



Full wwPDB EM Validation Report ⓘ

Mar 4, 2024 – 08:31 AM EST

PDB ID : 6CSX
EMDB ID : EMD-7609
Title : Single particles Cryo-EM structure of AcrB D407A associated with lipid bilayer at 3.0 Angstrom
Authors : Qiu, W.; Fu, Z.; Guo, Y.
Deposited on : 2018-03-21
Resolution : 3.00 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.dev70
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 : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

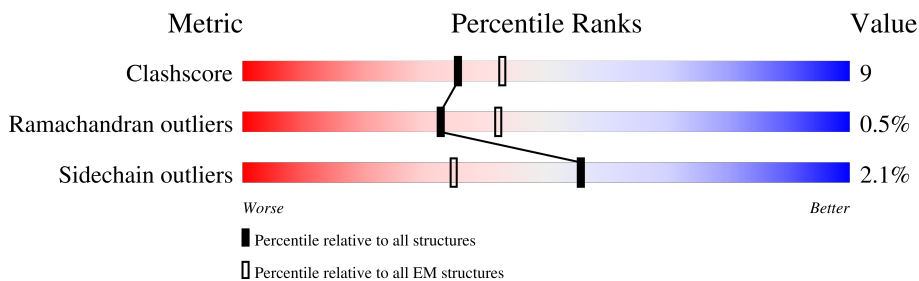
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	1057	
1	B	1057	
1	C	1057	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23232 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 efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	1019	7735	4979	1275	1437	44	0	0
1	C	1015	7685	4944	1269	1428	44	0	0
1	A	965	7305	4710	1194	1360	41	0	0

There are 27 discrepancies between the modelled and reference sequences:

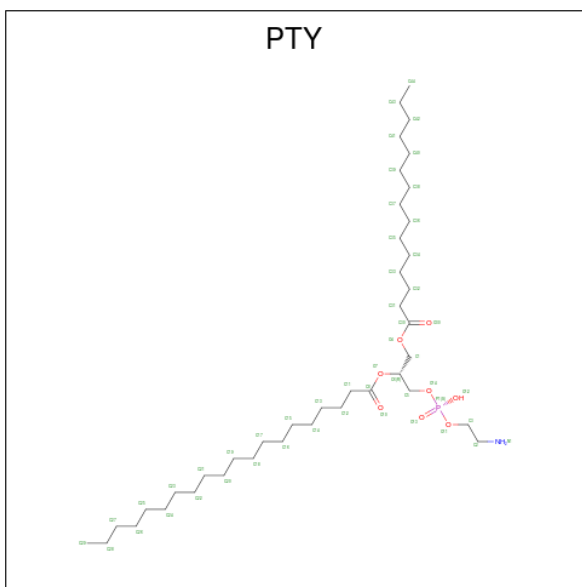
Chain	Residue	Modelled	Actual	Comment	Reference
B	407	ALA	ASP	engineered mutation	UNP P31224
B	1050	LEU	-	expression tag	UNP P31224
B	1051	GLU	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
B	1054	HIS	-	expression tag	UNP P31224
B	1055	HIS	-	expression tag	UNP P31224
B	1056	HIS	-	expression tag	UNP P31224
B	1057	HIS	-	expression tag	UNP P31224
C	407	ALA	ASP	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224
A	407	ALA	ASP	engineered mutation	UNP P31224
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C₄₀H₈₀NO₈P).



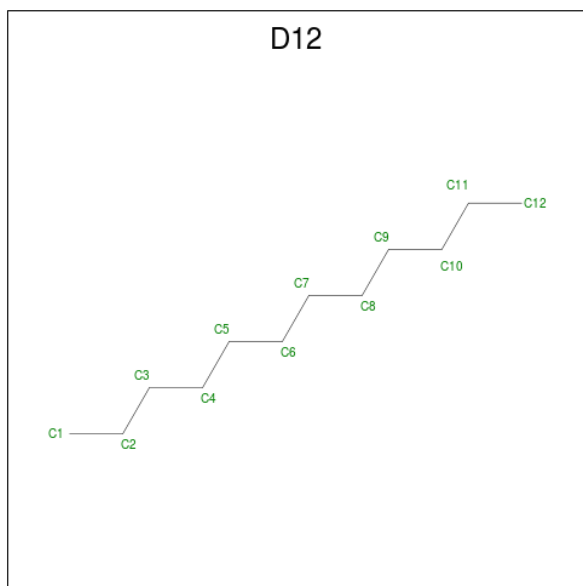
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	B	1	31	21	1	8	1	0
2	B	1	23	19		4		0
2	B	1	30	20	1	8	1	0
2	B	1	38	28	1	8	1	0
2	B	1	28	18	1	8	1	0
2	B	1	37	29	1	6	1	0
2	B	1	17	14		3		0
2	C	1	18	15		3		0
2	C	1	30	20	1	8	1	0

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Mol	Chain	Residues	Atoms	AltConf
2	C	1	Total C O 29 25 4	0
2	C	1	Total C N O P 34 24 1 8 1	0
2	A	1	Total C O P 28 19 8 1	0
2	A	1	Total C 20 20	0
2	A	1	Total C N O P 25 15 1 8 1	0
2	A	1	Total C N O P 32 23 1 7 1	0
2	A	1	Total C O 13 11 2	0
2	A	1	Total C O P 37 28 8 1	0
2	A	1	Total C N O P 25 15 1 8 1	0

- Molecule 3 is DODECANE (three-letter code: D12) (formula: C₁₂H₂₆).

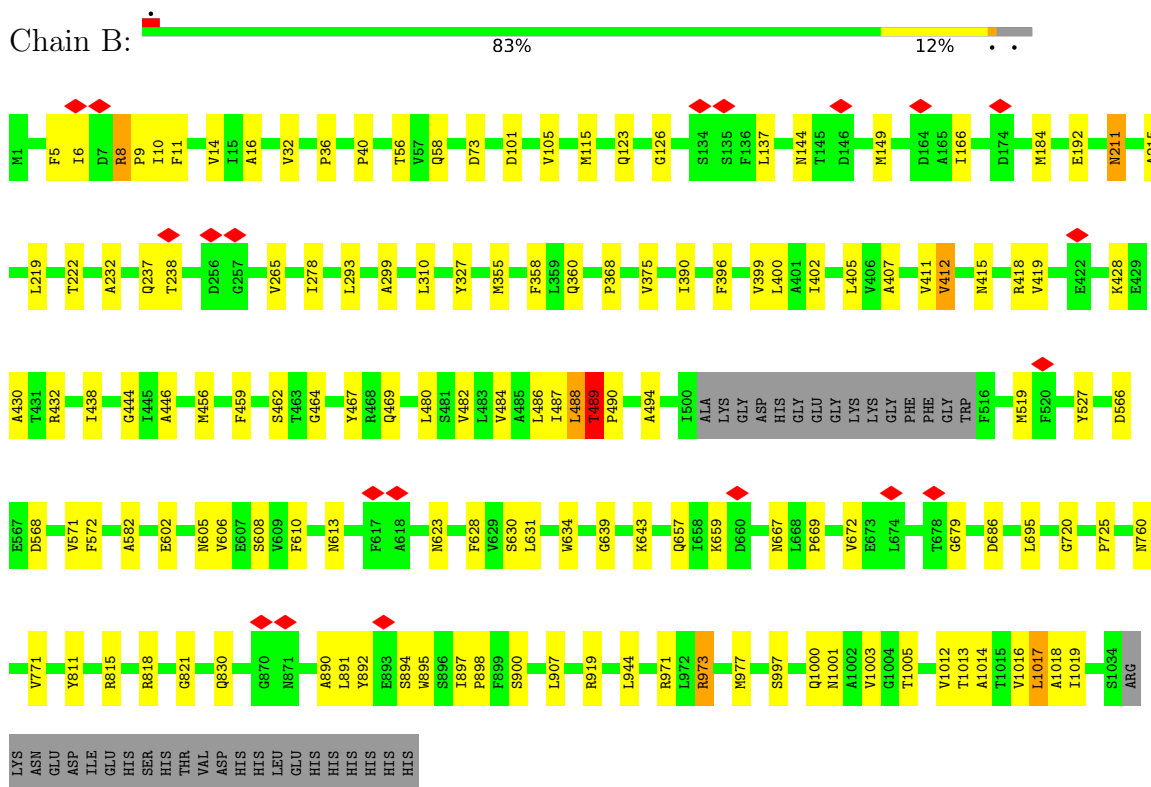


Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total C 12 12	0

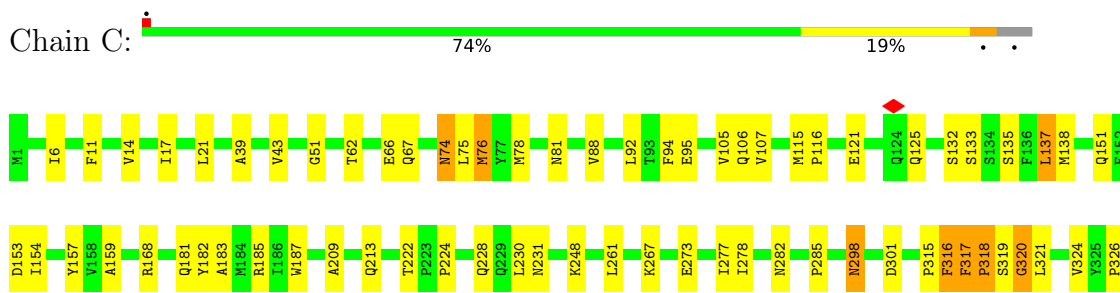
3 Residue-property plots

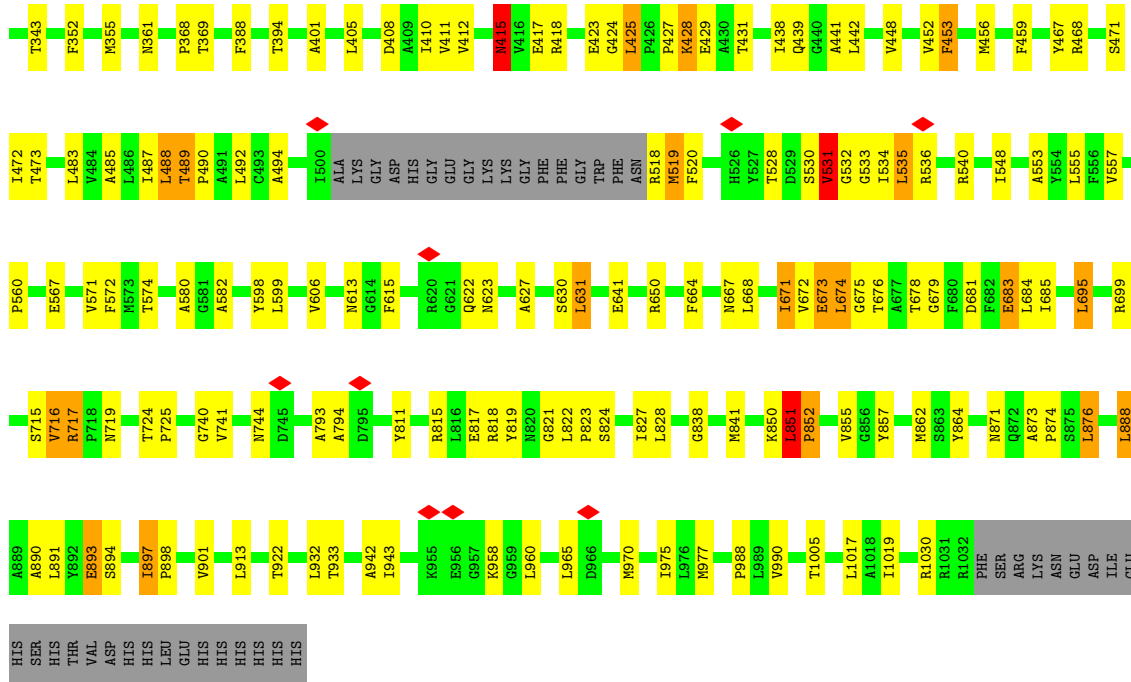
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

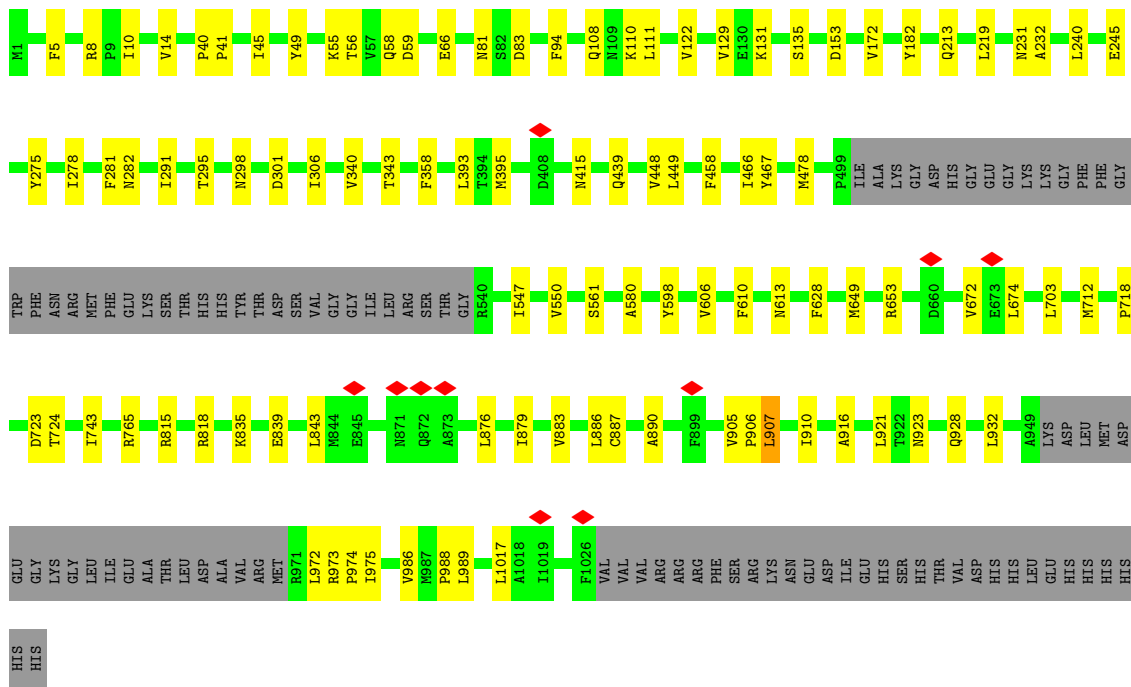
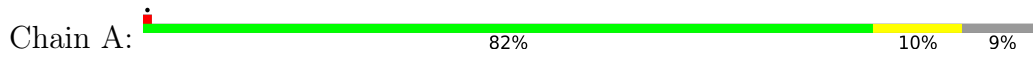


- Molecule 1: Multidrug efflux pump subunit AcrB





● Molecule 1: Multidrug efflux pump subunit AcrB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41190	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	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	0.165	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	273.28, 273.28, 273.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.854, 0.854, 0.854	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	0.40	0/7442	0.58	0/10118
1	B	0.38	0/7879	0.58	0/10703
1	C	0.42	0/7827	0.64	0/10636
All	All	0.40	0/23148	0.60	0/31457

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	7305	0	7459	74	0
1	B	7735	0	7899	126	0
1	C	7685	0	7842	214	0
2	A	180	0	210	12	0
2	B	204	0	245	10	0
2	C	111	0	134	5	0
3	B	12	0	26	0	0
All	All	23232	0	23815	404	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 (404) 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:C:317:PHE:CE2	1:C:321:LEU:HD23	1.61	1.32
1:C:452:VAL:O	1:C:453:PHE:CD2	1.82	1.31
1:C:317:PHE:CE2	1:C:321:LEU:CD2	2.23	1.21
1:C:317:PHE:CZ	1:C:321:LEU:CD2	2.29	1.14
1:C:531:VAL:HG23	1:C:965:LEU:CD2	1.83	1.07
1:A:907:LEU:CD2	1:A:1017:LEU:HB3	1.84	1.06
1:C:685:ILE:HG22	1:C:824:SER:HB3	1.15	1.05
1:C:531:VAL:HA	1:C:533:GLY:H	1.14	1.05
1:C:531:VAL:HB	1:C:532:GLY:HA2	1.28	1.05
1:B:5:PHE:CE2	1:B:487:ILE:HG23	1.91	1.04
1:A:439:GLN:HB3	2:A:1105:PTY:C8	1.86	1.03
1:B:894:SER:HB3	1:B:897:ILE:HG12	1.38	1.02
1:A:907:LEU:HD21	1:A:1017:LEU:HB3	1.06	1.02
1:B:407:ALA:O	1:B:411:VAL:HG23	1.62	1.00
1:B:411:VAL:HG13	1:B:971:ARG:HH12	1.23	0.99
1:C:532:GLY:HA3	1:C:535:LEU:HB2	1.43	0.99
1:C:315:PRO:HG2	1:C:316:PHE:CE1	1.99	0.98
1:C:317:PHE:CG	1:C:318:PRO:HD2	1.99	0.97
1:A:907:LEU:HD21	1:A:1017:LEU:CB	1.96	0.95
1:C:317:PHE:HE2	1:C:321:LEU:HD23	1.31	0.94
1:C:157:TYR:HE2	1:C:317:PHE:HE1	1.10	0.93
1:C:671:ILE:HD12	1:C:862:MET:SD	2.08	0.93
1:C:459:PHE:HE2	1:C:876:LEU:CD2	1.81	0.93
1:C:157:TYR:HE2	1:C:317:PHE:CE1	1.87	0.93
1:B:396:PHE:HA	1:B:399:VAL:HG22	1.51	0.92
1:B:10:ILE:HD12	1:C:893:GLU:O	1.69	0.91
1:C:456:MET:HB3	1:C:467:TYR:HB3	1.54	0.90
1:C:671:ILE:HB	1:C:674:LEU:HB2	1.55	0.89
1:C:452:VAL:O	1:C:453:PHE:HD2	1.27	0.88
1:B:1014:ALA:O	1:B:1018:ALA:HB3	1.73	0.88
1:C:157:TYR:CE2	1:C:317:PHE:CE1	2.61	0.88
1:C:317:PHE:CZ	1:C:321:LEU:HD22	2.06	0.88
1:C:317:PHE:CD1	1:C:318:PRO:HD2	2.10	0.87
1:C:532:GLY:CA	1:C:535:LEU:HB2	2.05	0.86
1:A:905:VAL:HG23	1:A:906:PRO:HD3	1.57	0.86
1:C:531:VAL:HG23	1:C:965:LEU:HD21	1.58	0.86
1:C:415:ASN:O	1:C:418:ARG:HG2	1.77	0.84
1:C:448:VAL:O	1:C:452:VAL:HG22	1.78	0.83
1:A:439:GLN:CB	2:A:1105:PTY:C8	2.56	0.82
1:C:685:ILE:CG2	1:C:824:SER:HB3	2.06	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:PHE:CE2	1:C:321:LEU:HD22	2.13	0.81
1:C:671:ILE:CD1	1:C:862:MET:SD	2.69	0.81
1:B:396:PHE:HA	1:B:399:VAL:CG2	2.10	0.80
1:C:137:LEU:O	1:C:137:LEU:HD22	1.82	0.79
1:C:157:TYR:CE2	1:C:317:PHE:HE1	1.98	0.78
1:B:897:ILE:N	1:B:898:PRO:CD	2.47	0.78
1:A:907:LEU:CD2	1:A:1017:LEU:CB	2.59	0.78
1:C:74:ASN:O	1:C:94:PHE:HD1	1.67	0.78
1:C:531:VAL:HB	1:C:532:GLY:CA	2.12	0.78
1:B:411:VAL:HG13	1:B:971:ARG:NH1	1.99	0.77
1:B:11:PHE:HD1	1:C:890:ALA:HB1	1.50	0.77
1:B:10:ILE:CD1	1:C:893:GLU:O	2.32	0.76
1:C:459:PHE:CE2	1:C:876:LEU:HG	2.19	0.76
1:C:531:VAL:CA	1:C:533:GLY:H	1.97	0.76
1:C:456:MET:HB3	1:C:467:TYR:CB	2.15	0.76
1:B:5:PHE:CZ	1:B:487:ILE:HG23	2.20	0.75
1:C:531:VAL:HA	1:C:533:GLY:N	1.97	0.75
1:B:400:LEU:HD21	1:B:1003:VAL:HG22	1.69	0.75
1:C:685:ILE:HD12	1:C:822:LEU:HD21	1.69	0.74
1:C:667:ASN:O	1:C:678:THR:HG22	1.88	0.74
1:A:972:LEU:HD13	1:A:972:LEU:O	1.87	0.74
1:C:213:GLN:HE21	1:A:56:THR:HG22	1.54	0.73
1:A:905:VAL:CG2	1:A:906:PRO:HD3	2.18	0.73
1:B:892:TYR:CB	1:B:897:ILE:HG21	2.18	0.72
1:C:685:ILE:HG22	1:C:824:SER:CB	2.09	0.72
1:B:407:ALA:O	1:B:411:VAL:CG2	2.38	0.72
1:B:8:ARG:HH12	2:B:1103:PTY:C30	2.03	0.72
1:B:399:VAL:O	1:B:402:ILE:HG13	1.89	0.72
1:B:412:VAL:CG2	1:B:438:ILE:HB	2.21	0.71
1:B:488:LEU:HD13	1:B:488:LEU:O	1.91	0.71
1:B:897:ILE:H	1:B:898:PRO:CD	2.03	0.71
1:C:459:PHE:CE2	1:C:876:LEU:CD2	2.70	0.71
1:C:319:SER:O	1:C:321:LEU:N	2.24	0.71
1:C:411:VAL:HB	1:C:442:LEU:HD21	1.71	0.71
1:C:459:PHE:CE2	1:C:876:LEU:HD23	2.26	0.71
1:C:683:GLU:HG2	1:C:824:SER:HB2	1.73	0.70
1:B:400:LEU:HD21	1:B:1003:VAL:CG2	2.21	0.70
1:B:489:THR:HB	1:B:490:PRO:HD3	1.72	0.70
1:C:851:LEU:HD22	1:C:852:PRO:HD3	1.72	0.70
1:C:467:TYR:O	1:C:471:SER:N	2.23	0.70
1:B:11:PHE:CD1	1:C:890:ALA:HB1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:GLU:OE1	1:C:417:GLU:HA	1.92	0.70
1:C:459:PHE:HE2	1:C:876:LEU:HD23	1.56	0.69
1:C:317:PHE:CD1	1:C:318:PRO:CD	2.76	0.69
1:B:1017:LEU:HD12	1:B:1017:LEU:C	2.14	0.69
1:B:892:TYR:CG	1:B:897:ILE:HG21	2.27	0.68
1:C:76:MET:SD	1:C:864:TYR:CE2	2.86	0.68
1:B:1012:VAL:O	1:B:1016:VAL:HG12	1.93	0.68
1:C:278:ILE:HG23	1:C:613:ASN:HB3	1.75	0.68
1:B:411:VAL:HG11	1:B:944:LEU:HD13	1.76	0.67
1:B:480:LEU:O	1:B:484:VAL:HG23	1.95	0.67
1:C:876:LEU:HD13	1:C:932:LEU:HD11	1.75	0.67
1:C:456:MET:CB	1:C:467:TYR:HB3	2.23	0.66
1:C:14:VAL:HG13	1:A:886:LEU:HB3	1.77	0.66
1:C:412:VAL:HG11	1:C:489:THR:HB	1.77	0.66
1:C:459:PHE:HE2	1:C:876:LEU:CG	2.09	0.65
1:C:452:VAL:O	1:C:453:PHE:CG	2.47	0.65
1:C:78:MET:HG2	1:C:92:LEU:HD13	1.79	0.65
1:A:343:THR:HG23	1:A:988:PRO:HB2	1.77	0.64
1:C:851:LEU:HB3	1:C:852:PRO:CD	2.27	0.64
1:B:1014:ALA:O	1:B:1018:ALA:CB	2.46	0.64
1:C:423:GLU:O	1:C:423:GLU:HG2	1.96	0.64
1:B:6:ILE:HG13	1:B:432:ARG:HH11	1.61	0.64
1:C:684:LEU:HD12	1:C:695:LEU:HD21	1.80	0.64
1:C:531:VAL:CB	1:C:532:GLY:HA2	2.15	0.63
1:C:66:GLU:OE1	1:C:818:ARG:NH1	2.32	0.63
1:A:58:GLN:HE21	1:A:818:ARG:HD2	1.64	0.63
1:B:58:GLN:HE21	1:B:818:ARG:HD2	1.64	0.62
1:C:415:ASN:CG	1:C:438:ILE:HD13	2.20	0.62
1:C:415:ASN:OD1	1:C:438:ILE:CD1	2.46	0.62
1:B:484:VAL:HG12	1:B:484:VAL:O	1.99	0.61
1:B:892:TYR:CD2	1:B:897:ILE:HG22	2.36	0.61
1:B:1017:LEU:HD12	1:B:1017:LEU:O	2.01	0.61
1:C:459:PHE:CE2	1:C:876:LEU:CG	2.83	0.61
1:C:667:ASN:O	1:C:678:THR:CG2	2.49	0.60
1:C:685:ILE:HD12	1:C:822:LEU:CD2	2.30	0.60
1:C:716:VAL:HG12	1:C:717:ARG:N	2.15	0.60
1:A:649:MET:SD	1:A:653:ARG:NH1	2.75	0.60
1:C:74:ASN:O	1:C:94:PHE:CD1	2.54	0.60
1:C:317:PHE:CG	1:C:318:PRO:CD	2.81	0.60
1:C:855:VAL:HG12	1:C:855:VAL:O	2.01	0.60
1:B:894:SER:CB	1:B:897:ILE:HG12	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:873:ALA:N	1:C:874:PRO:HD2	2.17	0.60
1:C:319:SER:OG	1:C:320:GLY:N	2.35	0.59
1:C:452:VAL:O	1:C:452:VAL:HG23	2.00	0.59
1:A:973:ARG:N	1:A:974:PRO:CD	2.64	0.59
1:B:890:ALA:HB2	1:A:14:VAL:HG21	1.85	0.59
1:C:248:LYS:HA	1:C:261:LEU:HD23	1.85	0.59
1:C:571:VAL:HG23	1:C:630:SER:HA	1.83	0.59
1:C:675:GLY:HA3	1:C:862:MET:HG2	1.83	0.59
1:B:375:VAL:HG22	1:B:484:VAL:HG21	1.85	0.59
1:B:489:THR:CB	1:B:490:PRO:HD3	2.32	0.59
1:B:907:LEU:HD22	1:B:1017:LEU:HD11	1.83	0.59
1:C:317:PHE:CZ	1:C:321:LEU:HD21	2.35	0.59
1:B:897:ILE:H	1:B:898:PRO:HD3	1.67	0.58
1:B:8:ARG:NH1	2:B:1103:PTY:C30	2.65	0.58
1:C:326:PRO:O	1:C:630:SER:HB3	2.02	0.58
1:C:897:ILE:HB	1:C:898:PRO:HD3	1.85	0.58
1:C:74:ASN:HB3	1:C:95:GLU:HG2	1.86	0.58
1:A:975:ILE:HD12	1:A:975:ILE:H	1.69	0.57
1:C:572:PHE:HE1	1:C:631:LEU:HD11	1.70	0.57
1:B:115:MET:O	1:B:123:GLN:NE2	2.38	0.57
1:C:43:VAL:HG11	1:C:107:VAL:HG11	1.85	0.57
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.86	0.57
1:C:6:ILE:HG22	1:C:428:LYS:HD3	1.86	0.57
1:B:602:GLU:OE2	1:B:605:ASN:ND2	2.38	0.57
1:B:184:MET:HB3	1:B:771:VAL:HG22	1.86	0.57
1:B:222:THR:OG1	1:C:622:GLN:NE2	2.37	0.57
1:B:360:GLN:NE2	1:B:519:MET:SD	2.77	0.57
1:C:187:TRP:HB2	1:C:267:LYS:HB2	1.85	0.56
1:C:567:GLU:O	1:C:667:ASN:ND2	2.35	0.56
1:B:610:PHE:HB3	1:B:628:PHE:HB2	1.86	0.56
1:C:316:PHE:CD1	1:C:316:PHE:N	2.73	0.56
1:B:412:VAL:HG23	1:B:438:ILE:HG21	1.87	0.56
1:C:815:ARG:NH1	1:C:817:GLU:OE2	2.38	0.56
1:B:411:VAL:CG1	1:B:971:ARG:HH12	2.07	0.56
1:A:835:LYS:HB2	1:A:839:GLU:HG3	1.87	0.56
1:C:76:MET:CE	1:C:864:TYR:HE2	2.18	0.56
1:C:553:ALA:O	1:C:557:VAL:HG23	2.06	0.56
1:B:897:ILE:N	1:B:898:PRO:HD2	2.21	0.56
1:B:215:ALA:HA	1:C:51:GLY:HA3	1.87	0.55
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.88	0.55
1:A:8:ARG:NH2	2:A:1101:PTY:O11	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ASP:OD1	1:C:182:TYR:OH	2.24	0.55
1:B:211:ASN:HB3	1:B:760:ASN:HD21	1.70	0.55
1:C:684:LEU:HD12	1:C:684:LEU:O	2.07	0.55
1:B:412:VAL:CG2	1:B:438:ILE:CB	2.84	0.54
1:B:919:ARG:NH1	1:B:1005:THR:OG1	2.39	0.54
1:C:719:ASN:HB2	1:C:828:LEU:HD23	1.89	0.54
1:A:467:TYR:OH	1:A:928:GLN:OE1	2.25	0.54
1:C:209:ALA:HB1	1:A:743:ILE:HD11	1.89	0.54
1:B:16:ALA:HB2	1:B:488:LEU:HG	1.90	0.54
1:B:166:ILE:HD11	1:B:310:LEU:HD21	1.88	0.54
1:B:237:GLN:NE2	1:B:238:THR:O	2.36	0.54
1:C:671:ILE:HD11	1:C:862:MET:SD	2.47	0.54
1:A:458:PHE:HE1	2:A:1106:PTY:H112	1.73	0.54
1:A:153:ASP:OD1	1:A:182:TYR:OH	2.26	0.54
1:A:561:SER:HA	1:A:923:ASN:HB3	1.89	0.53
1:B:144:ASN:ND2	1:B:149:MET:O	2.41	0.53
1:A:975:ILE:HD12	1:A:975:ILE:N	2.23	0.53
1:B:412:VAL:HA	1:B:415:ASN:HB3	1.91	0.53
1:C:685:ILE:HG21	1:C:819:TYR:HB3	1.89	0.53
1:C:394:THR:HG23	1:C:473:THR:HG21	1.91	0.53
1:C:428:LYS:HG2	1:C:494:ALA:HB1	1.89	0.53
1:C:121:GLU:O	1:C:125:GLN:NE2	2.43	0.52
1:B:105:VAL:HG21	1:C:105:VAL:HB	1.91	0.52
1:C:425:LEU:HD23	1:C:429:GLU:HB3	1.91	0.52
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.92	0.52
1:C:415:ASN:ND2	1:C:438:ILE:HD13	2.25	0.52
1:C:894:SER:HB2	1:C:897:ILE:HG12	1.91	0.52
1:C:62:THR:HG22	1:C:88:VAL:HG21	1.92	0.52
1:C:14:VAL:HA	1:C:17:ILE:HG22	1.91	0.52
1:A:298:ASN:HB3	1:A:301:ASP:HB2	1.91	0.52
1:C:315:PRO:HG2	1:C:316:PHE:CD1	2.44	0.52
1:A:449:LEU:HB3	1:A:478:MET:HE1	1.92	0.52
1:C:818:ARG:NH2	1:C:821:GLY:O	2.42	0.51
1:B:56:THR:HG23	1:A:213:GLN:HG3	1.93	0.51
1:B:639:GLY:O	1:B:643:LYS:NZ	2.42	0.51
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.93	0.51
1:A:41:PRO:HB3	1:A:295:THR:HG21	1.93	0.51
1:B:396:PHE:CA	1:B:399:VAL:HG22	2.34	0.51
1:C:318:PRO:HG2	1:C:321:LEU:HD13	1.91	0.51
1:B:606:VAL:HA	1:B:631:LEU:HA	1.92	0.51
1:B:375:VAL:CG1	1:B:405:LEU:HD21	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:TYR:CD2	1:B:897:ILE:CG2	2.94	0.51
1:C:453:PHE:HZ	1:C:933:THR:HB	1.75	0.51
1:C:423:GLU:HG2	1:C:425:LEU:HD12	1.93	0.51
1:A:610:PHE:HB3	1:A:628:PHE:HB2	1.93	0.50
2:B:1103:PTY:H112	2:B:1103:PTY:H321	1.93	0.50
1:C:78:MET:HG2	1:C:92:LEU:CD1	2.39	0.50
1:B:1013:THR:O	1:B:1017:LEU:HG	2.12	0.50
1:C:277:ILE:HD12	1:C:615:PHE:HB2	1.94	0.50
1:C:818:ARG:HA	1:C:823:PRO:HA	1.93	0.50
1:C:684:LEU:HA	1:C:857:TYR:HA	1.94	0.50
1:C:168:ARG:NH2	1:A:66:GLU:O	2.45	0.50
1:C:159:ALA:HB3	1:C:181:GLN:HB3	1.93	0.49
1:C:151:GLN:HA	1:C:154:ILE:HG22	1.93	0.49
1:C:678:THR:OG1	1:C:679:GLY:N	2.45	0.49
1:B:412:VAL:HG21	1:B:438:ILE:HB	1.95	0.49
2:A:1103:PTY:H131	2:A:1105:PTY:H151	1.93	0.49
1:B:411:VAL:HG11	1:B:944:LEU:CD1	2.40	0.49
1:B:895:TRP:NE1	1:A:10:ILE:HG22	2.28	0.49
2:B:1104:PTY:H152	2:C:1102:PTY:H121	1.95	0.49
2:C:1103:PTY:H161	2:A:1106:PTY:H332	1.94	0.49
1:A:135:SER:OG	1:A:672:VAL:O	2.29	0.49
2:B:1102:PTY:H332	2:B:1104:PTY:H391	1.94	0.49
1:C:441:ALA:O	1:C:442:LEU:HB2	2.12	0.49
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.95	0.49
1:B:73:ASP:OD2	1:A:131:LYS:NZ	2.46	0.49
1:B:415:ASN:OD1	1:B:418:ARG:NH1	2.46	0.49
1:A:547:ILE:HA	1:A:550:VAL:HG12	1.95	0.49
1:C:415:ASN:OD1	1:C:438:ILE:HD12	2.11	0.49
1:C:641:GLU:OE2	1:C:650:ARG:NH2	2.46	0.48
1:B:358:PHE:CD2	1:B:977:MET:HG2	2.48	0.48
1:C:151:GLN:HG3	1:C:285:PRO:HB3	1.95	0.48
1:C:418:ARG:NH2	1:C:970:MET:O	2.45	0.48
1:C:560:PRO:HG2	1:C:922:THR:HG22	1.95	0.48
2:C:1103:PTY:H381	1:A:883:VAL:HG11	1.95	0.48
1:B:137:LEU:HD22	1:B:293:LEU:HD23	1.95	0.48
1:C:681:ASP:OD1	1:C:681:ASP:N	2.47	0.48
1:B:566:ASP:OD1	1:B:667:ASN:ND2	2.47	0.48
1:B:892:TYR:CG	1:B:897:ILE:CG2	2.95	0.48
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.94	0.48
1:B:14:VAL:HG21	1:C:890:ALA:HB2	1.96	0.48
2:B:1104:PTY:H122	2:C:1102:PTY:HC6	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:MET:HB3	1:C:467:TYR:CG	2.49	0.48
1:A:986:VAL:HG23	1:A:989:LEU:HD12	1.96	0.48
1:B:36:PRO:HG3	1:B:469:GLN:HG3	1.95	0.48
1:B:568:ASP:OD2	1:B:634:TRP:NE1	2.41	0.48
1:C:489:THR:OG1	1:C:490:PRO:CD	2.62	0.48
1:B:582:ALA:HB3	1:B:623:ASN:HB3	1.96	0.47
1:C:488:LEU:O	1:C:488:LEU:HD22	2.14	0.47
1:C:671:ILE:HD13	1:C:674:LEU:HD12	1.96	0.47
1:A:598:TYR:HB3	1:A:606:VAL:HG11	1.96	0.47
1:A:712:MET:HG2	1:A:843:LEU:HD22	1.96	0.47
1:B:657:GLN:O	1:B:659:LYS:NZ	2.43	0.47
1:B:892:TYR:HB3	1:B:897:ILE:HG21	1.96	0.47
1:C:531:VAL:HG23	1:C:965:LEU:HD22	1.87	0.47
1:B:527:TYR:OH	1:B:1019:ILE:O	2.26	0.47
1:C:183:ALA:HB2	1:C:273:GLU:HG2	1.95	0.47
1:A:703:LEU:HD11	1:A:718:PRO:HG3	1.97	0.47
1:C:685:ILE:CG2	1:C:819:TYR:HB3	2.45	0.47
1:C:324:VAL:HG12	1:C:326:PRO:HG3	1.97	0.47
1:C:876:LEU:O	1:C:876:LEU:HD22	2.15	0.47
1:A:972:LEU:HA	1:A:975:ILE:HD13	1.97	0.47
1:B:669:PRO:HG2	1:B:672:VAL:HA	1.97	0.47
1:C:699:ARG:HG2	1:C:827:ILE:HD11	1.96	0.47
1:C:888:LEU:HD12	1:C:888:LEU:HA	1.77	0.47
1:A:973:ARG:N	1:A:974:PRO:HD2	2.29	0.47
1:B:608:SER:OG	1:B:630:SER:OG	2.32	0.47
2:C:1104:PTY:H331	2:C:1104:PTY:H362	1.72	0.47
1:C:282:ASN:HD22	1:C:599:LEU:HD11	1.81	0.46
1:B:126:GLY:HA3	1:C:116:PRO:HG3	1.96	0.46
1:B:489:THR:H	1:B:490:PRO:CD	2.29	0.46
1:C:425:LEU:CD2	1:C:429:GLU:HB3	2.45	0.46
1:C:838:GLY:HA2	1:C:841:MET:HG2	1.96	0.46
1:C:81:ASN:HD22	1:C:815:ARG:HH21	1.62	0.46
1:C:897:ILE:HG22	1:C:898:PRO:N	2.30	0.46
1:A:358:PHE:HD1	1:A:973:ARG:HD2	1.80	0.46
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.97	0.46
1:C:684:LEU:CD1	1:C:695:LEU:HD21	2.46	0.46
1:C:408:ASP:HB3	1:C:485:ALA:HB2	1.97	0.46
2:B:1103:PTY:H351	1:C:890:ALA:O	2.16	0.45
1:B:219:LEU:HD12	1:B:232:ALA:HB3	1.97	0.45
1:B:459:PHE:O	1:B:464:GLY:HA3	2.16	0.45
1:A:281:PHE:O	1:A:282:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:PHE:HD1	1:A:890:ALA:HB1	1.82	0.45
1:B:327:TYR:HD1	1:B:571:VAL:HG11	1.82	0.45
1:B:375:VAL:HG11	1:B:405:LEU:HD21	1.99	0.45
1:C:355:MET:HG2	1:C:368:PRO:HG2	1.98	0.45
1:C:483:LEU:O	1:C:487:ILE:HB	2.17	0.45
1:B:444:GLY:HA3	1:B:891:LEU:HD12	1.99	0.45
1:A:278:ILE:O	1:A:613:ASN:N	2.47	0.45
2:A:1105:PTY:H111	2:A:1105:PTY:H142	1.76	0.45
1:B:32:VAL:HG22	1:B:390:ILE:HB	1.99	0.45
1:C:675:GLY:HA3	1:C:862:MET:CG	2.45	0.45
1:C:897:ILE:HD13	1:C:897:ILE:HA	1.73	0.45
1:C:415:ASN:CG	1:C:438:ILE:CD1	2.85	0.45
1:C:427:PRO:O	1:C:431:THR:OG1	2.22	0.45
1:C:715:SER:O	1:C:715:SER:OG	2.28	0.45
1:B:32:VAL:O	1:B:299:ALA:N	2.43	0.45
1:C:901:VAL:HG11	1:C:943:ILE:HD11	1.99	0.45
1:B:818:ARG:NH2	1:B:821:GLY:O	2.43	0.44
1:C:574:THR:HB	1:C:627:ALA:HB3	1.99	0.44
1:C:671:ILE:O	1:C:674:LEU:N	2.42	0.44
1:C:695:LEU:O	1:C:695:LEU:HD22	2.17	0.44
1:A:81:ASN:HD22	1:A:815:ARG:HH22	1.65	0.44
1:A:916:ALA:HA	1:A:921:LEU:HD12	2.00	0.44
1:B:278:ILE:HG23	1:B:613:ASN:HB3	1.98	0.44
1:C:222:THR:HA	1:C:224:PRO:HD3	2.00	0.44
1:A:580:ALA:HB1	1:A:724:THR:HG22	1.98	0.44
1:C:531:VAL:HG23	1:C:965:LEU:HD23	1.85	0.44
1:B:895:TRP:NE1	1:A:10:ILE:CG2	2.80	0.44
1:C:317:PHE:CZ	1:C:321:LEU:HD23	2.09	0.44
1:C:532:GLY:HA2	1:C:535:LEU:HB2	1.97	0.44
1:A:723:ASP:OD1	1:A:723:ASP:N	2.48	0.44
2:A:1103:PTY:H111	2:A:1103:PTY:HC6	1.79	0.44
1:B:572:PHE:HE1	1:B:631:LEU:HD21	1.82	0.44
1:B:419:VAL:HG23	1:B:430:ALA:HB1	2.00	0.44
2:B:1101:PTY:H342	2:A:1101:PTY:H122	2.00	0.44
1:A:41:PRO:HG2	1:A:94:PHE:HB2	2.00	0.44
1:C:519:MET:SD	1:C:520:PHE:N	2.89	0.43
1:A:876:LEU:HD21	1:A:932:LEU:HD11	2.00	0.43
2:A:1107:PTY:H111	2:A:1107:PTY:H332	1.99	0.43
1:B:412:VAL:HG23	1:B:438:ILE:HG13	2.01	0.43
1:B:396:PHE:O	1:B:399:VAL:HG23	2.18	0.43
1:C:352:PHE:HD1	1:C:369:THR:HG21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:ALA:O	1:C:405:LEU:N	2.49	0.43
1:A:55:LYS:NZ	1:A:59:ASP:OD2	2.48	0.43
1:B:686:ASP:HB3	1:B:695:LEU:HD13	1.99	0.43
1:C:137:LEU:O	1:C:138:MET:HB3	2.17	0.43
1:C:671:ILE:H	1:C:671:ILE:HG13	1.60	0.43
1:B:412:VAL:HG23	1:B:438:ILE:CB	2.49	0.43
1:C:78:MET:HE3	1:C:92:LEU:HD11	2.01	0.43
1:B:1000:GLN:HA	1:B:1003:VAL:HG12	2.00	0.43
1:C:664:PHE:CE1	1:C:715:SER:HB2	2.54	0.43
1:C:535:LEU:O	1:C:536:ARG:C	2.55	0.43
1:C:548:ILE:HD13	1:C:1017:LEU:HD21	2.00	0.43
1:B:489:THR:N	1:B:490:PRO:CD	2.81	0.42
1:C:528:THR:C	1:C:530:SER:H	2.23	0.42
1:C:674:LEU:HD23	1:C:674:LEU:HA	1.76	0.42
1:C:185:ARG:HA	1:C:185:ARG:HD3	1.84	0.42
1:C:532:GLY:C	1:C:534:ILE:N	2.73	0.42
1:A:975:ILE:H	1:A:975:ILE:CD1	2.30	0.42
1:C:298:ASN:HB3	1:C:301:ASP:HB2	2.01	0.42
1:C:851:LEU:CB	1:C:852:PRO:CD	2.97	0.42
1:C:975:ILE:HG21	1:C:1019:ILE:HD12	2.00	0.42
1:C:990:VAL:HG13	1:C:1005:THR:HG22	2.02	0.42
1:A:108:GLN:HA	1:A:111:LEU:HB3	1.99	0.42
1:A:393:LEU:HD11	1:A:466:ILE:HG23	2.01	0.42
1:B:101:ASP:OD2	1:C:106:GLN:NE2	2.52	0.42
1:C:39:ALA:CB	1:C:673:GLU:OE1	2.67	0.42
1:A:45:ILE:HG12	1:A:129:VAL:HG22	2.01	0.42
1:B:355:MET:SD	1:B:368:PRO:HG2	2.60	0.42
1:C:468:ARG:HA	1:C:471:SER:OG	2.20	0.42
1:C:725:PRO:HG3	1:C:811:TYR:HE1	1.84	0.42
1:C:897:ILE:CB	1:C:898:PRO:HD3	2.48	0.42
1:B:489:THR:H	1:B:490:PRO:HD2	1.85	0.42
1:C:555:LEU:HB3	1:C:913:LEU:HD13	2.01	0.42
1:C:132:SER:OG	1:C:133:SER:N	2.53	0.42
1:C:683:GLU:HG2	1:C:824:SER:CB	2.46	0.42
2:B:1104:PTY:H112	2:B:1104:PTY:H321	2.01	0.42
1:C:388:PHE:HE2	1:C:472:ILE:HG13	1.85	0.42
1:C:582:ALA:HB3	1:C:623:ASN:HB3	2.02	0.42
1:C:228:GLN:HE21	1:C:230:LEU:HB3	1.84	0.42
1:C:488:LEU:HD22	1:C:492:LEU:HG	2.02	0.42
1:C:851:LEU:HD23	1:C:851:LEU:HA	1.77	0.42
1:B:428:LYS:HG2	1:B:494:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:VAL:HG13	1:B:480:LEU:HB2	2.02	0.41
1:C:598:TYR:HB3	1:C:606:VAL:HG11	2.02	0.41
1:C:685:ILE:HD12	1:C:822:LEU:CG	2.50	0.41
1:A:907:LEU:O	1:A:910:ILE:HG22	2.19	0.41
1:B:8:ARG:NH1	2:B:1103:PTY:O30	2.52	0.41
1:B:192:GLU:HB3	1:B:265:VAL:HG12	2.02	0.41
1:B:720:GLY:HA2	1:B:815:ARG:HH21	1.86	0.41
1:B:725:PRO:HG3	1:B:811:TYR:HE1	1.85	0.41
1:A:291:ILE:HD13	1:A:306:ILE:HD13	2.03	0.41
1:B:456:MET:HG2	1:B:467:TYR:HB3	2.02	0.41
1:A:40:PRO:HD2	1:A:674:LEU:HD21	2.03	0.41
1:B:973:ARG:O	1:B:977:MET:HG3	2.20	0.41
1:C:960:LEU:HD21	1:C:1030:ARG:HG2	2.01	0.41
1:B:679:GLY:HA2	1:B:830:GLN:HA	2.01	0.41
1:B:9:PRO:HD2	1:C:893:GLU:OE2	2.20	0.41
1:C:185:ARG:NH2	1:C:273:GLU:O	2.53	0.41
1:C:410:ILE:HG21	1:C:977:MET:HB3	2.02	0.41
1:B:997:SER:O	1:B:1001:ASN:ND2	2.54	0.41
1:C:740:GLY:O	1:C:794:ALA:N	2.51	0.41
1:A:49:TYR:HB2	1:A:122:VAL:HG22	2.02	0.41
1:A:83:ASP:N	1:A:83:ASP:OD1	2.54	0.41
1:A:240:LEU:HD22	1:A:245:GLU:HB3	2.03	0.41
1:A:972:LEU:HD22	1:A:975:ILE:HB	2.03	0.41
1:C:21:LEU:HD11	1:A:879:ILE:HD11	2.03	0.41
1:C:319:SER:O	1:C:320:GLY:C	2.60	0.40
1:C:741:VAL:HG12	1:C:793:ALA:HA	2.03	0.40
1:B:40:PRO:HD3	1:B:462:SER:HB3	2.03	0.40
1:A:219:LEU:HD12	1:A:232:ALA:HB3	2.03	0.40
1:A:439:GLN:HB2	2:A:1105:PTY:C8	2.44	0.40
1:A:448:VAL:HG22	1:A:887:CYS:HB3	2.03	0.40
1:B:355:MET:HG2	1:B:977:MET:HE1	2.02	0.40
1:B:897:ILE:H	1:B:898:PRO:HD2	1.79	0.40
1:B:907:LEU:HB3	1:B:1017:LEU:HD11	2.03	0.40
1:A:5:PHE:HZ	2:A:1102:PTY:H152	1.86	0.40
1:B:412:VAL:HA	1:B:415:ASN:CB	2.51	0.40
1:A:972:LEU:HD22	1:A:975:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	959/1057 (91%)	928 (97%)	31 (3%)	0	100	100
1	B	1015/1057 (96%)	961 (95%)	51 (5%)	3 (0%)	41	76
1	C	1011/1057 (96%)	907 (90%)	91 (9%)	13 (1%)	12	45
All	All	2985/3171 (94%)	2796 (94%)	173 (6%)	16 (0%)	32	68

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	320	GLY
1	C	424	GLY
1	C	453	PHE
1	B	489	THR
1	C	318	PRO
1	C	672	VAL
1	C	893	GLU
1	C	74	ASN
1	C	415	ASN
1	C	716	VAL
1	C	852	PRO
1	B	900	SER
1	C	535	LEU
1	C	851	LEU
1	B	412	VAL
1	C	531	VAL

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	783/862 (91%)	777 (99%)	6 (1%)	81	93
1	B	829/862 (96%)	822 (99%)	7 (1%)	81	93
1	C	821/862 (95%)	782 (95%)	39 (5%)	25	62
All	All	2433/2586 (94%)	2381 (98%)	52 (2%)	56	82

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	ARG
1	B	211	ASN
1	B	486	LEU
1	B	488	LEU
1	B	489	THR
1	B	973	ARG
1	B	1017	LEU
1	C	67	GLN
1	C	75	LEU
1	C	76	MET
1	C	115	MET
1	C	135	SER
1	C	137	LEU
1	C	231	ASN
1	C	298	ASN
1	C	316	PHE
1	C	317	PHE
1	C	361	ASN
1	C	415	ASN
1	C	425	LEU
1	C	428	LYS
1	C	439	GLN
1	C	488	LEU
1	C	489	THR
1	C	518	ARG
1	C	519	MET
1	C	531	VAL
1	C	540	ARG
1	C	631	LEU
1	C	668	LEU
1	C	671	ILE
1	C	673	GLU

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Mol	Chain	Res	Type
1	C	674	LEU
1	C	676	THR
1	C	683	GLU
1	C	695	LEU
1	C	717	ARG
1	C	744	ASN
1	C	850	LYS
1	C	851	LEU
1	C	871	ASN
1	C	876	LEU
1	C	888	LEU
1	C	891	LEU
1	C	897	ILE
1	C	958	LYS
1	A	110	LYS
1	A	231	ASN
1	A	275	TYR
1	A	415	ASN
1	A	765	ARG
1	A	907	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	58	GLN
1	B	211	ASN
1	B	298	ASN
1	B	760	ASN
1	C	74	ASN
1	C	213	GLN
1	C	231	ASN
1	C	282	ASN
1	C	298	ASN
1	C	361	ASN
1	C	469	GLN
1	C	744	ASN
1	A	58	GLN
1	A	231	ASN
1	A	415	ASN
1	A	469	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	1102	-	22,22,49	1.31	4 (18%)	24,24,54	1.53	3 (12%)
2	PTY	A	1107	-	24,24,49	1.22	4 (16%)	27,29,54	1.21	2 (7%)
2	PTY	A	1102	-	18,18,49	0.28	0	16,16,54	0.79	0
2	PTY	C	1104	-	33,33,49	1.04	4 (12%)	36,38,54	1.13	2 (5%)
2	PTY	B	1103	-	29,29,49	1.11	3 (10%)	32,34,54	1.13	2 (6%)
2	PTY	C	1102	-	29,29,49	1.12	4 (13%)	32,34,54	1.11	2 (6%)
2	PTY	A	1106	-	36,36,49	1.05	5 (13%)	40,41,54	1.16	2 (5%)
2	PTY	B	1105	-	27,27,49	1.17	4 (14%)	30,32,54	1.22	2 (6%)
3	D12	B	1108	-	11,11,11	0.28	0	10,10,10	0.85	0
2	PTY	B	1104	-	37,37,49	1.00	4 (10%)	40,42,54	1.24	2 (5%)
2	PTY	A	1104	-	31,31,49	0.87	2 (6%)	33,35,54	1.07	1 (3%)
2	PTY	A	1103	-	24,24,49	1.23	4 (16%)	27,29,54	1.21	2 (7%)
2	PTY	B	1107	-	16,16,49	0.88	1 (6%)	16,16,54	1.00	1 (6%)
2	PTY	B	1101	-	30,30,49	1.08	4 (13%)	33,35,54	1.12	2 (6%)
2	PTY	C	1103	-	28,28,49	0.94	2 (7%)	29,29,54	1.05	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PTY	B	1106	-	35,35,49	0.76	1 (2%)	36,37,54	0.89	1 (2%)
2	PTY	A	1101	-	27,27,49	1.21	5 (18%)	31,32,54	1.29	2 (6%)
2	PTY	A	1105	-	11,12,49	0.50	0	11,12,54	1.06	1 (9%)
2	PTY	C	1101	-	16,16,49	0.92	2 (12%)	15,15,54	0.97	1 (6%)

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	1102	-	-	7/23/23/53	-
2	PTY	A	1107	-	-	19/28/28/53	-
2	PTY	A	1102	-	-	6/14/14/53	-
2	PTY	C	1104	-	-	14/37/37/53	-
2	PTY	B	1103	-	-	18/33/33/53	-
2	PTY	C	1102	-	-	8/33/33/53	-
2	PTY	A	1106	-	-	22/38/38/53	-
2	PTY	B	1105	-	-	18/31/31/53	-
3	D12	B	1108	-	-	1/9/9/9	-
2	PTY	B	1104	-	-	21/41/41/53	-
2	PTY	A	1104	-	-	17/34/34/53	-
2	PTY	A	1103	-	-	13/28/28/53	-
2	PTY	B	1107	-	-	6/15/15/53	-
2	PTY	B	1101	-	-	16/34/34/53	-
2	PTY	C	1103	-	-	13/28/28/53	-
2	PTY	B	1106	-	-	17/34/34/53	-
2	PTY	A	1101	-	-	13/29/29/53	-
2	PTY	A	1105	-	-	5/11/11/53	-
2	PTY	C	1101	-	-	6/13/13/53	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1102	PTY	O7-C6	-3.93	1.40	1.47
2	A	1106	PTY	P1-O11	2.70	1.65	1.54
2	A	1101	PTY	P1-O11	2.67	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	PTY	O7-C6	-2.67	1.39	1.46
2	B	1103	PTY	O7-C6	-2.59	1.40	1.46
2	C	1102	PTY	O7-C6	-2.56	1.40	1.46
2	A	1103	PTY	O4-C30	2.55	1.40	1.33
2	A	1107	PTY	O7-C6	-2.55	1.40	1.46
2	A	1101	PTY	O7-C6	-2.52	1.40	1.46
2	B	1105	PTY	O4-C30	2.51	1.40	1.33
2	C	1103	PTY	O4-C30	2.47	1.40	1.33
2	C	1102	PTY	O4-C30	2.47	1.40	1.33
2	A	1106	PTY	O7-C6	-2.47	1.40	1.46
2	B	1105	PTY	O7-C8	2.45	1.41	1.34
2	C	1104	PTY	O7-C6	-2.44	1.40	1.46
2	B	1104	PTY	O7-C8	2.44	1.41	1.34
2	C	1103	PTY	O7-C8	2.42	1.40	1.33
2	B	1104	PTY	O4-C30	2.41	1.40	1.33
2	B	1102	PTY	O4-C30	2.40	1.40	1.33
2	A	1103	PTY	O7-C6	-2.40	1.40	1.46
2	B	1103	PTY	O4-C30	2.39	1.40	1.33
2	C	1101	PTY	O4-C30	2.39	1.40	1.33
2	A	1104	PTY	O7-C6	-2.38	1.40	1.46
2	B	1101	PTY	O4-C30	2.37	1.40	1.33
2	B	1107	PTY	O4-C30	2.34	1.40	1.33
2	A	1101	PTY	O4-C30	2.34	1.40	1.33
2	A	1106	PTY	O4-C30	2.32	1.40	1.33
2	A	1107	PTY	O4-C30	2.30	1.40	1.33
2	C	1104	PTY	O4-C30	2.25	1.39	1.33
2	A	1103	PTY	O7-C8	2.24	1.40	1.34
2	A	1107	PTY	O4-C1	-2.23	1.40	1.45
2	C	1104	PTY	O7-C8	2.22	1.40	1.34
2	B	1102	PTY	O7-C8	2.20	1.40	1.34
2	A	1104	PTY	O7-C8	2.19	1.40	1.34
2	B	1106	PTY	O7-C8	2.18	1.39	1.33
2	A	1106	PTY	O7-C8	2.18	1.40	1.34
2	C	1104	PTY	O4-C1	-2.14	1.40	1.45
2	B	1104	PTY	O4-C1	-2.12	1.40	1.45
2	A	1107	PTY	O7-C8	2.11	1.40	1.34
2	A	1101	PTY	O7-C8	2.11	1.40	1.34
2	A	1106	PTY	O4-C1	-2.07	1.40	1.45
2	C	1102	PTY	O7-C8	2.06	1.40	1.34
2	C	1102	PTY	O4-C1	-2.06	1.40	1.45
2	B	1103	PTY	O4-C1	-2.05	1.40	1.45
2	B	1105	PTY	O4-C1	-2.04	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1105	PTY	O7-C6	-2.04	1.41	1.46
2	A	1103	PTY	O4-C1	-2.04	1.40	1.45
2	C	1101	PTY	O4-C1	-2.03	1.40	1.45
2	B	1101	PTY	O7-C8	2.03	1.40	1.34
2	B	1102	PTY	O4-C1	-2.02	1.40	1.45
2	A	1101	PTY	O4-C1	-2.02	1.40	1.45
2	B	1101	PTY	O4-C1	-2.02	1.40	1.45
2	B	1104	PTY	O7-C6	-2.02	1.41	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1104	PTY	O7-C8-C11	4.89	122.04	111.50
2	A	1103	PTY	O7-C8-C11	4.54	121.29	111.50
2	A	1101	PTY	O7-C8-C11	4.21	120.58	111.50
2	B	1105	PTY	O7-C8-C11	4.15	120.45	111.50
2	C	1104	PTY	O7-C8-C11	4.07	120.26	111.50
2	B	1102	PTY	O7-C8-C11	4.00	120.13	111.50
2	A	1104	PTY	O7-C8-C11	3.90	119.90	111.50
2	A	1106	PTY	O7-C8-C11	3.85	119.80	111.50
2	A	1107	PTY	O7-C8-C11	3.77	119.62	111.50
2	B	1103	PTY	O7-C8-C11	3.74	119.57	111.50
2	C	1102	PTY	O7-C8-C11	3.67	119.40	111.50
2	B	1101	PTY	O7-C8-C11	3.57	119.20	111.50
2	B	1102	PTY	C6-O7-C8	-3.26	113.68	117.88
2	B	1105	PTY	O4-C30-C31	2.93	121.09	111.91
2	A	1101	PTY	O4-C30-C31	2.87	120.93	111.91
2	B	1102	PTY	O4-C30-C31	2.70	120.37	111.91
2	B	1103	PTY	O4-C30-C31	2.69	120.35	111.91
2	A	1106	PTY	O4-C30-C31	2.68	120.32	111.91
2	B	1106	PTY	O7-C8-C11	2.63	120.17	111.91
2	B	1101	PTY	O4-C30-C31	2.61	120.10	111.91
2	C	1102	PTY	O4-C30-C31	2.58	120.01	111.91
2	A	1107	PTY	O4-C30-C31	2.50	119.76	111.91
2	C	1104	PTY	O4-C30-C31	2.49	119.72	111.91
2	C	1103	PTY	O4-C30-C31	2.47	119.66	111.91
2	A	1105	PTY	O7-C8-C11	2.40	117.98	109.56
2	B	1104	PTY	O4-C30-C31	2.40	119.44	111.91
2	C	1103	PTY	O7-C8-C11	2.34	119.27	111.91
2	A	1103	PTY	O4-C30-C31	2.21	118.83	111.91
2	B	1107	PTY	O4-C30-C31	2.18	118.75	111.91
2	C	1101	PTY	O4-C30-C31	2.14	120.70	112.23

There are no chirality outliers.

All (240) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	PTY	O10-C8-O7-C6
2	B	1101	PTY	C3-O11-P1-O14
2	B	1101	PTY	C5-O14-P1-O11
2	B	1101	PTY	C5-O14-P1-O12
2	B	1101	PTY	C5-O14-P1-O13
2	B	1102	PTY	O10-C8-O7-C6
2	B	1102	PTY	C11-C8-O7-C6
2	B	1103	PTY	C3-O11-P1-O12
2	B	1103	PTY	C3-O11-P1-O13
2	B	1103	PTY	C5-O14-P1-O13
2	B	1104	PTY	C11-C8-O7-C6
2	B	1105	PTY	C11-C8-O7-C6
2	B	1105	PTY	C3-O11-P1-O12
2	B	1105	PTY	C3-O11-P1-O13
2	B	1105	PTY	C5-O14-P1-O12
2	B	1106	PTY	N1-C2-C3-O11
2	B	1106	PTY	C5-O14-P1-O12
2	C	1101	PTY	C31-C30-O4-C1
2	C	1104	PTY	C11-C8-O7-C6
2	C	1104	PTY	C3-O11-P1-O12
2	C	1104	PTY	C3-O11-P1-O14
2	C	1104	PTY	C5-O14-P1-O11
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-O12
2	A	1103	PTY	C5-O14-P1-O13
2	A	1104	PTY	N1-C2-C3-O11
2	A	1104	PTY	C11-C8-O7-C6
2	A	1104	PTY	C3-O11-P1-O13
2	A	1106	PTY	C11-C8-O7-C6
2	A	1106	PTY	C5-O14-P1-O12
2	A	1106	PTY	C5-O14-P1-O13
2	A	1107	PTY	C3-O11-P1-O12
2	A	1107	PTY	C5-O14-P1-O13
2	B	1105	PTY	O30-C30-O4-C1
2	C	1101	PTY	O30-C30-O4-C1
2	B	1105	PTY	C31-C30-O4-C1
2	A	1106	PTY	O30-C30-O4-C1
2	B	1104	PTY	O10-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
2	B	1105	PTY	O10-C8-O7-C6
2	C	1102	PTY	O10-C8-O7-C6
2	C	1104	PTY	O10-C8-O7-C6
2	A	1106	PTY	O10-C8-O7-C6
2	A	1106	PTY	C31-C30-O4-C1
2	B	1101	PTY	C11-C8-O7-C6
2	A	1104	PTY	O10-C8-O7-C6
2	C	1102	PTY	C11-C8-O7-C6
2	B	1106	PTY	C11-C8-O7-C6
2	B	1101	PTY	O4-C1-C6-O7
2	B	1106	PTY	O10-C8-O7-C6
2	C	1104	PTY	C31-C30-O4-C1
2	A	1106	PTY	C8-C11-C12-C13
2	B	1102	PTY	C8-C11-C12-C13
2	C	1104	PTY	O30-C30-O4-C1
2	A	1101	PTY	C11-C8-O7-C6
2	A	1107	PTY	C11-C8-O7-C6
2	B	1103	PTY	C3-O11-P1-O14
2	B	1103	PTY	C5-O14-P1-O11
2	B	1104	PTY	C5-O14-P1-O11
2	B	1105	PTY	C3-O11-P1-O14
2	B	1105	PTY	C5-O14-P1-O11
2	B	1106	PTY	C5-O14-P1-O11
2	A	1103	PTY	C3-O11-P1-O14
2	A	1104	PTY	C5-O14-P1-O11
2	A	1107	PTY	C3-O11-P1-O14
2	A	1106	PTY	C30-C31-C32-C33
2	A	1101	PTY	O10-C8-O7-C6
2	A	1107	PTY	O10-C8-O7-C6
2	A	1104	PTY	C15-C16-C17-C18
2	B	1106	PTY	C14-C15-C16-C17
2	B	1103	PTY	C12-C13-C14-C15
2	C	1103	PTY	C34-C35-C36-C37
2	C	1103	PTY	C30-C31-C32-C33
2	A	1107	PTY	O4-C1-C6-O7
2	C	1103	PTY	O4-C1-C6-O7
2	C	1103	PTY	C12-C13-C14-C15
2	A	1104	PTY	C19-C20-C21-C22
2	B	1104	PTY	C11-C12-C13-C14
2	A	1101	PTY	C33-C34-C35-C36
2	A	1102	PTY	C14-C15-C16-C17
2	C	1101	PTY	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
2	B	1105	PTY	C32-C33-C34-C35
2	A	1101	PTY	C34-C35-C36-C37
2	A	1106	PTY	C18-C19-C20-C21
2	A	1106	PTY	C19-C20-C21-C22
2	B	1102	PTY	C13-C14-C15-C16
2	B	1103	PTY	C11-C12-C13-C14
2	B	1101	PTY	C8-C11-C12-C13
2	C	1103	PTY	C13-C14-C15-C16
2	B	1107	PTY	C33-C34-C35-C36
2	A	1101	PTY	C12-C13-C14-C15
2	B	1104	PTY	O4-C1-C6-C5
2	A	1106	PTY	C11-C12-C13-C14
2	C	1103	PTY	C11-C8-O7-C6
2	B	1103	PTY	C11-C8-O7-C6
2	A	1104	PTY	C20-C21-C22-C23
2	A	1104	PTY	C16-C17-C18-C19
2	C	1103	PTY	C8-C11-C12-C13
2	C	1103	PTY	C16-C17-C18-C19
2	C	1101	PTY	C31-C32-C33-C34
2	C	1103	PTY	C33-C34-C35-C36
2	C	1103	PTY	O10-C8-O7-C6
2	B	1103	PTY	O10-C8-O7-C6
2	B	1104	PTY	C8-C11-C12-C13
2	A	1101	PTY	C8-C11-C12-C13
2	A	1105	PTY	C12-C11-C8-O7
2	B	1106	PTY	C15-C16-C17-C18
2	A	1106	PTY	C31-C32-C33-C34
2	B	1106	PTY	C33-C34-C35-C36
2	B	1104	PTY	C37-C38-C39-C40
2	C	1101	PTY	C32-C33-C34-C35
2	A	1103	PTY	C5-O14-P1-O11
2	A	1104	PTY	C3-O11-P1-O14
2	A	1107	PTY	O14-C5-C6-C1
2	B	1104	PTY	C31-C30-O4-C1
2	B	1104	PTY	C33-C34-C35-C36
2	A	1106	PTY	C20-C21-C22-C23
2	C	1104	PTY	O4-C1-C6-C5
2	A	1101	PTY	O4-C1-C6-C5
2	A	1106	PTY	O4-C1-C6-C5
2	A	1107	PTY	O4-C1-C6-C5
2	A	1106	PTY	C17-C18-C19-C20
2	A	1107	PTY	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	B	1104	PTY	O4-C30-C31-C32
2	A	1103	PTY	C8-C11-C12-C13
2	B	1105	PTY	C1-C6-O7-C8
2	B	1101	PTY	O14-C5-C6-O7
2	B	1104	PTY	O30-C30-O4-C1
2	C	1103	PTY	C32-C33-C34-C35
2	A	1102	PTY	C12-C13-C14-C15
2	B	1103	PTY	O14-C5-C6-C1
2	B	1105	PTY	O14-C5-C6-C1
2	B	1107	PTY	O4-C1-C6-O7
2	A	1104	PTY	C14-C15-C16-C17
2	B	1106	PTY	C8-C11-C12-C13
3	B	1108	D12	C6-C7-C8-C9
2	A	1107	PTY	C6-C5-O14-P1
2	B	1107	PTY	C32-C33-C34-C35
2	B	1101	PTY	O4-C1-C6-C5
2	C	1102	PTY	C11-C12-C13-C14
2	B	1103	PTY	O14-C5-C6-O7
2	A	1106	PTY	C23-C24-C25-C26
2	A	1106	PTY	O4-C1-C6-O7
2	B	1105	PTY	C6-C5-O14-P1
2	A	1103	PTY	O14-C5-C6-C1
2	B	1106	PTY	C13-C14-C15-C16
2	B	1107	PTY	C34-C35-C36-C37
2	A	1106	PTY	C5-O14-P1-O11
2	B	1101	PTY	C31-C30-O4-C1
2	B	1104	PTY	C1-C6-O7-C8
2	A	1102	PTY	C34-C35-C36-C37
2	A	1104	PTY	C6-C1-O4-C30
2	B	1103	PTY	C30-C31-C32-C33
2	B	1105	PTY	O14-C5-C6-O7
2	B	1104	PTY	O4-C1-C6-O7
2	B	1105	PTY	O4-C1-C6-O7
2	C	1104	PTY	O4-C1-C6-O7
2	B	1103	PTY	C13-C14-C15-C16
2	A	1102	PTY	C11-C12-C13-C14
2	A	1105	PTY	C11-C8-O7-C6
2	C	1103	PTY	C11-C12-C13-C14
2	B	1106	PTY	C3-O11-P1-O14
2	C	1102	PTY	C5-O14-P1-O11
2	A	1106	PTY	C6-C5-O14-P1
2	B	1104	PTY	C5-O14-P1-O12

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Mol	Chain	Res	Type	Atoms
2	B	1105	PTY	C5-O14-P1-O13
2	B	1106	PTY	C5-O14-P1-O13
2	C	1102	PTY	C5-O14-P1-O12
2	C	1102	PTY	C5-O14-P1-O13
2	C	1104	PTY	C3-O11-P1-O13
2	C	1104	PTY	C5-O14-P1-O12
2	A	1104	PTY	C3-O11-P1-O12
2	A	1104	PTY	C5-O14-P1-O13
2	A	1107	PTY	C3-O11-P1-O13
2	B	1101	PTY	O14-C5-C6-C1
2	B	1102	PTY	C34-C35-C36-C37
2	C	1104	PTY	C2-C3-O11-P1
2	A	1104	PTY	C2-C3-O11-P1
2	B	1101	PTY	O30-C30-O4-C1
2	A	1101	PTY	O14-C5-C6-O7
2	A	1103	PTY	O14-C5-C6-O7
2	A	1107	PTY	C8-C11-C12-C13
2	B	1104	PTY	C16-C17-C18-C19
2	B	1106	PTY	C31-C32-C33-C34
2	B	1105	PTY	O4-C1-C6-C5
2	C	1104	PTY	C34-C35-C36-C37
2	C	1103	PTY	C12-C11-C8-O7
2	A	1101	PTY	C13-C14-C15-C16
2	C	1102	PTY	C31-C30-O4-C1
2	C	1102	PTY	O30-C30-O4-C1
2	A	1107	PTY	O14-C5-C6-O7
2	A	1101	PTY	C35-C36-C37-C38
2	A	1101	PTY	O4-C1-C6-O7
2	B	1104	PTY	C3-O11-P1-O14
2	A	1103	PTY	O4-C1-C6-C5
2	B	1104	PTY	O30-C30-C31-C32
2	B	1104	PTY	C36-C37-C38-C39
2	B	1101	PTY	C31-C32-C33-C34
2	A	1101	PTY	C6-C5-O14-P1
2	A	1107	PTY	C31-C30-O4-C1
2	B	1103	PTY	C8-C11-C12-C13
2	A	1107	PTY	O30-C30-O4-C1
2	A	1106	PTY	C15-C16-C17-C18
2	B	1107	PTY	C37-C38-C39-C40
2	B	1103	PTY	C32-C33-C34-C35
2	A	1102	PTY	C32-C33-C34-C35
2	A	1101	PTY	O14-C5-C6-C1

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Mol	Chain	Res	Type	Atoms
2	B	1104	PTY	C15-C16-C17-C18
2	B	1103	PTY	N1-C2-C3-O11
2	B	1103	PTY	C31-C32-C33-C34
2	A	1105	PTY	O14-C5-C6-O7
2	B	1101	PTY	C12-C11-C8-O7
2	B	1104	PTY	C12-C11-C8-O7
2	A	1102	PTY	C33-C34-C35-C36
2	B	1106	PTY	C16-C17-C18-C19
2	B	1106	PTY	C12-C11-C8-O7
2	B	1102	PTY	C12-C11-C8-O7
2	C	1101	PTY	C35-C36-C37-C38
2	A	1106	PTY	C12-C11-C8-O7
2	B	1105	PTY	C30-C31-C32-C33
2	B	1104	PTY	C38-C39-C40-C41
2	A	1107	PTY	C12-C11-C8-O7
2	A	1105	PTY	C13-C14-C15-C16
2	B	1106	PTY	C12-C11-C8-O10
2	B	1101	PTY	C12-C11-C8-O10
2	A	1106	PTY	C12-C11-C8-O10
2	B	1103	PTY	O4-C30-C31-C32
2	C	1104	PTY	C11-C12-C13-C14
2	A	1107	PTY	C2-C3-O11-P1
2	B	1102	PTY	C12-C11-C8-O10
2	A	1103	PTY	C12-C11-C8-O7
2	B	1107	PTY	C35-C36-C37-C38
2	A	1105	PTY	O14-C5-C6-C1
2	A	1104	PTY	C12-C11-C8-O7
2	A	1104	PTY	C12-C11-C8-O10
2	A	1107	PTY	C12-C11-C8-O10
2	B	1106	PTY	C11-C12-C13-C14
2	A	1103	PTY	C12-C11-C8-O10
2	A	1107	PTY	O4-C30-C31-C32

There are no ring outliers.

13 monomers are involved in 23 short contacts:

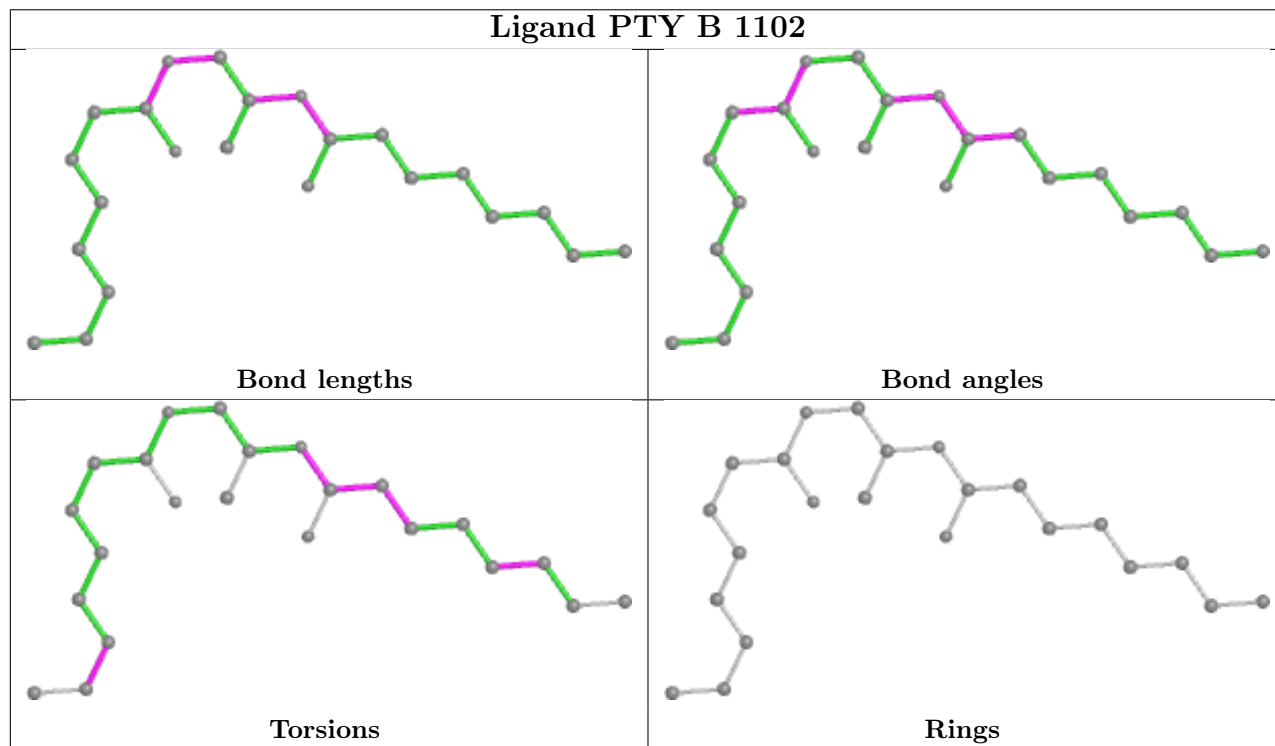
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1102	PTY	1	0
2	A	1107	PTY	1	0
2	A	1102	PTY	1	0
2	C	1104	PTY	1	0
2	B	1103	PTY	5	0

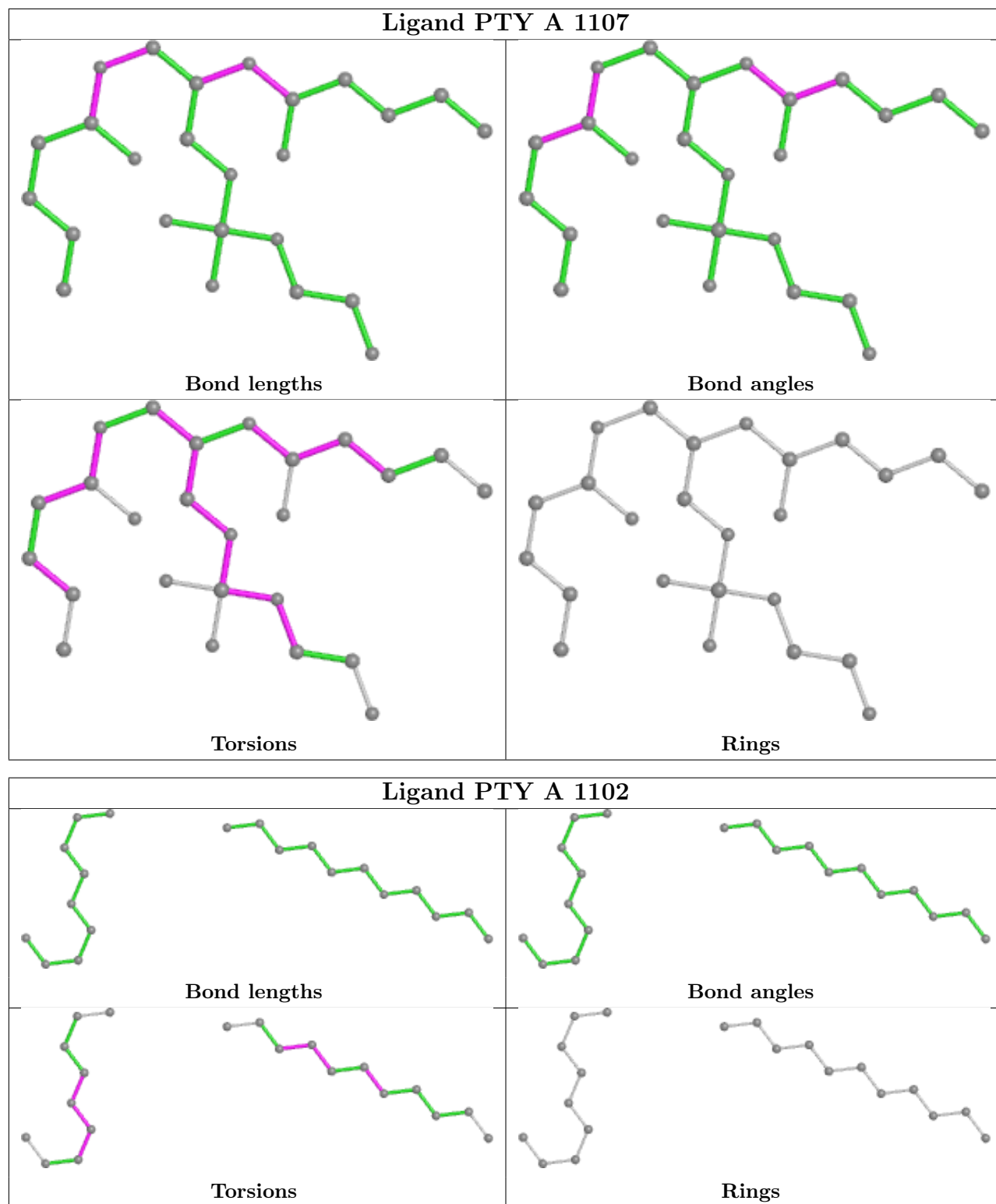
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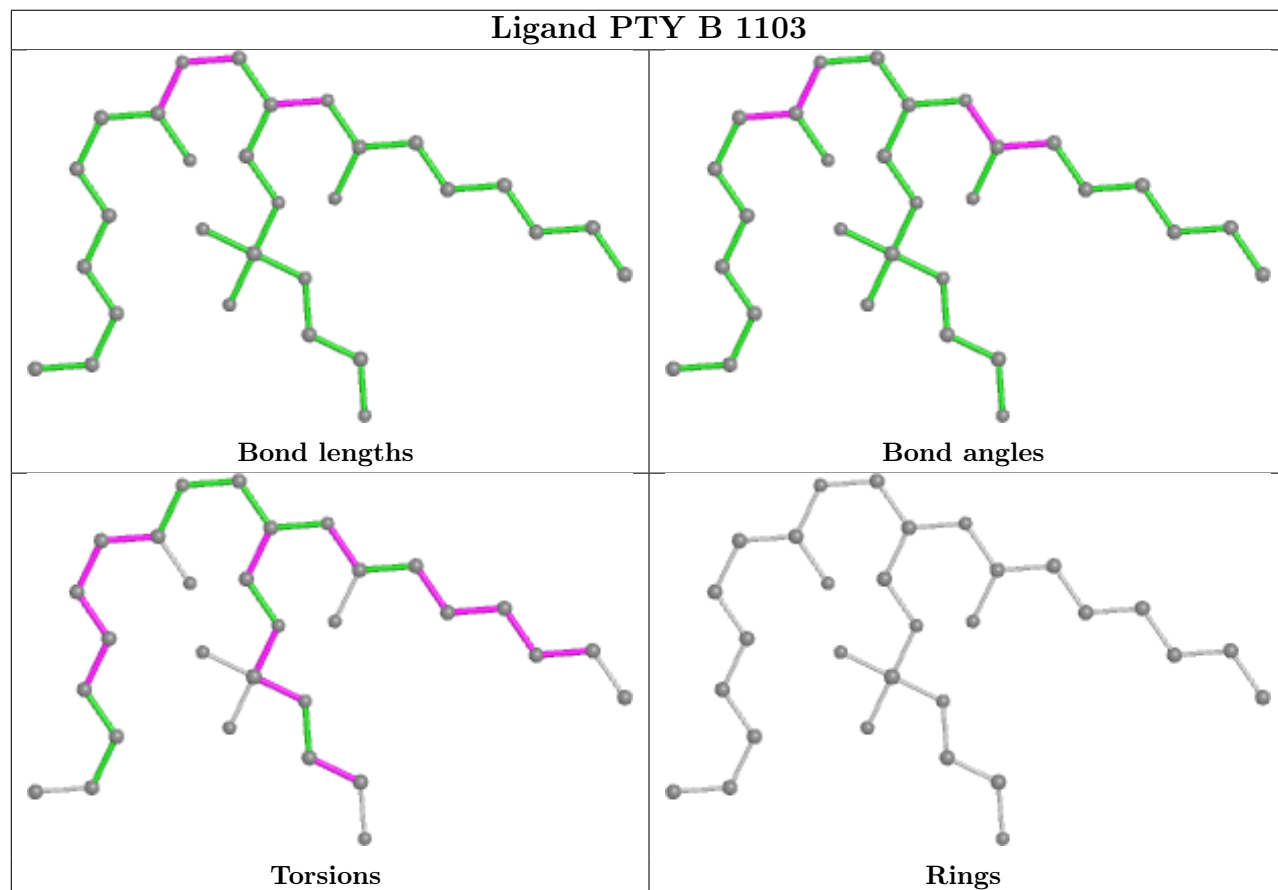
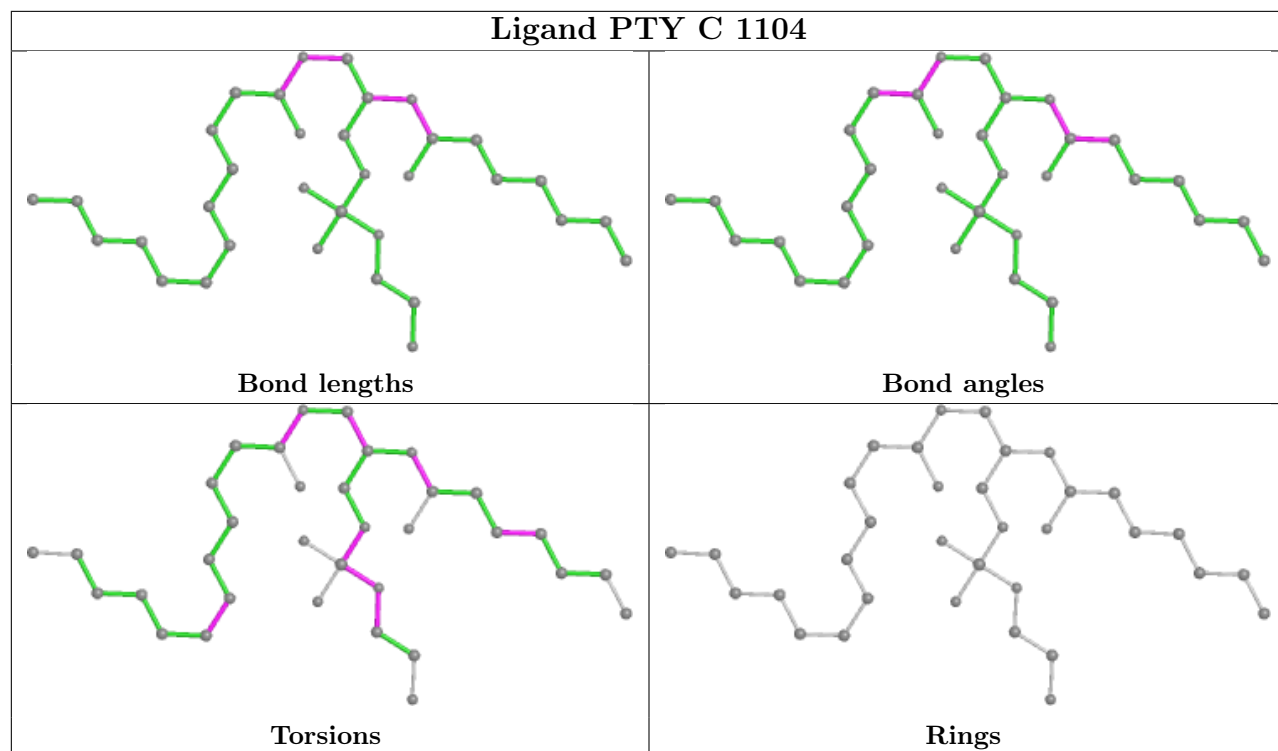
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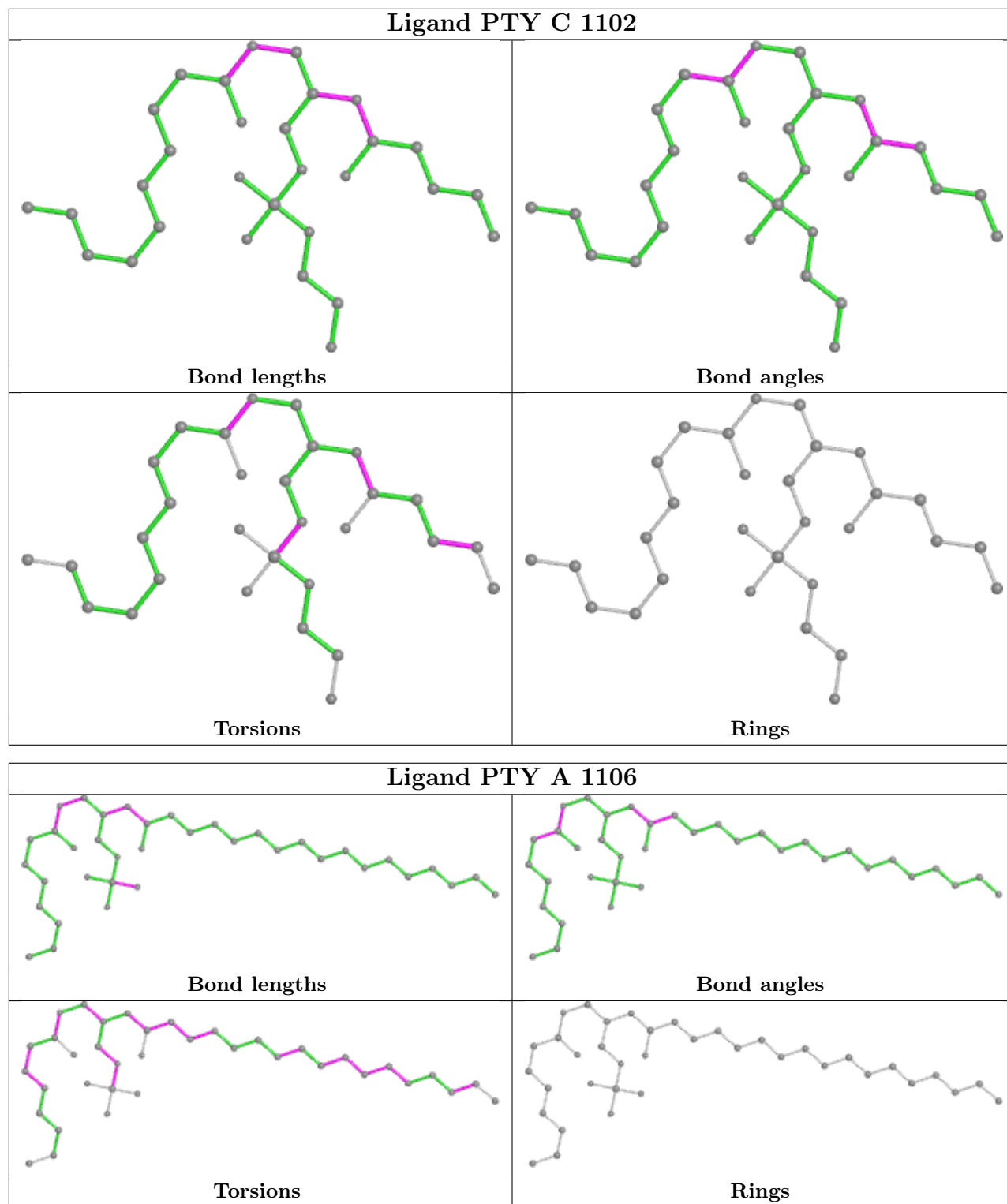
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1102	PTY	2	0
2	A	1106	PTY	2	0
2	B	1104	PTY	4	0
2	A	1103	PTY	2	0
2	B	1101	PTY	1	0
2	C	1103	PTY	2	0
2	A	1101	PTY	2	0
2	A	1105	PTY	5	0

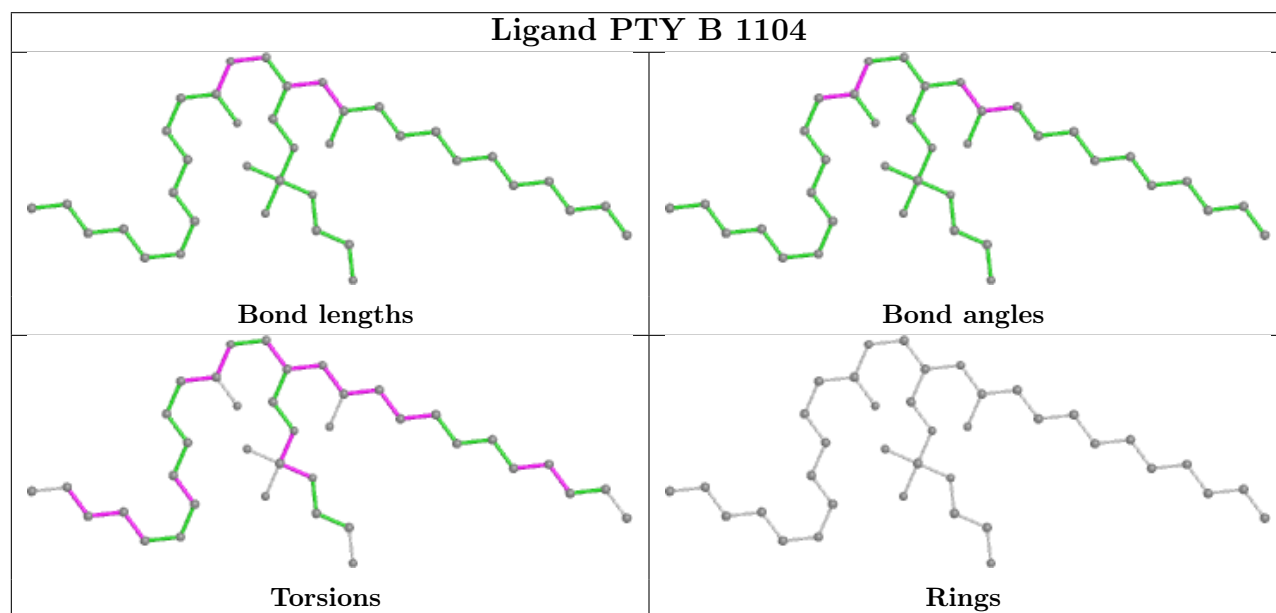
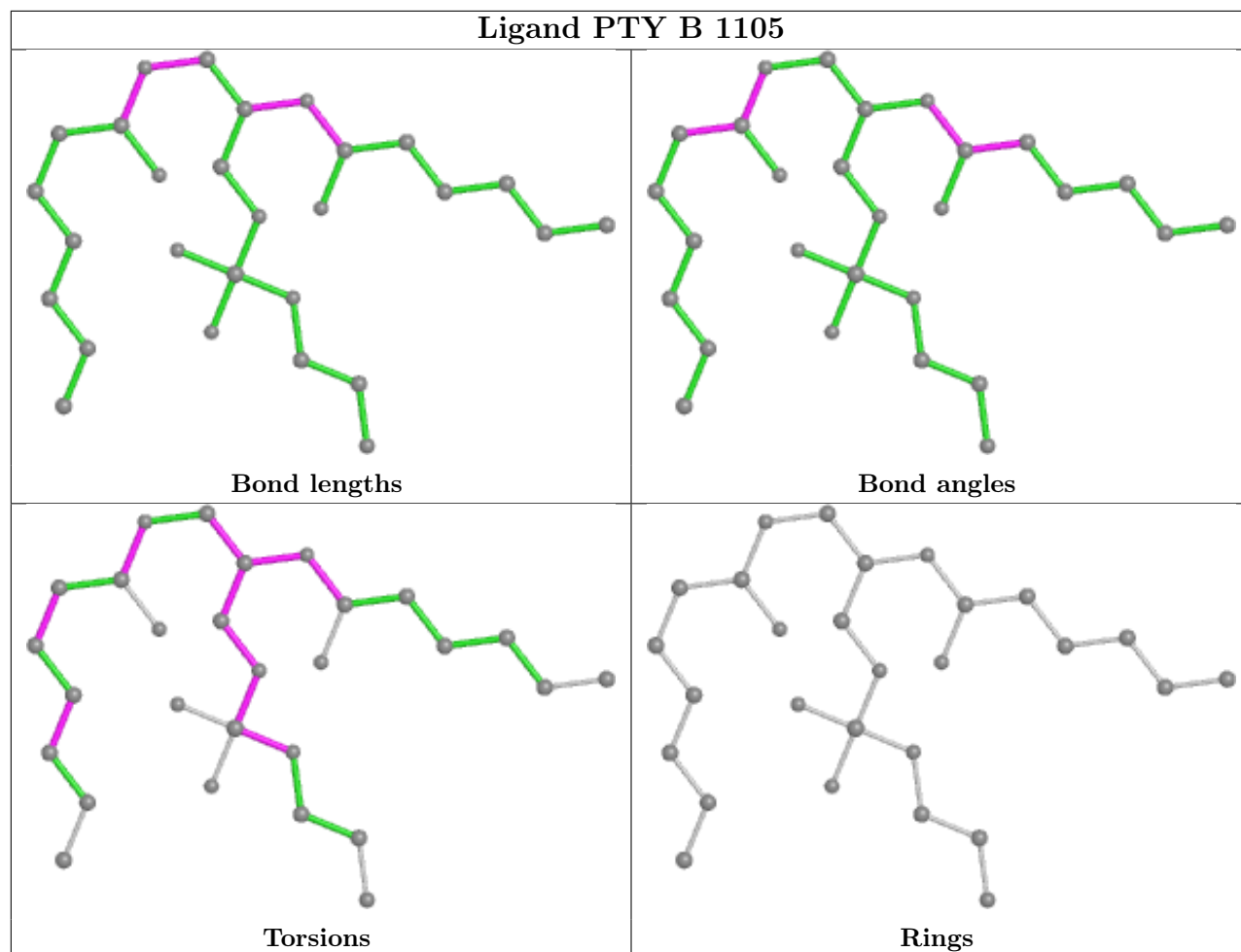
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

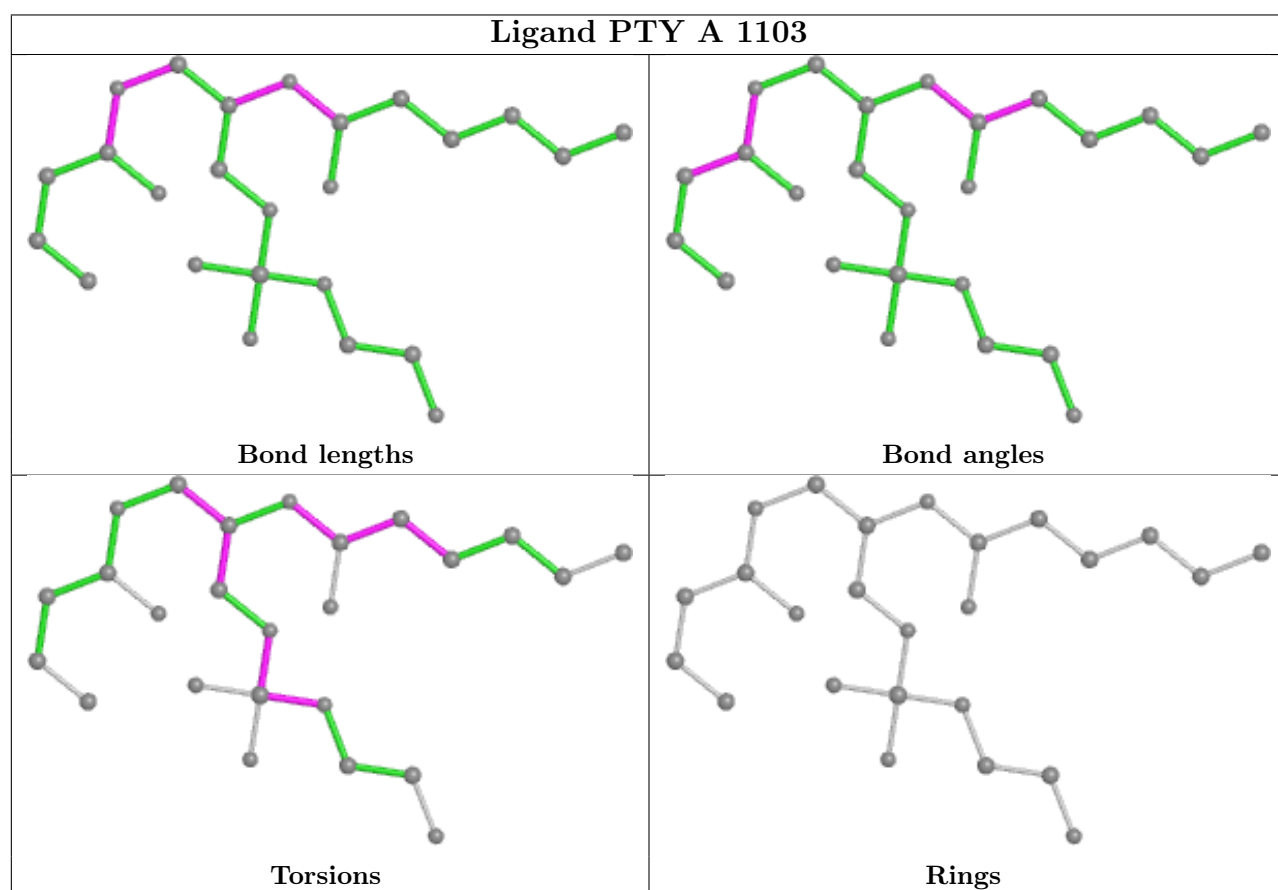
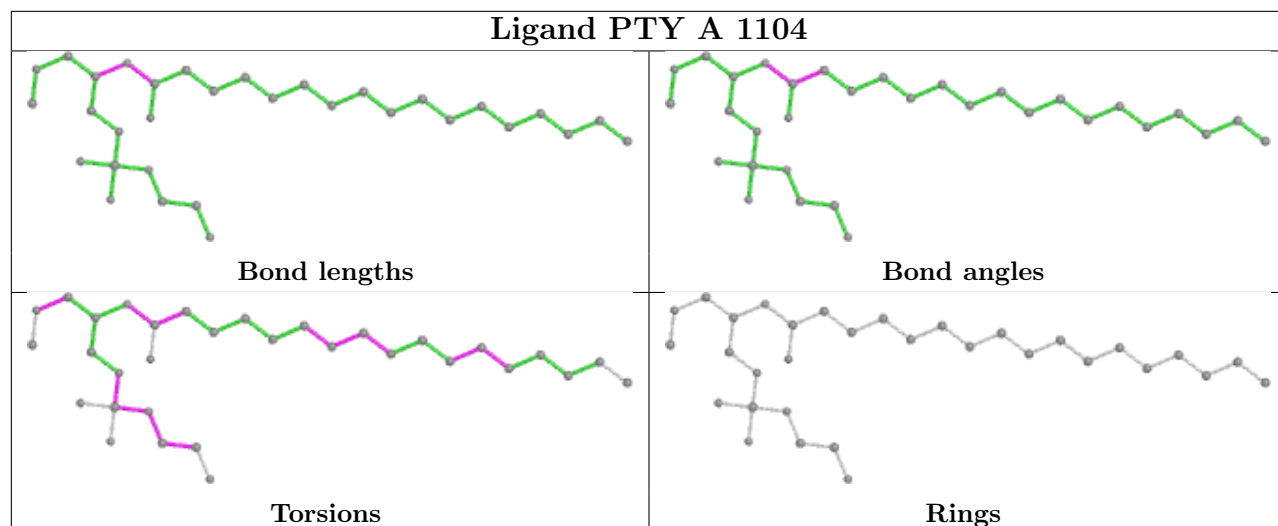


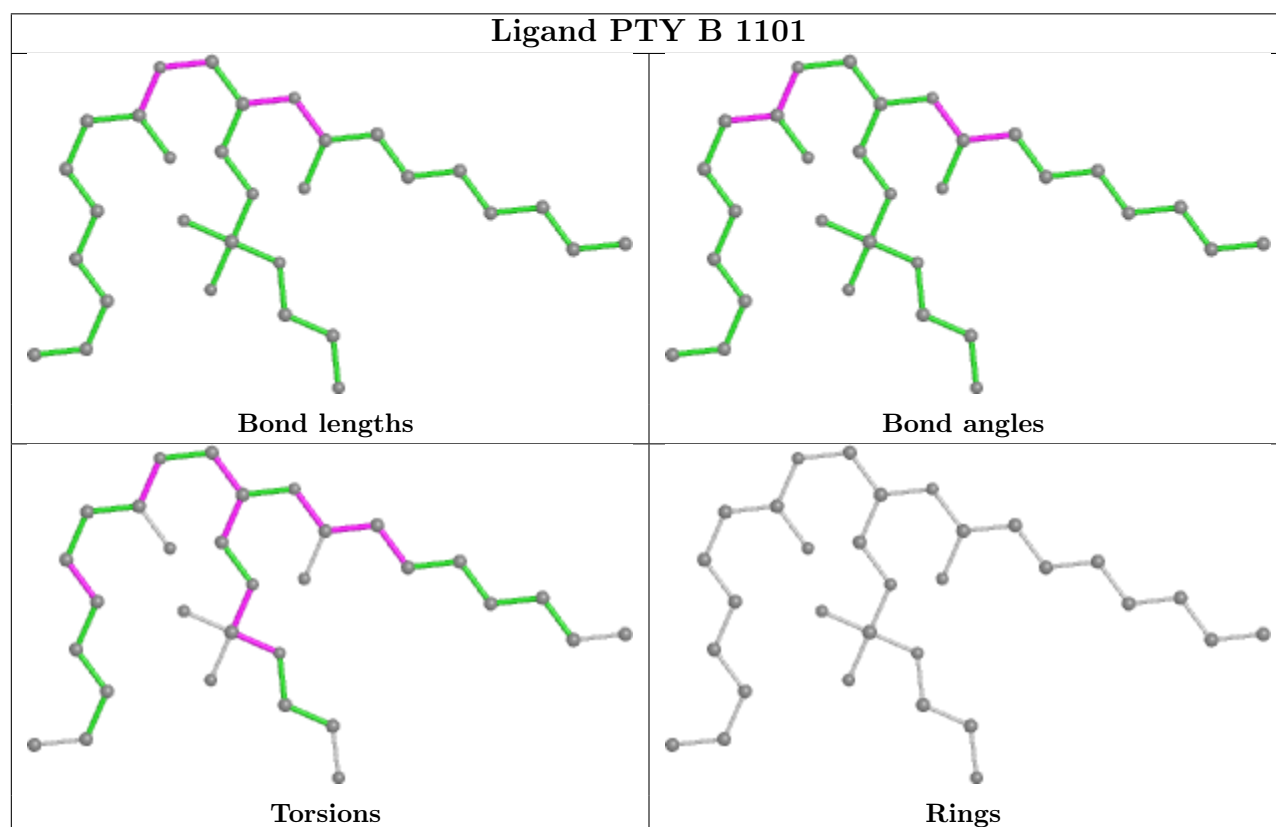
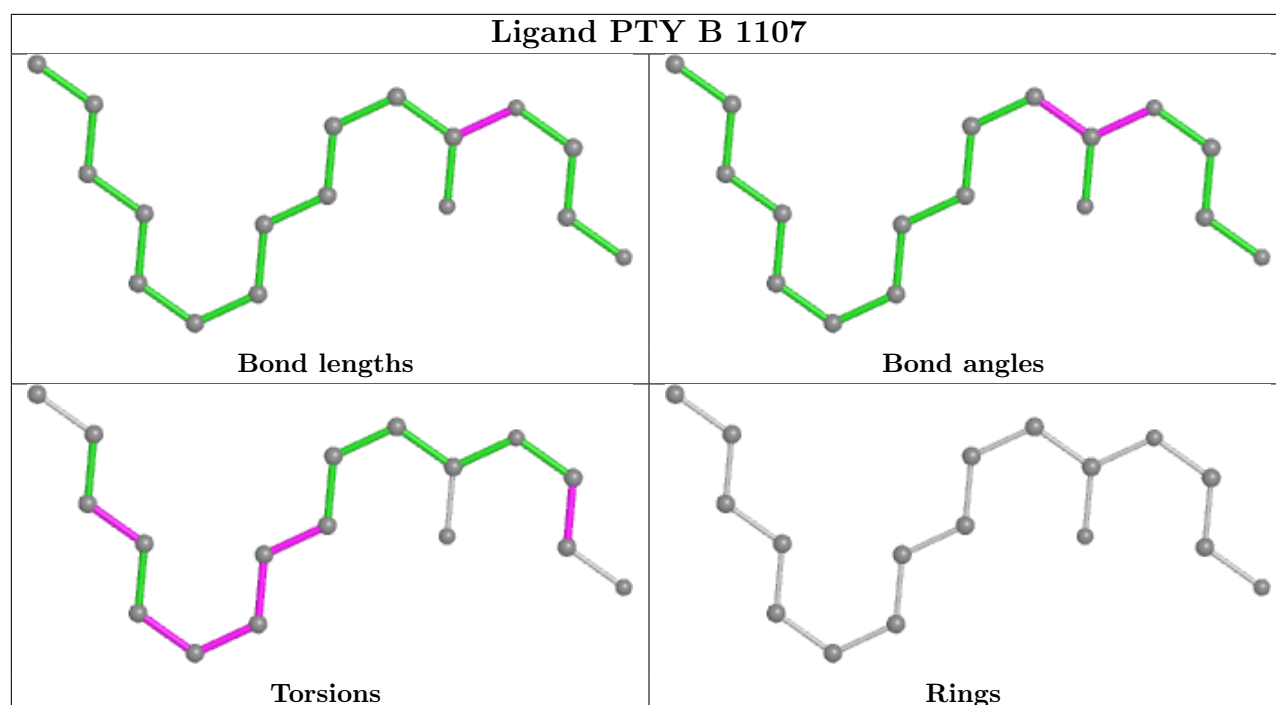


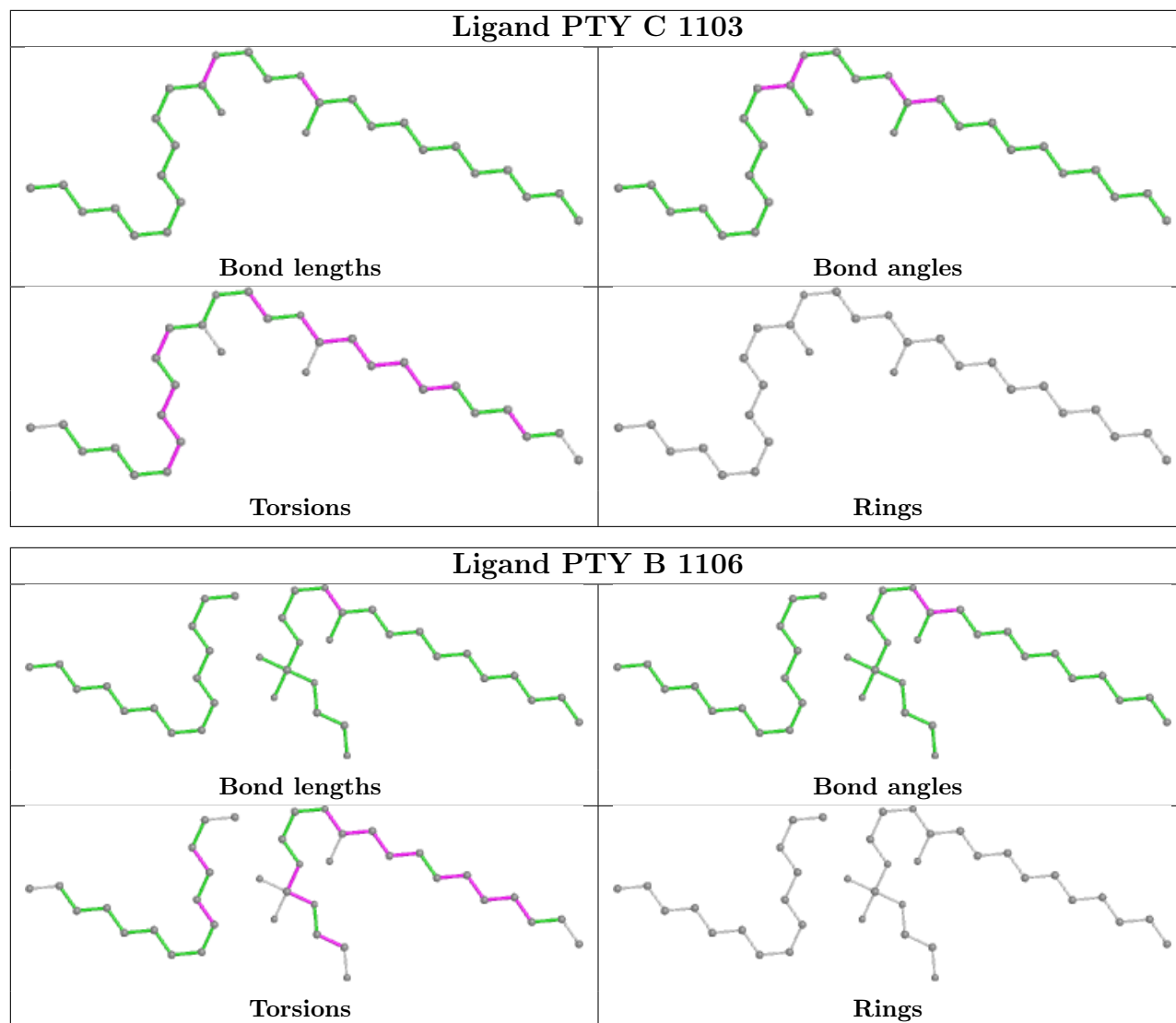


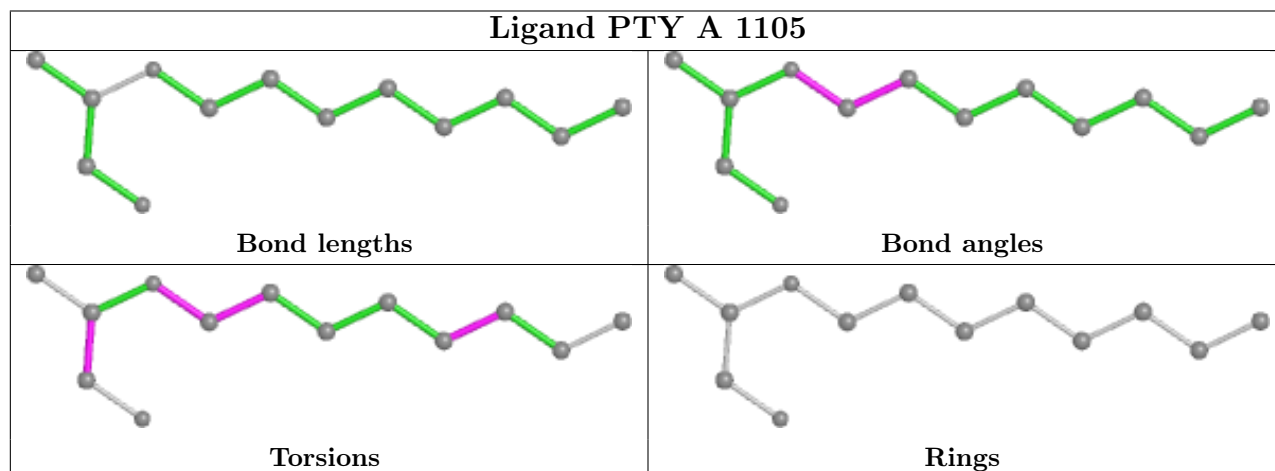
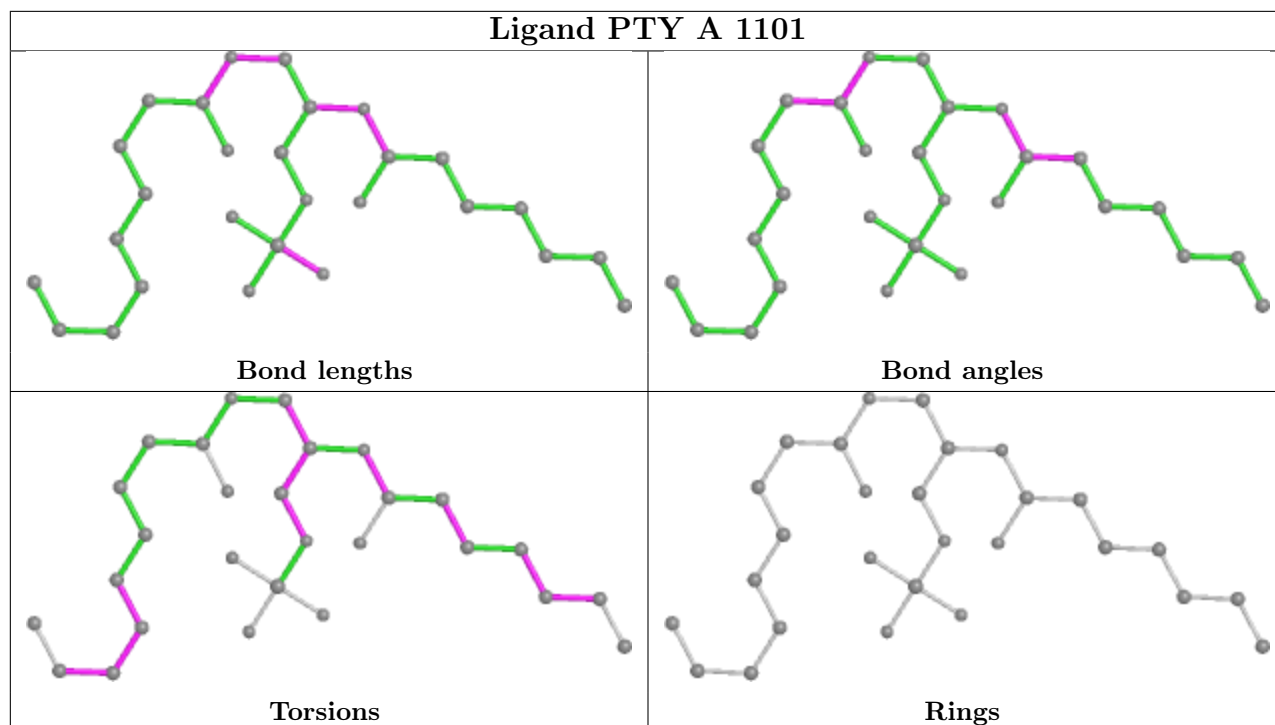


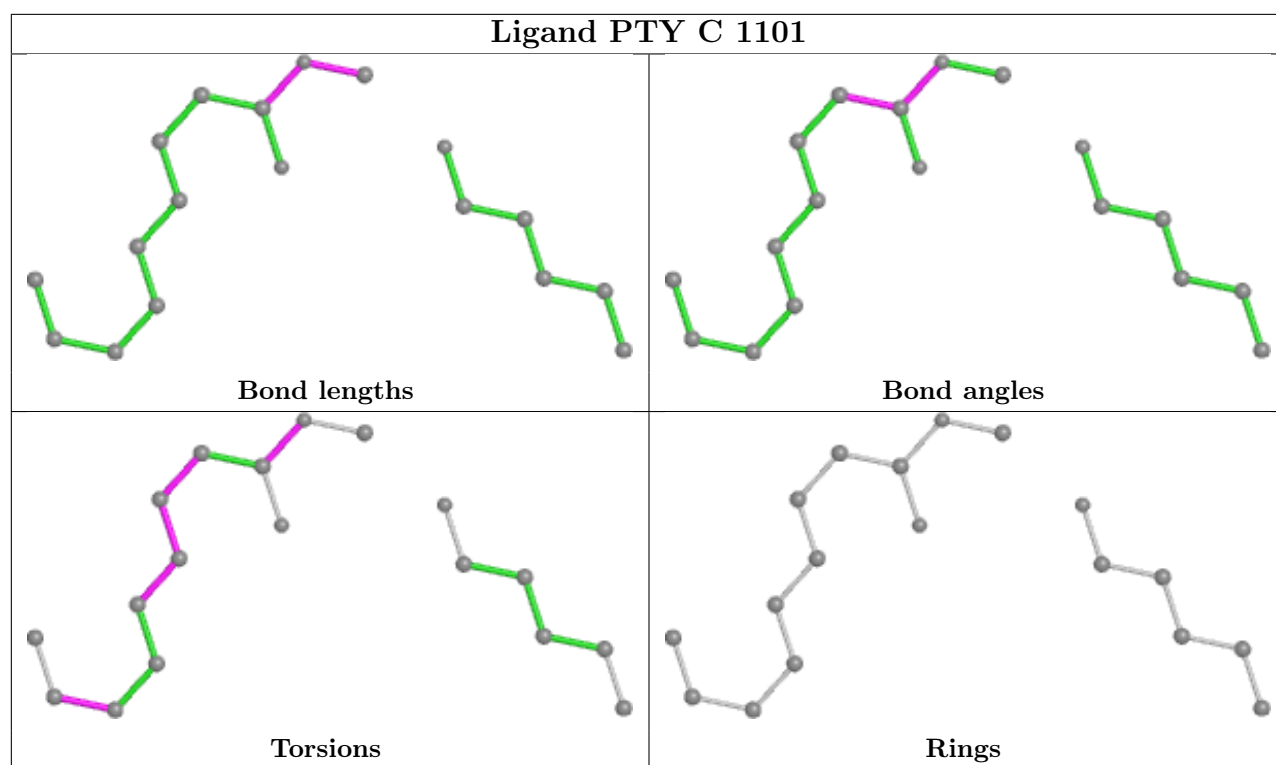












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

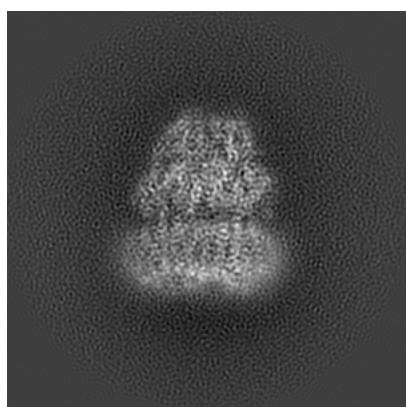
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7609. These allow visual inspection of the internal detail of the map and identification of artifacts.

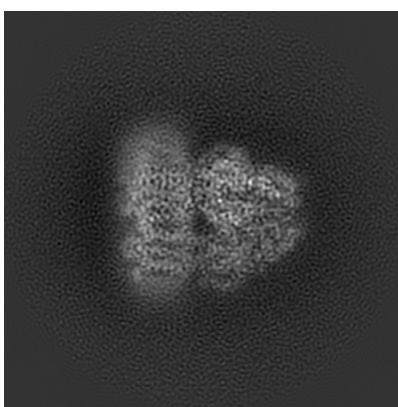
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

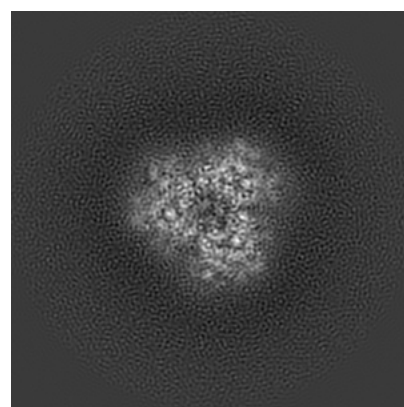
6.1.1 Primary map



X



Y

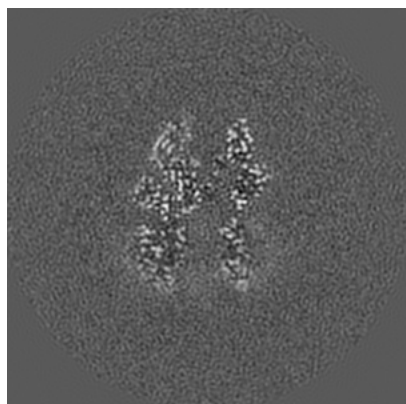


Z

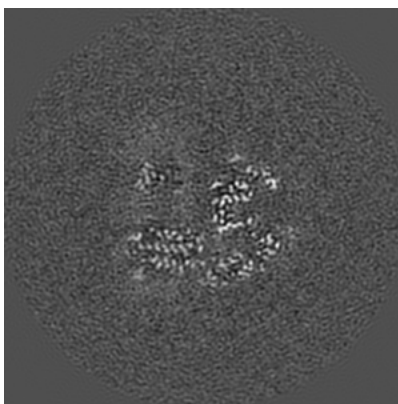
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

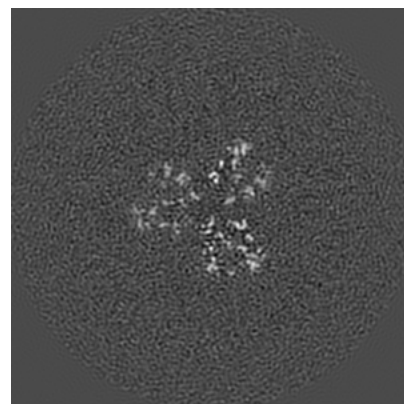
6.2.1 Primary map



X Index: 160



Y Index: 160

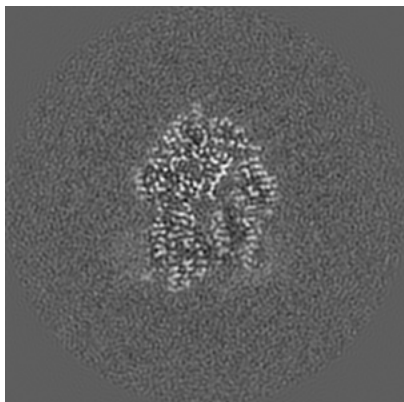


Z Index: 160

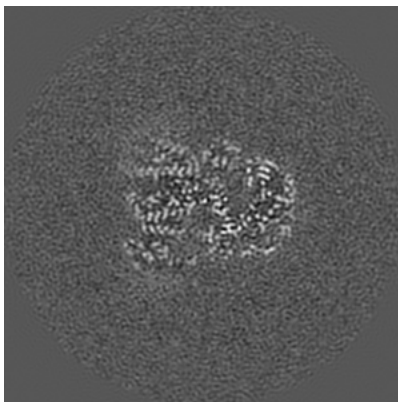
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

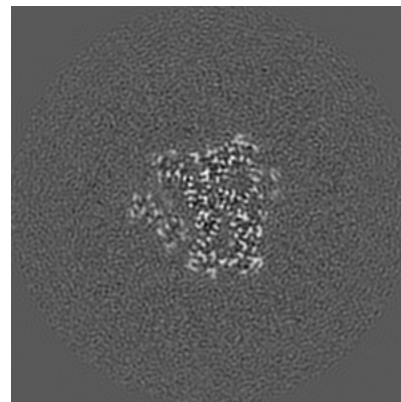
6.3.1 Primary map



X Index: 182



Y Index: 181

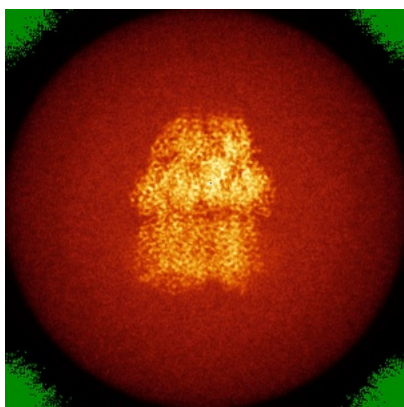


Z Index: 176

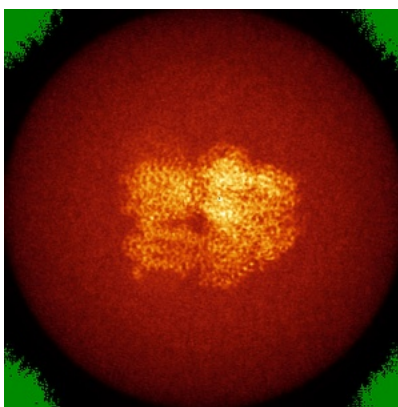
The images above show the largest variance slices of the map in three orthogonal directions.

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

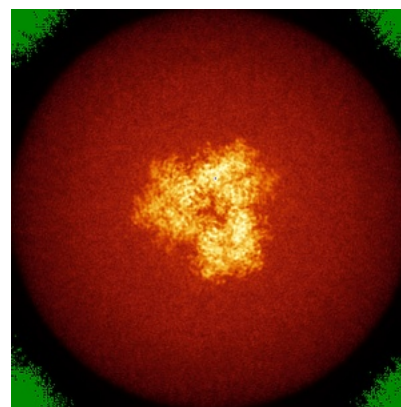
6.4.1 Primary map



X



Y

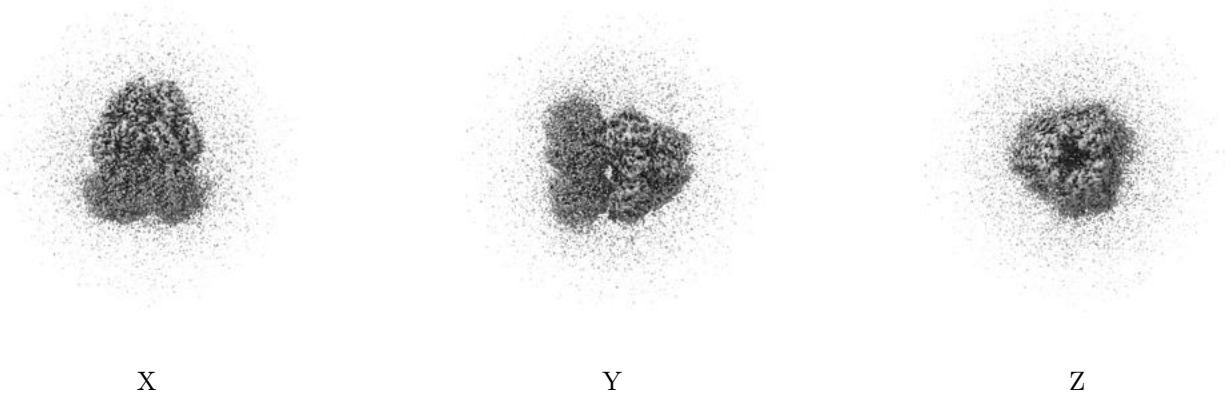


Z

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

6.5 Orthogonal surface views [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.

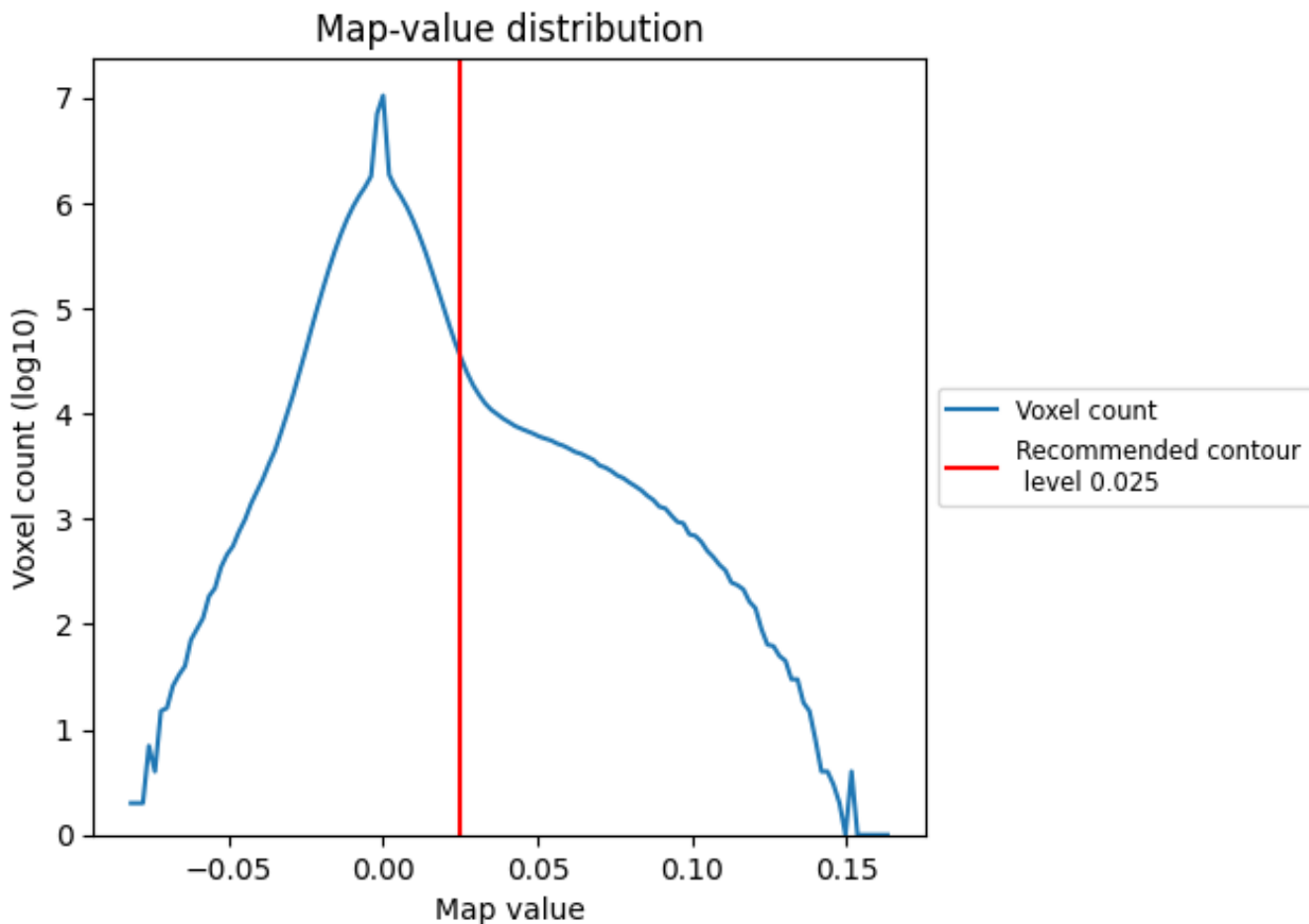
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

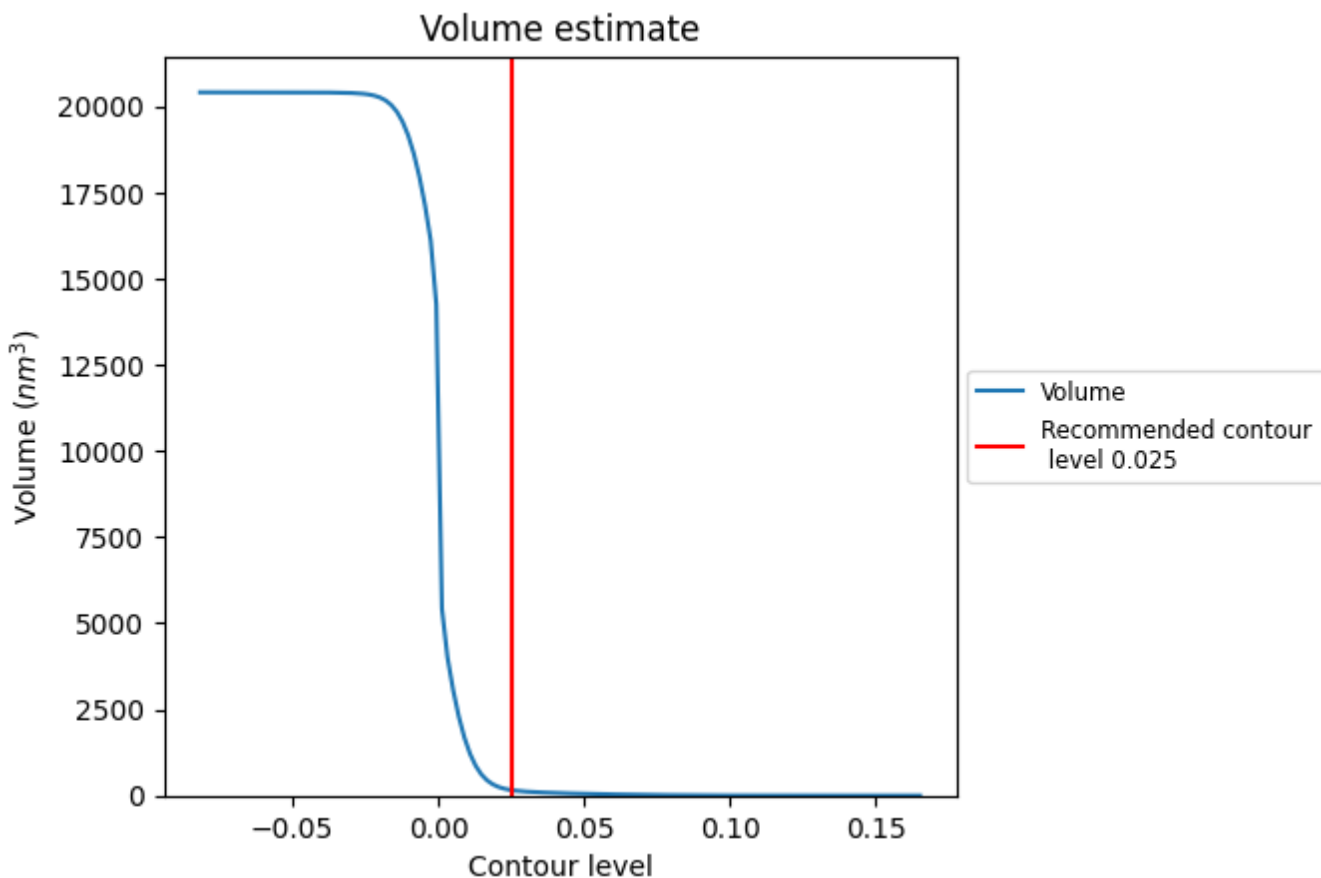
This section contains the results of statistical analysis of the map.

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.

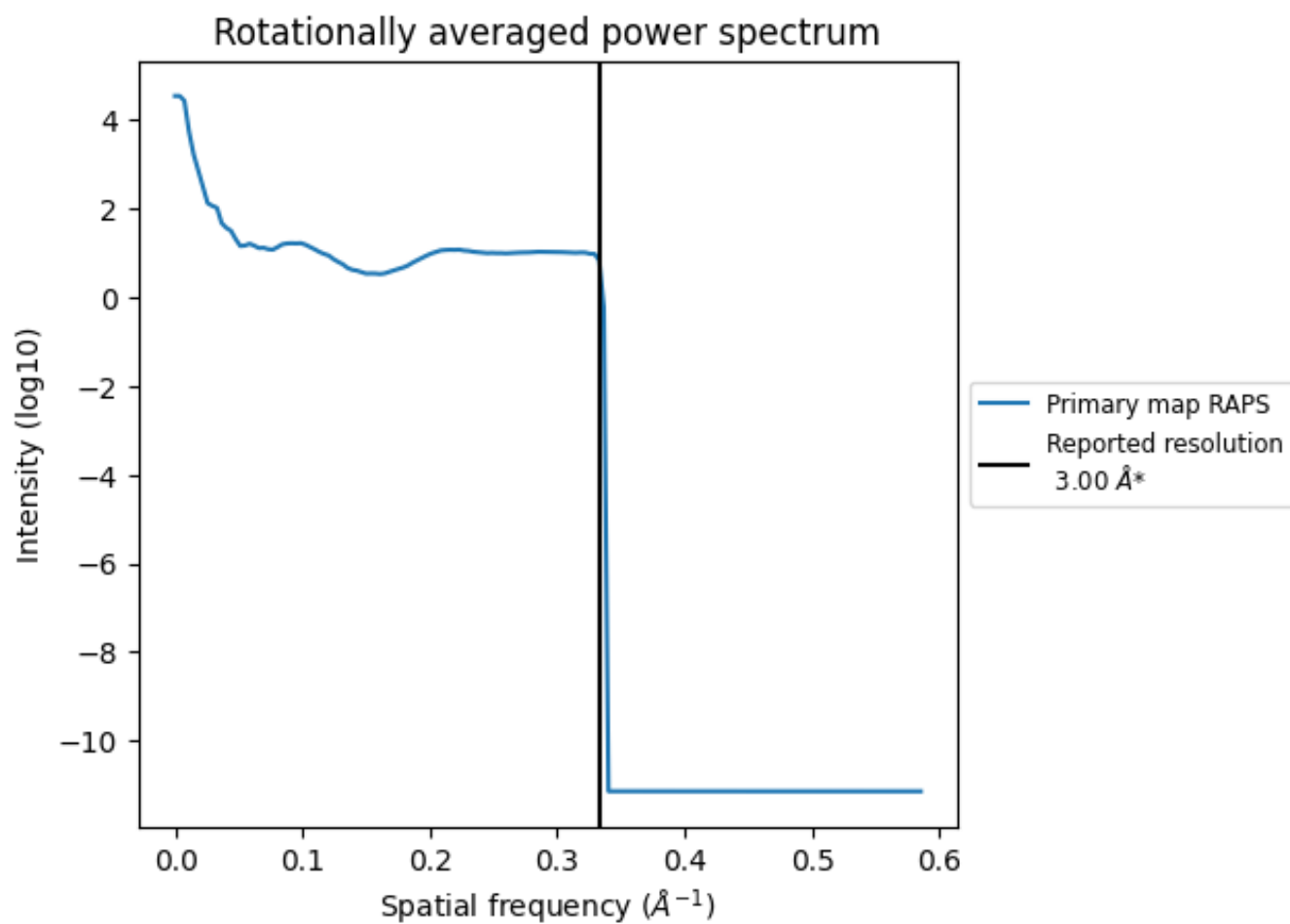
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 161 nm³; this corresponds to an approximate mass of 145 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 0.333 Å⁻¹

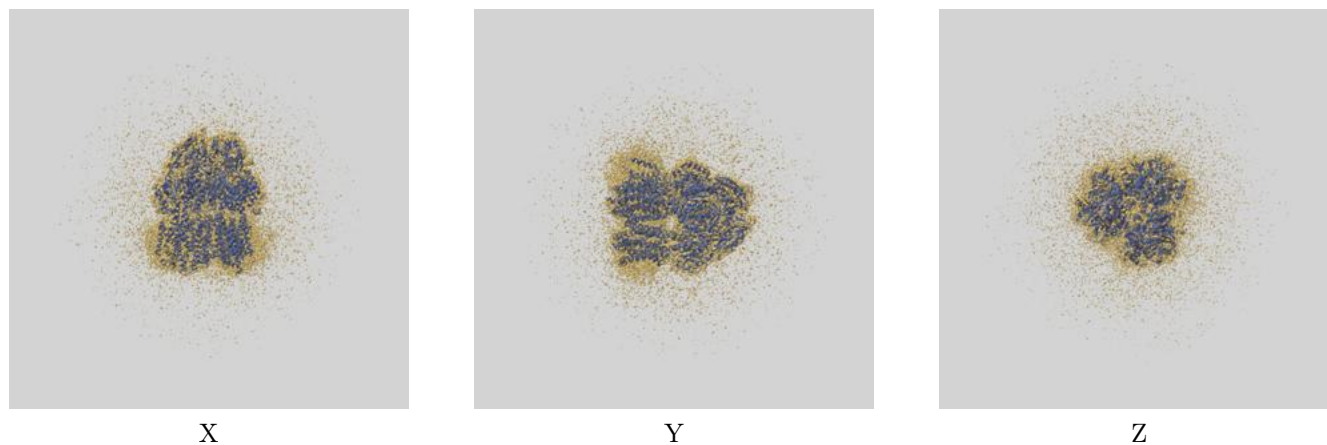
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

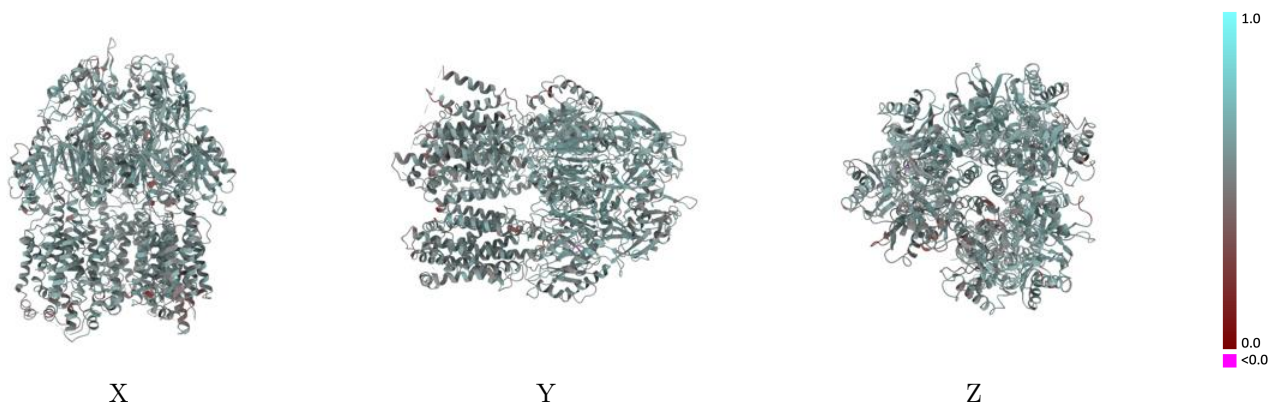
This section contains information regarding the fit between EMDB map EMD-7609 and PDB model 6CSX. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



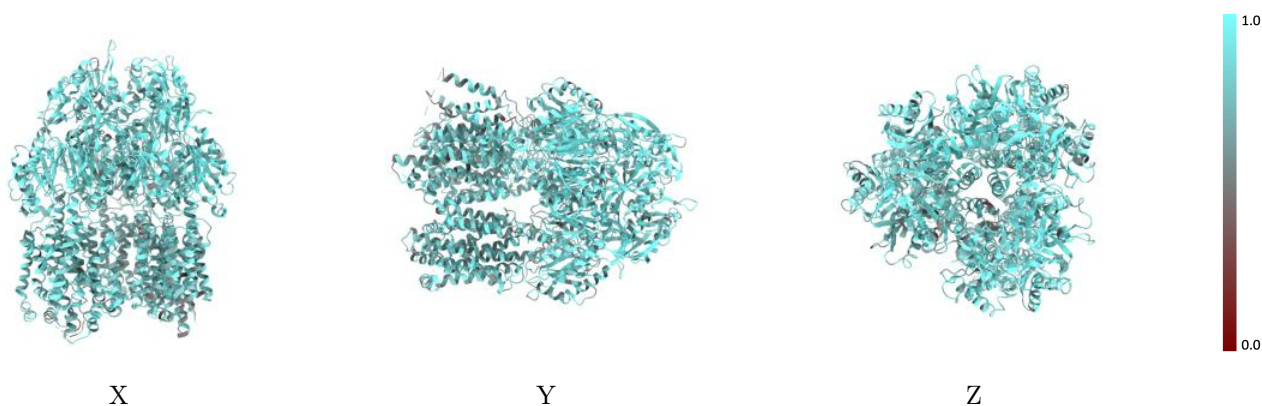
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



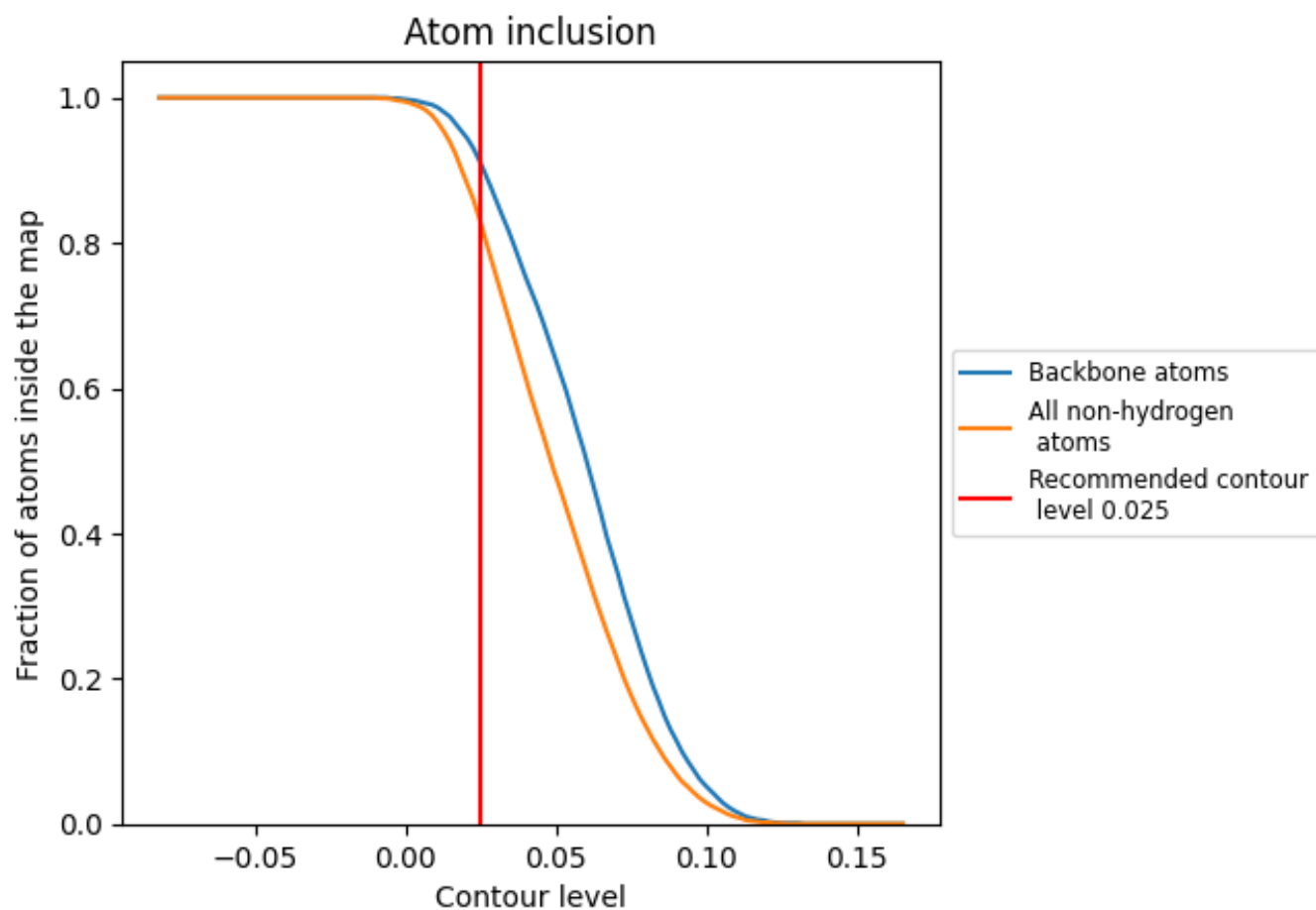
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 91% of all backbone atoms, 83% 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	 0.8280	 0.5530
A	 0.8340	 0.5610
B	 0.8040	 0.5440
C	 0.8450	 0.5550

