



Full wwPDB EM Validation Report ⓘ

Jun 15, 2026 – 01:49 PM EDT

PDB ID : 9Q1E / pdb_00009q1e
EMDB ID : EMD-72125
Title : Cryo-EM Structure of the MgtA Tetramer at 2.7 Å Resolution
Authors : Khan, M.B.; Primeau, J.O.; Basu, P.C.; Morth, J.P.; Lemieux, M.J.; Young, H.S.
Deposited on : 2025-08-13
Resolution : 2.69 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:

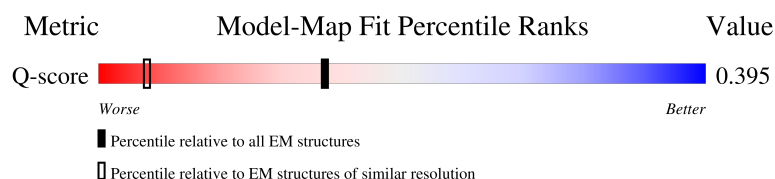
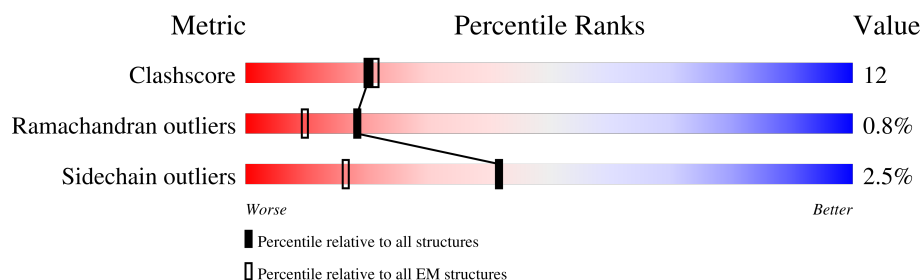
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.69 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	9309 (2.19 - 3.19)

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	921	
1	B	921	
1	C	921	
1	D	921	

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
3	BEF	A	1002	-	-	X	-
3	BEF	B	1002	-	-	X	-
3	BEF	C	1001	-	-	X	-
3	BEF	D	1003	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28466 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 Magnesium-transporting ATPase, P-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	889	Total	C	N	O	S	0	0
			6837	4403	1106	1286	42		
1	B	889	Total	C	N	O	S	0	0
			6837	4403	1106	1286	42		
1	C	889	Total	C	N	O	S	0	0
			6837	4403	1106	1286	42		
1	D	889	Total	C	N	O	S	0	0
			6837	4403	1106	1286	42		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP A0A1V0NGB6
A	-9	HIS	-	expression tag	UNP A0A1V0NGB6
A	-8	HIS	-	expression tag	UNP A0A1V0NGB6
A	-7	HIS	-	expression tag	UNP A0A1V0NGB6
A	-6	HIS	-	expression tag	UNP A0A1V0NGB6
A	-5	HIS	-	expression tag	UNP A0A1V0NGB6
A	-4	HIS	-	expression tag	UNP A0A1V0NGB6
A	-3	HIS	-	expression tag	UNP A0A1V0NGB6
A	-2	HIS	-	expression tag	UNP A0A1V0NGB6
A	-1	LEU	-	expression tag	UNP A0A1V0NGB6
A	0	GLU	-	expression tag	UNP A0A1V0NGB6
A	216	ALA	ASP	conflict	UNP A0A1V0NGB6
A	217	ALA	GLU	conflict	UNP A0A1V0NGB6
A	218	ALA	LYS	conflict	UNP A0A1V0NGB6
A	219	ALA	ASP	conflict	UNP A0A1V0NGB6
A	220	ALA	ASP	conflict	UNP A0A1V0NGB6
A	603	ALA	LYS	conflict	UNP A0A1V0NGB6
A	606	ALA	LYS	conflict	UNP A0A1V0NGB6
A	607	ALA	GLU	conflict	UNP A0A1V0NGB6
B	-10	MET	-	initiating methionine	UNP A0A1V0NGB6
B	-9	HIS	-	expression tag	UNP A0A1V0NGB6
B	-8	HIS	-	expression tag	UNP A0A1V0NGB6

Continued on next page...

Continued from previous page...

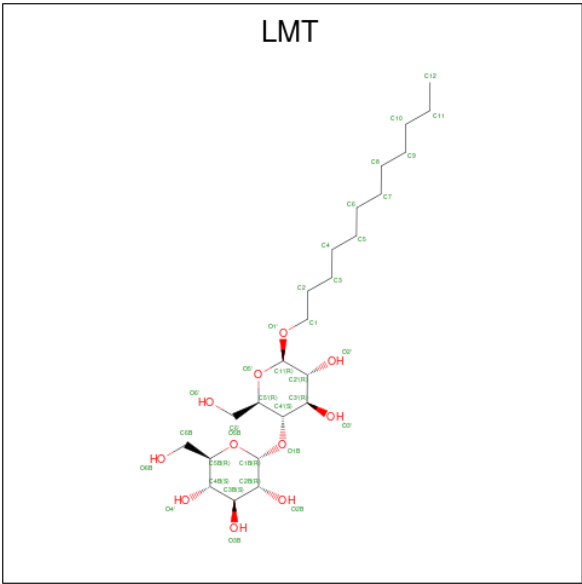
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP A0A1V0NGB6
B	-6	HIS	-	expression tag	UNP A0A1V0NGB6
B	-5	HIS	-	expression tag	UNP A0A1V0NGB6
B	-4	HIS	-	expression tag	UNP A0A1V0NGB6
B	-3	HIS	-	expression tag	UNP A0A1V0NGB6
B	-2	HIS	-	expression tag	UNP A0A1V0NGB6
B	-1	LEU	-	expression tag	UNP A0A1V0NGB6
B	0	GLU	-	expression tag	UNP A0A1V0NGB6
B	216	ALA	ASP	conflict	UNP A0A1V0NGB6
B	217	ALA	GLU	conflict	UNP A0A1V0NGB6
B	218	ALA	LYS	conflict	UNP A0A1V0NGB6
B	219	ALA	ASP	conflict	UNP A0A1V0NGB6
B	220	ALA	ASP	conflict	UNP A0A1V0NGB6
B	603	ALA	LYS	conflict	UNP A0A1V0NGB6
B	606	ALA	LYS	conflict	UNP A0A1V0NGB6
B	607	ALA	GLU	conflict	UNP A0A1V0NGB6
C	-10	MET	-	initiating methionine	UNP A0A1V0NGB6
C	-9	HIS	-	expression tag	UNP A0A1V0NGB6
C	-8	HIS	-	expression tag	UNP A0A1V0NGB6
C	-7	HIS	-	expression tag	UNP A0A1V0NGB6
C	-6	HIS	-	expression tag	UNP A0A1V0NGB6
C	-5	HIS	-	expression tag	UNP A0A1V0NGB6
C	-4	HIS	-	expression tag	UNP A0A1V0NGB6
C	-3	HIS	-	expression tag	UNP A0A1V0NGB6
C	-2	HIS	-	expression tag	UNP A0A1V0NGB6
C	-1	LEU	-	expression tag	UNP A0A1V0NGB6
C	0	GLU	-	expression tag	UNP A0A1V0NGB6
C	216	ALA	ASP	conflict	UNP A0A1V0NGB6
C	217	ALA	GLU	conflict	UNP A0A1V0NGB6
C	218	ALA	LYS	conflict	UNP A0A1V0NGB6
C	219	ALA	ASP	conflict	UNP A0A1V0NGB6
C	220	ALA	ASP	conflict	UNP A0A1V0NGB6
C	603	ALA	LYS	conflict	UNP A0A1V0NGB6
C	606	ALA	LYS	conflict	UNP A0A1V0NGB6
C	607	ALA	GLU	conflict	UNP A0A1V0NGB6
D	-10	MET	-	initiating methionine	UNP A0A1V0NGB6
D	-9	HIS	-	expression tag	UNP A0A1V0NGB6
D	-8	HIS	-	expression tag	UNP A0A1V0NGB6
D	-7	HIS	-	expression tag	UNP A0A1V0NGB6
D	-6	HIS	-	expression tag	UNP A0A1V0NGB6
D	-5	HIS	-	expression tag	UNP A0A1V0NGB6
D	-4	HIS	-	expression tag	UNP A0A1V0NGB6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	HIS	-	expression tag	UNP A0A1V0NGB6
D	-2	HIS	-	expression tag	UNP A0A1V0NGB6
D	-1	LEU	-	expression tag	UNP A0A1V0NGB6
D	0	GLU	-	expression tag	UNP A0A1V0NGB6
D	216	ALA	ASP	conflict	UNP A0A1V0NGB6
D	217	ALA	GLU	conflict	UNP A0A1V0NGB6
D	218	ALA	LYS	conflict	UNP A0A1V0NGB6
D	219	ALA	ASP	conflict	UNP A0A1V0NGB6
D	220	ALA	ASP	conflict	UNP A0A1V0NGB6
D	603	ALA	LYS	conflict	UNP A0A1V0NGB6
D	606	ALA	LYS	conflict	UNP A0A1V0NGB6
D	607	ALA	GLU	conflict	UNP A0A1V0NGB6

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



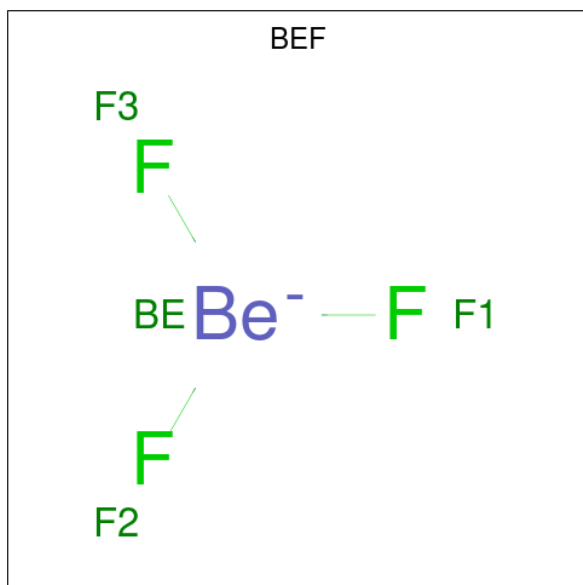
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	24	11	
2	B	1	Total	C	O	0
			35	24	11	
2	C	1	Total	C	O	0
			35	24	11	
2	C	1	Total	C	O	0
			35	24	11	
2	D	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

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

- Molecule 3 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	Be	F	0
			4	1	3	
3	B	1	Total	Be	F	0
			4	1	3	
3	C	1	Total	Be	F	0
			4	1	3	
3	D	1	Total	Be	F	0
			4	1	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

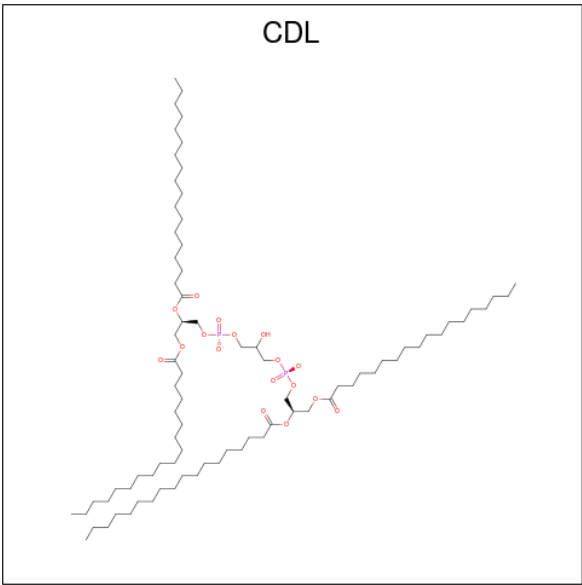
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	
4	B	2	Total	Mg	0
			2	2	
4	C	2	Total	Mg	0
			2	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
4	D	2	Total	Mg	0
			2	2	

- Molecule 5 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).

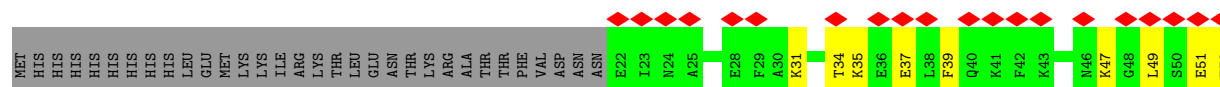


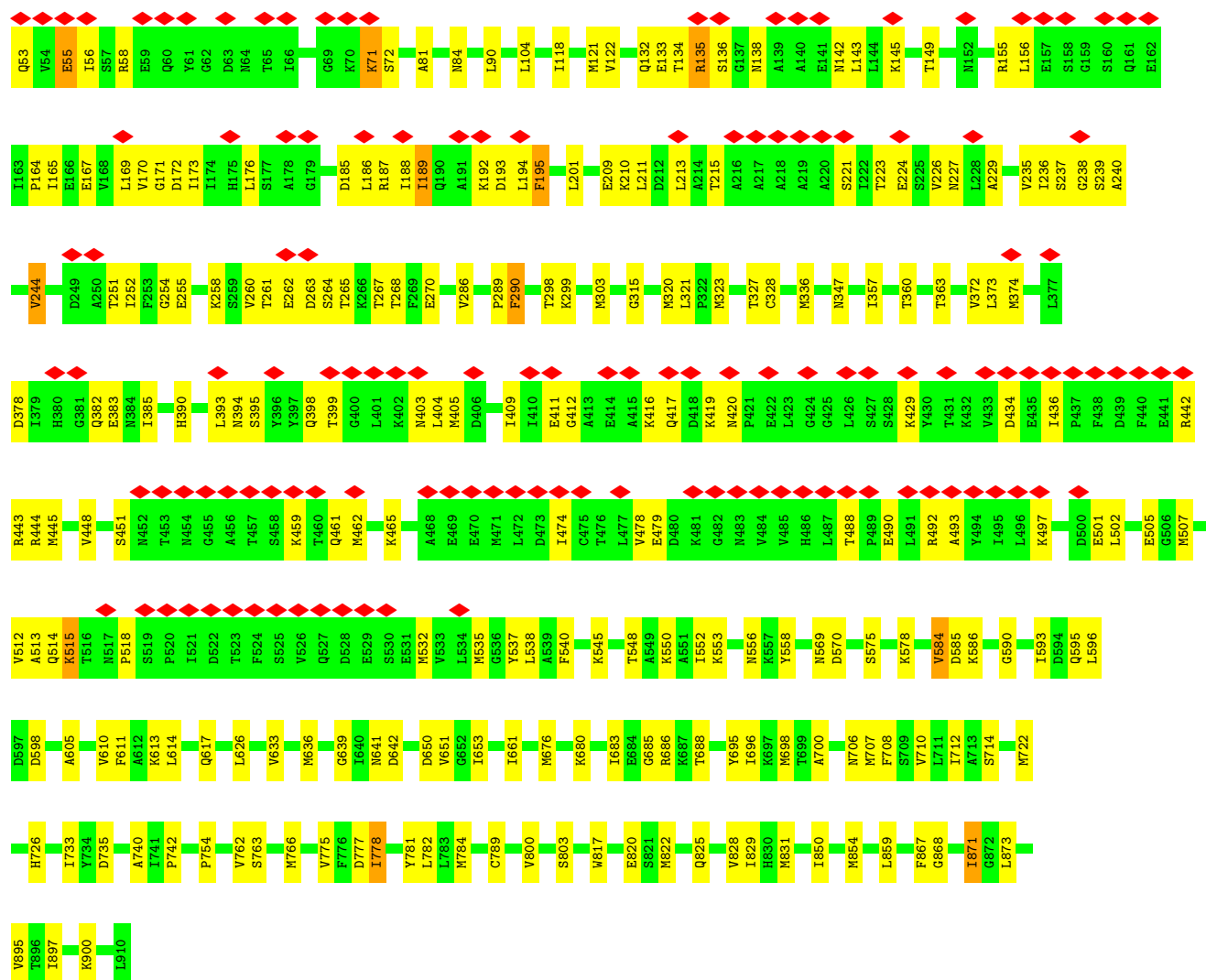
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			52	33	17	2	
5	A	1	Total	C	O	P	0
			52	33	17	2	
5	A	1	Total	C	O	P	0
			52	33	17	2	
5	A	1	Total	C	O	P	0
			52	33	17	2	
5	B	1	Total	C	O	P	0
			52	33	17	2	
5	B	1	Total	C	O	P	0
			52	33	17	2	
5	B	1	Total	C	O	P	0
			52	33	17	2	
5	B	1	Total	C	O	P	0
			52	33	17	2	
5	B	1	Total	C	O	P	0
			52	33	17	2	

Continued on next page...

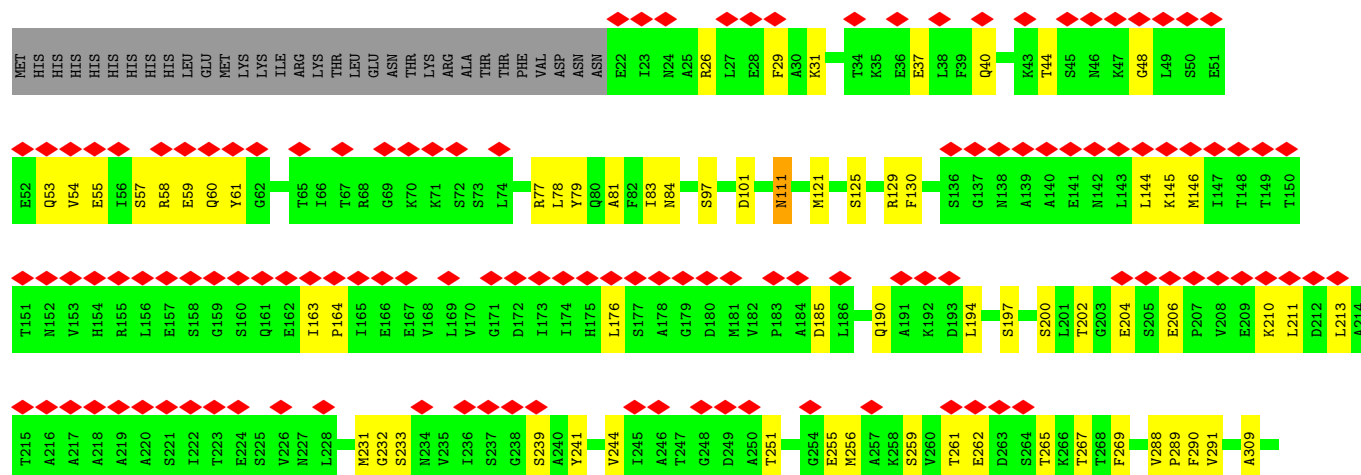
Continued from previous page...

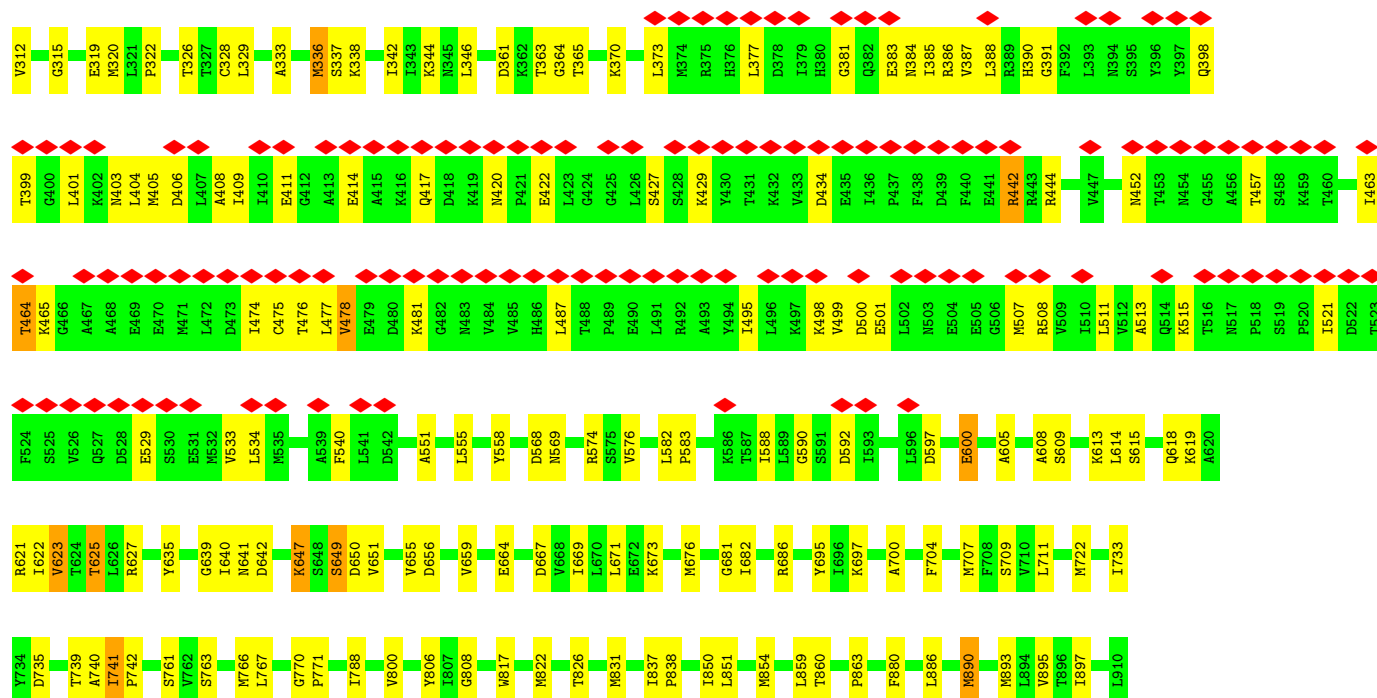
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	O	P	0
			52	33	17	2	
5	C	1	Total	C	O	P	0
			52	33	17	2	
5	C	1	Total	C	O	P	0
			52	33	17	2	
5	C	1	Total	C	O	P	0
			52	33	17	2	
5	C	1	Total	C	O	P	0
			52	33	17	2	
5	D	1	Total	C	O	P	0
			52	33	17	2	
5	D	1	Total	C	O	P	0
			52	33	17	2	





• Molecule 1: Magnesium-transporting ATPase, P-type 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105182	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.787	Depositor
Minimum map value	-0.333	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.113	Depositor
Map size ($\text{\AA}$)	399.9, 399.9, 399.9	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.93, 0.93, 0.93	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: BEF, LMT, CDL, MG

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	0.15	0/6956	0.41	2/9426 (0.0%)
1	B	0.15	0/6956	0.39	1/9426 (0.0%)
1	C	0.14	0/6956	0.41	3/9426 (0.0%)
1	D	0.14	0/6956	0.39	0/9426
All	All	0.14	0/27824	0.40	6/37704 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	VAL	N-CA-C	-5.72	106.82	111.91
1	A	158	SER	CB-CA-C	-5.47	110.25	116.54
1	A	72	SER	CB-CA-C	-5.33	109.45	115.79
1	B	199	ALA	CB-CA-C	-5.29	110.45	116.54
1	C	740	ALA	CA-C-N	5.09	123.45	120.24
1	C	740	ALA	C-N-CA	5.09	123.45	120.24

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	6837	0	7054	174	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6837	0	7053	171	0
1	C	6837	0	7054	194	0
1	D	6837	0	7054	157	0
2	A	35	0	46	0	0
2	B	35	0	46	0	0
2	C	70	0	92	0	0
2	D	70	0	92	0	0
3	A	4	0	0	4	0
3	B	4	0	0	8	0
3	C	4	0	0	4	0
3	D	4	0	0	6	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	208	0	192	9	0
5	B	312	0	286	16	0
5	C	260	0	240	6	0
5	D	104	0	96	3	0
All	All	28466	0	29305	705	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 12.

All (705) 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:D:363:THR:OG1	3:D:1003:BEF:F3	1.50	1.17
1:A:566:THR:HA	3:A:1002:BEF:F2	1.39	1.10
1:B:363:THR:HG23	3:B:1002:BEF:F3	1.52	0.97
1:D:363:THR:O	3:D:1003:BEF:F2	1.74	0.95
1:C:363:THR:O	3:C:1001:BEF:F2	1.74	0.94
1:C:363:THR:HB	3:C:1001:BEF:F2	1.55	0.93
1:A:619:LYS:NZ	3:A:1002:BEF:F2	1.93	0.90
1:B:508:ARG:HE	1:B:540:PHE:HB2	1.35	0.90
1:A:831:MET:HE3	1:A:892:MET:HG3	1.59	0.85
1:B:347:ASN:C	1:B:347:ASN:HD22	1.85	0.85
1:C:71:LYS:HG2	1:C:72:SER:H	1.41	0.85
1:B:363:THR:CG2	3:B:1002:BEF:F3	2.15	0.83
1:A:401:LEU:HD12	1:A:403:ASN:HB3	1.60	0.83
1:A:507:MET:HE2	1:A:540:PHE:HB3	1.60	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:MET:HG3	1:C:465:LYS:HE3	1.60	0.82
1:C:390:HIS:HE1	1:C:515:LYS:HB2	1.45	0.81
1:C:479:GLU:OE2	1:C:479:GLU:N	2.12	0.80
1:D:44:THR:HG22	1:D:53:GLN:HE21	1.46	0.80
1:B:389:ARG:O	1:B:392:PHE:HB3	1.81	0.79
1:A:545:LYS:HE2	1:A:576:VAL:HG23	1.65	0.78
1:D:695:TYR:OH	1:D:735:ASP:OD2	2.02	0.78
1:D:255:GLU:N	1:D:255:GLU:OE2	2.17	0.77
1:B:145:LYS:HG3	1:B:147:ILE:H	1.49	0.77
1:B:298:THR:HG22	5:B:1008:CDL:H121	1.66	0.77
1:C:445:MET:HG2	1:C:465:LYS:H	1.50	0.76
1:D:97:SER:O	1:D:101:ASP:HB2	1.84	0.76
1:C:194:LEU:HG	1:C:239:SER:H	1.49	0.76
1:A:187:ARG:HD2	1:A:189:ILE:HD12	1.68	0.75
1:A:507:MET:HE3	1:A:508:ARG:H	1.51	0.74
1:B:347:ASN:O	1:B:347:ASN:ND2	2.16	0.74
1:D:639:GLY:HA3	3:D:1003:BEF:F1	1.79	0.73
1:A:542:ASP:OD2	1:A:575:SER:OG	2.07	0.72
1:B:141:GLU:N	1:B:141:GLU:OE2	2.22	0.72
1:B:153:VAL:HG13	1:B:155:ARG:HG2	1.71	0.72
1:B:413:ALA:HA	1:B:416:LYS:HE2	1.72	0.72
1:B:585:ASP:OD1	1:B:586:LYS:N	2.23	0.71
1:C:710:VAL:O	1:C:714:SER:HB3	1.89	0.71
1:A:485:VAL:HG13	1:A:487:LEU:H	1.55	0.71
1:C:49:LEU:H	1:C:53:GLN:HG2	1.55	0.71
1:A:694:LYS:NZ	1:A:744:ASP:OD2	2.23	0.71
1:B:52:GLU:HA	1:B:55:GLU:HB2	1.73	0.70
1:A:51:GLU:OE2	1:A:51:GLU:N	2.22	0.70
1:C:403:ASN:ND2	1:C:405:MET:SD	2.65	0.70
1:B:221:SER:O	1:B:223:THR:N	2.22	0.69
1:D:398:GLN:HG2	1:D:399:THR:HG22	1.74	0.69
1:A:566:THR:CA	3:A:1002:BEF:F2	2.26	0.69
1:B:147:ILE:HG22	1:B:148:THR:HG23	1.75	0.69
1:C:81:ALA:O	1:C:84:ASN:ND2	2.25	0.69
1:D:740:ALA:HB2	1:D:851:LEU:HD12	1.74	0.69
1:C:55:GLU:OE2	1:C:56:ILE:N	2.26	0.69
1:C:390:HIS:CE1	1:C:515:LYS:HB2	2.27	0.68
1:D:231:MET:HE1	1:D:251:THR:HG21	1.76	0.68
1:C:176:LEU:HD13	1:C:235:VAL:HG11	1.75	0.68
1:C:778:ILE:HD13	1:C:784:MET:HG3	1.74	0.68
1:A:394:ASN:HB2	1:A:428:SER:HB3	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:O	1:A:407:LEU:HB2	1.94	0.67
1:D:288:VAL:HG13	1:D:309:ALA:HB1	1.76	0.67
1:B:706:ASN:ND2	1:B:825:GLN:OE1	2.28	0.67
1:C:210:LYS:HD2	1:C:226:VAL:HA	1.76	0.67
1:A:462:MET:HE2	1:A:530:SER:HA	1.76	0.67
1:A:517:ASN:ND2	1:A:519:SER:O	2.26	0.66
1:A:442:ARG:HH22	1:A:443:ARG:HE	1.41	0.66
1:C:192:LYS:H	1:C:239:SER:HA	1.59	0.66
1:D:185:ASP:HB2	1:D:244:VAL:HG23	1.77	0.66
1:A:327:THR:HA	1:A:330:ALA:HB3	1.78	0.65
1:A:366:LEU:HB3	1:A:545:LYS:HG2	1.79	0.65
1:C:188:ILE:O	1:C:239:SER:OG	2.14	0.65
1:B:141:GLU:O	1:B:142:ASN:ND2	2.29	0.65
1:A:81:ALA:O	1:A:84:ASN:ND2	2.28	0.64
1:B:837:ILE:HB	1:B:841:GLN:HG3	1.80	0.64
1:D:163:ILE:HD12	1:D:164:PRO:HD2	1.78	0.64
1:D:381:GLY:HA2	1:D:386:ARG:HH12	1.62	0.64
1:A:538:LEU:HB2	1:A:540:PHE:HE1	1.63	0.64
1:C:268:THR:OG1	1:C:650:ASP:OD2	2.10	0.64
1:C:55:GLU:CD	1:C:56:ILE:H	2.05	0.64
1:B:153:VAL:HG11	1:B:161:GLN:HE22	1.63	0.63
1:D:261:THR:HA	1:D:647:LYS:HZ1	1.62	0.63
1:A:71:LYS:HE3	1:A:77:ARG:HH12	1.63	0.63
1:B:303:MET:HA	1:B:303:MET:HE2	1.80	0.63
1:C:176:LEU:HD12	1:C:240:ALA:HA	1.81	0.63
1:A:361:ASP:O	1:A:365:THR:OG1	2.16	0.63
1:B:176:LEU:HD22	1:B:235:VAL:HG11	1.80	0.63
1:D:649:SER:OG	1:D:650:ASP:N	2.29	0.63
1:B:197:SER:HA	1:B:207:PRO:HA	1.80	0.63
1:A:577:CYS:HA	1:A:580:VAL:HG22	1.80	0.63
5:B:1009:CDL:HA31	5:B:1009:CDL:HB21	1.79	0.63
1:C:706:ASN:ND2	1:C:825:GLN:OE1	2.32	0.63
1:A:598:ASP:HA	1:A:601:LEU:HB3	1.79	0.63
1:D:267:THR:OG1	1:D:627:ARG:NH2	2.32	0.62
1:B:31:LYS:NZ	1:B:219:ALA:O	2.31	0.62
1:C:289:PRO:HB3	1:D:289:PRO:HB3	1.81	0.62
1:D:656:ASP:OD1	1:D:673:LYS:NZ	2.33	0.62
1:D:722:MET:HG3	1:D:817:TRP:HE3	1.64	0.62
1:A:38:LEU:O	1:A:40:GLN:NE2	2.33	0.62
1:D:190:GLN:NE2	1:D:239:SER:O	2.33	0.62
1:C:192:LYS:HD3	1:C:193:ASP:HB2	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ASP:O	1:A:420:ASN:ND2	2.33	0.62
1:C:255:GLU:HB2	1:C:617:GLN:HE21	1.64	0.62
1:D:363:THR:C	3:D:1003:BEF:F2	2.32	0.62
1:C:255:GLU:HA	1:C:258:LYS:HG3	1.82	0.62
1:A:171:GLY:HA2	1:A:239:SER:HB2	1.80	0.61
1:B:393:LEU:HG	1:B:397:TYR:HB2	1.82	0.61
1:C:215:THR:OG1	1:C:227:ASN:OD1	2.19	0.61
1:C:443:ARG:O	1:C:443:ARG:HD3	2.00	0.61
1:C:411:GLU:OE2	1:C:411:GLU:HA	2.01	0.61
1:C:459:LYS:NZ	1:C:518:PRO:O	2.33	0.61
1:D:583:PRO:O	1:D:609:SER:OG	2.19	0.61
1:D:507:MET:HE3	1:D:507:MET:HA	1.83	0.60
1:A:103:ILE:HG22	1:A:104:LEU:HD22	1.83	0.60
1:C:575:SER:HA	1:C:578:LYS:HE3	1.84	0.60
1:C:782:LEU:C	1:C:784:MET:H	2.10	0.60
5:A:1005:CDL:H531	5:A:1005:CDL:HB62	1.83	0.60
1:B:822:MET:HG2	1:B:859:LEU:HD13	1.83	0.60
1:D:54:VAL:HG12	1:D:58:ARG:HE	1.66	0.59
1:C:443:ARG:O	1:C:444:ARG:NE	2.34	0.59
1:A:507:MET:HE3	1:A:508:ARG:HB3	1.84	0.59
1:B:288:VAL:HG13	1:B:309:ALA:HB1	1.85	0.59
1:B:362:LYS:HA	1:B:366:LEU:HD13	1.85	0.59
1:D:417:GLN:HA	1:D:420:ASN:HB2	1.84	0.59
1:B:200:SER:OG	1:B:201:LEU:N	2.34	0.59
1:B:374:MET:SD	1:B:540:PHE:HA	2.43	0.59
1:C:505:GLU:OE2	1:C:507:MET:HB3	2.03	0.59
1:D:145:LYS:H	1:D:145:LYS:HE2	1.68	0.59
1:B:893:MET:HB3	1:D:886:LEU:HD11	1.83	0.59
1:C:676:MET:HE2	1:C:676:MET:N	2.18	0.59
1:D:121:MET:HG2	1:D:320:MET:HE3	1.84	0.59
1:C:419:LYS:HG2	1:C:420:ASN:H	1.68	0.58
1:A:371:VAL:HG12	1:A:542:ASP:HA	1.84	0.58
1:A:640:ILE:HG13	1:A:659:VAL:HG21	1.85	0.58
1:A:837:ILE:HB	1:A:841:GLN:HG3	1.85	0.58
1:D:206:GLU:N	1:D:206:GLU:OE2	2.30	0.58
1:B:459:LYS:HB2	1:B:518:PRO:HG2	1.85	0.58
1:B:641:ASN:OD1	3:B:1002:BEF:F1	2.11	0.58
1:C:134:THR:HG22	1:C:136:SER:H	1.66	0.58
1:C:195:PHE:HB2	1:C:236:ILE:HB	1.86	0.58
1:A:363:THR:OG1	4:A:1004:MG:MG	1.44	0.58
1:A:909:LEU:O	1:A:910:LEU:HB2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:GLN:OE1	1:C:398:GLN:N	2.36	0.58
1:A:320:MET:HB3	1:A:323:MET:HE2	1.86	0.58
1:B:23:ILE:HG23	1:B:24:ASN:H	1.68	0.58
1:C:194:LEU:HG	1:C:239:SER:N	2.17	0.58
1:A:717:LEU:HD13	1:A:721:PRO:HG3	1.86	0.58
1:C:194:LEU:H	1:C:238:GLY:HA3	1.67	0.58
1:A:186:LEU:HD23	1:A:187:ARG:H	1.68	0.58
1:C:51:GLU:O	1:C:58:ARG:NH2	2.37	0.58
1:D:373:LEU:HD11	1:D:409:ILE:HD13	1.86	0.58
1:A:489:PRO:O	1:A:491:LEU:N	2.36	0.57
1:C:164:PRO:HG2	1:C:167:GLU:HB2	1.85	0.57
5:B:1010:CDL:HB62	1:D:837:ILE:HD12	1.86	0.57
1:A:261:THR:OG1	1:A:262:GLU:OE1	2.21	0.57
1:A:695:TYR:OH	1:A:735:ASP:OD1	2.19	0.57
1:B:117:ILE:HG22	1:B:121:MET:HE3	1.86	0.57
1:C:493:ALA:HB1	1:C:497:LYS:HG2	1.86	0.57
1:B:275:SER:HB2	1:B:759:ALA:HB2	1.84	0.57
1:C:416:LYS:O	1:C:417:GLN:NE2	2.37	0.57
1:D:37:GLU:OE1	1:D:40:GLN:NE2	2.36	0.57
1:D:597:ASP:HB3	1:D:600:GLU:HG2	1.87	0.57
1:C:822:MET:HG2	1:C:859:LEU:HD13	1.85	0.57
1:D:442:ARG:NE	1:D:444:ARG:O	2.37	0.57
1:A:472:LEU:HD11	1:A:533:VAL:HG22	1.87	0.57
1:C:405:MET:HE3	1:C:405:MET:N	2.20	0.57
1:D:211:LEU:HD23	1:D:211:LEU:H	1.70	0.56
1:C:195:PHE:HB2	1:C:237:SER:H	1.71	0.56
5:C:1007:CDL:H1	5:C:1007:CDL:H732	1.87	0.56
1:B:486:HIS:HB2	1:B:488:THR:HG23	1.88	0.56
5:B:1010:CDL:HB4	5:B:1010:CDL:OA3	2.05	0.56
1:C:461:GLN:NE2	1:C:462:MET:O	2.38	0.56
1:D:405:MET:HE2	1:D:405:MET:H	1.71	0.56
1:C:224:GLU:OE1	1:C:224:GLU:N	2.36	0.56
1:D:822:MET:HG2	1:D:859:LEU:HD13	1.88	0.56
1:B:393:LEU:HA	1:B:397:TYR:HD1	1.71	0.56
1:B:347:ASN:C	1:B:347:ASN:ND2	2.57	0.56
1:C:194:LEU:HA	1:C:235:VAL:HG12	1.88	0.55
1:D:508:ARG:HB2	1:D:540:PHE:HZ	1.70	0.55
1:A:752:VAL:HG23	1:A:753:VAL:HG23	1.88	0.55
1:B:475:CYS:SG	1:B:492:ARG:NH1	2.76	0.55
1:B:501:GLU:CD	1:B:501:GLU:H	2.13	0.55
1:C:512:VAL:HG11	1:C:538:LEU:HD12	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:ASN:OD1	1:C:641:ASN:N	2.40	0.55
1:D:478:VAL:HB	1:D:533:VAL:HG21	1.88	0.55
1:B:445:MET:HE2	1:B:445:MET:HA	1.87	0.55
1:A:176:LEU:HD21	1:A:180:ASP:OD2	2.06	0.55
1:B:190:GLN:HE22	1:B:241:TYR:H	1.53	0.55
1:C:71:LYS:HG2	1:C:72:SER:N	2.17	0.55
1:C:186:LEU:HB2	1:C:229:ALA:HB3	1.88	0.55
1:B:399:THR:HG21	1:B:435:GLU:HG2	1.87	0.55
1:B:388:LEU:HD23	1:B:389:ARG:HH21	1.71	0.55
1:C:262:GLU:O	1:C:264:SER:N	2.40	0.55
1:C:360:THR:HG23	1:C:636:MET:HE3	1.89	0.55
1:D:364:GLY:HA3	3:D:1003:BEF:F2	1.97	0.55
1:A:102:ILE:HD11	1:A:112:PRO:HB3	1.88	0.54
1:B:582:LEU:HD12	1:B:583:PRO:HD2	1.89	0.54
1:B:588:ILE:HD13	1:B:593:ILE:HD11	1.88	0.54
1:D:568:ASP:OD1	1:D:569:ASN:ND2	2.41	0.54
1:A:170:VAL:HG13	1:A:172:ASP:H	1.72	0.54
1:A:505:GLU:HA	1:A:571:LYS:HE3	1.88	0.54
1:B:352:LEU:HD13	1:B:651:VAL:HG11	1.89	0.54
1:B:570:ASP:HB2	1:B:574:ARG:HH12	1.73	0.54
1:B:641:ASN:OD1	1:B:641:ASN:N	2.36	0.54
1:C:133:GLU:O	1:C:138:ASN:ND2	2.40	0.54
1:C:850:ILE:O	1:C:854:MET:HG3	2.07	0.54
1:A:596:LEU:H	1:A:596:LEU:HD23	1.71	0.54
1:B:741:ILE:HG22	1:B:742:PRO:HD3	1.89	0.54
1:D:704:PHE:HE2	1:D:771:PRO:HD3	1.73	0.54
1:A:37:GLU:HB3	1:A:187:ARG:HG2	1.90	0.54
1:D:144:LEU:H	1:D:145:LYS:HZ3	1.54	0.54
1:D:498:LYS:HD2	1:D:499:VAL:HG23	1.87	0.54
1:A:444:ARG:CD	1:A:444:ARG:H	2.20	0.54
1:A:834:THR:HG21	1:A:842:SER:HB3	1.90	0.54
1:B:886:LEU:HD11	1:D:893:MET:HB3	1.89	0.54
1:A:261:THR:OG1	1:A:262:GLU:N	2.29	0.54
1:B:342:ILE:HD13	1:B:671:LEU:HD21	1.90	0.54
1:C:221:SER:O	1:C:223:THR:N	2.37	0.54
1:D:500:ASP:O	1:D:501:GLU:HG2	2.08	0.54
1:A:77:ARG:HG3	1:A:77:ARG:HH11	1.73	0.54
1:A:565:LEU:HD12	1:A:635:TYR:HE2	1.72	0.54
1:B:629:SER:OG	1:B:631:ASN:OD1	2.25	0.54
1:D:618:GLN:O	1:D:622:ILE:HG12	2.08	0.54
1:A:186:LEU:HD23	1:A:187:ARG:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:MET:SD	1:A:405:MET:N	2.73	0.53
1:A:743:TRP:HZ2	5:A:1008:CDL:H121	1.73	0.53
1:C:195:PHE:N	1:C:237:SER:O	2.40	0.53
1:C:448:VAL:HG22	1:C:462:MET:HG3	1.90	0.53
1:D:558:TYR:HB3	1:D:686:ARG:HH12	1.73	0.53
1:B:157:GLU:OE2	1:B:158:SER:OG	2.24	0.53
1:A:225:SER:O	1:A:225:SER:OG	2.23	0.53
1:A:228:LEU:HD12	1:A:230:PHE:CE1	2.43	0.53
1:C:445:MET:SD	1:C:445:MET:N	2.82	0.53
1:C:570:ASP:OD1	1:C:570:ASP:N	2.37	0.53
1:A:354:SER:O	1:A:354:SER:OG	2.25	0.53
5:B:1010:CDL:HB21	5:B:1010:CDL:HB61	1.90	0.53
1:D:259:SER:O	1:D:259:SER:OG	2.27	0.53
1:D:291:VAL:HB	1:D:711:LEU:HD12	1.89	0.53
1:B:231:MET:C	1:B:231:MET:HE3	2.33	0.53
1:D:695:TYR:HB2	1:D:741:ILE:HG21	1.91	0.53
1:A:373:LEU:HD11	1:A:540:PHE:CD2	2.44	0.53
1:C:145:LYS:HE2	1:C:661:ILE:HD11	1.90	0.53
1:D:697:LYS:NZ	1:D:761:SER:OG	2.42	0.53
1:C:315:GLY:HA3	1:C:707:MET:HE2	1.90	0.53
1:D:204:GLU:OE1	1:D:204:GLU:N	2.42	0.53
1:B:121:MET:SD	1:B:319:GLU:HB3	2.48	0.53
1:B:722:MET:HG2	1:B:726:HIS:HB2	1.90	0.53
1:A:146:MET:SD	1:A:146:MET:N	2.82	0.53
1:C:488:THR:HG22	1:C:490:GLU:H	1.74	0.53
1:A:368:GLN:OE1	1:A:368:GLN:N	2.42	0.52
1:C:263:ASP:C	1:C:263:ASP:OD2	2.51	0.52
1:C:700:ALA:HB1	1:C:766:MET:SD	2.49	0.52
1:A:238:GLY:N	1:A:441:GLU:OE2	2.42	0.52
1:A:369:ASP:OD2	1:A:370:LYS:HD3	2.08	0.52
1:C:194:LEU:H	1:C:238:GLY:CA	2.22	0.52
1:D:262:GLU:O	1:D:265:THR:OG1	2.26	0.52
1:D:500:ASP:OD1	1:D:501:GLU:N	2.43	0.52
1:A:39:PHE:CZ	1:A:166:GLU:HG2	2.44	0.52
1:B:733:ILE:HD12	1:B:859:LEU:HD12	1.90	0.52
1:D:806:TYR:O	1:D:808:GLY:N	2.39	0.52
1:B:507:MET:HG2	1:B:541:LEU:HD23	1.91	0.52
1:D:850:ILE:O	1:D:854:MET:HG3	2.09	0.52
1:B:698:MET:HE3	1:B:829:ILE:HG12	1.92	0.52
1:C:374:MET:HG3	1:C:540:PHE:CE1	2.45	0.52
1:C:497:LYS:NZ	1:C:501:GLU:OE2	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LYS:HD3	1:A:47:LYS:HE2	1.91	0.52
1:B:547:SER:OG	1:B:674:ASP:O	2.15	0.52
1:C:221:SER:HB2	1:C:224:GLU:OE2	2.10	0.52
1:A:282:ARG:HH12	5:A:1006:CDL:H1	1.75	0.52
1:B:249:ASP:OD2	1:B:249:ASP:C	2.52	0.52
1:C:390:HIS:CD2	1:C:394:ASN:HD22	2.28	0.52
1:D:700:ALA:HB1	1:D:766:MET:SD	2.50	0.52
1:C:492:ARG:H	1:C:492:ARG:HD2	1.73	0.52
1:D:213:LEU:HD23	1:D:213:LEU:H	1.75	0.52
1:C:569:ASN:HA	1:C:613:LYS:HZ3	1.75	0.52
1:A:34:THR:OG1	1:A:187:ARG:NH2	2.43	0.51
1:C:636:MET:HB2	1:C:653:ILE:HB	1.91	0.51
1:D:48:GLY:N	1:D:53:GLN:HE22	2.08	0.51
1:A:136:SER:OG	1:A:140:ALA:O	2.24	0.51
1:A:570:ASP:O	1:A:574:ARG:HG2	2.11	0.51
1:B:469:GLU:HG2	1:B:511:LEU:HD23	1.92	0.51
1:C:686:ARG:HH22	1:C:754:PRO:HD3	1.75	0.51
1:C:698:MET:HE3	1:C:829:ILE:HG12	1.92	0.51
1:A:446:SER:HB2	1:A:465:LYS:HG3	1.91	0.51
1:C:363:THR:CB	3:C:1001:BEF:F2	2.39	0.51
1:C:465:LYS:HB2	1:C:513:ALA:H	1.74	0.51
1:C:733:ILE:HD12	1:C:859:LEU:HD12	1.92	0.51
1:B:584:VAL:HG12	1:B:610:VAL:HG21	1.92	0.51
1:A:342:ILE:HB	1:A:669:ILE:HG12	1.93	0.51
1:A:488:THR:OG1	1:A:491:LEU:O	2.28	0.51
1:C:584:VAL:HG12	1:C:585:ASP:H	1.75	0.51
1:B:594:ASP:OD1	1:B:594:ASP:N	2.38	0.51
1:A:831:MET:SD	1:A:838:PRO:HG2	2.51	0.50
1:A:198:GLN:OE1	1:A:230:PHE:HB2	2.10	0.50
1:B:363:THR:O	3:B:1002:BEF:F3	2.19	0.50
1:B:231:MET:HE2	1:B:253:PHE:HB2	1.94	0.50
1:B:493:ALA:HB1	1:B:499:VAL:HB	1.92	0.50
1:A:165:ILE:HG13	1:A:243:VAL:HG21	1.94	0.50
1:A:889:VAL:O	1:A:893:MET:HG2	2.11	0.50
1:D:315:GLY:HA3	1:D:707:MET:HE3	1.93	0.50
5:B:1010:CDL:HB62	1:D:837:ILE:CD1	2.42	0.50
1:C:263:ASP:OD2	1:C:265:THR:N	2.41	0.50
1:C:374:MET:SD	1:C:374:MET:N	2.85	0.50
1:C:558:TYR:CZ	1:C:683:ILE:HD11	2.47	0.50
1:B:113:GLN:O	1:B:117:ILE:HG13	2.11	0.50
1:A:479:GLU:HG2	1:A:480:ASP:H	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:THR:O	1:B:34:THR:N	2.45	0.50
5:B:1010:CDL:H512	1:D:838:PRO:HD2	1.94	0.50
1:C:142:ASN:O	1:C:143:LEU:HD12	2.12	0.50
1:A:35:LYS:HG3	1:A:42:PHE:HD2	1.77	0.50
1:C:395:SER:HB2	1:C:409:ILE:HG21	1.94	0.50
1:D:31:LYS:HD2	1:D:31:LYS:C	2.37	0.50
1:D:48:GLY:H	1:D:53:GLN:HE22	1.60	0.50
1:A:336:MET:HG3	1:A:349:ILE:HD11	1.93	0.49
1:A:700:ALA:HB1	1:A:766:MET:SD	2.51	0.49
1:C:412:GLY:O	1:C:416:LYS:HB3	2.11	0.49
1:D:81:ALA:HB1	1:D:129:ARG:HG2	1.92	0.49
1:B:291:VAL:HG21	1:B:312:VAL:HG21	1.94	0.49
1:D:194:LEU:HD11	1:D:210:LYS:HB3	1.95	0.49
1:C:267:THR:OG1	1:C:270:GLU:OE1	2.29	0.49
1:A:237:SER:HB3	1:A:441:GLU:OE2	2.13	0.49
1:B:187:ARG:HG3	1:B:189:ILE:HG23	1.93	0.49
1:B:641:ASN:ND2	3:B:1002:BEF:F1	2.35	0.49
1:A:251:THR:HG22	1:A:252:ILE:HG12	1.95	0.49
1:B:722:MET:HE3	1:B:727:ILE:HG12	1.94	0.49
1:C:390:HIS:O	1:C:394:ASN:ND2	2.45	0.49
1:A:507:MET:HE3	1:A:508:ARG:N	2.24	0.49
1:B:188:ILE:O	1:B:190:GLN:N	2.46	0.49
1:B:779:THR:HG23	1:D:897:ILE:HG21	1.94	0.49
1:D:434:ASP:OD2	1:D:521:ILE:HG21	2.13	0.49
1:A:387:VAL:HG11	1:A:538:LEU:HD11	1.94	0.49
1:A:514:GLN:HG2	1:A:515:LYS:N	2.28	0.49
1:C:121:MET:HG2	1:C:320:MET:HE3	1.95	0.49
1:D:390:HIS:CE1	1:D:465:LYS:HD3	2.48	0.49
1:A:401:LEU:HD13	1:A:401:LEU:O	2.12	0.49
1:A:847:PRO:HG3	5:A:1008:CDL:H511	1.93	0.49
5:B:1010:CDL:HA61	5:B:1010:CDL:H311	1.59	0.48
1:C:320:MET:HE2	1:C:320:MET:HA	1.94	0.48
1:B:622:ILE:HA	1:B:625:THR:HG22	1.94	0.48
1:C:104:LEU:HB3	1:C:303:MET:HE1	1.95	0.48
1:D:200:SER:OG	1:D:232:GLY:O	2.24	0.48
1:D:403:ASN:OD1	1:D:405:MET:HE2	2.14	0.48
1:D:475:CYS:HA	1:D:533:VAL:HG22	1.95	0.48
1:B:436:ILE:HD12	1:B:445:MET:HG3	1.95	0.48
1:C:639:GLY:N	1:C:642:ASP:OD2	2.45	0.48
1:C:778:ILE:H	1:C:820:GLU:CD	2.21	0.48
1:B:187:ARG:HH11	1:B:187:ARG:HA	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:THR:HA	1:B:544:PRO:HA	1.95	0.48
1:B:406:ASP:O	1:B:409:ILE:HG13	2.13	0.48
1:C:383:GLU:OE2	1:C:385:ILE:HG22	2.12	0.48
1:D:26:ARG:NH2	1:D:29:PHE:O	2.47	0.48
1:D:391:GLY:HA3	1:D:409:ILE:HG21	1.95	0.48
1:D:403:ASN:HB3	1:D:406:ASP:OD1	2.14	0.48
5:A:1005:CDL:HB4	5:A:1005:CDL:HA31	1.95	0.48
1:B:268:THR:HG21	1:B:632:SER:HB2	1.94	0.48
1:C:722:MET:HG2	1:C:726:HIS:HB2	1.95	0.48
1:D:767:LEU:HD22	5:D:1007:CDL:H141	1.95	0.48
1:C:708:PHE:O	1:C:712:ILE:HG12	2.14	0.48
1:D:605:ALA:HA	1:D:608:ALA:HB2	1.94	0.48
1:B:81:ALA:O	1:B:84:ASN:ND2	2.37	0.48
1:C:416:LYS:NZ	1:C:419:LYS:HB2	2.28	0.48
1:C:465:LYS:NZ	1:C:514:GLN:HE21	2.11	0.48
1:C:685:GLY:HA2	1:C:688:THR:HB	1.94	0.48
1:D:336:MET:SD	1:D:681:GLY:HA2	2.53	0.48
1:A:347:ASN:OD1	1:A:347:ASN:N	2.39	0.48
1:D:387:VAL:HG23	1:D:388:LEU:HD23	1.96	0.48
1:D:176:LEU:HD12	1:D:241:TYR:HD1	1.79	0.48
1:A:37:GLU:CD	1:A:187:ARG:HE	2.22	0.48
1:B:315:GLY:HA3	1:B:707:MET:HE3	1.95	0.48
1:C:461:GLN:NE2	1:C:515:LYS:O	2.47	0.48
1:C:867:PHE:HB3	5:C:1010:CDL:HB31	1.96	0.48
1:A:316:LEU:HG	1:A:707:MET:HG3	1.96	0.47
1:A:475:CYS:HB2	1:A:532:MET:HE1	1.96	0.47
1:B:185:ASP:HB3	1:B:246:ALA:HB3	1.96	0.47
1:B:636:MET:HG3	1:B:653:ILE:HB	1.96	0.47
1:D:639:GLY:CA	3:D:1003:BEF:F1	2.49	0.47
1:A:163:ILE:HD12	1:A:164:PRO:HD2	1.95	0.47
1:B:384:ASN:O	1:B:386:ARG:N	2.47	0.47
1:C:626:LEU:HB3	1:C:633:VAL:HG21	1.97	0.47
1:D:463:ILE:HD12	1:D:465:LYS:H	1.79	0.47
1:B:498:LYS:C	1:B:500:ASP:H	2.23	0.47
1:A:328:CYS:SG	1:A:742:PRO:HG3	2.54	0.47
1:C:695:TYR:OH	1:C:735:ASP:OD1	2.29	0.47
1:D:427:SER:HA	1:D:457:THR:HB	1.96	0.47
1:A:475:CYS:O	1:A:477:LEU:N	2.47	0.47
1:C:51:GLU:HG2	1:C:52:GLU:HG2	1.96	0.47
1:C:374:MET:HE2	1:C:374:MET:H	1.79	0.47
1:A:68:ARG:HA	1:A:68:ARG:HD3	1.74	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ILE:HD11	1:B:112:PRO:HB3	1.96	0.47
1:B:323:MET:O	1:B:327:THR:OG1	2.32	0.47
1:B:392:PHE:O	1:B:395:SER:HB2	2.15	0.47
1:B:627:ARG:NH1	1:B:650:ASP:OD1	2.48	0.47
1:B:103:ILE:HG22	1:B:104:LEU:HD23	1.97	0.47
5:B:1008:CDL:H112	5:C:1006:CDL:HB31	1.96	0.47
1:D:623:VAL:HG11	1:D:649:SER:HA	1.96	0.47
1:A:514:GLN:HG2	1:A:515:LYS:H	1.80	0.47
1:B:531:GLU:O	1:B:532:MET:HG2	2.15	0.47
1:C:185:ASP:O	1:C:186:LEU:HD23	2.15	0.47
1:C:552:ILE:O	1:C:556:ASN:ND2	2.48	0.47
1:C:726:HIS:NE2	1:C:871:ILE:O	2.36	0.47
1:C:777:ASP:O	1:C:781:TYR:N	2.39	0.47
1:D:568:ASP:H	1:D:613:LYS:H	1.63	0.47
1:A:374:MET:SD	1:A:374:MET:N	2.88	0.47
1:B:558:TYR:HE2	1:B:679:GLU:OE2	1.98	0.47
1:B:767:LEU:HD13	5:B:1007:CDL:HA31	1.97	0.47
1:C:192:LYS:N	1:C:238:GLY:O	2.47	0.47
1:C:442:ARG:HG3	1:C:444:ARG:HG2	1.97	0.47
1:D:55:GLU:O	1:D:59:GLU:HG2	2.15	0.47
1:A:77:ARG:HG3	1:A:77:ARG:NH1	2.30	0.46
1:A:567:GLY:HA2	1:A:614:LEU:H	1.80	0.46
1:B:570:ASP:N	1:B:570:ASP:OD1	2.47	0.46
1:B:623:VAL:HG11	1:B:649:SER:HB3	1.97	0.46
1:C:172:ASP:OD1	1:C:173:ILE:N	2.48	0.46
1:C:490:GLU:HA	1:C:493:ALA:HB3	1.97	0.46
1:C:550:LYS:C	1:C:552:ILE:H	2.23	0.46
1:D:383:GLU:OE1	1:D:384:ASN:N	2.35	0.46
1:D:682:ILE:O	1:D:686:ARG:HG3	2.16	0.46
1:B:137:GLY:O	1:B:344:LYS:NZ	2.49	0.46
1:C:90:LEU:HB3	1:C:122:VAL:HG22	1.95	0.46
1:C:188:ILE:C	1:C:189:ILE:HG13	2.41	0.46
1:A:282:ARG:HH22	5:A:1006:CDL:HB31	1.80	0.46
1:B:58:ARG:HD2	1:B:58:ARG:HA	1.70	0.46
1:C:193:ASP:OD1	1:C:237:SER:HA	2.14	0.46
1:D:403:ASN:OD1	1:D:404:LEU:N	2.48	0.46
1:B:695:TYR:HB2	1:B:741:ILE:HG21	1.96	0.46
1:C:639:GLY:N	3:C:1001:BEF:F1	2.39	0.46
1:B:700:ALA:HB1	1:B:766:MET:SD	2.55	0.46
1:D:111:ASN:HD22	1:D:111:ASN:C	2.22	0.46
1:D:474:ILE:HG22	1:D:475:CYS:H	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:SER:HB3	1:A:825:GLN:HG2	1.98	0.46
1:A:850:ILE:O	1:A:854:MET:HG3	2.16	0.46
1:B:360:THR:HG23	1:B:636:MET:HB3	1.96	0.46
1:B:577:CYS:SG	1:B:582:LEU:HB3	2.56	0.46
1:C:49:LEU:HD13	1:C:53:GLN:HA	1.98	0.46
1:C:378:ASP:H	1:C:382:GLN:H	1.63	0.46
1:C:598:ASP:OD1	1:C:598:ASP:N	2.48	0.46
1:B:189:ILE:HG13	1:B:190:GLN:H	1.80	0.46
1:B:346:LEU:C	1:B:348:SER:H	2.23	0.46
1:B:558:TYR:CZ	1:B:683:ILE:HD11	2.50	0.46
1:B:287:MET:HE3	1:B:711:LEU:HD13	1.97	0.46
1:C:71:LYS:CG	1:C:72:SER:H	2.21	0.46
1:C:169:LEU:HG	1:C:170:VAL:H	1.81	0.46
1:C:251:THR:HG23	1:C:254:GLY:H	1.80	0.46
1:C:336:MET:HE3	1:C:336:MET:HB3	1.86	0.46
1:C:585:ASP:O	1:C:586:LYS:HG2	2.16	0.46
1:C:676:MET:HE2	1:C:676:MET:H	1.80	0.46
1:D:57:SER:HA	1:D:60:GLN:HG2	1.98	0.46
1:D:568:ASP:OD1	1:D:569:ASN:N	2.46	0.46
1:D:640:ILE:HG13	1:D:659:VAL:HG21	1.97	0.46
1:A:37:GLU:OE2	1:A:167:GLU:OE2	2.33	0.46
1:A:156:LEU:H	1:A:156:LEU:HD23	1.80	0.46
1:A:596:LEU:HD11	1:A:604:VAL:HG21	1.98	0.46
1:C:502:LEU:HD12	1:C:505:GLU:HG2	1.98	0.46
5:C:1008:CDL:H111	5:C:1008:CDL:HA4	1.54	0.46
1:A:282:ARG:O	1:A:286:VAL:HG23	2.16	0.45
1:C:442:ARG:HE	1:C:444:ARG:HG3	1.80	0.45
1:C:722:MET:HB2	1:C:817:TRP:CE3	2.51	0.45
1:D:344:LYS:NZ	1:D:664:GLU:O	2.39	0.45
1:D:635:TYR:HE1	1:D:642:ASP:HB3	1.81	0.45
1:B:308:PHE:CZ	1:B:720:ILE:HA	2.51	0.45
1:B:374:MET:HE2	1:B:376:HIS:CE1	2.51	0.45
1:B:387:VAL:O	1:B:390:HIS:HB3	2.16	0.45
1:B:509:VAL:HG13	1:B:537:TYR:HB2	1.99	0.45
1:A:326:THR:C	1:A:328:CYS:H	2.23	0.45
1:C:286:VAL:O	1:C:290:PHE:HB2	2.16	0.45
1:C:762:VAL:O	1:C:766:MET:HG3	2.16	0.45
5:A:1006:CDL:H711	1:B:302:TRP:CZ2	2.52	0.45
1:C:434:ASP:OD1	1:C:434:ASP:N	2.49	0.45
1:A:369:ASP:OD2	1:A:370:LYS:N	2.49	0.45
1:A:375:ARG:HA	1:A:375:ARG:HD2	1.71	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:LYS:HB2	1:D:452:ASN:HA	1.97	0.45
1:D:722:MET:HG3	1:D:817:TRP:CE3	2.47	0.45
1:B:155:ARG:HA	1:B:155:ARG:HD3	1.73	0.45
1:D:741:ILE:HG22	1:D:742:PRO:HD3	1.98	0.45
1:D:851:LEU:HD23	1:D:854:MET:HE2	1.98	0.45
1:A:641:ASN:OD1	1:A:641:ASN:N	2.48	0.45
1:B:360:THR:HG23	1:B:636:MET:HE3	1.98	0.45
1:B:363:THR:CB	3:B:1002:BEF:F3	2.55	0.45
1:C:328:CYS:SG	1:C:742:PRO:HG3	2.57	0.45
1:C:722:MET:HB2	1:C:817:TRP:HE3	1.82	0.45
1:C:831:MET:HE3	1:C:831:MET:HB3	1.80	0.45
1:A:476:THR:OG1	1:A:477:LEU:N	2.50	0.45
1:B:348:SER:O	1:B:352:LEU:N	2.49	0.45
1:C:195:PHE:HE1	1:C:209:GLU:HB2	1.82	0.45
1:D:481:LYS:H	1:D:481:LYS:HD3	1.81	0.45
1:A:39:PHE:HZ	1:A:166:GLU:HG2	1.81	0.45
1:A:480:ASP:OD1	1:A:481:LYS:N	2.49	0.45
1:C:390:HIS:HA	1:C:393:LEU:HG	1.98	0.45
1:B:510:ILE:HD12	1:B:510:ILE:O	2.17	0.44
5:C:1006:CDL:HA32	5:D:1007:CDL:HA22	1.99	0.44
1:D:60:GLN:HG3	1:D:61:TYR:CD2	2.52	0.44
1:B:590:GLY:HA3	1:B:613:LYS:O	2.17	0.44
1:C:187:ARG:HD3	1:C:187:ARG:HA	1.75	0.44
1:C:298:THR:HG22	1:C:299:LYS:HD3	1.99	0.44
1:C:405:MET:O	1:C:409:ILE:HG12	2.17	0.44
1:C:436:ILE:HD13	1:C:448:VAL:HG23	1.99	0.44
1:D:320:MET:HA	1:D:320:MET:HE2	2.00	0.44
1:B:497:LYS:HD2	1:B:497:LYS:HA	1.62	0.44
1:B:511:LEU:HB3	1:B:534:LEU:HD13	1.99	0.44
5:B:1008:CDL:H122	5:C:1006:CDL:H542	1.99	0.44
1:D:84:ASN:OD1	1:D:84:ASN:N	2.51	0.44
1:D:346:LEU:HD23	1:D:346:LEU:HA	1.81	0.44
1:A:387:VAL:HA	1:A:390:HIS:ND1	2.32	0.44
1:A:546:GLU:OE2	1:A:547:SER:N	2.49	0.44
1:A:649:SER:OG	1:A:651:VAL:O	2.33	0.44
1:B:336:MET:HE2	1:B:336:MET:HA	1.99	0.44
1:B:570:ASP:HA	1:B:573:THR:HG22	1.99	0.44
1:B:639:GLY:N	1:B:642:ASP:OD2	2.29	0.44
1:C:545:LYS:O	1:C:548:THR:HG22	2.18	0.44
1:D:477:LEU:HD23	1:D:487:LEU:HD23	1.99	0.44
1:B:377:LEU:HD12	1:B:377:LEU:HA	1.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ILE:O	1:C:255:GLU:HG2	2.16	0.44
1:D:328:CYS:SG	1:D:742:PRO:HG3	2.57	0.44
1:A:390:HIS:CD2	1:A:390:HIS:C	2.95	0.44
1:C:193:ASP:H	1:C:239:SER:C	2.26	0.44
1:D:831:MET:HE3	1:D:831:MET:HB3	1.84	0.44
1:A:363:THR:OG1	1:A:363:THR:O	2.34	0.44
5:A:1006:CDL:H112	5:A:1006:CDL:HA4	1.34	0.44
1:D:77:ARG:HE	1:D:130:PHE:HE1	1.66	0.44
1:A:507:MET:CE	1:A:508:ARG:H	2.24	0.44
1:A:565:LEU:HD11	1:A:622:ILE:HD11	2.00	0.44
1:B:201:LEU:HD21	1:B:616:PRO:HG2	1.99	0.44
1:B:378:ASP:HB2	1:B:382:GLN:O	2.18	0.44
1:C:596:LEU:HD23	1:C:596:LEU:H	1.83	0.44
1:D:312:VAL:HA	1:D:707:MET:SD	2.57	0.44
1:D:788:ILE:HD13	1:D:880:PHE:HD1	1.82	0.44
5:B:1009:CDL:HB31	5:B:1009:CDL:HA32	1.99	0.44
1:C:512:VAL:HB	1:C:514:GLN:NE2	2.33	0.44
1:C:636:MET:HE2	1:C:636:MET:HB3	1.86	0.44
1:D:79:TYR:O	1:D:83:ILE:HG12	2.18	0.44
1:D:197:SER:O	1:D:233:SER:OG	2.36	0.44
5:D:1007:CDL:HA21	5:D:1007:CDL:HA62	2.00	0.44
1:A:135:ARG:HE	1:A:135:ARG:HB3	1.64	0.43
1:A:368:GLN:H	1:A:368:GLN:CD	2.26	0.43
1:A:389:ARG:HA	1:A:389:ARG:HD3	1.60	0.43
1:C:800:VAL:O	1:C:803:SER:OG	2.28	0.43
1:A:353:GLY:HA3	1:A:685:GLY:HA3	2.00	0.43
1:A:693:ILE:HA	1:A:693:ILE:HD12	1.83	0.43
1:D:621:ARG:O	1:D:625:THR:OG1	2.27	0.43
1:D:733:ILE:HD12	1:D:859:LEU:HD12	2.00	0.43
1:A:89:ILE:H	1:A:89:ILE:HG13	1.61	0.43
1:A:164:PRO:HG3	1:A:246:ALA:HA	2.00	0.43
1:B:283:PHE:CE1	5:B:1009:CDL:HB62	2.53	0.43
1:B:588:ILE:HD11	1:B:611:PHE:CD2	2.53	0.43
1:B:611:PHE:HD1	1:B:611:PHE:H	1.66	0.43
1:C:492:ARG:HD2	1:C:492:ARG:N	2.33	0.43
1:D:411:GLU:HA	1:D:414:GLU:HG3	2.00	0.43
1:A:226:VAL:HG13	1:A:227:ASN:OD1	2.19	0.43
1:A:779:THR:HG23	1:C:897:ILE:HG21	2.00	0.43
1:B:272:GLY:O	1:B:275:SER:OG	2.33	0.43
1:B:328:CYS:SG	1:B:742:PRO:HG3	2.57	0.43
1:C:135:ARG:HG3	1:C:135:ARG:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:LYS:HB3	1:C:429:LYS:HE3	1.70	0.43
1:C:782:LEU:C	1:C:784:MET:N	2.76	0.43
1:C:261:THR:C	1:C:262:GLU:HG3	2.44	0.43
1:A:221:SER:OG	1:A:224:GLU:OE1	2.26	0.43
1:A:288:VAL:HG13	1:A:309:ALA:HB1	2.00	0.43
1:A:471:MET:C	1:A:471:MET:HE2	2.43	0.43
1:B:362:LYS:HA	1:B:366:LEU:CD1	2.47	0.43
1:D:319:GLU:H	1:D:319:GLU:HG2	1.57	0.43
1:A:496:LEU:HB3	1:A:501:GLU:HA	2.00	0.43
1:B:893:MET:HB2	1:D:890:MET:SD	2.58	0.43
1:C:118:ILE:O	1:C:122:VAL:HG23	2.19	0.43
1:D:125:SER:HB2	1:D:322:PRO:HG2	2.01	0.43
1:D:641:ASN:OD1	1:D:641:ASN:N	2.51	0.43
1:A:209:GLU:OE2	1:A:211:LEU:HG	2.19	0.43
1:C:193:ASP:HA	1:C:237:SER:HA	2.01	0.43
1:C:595:GLN:N	1:C:595:GLN:OE1	2.51	0.43
1:D:377:LEU:HD23	1:D:377:LEU:HA	1.81	0.43
1:B:695:TYR:HB2	1:B:741:ILE:HD13	2.01	0.43
1:B:761:SER:HA	1:B:764:LYS:HE2	2.01	0.43
1:C:252:ILE:HA	1:C:255:GLU:OE2	2.19	0.43
1:C:590:GLY:O	1:C:593:ILE:HG13	2.18	0.43
1:A:168:VAL:HG11	1:A:246:ALA:HB2	2.00	0.43
1:A:860:THR:O	1:A:863:PRO:HD2	2.19	0.43
5:B:1010:CDL:H541	5:B:1010:CDL:H511	1.54	0.43
1:D:269:PHE:CZ	1:D:329:LEU:HD11	2.54	0.43
1:D:326:THR:C	1:D:328:CYS:H	2.26	0.43
1:A:227:ASN:O	1:A:227:ASN:ND2	2.52	0.42
1:B:287:MET:HE2	1:B:287:MET:HB3	1.86	0.42
1:C:211:LEU:HG	1:C:213:LEU:H	1.84	0.42
1:A:213:LEU:HG	1:A:215:THR:H	1.84	0.42
1:A:888:VAL:O	1:A:892:MET:HE2	2.19	0.42
1:C:868:GLY:O	1:C:873:LEU:HB2	2.19	0.42
1:D:588:ILE:HG22	1:D:590:GLY:H	1.84	0.42
1:A:51:GLU:O	1:A:55:GLU:HG2	2.19	0.42
1:A:385:ILE:HD11	1:A:389:ARG:NH2	2.34	0.42
1:A:865:THR:O	1:A:869:HIS:ND1	2.41	0.42
1:C:357:ILE:HB	1:C:633:VAL:HG22	2.00	0.42
1:D:111:ASN:O	1:D:111:ASN:ND2	2.35	0.42
1:A:312:VAL:HA	1:A:707:MET:SD	2.60	0.42
1:A:566:THR:OG1	3:A:1002:BEF:F3	2.18	0.42
1:A:697:LYS:HD3	1:A:910:LEU:HD12	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:667:ASP:N	1:D:667:ASP:OD1	2.51	0.42
1:A:361:ASP:HB3	1:A:637:GLY:HA2	2.02	0.42
1:A:442:ARG:NH2	1:A:443:ARG:HE	2.12	0.42
1:B:118:ILE:O	1:B:122:VAL:HG23	2.19	0.42
1:C:34:THR:HG23	1:C:37:GLU:H	1.85	0.42
1:D:342:ILE:HB	1:D:669:ILE:HB	2.01	0.42
1:A:352:LEU:HD12	1:A:355:MET:HE2	2.02	0.42
1:A:614:LEU:HD23	1:A:614:LEU:HA	1.83	0.42
1:B:32:THR:HG23	1:B:34:THR:HG23	2.00	0.42
1:B:336:MET:HB3	1:B:343:ILE:HD11	2.01	0.42
1:C:605:ALA:HA	1:C:611:PHE:HZ	1.83	0.42
1:C:323:MET:O	1:C:327:THR:OG1	2.36	0.42
1:D:338:LYS:HB2	1:D:338:LYS:HE3	1.75	0.42
1:D:574:ARG:C	1:D:576:VAL:H	2.28	0.42
1:D:582:LEU:HD12	1:D:582:LEU:HA	1.81	0.42
1:B:359:CYS:HB3	1:B:565:LEU:HD22	2.02	0.42
1:C:535:MET:HE3	1:C:535:MET:HB2	1.90	0.42
1:C:553:LYS:HE2	1:C:553:LYS:HB2	1.87	0.42
1:D:704:PHE:HD2	1:D:770:GLY:HA3	1.85	0.42
1:A:251:THR:O	1:A:253:PHE:N	2.52	0.42
1:C:255:GLU:HG3	1:C:617:GLN:HB2	2.02	0.42
1:C:372:VAL:HG22	1:C:373:LEU:H	1.84	0.42
1:D:422:GLU:CD	1:D:422:GLU:H	2.28	0.42
1:A:391:GLY:O	1:A:409:ILE:HG21	2.20	0.42
1:A:445:MET:HE1	1:A:463:ILE:HB	2.02	0.42
1:B:321:LEU:N	1:B:322:PRO:HD2	2.34	0.42
1:C:132:GLN:O	1:C:133:GLU:HG2	2.20	0.42
1:C:149:THR:O	1:C:165:ILE:HG12	2.20	0.42
1:D:26:ARG:HA	1:D:26:ARG:NE	2.34	0.42
1:D:408:ALA:O	1:D:411:GLU:HG3	2.20	0.42
1:B:136:SER:HA	1:B:139:ALA:O	2.20	0.41
1:C:478:VAL:HB	1:C:532:MET:HE1	2.02	0.41
1:D:342:ILE:HD11	1:D:671:LEU:HD21	2.02	0.41
1:A:444:ARG:H	1:A:444:ARG:HD2	1.85	0.41
1:B:192:LYS:HD3	1:B:192:LYS:N	2.35	0.41
1:B:269:PHE:CD2	1:B:347:ASN:HB2	2.55	0.41
1:C:261:THR:O	1:C:262:GLU:HG3	2.20	0.41
1:A:362:LYS:HE3	1:A:362:LYS:HB3	1.77	0.41
1:B:44:THR:HG21	1:B:171:GLY:HA3	2.01	0.41
1:C:31:LYS:O	1:C:227:ASN:ND2	2.44	0.41
1:C:321:LEU:HD11	1:C:696:ILE:HG12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:LEU:HB3	1:C:405:MET:HE3	2.03	0.41
1:C:443:ARG:HH11	1:C:443:ARG:C	2.27	0.41
1:D:495:ILE:HA	1:D:498:LYS:HE3	2.02	0.41
1:A:831:MET:HE2	1:A:831:MET:HB2	1.85	0.41
1:A:837:ILE:HG21	1:A:840:LEU:HB2	2.02	0.41
1:B:558:TYR:HB3	1:B:686:ARG:HH12	1.86	0.41
1:C:680:LYS:HZ2	1:C:680:LYS:HG2	1.78	0.41
1:D:464:THR:HG21	1:D:529:GLU:HA	2.02	0.41
1:A:622:ILE:HA	1:A:625:THR:HG22	2.01	0.41
1:A:667:ASP:OD1	1:A:667:ASP:N	2.53	0.41
1:A:883:TRP:HZ2	1:C:900:LYS:HD3	1.86	0.41
1:B:43:LYS:HB3	1:B:43:LYS:HE2	1.66	0.41
1:B:105:ALA:HB3	1:B:110:LYS:HG2	2.03	0.41
1:B:851:LEU:HD12	1:B:851:LEU:HA	1.89	0.41
1:D:256:MET:HE2	1:D:256:MET:HA	2.02	0.41
1:D:333:ALA:O	1:D:337:SER:OG	2.35	0.41
1:D:344:LYS:HB3	1:D:344:LYS:HE3	1.73	0.41
1:A:253:PHE:CD1	1:A:253:PHE:C	2.99	0.41
1:A:566:THR:OG1	1:A:568:ASP:OD1	2.39	0.41
5:A:1006:CDL:HB4	5:A:1006:CDL:H522	2.03	0.41
1:B:52:GLU:O	1:B:56:ILE:HG23	2.20	0.41
1:B:324:ILE:HG13	1:B:695:TYR:CZ	2.55	0.41
1:B:641:ASN:CG	3:B:1002:BEF:F1	2.54	0.41
1:B:800:VAL:HG13	1:B:803:SER:HB3	2.02	0.41
1:C:611:PHE:HB3	1:C:614:LEU:HD11	2.03	0.41
1:C:784:MET:O	1:C:789:CYS:HB2	2.21	0.41
1:A:407:LEU:HD23	1:A:410:ILE:HD13	2.03	0.41
1:A:534:LEU:HD12	1:A:534:LEU:HA	1.88	0.41
1:B:320:MET:HB3	1:B:323:MET:HE3	2.03	0.41
1:B:360:THR:HG22	1:B:361:ASP:H	1.85	0.41
1:B:363:THR:OG1	3:B:1002:BEF:F3	2.19	0.41
1:B:600:GLU:O	1:B:604:VAL:HG12	2.20	0.41
1:D:361:ASP:O	1:D:365:THR:OG1	2.37	0.41
1:D:481:LYS:HE2	1:D:481:LYS:HB2	1.91	0.41
1:A:37:GLU:H	1:A:37:GLU:HG2	1.64	0.41
1:A:132:GLN:NE2	1:A:326:THR:OG1	2.49	0.41
1:B:88:ILE:CG2	5:B:1006:CDL:H322	2.51	0.41
1:B:137:GLY:HA3	1:B:344:LYS:HB3	2.03	0.41
1:C:55:GLU:CG	1:C:56:ILE:H	2.33	0.41
1:C:171:GLY:H	1:C:244:VAL:HG13	1.86	0.41
1:D:370:LYS:HB2	1:D:370:LYS:HE2	1.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:511:LEU:HD21	1:D:534:LEU:HD23	2.02	0.41
1:D:615:SER:O	1:D:619:LYS:HB2	2.21	0.41
1:D:822:MET:O	1:D:826:THR:HG22	2.20	0.41
1:A:479:GLU:OE1	1:A:532:MET:HE3	2.21	0.41
1:B:661:ILE:HD12	1:B:664:GLU:OE2	2.21	0.41
1:D:635:TYR:CE1	1:D:642:ASP:HB3	2.56	0.41
1:A:383:GLU:OE1	1:A:385:ILE:HG22	2.21	0.40
1:B:596:LEU:HD23	1:B:596:LEU:H	1.86	0.40
1:C:399:THR:O	1:C:399:THR:OG1	2.33	0.40
1:C:512:VAL:O	1:C:512:VAL:HG23	2.21	0.40
1:D:383:GLU:OE1	1:D:385:ILE:HG23	2.22	0.40
1:D:403:ASN:OD1	1:D:403:ASN:C	2.64	0.40
1:D:513:ALA:HB1	1:D:515:LYS:HE2	2.02	0.40
1:A:626:LEU:HD23	1:A:626:LEU:HA	1.95	0.40
1:B:596:LEU:HD11	1:B:601:LEU:HD13	2.03	0.40
1:C:134:THR:HA	1:C:138:ASN:HB2	2.04	0.40
1:D:614:LEU:HD23	1:D:614:LEU:HA	1.93	0.40
1:B:192:LYS:HD3	1:B:192:LYS:H	1.87	0.40
1:B:481:LYS:HE2	1:B:481:LYS:HB2	1.90	0.40
1:B:764:LYS:HE2	1:B:764:LYS:HB2	1.85	0.40
1:C:35:LYS:HE3	1:C:39:PHE:CE2	2.56	0.40
1:D:551:ALA:O	1:D:555:LEU:HB2	2.22	0.40
1:D:860:THR:O	1:D:863:PRO:HD2	2.22	0.40
1:A:64:ASN:HB3	1:A:249:ASP:OD2	2.21	0.40
1:A:340:LYS:HD3	1:A:340:LYS:HA	1.96	0.40
1:B:66:ILE:HG22	1:B:248:GLY:HA2	2.04	0.40
1:B:282:ARG:HH21	5:B:1009:CDL:HB4	1.86	0.40
1:C:47:LYS:HD2	1:C:155:ARG:HH12	1.86	0.40
1:D:476:THR:HB	1:D:477:LEU:H	1.60	0.40
1:D:623:VAL:C	1:D:625:THR:H	2.28	0.40
1:A:31:LYS:HD3	1:A:187:ARG:HH12	1.85	0.40
1:B:76:LYS:HD2	1:B:76:LYS:HA	1.75	0.40
1:B:348:SER:HA	1:B:351:ASN:HB2	2.02	0.40
1:B:410:ILE:O	1:B:414:GLU:HG2	2.21	0.40
1:C:188:ILE:HG13	1:C:194:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	887/921 (96%)	828 (93%)	53 (6%)	6 (1%)	18	41
1	B	887/921 (96%)	819 (92%)	57 (6%)	11 (1%)	10	27
1	C	887/921 (96%)	790 (89%)	90 (10%)	7 (1%)	16	37
1	D	887/921 (96%)	808 (91%)	76 (9%)	3 (0%)	36	60
All	All	3548/3684 (96%)	3245 (92%)	276 (8%)	27 (1%)	18	37

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	VAL
1	B	189	ILE
1	B	499	VAL
1	D	649	SER
1	A	476	THR
1	A	490	GLU
1	A	643	ALA
1	B	23	ILE
1	B	222	ILE
1	B	385	ILE
1	C	778	ILE
1	B	147	ILE
1	D	592	ASP
1	A	479	GLU
1	B	33	SER
1	C	474	ILE
1	B	533	VAL
1	B	651	VAL
1	C	55	GLU
1	C	451	SER
1	B	145	LYS
1	B	484	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	515	LYS
1	D	478	VAL
1	A	521	ILE
1	C	871	ILE
1	C	189	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	764/795 (96%)	744 (97%)	20 (3%)	40	70
1	B	764/795 (96%)	747 (98%)	17 (2%)	45	74
1	C	764/795 (96%)	748 (98%)	16 (2%)	47	75
1	D	764/795 (96%)	741 (97%)	23 (3%)	36	66
All	All	3056/3180 (96%)	2980 (98%)	76 (2%)	42	71

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	67	THR
1	A	75	ILE
1	A	271	LYS
1	A	328	CYS
1	A	355	MET
1	A	380	HIS
1	A	390	HIS
1	A	405	MET
1	A	477	LEU
1	A	633	VAL
1	A	651	VAL
1	A	730	LEU
1	A	737	SER
1	A	739	THR
1	A	828	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	851	LEU
1	A	892	MET
1	A	908	GLU
1	A	909	LEU
1	B	44	THR
1	B	316	LEU
1	B	323	MET
1	B	347	ASN
1	B	360	THR
1	B	362	LYS
1	B	363	THR
1	B	368	GLN
1	B	390	HIS
1	B	447	VAL
1	B	465	LYS
1	B	610	VAL
1	B	641	ASN
1	B	650	ASP
1	B	655	VAL
1	B	709	SER
1	B	741	ILE
1	C	71	LYS
1	C	135	ARG
1	C	156	LEU
1	C	195	PHE
1	C	201	LEU
1	C	244	VAL
1	C	290	PHE
1	C	347	ASN
1	C	537	TYR
1	C	584	VAL
1	C	610	VAL
1	C	651	VAL
1	C	763	SER
1	C	775	VAL
1	C	828	VAL
1	C	895	VAL
1	D	78	LEU
1	D	111	ASN
1	D	146	MET
1	D	202	THR
1	D	290	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	336	MET
1	D	401	LEU
1	D	442	ARG
1	D	464	THR
1	D	600	GLU
1	D	623	VAL
1	D	625	THR
1	D	647	LYS
1	D	651	VAL
1	D	655	VAL
1	D	676	MET
1	D	709	SER
1	D	739	THR
1	D	741	ILE
1	D	763	SER
1	D	800	VAL
1	D	890	MET
1	D	895	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	132	GLN
1	A	384	ASN
1	A	420	ASN
1	A	452	ASN
1	B	142	ASN
1	B	152	ASN
1	B	161	GLN
1	B	390	HIS
1	B	503	ASN
1	C	53	GLN
1	C	198	GLN
1	C	380	HIS
1	C	390	HIS
1	C	394	ASN
1	C	461	GLN
1	C	514	GLN
1	D	53	GLN
1	D	152	ASN
1	D	345	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	347	ASN
1	D	390	HIS
1	D	420	ASN
1	D	452	ASN
1	D	579	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 8 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	CDL	C	1010	-	51,51,99	0.37	0	57,63,111	0.42	0
5	CDL	D	1006	-	51,51,99	0.38	0	57,63,111	0.47	0
2	LMT	D	1001	-	36,36,36	0.54	0	47,47,47	0.73	0
3	BEF	B	1002	-	0,3,3	-	-	-		
5	CDL	B	1008	-	51,51,99	0.37	0	57,63,111	0.45	0
5	CDL	B	1010	-	51,51,99	0.39	0	57,63,111	0.44	0
5	CDL	C	1007	-	51,51,99	0.42	0	57,63,111	0.54	0
5	CDL	A	1007	-	51,51,99	0.37	0	57,63,111	0.47	0
2	LMT	C	1003	-	36,36,36	0.16	0	47,47,47	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LMT	D	1002	-	36,36,36	0.14	0	47,47,47	0.23	0
5	CDL	C	1009	-	51,51,99	0.40	0	57,63,111	0.45	0
3	BEF	C	1001	-	0,3,3	-	-	-		
5	CDL	A	1005	-	51,51,99	0.39	0	57,63,111	0.49	0
5	CDL	C	1006	-	51,51,99	0.39	0	57,63,111	0.41	0
3	BEF	A	1002	-	0,3,3	-	-	-		
5	CDL	B	1009	-	51,51,99	0.38	0	57,63,111	0.44	0
5	CDL	A	1006	-	51,51,99	0.37	0	57,63,111	0.44	0
5	CDL	B	1007	-	51,51,99	0.39	0	57,63,111	0.54	0
5	CDL	C	1008	-	51,51,99	0.40	0	57,63,111	0.47	0
5	CDL	A	1008	-	51,51,99	0.37	0	57,63,111	0.40	0
5	CDL	B	1006	-	51,51,99	0.39	0	57,63,111	3.38	3 (5%)
2	LMT	C	1002	-	36,36,36	0.13	0	47,47,47	0.30	0
2	LMT	B	1001	-	36,36,36	0.14	0	47,47,47	0.24	0
5	CDL	D	1007	-	51,51,99	0.40	0	57,63,111	0.42	0
3	BEF	D	1003	-	0,3,3	-	-	-		
5	CDL	B	1005	-	51,51,99	0.40	0	57,63,111	0.51	0
2	LMT	A	1001	-	36,36,36	0.15	0	47,47,47	0.25	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
5	CDL	C	1010	-	-	21/62/62/110	-
5	CDL	D	1006	-	-	31/62/62/110	-
2	LMT	D	1001	-	-	7/21/61/61	0/2/2/2
5	CDL	B	1008	-	-	27/62/62/110	-
5	CDL	B	1010	-	-	28/62/62/110	-
5	CDL	C	1007	-	-	31/62/62/110	-
5	CDL	A	1007	-	-	32/62/62/110	-
2	LMT	C	1003	-	-	14/21/61/61	0/2/2/2
2	LMT	D	1002	-	-	11/21/61/61	0/2/2/2
5	CDL	C	1009	-	-	32/62/62/110	-
5	CDL	A	1005	-	-	32/62/62/110	-
5	CDL	C	1006	-	-	34/62/62/110	-
5	CDL	B	1009	-	-	28/62/62/110	-
5	CDL	A	1006	-	-	39/62/62/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CDL	B	1007	-	-	31/62/62/110	-
5	CDL	C	1008	-	-	36/62/62/110	-
5	CDL	A	1008	-	-	26/62/62/110	-
5	CDL	B	1006	-	-	40/62/62/110	-
2	LMT	C	1002	-	-	13/21/61/61	0/2/2/2
2	LMT	B	1001	-	-	13/21/61/61	0/2/2/2
5	CDL	D	1007	-	-	39/62/62/110	-
5	CDL	B	1005	-	-	32/62/62/110	-
2	LMT	A	1001	-	-	16/21/61/61	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1006	CDL	OA9-CA7-C31	-21.41	40.05	123.78
5	B	1006	CDL	OA8-CA7-OA9	-10.67	96.94	123.63
5	B	1006	CDL	OA8-CA7-C31	8.25	136.99	111.83

There are no chirality outliers.

All (613) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	LMT	C2-C1-O1'-C1'
2	C	1003	LMT	C2'-C1'-O1'-C1
5	A	1005	CDL	CB2-C1-CA2-OA2
5	A	1005	CDL	CA3-OA5-PA1-OA2
5	A	1005	CDL	CA3-OA5-PA1-OA3
5	A	1005	CDL	CB2-OB2-PB2-OB3
5	A	1005	CDL	C51-CB5-OB6-CB4
5	A	1006	CDL	CA2-OA2-PA1-OA3
5	A	1006	CDL	CA2-OA2-PA1-OA4
5	A	1006	CDL	CA2-OA2-PA1-OA5
5	A	1006	CDL	CA3-OA5-PA1-OA2
5	A	1006	CDL	OA7-CA5-OA6-CA4
5	A	1006	CDL	C11-CA5-OA6-CA4
5	A	1006	CDL	OB7-CB5-OB6-CB4
5	A	1007	CDL	CB2-C1-CA2-OA2
5	A	1007	CDL	CA2-C1-CB2-OB2
5	A	1007	CDL	CA2-OA2-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1007	CDL	CA2-OA2-PA1-OA5
5	A	1007	CDL	CA3-OA5-PA1-OA2
5	A	1007	CDL	CA3-OA5-PA1-OA4
5	A	1007	CDL	CB3-OB5-PB2-OB2
5	A	1007	CDL	CB3-OB5-PB2-OB4
5	A	1007	CDL	OB9-CB7-OB8-CB6
5	A	1007	CDL	C71-CB7-OB8-CB6
5	A	1008	CDL	CA2-OA2-PA1-OA3
5	A	1008	CDL	CA2-OA2-PA1-OA4
5	A	1008	CDL	CA2-OA2-PA1-OA5
5	A	1008	CDL	CB2-OB2-PB2-OB5
5	A	1008	CDL	CB3-OB5-PB2-OB2
5	A	1008	CDL	CB3-OB5-PB2-OB3
5	A	1008	CDL	CB3-OB5-PB2-OB4
5	B	1005	CDL	CA2-OA2-PA1-OA3
5	B	1005	CDL	CA2-OA2-PA1-OA4
5	B	1005	CDL	CA2-OA2-PA1-OA5
5	B	1005	CDL	CA3-OA5-PA1-OA4
5	B	1005	CDL	C11-CA5-OA6-CA4
5	B	1005	CDL	CB3-OB5-PB2-OB2
5	B	1005	CDL	C51-CB5-OB6-CB4
5	B	1006	CDL	CA2-OA2-PA1-OA3
5	B	1006	CDL	CA3-OA5-PA1-OA2
5	B	1006	CDL	CA3-OA5-PA1-OA3
5	B	1006	CDL	CA3-OA5-PA1-OA4
5	B	1006	CDL	C11-CA5-OA6-CA4
5	B	1006	CDL	CB2-OB2-PB2-OB3
5	B	1006	CDL	CB2-OB2-PB2-OB5
5	B	1006	CDL	CB3-OB5-PB2-OB3
5	B	1006	CDL	CB3-OB5-PB2-OB4
5	B	1007	CDL	CA2-OA2-PA1-OA4
5	B	1007	CDL	CA2-OA2-PA1-OA5
5	B	1007	CDL	CA3-OA5-PA1-OA2
5	B	1007	CDL	CA3-OA5-PA1-OA4
5	B	1007	CDL	CA4-CA3-OA5-PA1
5	B	1007	CDL	C11-CA5-OA6-CA4
5	B	1007	CDL	OB6-CB4-CB6-OB8
5	B	1007	CDL	C51-CB5-OB6-CB4
5	B	1008	CDL	CA3-OA5-PA1-OA3
5	B	1008	CDL	CB3-OB5-PB2-OB2
5	B	1008	CDL	CB3-OB5-PB2-OB4
5	B	1008	CDL	OB5-CB3-CB4-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1008	CDL	OB7-CB5-OB6-CB4
5	B	1008	CDL	C51-CB5-OB6-CB4
5	B	1009	CDL	CB2-C1-CA2-OA2
5	B	1009	CDL	CA2-OA2-PA1-OA4
5	B	1009	CDL	CA2-OA2-PA1-OA5
5	B	1009	CDL	CA3-OA5-PA1-OA2
5	B	1009	CDL	CA3-OA5-PA1-OA3
5	B	1009	CDL	CB2-OB2-PB2-OB3
5	B	1009	CDL	C51-CB5-OB6-CB4
5	B	1010	CDL	CA2-OA2-PA1-OA3
5	B	1010	CDL	CA2-OA2-PA1-OA4
5	B	1010	CDL	CA2-OA2-PA1-OA5
5	B	1010	CDL	CA3-OA5-PA1-OA4
5	B	1010	CDL	OA9-CA7-OA8-CA6
5	B	1010	CDL	C31-CA7-OA8-CA6
5	B	1010	CDL	CB3-OB5-PB2-OB2
5	B	1010	CDL	CB3-OB5-PB2-OB4
5	C	1006	CDL	OA5-CA3-CA4-OA6
5	C	1006	CDL	CB2-OB2-PB2-OB4
5	C	1006	CDL	CB2-OB2-PB2-OB5
5	C	1006	CDL	CB3-OB5-PB2-OB2
5	C	1006	CDL	CB3-OB5-PB2-OB3
5	C	1006	CDL	CB3-OB5-PB2-OB4
5	C	1007	CDL	CA2-OA2-PA1-OA4
5	C	1007	CDL	CA2-OA2-PA1-OA5
5	C	1007	CDL	OA5-CA3-CA4-OA6
5	C	1007	CDL	OA7-CA5-OA6-CA4
5	C	1007	CDL	C11-CA5-OA6-CA4
5	C	1007	CDL	CB2-OB2-PB2-OB5
5	C	1007	CDL	CB3-OB5-PB2-OB3
5	C	1007	CDL	CB3-OB5-PB2-OB4
5	C	1007	CDL	OB7-CB5-OB6-CB4
5	C	1008	CDL	CA2-OA2-PA1-OA3
5	C	1008	CDL	CA2-OA2-PA1-OA4
5	C	1008	CDL	CA3-OA5-PA1-OA3
5	C	1008	CDL	OA7-CA5-OA6-CA4
5	C	1008	CDL	C11-CA5-OA6-CA4
5	C	1008	CDL	CB2-OB2-PB2-OB3
5	C	1008	CDL	CB2-OB2-PB2-OB5
5	C	1009	CDL	CA3-OA5-PA1-OA2
5	C	1009	CDL	CA3-OA5-PA1-OA3
5	C	1009	CDL	CA3-OA5-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1009	CDL	CB3-OB5-PB2-OB3
5	C	1010	CDL	CA3-OA5-PA1-OA2
5	C	1010	CDL	CA3-OA5-PA1-OA3
5	C	1010	CDL	CA3-OA5-PA1-OA4
5	C	1010	CDL	CB3-OB5-PB2-OB2
5	C	1010	CDL	CB3-OB5-PB2-OB3
5	C	1010	CDL	CB3-OB5-PB2-OB4
5	C	1010	CDL	OB6-CB4-CB6-OB8
5	D	1006	CDL	CA2-OA2-PA1-OA3
5	D	1006	CDL	CA2-OA2-PA1-OA4
5	D	1006	CDL	CA2-OA2-PA1-OA5
5	D	1006	CDL	CA3-OA5-PA1-OA3
5	D	1006	CDL	CA3-OA5-PA1-OA4
5	D	1006	CDL	CB2-OB2-PB2-OB3
5	D	1006	CDL	CB3-OB5-PB2-OB2
5	D	1006	CDL	CB3-OB5-PB2-OB4
5	D	1007	CDL	CA2-OA2-PA1-OA3
5	D	1007	CDL	CA3-OA5-PA1-OA2
5	D	1007	CDL	CA3-OA5-PA1-OA3
5	D	1007	CDL	CA3-OA5-PA1-OA4
5	D	1007	CDL	CB2-OB2-PB2-OB3
5	D	1007	CDL	CB2-OB2-PB2-OB5
2	C	1003	LMT	O5B-C1B-O1B-C4'
5	A	1006	CDL	OB9-CB7-OB8-CB6
5	B	1006	CDL	OA9-CA7-OA8-CA6
5	B	1008	CDL	OB9-CB7-OB8-CB6
5	A	1005	CDL	OB9-CB7-OB8-CB6
5	C	1008	CDL	OA9-CA7-OA8-CA6
5	D	1006	CDL	OB9-CB7-OB8-CB6
2	C	1003	LMT	C4'-C5'-C6'-O6'
2	D	1001	LMT	C3'-C4'-O1B-C1B
5	A	1005	CDL	OB7-CB5-OB6-CB4
5	B	1005	CDL	OA7-CA5-OA6-CA4
5	B	1005	CDL	OB7-CB5-OB6-CB4
5	B	1006	CDL	OA7-CA5-OA6-CA4
5	B	1007	CDL	OA7-CA5-OA6-CA4
5	B	1007	CDL	OB7-CB5-OB6-CB4
5	B	1009	CDL	OB7-CB5-OB6-CB4
5	C	1006	CDL	OA7-CA5-OA6-CA4
2	D	1002	LMT	C1-C2-C3-C4
5	A	1005	CDL	C31-CA7-OA8-CA6
5	A	1006	CDL	C71-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1008	CDL	C71-CB7-OB8-CB6
5	C	1008	CDL	C71-CB7-OB8-CB6
5	D	1006	CDL	C71-CB7-OB8-CB6
5	A	1006	CDL	C51-CB5-OB6-CB4
5	C	1006	CDL	C11-CA5-OA6-CA4
5	C	1007	CDL	C51-CB5-OB6-CB4
2	C	1002	LMT	C3'-C4'-O1B-C1B
5	A	1005	CDL	C71-CB7-OB8-CB6
5	B	1006	CDL	C71-CB7-OB8-CB6
5	B	1007	CDL	C71-CB7-OB8-CB6
5	B	1009	CDL	C31-CA7-OA8-CA6
5	C	1008	CDL	C31-CA7-OA8-CA6
5	D	1007	CDL	C31-CA7-OA8-CA6
2	B	1001	LMT	O5B-C5B-C6B-O6B
5	A	1005	CDL	OA9-CA7-OA8-CA6
5	B	1005	CDL	OA9-CA7-OA8-CA6
5	B	1006	CDL	OB9-CB7-OB8-CB6
5	B	1007	CDL	OB9-CB7-OB8-CB6
5	C	1008	CDL	OB9-CB7-OB8-CB6
5	D	1007	CDL	OA9-CA7-OA8-CA6
2	A	1001	LMT	O5B-C5B-C6B-O6B
2	C	1003	LMT	O5'-C5'-C6'-O6'
5	B	1009	CDL	C31-C32-C33-C34
5	A	1007	CDL	O1-C1-CB2-OB2
5	B	1008	CDL	O1-C1-CA2-OA2
5	B	1008	CDL	O1-C1-CB2-OB2
5	B	1009	CDL	O1-C1-CA2-OA2
5	B	1009	CDL	O1-C1-CB2-OB2
5	B	1005	CDL	C31-CA7-OA8-CA6
2	A	1001	LMT	O5'-C5'-C6'-O6'
2	A	1001	LMT	C4B-C5B-C6B-O6B
2	B	1001	LMT	C4B-C5B-C6B-O6B
2	C	1003	LMT	O5B-C5B-C6B-O6B
2	C	1003	LMT	C4B-C5B-C6B-O6B
2	D	1002	LMT	C4B-C5B-C6B-O6B
2	B	1001	LMT	C1-C2-C3-C4
5	B	1009	CDL	OA9-CA7-OA8-CA6
2	A	1001	LMT	O5'-C1'-O1'-C1
2	A	1001	LMT	C6-C7-C8-C9
5	A	1006	CDL	C32-C33-C34-C35
2	D	1002	LMT	O5B-C5B-C6B-O6B
2	B	1001	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1001	LMT	C7-C8-C9-C10
5	B	1010	CDL	C51-C52-C53-C54
2	C	1003	LMT	C1-C2-C3-C4
5	B	1006	CDL	CA2-C1-CB2-OB2
5	B	1008	CDL	CA2-C1-CB2-OB2
5	D	1007	CDL	CB2-C1-CA2-OA2
5	D	1007	CDL	CA2-C1-CB2-OB2
5	C	1009	CDL	C71-CB7-OB8-CB6
2	B	1001	LMT	C4'-C5'-C6'-O6'
2	C	1002	LMT	C7-C8-C9-C10
5	A	1005	CDL	C31-C32-C33-C34
2	A	1001	LMT	C2'-C1'-O1'-C1
5	A	1005	CDL	O1-C1-CB2-OB2
5	B	1006	CDL	O1-C1-CB2-OB2
5	D	1007	CDL	O1-C1-CB2-OB2
5	B	1010	CDL	CA7-C31-C32-C33
5	C	1009	CDL	OB9-CB7-OB8-CB6
5	A	1005	CDL	CA5-C11-C12-C13
5	A	1008	CDL	CB7-C71-C72-C73
2	C	1002	LMT	C5-C6-C7-C8
5	B	1008	CDL	C32-C33-C34-C35
5	A	1006	CDL	CB7-C71-C72-C73
2	A	1001	LMT	C4'-C5'-C6'-O6'
2	D	1002	LMT	C5-C6-C7-C8
5	B	1007	CDL	CA7-C31-C32-C33
5	B	1009	CDL	CA7-C31-C32-C33
5	C	1006	CDL	CB7-C71-C72-C73
5	C	1007	CDL	CB7-C71-C72-C73
5	C	1009	CDL	C51-CB5-OB6-CB4
5	A	1005	CDL	CB7-C71-C72-C73
5	B	1007	CDL	CB7-C71-C72-C73
5	C	1008	CDL	CB7-C71-C72-C73
5	C	1009	CDL	CA7-C31-C32-C33
5	C	1009	CDL	CB7-C71-C72-C73
5	C	1010	CDL	C31-C32-C33-C34
5	A	1005	CDL	O1-C1-CA2-OA2
5	A	1006	CDL	O1-C1-CB2-OB2
5	B	1006	CDL	O1-C1-CA2-OA2
5	C	1008	CDL	O1-C1-CB2-OB2
5	D	1007	CDL	O1-C1-CA2-OA2
5	D	1006	CDL	C31-CA7-OA8-CA6
5	A	1005	CDL	CA7-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1007	CDL	CB5-C51-C52-C53
5	B	1010	CDL	CA5-C11-C12-C13
5	B	1010	CDL	CB7-C71-C72-C73
5	C	1006	CDL	CB5-C51-C52-C53
5	B	1009	CDL	C71-CB7-OB8-CB6
5	C	1009	CDL	OB7-CB5-OB6-CB4
5	A	1006	CDL	CA2-C1-CB2-OB2
5	B	1006	CDL	CB2-C1-CA2-OA2
5	B	1008	CDL	CB2-C1-CA2-OA2
5	C	1008	CDL	CA2-C1-CB2-OB2
2	A	1001	LMT	O1'-C1-C2-C3
5	B	1007	CDL	C12-C13-C14-C15
5	C	1006	CDL	C71-CB7-OB8-CB6
5	C	1009	CDL	C31-CA7-OA8-CA6
5	D	1006	CDL	CA5-C11-C12-C13
5	C	1008	CDL	C51-CB5-OB6-CB4
5	D	1007	CDL	C11-CA5-OA6-CA4
5	C	1008	CDL	OB7-CB5-OB6-CB4
5	D	1007	CDL	OA7-CA5-OA6-CA4
2	D	1001	LMT	C2'-C1'-O1'-C1
5	B	1006	CDL	CB5-C51-C52-C53
5	A	1007	CDL	O1-C1-CA2-OA2
5	A	1008	CDL	CA4-CA3-OA5-PA1
5	B	1005	CDL	C1-CA2-OA2-PA1
5	B	1009	CDL	OB9-CB7-OB8-CB6
5	C	1008	CDL	CA5-C11-C12-C13
5	A	1005	CDL	CB6-CB4-OB6-CB5
5	B	1007	CDL	CA3-CA4-OA6-CA5
5	D	1006	CDL	OA9-CA7-OA8-CA6
2	A	1001	LMT	C1-C2-C3-C4
2	D	1001	LMT	O5'-C1'-O1'-C1
5	C	1009	CDL	C11-CA5-OA6-CA4
2	D	1002	LMT	C3-C4-C5-C6
5	B	1006	CDL	OB6-CB4-CB6-OB8
5	B	1005	CDL	C71-CB7-OB8-CB6
5	C	1007	CDL	C31-CA7-OA8-CA6
5	C	1007	CDL	CA5-C11-C12-C13
2	C	1002	LMT	C11-C10-C9-C8
5	A	1007	CDL	C31-C32-C33-C34
5	B	1006	CDL	C11-C12-C13-C14
5	B	1006	CDL	C32-C33-C34-C35
5	B	1008	CDL	C31-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1001	LMT	C3-C4-C5-C6
5	A	1005	CDL	C32-C33-C34-C35
5	C	1006	CDL	C51-C52-C53-C54
5	B	1006	CDL	C51-CB5-OB6-CB4
5	B	1009	CDL	C11-CA5-OA6-CA4
5	B	1010	CDL	C11-CA5-OA6-CA4
5	C	1006	CDL	C51-CB5-OB6-CB4
5	C	1009	CDL	CA5-C11-C12-C13
5	C	1007	CDL	C71-CB7-OB8-CB6
2	A	1001	LMT	C11-C10-C9-C8
2	B	1001	LMT	C5-C6-C7-C8
5	D	1007	CDL	CA7-C31-C32-C33
5	C	1006	CDL	OB9-CB7-OB8-CB6
5	B	1006	CDL	C31-CA7-OA8-CA6
5	B	1005	CDL	CA3-CA4-CA6-OA8
5	C	1010	CDL	CA3-CA4-CA6-OA8
2	B	1001	LMT	C4-C5-C6-C7
5	A	1006	CDL	CA5-C11-C12-C13
5	B	1006	CDL	CA5-C11-C12-C13
5	B	1009	CDL	CA5-C11-C12-C13
5	D	1006	CDL	CB5-C51-C52-C53
2	C	1003	LMT	C7-C8-C9-C10
5	A	1007	CDL	C11-C12-C13-C14
5	C	1009	CDL	OA9-CA7-OA8-CA6
5	C	1007	CDL	C31-C32-C33-C34
5	A	1008	CDL	CB5-C51-C52-C53
5	C	1007	CDL	OA9-CA7-OA8-CA6
5	D	1007	CDL	C31-C32-C33-C34
5	C	1009	CDL	C32-C33-C34-C35
5	B	1005	CDL	CA5-C11-C12-C13
5	B	1007	CDL	CA5-C11-C12-C13
5	B	1009	CDL	C52-C53-C54-C55
5	B	1005	CDL	OB9-CB7-OB8-CB6
5	B	1008	CDL	OA9-CA7-OA8-CA6
5	C	1007	CDL	OB9-CB7-OB8-CB6
2	C	1002	LMT	C6-C7-C8-C9
5	B	1006	CDL	OB7-CB5-OB6-CB4
5	B	1009	CDL	OA7-CA5-OA6-CA4
5	B	1010	CDL	OA7-CA5-OA6-CA4
5	C	1009	CDL	OA7-CA5-OA6-CA4
2	B	1001	LMT	C9-C10-C11-C12
5	B	1006	CDL	C52-C53-C54-C55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1006	CDL	C31-CA7-OA8-CA6
2	C	1003	LMT	C5-C6-C7-C8
2	D	1002	LMT	C2-C3-C4-C5
5	C	1007	CDL	C11-C12-C13-C14
2	C	1002	LMT	C3-C4-C5-C6
5	A	1005	CDL	C11-C12-C13-C14
2	A	1001	LMT	C5-C6-C7-C8
2	A	1001	LMT	C7-C8-C9-C10
5	C	1008	CDL	C11-C12-C13-C14
2	C	1002	LMT	O5'-C5'-C6'-O6'
5	A	1005	CDL	C11-CA5-OA6-CA4
5	B	1010	CDL	C51-CB5-OB6-CB4
5	D	1007	CDL	C51-CB5-OB6-CB4
5	C	1006	CDL	OB7-CB5-OB6-CB4
5	D	1007	CDL	OB7-CB5-OB6-CB4
5	C	1006	CDL	CA5-C11-C12-C13
5	B	1010	CDL	C31-C32-C33-C34
5	C	1006	CDL	C11-C12-C13-C14
2	D	1001	LMT	O1'-C1-C2-C3
5	A	1006	CDL	OA5-CA3-CA4-OA6
5	A	1006	CDL	OB5-CB3-CB4-OB6
5	D	1006	CDL	C51-CB5-OB6-CB4
5	C	1010	CDL	OA6-CA4-CA6-OA8
2	C	1002	LMT	C4'-C5'-C6'-O6'
2	D	1001	LMT	O5B-C5B-C6B-O6B
5	C	1006	CDL	C1-CB2-OB2-PB2
5	B	1009	CDL	CA2-C1-CB2-OB2
5	C	1009	CDL	CB2-C1-CA2-OA2
2	C	1003	LMT	C11-C10-C9-C8
5	B	1005	CDL	C11-C12-C13-C14
5	A	1005	CDL	C51-C52-C53-C54
5	C	1009	CDL	C11-C12-C13-C14
5	D	1007	CDL	C32-C33-C34-C35
2	B	1001	LMT	C11-C10-C9-C8
5	C	1009	CDL	C51-C52-C53-C54
5	A	1008	CDL	OA5-CA3-CA4-CA6
5	C	1006	CDL	OA5-CA3-CA4-CA6
5	D	1006	CDL	OA5-CA3-CA4-CA6
5	D	1007	CDL	OB5-CB3-CB4-CB6
5	B	1008	CDL	CA7-C31-C32-C33
5	A	1006	CDL	OA9-CA7-OA8-CA6
5	A	1007	CDL	C31-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1008	CDL	C71-CB7-OB8-CB6
5	B	1006	CDL	CB7-C71-C72-C73
5	A	1005	CDL	CA3-CA4-CA6-OA8
5	B	1005	CDL	CB3-CB4-CB6-OB8
5	B	1006	CDL	CB3-CB4-CB6-OB8
5	B	1007	CDL	CA3-CA4-CA6-OA8
5	C	1009	CDL	CB3-CB4-CB6-OB8
5	C	1010	CDL	C71-CB7-OB8-CB6
5	D	1006	CDL	C11-C12-C13-C14
5	A	1006	CDL	CA4-CA3-OA5-PA1
5	A	1005	CDL	OA7-CA5-OA6-CA4
5	D	1006	CDL	CA7-C31-C32-C33
2	C	1003	LMT	C3-C4-C5-C6
5	B	1008	CDL	C51-C52-C53-C54
5	D	1007	CDL	C11-C12-C13-C14
5	A	1007	CDL	CB5-C51-C52-C53
5	B	1005	CDL	CA6-CA4-OA6-CA5
5	B	1008	CDL	CB6-CB4-OB6-CB5
5	A	1007	CDL	C51-C52-C53-C54
2	D	1002	LMT	C6-C7-C8-C9
5	A	1006	CDL	CB5-C51-C52-C53
5	A	1005	CDL	CA2-C1-CB2-OB2
5	C	1008	CDL	OB5-CB3-CB4-OB6
5	C	1006	CDL	C52-C53-C54-C55
2	A	1001	LMT	C4-C5-C6-C7
5	C	1009	CDL	C12-C13-C14-C15
5	B	1008	CDL	C11-C12-C13-C14
5	B	1008	CDL	C71-C72-C73-C74
5	C	1009	CDL	C71-C72-C73-C74
5	A	1008	CDL	C31-C32-C33-C34
5	C	1008	CDL	C52-C53-C54-C55
2	C	1002	LMT	C9-C10-C11-C12
5	C	1007	CDL	C52-C53-C54-C55
5	B	1005	CDL	C12-C13-C14-C15
5	B	1007	CDL	C52-C53-C54-C55
5	B	1009	CDL	C33-C34-C35-C36
5	D	1006	CDL	C12-C13-C14-C15
5	A	1007	CDL	CA5-C11-C12-C13
5	D	1007	CDL	C71-CB7-OB8-CB6
2	C	1003	LMT	C6-C7-C8-C9
5	B	1010	CDL	OB7-CB5-OB6-CB4
2	B	1001	LMT	C2-C1-O1'-C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	1002	LMT	C2-C1-O1'-C1'
5	C	1010	CDL	C11-C12-C13-C14
2	C	1002	LMT	C4-C5-C6-C7
5	A	1006	CDL	OA5-CA3-CA4-CA6
5	A	1006	CDL	OB5-CB3-CB4-CB6
5	B	1007	CDL	OA5-CA3-CA4-CA6
5	B	1008	CDL	OB5-CB3-CB4-CB6
5	B	1009	CDL	OA5-CA3-CA4-CA6
5	C	1007	CDL	OA5-CA3-CA4-CA6
5	C	1007	CDL	OB5-CB3-CB4-CB6
5	C	1008	CDL	OB5-CB3-CB4-CB6
5	C	1009	CDL	OA5-CA3-CA4-CA6
5	D	1006	CDL	OB5-CB3-CB4-CB6
5	C	1010	CDL	OB9-CB7-OB8-CB6
5	A	1006	CDL	C71-C72-C73-C74
5	A	1007	CDL	OA9-CA7-OA8-CA6
5	A	1008	CDL	OB9-CB7-OB8-CB6
5	B	1010	CDL	C52-C53-C54-C55
5	B	1005	CDL	C71-C72-C73-C74
5	C	1006	CDL	C31-CA7-OA8-CA6
5	A	1008	CDL	CB3-CB4-CB6-OB8
5	B	1007	CDL	CB3-CB4-CB6-OB8
5	B	1010	CDL	CA3-CA4-CA6-OA8
5	C	1006	CDL	CA3-CA4-CA6-OA8
5	D	1006	CDL	OB7-CB5-OB6-CB4
5	B	1009	CDL	OA5-CA3-CA4-OA6
5	D	1006	CDL	OB5-CB3-CB4-OB6
5	D	1007	CDL	OB5-CB3-CB4-OB6
5	C	1009	CDL	O1-C1-CA2-OA2
5	A	1007	CDL	C1-CB2-OB2-PB2
5	C	1007	CDL	C1-CA2-OA2-PA1
5	C	1007	CDL	C1-CB2-OB2-PB2
5	C	1009	CDL	CA4-CA3-OA5-PA1
5	A	1008	CDL	OA6-CA4-CA6-OA8
5	A	1008	CDL	OB6-CB4-CB6-OB8
2	B	1001	LMT	C6-C7-C8-C9
2	D	1002	LMT	C7-C8-C9-C10
5	C	1008	CDL	C32-C33-C34-C35
5	A	1006	CDL	C52-C53-C54-C55
2	D	1002	LMT	C9-C10-C11-C12
5	A	1006	CDL	O1-C1-CA2-OA2
2	A	1001	LMT	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1010	CDL	CB2-C1-CA2-OA2
5	C	1007	CDL	C71-C72-C73-C74
2	C	1002	LMT	C5'-C4'-O1B-C1B
5	A	1006	CDL	CA7-C31-C32-C33
5	D	1007	CDL	OB9-CB7-OB8-CB6
5	C	1006	CDL	OA9-CA7-OA8-CA6
5	C	1008	CDL	C12-C13-C14-C15
5	C	1010	CDL	C52-C53-C54-C55
5	A	1005	CDL	OA5-CA3-CA4-OA6
5	A	1008	CDL	OA5-CA3-CA4-OA6
5	B	1005	CDL	OA5-CA3-CA4-OA6
5	B	1007	CDL	OA5-CA3-CA4-OA6
5	B	1010	CDL	OA5-CA3-CA4-OA6
5	C	1007	CDL	OB5-CB3-CB4-OB6
5	C	1009	CDL	OA5-CA3-CA4-OA6
5	C	1008	CDL	C51-C52-C53-C54
5	B	1008	CDL	CB3-CB4-CB6-OB8
5	C	1010	CDL	CB3-CB4-CB6-OB8
5	A	1008	CDL	CA7-C31-C32-C33
5	A	1006	CDL	C11-C12-C13-C14
5	A	1006	CDL	OB6-CB4-CB6-OB8
5	B	1005	CDL	OA6-CA4-CA6-OA8
5	B	1005	CDL	OB6-CB4-CB6-OB8
5	B	1007	CDL	OA6-CA4-CA6-OA8
5	C	1008	CDL	OA6-CA4-CA6-OA8
5	C	1008	CDL	OB6-CB4-CB6-OB8
5	C	1009	CDL	OB6-CB4-CB6-OB8
5	D	1007	CDL	OB6-CB4-CB6-OB8
2	C	1002	LMT	C2-C1-O1'-C1'
2	C	1003	LMT	C2-C1-O1'-C1'
5	B	1005	CDL	OA5-CA3-CA4-CA6
5	B	1010	CDL	OA5-CA3-CA4-CA6
5	C	1010	CDL	OA5-CA3-CA4-CA6
5	B	1009	CDL	C12-C13-C14-C15
5	A	1008	CDL	C11-C12-C13-C14
5	B	1005	CDL	CA4-CA3-OA5-PA1
5	D	1007	CDL	CB4-CB3-OB5-PB2
5	C	1010	CDL	OA5-CA3-CA4-OA6
5	D	1006	CDL	OA5-CA3-CA4-OA6
5	B	1008	CDL	C52-C53-C54-C55
5	A	1005	CDL	OA6-CA4-CA6-OA8
5	A	1007	CDL	OA6-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1006	CDL	OA6-CA4-CA6-OA8
5	B	1008	CDL	OB6-CB4-CB6-OB8
5	B	1010	CDL	OA6-CA4-CA6-OA8
5	C	1007	CDL	OA6-CA4-CA6-OA8
5	A	1006	CDL	CB3-CB4-CB6-OB8
5	A	1008	CDL	CA3-CA4-CA6-OA8
5	C	1007	CDL	CA3-CA4-CA6-OA8
5	C	1008	CDL	CA3-CA4-CA6-OA8
5	A	1006	CDL	C12-C13-C14-C15
2	D	1001	LMT	C7-C8-C9-C10
5	B	1010	CDL	C12-C13-C14-C15
5	D	1007	CDL	CB7-C71-C72-C73
5	A	1005	CDL	CA3-OA5-PA1-OA4
5	A	1005	CDL	CB2-OB2-PB2-OB4
5	A	1005	CDL	CB2-OB2-PB2-OB5
5	A	1006	CDL	CA3-OA5-PA1-OA3
5	A	1006	CDL	CB2-OB2-PB2-OB3
5	A	1007	CDL	CA2-OA2-PA1-OA4
5	A	1007	CDL	CA3-OA5-PA1-OA3
5	A	1008	CDL	CB2-OB2-PB2-OB3
5	B	1005	CDL	CA3-OA5-PA1-OA2
5	B	1005	CDL	CB2-OB2-PB2-OB3
5	B	1006	CDL	CA2-OA2-PA1-OA4
5	B	1006	CDL	CB3-OB5-PB2-OB2
5	B	1008	CDL	CA2-OA2-PA1-OA5
5	B	1009	CDL	CA3-OA5-PA1-OA4
5	C	1006	CDL	CA2-OA2-PA1-OA3
5	C	1006	CDL	CA3-OA5-PA1-OA2
5	C	1006	CDL	CA3-OA5-PA1-OA3
5	C	1006	CDL	CA3-OA5-PA1-OA4
5	C	1007	CDL	CB2-OB2-PB2-OB3
5	C	1007	CDL	CB2-OB2-PB2-OB4
5	C	1007	CDL	CB3-OB5-PB2-OB2
5	C	1008	CDL	CA2-OA2-PA1-OA5
5	C	1008	CDL	CA3-OA5-PA1-OA2
5	C	1008	CDL	CA3-OA5-PA1-OA4
5	C	1009	CDL	CB3-OB5-PB2-OB2
5	D	1006	CDL	CA3-OA5-PA1-OA2
5	D	1006	CDL	CB2-OB2-PB2-OB4
5	D	1006	CDL	CB2-OB2-PB2-OB5
5	D	1006	CDL	CB3-OB5-PB2-OB3
5	D	1007	CDL	CA2-OA2-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	1007	CDL	CA2-OA2-PA1-OA5
5	D	1007	CDL	CB2-OB2-PB2-OB4
5	B	1006	CDL	C31-C32-C33-C34
5	A	1006	CDL	C1-CA2-OA2-PA1
5	A	1007	CDL	CB4-CB3-OB5-PB2
5	B	1008	CDL	C1-CB2-OB2-PB2
5	C	1006	CDL	C1-CA2-OA2-PA1
5	C	1006	CDL	CB4-CB3-OB5-PB2
5	C	1009	CDL	C1-CA2-OA2-PA1
5	B	1005	CDL	C51-C52-C53-C54
5	D	1007	CDL	C12-C13-C14-C15
5	C	1007	CDL	CA7-C31-C32-C33
5	C	1008	CDL	C71-C72-C73-C74
5	A	1008	CDL	C12-C13-C14-C15
5	C	1009	CDL	CB6-CB4-OB6-CB5
5	B	1007	CDL	C32-C31-CA7-OA8
5	B	1007	CDL	C31-C32-C33-C34
5	B	1005	CDL	C33-C34-C35-C36
5	B	1006	CDL	CA3-CA4-CA6-OA8
5	B	1006	CDL	C33-C34-C35-C36
5	C	1006	CDL	C12-C13-C14-C15
5	D	1006	CDL	C32-C31-CA7-OA8
5	D	1006	CDL	C52-C51-CB5-OB6
5	B	1010	CDL	C71-CB7-OB8-CB6
5	D	1006	CDL	C52-C53-C54-C55
5	B	1007	CDL	C71-C72-C73-C74
5	A	1006	CDL	CB2-C1-CA2-OA2
5	C	1008	CDL	CB4-CB3-OB5-PB2
5	B	1010	CDL	OB9-CB7-OB8-CB6
2	D	1001	LMT	C5'-C4'-O1B-C1B
5	A	1007	CDL	C32-C33-C34-C35
5	C	1010	CDL	C52-C51-CB5-OB6
5	D	1007	CDL	C33-C34-C35-C36
5	D	1007	CDL	C52-C53-C54-C55
5	D	1007	CDL	CA4-CA3-OA5-PA1
5	A	1005	CDL	OA5-CA3-CA4-CA6
5	B	1005	CDL	CB7-C71-C72-C73
5	B	1010	CDL	C32-C33-C34-C35
5	A	1008	CDL	C1-CB2-OB2-PB2
5	B	1010	CDL	C33-C34-C35-C36
5	C	1009	CDL	C52-C53-C54-C55
5	B	1006	CDL	OB5-CB3-CB4-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1010	CDL	C72-C71-CB7-OB8
5	B	1005	CDL	CB5-C51-C52-C53
5	B	1006	CDL	OA5-CA3-CA4-CA6
5	C	1006	CDL	OA6-CA4-CA6-OA8
5	B	1007	CDL	CB4-CB3-OB5-PB2
5	C	1010	CDL	O1-C1-CA2-OA2
5	C	1009	CDL	C12-C11-CA5-OA6
5	D	1007	CDL	CA6-CA4-OA6-CA5
5	B	1008	CDL	C31-C32-C33-C34
5	B	1006	CDL	C1-CA2-OA2-PA1
5	C	1006	CDL	OB5-CB3-CB4-OB6
5	B	1007	CDL	C31-CA7-OA8-CA6
5	C	1008	CDL	CB3-CB4-CB6-OB8
5	D	1007	CDL	CB3-CB4-CB6-OB8
5	B	1007	CDL	OA9-CA7-OA8-CA6
5	A	1005	CDL	C33-C34-C35-C36
5	B	1006	CDL	OB5-CB3-CB4-CB6
5	C	1006	CDL	OB5-CB3-CB4-CB6
5	D	1007	CDL	C52-C51-CB5-OB6
5	D	1007	CDL	C72-C71-CB7-OB8
5	B	1006	CDL	C72-C71-CB7-OB8
2	B	1001	LMT	C3-C4-C5-C6
5	A	1007	CDL	C52-C53-C54-C55
5	A	1007	CDL	C32-C31-CA7-OA8
5	C	1010	CDL	OA7-CA5-OA6-CA4
2	C	1003	LMT	C9-C10-C11-C12
5	B	1007	CDL	C32-C33-C34-C35
5	A	1007	CDL	CA3-CA4-CA6-OA8
5	A	1008	CDL	C52-C53-C54-C55
5	A	1006	CDL	C52-C51-CB5-OB6
5	C	1008	CDL	C31-C32-C33-C34
5	C	1006	CDL	CB3-CB4-OB6-CB5
5	B	1009	CDL	C11-C12-C13-C14
5	A	1007	CDL	OA7-CA5-OA6-CA4
5	A	1005	CDL	C1-CA2-OA2-PA1
5	D	1006	CDL	C1-CA2-OA2-PA1
5	B	1006	CDL	C72-C71-CB7-OB9
2	D	1002	LMT	C4'-C5'-C6'-O6'
5	B	1009	CDL	C12-C11-CA5-OA6
5	A	1006	CDL	C52-C51-CB5-OB7
5	C	1008	CDL	C12-C11-CA5-OA6
5	D	1007	CDL	C72-C71-CB7-OB9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1008	CDL	OB7-CB5-OB6-CB4
5	A	1006	CDL	OA6-CA4-CA6-OA8
5	A	1007	CDL	C32-C31-CA7-OA9
5	A	1007	CDL	C72-C71-CB7-OB8
5	A	1006	CDL	CA3-CA4-CA6-OA8
5	A	1007	CDL	C11-CA5-OA6-CA4
2	C	1002	LMT	O1'-C1-C2-C3
5	C	1008	CDL	C12-C11-CA5-OA7

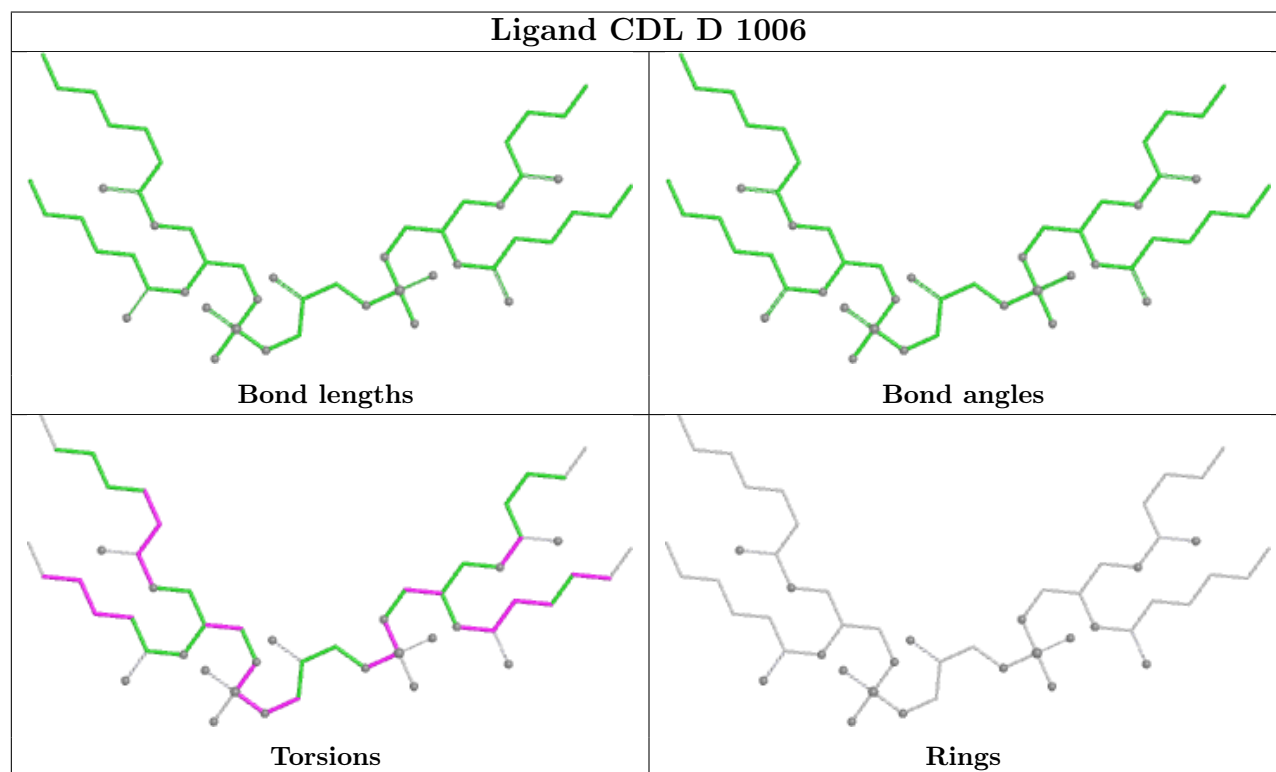
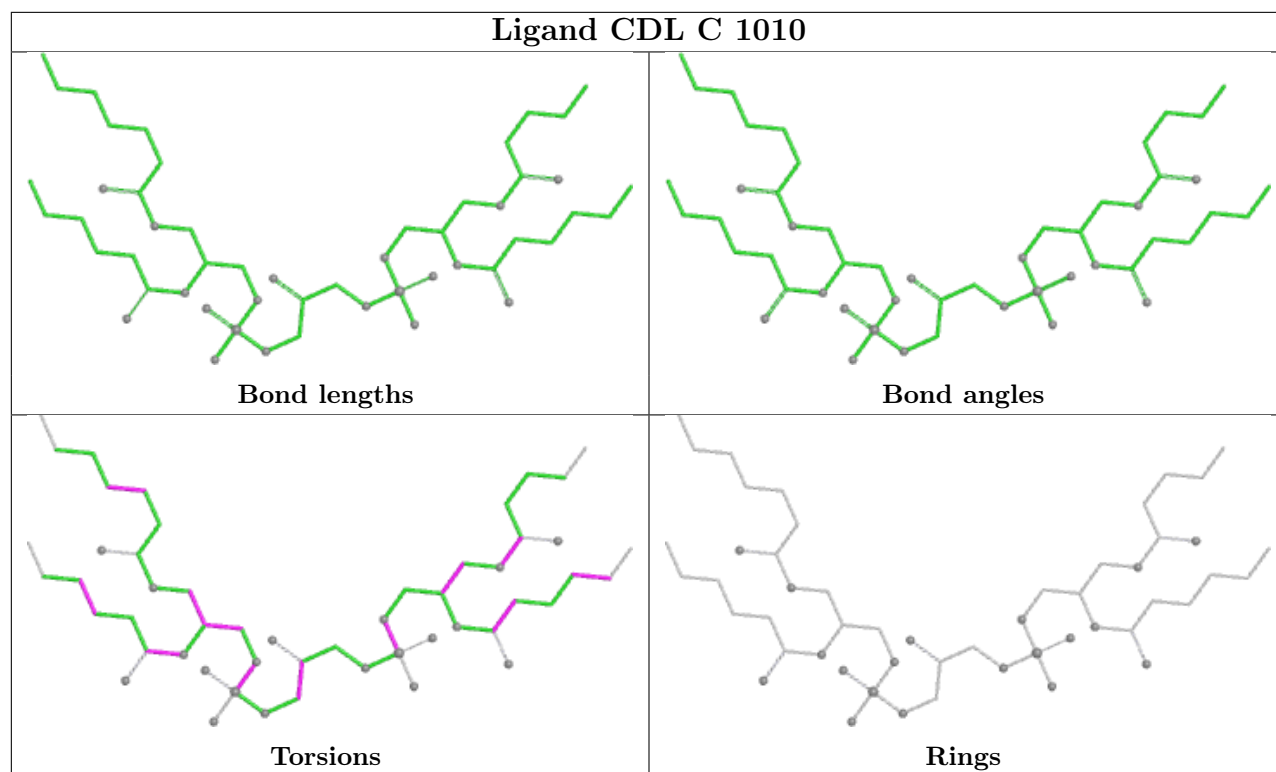
There are no ring outliers.

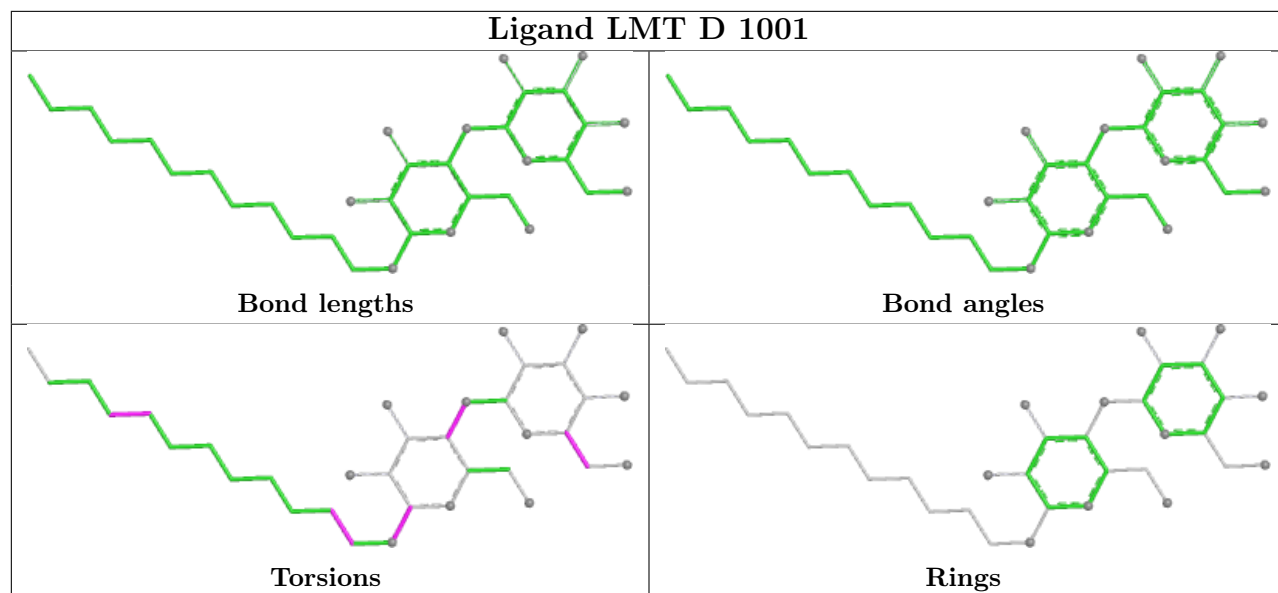
17 monomers are involved in 53 short contacts:

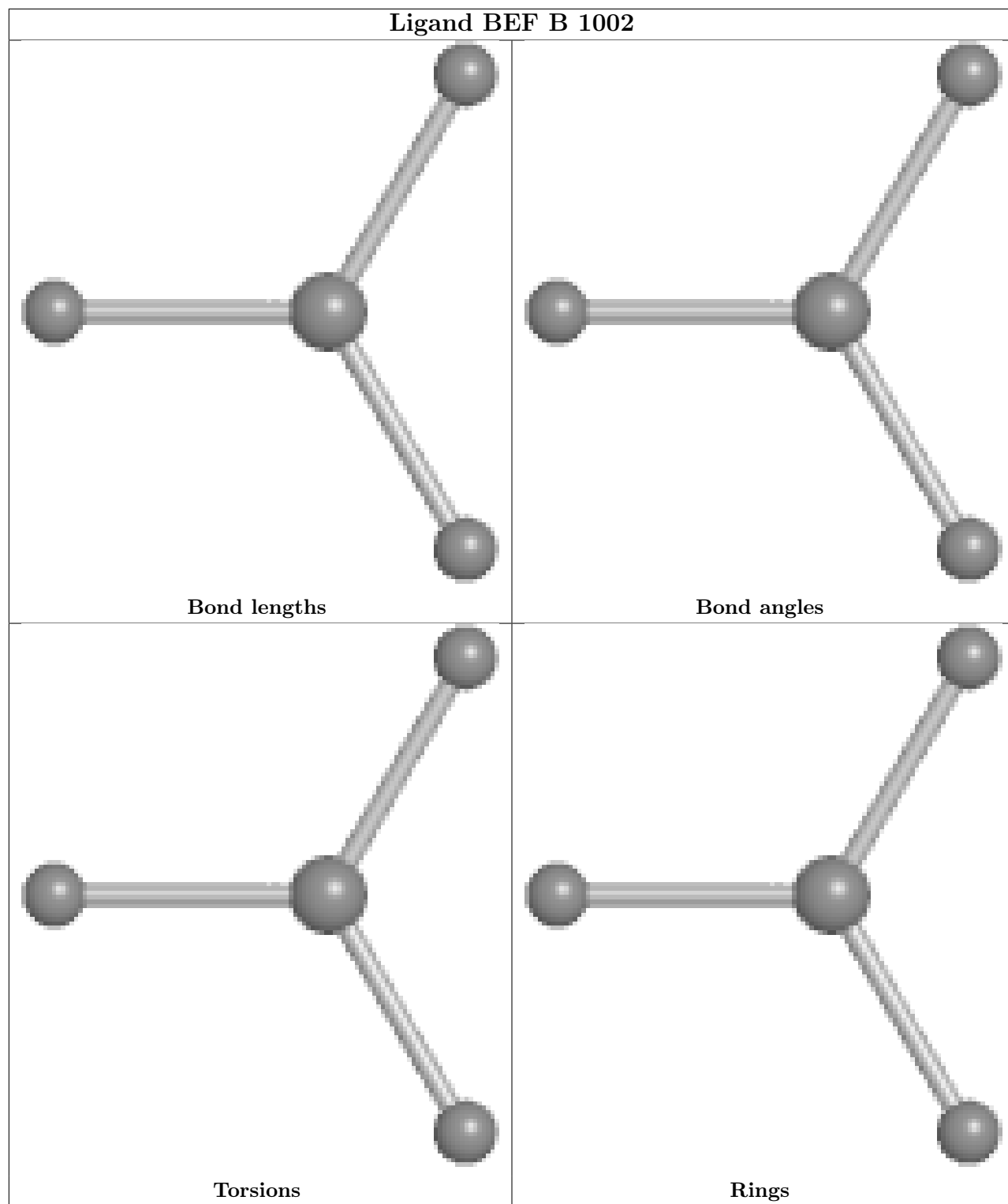
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1010	CDL	1	0
3	B	1002	BEF	8	0
5	B	1008	CDL	3	0
5	B	1010	CDL	7	0
5	C	1007	CDL	1	0
3	C	1001	BEF	4	0
5	A	1005	CDL	2	0
5	C	1006	CDL	3	0
3	A	1002	BEF	4	0
5	B	1009	CDL	4	0
5	A	1006	CDL	5	0
5	B	1007	CDL	1	0
5	C	1008	CDL	1	0
5	A	1008	CDL	2	0
5	B	1006	CDL	1	0
5	D	1007	CDL	3	0
3	D	1003	BEF	6	0

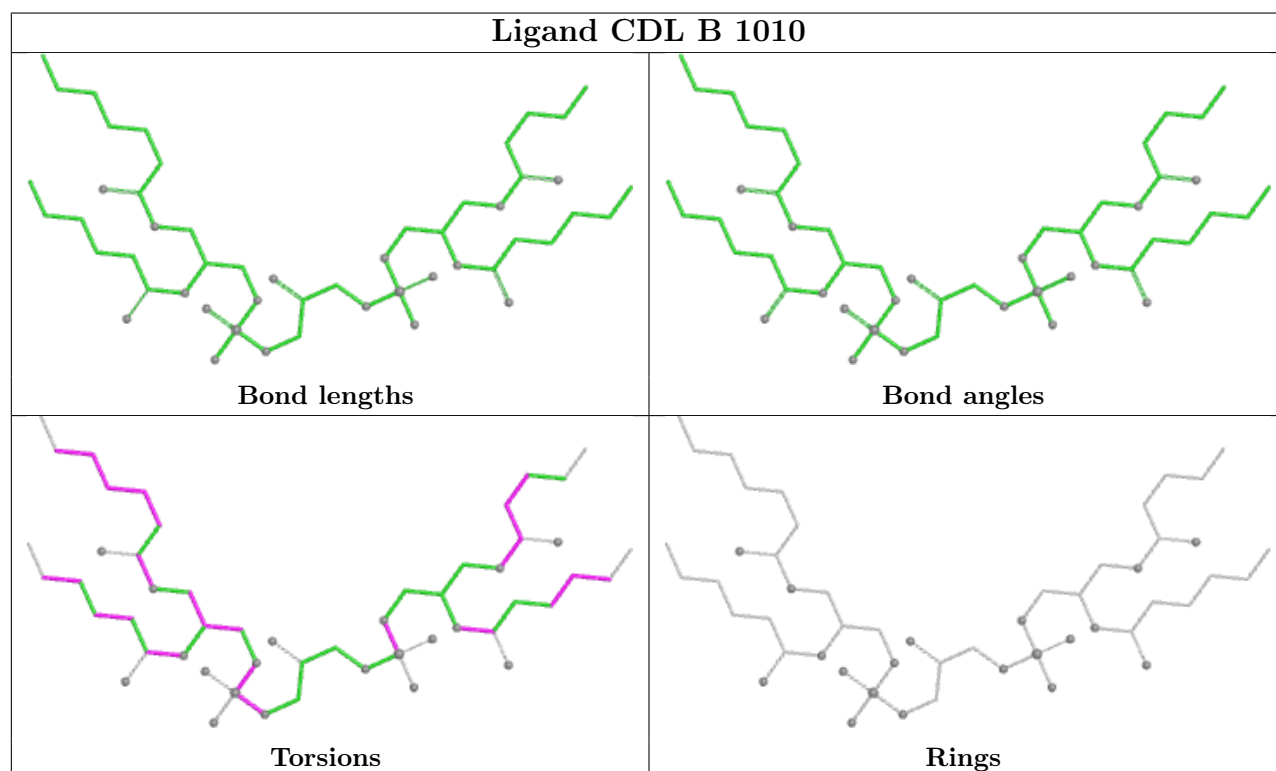
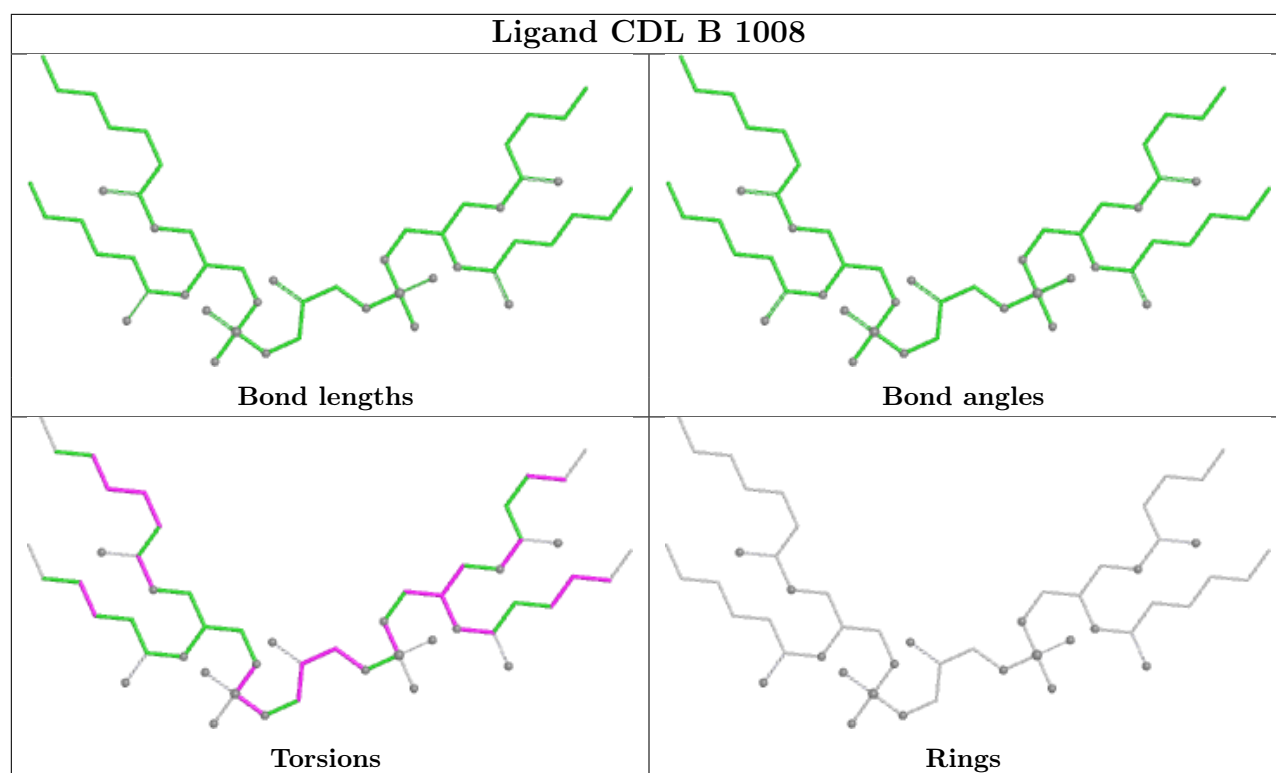
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

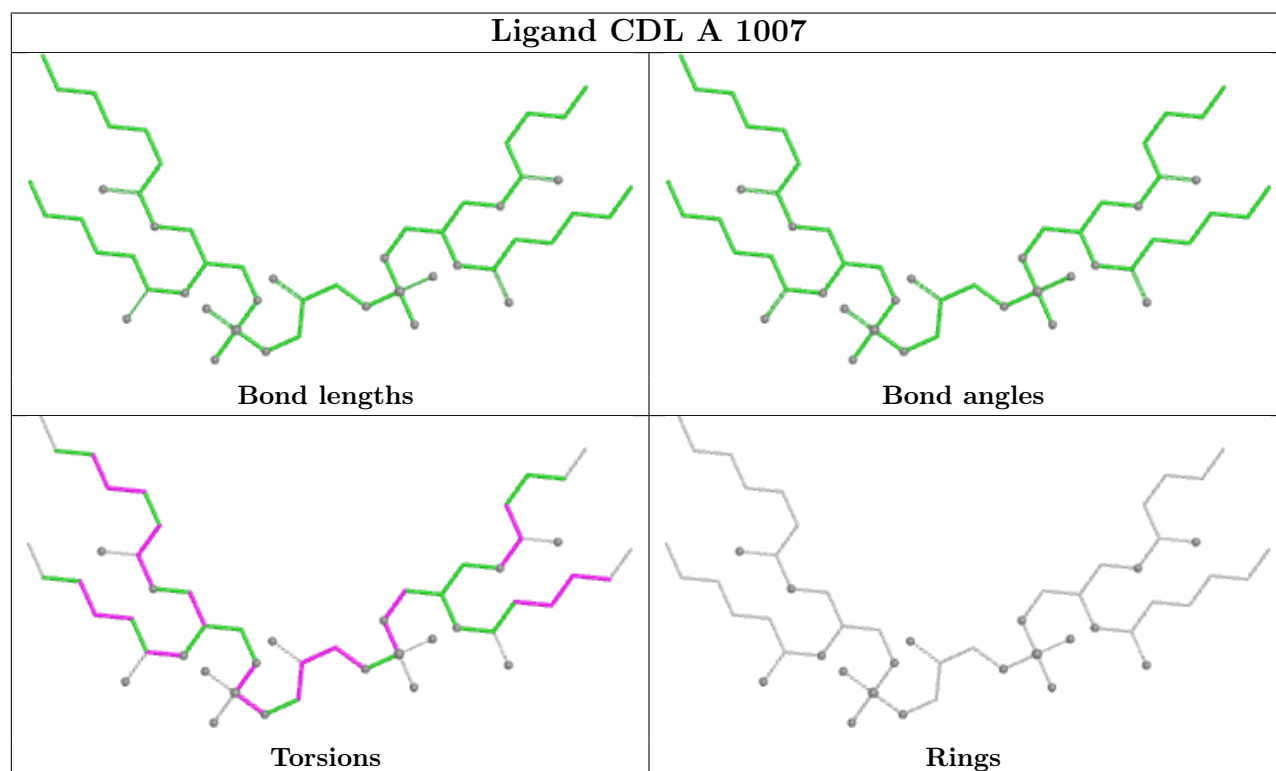
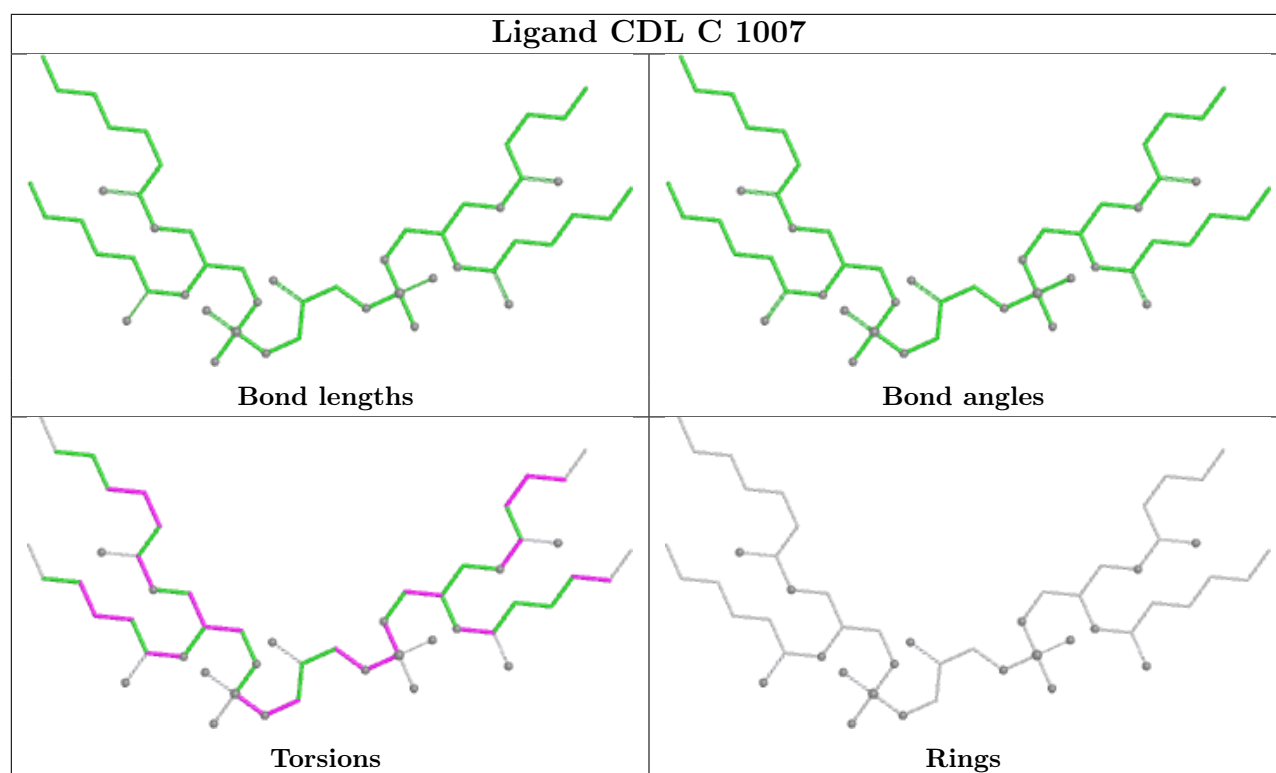
equivalents in the CSD to analyse the geometry.

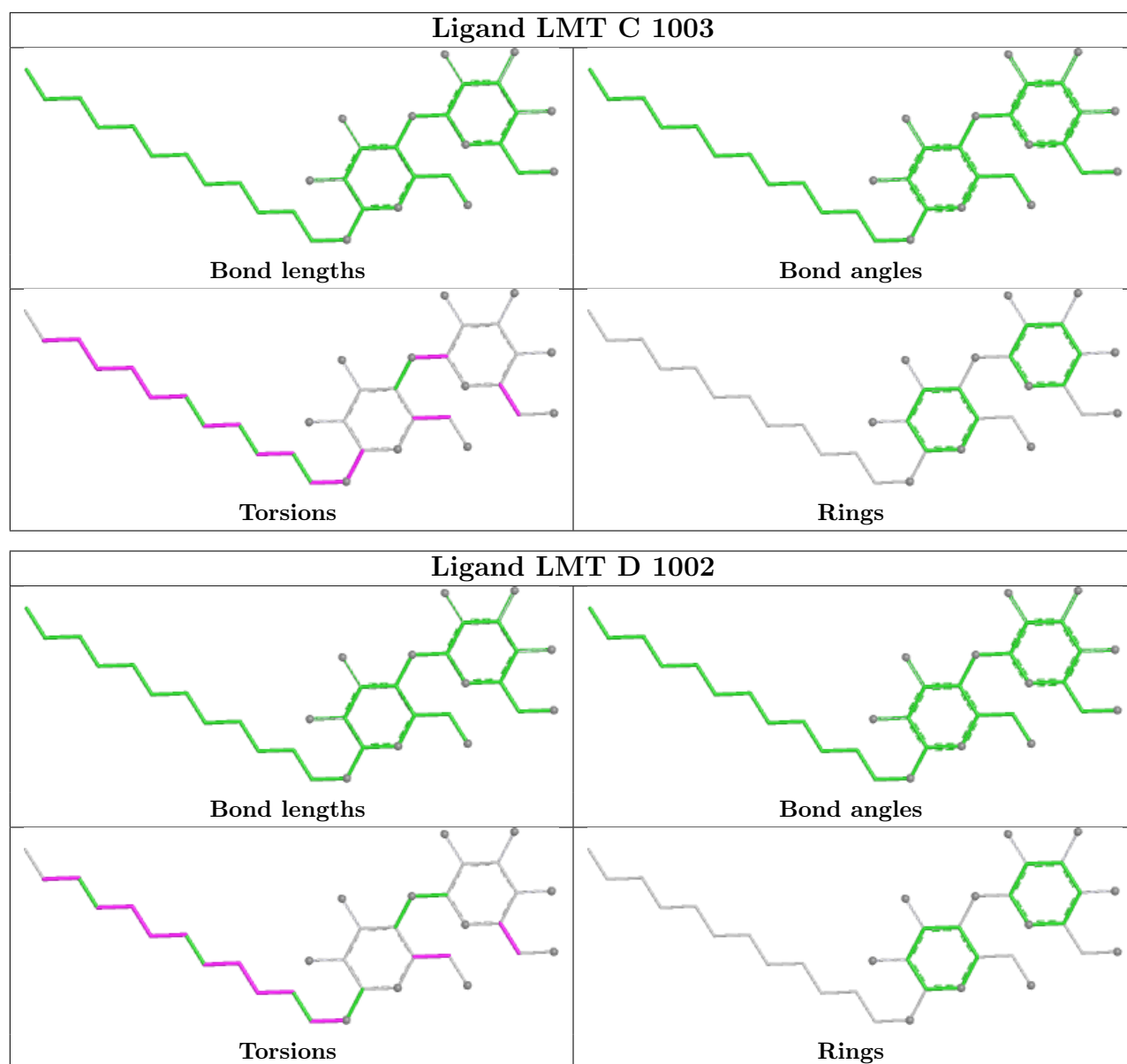


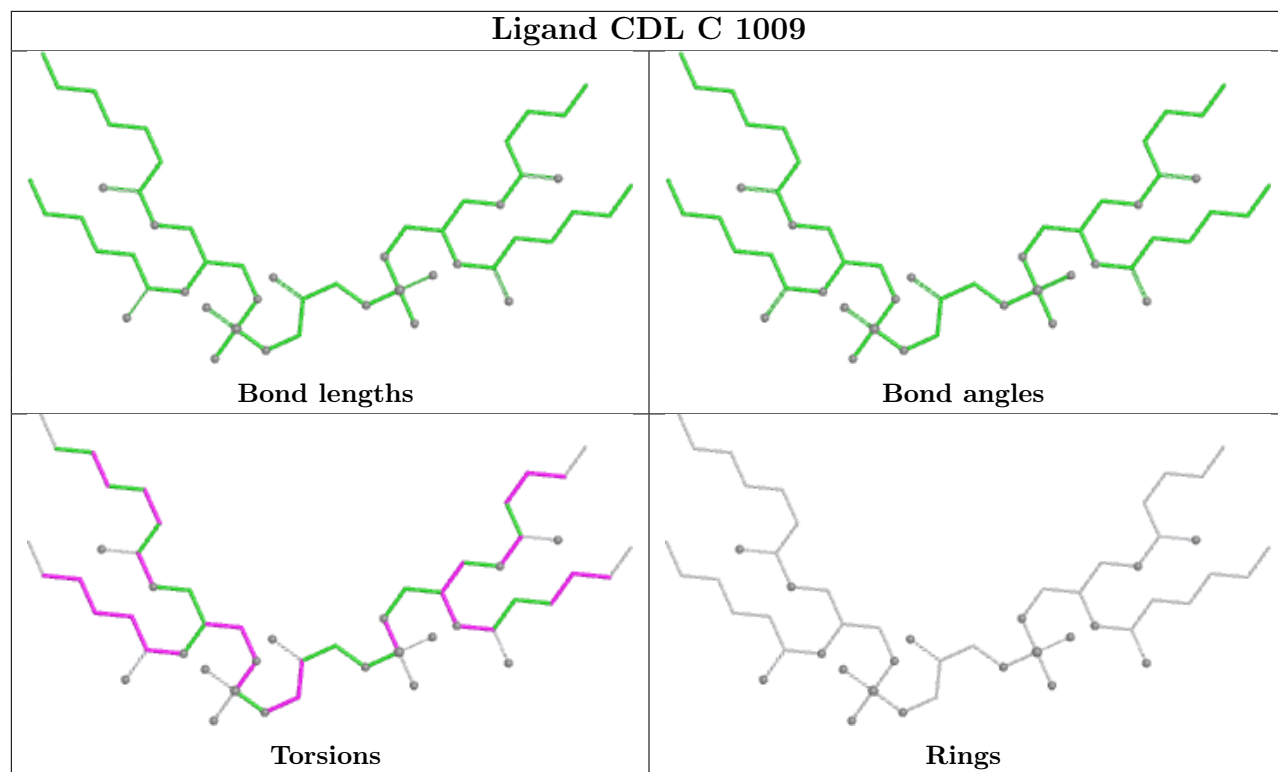


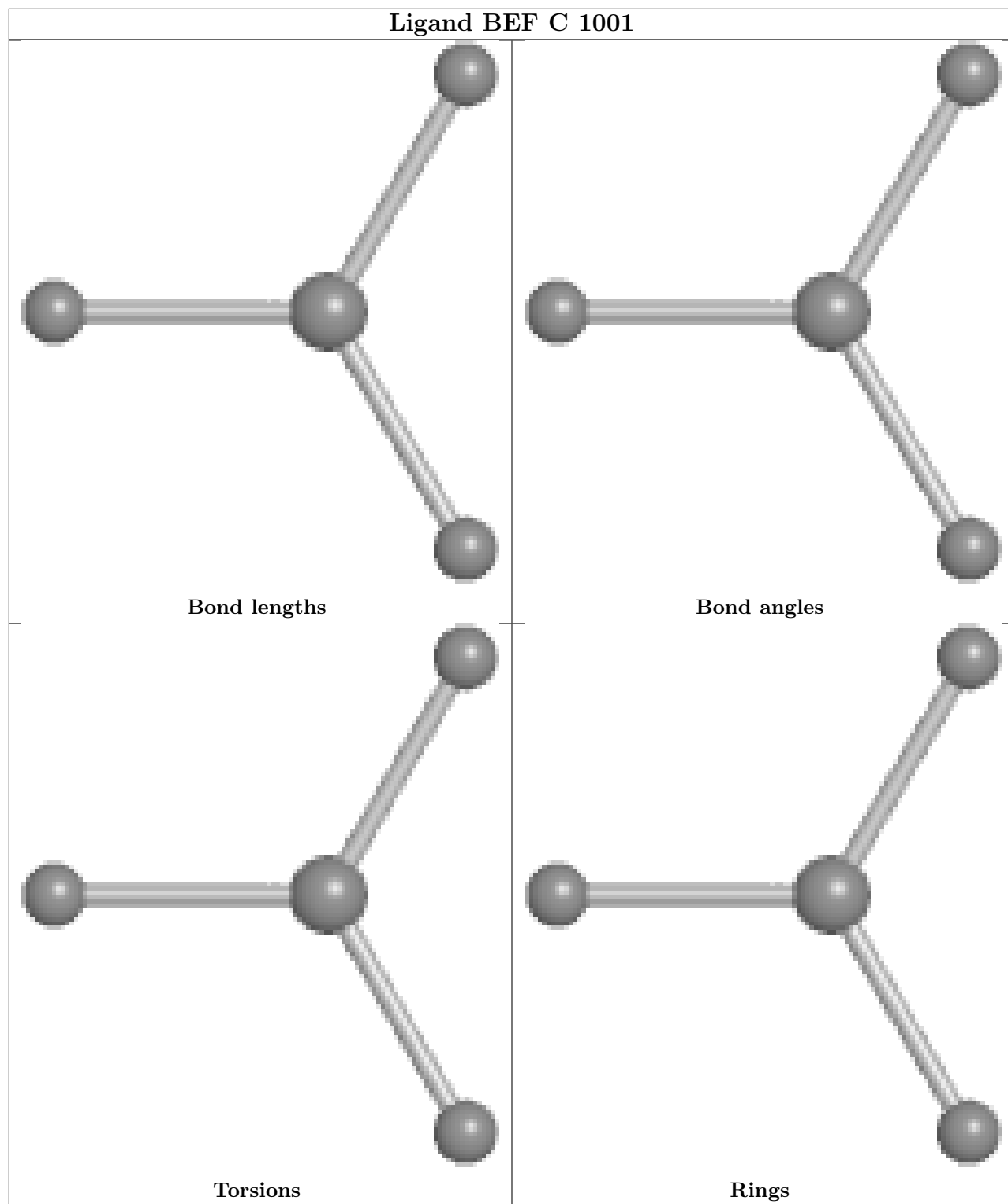


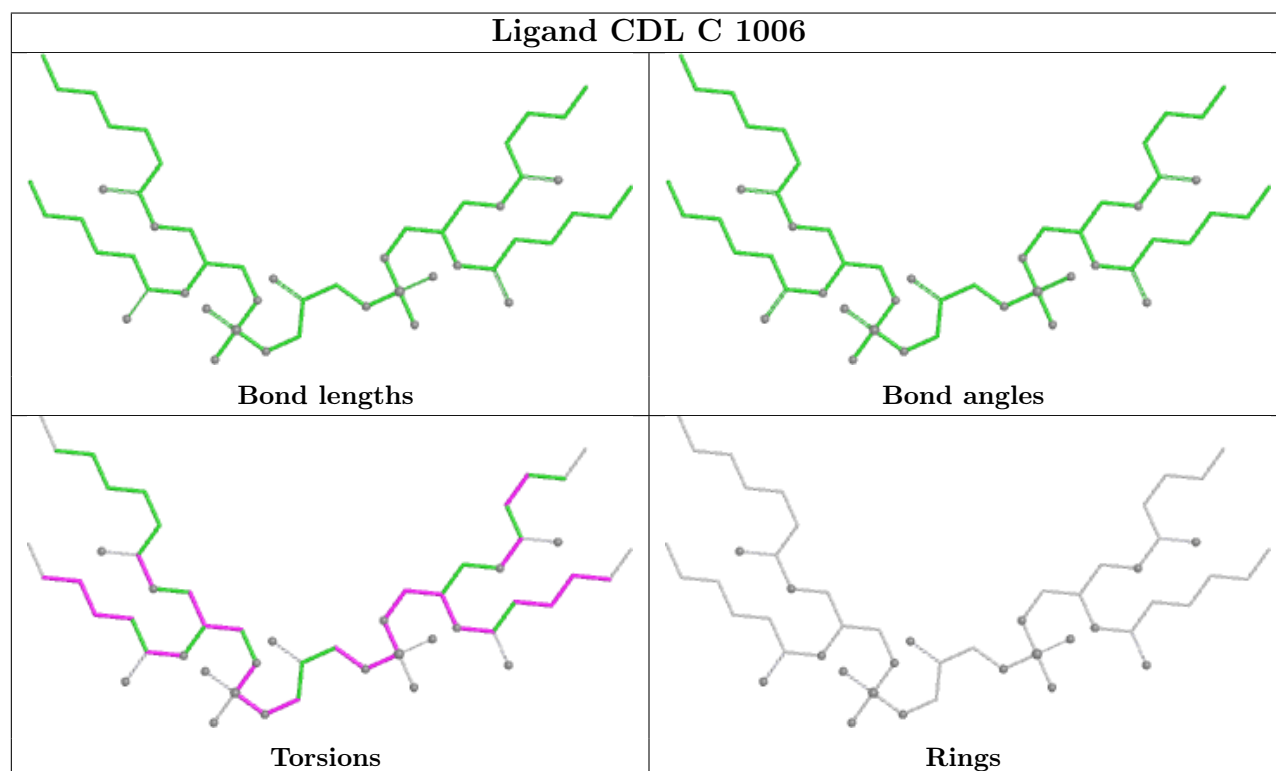
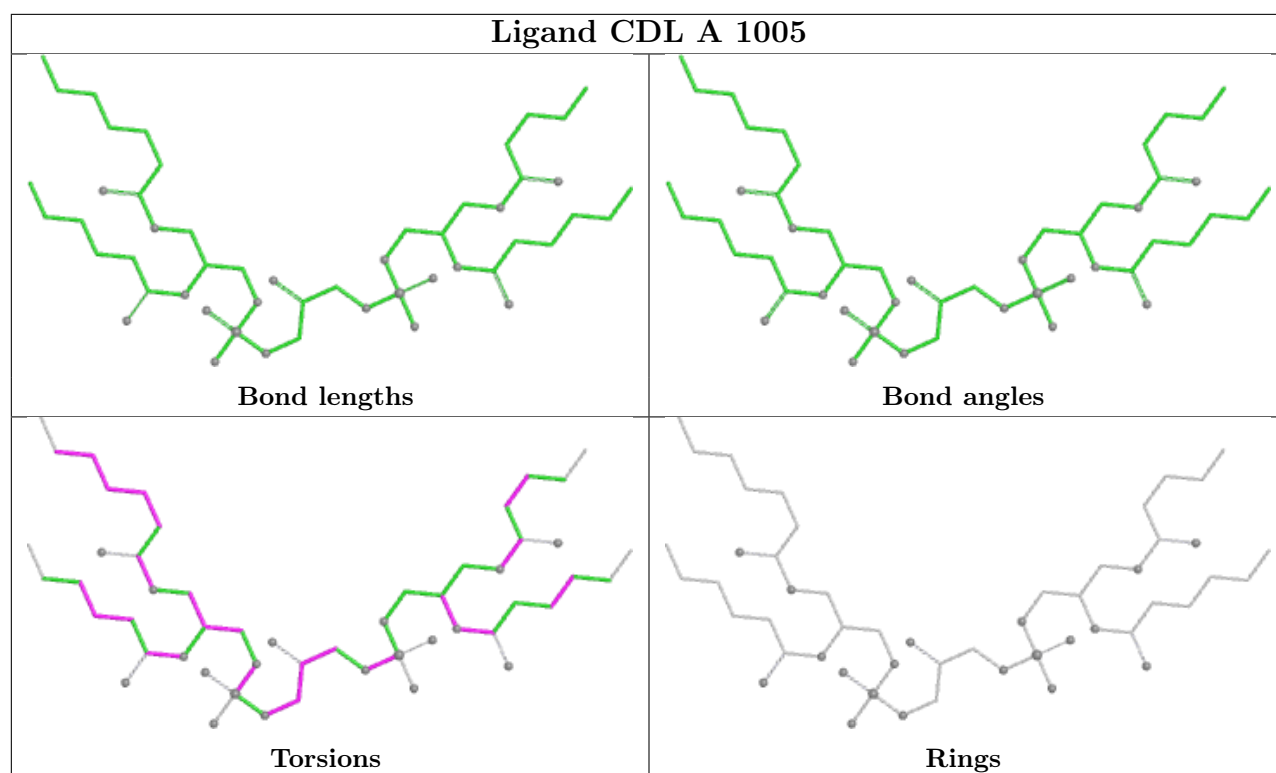


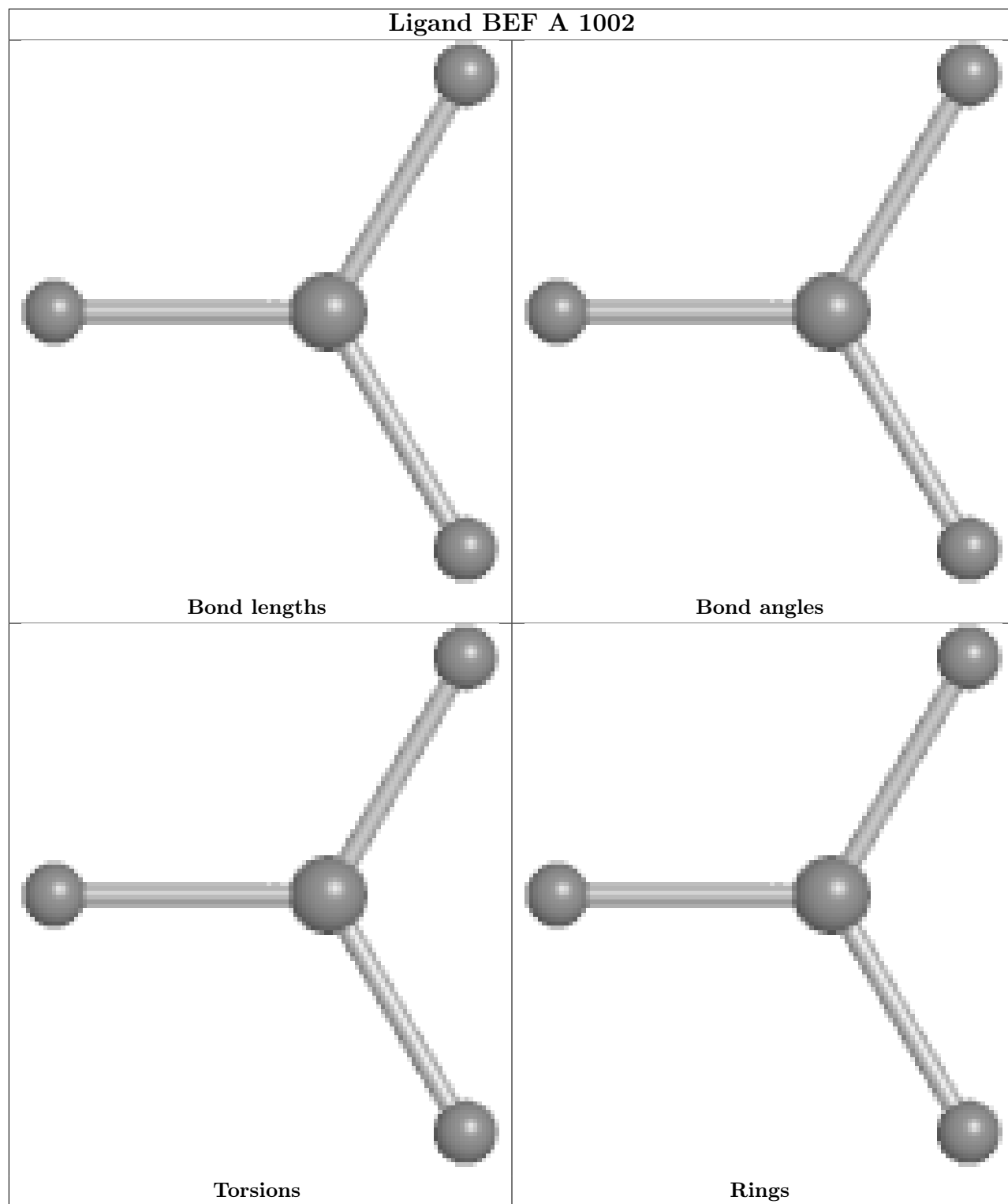


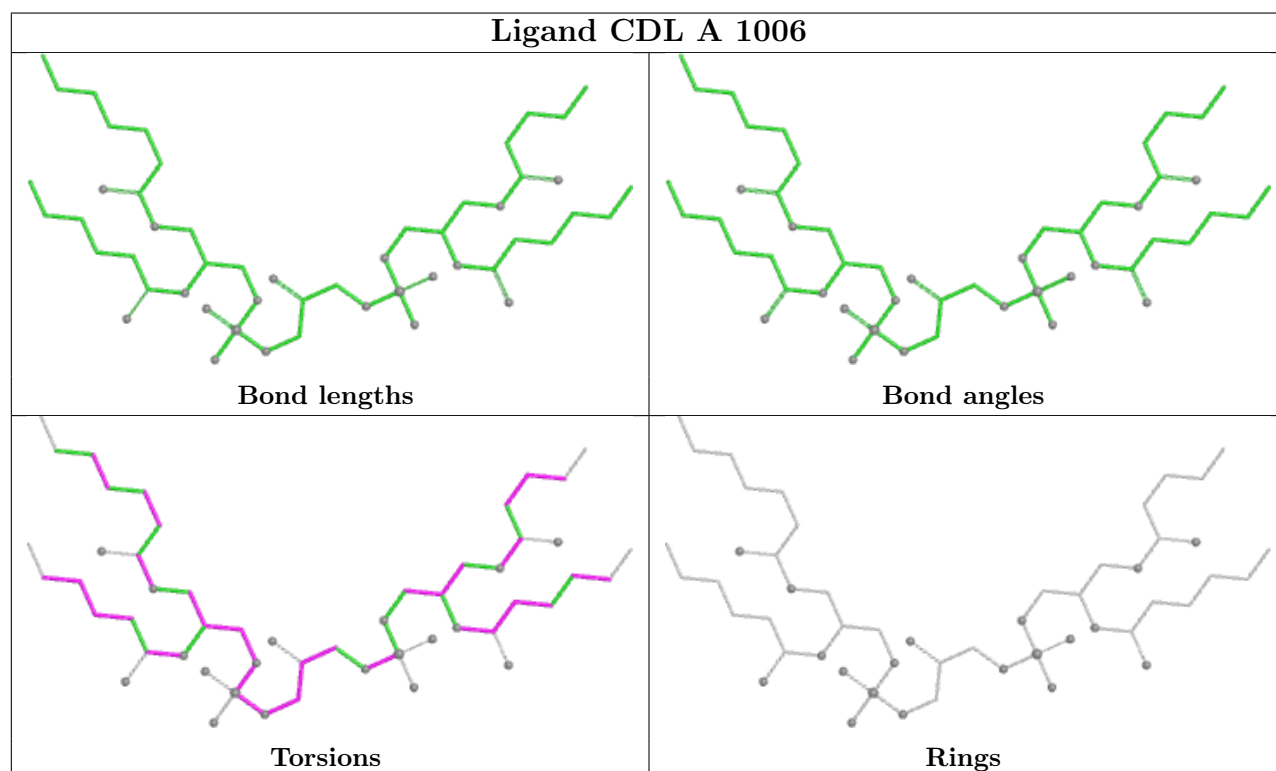
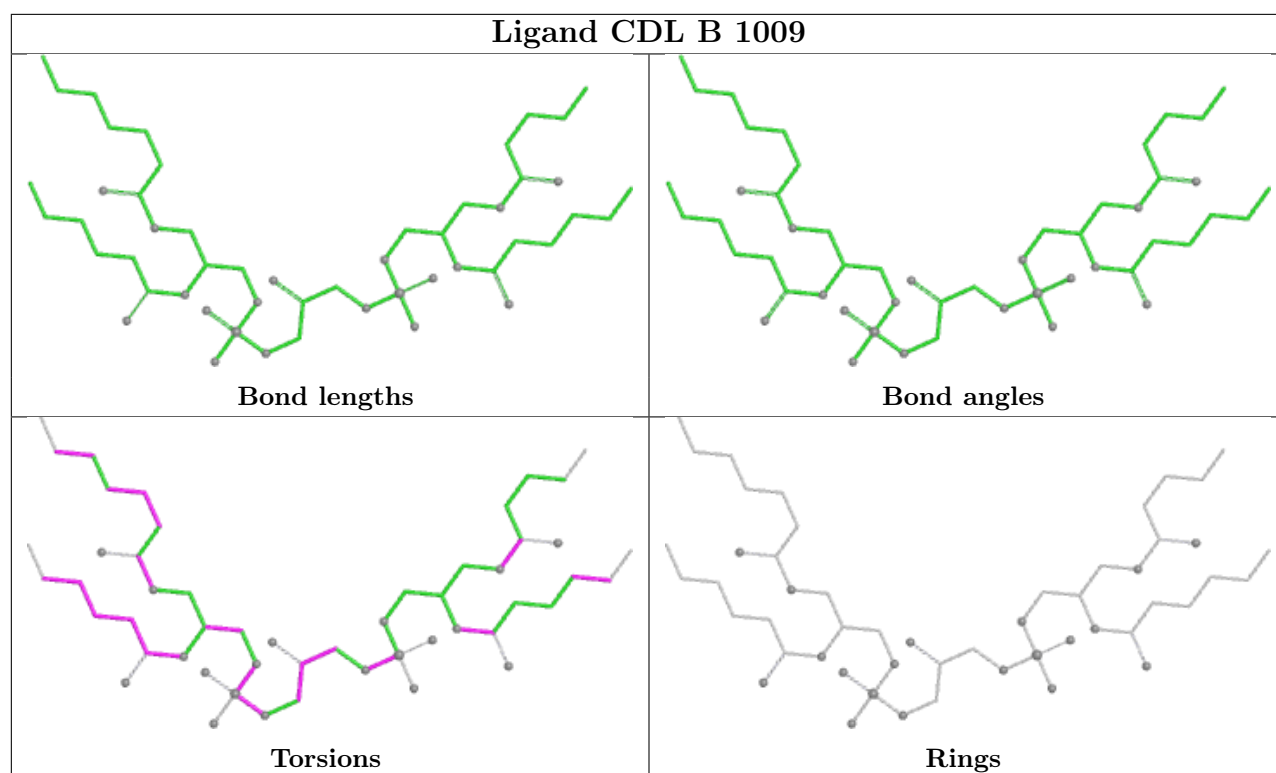


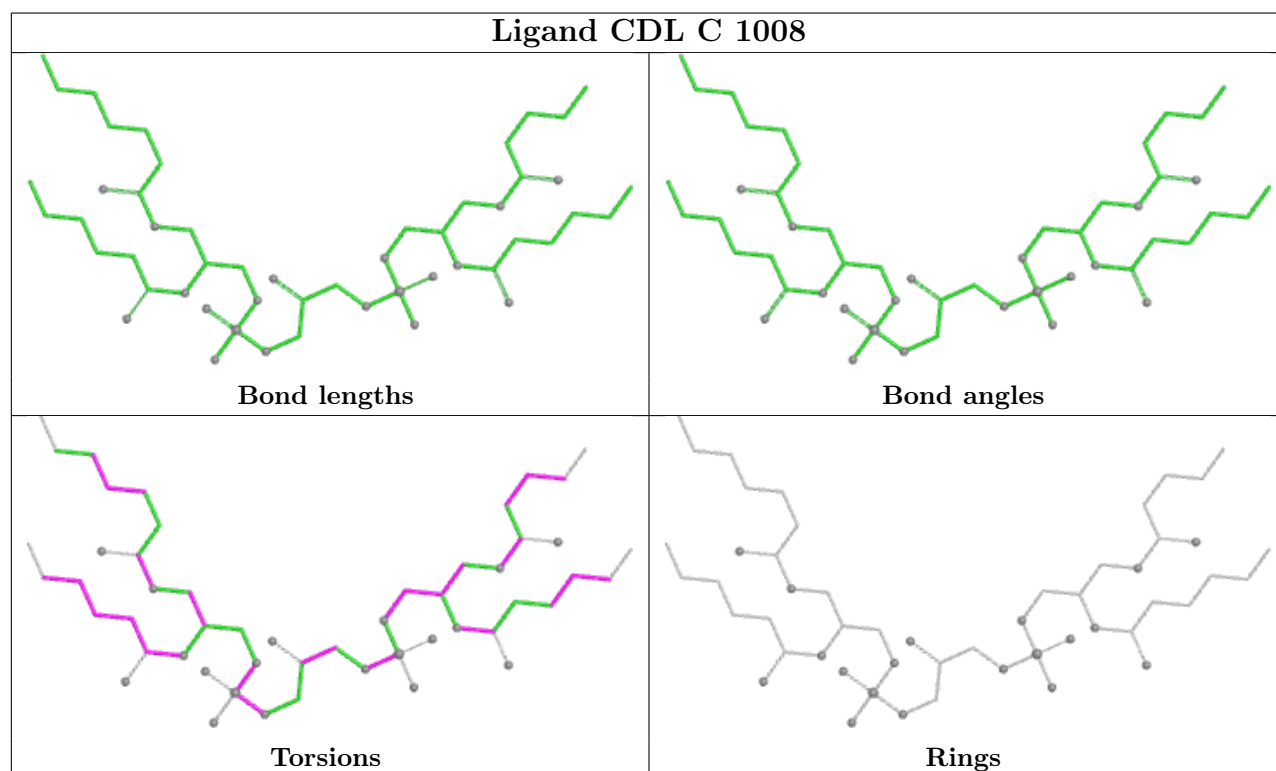
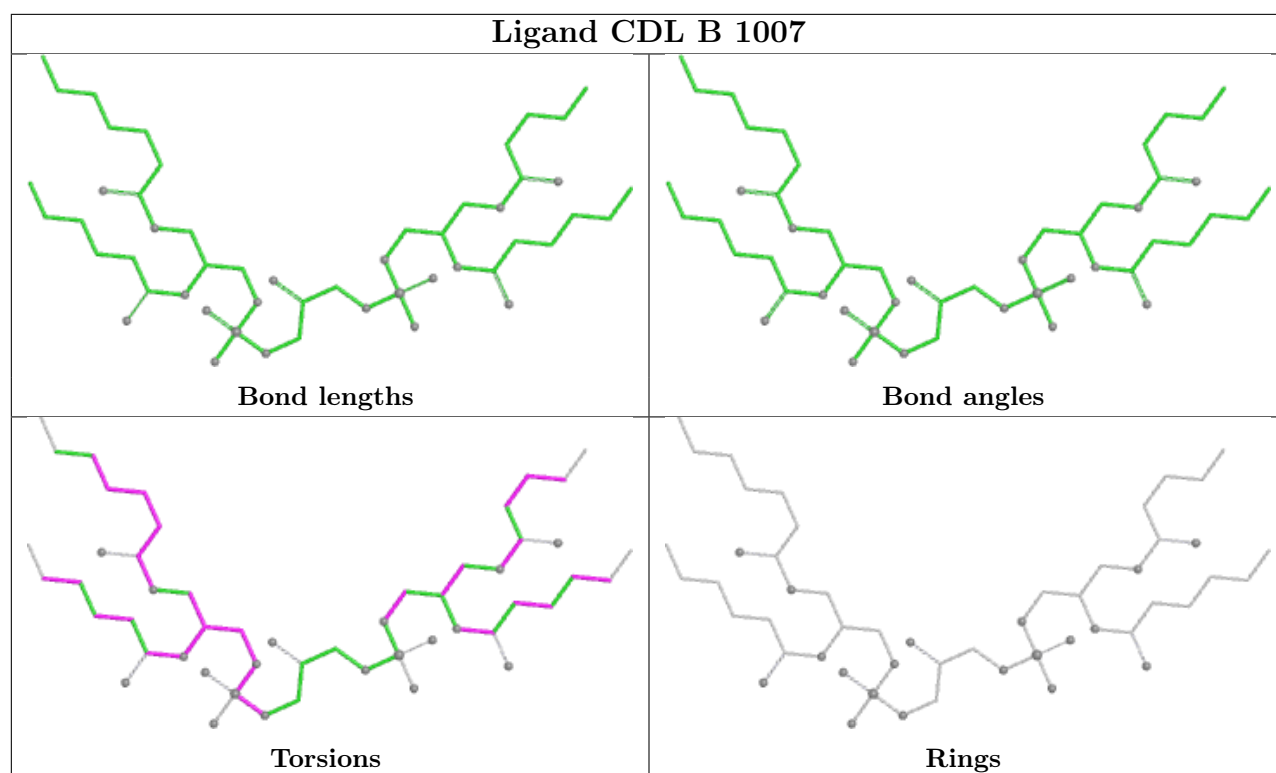


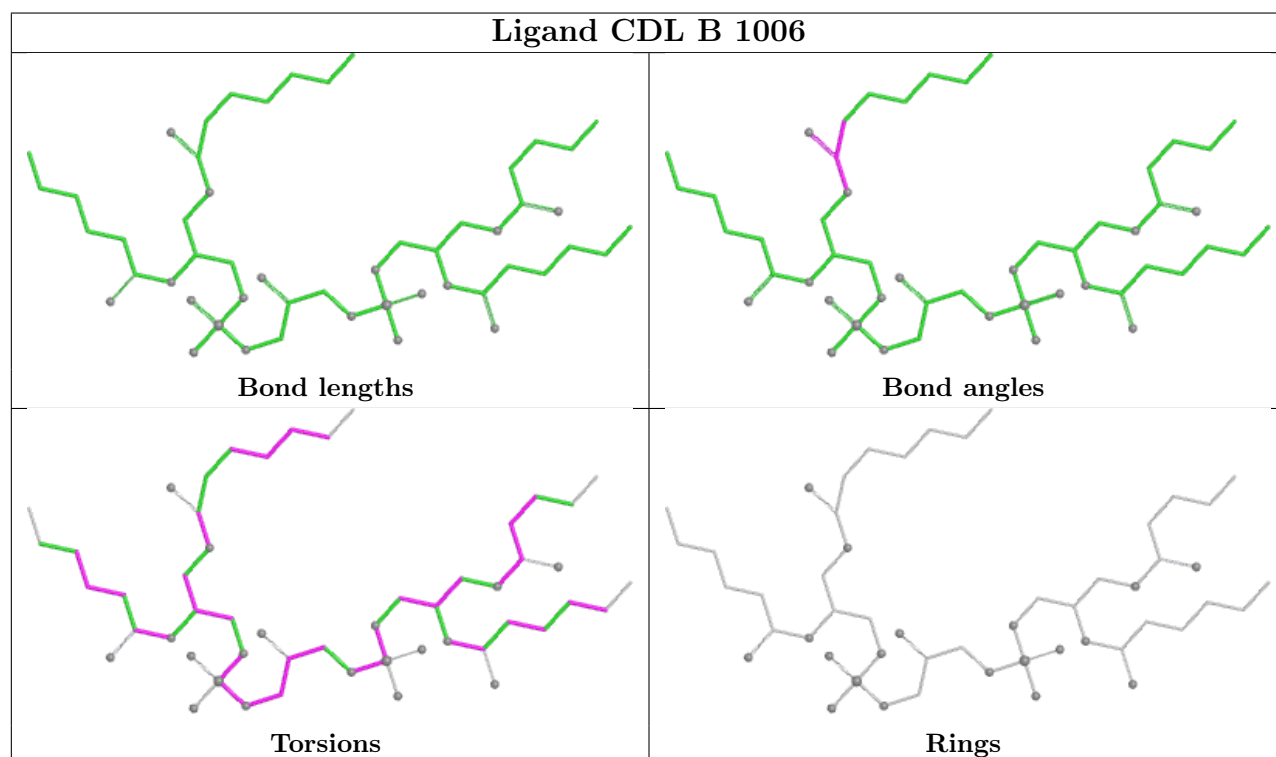
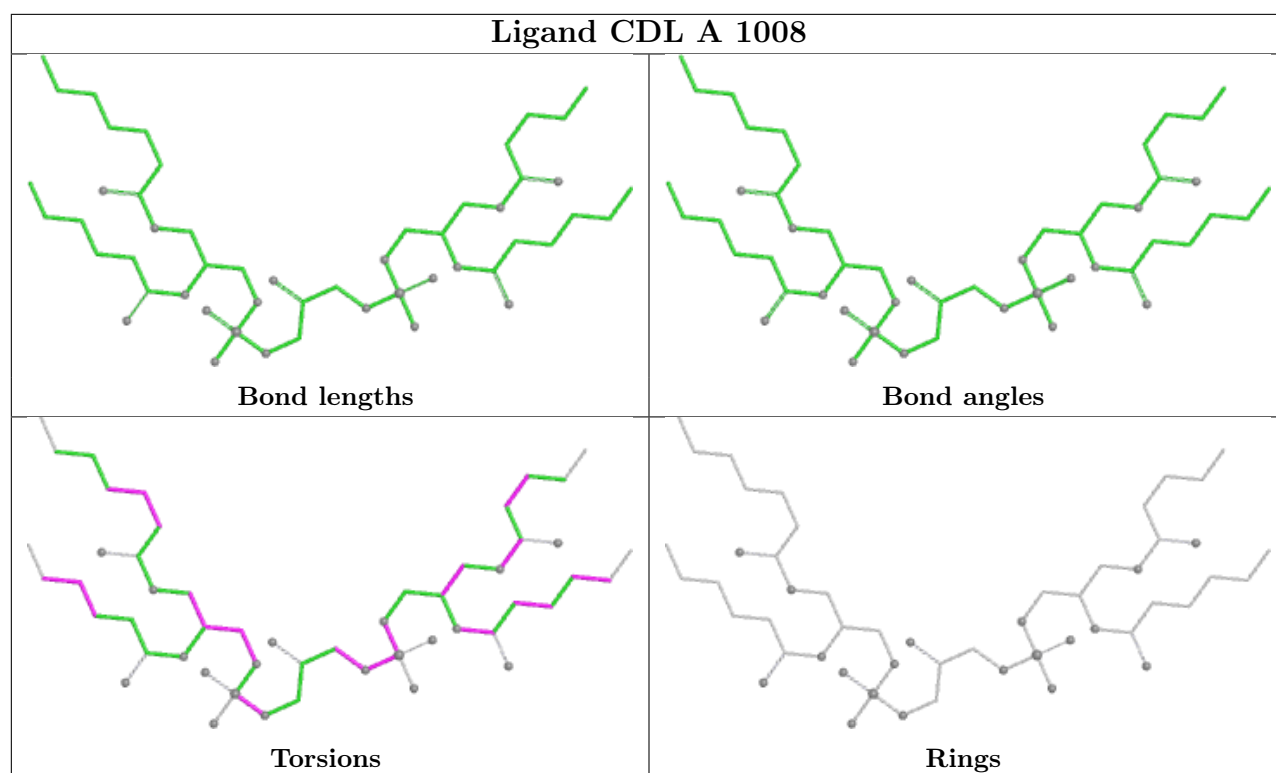


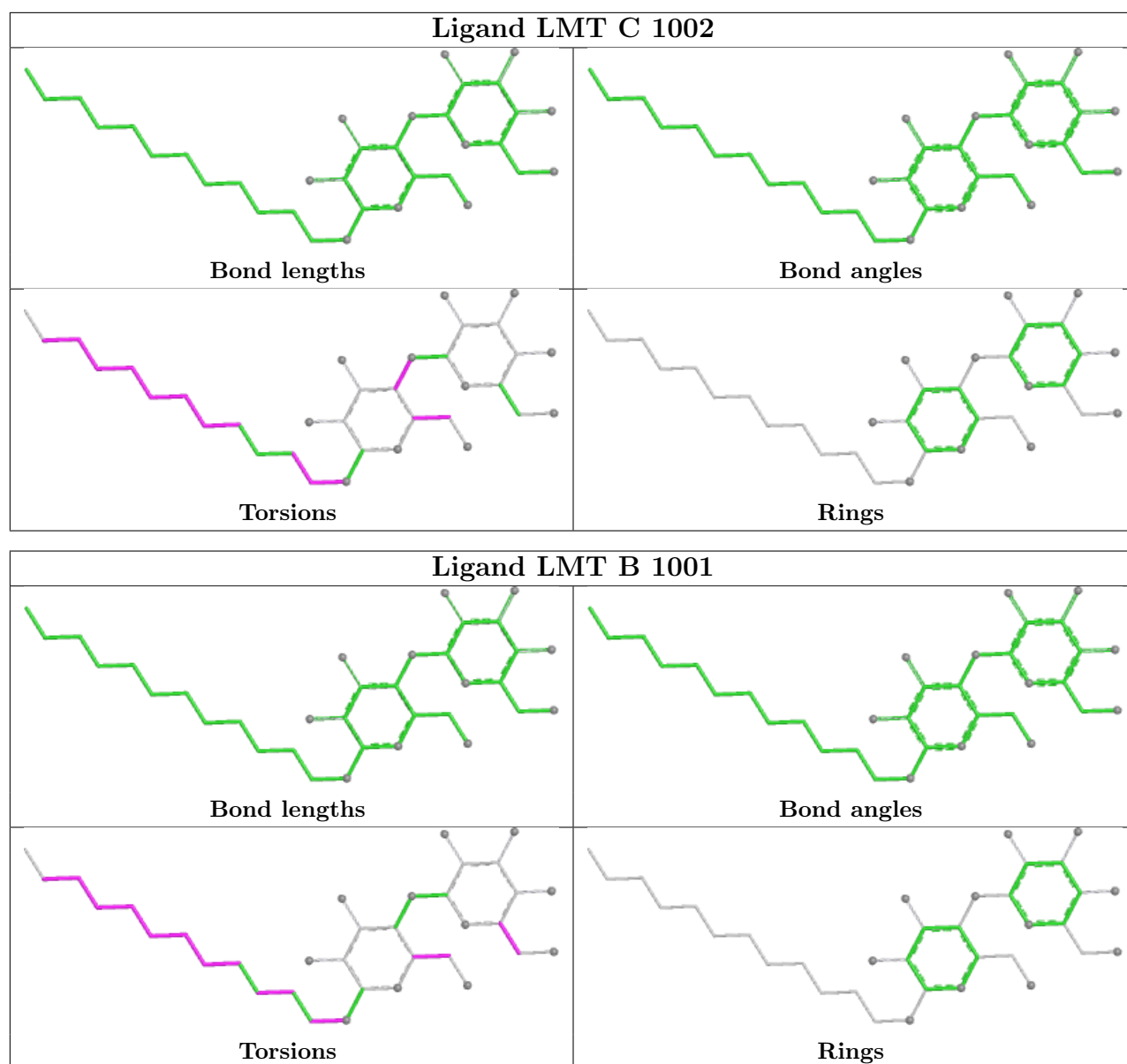


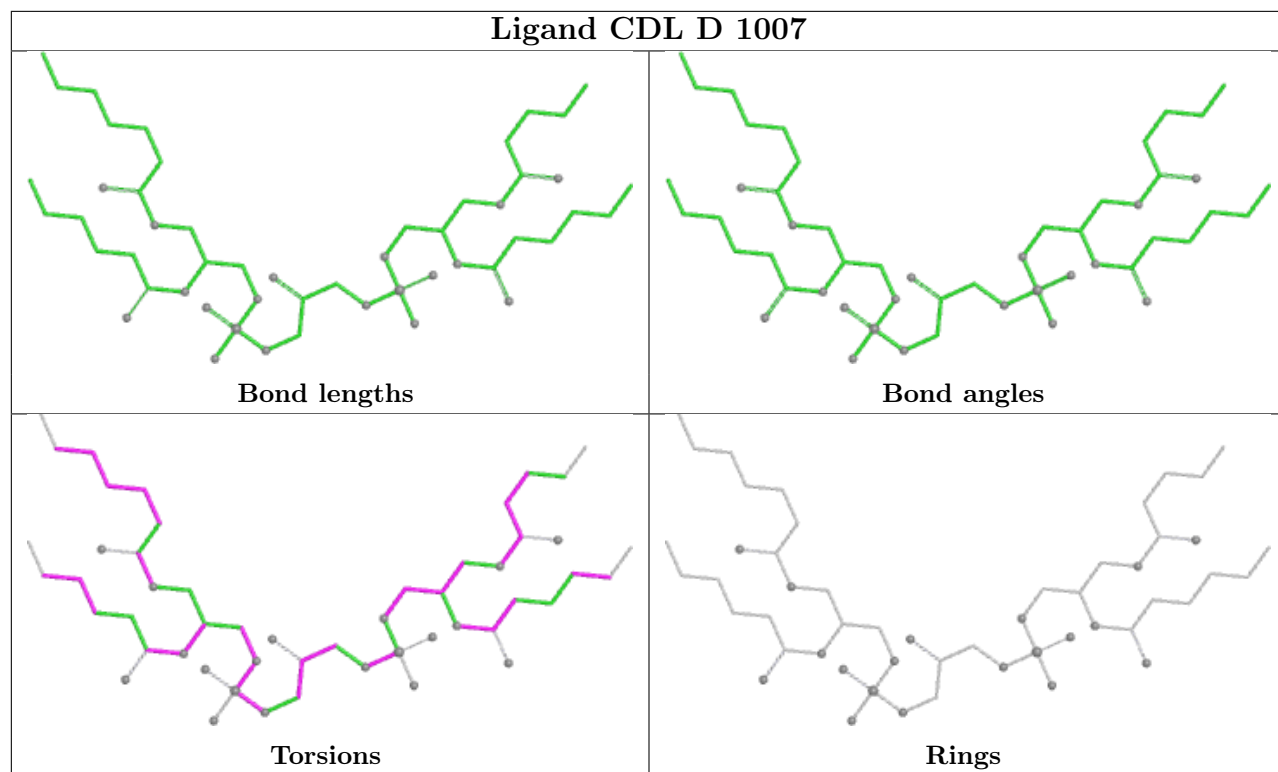


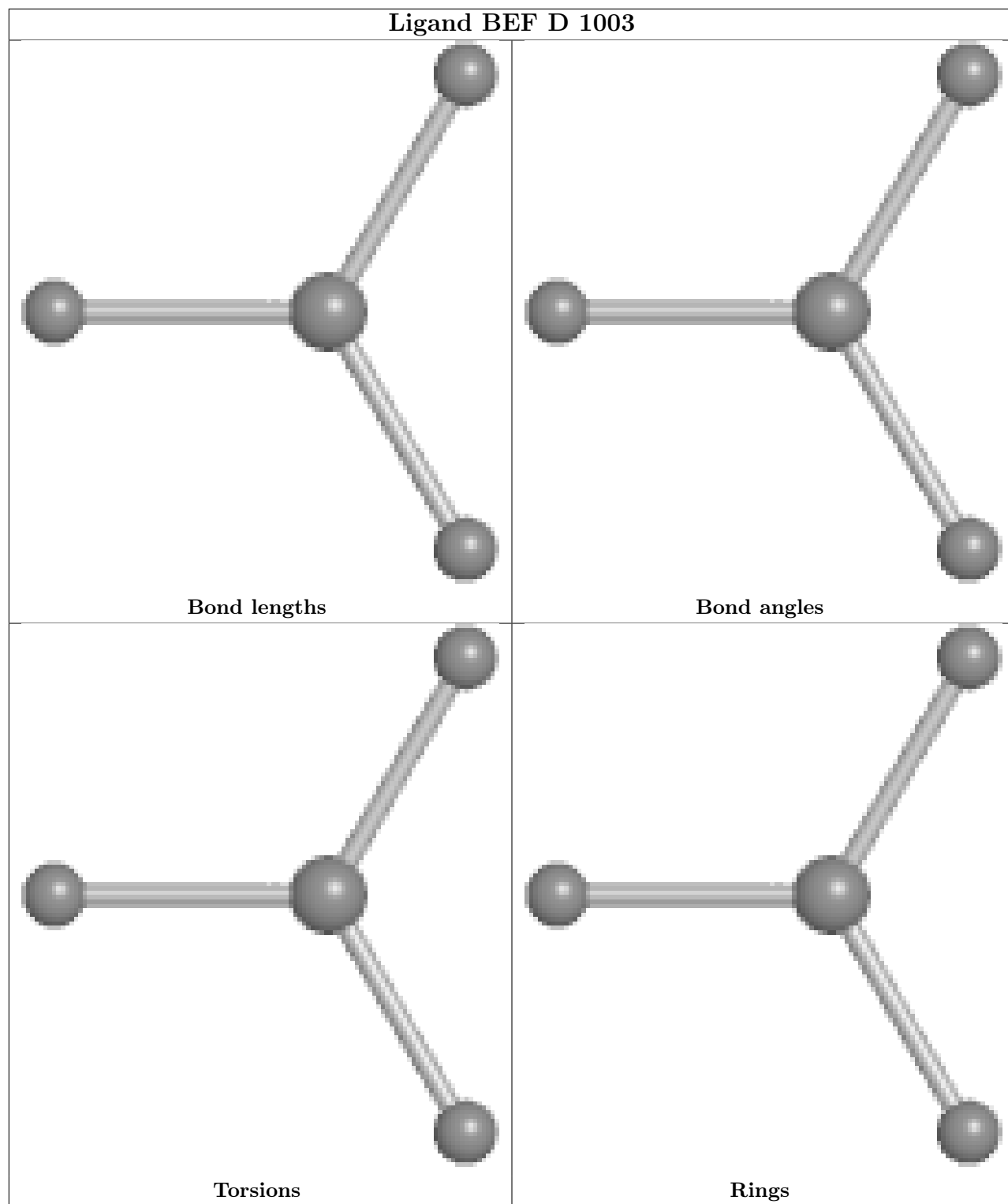


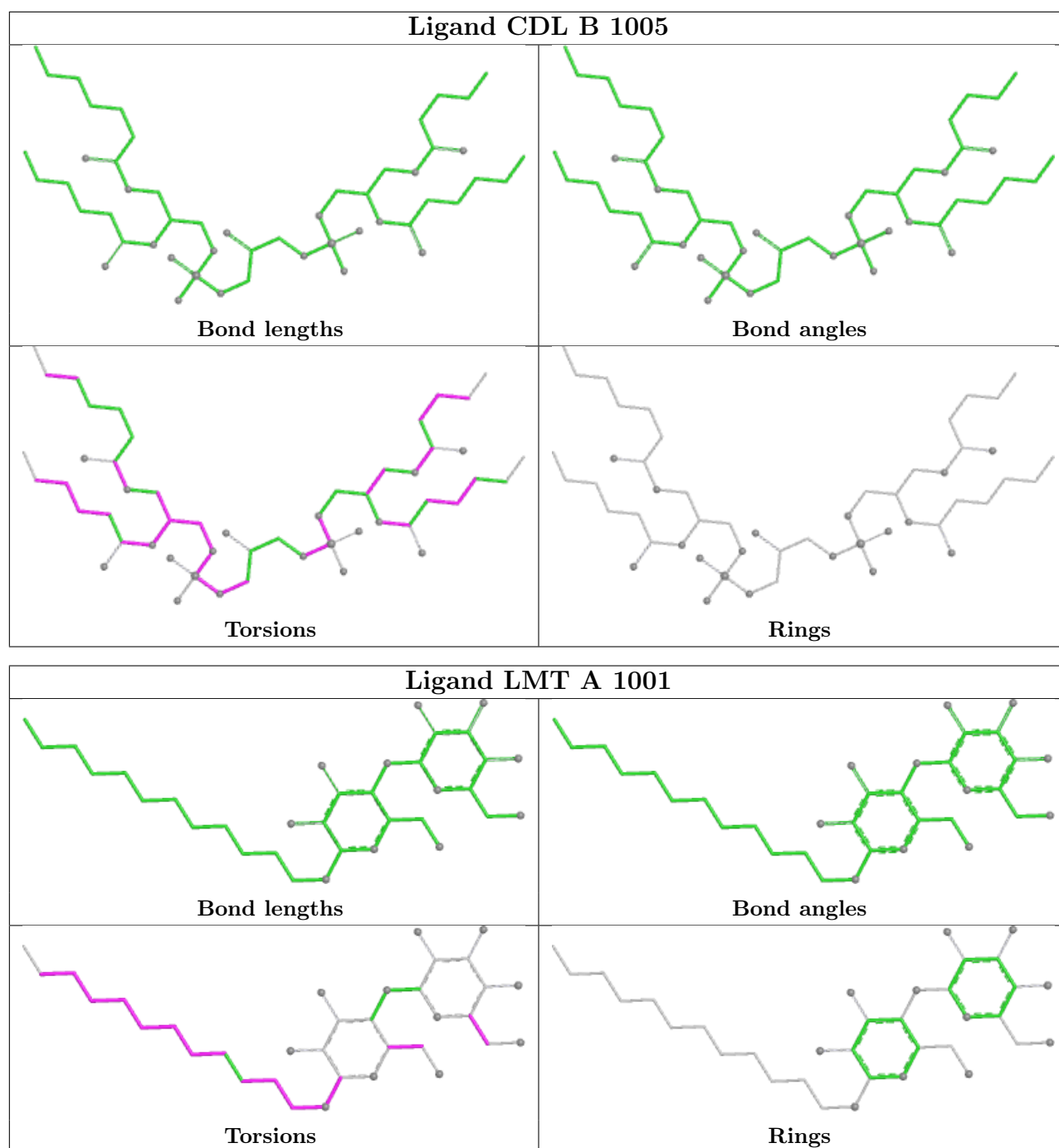












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

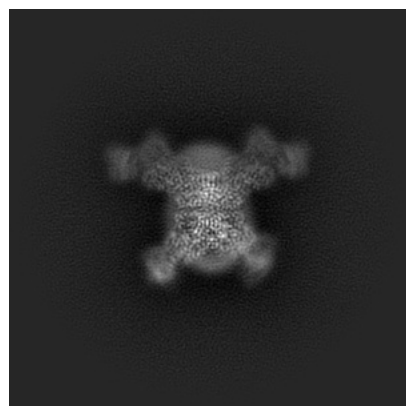
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72125. These allow visual inspection of the internal detail of the map and identification of artifacts.

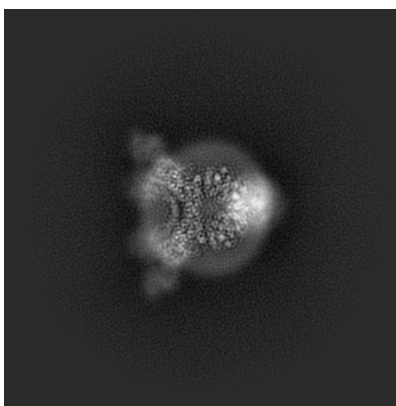
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

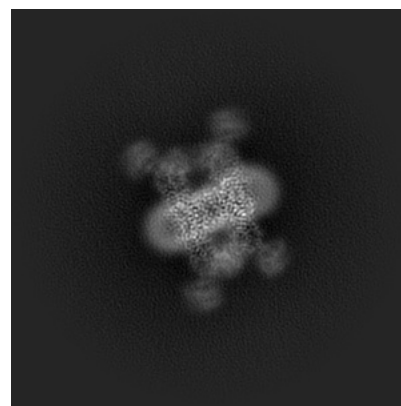
6.1.1 Primary map



X

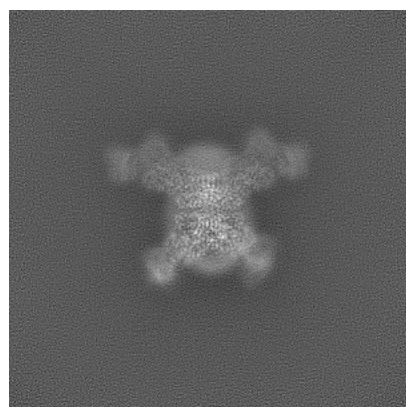


Y

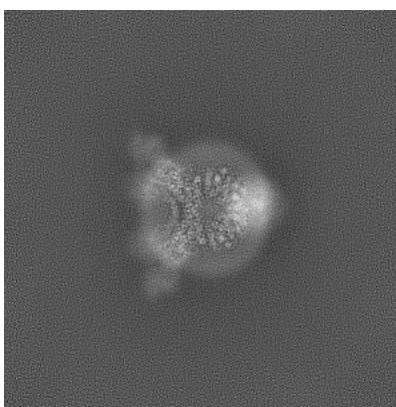


Z

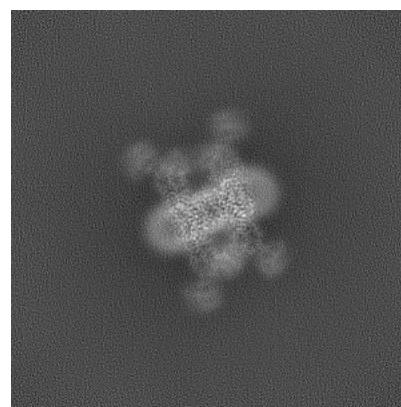
6.1.2 Raw map



X



Y

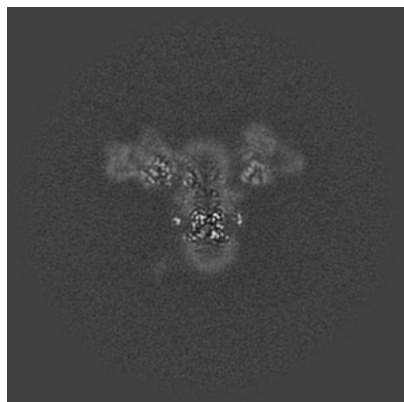


Z

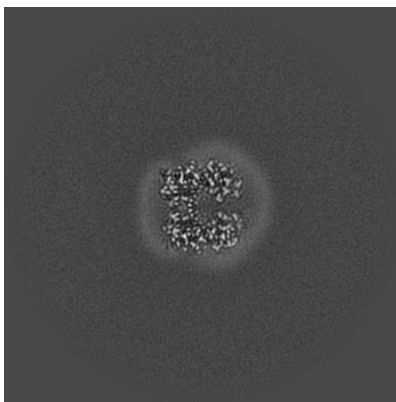
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

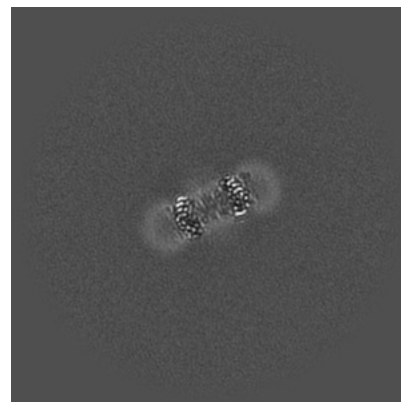
6.2.1 Primary map



X Index: 215

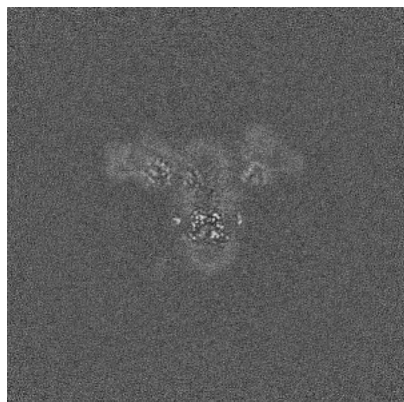


Y Index: 215

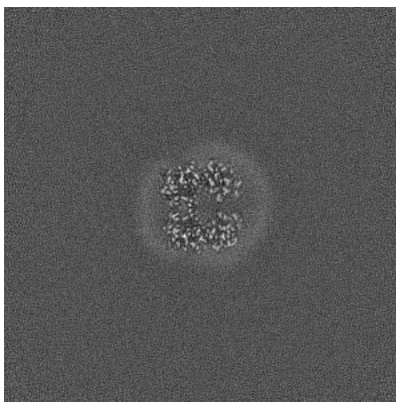


Z Index: 215

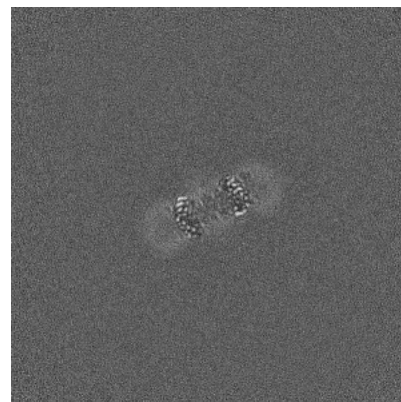
6.2.2 Raw map



X Index: 215



Y Index: 215

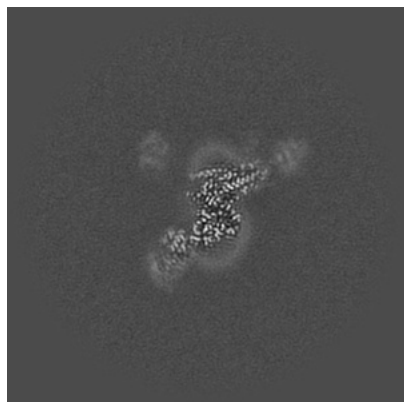


Z Index: 215

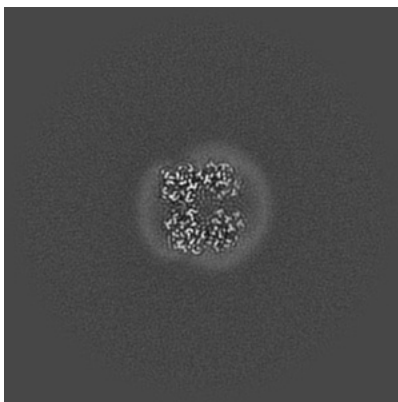
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

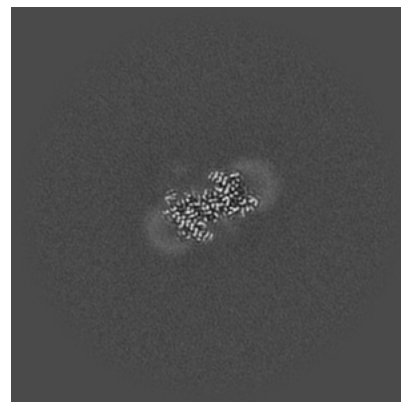
6.3.1 Primary map



X Index: 240

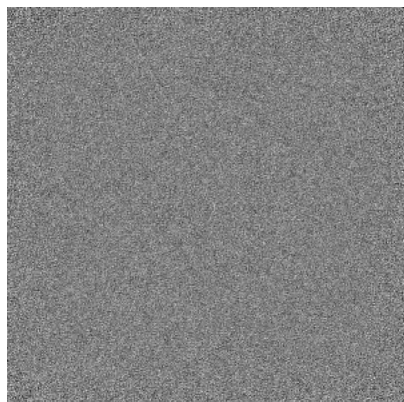


Y Index: 213

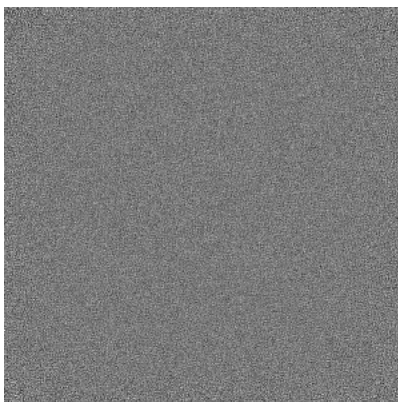


Z Index: 200

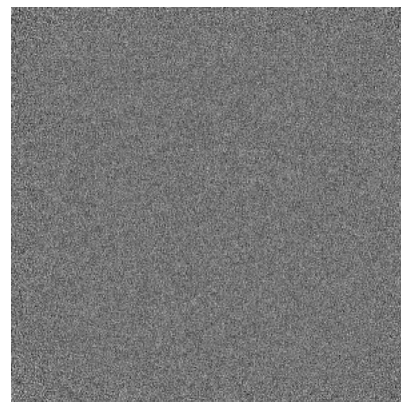
6.3.2 Raw map



X Index: 0



Y Index: 0

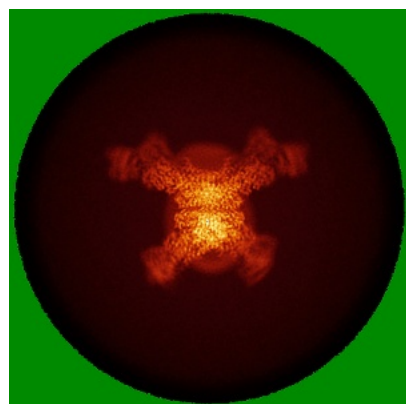


Z Index: 0

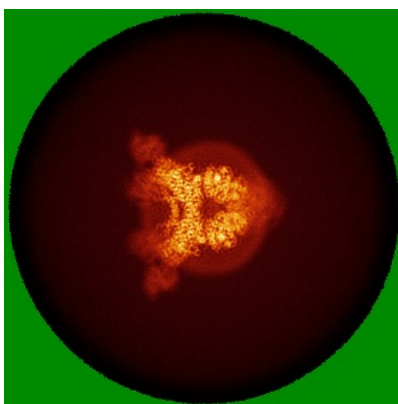
The images above show the largest variance slices of the map in three orthogonal directions.

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

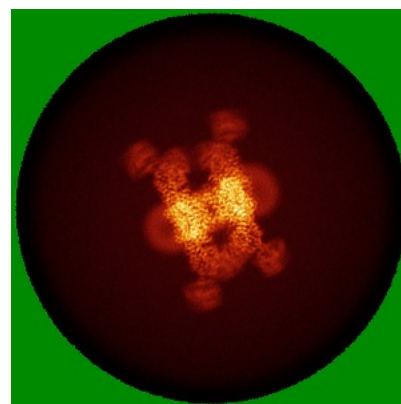
6.4.1 Primary map



X

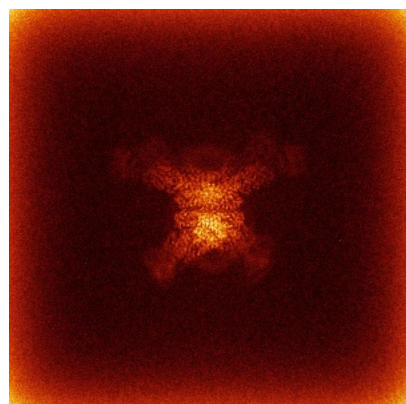


Y

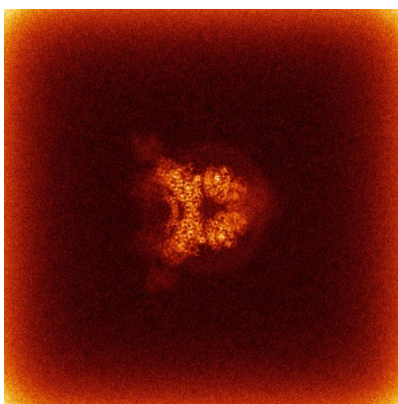


Z

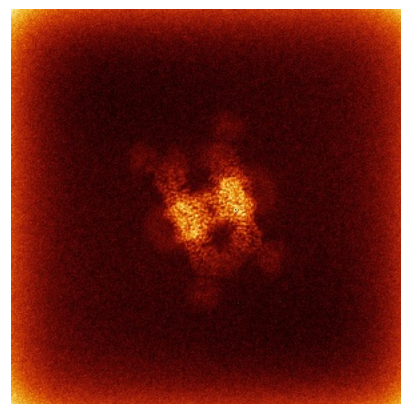
6.4.2 Raw map



X



Y

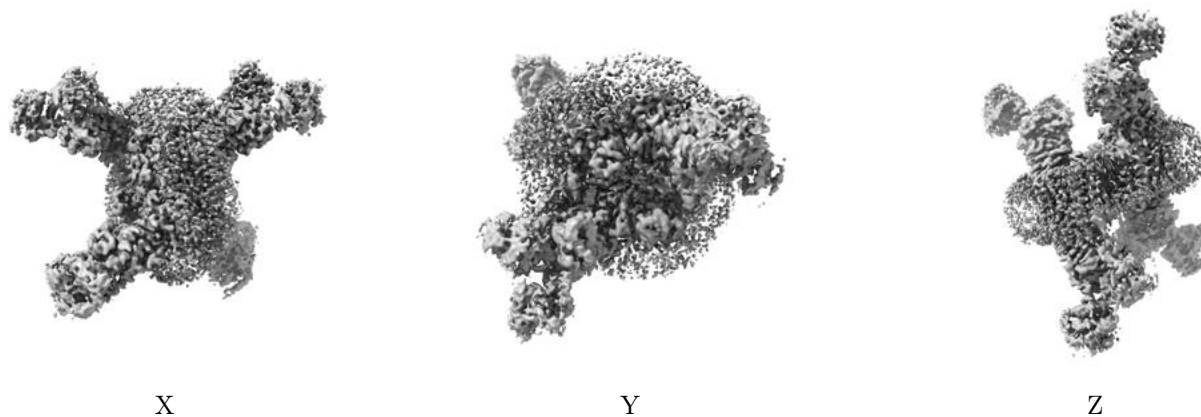


Z

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

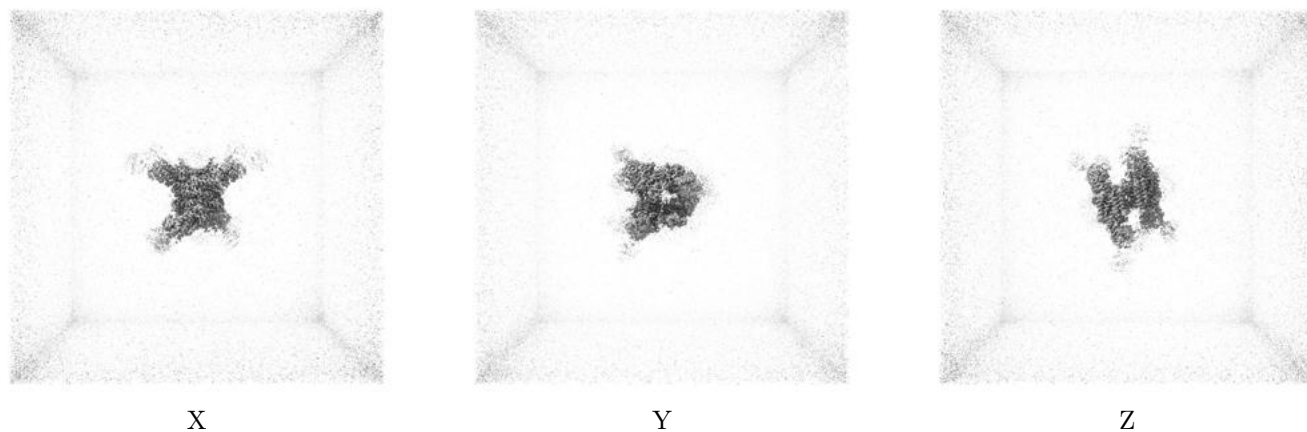
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.113. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

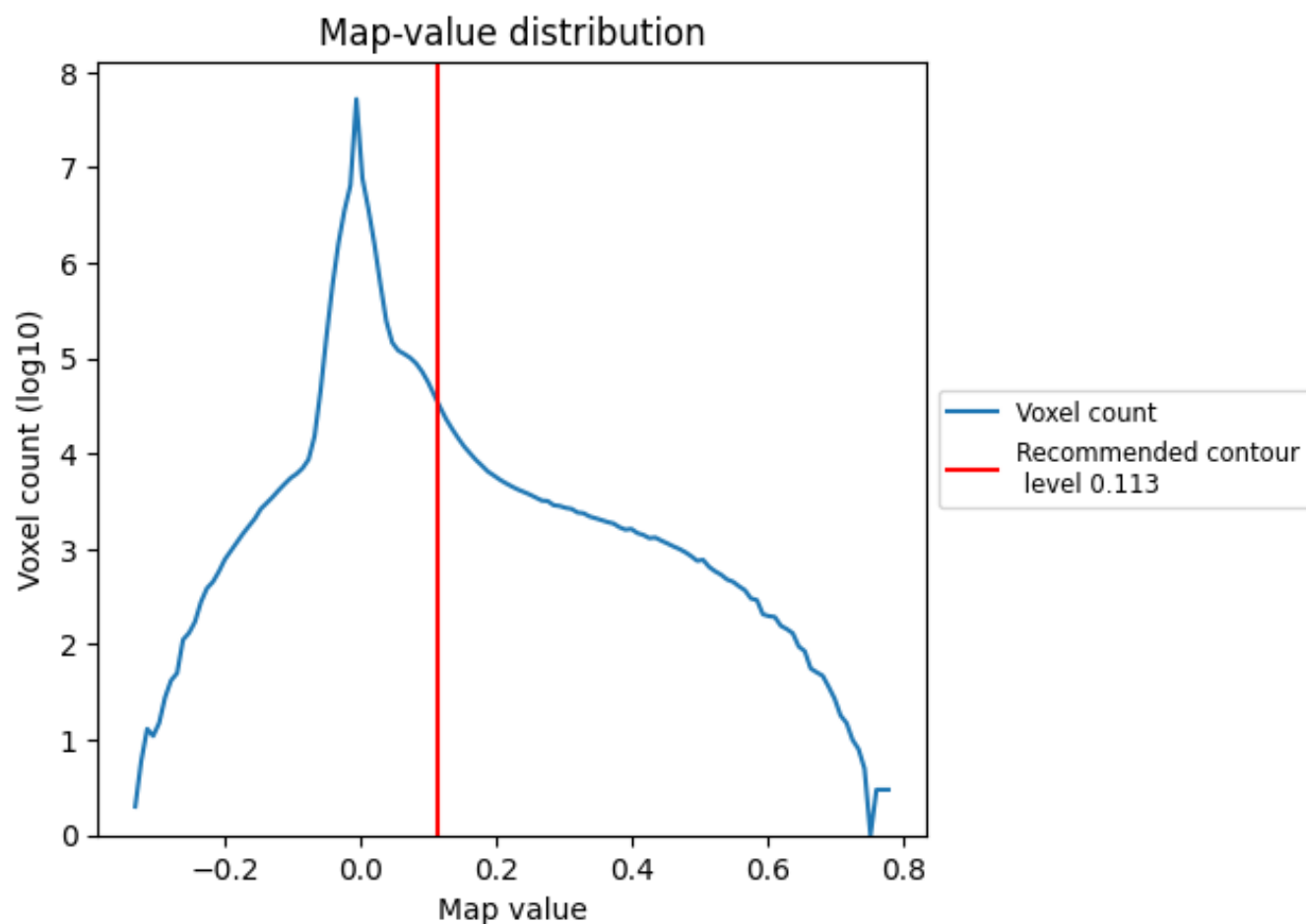
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

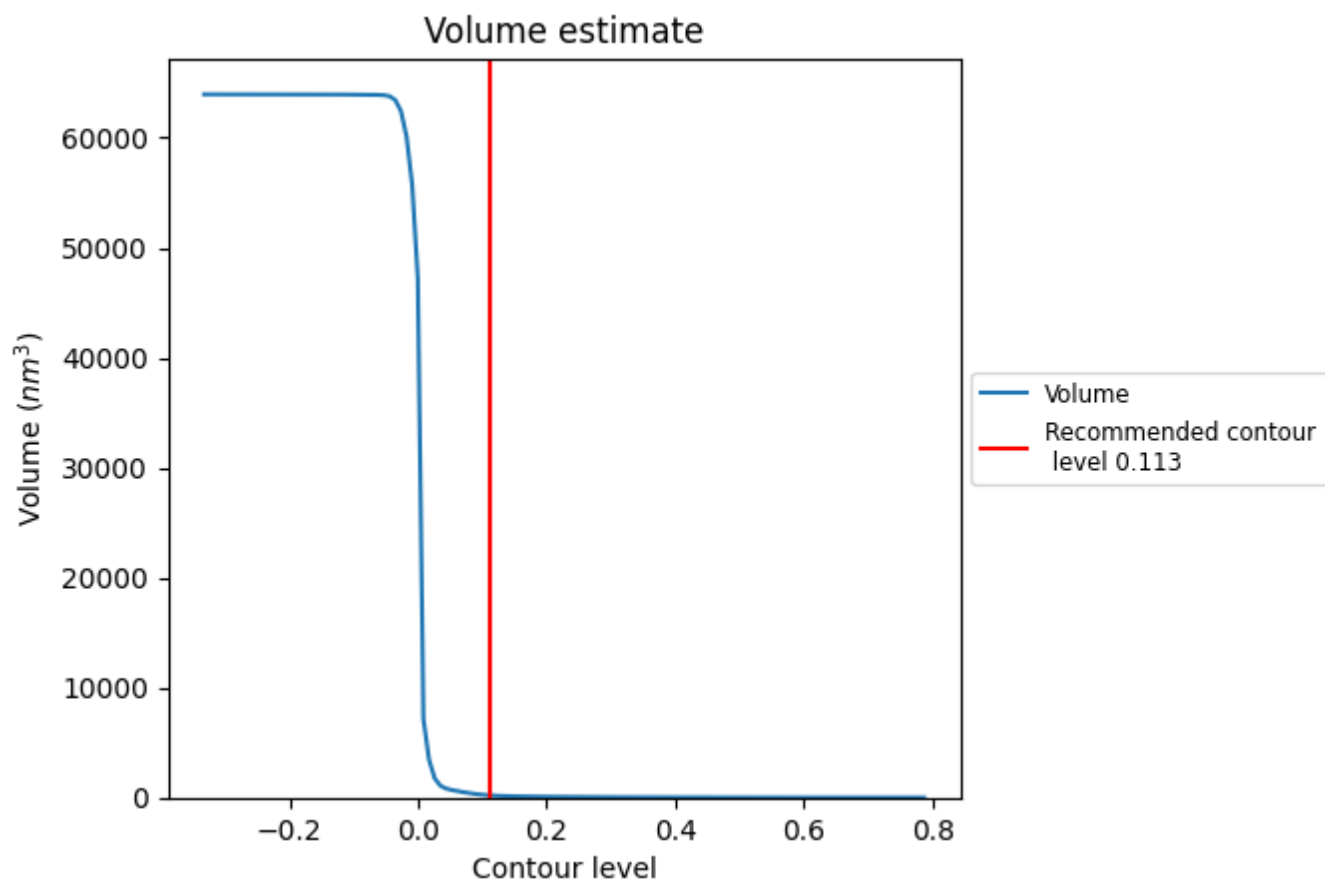
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

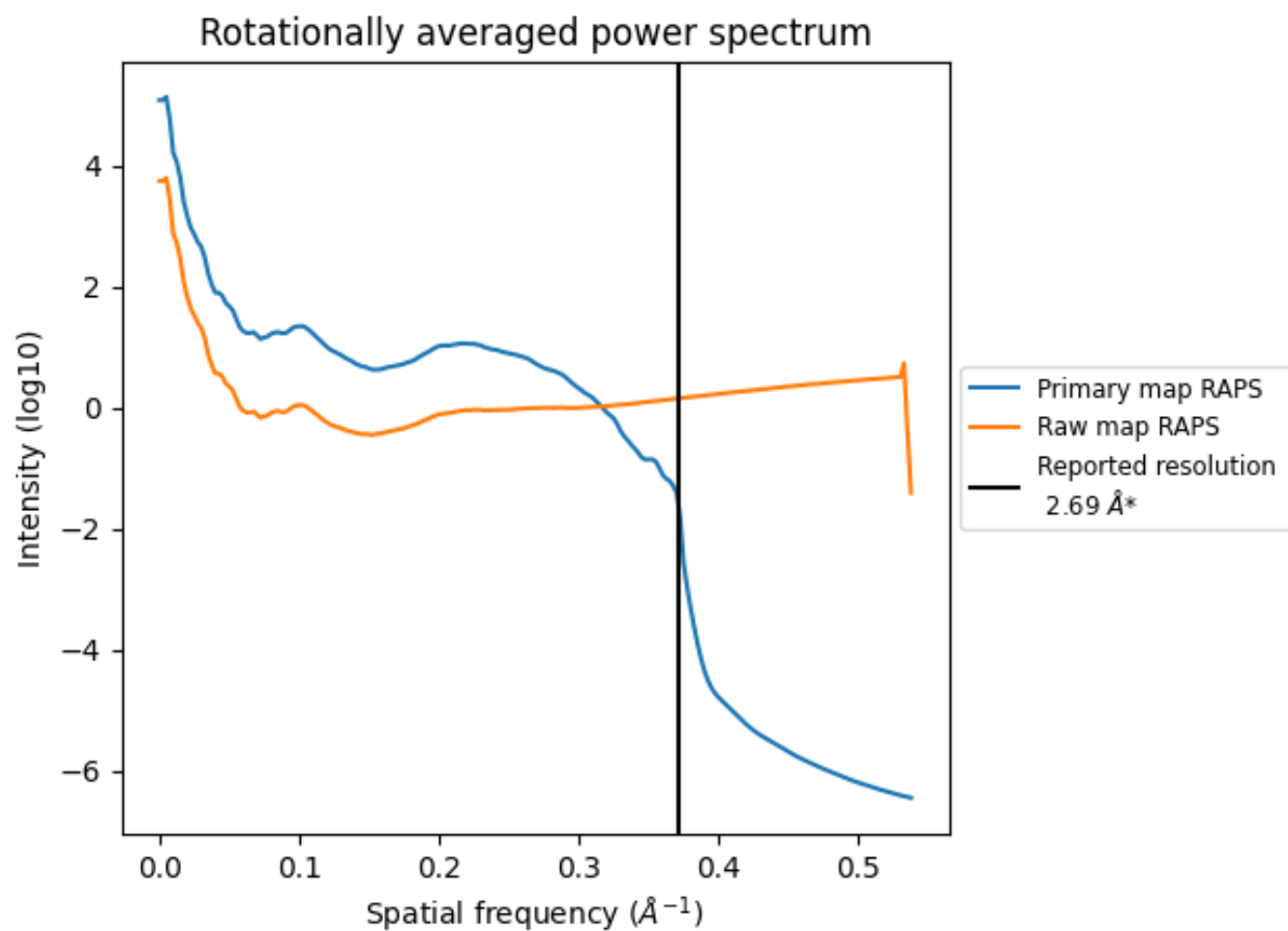
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 194 nm³; this corresponds to an approximate mass of 175 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 ⓘ

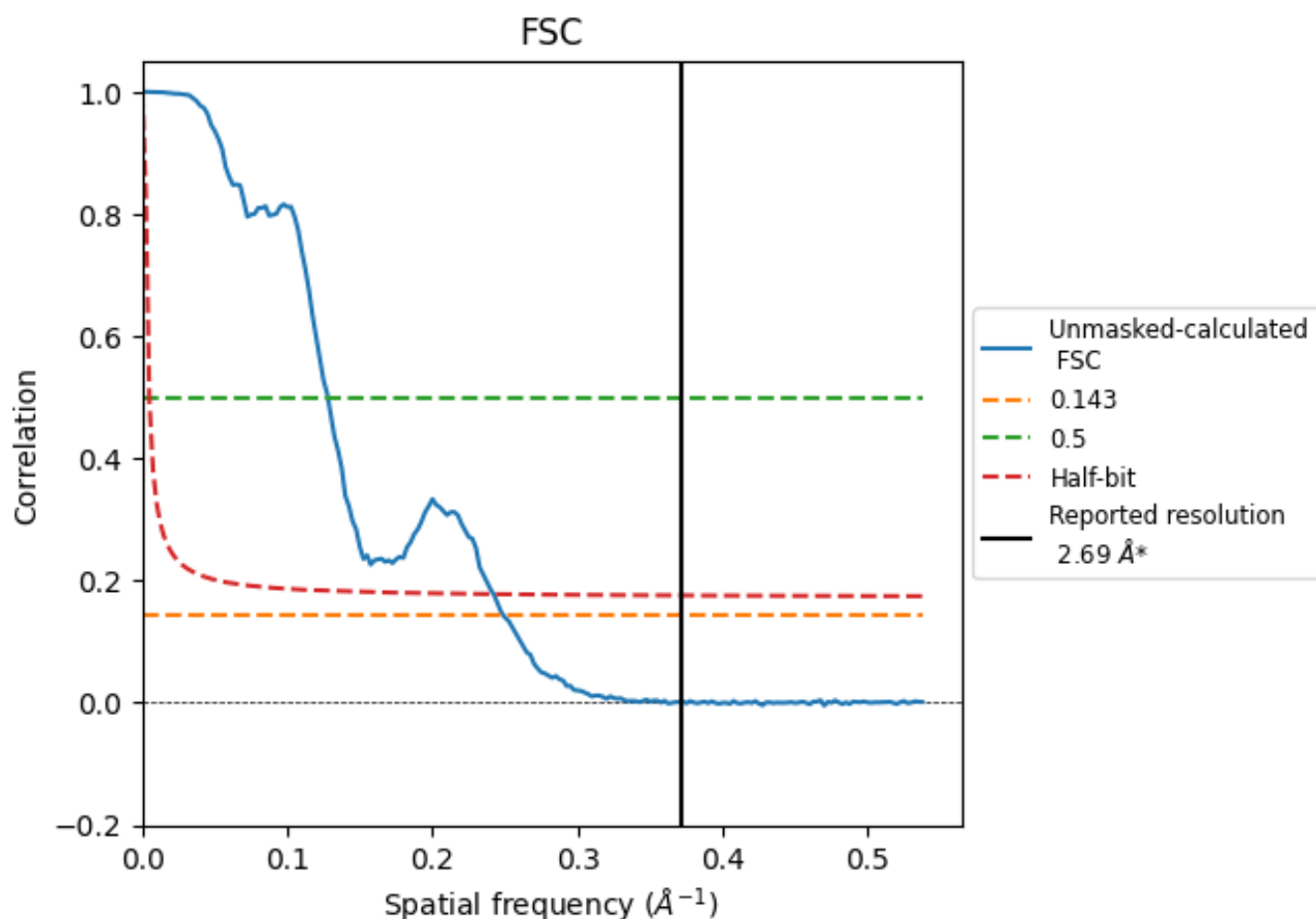


*Reported resolution corresponds to spatial frequency of 0.372 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.372 Å⁻¹

8.2 Resolution estimates [i](#)

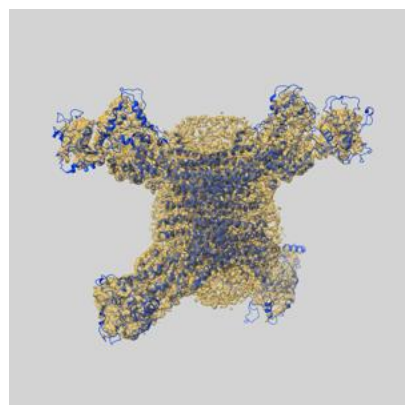
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	7.82	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 2.69 by more than 10 %

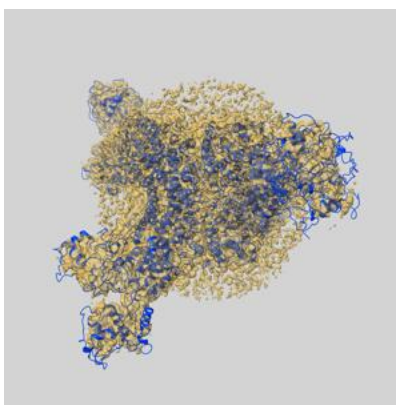
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72125 and PDB model 9Q1E. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

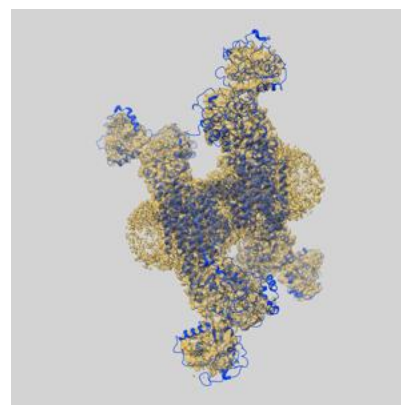
9.1 Map-model overlay [i](#)



X



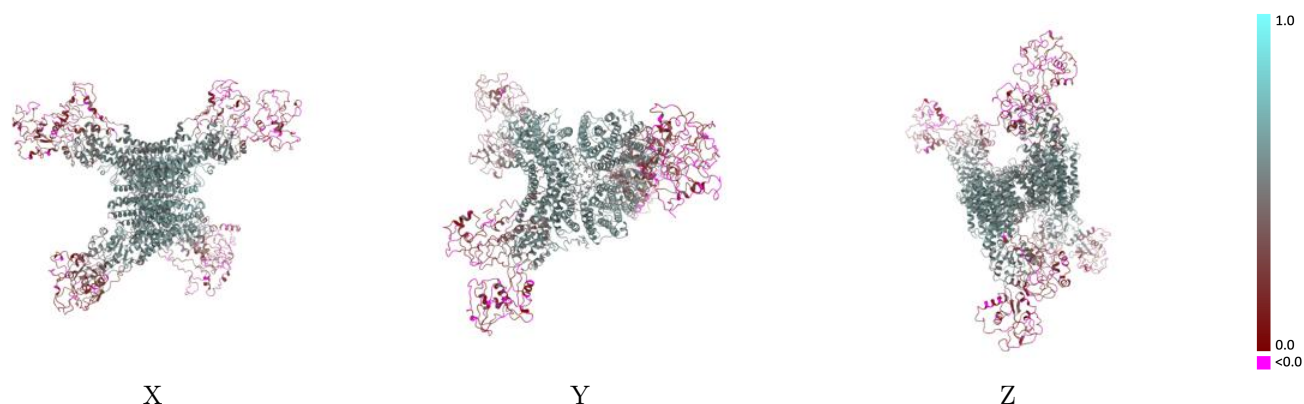
Y



Z

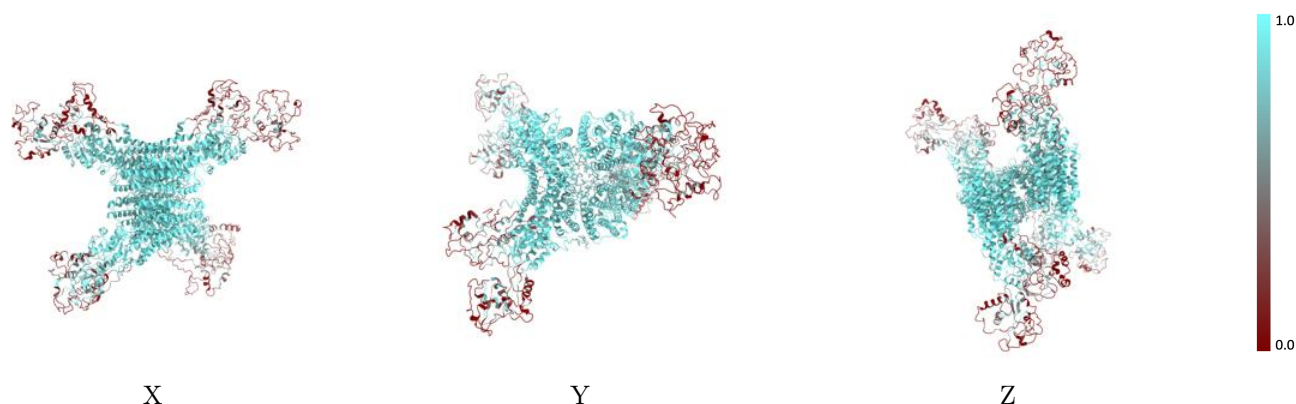
The images above show the 3D surface view of the map at the recommended contour level 0.113 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



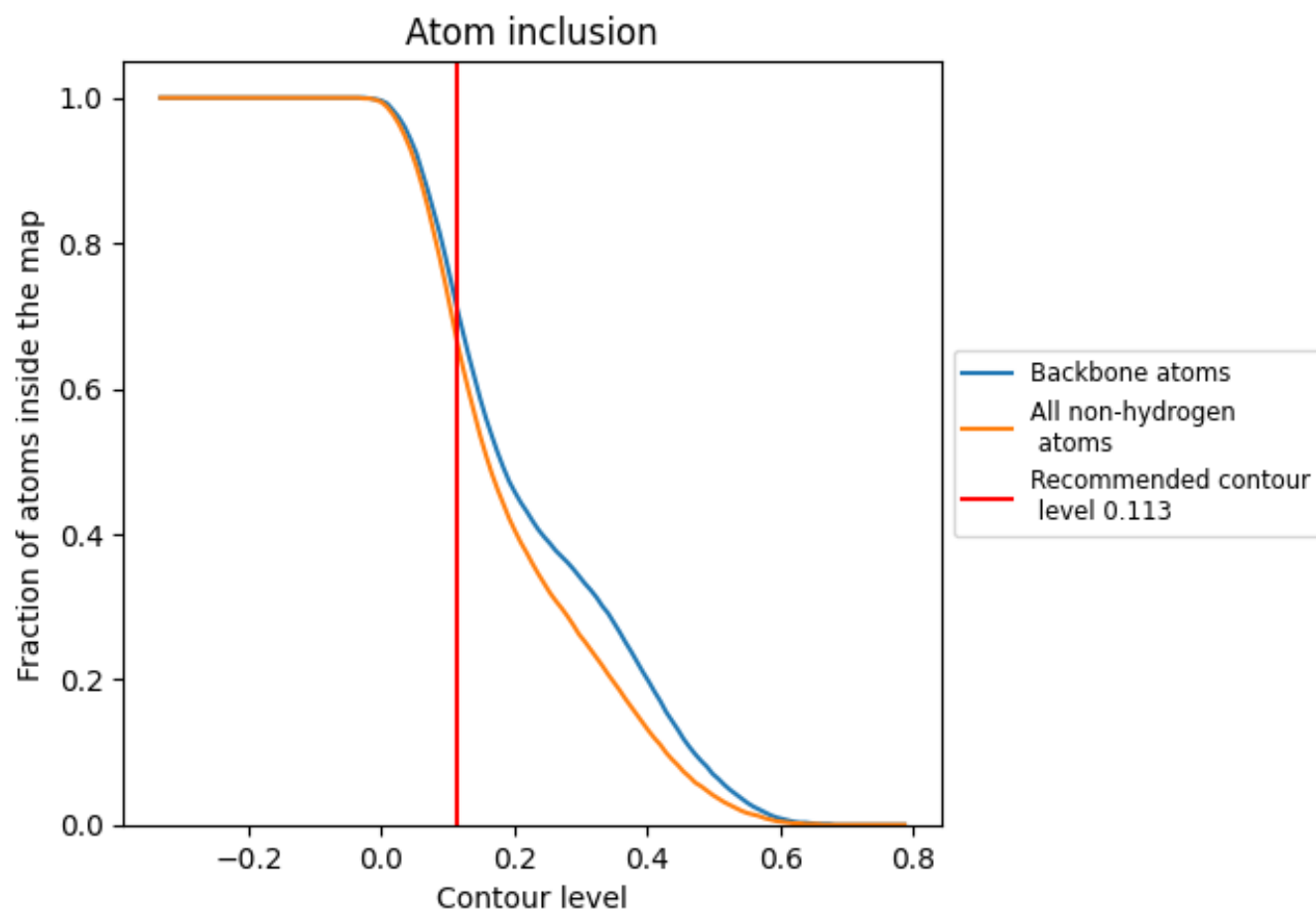
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.113).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 67% 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 (0.113) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6670	0.3950
A	0.6100	0.3650
B	0.6490	0.3910
C	0.7550	0.4420
D	0.6550	0.3790

