



Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 10:27 am BST

PDB ID : 9QPS / pdb_00009qps
EMDB ID : EMD-53282
Title : Single particle cryo-EM structure of MdtF V610F
Authors : Lawrence, R.; Adams, C.; Sousa, J.S.; Ahdash, Z.; Reading, E.
Deposited on : 2025-03-28
Resolution : 3.28 Å(reported)
Based on initial model : 9QPR

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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

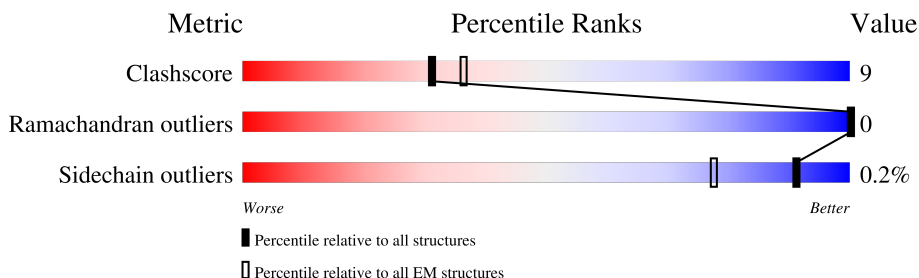
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.28 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1055	
1	B	1055	
1	C	1055	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24003 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 Multidrug resistance protein MdtF.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1024	Total	C	N	O	S	0	0
			7748	4977	1272	1457	42		
1	B	1016	Total	C	N	O	S	0	0
			7674	4926	1257	1449	42		
1	C	1016	Total	C	N	O	S	0	0
			7680	4929	1260	1449	42		

There are 57 discrepancies between the modelled and reference sequences:

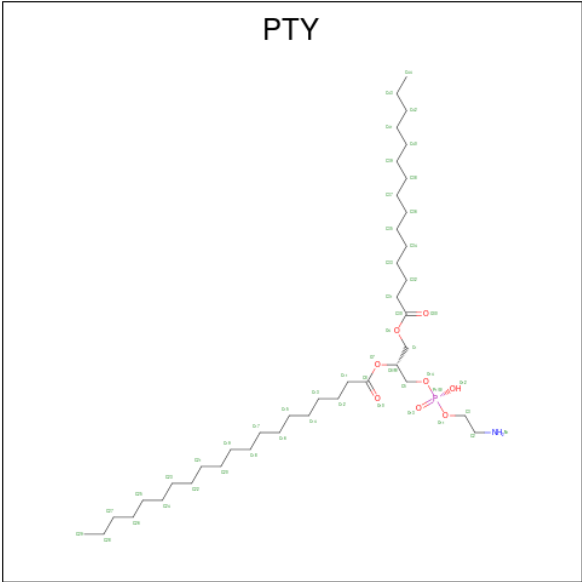
Chain	Residue	Modelled	Actual	Comment	Reference
A	610	PHE	VAL	engineered mutation	UNP P37637
A	1038	ALA	-	expression tag	UNP P37637
A	1039	SER	-	expression tag	UNP P37637
A	1040	GLY	-	expression tag	UNP P37637
A	1041	GLU	-	expression tag	UNP P37637
A	1042	ASN	-	expression tag	UNP P37637
A	1043	LEU	-	expression tag	UNP P37637
A	1044	TYR	-	expression tag	UNP P37637
A	1045	PHE	-	expression tag	UNP P37637
A	1046	GLN	-	expression tag	UNP P37637
A	1047	SER	-	expression tag	UNP P37637
A	1048	LEU	-	expression tag	UNP P37637
A	1049	GLU	-	expression tag	UNP P37637
A	1050	HIS	-	expression tag	UNP P37637
A	1051	HIS	-	expression tag	UNP P37637
A	1052	HIS	-	expression tag	UNP P37637
A	1053	HIS	-	expression tag	UNP P37637
A	1054	HIS	-	expression tag	UNP P37637
A	1055	HIS	-	expression tag	UNP P37637
B	610	PHE	VAL	engineered mutation	UNP P37637
B	1038	ALA	-	expression tag	UNP P37637
B	1039	SER	-	expression tag	UNP P37637
B	1040	GLY	-	expression tag	UNP P37637
B	1041	GLU	-	expression tag	UNP P37637

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1042	ASN	-	expression tag	UNP P37637
B	1043	LEU	-	expression tag	UNP P37637
B	1044	TYR	-	expression tag	UNP P37637
B	1045	PHE	-	expression tag	UNP P37637
B	1046	GLN	-	expression tag	UNP P37637
B	1047	SER	-	expression tag	UNP P37637
B	1048	LEU	-	expression tag	UNP P37637
B	1049	GLU	-	expression tag	UNP P37637
B	1050	HIS	-	expression tag	UNP P37637
B	1051	HIS	-	expression tag	UNP P37637
B	1052	HIS	-	expression tag	UNP P37637
B	1053	HIS	-	expression tag	UNP P37637
B	1054	HIS	-	expression tag	UNP P37637
B	1055	HIS	-	expression tag	UNP P37637
C	610	PHE	VAL	engineered mutation	UNP P37637
C	1038	ALA	-	expression tag	UNP P37637
C	1039	SER	-	expression tag	UNP P37637
C	1040	GLY	-	expression tag	UNP P37637
C	1041	GLU	-	expression tag	UNP P37637
C	1042	ASN	-	expression tag	UNP P37637
C	1043	LEU	-	expression tag	UNP P37637
C	1044	TYR	-	expression tag	UNP P37637
C	1045	PHE	-	expression tag	UNP P37637
C	1046	GLN	-	expression tag	UNP P37637
C	1047	SER	-	expression tag	UNP P37637
C	1048	LEU	-	expression tag	UNP P37637
C	1049	GLU	-	expression tag	UNP P37637
C	1050	HIS	-	expression tag	UNP P37637
C	1051	HIS	-	expression tag	UNP P37637
C	1052	HIS	-	expression tag	UNP P37637
C	1053	HIS	-	expression tag	UNP P37637
C	1054	HIS	-	expression tag	UNP P37637
C	1055	HIS	-	expression tag	UNP P37637

- Molecule 2 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



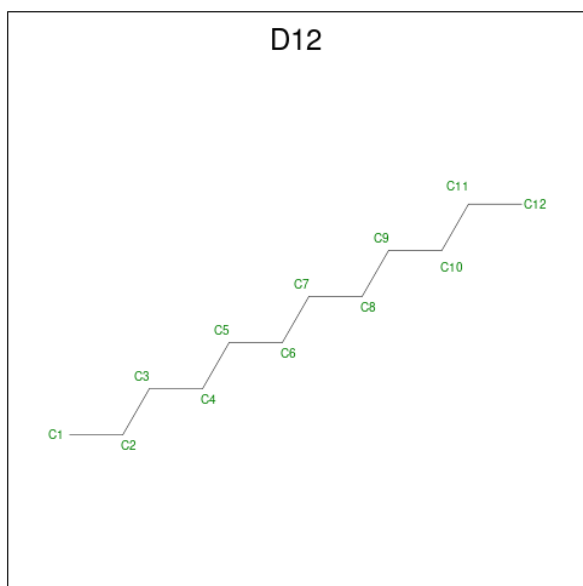
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	A	1	Total	C	N	O	P	0
			29	19	1	8	1	
2	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
2	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	B	1	Total	C	N	O	P	0
			50	40	1	8	1	
2	B	1	Total	C	N	O	P	0
			29	20	1	7	1	
2	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	B	1	Total	C	N	O	P	0
			27	17	1	8	1	
2	B	1	Total	C	N	O	P	0
			30	20	1	8	1	
2	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	B	1	Total	C	N	O	P	0
			37	27	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			38	28	1	8	1	
2	B	1	Total	C	N	O	P	0
			24	14	1	8	1	
2	B	1	Total	C	N	O	P	0
			33	23	1	8	1	
2	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
2	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
2	C	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	C	1	Total	C	N	O	P	0
			25	15	1	8	1	
2	C	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 3 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	C	0
			8	8	
3	A	1	Total	C	0
			10	10	
3	A	1	Total	C	0
			8	8	

Continued on next page...

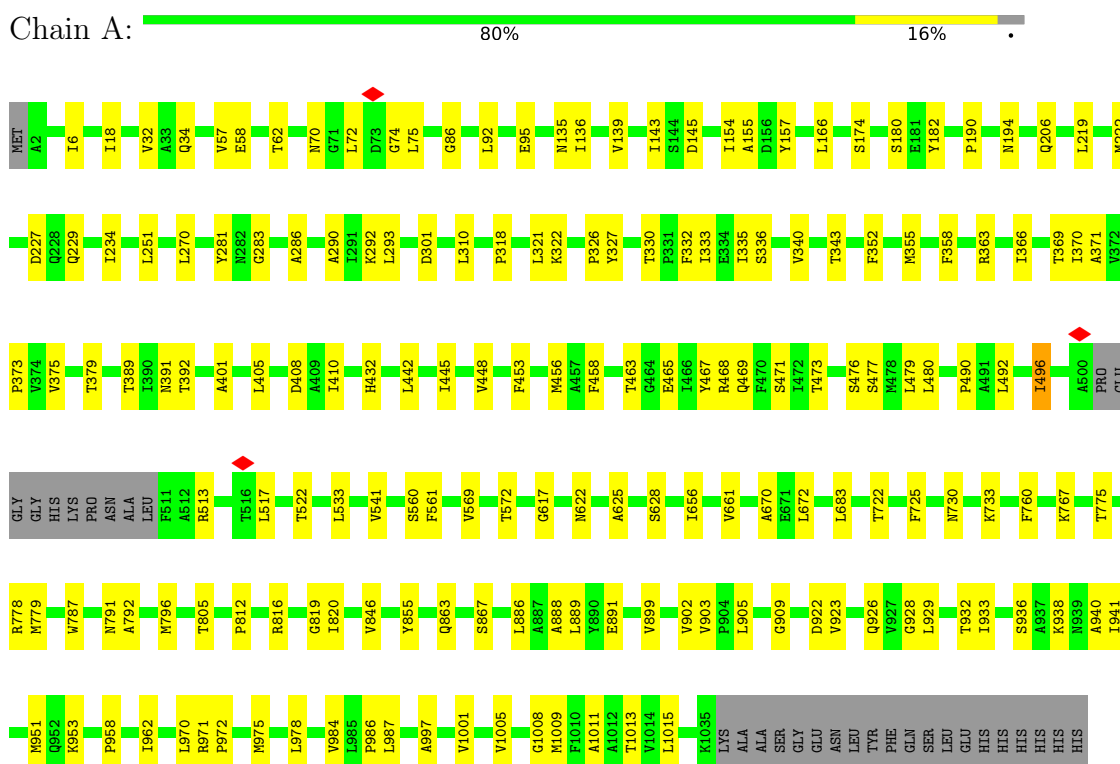
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C 8 8	0
3	B	1	Total C 10 10	0
3	B	1	Total C 12 12	0
3	B	1	Total C 7 7	0
3	C	1	Total C 8 8	0
3	C	1	Total C 12 12	0
3	C	1	Total C 8 8	0
3	C	1	Total C 11 11	0

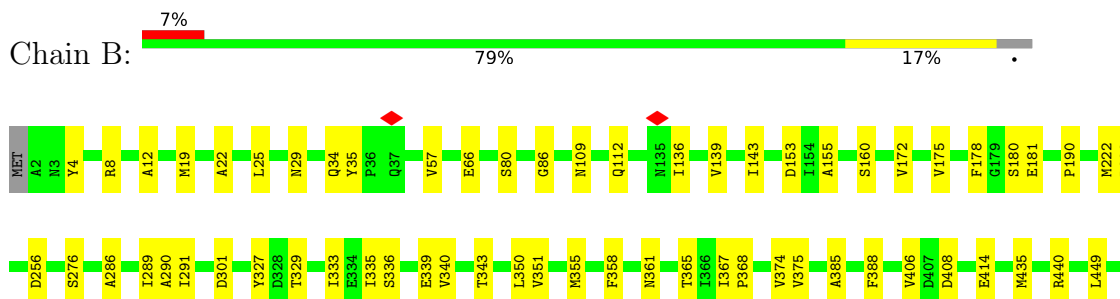
3 Residue-property plots

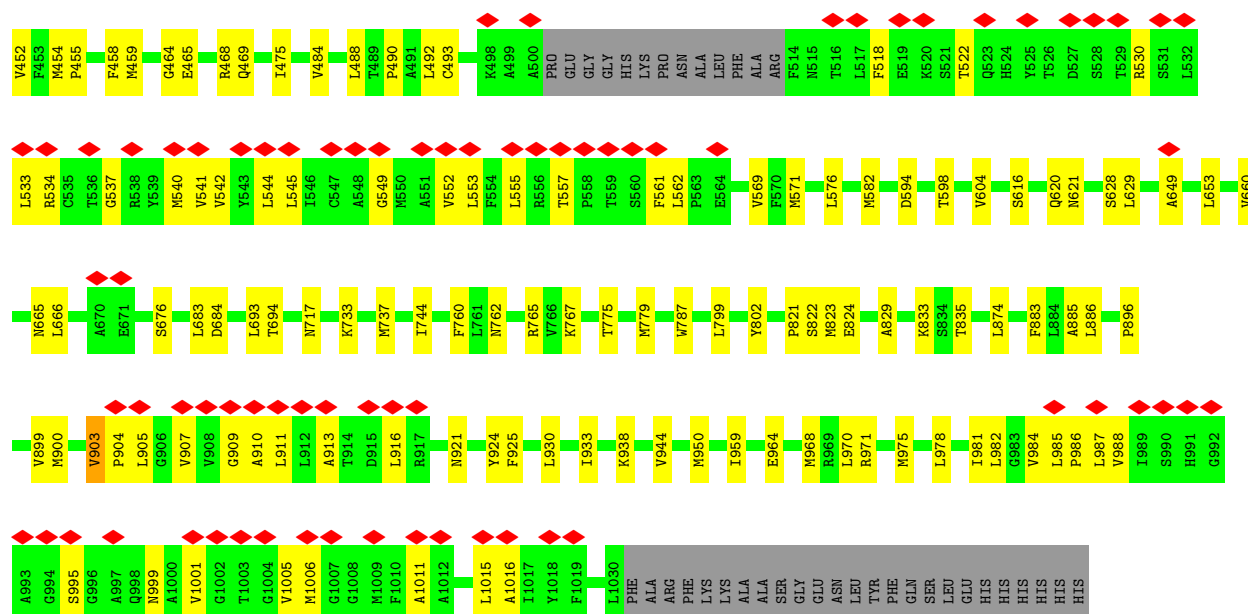
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Multidrug resistance protein MdtF

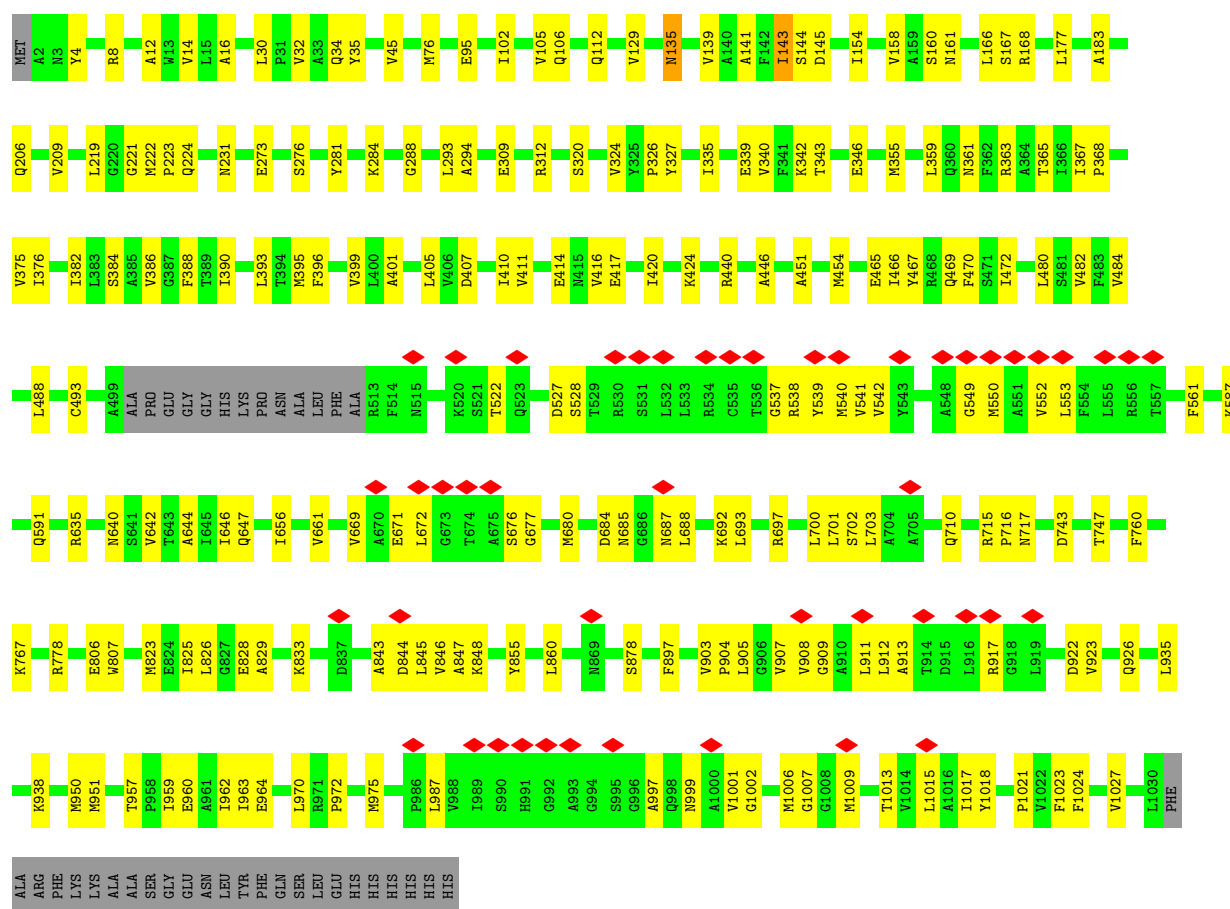
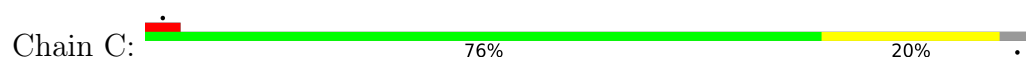


• Molecule 1: Multidrug resistance protein MdtF





• Molecule 1: Multidrug resistance protein MdtF



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1446003	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.25	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	150000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.299	Depositor
Minimum map value	-0.205	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	246.22, 246.22, 246.22	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.947, 0.947, 0.947	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: PTY, D12

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	0.13	0/7892	0.30	1/10738 (0.0%)
1	B	0.13	0/7815	0.32	0/10637
1	C	0.14	0/7821	0.34	0/10644
All	All	0.13	0/23528	0.32	1/32019 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	VAL	N-CA-C	-5.21	107.75	112.96

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	7748	0	7885	115	0
1	B	7674	0	7809	128	0
1	C	7680	0	7817	148	0
2	A	261	0	336	14	0
2	B	347	0	432	35	0
2	C	191	0	253	13	0
3	A	34	0	64	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	29	0	58	2	0
3	C	39	0	77	7	0
All	All	24003	0	24731	419	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 (419) 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:984:VAL:HG11	1:B:1006:MET:HB2	1.59	0.84
1:C:135:ASN:O	1:C:135:ASN:ND2	2.11	0.84
1:B:905:LEU:HD21	1:B:1015:LEU:HB3	1.61	0.81
1:C:340:VAL:HG21	1:C:395:MET:HB3	1.63	0.81
1:B:924:TYR:HB3	1:B:1001:VAL:HB	1.65	0.78
1:B:950:MET:HE1	1:B:964:GLU:HB3	1.66	0.77
1:A:463:THR:HG21	1:A:867:SER:HB2	1.67	0.77
2:C:1102:PTY:H342	2:C:1102:PTY:H151	1.69	0.75
1:A:389:THR:OG1	1:A:391:ASN:ND2	2.20	0.75
1:A:405:LEU:HD21	1:A:477:SER:HB3	1.70	0.74
1:A:492:LEU:HD22	1:A:496:ILE:HD11	1.72	0.71
1:A:72:LEU:HD12	1:A:75:LEU:HD22	1.72	0.70
1:C:160:SER:OG	1:C:161:ASN:OD1	2.10	0.70
2:C:1101:PTY:H402	2:C:1102:PTY:H212	1.71	0.69
1:C:700:LEU:HD23	1:C:701:LEU:HD12	1.74	0.69
1:B:717:ASN:HB3	1:B:824:GLU:HB3	1.75	0.68
1:A:467:TYR:OH	1:A:926:GLN:NE2	2.26	0.68
1:A:905:LEU:HD13	1:A:1015:LEU:HB3	1.75	0.67
2:A:1109:PTY:HC11	2:A:1109:PTY:HN11	1.59	0.67
1:C:145:ASP:HB2	1:C:320:SER:HB2	1.75	0.67
1:A:135:ASN:ND2	1:A:670:ALA:O	2.30	0.65
2:B:2003:PTY:H331	1:C:454:MET:HG3	1.79	0.64
1:C:472:ILE:HD12	2:C:1102:PTY:H141	1.79	0.64
1:C:950:MET:HE1	1:C:964:GLU:HB3	1.78	0.64
2:B:2005:PTY:H111	2:B:2006:PTY:H321	1.79	0.64
1:B:375:VAL:HG22	1:B:484:VAL:HG21	1.80	0.64
1:C:635:ARG:HB3	1:C:640:ASN:HB3	1.80	0.64
1:B:335:ILE:O	1:B:339:GLU:HG2	1.98	0.63
1:C:144:SER:HB3	1:C:154:ILE:HD11	1.80	0.63
1:B:358:PHE:HE1	1:B:978:LEU:HD23	1.62	0.62
1:C:143:ILE:HD12	1:C:281:TYR:HD2	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2001:PTY:H321	2:B:2001:PTY:H121	1.80	0.62
1:B:181:GLU:OE2	1:B:767:LYS:NZ	2.30	0.62
1:B:465:GLU:OE1	1:B:469:GLN:NE2	2.27	0.61
1:C:917:ARG:HH21	1:C:999:ASN:HD21	1.48	0.61
1:A:791:ASN:OD1	1:A:792:ALA:N	2.31	0.61
1:C:324:VAL:HG23	1:C:326:PRO:HD3	1.81	0.61
1:C:550:MET:HB2	1:C:908:VAL:HG22	1.81	0.61
1:B:582:MET:HG2	1:B:620:GLN:HG2	1.81	0.61
1:C:343:THR:HG21	1:C:399:VAL:HG13	1.83	0.61
1:C:717:ASN:HB2	1:C:826:LEU:HD22	1.82	0.60
1:B:530:ARG:HH12	1:B:534:ARG:HH11	1.50	0.60
1:C:446:ALA:HB2	1:C:482:VAL:HG21	1.83	0.60
1:C:375:VAL:HB	1:C:405:LEU:HD13	1.82	0.59
1:C:959:ILE:O	1:C:963:ILE:HG13	2.01	0.59
1:A:34:GLN:HB2	1:A:333:ILE:HG23	1.84	0.59
1:C:684:ASP:OD1	1:C:685:ASN:N	2.35	0.59
1:A:902:VAL:HG12	1:A:936:SER:HB3	1.85	0.59
1:C:701:LEU:HD21	1:C:716:PRO:HD3	1.84	0.59
1:B:223:PRO:HD2	1:C:778:ARG:HH22	1.68	0.59
1:B:29:ASN:HD21	2:B:2003:PTY:HN11	1.50	0.58
1:A:730:ASN:HD22	1:A:733:LYS:HE2	1.68	0.58
1:C:951:MET:HE1	1:C:1024:PHE:HZ	1.69	0.58
1:A:672:LEU:HD21	1:A:863:GLN:HG3	1.85	0.58
2:B:2001:PTY:H432	2:B:2001:PTY:H261	1.86	0.57
1:C:393:LEU:HD13	1:C:466:ILE:HG23	1.87	0.57
1:A:888:ALA:HB2	1:C:14:VAL:HG11	1.86	0.57
1:B:350:LEU:HD22	1:B:982:LEU:HD23	1.86	0.57
1:A:139:VAL:HB	1:A:327:TYR:HB3	1.86	0.57
2:A:1107:PTY:HC52	2:A:1108:PTY:H152	1.85	0.57
1:C:143:ILE:HD11	1:C:284:LYS:HB2	1.87	0.57
2:B:2005:PTY:HC21	2:B:2006:PTY:HC21	1.86	0.57
1:C:390:ILE:HG23	1:C:395:MET:HE3	1.86	0.57
1:B:530:ARG:HH12	1:B:534:ARG:NH1	2.02	0.57
1:B:549:GLY:O	1:B:552:VAL:HG12	2.05	0.57
1:C:904:PRO:HA	1:C:907:VAL:HG12	1.87	0.57
1:C:416:VAL:HG11	1:C:493:CYS:HB3	1.87	0.56
1:A:343:THR:HG23	1:A:986:PRO:HB2	1.86	0.56
1:B:465:GLU:HA	1:B:468:ARG:HH12	1.71	0.56
1:A:363:ARG:HD3	1:A:496:ILE:HG22	1.87	0.56
1:A:465:GLU:O	1:A:469:GLN:HG2	2.06	0.56
1:A:846:VAL:HG11	1:A:855:TYR:HB3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:GLU:O	1:C:469:GLN:HG2	2.05	0.56
1:A:375:VAL:HB	1:A:405:LEU:HD13	1.88	0.56
1:A:617:GLY:O	1:A:622:ASN:ND2	2.37	0.56
1:A:683:LEU:HD13	1:A:820:ILE:HD11	1.88	0.55
1:A:448:VAL:HG21	1:A:941:ILE:HD11	1.88	0.55
1:B:913:ALA:HA	1:B:916:LEU:HB3	1.87	0.55
1:B:139:VAL:HB	1:B:327:TYR:HB3	1.89	0.55
2:B:2009:PTY:H141	2:B:2009:PTY:H322	1.89	0.55
1:A:778:ARG:HH22	1:C:223:PRO:HD2	1.72	0.54
1:C:553:LEU:HB3	1:C:911:LEU:HD13	1.89	0.54
1:C:183:ALA:HB2	1:C:273:GLU:HG2	1.89	0.54
1:B:987:LEU:HD13	1:B:1001:VAL:HG13	1.89	0.54
1:C:909:GLY:HA2	1:C:912:LEU:HD12	1.88	0.54
2:A:1108:PTY:H391	2:C:1105:PTY:H121	1.89	0.54
1:B:34:GLN:HB2	1:B:333:ILE:HG12	1.90	0.54
1:C:355:MET:HE2	1:C:368:PRO:HG2	1.90	0.54
1:B:358:PHE:CE1	1:B:978:LEU:HD23	2.43	0.54
1:B:909:GLY:HA3	1:B:1011:ALA:HB2	1.88	0.54
1:B:660:VAL:HG12	1:B:660:VAL:O	2.08	0.54
1:C:677:GLY:HA2	1:C:828:GLU:HA	1.90	0.54
1:B:964:GLU:O	1:B:968:MET:HG2	2.07	0.53
1:C:553:LEU:HD23	1:C:911:LEU:HB3	1.91	0.53
1:C:1009:MET:O	1:C:1013:THR:HG22	2.08	0.53
1:C:401:ALA:O	1:C:405:LEU:HG	2.09	0.53
1:A:401:ALA:O	1:A:405:LEU:HG	2.09	0.53
1:B:522:THR:HG22	1:B:970:LEU:HD23	1.91	0.53
1:A:816:ARG:NH2	1:A:819:GLY:O	2.37	0.53
1:C:715:ARG:HH11	1:C:715:ARG:HG2	1.73	0.53
1:C:987:LEU:HD13	1:C:1001:VAL:HG13	1.90	0.53
1:B:569:VAL:HG12	1:B:628:SER:HA	1.91	0.53
1:C:671:GLU:HG3	1:C:672:LEU:HD23	1.91	0.53
1:C:688:LEU:HD12	1:C:692:LYS:HB3	1.91	0.53
1:B:604:VAL:HA	1:B:629:LEU:HA	1.90	0.53
1:C:222:MET:SD	1:C:224:GLN:NE2	2.82	0.53
1:C:669:VAL:HG22	1:C:671:GLU:H	1.73	0.53
1:A:410:ILE:HG23	1:A:975:MET:HE2	1.91	0.52
1:A:928:GLY:O	1:A:932:THR:HG23	2.09	0.52
1:C:951:MET:HE1	1:C:1024:PHE:CZ	2.44	0.52
1:A:473:THR:O	1:A:477:SER:OG	2.23	0.52
1:A:32:VAL:HG12	1:A:32:VAL:O	2.09	0.52
1:C:844:ASP:HA	1:C:847:ALA:HB3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:LEU:O	1:B:549:GLY:N	2.36	0.51
2:B:2001:PTY:H412	2:B:2001:PTY:H222	1.91	0.51
2:B:2010:PTY:H312	3:C:1106:D12:H32	1.93	0.51
1:C:957:THR:OG1	1:C:960:GLU:OE2	2.25	0.51
1:B:112:GLN:HG3	1:C:112:GLN:OE1	2.10	0.51
1:B:465:GLU:HA	1:B:468:ARG:NH1	2.26	0.51
1:C:34:GLN:HG2	1:C:35:TYR:CD1	2.45	0.51
1:B:459:MET:HB3	1:B:464:GLY:HA2	1.92	0.51
3:C:1108:D12:H71	2:C:1109:PTY:H341	1.92	0.51
1:C:1023:PHE:O	1:C:1027:VAL:HG23	2.11	0.51
1:A:194:ASN:HA	1:A:796:MET:HE2	1.93	0.51
1:B:995:SER:O	1:B:999:ASN:ND2	2.44	0.51
1:A:375:VAL:HG13	1:A:480:LEU:HB2	1.93	0.50
1:C:522:THR:HG22	1:C:970:LEU:HD23	1.93	0.50
1:B:136:ILE:HG21	1:B:290:ALA:HB1	1.92	0.50
1:C:700:LEU:O	1:C:701:LEU:HB2	2.11	0.50
1:C:703:LEU:HB3	1:C:845:LEU:HD11	1.93	0.50
1:A:336:SER:O	1:A:340:VAL:HG23	2.12	0.50
1:A:1009:MET:O	1:A:1013:THR:HG22	2.12	0.50
1:C:16:ALA:HB2	1:C:488:LEU:HD22	1.92	0.50
1:A:6:ILE:HG22	1:A:490:PRO:HB2	1.93	0.50
1:A:656:ILE:HD13	1:A:661:VAL:HG21	1.92	0.50
1:B:561:PHE:O	1:B:562:LEU:HD23	2.12	0.50
1:C:440:ARG:HD2	2:C:1103:PTY:HC21	1.94	0.50
1:C:905:LEU:HD22	1:C:1015:LEU:HD13	1.94	0.50
1:C:32:VAL:HG12	1:C:390:ILE:HB	1.94	0.50
1:C:45:VAL:HG22	1:C:129:VAL:HG22	1.93	0.50
1:B:533:LEU:HD13	1:B:959:ILE:HD11	1.94	0.49
1:B:874:LEU:HD21	2:B:2001:PTY:HC51	1.93	0.49
1:C:844:ASP:O	1:C:848:LYS:HG2	2.12	0.49
1:B:553:LEU:HB2	1:B:911:LEU:HD13	1.94	0.49
1:B:1001:VAL:O	1:B:1005:VAL:HG23	2.13	0.49
1:A:281:TYR:O	1:A:283:GLY:N	2.44	0.49
1:B:388:PHE:HE2	1:B:469:GLN:HA	1.78	0.49
1:C:139:VAL:O	1:C:139:VAL:HG12	2.13	0.49
1:C:656:ILE:HG13	1:C:661:VAL:HG11	1.93	0.49
1:A:513:ARG:O	1:A:517:LEU:HD12	2.13	0.49
1:B:57:VAL:HG21	1:B:86:GLY:HA2	1.95	0.49
1:C:710:GLN:HG2	1:C:833:LYS:HE2	1.95	0.49
1:A:358:PHE:HE1	1:A:978:LEU:HD23	1.77	0.49
1:B:649:ALA:O	1:B:653:LEU:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:VAL:O	1:C:646:ILE:HG23	2.13	0.49
1:C:997:ALA:O	1:C:1001:VAL:HG12	2.12	0.49
1:B:25:LEU:HD12	3:B:2004:D12:H82	1.95	0.49
1:B:518:PHE:O	1:B:522:THR:HG23	2.12	0.49
1:A:206:GLN:HG3	1:A:251:LEU:HA	1.94	0.49
1:B:440:ARG:HG2	2:B:2002:PTY:O12	2.13	0.49
1:C:407:ASP:O	1:C:411:VAL:HG12	2.13	0.49
1:B:744:ILE:HG23	1:B:799:LEU:HD11	1.94	0.48
1:B:985:LEU:N	1:B:986:PRO:HD2	2.29	0.48
1:C:1017:ILE:HG13	1:C:1018:TYR:CD1	2.48	0.48
1:A:997:ALA:O	1:A:1001:VAL:HG22	2.13	0.48
1:B:885:ALA:HA	2:B:2002:PTY:H371	1.94	0.48
1:A:722:THR:HG22	1:A:812:PRO:HD3	1.95	0.48
2:A:1103:PTY:H151	3:C:1106:D12:H62	1.96	0.48
1:B:616:SER:O	1:B:616:SER:OG	2.28	0.48
1:C:1013:THR:O	1:C:1017:ILE:HG12	2.14	0.48
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.94	0.48
1:C:414:GLU:CD	1:C:972:PRO:HG3	2.39	0.48
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.96	0.48
1:A:281:TYR:HE1	1:A:326:PRO:HB3	1.78	0.48
1:A:522:THR:HG22	1:A:970:LEU:HD23	1.96	0.48
1:C:760:PHE:CE1	1:C:767:LYS:HB2	2.49	0.48
1:C:537:GLY:O	1:C:540:MET:HB3	2.13	0.48
1:C:700:LEU:C	1:C:702:SER:H	2.21	0.48
1:A:6:ILE:HD11	1:A:432:HIS:NE2	2.29	0.48
1:B:775:THR:HG23	1:B:779:MET:HE3	1.96	0.48
1:C:396:PHE:HD2	1:C:470:PHE:CE1	2.32	0.48
1:B:343:THR:HG23	1:B:986:PRO:HB2	1.95	0.48
1:B:988:VAL:HA	1:B:999:ASN:HA	1.96	0.48
3:B:2004:D12:H13	2:B:2006:PTY:H322	1.96	0.48
1:C:913:ALA:CB	1:C:1007:GLY:HA3	2.44	0.47
1:B:799:LEU:HD12	1:B:802:TYR:HE1	1.79	0.47
1:B:155:ALA:HB1	1:B:180:SER:H	1.80	0.47
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.96	0.47
1:B:458:PHE:CD2	2:B:2001:PTY:H112	2.49	0.47
1:B:518:PHE:CE2	1:B:971:ARG:HG3	2.50	0.47
1:A:6:ILE:HD11	1:A:432:HIS:CE1	2.50	0.47
1:B:910:ALA:HB1	1:B:925:PHE:CE2	2.50	0.47
1:C:293:LEU:HG	1:C:294:ALA:H	1.79	0.47
1:C:672:LEU:CB	1:C:860:LEU:HD11	2.45	0.47
1:A:987:LEU:HD13	1:A:1001:VAL:HG23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1107:PTY:H361	2:B:2012:PTY:H152	1.97	0.47
1:A:889:LEU:HA	2:A:1105:PTY:H311	1.96	0.46
1:C:375:VAL:HG22	1:C:484:VAL:HG21	1.96	0.46
1:B:557:THR:HB	1:B:921:ASN:ND2	2.30	0.46
1:B:684:ASP:HB3	1:B:821:PRO:HG2	1.96	0.46
1:B:883:PHE:HB2	1:B:900:MET:HE2	1.97	0.46
1:C:361:ASN:O	1:C:365:THR:HG23	2.16	0.46
1:A:379:THR:HG23	1:A:476:SER:HB2	1.96	0.46
1:A:445:ILE:HG23	1:A:938:LYS:HG3	1.97	0.46
2:A:1109:PTY:H132	2:A:1109:PTY:H331	1.97	0.46
2:A:1109:PTY:H351	2:A:1109:PTY:H151	1.97	0.46
1:B:256:ASP:OD1	1:B:256:ASP:N	2.43	0.46
1:C:697:ARG:HG3	1:C:825:ILE:HD11	1.97	0.46
1:B:475:ILE:HG21	2:B:2008:PTY:H362	1.97	0.46
2:B:2001:PTY:H262	2:B:2002:PTY:H141	1.98	0.46
2:B:2008:PTY:O30	2:B:2012:PTY:N1	2.47	0.46
1:B:886:LEU:HB3	1:B:896:PRO:HB3	1.98	0.46
1:C:309:GLU:HG2	1:C:312:ARG:HH21	1.81	0.46
1:C:905:LEU:HD13	1:C:1015:LEU:HB3	1.97	0.46
1:B:153:ASP:OD1	1:B:153:ASP:N	2.49	0.46
1:C:539:TYR:HA	1:C:542:VAL:HB	1.96	0.46
1:A:58:GLU:HA	1:A:62:THR:HB	1.97	0.46
1:A:332:PHE:HA	1:A:335:ILE:HG22	1.98	0.46
1:A:458:PHE:HB2	2:A:1102:PTY:H122	1.97	0.46
1:A:899:VAL:HG13	1:A:940:ALA:HB3	1.97	0.46
1:C:359:LEU:HD13	1:C:417:GLU:HG3	1.98	0.46
1:C:1002:GLY:O	1:C:1006:MET:HB3	2.16	0.46
1:B:19:MET:HE2	1:B:374:VAL:HG12	1.96	0.45
1:B:408:ASP:OD1	1:B:938:LYS:NZ	2.39	0.45
2:B:2010:PTY:H201	3:C:1106:D12:H61	1.98	0.45
1:C:158:VAL:HG13	1:C:177:LEU:HD11	1.97	0.45
3:C:1108:D12:H22	2:C:1109:PTY:H311	1.99	0.45
1:A:456:MET:HB2	1:A:467:TYR:HB3	1.97	0.45
1:B:12:ALA:HB1	1:B:488:LEU:HA	1.99	0.45
1:C:166:LEU:C	1:C:168:ARG:H	2.25	0.45
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.98	0.45
1:C:959:ILE:O	1:C:962:ILE:HG22	2.17	0.45
1:B:981:ILE:O	1:B:984:VAL:HB	2.17	0.45
1:A:366:ILE:HA	1:A:369:THR:HG22	1.98	0.45
1:A:468:ARG:HH22	2:A:1108:PTY:HN11	1.63	0.45
1:A:775:THR:HG23	1:A:779:MET:HE3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PHE:CG	1:B:975:MET:HG3	2.51	0.45
2:B:2003:PTY:H312	1:C:454:MET:HB2	1.99	0.45
2:B:2006:PTY:H181	2:B:2006:PTY:H122	1.99	0.45
1:A:70:ASN:HB2	1:C:167:SER:HB3	1.99	0.45
1:A:222:MET:HE3	1:A:222:MET:HB3	1.83	0.45
1:A:453:PHE:O	1:A:471:SER:HB2	2.16	0.45
1:B:4:TYR:HD2	1:B:8:ARG:HE	1.64	0.45
1:C:206:GLN:HA	1:C:209:VAL:HG12	1.97	0.45
1:C:451:ALA:O	1:C:878:SER:OG	2.24	0.45
1:B:594:ASP:O	1:B:598:THR:HG22	2.17	0.45
1:C:76:MET:HG3	1:C:95:GLU:HG2	1.98	0.45
2:C:1109:PTY:HC11	2:C:1109:PTY:H312	1.81	0.45
2:A:1108:PTY:H182	2:A:1108:PTY:H351	1.98	0.44
1:B:143:ILE:HG22	1:B:286:ALA:HB2	1.99	0.44
1:B:172:VAL:HG13	1:B:291:ILE:HG23	1.98	0.44
1:B:449:LEU:HA	1:B:452:VAL:HG12	1.99	0.44
1:B:905:LEU:HD11	1:B:1015:LEU:HG	1.99	0.44
1:A:903:VAL:HG13	1:A:933:ILE:HG12	1.99	0.44
2:B:2001:PTY:H222	2:B:2001:PTY:H381	1.99	0.44
1:C:561:PHE:HD2	1:C:672:LEU:HD11	1.82	0.44
1:B:549:GLY:O	1:B:553:LEU:HD12	2.18	0.44
1:A:154:ILE:HG23	1:A:321:LEU:HD11	1.99	0.44
1:B:222:MET:HG3	1:C:276:SER:HA	2.00	0.44
1:C:416:VAL:O	1:C:420:ILE:HG13	2.17	0.44
1:A:330:THR:HA	1:A:333:ILE:HD12	2.00	0.44
1:A:572:THR:HB	1:A:625:ALA:HB3	1.99	0.44
1:B:665:ASN:OD1	1:B:666:LEU:N	2.51	0.44
1:B:930:LEU:HD12	1:B:930:LEU:HA	1.81	0.44
1:C:281:TYR:CZ	1:C:324:VAL:HG21	2.52	0.44
1:A:157:TYR:CZ	1:A:318:PRO:HD3	2.53	0.44
1:A:408:ASP:HB3	1:A:442:LEU:HD22	1.99	0.44
1:A:560:SER:OG	1:A:561:PHE:N	2.51	0.44
1:C:141:ALA:HA	1:C:288:GLY:HA2	2.00	0.44
1:C:911:LEU:HD23	1:C:911:LEU:HA	1.79	0.44
1:A:569:VAL:HG12	1:A:628:SER:HA	1.99	0.44
1:B:22:ALA:HB1	2:B:2005:PTY:HC11	1.99	0.44
1:B:541:VAL:O	1:B:544:LEU:HB3	2.18	0.44
1:A:886:LEU:HD21	1:A:941:ILE:HD11	2.00	0.44
1:B:518:PHE:CZ	1:B:971:ARG:HG3	2.52	0.44
1:B:676:SER:HA	1:B:835:THR:HG22	1.99	0.44
1:C:12:ALA:HB1	1:C:488:LEU:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:PHE:HB2	1:C:1027:VAL:HG11	2.00	0.44
1:A:932:THR:HG21	1:A:1008:GLY:HA3	2.00	0.44
1:B:910:ALA:HB1	1:B:925:PHE:HE2	1.83	0.44
2:B:2003:PTY:H201	2:C:1102:PTY:H382	2.00	0.44
1:A:389:THR:HG1	1:A:391:ASN:HD21	1.59	0.43
1:B:361:ASN:O	1:B:365:THR:HG22	2.18	0.43
2:B:2009:PTY:H392	2:B:2009:PTY:H361	1.85	0.43
1:A:222:MET:HG3	1:B:276:SER:HA	1.99	0.43
1:B:435:MET:HG3	1:B:490:PRO:HB3	2.00	0.43
1:B:569:VAL:HG23	1:B:666:LEU:HD11	2.00	0.43
1:B:833:LYS:HE2	1:B:833:LYS:HB3	1.82	0.43
1:B:351:VAL:HG21	1:B:406:VAL:HG21	1.98	0.43
1:C:335:ILE:O	1:C:339:GLU:HG2	2.18	0.43
1:C:684:ASP:HB3	1:C:693:LEU:HD22	1.99	0.43
1:C:903:VAL:N	1:C:904:PRO:HD2	2.33	0.43
1:B:66:GLU:OE2	1:B:80:SER:OG	2.28	0.43
1:C:102:ILE:O	1:C:106:GLN:HG3	2.19	0.43
1:C:143:ILE:HD12	1:C:281:TYR:CD2	2.50	0.43
1:C:951:MET:HE3	1:C:951:MET:HB2	1.92	0.43
1:B:537:GLY:O	1:B:540:MET:HB3	2.19	0.43
1:A:725:PHE:CZ	1:A:805:THR:HB	2.53	0.43
1:B:329:THR:O	1:B:333:ILE:HG13	2.18	0.43
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.92	0.43
1:A:479:LEU:HD13	3:A:1104:D12:H32	2.01	0.43
1:B:899:VAL:HG22	1:B:944:VAL:HG21	1.99	0.43
1:C:407:ASP:OD2	1:C:935:LEU:HD22	2.19	0.43
1:A:155:ALA:HB1	1:A:180:SER:H	1.84	0.43
1:A:182:TYR:CD1	1:A:270:LEU:HG	2.54	0.43
1:A:480:LEU:HD23	2:A:1107:PTY:H242	2.01	0.43
1:A:533:LEU:HD12	1:A:533:LEU:HA	1.88	0.43
1:C:480:LEU:HD13	2:C:1102:PTY:H231	2.00	0.43
1:C:644:ALA:HA	1:C:647:GLN:HG2	2.01	0.43
1:C:843:ALA:O	1:C:844:ASP:HB2	2.19	0.43
1:A:18:ILE:HD13	2:B:2001:PTY:H211	2.00	0.42
1:A:174:SER:HB3	1:A:292:LYS:HB2	2.01	0.42
1:B:4:TYR:HB2	1:B:8:ARG:HE	1.84	0.42
1:C:219:LEU:O	1:C:231:ASN:HA	2.19	0.42
1:C:697:ARG:HD3	1:C:823:MET:SD	2.58	0.42
1:A:74:GLY:O	1:A:95:GLU:N	2.51	0.42
1:A:340:VAL:HG21	1:A:392:THR:HG23	2.00	0.42
2:A:1109:PTY:H311	2:A:1109:PTY:H342	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:VAL:HG22	1:B:933:ILE:HD11	2.00	0.42
1:C:587:LYS:O	1:C:591:GLN:HG2	2.18	0.42
1:A:909:GLY:HA3	1:A:1011:ALA:CB	2.49	0.42
1:B:355:MET:SD	1:B:368:PRO:HG2	2.59	0.42
1:C:922:ASP:O	1:C:926:GLN:NE2	2.53	0.42
2:C:1103:PTY:H362	3:C:1104:D12:H81	2.00	0.42
1:A:370:ILE:O	1:A:373:PRO:HD2	2.19	0.42
1:B:490:PRO:HA	1:B:493:CYS:SG	2.59	0.42
1:C:386:VAL:HG23	1:C:388:PHE:HD2	1.84	0.42
1:C:806:GLU:HG2	1:C:807:TRP:N	2.34	0.42
1:A:136:ILE:HG12	1:A:290:ALA:HB1	2.02	0.42
1:A:962:ILE:HD12	1:A:962:ILE:HA	1.89	0.42
1:B:190:PRO:HG3	1:B:787:TRP:CE2	2.54	0.42
2:B:2001:PTY:H432	2:B:2001:PTY:H231	2.00	0.42
1:B:414:GLU:OE1	1:B:971:ARG:NE	2.53	0.42
1:B:683:LEU:HD12	1:B:822:SER:HB2	2.02	0.42
1:B:694:THR:HB	1:B:823:MET:HE1	2.01	0.42
1:A:371:ALA:O	1:A:375:VAL:HG23	2.20	0.42
1:A:951:MET:C	1:A:953:LYS:H	2.28	0.42
1:A:971:ARG:HB3	1:A:972:PRO:HD3	2.02	0.42
1:C:410:ILE:HG23	1:C:975:MET:HE3	2.02	0.42
1:C:743:ASP:O	1:C:747:THR:HG23	2.18	0.42
1:C:846:VAL:HG11	1:C:855:TYR:HB3	2.02	0.42
1:A:984:VAL:HG21	1:A:1005:VAL:HG23	2.01	0.42
1:B:336:SER:O	1:B:340:VAL:HG23	2.20	0.42
1:B:385:ALA:HB2	2:B:2005:PTY:O10	2.20	0.42
1:A:760:PHE:CE1	1:A:767:LYS:HB2	2.54	0.42
1:A:929:LEU:HD23	1:A:929:LEU:HA	1.82	0.42
1:B:555:LEU:HD23	1:B:555:LEU:HA	1.85	0.42
1:B:762:ASN:HB3	1:B:767:LYS:HE2	2.01	0.42
1:C:30:LEU:HD21	1:C:384:SER:HA	2.02	0.42
1:C:561:PHE:CE2	1:C:672:LEU:HD21	2.55	0.42
1:A:366:ILE:O	1:A:370:ILE:HG13	2.20	0.41
1:A:932:THR:CG2	1:A:1008:GLY:HA3	2.50	0.41
1:B:454:MET:N	1:B:455:PRO:HD2	2.35	0.41
1:B:760:PHE:CE1	1:B:767:LYS:HB2	2.55	0.41
1:C:676:SER:HB2	1:C:829:ALA:HB3	2.01	0.41
1:B:903:VAL:HG22	1:B:904:PRO:HD3	2.02	0.41
1:C:467:TYR:CE1	1:C:923:VAL:HG13	2.55	0.41
1:C:687:ASN:HD22	1:C:687:ASN:HA	1.71	0.41
1:B:984:VAL:HG22	1:B:1005:VAL:HB	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HD13	1:A:234:ILE:HD11	2.01	0.41
1:A:352:PHE:HA	1:A:355:MET:HE2	2.03	0.41
1:A:922:ASP:N	1:A:922:ASP:OD1	2.43	0.41
2:A:1101:PTY:H172	2:B:2001:PTY:H401	2.02	0.41
1:B:160:SER:HB3	1:B:765:ARG:HD3	2.01	0.41
1:C:221:GLY:O	1:C:224:GLN:HB3	2.20	0.41
1:C:342:LYS:O	1:C:346:GLU:HG3	2.20	0.41
1:C:527:ASP:OD1	1:C:528:SER:N	2.53	0.41
1:C:917:ARG:HH21	1:C:999:ASN:ND2	2.17	0.41
1:A:301:ASP:OD1	1:A:301:ASP:N	2.52	0.41
1:B:175:VAL:HG13	1:B:289:ILE:HG23	2.03	0.41
1:B:542:VAL:O	1:B:545:LEU:HG	2.20	0.41
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.89	0.41
1:A:778:ARG:NH2	1:C:223:PRO:HD2	2.36	0.41
1:B:355:MET:HE3	1:B:355:MET:HB2	1.64	0.41
1:B:571:MET:HE2	1:B:571:MET:HB3	1.78	0.41
1:C:407:ASP:OD1	1:C:938:LYS:NZ	2.54	0.41
1:C:424:LYS:HA	1:C:424:LYS:HD3	1.89	0.41
1:A:145:ASP:OD2	1:A:322:LYS:HE2	2.20	0.41
1:B:492:LEU:HD23	1:B:492:LEU:HA	1.94	0.41
2:B:2008:PTY:H121	2:B:2008:PTY:H151	1.84	0.41
1:C:367:ILE:HB	1:C:368:PRO:HD3	2.02	0.41
1:A:923:VAL:HA	1:A:926:GLN:NE2	2.36	0.41
1:B:978:LEU:HD12	1:B:982:LEU:HD13	2.03	0.41
1:C:680:MET:HG2	1:C:825:ILE:O	2.21	0.41
1:A:891:GLU:CD	1:C:8:ARG:HB3	2.45	0.41
1:B:178:PHE:CZ	1:B:290:ALA:HB2	2.56	0.41
1:B:576:LEU:HB2	1:B:621:ASN:HB2	2.03	0.41
1:B:733:LYS:O	1:B:737:MET:HG3	2.21	0.41
1:C:139:VAL:O	1:C:139:VAL:CG1	2.68	0.41
1:C:376:ILE:HD13	1:C:376:ILE:HA	1.92	0.41
1:A:190:PRO:HG3	1:A:787:TRP:CE2	2.56	0.41
1:B:676:SER:OG	1:B:829:ALA:HB3	2.21	0.41
2:B:2010:PTY:H182	3:C:1106:D12:H51	2.02	0.41
2:B:2011:PTY:H312	2:B:2011:PTY:H111	2.03	0.41
1:A:75:LEU:HD11	1:A:92:LEU:HB3	2.03	0.40
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.89	0.40
1:B:454:MET:SD	2:B:2008:PTY:H341	2.61	0.40
1:B:684:ASP:HB2	1:B:693:LEU:HD22	2.02	0.40
2:B:2012:PTY:H311	2:B:2012:PTY:HC12	1.90	0.40
1:C:102:ILE:O	1:C:105:VAL:HG12	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:VAL:HB	1:C:327:TYR:HB3	2.03	0.40
1:C:549:GLY:O	1:C:552:VAL:HG12	2.21	0.40
1:C:672:LEU:HB2	1:C:860:LEU:HD11	2.02	0.40
1:C:935:LEU:HD23	1:C:935:LEU:HA	1.88	0.40
1:C:962:ILE:HG12	1:C:1021:PRO:HA	2.03	0.40
1:B:905:LEU:HD22	1:B:1016:ALA:HB2	2.02	0.40
2:B:2003:PTY:H322	1:C:451:ALA:HA	2.02	0.40
1:A:227:ASP:O	1:A:229:GLN:HG2	2.22	0.40
1:C:30:LEU:HD23	1:C:30:LEU:HA	1.86	0.40
1:B:35:TYR:CZ	1:B:562:LEU:HD13	2.56	0.40
1:B:301:ASP:OD1	1:B:301:ASP:N	2.54	0.40
1:C:538:ARG:O	1:C:541:VAL:HG12	2.22	0.40
1:A:465:GLU:HG2	1:A:468:ARG:HH21	1.86	0.40
1:A:938:LYS:HB3	1:A:938:LYS:HE3	1.90	0.40
1:A:951:MET:SD	1:A:958:PRO:HB3	2.60	0.40
1:C:363:ARG:H	1:C:363:ARG:HG2	1.53	0.40
1:C:382:ILE:HG13	2:C:1101:PTY:H232	2.04	0.40
1:C:715:ARG:HG2	1:C:715:ARG:NH1	2.36	0.40
2:C:1109:PTY:H151	2:C:1109:PTY:H182	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1020/1055 (97%)	992 (97%)	28 (3%)	0	100	100
1	B	1012/1055 (96%)	963 (95%)	49 (5%)	0	100	100
1	C	1012/1055 (96%)	955 (94%)	57 (6%)	0	100	100
All	All	3044/3165 (96%)	2910 (96%)	134 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	837/862 (97%)	836 (100%)	1 (0%)	92	96
1	B	831/862 (96%)	829 (100%)	2 (0%)	92	96
1	C	832/862 (96%)	829 (100%)	3 (0%)	89	93
All	All	2500/2586 (97%)	2494 (100%)	6 (0%)	91	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	496	ILE
1	B	109	ASN
1	B	903	VAL
1	C	4	TYR
1	C	135	ASN
1	C	143	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	161	ASN
1	A	391	ASN
1	A	603	ASN
1	A	618	GLN
1	A	685	ASN
1	A	728	ASN
1	A	730	ASN
1	A	762	ASN
1	A	772	GLN
1	A	926	GLN
1	A	1029	HIS
1	B	34	GLN
1	B	437	GLN
1	B	523	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	618	GLN
1	B	621	ASN
1	B	685	ASN
1	B	687	ASN
1	B	772	GLN
1	B	783	ASN
1	C	68	ASN
1	C	112	GLN
1	C	176	GLN
1	C	231	ASN
1	C	237	GLN
1	C	311	ASN
1	C	415	ASN
1	C	523	GLN
1	C	618	GLN
1	C	620	GLN
1	C	622	ASN
1	C	710	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

33 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	$\# Z > 2$
2	PTY	B	2009	-	36,36,49	0.53	0	39,41,54	0.42	0
2	PTY	A	1109	-	36,36,49	0.51	0	39,41,54	0.48	0
2	PTY	A	1107	-	40,40,49	0.49	0	43,45,54	0.55	0
2	PTY	C	1105	-	24,24,49	0.60	0	27,29,54	0.65	1 (3%)
3	D12	B	2004	-	9,9,11	0.23	0	8,8,10	0.24	0
2	PTY	B	2005	-	26,26,49	0.59	0	29,31,54	0.63	1 (3%)
2	PTY	C	1103	-	31,31,49	0.56	0	34,36,54	0.44	0
3	D12	C	1104	-	7,7,11	0.24	0	6,6,10	0.19	0
3	D12	A	1111	-	7,7,11	0.25	0	6,6,10	0.16	0
2	PTY	A	1102	-	31,31,49	0.56	0	34,36,54	0.48	0
3	D12	B	2013	-	6,6,11	0.26	0	5,5,10	0.17	0
3	D12	B	2007	-	11,11,11	0.23	0	10,10,10	0.22	0
2	PTY	B	2008	-	39,39,49	0.51	0	42,44,54	0.42	0
3	D12	A	1104	-	7,7,11	0.26	0	6,6,10	0.15	0
2	PTY	B	2012	-	32,32,49	0.56	0	35,37,54	0.44	0
3	D12	C	1108	-	10,10,11	0.24	0	9,9,10	0.19	0
2	PTY	B	2001	-	49,49,49	0.46	0	52,54,54	0.39	0
2	PTY	B	2003	-	38,38,49	0.50	0	41,43,54	0.49	0
2	PTY	C	1101	-	46,46,49	0.48	0	49,51,54	0.38	0
2	PTY	A	1103	-	28,28,49	0.58	0	31,33,54	0.52	0
2	PTY	B	2010	-	37,37,49	0.52	0	40,42,54	0.41	0
2	PTY	B	2011	-	23,23,49	0.64	0	26,28,54	0.48	0
2	PTY	C	1102	-	46,46,49	0.46	0	49,51,54	0.50	1 (2%)
3	D12	A	1106	-	9,9,11	0.23	0	8,8,10	0.22	0
2	PTY	A	1101	-	38,38,49	0.51	0	41,43,54	0.46	0
2	PTY	A	1108	-	45,45,49	0.48	0	48,50,54	0.42	0
3	D12	C	1107	-	7,7,11	0.25	0	6,6,10	0.19	0
2	PTY	B	2006	-	29,29,49	0.57	0	32,34,54	0.48	0
3	D12	C	1106	-	11,11,11	0.23	0	10,10,10	0.21	0
2	PTY	B	2002	-	28,28,49	0.84	1 (3%)	30,32,54	0.57	0
2	PTY	A	1105	-	36,36,49	0.53	0	39,41,54	0.43	0
2	PTY	C	1109	-	39,39,49	0.50	0	42,44,54	0.42	0
3	D12	A	1110	-	7,7,11	0.25	0	6,6,10	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTY	B	2009	-	-	23/40/40/53	-
2	PTY	A	1109	-	-	21/40/40/53	-
2	PTY	A	1107	-	-	20/44/44/53	-
2	PTY	C	1105	-	-	18/28/28/53	-
3	D12	B	2004	-	-	3/7/7/9	-
2	PTY	B	2005	-	-	19/30/30/53	-
2	PTY	C	1103	-	-	19/35/35/53	-
3	D12	C	1104	-	-	4/5/5/9	-
3	D12	A	1111	-	-	2/5/5/9	-
2	PTY	A	1102	-	-	11/35/35/53	-
3	D12	B	2013	-	-	1/4/4/9	-
3	D12	B	2007	-	-	2/9/9/9	-
2	PTY	B	2008	-	-	24/43/43/53	-
3	D12	A	1104	-	-	3/5/5/9	-
2	PTY	B	2012	-	-	24/36/36/53	-
3	D12	C	1108	-	-	0/8/8/9	-
2	PTY	B	2001	-	-	15/53/53/53	-
2	PTY	B	2003	-	-	21/42/42/53	-
2	PTY	C	1101	-	-	24/50/50/53	-
2	PTY	A	1103	-	-	16/32/32/53	-
2	PTY	B	2010	-	-	20/41/41/53	-
2	PTY	B	2011	-	-	18/27/27/53	-
2	PTY	C	1102	-	-	20/50/50/53	-
3	D12	A	1106	-	-	5/7/7/9	-
2	PTY	A	1101	-	-	21/42/42/53	-
2	PTY	A	1108	-	-	27/49/49/53	-
3	D12	C	1107	-	-	1/5/5/9	-
2	PTY	B	2006	-	-	18/33/33/53	-
3	D12	C	1106	-	-	5/9/9/9	-
2	PTY	B	2002	-	-	15/31/31/53	-
2	PTY	A	1105	-	-	16/40/40/53	-
2	PTY	C	1109	-	-	24/43/43/53	-
3	D12	A	1110	-	-	1/5/5/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	PTY	O7-C8	-3.45	1.33	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2005	PTY	C6-O7-C8	2.16	123.11	117.79
2	C	1105	PTY	C6-O7-C8	2.11	122.99	117.79
2	C	1102	PTY	C6-O7-C8	2.09	122.94	117.79

There are no chirality outliers.

All (461) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	PTY	C2-C3-O11-P1
2	A	1101	PTY	C11-C8-O7-C6
2	A	1101	PTY	C3-O11-P1-O12
2	A	1101	PTY	C5-O14-P1-O13
2	A	1102	PTY	C3-O11-P1-O12
2	A	1102	PTY	C3-O11-P1-O13
2	A	1102	PTY	C3-O11-P1-O14
2	A	1103	PTY	C2-C3-O11-P1
2	A	1103	PTY	O10-C8-O7-C6
2	A	1103	PTY	C11-C8-O7-C6
2	A	1103	PTY	C3-O11-P1-O12
2	A	1103	PTY	C5-O14-P1-O13
2	A	1105	PTY	C3-O11-P1-O14
2	A	1107	PTY	C5-O14-P1-O13
2	A	1108	PTY	O10-C8-O7-C6
2	A	1108	PTY	C3-O11-P1-O12
2	A	1108	PTY	C5-O14-P1-O11
2	A	1109	PTY	C5-O14-P1-O13
2	B	2001	PTY	N1-C2-C3-O11
2	B	2001	PTY	C3-O11-P1-O13
2	B	2002	PTY	N1-C2-C3-O11
2	B	2002	PTY	C3-O11-P1-O12
2	B	2002	PTY	C3-O11-P1-O13
2	B	2002	PTY	C3-O11-P1-O14
2	B	2003	PTY	N1-C2-C3-O11
2	B	2003	PTY	C11-C8-O7-C6
2	B	2003	PTY	C5-O14-P1-O13
2	B	2005	PTY	N1-C2-C3-O11
2	B	2006	PTY	N1-C2-C3-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2006	PTY	C11-C8-O7-C6
2	B	2006	PTY	C3-O11-P1-O13
2	B	2006	PTY	C3-O11-P1-O14
2	B	2006	PTY	C5-O14-P1-O13
2	B	2008	PTY	N1-C2-C3-O11
2	B	2008	PTY	O10-C8-O7-C6
2	B	2008	PTY	C11-C8-O7-C6
2	B	2008	PTY	C3-O11-P1-O13
2	B	2008	PTY	C5-O14-P1-O11
2	B	2008	PTY	C5-O14-P1-O12
2	B	2008	PTY	C5-O14-P1-O13
2	B	2009	PTY	N1-C2-C3-O11
2	B	2009	PTY	C2-C3-O11-P1
2	B	2009	PTY	C11-C8-O7-C6
2	B	2009	PTY	C3-O11-P1-O12
2	B	2009	PTY	C5-O14-P1-O13
2	B	2010	PTY	C3-O11-P1-O12
2	B	2010	PTY	C3-O11-P1-O13
2	B	2010	PTY	C3-O11-P1-O14
2	B	2011	PTY	O10-C8-O7-C6
2	B	2011	PTY	C3-O11-P1-O13
2	B	2012	PTY	C3-O11-P1-O13
2	C	1101	PTY	O10-C8-O7-C6
2	C	1101	PTY	C11-C8-O7-C6
2	C	1101	PTY	C3-O11-P1-O12
2	C	1101	PTY	C3-O11-P1-O13
2	C	1102	PTY	N1-C2-C3-O11
2	C	1102	PTY	C11-C8-O7-C6
2	C	1102	PTY	C5-O14-P1-O11
2	C	1102	PTY	C5-O14-P1-O12
2	C	1102	PTY	C5-O14-P1-O13
2	C	1103	PTY	O4-C1-C6-O7
2	C	1103	PTY	C11-C8-O7-C6
2	C	1103	PTY	C5-O14-P1-O13
2	C	1105	PTY	N1-C2-C3-O11
2	C	1105	PTY	C11-C8-O7-C6
2	C	1105	PTY	C5-O14-P1-O12
2	C	1109	PTY	N1-C2-C3-O11
2	C	1109	PTY	C2-C3-O11-P1
2	A	1107	PTY	O30-C30-O4-C1
2	A	1108	PTY	O30-C30-O4-C1
2	B	2009	PTY	O30-C30-O4-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2012	PTY	O30-C30-O4-C1
2	C	1101	PTY	O30-C30-O4-C1
2	C	1103	PTY	O30-C30-O4-C1
2	C	1105	PTY	O30-C30-O4-C1
2	C	1109	PTY	O30-C30-O4-C1
2	A	1101	PTY	O10-C8-O7-C6
2	A	1109	PTY	O10-C8-O7-C6
2	B	2003	PTY	O10-C8-O7-C6
2	B	2009	PTY	O10-C8-O7-C6
2	C	1102	PTY	O10-C8-O7-C6
2	C	1103	PTY	O10-C8-O7-C6
2	C	1105	PTY	O10-C8-O7-C6
2	A	1107	PTY	C31-C30-O4-C1
2	A	1108	PTY	C31-C30-O4-C1
2	B	2008	PTY	C31-C30-O4-C1
2	B	2012	PTY	C31-C30-O4-C1
2	C	1101	PTY	C31-C30-O4-C1
2	C	1103	PTY	C31-C30-O4-C1
2	C	1109	PTY	C31-C30-O4-C1
2	A	1108	PTY	C11-C8-O7-C6
2	A	1109	PTY	C11-C8-O7-C6
2	B	2011	PTY	C11-C8-O7-C6
2	A	1109	PTY	O30-C30-O4-C1
2	A	1101	PTY	C31-C30-O4-C1
2	A	1109	PTY	C31-C30-O4-C1
2	B	2006	PTY	C31-C30-O4-C1
2	B	2009	PTY	C31-C30-O4-C1
2	C	1105	PTY	C31-C30-O4-C1
2	B	2011	PTY	C8-C11-C12-C13
2	B	2006	PTY	O10-C8-O7-C6
2	A	1101	PTY	O30-C30-O4-C1
2	B	2008	PTY	O30-C30-O4-C1
2	C	1109	PTY	C11-C8-O7-C6
2	B	2006	PTY	O30-C30-O4-C1
2	C	1109	PTY	O10-C8-O7-C6
2	B	2002	PTY	C31-C30-O4-C1
2	B	2005	PTY	C31-C30-O4-C1
2	B	2011	PTY	C31-C30-O4-C1
2	A	1101	PTY	C15-C16-C17-C18
2	C	1101	PTY	O4-C1-C6-O7
2	B	2002	PTY	O30-C30-O4-C1
2	B	2005	PTY	O30-C30-O4-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2011	PTY	O30-C30-O4-C1
2	A	1105	PTY	C30-C31-C32-C33
2	B	2005	PTY	C8-C11-C12-C13
2	C	1105	PTY	C30-C31-C32-C33
2	A	1101	PTY	C8-C11-C12-C13
2	A	1101	PTY	C30-C31-C32-C33
2	C	1109	PTY	C8-C11-C12-C13
2	A	1101	PTY	C3-O11-P1-O14
2	A	1103	PTY	C3-O11-P1-O14
2	A	1103	PTY	C5-O14-P1-O11
2	A	1108	PTY	C3-O11-P1-O14
2	A	1109	PTY	C5-O14-P1-O11
2	B	2002	PTY	C5-O14-P1-O11
2	B	2003	PTY	C3-O11-P1-O14
2	B	2005	PTY	C3-O11-P1-O14
2	B	2006	PTY	C5-O14-P1-O11
2	B	2009	PTY	C3-O11-P1-O14
2	B	2011	PTY	C5-O14-P1-O11
2	B	2012	PTY	C5-O14-P1-O11
2	C	1101	PTY	C3-O11-P1-O14
2	C	1105	PTY	C5-O14-P1-O11
2	C	1109	PTY	C3-O11-P1-O14
2	C	1109	PTY	C5-O14-P1-O11
2	B	2012	PTY	C13-C14-C15-C16
2	B	2005	PTY	C13-C14-C15-C16
2	B	2008	PTY	C22-C23-C24-C25
2	A	1105	PTY	C12-C13-C14-C15
2	B	2001	PTY	C33-C34-C35-C36
2	B	2010	PTY	C11-C12-C13-C14
2	B	2010	PTY	C15-C16-C17-C18
2	A	1103	PTY	C31-C32-C33-C34
2	C	1103	PTY	C33-C34-C35-C36
2	C	1109	PTY	C33-C34-C35-C36
2	C	1109	PTY	C37-C38-C39-C40
2	A	1109	PTY	C14-C15-C16-C17
2	B	2008	PTY	C16-C17-C18-C19
2	C	1101	PTY	C38-C39-C40-C41
3	A	1111	D12	C6-C7-C8-C9
2	B	2005	PTY	C11-C12-C13-C14
2	C	1101	PTY	C20-C21-C22-C23
2	C	1103	PTY	C30-C31-C32-C33
3	C	1106	D12	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1101	PTY	C11-C12-C13-C14
2	A	1101	PTY	C31-C32-C33-C34
2	A	1107	PTY	C35-C36-C37-C38
2	B	2008	PTY	C33-C34-C35-C36
2	B	2012	PTY	C14-C15-C16-C17
2	A	1108	PTY	C21-C22-C23-C24
2	A	1109	PTY	C31-C32-C33-C34
2	A	1108	PTY	C13-C14-C15-C16
2	A	1108	PTY	C36-C37-C38-C39
3	C	1106	D12	C6-C7-C8-C9
2	A	1105	PTY	C36-C37-C38-C39
2	B	2003	PTY	C33-C34-C35-C36
2	B	2010	PTY	C33-C34-C35-C36
2	C	1109	PTY	C31-C32-C33-C34
3	A	1106	D12	C6-C7-C8-C9
2	B	2001	PTY	O14-C5-C6-C1
2	A	1107	PTY	C14-C15-C16-C17
2	B	2008	PTY	C21-C22-C23-C24
2	A	1102	PTY	N1-C2-C3-O11
2	C	1101	PTY	C11-C12-C13-C14
2	C	1101	PTY	C13-C14-C15-C16
2	C	1103	PTY	C11-C12-C13-C14
2	A	1105	PTY	C33-C34-C35-C36
2	B	2009	PTY	C31-C32-C33-C34
3	B	2004	D12	C4-C5-C6-C7
2	A	1109	PTY	C19-C20-C21-C22
2	A	1103	PTY	O4-C1-C6-C5
2	B	2005	PTY	O4-C1-C6-C5
2	A	1108	PTY	C18-C19-C20-C21
2	A	1108	PTY	C16-C17-C18-C19
2	B	2003	PTY	C36-C37-C38-C39
2	C	1102	PTY	C35-C36-C37-C38
2	C	1103	PTY	C34-C35-C36-C37
2	C	1103	PTY	C31-C32-C33-C34
2	A	1108	PTY	C24-C25-C26-C27
2	B	2008	PTY	C11-C12-C13-C14
2	B	2008	PTY	C32-C33-C34-C35
2	C	1101	PTY	C15-C16-C17-C18
2	B	2012	PTY	C11-C8-O7-C6
2	C	1101	PTY	C17-C18-C19-C20
2	C	1109	PTY	C30-C31-C32-C33
2	A	1108	PTY	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2009	PTY	C30-C31-C32-C33
2	C	1103	PTY	C8-C11-C12-C13
2	B	2006	PTY	C14-C15-C16-C17
3	A	1106	D12	C2-C3-C4-C5
2	A	1101	PTY	C33-C34-C35-C36
2	B	2006	PTY	C8-C11-C12-C13
2	A	1105	PTY	C11-C8-O7-C6
2	B	2010	PTY	C11-C8-O7-C6
2	B	2011	PTY	O14-C5-C6-O7
2	C	1102	PTY	C15-C16-C17-C18
2	B	2009	PTY	C34-C35-C36-C37
3	C	1104	D12	C6-C7-C8-C9
2	B	2012	PTY	O10-C8-O7-C6
2	A	1108	PTY	C20-C21-C22-C23
2	B	2002	PTY	O4-C1-C6-O7
2	A	1107	PTY	C8-C11-C12-C13
2	A	1107	PTY	C20-C21-C22-C23
3	B	2004	D12	C6-C7-C8-C9
2	A	1101	PTY	C5-O14-P1-O11
2	A	1107	PTY	C5-O14-P1-O11
2	B	2011	PTY	C3-O11-P1-O14
2	B	2012	PTY	C30-C31-C32-C33
2	B	2003	PTY	C13-C14-C15-C16
2	B	2002	PTY	O14-C5-C6-C1
2	B	2012	PTY	O14-C5-C6-C1
2	C	1102	PTY	O14-C5-C6-C1
2	B	2012	PTY	C32-C33-C34-C35
2	C	1109	PTY	C11-C12-C13-C14
2	C	1109	PTY	C36-C37-C38-C39
2	A	1102	PTY	O4-C1-C6-C5
2	B	2012	PTY	O4-C1-C6-C5
2	C	1101	PTY	O4-C1-C6-C5
2	C	1103	PTY	O4-C1-C6-C5
3	A	1111	D12	C5-C6-C7-C8
2	C	1102	PTY	C31-C32-C33-C34
2	A	1105	PTY	C31-C32-C33-C34
3	C	1104	D12	C7-C8-C9-C10
2	B	2010	PTY	C31-C30-O4-C1
2	B	2003	PTY	C5-C6-O7-C8
2	A	1102	PTY	C14-C15-C16-C17
3	C	1106	D12	C2-C3-C4-C5
2	A	1109	PTY	C6-C5-O14-P1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1109	PTY	O14-C5-C6-O7
2	B	2010	PTY	O30-C30-O4-C1
2	A	1107	PTY	C34-C35-C36-C37
2	C	1101	PTY	C34-C35-C36-C37
2	B	2003	PTY	C31-C30-O4-C1
2	C	1101	PTY	C40-C41-C42-C43
2	A	1105	PTY	O10-C8-O7-C6
2	B	2010	PTY	O10-C8-O7-C6
2	B	2012	PTY	C33-C34-C35-C36
3	A	1104	D12	C1-C2-C3-C4
3	A	1110	D12	C5-C6-C7-C8
2	B	2003	PTY	O14-C5-C6-C1
2	B	2011	PTY	O14-C5-C6-C1
2	C	1105	PTY	O14-C5-C6-C1
2	B	2008	PTY	C8-C11-C12-C13
2	A	1105	PTY	N1-C2-C3-O11
2	C	1101	PTY	N1-C2-C3-O11
2	C	1103	PTY	N1-C2-C3-O11
2	B	2012	PTY	C12-C13-C14-C15
2	A	1103	PTY	C30-C31-C32-C33
2	C	1102	PTY	C39-C40-C41-C42
2	A	1109	PTY	O4-C1-C6-C5
2	B	2002	PTY	O4-C1-C6-C5
2	B	2008	PTY	O4-C1-C6-C5
2	B	2009	PTY	O4-C1-C6-C5
3	B	2007	D12	C11-C10-C9-C8
2	C	1102	PTY	C34-C35-C36-C37
2	A	1101	PTY	C14-C15-C16-C17
2	A	1108	PTY	C12-C13-C14-C15
2	B	2006	PTY	C16-C17-C18-C19
2	B	2001	PTY	C34-C35-C36-C37
2	B	2001	PTY	O14-C5-C6-O7
2	B	2002	PTY	O14-C5-C6-O7
2	B	2003	PTY	O14-C5-C6-O7
2	B	2012	PTY	O14-C5-C6-O7
2	C	1102	PTY	O14-C5-C6-O7
2	B	2003	PTY	O30-C30-O4-C1
2	B	2009	PTY	O4-C1-C6-O7
2	B	2010	PTY	O4-C1-C6-O7
2	C	1105	PTY	O4-C1-C6-O7
2	B	2009	PTY	C14-C15-C16-C17
2	B	2008	PTY	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1103	PTY	C12-C13-C14-C15
2	C	1109	PTY	C35-C36-C37-C38
2	B	2006	PTY	C6-C5-O14-P1
2	B	2012	PTY	C6-C5-O14-P1
2	A	1102	PTY	C12-C13-C14-C15
2	B	2011	PTY	C11-C12-C13-C14
3	A	1106	D12	C1-C2-C3-C4
2	B	2009	PTY	C12-C13-C14-C15
2	A	1109	PTY	O14-C5-C6-C1
2	C	1102	PTY	C11-C12-C13-C14
2	C	1109	PTY	C12-C13-C14-C15
2	C	1101	PTY	C37-C38-C39-C40
2	A	1107	PTY	C5-C6-O7-C8
2	A	1109	PTY	C5-C6-O7-C8
2	B	2008	PTY	C5-C6-O7-C8
2	B	2002	PTY	C6-C5-O14-P1
2	C	1105	PTY	O4-C1-C6-C5
2	C	1105	PTY	C6-C5-O14-P1
2	A	1109	PTY	O14-C5-C6-O7
2	B	2006	PTY	O14-C5-C6-O7
2	C	1105	PTY	O14-C5-C6-O7
2	A	1109	PTY	O4-C1-C6-O7
2	B	2003	PTY	C12-C13-C14-C15
2	A	1107	PTY	O10-C8-O7-C6
2	A	1107	PTY	C11-C8-O7-C6
2	C	1103	PTY	C5-O14-P1-O11
2	A	1101	PTY	C5-O14-P1-O12
2	A	1103	PTY	C5-O14-P1-O12
2	A	1105	PTY	C3-O11-P1-O13
2	A	1108	PTY	C5-O14-P1-O12
2	A	1109	PTY	C5-O14-P1-O12
2	B	2002	PTY	C5-O14-P1-O13
2	B	2003	PTY	C3-O11-P1-O13
2	B	2005	PTY	C3-O11-P1-O13
2	B	2011	PTY	C3-O11-P1-O12
2	B	2011	PTY	C5-O14-P1-O13
2	B	2012	PTY	C5-O14-P1-O13
2	C	1105	PTY	C5-O14-P1-O13
2	C	1109	PTY	C3-O11-P1-O13
2	C	1109	PTY	C5-O14-P1-O13
2	A	1108	PTY	C15-C16-C17-C18
2	B	2005	PTY	O14-C5-C6-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2006	PTY	O14-C5-C6-C1
3	B	2007	D12	C5-C6-C7-C8
2	A	1102	PTY	C2-C3-O11-P1
2	B	2005	PTY	C2-C3-O11-P1
2	C	1101	PTY	C2-C3-O11-P1
2	A	1105	PTY	C8-C11-C12-C13
3	B	2013	D12	C1-C2-C3-C4
2	C	1101	PTY	C35-C36-C37-C38
2	B	2005	PTY	O14-C5-C6-O7
2	A	1109	PTY	C12-C13-C14-C15
2	B	2009	PTY	C36-C37-C38-C39
2	B	2001	PTY	C17-C18-C19-C20
2	A	1102	PTY	O4-C1-C6-O7
2	A	1103	PTY	O4-C1-C6-O7
2	B	2005	PTY	O4-C1-C6-O7
2	B	2012	PTY	O4-C1-C6-O7
3	C	1104	D12	C9-C10-C11-C12
2	A	1103	PTY	C11-C12-C13-C14
2	A	1108	PTY	C14-C15-C16-C17
2	B	2001	PTY	C37-C38-C39-C40
2	A	1108	PTY	C26-C27-C28-C29
2	B	2008	PTY	C31-C32-C33-C34
2	A	1103	PTY	C1-C6-O7-C8
2	C	1105	PTY	C5-C6-O7-C8
2	B	2010	PTY	O14-C5-C6-O7
3	C	1107	D12	C9-C10-C11-C12
2	A	1109	PTY	C3-O11-P1-O14
2	B	2001	PTY	C3-O11-P1-O14
2	B	2001	PTY	C5-O14-P1-O11
2	B	2003	PTY	C5-O14-P1-O11
2	B	2005	PTY	C5-O14-P1-O11
2	B	2008	PTY	C3-O11-P1-O14
2	B	2009	PTY	C5-O14-P1-O11
2	B	2010	PTY	C5-O14-P1-O11
2	B	2012	PTY	C3-O11-P1-O14
2	C	1101	PTY	C5-O14-P1-O11
2	C	1103	PTY	C3-O11-P1-O14
2	A	1108	PTY	C11-C12-C13-C14
2	A	1102	PTY	C6-C5-O14-P1
2	A	1108	PTY	C6-C5-O14-P1
2	C	1109	PTY	O14-C5-C6-C1
2	B	2010	PTY	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1104	D12	C2-C3-C4-C5
2	A	1105	PTY	C15-C16-C17-C18
2	B	2001	PTY	O4-C1-C6-O7
2	B	2006	PTY	O4-C1-C6-O7
2	C	1101	PTY	C39-C40-C41-C42
2	B	2008	PTY	C6-C5-O14-P1
2	A	1108	PTY	C17-C18-C19-C20
3	C	1106	D12	C4-C5-C6-C7
2	B	2010	PTY	O4-C1-C6-C5
3	A	1106	D12	C5-C6-C7-C8
2	B	2005	PTY	C1-C6-O7-C8
2	A	1103	PTY	C32-C33-C34-C35
2	B	2003	PTY	C35-C36-C37-C38
2	B	2009	PTY	O14-C5-C6-C1
2	B	2009	PTY	C33-C34-C35-C36
2	B	2008	PTY	O4-C1-C6-O7
3	A	1106	D12	C7-C8-C9-C10
2	A	1105	PTY	O4-C30-C31-C32
2	A	1105	PTY	C32-C33-C34-C35
2	A	1109	PTY	C13-C14-C15-C16
3	B	2004	D12	C3-C4-C5-C6
2	A	1107	PTY	C12-C13-C14-C15
2	A	1101	PTY	C18-C19-C20-C21
2	B	2001	PTY	C35-C36-C37-C38
2	B	2010	PTY	N1-C2-C3-O11
2	B	2011	PTY	N1-C2-C3-O11
2	B	2010	PTY	C14-C15-C16-C17
2	A	1101	PTY	C6-C1-O4-C30
2	B	2009	PTY	O4-C30-C31-C32
2	A	1109	PTY	C16-C17-C18-C19
3	A	1104	D12	C4-C5-C6-C7
2	A	1107	PTY	C16-C17-C18-C19
2	B	2011	PTY	C12-C11-C8-O7
2	C	1102	PTY	O4-C30-C31-C32
2	C	1109	PTY	O4-C30-C31-C32
2	B	2012	PTY	C1-C6-O7-C8
2	B	2012	PTY	C5-C6-O7-C8
2	C	1102	PTY	C5-C6-O7-C8
2	B	2012	PTY	C31-C32-C33-C34
2	C	1105	PTY	C12-C11-C8-O7
2	A	1103	PTY	C6-C5-O14-P1
2	B	2011	PTY	O4-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1109	PTY	C19-C20-C21-C22
2	B	2005	PTY	C12-C11-C8-O7
2	A	1105	PTY	C14-C15-C16-C17
2	A	1101	PTY	C13-C14-C15-C16
2	A	1109	PTY	C18-C19-C20-C21
2	B	2002	PTY	C35-C36-C37-C38
2	B	2003	PTY	O4-C1-C6-O7
2	A	1107	PTY	C32-C33-C34-C35
2	A	1107	PTY	O4-C30-C31-C32
2	B	2003	PTY	C12-C11-C8-O7
2	B	2005	PTY	C14-C15-C16-C17
2	B	2012	PTY	C12-C11-C8-O7
2	B	2001	PTY	C13-C14-C15-C16
3	C	1104	D12	C5-C6-C7-C8
2	B	2009	PTY	C11-C12-C13-C14
2	B	2011	PTY	C12-C11-C8-O10
2	C	1109	PTY	O30-C30-C31-C32
2	C	1101	PTY	C14-C15-C16-C17
2	A	1102	PTY	C8-C11-C12-C13
2	B	2003	PTY	C30-C31-C32-C33
2	B	2009	PTY	O30-C30-C31-C32
2	B	2011	PTY	O30-C30-C31-C32
2	C	1102	PTY	O30-C30-C31-C32
2	A	1108	PTY	C25-C26-C27-C28
2	A	1107	PTY	C33-C34-C35-C36
2	A	1107	PTY	C18-C19-C20-C21
2	B	2005	PTY	C12-C11-C8-O10
2	C	1105	PTY	C12-C11-C8-O10
2	B	2005	PTY	C3-O11-P1-O12
2	B	2010	PTY	C5-O14-P1-O13
2	C	1103	PTY	C3-O11-P1-O13
2	A	1107	PTY	O30-C30-C31-C32
2	B	2010	PTY	O14-C5-C6-C1
2	B	2008	PTY	C12-C13-C14-C15
2	C	1105	PTY	C31-C32-C33-C34
2	A	1101	PTY	C12-C11-C8-O7
2	A	1108	PTY	C12-C11-C8-O7
2	A	1105	PTY	C2-C3-O11-P1
2	A	1107	PTY	C2-C3-O11-P1
2	B	2002	PTY	C2-C3-O11-P1
2	C	1102	PTY	C2-C3-O11-P1
2	C	1102	PTY	C1-C6-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1103	PTY	C2-C3-O11-P1
2	B	2006	PTY	C13-C14-C15-C16
2	B	2001	PTY	O4-C30-C31-C32
3	C	1106	D12	C7-C8-C9-C10
2	B	2010	PTY	C12-C11-C8-O7
2	B	2012	PTY	C12-C11-C8-O10
2	A	1108	PTY	C12-C11-C8-O10
2	B	2003	PTY	C12-C11-C8-O10
2	B	2006	PTY	C12-C13-C14-C15
2	A	1108	PTY	C37-C38-C39-C40
2	B	2001	PTY	O30-C30-C31-C32
2	C	1102	PTY	C12-C11-C8-O7

There are no ring outliers.

27 monomers are involved in 60 short contacts:

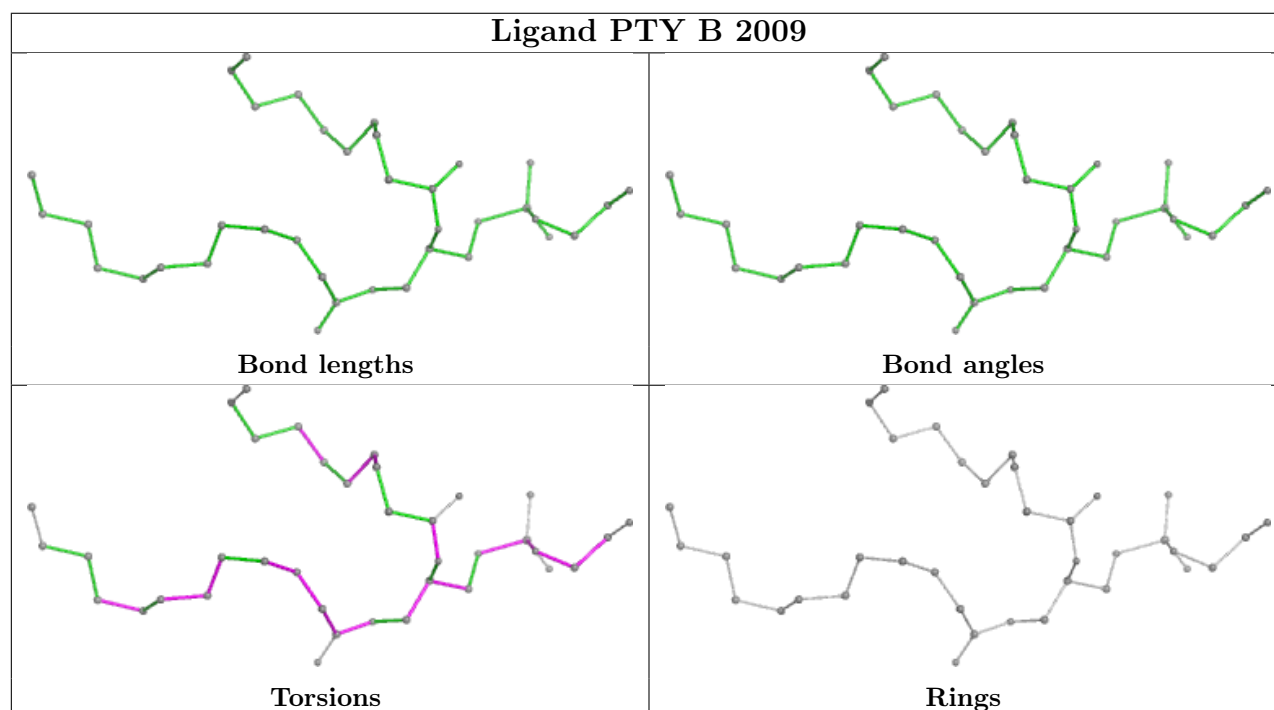
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2009	PTY	2	0
2	A	1109	PTY	4	0
2	A	1107	PTY	3	0
2	C	1105	PTY	1	0
3	B	2004	D12	2	0
2	B	2005	PTY	4	0
2	C	1103	PTY	2	0
3	C	1104	D12	1	0
2	A	1102	PTY	1	0
2	B	2008	PTY	4	0
3	A	1104	D12	1	0
2	B	2012	PTY	3	0
3	C	1108	D12	2	0
2	B	2001	PTY	10	0
2	B	2003	PTY	5	0
2	C	1101	PTY	2	0
2	A	1103	PTY	1	0
2	B	2010	PTY	3	0
2	B	2011	PTY	1	0
2	C	1102	PTY	5	0
2	A	1101	PTY	1	0
2	A	1108	PTY	4	0
2	B	2006	PTY	4	0
3	C	1106	D12	4	0
2	B	2002	PTY	3	0

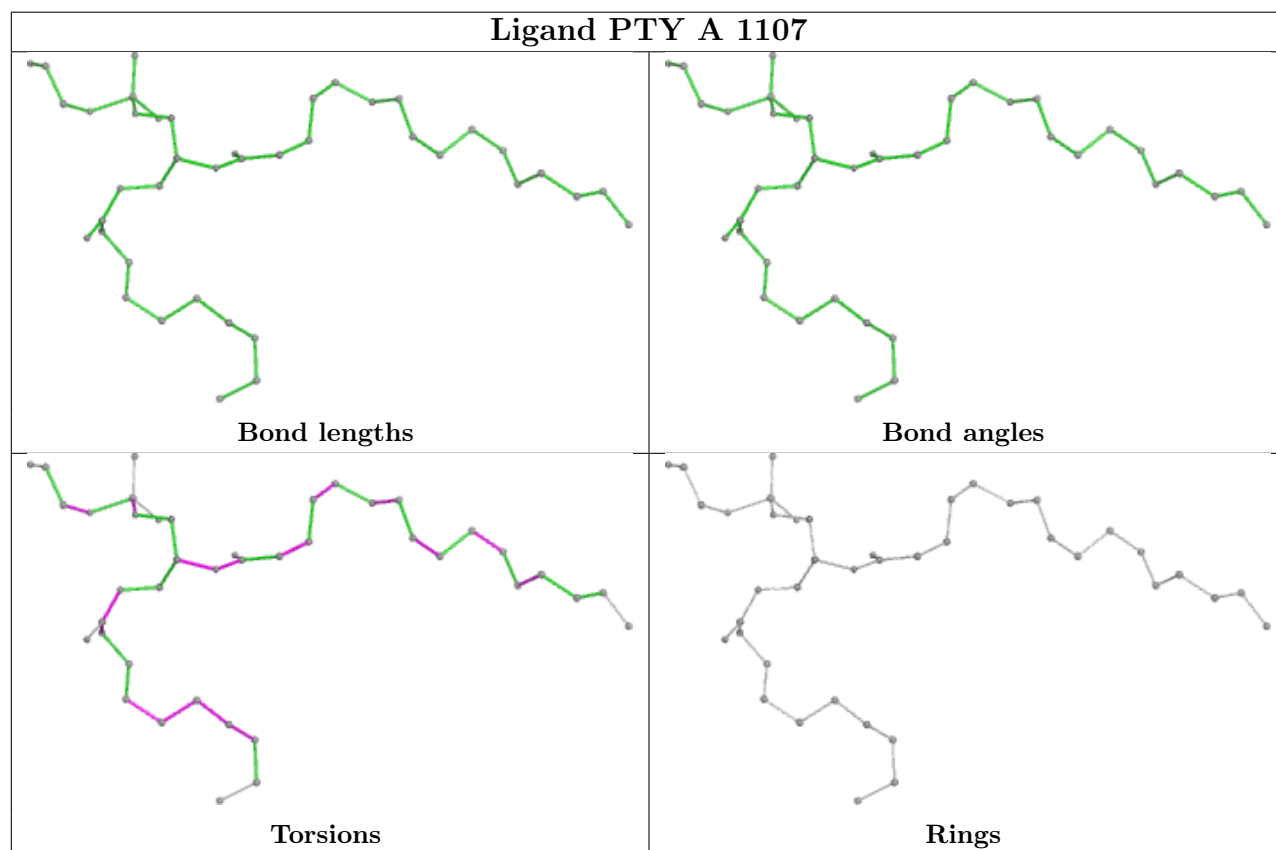
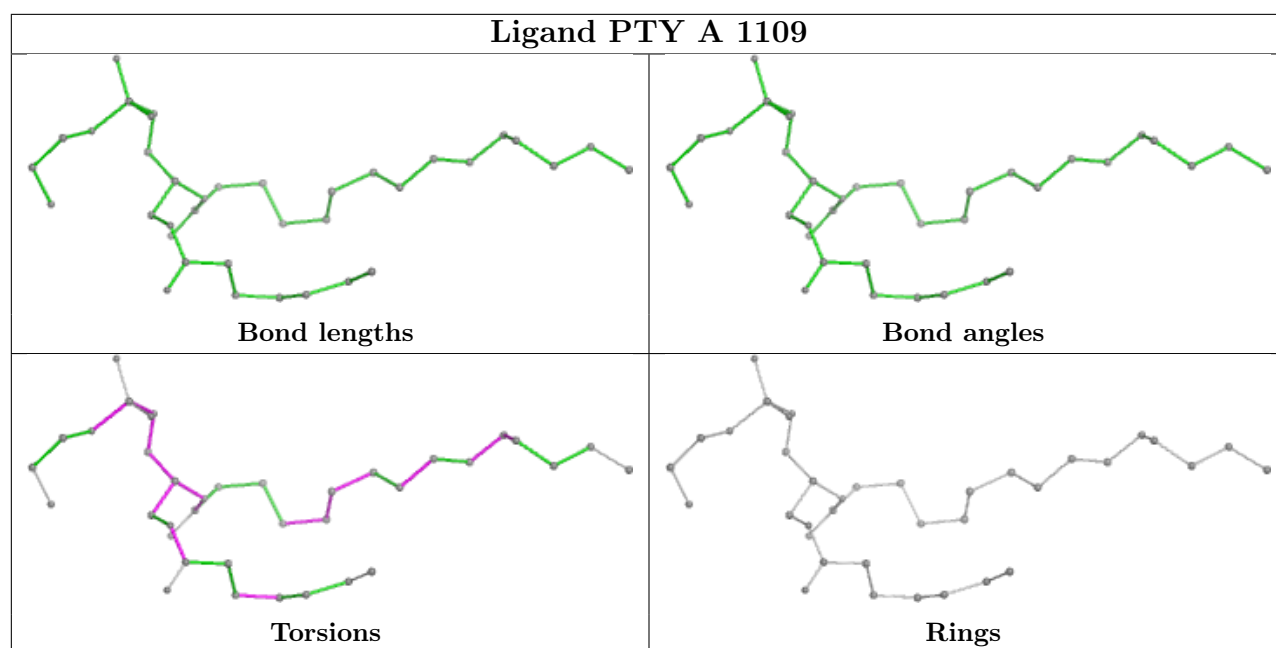
Continued on next page...

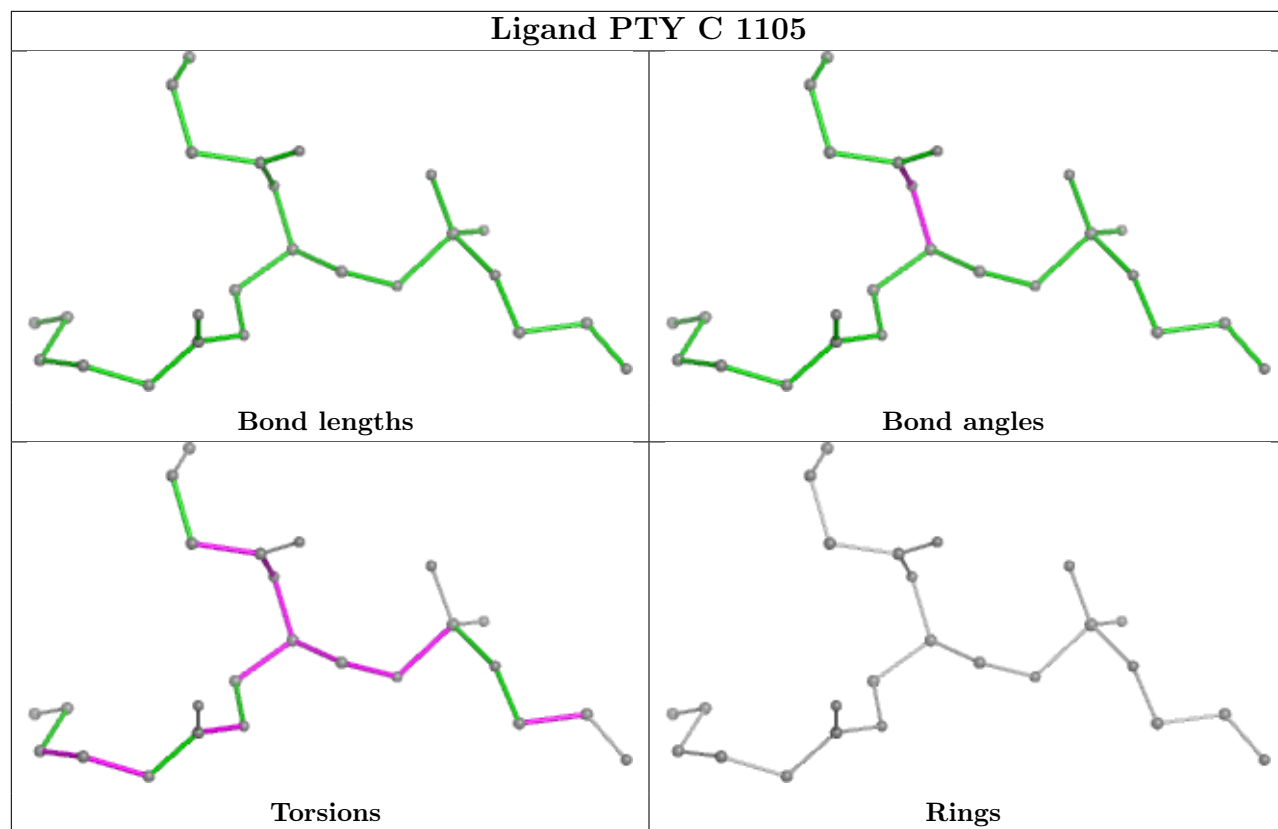
Continued from previous page...

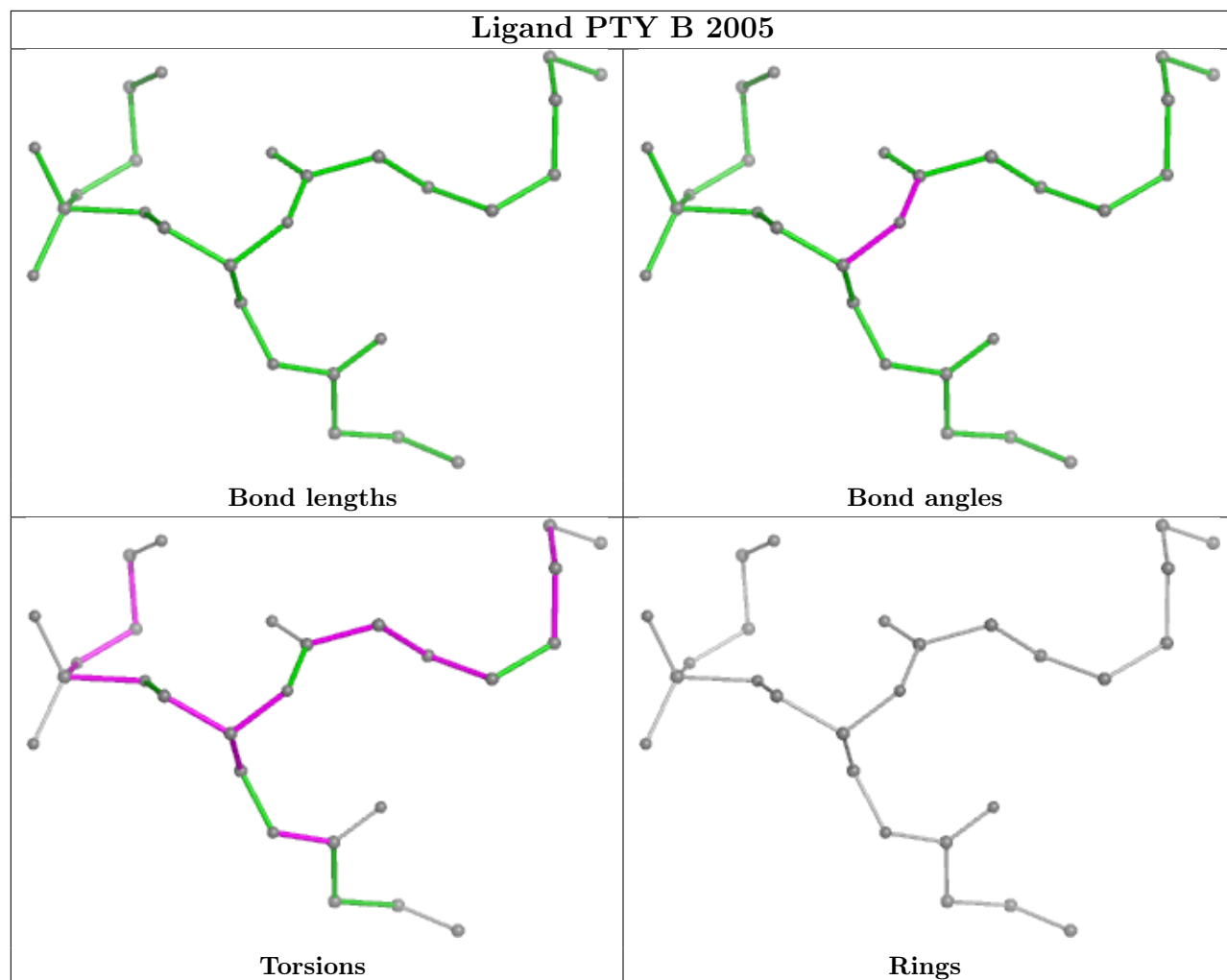
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1105	PTY	1	0
2	C	1109	PTY	4	0

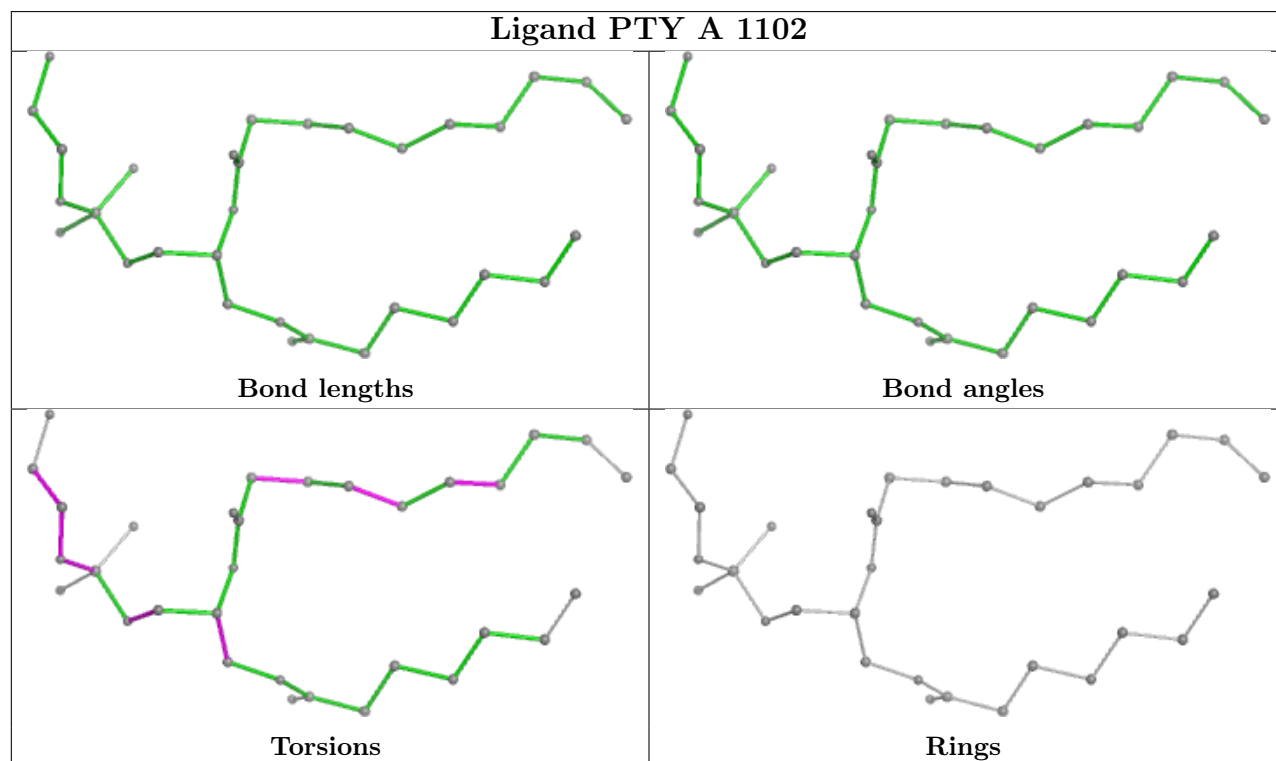
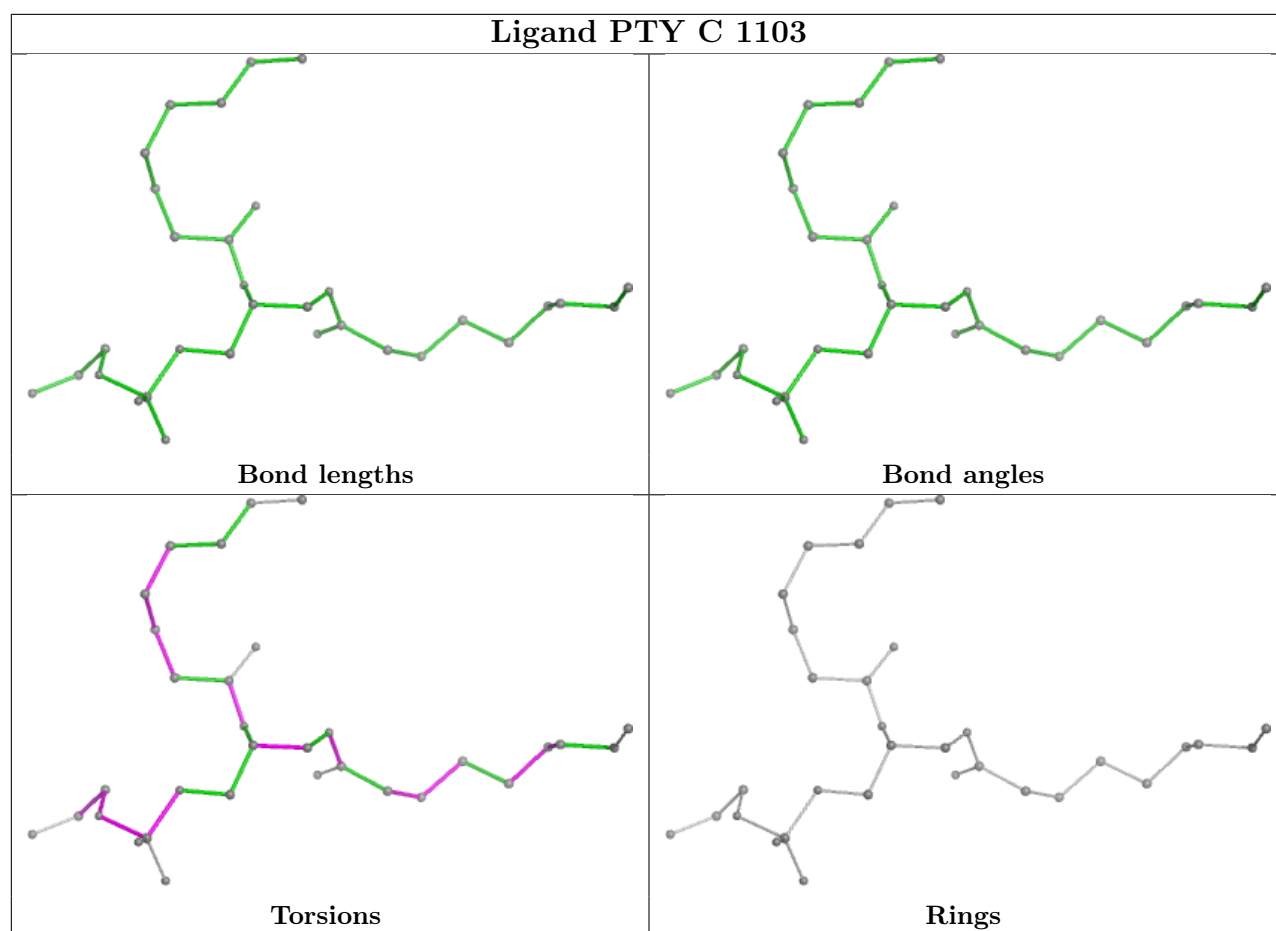
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

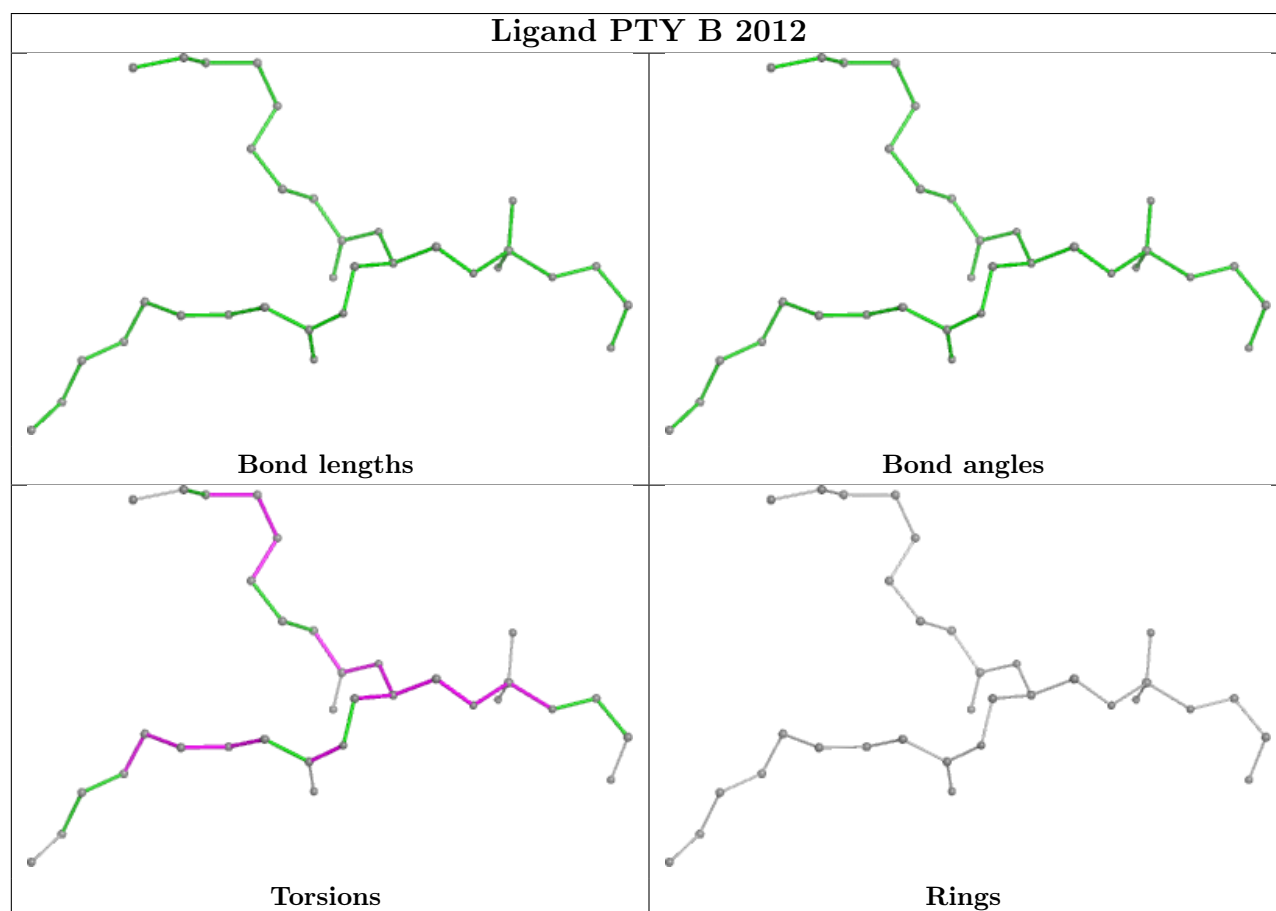
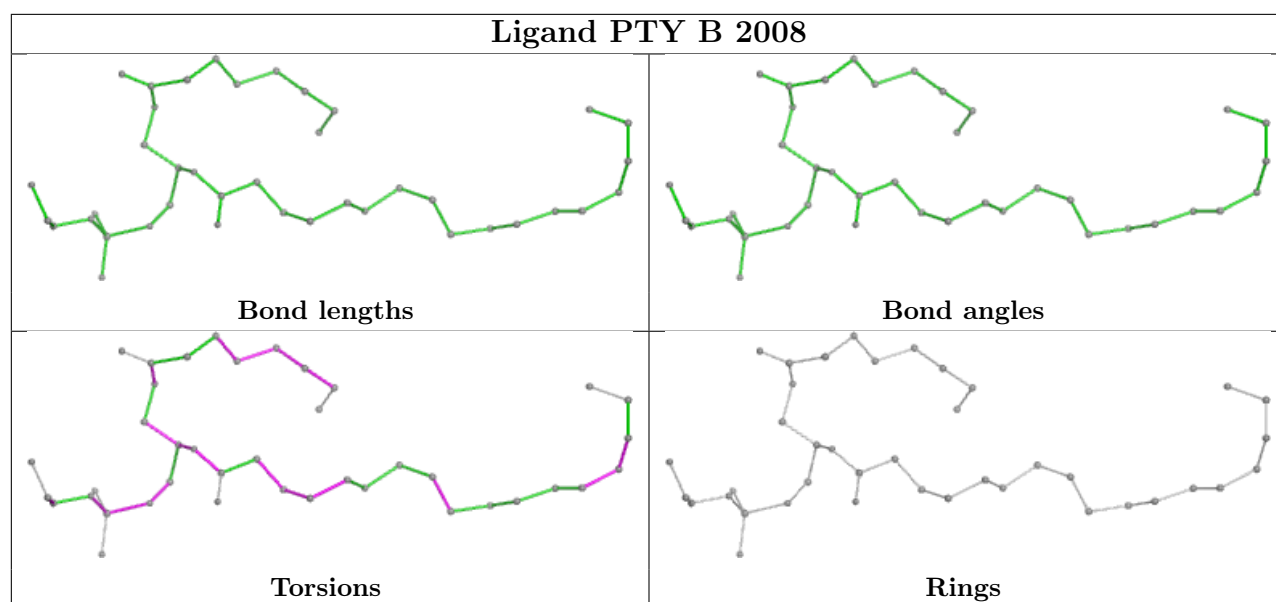


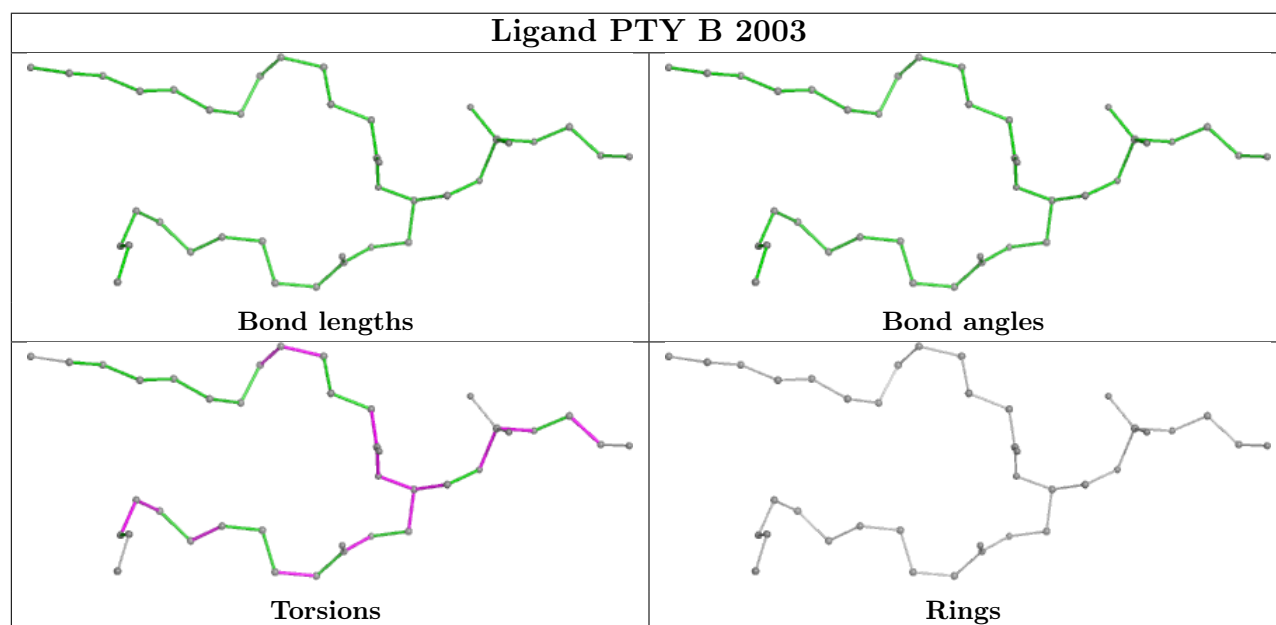
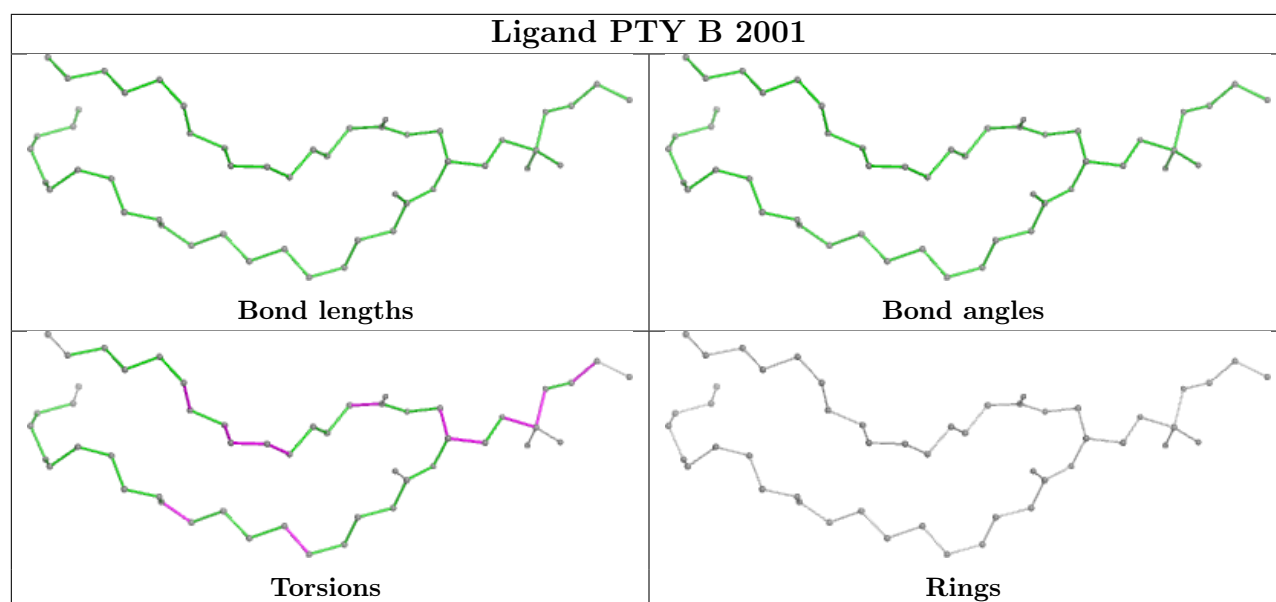


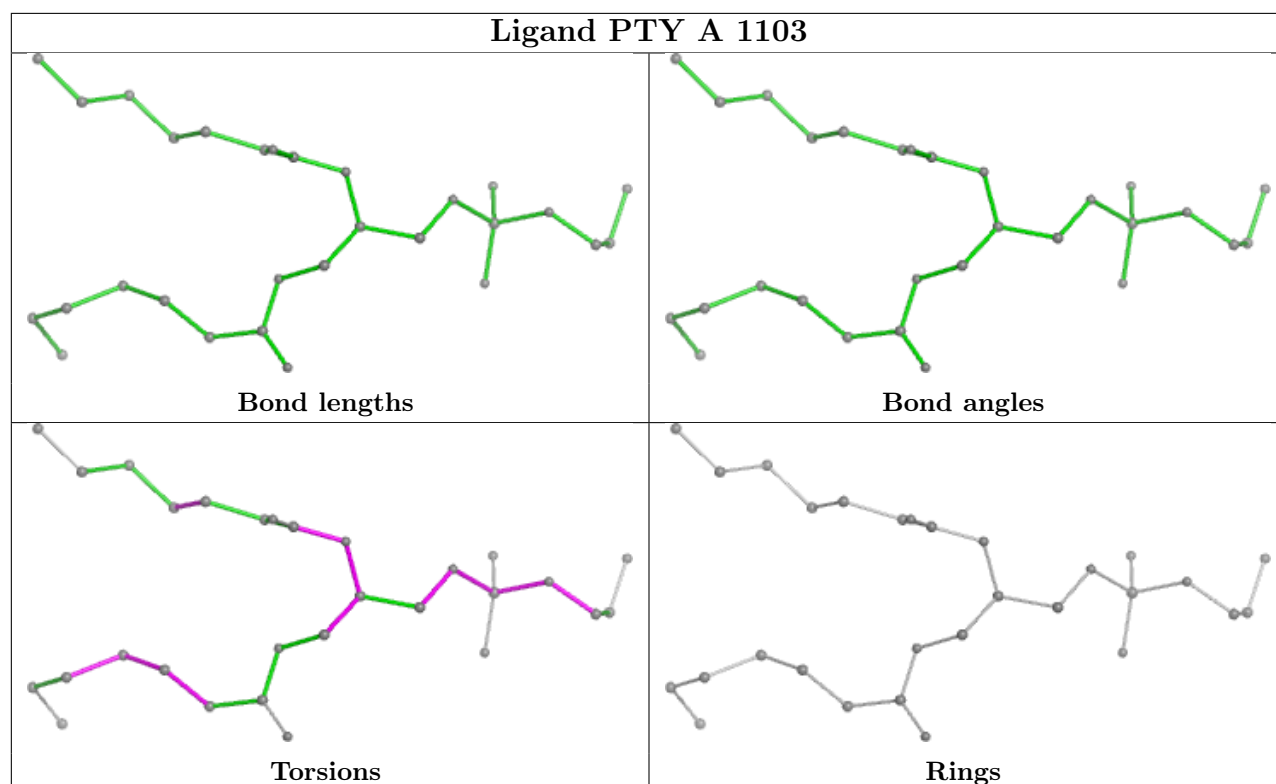
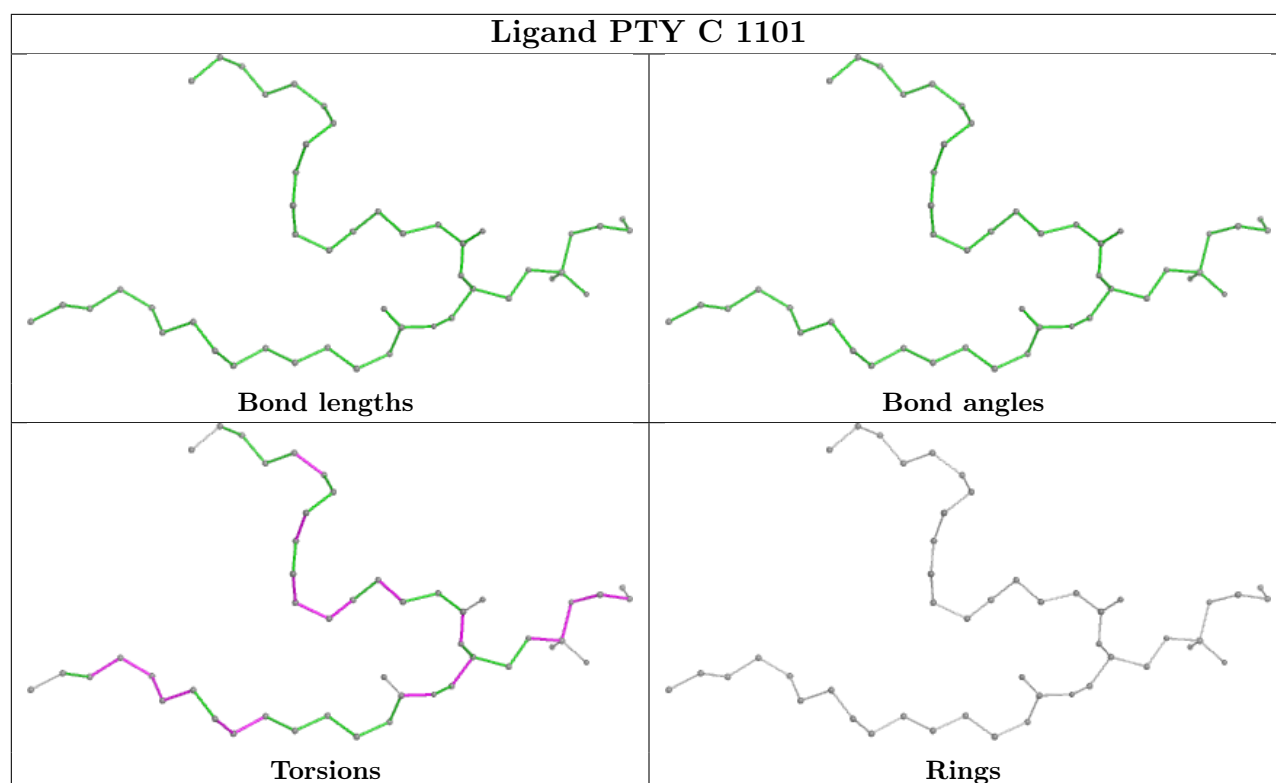


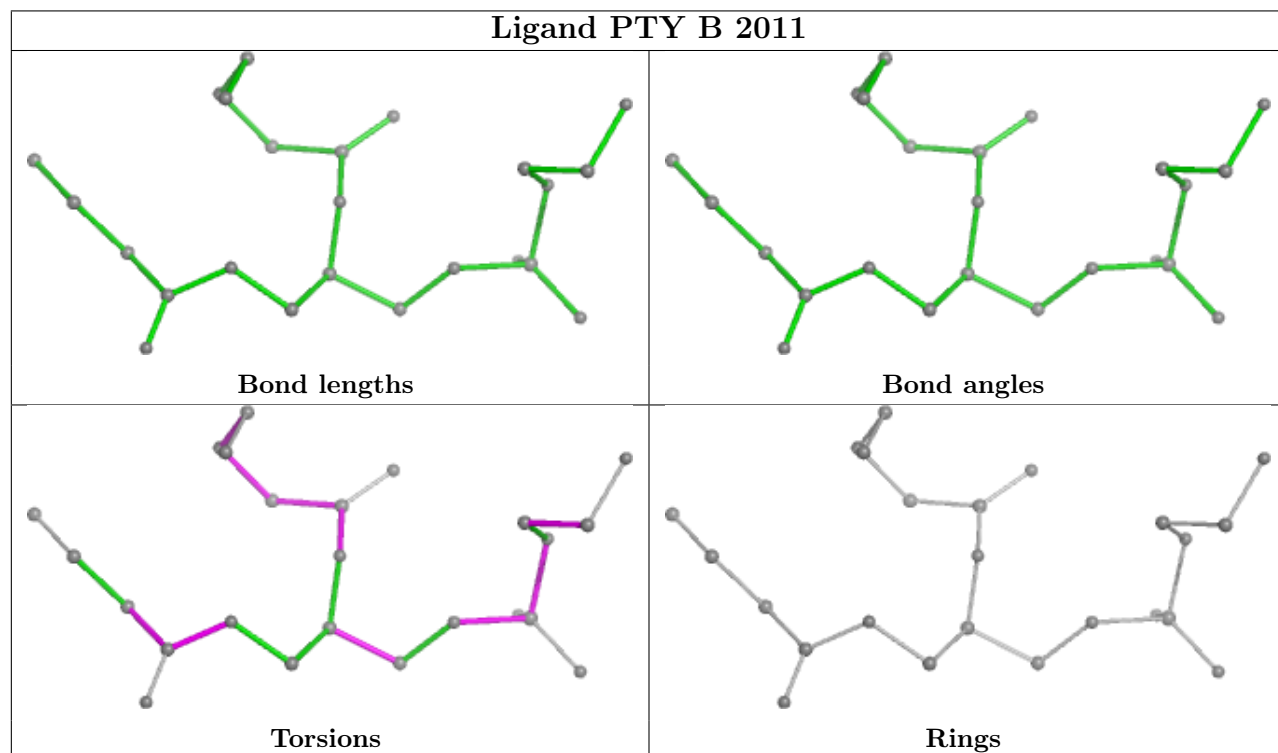
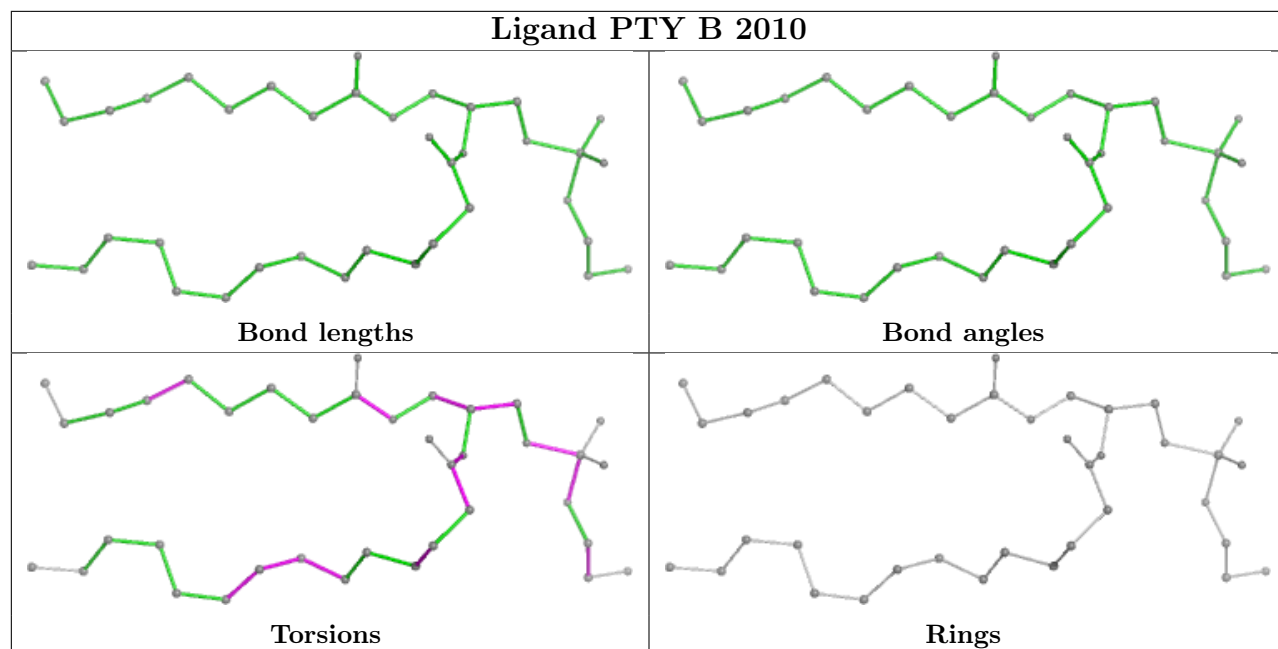


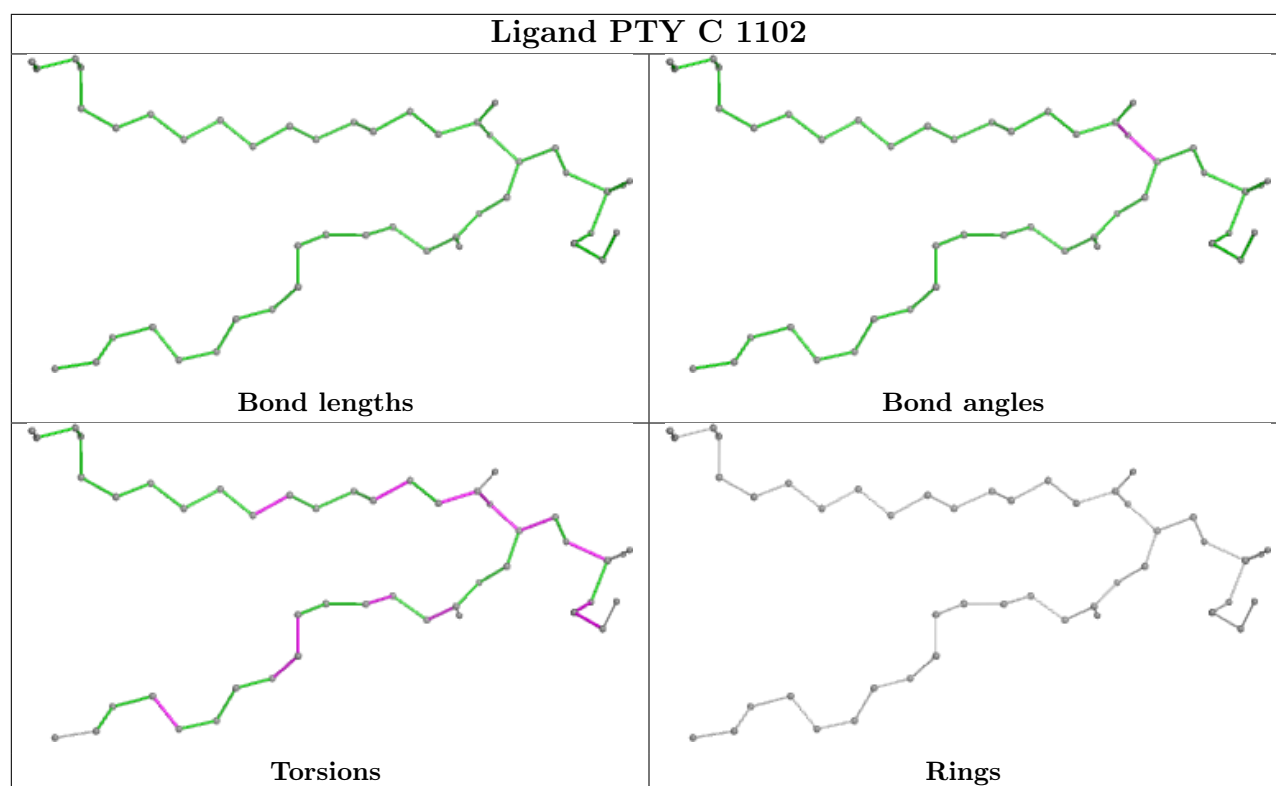


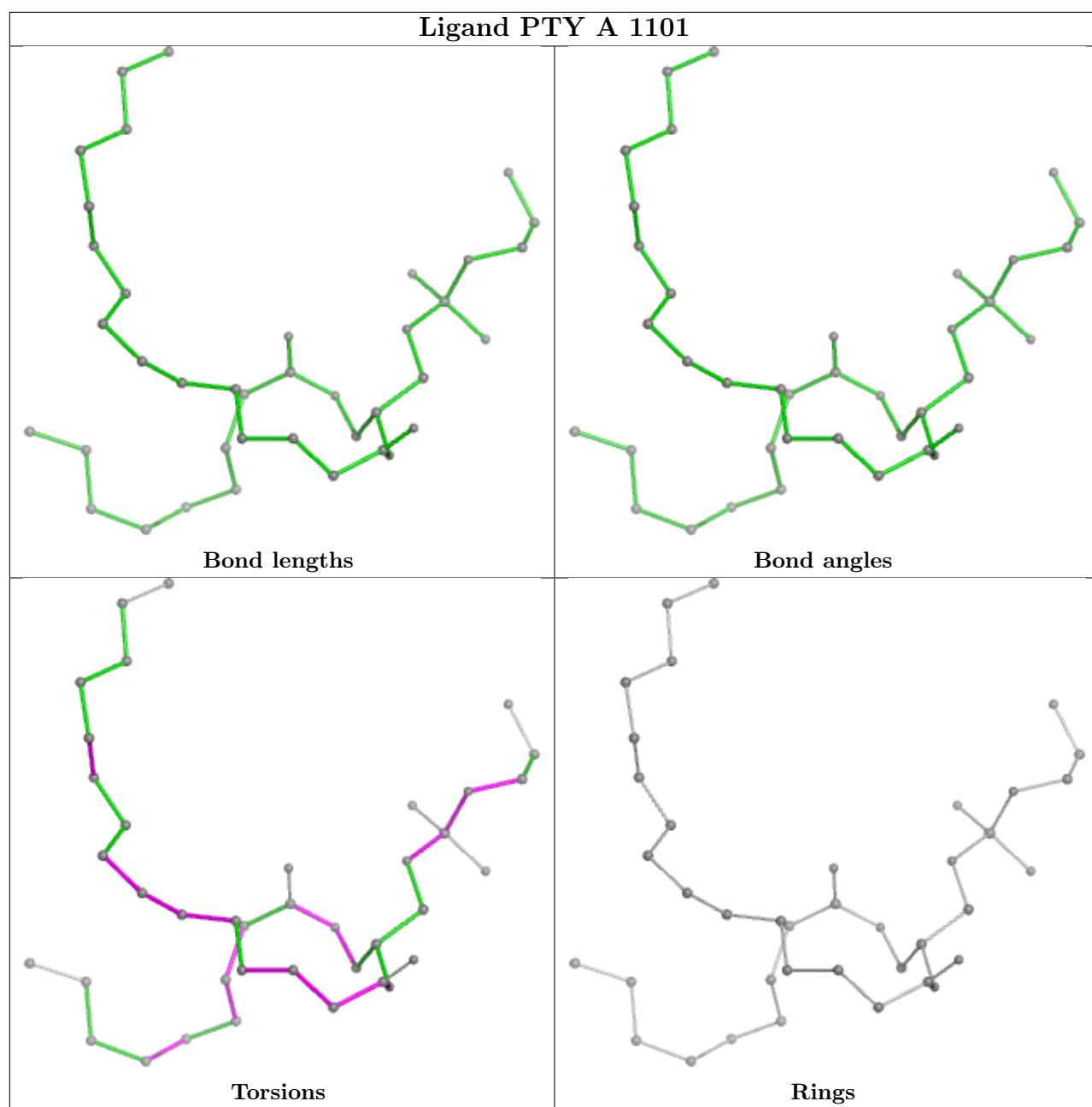


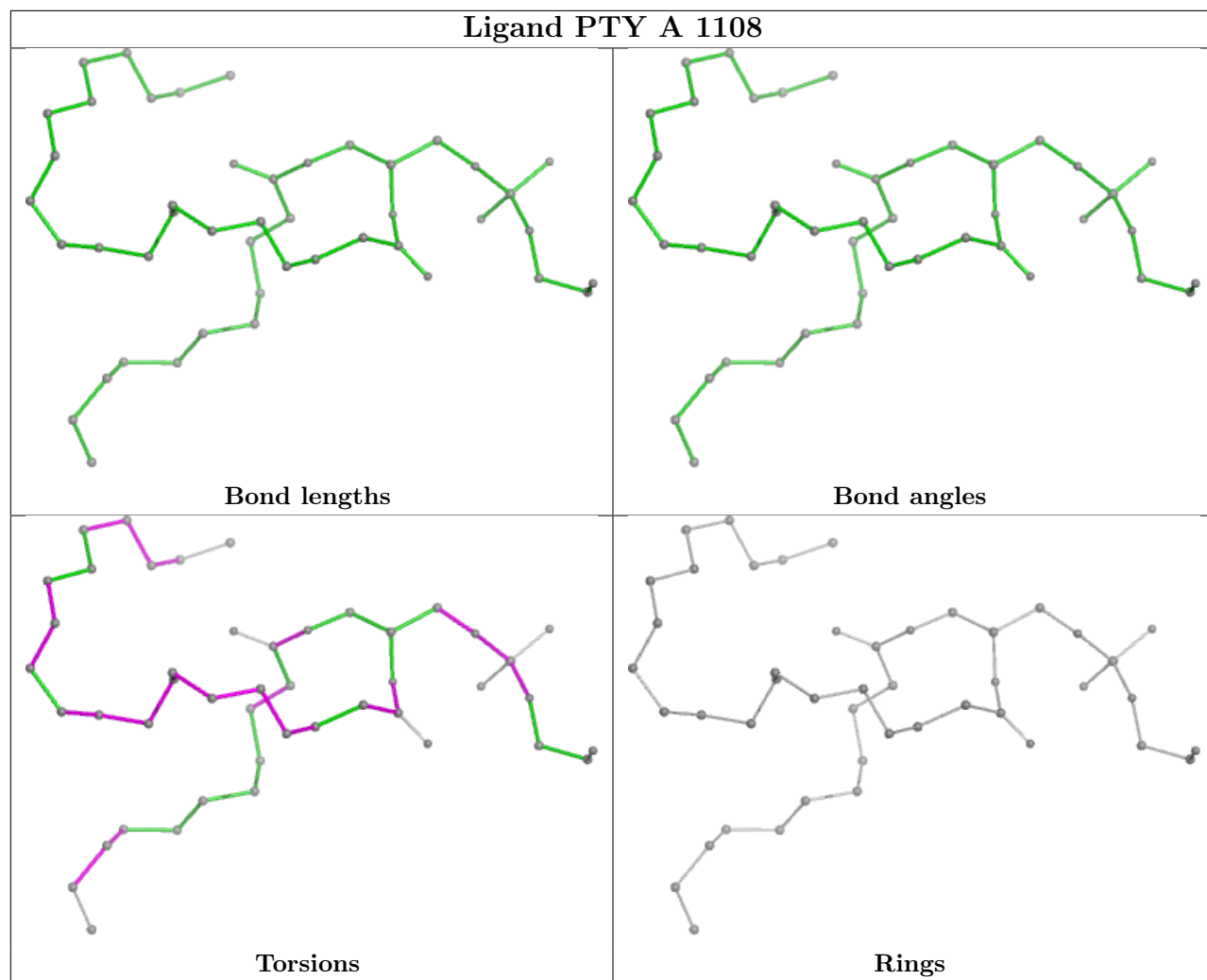


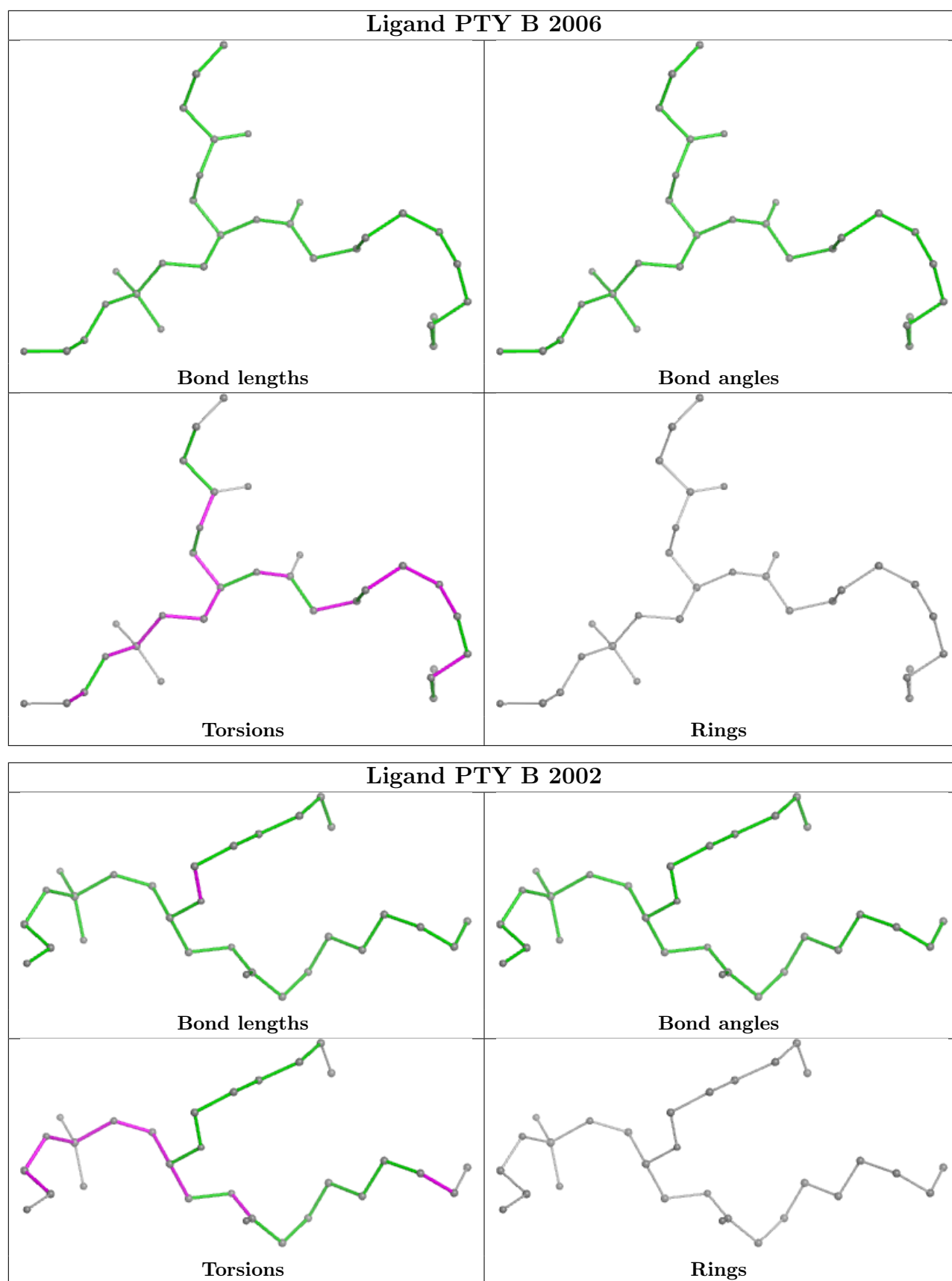


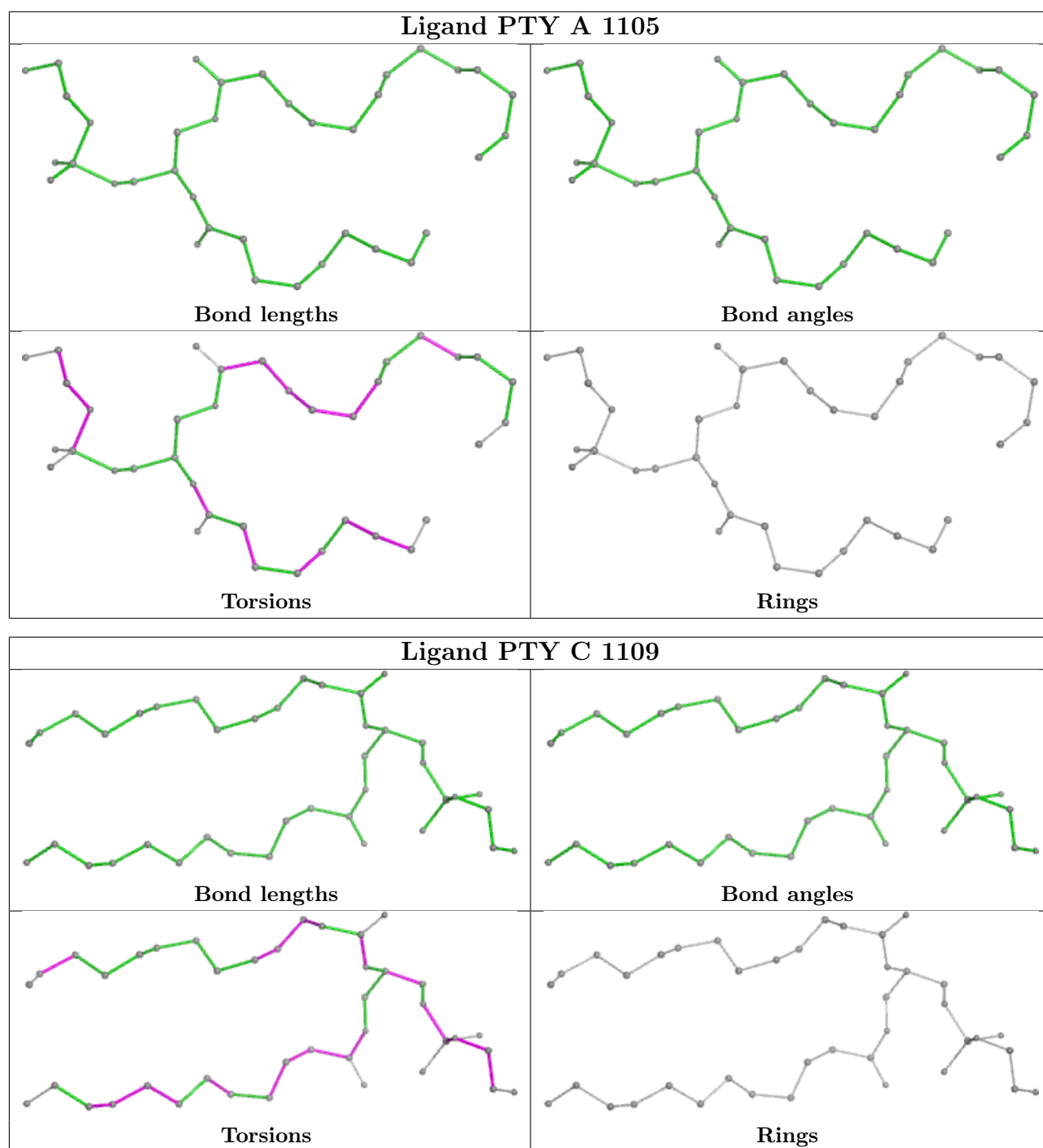












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

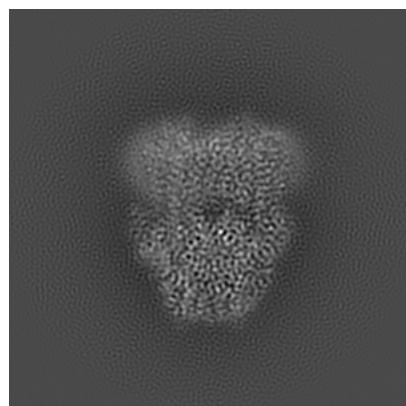
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53282. These allow visual inspection of the internal detail of the map and identification of artifacts.

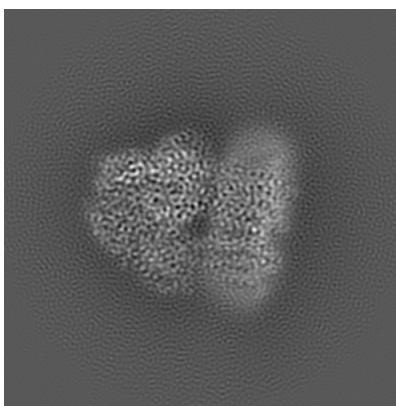
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

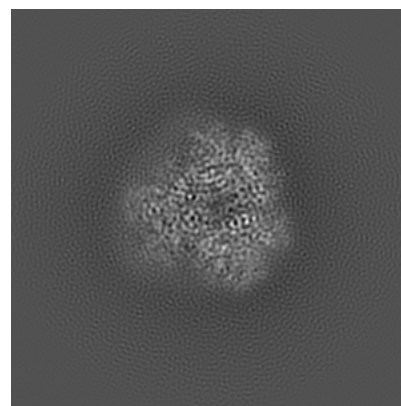
6.1.1 Primary map



X

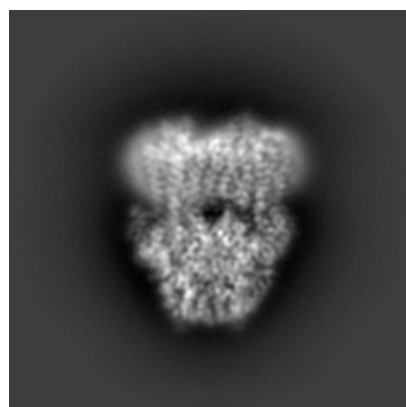


Y

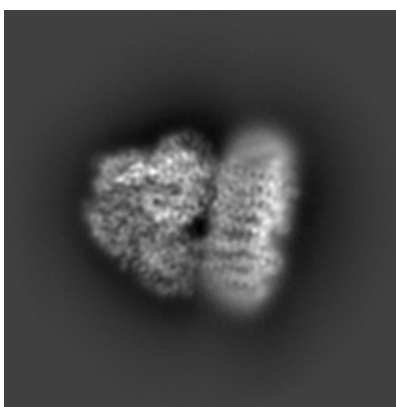


Z

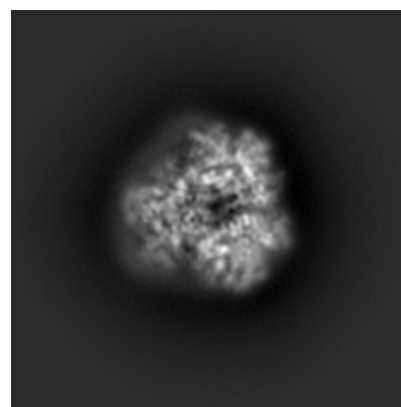
6.1.2 Raw map



X



Y

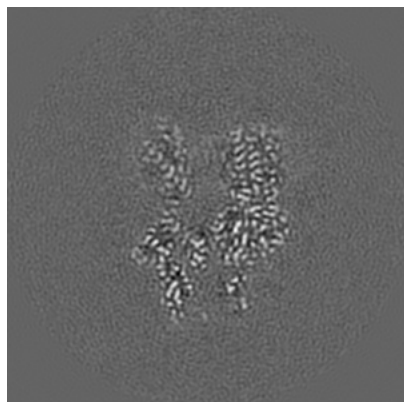


Z

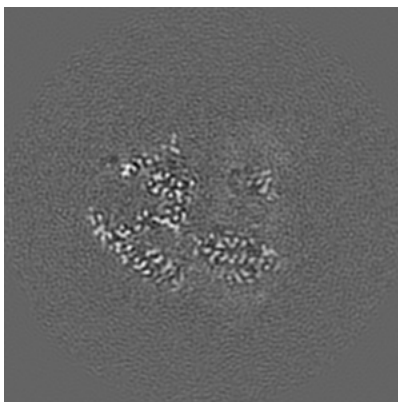
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

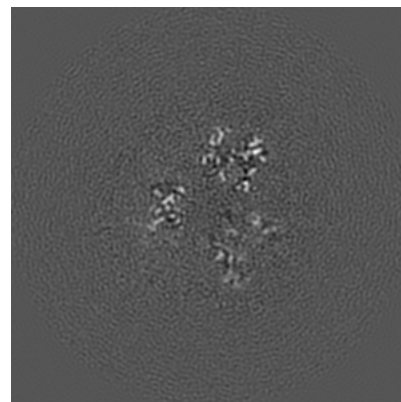
6.2.1 Primary map



X Index: 130

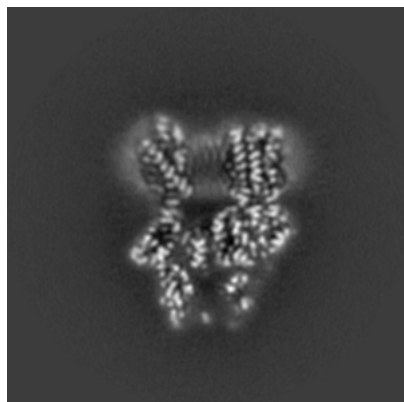


Y Index: 130

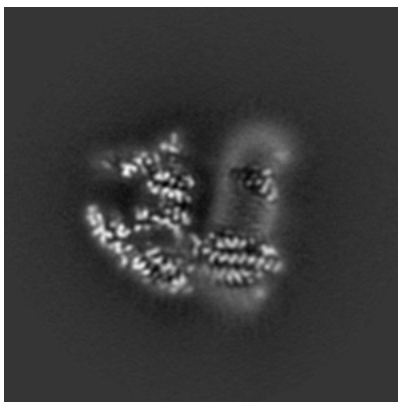


Z Index: 130

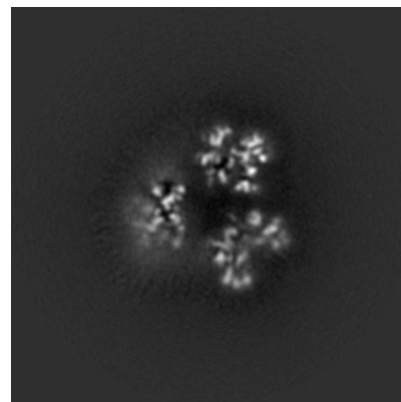
6.2.2 Raw map



X Index: 130



Y Index: 130

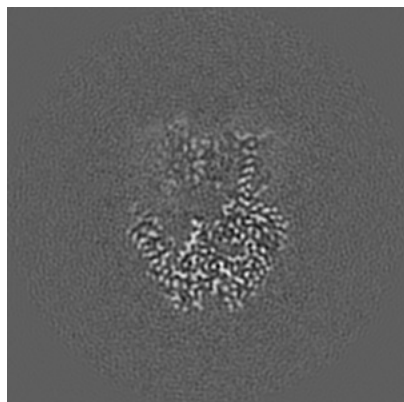


Z Index: 130

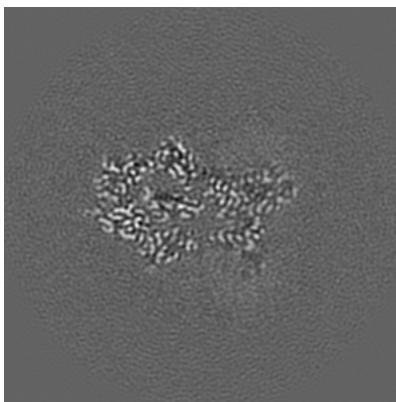
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

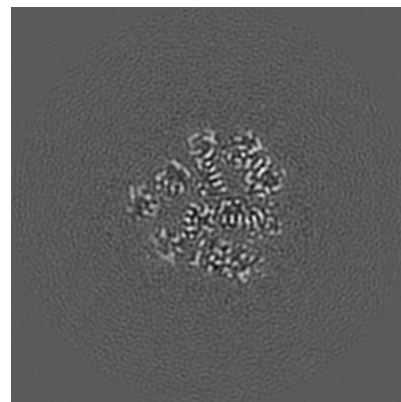
6.3.1 Primary map



X Index: 153

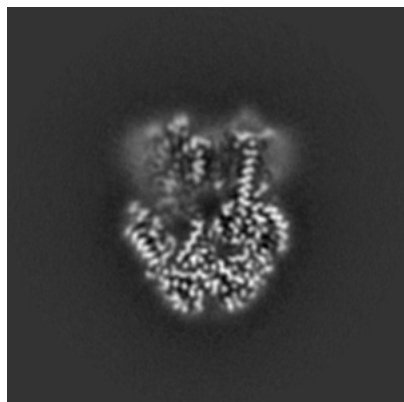


Y Index: 148

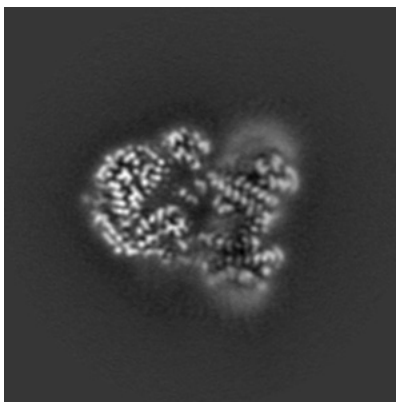


Z Index: 107

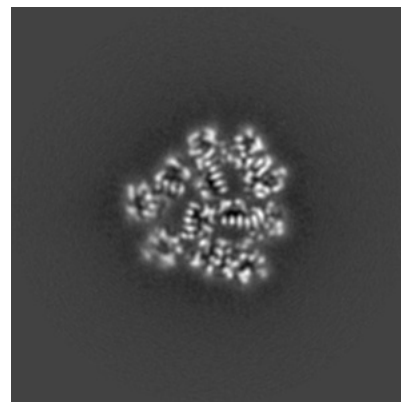
6.3.2 Raw map



X Index: 153



Y Index: 115

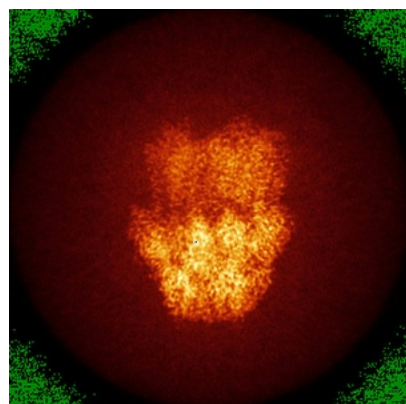


Z Index: 107

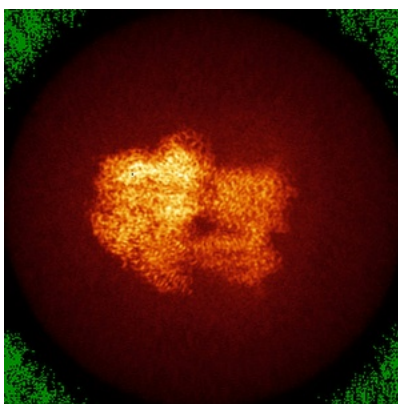
The images above show the largest variance slices of the map in three orthogonal directions.

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

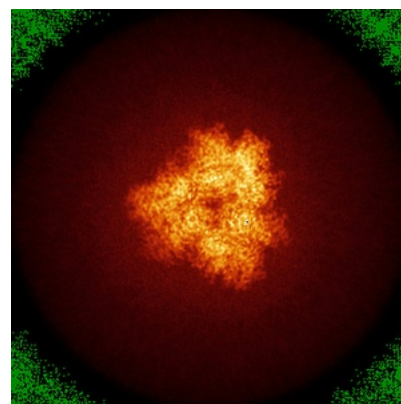
6.4.1 Primary map



X

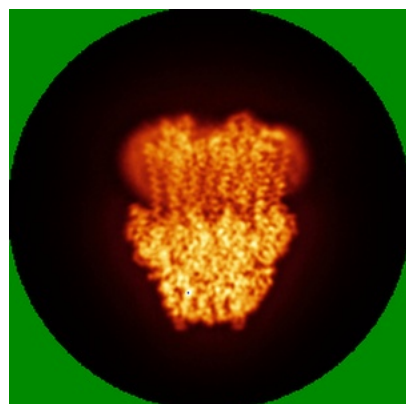


Y

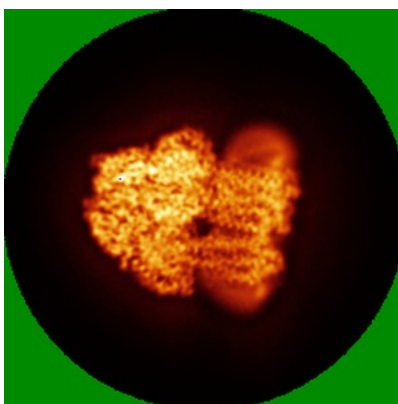


Z

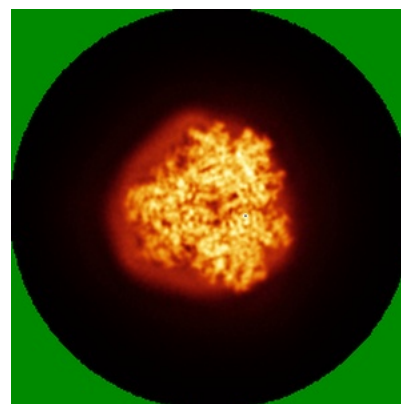
6.4.2 Raw map



X



Y

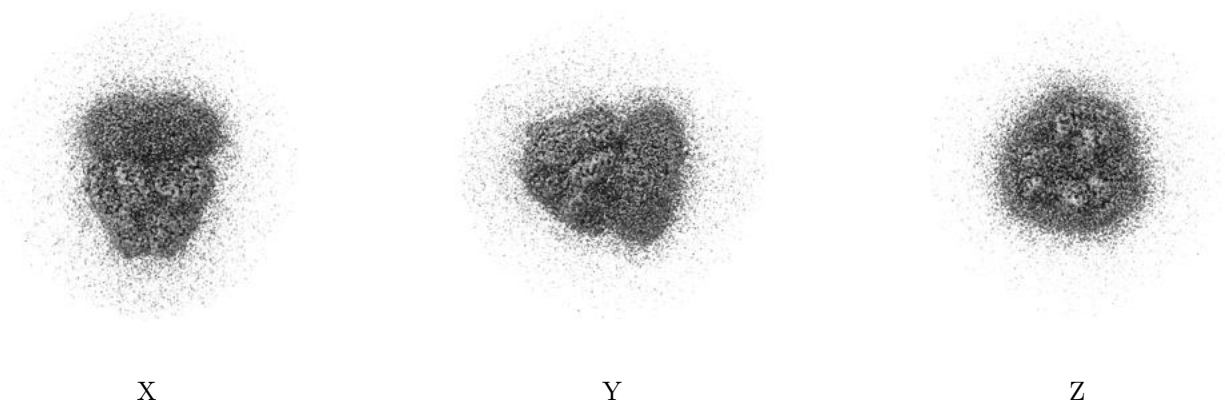


Z

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

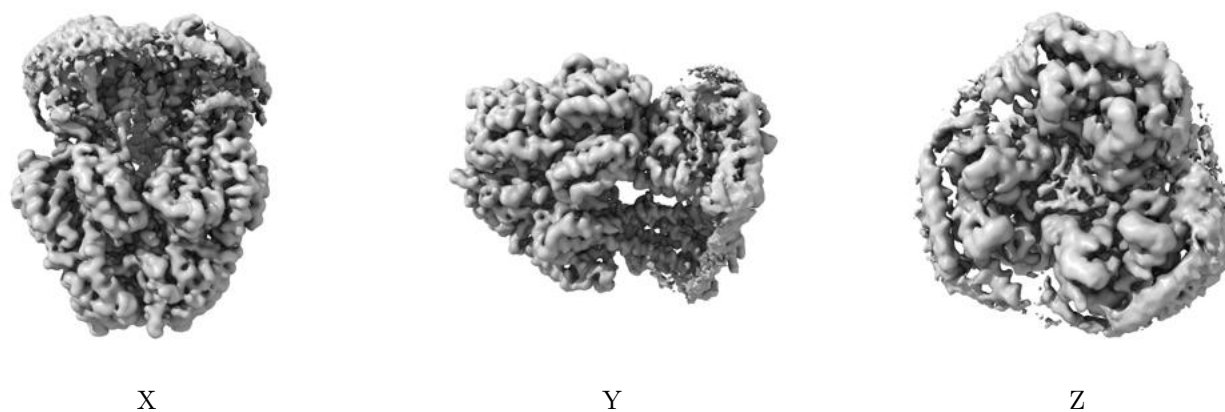
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

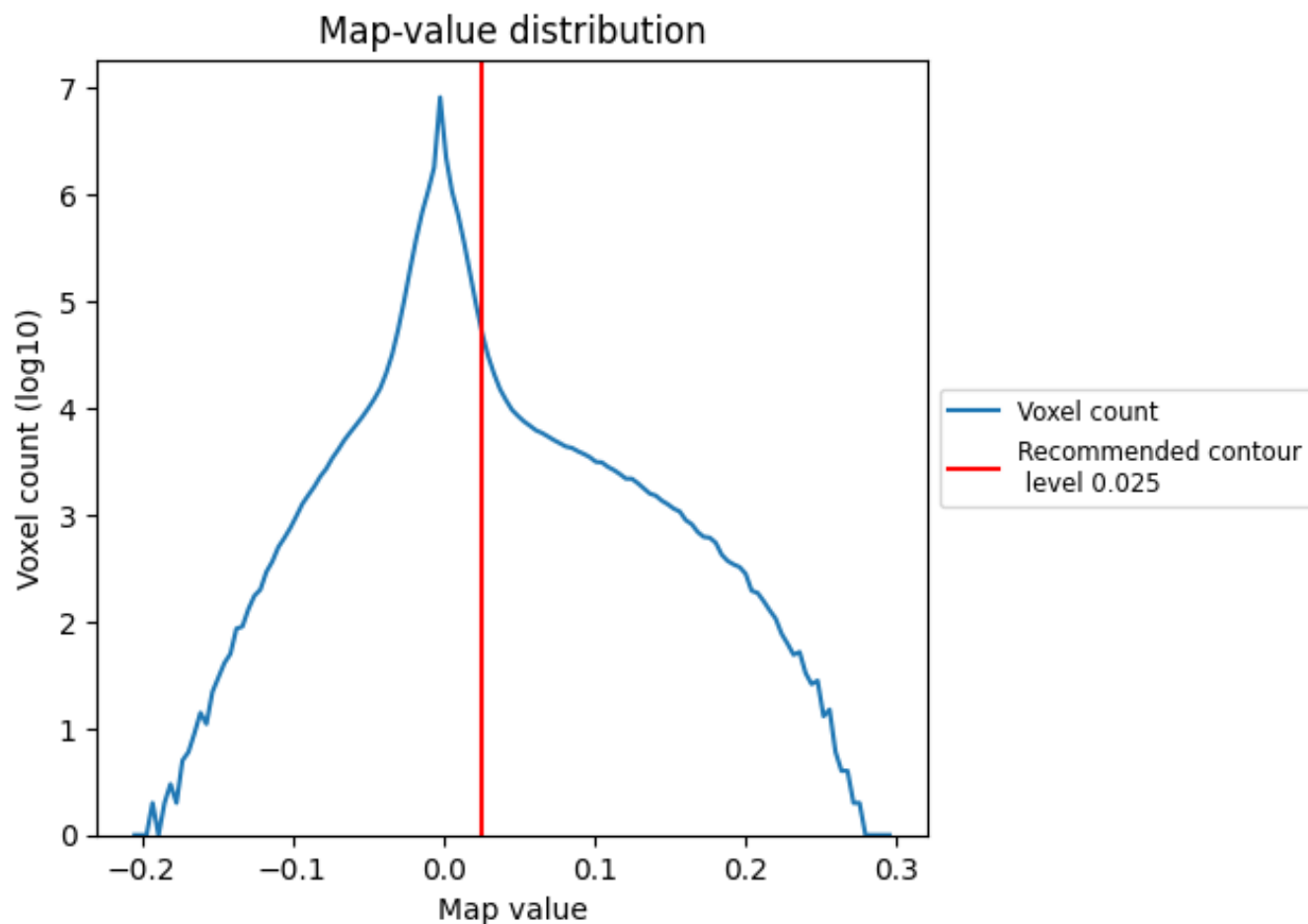
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

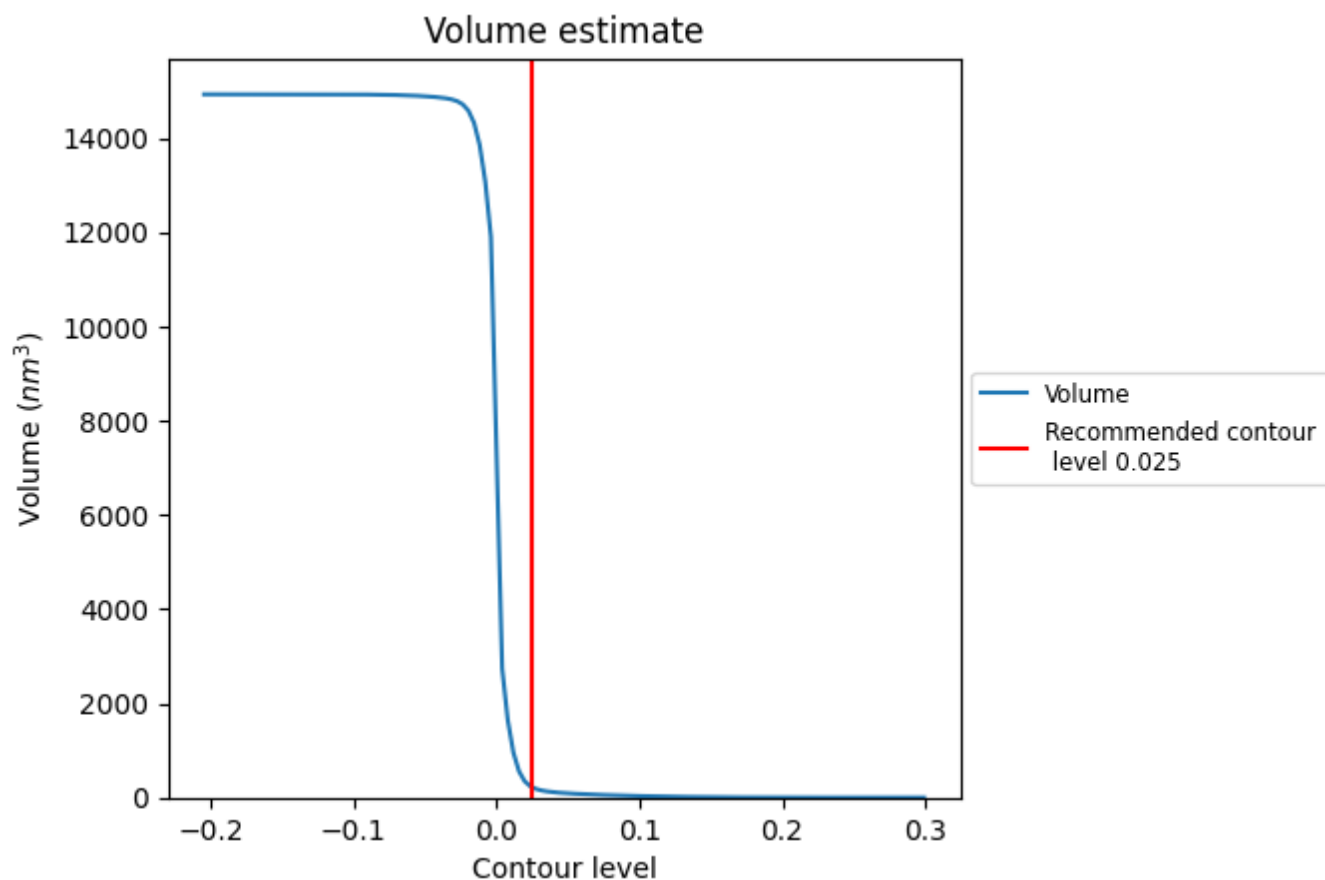
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

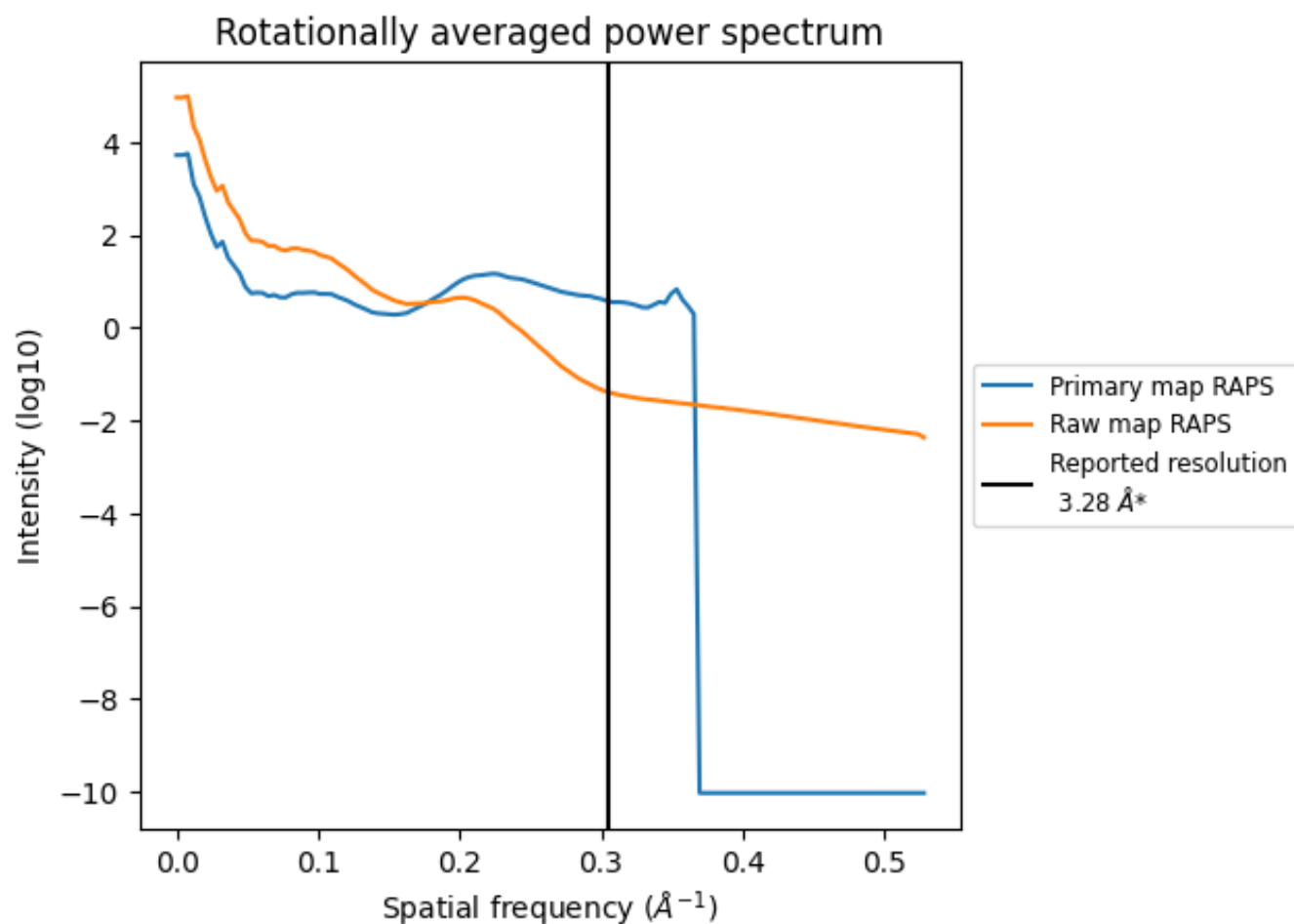
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 221 nm³; this corresponds to an approximate mass of 199 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

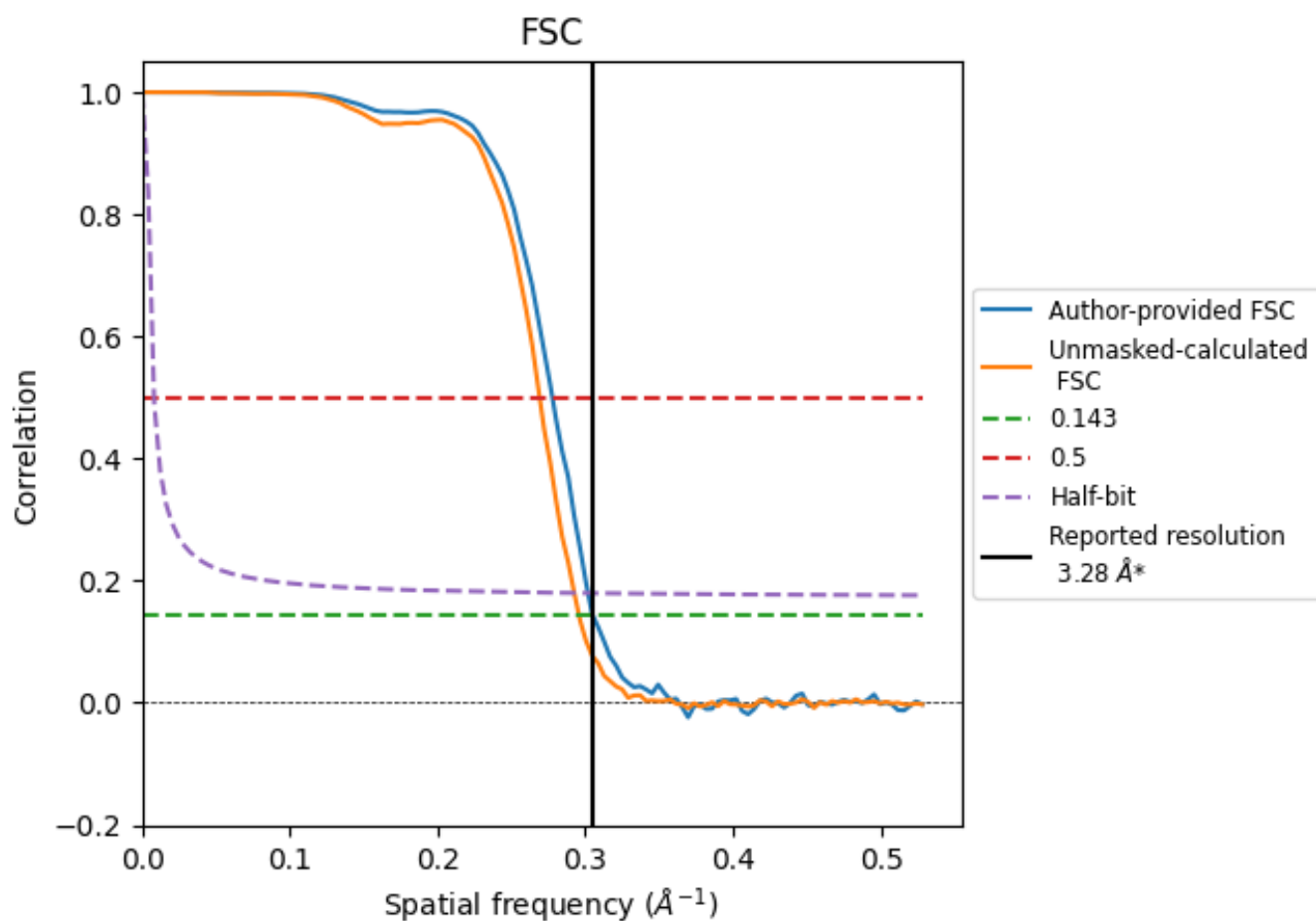


*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

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 0.305 \AA^{-1}

8.2 Resolution estimates [i](#)

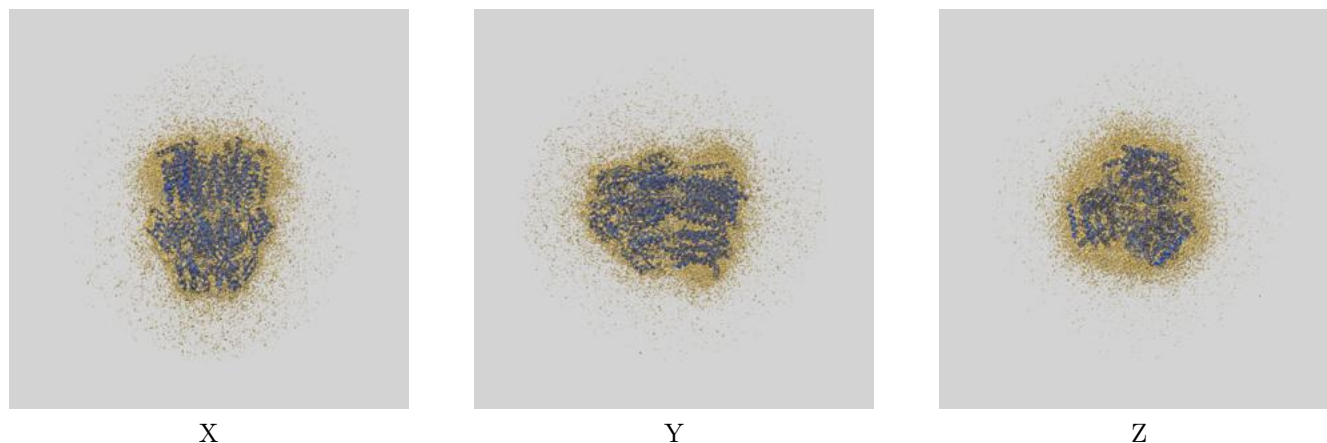
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.28	3.60	3.31
Unmasked-calculated*	3.38	3.72	3.42

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

9 Map-model fit [i](#)

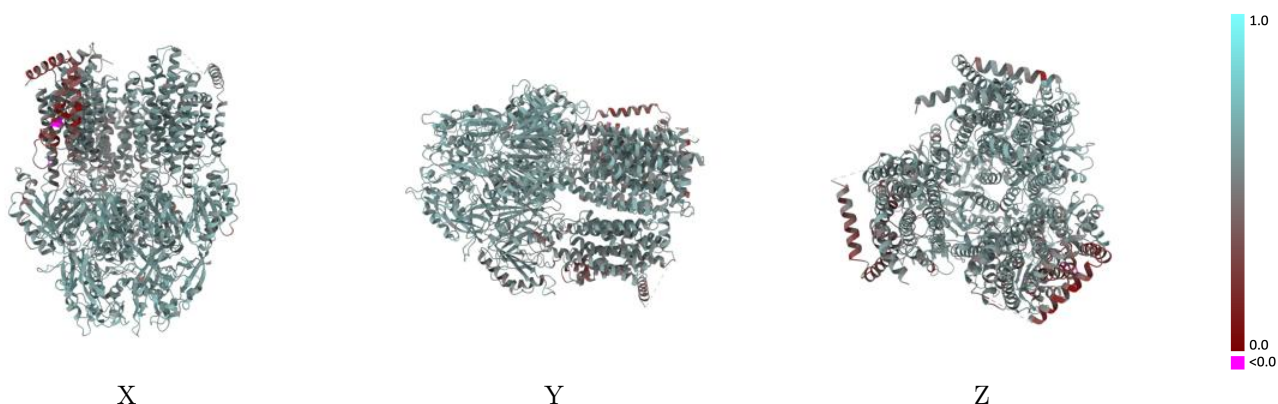
This section contains information regarding the fit between EMDB map EMD-53282 and PDB model 9QPS. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



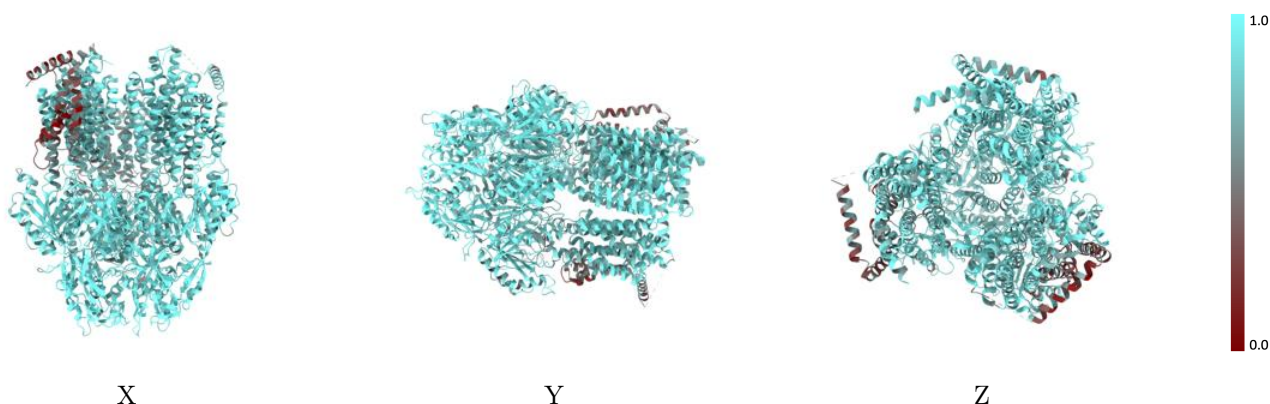
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



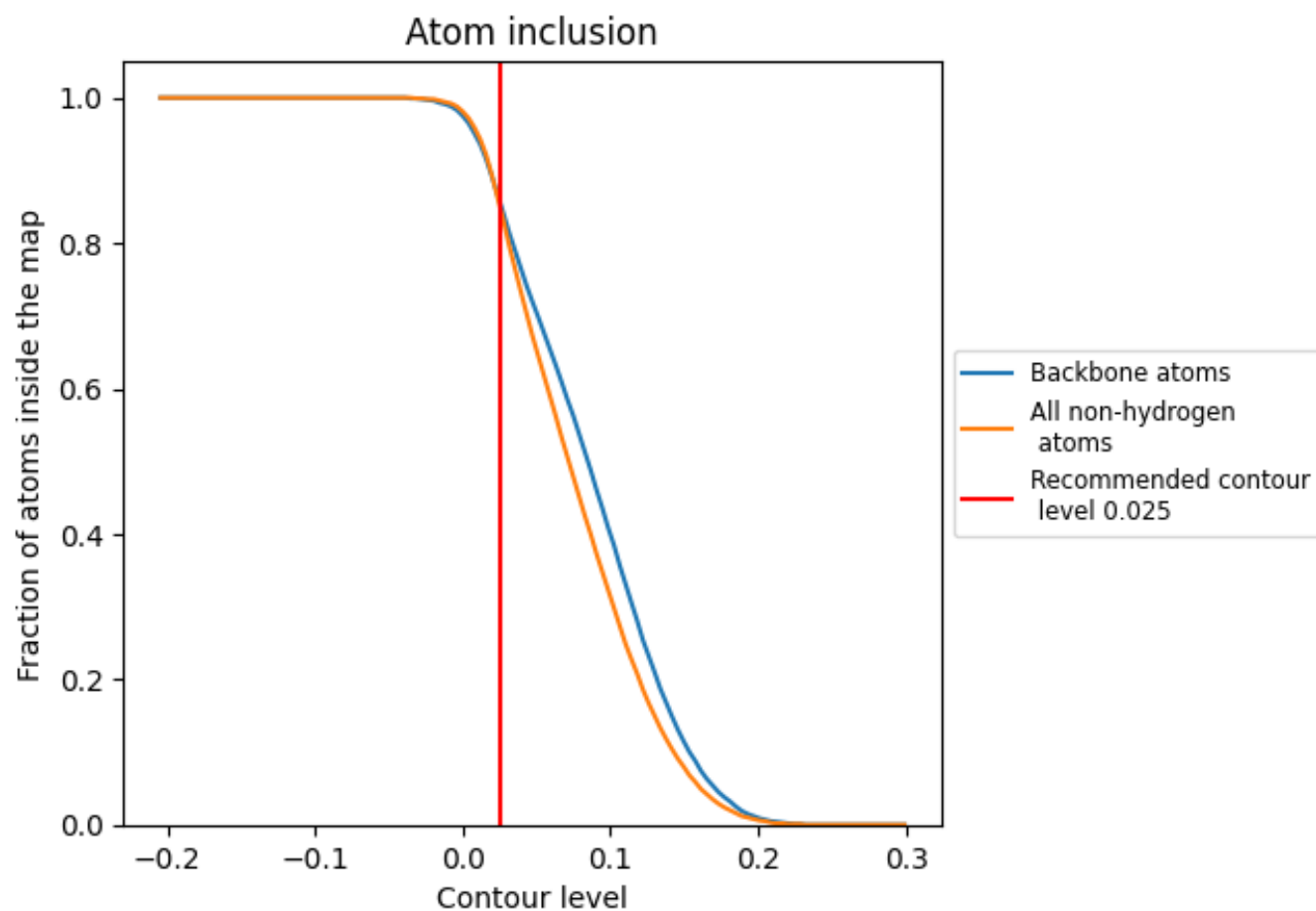
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8520	<div><div></div></div> 0.5540
A	<div><div></div></div> 0.9010	<div><div></div></div> 0.5810
B	<div><div></div></div> 0.8180	<div><div></div></div> 0.5330
C	<div><div></div></div> 0.8380	<div><div></div></div> 0.5460

