



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:11 am BST

PDB ID : 1E14
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH PHE M197 REPLACED WITH ARG (CHAIN M, FM197R) AND GLY M203 REPLACED WITH ASP (CHAIN M, GM203D)
Authors : Fyfe, P.K.; Ridge, J.P.; McAuley, K.E.; Cogdell, R.J.; Isaacs, N.W.; Jones, M.R.
Deposited on : 2000-04-18
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

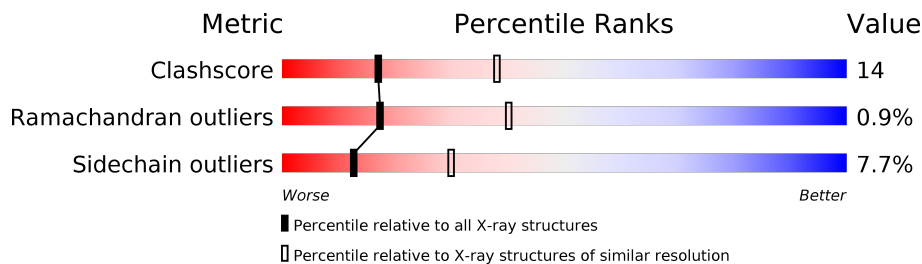
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	260	
2	L	281	
3	M	307	

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
5	BCL	M	1301	X	-	-	-
6	BPH	L	401	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7250 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	241	1830	1169	315	337	9	0	0	1

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	281	2232	1507	355	362	8	0	0	0

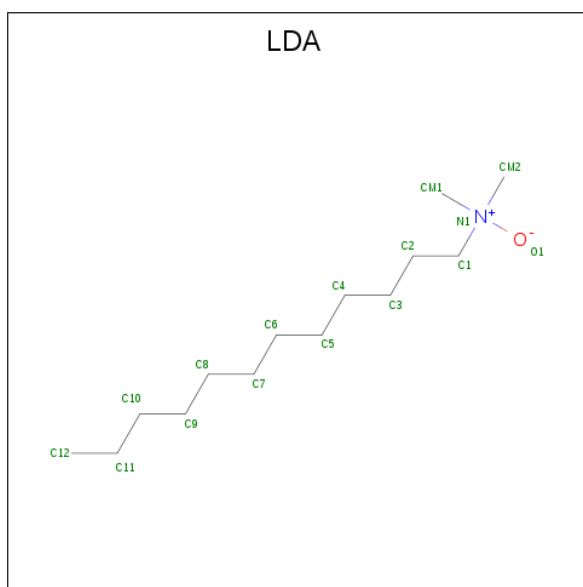
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2413	1606	398	399	10	0	0	1

There are 2 discrepancies between the modelled and reference sequences:

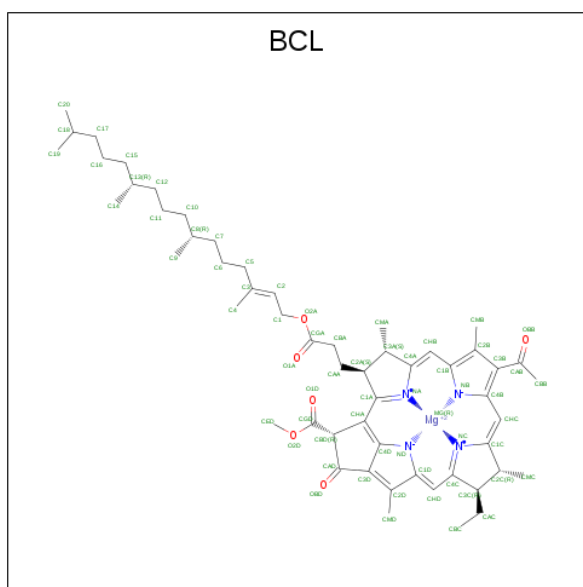
Chain	Residue	Modelled	Actual	Comment	Reference
M	197	ARG	PHE	conflict	UNP P0C0Y9
M	203	ASP	GLY	conflict	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



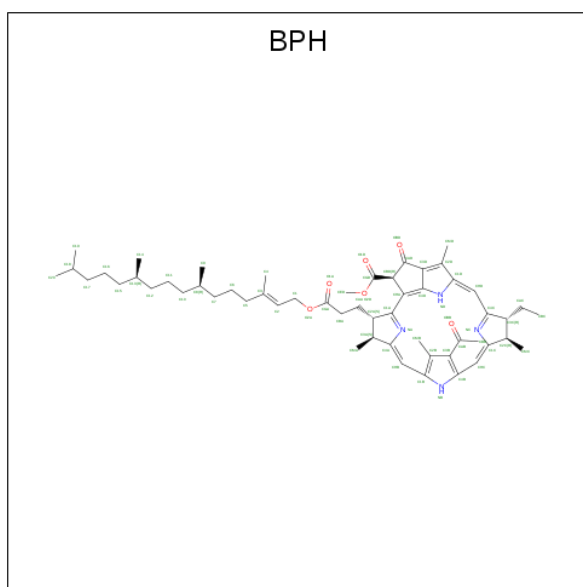
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

Continued on next page...

Continued from previous page...

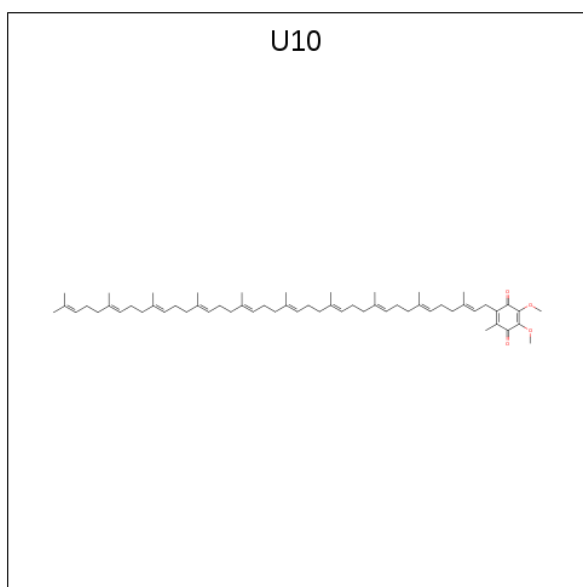
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

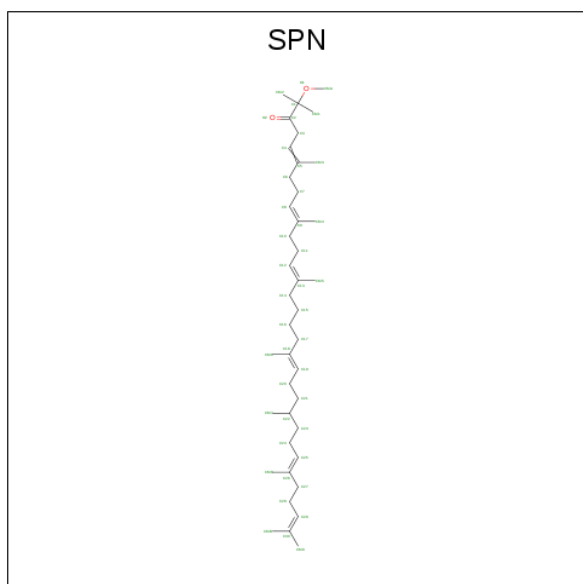


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	22	0
			48	44	4		
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

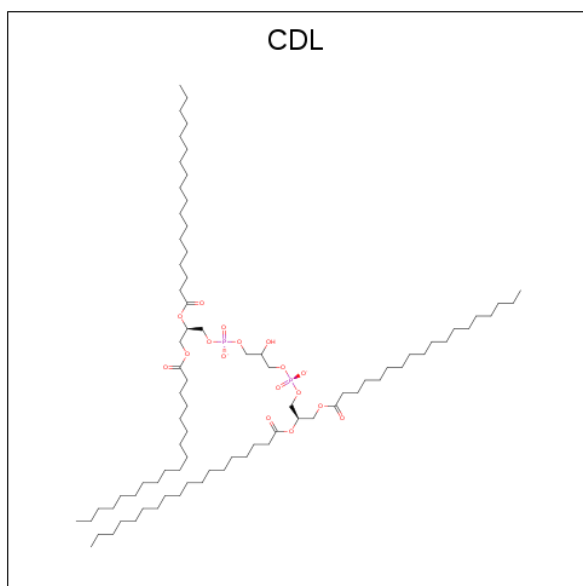
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is SPEROIDENONE (three-letter code: SPN) (formula: C₄₁H₇₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			43	41	2		

- Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	42	Total	O	0	0
			42	42		
11	L	28	Total	O	0	0
			28	28		
11	M	42	Total	O	0	0
			42	42		

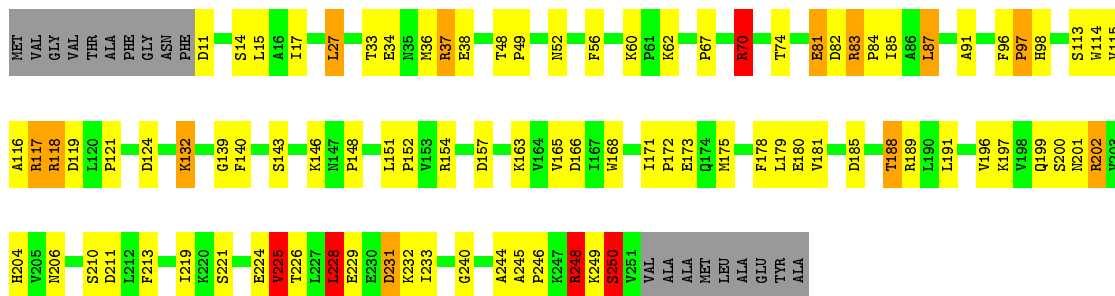
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

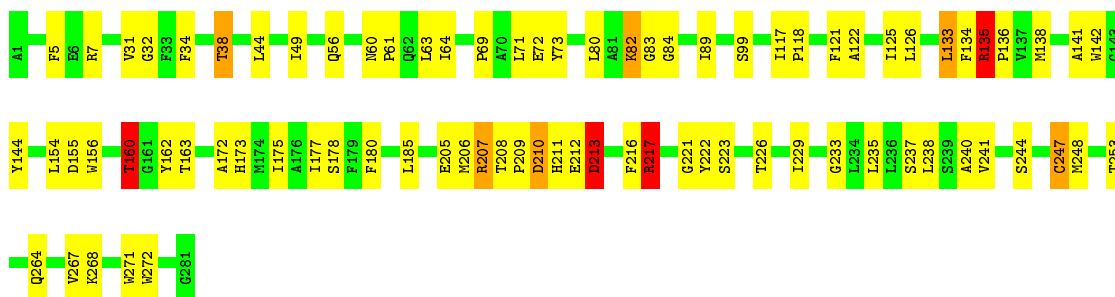
- Molecule 1: Reaction center protein H chain

Chain H: 



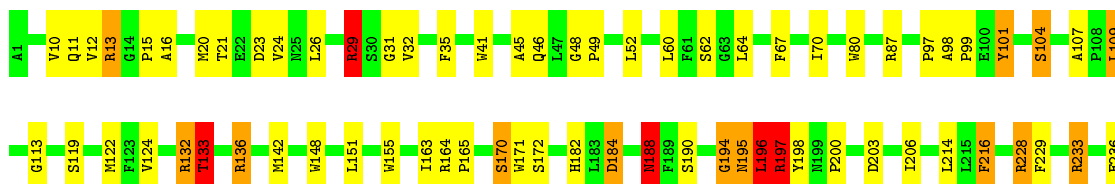
- Molecule 2: Reaction center protein L chain

Chain L: 



- Molecule 3: Reaction center protein M chain

Chain M: 





4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.00Å 140.00Å 184.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	92.6 (30.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7250	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

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: BCL, LDA, CDL, BPH, FE, SPN, U10

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	H	0.66	0/1878	1.75	30/2555 (1.2%)
2	L	0.63	0/2320	1.48	12/3175 (0.4%)
3	M	0.61	0/2504	1.56	36/3419 (1.1%)
All	All	0.63	0/6702	1.59	78/9149 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	7
2	L	0	5
3	M	0	2
All	All	0	14

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	70	ARG	NE-CZ-NH2	-21.92	109.34	120.30
3	M	247	ARG	NE-CZ-NH1	17.87	129.24	120.30
2	L	135	ARG	NE-CZ-NH1	16.24	128.42	120.30
2	L	135	ARG	CD-NE-CZ	15.24	144.93	123.60
2	L	135	ARG	NE-CZ-NH2	-14.98	112.81	120.30
1	H	117	ARG	NE-CZ-NH2	-14.97	112.82	120.30
1	H	37	ARG	NE-CZ-NH1	-14.23	113.18	120.30
3	M	132	ARG	NE-CZ-NH1	-14.16	113.22	120.30
2	L	217	ARG	NE-CZ-NH1	14.12	127.36	120.30
3	M	241	ARG	NE-CZ-NH2	-13.14	113.73	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	202	ARG	NE-CZ-NH1	11.98	126.29	120.30
1	H	118	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	H	70	ARG	NE-CZ-NH1	11.11	125.85	120.30
1	H	83	ARG	CD-NE-CZ	11.06	139.08	123.60
2	L	217	ARG	CD-NE-CZ	10.66	138.53	123.60
3	M	241	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	H	70	ARG	CD-NE-CZ	10.20	137.88	123.60
3	M	29	ARG	NE-CZ-NH2	-10.11	115.25	120.30
3	M	13	ARG	NE-CZ-NH2	-9.97	115.32	120.30
2	L	155	ASP	CB-CG-OD2	-9.91	109.38	118.30
3	M	198	TYR	CB-CG-CD2	9.38	126.63	121.00
1	H	117	ARG	CD-NE-CZ	8.52	135.52	123.60
3	M	253	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	H	189	ARG	CD-NE-CZ	8.27	135.18	123.60
1	H	224	GLU	OE1-CD-OE2	8.22	133.17	123.30
3	M	247	ARG	CD-NE-CZ	8.17	135.03	123.60
1	H	211	ASP	CB-CG-OD2	-8.06	111.04	118.30
3	M	241	ARG	CD-NE-CZ	8.02	134.83	123.60
3	M	136	ARG	NE-CZ-NH1	7.80	124.20	120.30
2	L	213	ASP	CB-CG-OD2	7.72	125.25	118.30
3	M	247	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	H	37	ARG	NE-CZ-NH2	7.54	124.07	120.30
3	M	188	ASN	OD1-CG-ND2	7.39	138.89	121.90
2	L	31	VAL	CA-C-N	7.36	130.93	116.20
3	M	136	ARG	NE-CZ-NH2	7.27	123.93	120.30
3	M	132	ARG	NE-CZ-NH2	7.21	123.91	120.30
3	M	198	TYR	CG-CD1-CE1	7.09	126.97	121.30
3	M	228	ARG	NE-CZ-NH1	-6.97	116.82	120.30
3	M	136	ARG	NH1-CZ-NH2	-6.86	111.86	119.40
2	L	217	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	H	231	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	H	225	VAL	CB-CA-C	-6.44	99.16	111.40
1	H	228	LEU	CA-CB-CG	6.42	130.08	115.30
1	H	211	ASP	CB-CG-OD1	6.34	124.01	118.30
3	M	29	ARG	NE-CZ-NH1	6.33	123.46	120.30
3	M	23	ASP	CB-CG-OD2	-6.28	112.64	118.30
1	H	81	GLU	OE1-CD-OE2	6.19	130.73	123.30
3	M	253	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	L	31	VAL	C-N-CA	-6.11	109.47	122.30
1	H	163	LYS	CA-CB-CG	6.03	126.66	113.40
3	M	29	ARG	CD-NE-CZ	6.03	132.04	123.60
3	M	233	ARG	NE-CZ-NH2	-6.01	117.30	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	101	TYR	CB-CG-CD1	5.95	124.57	121.00
1	H	119	ASP	C-N-CA	5.92	136.50	121.70
3	M	246	GLU	CG-CD-OE2	-5.88	106.53	118.30
3	M	101	TYR	CB-CG-CD2	-5.71	117.57	121.00
3	M	133	THR	CA-CB-CG2	5.68	120.35	112.40
1	H	175	MET	CA-CB-CG	5.62	122.86	113.30
3	M	12	VAL	N-CA-CB	-5.61	99.15	111.50
3	M	236	GLU	OE1-CD-OE2	-5.61	116.57	123.30
3	M	87	ARG	NE-CZ-NH1	-5.58	117.51	120.30
3	M	188	ASN	CA-CB-CG	-5.54	101.21	113.40
3	M	182	HIS	CA-CB-CG	5.53	123.00	113.60
1	H	117	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	H	67	PRO	N-CA-C	5.49	126.37	112.10
3	M	184	ASP	CB-CG-OD1	5.41	123.17	118.30
2	L	31	VAL	O-C-N	-5.33	114.14	123.20
1	H	132	LYS	CB-CA-C	-5.29	99.81	110.40
1	H	202	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	H	11	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	H	152	PRO	N-CA-CB	5.26	109.62	103.30
1	H	248	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	L	222	TYR	CB-CG-CD2	5.23	124.14	121.00
3	M	292	ASP	CB-CG-OD2	-5.15	113.67	118.30
3	M	197	ARG	NE-CZ-NH1	5.13	122.87	120.30
3	M	188	ASN	CB-CG-OD1	-5.11	111.38	121.60
1	H	118	ARG	CD-NE-CZ	-5.08	116.48	123.60
1	H	97	PRO	N-CA-CB	5.02	109.33	103.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	113	SER	Mainchain
1	H	114	TRP	Mainchain
1	H	115	VAL	Mainchain
1	H	185	ASP	Mainchain
1	H	250	SER	Mainchain
1	H	87	LEU	Mainchain
1	H	91	ALA	Mainchain
2	L	141	ALA	Mainchain
2	L	160	THR	Mainchain
2	L	162	TYR	Mainchain
2	L	213	ASP	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	L	253	THR	Mainchain
3	M	196	LEU	Mainchain
3	M	29	ARG	Mainchain

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	H	1830	0	1836	61	0
2	L	2232	0	2187	59	0
3	M	2413	0	2326	58	0
4	H	16	0	31	0	0
4	M	32	0	62	5	0
5	L	132	0	148	15	0
5	M	132	0	148	10	0
6	L	65	0	76	10	0
6	M	65	0	76	3	0
7	L	48	0	58	1	0
7	M	48	0	63	0	0
8	M	1	0	0	0	0
9	M	43	0	69	5	0
10	M	81	0	106	16	0
11	H	42	0	0	3	0
11	L	28	0	0	1	0
11	M	42	0	0	1	0
All	All	7250	0	7186	200	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 14.

All (200) 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)
10:M:800:CDL:CA6	10:M:800:CDL:HB4	1.62	1.28
10:M:800:CDL:HA61	10:M:800:CDL:HB4	1.10	1.10
10:M:800:CDL:CB4	10:M:800:CDL:HA61	1.83	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:LEU:HD23	10:M:800:CDL:H132	1.51	0.92
2:L:206:MET:HE1	3:M:239:ALA:HB2	1.51	0.89
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.57	0.86
10:M:800:CDL:HA62	10:M:800:CDL:HB4	1.55	0.86
10:M:800:CDL:CA7	10:M:800:CDL:OB7	2.25	0.84
3:M:31:GLY:H	4:M:702:LDA:H92	1.40	0.84
3:M:197:ARG:HH11	3:M:197:ARG:HG3	1.44	0.81
1:H:154:ARG:HE	1:H:204:HIS:HD2	1.29	0.80
10:M:800:CDL:HA61	10:M:800:CDL:CB6	2.13	0.78
3:M:197:ARG:HG3	3:M:197:ARG:NH1	1.97	0.77
1:H:154:ARG:HE	1:H:204:HIS:CD2	2.03	0.76
2:L:154:LEU:HB3	3:M:197:ARG:HG2	1.67	0.76
10:M:800:CDL:C31	10:M:800:CDL:OB7	2.34	0.75
1:H:132:LYS:HG3	1:H:171:ILE:HD13	1.72	0.72
1:H:70:ARG:O	1:H:118:ARG:NH2	2.24	0.71
1:H:96:PHE:HB3	1:H:97:PRO:CD	2.20	0.70
3:M:203:ASP:HB2	4:M:703:LDA:HM11	1.73	0.68
5:M:1303:BCL:HBB3	5:M:1303:BCL:HMB1	1.76	0.68
2:L:221:GLY:HA3	4:M:702:LDA:HM21	1.75	0.67
2:L:267:VAL:HG13	2:L:268:LYS:HD3	1.76	0.66
5:L:1302:BCL:OBB	5:L:1302:BCL:HHC	1.93	0.66
2:L:208:THR:HB	2:L:209:PRO:HD2	1.77	0.66
3:M:190:SER:HA	3:M:196:LEU:HD13	1.78	0.65
1:H:171:ILE:N	1:H:172:PRO:HD2	2.11	0.65
2:L:135:ARG:HB2	2:L:136:PRO:HD3	1.78	0.65
2:L:221:GLY:HA3	4:M:702:LDA:CM2	2.26	0.65
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.44	0.64
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.16	0.63
5:L:1304:BCL:C1C	5:L:1304:BCL:CBC	2.77	0.63
1:H:96:PHE:HB3	1:H:97:PRO:HD2	1.79	0.63
2:L:34:PHE:O	2:L:38:THR:HG23	1.99	0.62
2:L:49:ILE:HG12	2:L:89:ILE:HD13	1.79	0.62
2:L:71:LEU:H	2:L:71:LEU:HD12	1.64	0.62
5:L:1302:BCL:HBD	5:L:1304:BCL:HAC1	1.81	0.62
1:H:197:LYS:NZ	1:H:199:GLN:HE21	1.98	0.62
5:M:1303:BCL:CBB	5:M:1303:BCL:HMB1	2.29	0.62
1:H:14:SER:HA	1:H:17:ILE:HG22	1.82	0.60
2:L:264:GLN:HA	2:L:267:VAL:HG12	1.83	0.60
3:M:197:ARG:HH11	3:M:197:ARG:CG	2.13	0.60
1:H:132:LYS:HG3	1:H:171:ILE:CD1	2.32	0.60
5:M:1301:BCL:H61	5:M:1303:BCL:H18	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:101:TYR:O	3:M:104:SER:HB3	2.02	0.59
2:L:156:TRP:O	2:L:160:THR:HG23	2.02	0.59
2:L:5:PHE:CD1	3:M:246:GLU:HG2	2.37	0.59
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.84	0.59
10:M:800:CDL:OB7	10:M:800:CDL:H312	2.03	0.58
3:M:70:ILE:HD13	9:M:600:SPN:H102	1.86	0.58
5:M:1301:BCL:HHC	5:M:1301:BCL:OBB	2.04	0.57
2:L:5:PHE:CE1	3:M:246:GLU:HG2	2.40	0.57
1:H:219:ILE:HG21	1:H:225:VAL:HG13	1.86	0.56
10:M:800:CDL:HA61	10:M:800:CDL:HB61	1.86	0.56
3:M:233:ARG:HA	11:M:2031:HOH:O	2.06	0.56
1:H:117:ARG:HD3	3:M:242:GLY:CA	2.36	0.56
5:L:1304:BCL:HBB2	5:L:1304:BCL:HMB1	1.88	0.56
2:L:229:ILE:HG13	2:L:229:ILE:O	2.06	0.55
3:M:16:ALA:HB1	3:M:32:VAL:HG21	1.89	0.55
1:H:121:PRO:HB3	1:H:225:VAL:O	2.06	0.55
3:M:170:SER:HG	3:M:172:SER:HG	1.53	0.55
1:H:34:GLU:OE1	1:H:37:ARG:NH1	2.40	0.55
2:L:156:TRP:CE2	2:L:160:THR:HG21	2.42	0.55
2:L:49:ILE:CG1	2:L:89:ILE:HD13	2.37	0.55
2:L:121:PHE:CE2	2:L:125:ILE:HD11	2.43	0.54
3:M:21:THR:HG23	3:M:26:LEU:HD11	1.87	0.54
5:L:1302:BCL:HBB3	5:L:1302:BCL:HMB1	1.89	0.54
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.89	0.54
1:H:249:LYS:O	1:H:250:SER:HB2	2.08	0.54
6:L:401:BPH:OBB	6:L:401:BPH:HHC	2.08	0.54
3:M:97:PRO:HG2	3:M:171:TRP:HB2	1.90	0.54
6:M:402:BPH:HHH	6:M:402:BPH:HBC3	1.90	0.53
1:H:146:LYS:HE2	1:H:200:SER:O	2.09	0.52
1:H:139:GLY:HA3	3:M:15:PRO:HD3	1.91	0.52
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.90	0.52
1:H:226:THR:OG1	1:H:229:GLU:HG3	2.09	0.52
2:L:241:VAL:HG21	6:L:401:BPH:HAC2	1.92	0.52
1:H:228:LEU:O	1:H:232:LYS:HG3	2.09	0.52
3:M:119:SER:HB3	9:M:600:SPN:H232	1.91	0.52
1:H:245:ALA:HB3	1:H:246:PRO:HD3	1.92	0.52
1:H:62:LYS:HE3	11:H:2006:HOH:O	2.09	0.52
3:M:98:ALA:HB1	3:M:99:PRO:HD2	1.92	0.51
2:L:60:ASN:O	2:L:64:ILE:HG13	2.10	0.51
3:M:109:LEU:HA	3:M:113:GLY:HA3	1.93	0.51
3:M:293:ASN:OD1	3:M:295:TYR:HB3	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:80:LEU:HA	2:L:84:GLY:HA3	1.91	0.51
1:H:83:ARG:HB2	1:H:84:PRO:HD2	1.92	0.51
2:L:135:ARG:HD3	2:L:248:MET:O	2.11	0.51
2:L:135:ARG:CB	2:L:136:PRO:HD3	2.39	0.51
3:M:148:TRP:CD1	10:M:800:CDL:H511	2.46	0.50
3:M:67:PHE:CE1	9:M:600:SPN:H61	2.46	0.50
2:L:154:LEU:HD13	3:M:197:ARG:HG2	1.94	0.50
1:H:132:LYS:NZ	11:H:2028:HOH:O	2.45	0.50
1:H:197:LYS:HZ3	1:H:199:GLN:HE21	1.59	0.50
3:M:101:TYR:CG	3:M:107:ALA:HB2	2.47	0.50
2:L:69:PRO:HG2	2:L:142:TRP:CB	2.42	0.49
2:L:122:ALA:O	2:L:126:LEU:HG	2.12	0.49
6:L:401:BPH:CMB	6:L:401:BPH:HBB3	2.42	0.49
2:L:233:GLY:HA3	3:M:216:PHE:CE1	2.47	0.49
5:L:1304:BCL:C1C	5:L:1304:BCL:HBC2	2.43	0.48
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.47	0.48
2:L:73:TYR:OH	2:L:82:LYS:HD2	2.12	0.48
5:L:1302:BCL:H42	5:L:1304:BCL:HBC3	1.95	0.48
3:M:197:ARG:NH2	5:M:1303:BCL:OBB	2.46	0.48
3:M:24:VAL:HG11	3:M:29:ARG:NH2	2.28	0.48
3:M:194:GLY:O	3:M:195:ASN:CB	2.61	0.48
1:H:191:LEU:HD11	1:H:213:PHE:CE2	2.49	0.48
5:L:1302:BCL:OBB	5:L:1302:BCL:CHC	2.62	0.48
2:L:32:GLY:HA3	11:L:2016:HOH:O	2.13	0.48
1:H:201:ASN:O	1:H:202:ARG:HB3	2.13	0.47
1:H:33:THR:O	1:H:36:MET:HB2	2.14	0.47
1:H:171:ILE:N	1:H:172:PRO:CD	2.78	0.47
2:L:154:LEU:HD13	3:M:197:ARG:CG	2.45	0.47
1:H:140:PHE:HA	3:M:13:ARG:O	2.15	0.47
3:M:155:TRP:CD2	10:M:800:CDL:H812	2.50	0.47
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.96	0.47
2:L:172:ALA:HB3	2:L:247:CYS:HA	1.95	0.47
3:M:148:TRP:CE2	10:M:800:CDL:H511	2.50	0.47
1:H:37:ARG:HD2	1:H:37:ARG:HH11	1.46	0.46
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.80	0.46
2:L:233:GLY:HA3	3:M:216:PHE:CD1	2.50	0.46
2:L:210:ASP:HB2	3:M:20:MET:HE3	1.97	0.46
2:L:117:ILE:HB	2:L:118:PRO:HD3	1.97	0.46
2:L:134:PHE:O	2:L:138:MET:HG3	2.15	0.46
1:H:206:ASN:HD21	1:H:248:ARG:HD3	1.81	0.46
2:L:208:THR:O	2:L:211:HIS:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.51	0.46
1:H:121:PRO:HA	1:H:226:THR:HA	1.98	0.45
5:L:1304:BCL:CBB	5:L:1304:BCL:HMB1	2.46	0.45
3:M:35:PHE:CE1	3:M:46:GLN:HB2	2.51	0.45
5:L:1304:BCL:HMD1	3:M:206:ILE:HD13	1.98	0.45
1:H:197:LYS:HD3	1:H:199:GLN:NE2	2.30	0.45
1:H:206:ASN:O	1:H:248:ARG:NH1	2.49	0.45
2:L:117:ILE:HB	2:L:118:PRO:CD	2.46	0.45
5:M:1301:BCL:H141	5:M:1301:BCL:H162	1.65	0.45
1:H:180:GLU:OE2	1:H:188:THR:HG21	2.16	0.45
2:L:175:ILE:O	2:L:178:SER:HB2	2.16	0.45
1:H:199:GLN:HB2	1:H:202:ARG:O	2.17	0.45
3:M:132:ARG:O	3:M:133:THR:C	2.52	0.45
1:H:165:VAL:O	1:H:166:ASP:HB2	2.17	0.45
1:H:87:LEU:HD13	1:H:98:HIS:HB2	1.99	0.44
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.98	0.44
1:H:38:GLU:OE1	3:M:241:ARG:NH1	2.47	0.44
3:M:270:ILE:HD13	10:M:800:CDL:H711	1.98	0.44
6:M:402:BPH:H9C2	6:M:402:BPH:H6C1	1.73	0.44
1:H:240:GLY:O	1:H:244:ALA:HB3	2.18	0.44
1:H:34:GLU:CD	1:H:37:ARG:HH12	2.22	0.43
1:H:229:GLU:O	1:H:233:ILE:HD12	2.18	0.43
1:H:62:LYS:O	1:H:74:THR:HA	2.17	0.43
2:L:241:VAL:HG21	6:L:401:BPH:H2C	2.00	0.43
6:L:401:BPH:ND	3:M:214:LEU:HD13	2.34	0.43
2:L:209:PRO:O	2:L:212:GLU:HB2	2.19	0.43
6:L:401:BPH:H141	6:L:401:BPH:H162	1.72	0.43
6:M:402:BPH:H4C1	6:M:402:BPH:H6C1	1.34	0.43
3:M:200:PRO:HA	4:M:703:LDA:HM12	2.00	0.43
3:M:228:ARG:HG3	3:M:229:PHE:CE2	2.54	0.43
5:L:1302:BCL:H2C	5:M:1303:BCL:H2C	2.00	0.43
1:H:82:ASP:O	1:H:83:ARG:HB3	2.18	0.43
2:L:38:THR:HG22	2:L:99:SER:CB	2.49	0.43
5:M:1301:BCL:CBB	5:M:1301:BCL:HMB1	2.48	0.43
5:M:1303:BCL:HHC	5:M:1303:BCL:OBB	2.19	0.43
10:M:800:CDL:H522	10:M:800:CDL:H311	2.00	0.43
1:H:168:TRP:CZ3	1:H:225:VAL:HG22	2.53	0.42
5:L:1304:BCL:H203	6:L:401:BPH:H112	2.00	0.42
1:H:124:ASP:HB2	2:L:210:ASP:OD2	2.19	0.42
2:L:238:LEU:HD23	6:L:401:BPH:CBC	2.50	0.42
3:M:184:ASP:O	3:M:188:ASN:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:226:THR:HG22	7:L:501:U10:H3M2	2.02	0.42
5:L:1302:BCL:H122	6:L:401:BPH:H3A	2.01	0.42
2:L:247:CYS:SG	2:L:248:MET:HG2	2.59	0.42
1:H:228:LEU:HD22	1:H:232:LYS:HE3	2.01	0.42
1:H:225:VAL:HG12	1:H:229:GLU:HB2	2.01	0.42
1:H:179:LEU:HD11	1:H:196:VAL:HG21	2.01	0.41
6:L:401:BPH:CMB	6:L:401:BPH:CBB	2.98	0.41
3:M:163:ILE:HG22	3:M:285:LEU:HD11	2.03	0.41
1:H:98:HIS:HE1	11:H:2019:HOH:O	2.02	0.41
1:H:36:MET:CE	1:H:56:PHE:HB2	2.50	0.41
10:M:800:CDL:C52	10:M:800:CDL:H312	2.50	0.41
2:L:69:PRO:HD3	2:L:83:GLY:O	2.21	0.41
3:M:243:THR:O	3:M:247:ARG:HG2	2.20	0.41
3:M:11:GLN:NE2	3:M:41:TRP:CD2	2.88	0.41
5:L:1302:BCL:H2C	5:L:1302:BCL:HBC2	1.89	0.41
2:L:207:ARG:HG2	3:M:142:MET:HG2	2.02	0.41
2:L:133:LEU:HD12	2:L:133:LEU:O	2.20	0.41
5:L:1302:BCL:CBB	5:L:1302:BCL:HMB1	2.49	0.41
2:L:163:THR:O	2:L:163:THR:HG22	2.21	0.41
2:L:213:ASP:O	2:L:217:ARG:HG3	2.20	0.41
3:M:241:ARG:HG3	3:M:245:ALA:HB3	2.03	0.41
2:L:60:ASN:HA	2:L:61:PRO:HD3	1.82	0.41
3:M:122:MET:SD	9:M:600:SPN:H19	2.60	0.41
5:M:1301:BCL:H193	5:M:1301:BCL:H161	1.86	0.40
2:L:241:VAL:O	2:L:244:SER:HB2	2.20	0.40
3:M:48:GLY:HA2	3:M:49:PRO:C	2.42	0.40
1:H:48:THR:HB	1:H:49:PRO:HD2	2.02	0.40
2:L:71:LEU:HD23	2:L:144:TYR:CZ	2.56	0.40
2:L:210:ASP:CB	3:M:20:MET:HE3	2.52	0.40
3:M:60:LEU:HD23	3:M:64:LEU:HD11	2.04	0.40
1:H:157:ASP:OD2	1:H:210:SER:OG	2.33	0.40
3:M:35:PHE:HA	3:M:45:ALA:O	2.21	0.40
3:M:67:PHE:CZ	9:M:600:SPN:H61	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	H	239/260 (92%)	224 (94%)	13 (5%)	2 (1%)	19	43
2	L	279/281 (99%)	262 (94%)	17 (6%)	0	100	100
3	M	301/307 (98%)	275 (91%)	21 (7%)	5 (2%)	9	23
All	All	819/848 (97%)	761 (93%)	51 (6%)	7 (1%)	17	40

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	250	SER
1	H	116	ALA
3	M	195	ASN
3	M	301	HIS
3	M	80	TRP
3	M	194	GLY
3	M	302	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	H	195/208 (94%)	182 (93%)	13 (7%)	16	37
2	L	220/220 (100%)	199 (90%)	21 (10%)	8	20
3	M	237/241 (98%)	221 (93%)	16 (7%)	16	36
All	All	652/669 (98%)	602 (92%)	50 (8%)	13	30

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	15	LEU
1	H	27	LEU
1	H	52	ASN
1	H	60	LYS
1	H	70	ARG
1	H	143	SER
1	H	173	GLU
1	H	188	THR
1	H	221	SER
1	H	225	VAL
1	H	228	LEU
1	H	231	ASP
1	H	248	ARG
2	L	38	THR
2	L	44	LEU
2	L	56	GLN
2	L	63	LEU
2	L	72	GLU
2	L	82	LYS
2	L	133	LEU
2	L	135	ARG
2	L	160	THR
2	L	185	LEU
2	L	205	GLU
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	217	ARG
2	L	223	SER
2	L	235	LEU
2	L	237	SER
2	L	247	CYS
2	L	271	TRP
2	L	272	TRP
3	M	10	VAL
3	M	52	LEU
3	M	62	SER
3	M	104	SER
3	M	109	LEU
3	M	124	VAL
3	M	133	THR
3	M	136	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	151	LEU
3	M	170	SER
3	M	188	ASN
3	M	196	LEU
3	M	197	ARG
3	M	216	PHE
3	M	247	ARG
3	M	259	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	126	HIS
1	H	199	GLN
1	H	204	HIS
1	H	206	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	LDA	M	703	-	12,15,15	2.42	1 (8%)	14,17,17	0.81	1 (7%)
4	LDA	M	702	-	12,15,15	2.45	1 (8%)	14,17,17	0.85	1 (7%)
5	BCL	M	1303	3	58,74,74	1.64	11 (18%)	69,115,115	1.97	23 (33%)
5	BCL	L	1304	2	58,74,74	1.60	7 (12%)	69,115,115	2.96	23 (33%)
10	CDL	M	800	-	80,80,99	0.50	0	86,92,111	0.90	3 (3%)
9	SPN	M	600	-	40,42,42	3.79	18 (45%)	50,52,52	2.93	19 (38%)
7	U10	M	502	-	48,48,63	1.79	14 (29%)	58,61,79	1.51	13 (22%)
5	BCL	M	1301	3	58,74,74	1.61	8 (13%)	69,115,115	2.48	27 (39%)
6	BPH	M	402	-	64,70,70	1.22	7 (10%)	76,101,101	2.58	25 (32%)
4	LDA	H	701	-	12,15,15	2.46	1 (8%)	14,17,17	0.79	1 (7%)
7	U10	L	501	-	47,47,63	2.03	13 (27%)	54,58,79	2.66	21 (38%)
5	BCL	L	1302	2	58,74,74	1.66	10 (17%)	69,115,115	2.36	22 (31%)
6	BPH	L	401	-	64,70,70	1.40	7 (10%)	76,101,101	2.46	21 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	M	703	-	-	8/13/13/13	-
4	LDA	M	702	-	-	12/13/13/13	-
5	BCL	M	1303	3	-	6/37/137/137	-
5	BCL	L	1304	2	-	9/37/137/137	-
10	CDL	M	800	-	-	35/91/91/110	-
9	SPN	M	600	-	-	18/50/51/51	-
7	U10	M	502	-	-	6/45/69/87	0/1/1/1
5	BCL	M	1301	3	1/1/21/25	17/37/137/137	-
6	BPH	M	402	-	-	22/54/105/105	0/5/6/6
4	LDA	H	701	-	-	12/13/13/13	-
7	U10	L	501	-	-	15/41/65/87	0/1/1/1
5	BCL	L	1302	2	-	9/37/137/137	-
6	BPH	L	401	-	2/2/18/22	15/54/105/105	0/5/6/6

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	600	SPN	C4-C5	8.89	1.54	1.33
9	M	600	SPN	C8-C9	8.50	1.53	1.33
4	H	701	LDA	O1-N1	-8.48	1.22	1.42
4	M	702	LDA	O1-N1	-8.47	1.22	1.42
4	M	703	LDA	O1-N1	-8.38	1.22	1.42
9	M	600	SPN	C19-C18	8.30	1.52	1.33
9	M	600	SPN	C12-C13	8.08	1.52	1.33
9	M	600	SPN	C3-C4	-6.86	1.40	1.50
9	M	600	SPN	C10-C9	-6.61	1.37	1.51
9	M	600	SPN	C6-C5	-6.13	1.38	1.51
5	L	1302	BCL	MG-NA	6.05	2.20	2.06
5	L	1304	BCL	O2D-CGD	5.87	1.47	1.33
7	L	501	U10	C20-C19	-5.87	1.25	1.49
5	L	1302	BCL	O2D-CGD	5.85	1.47	1.33
5	M	1301	BCL	O2D-CGD	5.69	1.47	1.33
5	M	1303	BCL	C4B-NB	5.42	1.40	1.35
9	M	600	SPN	C17-C18	-5.26	1.40	1.51
9	M	600	SPN	C14-C13	-5.19	1.40	1.51
5	L	1304	BCL	C1B-NB	5.18	1.39	1.35
6	L	401	BPH	O2D-CGD	5.15	1.45	1.33
5	M	1303	BCL	MG-NA	5.12	2.18	2.06
7	L	501	U10	C7-C8	-5.03	1.43	1.50
6	L	401	BPH	O2A-CGA	4.89	1.47	1.33
5	M	1303	BCL	O2D-CGD	4.70	1.44	1.33
5	M	1301	BCL	MG-NA	4.56	2.17	2.06
5	M	1301	BCL	C1B-NB	4.38	1.39	1.35
5	L	1304	BCL	O2A-CGA	4.29	1.45	1.33
5	M	1301	BCL	O2A-CGA	4.24	1.45	1.33
6	M	402	BPH	O2D-CGD	4.17	1.43	1.33
7	M	502	U10	O4-C4	4.03	1.46	1.36
5	L	1304	BCL	MG-NA	4.02	2.15	2.06
7	L	501	U10	O4-C4	4.00	1.46	1.36
9	M	600	SPN	O1-CMA	4.00	1.55	1.43
6	M	402	BPH	O2A-CGA	3.82	1.44	1.33
7	L	501	U10	O3-C3	3.65	1.45	1.36
5	M	1303	BCL	O2A-CGA	3.61	1.43	1.33
7	L	501	U10	C13-C14	3.57	1.41	1.33
5	L	1302	BCL	C4B-NB	3.56	1.38	1.35
6	L	401	BPH	O2D-CED	-3.52	1.37	1.45
5	L	1302	BCL	O2A-CGA	3.51	1.43	1.33
5	M	1303	BCL	C1B-NB	3.50	1.38	1.35
7	M	502	U10	O3-C3	3.48	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	600	SPN	C20-C19	-3.47	1.39	1.50
9	M	600	SPN	C11-C12	-3.44	1.39	1.50
5	M	1301	BCL	C4B-NB	3.25	1.38	1.35
5	L	1304	BCL	C4B-NB	3.23	1.38	1.35
5	L	1302	BCL	C2-C3	3.21	1.40	1.33
7	M	502	U10	C7-C8	-3.11	1.46	1.50
9	M	600	SPN	C25-C26	3.07	1.40	1.33
7	M	502	U10	C33-C34	3.07	1.40	1.33
7	M	502	U10	C13-C14	2.99	1.40	1.33
5	M	1303	BCL	C2-C3	2.98	1.40	1.33
7	M	502	U10	C8-C9	2.98	1.40	1.33
7	L	501	U10	C28-C29	2.97	1.40	1.33
5	M	1301	BCL	C2-C3	2.85	1.39	1.33
9	M	600	SPN	C29-C30	2.82	1.40	1.32
5	L	1304	BCL	C2-C3	2.82	1.39	1.33
7	M	502	U10	C23-C24	2.78	1.39	1.33
7	L	501	U10	C37-C38	-2.77	1.41	1.50
5	L	1302	BCL	C1B-NB	2.71	1.37	1.35
5	L	1302	BCL	C2C-C3C	-2.71	1.46	1.54
7	M	502	U10	C28-C29	2.65	1.39	1.33
6	L	401	BPH	O1D-CGD	2.64	1.27	1.21
9	M	600	SPN	C7-C8	-2.62	1.41	1.50
6	M	402	BPH	O2D-CED	-2.61	1.39	1.45
7	M	502	U10	C38-C39	2.59	1.39	1.32
5	M	1303	BCL	MG-NC	2.58	2.12	2.06
9	M	600	SPN	C21-C22	-2.57	1.39	1.52
7	M	502	U10	C18-C19	2.56	1.39	1.33
5	M	1301	BCL	C3B-C2B	-2.53	1.34	1.39
7	L	501	U10	O3-C3M	-2.49	1.39	1.45
6	L	401	BPH	C2-C3	2.49	1.39	1.33
7	L	501	U10	C8-C9	2.48	1.38	1.33
5	M	1303	BCL	C2C-C3C	-2.48	1.47	1.54
6	M	402	BPH	C4-C3	2.46	1.57	1.50
6	M	402	BPH	C2-C3	2.42	1.38	1.33
5	L	1302	BCL	O2D-CED	-2.39	1.39	1.45
7	M	502	U10	O4-C4M	-2.30	1.39	1.45
9	M	600	SPN	CM4-C9	2.28	1.56	1.50
5	M	1303	BCL	O2D-CED	-2.26	1.40	1.45
5	L	1302	BCL	O1D-CGD	2.24	1.26	1.21
7	M	502	U10	C40-C39	2.22	1.56	1.50
7	L	501	U10	C43-C44	2.15	1.38	1.32
7	M	502	U10	C35-C34	2.12	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	600	SPN	C16-C15	-2.12	1.39	1.51
7	M	502	U10	O3-C3M	-2.10	1.40	1.45
6	L	401	BPH	C5-C3	2.09	1.55	1.51
7	L	501	U10	C42-C43	-2.08	1.43	1.50
5	M	1303	BCL	OBD-CAD	2.08	1.25	1.22
5	M	1301	BCL	CAA-C2A	2.07	1.57	1.54
6	L	401	BPH	OBD-CAD	2.06	1.25	1.22
7	L	501	U10	C33-C34	2.05	1.37	1.33
6	M	402	BPH	C4A-NA	2.04	1.40	1.35
5	L	1304	BCL	C2C-C3C	-2.04	1.48	1.54
6	M	402	BPH	O1D-CGD	2.03	1.26	1.21
7	L	501	U10	C32-C33	-2.02	1.43	1.50
5	L	1302	BCL	C3B-C2B	-2.02	1.35	1.39
5	M	1303	BCL	O1D-CGD	2.01	1.26	1.21

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	401	BPH	O2D-CGD-CBD	13.31	134.91	111.27
5	L	1304	BCL	O2D-CGD-CBD	11.19	131.15	111.27
7	L	501	U10	C37-C38-C39	10.29	152.45	127.66
6	M	402	BPH	O2D-CGD-CBD	9.94	128.94	111.27
5	L	1304	BCL	C1C-NC-C4C	9.36	110.92	106.71
5	L	1304	BCL	C4A-NA-C1A	8.33	110.45	106.71
5	M	1301	BCL	C1C-NC-C4C	8.07	110.33	106.71
5	L	1302	BCL	C4A-NA-C1A	7.25	109.97	106.71
9	M	600	SPN	CM6-C18-C17	7.22	127.41	115.27
7	L	501	U10	C32-C33-C34	7.18	144.94	127.66
9	M	600	SPN	C7-C8-C9	-7.00	110.81	127.66
6	M	402	BPH	C5-C3-C2	6.68	134.63	121.12
6	M	402	BPH	OBD-CAD-CBD	-6.62	116.44	125.89
6	M	402	BPH	O2D-CGD-O1D	-6.60	110.94	123.84
9	M	600	SPN	CM5-C13-C14	6.59	126.36	115.27
5	M	1303	BCL	C4A-NA-C1A	6.40	109.58	106.71
6	L	401	BPH	O1D-CGD-CBD	-6.35	111.50	124.48
5	L	1302	BCL	C1C-NC-C4C	6.15	109.47	106.71
5	M	1301	BCL	CMB-C2B-C1B	-5.81	119.54	128.46
9	M	600	SPN	CM3-C5-C6	5.55	124.60	115.27
5	L	1302	BCL	O2A-CGA-CBA	5.54	129.28	111.91
5	L	1304	BCL	O2D-CGD-O1D	-5.45	113.18	123.84
9	M	600	SPN	C14-C13-C12	-5.36	110.26	121.12
6	M	402	BPH	C1-C2-C3	-5.36	116.77	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	401	BPH	O2D-CGD-O1D	-5.36	113.36	123.84
9	M	600	SPN	C6-C5-C4	-5.23	110.53	121.12
5	L	1302	BCL	C4B-C3B-CAB	-5.21	117.07	127.13
7	L	501	U10	C42-C43-C44	5.18	145.47	127.75
5	M	1301	BCL	C4A-NA-C1A	5.12	109.01	106.71
9	M	600	SPN	C3-C4-C5	-5.11	118.28	126.79
5	M	1301	BCL	C4B-C3B-CAB	-5.04	117.40	127.13
5	L	1302	BCL	O2A-CGA-O1A	-4.93	111.15	123.59
5	L	1302	BCL	O2D-CGD-CBD	4.88	119.93	111.27
5	L	1304	BCL	CAC-C3C-C4C	-4.81	101.91	112.58
6	L	401	BPH	C1-O2A-CGA	-4.79	103.87	116.44
5	L	1304	BCL	O1D-CGD-CBD	-4.76	114.75	124.48
6	M	402	BPH	C3A-C4A-CHB	4.76	130.04	121.83
5	M	1301	BCL	CMB-C2B-C3B	4.72	133.50	124.68
6	L	401	BPH	O2A-CGA-O1A	-4.70	111.73	123.59
5	L	1302	BCL	C4B-CHC-C1C	-4.65	120.92	130.12
5	L	1304	BCL	O2A-CGA-O1A	-4.64	111.88	123.59
7	M	502	U10	C27-C28-C29	-4.54	116.74	127.66
5	L	1304	BCL	CMB-C2B-C1B	-4.52	121.52	128.46
7	L	501	U10	C20-C19-C18	4.44	163.06	126.37
5	M	1301	BCL	C4-C3-C5	-4.39	107.88	115.27
6	L	401	BPH	CHD-C4C-NC	-4.34	120.04	125.20
5	M	1303	BCL	C1C-NC-C4C	4.32	108.65	106.71
9	M	600	SPN	C7-C6-C5	4.29	127.11	112.98
5	L	1304	BCL	OBB-CAB-C3B	4.25	127.54	119.99
5	L	1302	BCL	CMD-C2D-C3D	4.18	132.50	124.68
6	M	402	BPH	OBD-CAD-C3D	4.08	134.76	127.98
5	M	1301	BCL	CAA-C2A-C3A	-4.01	101.79	112.78
6	M	402	BPH	O1D-CGD-CBD	-4.01	116.29	124.48
6	M	402	BPH	O2A-CGA-CBA	4.00	124.45	111.91
7	M	502	U10	C20-C19-C21	-4.00	108.55	115.27
9	M	600	SPN	O1-C1-C2	-3.98	100.61	108.78
5	M	1301	BCL	O2A-CGA-CBA	3.98	124.39	111.91
9	M	600	SPN	C17-C18-C19	-3.97	113.09	121.12
5	M	1301	BCL	CBC-CAC-C3C	-3.97	104.64	113.47
9	M	600	SPN	CM4-C9-C10	3.91	121.85	115.27
6	M	402	BPH	OBB-CAB-C3B	3.85	127.53	120.41
6	M	402	BPH	C2C-C3C-C4C	3.84	107.09	101.34
6	L	401	BPH	C4A-NA-C1A	3.84	111.24	108.14
5	M	1301	BCL	CAC-C3C-C4C	-3.84	104.07	112.58
5	L	1304	BCL	C4D-C3D-CAD	-3.75	106.38	108.47
5	L	1304	BCL	CAC-C3C-C2C	-3.75	104.90	114.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	501	U10	C3M-O3-C3	3.74	129.72	116.47
7	L	501	U10	C7-C8-C9	3.73	133.00	126.79
5	M	1303	BCL	OBB-CAB-C3B	3.72	126.58	119.99
6	M	402	BPH	CHD-C4C-NC	-3.70	120.80	125.20
5	M	1301	BCL	C1-O2A-CGA	3.69	126.14	116.44
7	L	501	U10	C31-C29-C28	3.62	128.44	121.12
9	M	600	SPN	CM7-C22-C21	3.58	124.27	111.29
9	M	600	SPN	C20-C19-C18	-3.56	119.08	127.66
5	M	1301	BCL	C1B-CHB-C4A	-3.53	123.14	130.12
7	L	501	U10	C35-C34-C36	-3.52	109.34	115.27
5	L	1304	BCL	CMB-C2B-C3B	3.49	131.22	124.68
5	L	1302	BCL	OBD-CAD-CBD	-3.49	120.91	125.89
5	L	1304	BCL	C4B-C3B-CAB	-3.47	120.43	127.13
9	M	600	SPN	C16-C17-C18	3.42	122.43	113.45
5	L	1302	BCL	O2D-CGD-O1D	-3.39	117.20	123.84
5	L	1304	BCL	CMD-C2D-C3D	3.38	131.00	124.68
6	M	402	BPH	C4-C3-C5	-3.35	109.63	115.27
5	M	1301	BCL	C2C-C3C-C4C	3.30	106.29	101.34
5	L	1302	BCL	C2A-C3A-C4A	3.29	107.19	101.87
6	L	401	BPH	O2A-CGA-CBA	3.29	122.24	111.91
5	L	1302	BCL	C2C-C3C-C4C	3.25	106.20	101.34
6	L	401	BPH	CMA-C3A-C4A	-3.18	102.91	112.36
5	M	1301	BCL	O2D-CGD-CBD	3.18	116.91	111.27
5	L	1302	BCL	C4D-C3D-CAD	-3.17	106.70	108.47
5	L	1304	BCL	CHD-C4C-NC	3.17	128.59	125.08
5	M	1303	BCL	C4B-CHC-C1C	-3.16	123.85	130.12
5	M	1303	BCL	OBB-CAB-CBB	-3.15	113.09	120.17
5	L	1302	BCL	CAC-C3C-C4C	-3.13	105.64	112.58
5	M	1303	BCL	OBD-CAD-CBD	-3.13	121.43	125.89
9	M	600	SPN	C16-C15-C14	3.11	124.37	113.19
6	M	402	BPH	C4-C3-C2	-3.10	115.73	123.68
6	L	401	BPH	C1C-NC-C4C	-3.07	107.84	110.54
9	M	600	SPN	C15-C14-C13	3.07	121.50	113.45
5	M	1303	BCL	C4D-C3D-CAD	-3.06	106.76	108.47
7	L	501	U10	C1M-C1-C6	-3.01	119.49	124.40
5	M	1303	BCL	C5-C3-C2	2.97	127.12	121.12
7	L	501	U10	C40-C39-C38	-2.96	116.07	123.68
9	M	600	SPN	C15-C16-C17	2.95	123.80	113.19
7	L	501	U10	O2-C2-C3	-2.95	114.68	120.93
5	L	1302	BCL	CBA-CAA-C2A	2.94	122.56	113.86
5	L	1304	BCL	CAA-C2A-C3A	-2.92	104.79	112.78
5	M	1301	BCL	OBB-CAB-C3B	2.89	125.11	119.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1303	BCL	C4B-C3B-CAB	-2.87	121.59	127.13
5	M	1303	BCL	O2D-CGD-CBD	2.86	116.36	111.27
10	M	800	CDL	CA4-OA6-CA5	-2.85	110.77	117.79
7	M	502	U10	C12-C13-C14	2.85	134.52	127.66
5	M	1303	BCL	O2A-CGA-CBA	2.80	120.71	111.91
7	M	502	U10	C25-C24-C23	2.80	130.86	123.68
5	M	1301	BCL	O2A-CGA-O1A	-2.79	116.54	123.59
5	M	1303	BCL	CAC-C3C-C4C	-2.79	106.39	112.58
7	L	501	U10	C36-C34-C33	2.79	126.76	121.12
6	M	402	BPH	CAA-C2A-C3A	-2.78	105.16	112.78
5	M	1303	BCL	CAC-C3C-C2C	-2.68	107.55	114.26
7	L	501	U10	O5-C5-C6	-2.68	116.85	121.55
5	L	1302	BCL	CHC-C1C-NC	2.67	128.20	124.51
7	M	502	U10	C20-C19-C18	2.66	130.50	123.68
5	L	1304	BCL	C2A-C3A-C4A	2.65	106.15	101.87
5	L	1304	BCL	C6-C5-C3	-2.64	106.52	113.45
5	M	1301	BCL	C4D-C3D-CAD	-2.64	107.00	108.47
7	L	501	U10	C41-C39-C38	2.63	126.44	121.12
5	M	1301	BCL	C4-C3-C2	2.63	130.42	123.68
5	M	1303	BCL	O2A-C1-C2	-2.61	101.77	108.64
9	M	600	SPN	C10-C9-C8	-2.60	115.85	121.12
7	L	501	U10	C30-C29-C28	-2.59	117.02	123.68
6	M	402	BPH	CBB-CAB-C3B	-2.58	114.92	120.43
5	M	1301	BCL	OBD-CAD-CBD	-2.57	122.22	125.89
5	L	1302	BCL	O2A-C1-C2	-2.57	101.89	108.64
6	M	402	BPH	C4D-CHA-C1A	-2.55	124.21	130.51
5	L	1302	BCL	CMA-C3A-C2A	-2.55	103.53	113.83
6	L	401	BPH	CMA-C3A-C2A	-2.54	103.57	113.83
5	L	1304	BCL	OBB-CAB-CBB	-2.54	114.45	120.17
5	M	1301	BCL	O2A-C1-C2	2.54	115.31	108.64
5	L	1304	BCL	CAA-CBA-CGA	2.53	120.66	113.25
7	M	502	U10	C6-C1-C2	2.53	121.18	119.18
4	M	702	LDA	CM2-N1-C1	-2.53	104.93	110.23
6	M	402	BPH	CMA-C3A-C2A	-2.51	103.69	113.83
5	L	1304	BCL	C2C-C3C-C4C	2.50	105.08	101.34
6	L	401	BPH	C2A-C3A-C4A	2.49	106.25	101.34
7	L	501	U10	C12-C13-C14	-2.45	121.76	127.66
6	M	402	BPH	C3A-C4A-NA	-2.44	108.88	113.05
5	M	1301	BCL	CAC-C3C-C2C	-2.44	108.17	114.26
4	H	701	LDA	CM1-N1-C1	-2.44	105.11	110.23
6	L	401	BPH	C3A-C4A-NA	-2.43	108.90	113.05
6	M	402	BPH	C6-C5-C3	-2.43	107.10	113.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1304	BCL	O2A-CGA-CBA	2.40	119.45	111.91
5	M	1303	BCL	O2A-CGA-O1A	-2.38	117.57	123.59
6	L	401	BPH	C4D-CHA-C1A	-2.38	124.64	130.51
5	M	1303	BCL	O1D-CGD-CBD	-2.37	119.63	124.48
7	M	502	U10	C25-C24-C26	-2.34	111.34	115.27
6	M	402	BPH	CHB-C4A-NA	-2.34	120.92	124.94
6	M	402	BPH	C1-O2A-CGA	2.33	122.55	116.44
5	L	1302	BCL	O1D-CGD-CBD	-2.32	119.73	124.48
10	M	800	CDL	OB8-CB7-OB9	-2.32	117.73	123.59
5	M	1301	BCL	C1D-CHD-C4C	-2.31	122.47	125.88
5	M	1303	BCL	C2A-C3A-C4A	2.27	105.54	101.87
6	L	401	BPH	CBB-CAB-C3B	-2.26	115.59	120.43
7	L	501	U10	C6-C1-C2	2.26	120.97	119.18
5	M	1301	BCL	CAA-CBA-CGA	2.24	119.81	113.25
5	M	1303	BCL	C6-C7-C8	2.24	123.15	115.92
5	M	1303	BCL	C2C-C3C-C4C	2.23	104.69	101.34
7	M	502	U10	C36-C34-C33	2.23	125.64	121.12
5	M	1303	BCL	C1B-CHB-C4A	-2.22	125.73	130.12
7	L	501	U10	C16-C14-C13	2.22	125.60	121.12
7	L	501	U10	C15-C14-C13	-2.21	118.01	123.68
10	M	800	CDL	OA6-CA5-C11	2.20	116.25	111.50
7	L	501	U10	C36-C37-C38	2.19	119.07	111.88
5	L	1302	BCL	CMA-C3A-C4A	-2.19	105.89	111.77
6	L	401	BPH	CMB-C2B-C1B	2.17	128.41	125.06
5	M	1301	BCL	C2A-C3A-C4A	2.16	105.36	101.87
6	L	401	BPH	CHB-C1B-C2B	-2.16	120.30	125.73
5	L	1302	BCL	CMC-C2C-C1C	-2.15	106.00	111.77
7	M	502	U10	C27-C26-C24	-2.13	105.95	112.98
9	M	600	SPN	CM6-C18-C19	-2.13	118.21	123.68
6	L	401	BPH	C2C-C3C-C4C	2.11	104.51	101.34
5	M	1301	BCL	C3C-C2C-C1C	2.11	105.28	101.87
5	L	1302	BCL	C3C-C2C-C1C	2.11	105.28	101.87
5	M	1301	BCL	CHA-C1A-NA	-2.11	121.57	126.40
6	L	401	BPH	OBB-CAB-C3B	2.08	124.26	120.41
5	M	1303	BCL	CAA-C2A-C3A	-2.08	107.08	112.78
7	L	501	U10	C4M-O4-C4	2.08	123.84	116.47
7	M	502	U10	C22-C21-C19	-2.08	106.15	112.98
5	L	1304	BCL	C4B-CHC-C1C	-2.07	126.01	130.12
6	L	401	BPH	C3C-C2C-C1C	2.07	105.22	101.87
5	M	1303	BCL	C3C-C2C-C1C	2.07	105.22	101.87
6	M	402	BPH	C11-C12-C13	-2.07	109.24	115.92
6	M	402	BPH	O1A-CGA-CBA	-2.05	115.73	123.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	703	LDA	CM1-N1-C1	-2.05	105.93	110.23
5	M	1303	BCL	CHA-C1A-NA	-2.04	121.72	126.40
7	M	502	U10	C30-C29-C31	2.04	118.70	115.27
5	M	1301	BCL	CHD-C4C-NC	2.04	127.34	125.08
7	M	502	U10	C26-C27-C28	-2.03	105.19	111.88
6	M	402	BPH	CED-O2D-CGD	2.02	120.52	115.94
7	M	502	U10	C4M-O4-C4	2.02	123.61	116.47
6	L	401	BPH	CAC-C3C-C2C	-2.00	109.25	114.26

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1301	BCL	C13
6	L	401	BPH	C8
6	L	401	BPH	C13

All (184) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	703	LDA	C2-C1-N1-O1
4	M	703	LDA	C2-C1-N1-CM1
4	M	703	LDA	C2-C1-N1-CM2
4	M	702	LDA	C2-C1-N1-O1
4	M	702	LDA	C2-C1-N1-CM1
4	M	702	LDA	C2-C1-N1-CM2
4	M	702	LDA	N1-C1-C2-C3
5	L	1304	BCL	C2C-C3C-CAC-CBC
10	M	800	CDL	CA2-OA2-PA1-OA3
10	M	800	CDL	CA2-OA2-PA1-OA4
9	M	600	SPN	CM3-C5-C6-C7
9	M	600	SPN	C11-C10-C9-CM4
9	M	600	SPN	C11-C12-C13-C14
9	M	600	SPN	CM5-C13-C14-C15
9	M	600	SPN	C16-C17-C18-CM6
5	M	1301	BCL	C1-C2-C3-C4
5	M	1301	BCL	C1-C2-C3-C5
5	M	1301	BCL	C11-C12-C13-C15
6	M	402	BPH	C4B-C3B-CAB-OBB
6	M	402	BPH	C2B-C3B-CAB-OBB
4	H	701	LDA	C2-C1-N1-O1
4	H	701	LDA	C2-C1-N1-CM2
4	H	701	LDA	N1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	L	501	U10	C17-C18-C19-C20
7	L	501	U10	C29-C31-C32-C33
7	L	501	U10	C36-C37-C38-C39
7	L	501	U10	C41-C42-C43-C44
6	L	401	BPH	C4C-C3C-CAC-CBC
6	L	401	BPH	O2A-C1-C2-C3
9	M	600	SPN	C14-C15-C16-C17
6	M	402	BPH	C4-C3-C5-C6
9	M	600	SPN	C4-C5-C6-C7
9	M	600	SPN	C11-C10-C9-C8
9	M	600	SPN	C12-C13-C14-C15
9	M	600	SPN	C16-C17-C18-C19
6	M	402	BPH	C2-C3-C5-C6
7	M	502	U10	C24-C26-C27-C28
7	L	501	U10	C9-C11-C12-C13
7	L	501	U10	C34-C36-C37-C38
5	M	1301	BCL	C14-C13-C15-C16
6	M	402	BPH	C6-C7-C8-C9
5	L	1302	BCL	C6-C7-C8-C9
6	L	401	BPH	C14-C13-C15-C16
10	M	800	CDL	C31-CA7-OA8-CA6
10	M	800	CDL	CA7-C31-C32-C33
10	M	800	CDL	CB7-C71-C72-C73
6	M	402	BPH	C15-C16-C17-C18
5	M	1301	BCL	C6-C7-C8-C10
6	M	402	BPH	C12-C13-C15-C16
6	L	401	BPH	C11-C10-C8-C7
5	M	1301	BCL	C5-C6-C7-C8
7	M	502	U10	C29-C31-C32-C33
10	M	800	CDL	OA9-CA7-OA8-CA6
5	M	1301	BCL	C8-C10-C11-C12
10	M	800	CDL	CA2-OA2-PA1-OA5
10	M	800	CDL	CA5-C11-C12-C13
10	M	800	CDL	C11-C12-C13-C14
6	M	402	BPH	C2B-C3B-CAB-CBB
5	M	1301	BCL	C13-C15-C16-C17
10	M	800	CDL	C78-C79-C80-C81
10	M	800	CDL	C79-C80-C81-C82
10	M	800	CDL	C51-C52-C53-C54
4	M	702	LDA	C6-C7-C8-C9
4	M	702	LDA	C7-C8-C9-C10
6	M	402	BPH	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	M	702	LDA	C5-C6-C7-C8
4	H	701	LDA	C4-C5-C6-C7
6	M	402	BPH	O1D-CGD-O2D-CED
9	M	600	SPN	C26-C27-C28-C29
10	M	800	CDL	C52-C53-C54-C55
4	M	703	LDA	C6-C7-C8-C9
6	M	402	BPH	CBA-CGA-O2A-C1
4	M	702	LDA	C11-C10-C9-C8
7	L	501	U10	C15-C14-C16-C17
7	L	501	U10	C40-C39-C41-C42
7	L	501	U10	C13-C14-C16-C17
10	M	800	CDL	C39-C40-C41-C42
5	M	1301	BCL	C2-C1-O2A-CGA
5	L	1304	BCL	C3-C5-C6-C7
10	M	800	CDL	C37-C38-C39-C40
7	M	502	U10	C30-C29-C31-C32
7	M	502	U10	C28-C29-C31-C32
6	M	402	BPH	C11-C10-C8-C7
7	L	501	U10	C38-C39-C41-C42
4	H	701	LDA	C1-C2-C3-C4
10	M	800	CDL	C21-C22-C23-C24
5	L	1302	BCL	C2A-CAA-CBA-CGA
4	H	701	LDA	C5-C6-C7-C8
4	M	703	LDA	C3-C4-C5-C6
5	L	1304	BCL	C6-C7-C8-C9
6	M	402	BPH	C11-C10-C8-C9
6	M	402	BPH	C14-C13-C15-C16
4	H	701	LDA	C6-C7-C8-C9
4	M	703	LDA	C1-C2-C3-C4
4	M	702	LDA	C2-C3-C4-C5
4	M	703	LDA	C11-C10-C9-C8
6	L	401	BPH	C2C-C3C-CAC-CBC
6	L	401	BPH	C2-C3-C5-C6
10	M	800	CDL	CB3-CB4-CB6-OB8
10	M	800	CDL	C81-C82-C83-C84
6	L	401	BPH	C10-C11-C12-C13
5	L	1302	BCL	C15-C16-C17-C18
6	L	401	BPH	C4-C3-C5-C6
6	L	401	BPH	C8-C10-C11-C12
4	M	702	LDA	C9-C10-C11-C12
6	L	401	BPH	C5-C6-C7-C8
5	M	1301	BCL	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	L	401	BPH	C11-C10-C8-C9
5	L	1302	BCL	CBD-CGD-O2D-CED
10	M	800	CDL	C71-C72-C73-C74
9	M	600	SPN	CM2-C1-C2-O2
9	M	600	SPN	CM2-C1-C2-C3
5	M	1301	BCL	C15-C16-C17-C18
4	M	702	LDA	C1-C2-C3-C4
10	M	800	CDL	OB6-CB4-CB6-OB8
9	M	600	SPN	C9-C10-C11-C12
5	M	1303	BCL	C5-C6-C7-C8
10	M	800	CDL	C40-C41-C42-C43
10	M	800	CDL	C53-C54-C55-C56
5	L	1302	BCL	C11-C12-C13-C15
5	L	1304	BCL	C13-C15-C16-C17
5	M	1303	BCL	CAD-CBD-CGD-O2D
4	H	701	LDA	C2-C3-C4-C5
10	M	800	CDL	OA5-CA3-CA4-OA6
10	M	800	CDL	C35-C36-C37-C38
4	H	701	LDA	C2-C1-N1-CM1
9	M	600	SPN	CM2-C1-O1-CMA
5	L	1302	BCL	C13-C15-C16-C17
5	M	1301	BCL	C11-C12-C13-C14
5	M	1303	BCL	C16-C17-C18-C19
10	M	800	CDL	C36-C37-C38-C39
7	L	501	U10	C2-C3-O3-C3M
5	L	1304	BCL	O1D-CGD-O2D-CED
10	M	800	CDL	CB5-C51-C52-C53
6	M	402	BPH	C13-C15-C16-C17
6	M	402	BPH	C8-C10-C11-C12
10	M	800	CDL	OA6-CA4-CA6-OA8
10	M	800	CDL	C75-C76-C77-C78
6	M	402	BPH	C11-C12-C13-C15
6	L	401	BPH	C11-C12-C13-C15
5	L	1302	BCL	C11-C12-C13-C14
6	M	402	BPH	C5-C6-C7-C8
5	L	1304	BCL	C16-C17-C18-C19
4	M	702	LDA	C4-C5-C6-C7
4	M	703	LDA	C9-C10-C11-C12
6	M	402	BPH	C2-C1-O2A-CGA
10	M	800	CDL	C80-C81-C82-C83
7	M	502	U10	C5-C4-O4-C4M
4	H	701	LDA	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	M	402	BPH	O2A-C1-C2-C3
6	M	402	BPH	C6-C7-C8-C10
6	L	401	BPH	C12-C13-C15-C16
5	M	1301	BCL	O1A-CGA-O2A-C1
5	M	1301	BCL	C3-C5-C6-C7
9	M	600	SPN	C2-C3-C4-C5
10	M	800	CDL	OA5-CA3-CA4-CA6
7	M	502	U10	C34-C36-C37-C38
6	L	401	BPH	C1-C2-C3-C4
7	L	501	U10	C4-C3-O3-C3M
7	L	501	U10	C30-C29-C31-C32
5	M	1301	BCL	CAD-CBD-CGD-O2D
5	L	1302	BCL	CAD-CBD-CGD-O2D
5	M	1301	BCL	CBA-CGA-O2A-C1
10	M	800	CDL	C32-C31-CA7-OA8
10	M	800	CDL	C72-C71-CB7-OB8
5	L	1304	BCL	CHA-CBD-CGD-O2D
6	M	402	BPH	CHA-CBD-CGD-O2D
6	L	401	BPH	CHA-CBD-CGD-O2D
7	L	501	U10	C28-C29-C31-C32
4	H	701	LDA	C7-C8-C9-C10
7	L	501	U10	C16-C17-C18-C19
4	H	701	LDA	C11-C10-C9-C8
5	M	1303	BCL	C11-C12-C13-C15
5	M	1301	BCL	C12-C13-C15-C16
10	M	800	CDL	C72-C71-CB7-OB9
9	M	600	SPN	C6-C7-C8-C9
5	L	1304	BCL	C16-C17-C18-C20
10	M	800	CDL	C32-C31-CA7-OA9
9	M	600	SPN	C18-C19-C20-C21
5	M	1303	BCL	CAA-CBA-CGA-O2A
5	M	1303	BCL	CAD-CBD-CGD-O1D
10	M	800	CDL	C19-C20-C21-C22
5	L	1304	BCL	C12-C13-C15-C16
5	L	1302	BCL	C11-C10-C8-C7

There are no ring outliers.

11 monomers are involved in 62 short contacts:

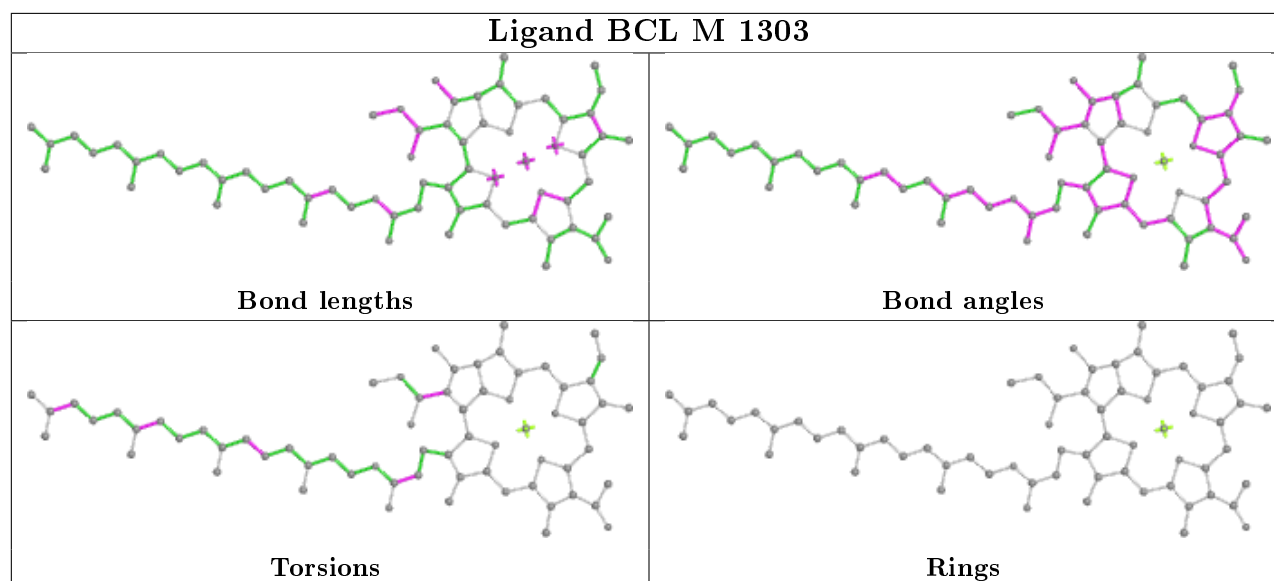
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	703	LDA	2	0
4	M	702	LDA	3	0

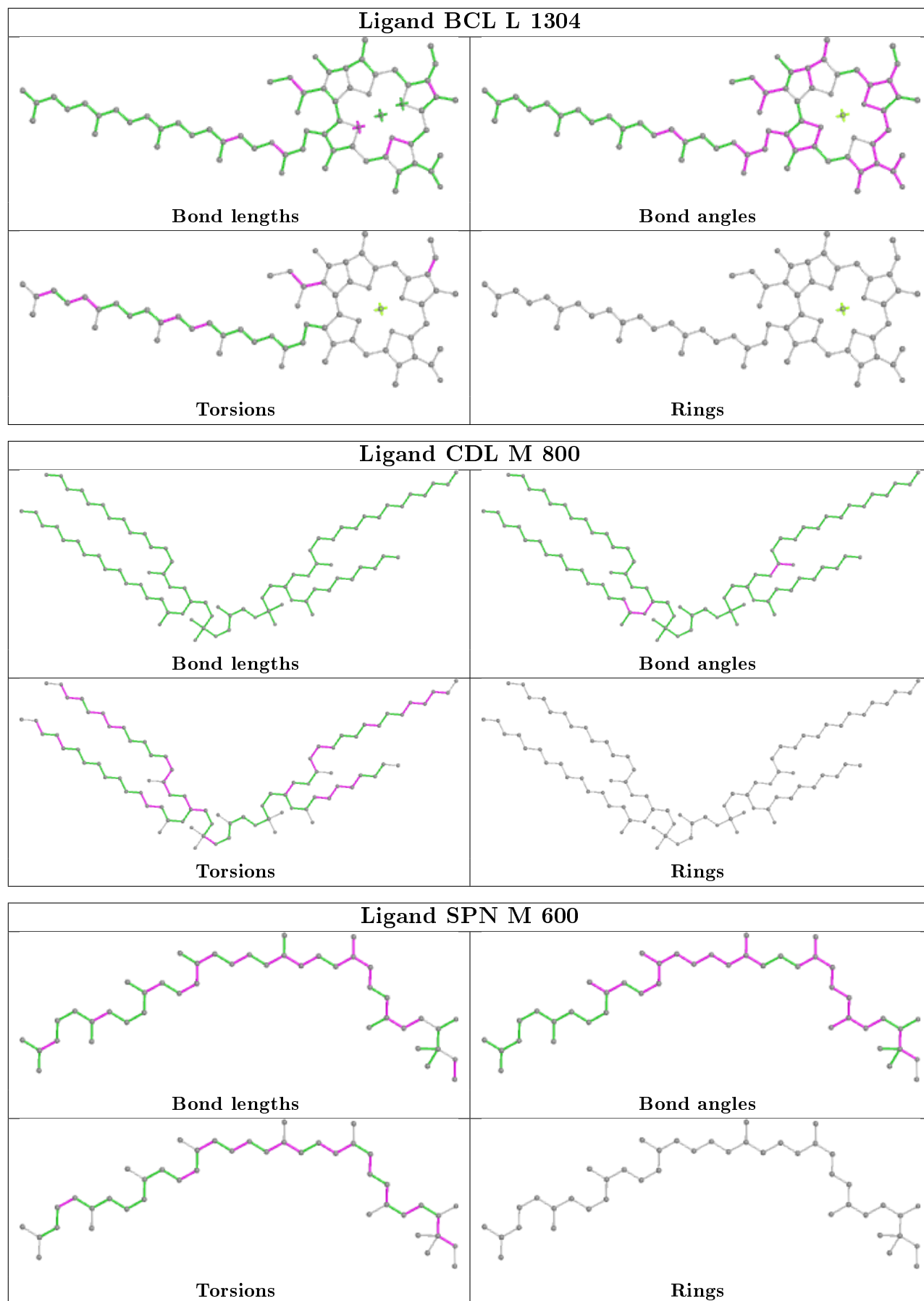
Continued on next page...

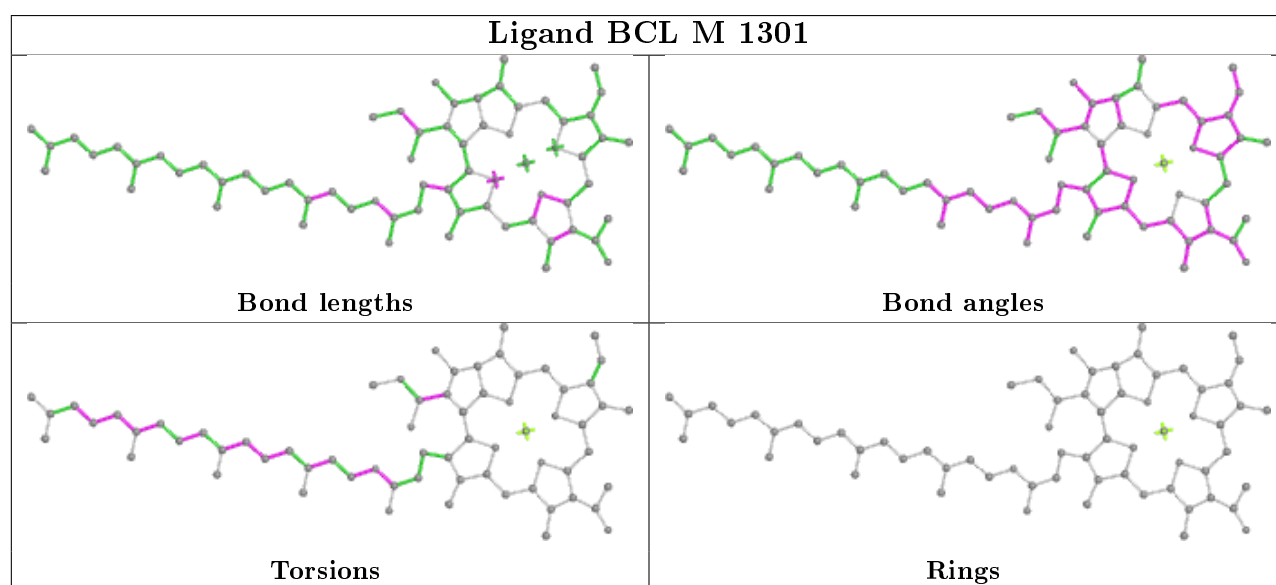
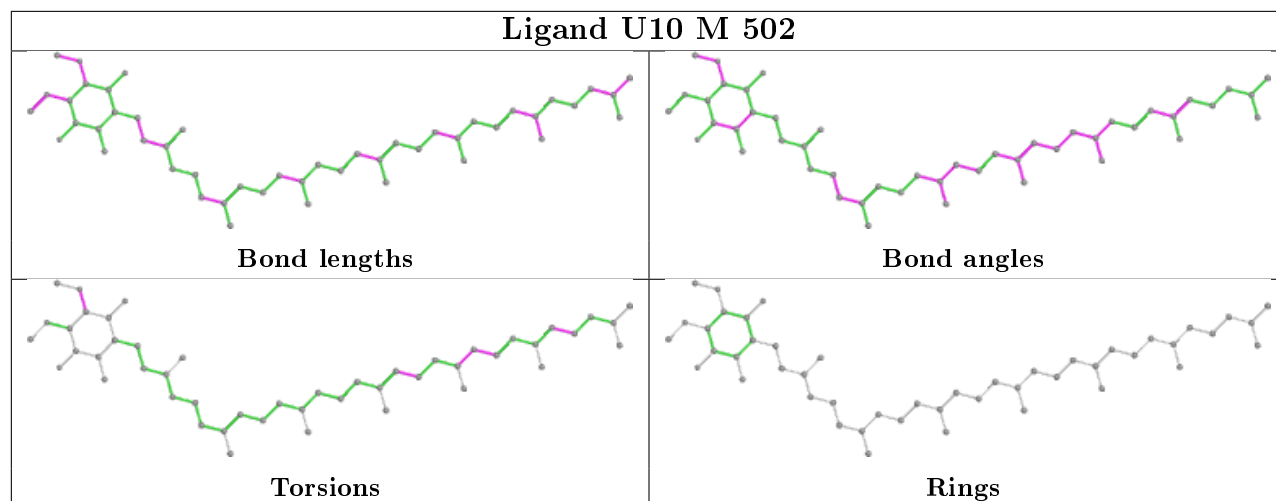
Continued from previous page...

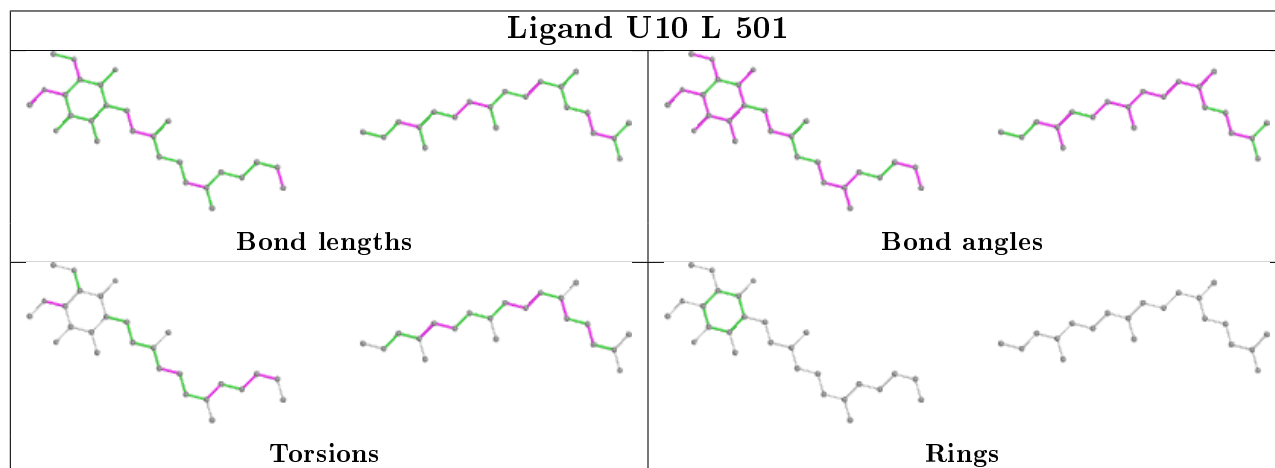
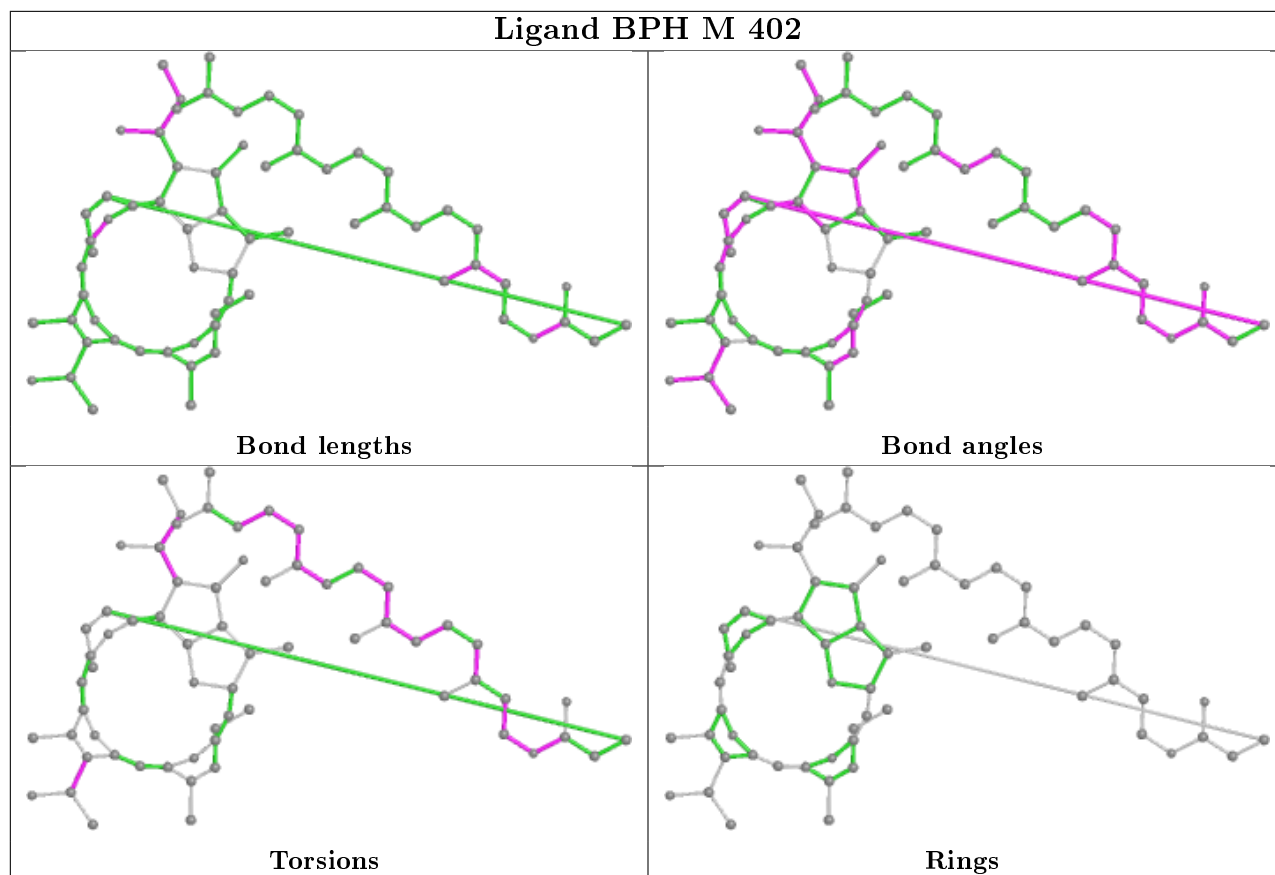
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1303	BCL	6	0
5	L	1304	BCL	8	0
10	M	800	CDL	16	0
9	M	600	SPN	5	0
5	M	1301	BCL	5	0
6	M	402	BPH	3	0
7	L	501	U10	1	0
5	L	1302	BCL	9	0
6	L	401	BPH	10	0

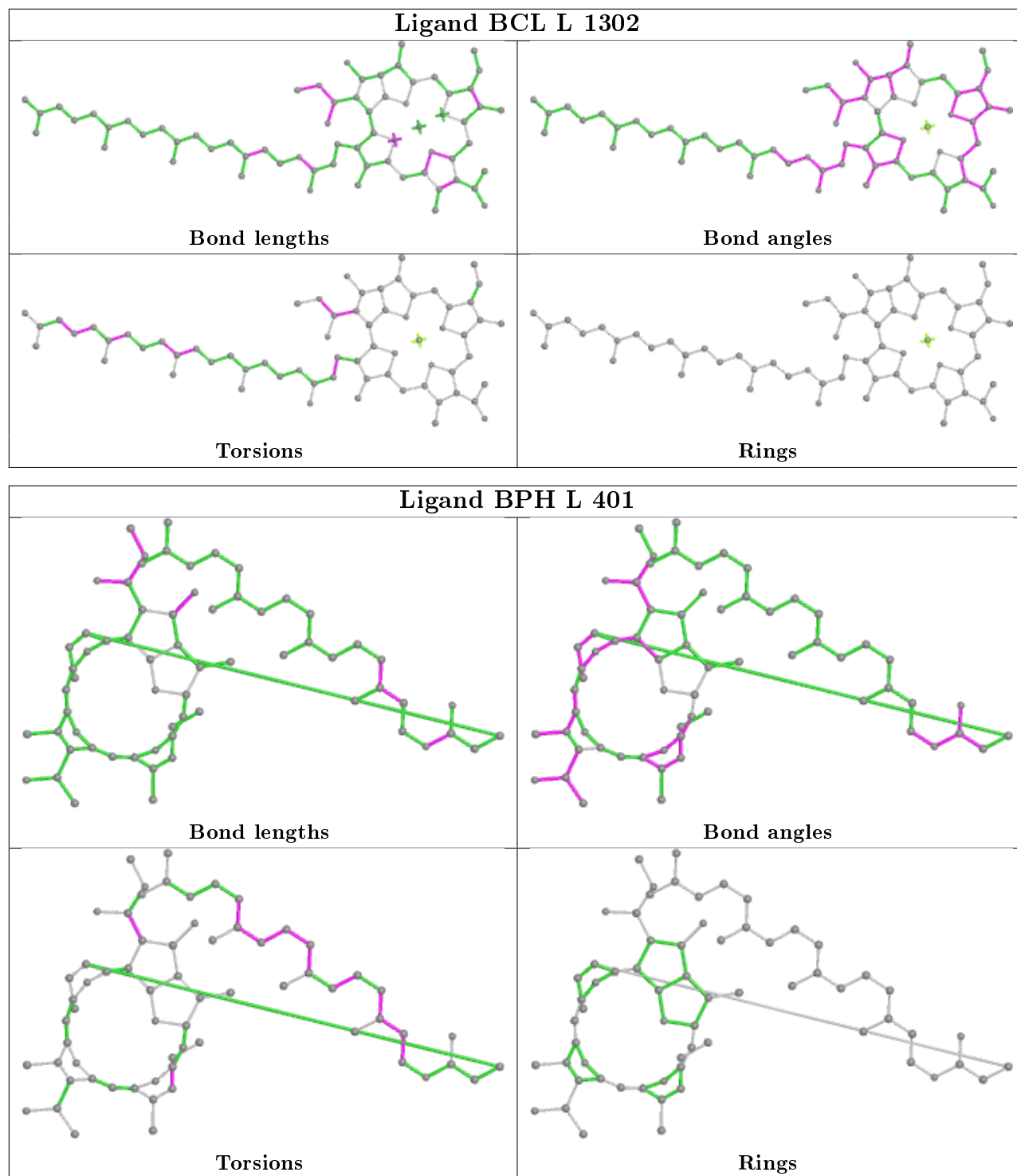
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.