



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 06:28 PM EST

PDB ID : 6UZ8
EMDB ID : EMD-20953
Title : Cryo-EM structure of human TRPC6 in complex with agonist AM-0883
Authors : Bai, Y.; Yu, X.; Huang, X.; Chen, H.
Deposited on : 2019-11-14
Resolution : 2.84 Å (reported)

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

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

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

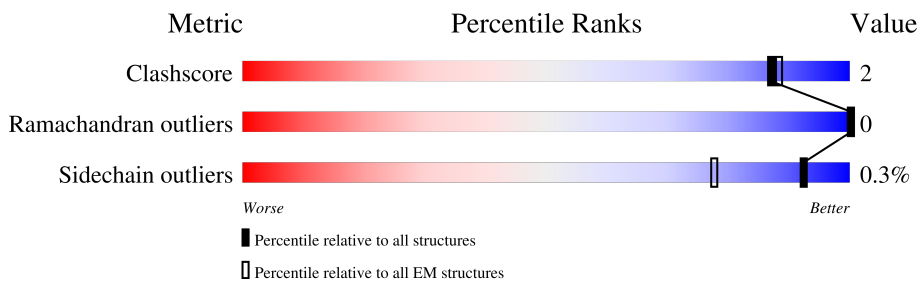
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	
1	B	847	
1	C	847	
1	D	847	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23320 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.

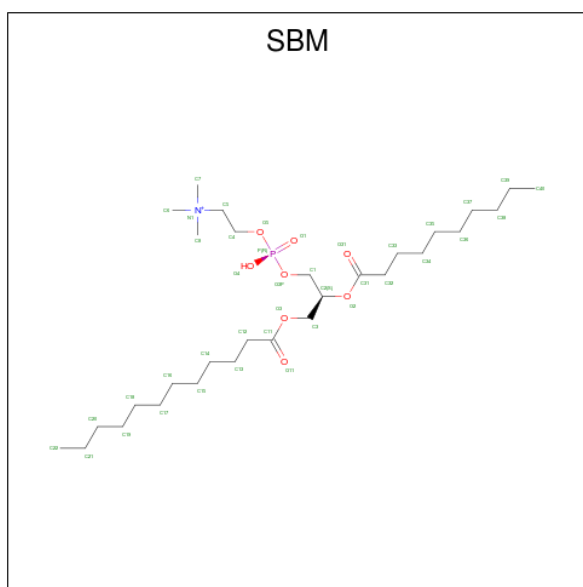
- Molecule 1 is a protein called Short transient receptor potential channel 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	734	5693	3707	954	997	35	1	0
1	D	734	5693	3707	954	997	35	1	0
1	B	734	5693	3707	954	997	35	1	0
1	C	734	5693	3707	954	997	35	1	0

There are 8 discrepancies between the modelled and reference sequences:

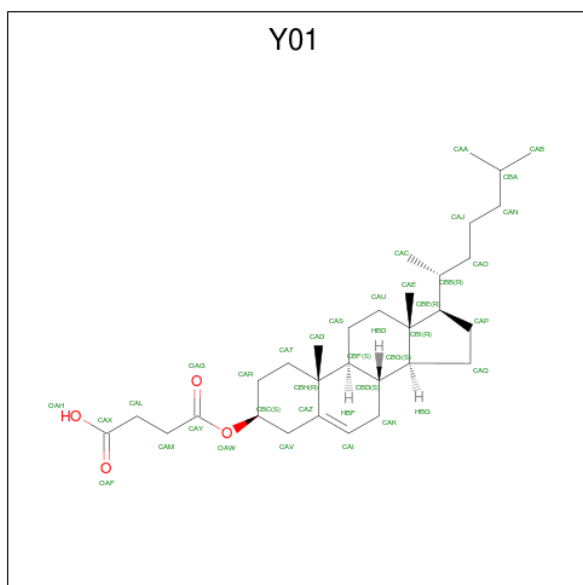
Chain	Residue	Modelled	Actual	Comment	Reference
A	867	THR	VAL	conflict	UNP Q9Y210
A	868	THR	LEU	conflict	UNP Q9Y210
D	867	THR	VAL	conflict	UNP Q9Y210
D	868	THR	LEU	conflict	UNP Q9Y210
B	867	THR	VAL	conflict	UNP Q9Y210
B	868	THR	LEU	conflict	UNP Q9Y210
C	867	THR	VAL	conflict	UNP Q9Y210
C	868	THR	LEU	conflict	UNP Q9Y210

- Molecule 2 is 2-[[[(2 {S})-2-decanoyloxy-3-dodecanoyloxy-propoxy]-oxidanyl-phosphoryl]oxy ethyl-trimethyl-azanium (three-letter code: SBM) (formula: C₃₀H₆₁NO₈P).



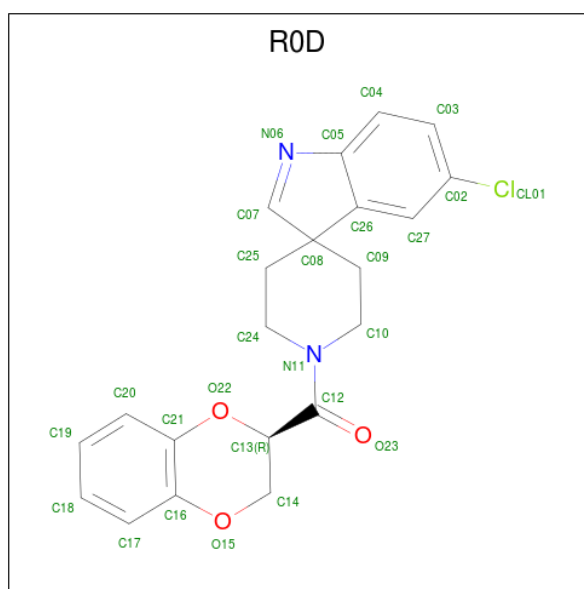
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		
2	A	1	Total	40	30	1	8	1	0
2	D	1	Total	40	30	1	8	1	0
2	B	1	Total	40	30	1	8	1	0
2	C	1	Total	40	30	1	8	1	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			70	62	8	
3	A	1	Total	C	O	0
			70	62	8	
3	D	1	Total	C	O	0
			70	62	8	
3	D	1	Total	C	O	0
			70	62	8	
3	B	1	Total	C	O	0
			70	62	8	
3	B	1	Total	C	O	0
			70	62	8	
3	C	1	Total	C	O	0
			70	62	8	
3	C	1	Total	C	O	0
			70	62	8	

- Molecule 4 is (5-chloro-1'-H-spiro[indole-3,4'-piperidin]-1'-yl)[(2R)-2,3-dihydro-1,4-benzodioxin-2-yl]methanone (three-letter code: R0D) (formula: C₂₁H₁₉ClN₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	Cl	N	O	0
			27	21	1	2	3	
4	D	1	Total	C	Cl	N	O	0
			27	21	1	2	3	
4	B	1	Total	C	Cl	N	O	0
			27	21	1	2	3	

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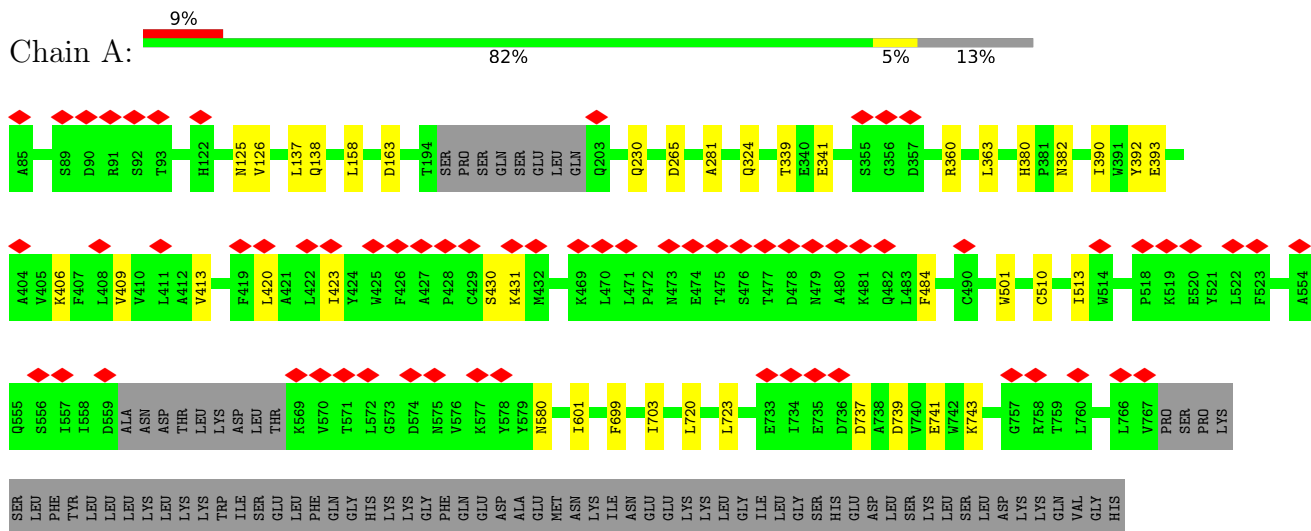
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
4	C	1	27	21	1	2	3	0

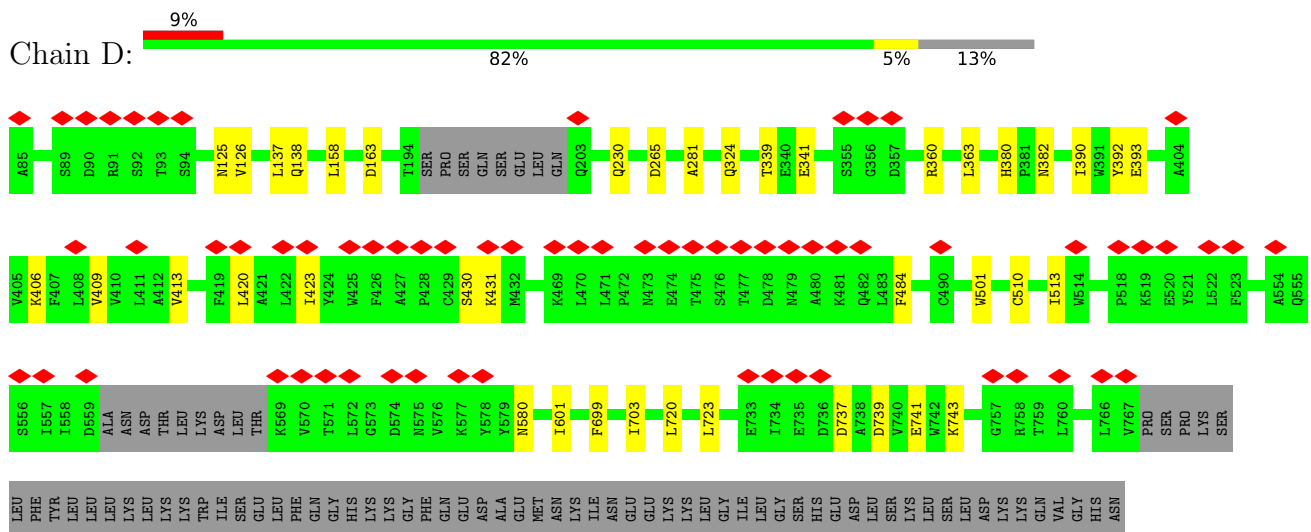
3 Residue-property plots

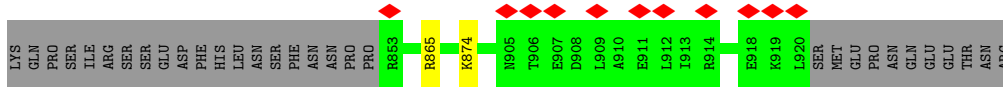
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Short transient receptor potential channel 6

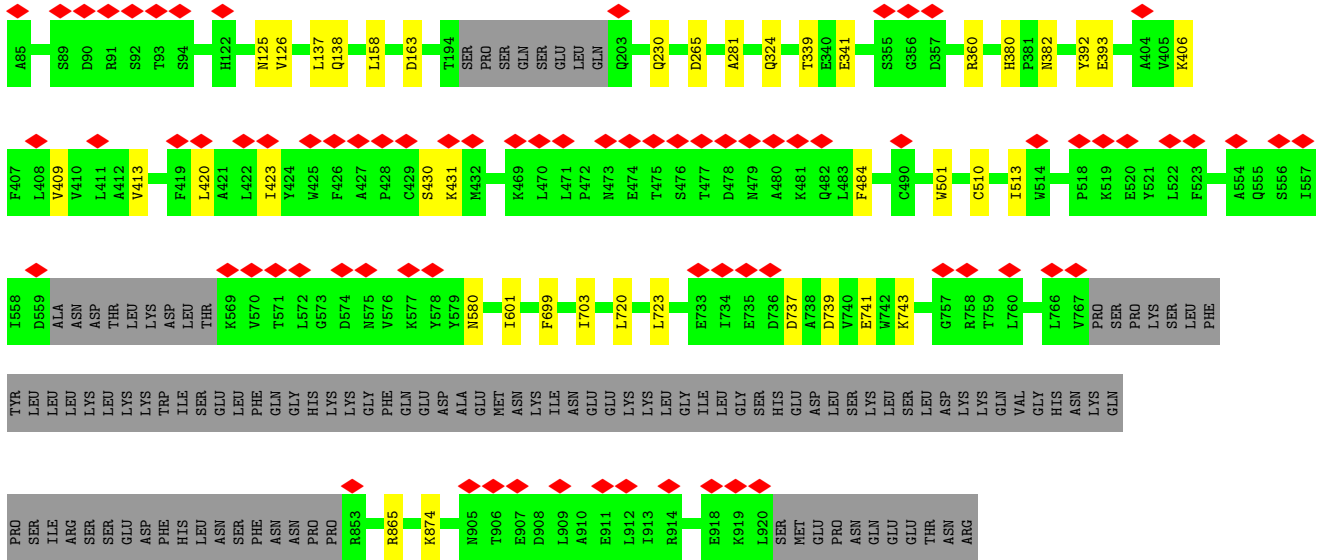
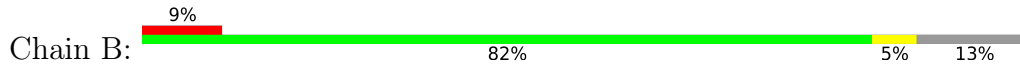


- Molecule 1: Short transient receptor potential channel 6

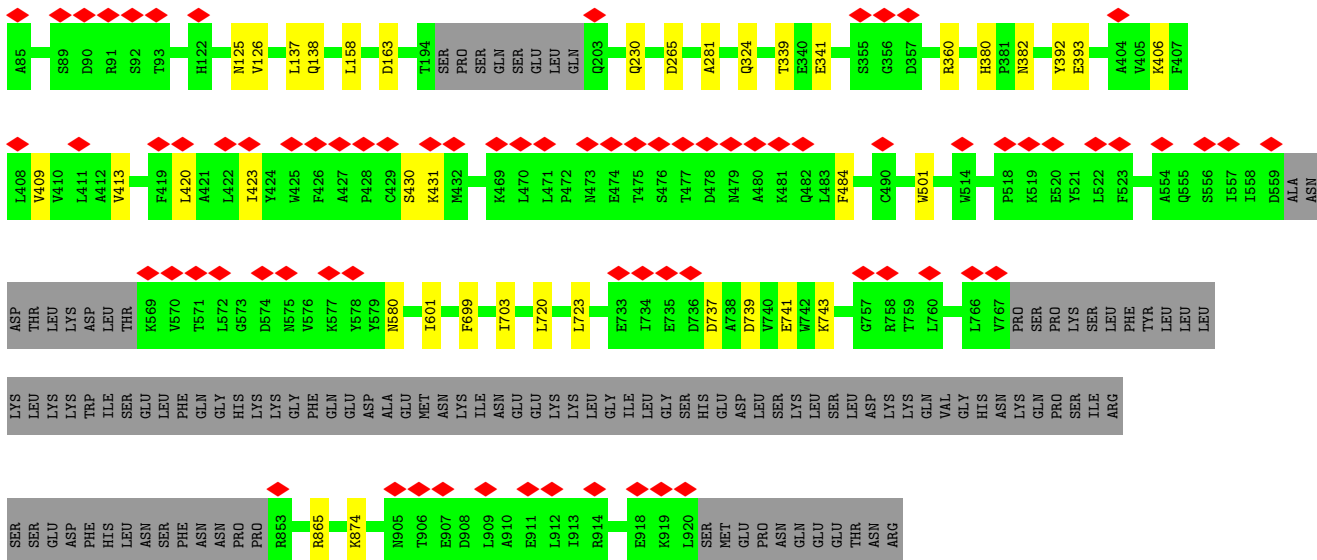
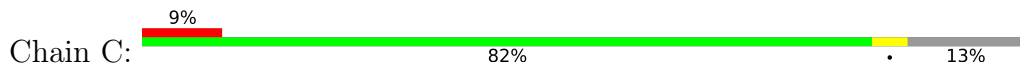




- Molecule 1: Short transient receptor potential channel 6



- 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	68553	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	37.391	Depositor
Minimum map value	-18.938	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.3	Depositor
Map size (Å)	329.47202, 329.47202, 329.47202	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.248, 1.248, 1.248	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: Y01, R0D, SBM

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	0.31	0/5821	0.52	1/7889 (0.0%)
1	B	0.31	0/5821	0.52	1/7889 (0.0%)
1	C	0.31	0/5821	0.52	1/7889 (0.0%)
1	D	0.31	0/5821	0.52	1/7889 (0.0%)
All	All	0.31	0/23284	0.52	4/31556 (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	C	125	ASN	N-CA-CB	-5.26	101.14	110.60
1	D	125	ASN	N-CA-CB	-5.25	101.15	110.60
1	A	125	ASN	N-CA-CB	-5.25	101.16	110.60
1	B	125	ASN	N-CA-CB	-5.25	101.16	110.60

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	5693	0	5570	24	0
1	B	5693	0	5570	23	0
1	C	5693	0	5570	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5693	0	5570	24	0
2	A	40	0	0	0	0
2	B	40	0	0	0	0
2	C	40	0	0	0	0
2	D	40	0	0	0	0
3	A	70	0	98	3	0
3	B	70	0	98	6	0
3	C	70	0	98	4	0
3	D	70	0	98	5	0
4	A	27	0	0	0	0
4	B	27	0	0	0	0
4	C	27	0	0	0	0
4	D	27	0	0	0	0
All	All	23320	0	22672	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (91) 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:601:ILE:HD11	1:C:703:ILE:HD12	1.79	0.65
1:A:601:ILE:HD11	1:B:703:ILE:HD12	1.79	0.64
1:A:703:ILE:HD12	1:D:601:ILE:HD11	1.79	0.63
1:D:703:ILE:HD12	1:C:601:ILE:HD11	1.79	0.63
1:B:138:GLN:NE2	1:B:163:ASP:OD2	2.37	0.54
1:C:138:GLN:NE2	1:C:163:ASP:OD2	2.37	0.53
1:D:138:GLN:NE2	1:D:163:ASP:OD2	2.37	0.53
1:C:699:PHE:HA	3:C:1002:Y01:HAR1	1.91	0.52
1:D:699:PHE:HA	3:D:1004:Y01:HAR1	1.92	0.52
1:B:739:ASP:OD1	1:B:743:LYS:NZ	2.43	0.52
1:D:739:ASP:OD1	1:D:743:LYS:NZ	2.43	0.52
1:C:739:ASP:OD1	1:C:743:LYS:NZ	2.43	0.51
1:B:430:SER:OG	1:B:431:LYS:N	2.44	0.51
1:A:138:GLN:NE2	1:A:163:ASP:OD2	2.37	0.51
1:A:699:PHE:HA	3:A:1004:Y01:HAR1	1.91	0.51
1:A:430:SER:OG	1:A:431:LYS:N	2.44	0.51
1:A:739:ASP:OD1	1:A:743:LYS:NZ	2.43	0.50
1:B:699:PHE:HA	3:B:1002:Y01:HAR1	1.92	0.50
1:C:430:SER:OG	1:C:431:LYS:N	2.44	0.50
1:D:430:SER:OG	1:D:431:LYS:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:LEU:HD22	1:D:158:LEU:HD13	1.94	0.49
1:B:230:GLN:O	1:B:874:LYS:NZ	2.46	0.49
1:C:230:GLN:O	1:C:874:LYS:NZ	2.46	0.49
1:A:137:LEU:HD22	1:A:158:LEU:HD13	1.94	0.49
3:B:1004:Y01:HAP1	3:B:1004:Y01:HAO2	1.67	0.48
1:B:281:ALA:O	1:B:324:GLN:NE2	2.47	0.48
1:A:281:ALA:O	1:A:324:GLN:NE2	2.47	0.48
1:B:137:LEU:HD22	1:B:158:LEU:HD13	1.94	0.48
3:A:1004:Y01:HAO2	3:A:1004:Y01:HAP1	1.56	0.48
1:C:137:LEU:HD22	1:C:158:LEU:HD13	1.94	0.48
1:A:230:GLN:O	1:A:874:LYS:NZ	2.46	0.48
1:A:420:LEU:HA	1:A:423:ILE:HG12	1.96	0.48
1:C:281:ALA:O	1:C:324:GLN:NE2	2.47	0.47
1:B:420:LEU:HA	1:B:423:ILE:HG12	1.96	0.47
3:B:1002:Y01:HAE2	3:B:1002:Y01:HBB	1.76	0.47
1:B:339:THR:OG1	1:C:265:ASP:OD1	2.30	0.47
1:D:230:GLN:O	1:D:874:LYS:NZ	2.46	0.47
1:D:281:ALA:O	1:D:324:GLN:NE2	2.47	0.47
1:D:420:LEU:HA	1:D:423:ILE:HG12	1.96	0.47
1:B:413:VAL:HG13	1:B:420:LEU:HD21	1.96	0.47
1:D:413:VAL:HG13	1:D:420:LEU:HD21	1.96	0.46
1:A:413:VAL:HG13	1:A:420:LEU:HD21	1.96	0.46
1:C:413:VAL:HG13	1:C:420:LEU:HD21	1.96	0.46
1:C:420:LEU:HA	1:C:423:ILE:HG12	1.96	0.46
1:A:484:PHE:HB3	1:A:580:ASN:HA	1.98	0.46
1:C:484:PHE:HB3	1:C:580:ASN:HA	1.98	0.45
1:D:265:ASP:OD1	1:C:339:THR:OG1	2.30	0.45
1:A:341:GLU:OE1	1:A:865:ARG:NH1	2.49	0.45
3:D:1004:Y01:HAO2	3:D:1004:Y01:HAP1	1.56	0.45
1:A:339:THR:OG1	1:B:265:ASP:OD1	2.30	0.45
1:B:341:GLU:OE1	1:B:865:ARG:NH1	2.49	0.45
1:D:341:GLU:OE1	1:D:865:ARG:NH1	2.49	0.44
1:B:484:PHE:HB3	1:B:580:ASN:HA	1.98	0.44
1:A:406:LYS:HA	1:A:409:VAL:HG12	2.00	0.44
3:B:1004:Y01:HAE2	3:B:1004:Y01:HBB	1.87	0.44
1:B:406:LYS:HA	1:B:409:VAL:HG12	2.00	0.44
1:D:484:PHE:HB3	1:D:580:ASN:HA	1.98	0.43
3:C:1004:Y01:HAP1	3:C:1004:Y01:HAO2	1.67	0.43
1:A:392:TYR:OH	3:A:1002:Y01:OAF	2.36	0.43
1:D:406:LYS:HA	1:D:409:VAL:HG12	2.00	0.43
3:D:1002:Y01:HAP1	3:D:1002:Y01:HAO2	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:LYS:HA	1:C:409:VAL:HG12	2.00	0.42
1:A:720:LEU:HD22	1:D:723:LEU:HD13	2.02	0.42
1:C:360:ARG:NH1	1:C:393:GLU:OE1	2.51	0.42
1:D:720:LEU:HD22	1:C:723:LEU:HD13	2.02	0.42
3:B:1002:Y01:HAP1	3:B:1002:Y01:HAO2	1.56	0.42
3:C:1004:Y01:HAE2	3:C:1004:Y01:HBB	1.87	0.42
1:A:265:ASP:OD1	1:D:339:THR:OG1	2.30	0.42
1:B:392:TYR:OH	3:B:1004:Y01:OAF	2.36	0.42
1:D:380:HIS:HD2	1:D:382:ASN:H	1.68	0.42
1:C:392:TYR:OH	3:C:1004:Y01:OAF	2.36	0.42
1:A:380:HIS:HD2	1:A:382:ASN:H	1.68	0.42
1:A:360:ARG:NH1	1:A:393:GLU:OE1	2.51	0.41
1:B:723:LEU:HD13	1:C:720:LEU:HD22	2.02	0.41
1:B:380:HIS:HD2	1:B:382:ASN:H	1.68	0.41
1:A:723:LEU:HD13	1:B:720:LEU:HD22	2.02	0.41
1:A:510:CYS:HA	1:A:513:ILE:HG22	2.03	0.41
1:D:510:CYS:HA	1:D:513:ILE:HG22	2.03	0.41
3:D:1004:Y01:HAE2	3:D:1004:Y01:HBB	1.76	0.41
1:B:737:ASP:O	1:B:741:GLU:HG2	2.21	0.41
1:A:737:ASP:O	1:A:741:GLU:HG2	2.21	0.41
1:C:380:HIS:HD2	1:C:382:ASN:H	1.68	0.41
1:D:392:TYR:OH	3:D:1002:Y01:OAF	2.36	0.41
1:D:737:ASP:O	1:D:741:GLU:HG2	2.21	0.41
1:C:341:GLU:OE1	1:C:865:ARG:NH1	2.49	0.41
1:C:737:ASP:O	1:C:741:GLU:HG2	2.21	0.41
1:B:360:ARG:NH1	1:B:393:GLU:OE1	2.51	0.40
1:A:363:LEU:HD21	1:A:390:ILE:HD13	2.04	0.40
1:D:360:ARG:NH1	1:D:393:GLU:OE1	2.51	0.40
1:D:363:LEU:HD21	1:D:390:ILE:HD13	2.04	0.40
1:B:510:CYS:HA	1:B:513:ILE:HG22	2.03	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	727/847 (86%)	696 (96%)	31 (4%)	0	100	100
1	B	727/847 (86%)	696 (96%)	31 (4%)	0	100	100
1	C	727/847 (86%)	696 (96%)	31 (4%)	0	100	100
1	D	727/847 (86%)	696 (96%)	31 (4%)	0	100	100
All	All	2908/3388 (86%)	2784 (96%)	124 (4%)	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	573/748 (77%)	571 (100%)	2 (0%)	92	96
1	B	573/748 (77%)	571 (100%)	2 (0%)	92	96
1	C	573/748 (77%)	571 (100%)	2 (0%)	92	96
1	D	573/748 (77%)	571 (100%)	2 (0%)	92	96
All	All	2292/2992 (77%)	2284 (100%)	8 (0%)	92	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	VAL
1	A	501	TRP
1	D	126	VAL
1	D	501	TRP
1	B	126	VAL
1	B	501	TRP
1	C	126	VAL
1	C	501	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	ASN
1	A	380	HIS
1	A	732	GLN
1	D	259	ASN
1	D	380	HIS
1	D	732	GLN
1	B	259	ASN
1	B	380	HIS
1	B	732	GLN
1	C	380	HIS
1	C	732	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	Y01	D	1002	-	38,38,38	1.80	8 (21%)	57,57,57	2.21	16 (28%)
2	SBM	C	1003	-	39,39,39	1.30	3 (7%)	45,47,47	1.07	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	R0D	C	1001	-	29,31,31	1.28	4 (13%)	36,46,46	1.49	7 (19%)
4	R0D	B	1001	-	29,31,31	1.28	4 (13%)	36,46,46	1.49	7 (19%)
3	Y01	C	1004	-	38,38,38	1.80	8 (21%)	57,57,57	2.21	16 (28%)
3	Y01	A	1002	-	38,38,38	1.80	8 (21%)	57,57,57	2.21	16 (28%)
2	SBM	D	1001	-	39,39,39	1.30	3 (7%)	45,47,47	1.07	3 (6%)
2	SBM	A	1001	-	39,39,39	1.30	3 (7%)	45,47,47	1.07	3 (6%)
3	Y01	C	1002	-	38,38,38	2.10	9 (23%)	57,57,57	2.38	27 (47%)
3	Y01	B	1004	-	38,38,38	1.80	8 (21%)	57,57,57	2.21	17 (29%)
3	Y01	D	1004	-	38,38,38	2.09	9 (23%)	57,57,57	2.39	27 (47%)
2	SBM	B	1003	-	39,39,39	1.30	3 (7%)	45,47,47	1.07	3 (6%)
3	Y01	A	1004	-	38,38,38	2.10	9 (23%)	57,57,57	2.38	27 (47%)
4	R0D	A	1003	-	29,31,31	1.28	4 (13%)	36,46,46	1.49	7 (19%)
3	Y01	B	1002	-	38,38,38	2.10	9 (23%)	57,57,57	2.38	27 (47%)
4	R0D	D	1003	-	29,31,31	1.28	4 (13%)	36,46,46	1.48	7 (19%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Y01	D	1002	-	-	13/19/77/77	0/4/4/4
2	SBM	C	1003	-	-	22/43/43/43	-
4	R0D	C	1001	-	-	1/7/41/41	0/5/5/5
4	R0D	B	1001	-	-	1/7/41/41	0/5/5/5
3	Y01	C	1004	-	-	13/19/77/77	0/4/4/4
3	Y01	A	1002	-	-	13/19/77/77	0/4/4/4
2	SBM	D	1001	-	-	22/43/43/43	-
2	SBM	A	1001	-	-	22/43/43/43	-
3	Y01	C	1002	-	-	11/19/77/77	0/4/4/4
3	Y01	B	1004	-	-	13/19/77/77	0/4/4/4
3	Y01	D	1004	-	-	11/19/77/77	0/4/4/4
2	SBM	B	1003	-	-	22/43/43/43	-
3	Y01	A	1004	-	-	11/19/77/77	0/4/4/4
4	R0D	A	1003	-	-	1/7/41/41	0/5/5/5
3	Y01	B	1002	-	-	11/19/77/77	0/4/4/4
4	R0D	D	1003	-	-	1/7/41/41	0/5/5/5

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1004	Y01	CBH-CBF	6.12	1.66	1.56
3	B	1002	Y01	CBH-CBF	6.12	1.66	1.56
3	C	1002	Y01	CBH-CBF	6.12	1.66	1.56
3	D	1004	Y01	CBH-CBF	6.09	1.66	1.56
2	C	1003	SBM	P-O5	4.65	1.78	1.59
2	A	1001	SBM	P-O5	4.64	1.78	1.59
2	D	1001	SBM	P-O5	4.64	1.78	1.59
2	B	1003	SBM	P-O5	4.64	1.78	1.59
3	A	1002	Y01	CBH-CBF	4.43	1.63	1.56
3	D	1002	Y01	CBH-CBF	4.43	1.63	1.56
3	B	1004	Y01	CBH-CBF	4.43	1.63	1.56
3	C	1004	Y01	CBH-CBF	4.43	1.63	1.56
4	D	1003	R0D	C12-N11	4.33	1.41	1.34
4	A	1003	R0D	C12-N11	4.32	1.41	1.34
4	B	1001	R0D	C12-N11	4.32	1.41	1.34
4	C	1001	R0D	C12-N11	4.32	1.41	1.34
3	A	1004	Y01	CAL-CAX	4.24	1.60	1.50
3	D	1004	Y01	CAL-CAX	4.20	1.60	1.50
3	B	1002	Y01	CAL-CAX	4.20	1.60	1.50
3	C	1002	Y01	CAL-CAX	4.20	1.60	1.50
3	D	1004	Y01	CBI-CBE	4.19	1.63	1.55
3	B	1002	Y01	CBI-CBE	4.19	1.63	1.55
3	C	1002	Y01	CBI-CBE	4.19	1.63	1.55
3	A	1004	Y01	CBI-CBE	4.16	1.62	1.55
3	A	1002	Y01	CAL-CAX	3.79	1.59	1.50
3	D	1002	Y01	CAL-CAX	3.79	1.59	1.50
3	B	1004	Y01	CAL-CAX	3.79	1.59	1.50
3	C	1004	Y01	CAL-CAX	3.78	1.59	1.50
3	A	1004	Y01	CAV-CBC	3.45	1.60	1.52
3	D	1004	Y01	CAV-CBC	3.45	1.60	1.52
3	B	1002	Y01	CAV-CBC	3.45	1.60	1.52
3	C	1002	Y01	CAV-CBC	3.45	1.60	1.52
3	D	1004	Y01	CBD-CBG	3.40	1.60	1.53
3	D	1002	Y01	CBI-CBE	3.39	1.61	1.55
3	A	1004	Y01	CBD-CBG	3.38	1.60	1.53
3	B	1002	Y01	CBD-CBG	3.38	1.60	1.53
3	C	1002	Y01	CBD-CBG	3.38	1.60	1.53
3	A	1004	Y01	CBB-CBE	3.37	1.60	1.54
3	D	1004	Y01	CBB-CBE	3.37	1.60	1.54
3	B	1002	Y01	CBB-CBE	3.37	1.60	1.54
3	C	1002	Y01	CBB-CBE	3.37	1.60	1.54
3	B	1002	Y01	CAV-CAZ	3.36	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	Y01	CAV-CAZ	3.36	1.59	1.51
3	A	1002	Y01	CBI-CBE	3.35	1.61	1.55
3	B	1004	Y01	CBI-CBE	3.35	1.61	1.55
3	C	1004	Y01	CBI-CBE	3.35	1.61	1.55
3	A	1004	Y01	CAV-CAZ	3.34	1.58	1.51
3	D	1004	Y01	CAV-CAZ	3.34	1.58	1.51
3	A	1002	Y01	CBD-CBG	3.30	1.59	1.53
3	D	1002	Y01	CBD-CBG	3.30	1.59	1.53
3	C	1004	Y01	CBD-CBG	3.30	1.59	1.53
3	B	1004	Y01	CBD-CBG	3.29	1.59	1.53
3	D	1002	Y01	CBB-CBE	3.05	1.59	1.54
3	C	1004	Y01	CBB-CBE	3.05	1.59	1.54
3	A	1002	Y01	CAV-CAZ	3.04	1.58	1.51
3	B	1004	Y01	CAV-CAZ	3.04	1.58	1.51
3	C	1004	Y01	CAV-CAZ	3.04	1.58	1.51
3	A	1002	Y01	CBB-CBE	3.03	1.59	1.54
3	B	1004	Y01	CBB-CBE	3.03	1.59	1.54
3	D	1002	Y01	CAV-CAZ	3.03	1.58	1.51
3	A	1002	Y01	CAV-CBC	3.01	1.59	1.52
3	D	1002	Y01	CAV-CBC	3.01	1.59	1.52
3	B	1004	Y01	CAV-CBC	3.01	1.59	1.52
3	C	1004	Y01	CAV-CBC	3.01	1.59	1.52
2	D	1001	SBM	C3-C2	2.64	1.58	1.50
2	A	1001	SBM	C3-C2	2.63	1.58	1.50
2	B	1003	SBM	C3-C2	2.63	1.58	1.50
2	C	1003	SBM	C3-C2	2.63	1.58	1.50
3	A	1004	Y01	CBD-CBF	2.56	1.58	1.53
3	D	1004	Y01	CBD-CBF	2.56	1.58	1.53
3	B	1002	Y01	CBD-CBF	2.56	1.58	1.53
3	C	1002	Y01	CBD-CBF	2.56	1.58	1.53
3	D	1002	Y01	CBD-CBF	2.53	1.58	1.53
3	A	1002	Y01	CBD-CBF	2.51	1.58	1.53
3	B	1004	Y01	CBD-CBF	2.51	1.58	1.53
3	C	1004	Y01	CBD-CBF	2.51	1.58	1.53
4	A	1003	R0D	C14-C13	2.49	1.54	1.51
4	D	1003	R0D	C14-C13	2.49	1.54	1.51
4	B	1001	R0D	C14-C13	2.49	1.54	1.51
4	C	1001	R0D	C14-C13	2.49	1.54	1.51
3	D	1004	Y01	CAU-CAS	2.23	1.58	1.53
3	A	1004	Y01	CAU-CAS	2.21	1.58	1.53
3	B	1002	Y01	CAU-CAS	2.21	1.58	1.53
3	C	1002	Y01	CAU-CAS	2.21	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	SBM	O5-C4	-2.12	1.36	1.44
2	D	1001	SBM	O5-C4	-2.12	1.36	1.44
2	B	1003	SBM	O5-C4	-2.12	1.36	1.44
2	C	1003	SBM	O5-C4	-2.12	1.36	1.44
4	A	1003	R0D	C05-C26	2.12	1.42	1.39
4	D	1003	R0D	C05-C26	2.12	1.42	1.39
4	B	1001	R0D	C05-C26	2.12	1.42	1.39
4	C	1001	R0D	C05-C26	2.12	1.42	1.39
4	A	1003	R0D	C08-C07	2.05	1.56	1.48
4	D	1003	R0D	C08-C07	2.05	1.56	1.48
4	B	1001	R0D	C08-C07	2.05	1.56	1.48
4	C	1001	R0D	C08-C07	2.05	1.56	1.48

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1004	Y01	OAW-CAY-CAM	7.02	126.63	111.50
3	B	1002	Y01	OAW-CAY-CAM	7.02	126.63	111.50
3	C	1002	Y01	OAW-CAY-CAM	7.02	126.63	111.50
3	D	1004	Y01	OAW-CAY-CAM	7.02	126.62	111.50
3	A	1002	Y01	OAW-CAY-CAM	6.84	126.25	111.50
3	D	1002	Y01	OAW-CAY-CAM	6.84	126.25	111.50
3	B	1004	Y01	OAW-CAY-CAM	6.84	126.25	111.50
3	C	1004	Y01	OAW-CAY-CAM	6.84	126.25	111.50
3	A	1004	Y01	CBC-CAV-CAZ	5.91	120.70	111.52
3	D	1004	Y01	CBC-CAV-CAZ	5.91	120.70	111.52
3	B	1002	Y01	CBC-CAV-CAZ	5.90	120.68	111.52
3	C	1002	Y01	CBC-CAV-CAZ	5.90	120.68	111.52
3	A	1002	Y01	CBC-CAV-CAZ	5.44	119.97	111.52
3	B	1004	Y01	CBC-CAV-CAZ	5.44	119.97	111.52
3	C	1004	Y01	CBC-CAV-CAZ	5.44	119.97	111.52
3	D	1002	Y01	CBC-CAV-CAZ	5.42	119.95	111.52
3	A	1004	Y01	CAE-CBI-CAU	-4.77	103.05	110.59
3	D	1004	Y01	CAE-CBI-CAU	-4.77	103.05	110.59
3	B	1002	Y01	CAE-CBI-CAU	-4.77	103.05	110.59
3	C	1002	Y01	CAE-CBI-CAU	-4.75	103.09	110.59
3	A	1002	Y01	CAE-CBI-CAU	-4.71	103.15	110.59
3	D	1002	Y01	CAE-CBI-CAU	-4.71	103.15	110.59
3	B	1004	Y01	CAE-CBI-CAU	-4.69	103.18	110.59
3	C	1004	Y01	CAE-CBI-CAU	-4.69	103.19	110.59
3	D	1004	Y01	CAK-CBD-CBG	4.42	117.31	110.91
3	A	1004	Y01	CAK-CBD-CBG	4.40	117.29	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	Y01	CAK-CBD-CBG	4.40	117.29	110.91
3	C	1002	Y01	CAK-CBD-CBG	4.40	117.29	110.91
4	A	1003	R0D	C08-C26-C05	4.35	110.72	107.19
4	D	1003	R0D	C08-C26-C05	4.35	110.72	107.19
4	B	1001	R0D	C08-C26-C05	4.35	110.72	107.19
4	C	1001	R0D	C08-C26-C05	4.35	110.72	107.19
3	A	1004	Y01	OAW-CAY-OAG	-4.16	113.64	123.70
3	B	1002	Y01	OAW-CAY-OAG	-4.16	113.64	123.70
3	C	1002	Y01	OAW-CAY-OAG	-4.16	113.64	123.70
3	D	1004	Y01	OAW-CAY-OAG	-4.16	113.65	123.70
3	A	1002	Y01	OAW-CAY-OAG	-4.07	113.87	123.70
3	D	1002	Y01	OAW-CAY-OAG	-4.07	113.87	123.70
3	B	1004	Y01	OAW-CAY-OAG	-4.07	113.87	123.70
3	C	1004	Y01	OAW-CAY-OAG	-4.07	113.87	123.70
3	D	1004	Y01	CBF-CBH-CAZ	3.79	115.60	109.65
3	A	1004	Y01	CBF-CBH-CAZ	3.77	115.57	109.65
3	B	1002	Y01	CBF-CBH-CAZ	3.77	115.57	109.65
3	C	1002	Y01	CBF-CBH-CAZ	3.77	115.57	109.65
3	D	1002	Y01	CAV-CAZ-CAI	3.69	125.93	120.61
3	A	1002	Y01	CAV-CAZ-CAI	3.69	125.92	120.61
3	B	1004	Y01	CAV-CAZ-CAI	3.69	125.92	120.61
3	C	1004	Y01	CAV-CAZ-CAI	3.69	125.92	120.61
3	A	1002	Y01	CAQ-CBG-CBI	-3.66	99.44	103.84
3	B	1004	Y01	CAQ-CBG-CBI	-3.66	99.44	103.84
2	D	1001	SBM	O2-C31-C32	3.64	119.35	111.50
3	D	1002	Y01	CAQ-CBG-CBI	-3.64	99.46	103.84
3	C	1004	Y01	CAQ-CBG-CBI	-3.64	99.46	103.84
2	A	1001	SBM	O2-C31-C32	3.62	119.31	111.50
2	B	1003	SBM	O2-C31-C32	3.62	119.31	111.50
2	C	1003	SBM	O2-C31-C32	3.62	119.31	111.50
4	A	1003	R0D	C24-C25-C08	3.42	116.90	112.47
4	D	1003	R0D	C24-C25-C08	3.42	116.90	112.47
4	B	1001	R0D	C24-C25-C08	3.42	116.90	112.47
4	C	1001	R0D	C24-C25-C08	3.42	116.90	112.47
3	A	1004	Y01	CAQ-CBG-CBI	-3.39	99.76	103.84
3	D	1004	Y01	CAQ-CBG-CBI	-3.39	99.76	103.84
3	B	1002	Y01	CAQ-CBG-CBI	-3.39	99.76	103.84
3	C	1002	Y01	CAQ-CBG-CBI	-3.38	99.76	103.84
3	B	1004	Y01	CAD-CBH-CAZ	-3.38	102.87	108.34
3	A	1002	Y01	CAD-CBH-CAZ	-3.37	102.88	108.34
3	D	1002	Y01	CAD-CBH-CAZ	-3.37	102.88	108.34
3	C	1004	Y01	CAD-CBH-CAZ	-3.35	102.92	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1004	Y01	CAK-CBD-CBG	3.30	115.68	110.91
3	A	1002	Y01	CAK-CBD-CBG	3.29	115.68	110.91
3	D	1002	Y01	CAK-CBD-CBG	3.29	115.68	110.91
3	C	1004	Y01	CAK-CBD-CBG	3.29	115.68	110.91
3	B	1002	Y01	CAV-CAZ-CBH	-3.18	112.19	116.42
3	C	1002	Y01	CAV-CAZ-CBH	-3.18	112.19	116.42
3	A	1004	Y01	CAV-CAZ-CBH	-3.18	112.20	116.42
3	D	1004	Y01	CAV-CAZ-CBH	-3.16	112.22	116.42
2	C	1003	SBM	O4-P-O1	3.10	127.58	112.24
2	A	1001	SBM	O4-P-O1	3.10	127.55	112.24
2	D	1001	SBM	O4-P-O1	3.10	127.55	112.24
2	B	1003	SBM	O4-P-O1	3.09	127.53	112.24
3	A	1004	Y01	CBG-CBI-CBE	3.08	103.72	100.07
3	D	1004	Y01	CBG-CBI-CBE	3.06	103.70	100.07
3	B	1002	Y01	CBG-CBI-CBE	3.06	103.70	100.07
3	C	1002	Y01	CBG-CBI-CBE	3.04	103.68	100.07
3	A	1002	Y01	CAU-CBI-CBE	3.03	121.11	116.57
3	C	1004	Y01	CAU-CBI-CBE	3.03	121.11	116.57
3	D	1002	Y01	CAU-CBI-CBE	3.03	121.10	116.57
3	B	1004	Y01	CAU-CBI-CBE	3.02	121.09	116.57
3	A	1004	Y01	CAU-CBI-CBE	2.88	120.89	116.57
3	D	1004	Y01	CAU-CBI-CBE	2.88	120.88	116.57
3	B	1002	Y01	CAU-CBI-CBE	2.88	120.88	116.57
3	A	1002	Y01	CBF-CBH-CAZ	2.87	114.16	109.65
3	D	1002	Y01	CBF-CBH-CAZ	2.87	114.16	109.65
3	C	1004	Y01	CBF-CBH-CAZ	2.87	114.15	109.65
3	C	1002	Y01	CAU-CBI-CBE	2.87	120.86	116.57
3	B	1004	Y01	CBF-CBH-CAZ	2.86	114.13	109.65
3	C	1002	Y01	OAW-CBC-CAV	2.85	113.96	108.12
3	D	1004	Y01	CAD-CBH-CAZ	-2.85	103.73	108.34
3	A	1004	Y01	OAW-CBC-CAV	2.84	113.94	108.12
3	D	1004	Y01	OAW-CBC-CAV	2.84	113.94	108.12
3	B	1002	Y01	OAW-CBC-CAV	2.84	113.94	108.12
3	D	1004	Y01	CAT-CBH-CBF	2.84	112.69	108.73
3	A	1004	Y01	CAT-CBH-CBF	2.83	112.67	108.73
3	B	1002	Y01	CAT-CBH-CBF	2.83	112.67	108.73
3	C	1002	Y01	CAT-CBH-CBF	2.83	112.67	108.73
3	A	1004	Y01	CAD-CBH-CAZ	-2.82	103.77	108.34
3	B	1002	Y01	CAD-CBH-CAZ	-2.82	103.77	108.34
3	C	1002	Y01	CAD-CBH-CAZ	-2.82	103.77	108.34
3	A	1002	Y01	OAW-CBC-CAV	2.79	113.83	108.12
3	D	1002	Y01	OAW-CBC-CAV	2.79	113.83	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1004	Y01	OAW-CBC-CAV	2.79	113.83	108.12
3	C	1004	Y01	OAW-CBC-CAV	2.79	113.83	108.12
3	B	1002	Y01	CAV-CAZ-CAI	2.74	124.55	120.61
3	C	1002	Y01	CAV-CAZ-CAI	2.74	124.55	120.61
3	D	1004	Y01	CAU-CAS-CBF	2.73	117.84	113.11
3	A	1004	Y01	CAV-CAZ-CAI	2.72	124.53	120.61
3	D	1004	Y01	CAV-CAZ-CAI	2.72	124.53	120.61
3	A	1004	Y01	CAR-CAT-CBH	2.72	118.64	112.74
3	A	1004	Y01	CAU-CAS-CBF	2.71	117.82	113.11
3	B	1002	Y01	CAU-CAS-CBF	2.71	117.82	113.11
3	C	1002	Y01	CAU-CAS-CBF	2.71	117.82	113.11
3	D	1004	Y01	CAR-CAT-CBH	2.71	118.61	112.74
3	B	1002	Y01	CAR-CAT-CBH	2.71	118.61	112.74
3	C	1002	Y01	CAR-CAT-CBH	2.71	118.61	112.74
3	D	1004	Y01	CBH-CAZ-CAI	-2.71	118.76	122.90
3	A	1004	Y01	CBH-CAZ-CAI	-2.69	118.79	122.90
3	B	1002	Y01	CBH-CAZ-CAI	-2.69	118.79	122.90
3	C	1002	Y01	CBH-CAZ-CAI	-2.69	118.79	122.90
3	A	1004	Y01	CAT-CAR-CBC	2.68	114.91	110.33
3	D	1004	Y01	CAT-CAR-CBC	2.68	114.90	110.33
3	B	1002	Y01	CAT-CAR-CBC	2.68	114.90	110.33
3	C	1002	Y01	CAT-CAR-CBC	2.68	114.90	110.33
3	D	1004	Y01	CAD-CBH-CBF	-2.61	108.57	111.68
3	A	1004	Y01	CAD-CBH-CBF	-2.58	108.60	111.68
3	B	1002	Y01	CAD-CBH-CBF	-2.58	108.60	111.68
3	C	1002	Y01	CAD-CBH-CBF	-2.58	108.60	111.68
3	A	1002	Y01	CAD-CBH-CAT	-2.58	105.36	109.43
3	D	1002	Y01	CAD-CBH-CAT	-2.58	105.36	109.43
3	C	1004	Y01	CAD-CBH-CAT	-2.58	105.36	109.43
3	A	1002	Y01	CAR-CBC-CAV	-2.57	107.15	110.99
3	D	1002	Y01	CAR-CBC-CAV	-2.57	107.15	110.99
3	C	1004	Y01	CAR-CBC-CAV	-2.57	107.15	110.99
3	B	1004	Y01	CAD-CBH-CAT	-2.57	105.38	109.43
3	B	1004	Y01	CAR-CBC-CAV	-2.56	107.17	110.99
4	A	1003	R0D	C27-C26-C05	-2.44	118.61	120.75
4	B	1001	R0D	C27-C26-C05	-2.44	118.61	120.75
4	C	1001	R0D	C27-C26-C05	-2.44	118.61	120.75
4	A	1003	R0D	O23-C12-N11	-2.44	118.81	121.67
4	B	1001	R0D	O23-C12-N11	-2.44	118.81	121.67
4	C	1001	R0D	O23-C12-N11	-2.44	118.81	121.67
3	D	1004	Y01	CBI-CBE-CBB	-2.44	115.67	119.49
3	B	1002	Y01	CBI-CBE-CBB	-2.44	115.67	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	Y01	CBI-CBE-CBB	-2.44	115.67	119.49
3	A	1002	Y01	CAT-CBH-CBF	2.43	112.12	108.73
3	D	1002	Y01	CAT-CBH-CBF	2.43	112.12	108.73
3	C	1004	Y01	CAT-CBH-CBF	2.43	112.12	108.73
3	B	1004	Y01	CAT-CBH-CBF	2.42	112.11	108.73
3	A	1004	Y01	CBI-CBE-CBB	-2.42	115.70	119.49
4	D	1003	R0D	O23-C12-N11	-2.40	118.86	121.67
4	D	1003	R0D	C27-C26-C05	-2.40	118.65	120.75
4	A	1003	R0D	C17-C16-C21	2.30	122.80	119.70
4	B	1001	R0D	C17-C16-C21	2.30	122.80	119.70
4	C	1001	R0D	C17-C16-C21	2.30	122.80	119.70
4	D	1003	R0D	C17-C16-C21	2.28	122.77	119.70
4	A	1003	R0D	C10-C09-C08	2.25	115.38	112.47
4	D	1003	R0D	C10-C09-C08	2.25	115.38	112.47
4	B	1001	R0D	C10-C09-C08	2.25	115.38	112.47
4	C	1001	R0D	C10-C09-C08	2.25	115.38	112.47
3	C	1004	Y01	CAR-CAT-CBH	2.20	117.50	112.74
3	A	1002	Y01	CAR-CAT-CBH	2.18	117.47	112.74
3	B	1004	Y01	CAR-CAT-CBH	2.18	117.47	112.74
3	D	1002	Y01	CAR-CAT-CBH	2.18	117.45	112.74
2	C	1003	SBM	O5-P-O1	-2.17	100.58	109.07
2	A	1001	SBM	O5-P-O1	-2.17	100.61	109.07
2	D	1001	SBM	O5-P-O1	-2.17	100.61	109.07
2	B	1003	SBM	O5-P-O1	-2.17	100.61	109.07
3	C	1002	Y01	CBC-OAW-CAY	2.14	123.07	117.79
3	D	1004	Y01	CAS-CBF-CBH	2.14	115.90	113.08
3	A	1004	Y01	CAQ-CBG-CBD	2.14	122.60	119.08
3	B	1002	Y01	CAQ-CBG-CBD	2.14	122.60	119.08
3	C	1002	Y01	CAQ-CBG-CBD	2.14	122.60	119.08
3	D	1004	Y01	CBC-OAW-CAY	2.13	123.05	117.79
3	A	1004	Y01	CBC-OAW-CAY	2.13	123.04	117.79
3	B	1002	Y01	CBC-OAW-CAY	2.13	123.04	117.79
3	A	1004	Y01	CAD-CBH-CAT	-2.13	106.06	109.43
3	D	1004	Y01	CAD-CBH-CAT	-2.13	106.06	109.43
3	B	1002	Y01	CAD-CBH-CAT	-2.13	106.06	109.43
3	C	1002	Y01	CAD-CBH-CAT	-2.13	106.06	109.43
3	D	1004	Y01	CAC-CBB-CAO	2.13	113.70	110.36
4	A	1003	R0D	O22-C21-C20	2.12	120.08	116.29
4	B	1001	R0D	O22-C21-C20	2.12	120.08	116.29
4	C	1001	R0D	O22-C21-C20	2.12	120.08	116.29
3	A	1004	Y01	CAS-CBF-CBH	2.12	115.88	113.08
3	B	1002	Y01	CAS-CBF-CBH	2.12	115.88	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	Y01	CAS-CBF-CBH	2.12	115.88	113.08
3	D	1004	Y01	CAQ-CBG-CBD	2.12	122.57	119.08
4	D	1003	R0D	O22-C21-C20	2.11	120.06	116.29
3	C	1004	Y01	CAU-CAS-CBF	2.11	116.77	113.11
3	A	1004	Y01	CAC-CBB-CAO	2.11	113.67	110.36
3	B	1002	Y01	CAC-CBB-CAO	2.11	113.67	110.36
3	C	1002	Y01	CAC-CBB-CAO	2.11	113.67	110.36
3	A	1002	Y01	CAU-CAS-CBF	2.09	116.74	113.11
3	D	1002	Y01	CAU-CAS-CBF	2.09	116.74	113.11
3	B	1004	Y01	CAU-CAS-CBF	2.09	116.74	113.11
3	A	1004	Y01	CAR-CBC-CAV	-2.05	107.93	110.99
3	D	1004	Y01	CAR-CBC-CAV	-2.05	107.93	110.99
3	B	1002	Y01	CAR-CBC-CAV	-2.05	107.93	110.99
3	C	1002	Y01	CAR-CBC-CAV	-2.05	107.93	110.99
3	A	1004	Y01	CAO-CBB-CBE	2.04	114.51	110.28
3	D	1004	Y01	CAO-CBB-CBE	2.04	114.51	110.28
3	B	1002	Y01	CAO-CBB-CBE	2.04	114.51	110.28
3	C	1002	Y01	CAO-CBB-CBE	2.04	114.51	110.28
3	B	1004	Y01	CAV-CAZ-CBH	-2.02	113.74	116.42

There are no chirality outliers.

All (188) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	SBM	C1-O3P-P-O4
2	A	1001	SBM	C1-O3P-P-O5
2	A	1001	SBM	C4-O5-P-O3P
2	A	1001	SBM	C4-O5-P-O1
2	A	1001	SBM	C4-O5-P-O4
2	D	1001	SBM	C1-O3P-P-O4
2	D	1001	SBM	C1-O3P-P-O5
2	D	1001	SBM	C4-O5-P-O3P
2	D	1001	SBM	C4-O5-P-O1
2	D	1001	SBM	C4-O5-P-O4
2	B	1003	SBM	C1-O3P-P-O4
2	B	1003	SBM	C1-O3P-P-O5
2	B	1003	SBM	C4-O5-P-O3P
2	B	1003	SBM	C4-O5-P-O1
2	B	1003	SBM	C4-O5-P-O4
2	C	1003	SBM	C1-O3P-P-O4
2	C	1003	SBM	C1-O3P-P-O5
2	C	1003	SBM	C4-O5-P-O3P

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Mol	Chain	Res	Type	Atoms
2	C	1003	SBM	C4-O5-P-O1
2	C	1003	SBM	C4-O5-P-O4
3	A	1004	Y01	CAO-CBB-CBE-CAP
3	A	1004	Y01	CAO-CBB-CBE-CBI
3	A	1004	Y01	CAC-CBB-CBE-CBI
3	D	1004	Y01	CAO-CBB-CBE-CAP
3	D	1004	Y01	CAO-CBB-CBE-CBI
3	D	1004	Y01	CAC-CBB-CBE-CBI
3	B	1002	Y01	CAO-CBB-CBE-CAP
3	B	1002	Y01	CAO-CBB-CBE-CBI
3	B	1002	Y01	CAC-CBB-CBE-CBI
3	C	1002	Y01	CAO-CBB-CBE-CAP
3	C	1002	Y01	CAO-CBB-CBE-CBI
3	C	1002	Y01	CAC-CBB-CBE-CBI
4	A	1003	R0D	O23-C12-C13-O22
4	D	1003	R0D	O23-C12-C13-O22
4	B	1001	R0D	O23-C12-C13-O22
4	C	1001	R0D	O23-C12-C13-O22
3	A	1004	Y01	CAJ-CAO-CBB-CAC
3	D	1004	Y01	CAJ-CAO-CBB-CAC
3	B	1002	Y01	CAJ-CAO-CBB-CAC
3	C	1002	Y01	CAJ-CAO-CBB-CAC
3	A	1004	Y01	CAC-CBB-CBE-CAP
3	D	1004	Y01	CAC-CBB-CBE-CAP
3	B	1002	Y01	CAC-CBB-CBE-CAP
3	C	1002	Y01	CAC-CBB-CBE-CAP
3	A	1002	Y01	CAO-CBB-CBE-CBI
3	D	1002	Y01	CAO-CBB-CBE-CBI
3	B	1004	Y01	CAO-CBB-CBE-CBI
3	C	1004	Y01	CAO-CBB-CBE-CBI
2	A	1001	SBM	C33-C34-C35-C36
2	D	1001	SBM	C33-C34-C35-C36
2	B	1003	SBM	C33-C34-C35-C36
2	C	1003	SBM	C33-C34-C35-C36
3	A	1002	Y01	CAJ-CAO-CBB-CBE
3	D	1002	Y01	CAJ-CAO-CBB-CBE
3	B	1004	Y01	CAJ-CAO-CBB-CBE
3	C	1004	Y01	CAJ-CAO-CBB-CBE
3	A	1002	Y01	CAO-CAJ-CAN-CBA
3	D	1002	Y01	CAO-CAJ-CAN-CBA
3	B	1004	Y01	CAO-CAJ-CAN-CBA
3	C	1004	Y01	CAO-CAJ-CAN-CBA

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Mol	Chain	Res	Type	Atoms
3	A	1004	Y01	CAN-CAJ-CAO-CBB
3	D	1004	Y01	CAN-CAJ-CAO-CBB
3	B	1002	Y01	CAN-CAJ-CAO-CBB
3	C	1002	Y01	CAN-CAJ-CAO-CBB
3	A	1002	Y01	CAO-CBB-CBE-CAP
3	D	1002	Y01	CAO-CBB-CBE-CAP
3	B	1004	Y01	CAO-CBB-CBE-CAP
3	C	1004	Y01	CAO-CBB-CBE-CAP
2	A	1001	SBM	C31-C32-C33-C34
2	D	1001	SBM	C31-C32-C33-C34
2	B	1003	SBM	C31-C32-C33-C34
2	C	1003	SBM	C31-C32-C33-C34
2	A	1001	SBM	C32-C33-C34-C35
2	D	1001	SBM	C32-C33-C34-C35
2	B	1003	SBM	C32-C33-C34-C35
2	C	1003	SBM	C32-C33-C34-C35
3	A	1002	Y01	CAJ-CAO-CBB-CAC
3	D	1002	Y01	CAJ-CAO-CBB-CAC
3	B	1004	Y01	CAJ-CAO-CBB-CAC
3	C	1004	Y01	CAJ-CAO-CBB-CAC
3	A	1002	Y01	CAJ-CAN-CBA-CAA
3	D	1002	Y01	CAJ-CAN-CBA-CAA
3	B	1004	Y01	CAJ-CAN-CBA-CAA
3	C	1004	Y01	CAJ-CAN-CBA-CAA
2	A	1001	SBM	C32-C31-O2-C2
2	D	1001	SBM	C32-C31-O2-C2
2	B	1003	SBM	C32-C31-O2-C2
2	C	1003	SBM	C32-C31-O2-C2
2	A	1001	SBM	O31-C31-O2-C2
2	D	1001	SBM	O31-C31-O2-C2
2	B	1003	SBM	O31-C31-O2-C2
2	C	1003	SBM	O31-C31-O2-C2
3	A	1002	Y01	CAC-CBB-CBE-CBI
3	D	1002	Y01	CAC-CBB-CBE-CBI
3	B	1004	Y01	CAC-CBB-CBE-CBI
3	C	1004	Y01	CAC-CBB-CBE-CBI
2	A	1001	SBM	O2-C2-C3-O3
2	D	1001	SBM	O2-C2-C3-O3
2	B	1003	SBM	O2-C2-C3-O3
2	C	1003	SBM	O2-C2-C3-O3
2	A	1001	SBM	C16-C17-C18-C19
2	D	1001	SBM	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
2	B	1003	SBM	C16-C17-C18-C19
2	C	1003	SBM	C16-C17-C18-C19
3	A	1002	Y01	CAC-CBB-CBE-CAP
3	D	1002	Y01	CAC-CBB-CBE-CAP
3	B	1004	Y01	CAC-CBB-CBE-CAP
3	C	1004	Y01	CAC-CBB-CBE-CAP
2	A	1001	SBM	C15-C16-C17-C18
2	D	1001	SBM	C15-C16-C17-C18
2	C	1003	SBM	C15-C16-C17-C18
2	B	1003	SBM	C15-C16-C17-C18
3	A	1002	Y01	CAJ-CAN-CBA-CAB
3	D	1002	Y01	CAJ-CAN-CBA-CAB
3	B	1004	Y01	CAJ-CAN-CBA-CAB
3	C	1004	Y01	CAJ-CAN-CBA-CAB
2	A	1001	SBM	C17-C18-C19-C20
2	D	1001	SBM	C17-C18-C19-C20
2	B	1003	SBM	C17-C18-C19-C20
2	C	1003	SBM	C17-C18-C19-C20
2	A	1001	SBM	C35-C36-C37-C38
2	D	1001	SBM	C35-C36-C37-C38
2	B	1003	SBM	C35-C36-C37-C38
2	C	1003	SBM	C35-C36-C37-C38
2	A	1001	SBM	C1-O3P-P-O1
2	D	1001	SBM	C1-O3P-P-O1
2	B	1003	SBM	C1-O3P-P-O1
2	C	1003	SBM	C1-O3P-P-O1
2	A	1001	SBM	C1-C2-C3-O3
2	A	1001	SBM	O5-C4-C5-N1
2	D	1001	SBM	C1-C2-C3-O3
2	D	1001	SBM	O5-C4-C5-N1
2	B	1003	SBM	C1-C2-C3-O3
2	B	1003	SBM	O5-C4-C5-N1
2	C	1003	SBM	C1-C2-C3-O3
2	C	1003	SBM	O5-C4-C5-N1
2	C	1003	SBM	C19-C20-C21-C22
2	A	1001	SBM	C19-C20-C21-C22
2	D	1001	SBM	C19-C20-C21-C22
2	B	1003	SBM	C19-C20-C21-C22
2	A	1001	SBM	C14-C15-C16-C17
2	D	1001	SBM	C14-C15-C16-C17
2	B	1003	SBM	C14-C15-C16-C17
2	C	1003	SBM	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	A	1002	Y01	CAM-CAL-CAX-OAF
3	D	1002	Y01	CAM-CAL-CAX-OAF
3	B	1004	Y01	CAM-CAL-CAX-OAF
3	C	1004	Y01	CAM-CAL-CAX-OAF
3	A	1002	Y01	CAM-CAL-CAX-OAH
3	D	1002	Y01	CAM-CAL-CAX-OAH
3	B	1004	Y01	CAM-CAL-CAX-OAH
3	C	1004	Y01	CAM-CAL-CAX-OAH
3	A	1002	Y01	OAG-CAY-OAW-CBC
3	D	1002	Y01	OAG-CAY-OAW-CBC
3	B	1004	Y01	OAG-CAY-OAW-CBC
3	C	1004	Y01	OAG-CAY-OAW-CBC
2	A	1001	SBM	C18-C19-C20-C21
2	B	1003	SBM	C18-C19-C20-C21
2	C	1003	SBM	C18-C19-C20-C21
2	D	1001	SBM	C18-C19-C20-C21
2	A	1001	SBM	C34-C35-C36-C37
2	D	1001	SBM	C34-C35-C36-C37
2	C	1003	SBM	C34-C35-C36-C37
3	A	1004	Y01	CAM-CAL-CAX-OAH
3	D	1004	Y01	CAM-CAL-CAX-OAH
3	B	1002	Y01	CAM-CAL-CAX-OAH
3	C	1002	Y01	CAM-CAL-CAX-OAH
2	B	1003	SBM	C34-C35-C36-C37
3	A	1004	Y01	CAM-CAL-CAX-OAF
3	D	1004	Y01	CAM-CAL-CAX-OAF
3	B	1002	Y01	CAM-CAL-CAX-OAF
3	C	1002	Y01	CAM-CAL-CAX-OAF
3	A	1004	Y01	CAJ-CAN-CBA-CAB
3	D	1004	Y01	CAJ-CAN-CBA-CAB
3	C	1002	Y01	CAJ-CAN-CBA-CAB
3	B	1002	Y01	CAJ-CAN-CBA-CAB
3	A	1004	Y01	CAJ-CAO-CBB-CBE
3	D	1004	Y01	CAJ-CAO-CBB-CBE
3	B	1002	Y01	CAJ-CAO-CBB-CBE
3	C	1002	Y01	CAJ-CAO-CBB-CBE
3	A	1002	Y01	CAM-CAY-OAW-CBC
3	D	1002	Y01	CAM-CAY-OAW-CBC
3	B	1004	Y01	CAM-CAY-OAW-CBC
3	C	1004	Y01	CAM-CAY-OAW-CBC
3	C	1002	Y01	CAO-CAJ-CAN-CBA
3	A	1004	Y01	CAO-CAJ-CAN-CBA

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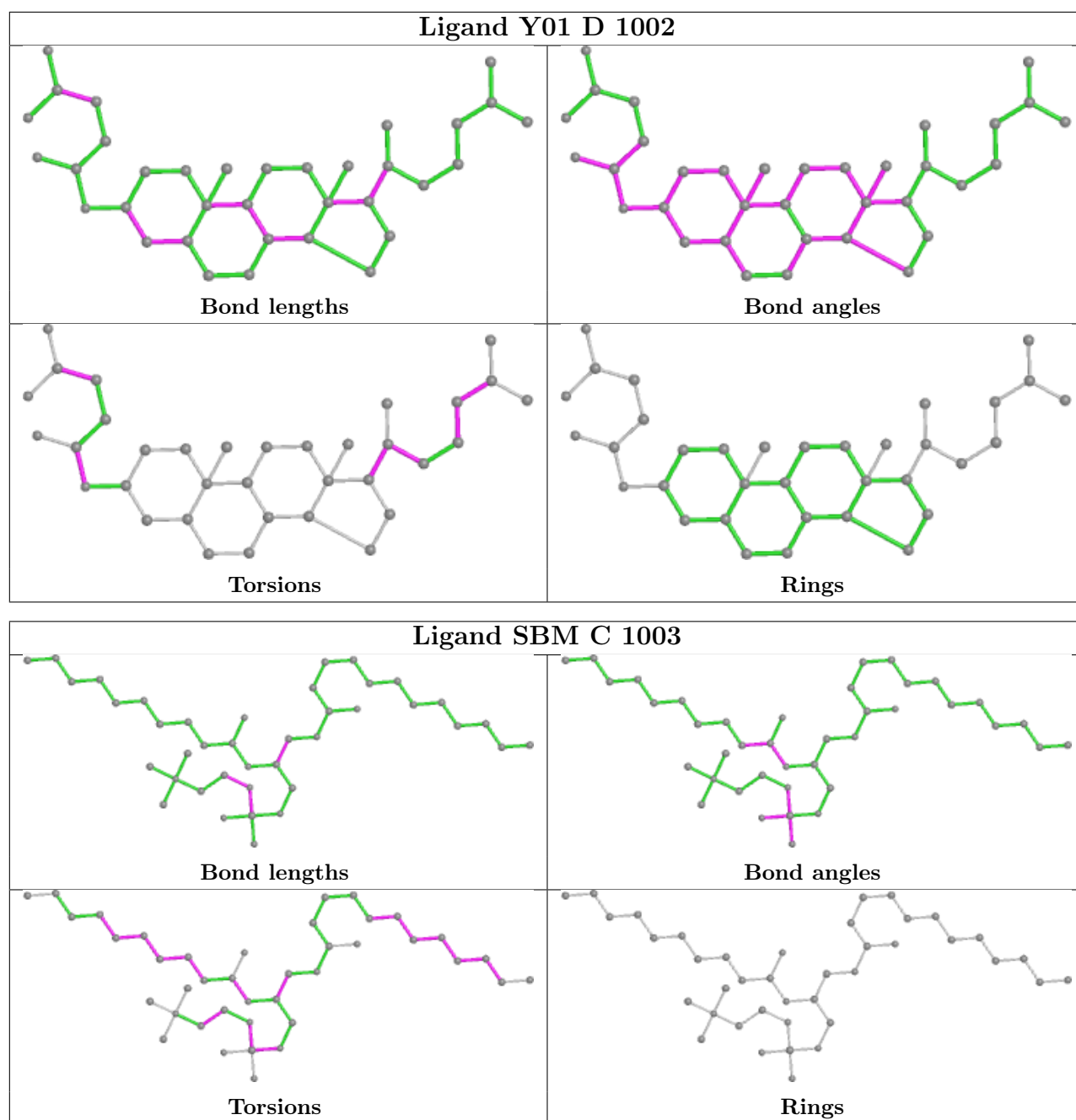
Mol	Chain	Res	Type	Atoms
3	B	1002	Y01	CAO-CAJ-CAN-CBA
3	D	1004	Y01	CAO-CAJ-CAN-CBA

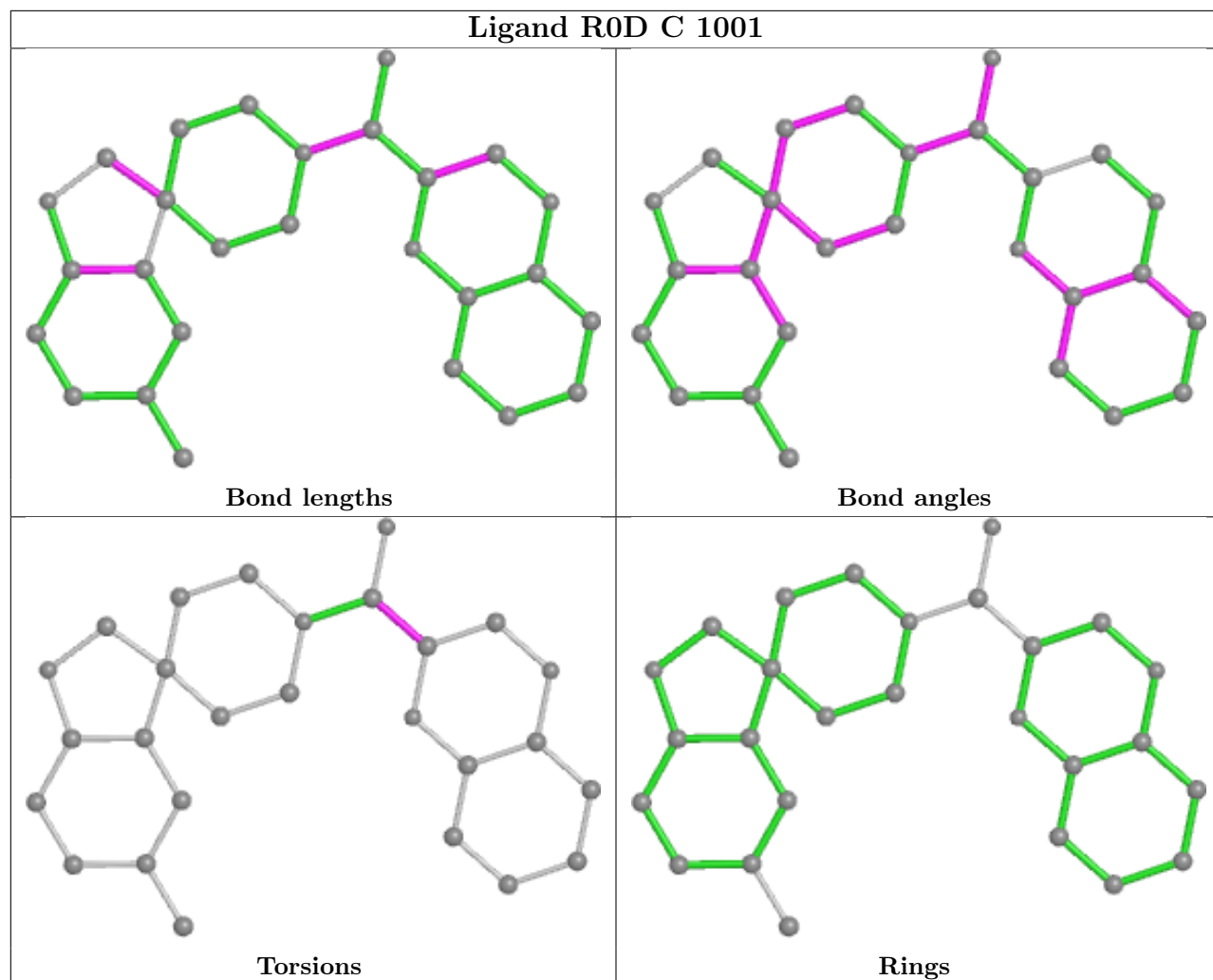
There are no ring outliers.

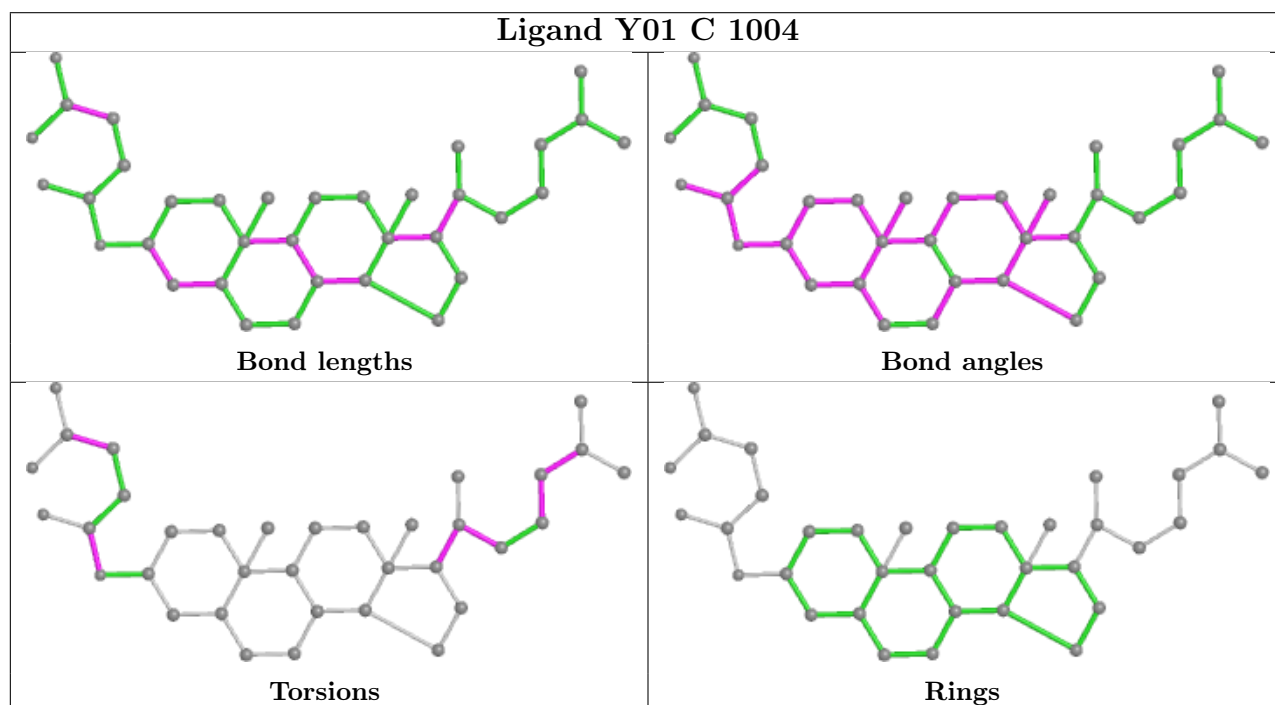
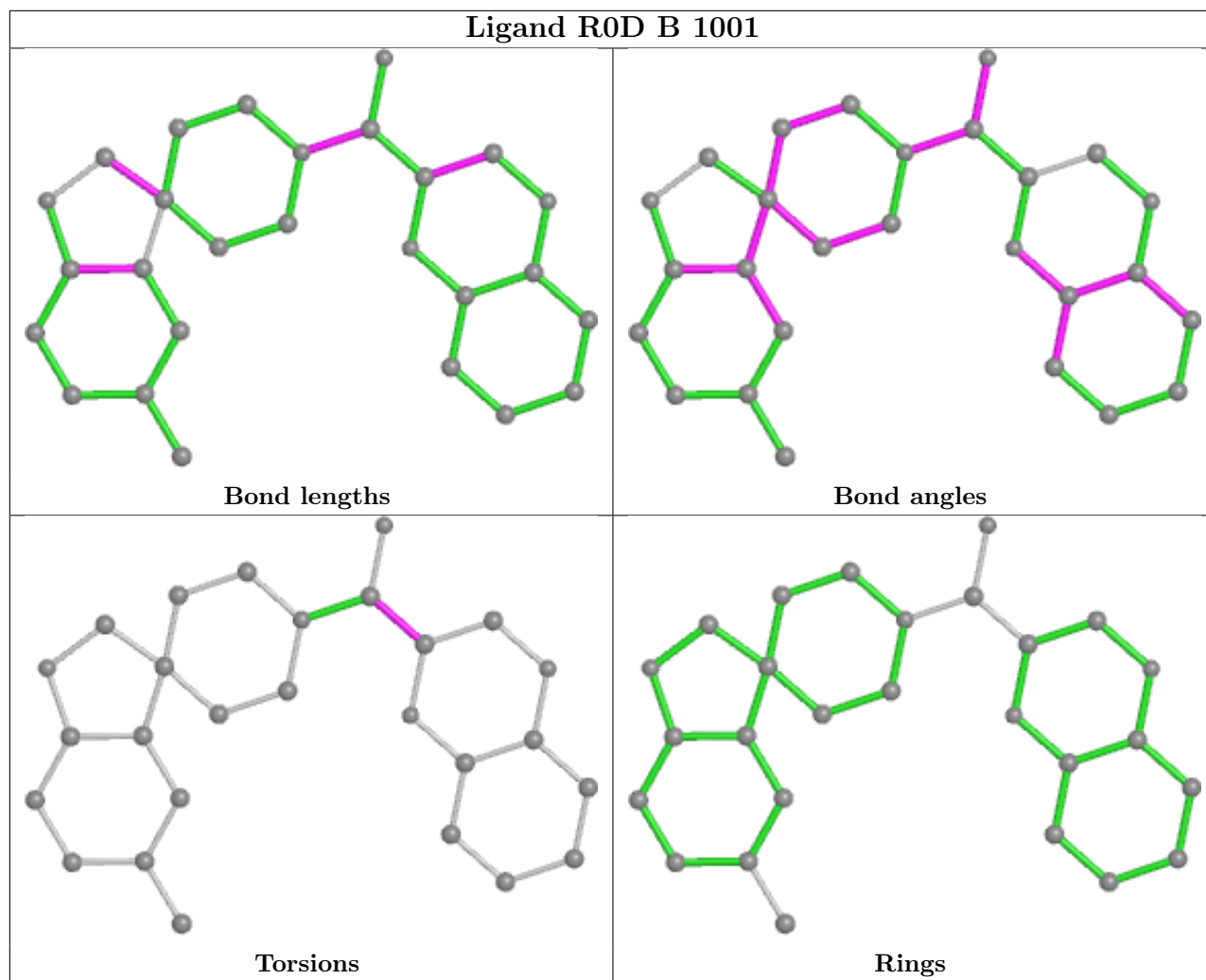
8 monomers are involved in 18 short contacts:

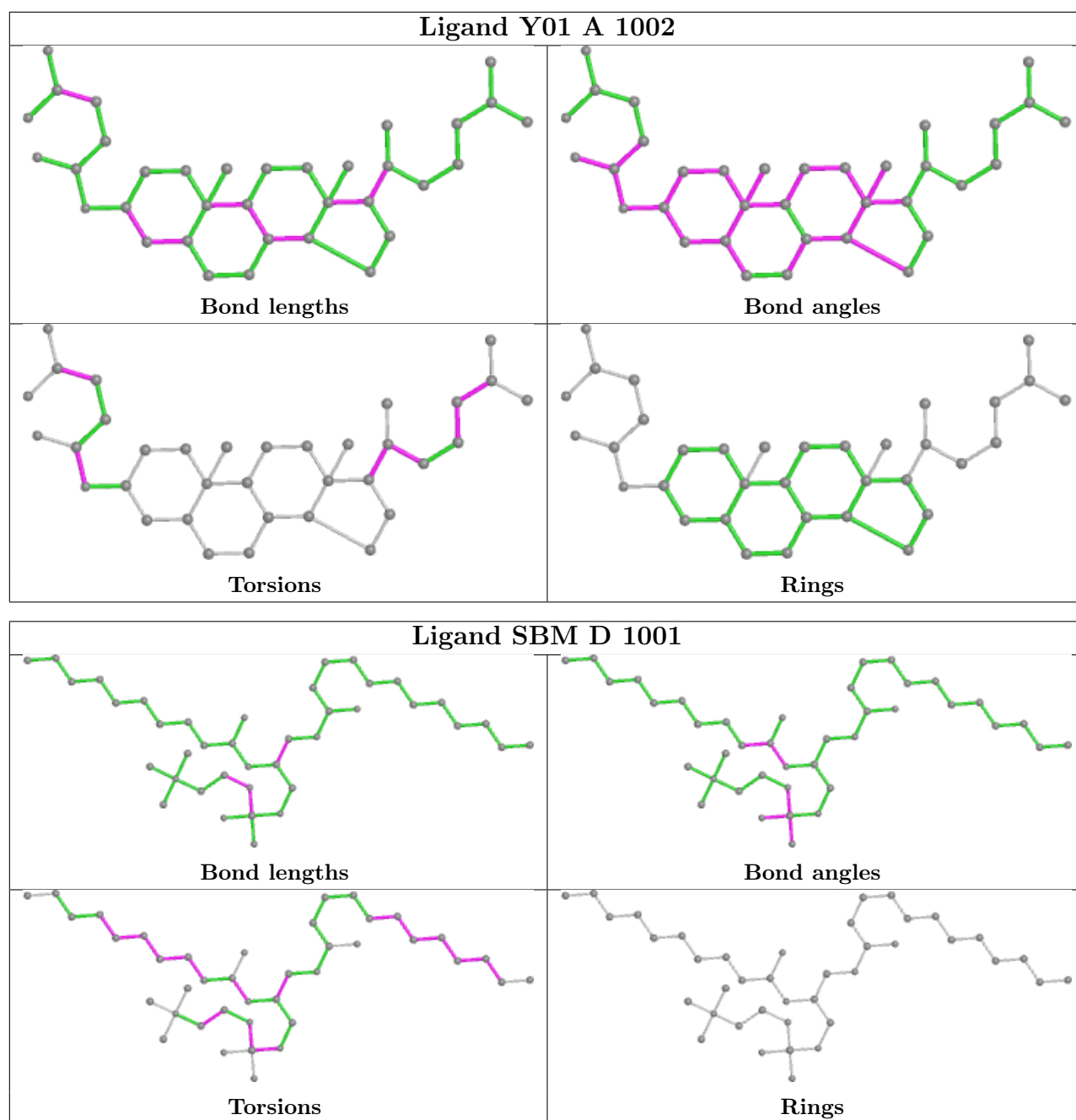
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1002	Y01	2	0
3	C	1004	Y01	3	0
3	A	1002	Y01	1	0
3	C	1002	Y01	1	0
3	B	1004	Y01	3	0
3	D	1004	Y01	3	0
3	A	1004	Y01	2	0
3	B	1002	Y01	3	0

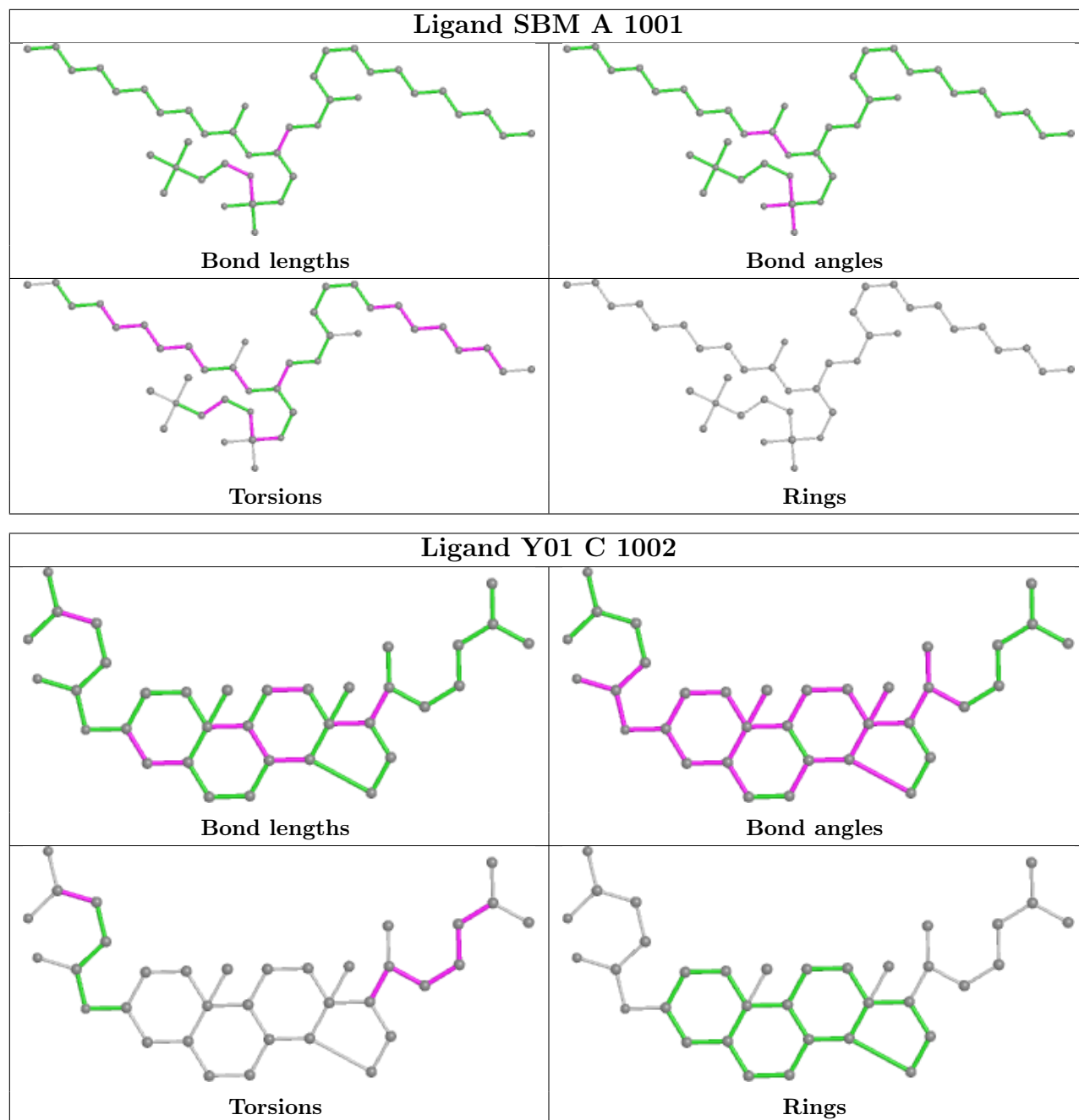
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

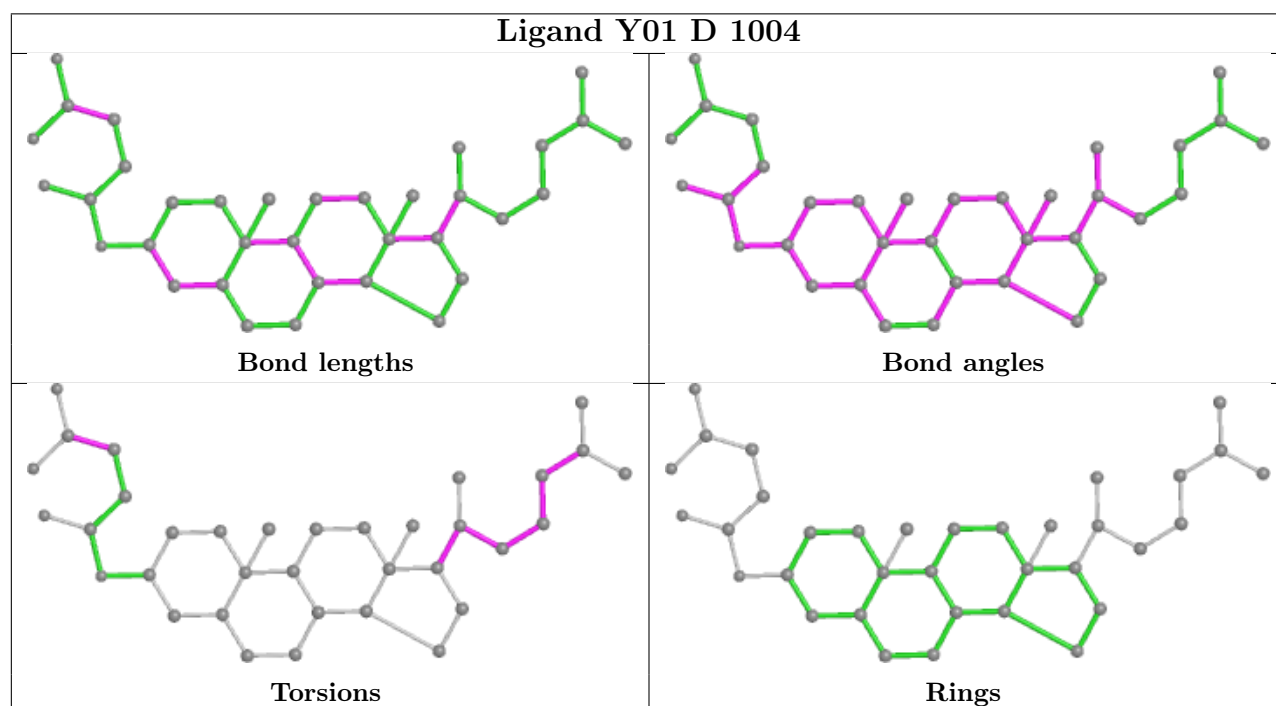
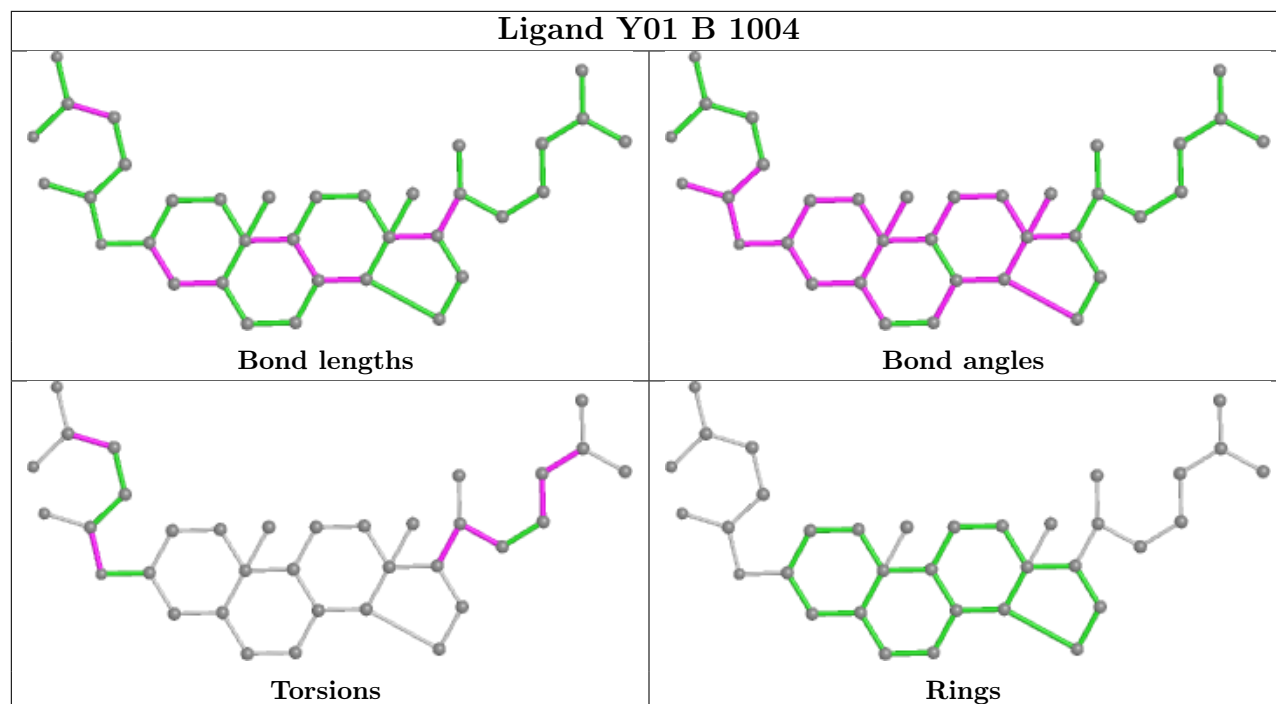


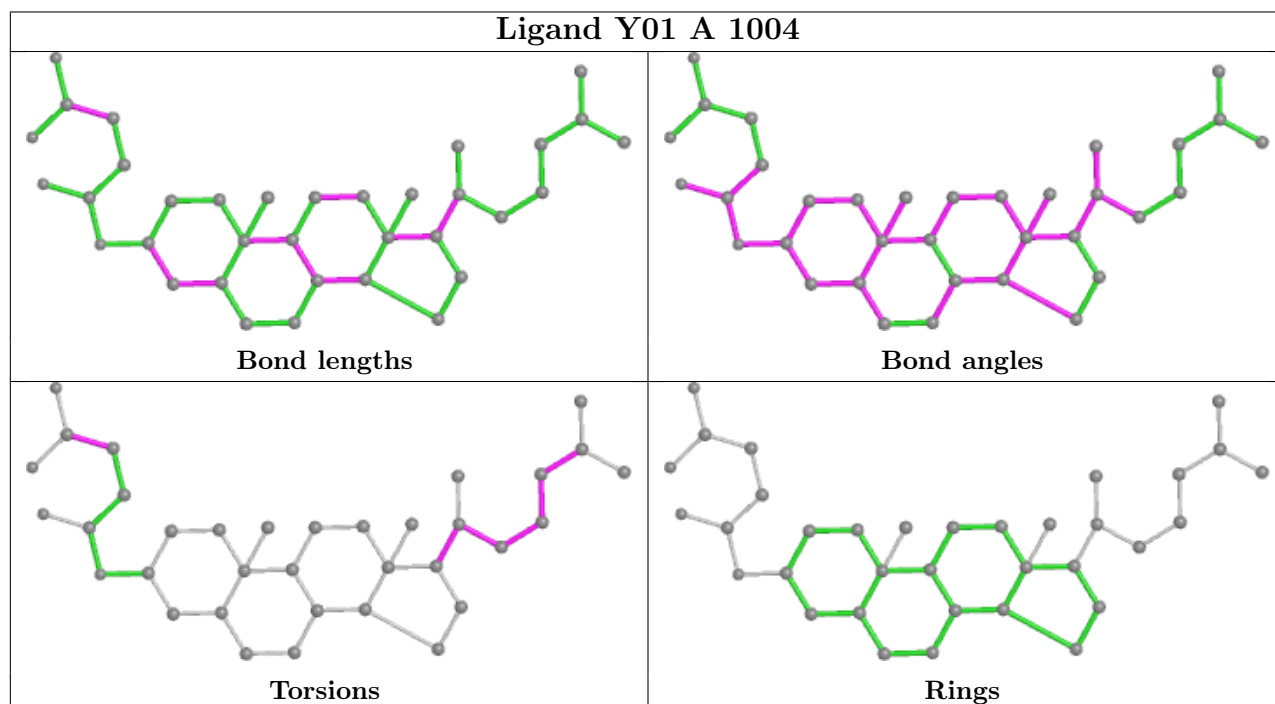
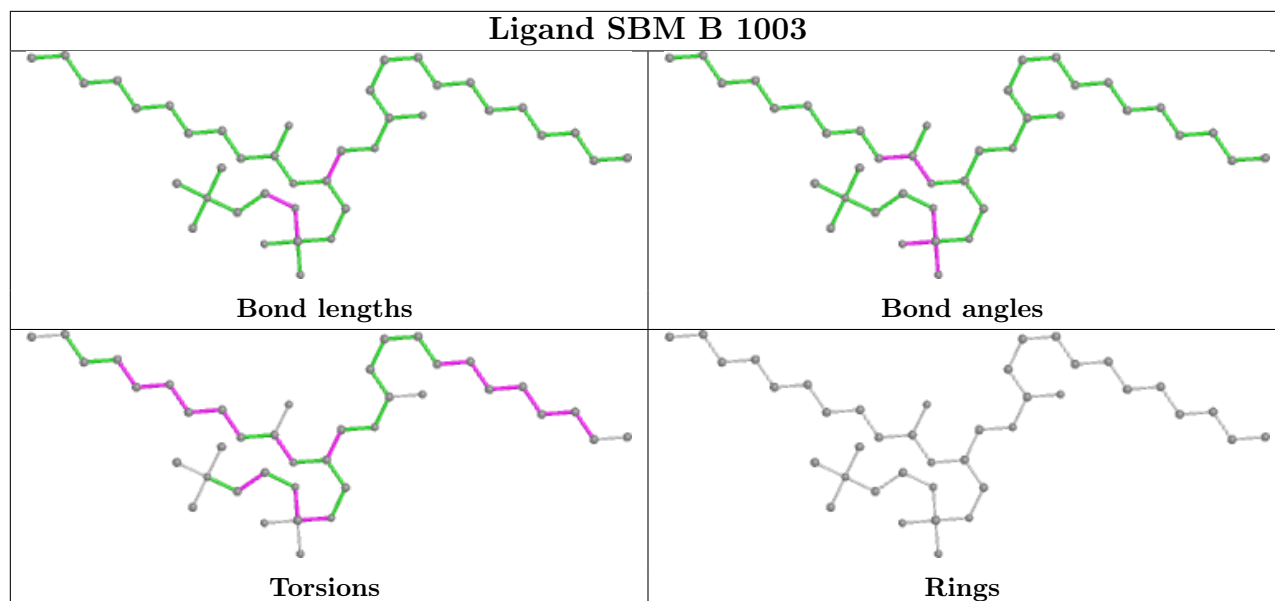


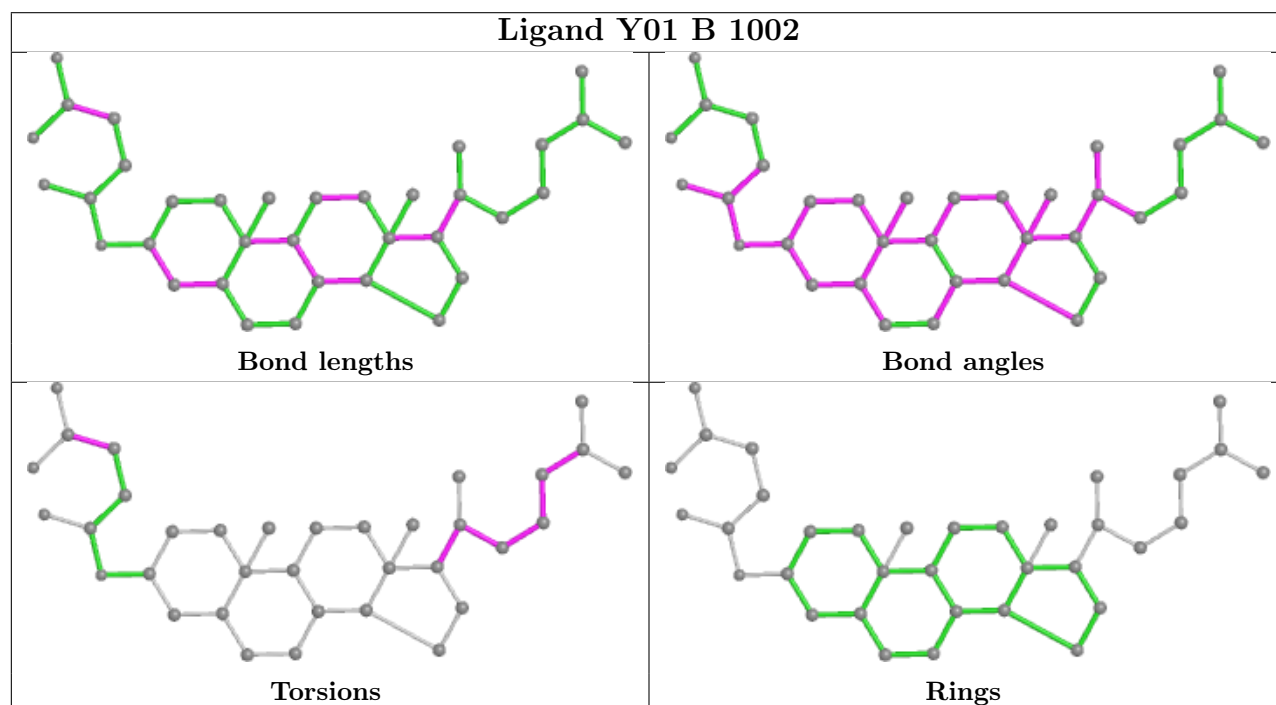
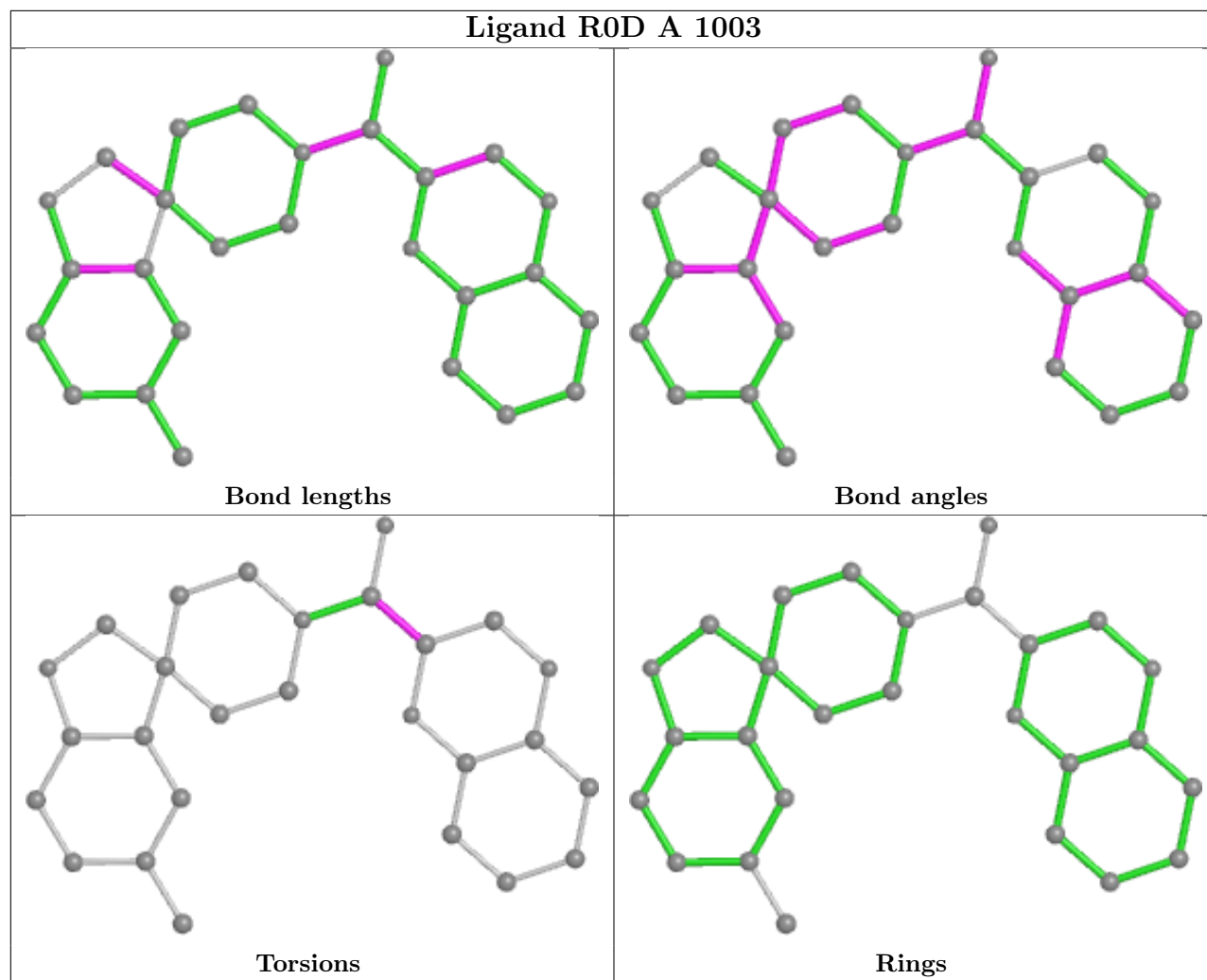


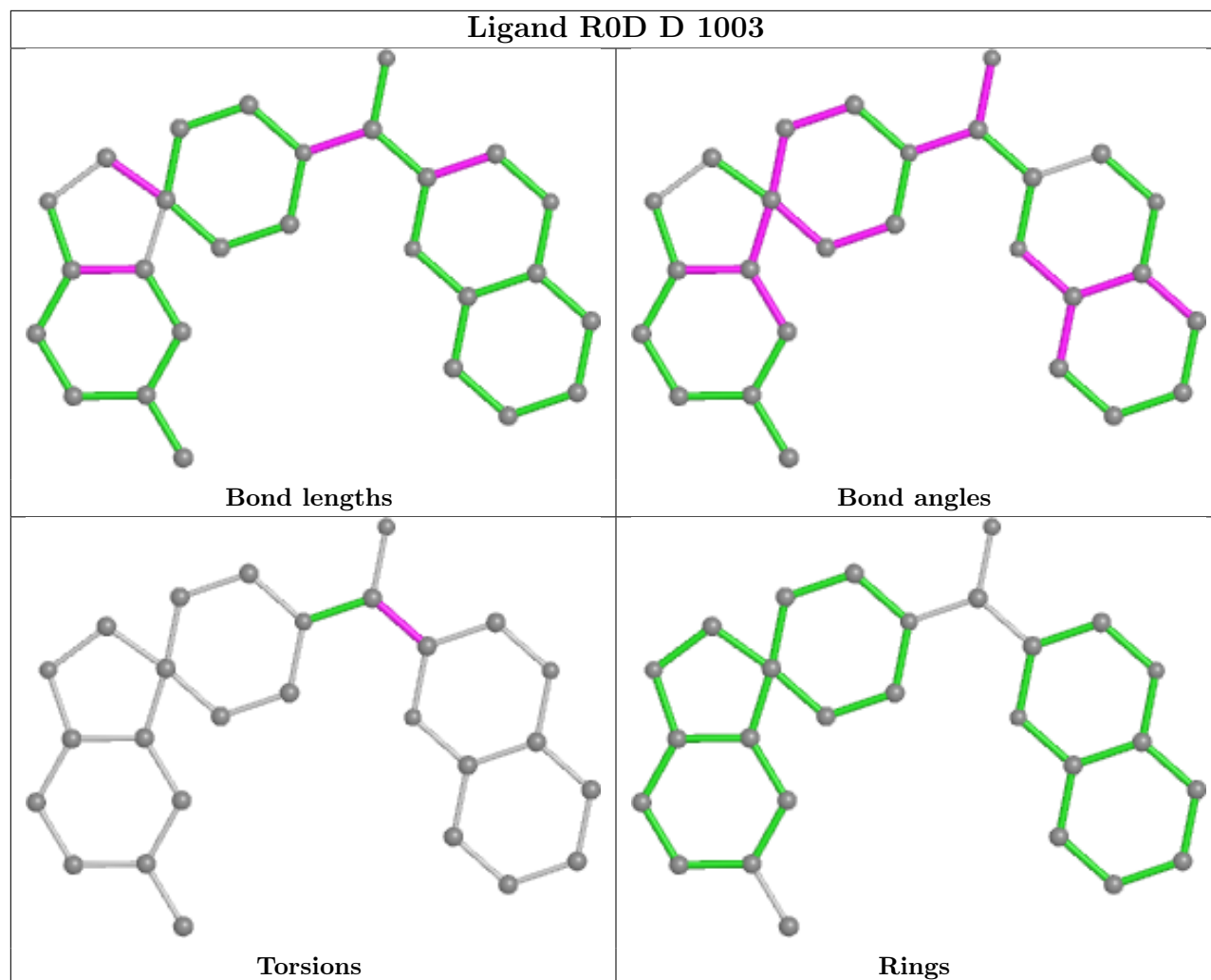












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

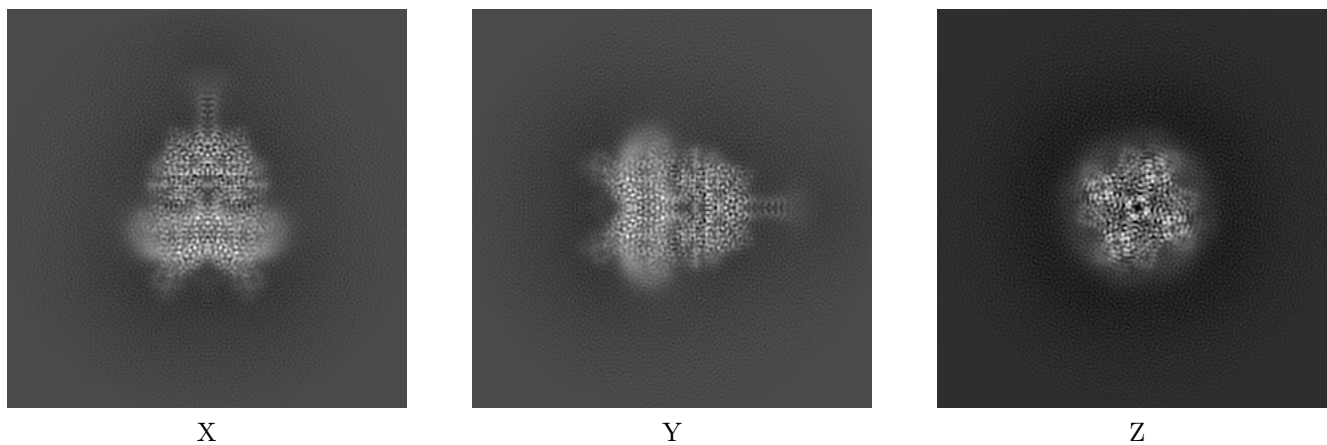
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20953. 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](#)

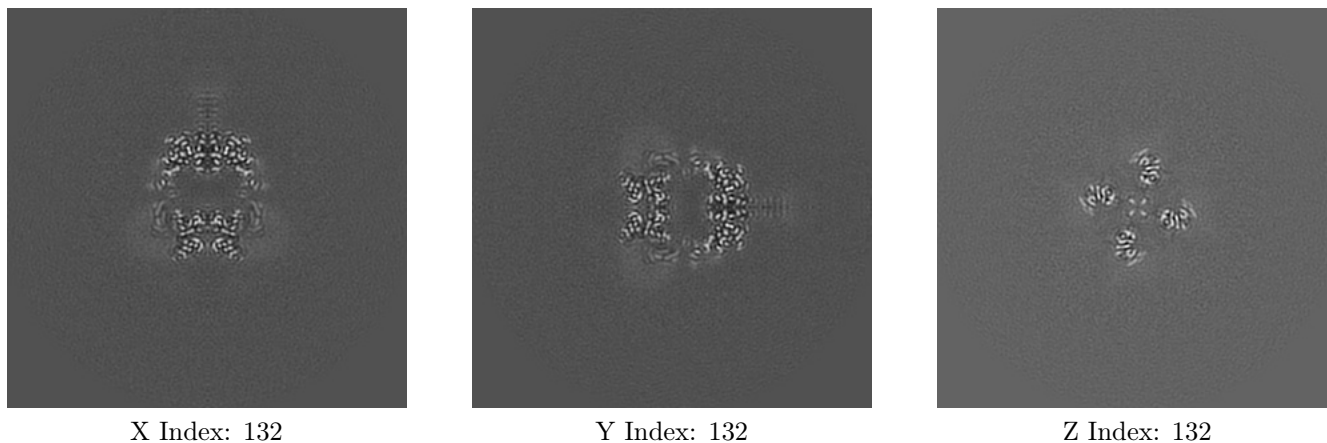
6.1.1 Primary map



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

6.2 Central slices [i](#)

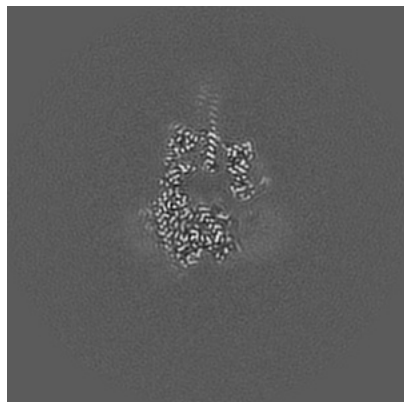
6.2.1 Primary map



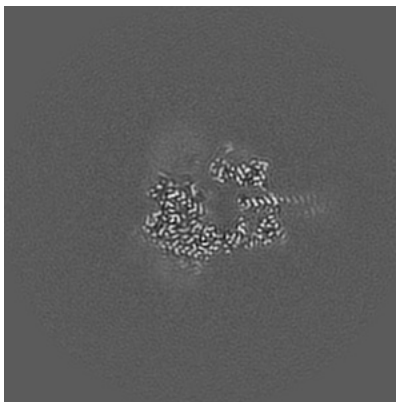
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

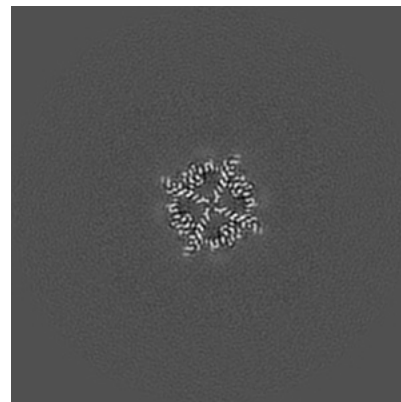
6.3.1 Primary map



X Index: 125



Y Index: 139

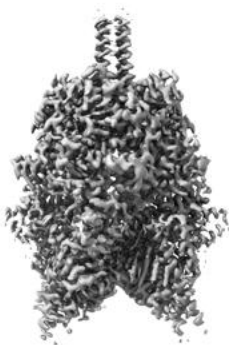


Z Index: 155

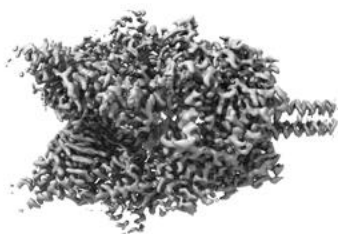
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

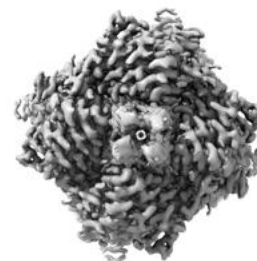
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

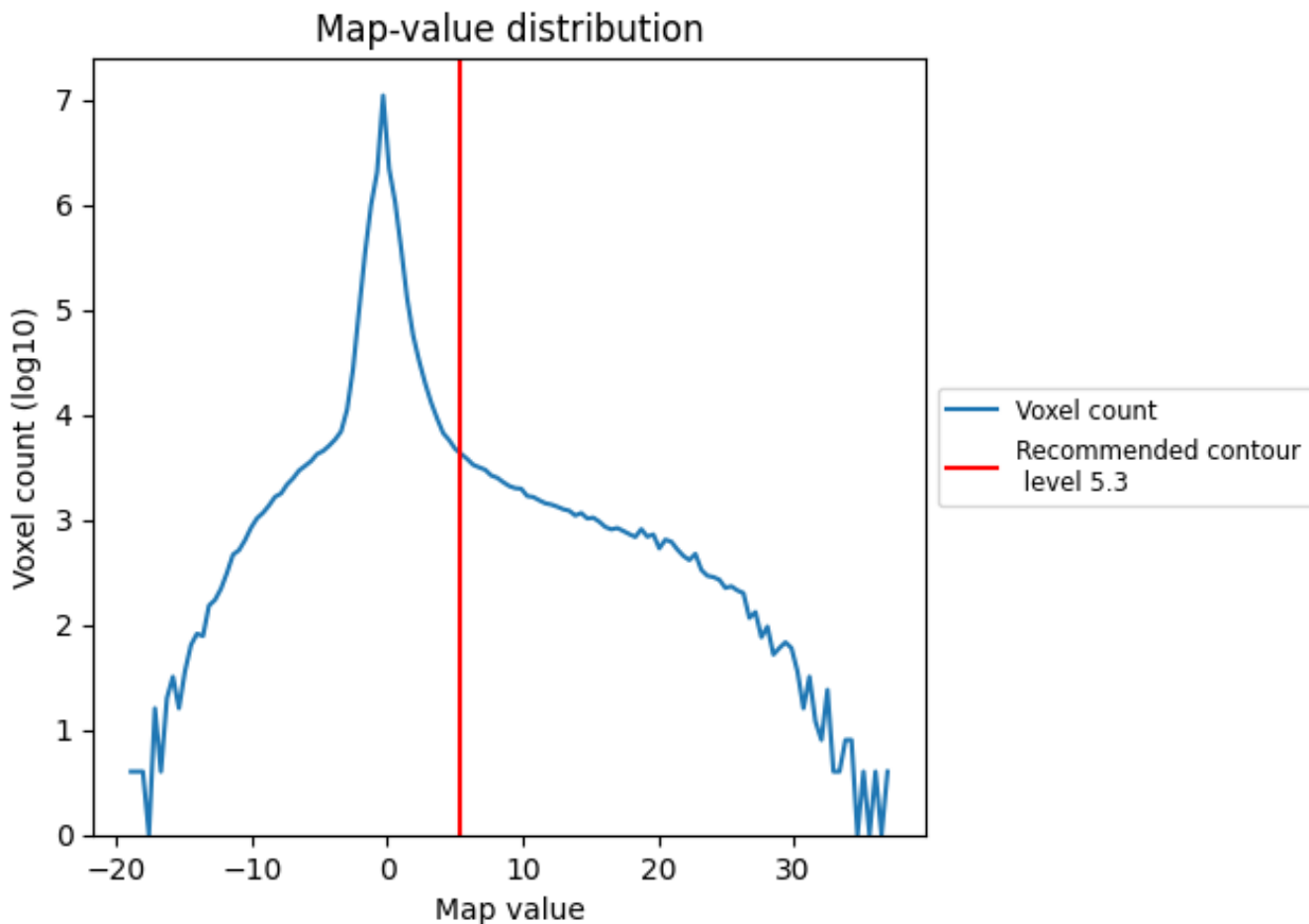
6.5 Mask visualisation

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

7 Map analysis [i](#)

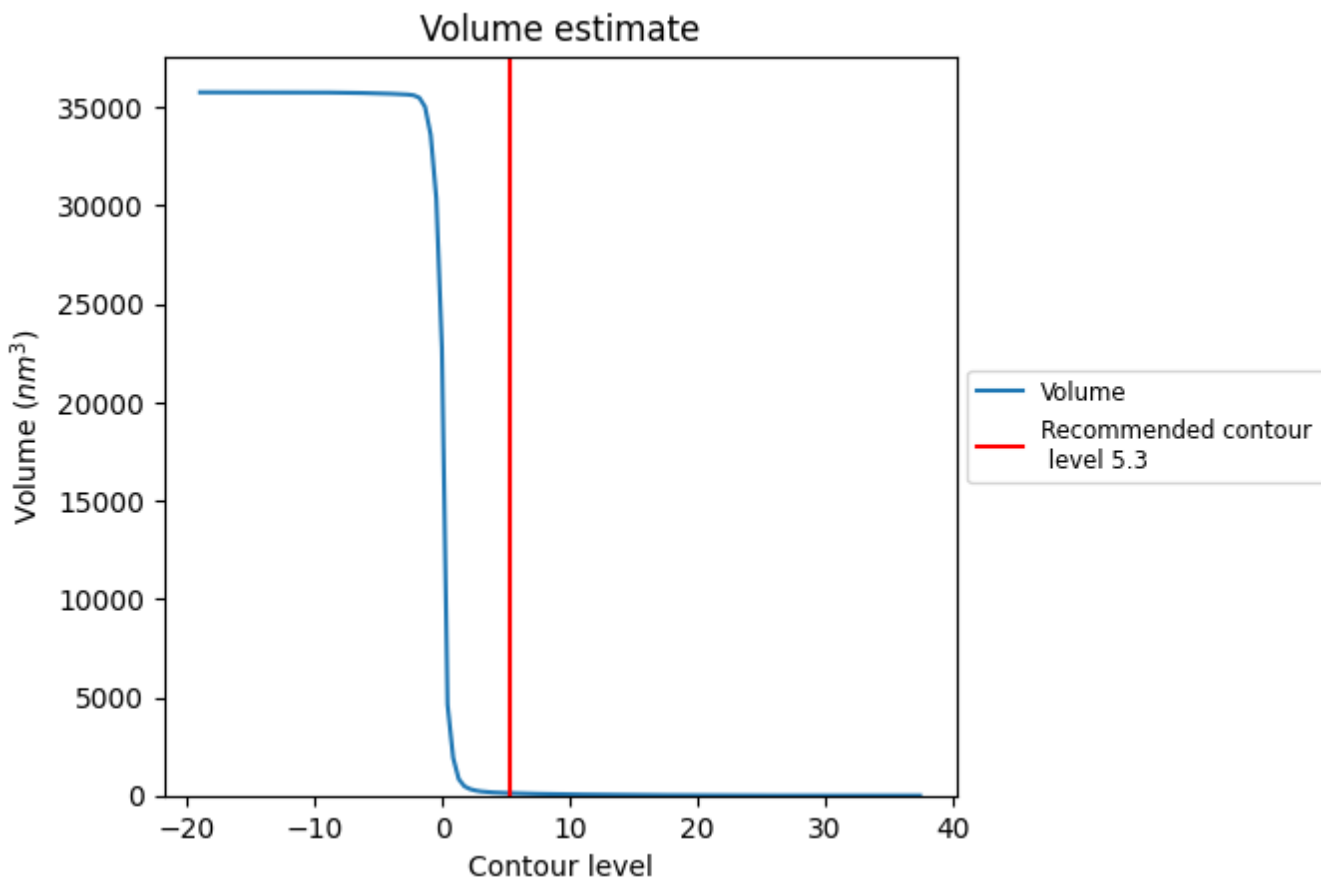
This section contains the results of statistical analysis of the map.

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.

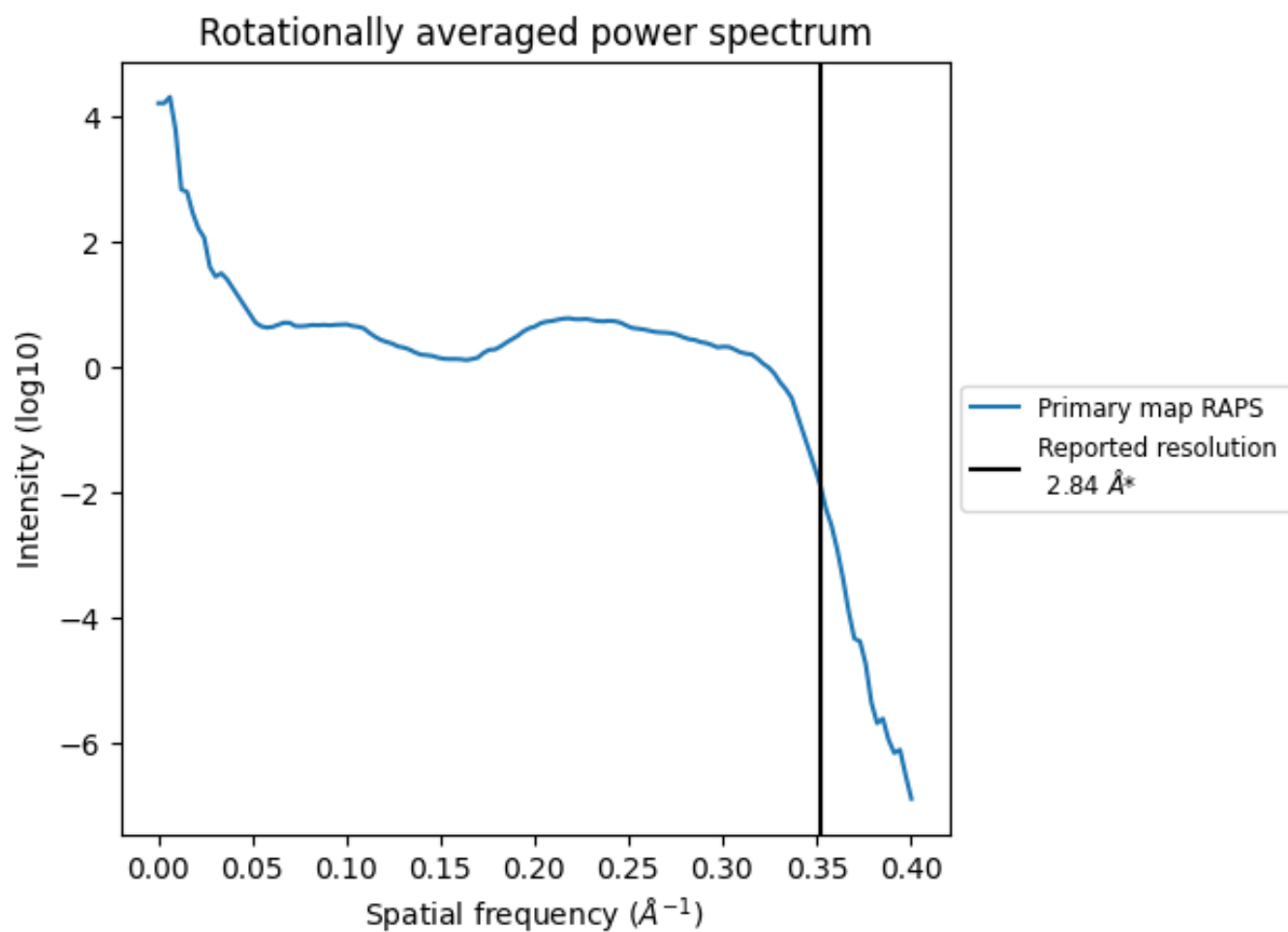
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 122 nm^3 ; this corresponds to an approximate mass of 110 kDa.

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

7.3 Rotationally averaged power spectrum i

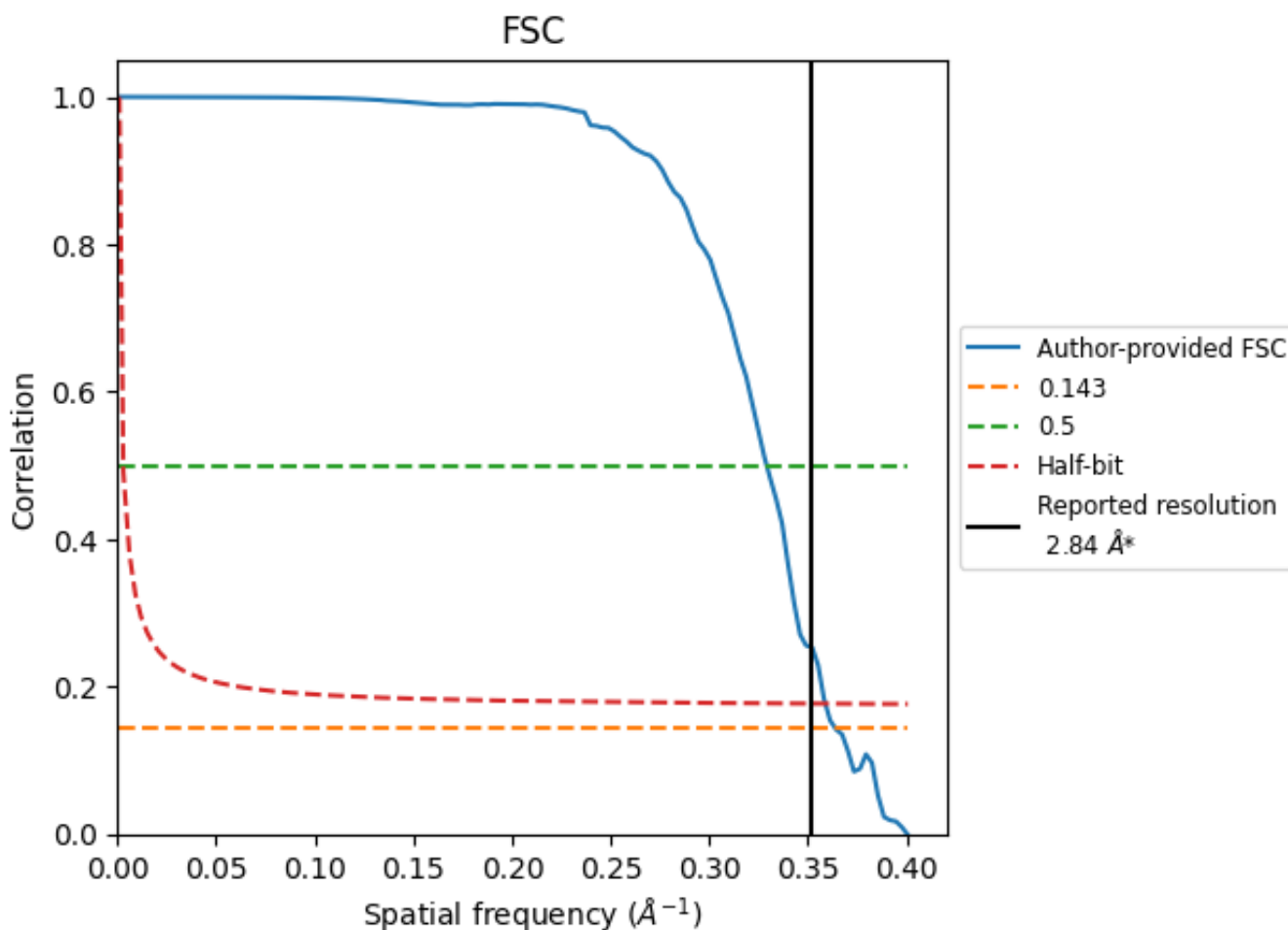


*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

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 0.352 Å⁻¹

8.2 Resolution estimates [i](#)

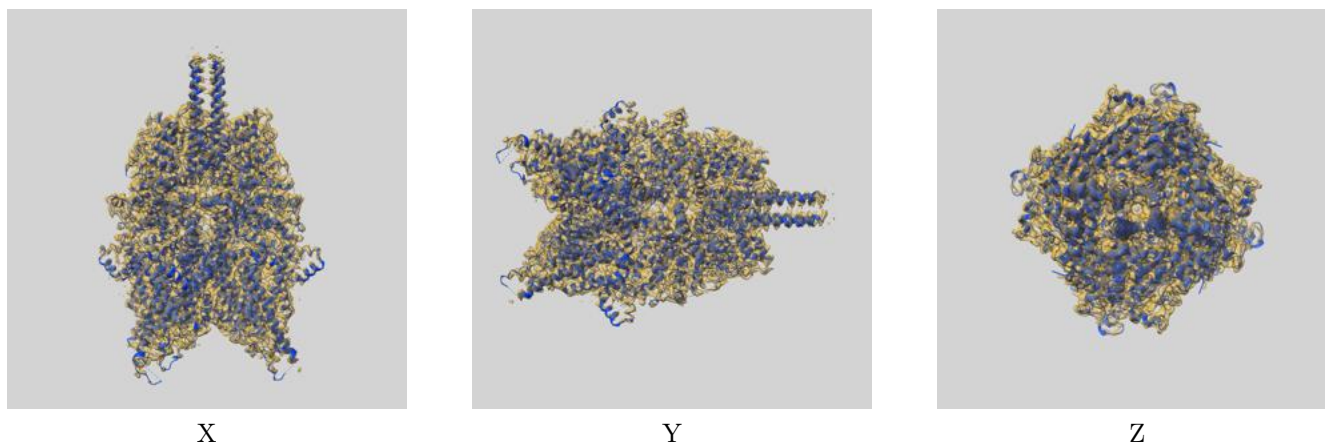
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.75	3.04	2.79
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

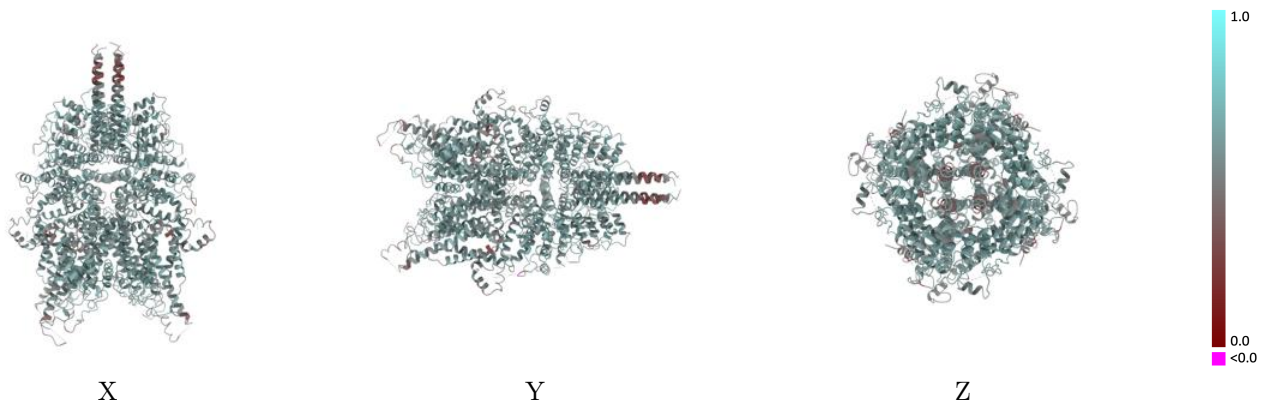
This section contains information regarding the fit between EMDB map EMD-20953 and PDB model 6UZ8. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



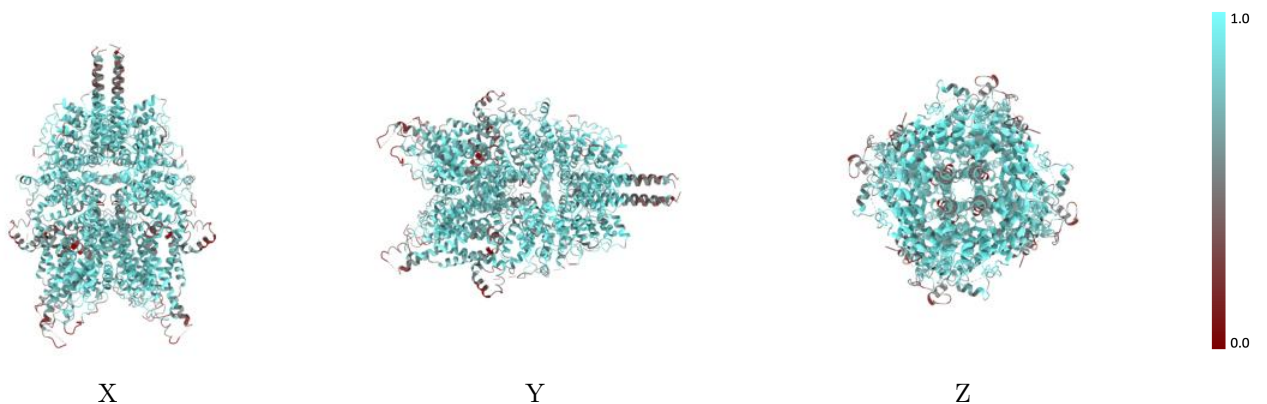
The images above show the 3D surface view of the map at the recommended contour level 5.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



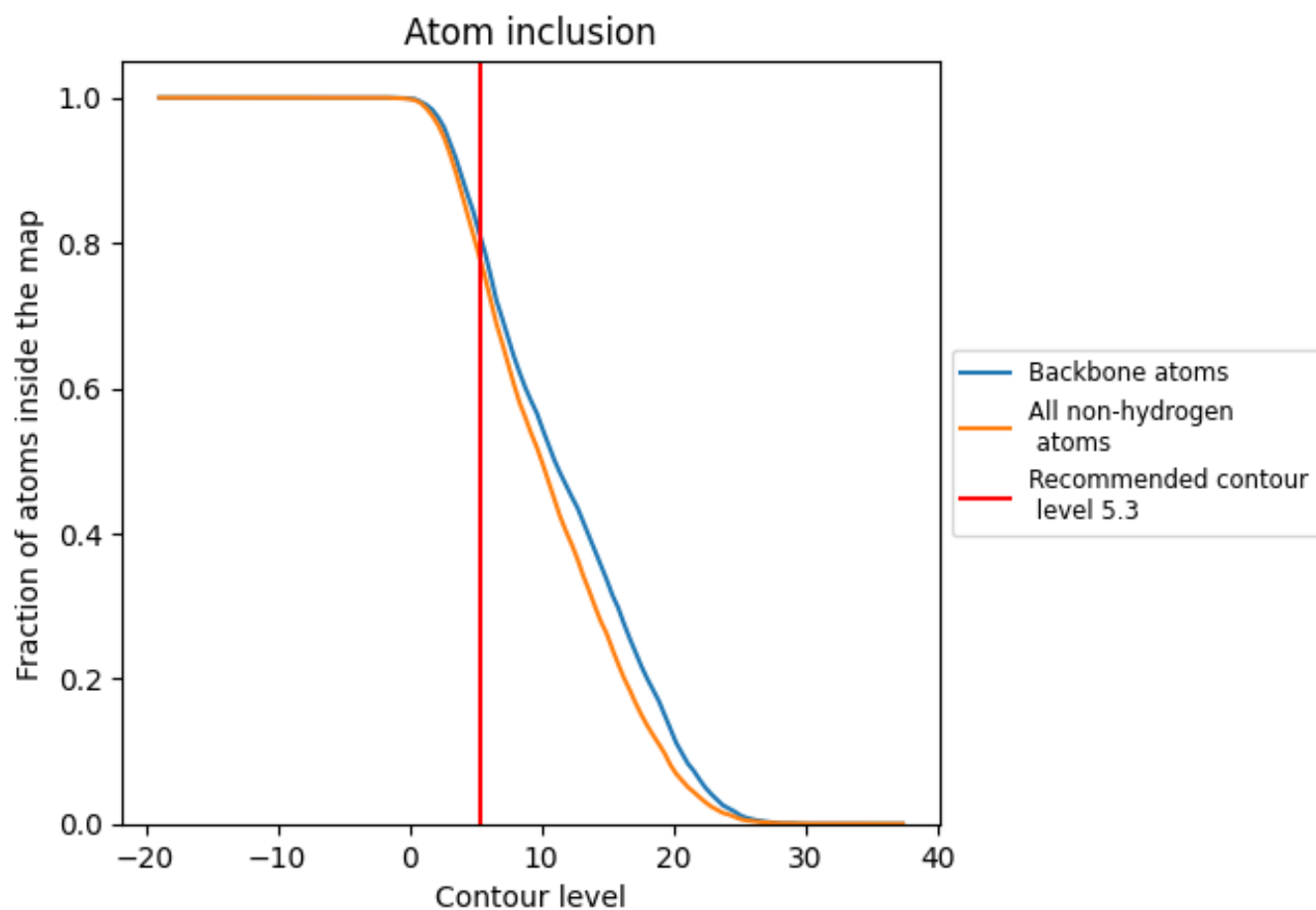
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.3).






9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

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

The table lists the average atom inclusion at the recommended contour level (5.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7823	 0.5730
A	 0.7824	 0.5730
B	 0.7823	 0.5740
C	 0.7823	 0.5730
D	 0.7821	 0.5730

