



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 02:39 AM JST

PDB ID : 7DXG
EMDB ID : EMD-30908
Title : Structure of SAR7334-bound TRPC6 at 2.9 angstrom
Authors : Chen, L.; Guo, W.
Deposited on : 2021-01-18
Resolution : 2.90 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) : 2.31.3

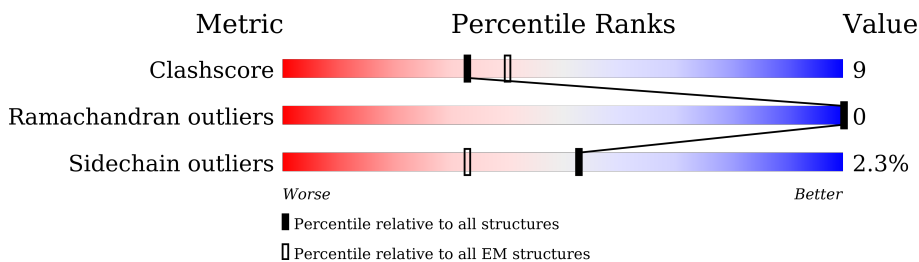
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	931	
1	B	931	
1	C	931	
1	D	931	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 23432 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	698	5603	3639	922	1006	36	0	0
1	B	698	5603	3639	922	1006	36	0	0
1	C	698	5603	3639	922	1006	36	0	0
1	D	698	5603	3639	922	1006	36	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0
2	D	1	Total 1	Zn 1	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

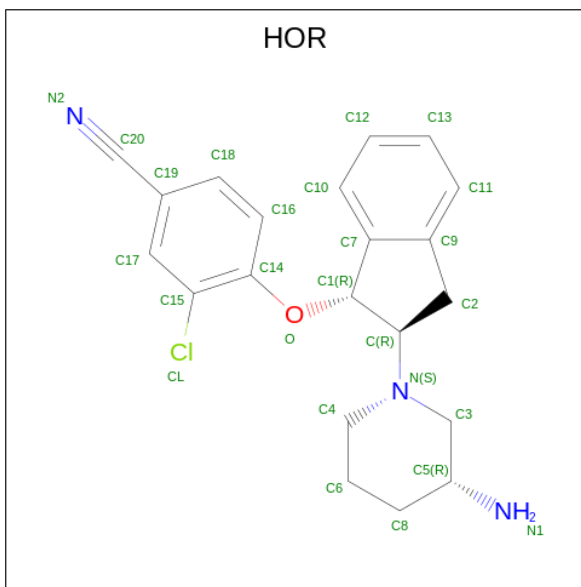
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total 2	Ca 2	0
3	B	2	Total 2	Ca 2	0
3	C	2	Total 2	Ca 2	0
3	D	2	Total 2	Ca 2	0

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).

Continued from previous page...

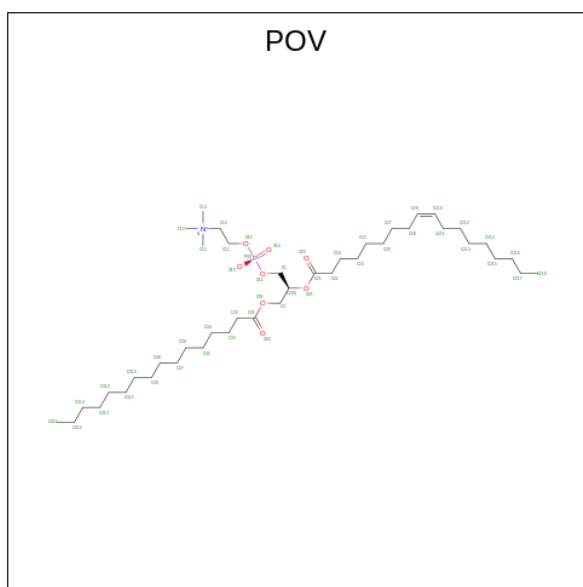
Mol	Chain	Residues	Atoms			AltConf
4	D	1	Total	C	O	0
			140	124	16	
4	D	1	Total	C	O	0
			140	124	16	

- Molecule 5 is 4-[[[(1R,2R)-2-[(3R)-3-azanyl piperidin-1-yl]-2,3-dihydro-1H-inden-1-yl]oxy]-3-chloranyl-benzenecarbonitrile (three-letter code: HOR) (formula: $C_{21}H_{22}ClN_3O$) (labeled as "Ligand of Interest" by depositor).



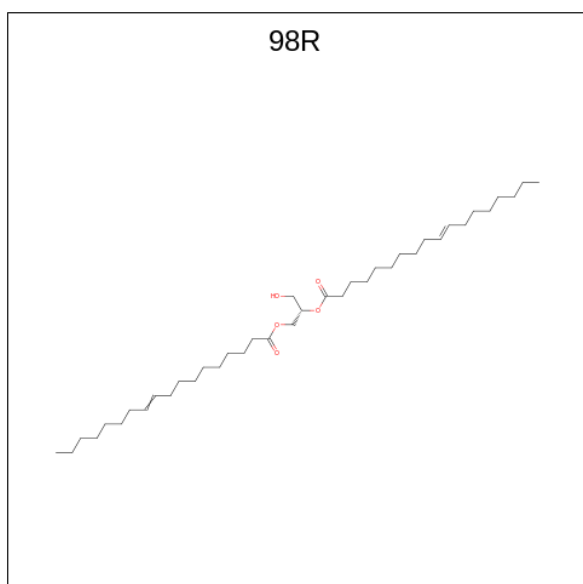
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	Cl	N	O	0
			26	21	1	3	1	
5	B	1	Total	C	Cl	N	O	0
			26	21	1	3	1	
5	C	1	Total	C	Cl	N	O	0
			26	21	1	3	1	
5	D	1	Total	C	Cl	N	O	0
			26	21	1	3	1	

- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	Total 46	C 36	N 1	O 8	P 1	0
6	B	1	Total 46	C 36	N 1	O 8	P 1	0
6	C	1	Total 46	C 36	N 1	O 8	P 1	0
6	D	1	Total 46	C 36	N 1	O 8	P 1	0

- Molecule 7 is [(2S)-2-[(E)-octadec-10-enoyl]oxy-3-oxidanyl-propyl] octadec-10-enoate (three-letter code: 98R) (formula: C₃₉H₇₂O₅).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total 80	C 70	O 10	0
7	A	1	Total 80	C 70	O 10	0
7	B	1	Total 80	C 70	O 10	0
7	B	1	Total 80	C 70	O 10	0

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82862	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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	7.189	Depositor
Minimum map value	-3.936	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.239	Depositor
Recommended contour level	0.96	Depositor
Map size (\AA)	292.59998, 292.59998, 292.59998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.045, 1.045, 1.045	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: CA, ZN, POV, HOR, Y01, 98R

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/5726	0.38	0/7735
1	B	0.26	0/5726	0.38	0/7735
1	C	0.26	0/5726	0.38	0/7735
1	D	0.26	0/5726	0.38	0/7735
All	All	0.26	0/22904	0.38	0/30940

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	5603	0	5585	113	0
1	B	5603	0	5585	109	0
1	C	5603	0	5585	110	0
1	D	5603	0	5585	112	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	140	0	196	25	0
4	B	140	0	196	26	0
4	C	140	0	196	27	0
4	D	140	0	196	27	0
5	A	26	0	0	0	0
5	B	26	0	0	0	0
5	C	26	0	0	0	0
5	D	26	0	0	0	0
6	A	46	0	64	2	0
6	B	46	0	64	3	0
6	C	46	0	64	3	0
6	D	46	0	64	2	0
7	A	80	0	0	2	0
7	B	80	0	0	2	0
All	All	23432	0	23380	432	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 9.

All (432) 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:879:VAL:HG11	1:C:884:LEU:HD22	1.35	1.09
1:B:884:LEU:HD22	1:D:879:VAL:HG11	1.35	1.07
1:A:884:LEU:HD22	1:C:879:VAL:HG11	1.35	1.06
1:A:879:VAL:HG11	1:D:884:LEU:HD22	1.35	1.05
4:A:1003:Y01:HAB1	4:A:1003:Y01:HAC3	1.52	0.92
4:C:1004:Y01:HAB1	4:C:1004:Y01:HAC3	1.52	0.91
4:D:1004:Y01:HAB1	4:D:1004:Y01:HAC3	1.52	0.91
4:B:1003:Y01:HAB1	4:B:1003:Y01:HAC3	1.52	0.91
1:B:884:LEU:HD22	1:D:879:VAL:CG1	2.12	0.79
1:B:879:VAL:CG1	1:C:884:LEU:HD22	2.12	0.78
1:A:884:LEU:HD22	1:C:879:VAL:CG1	2.12	0.78
1:A:879:VAL:CG1	1:D:884:LEU:HD22	2.12	0.78
1:B:728:ASN:HD21	1:D:730:SER:HB2	1.49	0.78
1:A:730:SER:HB2	1:D:728:ASN:HD21	1.49	0.77
1:B:730:SER:HB2	1:C:728:ASN:HD21	1.49	0.76
1:A:884:LEU:HG	1:C:887:ILE:CD1	2.16	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:ILE:CD1	1:D:884:LEU:HG	2.16	0.75
1:D:190:LYS:H	1:D:191:ARG:NH1	1.85	0.75
1:B:190:LYS:H	1:B:191:ARG:NH1	1.85	0.75
1:A:190:LYS:H	1:A:191:ARG:NH1	1.85	0.74
1:B:884:LEU:HG	1:D:887:ILE:CD1	2.16	0.74
1:B:887:ILE:CD1	1:C:884:LEU:HG	2.16	0.74
1:A:728:ASN:HD21	1:C:730:SER:HB2	1.49	0.74
1:C:190:LYS:H	1:C:191:ARG:NH1	1.85	0.74
1:D:880:ASN:H	1:D:880:ASN:HD22	1.36	0.73
1:A:880:ASN:HD22	1:A:880:ASN:H	1.36	0.73
4:B:1003:Y01:HAC2	4:B:1003:Y01:CAE	2.19	0.72
1:B:880:ASN:H	1:B:880:ASN:HD22	1.36	0.71
4:D:1004:Y01:CAE	4:D:1004:Y01:HAC2	2.19	0.71
4:C:1004:Y01:HAC2	4:C:1004:Y01:CAE	2.19	0.71
4:A:1003:Y01:HAC2	4:A:1003:Y01:CAE	2.20	0.71
1:C:880:ASN:HD22	1:C:880:ASN:H	1.36	0.70
1:A:884:LEU:HG	1:C:887:ILE:HD11	1.73	0.70
1:B:884:LEU:HG	1:D:887:ILE:HD11	1.73	0.69
1:B:887:ILE:HD11	1:C:884:LEU:HG	1.73	0.69
1:A:887:ILE:HD11	1:D:884:LEU:HG	1.73	0.67
4:B:1003:Y01:HAC2	4:B:1003:Y01:HAE3	1.77	0.66
4:D:1004:Y01:HAC2	4:D:1004:Y01:HAE3	1.77	0.65
4:C:1004:Y01:HAC2	4:C:1004:Y01:HAE3	1.77	0.64
4:A:1003:Y01:HAC2	4:A:1003:Y01:HAE3	1.77	0.64
1:A:888:LYS:HE2	1:C:886:GLU:OE2	1.98	0.64
1:B:886:GLU:OE2	1:C:888:LYS:HE2	1.98	0.63
1:B:888:LYS:HE2	1:D:886:GLU:OE2	1.98	0.63
1:D:98:GLU:OE1	1:D:101:ARG:NH1	2.31	0.63
1:A:886:GLU:OE2	1:D:888:LYS:HE2	1.98	0.63
1:C:98:GLU:OE1	1:C:101:ARG:NH1	2.31	0.62
1:A:884:LEU:HD11	1:C:887:ILE:HD12	1.82	0.62
1:B:887:ILE:HD12	1:C:884:LEU:HD11	1.81	0.62
1:A:410:VAL:HG11	4:A:1003:Y01:HAI	1.81	0.62
1:B:98:GLU:OE1	1:B:101:ARG:NH1	2.31	0.62
1:C:410:VAL:HG11	4:C:1004:Y01:HAI	1.81	0.62
1:A:98:GLU:OE1	1:A:101:ARG:NH1	2.31	0.62
1:A:887:ILE:HD12	1:D:884:LEU:HD11	1.81	0.62
1:B:884:LEU:HD11	1:D:887:ILE:HD12	1.82	0.62
1:B:879:VAL:CG2	1:C:880:ASN:O	2.48	0.62
1:D:410:VAL:HG11	4:D:1004:Y01:HAI	1.81	0.62
1:B:880:ASN:O	1:D:879:VAL:CG2	2.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:VAL:HG11	4:B:1003:Y01:HAI	1.81	0.61
1:A:458:VAL:HG22	1:D:650:ILE:HD13	1.83	0.61
1:A:884:LEU:HD11	1:C:887:ILE:CD1	2.31	0.61
1:A:650:ILE:HD13	1:C:458:VAL:HG22	1.83	0.61
1:A:887:ILE:CD1	1:D:884:LEU:HD11	2.31	0.61
1:A:879:VAL:CG2	1:D:880:ASN:O	2.48	0.61
1:B:884:LEU:HD11	1:D:887:ILE:CD1	2.31	0.61
1:B:458:VAL:HG22	1:C:650:ILE:HD13	1.83	0.60
1:B:887:ILE:CD1	1:C:884:LEU:HD11	2.31	0.60
1:A:880:ASN:O	1:C:879:VAL:CG2	2.48	0.60
1:B:650:ILE:HD13	1:D:458:VAL:HG22	1.83	0.60
1:B:880:ASN:H	1:B:880:ASN:ND2	1.98	0.60
1:B:884:LEU:CD1	1:D:887:ILE:CD1	2.80	0.60
1:A:442:LYS:NZ	1:A:756:GLU:O	2.33	0.60
1:A:884:LEU:CD1	1:C:887:ILE:CD1	2.80	0.59
1:A:887:ILE:CD1	1:D:884:LEU:CD1	2.80	0.59
1:A:887:ILE:CD1	1:D:884:LEU:CG	2.81	0.59
1:B:887:ILE:CD1	1:C:884:LEU:CD1	2.80	0.59
1:B:463:ASP:OD1	1:B:463:ASP:N	2.33	0.59
1:C:880:ASN:H	1:C:880:ASN:ND2	1.98	0.59
1:D:880:ASN:H	1:D:880:ASN:ND2	1.98	0.59
1:A:880:ASN:H	1:A:880:ASN:ND2	1.98	0.59
1:A:884:LEU:CG	1:C:887:ILE:CD1	2.81	0.59
1:C:223:ILE:HB	1:C:243:ALA:HB1	1.85	0.59
1:D:223:ILE:HB	1:D:243:ALA:HB1	1.85	0.59
1:A:879:VAL:HG11	1:D:884:LEU:CD2	2.24	0.59
1:A:223:ILE:HB	1:A:243:ALA:HB1	1.85	0.58
1:B:884:LEU:CG	1:D:887:ILE:CD1	2.81	0.58
1:B:887:ILE:CD1	1:C:884:LEU:CG	2.81	0.58
1:A:887:ILE:HD12	1:D:884:LEU:CG	2.34	0.58
4:B:1006:Y01:HAI	4:B:1008:Y01:HAD3	1.86	0.58
1:B:223:ILE:HB	1:B:243:ALA:HB1	1.85	0.57
4:A:1006:Y01:HAI	4:A:1008:Y01:HAD3	1.86	0.57
1:B:330:VAL:HG21	1:B:376:LYS:HB3	1.86	0.57
1:A:884:LEU:CG	1:C:887:ILE:HD12	2.34	0.57
4:D:1007:Y01:HAI	4:D:1009:Y01:HAD3	1.86	0.57
1:C:330:VAL:HG21	1:C:376:LYS:HB3	1.86	0.57
1:B:884:LEU:CG	1:D:887:ILE:HD12	2.34	0.57
1:C:442:LYS:NZ	1:C:756:GLU:O	2.33	0.57
1:A:659:TYR:HB3	1:A:662:ALA:HB3	1.87	0.57
4:C:1007:Y01:HAI	4:C:1009:Y01:HAD3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:VAL:HG21	1:D:376:LYS:HB3	1.86	0.57
1:D:463:ASP:OD1	1:D:463:ASP:N	2.33	0.56
1:B:887:ILE:HD12	1:C:884:LEU:CG	2.34	0.56
4:B:1003:Y01:HAE2	4:B:1003:Y01:HAO2	1.88	0.56
1:D:659:TYR:HB3	1:D:662:ALA:HB3	1.87	0.56
4:D:1004:Y01:HAE2	4:D:1004:Y01:HAO2	1.88	0.56
1:B:880:ASN:HD22	1:B:880:ASN:N	1.99	0.56
1:D:442:LYS:NZ	1:D:756:GLU:O	2.33	0.56
1:A:330:VAL:HG21	1:A:376:LYS:HB3	1.86	0.56
1:C:463:ASP:OD1	1:C:463:ASP:N	2.33	0.56
1:C:659:TYR:HB3	1:C:662:ALA:HB3	1.87	0.56
1:B:659:TYR:HB3	1:B:662:ALA:HB3	1.87	0.56
1:A:634:ILE:HD11	1:D:720:LEU:HD23	1.89	0.55
1:A:884:LEU:CD2	1:C:879:VAL:CG1	2.84	0.55
4:C:1004:Y01:HAE2	4:C:1004:Y01:HAO2	1.88	0.55
4:A:1003:Y01:HAO2	4:A:1003:Y01:HAE2	1.88	0.55
1:B:884:LEU:CD2	1:D:879:VAL:HG11	2.24	0.55
1:B:720:LEU:HD23	1:D:634:ILE:HD11	1.89	0.55
1:D:889:GLN:OE1	1:D:889:GLN:HA	2.06	0.55
1:C:889:GLN:HA	1:C:889:GLN:OE1	2.06	0.55
4:B:1003:Y01:CAE	4:B:1003:Y01:CAC	2.85	0.55
1:B:739:ASP:OD2	1:B:743:LYS:NZ	2.40	0.54
1:B:884:LEU:CD2	1:D:879:VAL:CG1	2.84	0.54
1:D:739:ASP:OD2	1:D:743:LYS:NZ	2.40	0.54
7:B:1009:98R:C32	7:B:1009:98R:C3	2.85	0.54
1:A:720:LEU:HD23	1:C:634:ILE:HD11	1.89	0.54
1:A:879:VAL:CG1	1:D:884:LEU:CD2	2.84	0.54
1:A:889:GLN:OE1	1:A:889:GLN:HA	2.06	0.54
1:D:663:LYS:HB3	1:D:663:LYS:HZ3	1.72	0.54
1:B:889:GLN:OE1	1:B:889:GLN:HA	2.06	0.54
1:A:702:ASN:HD22	4:A:1010:Y01:HAL2	1.73	0.54
1:B:634:ILE:HD11	1:C:720:LEU:HD23	1.89	0.54
1:A:739:ASP:OD2	1:A:743:LYS:NZ	2.40	0.54
7:A:1011:98R:C3	7:A:1011:98R:C32	2.85	0.54
1:A:485:ARG:NH1	1:A:586:TRP:CE2	2.76	0.53
7:A:1009:98R:C32	7:A:1009:98R:C3	2.85	0.53
1:B:485:ARG:NH1	1:B:586:TRP:CE2	2.76	0.53
1:A:880:ASN:ND2	1:A:883:GLU:HB2	2.24	0.53
1:B:663:LYS:NZ	1:B:663:LYS:HB3	2.24	0.53
1:B:702:ASN:HD22	4:B:1010:Y01:HAL2	1.73	0.53
1:C:739:ASP:OD2	1:C:743:LYS:NZ	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:663:LYS:HB3	1:D:663:LYS:NZ	2.24	0.53
7:B:1011:98R:C32	7:B:1011:98R:C3	2.85	0.53
1:D:485:ARG:NH1	1:D:586:TRP:CE2	2.76	0.53
1:C:880:ASN:ND2	1:C:883:GLU:HB2	2.24	0.53
4:C:1004:Y01:CAE	4:C:1004:Y01:CAC	2.85	0.53
1:C:485:ARG:NH1	1:C:586:TRP:CE2	2.76	0.53
1:A:887:ILE:HD12	1:D:884:LEU:CD1	2.39	0.53
1:A:258:CYS:O	1:A:262:GLN:HG2	2.09	0.53
1:C:702:ASN:HD22	4:C:1001:Y01:HAL2	1.73	0.53
1:D:880:ASN:ND2	1:D:883:GLU:HB2	2.24	0.52
1:D:702:ASN:HD22	4:D:1001:Y01:HAL2	1.73	0.52
1:C:886:GLU:O	1:C:886:GLU:HG2	2.10	0.52
1:A:398:LEU:HD23	1:A:401:GLN:HG3	1.92	0.52
1:A:663:LYS:NZ	1:A:663:LYS:HB3	2.24	0.52
1:C:663:LYS:NZ	1:C:663:LYS:HB3	2.24	0.52
1:D:398:LEU:HD23	1:D:401:GLN:HG3	1.92	0.52
1:D:542:ILE:HD12	4:D:1009:Y01:HAU2	1.92	0.52
1:B:542:ILE:HD12	4:B:1008:Y01:HAU2	1.92	0.52
1:B:887:ILE:HD12	1:C:884:LEU:CD1	2.39	0.52
1:C:398:LEU:HD23	1:C:401:GLN:HG3	1.92	0.52
1:A:542:ILE:HD12	4:A:1008:Y01:HAU2	1.92	0.52
1:A:884:LEU:CD1	1:C:887:ILE:HD12	2.39	0.52
1:B:398:LEU:HD23	1:B:401:GLN:HG3	1.92	0.52
1:B:614:LEU:HG	1:B:620:PHE:HB3	1.91	0.52
1:C:258:CYS:O	1:C:262:GLN:HG2	2.09	0.52
1:A:191:ARG:HE	1:A:238:LEU:HD22	1.75	0.52
1:A:507:TRP:HD1	1:A:765:ASN:ND2	2.08	0.52
1:B:139:LEU:O	1:B:143:ASN:ND2	2.41	0.52
1:C:614:LEU:HG	1:C:620:PHE:HB3	1.91	0.52
1:D:191:ARG:HE	1:D:238:LEU:HD22	1.75	0.52
1:D:258:CYS:O	1:D:262:GLN:HG2	2.09	0.52
1:B:879:VAL:CG1	1:C:884:LEU:CD2	2.84	0.52
1:B:880:ASN:ND2	1:B:883:GLU:HB2	2.24	0.52
1:B:886:GLU:HG2	1:B:886:GLU:O	2.10	0.52
1:C:574:ASP:N	1:C:574:ASP:OD1	2.43	0.52
1:D:886:GLU:O	1:D:886:GLU:HG2	2.10	0.52
1:B:574:ASP:OD1	1:B:574:ASP:N	2.43	0.52
1:C:191:ARG:HE	1:C:238:LEU:HD22	1.75	0.52
1:C:542:ILE:HD12	4:C:1009:Y01:HAU2	1.92	0.52
1:D:507:TRP:HD1	1:D:765:ASN:ND2	2.08	0.52
1:B:191:ARG:HE	1:B:238:LEU:HD22	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ASP:OD1	1:A:574:ASP:N	2.43	0.51
4:A:1003:Y01:CAE	4:A:1003:Y01:CAC	2.85	0.51
4:D:1004:Y01:CAE	4:D:1004:Y01:CAC	2.85	0.51
1:B:884:LEU:CD1	1:D:887:ILE:HD12	2.39	0.51
1:A:886:GLU:OE2	1:D:888:LYS:CE	2.58	0.51
1:A:886:GLU:O	1:A:886:GLU:HG2	2.10	0.51
1:B:258:CYS:O	1:B:262:GLN:HG2	2.09	0.51
1:B:888:LYS:CE	1:D:886:GLU:OE2	2.58	0.51
1:D:574:ASP:OD1	1:D:574:ASP:N	2.43	0.51
1:C:139:LEU:O	1:C:143:ASN:ND2	2.41	0.51
1:D:880:ASN:HD22	1:D:880:ASN:N	1.99	0.51
1:A:888:LYS:CE	1:C:886:GLU:OE2	2.58	0.51
1:C:507:TRP:HD1	1:C:765:ASN:ND2	2.08	0.51
1:D:614:LEU:HG	1:D:620:PHE:HB3	1.91	0.51
1:A:614:LEU:HG	1:A:620:PHE:HB3	1.91	0.51
1:A:880:ASN:HD22	1:A:880:ASN:N	1.99	0.51
1:A:463:ASP:OD1	1:A:463:ASP:N	2.33	0.51
4:D:1004:Y01:HAC2	4:D:1004:Y01:HAE2	1.93	0.51
1:B:507:TRP:HD1	1:B:765:ASN:ND2	2.08	0.50
1:B:886:GLU:OE2	1:C:888:LYS:CE	2.58	0.50
1:B:509:GLU:HG3	1:B:534:LEU:HD12	1.94	0.50
1:C:489:SER:HB3	1:C:548:PHE:HA	1.94	0.50
1:D:489:SER:HB3	1:D:548:PHE:HA	1.94	0.50
1:A:489:SER:HB3	1:A:548:PHE:HA	1.94	0.50
1:B:440:PHE:HE1	4:B:1003:Y01:OAF	1.95	0.50
1:B:442:LYS:NZ	1:B:756:GLU:O	2.33	0.50
1:D:440:PHE:HE1	4:D:1004:Y01:OAF	1.95	0.50
1:B:489:SER:HB3	1:B:548:PHE:HA	1.94	0.50
1:D:509:GLU:HG3	1:D:534:LEU:HD12	1.94	0.49
1:C:485:ARG:HD3	1:C:579:TYR:HA	1.94	0.49
1:A:440:PHE:HE1	4:A:1003:Y01:OAF	1.95	0.49
1:B:485:ARG:HD3	1:B:579:TYR:HA	1.94	0.49
1:C:509:GLU:HG3	1:C:534:LEU:HD12	1.94	0.49
1:C:880:ASN:HD22	1:C:880:ASN:N	1.99	0.49
4:B:1003:Y01:HAC2	4:B:1003:Y01:HAE2	1.93	0.49
1:C:440:PHE:HE1	4:C:1004:Y01:OAF	1.95	0.49
1:A:505:MET:HG3	1:A:762:VAL:HG11	1.95	0.49
1:A:102:PHE:HD1	1:A:117:MET:HE3	1.78	0.48
1:A:485:ARG:HD3	1:A:579:TYR:HA	1.94	0.48
1:A:509:GLU:HG3	1:A:534:LEU:HD12	1.94	0.48
1:C:505:MET:HG3	1:C:762:VAL:HG11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:PHE:HD1	1:D:117:MET:HE3	1.78	0.48
1:D:485:ARG:HD3	1:D:579:TYR:HA	1.94	0.48
4:A:1008:Y01:HAE2	4:A:1008:Y01:HBB	1.66	0.48
1:B:102:PHE:HD1	1:B:117:MET:HE3	1.77	0.48
1:D:448:ALA:O	1:D:451:THR:HG22	2.14	0.48
1:B:505:MET:HG3	1:B:762:VAL:HG11	1.95	0.48
1:C:448:ALA:O	1:C:451:THR:HG22	2.14	0.48
1:D:139:LEU:O	1:D:143:ASN:ND2	2.41	0.48
1:D:505:MET:HG3	1:D:762:VAL:HG11	1.95	0.48
1:A:448:ALA:O	1:A:451:THR:HG22	2.14	0.48
1:C:102:PHE:HD1	1:C:117:MET:HE3	1.79	0.48
4:D:1004:Y01:OAG	4:D:1004:Y01:HAR1	2.14	0.48
4:A:1003:Y01:OAG	4:A:1003:Y01:HAR1	2.14	0.47
1:A:111:ILE:HG12	1:A:148:ILE:HG13	1.97	0.47
1:A:886:GLU:OE2	1:D:888:LYS:NZ	2.48	0.47
1:B:117:MET:HG2	1:B:121:CYS:SG	2.55	0.47
1:B:884:LEU:HG	1:D:887:ILE:HD12	1.94	0.47
1:C:431:LYS:HE2	1:C:435:ILE:HD11	1.96	0.47
1:C:613:ILE:HG22	4:C:1004:Y01:HAT1	1.97	0.47
6:C:1008:POV:H15A	6:C:1008:POV:H11A	1.69	0.47
1:D:117:MET:HG2	1:D:121:CYS:SG	2.55	0.47
1:A:139:LEU:O	1:A:143:ASN:ND2	2.41	0.47
1:B:448:ALA:O	1:B:451:THR:HG22	2.14	0.47
1:B:663:LYS:HB3	1:B:663:LYS:HZ3	1.78	0.47
1:C:117:MET:HG2	1:C:121:CYS:SG	2.55	0.47
1:B:451:THR:HB	4:B:1003:Y01:CAQ	2.45	0.47
1:B:878:GLU:OE1	1:C:878:GLU:OE2	2.33	0.47
1:D:451:THR:HB	4:D:1004:Y01:CAQ	2.45	0.47
4:C:1004:Y01:OAG	4:C:1004:Y01:HAR1	2.14	0.47
1:A:117:MET:HG2	1:A:121:CYS:SG	2.55	0.46
1:A:431:LYS:HE2	1:A:435:ILE:HD11	1.96	0.46
1:A:888:LYS:NZ	1:C:886:GLU:OE2	2.48	0.46
1:B:613:ILE:HG22	4:B:1003:Y01:HAT1	1.97	0.46
4:D:1009:Y01:HAE2	4:D:1009:Y01:HBB	1.65	0.46
1:D:111:ILE:HG12	1:D:148:ILE:HG13	1.97	0.46
1:A:451:THR:HB	4:A:1003:Y01:CAQ	2.45	0.46
1:B:111:ILE:HG12	1:B:148:ILE:HG13	1.97	0.46
1:B:888:LYS:NZ	1:D:886:GLU:OE2	2.48	0.46
1:C:880:ASN:ND2	1:C:880:ASN:N	2.60	0.46
4:C:1004:Y01:HAC2	4:C:1004:Y01:HAE2	1.93	0.46
4:B:1003:Y01:HAR1	4:B:1003:Y01:OAG	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:THR:HB	4:C:1004:Y01:CAQ	2.45	0.46
1:A:878:GLU:OE2	1:C:878:GLU:OE1	2.33	0.46
4:A:1010:Y01:HBB	4:A:1010:Y01:HAE2	1.70	0.46
1:B:431:LYS:HE2	1:B:435:ILE:HD11	1.96	0.46
4:C:1004:Y01:HAN1	4:C:1004:Y01:HBB	1.40	0.46
1:A:663:LYS:HB3	1:A:663:LYS:HZ3	1.80	0.46
1:D:431:LYS:HE2	1:D:435:ILE:HD11	1.96	0.46
1:B:878:GLU:OE2	1:D:878:GLU:OE1	2.33	0.46
1:A:613:ILE:HG22	4:A:1003:Y01:HAT1	1.97	0.46
4:A:1003:Y01:HAC2	4:A:1003:Y01:HAE2	1.93	0.46
1:B:886:GLU:OE2	1:C:888:LYS:NZ	2.48	0.46
1:C:702:ASN:ND2	4:C:1001:Y01:HAL2	2.31	0.46
4:B:1010:Y01:HAP1	4:B:1010:Y01:HAO1	1.70	0.46
4:C:1001:Y01:HAP1	4:C:1001:Y01:HAO1	1.70	0.46
1:D:613:ILE:HG22	4:D:1004:Y01:HAT1	1.97	0.46
1:D:880:ASN:ND2	1:D:880:ASN:N	2.60	0.46
1:A:878:GLU:OE1	1:D:878:GLU:OE2	2.33	0.45
1:A:384:GLN:HE21	1:A:746:ARG:HH21	1.64	0.45
4:B:1008:Y01:HAJ1	4:B:1008:Y01:HAC3	1.66	0.45
1:D:384:GLN:HE21	1:D:746:ARG:HH21	1.64	0.45
1:C:111:ILE:HG12	1:C:148:ILE:HG13	1.97	0.45
6:D:1008:POV:H15A	6:D:1008:POV:H11A	1.69	0.45
1:B:702:ASN:ND2	4:B:1010:Y01:HAL2	2.31	0.45
4:B:1003:Y01:HAC1	4:B:1003:Y01:HAP1	1.72	0.45
1:C:360:ARG:NH1	1:C:754:PHE:O	2.44	0.45
4:C:1009:Y01:HAD2	4:C:1009:Y01:HAS2	1.77	0.45
4:A:1003:Y01:HBA	6:D:1008:POV:H31C	1.98	0.45
1:B:183:HIS:CG	1:B:184:PRO:HD2	2.52	0.45
6:B:1007:POV:H39	6:B:1007:POV:H36	1.89	0.45
1:C:183:HIS:CG	1:C:184:PRO:HD2	2.52	0.45
4:C:1001:Y01:HBB	4:C:1001:Y01:HAE2	1.70	0.45
6:C:1008:POV:H39	6:C:1008:POV:H36	1.89	0.45
1:D:183:HIS:CG	1:D:184:PRO:HD2	2.52	0.45
1:D:363:LEU:HD11	1:D:390:ILE:HD13	1.99	0.45
1:A:208:ALA:HA	1:A:214:THR:HG22	2.00	0.44
1:C:533:MET:HB3	1:C:605:LEU:HB3	2.00	0.44
1:D:533:MET:HB3	1:D:605:LEU:HB3	2.00	0.44
1:A:360:ARG:NH1	1:A:754:PHE:O	2.44	0.44
1:B:338:ASN:HB2	1:C:265:ASP:OD2	2.18	0.44
1:B:349:ASP:O	1:B:353:LEU:HG	2.18	0.44
1:B:363:LEU:HD11	1:B:390:ILE:HD13	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:HD22	1:C:158:LEU:HD21	1.99	0.44
1:D:360:ARG:NH1	1:D:754:PHE:O	2.44	0.44
1:A:265:ASP:OD2	1:C:338:ASN:HB2	2.18	0.44
6:A:1007:POV:H31C	4:C:1004:Y01:HBA	1.98	0.44
1:B:728:ASN:O	1:B:732:GLN:HG2	2.18	0.44
1:A:363:LEU:HD11	1:A:390:ILE:HD13	1.99	0.44
1:C:349:ASP:O	1:C:353:LEU:HG	2.18	0.44
1:D:137:LEU:HD22	1:D:158:LEU:HD21	1.99	0.44
6:B:1007:POV:H31C	4:D:1004:Y01:HBA	1.98	0.44
1:C:384:GLN:HE21	1:C:746:ARG:HH21	1.64	0.44
1:D:208:ALA:HA	1:D:214:THR:HG22	1.99	0.44
1:D:376:LYS:HG3	1:D:740:VAL:HG21	2.00	0.44
4:D:1004:Y01:HAN1	4:D:1004:Y01:HBB	1.40	0.44
1:A:338:ASN:HB2	1:D:265:ASP:OD2	2.18	0.44
1:A:376:LYS:HG3	1:A:740:VAL:HG21	2.00	0.44
1:A:702:ASN:ND2	4:A:1010:Y01:HAL2	2.31	0.44
1:B:384:GLN:HE21	1:B:746:ARG:HH21	1.64	0.44
1:C:208:ALA:HA	1:C:214:THR:HG22	1.99	0.44
1:D:349:ASP:O	1:D:353:LEU:HG	2.18	0.44
1:D:702:ASN:ND2	4:D:1001:Y01:HAL2	2.31	0.44
1:B:533:MET:HB3	1:B:605:LEU:HB3	2.00	0.44
1:A:533:MET:HB3	1:A:605:LEU:HB3	2.00	0.44
1:A:728:ASN:O	1:A:732:GLN:HG2	2.18	0.43
6:A:1007:POV:H15A	6:A:1007:POV:H11A	1.69	0.43
4:B:1003:Y01:HAE3	4:B:1003:Y01:CAC	2.47	0.43
1:D:592:GLN:NE2	1:D:596:GLU:OE2	2.50	0.43
1:B:614:LEU:HD12	1:B:614:LEU:HA	1.88	0.43
4:B:1003:Y01:HBA	6:C:1008:POV:H31C	1.98	0.43
1:C:363:LEU:HD11	1:C:390:ILE:HD13	1.99	0.43
4:C:1009:Y01:HAC3	4:C:1009:Y01:HAJ1	1.66	0.43
1:B:137:LEU:HD22	1:B:158:LEU:HD21	1.99	0.43
4:B:1003:Y01:HAN1	4:B:1003:Y01:HBB	1.40	0.43
1:A:349:ASP:O	1:A:353:LEU:HG	2.18	0.43
1:C:728:ASN:O	1:C:732:GLN:HG2	2.18	0.43
1:D:728:ASN:O	1:D:732:GLN:HG2	2.18	0.43
1:A:880:ASN:O	1:C:879:VAL:HG22	2.18	0.43
1:C:376:LYS:HG3	1:C:740:VAL:HG21	2.00	0.43
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.90	0.43
1:B:265:ASP:OD2	1:D:338:ASN:HB2	2.18	0.43
1:C:357:ASP:HB2	1:C:360:ARG:HH21	1.84	0.43
1:C:592:GLN:NE2	1:C:596:GLU:OE2	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1007:Y01:HAD2	4:D:1007:Y01:HAS2	1.80	0.43
1:A:183:HIS:CG	1:A:184:PRO:HD2	2.52	0.43
1:A:357:ASP:HB2	1:A:360:ARG:HH21	1.84	0.43
1:B:208:ALA:HA	1:B:214:THR:HG22	2.00	0.43
1:D:357:ASP:HB2	1:D:360:ARG:HH21	1.84	0.43
4:D:1004:Y01:HAE1	4:D:1004:Y01:HBD	1.78	0.43
4:A:1008:Y01:HAD2	4:A:1008:Y01:HAS2	1.77	0.43
1:B:357:ASP:HB2	1:B:360:ARG:HH21	1.84	0.43
1:B:376:LYS:HG3	1:B:740:VAL:HG21	2.00	0.43
1:B:703:ILE:HD12	1:D:601:ILE:HD11	2.01	0.43
4:C:1004:Y01:HAP1	4:C:1004:Y01:HAC1	1.72	0.43
1:D:312:LYS:HZ2	1:D:315:LYS:HZ2	1.67	0.43
1:C:663:LYS:HB3	1:C:663:LYS:HZ3	1.83	0.43
1:A:592:GLN:NE2	1:A:596:GLU:OE2	2.50	0.42
1:A:703:ILE:HD12	1:C:601:ILE:HD11	2.01	0.42
1:A:879:VAL:HG22	1:D:880:ASN:O	2.18	0.42
1:B:507:TRP:HD1	1:B:765:ASN:HD22	1.66	0.42
1:B:880:ASN:O	1:D:879:VAL:HG22	2.18	0.42
1:D:614:LEU:HD12	1:D:614:LEU:HA	1.88	0.42
1:A:191:ARG:H	1:A:191:ARG:HG2	1.57	0.42
1:A:507:TRP:HD1	1:A:765:ASN:HD22	1.66	0.42
1:A:601:ILE:HD11	1:D:703:ILE:HD12	2.01	0.42
1:B:592:GLN:NE2	1:B:596:GLU:OE2	2.50	0.42
1:C:366:LEU:HD23	1:C:366:LEU:HA	1.90	0.42
4:B:1008:Y01:HAU2	4:B:1008:Y01:HAC1	2.02	0.42
1:B:601:ILE:HD11	1:C:703:ILE:HD12	2.01	0.42
1:C:191:ARG:HD3	1:C:243:ALA:HB2	2.02	0.42
1:C:454:LEU:O	1:C:458:VAL:HG23	2.20	0.42
1:D:507:TRP:HD1	1:D:765:ASN:HD22	1.66	0.42
1:B:191:ARG:H	1:B:191:ARG:HG2	1.57	0.42
1:B:366:LEU:HD23	1:B:366:LEU:HA	1.90	0.42
4:B:1008:Y01:HAE2	4:B:1008:Y01:HBB	1.66	0.42
1:A:137:LEU:HD22	1:A:158:LEU:HD21	1.99	0.42
4:B:1003:Y01:HAE1	4:B:1003:Y01:HBD	1.78	0.42
1:D:366:LEU:HD23	1:D:366:LEU:HA	1.90	0.42
4:D:1009:Y01:HAU2	4:D:1009:Y01:HAC1	2.02	0.42
1:A:454:LEU:O	1:A:458:VAL:HG23	2.20	0.42
1:D:760:LEU:HA	1:D:761:PRO:HD3	1.86	0.42
1:A:191:ARG:HD3	1:A:243:ALA:HB2	2.02	0.42
1:A:440:PHE:CE1	4:A:1003:Y01:OAF	2.73	0.42
1:A:642:ILE:HD13	1:A:642:ILE:HA	1.94	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:TRP:HD1	1:C:765:ASN:HD22	1.66	0.42
4:C:1009:Y01:HAE2	4:C:1009:Y01:HBB	1.66	0.42
1:B:320:LYS:HE3	1:B:320:LYS:HB2	1.79	0.41
1:B:542:ILE:HD12	4:B:1008:Y01:HAC1	2.03	0.41
1:A:398:LEU:HD23	1:A:398:LEU:HA	1.92	0.41
4:A:1003:Y01:HAC1	4:A:1003:Y01:HAP1	1.72	0.41
1:C:190:LYS:H	1:C:191:ARG:HH11	1.66	0.41
4:C:1004:Y01:HAE3	4:C:1004:Y01:CAC	2.47	0.41
1:D:454:LEU:O	1:D:458:VAL:HG23	2.20	0.41
4:D:1004:Y01:HAC3	4:D:1004:Y01:CAB	2.36	0.41
1:A:542:ILE:HD12	4:A:1008:Y01:HAC1	2.03	0.41
4:D:1004:Y01:HAC1	4:D:1004:Y01:HAP1	1.72	0.41
4:C:1009:Y01:HAU2	4:C:1009:Y01:HAC1	2.02	0.41
1:D:320:LYS:HE3	1:D:320:LYS:HB2	1.79	0.41
1:B:191:ARG:HD3	1:B:243:ALA:HB2	2.02	0.41
1:B:454:LEU:O	1:B:458:VAL:HG23	2.20	0.41
6:B:1007:POV:H11A	6:B:1007:POV:H15A	1.69	0.41
1:C:440:PHE:CE1	4:C:1004:Y01:OAF	2.73	0.41
1:C:542:ILE:HD12	4:C:1009:Y01:HAC1	2.03	0.41
1:D:542:ILE:HD12	4:D:1009:Y01:HAC1	2.03	0.41
1:A:760:LEU:HA	1:A:761:PRO:HD3	1.86	0.41
1:A:174:VAL:HG11	1:A:233:GLU:HG2	2.03	0.41
1:A:610:ILE:HG22	1:A:614:LEU:HD13	2.03	0.41
1:A:880:ASN:ND2	1:A:880:ASN:N	2.60	0.41
4:A:1008:Y01:HAU2	4:A:1008:Y01:HAC1	2.02	0.41
1:C:191:ARG:H	1:C:191:ARG:HG2	1.57	0.41
4:D:1004:Y01:HAE3	4:D:1004:Y01:CAC	2.47	0.41
4:A:1003:Y01:HAS2	4:A:1003:Y01:HAE1	1.94	0.41
1:B:209:TYR:HD2	1:B:209:TYR:H	1.69	0.41
1:C:174:VAL:HG11	1:C:233:GLU:HG2	2.03	0.40
1:D:398:LEU:HD13	1:D:440:PHE:HE2	1.86	0.40
4:D:1009:Y01:HAD2	4:D:1009:Y01:HAS2	1.77	0.40
1:B:360:ARG:NH1	1:B:754:PHE:O	2.44	0.40
1:C:297:ALA:HB3	1:C:329:VAL:HG23	2.04	0.40
1:D:398:LEU:HD23	1:D:398:LEU:HA	1.92	0.40
1:B:297:ALA:HB3	1:B:329:VAL:HG23	2.04	0.40
1:B:440:PHE:CE1	4:B:1003:Y01:OAF	2.73	0.40
1:B:905:ASN:ND2	1:C:906:THR:HG21	2.36	0.40
1:D:191:ARG:HD3	1:D:243:ALA:HB2	2.02	0.40
1:D:209:TYR:HD2	1:D:209:TYR:H	1.69	0.40
4:D:1001:Y01:HAE2	4:D:1001:Y01:HBB	1.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PRO:HD2	1:A:390:ILE:HD11	2.04	0.40
1:A:698:LYS:HA	1:A:698:LYS:HD3	1.91	0.40
1:A:906:THR:HG21	1:C:905:ASN:ND2	2.36	0.40
4:A:1003:Y01:HBB	4:A:1003:Y01:HAN1	1.40	0.40
1:C:450:PHE:HE2	1:C:610:ILE:HG12	1.86	0.40
1:C:880:ASN:ND2	1:C:883:GLU:OE1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	686/931 (74%)	669 (98%)	17 (2%)	0	100	100
1	B	686/931 (74%)	669 (98%)	17 (2%)	0	100	100
1	C	686/931 (74%)	669 (98%)	17 (2%)	0	100	100
1	D	686/931 (74%)	669 (98%)	17 (2%)	0	100	100
All	All	2744/3724 (74%)	2676 (98%)	68 (2%)	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	599/813 (74%)	585 (98%)	14 (2%)	50	80
1	B	599/813 (74%)	585 (98%)	14 (2%)	50	80
1	C	599/813 (74%)	585 (98%)	14 (2%)	50	80
1	D	599/813 (74%)	585 (98%)	14 (2%)	50	80
All	All	2396/3252 (74%)	2340 (98%)	56 (2%)	53	80

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	LEU
1	A	191	ARG
1	A	205	ASP
1	A	209	TYR
1	A	417	LEU
1	A	463	ASP
1	A	468	THR
1	A	501	TRP
1	A	537	PHE
1	A	558	ILE
1	A	614	LEU
1	A	627	LEU
1	A	758	ARG
1	A	880	ASN
1	B	166	LEU
1	B	191	ARG
1	B	205	ASP
1	B	209	TYR
1	B	417	LEU
1	B	463	ASP
1	B	468	THR
1	B	501	TRP
1	B	537	PHE
1	B	558	ILE
1	B	614	LEU
1	B	627	LEU
1	B	758	ARG
1	B	880	ASN
1	C	166	LEU
1	C	191	ARG
1	C	205	ASP
1	C	209	TYR
1	C	417	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	463	ASP
1	C	468	THR
1	C	501	TRP
1	C	537	PHE
1	C	558	ILE
1	C	614	LEU
1	C	627	LEU
1	C	758	ARG
1	C	880	ASN
1	D	166	LEU
1	D	191	ARG
1	D	205	ASP
1	D	209	TYR
1	D	417	LEU
1	D	463	ASP
1	D	468	THR
1	D	501	TRP
1	D	537	PHE
1	D	558	ILE
1	D	614	LEU
1	D	627	LEU
1	D	758	ARG
1	D	880	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	728	ASN
1	A	880	ASN
1	A	905	ASN
1	B	728	ASN
1	B	880	ASN
1	B	905	ASN
1	C	728	ASN
1	C	880	ASN
1	C	905	ASN
1	D	728	ASN
1	D	880	ASN
1	D	905	ASN

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](#)

Of 40 ligands modelled in this entry, 12 are monoatomic - leaving 28 for Mogul analysis.

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
4	Y01	A	1010	-	38,38,38	1.00	2 (5%)	57,57,57	1.36	7 (12%)
4	Y01	B	1008	-	38,38,38	0.97	2 (5%)	57,57,57	1.51	12 (21%)
6	POV	D	1008	-	45,45,51	1.01	2 (4%)	51,53,59	1.05	3 (5%)
4	Y01	A	1006	-	38,38,38	0.96	1 (2%)	57,57,57	1.20	5 (8%)
4	Y01	A	1008	-	38,38,38	0.97	2 (5%)	57,57,57	1.51	12 (21%)
4	Y01	D	1004	-	38,38,38	1.03	2 (5%)	57,57,57	1.74	17 (29%)
4	Y01	C	1001	-	38,38,38	1.00	2 (5%)	57,57,57	1.36	7 (12%)
6	POV	C	1008	-	45,45,51	1.01	2 (4%)	51,53,59	1.05	3 (5%)
4	Y01	D	1009	-	38,38,38	0.97	1 (2%)	57,57,57	1.51	12 (21%)
5	HOR	B	1004	-	29,29,29	1.92	5 (17%)	35,41,41	1.32	4 (11%)
4	Y01	D	1001	-	38,38,38	1.00	2 (5%)	57,57,57	1.36	7 (12%)
4	Y01	C	1009	-	38,38,38	0.97	2 (5%)	57,57,57	1.51	12 (21%)
7	98R	A	1011	-	39,39,43	0.97	2 (5%)	41,41,45	1.09	2 (4%)
6	POV	A	1007	-	45,45,51	1.01	2 (4%)	51,53,59	1.05	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	98R	A	1009	-	39,39,43	0.97	2 (5%)	41,41,45	1.09	2 (4%)
4	Y01	B	1003	-	38,38,38	1.03	2 (5%)	57,57,57	1.74	17 (29%)
4	Y01	D	1007	-	38,38,38	0.96	1 (2%)	57,57,57	1.20	5 (8%)
5	HOR	C	1005	-	29,29,29	1.92	5 (17%)	35,41,41	1.32	4 (11%)
6	POV	B	1007	-	45,45,51	1.01	2 (4%)	51,53,59	1.05	3 (5%)
4	Y01	B	1006	-	38,38,38	0.96	1 (2%)	57,57,57	1.20	5 (8%)
4	Y01	C	1007	-	38,38,38	0.96	1 (2%)	57,57,57	1.20	4 (7%)
7	98R	B	1009	-	39,39,43	0.97	2 (5%)	41,41,45	1.09	2 (4%)
4	Y01	A	1003	-	38,38,38	1.03	2 (5%)	57,57,57	1.74	17 (29%)
5	HOR	D	1005	-	29,29,29	1.92	5 (17%)	35,41,41	1.32	4 (11%)
4	Y01	B	1010	-	38,38,38	1.00	2 (5%)	57,57,57	1.36	6 (10%)
7	98R	B	1011	-	39,39,43	0.97	2 (5%)	41,41,45	1.09	2 (4%)
4	Y01	C	1004	-	38,38,38	1.03	2 (5%)	57,57,57	1.74	17 (29%)
5	HOR	A	1004	-	29,29,29	1.92	5 (17%)	35,41,41	1.32	4 (11%)

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
4	Y01	A	1010	-	-	7/19/77/77	0/4/4/4
4	Y01	B	1008	-	-	9/19/77/77	0/4/4/4
6	POV	D	1008	-	-	13/49/49/55	-
4	Y01	A	1006	-	-	9/19/77/77	0/4/4/4
4	Y01	A	1008	-	-	9/19/77/77	0/4/4/4
4	Y01	D	1004	-	-	12/19/77/77	0/4/4/4
4	Y01	C	1001	-	-	7/19/77/77	0/4/4/4
6	POV	C	1008	-	-	13/49/49/55	-
4	Y01	D	1009	-	-	9/19/77/77	0/4/4/4
5	HOR	B	1004	-	-	1/10/32/32	0/4/4/4
4	Y01	D	1001	-	-	7/19/77/77	0/4/4/4
4	Y01	C	1009	-	-	9/19/77/77	0/4/4/4
7	98R	A	1011	-	-	17/41/41/45	-
6	POV	A	1007	-	-	13/49/49/55	-
7	98R	A	1009	-	-	18/41/41/45	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Y01	B	1003	-	-	12/19/77/77	0/4/4/4
4	Y01	D	1007	-	-	9/19/77/77	0/4/4/4
5	HOR	C	1005	-	-	1/10/32/32	0/4/4/4
6	POV	B	1007	-	-	13/49/49/55	-
4	Y01	B	1006	-	-	9/19/77/77	0/4/4/4
4	Y01	C	1007	-	-	9/19/77/77	0/4/4/4
7	98R	B	1009	-	-	17/41/41/45	-
4	Y01	A	1003	-	-	12/19/77/77	0/4/4/4
5	HOR	D	1005	-	-	1/10/32/32	0/4/4/4
4	Y01	B	1010	-	-	7/19/77/77	0/4/4/4
7	98R	B	1011	-	-	17/41/41/45	-
4	Y01	C	1004	-	-	12/19/77/77	0/4/4/4
5	HOR	A	1004	-	-	1/10/32/32	0/4/4/4

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1005	HOR	C19-C20	-7.06	1.28	1.44
5	A	1004	HOR	C19-C20	-7.04	1.28	1.44
5	B	1004	HOR	C19-C20	-7.04	1.28	1.44
5	D	1005	HOR	C19-C20	-7.04	1.28	1.44
5	A	1004	HOR	C14-C15	5.03	1.48	1.39
5	B	1004	HOR	C14-C15	5.03	1.48	1.39
5	C	1005	HOR	C14-C15	5.03	1.48	1.39
5	D	1005	HOR	C14-C15	5.03	1.48	1.39
6	A	1007	POV	O31-C31	4.24	1.45	1.33
6	B	1007	POV	O31-C31	4.24	1.45	1.33
6	C	1008	POV	O31-C31	4.24	1.45	1.33
6	D	1008	POV	O31-C31	4.24	1.45	1.33
4	A	1008	Y01	OAW-CAY	4.16	1.46	1.34
4	B	1008	Y01	OAW-CAY	4.16	1.46	1.34
4	C	1009	Y01	OAW-CAY	4.16	1.46	1.34
6	A	1007	POV	O21-C21	4.14	1.46	1.34
6	B	1007	POV	O21-C21	4.14	1.46	1.34
6	C	1008	POV	O21-C21	4.14	1.46	1.34
6	D	1008	POV	O21-C21	4.14	1.46	1.34
4	D	1009	Y01	OAW-CAY	4.14	1.46	1.34
4	A	1006	Y01	OAW-CAY	4.12	1.45	1.34
4	B	1006	Y01	OAW-CAY	4.12	1.45	1.34
4	C	1007	Y01	OAW-CAY	4.12	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1007	Y01	OAW-CAY	4.12	1.45	1.34
4	A	1010	Y01	OAW-CAY	4.11	1.45	1.34
4	B	1010	Y01	OAW-CAY	4.11	1.45	1.34
4	C	1001	Y01	OAW-CAY	4.11	1.45	1.34
4	D	1001	Y01	OAW-CAY	4.11	1.45	1.34
7	A	1009	98R	O3-C11	4.09	1.45	1.33
7	A	1011	98R	O3-C11	4.09	1.45	1.33
7	B	1009	98R	O3-C11	4.09	1.45	1.33
7	B	1011	98R	O3-C11	4.09	1.45	1.33
4	A	1003	Y01	OAW-CAY	3.90	1.45	1.34
4	B	1003	Y01	OAW-CAY	3.90	1.45	1.34
4	C	1004	Y01	OAW-CAY	3.90	1.45	1.34
4	D	1004	Y01	OAW-CAY	3.90	1.45	1.34
5	A	1004	HOR	C9-C7	3.89	1.46	1.39
7	A	1009	98R	O2-C31	3.87	1.45	1.34
7	A	1011	98R	O2-C31	3.87	1.45	1.34
7	B	1009	98R	O2-C31	3.87	1.45	1.34
7	B	1011	98R	O2-C31	3.87	1.45	1.34
5	B	1004	HOR	C9-C7	3.85	1.46	1.39
5	C	1005	HOR	C9-C7	3.85	1.46	1.39
5	D	1005	HOR	C9-C7	3.85	1.46	1.39
5	A	1004	HOR	C15-CL	2.76	1.80	1.73
5	B	1004	HOR	C15-CL	2.76	1.80	1.73
5	C	1005	HOR	C15-CL	2.76	1.80	1.73
5	D	1005	HOR	C15-CL	2.76	1.80	1.73
4	C	1004	Y01	CBI-CBG	-2.25	1.50	1.55
4	A	1003	Y01	CBI-CBG	-2.24	1.50	1.55
4	B	1003	Y01	CBI-CBG	-2.24	1.50	1.55
4	D	1004	Y01	CBI-CBG	-2.24	1.50	1.55
5	D	1005	HOR	C7-C1	-2.13	1.47	1.51
5	A	1004	HOR	C7-C1	-2.09	1.47	1.51
5	B	1004	HOR	C7-C1	-2.09	1.47	1.51
5	C	1005	HOR	C7-C1	-2.09	1.47	1.51
4	A	1010	Y01	CBH-CBF	-2.08	1.52	1.56
4	B	1010	Y01	CBH-CBF	-2.08	1.52	1.56
4	C	1001	Y01	CBH-CBF	-2.08	1.52	1.56
4	D	1001	Y01	CBH-CBF	-2.08	1.52	1.56
4	A	1008	Y01	CBH-CBF	-2.02	1.52	1.56
4	B	1008	Y01	CBH-CBF	-2.02	1.52	1.56
4	C	1009	Y01	CBH-CBF	-2.01	1.52	1.56

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	Y01	CBD-CAK-CAI	-4.48	106.29	112.73
4	C	1004	Y01	CBD-CAK-CAI	-4.48	106.29	112.73
4	D	1004	Y01	CBD-CAK-CAI	-4.48	106.29	112.73
4	B	1003	Y01	CBD-CAK-CAI	-4.46	106.33	112.73
6	B	1007	POV	O21-C21-C22	4.39	120.96	111.50
6	A	1007	POV	O21-C21-C22	4.38	120.93	111.50
6	C	1008	POV	O21-C21-C22	4.38	120.93	111.50
6	D	1008	POV	O21-C21-C22	4.38	120.93	111.50
4	C	1004	Y01	CBI-CBG-CBD	-4.23	108.11	114.38
4	A	1003	Y01	CBI-CBG-CBD	-4.22	108.13	114.38
4	B	1003	Y01	CBI-CBG-CBD	-4.22	108.13	114.38
4	D	1004	Y01	CBI-CBG-CBD	-4.22	108.13	114.38
7	A	1009	98R	O2-C31-C32	4.11	120.37	111.50
7	A	1011	98R	O2-C31-C32	4.11	120.37	111.50
7	B	1009	98R	O2-C31-C32	4.11	120.37	111.50
7	B	1011	98R	O2-C31-C32	4.11	120.37	111.50
4	A	1006	Y01	OAW-CAY-CAM	4.04	120.21	111.50
4	C	1007	Y01	OAW-CAY-CAM	4.04	120.21	111.50
4	D	1007	Y01	OAW-CAY-CAM	4.04	120.21	111.50
4	B	1006	Y01	OAW-CAY-CAM	4.03	120.19	111.50
4	D	1009	Y01	CBI-CBE-CBB	-3.98	113.25	119.49
4	B	1008	Y01	CBI-CBE-CBB	-3.97	113.28	119.49
4	A	1008	Y01	CBI-CBE-CBB	-3.96	113.29	119.49
4	C	1009	Y01	CBI-CBE-CBB	-3.96	113.29	119.49
4	A	1010	Y01	OAW-CAY-CAM	3.96	120.03	111.50
4	B	1010	Y01	OAW-CAY-CAM	3.96	120.03	111.50
4	C	1001	Y01	OAW-CAY-CAM	3.96	120.03	111.50
4	D	1001	Y01	OAW-CAY-CAM	3.96	120.03	111.50
4	A	1003	Y01	OAW-CAY-CAM	3.93	119.97	111.50
4	B	1003	Y01	OAW-CAY-CAM	3.93	119.97	111.50
4	C	1004	Y01	OAW-CAY-CAM	3.93	119.97	111.50
4	D	1004	Y01	OAW-CAY-CAM	3.93	119.97	111.50
4	A	1008	Y01	OAW-CAY-CAM	3.90	119.90	111.50
4	B	1008	Y01	OAW-CAY-CAM	3.90	119.90	111.50
4	C	1009	Y01	OAW-CAY-CAM	3.90	119.90	111.50
4	D	1009	Y01	OAW-CAY-CAM	3.88	119.87	111.50
5	A	1004	HOR	O-C14-C15	3.73	119.41	116.13
5	C	1005	HOR	O-C14-C15	3.73	119.41	116.13
5	D	1005	HOR	O-C14-C15	3.73	119.41	116.13
5	B	1004	HOR	O-C14-C15	3.71	119.39	116.13
4	D	1001	Y01	CBI-CBE-CBB	-3.61	113.83	119.49
4	A	1010	Y01	CBI-CBE-CBB	-3.61	113.83	119.49
4	B	1010	Y01	CBI-CBE-CBB	-3.61	113.83	119.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1001	Y01	CBI-CBE-CBB	-3.61	113.83	119.49
4	C	1009	Y01	CBG-CBI-CBE	3.46	104.17	100.07
4	B	1008	Y01	CBG-CBI-CBE	3.45	104.16	100.07
4	A	1008	Y01	CBG-CBI-CBE	3.45	104.16	100.07
4	D	1009	Y01	CBG-CBI-CBE	3.43	104.13	100.07
4	A	1003	Y01	CAP-CBE-CBB	-2.93	107.61	112.15
4	B	1003	Y01	CAP-CBE-CBB	-2.93	107.62	112.15
4	C	1004	Y01	CAP-CBE-CBB	-2.93	107.62	112.15
4	D	1004	Y01	CAP-CBE-CBB	-2.93	107.62	112.15
4	A	1003	Y01	CAM-CAL-CAX	-2.89	107.38	113.60
4	B	1003	Y01	CAM-CAL-CAX	-2.89	107.38	113.60
4	D	1004	Y01	CAM-CAL-CAX	-2.89	107.38	113.60
5	A	1004	HOR	C12-C10-C7	-2.88	117.35	121.01
5	B	1004	HOR	C12-C10-C7	-2.88	117.35	121.01
5	D	1005	HOR	C12-C10-C7	-2.88	117.35	121.01
4	C	1004	Y01	CAM-CAL-CAX	-2.88	107.42	113.60
5	C	1005	HOR	C12-C10-C7	-2.87	117.37	121.01
4	A	1010	Y01	CAV-CAZ-CBH	2.86	120.21	116.42
4	B	1010	Y01	CAV-CAZ-CBH	2.86	120.21	116.42
4	C	1001	Y01	CAV-CAZ-CBH	2.86	120.21	116.42
4	D	1001	Y01	CAV-CAZ-CBH	2.86	120.21	116.42
4	A	1003	Y01	CBG-CBI-CBE	2.79	103.37	100.07
4	B	1003	Y01	CBG-CBI-CBE	2.79	103.37	100.07
4	D	1004	Y01	CBG-CBI-CBE	2.79	103.37	100.07
4	C	1004	Y01	CBG-CBI-CBE	2.77	103.36	100.07
4	D	1009	Y01	CAS-CBF-CBH	-2.73	109.48	113.08
4	C	1009	Y01	CAS-CBF-CBH	-2.73	109.48	113.08
4	A	1008	Y01	CAS-CBF-CBH	-2.72	109.50	113.08
4	B	1008	Y01	CAS-CBF-CBH	-2.72	109.50	113.08
7	A	1009	98R	O3-C11-C12	2.66	120.25	111.91
7	A	1011	98R	O3-C11-C12	2.66	120.25	111.91
7	B	1009	98R	O3-C11-C12	2.66	120.25	111.91
7	B	1011	98R	O3-C11-C12	2.66	120.25	111.91
4	A	1003	Y01	CAJ-CAO-CBB	-2.66	107.39	115.03
4	B	1003	Y01	CAJ-CAO-CBB	-2.66	107.39	115.03
4	C	1004	Y01	CAJ-CAO-CBB	-2.66	107.39	115.03
4	D	1004	Y01	CAJ-CAO-CBB	-2.66	107.39	115.03
6	A	1007	POV	O31-C31-C32	2.59	120.04	111.91
6	B	1007	POV	O31-C31-C32	2.59	120.04	111.91
6	C	1008	POV	O31-C31-C32	2.59	120.04	111.91
6	D	1008	POV	O31-C31-C32	2.58	120.01	111.91
5	A	1004	HOR	C13-C11-C9	-2.46	117.21	120.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1004	HOR	C13-C11-C9	-2.46	117.21	120.89
5	C	1005	HOR	C13-C11-C9	-2.46	117.21	120.89
5	D	1005	HOR	C13-C11-C9	-2.46	117.21	120.89
6	A	1007	POV	C2-O21-C21	-2.42	111.82	117.79
6	B	1007	POV	C2-O21-C21	-2.42	111.82	117.79
6	C	1008	POV	C2-O21-C21	-2.42	111.82	117.79
6	D	1008	POV	C2-O21-C21	-2.42	111.82	117.79
4	B	1003	Y01	CBF-CBH-CAZ	2.35	113.34	109.65
4	B	1003	Y01	CAD-CBH-CBF	-2.34	108.89	111.68
4	A	1003	Y01	CBF-CBH-CAZ	2.33	113.30	109.65
4	C	1004	Y01	CBF-CBH-CAZ	2.33	113.30	109.65
4	D	1004	Y01	CBF-CBH-CAZ	2.33	113.30	109.65
4	A	1003	Y01	CAD-CBH-CBF	-2.31	108.93	111.68
4	C	1004	Y01	CAD-CBH-CBF	-2.31	108.93	111.68
4	D	1004	Y01	CAD-CBH-CBF	-2.31	108.93	111.68
4	D	1009	Y01	CAE-CBI-CBE	-2.29	107.45	111.71
4	A	1008	Y01	CAE-CBI-CBE	-2.28	107.47	111.71
4	C	1009	Y01	CAE-CBI-CBE	-2.28	107.47	111.71
4	B	1008	Y01	CAE-CBI-CBE	-2.26	107.49	111.71
4	A	1008	Y01	CAJ-CAO-CBB	-2.23	108.61	115.03
4	B	1008	Y01	CAJ-CAO-CBB	-2.23	108.61	115.03
4	C	1009	Y01	CAJ-CAO-CBB	-2.23	108.61	115.03
4	D	1009	Y01	CAJ-CAO-CBB	-2.23	108.61	115.03
4	B	1010	Y01	CBH-CBF-CBD	-2.23	109.39	112.73
4	A	1003	Y01	CAQ-CBG-CBI	2.22	106.52	103.84
4	B	1003	Y01	CAQ-CBG-CBI	2.22	106.52	103.84
4	D	1004	Y01	CAQ-CBG-CBI	2.22	106.52	103.84
4	C	1004	Y01	CAQ-CBG-CBI	2.21	106.50	103.84
4	A	1003	Y01	OAH-CAX-CAL	2.21	121.13	114.03
4	B	1003	Y01	OAH-CAX-CAL	2.21	121.13	114.03
4	D	1004	Y01	OAH-CAX-CAL	2.21	121.13	114.03
4	C	1004	Y01	OAH-CAX-CAL	2.21	121.12	114.03
4	D	1007	Y01	CAS-CBF-CBH	-2.21	110.17	113.08
4	A	1010	Y01	CBH-CBF-CBD	-2.20	109.43	112.73
4	C	1001	Y01	CBH-CBF-CBD	-2.20	109.43	112.73
4	D	1001	Y01	CBH-CBF-CBD	-2.20	109.43	112.73
4	A	1006	Y01	CBC-OAW-CAY	-2.20	112.37	117.79
4	B	1006	Y01	CBC-OAW-CAY	-2.20	112.37	117.79
4	C	1007	Y01	CBC-OAW-CAY	-2.20	112.37	117.79
4	D	1007	Y01	CBC-OAW-CAY	-2.20	112.37	117.79
4	A	1008	Y01	CBH-CBF-CBD	-2.19	109.45	112.73
4	B	1010	Y01	CAS-CAU-CBI	-2.19	109.03	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1006	Y01	CAS-CBF-CBH	-2.19	110.19	113.08
4	B	1006	Y01	CAS-CBF-CBH	-2.19	110.19	113.08
4	B	1003	Y01	CAV-CAZ-CAI	-2.18	117.47	120.61
4	C	1004	Y01	CAV-CAZ-CAI	-2.18	117.47	120.61
4	D	1004	Y01	CAV-CAZ-CAI	-2.18	117.47	120.61
4	D	1001	Y01	CAS-CAU-CBI	-2.18	109.05	112.78
4	C	1007	Y01	CAS-CBF-CBH	-2.17	110.22	113.08
4	B	1008	Y01	CBH-CBF-CBD	-2.17	109.48	112.73
4	C	1001	Y01	CAS-CAU-CBI	-2.17	109.06	112.78
4	A	1010	Y01	CAS-CAU-CBI	-2.17	109.06	112.78
4	D	1009	Y01	CBH-CBF-CBD	-2.16	109.50	112.73
4	A	1003	Y01	CAV-CAZ-CAI	-2.16	117.50	120.61
4	B	1008	Y01	CAS-CAU-CBI	-2.16	109.08	112.78
4	C	1009	Y01	CAS-CAU-CBI	-2.16	109.08	112.78
4	D	1009	Y01	CAS-CAU-CBI	-2.16	109.08	112.78
4	C	1009	Y01	CBH-CBF-CBD	-2.16	109.50	112.73
4	D	1004	Y01	CBC-OAW-CAY	-2.15	112.50	117.79
4	A	1008	Y01	CAS-CAU-CBI	-2.14	109.11	112.78
4	A	1003	Y01	CBC-OAW-CAY	-2.13	112.53	117.79
4	B	1003	Y01	CBC-OAW-CAY	-2.13	112.53	117.79
4	C	1004	Y01	CBC-OAW-CAY	-2.13	112.53	117.79
4	D	1009	Y01	CBI-CBG-CBD	-2.12	111.24	114.38
4	A	1003	Y01	CAS-CAU-CBI	-2.11	109.15	112.78
4	B	1003	Y01	CAS-CAU-CBI	-2.11	109.15	112.78
4	D	1004	Y01	CAS-CAU-CBI	-2.11	109.15	112.78
4	C	1009	Y01	CBD-CAK-CAI	-2.11	109.70	112.73
4	A	1008	Y01	CAV-CAZ-CBH	2.11	119.22	116.42
4	B	1008	Y01	CAV-CAZ-CBH	2.11	119.22	116.42
4	C	1009	Y01	CAV-CAZ-CBH	2.11	119.22	116.42
4	A	1003	Y01	CAP-CBE-CBI	2.10	106.38	103.84
4	B	1003	Y01	CAP-CBE-CBI	2.10	106.38	103.84
4	C	1004	Y01	CAP-CBE-CBI	2.10	106.38	103.84
4	D	1004	Y01	CAP-CBE-CBI	2.10	106.38	103.84
4	A	1008	Y01	CBI-CBG-CBD	-2.10	111.27	114.38
4	B	1008	Y01	CBI-CBG-CBD	-2.10	111.27	114.38
4	C	1004	Y01	CAS-CAU-CBI	-2.10	109.18	112.78
4	A	1003	Y01	CBF-CBD-CBG	-2.09	106.29	109.09
4	B	1003	Y01	CBF-CBD-CBG	-2.09	106.29	109.09
4	C	1004	Y01	CBF-CBD-CBG	-2.09	106.29	109.09
4	D	1004	Y01	CBF-CBD-CBG	-2.09	106.29	109.09
4	C	1009	Y01	CBI-CBG-CBD	-2.09	111.29	114.38
4	B	1008	Y01	CBD-CAK-CAI	-2.08	109.74	112.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1009	Y01	CBD-CAK-CAI	-2.08	109.74	112.73
4	D	1009	Y01	CAV-CAZ-CBH	2.08	119.19	116.42
4	A	1008	Y01	CBD-CAK-CAI	-2.08	109.74	112.73
4	A	1006	Y01	OAW-CAY-OAG	-2.06	118.72	123.70
4	B	1006	Y01	OAW-CAY-OAG	-2.06	118.72	123.70
4	C	1007	Y01	OAW-CAY-OAG	-2.06	118.72	123.70
4	D	1007	Y01	OAW-CAY-OAG	-2.06	118.72	123.70
4	A	1010	Y01	OAH-CAX-CAL	2.05	120.63	114.03
4	B	1010	Y01	OAH-CAX-CAL	2.05	120.63	114.03
4	C	1001	Y01	OAH-CAX-CAL	2.05	120.63	114.03
4	D	1001	Y01	OAH-CAX-CAL	2.05	120.63	114.03
4	B	1003	Y01	CAK-CAI-CAZ	-2.04	121.30	125.06
4	A	1003	Y01	CAK-CAI-CAZ	-2.02	121.33	125.06
4	C	1004	Y01	CAK-CAI-CAZ	-2.02	121.33	125.06
4	D	1004	Y01	CAK-CAI-CAZ	-2.02	121.33	125.06
4	A	1008	Y01	OAH-CAX-CAL	2.01	120.50	114.03
4	C	1009	Y01	OAH-CAX-CAL	2.01	120.50	114.03
4	D	1001	Y01	CBC-OAW-CAY	-2.01	112.83	117.79
4	D	1009	Y01	OAH-CAX-CAL	2.01	120.49	114.03
5	A	1004	HOR	C17-C15-CL	2.01	121.74	118.49
5	B	1004	HOR	C17-C15-CL	2.01	121.74	118.49
5	C	1005	HOR	C17-C15-CL	2.01	121.74	118.49
5	D	1005	HOR	C17-C15-CL	2.01	121.74	118.49
4	D	1007	Y01	CBH-CBF-CBD	-2.01	109.73	112.73
4	B	1008	Y01	OAH-CAX-CAL	2.00	120.47	114.03
4	A	1006	Y01	CBH-CBF-CBD	-2.00	109.73	112.73
4	B	1006	Y01	CBH-CBF-CBD	-2.00	109.73	112.73
4	A	1010	Y01	CBC-OAW-CAY	-2.00	112.86	117.79
4	C	1001	Y01	CBC-OAW-CAY	-2.00	112.86	117.79

There are no chirality outliers.

All (273) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	Y01	CAR-CBC-OAW-CAY
4	A	1003	Y01	CAM-CAY-OAW-CBC
4	A	1008	Y01	CAM-CAY-OAW-CBC
4	B	1003	Y01	CAR-CBC-OAW-CAY
4	B	1003	Y01	CAM-CAY-OAW-CBC
4	B	1008	Y01	CAM-CAY-OAW-CBC
4	C	1004	Y01	CAR-CBC-OAW-CAY
4	C	1004	Y01	CAM-CAY-OAW-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	1009	Y01	CAM-CAY-OAW-CBC
4	D	1004	Y01	CAR-CBC-OAW-CAY
4	D	1004	Y01	CAM-CAY-OAW-CBC
4	D	1009	Y01	CAM-CAY-OAW-CBC
5	A	1004	HOR	C1-C-N-C4
5	B	1004	HOR	C1-C-N-C4
5	C	1005	HOR	C1-C-N-C4
5	D	1005	HOR	C1-C-N-C4
7	A	1009	98R	O3P-C1-C2-O2
7	A	1009	98R	C12-C11-O3-C3
7	A	1009	98R	O11-C11-O3-C3
7	A	1009	98R	O31-C31-O2-C2
7	A	1011	98R	O3P-C1-C2-O2
7	A	1011	98R	C12-C11-O3-C3
7	A	1011	98R	O11-C11-O3-C3
7	A	1011	98R	O31-C31-O2-C2
7	B	1009	98R	O3P-C1-C2-O2
7	B	1009	98R	C12-C11-O3-C3
7	B	1009	98R	O11-C11-O3-C3
7	B	1009	98R	O31-C31-O2-C2
7	B	1011	98R	O3P-C1-C2-O2
7	B	1011	98R	C12-C11-O3-C3
7	B	1011	98R	O11-C11-O3-C3
7	B	1011	98R	O31-C31-O2-C2
4	A	1010	Y01	CAC-CBB-CBE-CBI
4	B	1010	Y01	CAC-CBB-CBE-CBI
4	C	1001	Y01	CAC-CBB-CBE-CBI
4	D	1001	Y01	CAC-CBB-CBE-CBI
4	A	1003	Y01	OAG-CAY-OAW-CBC
4	A	1008	Y01	OAG-CAY-OAW-CBC
4	B	1003	Y01	OAG-CAY-OAW-CBC
4	B	1008	Y01	OAG-CAY-OAW-CBC
4	C	1004	Y01	OAG-CAY-OAW-CBC
4	C	1009	Y01	OAG-CAY-OAW-CBC
4	D	1004	Y01	OAG-CAY-OAW-CBC
4	D	1009	Y01	OAG-CAY-OAW-CBC
7	A	1009	98R	C32-C31-O2-C2
7	A	1011	98R	C32-C31-O2-C2
7	B	1009	98R	C32-C31-O2-C2
7	B	1011	98R	C32-C31-O2-C2
4	A	1010	Y01	CAC-CBB-CBE-CAP
4	B	1010	Y01	CAC-CBB-CBE-CAP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	1001	Y01	CAC-CBB-CBE-CAP
4	D	1001	Y01	CAC-CBB-CBE-CAP
4	A	1010	Y01	CAO-CBB-CBE-CBI
4	B	1010	Y01	CAO-CBB-CBE-CBI
4	C	1001	Y01	CAO-CBB-CBE-CBI
4	D	1001	Y01	CAO-CBB-CBE-CBI
4	A	1006	Y01	OAG-CAY-OAW-CBC
4	B	1006	Y01	OAG-CAY-OAW-CBC
4	C	1007	Y01	OAG-CAY-OAW-CBC
4	D	1007	Y01	OAG-CAY-OAW-CBC
4	A	1010	Y01	CAO-CBB-CBE-CAP
4	B	1010	Y01	CAO-CBB-CBE-CAP
4	C	1001	Y01	CAO-CBB-CBE-CAP
4	D	1001	Y01	CAO-CBB-CBE-CAP
4	A	1006	Y01	CAM-CAY-OAW-CBC
4	B	1006	Y01	CAM-CAY-OAW-CBC
4	C	1007	Y01	CAM-CAY-OAW-CBC
4	D	1007	Y01	CAM-CAY-OAW-CBC
6	A	1007	POV	C22-C21-O21-C2
6	B	1007	POV	C22-C21-O21-C2
6	C	1008	POV	C22-C21-O21-C2
6	D	1008	POV	C22-C21-O21-C2
4	A	1006	Y01	CAJ-CAO-CBB-CBE
4	B	1006	Y01	CAJ-CAO-CBB-CBE
4	C	1007	Y01	CAJ-CAO-CBB-CBE
4	D	1007	Y01	CAJ-CAO-CBB-CBE
4	A	1006	Y01	CAJ-CAO-CBB-CAC
4	B	1006	Y01	CAJ-CAO-CBB-CAC
4	C	1007	Y01	CAJ-CAO-CBB-CAC
4	D	1007	Y01	CAJ-CAO-CBB-CAC
6	A	1007	POV	O22-C21-O21-C2
6	B	1007	POV	O22-C21-O21-C2
6	C	1008	POV	O22-C21-O21-C2
6	D	1008	POV	O22-C21-O21-C2
4	A	1003	Y01	CAO-CBB-CBE-CBI
4	B	1003	Y01	CAO-CBB-CBE-CBI
4	C	1004	Y01	CAO-CBB-CBE-CBI
4	D	1004	Y01	CAO-CBB-CBE-CBI
4	A	1003	Y01	CAO-CBB-CBE-CAP
4	B	1003	Y01	CAO-CBB-CBE-CAP
4	C	1004	Y01	CAO-CBB-CBE-CAP
4	D	1004	Y01	CAO-CBB-CBE-CAP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1003	Y01	CAC-CBB-CBE-CAP
4	B	1003	Y01	CAC-CBB-CBE-CAP
4	C	1004	Y01	CAC-CBB-CBE-CAP
4	D	1004	Y01	CAC-CBB-CBE-CAP
4	A	1006	Y01	CAX-CAL-CAM-CAY
4	B	1006	Y01	CAX-CAL-CAM-CAY
4	C	1007	Y01	CAX-CAL-CAM-CAY
4	D	1007	Y01	CAX-CAL-CAM-CAY
6	A	1007	POV	C24-C25-C26-C27
6	B	1007	POV	C24-C25-C26-C27
6	C	1008	POV	C24-C25-C26-C27
6	D	1008	POV	C24-C25-C26-C27
7	A	1009	98R	C42-C43-C44-C45
7	A	1011	98R	C42-C43-C44-C45
7	B	1011	98R	C42-C43-C44-C45
7	B	1009	98R	C42-C43-C44-C45
4	A	1006	Y01	CAV-CBC-OAW-CAY
4	B	1006	Y01	CAV-CBC-OAW-CAY
4	C	1007	Y01	CAV-CBC-OAW-CAY
4	D	1007	Y01	CAV-CBC-OAW-CAY
4	A	1010	Y01	OAG-CAY-OAW-CBC
4	B	1010	Y01	OAG-CAY-OAW-CBC
4	C	1001	Y01	OAG-CAY-OAW-CBC
4	D	1001	Y01	OAG-CAY-OAW-CBC
4	A	1003	Y01	CAO-CAJ-CAN-CBA
4	B	1003	Y01	CAO-CAJ-CAN-CBA
4	C	1004	Y01	CAO-CAJ-CAN-CBA
4	D	1004	Y01	CAO-CAJ-CAN-CBA
4	A	1010	Y01	CAM-CAY-OAW-CBC
4	B	1010	Y01	CAM-CAY-OAW-CBC
4	C	1001	Y01	CAM-CAY-OAW-CBC
4	D	1001	Y01	CAM-CAY-OAW-CBC
4	A	1006	Y01	CAR-CBC-OAW-CAY
4	B	1006	Y01	CAR-CBC-OAW-CAY
4	C	1007	Y01	CAR-CBC-OAW-CAY
4	D	1007	Y01	CAR-CBC-OAW-CAY
4	A	1003	Y01	CAN-CAJ-CAO-CBB
4	B	1003	Y01	CAN-CAJ-CAO-CBB
4	C	1004	Y01	CAN-CAJ-CAO-CBB
4	D	1004	Y01	CAN-CAJ-CAO-CBB
4	A	1003	Y01	CAV-CBC-OAW-CAY
4	B	1003	Y01	CAV-CBC-OAW-CAY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	1004	Y01	CAV-CBC-OAW-CAY
4	D	1004	Y01	CAV-CBC-OAW-CAY
7	A	1009	98R	C14-C15-C16-C17
7	A	1011	98R	C14-C15-C16-C17
7	B	1011	98R	C14-C15-C16-C17
7	B	1009	98R	C14-C15-C16-C17
6	A	1007	POV	O21-C2-C3-O31
6	B	1007	POV	O21-C2-C3-O31
6	C	1008	POV	O21-C2-C3-O31
6	D	1008	POV	O21-C2-C3-O31
4	A	1008	Y01	CAO-CBB-CBE-CBI
4	B	1008	Y01	CAO-CBB-CBE-CBI
4	C	1009	Y01	CAO-CBB-CBE-CBI
4	D	1009	Y01	CAO-CBB-CBE-CBI
7	A	1009	98R	O3P-C1-C2-C3
7	A	1011	98R	O3P-C1-C2-C3
7	B	1009	98R	O3P-C1-C2-C3
7	B	1011	98R	O3P-C1-C2-C3
7	A	1011	98R	C12-C13-C14-C15
7	B	1009	98R	C12-C13-C14-C15
7	A	1009	98R	C12-C13-C14-C15
7	B	1011	98R	C12-C13-C14-C15
4	A	1008	Y01	CAC-CBB-CBE-CBI
4	B	1008	Y01	CAC-CBB-CBE-CBI
4	C	1009	Y01	CAC-CBB-CBE-CBI
4	D	1009	Y01	CAC-CBB-CBE-CBI
6	B	1007	POV	C34-C35-C36-C37
6	A	1007	POV	C34-C35-C36-C37
6	C	1008	POV	C34-C35-C36-C37
6	D	1008	POV	C34-C35-C36-C37
6	A	1007	POV	C35-C36-C37-C38
6	B	1007	POV	C35-C36-C37-C38
6	C	1008	POV	C35-C36-C37-C38
6	D	1008	POV	C35-C36-C37-C38
6	A	1007	POV	C11-O12-P-O11
6	B	1007	POV	C11-O12-P-O11
6	C	1008	POV	C11-O12-P-O11
6	D	1008	POV	C11-O12-P-O11
6	A	1007	POV	C21-C22-C23-C24
6	B	1007	POV	C21-C22-C23-C24
6	C	1008	POV	C21-C22-C23-C24
6	D	1008	POV	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1008	Y01	CAJ-CAN-CBA-CAB
4	B	1008	Y01	CAJ-CAN-CBA-CAB
4	C	1009	Y01	CAJ-CAN-CBA-CAB
4	D	1009	Y01	CAJ-CAN-CBA-CAB
6	A	1007	POV	C1-O11-P-O12
6	B	1007	POV	C1-O11-P-O12
6	C	1008	POV	C1-O11-P-O12
6	D	1008	POV	C1-O11-P-O12
6	A	1007	POV	C1-C2-C3-O31
6	B	1007	POV	C1-C2-C3-O31
6	C	1008	POV	C1-C2-C3-O31
6	D	1008	POV	C1-C2-C3-O31
7	A	1009	98R	C18-C19-C20-C21
7	A	1011	98R	C18-C19-C20-C21
7	B	1009	98R	C18-C19-C20-C21
7	B	1011	98R	C18-C19-C20-C21
7	B	1009	98R	C13-C14-C15-C16
7	A	1009	98R	C13-C14-C15-C16
7	A	1011	98R	C13-C14-C15-C16
7	B	1011	98R	C13-C14-C15-C16
7	A	1009	98R	C21-C22-C23-C24
7	A	1011	98R	C21-C22-C23-C24
7	B	1009	98R	C21-C22-C23-C24
7	B	1011	98R	C21-C22-C23-C24
4	A	1008	Y01	CAO-CBB-CBE-CAP
4	B	1008	Y01	CAO-CBB-CBE-CAP
4	C	1009	Y01	CAO-CBB-CBE-CAP
4	D	1009	Y01	CAO-CBB-CBE-CAP
7	A	1009	98R	C3-C2-O2-C31
7	A	1011	98R	C3-C2-O2-C31
7	B	1009	98R	C3-C2-O2-C31
7	B	1011	98R	C3-C2-O2-C31
4	A	1008	Y01	CAM-CAL-CAX-OAH
4	B	1008	Y01	CAM-CAL-CAX-OAH
4	C	1009	Y01	CAM-CAL-CAX-OAH
4	D	1009	Y01	CAM-CAL-CAX-OAH
4	A	1006	Y01	CAM-CAL-CAX-OAH
4	B	1006	Y01	CAM-CAL-CAX-OAH
4	C	1007	Y01	CAM-CAL-CAX-OAH
4	D	1007	Y01	CAM-CAL-CAX-OAH
4	A	1006	Y01	CAM-CAL-CAX-OAF
4	B	1006	Y01	CAM-CAL-CAX-OAF

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	1007	Y01	CAM-CAL-CAX-OAF
4	D	1007	Y01	CAM-CAL-CAX-OAF
4	A	1008	Y01	CAJ-CAN-CBA-CAA
4	B	1008	Y01	CAJ-CAN-CBA-CAA
4	C	1009	Y01	CAJ-CAN-CBA-CAA
4	D	1009	Y01	CAJ-CAN-CBA-CAA
6	A	1007	POV	C27-C28-C29-C210
6	B	1007	POV	C27-C28-C29-C210
6	C	1008	POV	C27-C28-C29-C210
6	D	1008	POV	C27-C28-C29-C210
7	A	1009	98R	C38-C39-C40-C41
7	A	1009	98R	C20-C21-C22-C23
7	A	1011	98R	C38-C39-C40-C41
7	A	1011	98R	C20-C21-C22-C23
7	B	1009	98R	C38-C39-C40-C41
7	B	1009	98R	C20-C21-C22-C23
7	B	1011	98R	C38-C39-C40-C41
7	B	1011	98R	C20-C21-C22-C23
7	A	1009	98R	C1-C2-O2-C31
7	A	1011	98R	C1-C2-O2-C31
7	B	1009	98R	C1-C2-O2-C31
7	B	1011	98R	C1-C2-O2-C31
4	A	1008	Y01	CAM-CAL-CAX-OAF
4	B	1008	Y01	CAM-CAL-CAX-OAF
4	C	1009	Y01	CAM-CAL-CAX-OAF
4	D	1009	Y01	CAM-CAL-CAX-OAF
6	A	1007	POV	C33-C34-C35-C36
6	B	1007	POV	C33-C34-C35-C36
6	C	1008	POV	C33-C34-C35-C36
6	D	1008	POV	C33-C34-C35-C36
4	A	1003	Y01	CAL-CAM-CAY-OAW
4	B	1003	Y01	CAL-CAM-CAY-OAW
4	C	1004	Y01	CAL-CAM-CAY-OAW
4	D	1004	Y01	CAL-CAM-CAY-OAW
4	A	1003	Y01	CAJ-CAN-CBA-CAA
4	B	1003	Y01	CAJ-CAN-CBA-CAA
4	C	1004	Y01	CAJ-CAN-CBA-CAA
4	D	1004	Y01	CAJ-CAN-CBA-CAA
4	A	1003	Y01	CAL-CAM-CAY-OAG
4	B	1003	Y01	CAL-CAM-CAY-OAG
4	C	1004	Y01	CAL-CAM-CAY-OAG
4	D	1004	Y01	CAL-CAM-CAY-OAG

Continued on next page...

Continued from previous page...

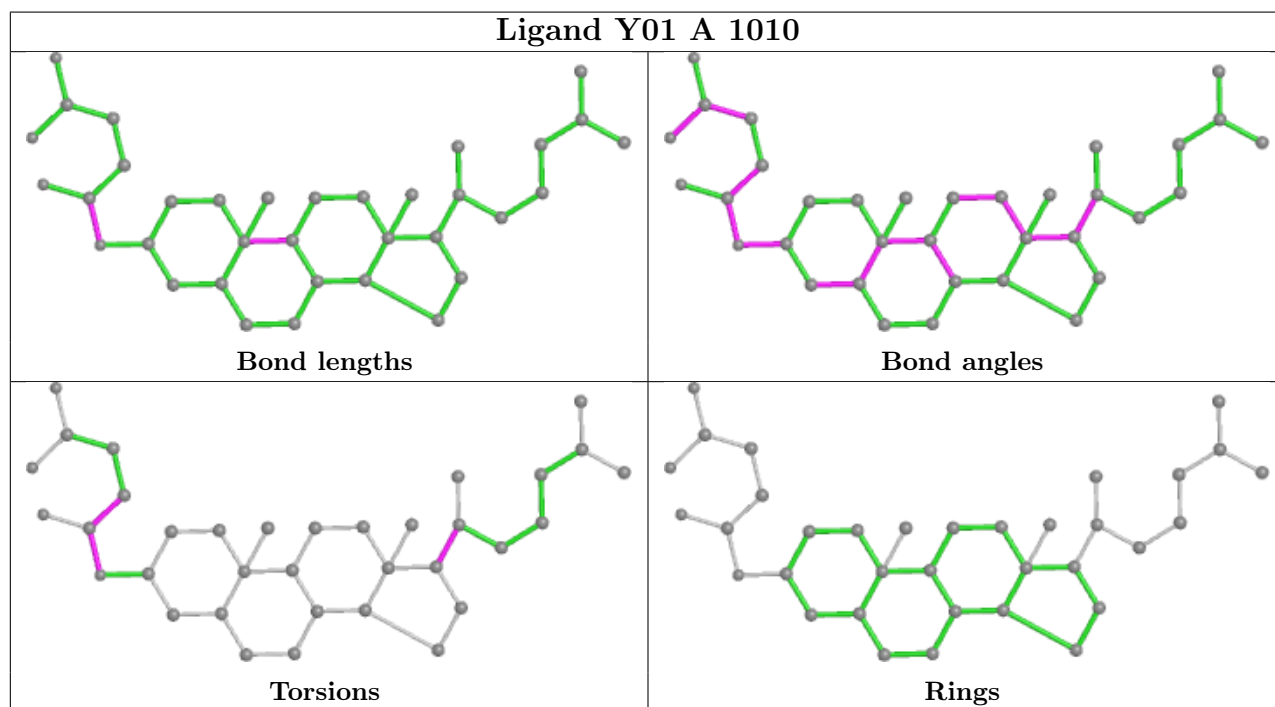
Mol	Chain	Res	Type	Atoms
7	B	1009	98R	C32-C33-C34-C35
7	A	1009	98R	C32-C33-C34-C35
7	B	1011	98R	C32-C33-C34-C35
7	A	1011	98R	C32-C33-C34-C35
4	A	1010	Y01	CAL-CAM-CAY-OAW
4	B	1010	Y01	CAL-CAM-CAY-OAW
4	C	1001	Y01	CAL-CAM-CAY-OAW
4	D	1001	Y01	CAL-CAM-CAY-OAW
6	A	1007	POV	C29-C210-C211-C212
6	B	1007	POV	C29-C210-C211-C212
6	C	1008	POV	C29-C210-C211-C212
6	D	1008	POV	C29-C210-C211-C212
7	A	1009	98R	C40-C41-C42-C43

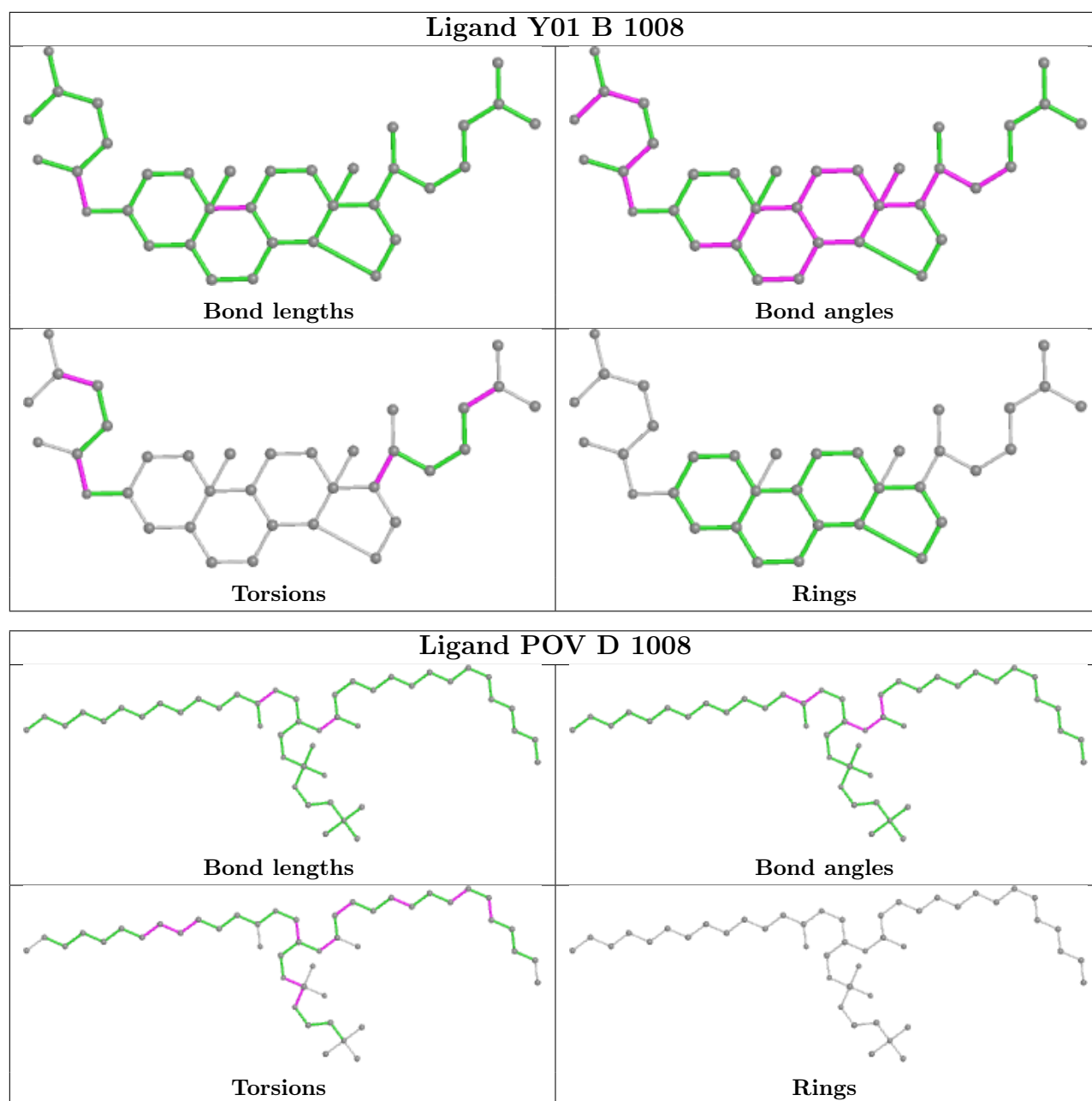
There are no ring outliers.

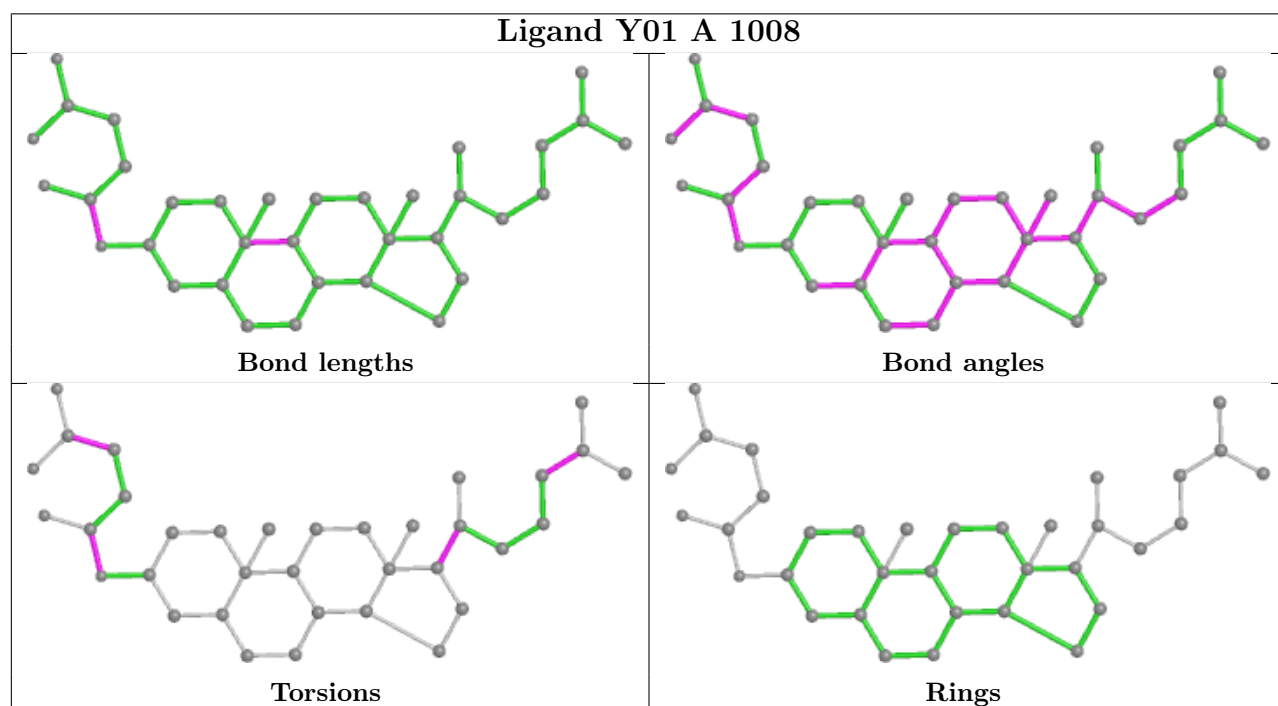
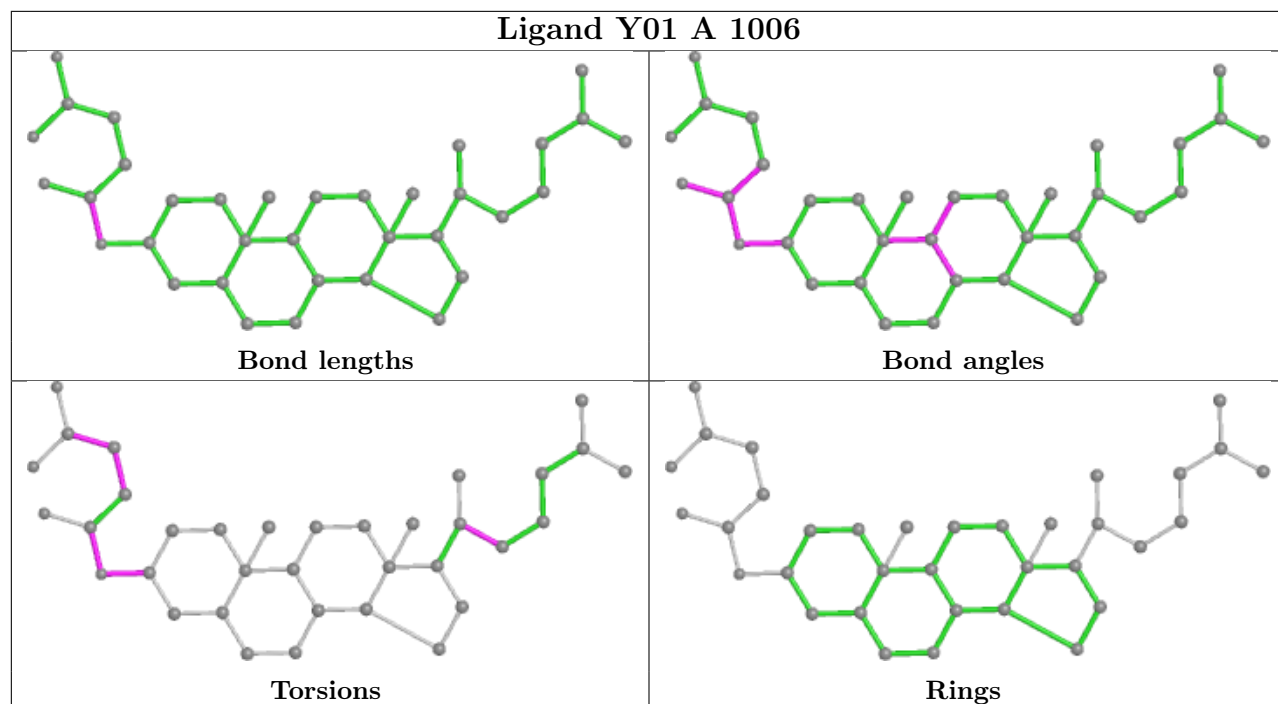
24 monomers are involved in 115 short contacts:

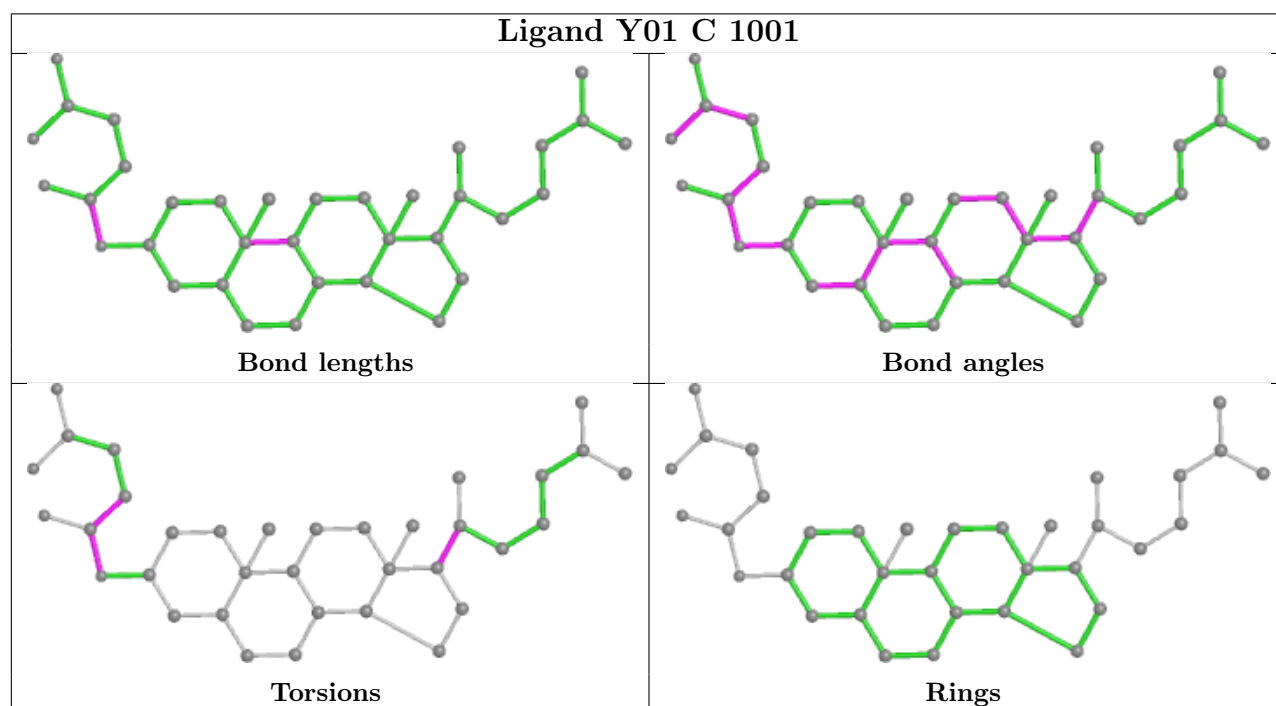
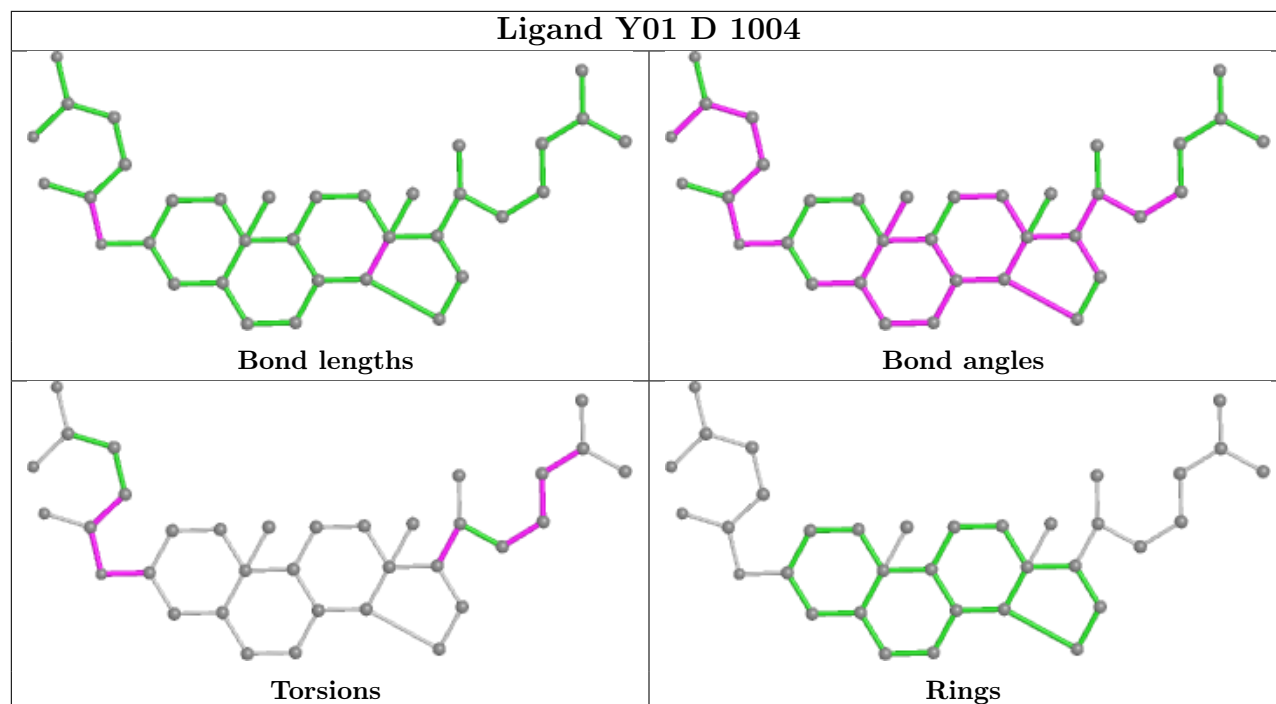
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1010	Y01	3	0
4	B	1008	Y01	6	0
6	D	1008	POV	2	0
4	A	1006	Y01	1	0
4	A	1008	Y01	6	0
4	D	1004	Y01	17	0
4	C	1001	Y01	4	0
6	C	1008	POV	3	0
4	D	1009	Y01	6	0
4	D	1001	Y01	3	0
4	C	1009	Y01	7	0
7	A	1011	98R	1	0
6	A	1007	POV	2	0
7	A	1009	98R	1	0
4	B	1003	Y01	17	0
4	D	1007	Y01	2	0
6	B	1007	POV	3	0
4	B	1006	Y01	1	0
4	C	1007	Y01	1	0
7	B	1009	98R	1	0
4	A	1003	Y01	16	0
4	B	1010	Y01	3	0
7	B	1011	98R	1	0
4	C	1004	Y01	16	0

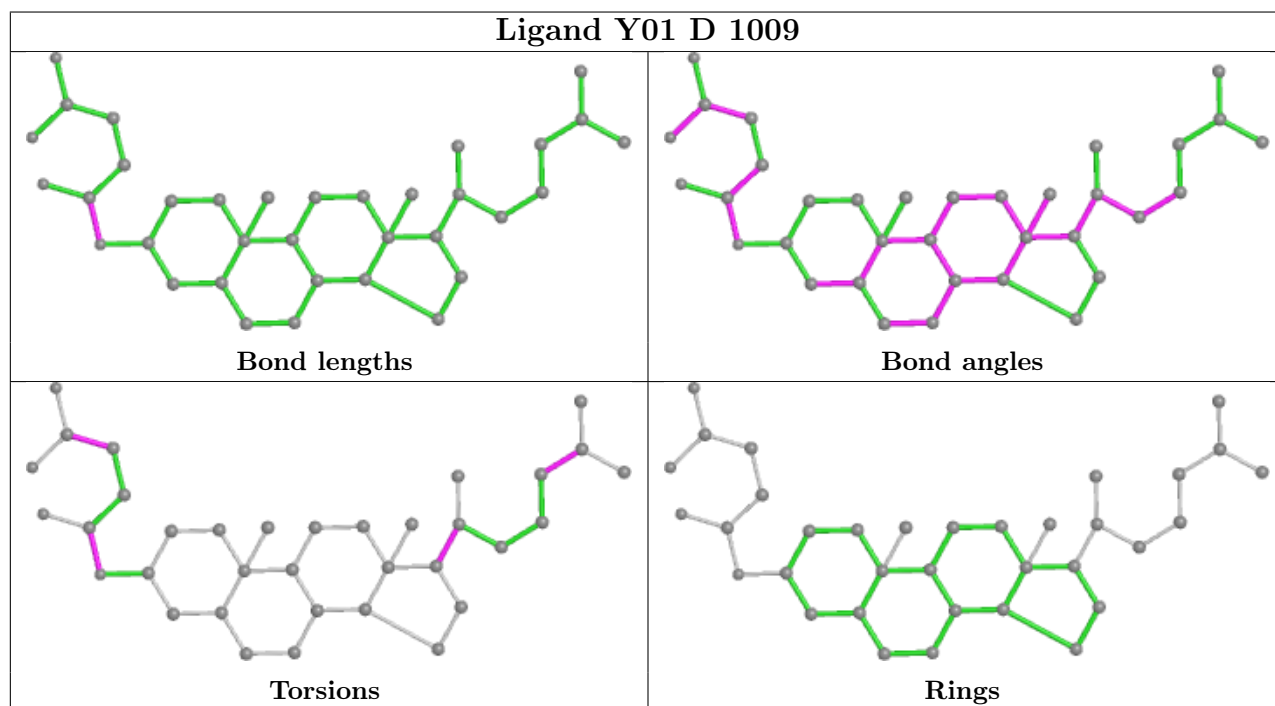
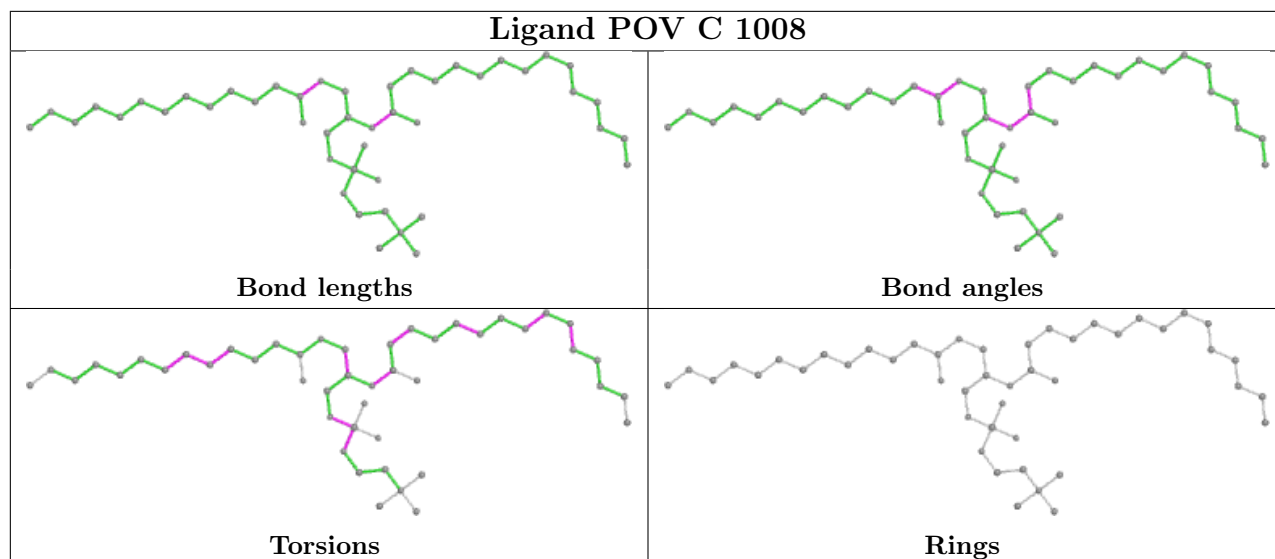
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

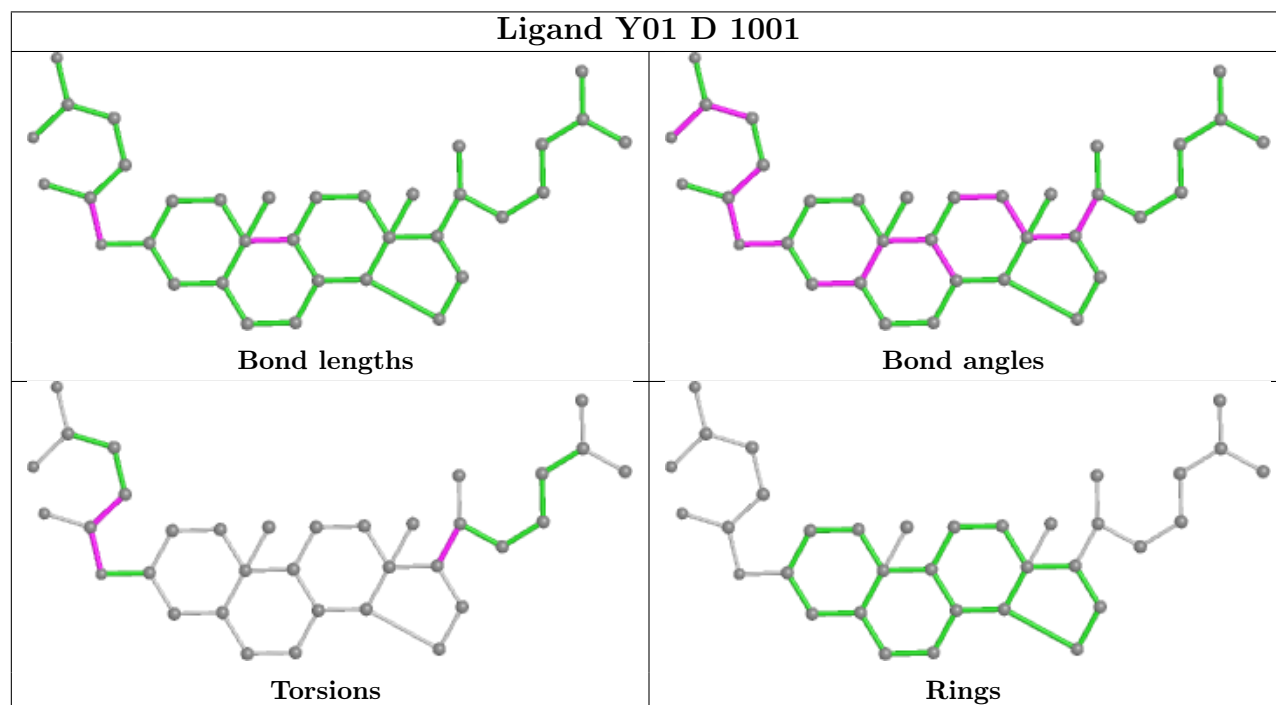
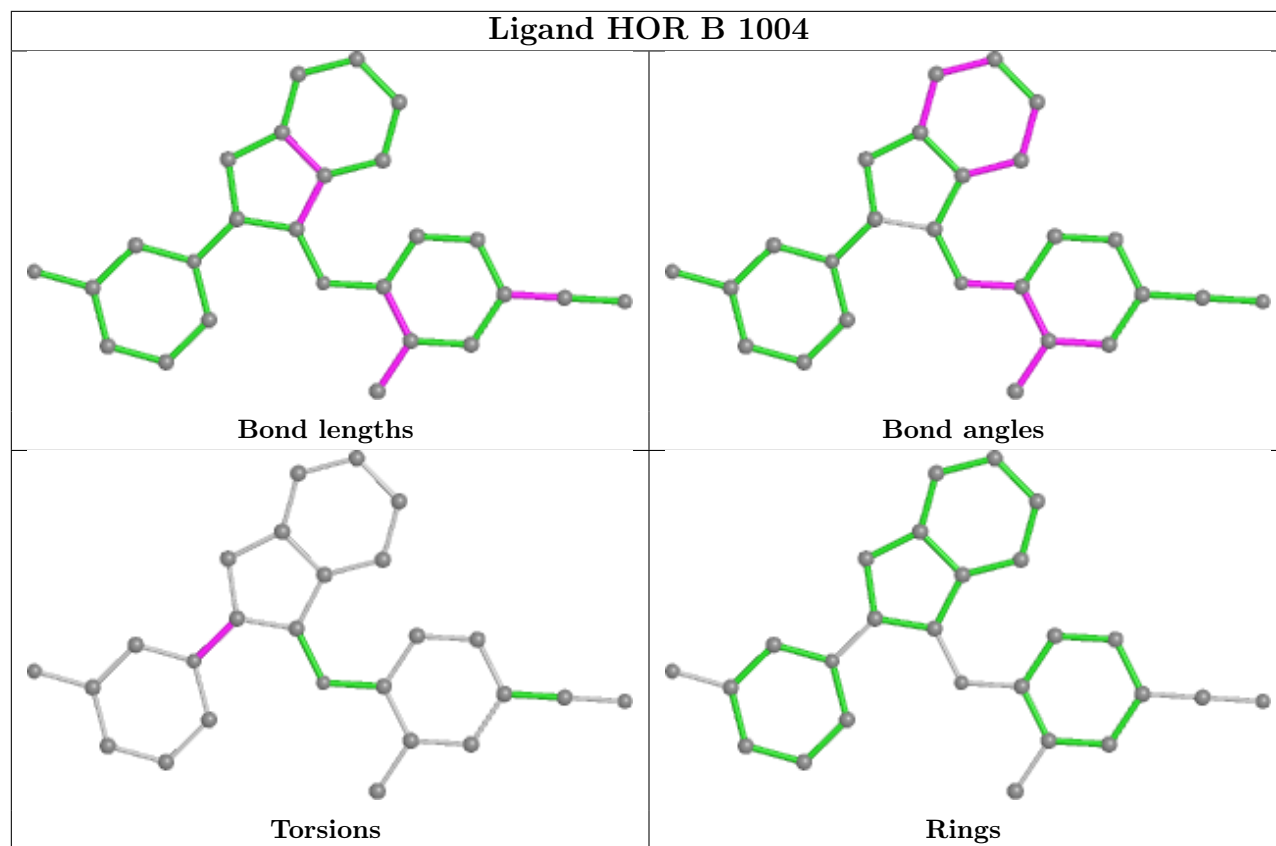


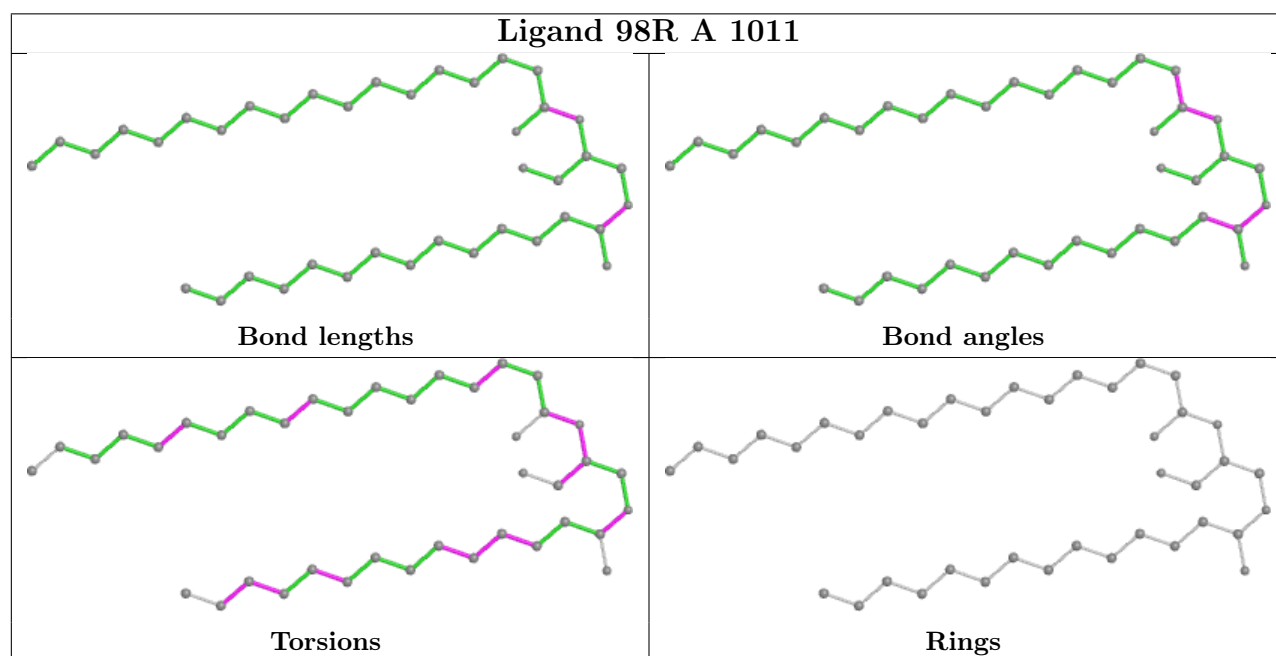
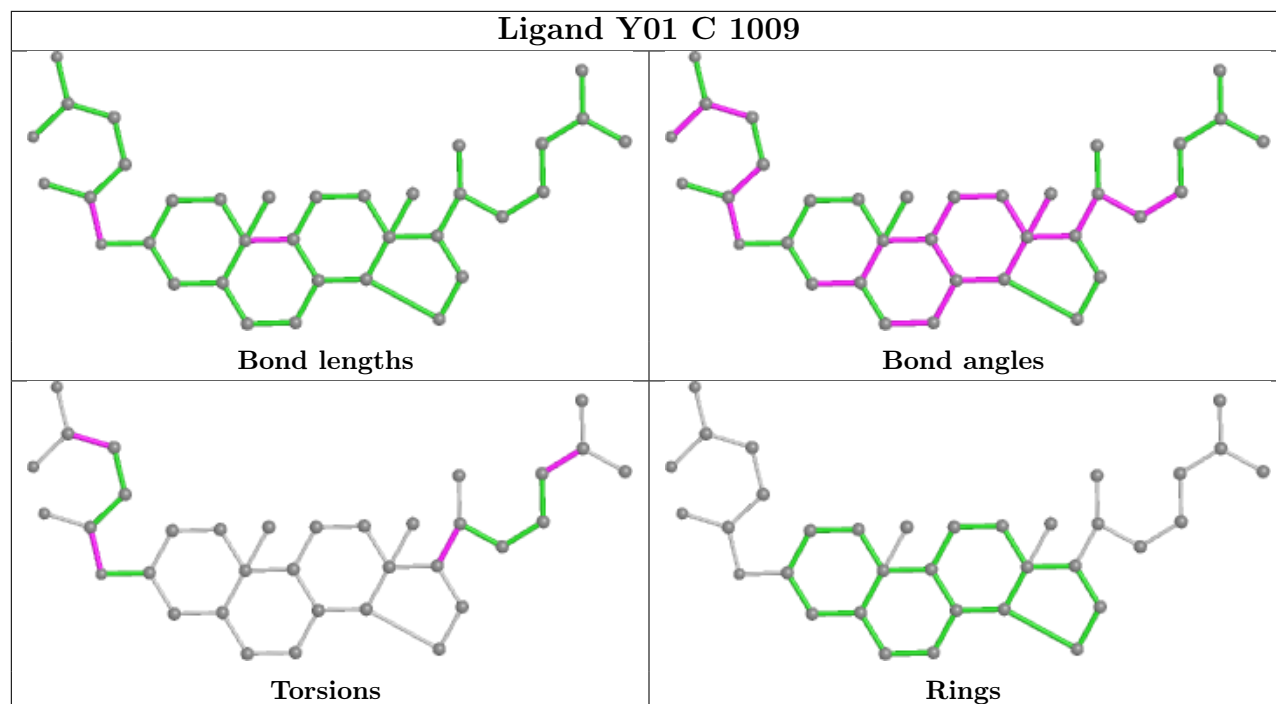


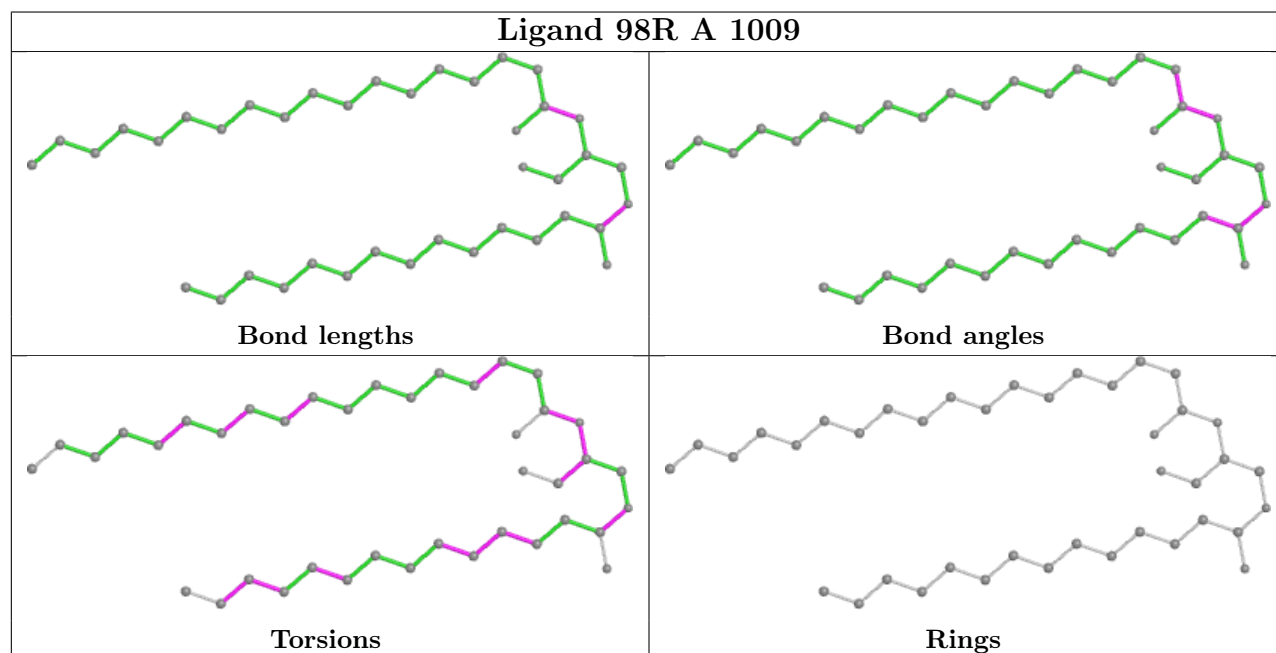
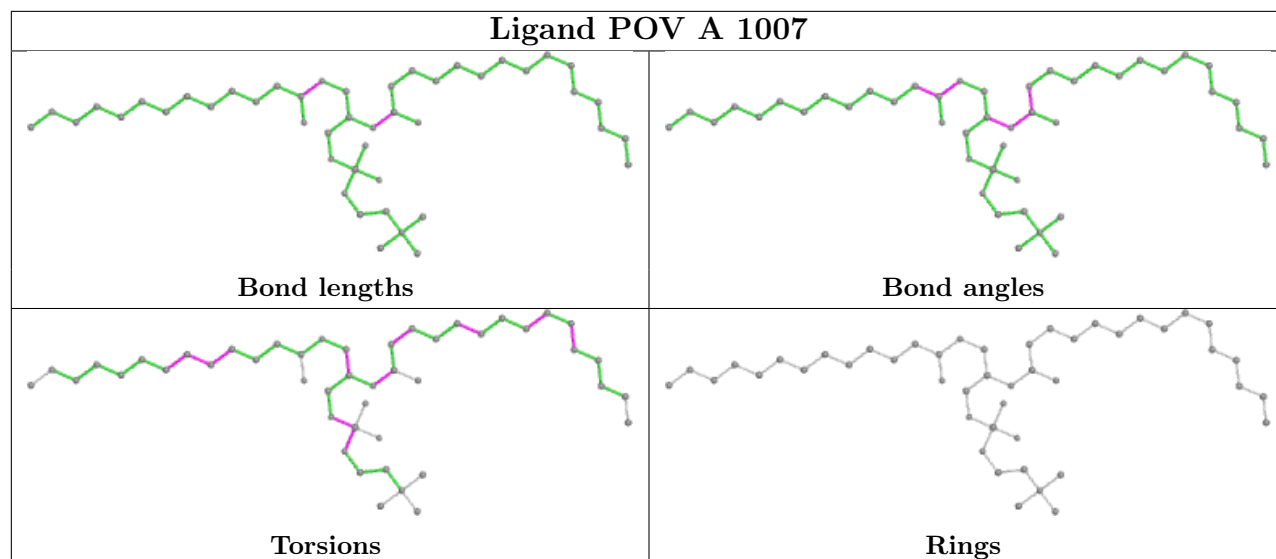


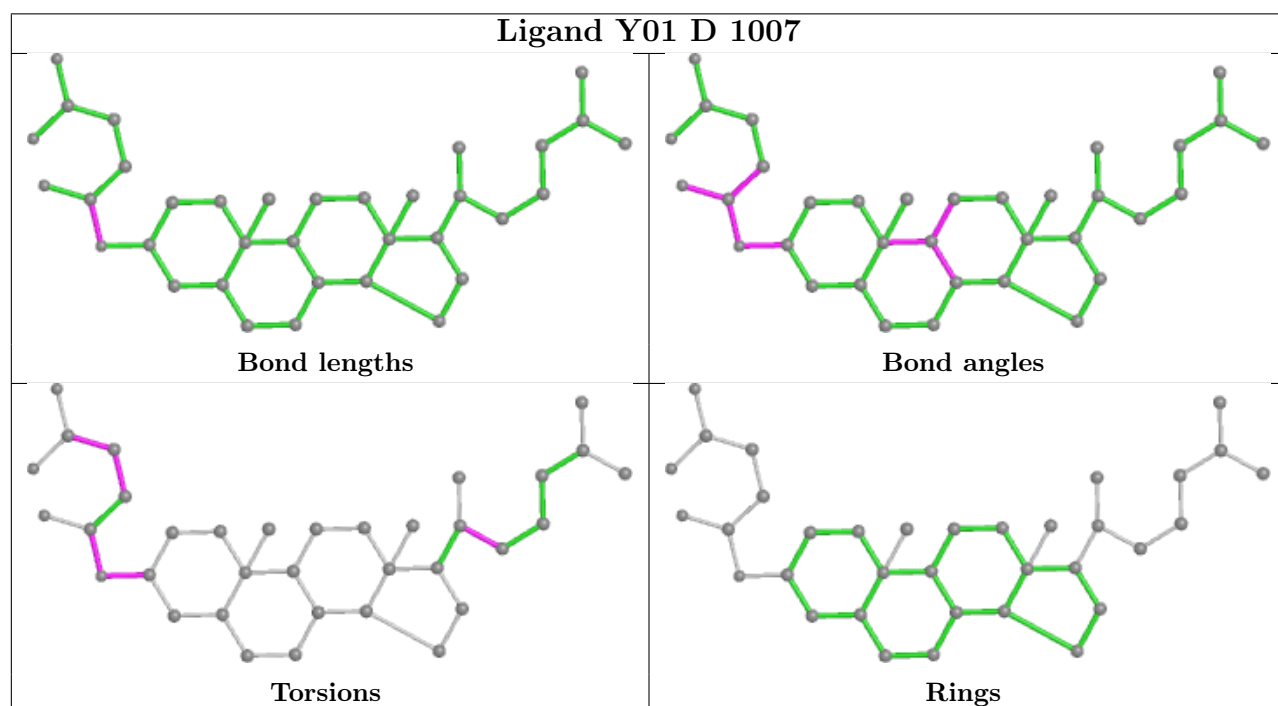
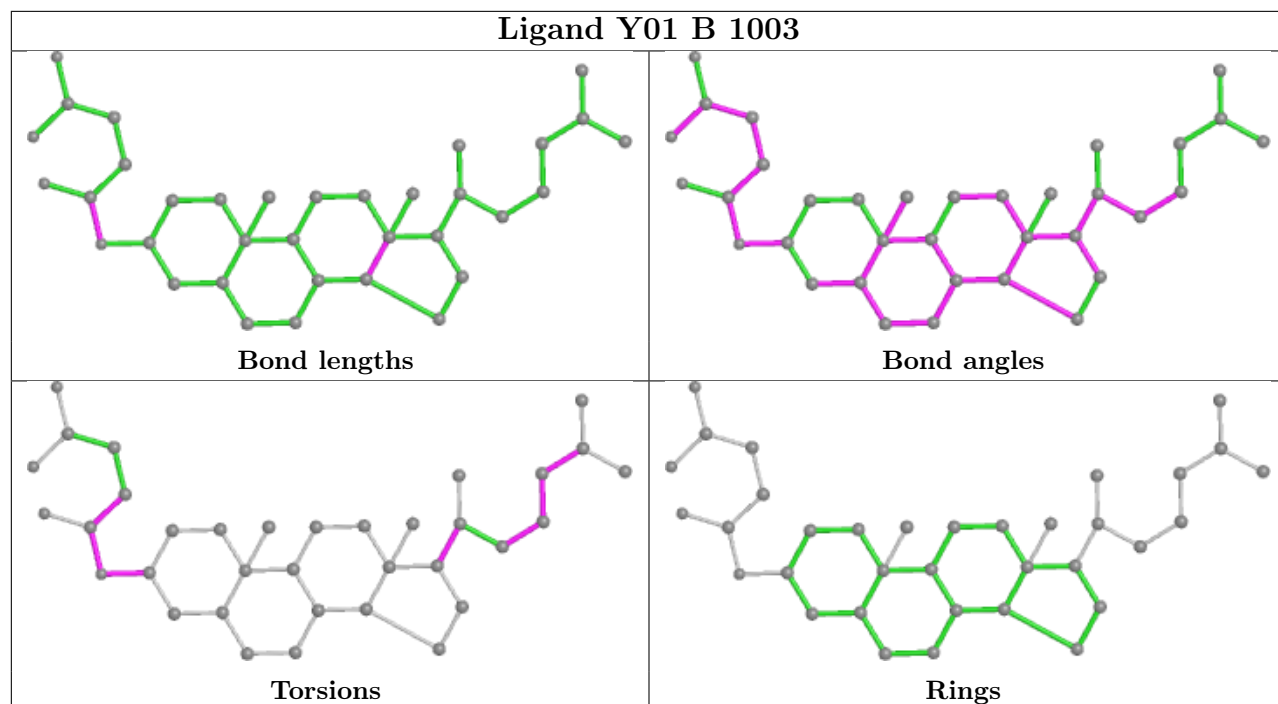


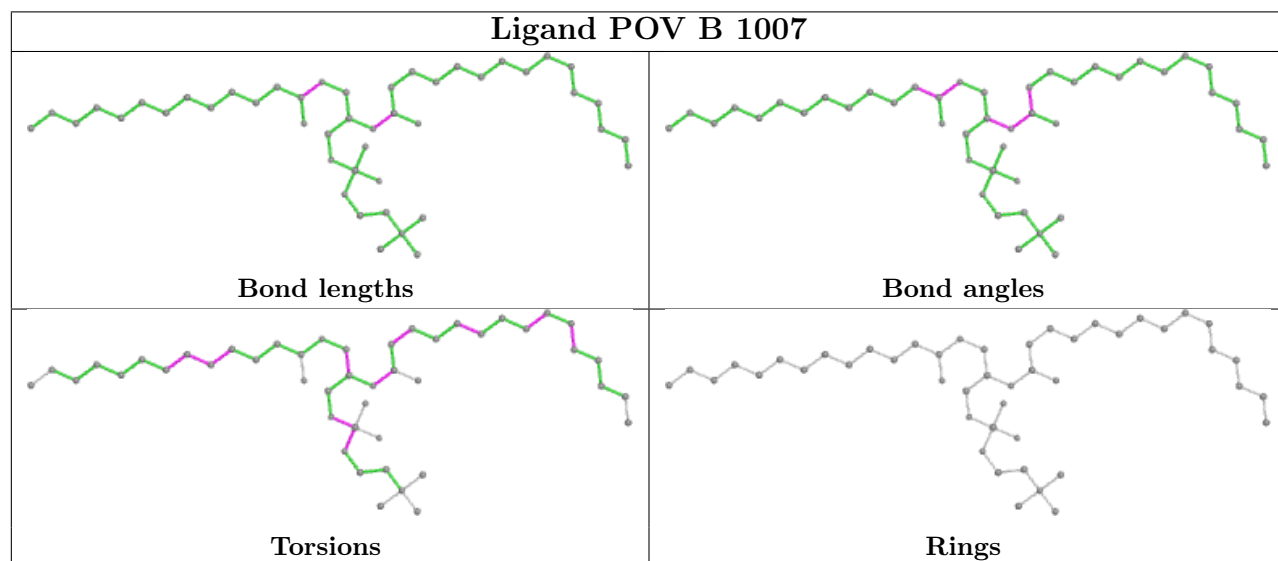
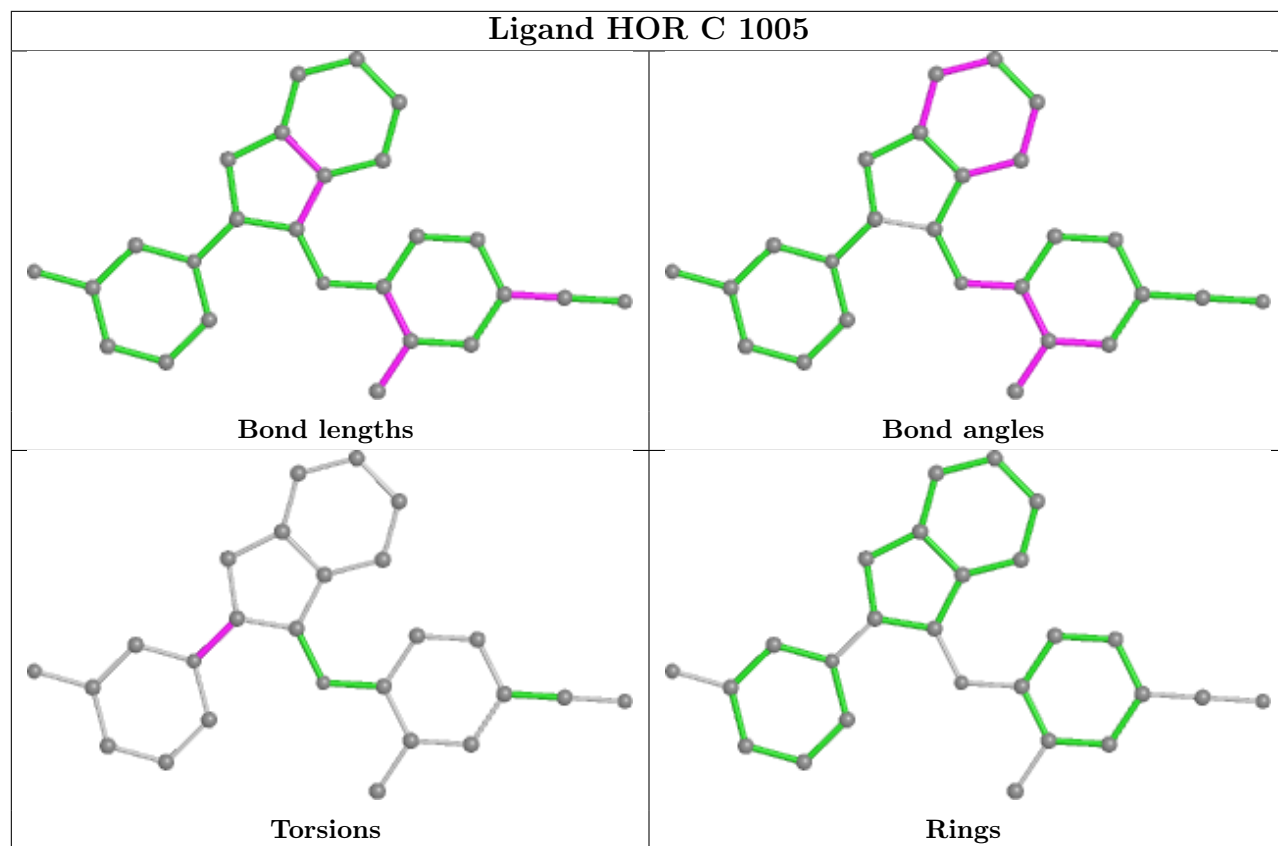


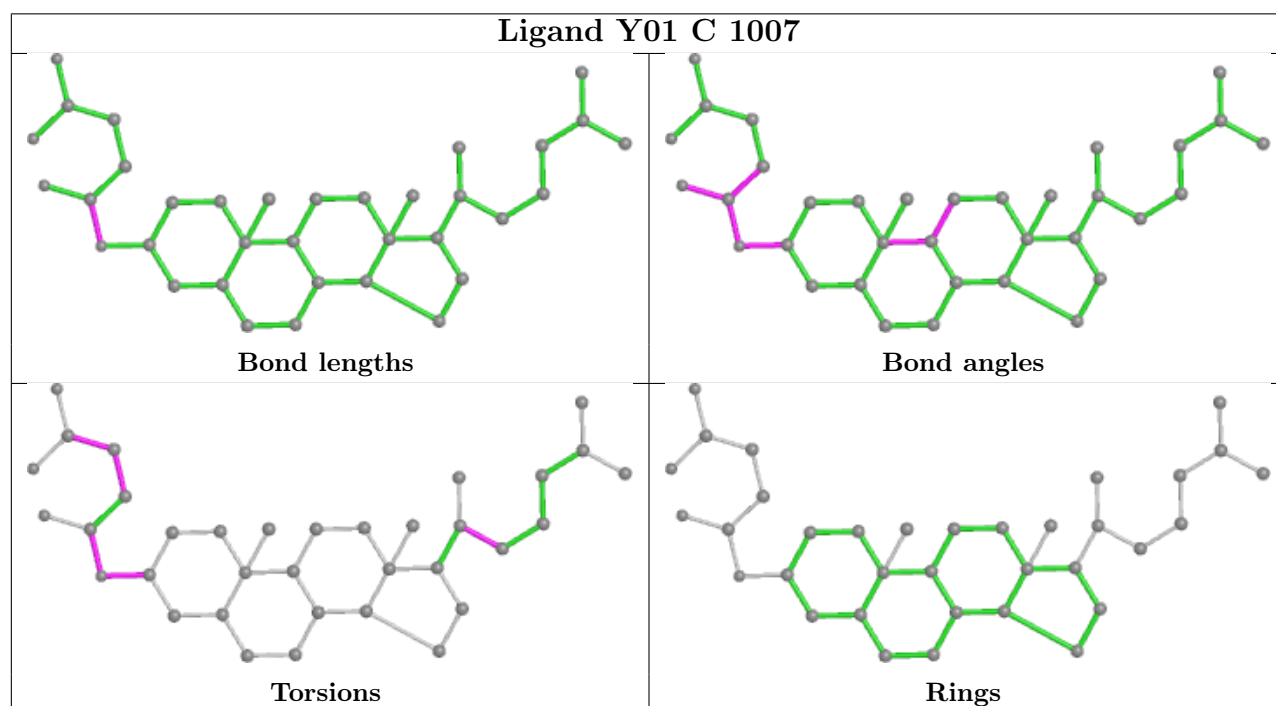
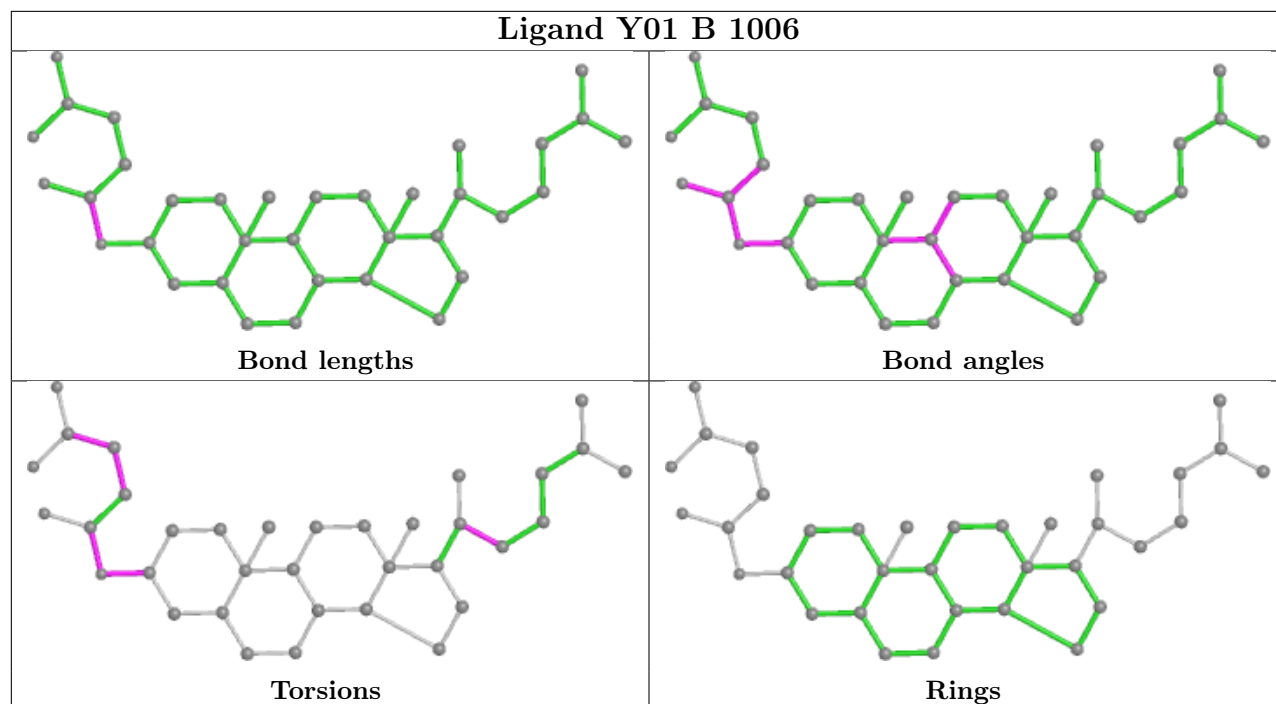


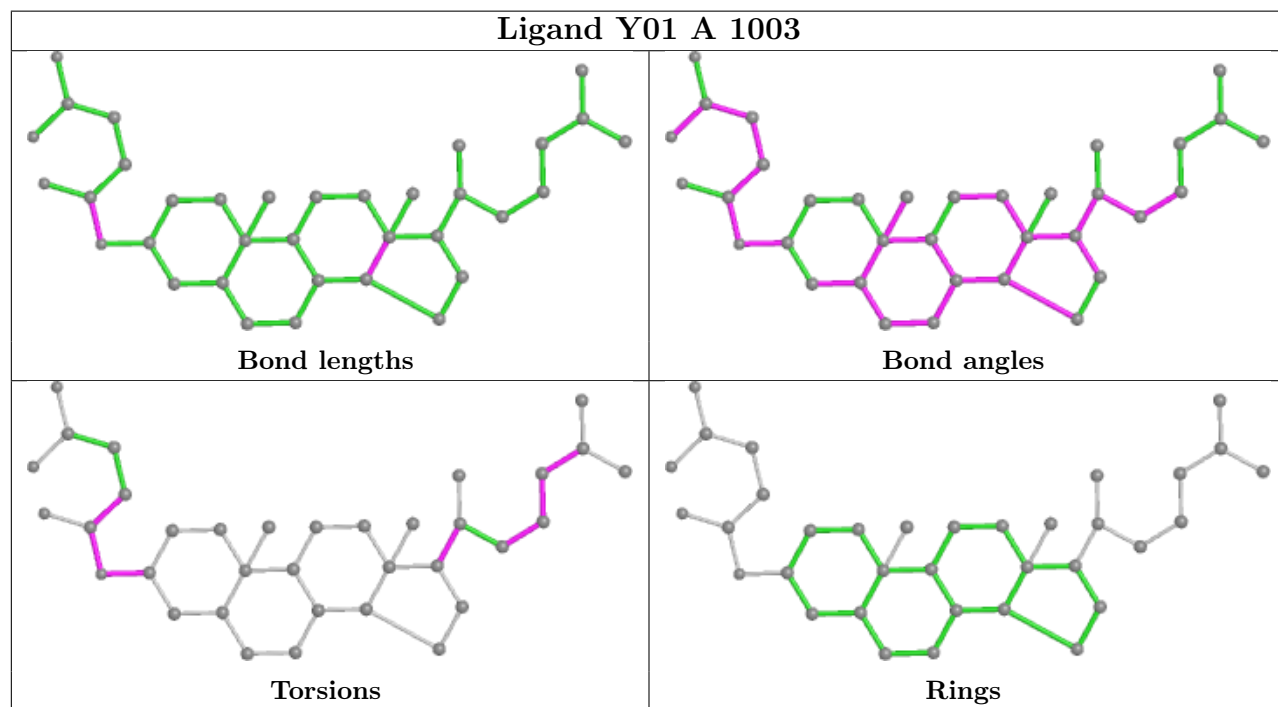
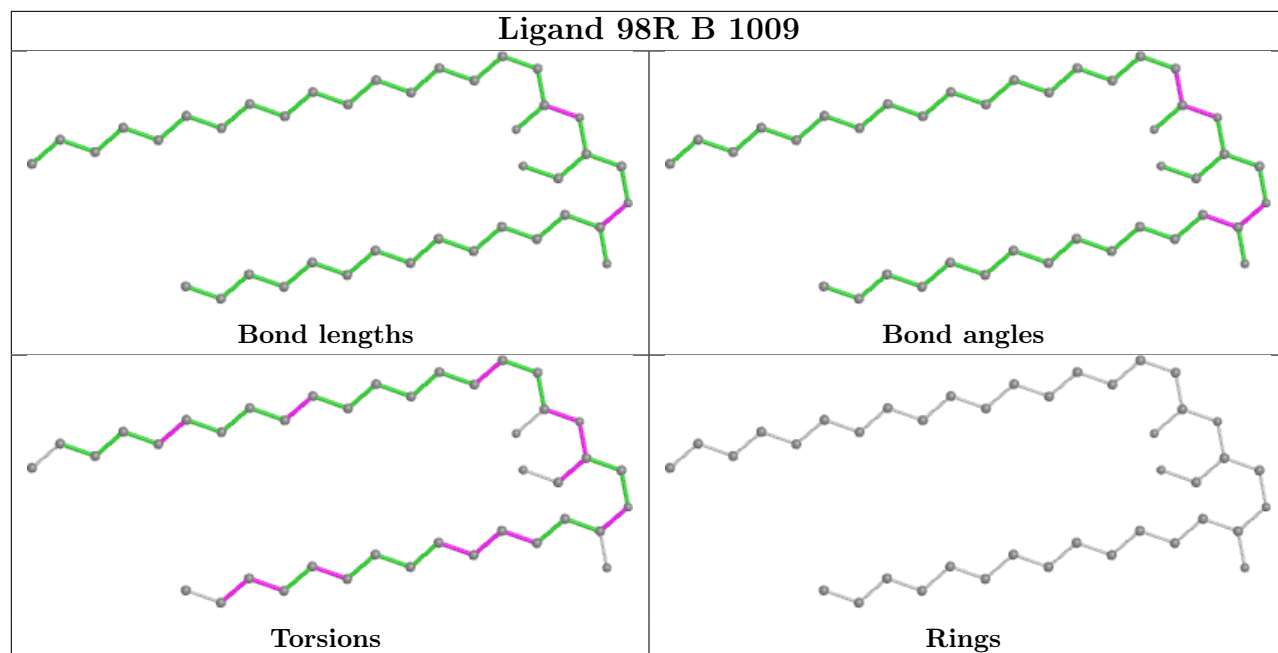


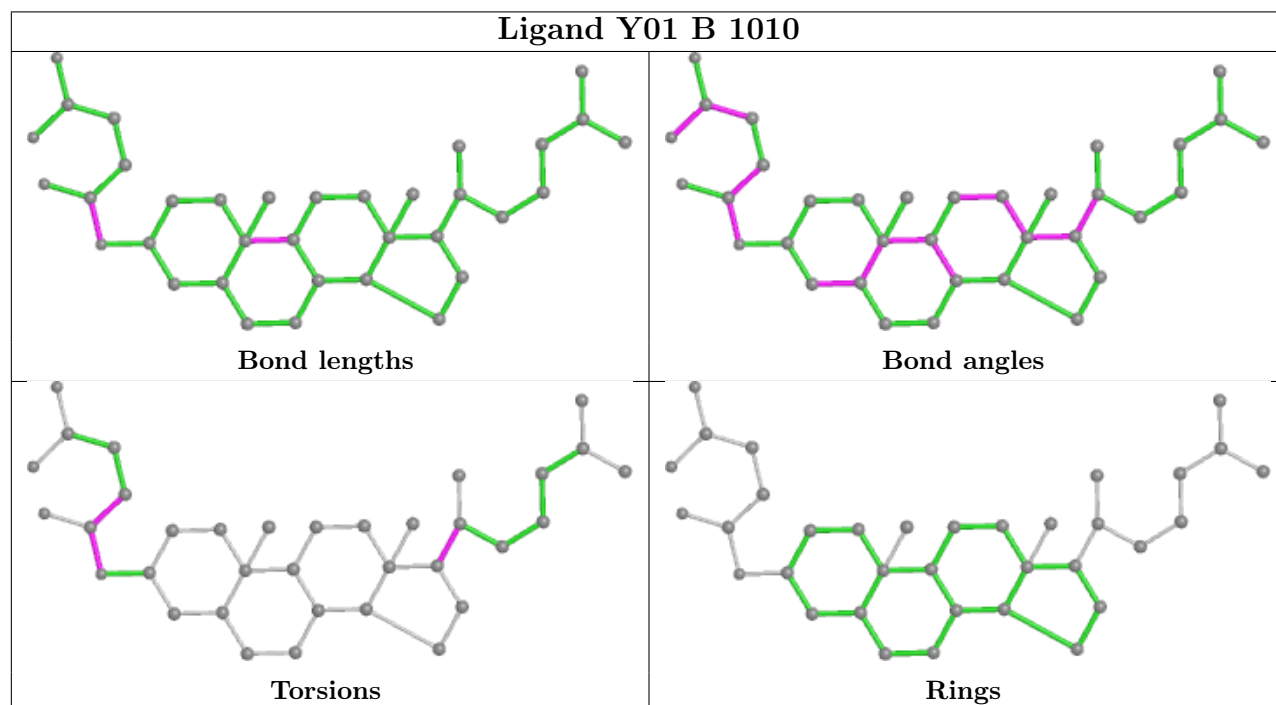
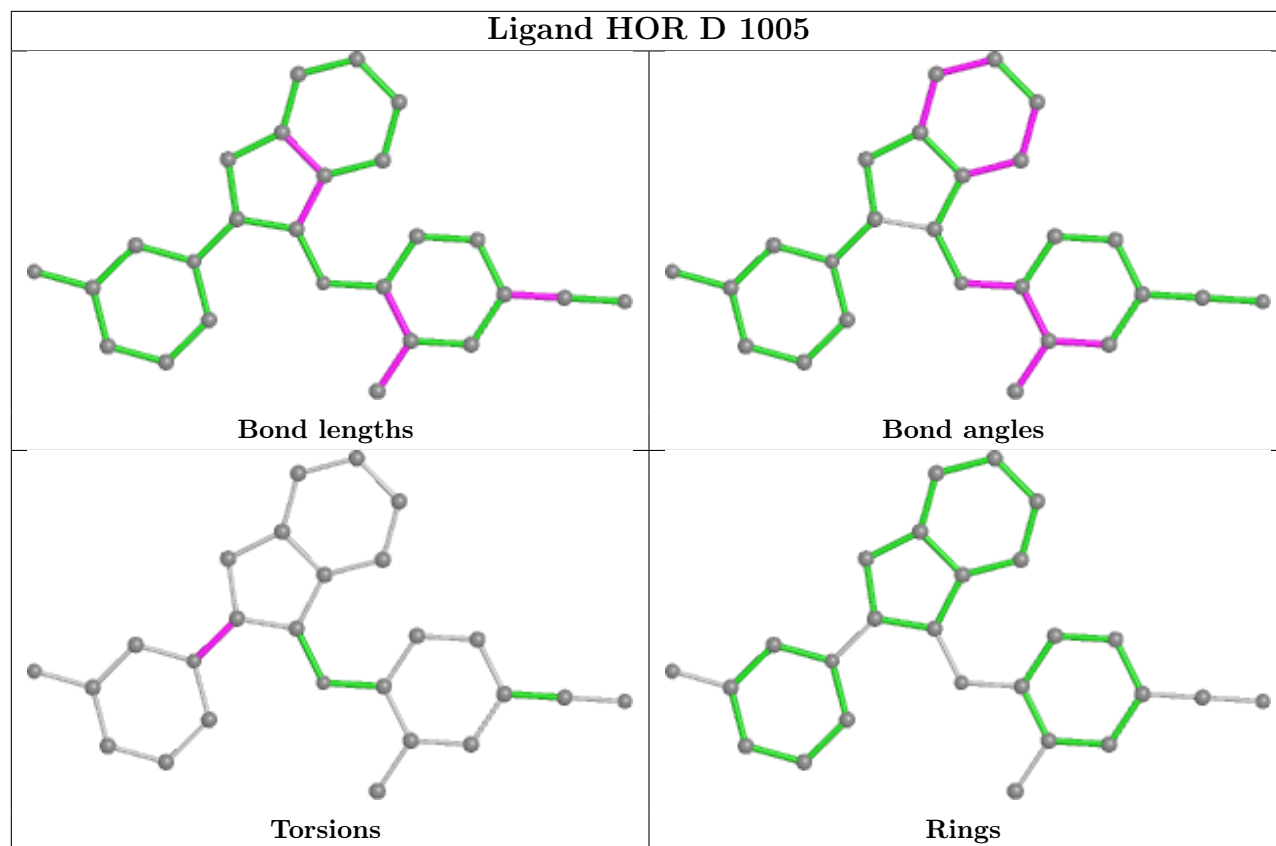


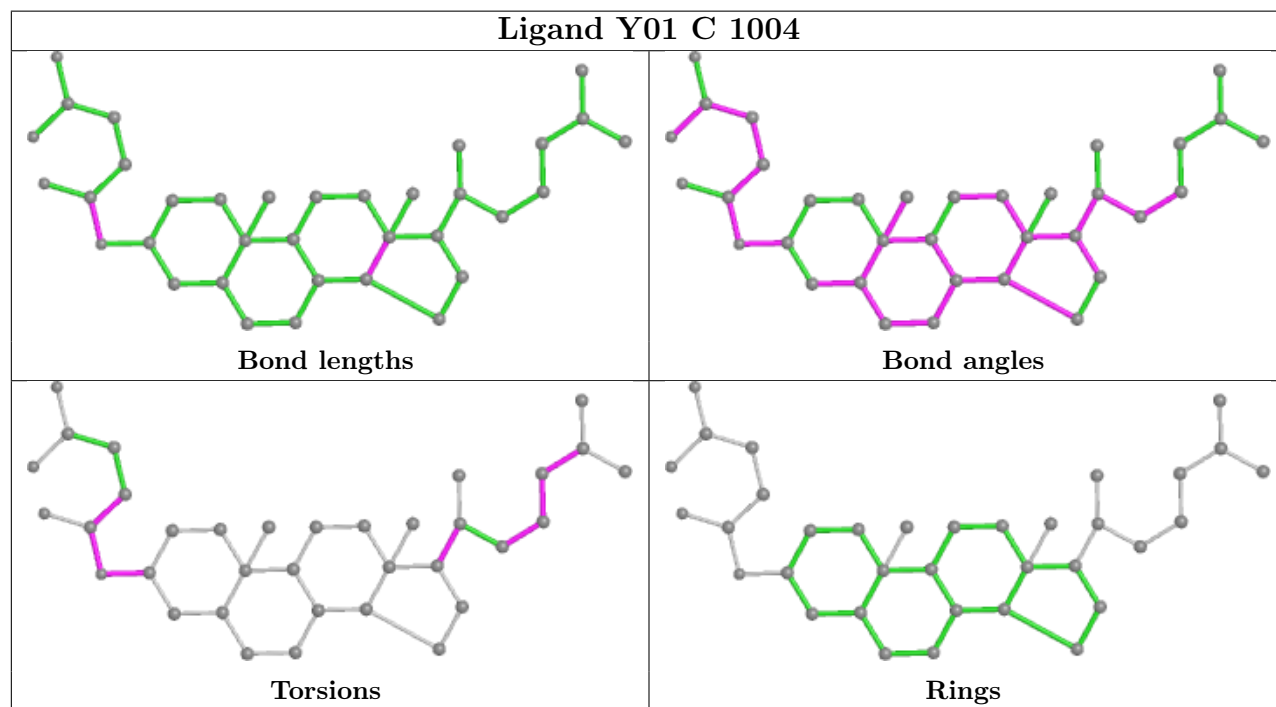
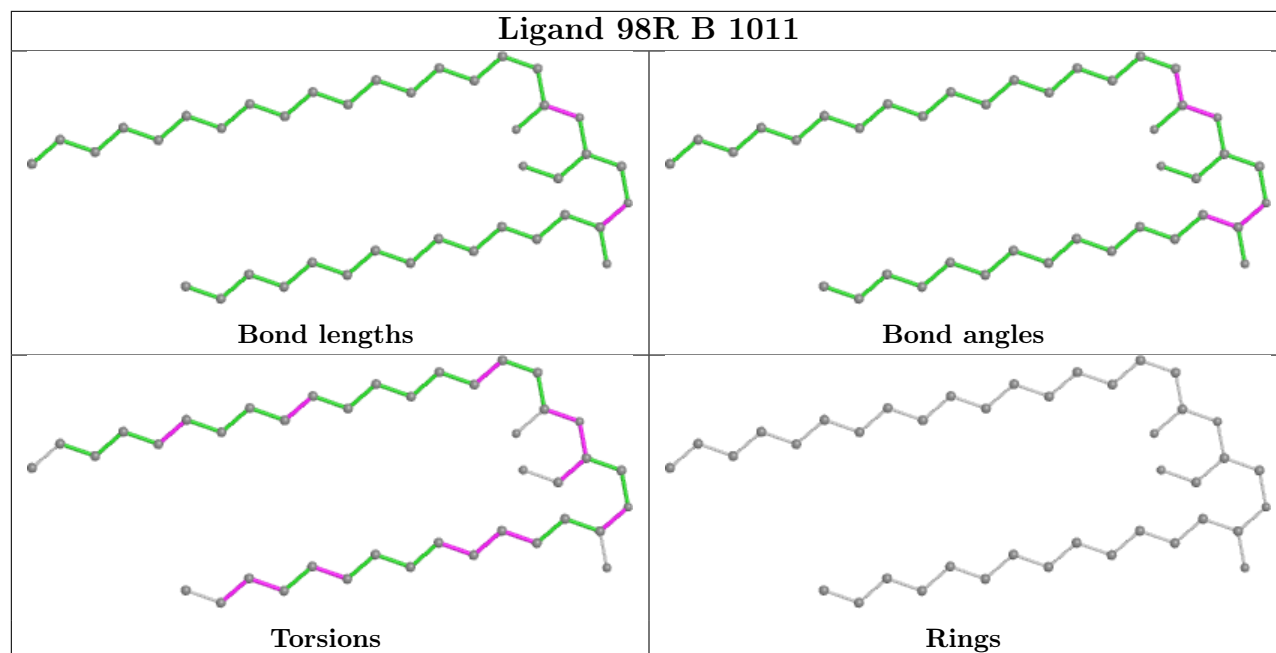


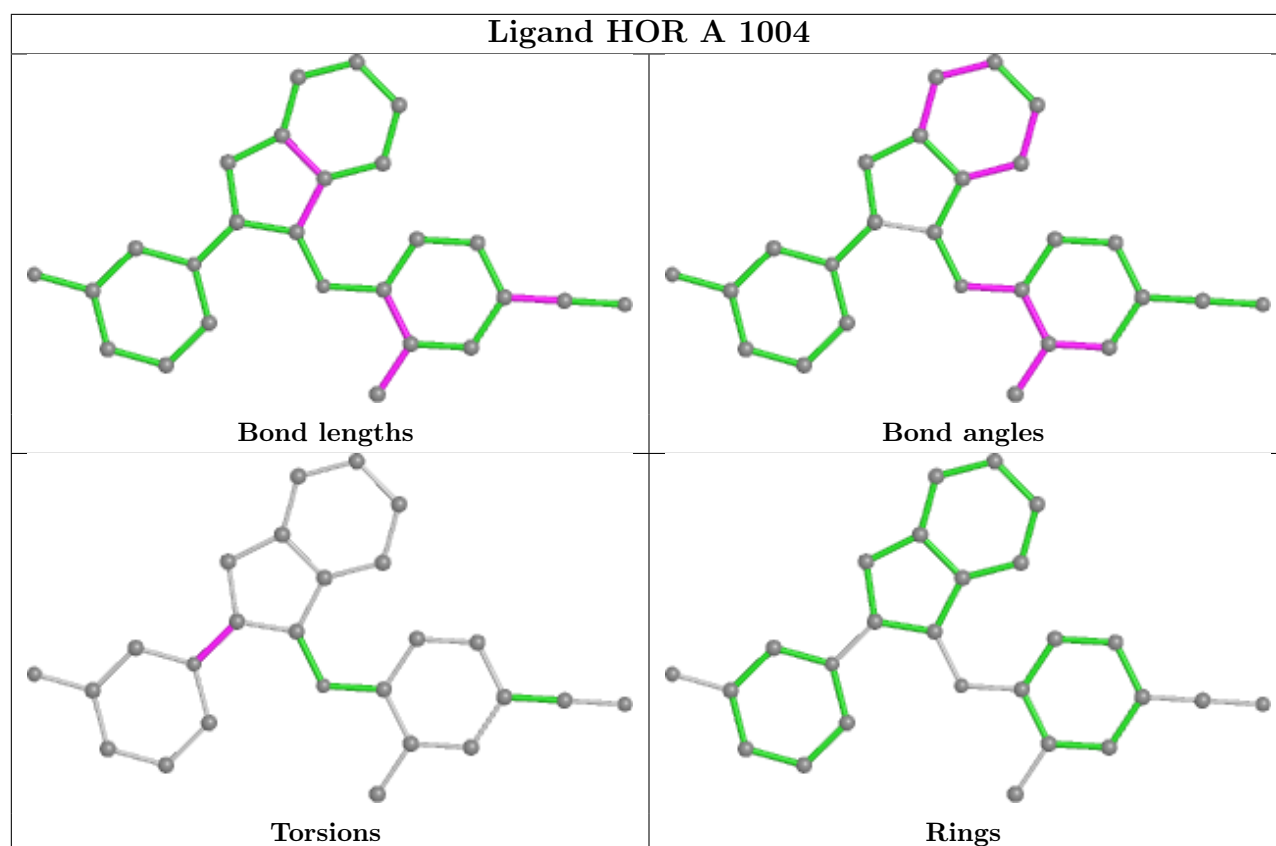












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

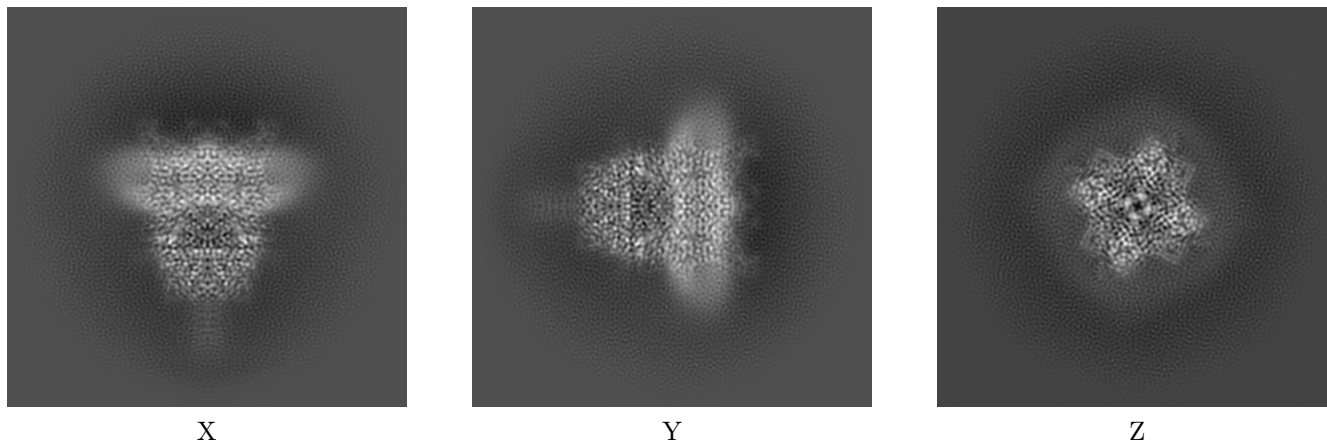
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30908. These allow visual inspection of the internal detail of the map and identification of artifacts.

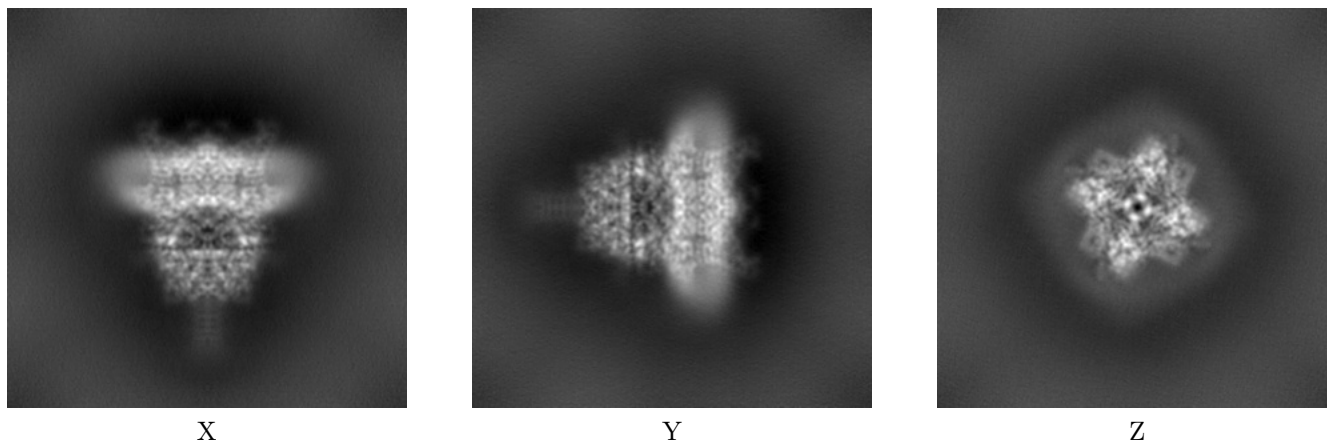
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



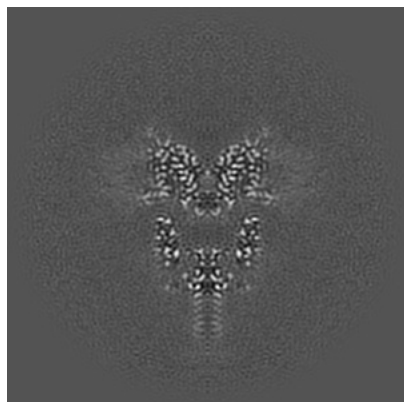
6.1.2 Raw map



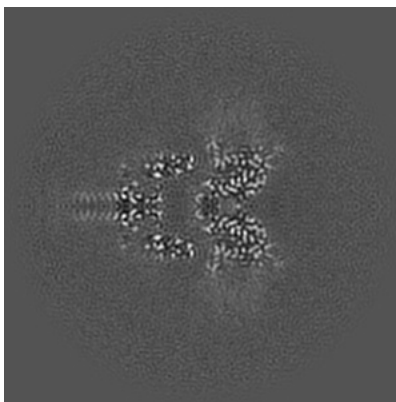
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

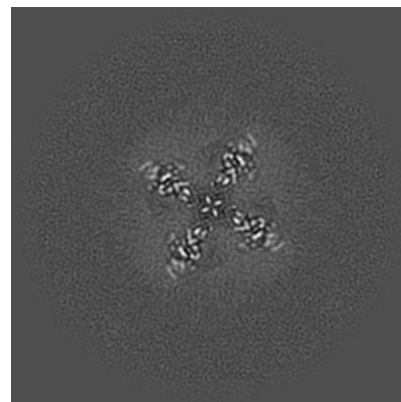
6.2.1 Primary map



X Index: 140

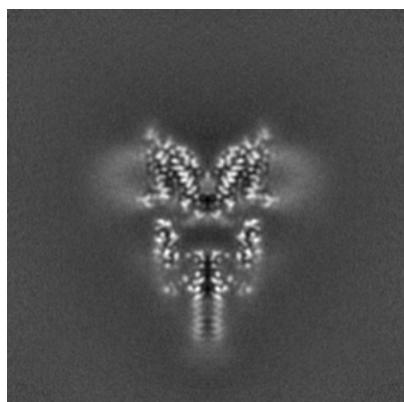


Y Index: 140

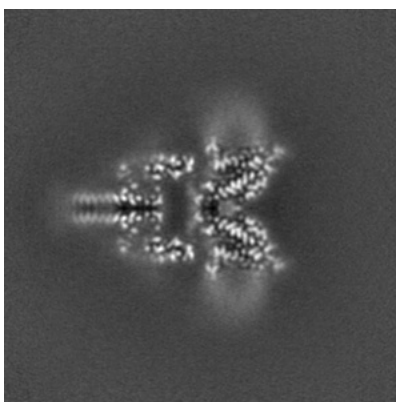


Z Index: 140

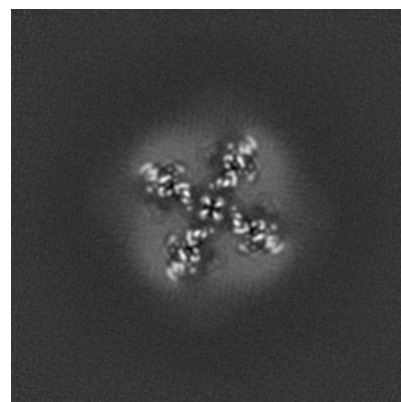
6.2.2 Raw map



X Index: 140



Y Index: 140

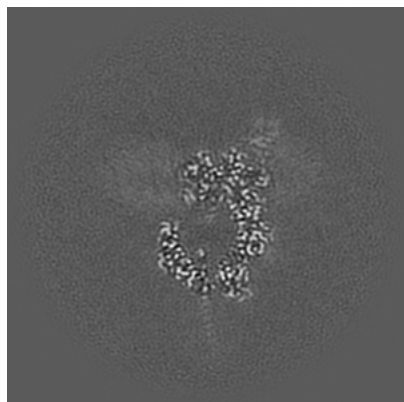


Z Index: 140

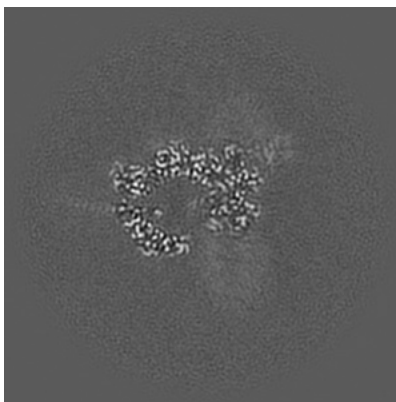
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

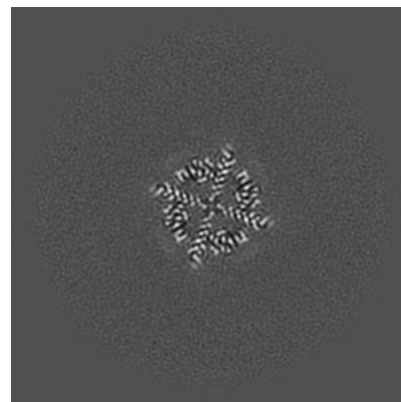
6.3.1 Primary map



X Index: 150

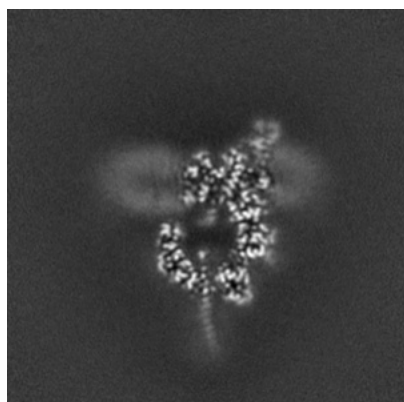


Y Index: 130

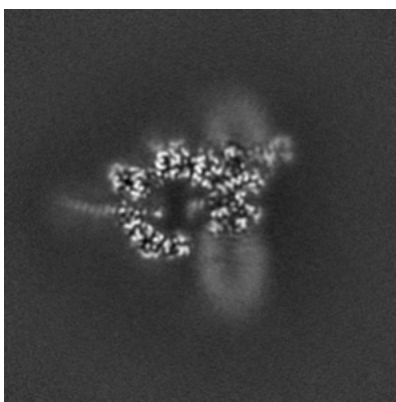


Z Index: 108

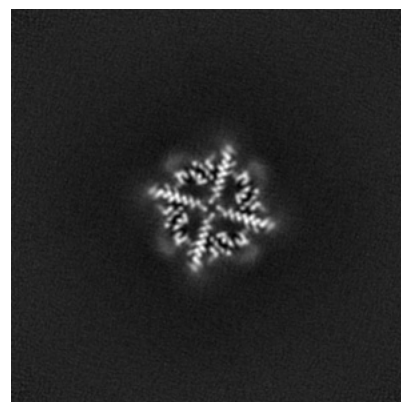
6.3.2 Raw map



X Index: 150



Y Index: 130

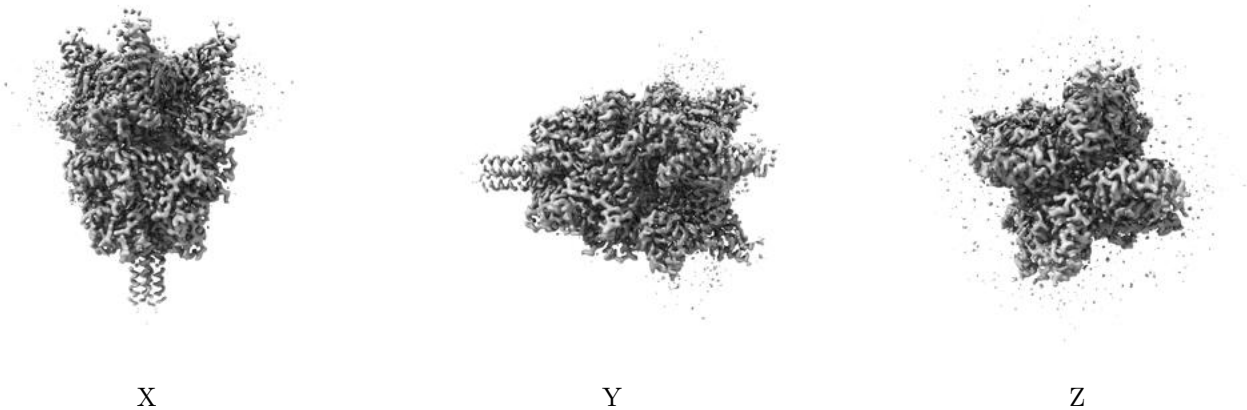


Z Index: 108

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

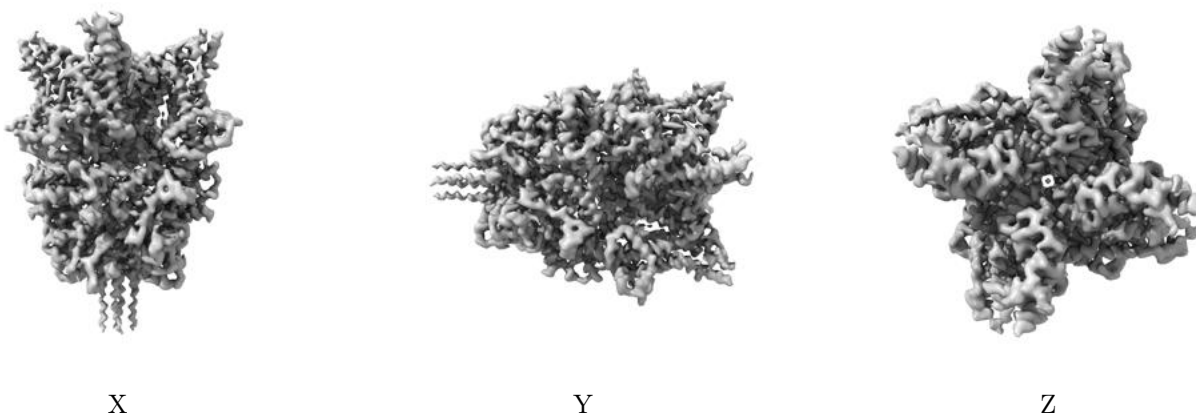
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.96. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

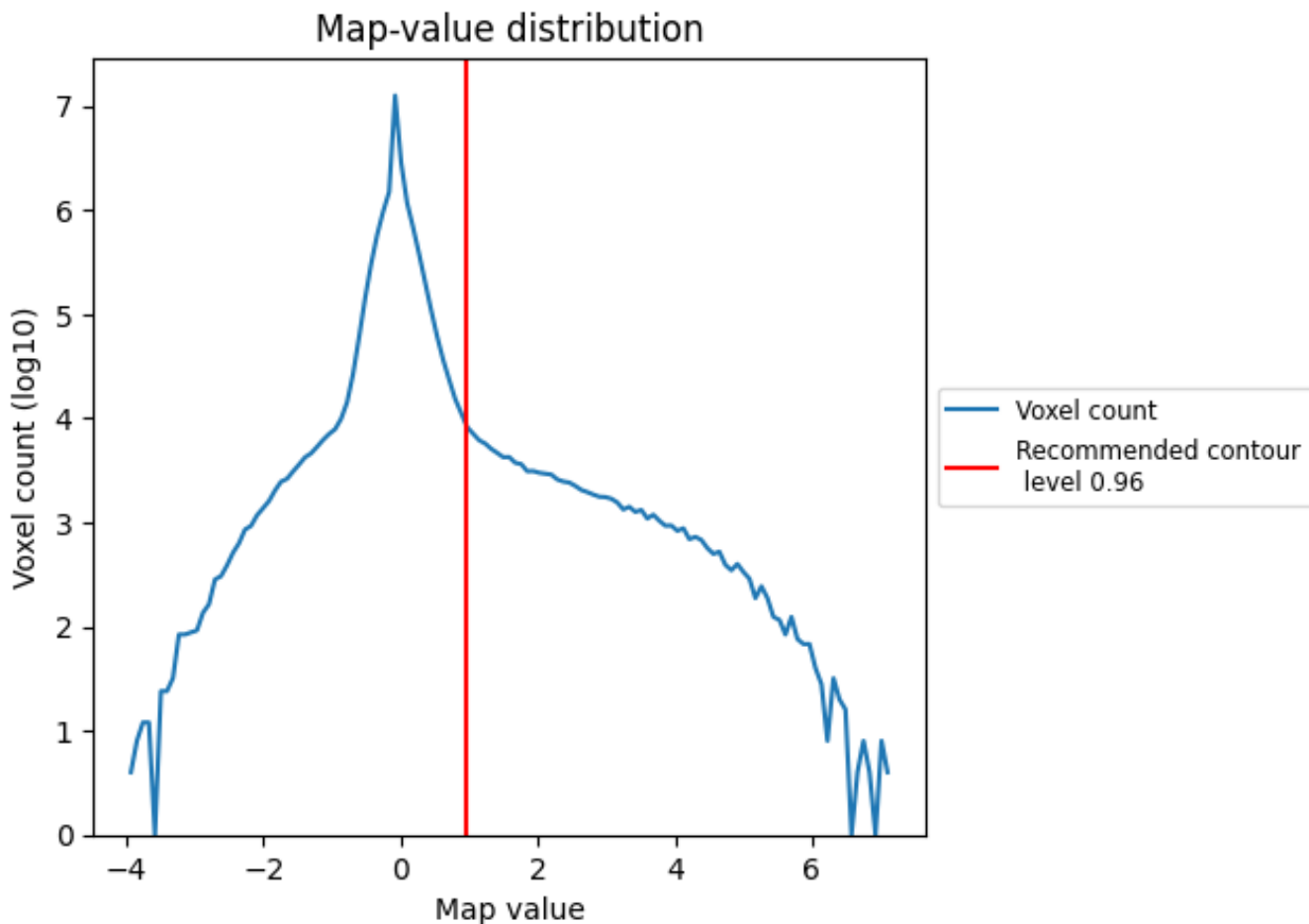
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

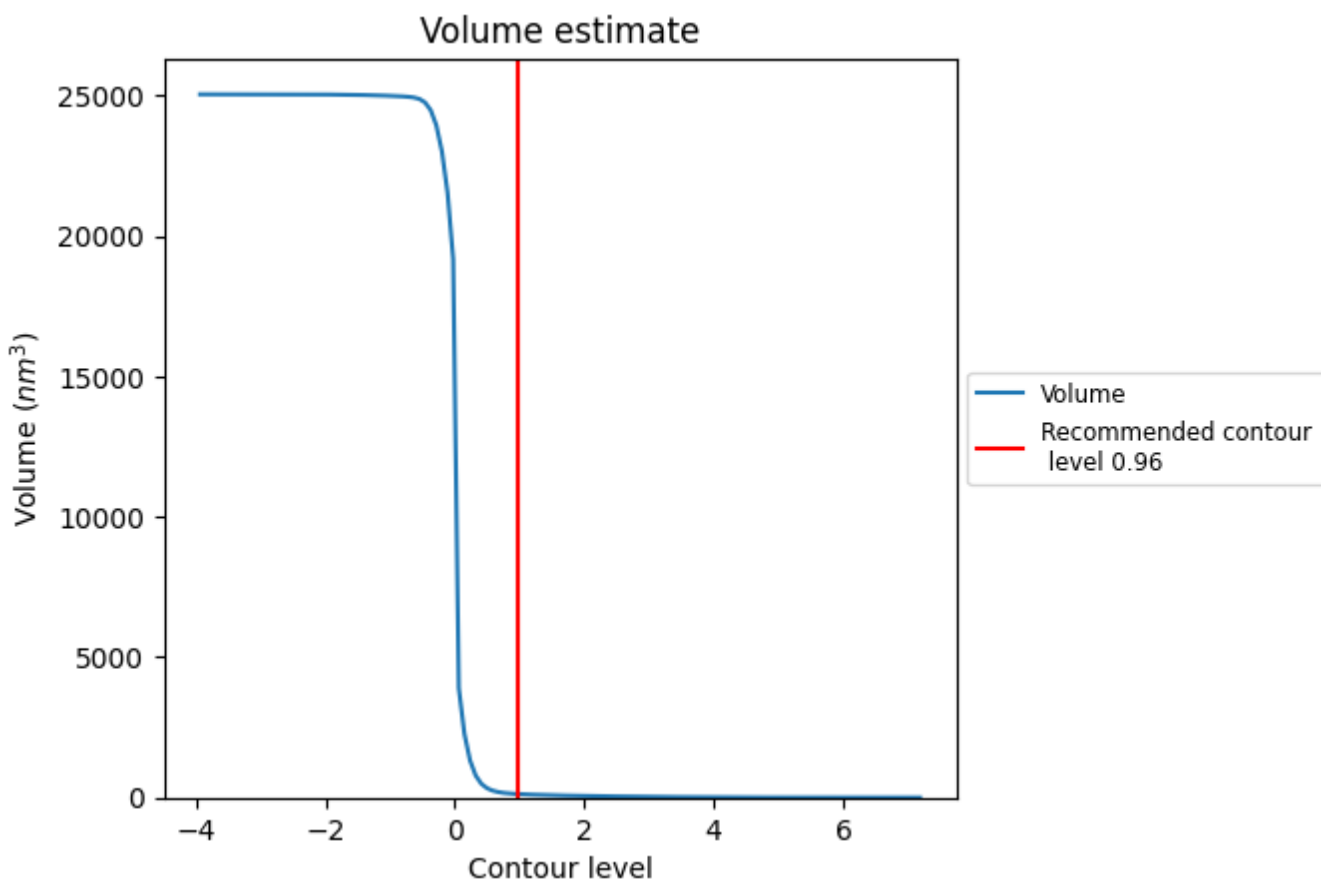
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

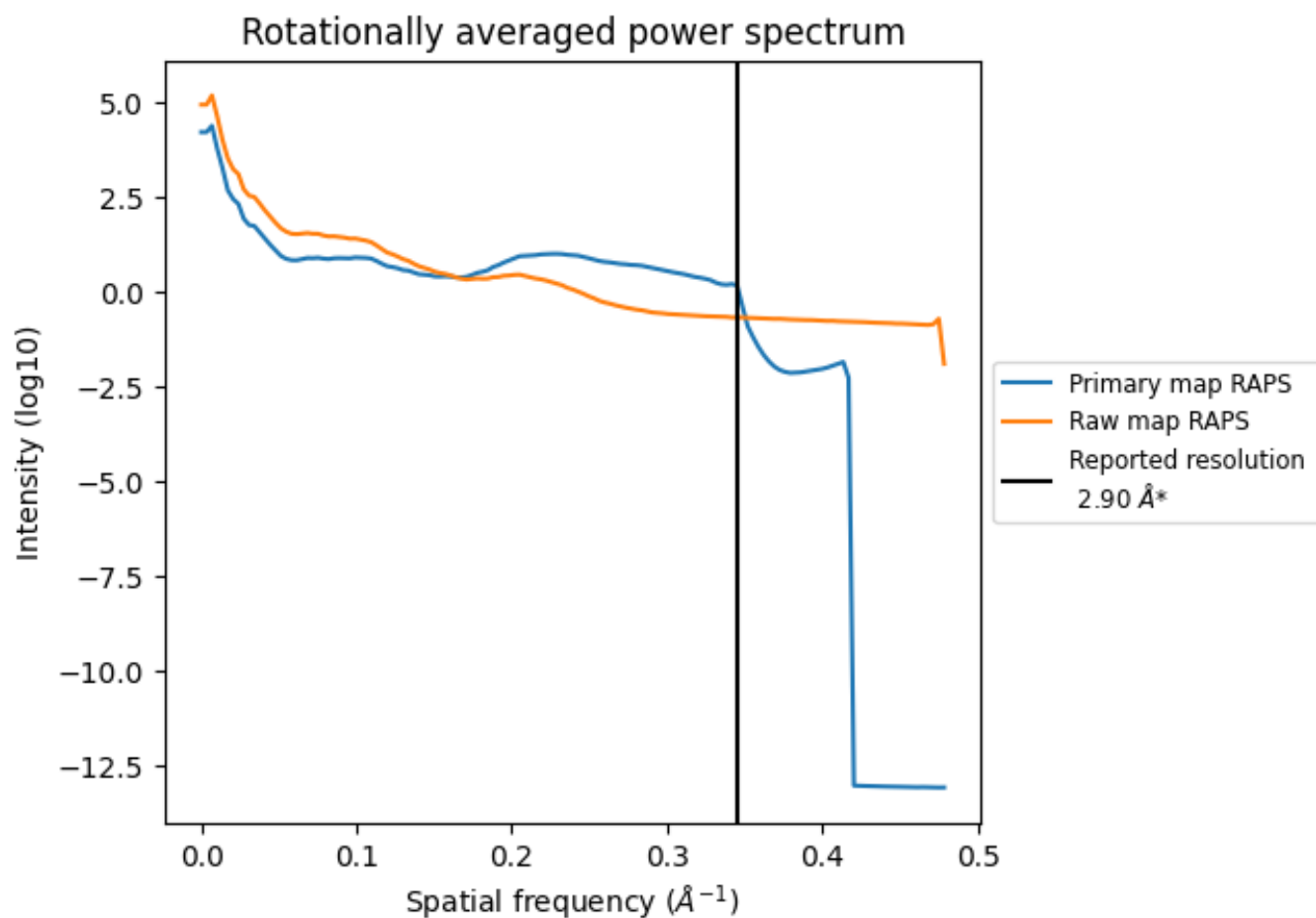
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm³; this corresponds to an approximate mass of 114 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

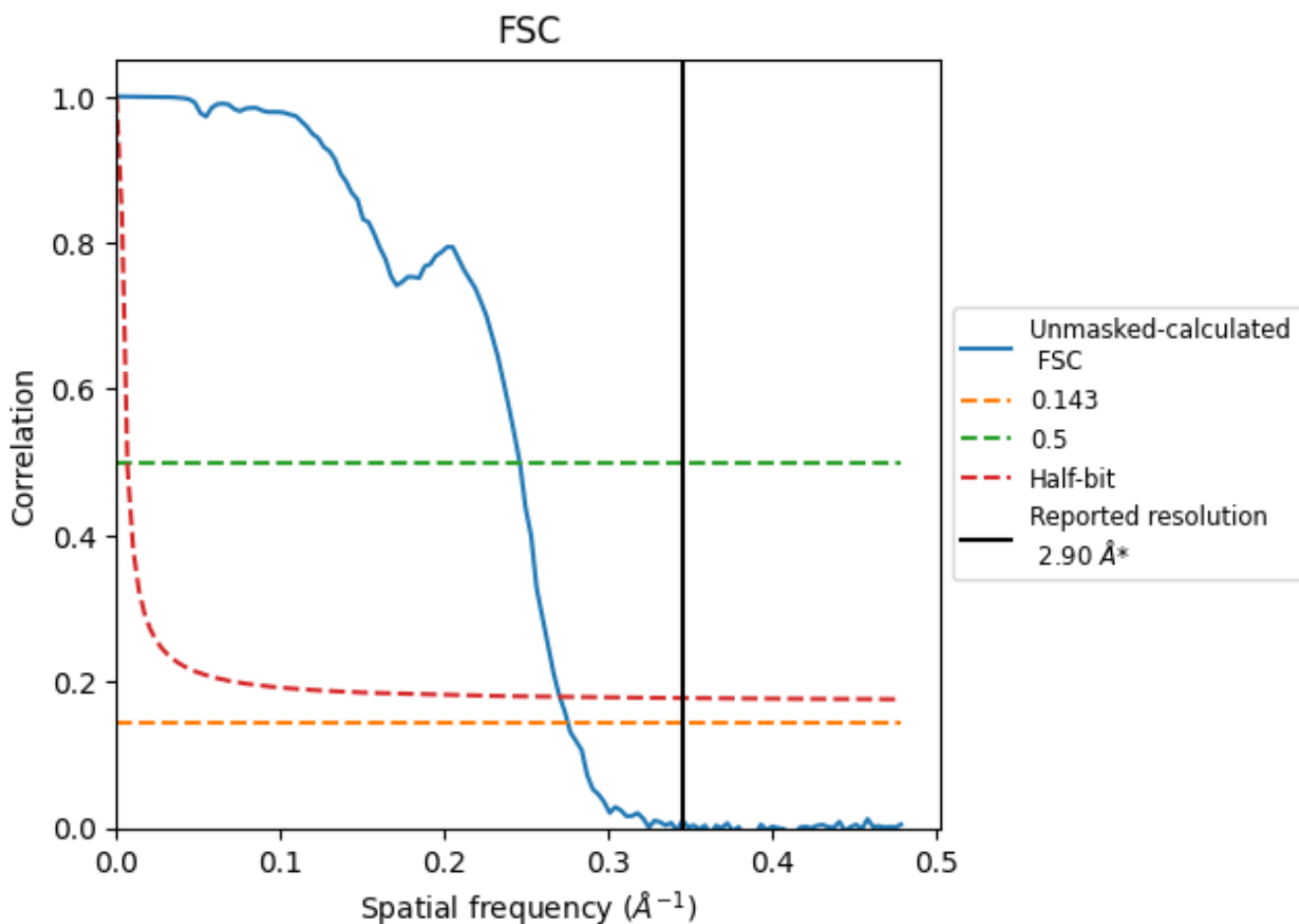


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

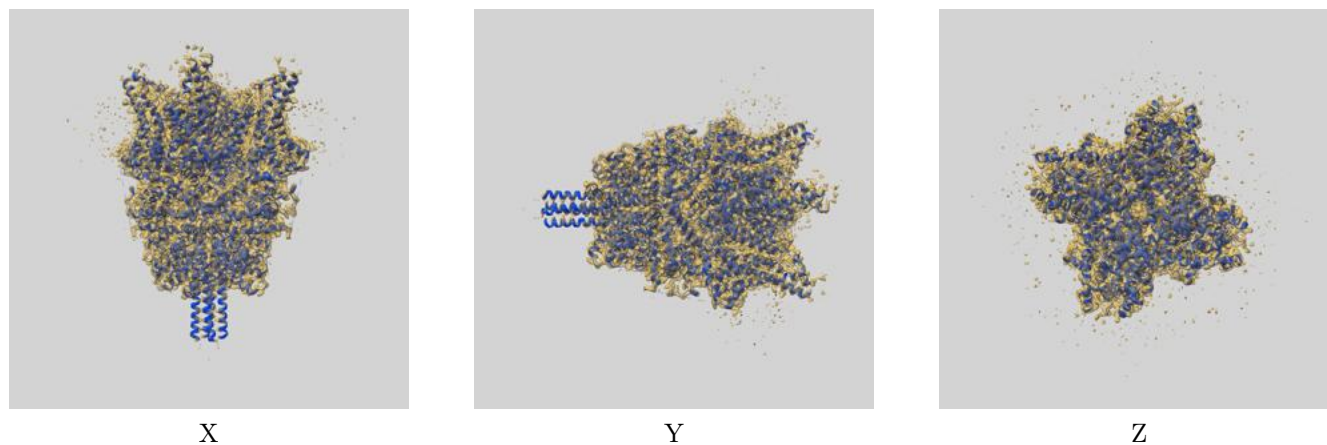
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.63	4.07	3.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.63 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

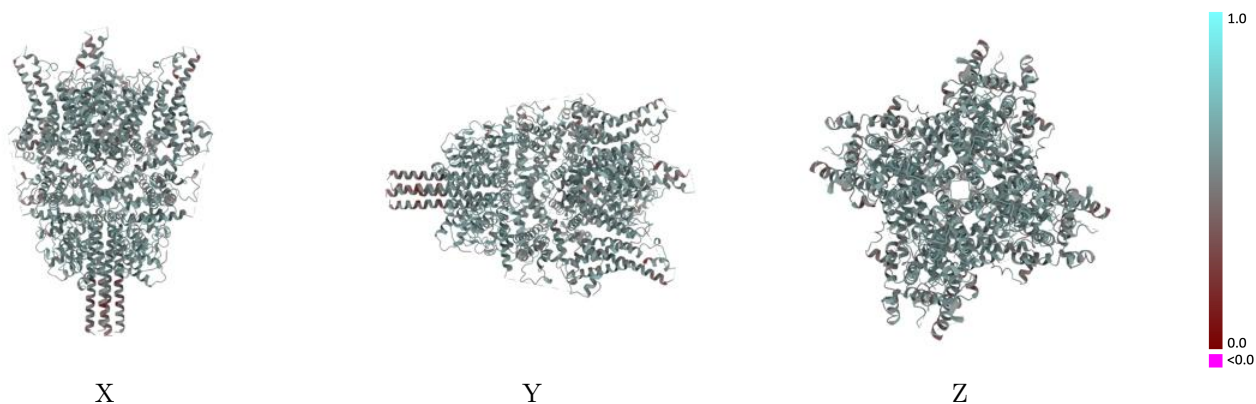
This section contains information regarding the fit between EMDB map EMD-30908 and PDB model 7DXG. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



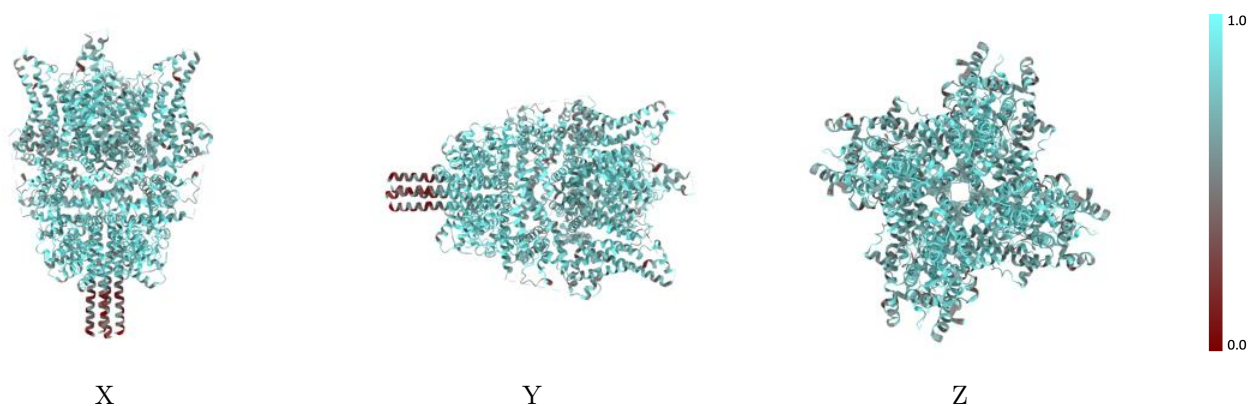
The images above show the 3D surface view of the map at the recommended contour level 0.96 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



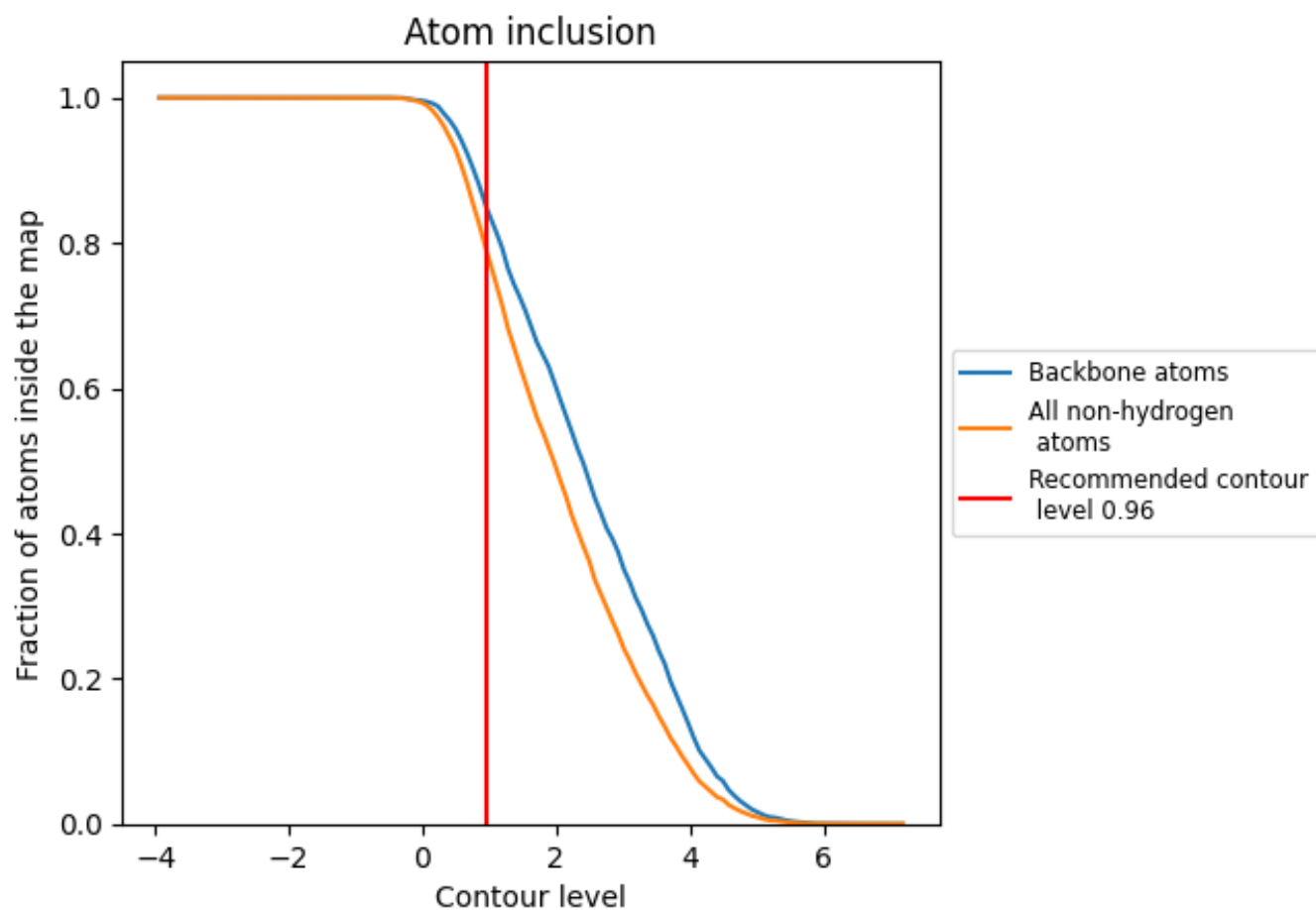
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.96).











9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.96) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7883	 0.5510
A	 0.7877	 0.5520
B	 0.7878	 0.5510
C	 0.7886	 0.5500
D	 0.7891	 0.5520

