



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:30 AM UTC

PDB ID : 7D3U / pdb_00007d3u
EMDB ID : EMD-30567
Title : Structure of Mrp complex from Dietzia sp. DQ12-45-1b
Authors : Li, B.; Zhang, K.D.; Wu, X.L.; Zhang, X.C.
Deposited on : 2020-09-21
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

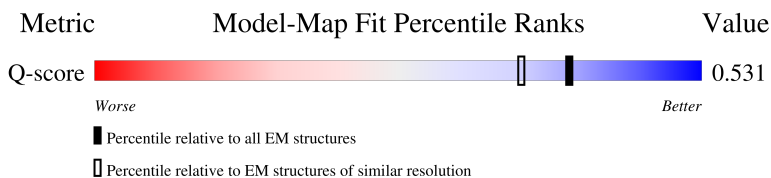
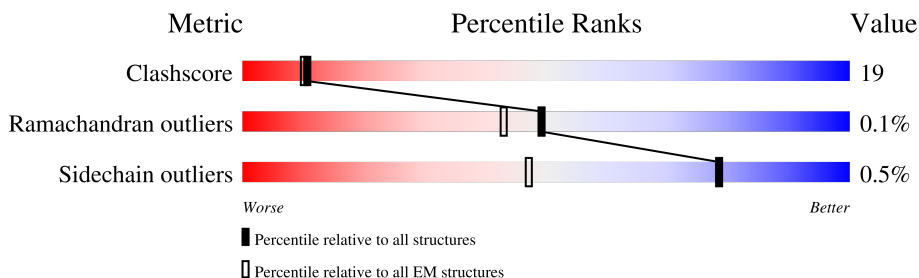
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	D	574	
2	A	958	
3	C	137	
4	F	85	

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Mol	Chain	Length	Quality of chain
5	G	125	
6	E	121	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	LMT	A	1207	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14333 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 Monovalent Na⁺/H⁺ antiporter subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	534	Total	C	N	O	S	0	0
			3897	2565	635	682	15		

- Molecule 2 is a protein called Monovalent Na⁺/H⁺ antiporter subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	904	Total	C	N	O	S	0	0
			6661	4367	1117	1148	29		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	expression tag	UNP A0A221C8X2

- Molecule 3 is a protein called Monovalent Na⁺/H⁺ antiporter subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	129	Total	C	N	O	S	0	0
			938	605	149	180	4		

- Molecule 4 is a protein called Monovalent Na⁺/H⁺ antiporter subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	85	Total	C	N	O	S	0	0
			629	414	108	104	3		

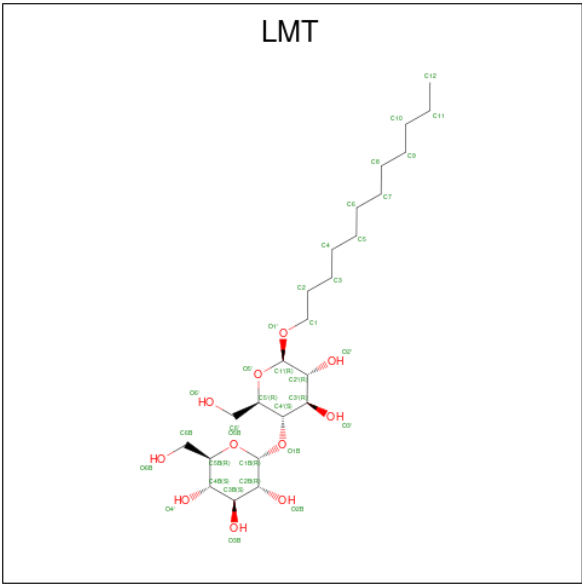
- Molecule 5 is a protein called Monovalent Na⁺/H⁺ antiporter subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	111	Total	C	N	O	S	0	0
			799	528	130	139	2		

- Molecule 6 is a protein called Cation antiporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	110	Total	C	N	O	S	0	0
			892	580	154	154	4		

- Molecule 7 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
7	D	1	Total	C		0
			12	12		
7	D	1	Total	C		0
			12	12		
7	D	1	Total	C	O	0
			35	24	11	
7	D	1	Total	C		0
			12	12		
7	D	1	Total	C		0
			12	12		
7	D	1	Total	C		0
			12	12		
7	D	1	Total	C	O	0
			35	24	11	
7	D	1	Total	C	O	0
			35	24	11	
7	D	1	Total	C		0
			12	12		

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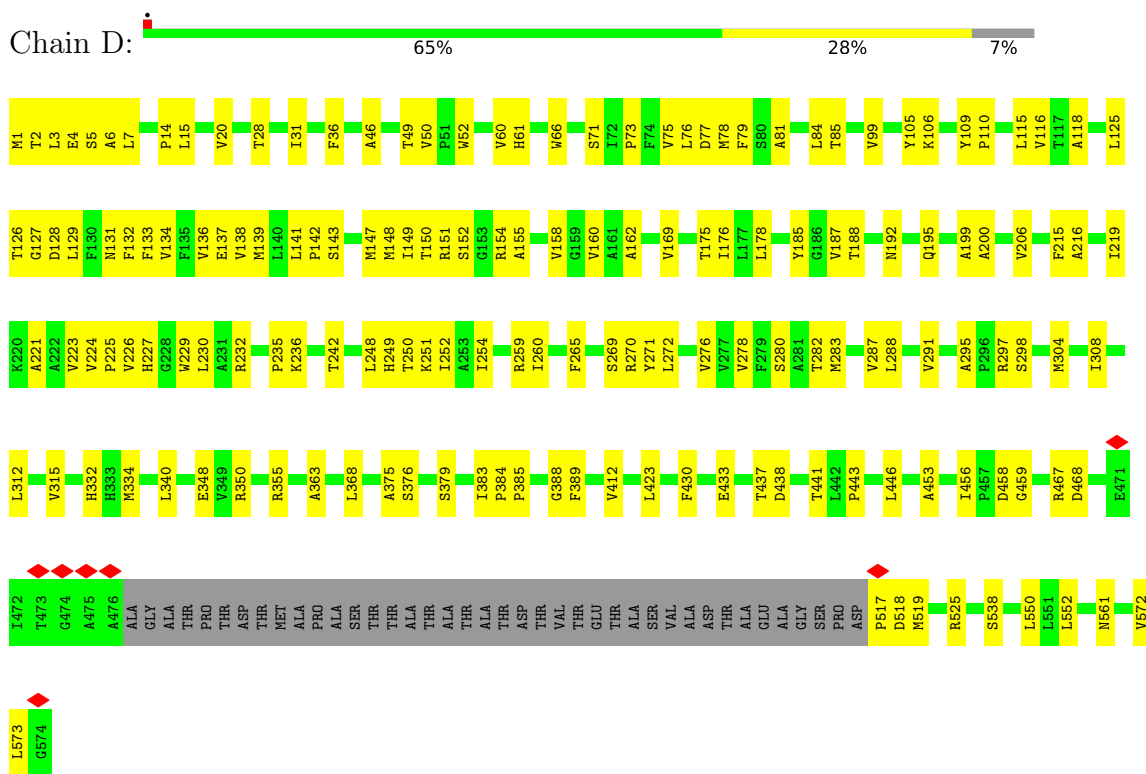
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Mol	Chain	Residues	Atoms	AltConf
7	D	1	Total C 12 12	0
7	A	1	Total C O 35 24 11	0
7	A	1	Total C O 35 24 11	0
7	A	1	Total C 12 12	0
7	A	1	Total C 12 12	0
7	A	1	Total C 12 12	0
7	A	1	Total C O 35 24 11	0
7	A	1	Total C 12 12	0
7	A	1	Total C 12 12	0
7	A	1	Total C O 35 24 11	0
7	A	1	Total C 9 9	0
7	A	1	Total C 12 12	0
7	A	1	Total C 12 12	0
7	A	1	Total C 12 12	0
7	A	1	Total C O 35 24 11	0
7	A	1	Total C 12 12	0
7	C	1	Total C 12 12	0
7	C	1	Total C 12 12	0

3 Residue-property plots

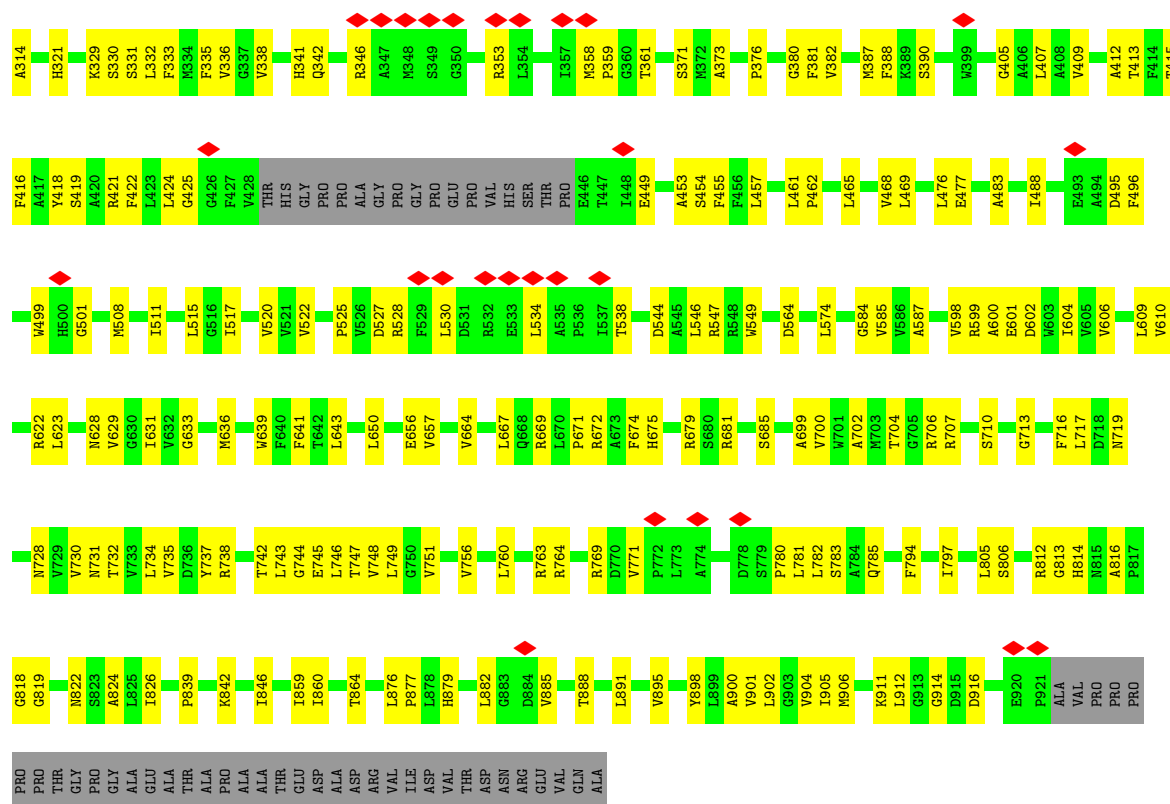
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Monovalent Na⁺/H⁺ antiporter subunit D

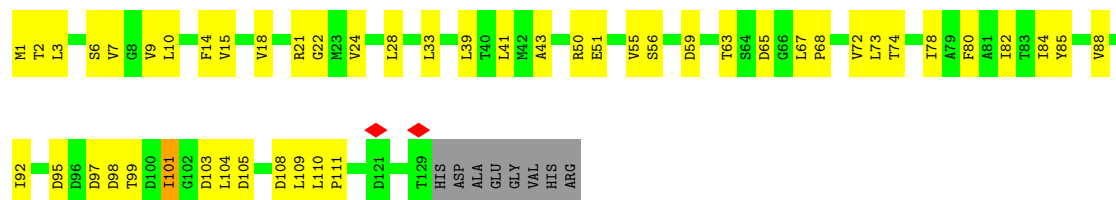


• Molecule 2: Monovalent Na⁺/H⁺ antiporter subunit A

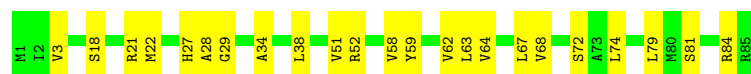




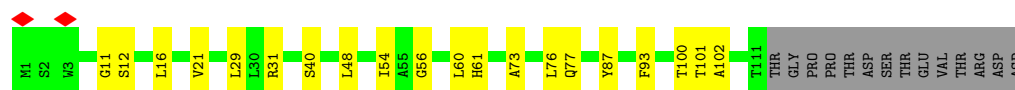
• Molecule 3: Monovalent Na⁺/H⁺ antiporter subunit C



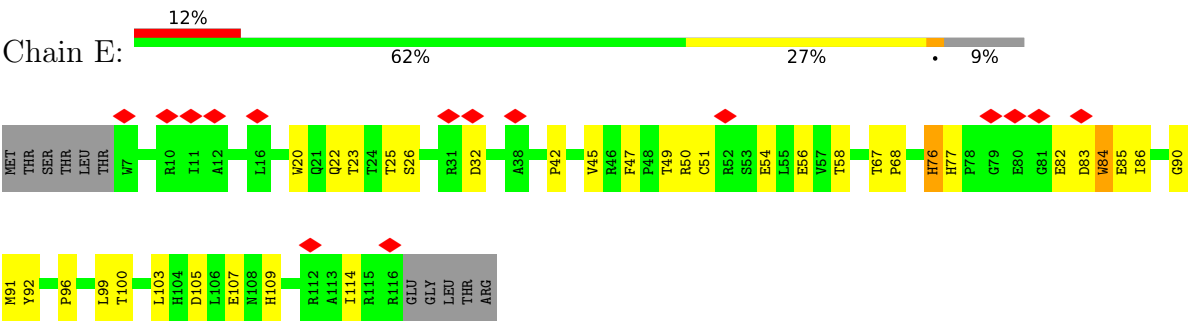
• Molecule 4: Monovalent Na⁺/H⁺ antiporter subunit F



• Molecule 5: Monovalent Na⁺/H⁺ antiporter subunit G



• Molecule 6: Cation antiporter



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93505	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 ($e^-/\text{\AA}^2$)	60	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	33.113	Depositor
Minimum map value	-18.337	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT

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	D	0.17	0/3977	0.35	1/5445 (0.0%)
2	A	0.17	0/6806	0.37	0/9312
3	C	0.17	0/957	0.34	0/1313
4	F	0.17	0/637	0.34	0/866
5	G	0.14	0/817	0.27	0/1116
6	E	0.22	0/923	0.45	0/1263
All	All	0.17	0/14117	0.36	1/19315 (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	D	517	PRO	N-CA-CB	6.77	110.44	103.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	D	3897	0	4109	151	0
2	A	6661	0	6938	340	0
3	C	938	0	953	72	0
4	F	629	0	688	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	799	0	829	28	0
6	E	892	0	867	32	0
7	A	292	0	447	29	0
7	C	24	0	46	1	0
7	D	201	0	320	4	0
All	All	14333	0	15197	553	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 19.

All (553) 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)
2:A:131:TRP:CZ2	2:A:213:LYS:HG3	1.65	1.32
2:A:44:TRP:CZ2	7:A:1209:LMT:H22	1.62	1.31
2:A:284:GLN:HE21	2:A:530:LEU:CD1	1.52	1.22
1:D:49:THR:CG2	1:D:76:LEU:HD21	1.74	1.17
1:D:49:THR:HG21	1:D:76:LEU:HD21	1.27	1.15
2:A:175:VAL:HG22	2:A:181:THR:HG22	1.28	1.11
2:A:734:LEU:HD11	3:C:73:LEU:HD23	1.25	1.10
2:A:288:LEU:HD12	2:A:346:ARG:HE	1.14	1.10
6:E:49:THR:HG22	6:E:51:CYS:SG	1.91	1.08
2:A:353:ARG:HD3	2:A:424:LEU:HB2	1.37	1.05
2:A:454:SER:HB3	7:A:1207:LMT:H101	1.38	1.03
1:D:28:THR:HG21	1:D:459:GLY:HA3	1.40	1.02
2:A:284:GLN:NE2	2:A:530:LEU:CD1	2.24	1.01
2:A:44:TRP:CH2	7:A:1209:LMT:C2	2.46	0.99
2:A:44:TRP:CH2	7:A:1209:LMT:H22	1.97	0.98
2:A:44:TRP:CZ2	7:A:1209:LMT:C2	2.46	0.98
1:D:412:VAL:HG22	2:A:165:LEU:HD21	1.46	0.97
1:D:224:VAL:O	1:D:227:HIS:HD2	1.46	0.96
2:A:284:GLN:NE2	2:A:530:LEU:HD12	1.78	0.96
2:A:131:TRP:CZ2	2:A:213:LYS:CG	2.48	0.96
2:A:175:VAL:CG2	2:A:181:THR:HG22	1.94	0.95
2:A:288:LEU:HD12	2:A:346:ARG:NE	1.82	0.94
1:D:552:LEU:CD1	2:A:61:LEU:HD13	1.96	0.94
1:D:187:VAL:CG2	1:D:206:VAL:HG22	2.00	0.91
2:A:284:GLN:HE21	2:A:530:LEU:HD11	1.33	0.91
1:D:28:THR:HG21	1:D:459:GLY:CA	2.01	0.91
2:A:760:LEU:HD23	3:C:92:ILE:HD11	1.53	0.90
2:A:763:ARG:HB2	3:C:92:ILE:HG21	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:PHE:CE1	3:C:18:VAL:HG21	2.07	0.90
6:E:32:ASP:OD1	6:E:92:TYR:HE2	1.55	0.90
2:A:353:ARG:HG2	2:A:425:GLY:H	1.35	0.89
1:D:552:LEU:HD13	2:A:61:LEU:HD13	1.54	0.89
2:A:132:GLU:HA	2:A:135:THR:HG22	1.55	0.89
1:D:412:VAL:HG22	2:A:165:LEU:CD2	2.03	0.88
2:A:598:VAL:HG21	3:C:1:MET:H3	1.38	0.88
1:D:141:LEU:HD22	2:A:748:VAL:HB	1.56	0.87
1:D:187:VAL:HG23	1:D:206:VAL:HG22	1.57	0.86
2:A:44:TRP:CH2	7:A:1209:LMT:H21	2.11	0.86
3:C:80:PHE:CZ	3:C:84:ILE:HD11	2.10	0.85
2:A:745:GLU:C	2:A:748:VAL:HG22	2.01	0.85
2:A:412:ALA:HA	2:A:415:THR:HG22	1.59	0.84
1:D:49:THR:HG21	1:D:76:LEU:CD2	2.06	0.84
2:A:636:MET:SD	3:C:39:LEU:HD11	2.18	0.84
6:E:105:ASP:O	6:E:109:HIS:CD2	2.30	0.84
2:A:131:TRP:CE2	2:A:213:LYS:HG3	2.12	0.84
5:G:56:GLY:O	5:G:60:LEU:HD13	1.78	0.84
2:A:288:LEU:HD11	2:A:346:ARG:HH21	1.42	0.83
2:A:598:VAL:CG2	3:C:1:MET:N	2.41	0.83
5:G:48:LEU:HD11	6:E:25:THR:HG22	1.62	0.82
1:D:224:VAL:O	1:D:227:HIS:CD2	2.32	0.82
2:A:636:MET:HE1	3:C:39:LEU:HG	1.62	0.81
2:A:745:GLU:O	2:A:748:VAL:HG22	1.78	0.81
2:A:763:ARG:HB2	3:C:92:ILE:CG2	2.10	0.81
2:A:763:ARG:CB	3:C:92:ILE:CG2	2.58	0.81
1:D:46:ALA:CB	1:D:85:THR:HG22	2.12	0.80
3:C:10:LEU:HD12	3:C:39:LEU:HD12	1.61	0.80
1:D:383:ILE:HG22	1:D:385:PRO:HD2	1.64	0.80
2:A:598:VAL:CG2	3:C:1:MET:H3	1.94	0.80
2:A:745:GLU:O	2:A:748:VAL:CG2	2.30	0.80
6:E:49:THR:CG2	6:E:51:CYS:SG	2.70	0.80
2:A:745:GLU:HA	2:A:748:VAL:HG22	1.63	0.79
1:D:552:LEU:HD13	2:A:61:LEU:CD1	2.13	0.79
2:A:707:ARG:HH22	2:A:710:SER:N	1.80	0.79
2:A:734:LEU:CD1	3:C:73:LEU:HD23	2.13	0.77
2:A:353:ARG:HD3	2:A:424:LEU:CB	2.14	0.77
2:A:284:GLN:HE21	2:A:530:LEU:HD12	1.35	0.77
6:E:32:ASP:OD1	6:E:92:TYR:CE2	2.38	0.77
2:A:353:ARG:CZ	2:A:424:LEU:HD13	2.15	0.76
2:A:131:TRP:HZ2	2:A:213:LYS:HG3	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:734:LEU:HD11	3:C:73:LEU:CD2	2.09	0.76
2:A:763:ARG:HB3	3:C:92:ILE:HG23	1.67	0.76
5:G:48:LEU:CD1	6:E:25:THR:HG22	2.15	0.76
2:A:745:GLU:CA	2:A:748:VAL:HG22	2.16	0.76
2:A:424:LEU:HD12	2:A:424:LEU:O	1.87	0.75
1:D:552:LEU:CD1	2:A:61:LEU:CD1	2.63	0.75
2:A:622:ARG:HD2	2:A:671:PRO:O	1.83	0.75
2:A:745:GLU:HA	2:A:748:VAL:CG2	2.17	0.75
1:D:552:LEU:HD11	2:A:61:LEU:HD13	1.71	0.73
2:A:453:ALA:O	2:A:457:LEU:HD12	1.89	0.73
2:A:600:ALA:HB3	4:F:52:ARG:HH11	1.54	0.73
2:A:263:TRP:O	2:A:267:LEU:HD13	1.88	0.72
1:D:412:VAL:CG2	2:A:165:LEU:HD21	2.19	0.72
1:D:443:PRO:HG2	1:D:446:LEU:HD13	1.71	0.72
1:D:148:MET:HE1	1:D:160:VAL:HG22	1.71	0.72
5:G:48:LEU:HD11	6:E:25:THR:CG2	2.20	0.72
2:A:131:TRP:HZ2	2:A:213:LYS:CG	2.01	0.72
1:D:49:THR:HG22	1:D:76:LEU:HD21	1.71	0.71
2:A:141:LEU:HD13	2:A:233:VAL:HG13	1.72	0.71
2:A:353:ARG:CD	2:A:424:LEU:HB2	2.18	0.70
2:A:361:THR:O	2:A:361:THR:HG22	1.89	0.70
1:D:187:VAL:HG21	1:D:206:VAL:HG22	1.74	0.70
1:D:223:VAL:HG23	1:D:225:PRO:HD2	1.74	0.70
2:A:453:ALA:O	2:A:457:LEU:CD1	2.40	0.70
7:D:607:LMT:H112	7:D:608:LMT:H91	1.73	0.69
1:D:46:ALA:HB1	1:D:85:THR:CG2	2.22	0.69
1:D:49:THR:CG2	1:D:76:LEU:CD2	2.64	0.69
2:A:108:MET:SD	2:A:233:VAL:HG22	2.33	0.69
2:A:44:TRP:CZ3	2:A:74:ARG:HG2	2.28	0.69
5:G:54:ILE:HG13	5:G:77:GLN:HE22	1.58	0.69
2:A:601:GLU:HB3	4:F:52:ARG:HD3	1.74	0.68
1:D:116:VAL:HG23	1:D:142:PRO:HB2	1.74	0.68
2:A:600:ALA:HB3	4:F:52:ARG:NH1	2.09	0.68
2:A:763:ARG:CB	3:C:92:ILE:HG23	2.23	0.68
1:D:295:ALA:HB3	1:D:298:SER:HB3	1.75	0.68
1:D:50:VAL:HG13	1:D:78:MET:HE1	1.75	0.67
2:A:44:TRP:CZ3	2:A:74:ARG:HD3	2.29	0.67
6:E:50:ARG:NH1	6:E:107:GLU:OE2	2.27	0.67
6:E:83:ASP:O	6:E:84:TRP:O	2.12	0.67
1:D:77:ASP:O	1:D:561:ASN:ND2	2.27	0.67
1:D:28:THR:CG2	1:D:459:GLY:HA3	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ALA:HB1	1:D:85:THR:HG22	1.76	0.67
2:A:263:TRP:CZ2	2:A:267:LEU:HD21	2.30	0.67
4:F:3:VAL:HG21	5:G:12:SER:OG	1.95	0.67
2:A:43:ILE:HA	2:A:47:ILE:HD12	1.77	0.67
2:A:876:LEU:HD12	2:A:877:PRO:HD2	1.76	0.66
2:A:288:LEU:CD1	2:A:346:ARG:HE	2.02	0.66
2:A:45:PHE:HE1	7:A:1210:LMT:H32	1.61	0.65
2:A:237:LEU:HA	2:A:241:ALA:HB3	1.79	0.65
2:A:405:GLY:O	2:A:409:VAL:HG23	1.96	0.65
2:A:44:TRP:HE1	7:A:1210:LMT:H51	1.61	0.65
2:A:342:GLN:NE2	2:A:449:GLU:O	2.29	0.65
2:A:744:GLY:O	2:A:748:VAL:HG13	1.96	0.65
1:D:141:LEU:HD22	2:A:748:VAL:CB	2.25	0.65
2:A:622:ARG:HD3	2:A:667:LEU:HD22	1.79	0.65
2:A:44:TRP:NE1	7:A:1210:LMT:H51	2.10	0.65
1:D:14:PRO:HB2	1:D:118:ALA:HB2	1.77	0.65
1:D:116:VAL:CG2	1:D:142:PRO:HB2	2.26	0.65
1:D:175:THR:HG21	3:C:33:LEU:HG	1.78	0.64
6:E:82:GLU:O	6:E:83:ASP:HB2	1.96	0.64
1:D:312:LEU:O	1:D:315:VAL:HG12	1.97	0.64
1:D:137:GLU:O	1:D:141:LEU:HD13	1.97	0.64
2:A:477:GLU:HG2	2:A:495:ASP:HA	1.79	0.64
2:A:763:ARG:CB	3:C:92:ILE:HG21	2.24	0.64
1:D:132:PHE:O	1:D:136:VAL:HG23	1.97	0.64
2:A:44:TRP:CE3	2:A:74:ARG:HG2	2.32	0.64
2:A:88:MET:HE1	2:A:108:MET:HB3	1.80	0.64
2:A:813:GLY:HA3	2:A:819:GLY:HA2	1.79	0.64
2:A:353:ARG:NH1	2:A:424:LEU:HD13	2.12	0.64
2:A:756:VAL:HG22	3:C:88:VAL:HG11	1.79	0.63
2:A:700:VAL:HG21	3:C:7:VAL:HG11	1.80	0.63
5:G:100:THR:HG22	5:G:102:ALA:H	1.63	0.63
1:D:384:PRO:HG2	2:A:132:GLU:HB2	1.80	0.63
1:D:141:LEU:CD2	2:A:748:VAL:HB	2.26	0.62
1:D:200:ALA:HB3	1:D:265:PHE:HA	1.81	0.62
3:C:14:PHE:CD1	3:C:18:VAL:HG21	2.34	0.62
2:A:707:ARG:NH2	2:A:710:SER:N	2.47	0.62
2:A:749:LEU:HD22	2:A:904:VAL:HG11	1.80	0.62
1:D:224:VAL:HB	1:D:282:THR:HA	1.82	0.62
2:A:260:VAL:HG23	2:A:263:TRP:HB3	1.82	0.62
2:A:599:ARG:HB2	2:A:602:ASP:OD2	2.01	0.61
2:A:73:ALA:O	2:A:77:THR:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:LEU:HD11	1:D:76:LEU:HD22	1.82	0.60
2:A:629:VAL:HG21	3:C:28:LEU:HD22	1.83	0.60
2:A:412:ALA:CA	2:A:415:THR:HG22	2.31	0.60
2:A:628:ASN:ND2	4:F:22:MET:SD	2.75	0.60
1:D:225:PRO:HG2	7:D:607:LMT:H122	1.82	0.60
2:A:763:ARG:HB3	3:C:92:ILE:CG2	2.27	0.60
2:A:453:ALA:O	2:A:457:LEU:HG	2.02	0.59
2:A:46:ALA:O	2:A:47:ILE:HG13	2.02	0.59
2:A:657:VAL:HG23	4:F:72:SER:HB3	1.83	0.59
5:G:56:GLY:O	5:G:60:LEU:CD1	2.49	0.59
2:A:44:TRP:CZ3	2:A:74:ARG:CD	2.85	0.59
4:F:59:TYR:HA	4:F:62:VAL:HB	1.85	0.59
2:A:610:VAL:HG22	3:C:9:VAL:HG21	1.85	0.59
2:A:303:LEU:HD21	2:A:321:HIS:HB3	1.85	0.59
2:A:454:SER:HB3	7:A:1207:LMT:C10	2.22	0.59
7:A:1213:LMT:H52	7:C:2201:LMT:H61	1.85	0.58
6:E:83:ASP:O	6:E:84:TRP:C	2.45	0.58
1:D:251:LYS:HG2	1:D:334:MET:HE2	1.85	0.58
2:A:373:ALA:HB2	2:A:419:SER:OG	2.04	0.58
1:D:106:LYS:NZ	1:D:458:ASP:OD2	2.36	0.58
1:D:270:ARG:NH2	1:D:271:TYR:OH	2.37	0.58
2:A:141:LEU:HD13	2:A:233:VAL:CG1	2.33	0.58
2:A:341:HIS:CD2	2:A:341:HIS:O	2.56	0.58
2:A:412:ALA:O	2:A:415:THR:HG22	2.03	0.58
1:D:340:LEU:HD13	1:D:376:SER:HB2	1.85	0.58
2:A:760:LEU:HD12	2:A:911:LYS:HB3	1.85	0.58
2:A:454:SER:CB	7:A:1207:LMT:H101	2.26	0.58
6:E:45:VAL:HG21	6:E:99:LEU:HD23	1.86	0.58
1:D:46:ALA:C	1:D:85:THR:HG22	2.29	0.58
2:A:189:ASP:HB3	2:A:191:VAL:HG12	1.86	0.58
2:A:288:LEU:HD11	2:A:346:ARG:NH2	2.18	0.58
2:A:132:GLU:CA	2:A:135:THR:HG22	2.29	0.57
1:D:384:PRO:HB3	2:A:129:VAL:HG22	1.85	0.57
2:A:806:SER:OG	2:A:826:ILE:HG23	2.04	0.57
1:D:552:LEU:HD11	2:A:61:LEU:CD1	2.32	0.57
2:A:66:ARG:HG2	2:A:122:ASP:HB3	1.86	0.57
2:A:175:VAL:HG22	2:A:181:THR:CG2	2.19	0.57
2:A:295:SER:OG	2:A:329:LYS:NZ	2.33	0.57
2:A:760:LEU:CD2	3:C:92:ILE:HD11	2.33	0.57
2:A:412:ALA:HA	2:A:415:THR:CG2	2.31	0.57
2:A:707:ARG:HH22	2:A:710:SER:CA	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:LEU:HD22	2:A:747:THR:HG21	1.88	0.56
2:A:585:VAL:HA	7:A:1212:LMT:H51	1.87	0.56
6:E:105:ASP:O	6:E:109:HIS:HD2	1.85	0.56
1:D:230:LEU:HD21	1:D:304:MET:HE3	1.86	0.56
2:A:132:GLU:HA	2:A:135:THR:CG2	2.32	0.56
1:D:160:VAL:HG21	2:A:763:ARG:HD3	1.88	0.56
2:A:771:VAL:O	4:F:84:ARG:NH1	2.38	0.56
2:A:601:GLU:OE1	4:F:52:ARG:NE	2.36	0.56
2:A:623:LEU:HD23	4:F:28:ALA:HB1	1.88	0.56
3:C:21:ARG:NH2	3:C:98:ASP:OD2	2.38	0.56
1:D:150:THR:HG22	1:D:151:ARG:N	2.19	0.56
2:A:469:LEU:HD13	2:A:476:LEU:HD11	1.88	0.56
1:D:363:ALA:HB2	1:D:430:PHE:HB3	1.88	0.56
5:G:40:SER:OG	6:E:91:MET:SD	2.61	0.56
2:A:598:VAL:HG23	3:C:1:MET:N	2.22	0.55
2:A:672:ARG:HE	2:A:769:ARG:HH22	1.54	0.55
2:A:135:THR:HB	2:A:213:LYS:NZ	2.22	0.55
3:C:10:LEU:CD1	3:C:39:LEU:HD12	2.33	0.55
6:E:77:HIS:HB3	6:E:84:TRP:HA	1.89	0.55
1:D:158:VAL:HG22	3:C:104:LEU:HG	1.89	0.55
1:D:423:LEU:HD11	2:A:157:LEU:HD23	1.89	0.55
2:A:141:LEU:HD22	2:A:233:VAL:HG21	1.88	0.55
2:A:151:GLN:NE2	2:A:547:ARG:HH22	2.05	0.54
1:D:128:ASP:OD1	1:D:131:ASN:HB3	2.08	0.54
2:A:818:GLY:HA2	2:A:822:ASN:ND2	2.21	0.54
1:D:154:ARG:NH2	1:D:468:ASP:OD2	2.40	0.54
2:A:288:LEU:CD1	2:A:346:ARG:HH21	2.19	0.54
6:E:42:PRO:HA	6:E:90:GLY:O	2.07	0.54
1:D:133:PHE:O	1:D:137:GLU:HG2	2.08	0.54
2:A:272:MET:HE2	2:A:407:LEU:HB3	1.88	0.54
5:G:73:ALA:O	5:G:77:GLN:HG3	2.07	0.54
2:A:76:PHE:HA	2:A:79:ILE:HG22	1.88	0.54
2:A:155:ARG:NH1	2:A:544:ASP:OD2	2.41	0.54
2:A:361:THR:O	2:A:361:THR:CG2	2.54	0.54
1:D:250:THR:O	1:D:254:ILE:HG12	2.07	0.54
2:A:650:LEU:HD21	4:F:64:VAL:HG21	1.90	0.54
2:A:285:ARG:O	2:A:421:ARG:NH1	2.41	0.54
3:C:55:VAL:HG12	3:C:56:SER:N	2.23	0.54
2:A:669:ARG:NH2	2:A:914:GLY:O	2.40	0.54
2:A:657:VAL:HB	4:F:68:VAL:HG13	1.90	0.53
1:D:453:ALA:HA	2:A:764:ARG:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:453:ALA:O	2:A:457:LEU:CG	2.56	0.53
1:D:49:THR:HG23	1:D:52:TRP:HE3	1.73	0.53
6:E:45:VAL:CG2	6:E:99:LEU:HD23	2.39	0.53
1:D:178:LEU:HD11	3:C:41:LEU:HD11	1.91	0.53
1:D:235:PRO:HG3	1:D:298:SER:HA	1.91	0.53
2:A:203:ALA:HB1	2:A:263:TRP:HB2	1.90	0.53
2:A:574:LEU:HD13	3:C:15:VAL:HG13	1.89	0.53
1:D:550:LEU:HB2	7:A:1214:LMT:H4B	1.91	0.53
2:A:331:SER:HB3	2:A:462:PRO:HB2	1.91	0.53
2:A:353:ARG:HG2	2:A:425:GLY:N	2.16	0.53
2:A:117:GLY:HA3	7:A:1214:LMT:H123	1.91	0.53
2:A:641:PHE:HZ	4:F:58:VAL:HG22	1.75	0.53
2:A:743:LEU:HD12	2:A:746:LEU:HD11	1.91	0.53
3:C:24:VAL:O	3:C:28:LEU:HG	2.09	0.53
2:A:636:MET:SD	3:C:39:LEU:HD21	2.49	0.52
3:C:68:PRO:O	3:C:72:VAL:HG12	2.09	0.52
1:D:412:VAL:HG22	2:A:165:LEU:HD23	1.90	0.52
2:A:415:THR:HA	2:A:418:TYR:CE2	2.44	0.52
2:A:606:VAL:HG21	3:C:2:THR:HB	1.91	0.52
1:D:150:THR:HG21	1:D:446:LEU:HD23	1.92	0.52
2:A:599:ARG:N	2:A:602:ASP:OD2	2.40	0.52
3:C:105:ASP:O	3:C:108:ASP:OD1	2.28	0.52
2:A:215:ALA:HB3	2:A:297:ILE:HG12	1.91	0.52
3:C:10:LEU:HD12	3:C:39:LEU:CD1	2.36	0.52
3:C:14:PHE:HE1	3:C:18:VAL:HG21	1.65	0.52
2:A:707:ARG:HH22	2:A:710:SER:H	1.58	0.51
6:E:47:PHE:HD2	6:E:86:ILE:HD11	1.75	0.51
6:E:20:TRP:HA	6:E:23:THR:HG22	1.93	0.51
2:A:17:SER:OG	2:A:18:PRO:HD3	2.11	0.51
2:A:141:LEU:HB3	2:A:233:VAL:HG11	1.91	0.51
1:D:219:ILE:HG12	1:D:226:VAL:HG21	1.92	0.51
1:D:375:ALA:HB3	1:D:538:SER:OG	2.11	0.51
4:F:34:ALA:O	4:F:38:LEU:HG	2.10	0.51
1:D:162:ALA:HB2	1:D:236:LYS:HD2	1.92	0.51
2:A:604:ILE:HG22	7:A:1202:LMT:H102	1.91	0.51
1:D:36:PHE:HE2	1:D:99:VAL:HG21	1.76	0.51
1:D:412:VAL:O	2:A:165:LEU:HD21	2.10	0.51
2:A:93:ARG:HH11	7:A:1208:LMT:H92	1.75	0.51
2:A:601:GLU:HB3	4:F:52:ARG:CD	2.40	0.51
3:C:14:PHE:CG	3:C:33:LEU:HB2	2.46	0.51
1:D:109:TYR:HB3	1:D:110:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:130:ALA:O	2:A:134:THR:HG23	2.11	0.50
3:C:22:GLY:H	3:C:99:THR:HG22	1.75	0.50
1:D:412:VAL:CG2	2:A:165:LEU:CD2	2.82	0.50
2:A:707:ARG:HH22	2:A:710:SER:HB3	1.76	0.50
1:D:199:ALA:O	1:D:206:VAL:HG11	2.11	0.50
1:D:254:ILE:HD12	1:D:312:LEU:HG	1.94	0.50
2:A:139:PHE:O	2:A:143:THR:HG23	2.12	0.50
2:A:263:TRP:NE1	2:A:267:LEU:HD22	2.26	0.50
2:A:306:THR:HG21	2:A:387:MET:HE2	1.92	0.50
1:D:76:LEU:HD11	1:D:81:ALA:HB2	1.92	0.50
1:D:232:ARG:NH1	3:C:103:ASP:OD1	2.45	0.50
2:A:745:GLU:O	2:A:748:VAL:HG23	2.09	0.50
2:A:44:TRP:CZ3	2:A:74:ARG:CG	2.95	0.50
2:A:138:SER:O	2:A:142:ILE:HG12	2.11	0.50
2:A:250:LEU:HD12	2:A:304:VAL:HG12	1.93	0.50
4:F:3:VAL:HG23	5:G:16:LEU:HG	1.93	0.50
1:D:28:THR:CG2	1:D:459:GLY:CA	2.84	0.49
2:A:609:LEU:HD23	3:C:6:SER:HB2	1.93	0.49
6:E:32:ASP:OD2	6:E:91:MET:HE1	2.12	0.49
1:D:77:ASP:OD2	1:D:259:ARG:NH1	2.37	0.49
4:F:74:LEU:HD22	5:G:87:TYR:HD2	1.76	0.49
2:A:32:LEU:HD13	2:A:109:THR:HG21	1.95	0.49
1:D:60:VAL:HG11	1:D:572:VAL:HA	1.95	0.49
2:A:376:PRO:HA	2:A:381:PHE:CG	2.48	0.49
1:D:84:LEU:HD11	1:D:125:LEU:HD21	1.93	0.49
1:D:199:ALA:O	1:D:206:VAL:CG1	2.61	0.49
2:A:622:ARG:HG2	2:A:674:PHE:CE1	2.47	0.49
1:D:384:PRO:HA	1:D:389:PHE:CG	2.46	0.49
2:A:202:ILE:HG22	2:A:257:LEU:HD11	1.95	0.49
2:A:314:ALA:HA	2:A:390:SER:OG	2.13	0.49
4:F:81:SER:OG	4:F:84:ARG:O	2.27	0.49
2:A:598:VAL:CG2	3:C:1:MET:H2	2.21	0.48
2:A:44:TRP:CD1	7:A:1210:LMT:H51	2.49	0.48
2:A:69:LEU:HG	2:A:69:LEU:O	2.13	0.48
2:A:412:ALA:C	2:A:415:THR:HG22	2.38	0.48
1:D:3:LEU:O	1:D:3:LEU:HD13	2.14	0.48
2:A:633:GLY:HA3	2:A:656:GLU:HG3	1.96	0.48
7:A:1209:LMT:H12	7:A:1209:LMT:H41	1.72	0.48
2:A:63:VAL:HG13	2:A:123:ASP:OD2	2.14	0.48
6:E:54:GLU:O	6:E:58:THR:HG22	2.14	0.48
1:D:66:TRP:HB2	1:D:71:SER:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:VAL:HG21	1:D:229:TRP:HB2	1.96	0.47
2:A:734:LEU:CD1	3:C:73:LEU:CD2	2.85	0.47
1:D:20:VAL:HA	2:A:859:ILE:HD11	1.96	0.47
3:C:85:TYR:HA	3:C:88:VAL:HG12	1.97	0.47
2:A:824:ALA:HB2	2:A:898:TYR:HA	1.95	0.47
5:G:11:GLY:C	5:G:60:LEU:HD11	2.40	0.47
2:A:78:MET:CE	7:A:1210:LMT:C9	2.92	0.47
4:F:59:TYR:O	4:F:63:LEU:N	2.38	0.47
4:F:67:LEU:HD21	5:G:76:LEU:HD13	1.97	0.47
6:E:114:ILE:HD12	6:E:114:ILE:O	2.13	0.47
2:A:199:ALA:HB1	2:A:257:LEU:CD2	2.44	0.47
2:A:742:THR:HA	2:A:745:GLU:HG2	1.97	0.47
1:D:126:THR:OG1	1:D:131:ASN:ND2	2.41	0.47
2:A:263:TRP:CE2	2:A:267:LEU:CD2	2.97	0.47
3:C:10:LEU:CD1	3:C:39:LEU:CD1	2.92	0.47
1:D:192:ASN:HB3	1:D:195:GLN:HG3	1.97	0.47
2:A:123:ASP:HB3	2:A:126:VAL:HG12	1.97	0.47
2:A:302:PHE:O	2:A:306:THR:HG22	2.15	0.47
2:A:346:ARG:HA	2:A:346:ARG:HD2	1.74	0.47
4:F:27:HIS:CD2	4:F:29:GLY:H	2.32	0.47
2:A:879:HIS:HA	2:A:888:THR:HA	1.95	0.47
3:C:14:PHE:CD1	3:C:18:VAL:CG2	2.98	0.47
2:A:338:VAL:HG23	2:A:455:PHE:CE2	2.50	0.47
2:A:601:GLU:O	2:A:601:GLU:HG2	2.14	0.47
1:D:142:PRO:HG3	2:A:751:VAL:HG21	1.97	0.46
2:A:373:ALA:HB1	2:A:416:PHE:HD1	1.79	0.46
2:A:44:TRP:CE2	7:A:1209:LMT:H22	2.35	0.46
2:A:115:MET:O	2:A:119:VAL:HG22	2.15	0.46
2:A:254:SER:O	2:A:258:HIS:HB3	2.16	0.46
2:A:263:TRP:CE2	2:A:267:LEU:HD21	2.49	0.46
2:A:584:GLY:HA2	2:A:587:ALA:HB3	1.96	0.46
2:A:636:MET:HE1	3:C:39:LEU:CG	2.37	0.46
6:E:76:HIS:O	6:E:85:GLU:HB2	2.16	0.46
1:D:143:SER:OG	1:D:249:HIS:CE1	2.67	0.46
2:A:132:GLU:O	2:A:135:THR:HG22	2.14	0.46
2:A:306:THR:O	2:A:314:ALA:HB1	2.15	0.46
2:A:424:LEU:HD12	2:A:424:LEU:C	2.40	0.46
2:A:88:MET:HE3	2:A:109:THR:HG22	1.97	0.46
2:A:131:TRP:NE1	2:A:213:LYS:HD3	2.30	0.46
2:A:681:ARG:O	2:A:685:SER:OG	2.26	0.46
1:D:46:ALA:HB3	1:D:85:THR:HG22	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:135:THR:HB	2:A:213:LYS:HZ3	1.80	0.46
2:A:409:VAL:O	2:A:413:THR:OG1	2.31	0.46
2:A:785:GLN:HG2	2:A:839:PRO:HB3	1.96	0.46
3:C:101:ILE:HD12	3:C:104:LEU:HD22	1.97	0.46
2:A:824:ALA:HB1	2:A:901:VAL:HB	1.97	0.46
1:D:46:ALA:C	1:D:85:THR:CG2	2.88	0.45
1:D:215:PHE:CZ	1:D:219:ILE:HD11	2.51	0.45
1:D:280:SER:HA	1:D:283:MET:HE2	1.97	0.45
1:D:297:ARG:HE	1:D:348:GLU:CD	2.24	0.45
2:A:534:LEU:HD12	2:A:534:LEU:HA	1.75	0.45
2:A:131:TRP:CE2	2:A:213:LYS:CG	2.90	0.45
2:A:255:GLU:HA	2:A:488:ILE:HA	1.97	0.45
1:D:28:THR:HG21	1:D:459:GLY:C	2.40	0.45
1:D:49:THR:HG22	1:D:49:THR:O	2.16	0.45
1:D:115:LEU:HD13	2:A:751:VAL:HG22	1.99	0.45
1:D:340:LEU:HD12	1:D:340:LEU:HA	1.84	0.45
2:A:699:ALA:HB2	7:A:1212:LMT:H81	1.97	0.45
1:D:134:VAL:O	1:D:138:VAL:HG23	2.15	0.45
1:D:149:ILE:HD13	1:D:456:ILE:HD13	1.98	0.45
2:A:216:GLN:NE2	2:A:274:THR:HG21	2.32	0.45
2:A:335:PHE:HA	2:A:338:VAL:HG12	1.98	0.45
2:A:675:HIS:HE1	3:C:97:ASP:OD1	1.99	0.45
2:A:734:LEU:O	2:A:742:THR:OG1	2.23	0.45
2:A:781:LEU:HD12	5:G:93:PHE:CD1	2.51	0.45
2:A:846:ILE:HG21	2:A:906:MET:HG2	1.98	0.45
2:A:332:LEU:O	2:A:336:VAL:HG23	2.17	0.45
2:A:664:VAL:HG22	4:F:79:LEU:HD22	1.99	0.45
2:A:763:ARG:HD3	3:C:92:ILE:HG22	1.98	0.45
2:A:842:LYS:HA	2:A:916:ASP:OD2	2.16	0.45
1:D:128:ASP:OD2	2:A:738:ARG:NH2	2.38	0.45
2:A:522:VAL:HG22	2:A:525:PRO:HG2	1.98	0.45
2:A:780:PRO:HB3	6:E:76:HIS:ND1	2.32	0.45
2:A:222:TRP:CH2	2:A:242:MET:HE3	2.52	0.45
2:A:707:ARG:HH22	2:A:710:SER:CB	2.29	0.45
4:F:51:VAL:HG22	5:G:61:HIS:CE1	2.52	0.45
5:G:100:THR:HG22	5:G:101:THR:N	2.32	0.45
2:A:131:TRP:HZ2	2:A:213:LYS:HG2	1.80	0.45
2:A:175:VAL:HG21	2:A:181:THR:HG22	1.91	0.45
2:A:716:PHE:HE2	3:C:67:LEU:HD13	1.82	0.45
7:A:1211:LMT:H21	3:C:1:MET:HE2	1.98	0.45
2:A:44:TRP:HB2	2:A:78:MET:SD	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:220:GLN:HE21	2:A:538:THR:HG22	1.81	0.45
1:D:150:THR:CG2	1:D:151:ARG:N	2.80	0.44
2:A:227:MET:HE1	2:A:333:PHE:CE1	2.52	0.44
2:A:601:GLU:CB	4:F:52:ARG:HD3	2.46	0.44
2:A:879:HIS:HB3	2:A:888:THR:HB	1.99	0.44
2:A:900:ALA:O	2:A:904:VAL:HG23	2.17	0.44
1:D:143:SER:O	1:D:147:MET:HG3	2.18	0.44
1:D:195:GLN:HG2	1:D:573:LEU:HD21	1.99	0.44
2:A:169:THR:HG21	7:A:1206:LMT:H72	1.98	0.44
2:A:415:THR:HA	2:A:418:TYR:CD2	2.53	0.44
1:D:105:TYR:O	1:D:459:GLY:N	2.50	0.44
1:D:139:MET:HE3	1:D:249:HIS:ND1	2.32	0.44
1:D:242:THR:HG21	1:D:297:ARG:HH11	1.83	0.44
2:A:546:LEU:HD12	2:A:549:TRP:HE3	1.83	0.44
2:A:731:ASN:O	2:A:735:VAL:HG12	2.18	0.44
1:D:77:ASP:C	1:D:79:PHE:H	2.25	0.44
2:A:220:GLN:NE2	2:A:538:THR:HG22	2.33	0.44
1:D:1:MET:HE1	1:D:6:ALA:HB2	1.99	0.44
1:D:141:LEU:HD23	2:A:748:VAL:O	2.17	0.44
2:A:387:MET:HE3	2:A:387:MET:HB2	1.74	0.44
4:F:21:ARG:NE	5:G:29:LEU:O	2.43	0.44
1:D:188:THR:HG23	1:D:206:VAL:HG21	1.99	0.44
2:A:46:ALA:C	2:A:47:ILE:HG13	2.41	0.44
2:A:679:ARG:C	2:A:681:ARG:H	2.25	0.44
1:D:169:VAL:HG21	1:D:229:TRP:CG	2.52	0.43
1:D:518:ASP:OD1	1:D:519:MET:N	2.51	0.43
2:A:782:LEU:HD23	2:A:782:LEU:HA	1.86	0.43
2:A:499:TRP:CD1	2:A:501:GLY:H	2.36	0.43
2:A:3:LEU:HD11	2:A:120:LEU:HD13	2.01	0.43
2:A:72:LEU:HA	2:A:483:ALA:HB1	2.00	0.43
2:A:231:THR:OG1	2:A:289:LYS:CE	2.65	0.43
2:A:382:VAL:HG21	2:A:496:PHE:HB3	2.00	0.43
2:A:749:LEU:HD23	2:A:749:LEU:HA	1.79	0.43
6:E:99:LEU:O	6:E:103:LEU:HG	2.18	0.43
2:A:598:VAL:O	7:A:1202:LMT:O3'	2.36	0.43
2:A:107:LEU:HD21	7:A:1204:LMT:H82	2.00	0.43
2:A:136:LEU:HD23	2:A:136:LEU:HA	1.88	0.43
2:A:231:THR:OG1	2:A:289:LYS:HE2	2.18	0.43
2:A:288:LEU:CD1	2:A:346:ARG:NH2	2.80	0.43
2:A:358:MET:N	2:A:359:PRO:HD2	2.33	0.43
5:G:54:ILE:CG1	5:G:77:GLN:HE22	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:782:LEU:O	2:A:783:SER:OG	2.30	0.43
7:A:1214:LMT:H71	7:A:1214:LMT:H42	1.92	0.43
2:A:107:LEU:HD21	7:A:1204:LMT:H101	2.00	0.43
2:A:300:LEU:O	2:A:304:VAL:HG22	2.18	0.43
2:A:465:LEU:HA	2:A:468:VAL:HG22	2.00	0.43
3:C:80:PHE:CE1	3:C:84:ILE:HD11	2.52	0.43
4:F:18:SER:HB3	4:F:38:LEU:HD21	1.99	0.43
5:G:11:GLY:HA2	5:G:56:GLY:HA2	2.00	0.43
1:D:129:LEU:HD21	1:D:260:ILE:HD11	2.00	0.43
2:A:91:SER:HA	2:A:94:TYR:HB3	2.01	0.43
2:A:719:ASN:O	2:A:737:TYR:OH	2.36	0.43
3:C:80:PHE:CE2	3:C:84:ILE:HD11	2.51	0.43
1:D:139:MET:O	1:D:143:SER:OG	2.35	0.43
1:D:248:LEU:O	1:D:252:ILE:HG12	2.19	0.43
1:D:433:GLU:HG2	2:A:147:PRO:HG3	2.00	0.43
2:A:131:TRP:HE1	2:A:213:LYS:HD3	1.83	0.43
1:D:379:SER:O	1:D:388:GLY:HA3	2.18	0.42
2:A:702:ALA:HA	2:A:706:ARG:HH21	1.84	0.42
2:A:730:VAL:O	2:A:734:LEU:HG	2.19	0.42
2:A:745:GLU:CA	2:A:748:VAL:CG2	2.87	0.42
2:A:891:LEU:O	2:A:895:VAL:HG23	2.19	0.42
5:G:11:GLY:HA3	5:G:60:LEU:CD1	2.49	0.42
1:D:276:VAL:O	1:D:280:SER:OG	2.31	0.42
2:A:746:LEU:HD12	2:A:747:THR:N	2.34	0.42
2:A:203:ALA:CA	2:A:257:LEU:HD13	2.49	0.42
2:A:371:SER:O	2:A:380:GLY:HA3	2.19	0.42
5:G:11:GLY:HA3	5:G:60:LEU:HD12	2.00	0.42
1:D:467:ARG:O	1:D:468:ASP:OD1	2.37	0.42
2:A:55:VAL:HG23	2:A:65:LEU:HB3	2.02	0.42
2:A:163:GLY:HA3	2:A:212:THR:OG1	2.19	0.42
2:A:312:PRO:HA	2:A:488:ILE:HD11	2.01	0.42
2:A:461:LEU:HB3	2:A:462:PRO:HD3	2.02	0.42
2:A:882:LEU:O	2:A:885:VAL:HG22	2.19	0.42
1:D:185:TYR:OH	3:C:65:ASP:OD2	2.28	0.42
2:A:195:ASP:OD1	2:A:195:ASP:N	2.51	0.42
3:C:95:ASP:OD1	3:C:95:ASP:N	2.41	0.42
1:D:2:THR:C	1:D:4:GLU:H	2.28	0.42
1:D:73:PRO:HG2	1:D:127:GLY:HA3	2.02	0.42
1:D:152:SER:OG	1:D:446:LEU:O	2.33	0.42
2:A:291:LEU:HD22	2:A:422:PHE:HD2	1.84	0.42
2:A:728:ASN:O	2:A:732:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:54:ILE:HG13	5:G:77:GLN:NE2	2.31	0.42
1:D:236:LYS:HE3	2:A:564:ASP:OD2	2.20	0.42
1:D:438:ASP:OD1	1:D:438:ASP:N	2.45	0.42
2:A:822:ASN:ND2	2:A:822:ASN:H	2.17	0.42
3:C:51:GLU:HB3	3:C:63:THR:HA	2.02	0.42
3:C:78:ILE:O	3:C:82:ILE:HG13	2.19	0.42
5:G:21:VAL:HG21	6:E:26:SER:HB3	2.00	0.42
1:D:36:PHE:CE2	1:D:99:VAL:HG21	2.54	0.42
1:D:46:ALA:HB1	1:D:85:THR:HG23	1.97	0.42
2:A:13:ILE:HG12	2:A:35:MET:SD	2.60	0.42
2:A:631:ILE:HD11	4:F:38:LEU:HD12	2.01	0.42
2:A:806:SER:OG	2:A:826:ILE:CG2	2.68	0.42
3:C:55:VAL:CG1	3:C:56:SER:N	2.82	0.42
2:A:108:MET:HB3	2:A:108:MET:HE3	1.92	0.42
2:A:284:GLN:HE22	2:A:534:LEU:HD22	1.85	0.42
2:A:231:THR:OG1	2:A:289:LYS:NZ	2.51	0.42
2:A:713:GLY:O	2:A:717:LEU:HG	2.19	0.42
2:A:763:ARG:HE	3:C:92:ILE:HG22	1.84	0.42
2:A:763:ARG:CD	3:C:92:ILE:HG22	2.50	0.42
2:A:794:PHE:CD1	2:A:797:ILE:HD11	2.55	0.41
4:F:18:SER:OG	5:G:29:LEU:HD12	2.20	0.41
2:A:517:ILE:HA	2:A:520:VAL:HG12	2.01	0.41
2:A:669:ARG:NH1	2:A:912:LEU:O	2.48	0.41
2:A:707:ARG:NH2	2:A:710:SER:HB3	2.36	0.41
1:D:221:ALA:O	1:D:308:ILE:HG21	2.21	0.41
2:A:672:ARG:HE	2:A:769:ARG:NH2	2.16	0.41
2:A:707:ARG:NH2	2:A:710:SER:CA	2.82	0.41
2:A:745:GLU:OE2	3:C:74:THR:HA	2.20	0.41
1:D:355:ARG:HG2	3:C:109:LEU:HD13	2.02	0.41
1:D:269:SER:HA	1:D:272:LEU:HG	2.02	0.41
1:D:278:VAL:HG11	7:D:607:LMT:H121	2.02	0.41
2:A:643:LEU:HA	3:C:50:ARG:HD2	2.02	0.41
1:D:350:ARG:O	1:D:441:THR:CG2	2.69	0.41
2:A:151:GLN:HE21	2:A:547:ARG:HH22	1.67	0.41
3:C:59:ASP:O	3:C:63:THR:HG23	2.20	0.41
2:A:132:GLU:C	2:A:135:THR:HG22	2.46	0.41
1:D:5:SER:HA	1:D:61:HIS:CE1	2.55	0.41
1:D:155:ALA:HB3	2:A:763:ARG:HG3	2.02	0.41
1:D:368:LEU:HD22	7:D:605:LMT:H51	2.02	0.41
2:A:90:TYR:HE2	2:A:232:PRO:HG3	1.85	0.41
2:A:217:PHE:HB3	2:A:218:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:291:LEU:HD12	2:A:421:ARG:HH11	1.85	0.41
4:F:81:SER:OG	4:F:81:SER:O	2.39	0.41
5:G:31:ARG:HE	5:G:31:ARG:HB2	1.71	0.41
6:E:51:CYS:HB3	6:E:56:GLU:HB2	2.02	0.41
1:D:31:ILE:HD12	1:D:110:PRO:HG2	2.03	0.41
1:D:176:ILE:HG22	1:D:216:ALA:HB2	2.03	0.41
2:A:388:PHE:HB3	2:A:508:MET:SD	2.61	0.41
2:A:902:LEU:HD12	2:A:902:LEU:HA	1.85	0.41
3:C:110:LEU:HB3	3:C:111:PRO:HD2	2.03	0.41
5:G:48:LEU:HD21	6:E:22:GLN:HE21	1.86	0.41
6:E:67:THR:HA	6:E:68:PRO:HD3	1.95	0.41
6:E:96:PRO:O	6:E:100:THR:HG23	2.21	0.41
1:D:60:VAL:HG22	1:D:75:VAL:HG12	2.03	0.41
1:D:437:THR:HG23	1:D:525:ARG:HH22	1.86	0.41
2:A:805:LEU:HD11	4:F:63:LEU:HG	2.03	0.41
2:A:901:VAL:O	2:A:905:ILE:HG12	2.20	0.41
2:A:511:ILE:HG23	2:A:515:LEU:HD13	2.03	0.40
2:A:622:ARG:HB3	2:A:667:LEU:HD13	2.02	0.40
1:D:260:ILE:HD13	1:D:260:ILE:HA	1.90	0.40
2:A:31:PRO:O	2:A:35:MET:N	2.54	0.40
2:A:84:GLY:O	2:A:88:MET:HG2	2.21	0.40
2:A:239:ALA:HB2	2:A:330:SER:HB2	2.03	0.40
5:G:21:VAL:CG2	6:E:26:SER:HB3	2.51	0.40
2:A:704:THR:HB	3:C:43:ALA:O	2.21	0.40
1:D:137:GLU:HG3	3:C:78:ILE:HG21	2.03	0.40
1:D:288:LEU:HD23	1:D:288:LEU:HA	1.93	0.40
2:A:7:LEU:HD11	2:A:117:GLY:HA2	2.03	0.40
2:A:527:ASP:OD1	2:A:528:ARG:N	2.55	0.40
1:D:287:VAL:O	1:D:291:VAL:HG13	2.21	0.40
2:A:812:ARG:HG3	2:A:816:ALA:HB3	2.04	0.40
2:A:860:ILE:O	2:A:864:THR:HG22	2.21	0.40
7:A:1202:LMT:H5B	7:A:1202:LMT:H6E	2.03	0.40
3:C:3:LEU:HD12	3:C:3:LEU:HA	1.80	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	D	530/574 (92%)	502 (95%)	28 (5%)	0	100	100
2	A	900/958 (94%)	845 (94%)	55 (6%)	0	100	100
3	C	127/137 (93%)	121 (95%)	6 (5%)	0	100	100
4	F	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
5	G	109/125 (87%)	105 (96%)	4 (4%)	0	100	100
6	E	108/121 (89%)	99 (92%)	8 (7%)	1 (1%)	14	48
All	All	1857/2000 (93%)	1750 (94%)	106 (6%)	1 (0%)	49	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	84	TRP

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	D	400/428 (94%)	399 (100%)	1 (0%)	86	91
2	A	672/717 (94%)	668 (99%)	4 (1%)	78	88
3	C	101/108 (94%)	100 (99%)	1 (1%)	68	84
4	F	65/65 (100%)	65 (100%)	0	100	100
5	G	77/90 (86%)	77 (100%)	0	100	100
6	E	96/107 (90%)	95 (99%)	1 (1%)	68	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1411/1515 (93%)	1404 (100%)	7 (0%)	78 89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	332	HIS
2	A	111	PHE
2	A	302	PHE
2	A	639	TRP
2	A	814	HIS
3	C	101	ILE
6	E	76	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	42	GLN
1	D	121	ASN
1	D	131	ASN
1	D	170	ASN
1	D	227	HIS
1	D	249	HIS
1	D	303	HIS
1	D	332	HIS
2	A	101	HIS
2	A	151	GLN
2	A	216	GLN
2	A	264	ASN
2	A	284	GLN
2	A	325	HIS
2	A	341	HIS
2	A	342	GLN
2	A	628	ASN
2	A	675	HIS
2	A	719	ASN
3	C	69	GLN
4	F	27	HIS
5	G	61	HIS
5	G	77	GLN
6	E	22	GLN
6	E	77	HIS

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Mol	Chain	Res	Type
6	E	109	HIS

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](#)

28 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	$\# Z > 2$
7	LMT	A	1208	-	11,11,36	0.31	0	10,10,47	0.77	0
7	LMT	D	611	-	11,11,36	0.34	0	10,10,47	0.78	0
7	LMT	A	1210	-	8,8,36	1.54	2 (25%)	7,7,47	1.76	2 (28%)
7	LMT	D	603	-	36,36,36	1.17	5 (13%)	47,47,47	1.11	3 (6%)
7	LMT	A	1204	-	11,11,36	0.33	0	10,10,47	0.76	0
7	LMT	A	1214	-	36,36,36	1.08	3 (8%)	47,47,47	1.15	2 (4%)
7	LMT	A	1201	-	36,36,36	1.12	5 (13%)	47,47,47	1.04	3 (6%)
7	LMT	A	1206	-	36,36,36	1.12	5 (13%)	47,47,47	1.08	2 (4%)
7	LMT	A	1203	-	11,11,36	0.33	0	10,10,47	0.78	0
7	LMT	A	1209	-	36,36,36	1.14	5 (13%)	47,47,47	1.05	3 (6%)
7	LMT	C	2201	-	11,11,36	0.32	0	10,10,47	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	LMT	A	1205	-	11,11,36	0.32	0	10,10,47	0.78	0
7	LMT	A	1207	-	11,11,36	2.43	5 (45%)	10,10,47	3.00	7 (70%)
7	LMT	D	608	-	36,36,36	1.18	6 (16%)	47,47,47	1.00	1 (2%)
7	LMT	D	610	-	11,11,36	0.32	0	10,10,47	0.80	0
7	LMT	D	606	-	11,11,36	0.34	0	10,10,47	0.78	0
7	LMT	D	609	-	36,36,36	1.13	4 (11%)	47,47,47	1.16	5 (10%)
7	LMT	D	605	-	11,11,36	0.32	0	10,10,47	0.78	0
7	LMT	A	1215	-	11,11,36	0.33	0	10,10,47	0.77	0
7	LMT	D	607	-	11,11,36	0.35	0	10,10,47	0.76	0
7	LMT	A	1213	-	11,11,36	0.34	0	10,10,47	0.78	0
7	LMT	A	1212	-	11,11,36	0.35	0	10,10,47	0.78	0
7	LMT	A	1211	-	11,11,36	0.32	0	10,10,47	0.78	0
7	LMT	D	601	-	11,11,36	0.32	0	10,10,47	0.76	0
7	LMT	D	604	-	11,11,36	0.32	0	10,10,47	0.79	0
7	LMT	D	602	-	11,11,36	0.32	0	10,10,47	0.77	0
7	LMT	A	1202	-	36,36,36	1.14	6 (16%)	47,47,47	1.04	2 (4%)
7	LMT	C	2202	-	11,11,36	0.33	0	10,10,47	0.79	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
7	LMT	A	1208	-	-	0/9/9/61	-
7	LMT	D	611	-	-	0/9/9/61	-
7	LMT	A	1210	-	-	2/6/6/61	-
7	LMT	D	603	-	-	11/21/61/61	0/2/2/2
7	LMT	A	1204	-	-	1/9/9/61	-
7	LMT	A	1214	-	-	12/21/61/61	0/2/2/2
7	LMT	A	1201	-	-	11/21/61/61	1/2/2/2
7	LMT	A	1206	-	-	5/21/61/61	0/2/2/2
7	LMT	A	1203	-	-	3/9/9/61	-
7	LMT	A	1209	-	-	5/21/61/61	0/2/2/2
7	LMT	C	2201	-	-	0/9/9/61	-
7	LMT	A	1205	-	-	3/9/9/61	-
7	LMT	A	1207	-	-	4/9/9/61	-
7	LMT	D	608	-	-	6/21/61/61	0/2/2/2
7	LMT	D	610	-	-	4/9/9/61	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LMT	D	606	-	-	2/9/9/61	-
7	LMT	D	609	-	-	3/21/61/61	0/2/2/2
7	LMT	D	605	-	-	4/9/9/61	-
7	LMT	A	1215	-	-	3/9/9/61	-
7	LMT	D	607	-	-	0/9/9/61	-
7	LMT	A	1213	-	-	4/9/9/61	-
7	LMT	A	1212	-	-	0/9/9/61	-
7	LMT	A	1211	-	-	2/9/9/61	-
7	LMT	D	601	-	-	2/9/9/61	-
7	LMT	D	604	-	-	1/9/9/61	-
7	LMT	D	602	-	-	1/9/9/61	-
7	LMT	A	1202	-	-	6/21/61/61	0/2/2/2
7	LMT	C	2202	-	-	3/9/9/61	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1207	LMT	C6-C5	-5.03	1.26	1.51
7	A	1207	LMT	C7-C6	-3.96	1.32	1.51
7	A	1201	LMT	O3'-C3'	-2.74	1.36	1.43
7	A	1207	LMT	C8-C7	-2.64	1.38	1.51
7	D	608	LMT	O3'-C3'	-2.57	1.36	1.43
7	A	1207	LMT	C5-C4	-2.53	1.39	1.51
7	A	1202	LMT	O3'-C3'	-2.51	1.36	1.43
7	D	603	LMT	O3'-C3'	-2.51	1.36	1.43
7	A	1209	LMT	O3'-C3'	-2.51	1.36	1.43
7	D	609	LMT	O3'-C3'	-2.45	1.36	1.43
7	A	1214	LMT	O3'-C3'	-2.42	1.37	1.43
7	A	1206	LMT	O3'-C3'	-2.39	1.37	1.43
7	A	1206	LMT	O2B-C2B	-2.30	1.37	1.43
7	D	608	LMT	O2'-C2'	-2.30	1.37	1.43
7	A	1201	LMT	O2'-C2'	-2.28	1.37	1.43
7	A	1202	LMT	O2B-C2B	-2.27	1.37	1.43
7	D	608	LMT	O2B-C2B	-2.27	1.37	1.43
7	A	1201	LMT	O3B-C3B	-2.25	1.37	1.43
7	D	609	LMT	O2B-C2B	-2.25	1.37	1.43
7	A	1202	LMT	O3B-C3B	-2.25	1.37	1.43
7	A	1209	LMT	O2B-C2B	-2.24	1.37	1.43
7	A	1210	LMT	C8-C7	-2.23	1.37	1.51
7	A	1214	LMT	O2B-C2B	-2.23	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1209	LMT	O2'-C2'	-2.23	1.37	1.43
7	D	608	LMT	O1'-C1'	-2.21	1.36	1.40
7	D	603	LMT	O2B-C2B	-2.21	1.37	1.43
7	D	603	LMT	O2'-C2'	-2.21	1.37	1.43
7	A	1201	LMT	O2B-C2B	-2.21	1.37	1.43
7	A	1206	LMT	O3B-C3B	-2.21	1.37	1.43
7	A	1209	LMT	O3B-C3B	-2.21	1.37	1.43
7	A	1207	LMT	C2-C3	-2.20	1.38	1.51
7	D	608	LMT	O3B-C3B	-2.18	1.37	1.43
7	D	609	LMT	O3B-C3B	-2.17	1.37	1.43
7	D	609	LMT	O2'-C2'	-2.17	1.37	1.43
7	A	1206	LMT	O2'-C2'	-2.16	1.37	1.43
7	A	1202	LMT	O2'-C2'	-2.15	1.37	1.43
7	D	603	LMT	O3B-C3B	-2.09	1.37	1.43
7	A	1206	LMT	O4'-C4B	-2.09	1.37	1.43
7	A	1214	LMT	O3B-C3B	-2.08	1.37	1.43
7	A	1209	LMT	O1'-C1'	-2.07	1.36	1.40
7	A	1202	LMT	O4'-C4B	-2.07	1.37	1.43
7	D	603	LMT	O1'-C1'	-2.06	1.36	1.40
7	A	1202	LMT	O1'-C1'	-2.05	1.36	1.40
7	D	608	LMT	O4'-C4B	-2.05	1.37	1.43
7	A	1210	LMT	C7-C6	-2.01	1.41	1.51
7	A	1201	LMT	O4'-C4B	-2.01	1.38	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1207	LMT	C7-C6-C5	-4.84	89.90	114.37
7	A	1207	LMT	C6-C5-C4	-3.86	94.85	114.37
7	A	1207	LMT	C5-C4-C3	3.79	133.51	114.37
7	A	1207	LMT	C10-C9-C8	3.71	133.15	114.37
7	A	1214	LMT	O5B-C5B-C4B	3.59	116.17	109.70
7	D	603	LMT	C3'-C4'-C5'	-3.40	103.39	110.93
7	A	1209	LMT	C1'-O5'-C5'	-3.28	107.32	113.72
7	A	1210	LMT	C8-C7-C6	-3.14	87.75	115.25
7	D	609	LMT	O5B-C5B-C4B	3.07	115.23	109.70
7	D	608	LMT	C1'-O5'-C5'	-2.98	107.89	113.72
7	A	1206	LMT	O5'-C5'-C6'	2.93	113.70	106.44
7	A	1201	LMT	C1'-O5'-C5'	-2.81	108.24	113.72
7	A	1202	LMT	C1'-O5'-C5'	-2.80	108.26	113.72
7	A	1202	LMT	C3'-C4'-C5'	-2.78	104.76	110.93
7	A	1207	LMT	C8-C7-C6	2.78	128.41	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	609	LMT	C1'-O5'-C5'	-2.72	108.42	113.72
7	A	1210	LMT	C6-C5-C4	2.68	127.90	114.37
7	A	1207	LMT	C1-C2-C3	2.46	129.95	113.36
7	D	609	LMT	C1B-O5B-C5B	2.39	118.40	113.72
7	A	1207	LMT	C9-C8-C7	2.38	126.41	114.37
7	D	609	LMT	O5B-C5B-C6B	2.36	112.29	106.44
7	D	609	LMT	C3'-C4'-C5'	-2.32	105.80	110.93
7	A	1201	LMT	O5B-C5B-C4B	2.31	113.87	109.70
7	A	1214	LMT	C1B-O5B-C5B	2.29	118.20	113.72
7	D	603	LMT	C1'-O5'-C5'	-2.28	109.26	113.72
7	A	1201	LMT	C3'-C4'-C5'	-2.19	106.08	110.93
7	A	1209	LMT	O5B-C5B-C4B	2.12	113.52	109.70
7	A	1206	LMT	C2'-C3'-C4'	2.09	114.43	109.68
7	D	603	LMT	O5'-C1'-O1'	-2.07	105.14	110.04
7	A	1209	LMT	C3'-C4'-C5'	-2.05	106.38	110.93

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	603	LMT	C2'-C1'-O1'-C1
7	D	603	LMT	O5'-C1'-O1'-C1
7	A	1201	LMT	O5'-C1'-O1'-C1
7	A	1214	LMT	O5'-C1'-O1'-C1
7	A	1214	LMT	C4'-C5'-C6'-O6'
7	A	1214	LMT	O5'-C5'-C6'-O6'
7	D	603	LMT	O5B-C5B-C6B-O6B
7	A	1201	LMT	C4'-C5'-C6'-O6'
7	A	1206	LMT	C4B-C5B-C6B-O6B
7	A	1206	LMT	O5B-C5B-C6B-O6B
7	A	1214	LMT	C4B-C5B-C6B-O6B
7	A	1201	LMT	O5'-C5'-C6'-O6'
7	D	603	LMT	C4'-C5'-C6'-O6'
7	D	603	LMT	C4B-C5B-C6B-O6B
7	D	608	LMT	O5'-C1'-O1'-C1
7	D	608	LMT	C2'-C1'-O1'-C1
7	A	1201	LMT	C2'-C1'-O1'-C1
7	A	1214	LMT	O5B-C5B-C6B-O6B
7	D	603	LMT	O5'-C5'-C6'-O6'
7	A	1214	LMT	C3'-C4'-O1B-C1B
7	A	1214	LMT	O1'-C1-C2-C3
7	A	1214	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
7	A	1214	LMT	C2'-C1'-O1'-C1
7	D	605	LMT	C7-C8-C9-C10
7	A	1201	LMT	C11-C10-C9-C8
7	A	1206	LMT	C2-C1-O1'-C1'
7	A	1209	LMT	C2-C1-O1'-C1'
7	D	602	LMT	C7-C8-C9-C10
7	A	1203	LMT	C6-C7-C8-C9
7	D	605	LMT	C2-C3-C4-C5
7	A	1211	LMT	C4-C5-C6-C7
7	D	609	LMT	O5'-C5'-C6'-O6'
7	D	608	LMT	C4-C5-C6-C7
7	A	1201	LMT	C1-C2-C3-C4
7	A	1202	LMT	C4-C5-C6-C7
7	D	601	LMT	C3-C4-C5-C6
7	D	603	LMT	C4-C5-C6-C7
7	D	608	LMT	C7-C8-C9-C10
7	A	1202	LMT	C5-C6-C7-C8
7	A	1204	LMT	C11-C10-C9-C8
7	A	1207	LMT	C11-C10-C9-C8
7	A	1206	LMT	C1-C2-C3-C4
7	A	1214	LMT	C1-C2-C3-C4
7	A	1209	LMT	C11-C10-C9-C8
7	A	1209	LMT	C5-C6-C7-C8
7	D	606	LMT	C11-C10-C9-C8
7	A	1207	LMT	C7-C8-C9-C10
7	A	1214	LMT	C2-C3-C4-C5
7	A	1201	LMT	C2B-C1B-O1B-C4'
7	D	603	LMT	C5-C6-C7-C8
7	A	1206	LMT	C4'-C5'-C6'-O6'
7	A	1201	LMT	O5B-C1B-O1B-C4'
7	A	1205	LMT	C9-C10-C11-C12
7	A	1203	LMT	C7-C8-C9-C10
7	D	606	LMT	C7-C8-C9-C10
7	D	605	LMT	C6-C7-C8-C9
7	D	608	LMT	C3-C4-C5-C6
7	D	603	LMT	C2-C1-O1'-C1'
7	A	1205	LMT	C3-C4-C5-C6
7	A	1201	LMT	O1'-C1-C2-C3
7	A	1210	LMT	C2-C3-C4-C5
7	D	610	LMT	C6-C7-C8-C9
7	D	610	LMT	C3-C4-C5-C6
7	A	1201	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	D	603	LMT	C2-C3-C4-C5
7	A	1213	LMT	C5-C6-C7-C8
7	A	1202	LMT	C7-C8-C9-C10
7	A	1210	LMT	C3-C4-C5-C6
7	D	609	LMT	C4B-C5B-C6B-O6B
7	A	1215	LMT	C1-C2-C3-C4
7	D	609	LMT	C2-C1-O1'-C1'
7	A	1213	LMT	C2-C3-C4-C5
7	A	1207	LMT	C5-C6-C7-C8
7	A	1202	LMT	C3-C4-C5-C6
7	D	610	LMT	C5-C6-C7-C8
7	C	2202	LMT	C2-C3-C4-C5
7	D	605	LMT	C1-C2-C3-C4
7	A	1214	LMT	C3-C4-C5-C6
7	A	1213	LMT	C7-C8-C9-C10
7	D	610	LMT	C1-C2-C3-C4
7	A	1211	LMT	C3-C4-C5-C6
7	D	604	LMT	C3-C4-C5-C6
7	A	1202	LMT	C2-C3-C4-C5
7	D	603	LMT	C3-C4-C5-C6
7	A	1215	LMT	C6-C7-C8-C9
7	A	1209	LMT	C5'-C4'-O1B-C1B
7	A	1201	LMT	C2-C1-O1'-C1'
7	A	1207	LMT	C6-C7-C8-C9
7	A	1205	LMT	C6-C7-C8-C9
7	C	2202	LMT	C11-C10-C9-C8
7	A	1215	LMT	C7-C8-C9-C10
7	C	2202	LMT	C3-C4-C5-C6
7	A	1209	LMT	C2-C3-C4-C5
7	A	1203	LMT	C3-C4-C5-C6
7	A	1202	LMT	C4B-C5B-C6B-O6B
7	D	601	LMT	C11-C10-C9-C8
7	A	1213	LMT	C3-C4-C5-C6
7	D	608	LMT	O1'-C1-C2-C3

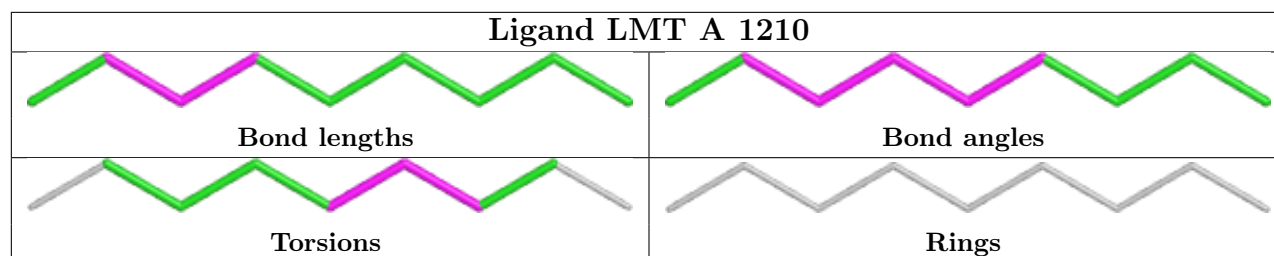
All (1) ring outliers are listed below:

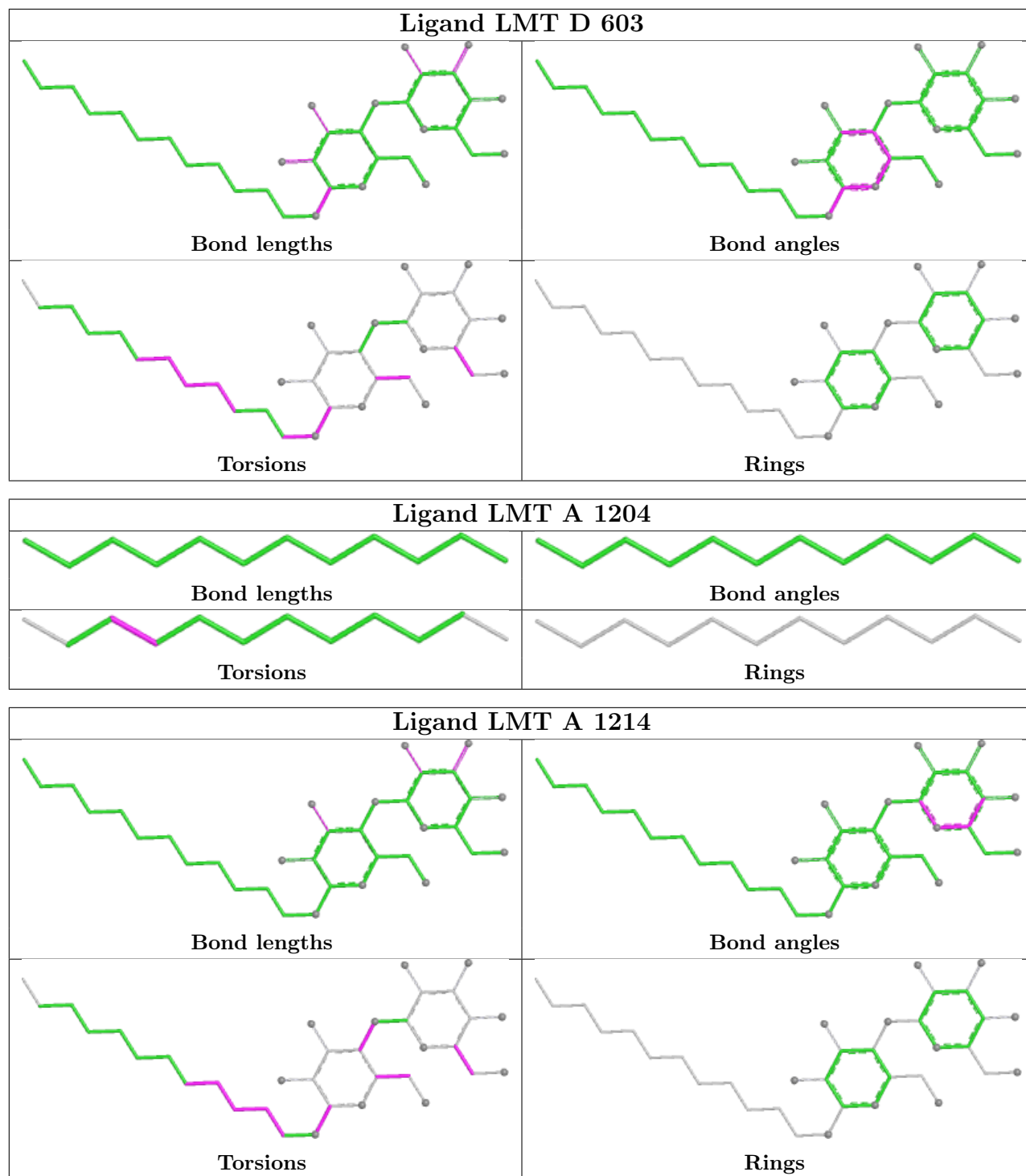
Mol	Chain	Res	Type	Atoms
7	A	1201	LMT	C1'-C2'-C3'-C4'-C5'-O5'

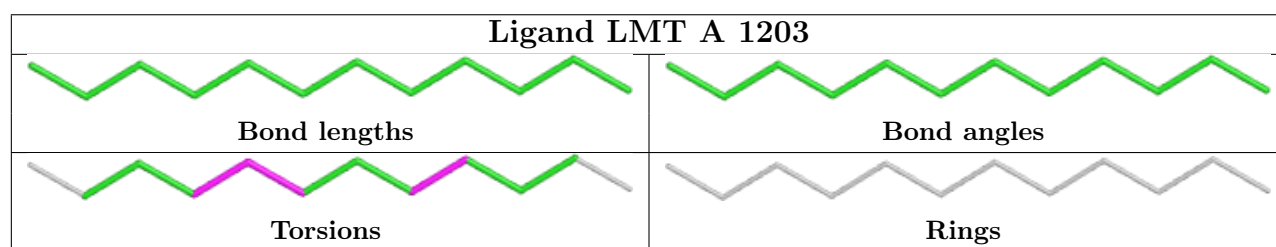
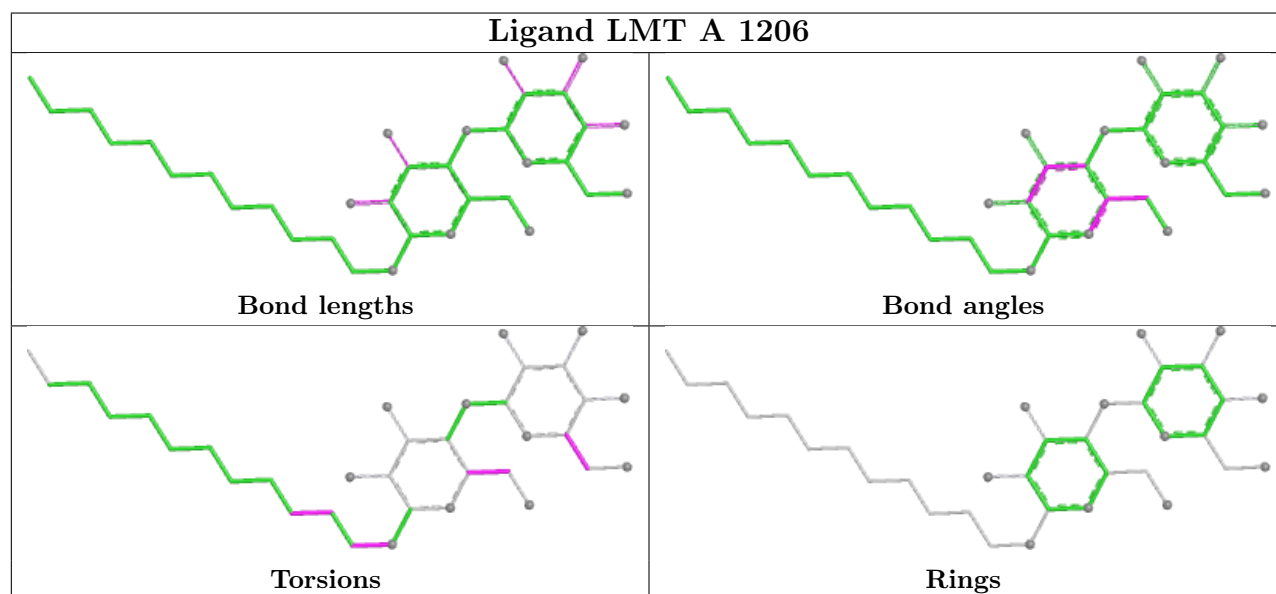
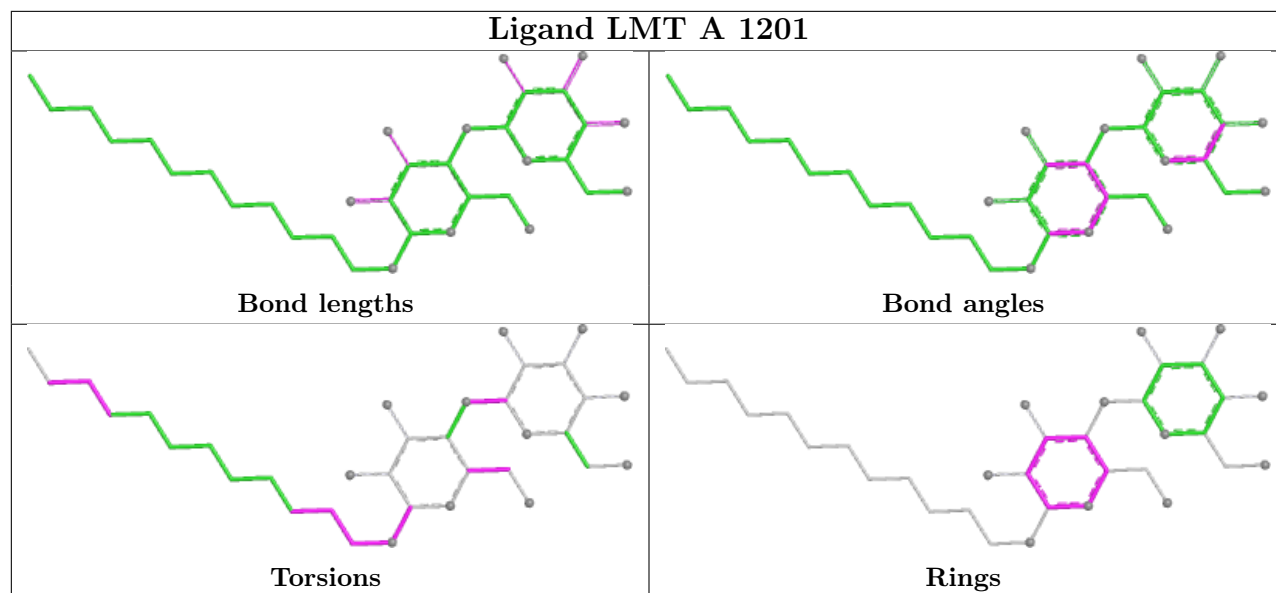
15 monomers are involved in 33 short contacts:

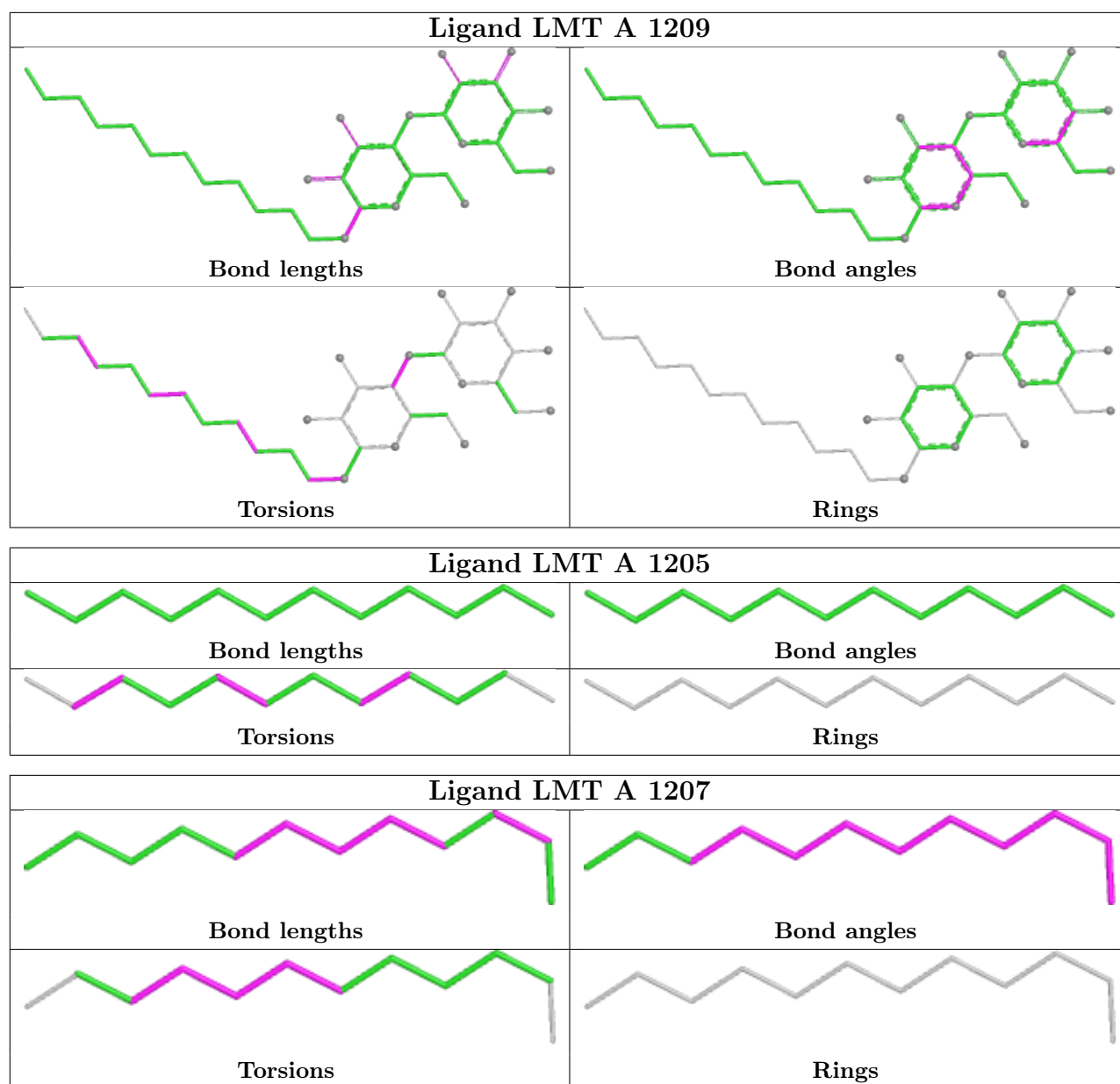
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1208	LMT	1	0
7	A	1210	LMT	5	0
7	A	1204	LMT	2	0
7	A	1214	LMT	3	0
7	A	1206	LMT	1	0
7	A	1209	LMT	7	0
7	C	2201	LMT	1	0
7	A	1207	LMT	3	0
7	D	608	LMT	1	0
7	D	605	LMT	1	0
7	D	607	LMT	3	0
7	A	1213	LMT	1	0
7	A	1212	LMT	2	0
7	A	1211	LMT	1	0
7	A	1202	LMT	3	0

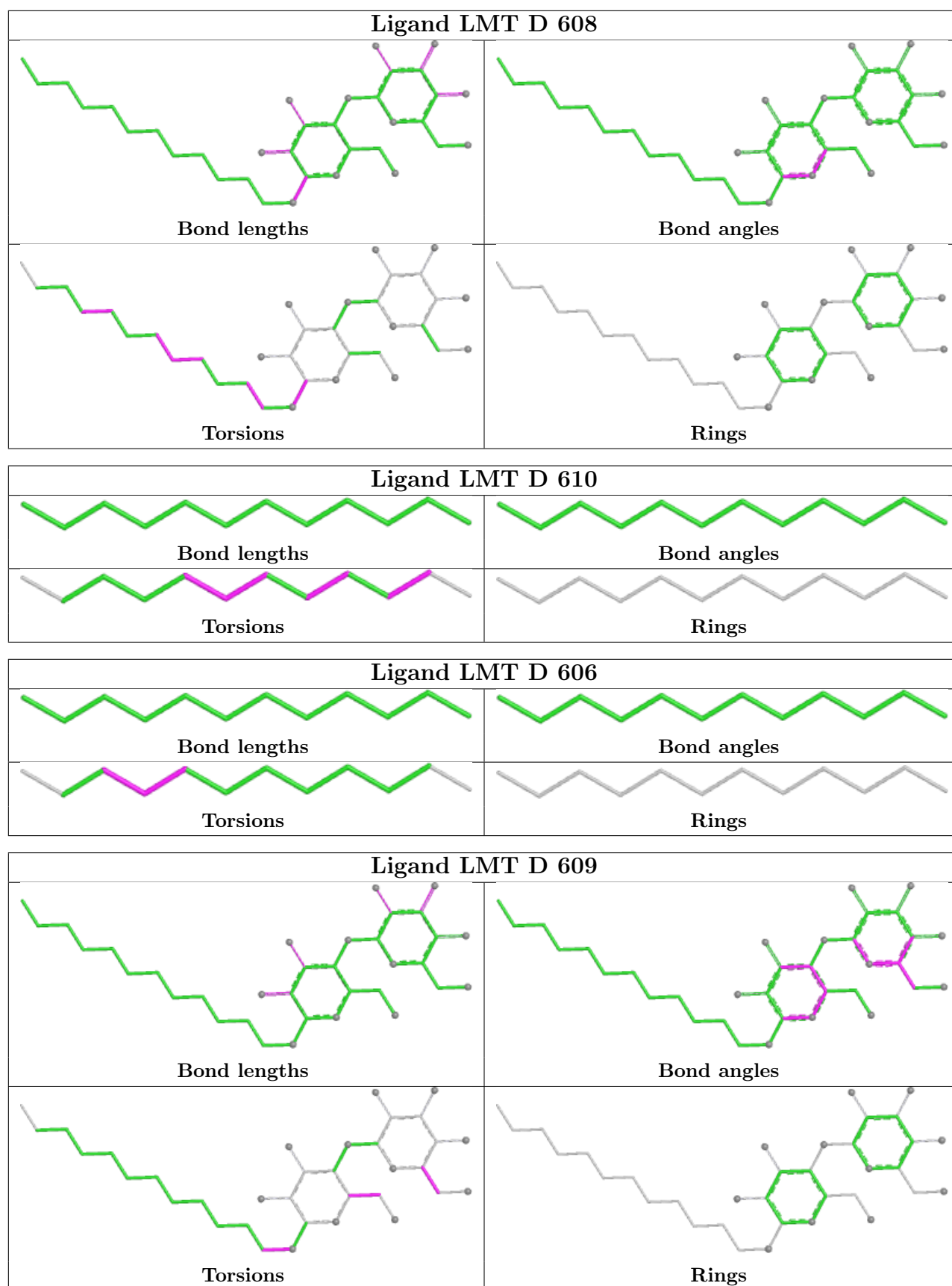
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











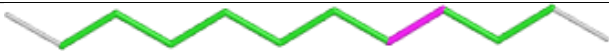
Ligand LMT D 605			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

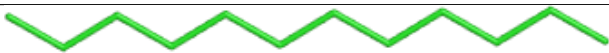
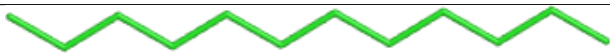
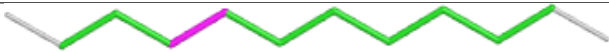
Ligand LMT A 1215			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

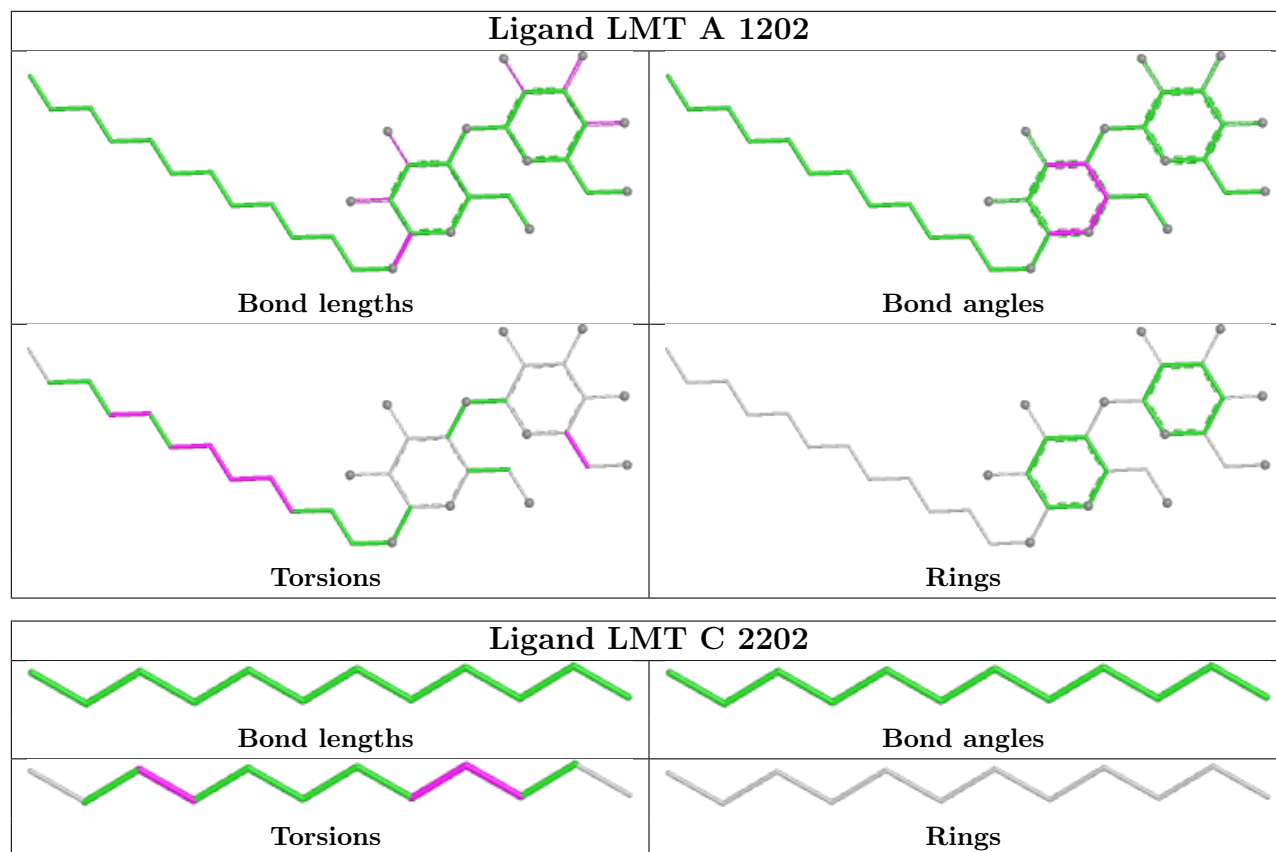
Ligand LMT A 1213			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand LMT A 1211			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand LMT D 601			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand LMT D 604			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand LMT D 602			
 Bond lengths		 Bond angles	
 Torsions		 Rings	



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.

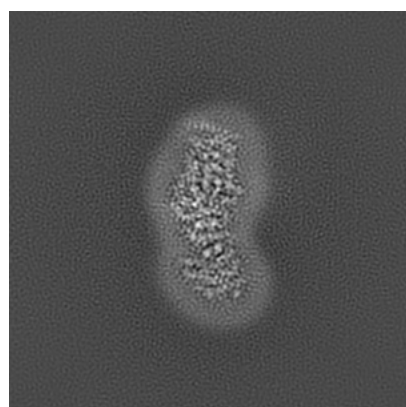
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30567. These allow visual inspection of the internal detail of the map and identification of artifacts.

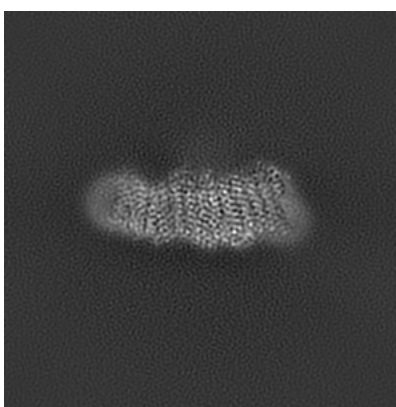
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

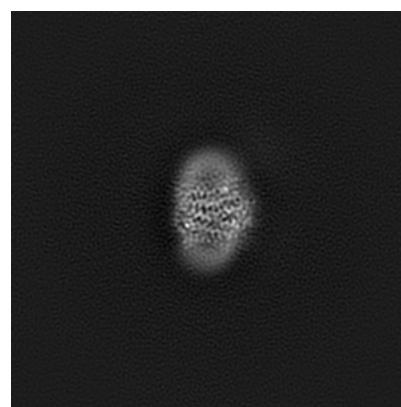
6.1.1 Primary map



X



Y

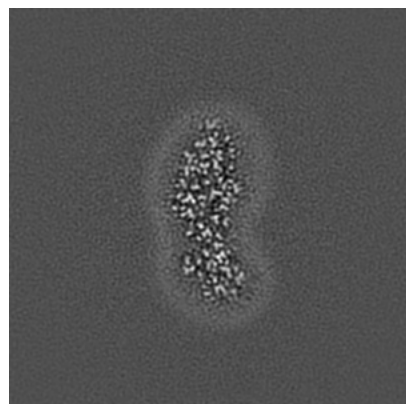


Z

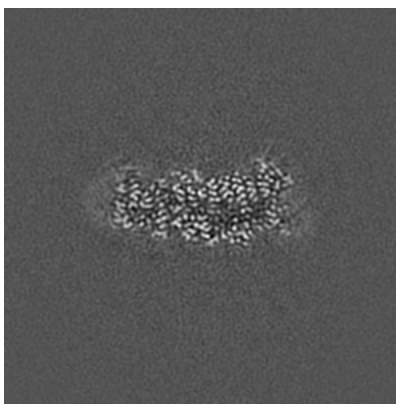
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

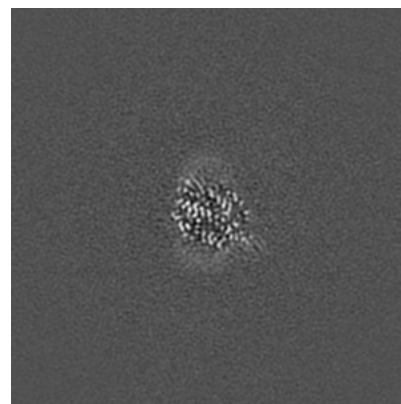
6.2.1 Primary map



X Index: 150



Y Index: 150

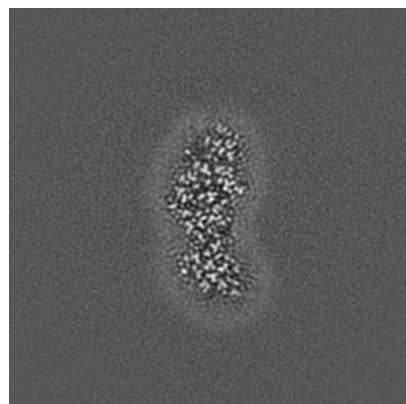


Z Index: 150

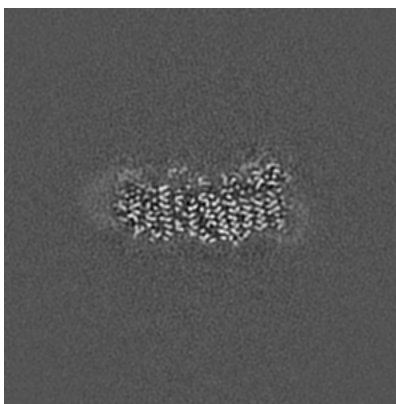
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

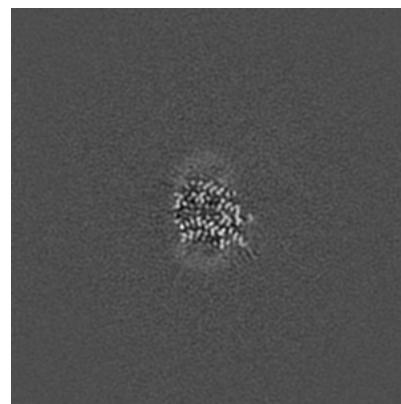
6.3.1 Primary map



X Index: 156



Y Index: 155

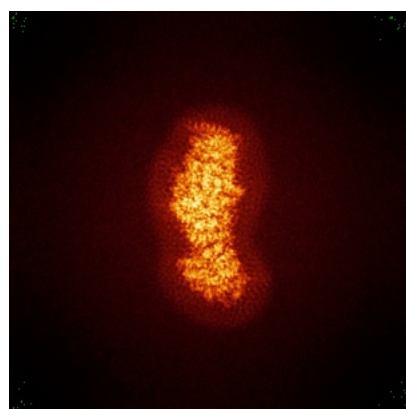


Z Index: 155

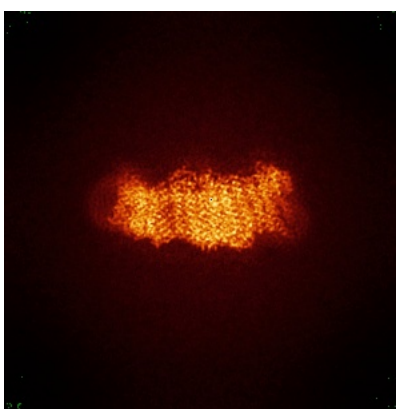
The images above show the largest variance slices of the map in three orthogonal directions.

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

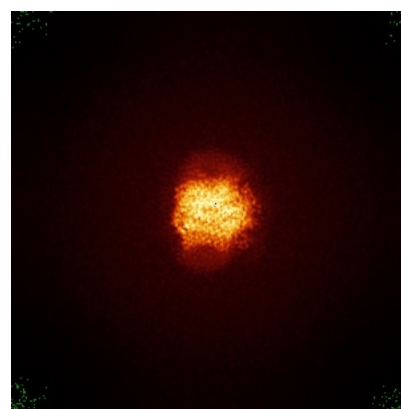
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

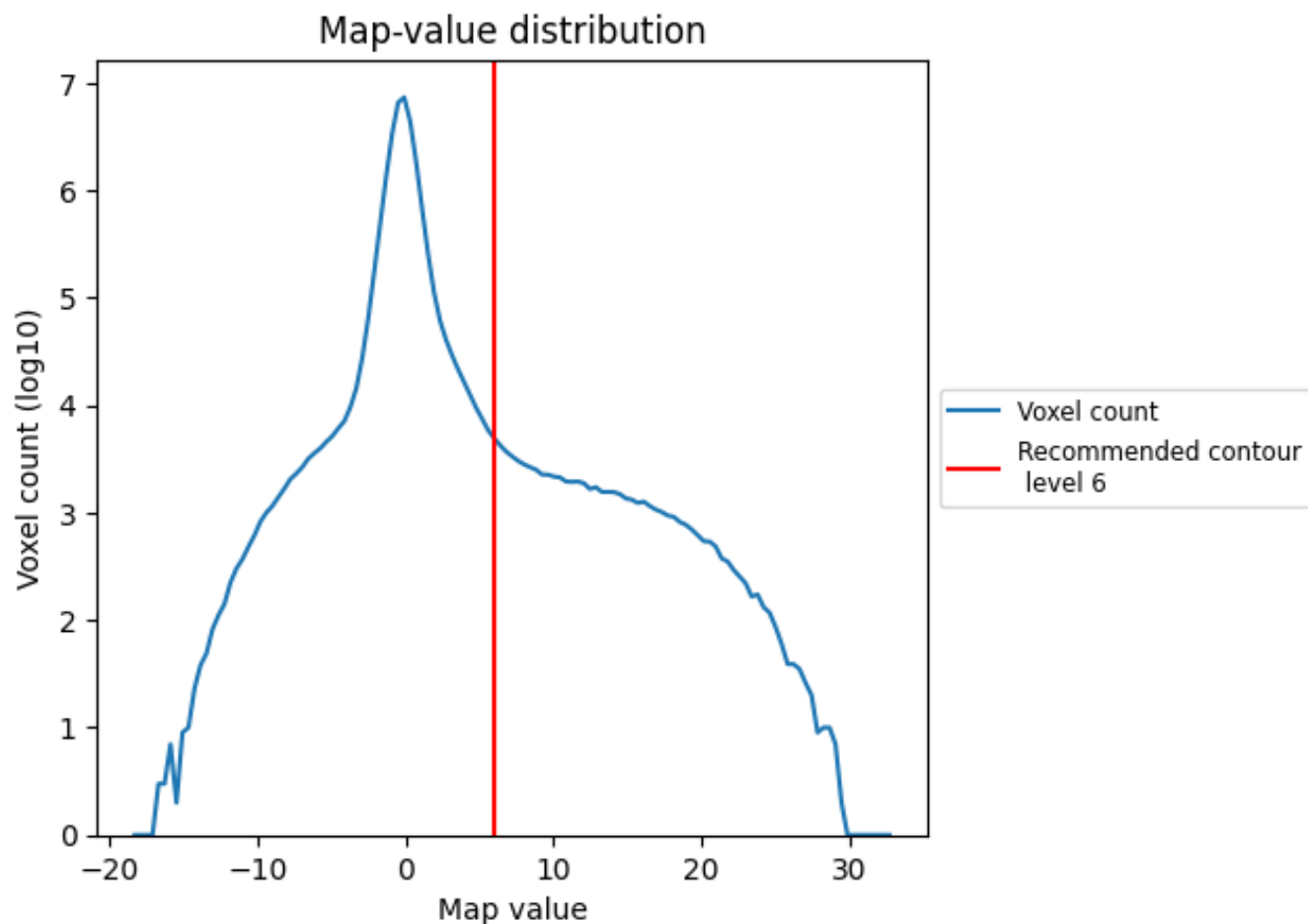
6.6 Mask visualisation

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

7 Map analysis [i](#)

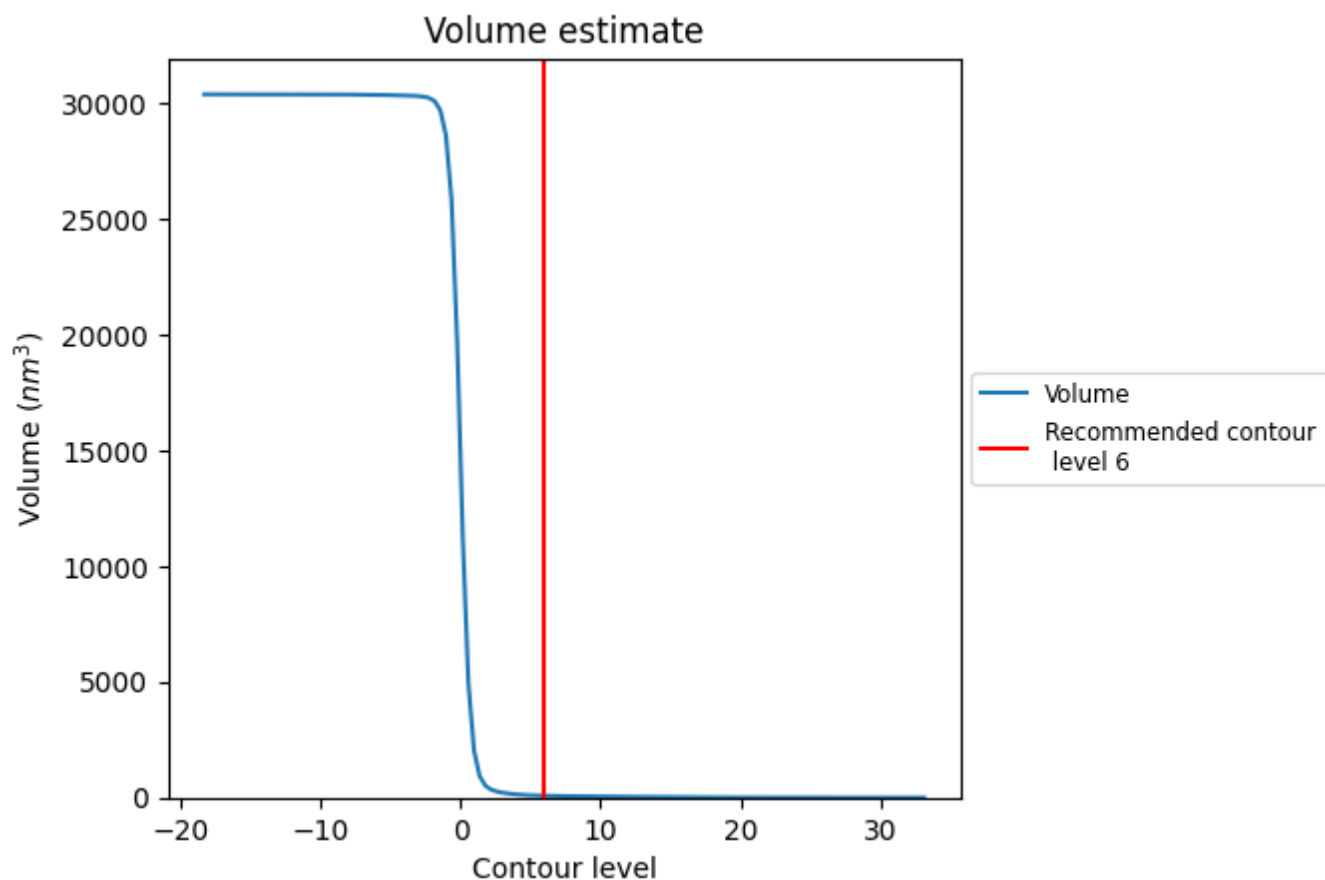
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

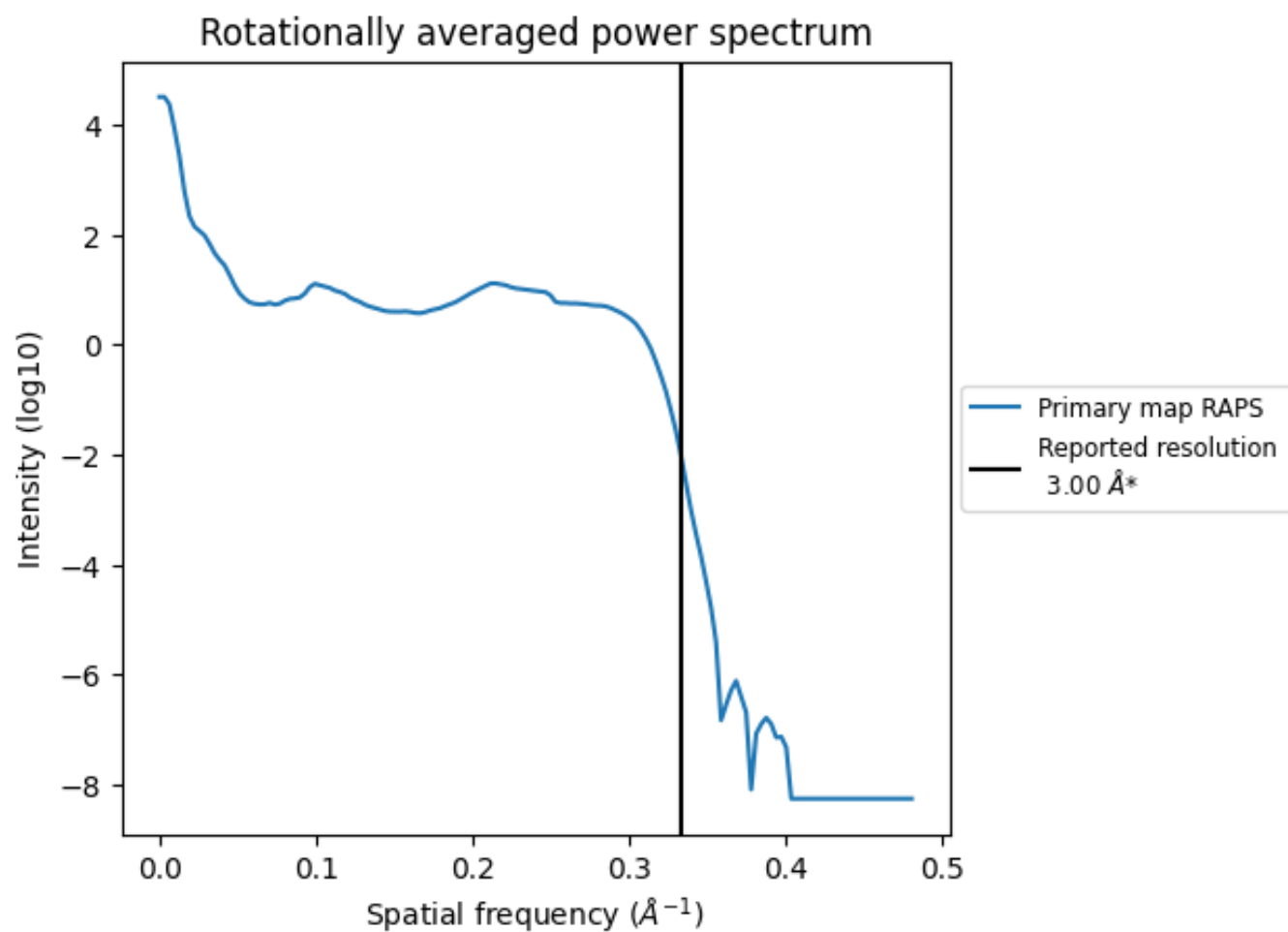
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm³; this corresponds to an approximate mass of 71 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 0.333 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

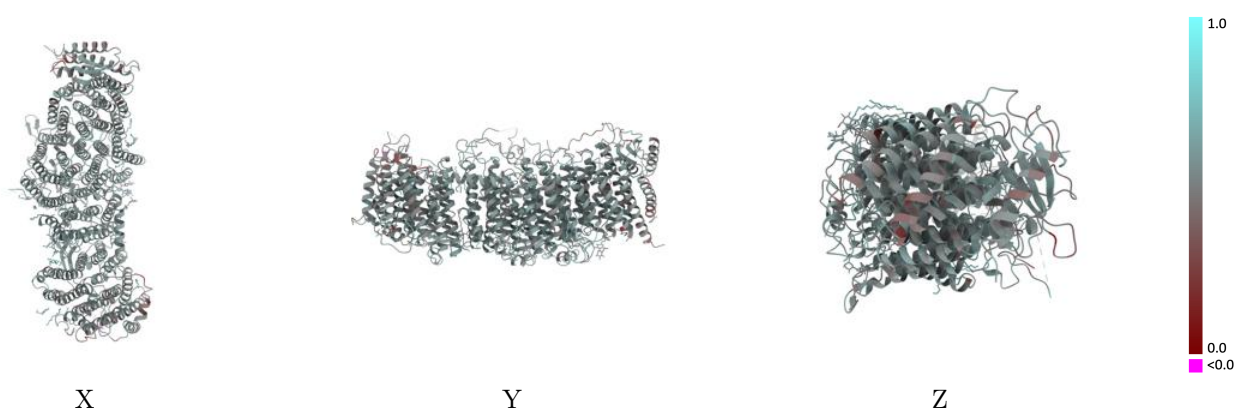
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30567 and PDB model 7D3U. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

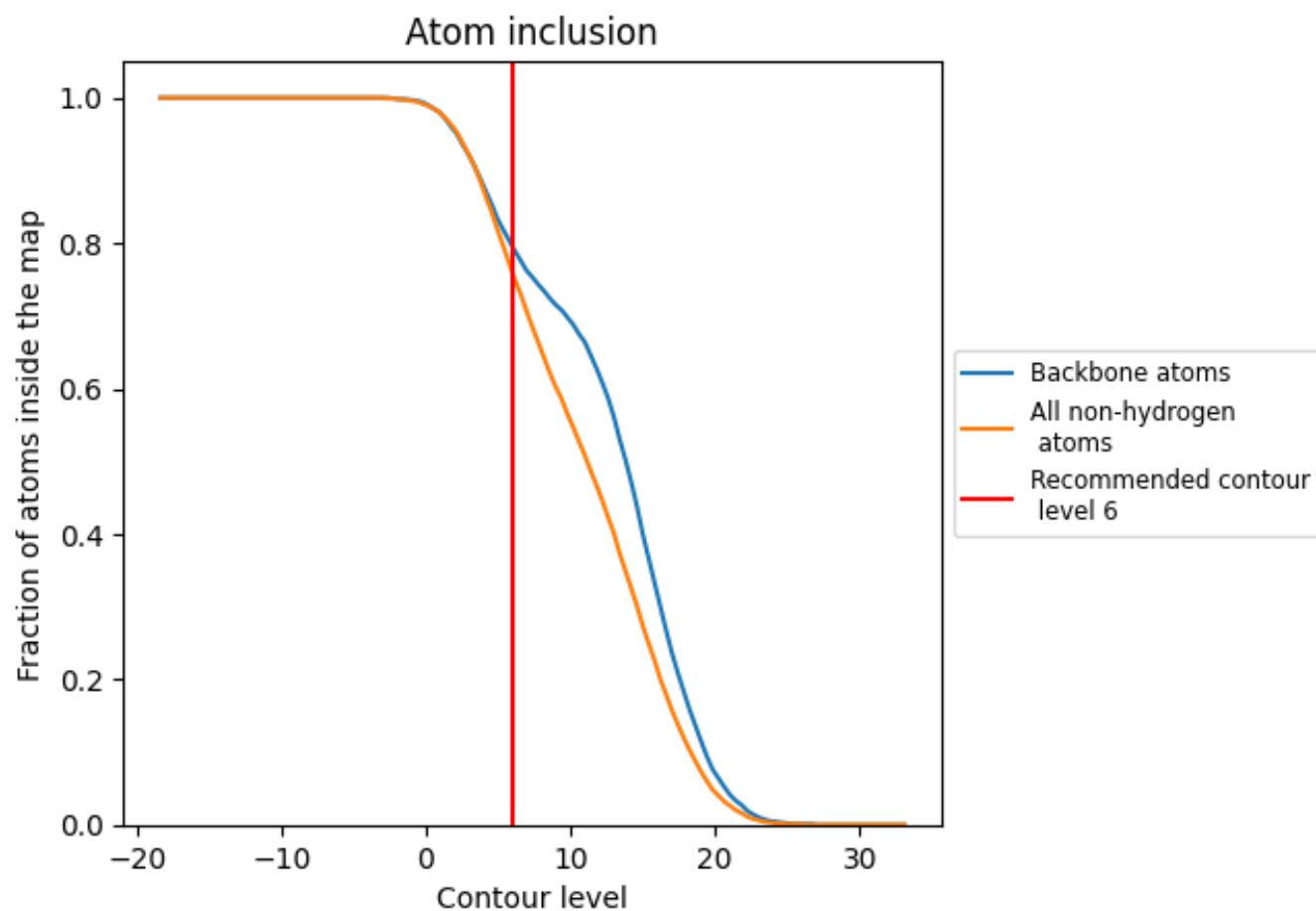


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7600	0.5310
A	0.7430	0.5270
C	0.7790	0.5430
D	0.8090	0.5500
E	0.6650	0.4910
F	0.7620	0.5230
G	0.7290	0.5090

1.0

0.0

<0.0