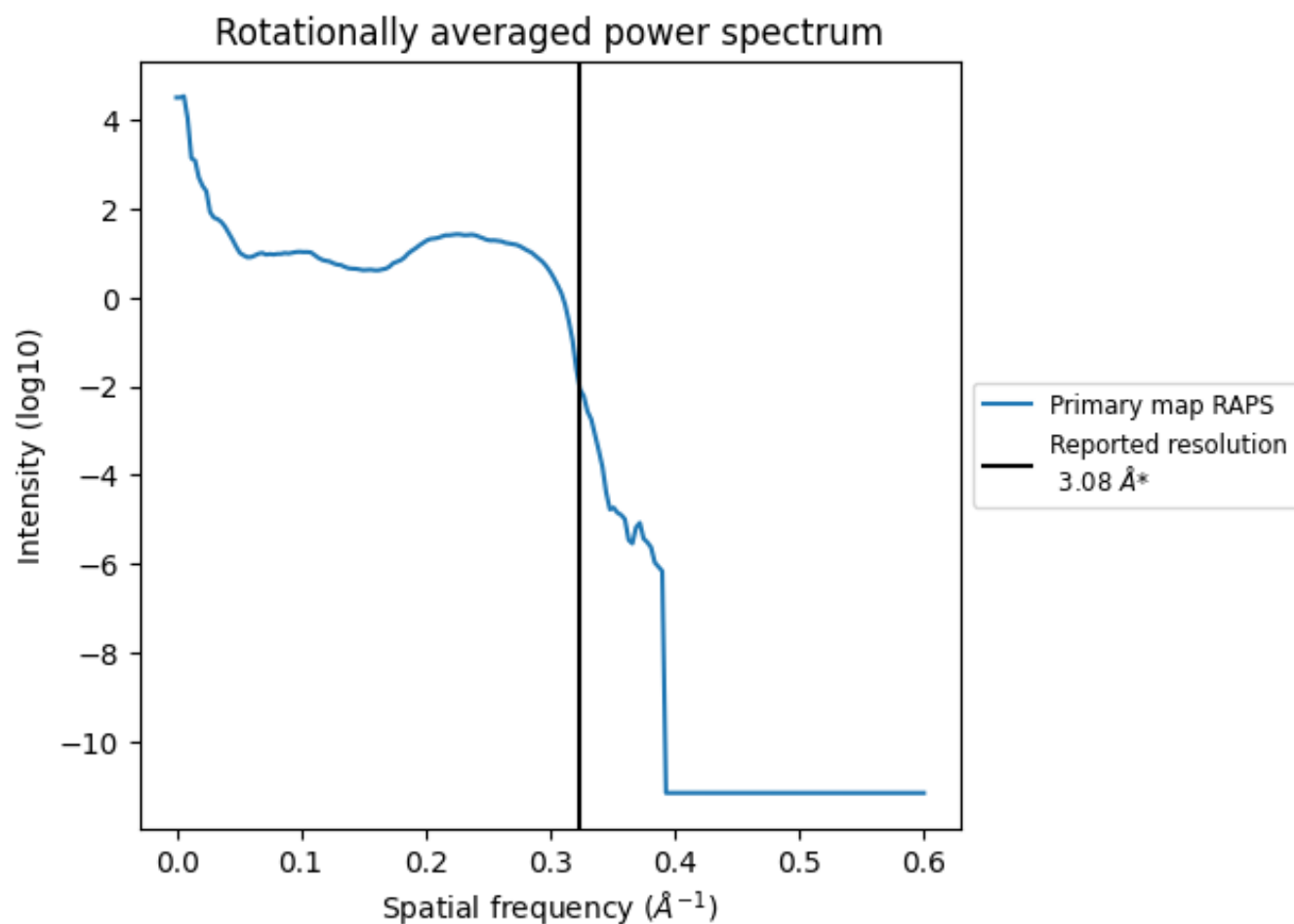
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 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 ⓘ

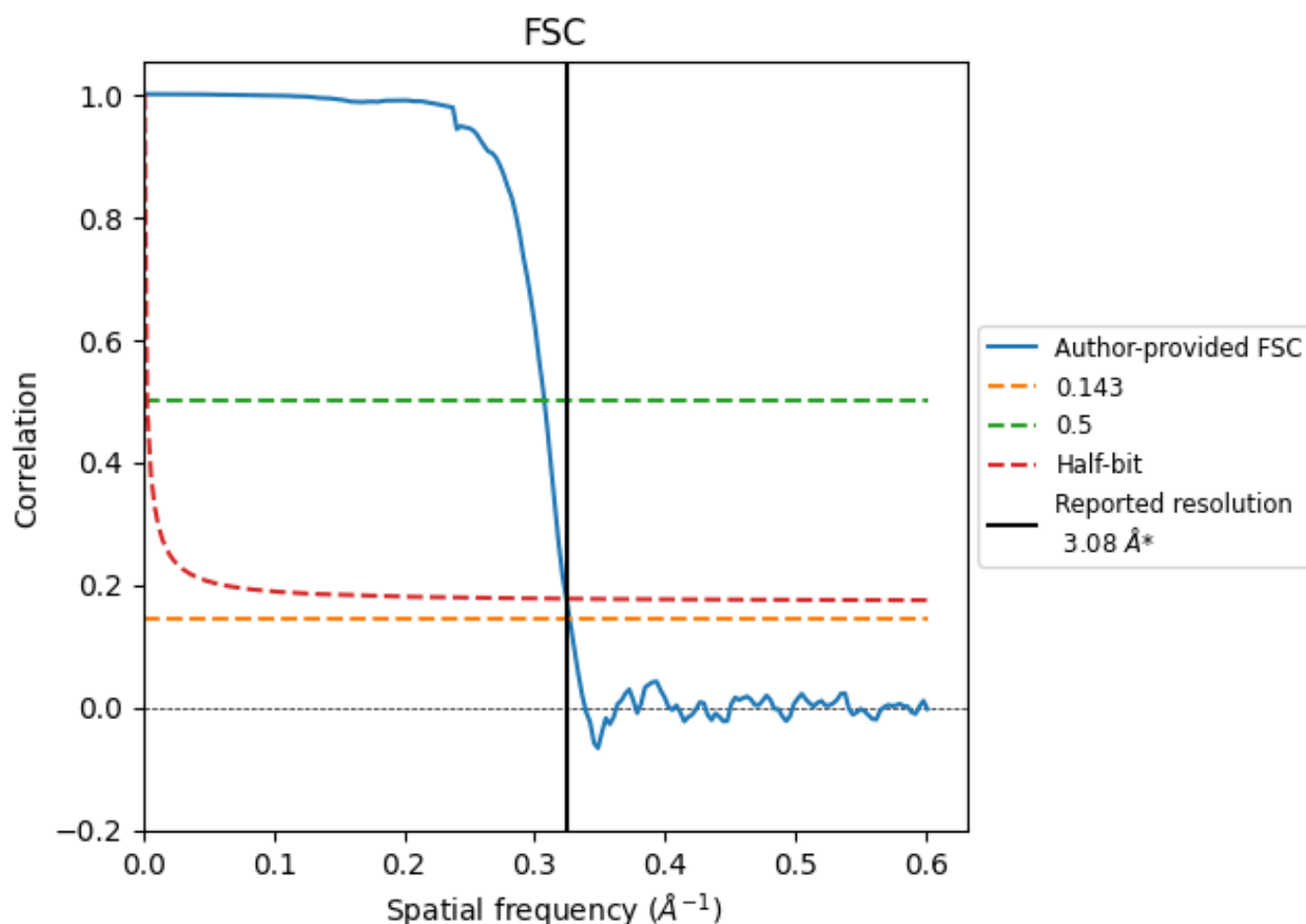


*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

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 0.325 Å⁻¹

8.2 Resolution estimates [i](#)

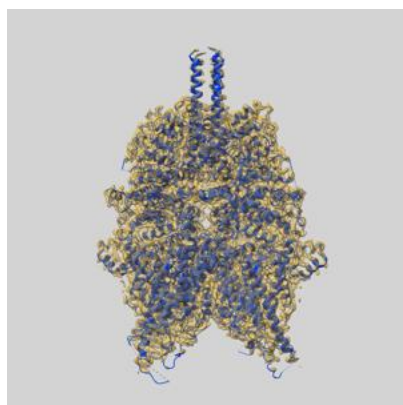
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.06	3.25	3.08
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

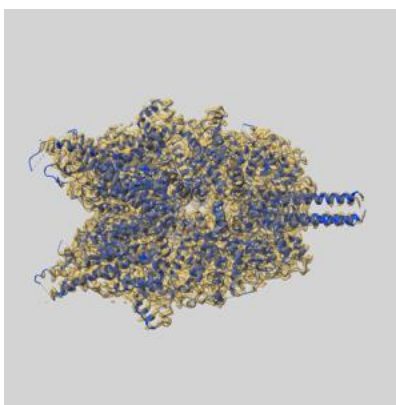
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20954 and PDB model 6UZA. Per-residue inclusion information can be found in section [3](#) on page [7](#).

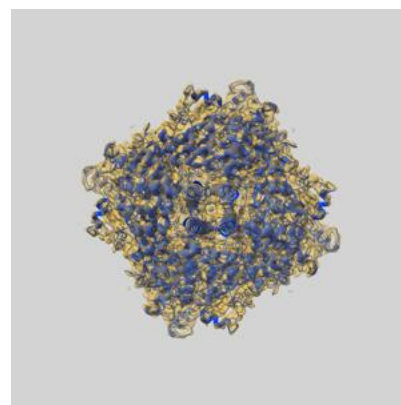
9.1 Map-model overlay [i](#)



X



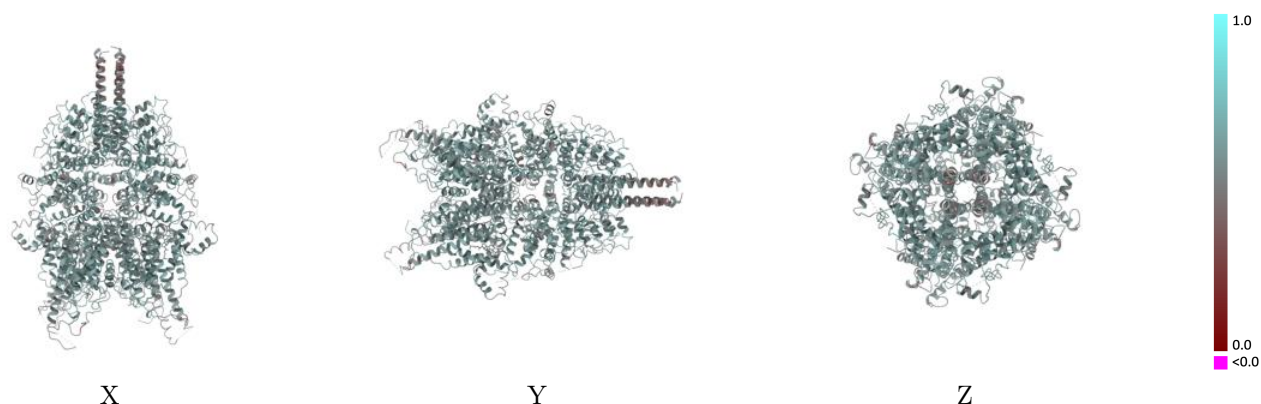
Y



Z

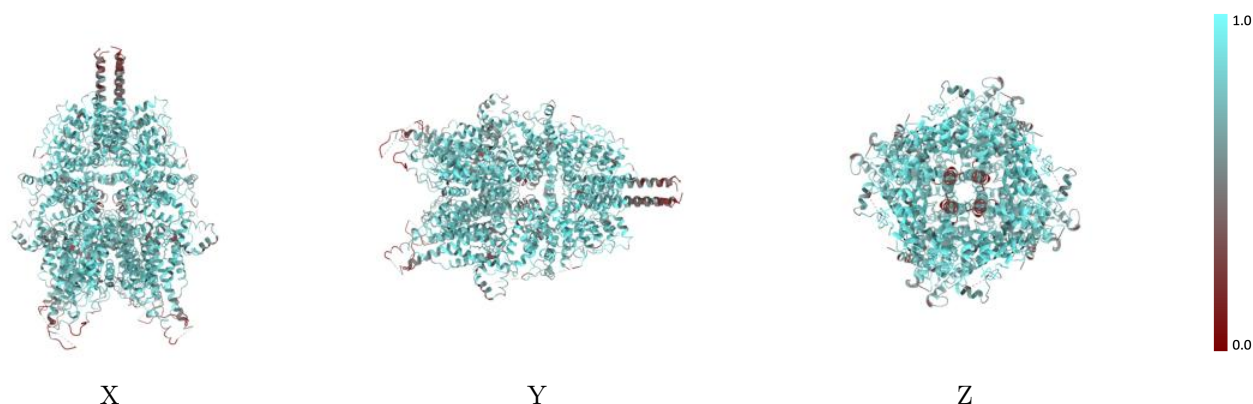
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



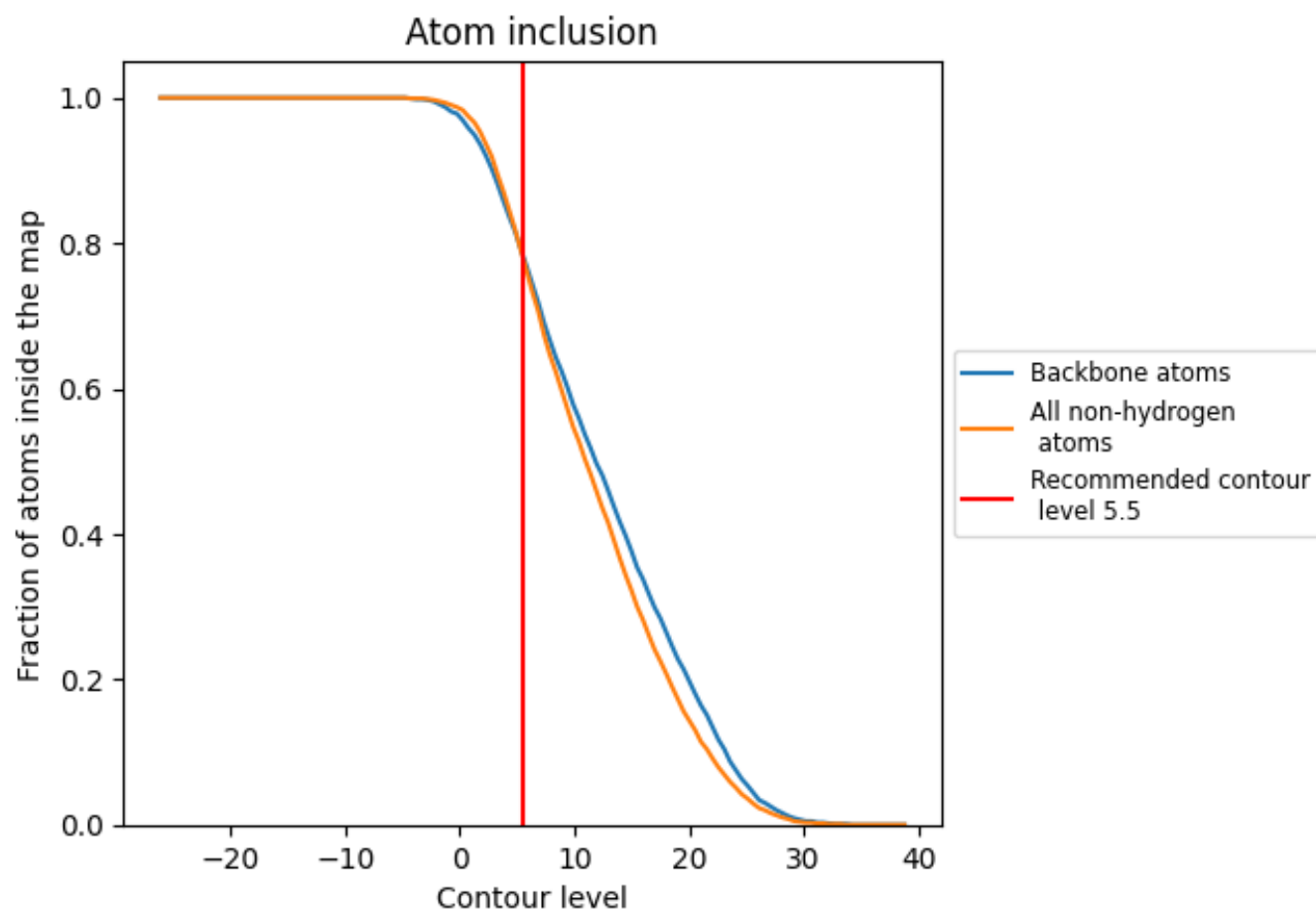
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7800	0.5680
A	0.7790	0.5680
B	0.7800	0.5680
C	0.7800	0.5690
D	0.7810	0.5680

