



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 06:53 PM EDT

PDB ID : 1RZZ
Title : PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG M233 REPLACED WITH CYS IN THE CHARGE-NEUTRAL DQAQB STATE (TETRAGONAL FORM)
Authors : Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.
Deposited on : 2003-12-29
Resolution : 2.40 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)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

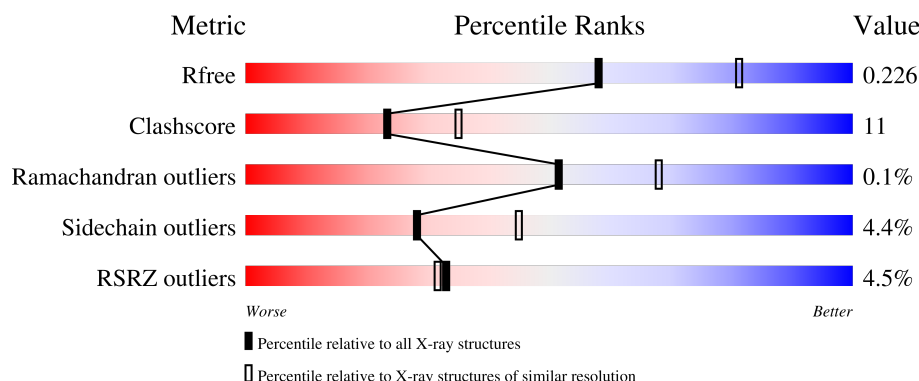
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	281	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>.</div> </div> </div>
1	R	281	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
2	M	307	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>..</div> </div> </div>
2	S	307	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>..</div> </div> </div>
3	H	260	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>5%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	T	260	

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	U10	R	2009	-	-	-	X
7	BPH	M	1005	X	-	-	-
7	BPH	M	1006	X	-	-	-
7	BPH	R	2006	X	-	-	-
7	BPH	S	2005	X	-	-	-
9	LDA	S	2011	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14481 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 L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	356	361	8			
1	R	281	Total	C	N	O	S	0	0	0
			2232	1507	356	361	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	213	ASN	ASP	engineered mutation	UNP P02954
R	213	ASN	ASP	engineered mutation	UNP P02954

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	299	Total	C	N	O	S	0	0	0
			2385	1594	388	392	11			
2	S	299	Total	C	N	O	S	0	0	0
			2385	1594	388	392	11			

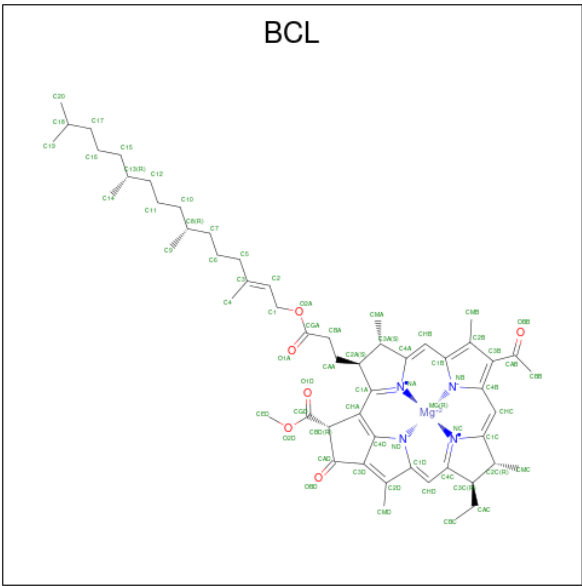
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	233	CYS	ARG	engineered mutation	UNP P02953
S	233	CYS	ARG	engineered mutation	UNP P02953

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

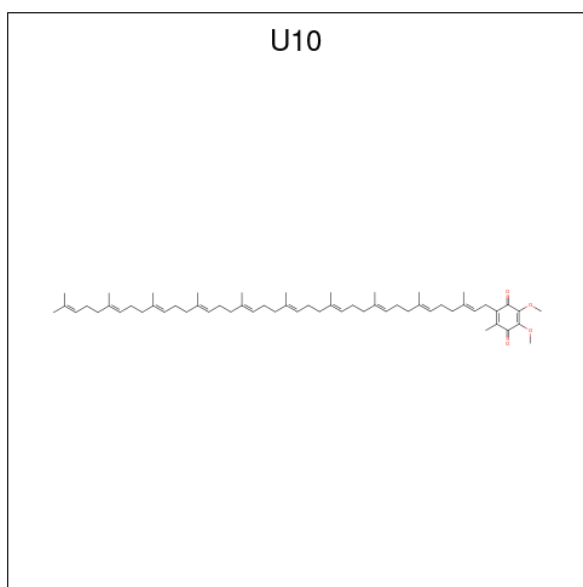
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			
3	T	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	S	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).

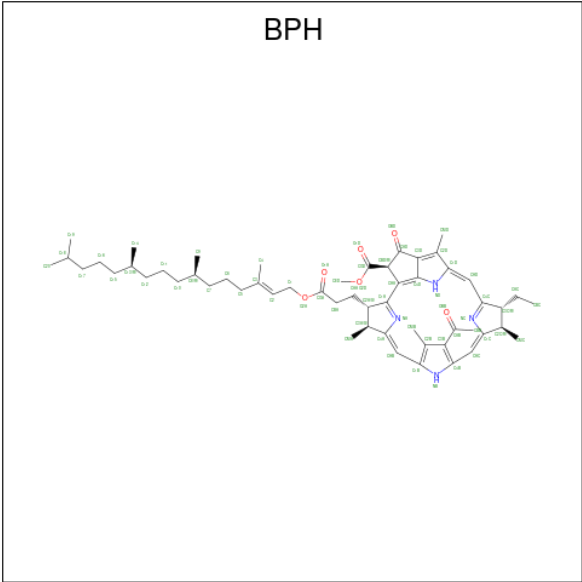


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			44	40	4		
5	M	1	Total	C	O	0	0
			38	34	4		
5	R	1	Total	C	O	0	0
			18	14	4		
5	S	1	Total	C	O	0	0
			32	28	4		

- Molecule 6 is FE (II) ION (three-letter code: FE2) (formula: Fe).

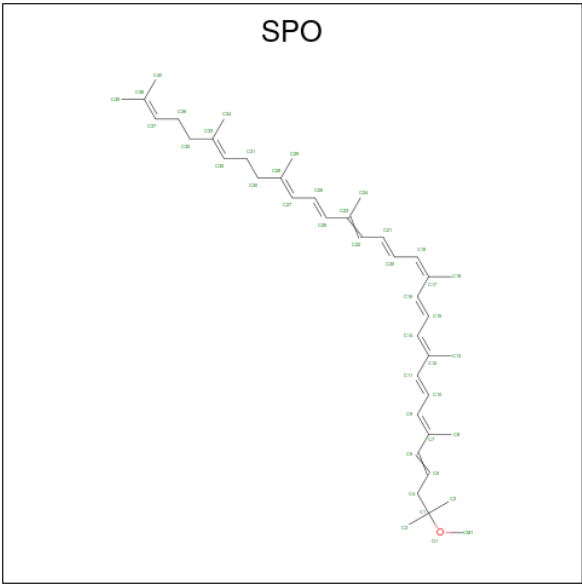
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Fe	0	0
			1	1		
6	S	1	Total	Fe	0	0
			1	1		

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



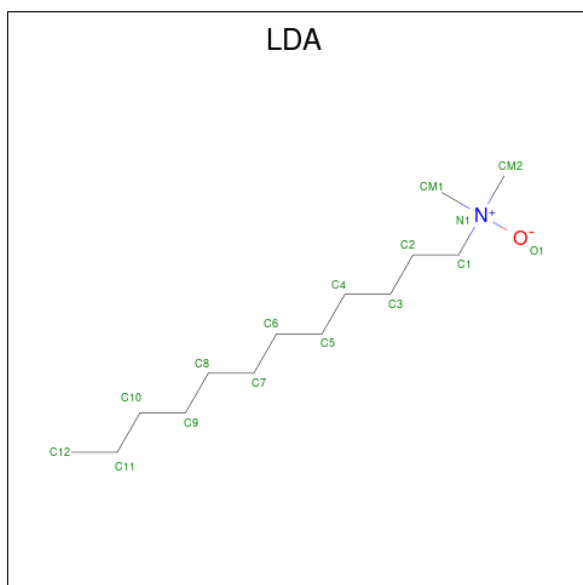
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			55	45	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		
7	R	1	Total	C	N	O	0	0
			65	55	4	6		
7	S	1	Total	C	N	O	0	0
			55	45	4	6		

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			42	41	1		
8	S	1	Total	C	O	0	0
			42	41	1		

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	S	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	72	Total	O	0	0
			72	72		
10	M	107	Total	O	0	0
			107	107		

Continued on next page...

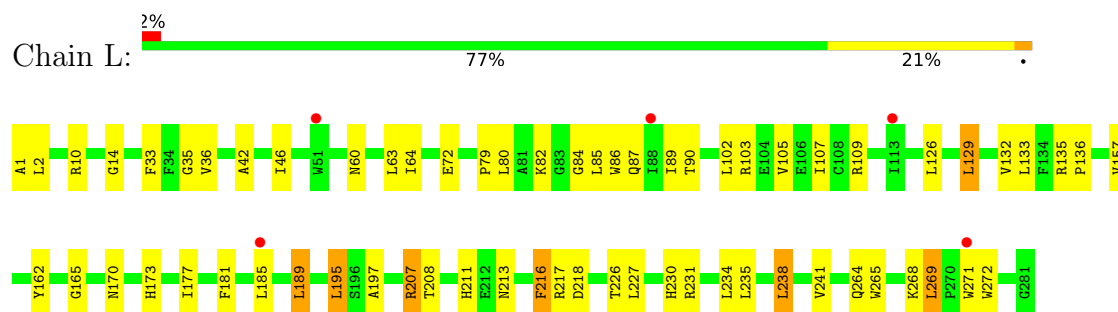
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	109	Total 109	O 109	0	0
10	R	47	Total 47	O 47	0	0
10	S	75	Total 75	O 75	0	0
10	T	63	Total 63	O 63	0	0

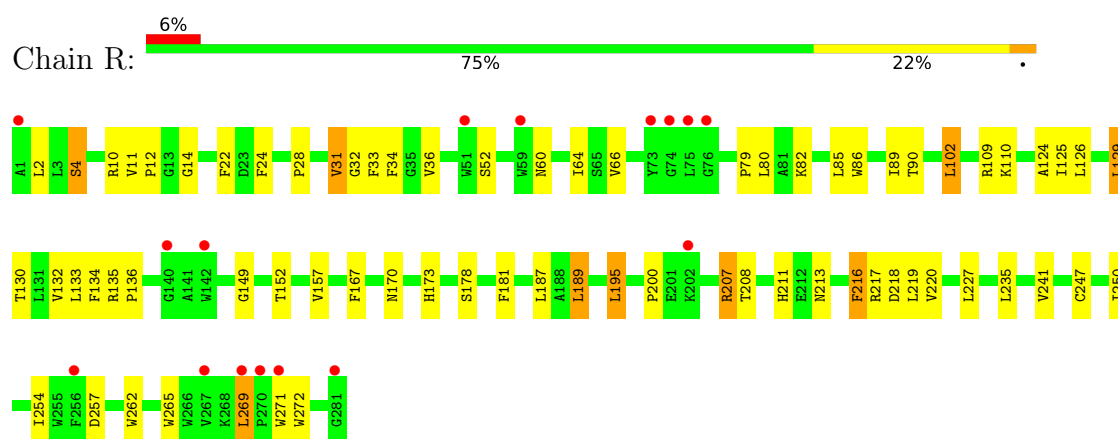
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

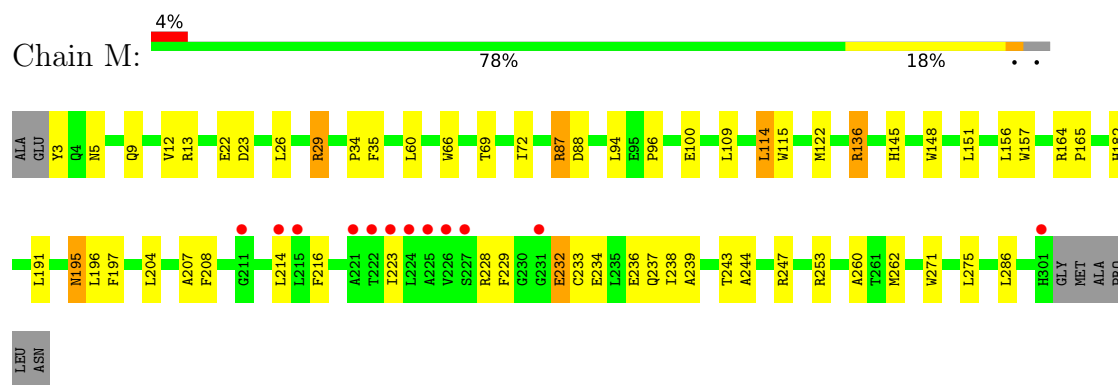
- Molecule 1: Reaction center protein L chain



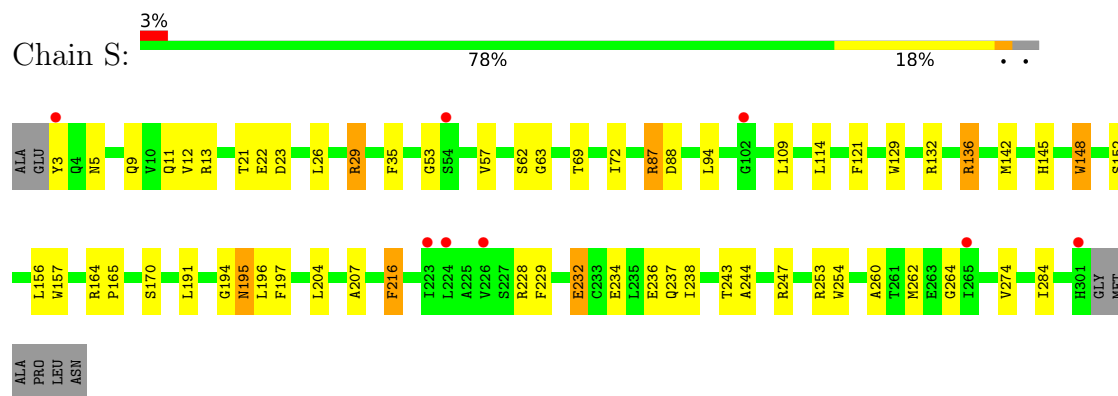
- Molecule 1: Reaction center protein L chain



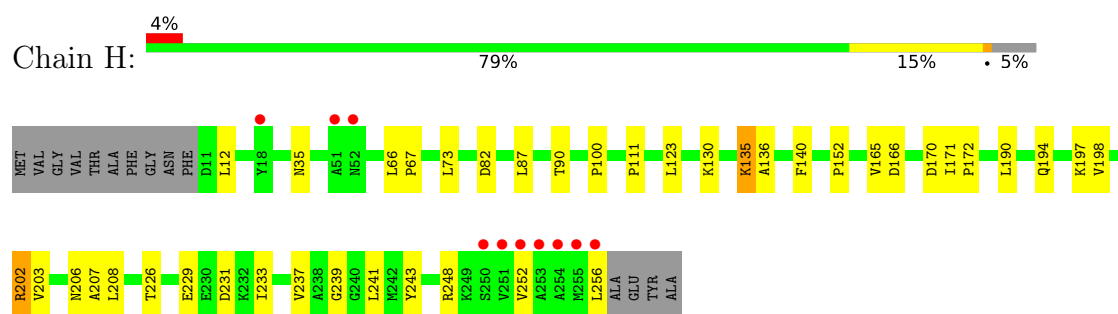
- Molecule 2: Reaction center protein M chain



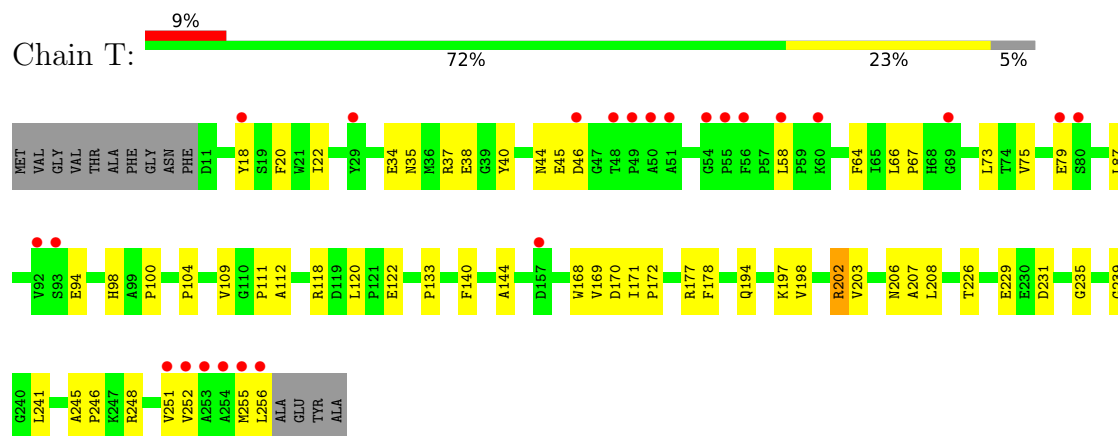
- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



- Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.58Å 139.58Å 274.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.76 – 2.40 39.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.76-2.40) 98.3 (39.76-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.238 0.200 , 0.226	Depositor DCC
R_{free} test set	5283 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14481	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BPH, U10, SPO, LDA, BCL, FE2

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	L	0.42	0/2320	0.57	0/3175
1	R	0.37	0/2320	0.55	0/3175
2	M	0.41	0/2477	0.56	0/3383
2	S	0.39	0/2477	0.53	0/3383
3	H	0.35	0/1917	0.60	0/2608
3	T	0.31	0/1917	0.56	0/2608
All	All	0.38	0/13428	0.56	0/18332

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	L	2232	0	2189	57	0
1	R	2232	0	2189	60	0
2	M	2385	0	2296	51	0
2	S	2385	0	2296	63	0
3	H	1869	0	1884	36	0
3	T	1869	0	1884	52	0
4	L	183	0	189	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	66	0	74	13	0
4	R	66	0	74	5	0
4	S	183	0	189	21	0
5	L	44	0	56	3	0
5	M	38	0	47	4	0
5	R	18	0	15	0	0
5	S	32	0	39	1	0
6	M	1	0	0	0	0
6	S	1	0	0	0	0
7	M	120	0	127	6	0
7	R	65	0	74	5	0
7	S	55	0	53	2	0
8	M	42	0	60	4	0
8	S	42	0	60	3	0
9	M	64	0	124	3	0
9	S	16	0	31	0	0
10	H	109	0	0	1	0
10	L	72	0	0	1	0
10	M	107	0	0	2	0
10	R	47	0	0	2	0
10	S	75	0	0	3	0
10	T	63	0	0	1	0
All	All	14481	0	13950	317	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 11.

All (317) 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:R:241:VAL:HG21	7:R:2006:BPH:HAC1	1.40	1.03
1:L:241:VAL:HG21	7:M:1006:BPH:HAC2	1.38	1.01
2:M:109:LEU:HD12	2:M:114:LEU:HD13	1.56	0.86
2:S:157:TRP:HB2	4:S:2003:BCL:H62	1.58	0.84
4:S:2001:BCL:HBC1	4:S:2003:BCL:CAD	2.09	0.82
1:R:79:PRO:HG2	1:R:82:LYS:HB2	1.61	0.82
1:R:208:THR:H	1:R:211:HIS:HD2	1.28	0.81
2:S:207:ALA:HA	4:S:2004:BCL:O1A	1.81	0.80
2:S:21:THR:HG23	2:S:26:LEU:HD11	1.63	0.80
1:R:227:LEU:HD13	2:S:232:GLU:HG2	1.64	0.80
2:S:13:ARG:HD2	2:S:35:PHE:CD2	2.18	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:208:THR:H	1:R:211:HIS:CD2	2.01	0.78
2:M:157:TRP:HB2	4:M:1003:BCL:H62	1.65	0.77
1:R:52:SER:HB2	1:R:85:LEU:HD23	1.66	0.77
1:L:189:LEU:HG	1:L:216:PHE:HZ	1.50	0.76
1:L:217:ARG:HD2	10:M:1043:HOH:O	1.85	0.75
5:M:1008:U10:H202	9:M:1012:LDA:H123	1.68	0.75
2:S:197:PHE:HZ	4:S:2003:BCL:HBB2	1.50	0.75
1:L:79:PRO:HG2	1:L:82:LYS:HB2	1.69	0.74
1:R:189:LEU:HG	1:R:216:PHE:HZ	1.53	0.73
1:R:2:LEU:HG	1:R:10:ARG:NH1	2.04	0.73
2:M:197:PHE:HZ	4:M:1003:BCL:HBB2	1.54	0.72
4:L:1001:BCL:HBB3	4:M:1003:BCL:H41	1.72	0.71
3:H:202:ARG:HG2	3:H:203:VAL:N	2.06	0.71
4:R:2002:BCL:HBD	4:S:2004:BCL:HBC1	1.73	0.70
1:R:217:ARG:HD2	10:S:2014:HOH:O	1.92	0.70
2:S:63:GLY:HA3	7:S:2005:BPH:H5C2	1.74	0.70
2:M:253:ARG:HD3	10:M:1016:HOH:O	1.91	0.69
4:L:1002:BCL:HBD	4:L:1004:BCL:CBC	2.21	0.69
2:S:136:ARG:HA	2:S:136:ARG:NE	2.07	0.69
3:H:252:VAL:O	3:H:256:LEU:HD13	1.92	0.68
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.75	0.68
4:L:1004:BCL:HMA1	4:L:1004:BCL:H121	1.76	0.68
3:T:226:THR:OG1	3:T:229:GLU:HG3	1.94	0.68
3:T:44:ASN:HB2	3:T:46:ASP:OD1	1.94	0.67
3:T:202:ARG:HG2	3:T:203:VAL:N	2.09	0.67
10:R:2021:HOH:O	2:S:253:ARG:HD3	1.94	0.67
1:L:105:VAL:O	1:L:109:ARG:HG3	1.94	0.67
2:S:228:ARG:HA	3:T:194:GLN:CG	2.25	0.66
2:S:243:THR:O	2:S:247:ARG:HG3	1.94	0.66
3:T:73:LEU:HD11	3:T:75:VAL:HG13	1.77	0.66
1:R:135:ARG:HB3	1:R:136:PRO:HD3	1.77	0.66
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.77	0.66
2:S:9:GLN:NE2	3:T:198:VAL:H	1.94	0.66
2:M:9:GLN:NE2	3:H:198:VAL:H	1.93	0.65
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.78	0.65
3:T:252:VAL:O	3:T:256:LEU:HD13	1.97	0.65
2:M:197:PHE:CZ	4:M:1003:BCL:HBB2	2.32	0.65
4:R:2002:BCL:HBD	4:S:2004:BCL:CBC	2.27	0.65
2:M:136:ARG:NE	2:M:136:ARG:HA	2.10	0.64
1:L:86:TRP:CH2	1:L:132:VAL:HG13	2.33	0.64
1:L:80:LEU:H	1:L:80:LEU:HD22	1.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:14:GLY:O	1:R:109:ARG:HD3	1.97	0.64
1:L:208:THR:H	1:L:211:HIS:CD2	2.16	0.63
2:M:13:ARG:HD2	2:M:35:PHE:CD2	2.33	0.63
1:L:185:LEU:HD23	4:L:1001:BCL:H42	1.80	0.63
4:S:2001:BCL:HBB3	4:S:2003:BCL:H41	1.79	0.63
2:S:109:LEU:HD12	2:S:114:LEU:HD13	1.80	0.63
1:L:33:PHE:O	1:L:36:VAL:HG22	1.98	0.62
4:L:1004:BCL:O1A	2:M:207:ALA:HA	1.99	0.62
4:L:1001:BCL:HBC1	4:M:1003:BCL:CBF	2.29	0.62
3:T:118:ARG:HD3	3:T:120:LEU:HD12	1.80	0.62
2:M:9:GLN:HE22	3:H:197:LYS:HA	1.64	0.61
1:L:189:LEU:HB3	5:L:1009:U10:H4M3	1.81	0.61
2:S:69:THR:O	2:S:72:ILE:HG22	2.00	0.61
2:S:195:ASN:ND2	2:S:197:PHE:H	1.98	0.61
4:L:1002:BCL:HBD	4:L:1004:BCL:HBC1	1.82	0.61
1:L:84:GLY:HA2	1:L:87:GLN:HE21	1.64	0.60
2:M:208:PHE:HE1	9:M:1014:LDA:H101	1.65	0.60
4:L:1004:BCL:H61	5:M:1008:U10:H203	1.84	0.60
1:L:86:TRP:CZ2	1:L:132:VAL:HG13	2.36	0.60
1:L:208:THR:H	1:L:211:HIS:HD2	1.48	0.60
2:S:236:GLU:HG3	3:T:122:GLU:OE2	2.01	0.60
1:L:60:ASN:CG	1:L:63:LEU:HD23	2.22	0.59
2:M:243:THR:O	2:M:247:ARG:HG3	2.03	0.59
1:L:265:TRP:O	1:L:269:LEU:HD13	2.02	0.59
2:M:228:ARG:HA	3:H:194:GLN:HG2	1.85	0.59
2:S:9:GLN:HE22	3:T:198:VAL:H	1.50	0.59
3:T:87:LEU:HD23	3:T:100:PRO:HA	1.84	0.58
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.05	0.57
1:L:14:GLY:O	1:L:109:ARG:HD3	2.05	0.57
3:T:194:GLN:CD	3:T:194:GLN:H	2.07	0.57
1:R:178:SER:HA	4:S:2001:BCL:O1A	2.05	0.57
2:M:69:THR:O	2:M:72:ILE:HG22	2.04	0.56
2:S:157:TRP:HB2	4:S:2003:BCL:C6	2.30	0.56
1:R:28:PRO:HB3	2:S:253:ARG:NH1	2.20	0.56
4:L:1002:BCL:HBD	4:L:1004:BCL:HBC3	1.85	0.56
3:H:135:LYS:NZ	3:H:135:LYS:HB3	2.20	0.56
3:T:37:ARG:O	3:T:38:GLU:HG2	2.06	0.56
3:T:133:PRO:HG3	3:T:168:TRP:CZ2	2.40	0.56
4:L:1001:BCL:HBC1	4:M:1003:BCL:HBD	1.88	0.56
2:S:228:ARG:HA	3:T:194:GLN:HG3	1.86	0.56
4:L:1001:BCL:HBC1	4:M:1003:BCL:CAD	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:218:ASP:OD1	2:M:29:ARG:HD2	2.05	0.56
2:S:197:PHE:CZ	4:S:2003:BCL:HBB2	2.35	0.56
3:T:133:PRO:HG3	3:T:168:TRP:CE2	2.41	0.56
1:L:60:ASN:O	1:L:64:ILE:HG13	2.06	0.56
2:M:157:TRP:HB2	4:M:1003:BCL:C6	2.35	0.56
1:L:157:VAL:HG11	4:M:1003:BCL:HBB1	1.87	0.55
3:T:45:GLU:HG3	3:T:94:GLU:OE1	2.06	0.55
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.71	0.55
2:S:264:GLY:HA3	3:T:35:ASN:OD1	2.06	0.55
1:L:60:ASN:ND2	1:L:63:LEU:HD23	2.22	0.55
1:R:218:ASP:OD1	2:S:29:ARG:HD2	2.07	0.55
3:T:73:LEU:CD1	3:T:75:VAL:HG13	2.35	0.55
2:S:12:VAL:HG21	3:T:169:VAL:HG21	1.89	0.54
2:S:195:ASN:C	2:S:195:ASN:HD22	2.09	0.54
1:R:170:ASN:HB3	1:R:173:HIS:CB	2.38	0.54
1:R:265:TRP:O	1:R:269:LEU:HD13	2.08	0.54
2:S:152:SER:HB2	2:S:274:VAL:HG13	1.89	0.54
1:L:269:LEU:HD23	1:L:271:TRP:CZ2	2.44	0.53
3:T:241:LEU:O	3:T:248:ARG:NH2	2.41	0.53
1:L:103:ARG:O	1:L:107:ILE:HG13	2.07	0.53
1:L:264:GLN:OE1	1:L:268:LYS:HE2	2.08	0.53
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.08	0.53
2:S:9:GLN:HE22	3:T:197:LYS:HA	1.73	0.53
3:T:37:ARG:HH11	3:T:37:ARG:HG2	1.73	0.53
1:R:213:ASN:O	1:R:217:ARG:HB2	2.08	0.53
3:T:251:VAL:O	3:T:255:MET:HG3	2.09	0.53
1:L:80:LEU:H	1:L:80:LEU:CD2	2.22	0.53
1:R:189:LEU:HG	1:R:216:PHE:CZ	2.41	0.52
4:L:1002:BCL:H122	7:M:1006:BPH:H3A	1.92	0.52
3:H:152:PRO:HG2	3:H:202:ARG:HB2	1.91	0.52
1:R:157:VAL:HG11	4:S:2003:BCL:HBB1	1.91	0.52
2:S:157:TRP:HD1	4:S:2001:BCL:HBB1	1.73	0.52
2:S:152:SER:CB	2:S:274:VAL:HG13	2.40	0.52
3:T:168:TRP:HB2	3:T:178:PHE:HB2	1.90	0.52
3:T:171:ILE:HB	3:T:172:PRO:HD3	1.92	0.52
3:H:66:LEU:HD22	3:H:66:LEU:N	2.25	0.52
1:L:213:ASN:O	1:L:217:ARG:HB2	2.10	0.51
1:L:238:LEU:HD12	7:M:1006:BPH:CBC	2.41	0.51
1:R:269:LEU:HD23	1:R:271:TRP:CZ2	2.45	0.51
2:M:271:TRP:O	2:M:275:LEU:HG	2.11	0.51
1:R:33:PHE:O	1:R:36:VAL:HG22	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:241:LEU:O	3:H:248:ARG:NH2	2.44	0.51
1:R:22:PHE:HA	1:R:24:PHE:CE2	2.45	0.51
1:R:257:ASP:HB3	10:R:2056:HOH:O	2.10	0.51
3:H:207:ALA:O	3:H:208:LEU:HD12	2.11	0.51
2:S:164:ARG:HB3	2:S:165:PRO:HD3	1.94	0.50
1:L:85:LEU:O	1:L:89:ILE:HG13	2.10	0.50
2:S:13:ARG:O	3:T:140:PHE:HA	2.11	0.50
2:S:284:ILE:HG12	4:S:2003:BCL:HED3	1.93	0.50
1:L:216:PHE:CE1	5:L:1009:U10:H4M2	2.46	0.50
3:H:194:GLN:CD	3:H:194:GLN:H	2.14	0.50
2:M:9:GLN:HE22	3:H:198:VAL:H	1.57	0.50
4:R:2002:BCL:H122	7:R:2006:BPH:H3A	1.93	0.50
1:L:189:LEU:HG	1:L:216:PHE:CZ	2.40	0.50
1:R:85:LEU:O	1:R:89:ILE:HG13	2.12	0.50
4:S:2004:BCL:H121	4:S:2004:BCL:HMA1	1.93	0.50
1:R:80:LEU:HB3	1:R:85:LEU:HD13	1.92	0.50
2:S:21:THR:HG23	2:S:26:LEU:CD1	2.38	0.50
1:L:72:GLU:HG3	10:L:1062:HOH:O	2.11	0.49
4:L:1001:BCL:HBB2	8:M:1010:SPO:H243	1.94	0.49
3:H:135:LYS:NZ	3:H:135:LYS:CB	2.75	0.49
2:M:195:ASN:ND2	2:M:197:PHE:H	2.10	0.49
1:L:231:ARG:HD2	2:M:5:ASN:O	2.13	0.49
3:H:82:ASP:OD1	3:H:82:ASP:N	2.45	0.49
1:R:28:PRO:HB3	2:S:253:ARG:HH11	1.75	0.49
4:R:2002:BCL:H52	7:R:2006:BPH:HBB2	1.94	0.49
2:S:3:TYR:CE1	2:S:9:GLN:HG3	2.47	0.49
3:T:37:ARG:HG2	3:T:37:ARG:NH1	2.28	0.49
1:L:1:ALA:C	1:L:2:LEU:HD12	2.34	0.49
3:H:66:LEU:HD22	3:H:66:LEU:H	1.77	0.49
4:L:1001:BCL:HBB2	4:L:1001:BCL:HHC	1.95	0.48
2:M:208:PHE:CE1	9:M:1014:LDA:H101	2.46	0.48
2:M:3:TYR:CE1	2:M:9:GLN:HG3	2.47	0.48
1:R:80:LEU:O	1:R:85:LEU:HB2	2.12	0.48
1:R:195:LEU:HB3	2:S:145:HIS:CD2	2.47	0.48
1:L:162:TYR:HA	1:L:165:GLY:O	2.13	0.48
1:R:80:LEU:H	1:R:80:LEU:HD22	1.78	0.48
3:T:170:ASP:HB2	3:T:177:ARG:HG3	1.96	0.48
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.94	0.48
1:R:133:LEU:C	1:R:133:LEU:HD23	2.34	0.48
4:S:2001:BCL:HBB2	8:S:2010:SPO:H243	1.95	0.48
3:T:118:ARG:HG2	3:T:120:LEU:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90:THR:CG2	1:L:132:VAL:HG11	2.44	0.48
2:M:195:ASN:HD22	2:M:195:ASN:C	2.17	0.48
3:T:206:ASN:HD21	3:T:248:ARG:HD2	1.79	0.47
2:M:114:LEU:HD12	2:M:114:LEU:HA	1.73	0.47
4:L:1002:BCL:HAA2	4:L:1004:BCL:HBC1	1.97	0.47
1:R:125:ILE:HG22	1:R:129:LEU:HD22	1.96	0.47
3:T:34:GLU:HA	3:T:34:GLU:OE1	2.13	0.47
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.50	0.47
2:M:237:GLN:HB2	2:M:262:MET:HG2	1.96	0.47
1:R:181:PHE:CZ	4:S:2003:BCL:O1A	2.68	0.47
1:R:241:VAL:CG2	7:R:2006:BPH:HAC1	2.30	0.47
4:R:2002:BCL:NC	4:S:2003:BCL:HBB3	2.30	0.47
1:R:170:ASN:HB3	1:R:173:HIS:HB2	1.96	0.47
1:L:170:ASN:HB3	1:L:173:HIS:CB	2.45	0.46
1:L:227:LEU:HD13	2:M:232:GLU:HG2	1.98	0.46
1:R:60:ASN:O	1:R:64:ILE:HG13	2.15	0.46
1:R:66:VAL:HG11	1:R:89:ILE:HD12	1.97	0.46
4:L:1001:BCL:CBC	4:M:1003:BCL:CAD	2.93	0.46
2:S:228:ARG:HA	3:T:194:GLN:HG2	1.96	0.46
2:M:234:GLU:O	2:M:238:ILE:HG13	2.14	0.46
3:T:111:PRO:HB2	3:T:239:GLY:HA2	1.98	0.46
3:H:111:PRO:HB2	3:H:239:GLY:HA2	1.97	0.46
4:S:2001:BCL:HBB3	4:S:2003:BCL:H61	1.97	0.46
1:R:11:VAL:HB	1:R:12:PRO:HD2	1.98	0.46
2:S:3:TYR:CZ	2:S:5:ASN:HA	2.51	0.46
1:R:80:LEU:H	1:R:80:LEU:CD2	2.29	0.46
2:S:204:LEU:HD13	3:T:20:PHE:CE2	2.51	0.46
3:T:87:LEU:HD22	3:T:98:HIS:O	2.15	0.46
3:H:233:ILE:O	3:H:237:VAL:HG23	2.16	0.46
1:L:35:GLY:HA2	1:L:103:ARG:HD2	1.98	0.46
1:L:80:LEU:HD22	1:L:80:LEU:N	2.28	0.45
4:L:1001:BCL:H41	5:L:1009:U10:H112	1.97	0.45
3:H:135:LYS:HB3	3:H:135:LYS:HZ3	1.82	0.45
4:S:2001:BCL:HBB2	4:S:2001:BCL:HHC	1.99	0.45
3:H:111:PRO:HD2	3:H:243:TYR:CE2	2.52	0.45
3:H:165:VAL:O	3:H:166:ASP:HB2	2.17	0.45
2:M:228:ARG:HA	3:H:194:GLN:CG	2.45	0.45
2:S:237:GLN:HB2	2:S:262:MET:HG2	1.98	0.45
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.16	0.45
2:S:194:GLY:O	2:S:195:ASN:HB3	2.17	0.45
3:T:40:TYR:HB3	3:T:58:LEU:HD21	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:LEU:HD13	7:M:1005:BPH:ND	2.32	0.45
4:L:1004:BCL:HBB3	7:M:1006:BPH:H152	1.99	0.45
2:M:286:LEU:CD2	3:H:12:LEU:HD12	2.48	0.44
1:R:170:ASN:HB3	1:R:173:HIS:HB3	1.97	0.44
1:R:149:GLY:HA3	1:R:152:THR:OG1	2.17	0.44
4:S:2001:BCL:CBB	8:S:2010:SPO:H243	2.47	0.44
2:M:195:ASN:HD22	2:M:197:PHE:H	1.64	0.44
1:R:34:PHE:CE1	1:R:102:LEU:HD23	2.52	0.44
1:R:211:HIS:HE1	2:S:22:GLU:OE1	2.00	0.44
1:L:207:ARG:HA	1:L:207:ARG:HD2	1.57	0.44
1:R:129:LEU:HB3	1:R:134:PHE:CE2	2.52	0.44
1:R:207:ARG:HG3	2:S:142:MET:HG2	1.99	0.44
2:S:148:TRP:HA	2:S:148:TRP:CE3	2.53	0.44
3:T:207:ALA:HA	3:T:241:LEU:HD23	2.00	0.44
1:L:226:THR:HG23	1:L:227:LEU:N	2.33	0.44
3:H:90:THR:HG22	10:H:290:HOH:O	2.16	0.44
2:S:229:PHE:HB2	2:S:244:ALA:HB2	2.00	0.44
3:H:66:LEU:HA	3:H:67:PRO:HD3	1.85	0.44
1:R:262:TRP:O	1:R:265:TRP:HD1	2.01	0.44
2:M:196:LEU:HD12	2:M:196:LEU:HA	1.85	0.44
3:H:12:LEU:HD13	3:H:12:LEU:C	2.38	0.44
3:T:18:TYR:O	3:T:22:ILE:HG12	2.18	0.44
3:T:64:PHE:HD2	3:T:73:LEU:HD12	1.82	0.44
2:S:87:ARG:HG3	2:S:88:ASP:N	2.33	0.43
2:S:148:TRP:HA	2:S:148:TRP:HE3	1.82	0.43
4:L:1001:BCL:HMB2	7:M:1005:BPH:HMB3	2.00	0.43
2:M:96:PRO:HB3	2:M:115:TRP:CE2	2.53	0.43
2:S:11:GLN:HB2	3:T:144:ALA:HB3	2.00	0.43
2:S:53:GLY:O	2:S:57:VAL:HG23	2.18	0.43
2:S:129:TRP:O	2:S:132:ARG:HB3	2.17	0.43
1:L:177:ILE:HG12	4:L:1002:BCL:HMB3	2.00	0.43
2:S:62:SER:HB3	2:S:121:PHE:O	2.18	0.43
2:S:236:GLU:OE1	3:T:122:GLU:HG2	2.18	0.43
3:T:112:ALA:HA	3:T:235:GLY:O	2.19	0.43
2:S:63:GLY:CA	7:S:2005:BPH:H5C2	2.47	0.43
2:M:13:ARG:O	3:H:140:PHE:HA	2.19	0.43
1:L:80:LEU:HD12	1:L:85:LEU:HD13	2.00	0.43
2:M:22:GLU:HB3	2:M:23:ASP:H	1.67	0.43
1:R:90:THR:HG23	1:R:132:VAL:HG11	2.01	0.43
2:M:87:ARG:HG3	2:M:88:ASP:N	2.34	0.42
1:R:86:TRP:CH2	1:R:132:VAL:HG13	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:234:GLU:O	2:S:238:ILE:HG13	2.18	0.42
1:R:227:LEU:HD13	2:S:232:GLU:CG	2.43	0.42
3:T:66:LEU:HA	3:T:67:PRO:HD3	1.84	0.42
1:L:197:ALA:HA	1:L:207:ARG:HB2	2.01	0.42
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.54	0.42
1:R:130:THR:HA	1:R:134:PHE:HD2	1.84	0.42
1:L:170:ASN:HB3	1:L:173:HIS:HB3	2.01	0.42
4:L:1004:BCL:H3A	4:L:1004:BCL:HBA2	1.73	0.42
2:M:214:LEU:HD21	5:M:1008:U10:H172	2.00	0.42
2:S:22:GLU:HB3	2:S:23:ASP:H	1.61	0.42
3:T:104:PRO:HA	3:T:109:VAL:HG22	2.01	0.42
2:M:182:HIS:CG	8:M:1010:SPO:H181	2.54	0.42
4:M:1003:BCL:CBB	4:M:1003:BCL:HHC	2.49	0.42
1:L:129:LEU:HD12	1:L:129:LEU:HA	1.86	0.42
1:L:185:LEU:HD12	1:L:185:LEU:O	2.19	0.42
2:M:13:ARG:HD2	2:M:35:PHE:CE2	2.54	0.42
1:R:133:LEU:HD22	1:R:134:PHE:CD1	2.54	0.42
3:T:206:ASN:ND2	10:T:312:HOH:O	2.48	0.42
3:H:194:GLN:H	3:H:194:GLN:NE2	2.18	0.42
2:S:114:LEU:HD12	2:S:114:LEU:HA	1.94	0.42
1:L:211:HIS:HE1	2:M:22:GLU:OE1	2.02	0.42
1:L:42:ALA:O	1:L:46:ILE:HG13	2.19	0.42
2:M:239:ALA:HB1	3:H:66:LEU:HD11	2.02	0.42
1:R:219:LEU:HG	1:R:220:VAL:HG13	2.01	0.42
2:S:170:SER:HB2	10:S:2022:HOH:O	2.20	0.42
5:M:1008:U10:H4M2	5:M:1008:U10:H3M3	2.02	0.41
1:L:195:LEU:HB3	2:M:145:HIS:CD2	2.55	0.41
1:R:250:ILE:HB	1:R:254:ILE:HD11	2.03	0.41
2:S:260:ALA:HB1	3:T:35:ASN:OD1	2.19	0.41
3:H:190:LEU:HB2	3:H:233:ILE:HD13	2.00	0.41
1:R:4:SER:O	3:T:79:GLU:HG2	2.20	0.41
1:R:110:LYS:HD2	2:S:254:TRP:CZ3	2.55	0.41
1:R:187:LEU:HD13	2:S:216:PHE:CG	2.55	0.41
2:S:195:ASN:HD22	2:S:196:LEU:N	2.18	0.41
8:S:2010:SPO:H15	8:S:2010:SPO:H131	1.85	0.41
10:S:2032:HOH:O	3:T:194:GLN:HB3	2.20	0.41
1:R:2:LEU:HG	1:R:10:ARG:HH12	1.83	0.41
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.85	0.41
3:T:73:LEU:HD13	3:T:73:LEU:C	2.41	0.41
3:H:135:LYS:HG2	3:H:136:ALA:N	2.36	0.41
3:T:73:LEU:HD11	3:T:75:VAL:CG1	2.47	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90:THR:HG23	1:L:132:VAL:HG11	2.01	0.41
1:L:234:LEU:O	1:L:238:LEU:HB2	2.21	0.41
2:M:233:CYS:O	2:M:236:GLU:HB3	2.21	0.41
1:L:135:ARG:N	1:L:136:PRO:CD	2.84	0.41
2:M:100:GLU:CD	2:M:100:GLU:H	2.25	0.41
2:M:204:LEU:O	2:M:207:ALA:HB3	2.20	0.41
8:M:1010:SPO:H15	8:M:1010:SPO:H131	1.88	0.41
1:R:31:VAL:HG12	1:R:32:GLY:N	2.36	0.41
3:T:245:ALA:N	3:T:246:PRO:CD	2.84	0.41
2:S:195:ASN:ND2	2:S:195:ASN:C	2.73	0.41
4:M:1003:BCL:H62	4:M:1003:BCL:H92	1.94	0.40
1:R:200:PRO:HB3	1:R:207:ARG:HD3	2.04	0.40
1:R:124:ALA:HB2	7:R:2006:BPH:HBC3	2.03	0.40
1:L:181:PHE:CZ	4:M:1003:BCL:O1A	2.74	0.40
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.56	0.40
4:L:1001:BCL:CBB	8:M:1010:SPO:H243	2.51	0.40
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.56	0.40
1:R:66:VAL:HG12	1:R:86:TRP:HB2	2.02	0.40
4:S:2004:BCL:H61	5:S:2008:U10:H203	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 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	L	279/281 (99%)	269 (96%)	10 (4%)	0	100	100
1	R	279/281 (99%)	263 (94%)	14 (5%)	2 (1%)	22	32
2	M	297/307 (97%)	285 (96%)	12 (4%)	0	100	100
2	S	297/307 (97%)	287 (97%)	10 (3%)	0	100	100
3	H	244/260 (94%)	236 (97%)	8 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	T	244/260 (94%)	235 (96%)	9 (4%)	0	100	100
All	All	1640/1696 (97%)	1575 (96%)	63 (4%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	4	SER
1	R	31	VAL

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 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	L	220/220 (100%)	207 (94%)	13 (6%)	19	32
1	R	220/220 (100%)	208 (94%)	12 (6%)	21	35
2	M	235/240 (98%)	220 (94%)	15 (6%)	17	28
2	S	235/240 (98%)	225 (96%)	10 (4%)	29	46
3	H	199/208 (96%)	194 (98%)	5 (2%)	47	67
3	T	199/208 (96%)	196 (98%)	3 (2%)	65	80
All	All	1308/1336 (98%)	1250 (96%)	58 (4%)	28	45

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	ARG
1	L	102	LEU
1	L	126	LEU
1	L	129	LEU
1	L	133	LEU
1	L	189	LEU
1	L	195	LEU
1	L	207	ARG
1	L	216	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	235	LEU
1	L	238	LEU
1	L	269	LEU
1	L	272	TRP
2	M	12	VAL
2	M	26	LEU
2	M	29	ARG
2	M	34	PRO
2	M	60	LEU
2	M	87	ARG
2	M	94	LEU
2	M	114	LEU
2	M	136	ARG
2	M	151	LEU
2	M	156	LEU
2	M	191	LEU
2	M	195	ASN
2	M	216	PHE
2	M	232	GLU
3	H	73	LEU
3	H	123	LEU
3	H	135	LYS
3	H	202	ARG
3	H	231	ASP
1	R	102	LEU
1	R	126	LEU
1	R	129	LEU
1	R	167	PHE
1	R	189	LEU
1	R	195	LEU
1	R	207	ARG
1	R	216	PHE
1	R	235	LEU
1	R	247	CYS
1	R	269	LEU
1	R	272	TRP
2	S	29	ARG
2	S	87	ARG
2	S	94	LEU
2	S	136	ARG
2	S	148	TRP
2	S	156	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	191	LEU
2	S	195	ASN
2	S	216	PHE
2	S	232	GLU
3	T	202	ARG
3	T	208	LEU
3	T	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	87	GLN
1	L	183	ASN
1	L	211	HIS
2	M	9	GLN
2	M	44	ASN
2	M	195	ASN
3	H	206	ASN
1	R	87	GLN
1	R	159	ASN
1	R	183	ASN
1	R	211	HIS
2	S	9	GLN
2	S	195	ASN
3	T	98	HIS
3	T	128	HIS
3	T	194	GLN
3	T	206	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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$
7	BPH	R	2006	-	64,70,70	1.54	11 (17%)	76,101,101	2.19	20 (26%)
4	BCL	R	2002	-	58,74,74	1.20	4 (6%)	69,115,115	2.06	22 (31%)
4	BCL	L	1002	-	58,74,74	1.10	4 (6%)	69,115,115	2.05	20 (28%)
5	U10	R	2009	-	18,18,63	2.26	7 (38%)	22,25,79	2.29	7 (31%)
8	SPO	S	2010	-	40,41,41	3.39	24 (60%)	47,50,50	4.13	14 (29%)
9	LDA	S	2011	-	12,15,15	2.06	1 (8%)	14,17,17	1.71	4 (28%)
7	BPH	M	1005	-	54,60,70	1.43	7 (12%)	64,89,101	2.23	20 (31%)
4	BCL	L	1001	-	43,59,74	1.61	7 (16%)	51,97,115	2.20	14 (27%)
4	BCL	M	1003	-	58,74,74	1.25	7 (12%)	69,115,115	2.03	23 (33%)
9	LDA	M	1012	-	12,15,15	2.10	1 (8%)	14,17,17	1.71	4 (28%)
7	BPH	S	2005	-	54,60,70	1.43	8 (14%)	64,89,101	2.35	22 (34%)
5	U10	L	1009	-	44,44,63	2.09	17 (38%)	53,56,79	2.96	16 (30%)
7	BPH	M	1006	-	64,70,70	1.48	8 (12%)	76,101,101	2.16	21 (27%)
5	U10	S	2008	-	32,32,63	1.98	10 (31%)	38,41,79	1.96	10 (26%)
4	BCL	S	2004	-	58,74,74	1.32	9 (15%)	69,115,115	1.99	22 (31%)
9	LDA	M	1014	-	12,15,15	2.11	1 (8%)	14,17,17	1.74	5 (35%)
4	BCL	S	2001	-	43,59,74	1.45	6 (13%)	51,97,115	2.18	14 (27%)
9	LDA	M	1013	-	12,15,15	2.08	1 (8%)	14,17,17	1.70	4 (28%)
9	LDA	M	1011	-	12,15,15	1.99	1 (8%)	14,17,17	1.66	4 (28%)
8	SPO	M	1010	-	40,41,41	3.47	24 (60%)	47,50,50	4.02	14 (29%)
4	BCL	L	1004	-	58,74,74	1.32	7 (12%)	69,115,115	2.10	21 (30%)
4	BCL	S	2003	-	58,74,74	1.23	4 (6%)	69,115,115	2.15	27 (39%)
5	U10	M	1008	-	38,38,63	1.98	11 (28%)	46,49,79	1.92	11 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BPH	R	2006	-	2/2/18/22	16/54/105/105	0/5/6/6
4	BCL	R	2002	-	-	5/37/137/137	-
4	BCL	L	1002	-	-	6/37/137/137	-
5	U10	R	2009	-	-	1/9/33/87	0/1/1/1
8	SPO	S	2010	-	-	12/47/47/47	-
9	LDA	S	2011	-	-	7/13/13/13	-
7	BPH	M	1005	-	1/1/16/22	11/42/93/105	0/5/6/6
4	BCL	L	1001	-	-	2/19/119/137	-
4	BCL	M	1003	-	-	10/37/137/137	-
9	LDA	M	1012	-	-	6/13/13/13	-
7	BPH	S	2005	-	1/1/16/22	14/42/93/105	0/5/6/6
5	U10	L	1009	-	-	7/41/65/87	0/1/1/1
7	BPH	M	1006	-	2/2/18/22	18/54/105/105	0/5/6/6
5	U10	S	2008	-	-	2/26/50/87	0/1/1/1
4	BCL	S	2004	-	-	7/37/137/137	-
9	LDA	M	1014	-	-	6/13/13/13	-
4	BCL	S	2001	-	-	3/19/119/137	-
9	LDA	M	1013	-	-	4/13/13/13	-
9	LDA	M	1011	-	-	6/13/13/13	-
8	SPO	M	1010	-	-	13/47/47/47	-
4	BCL	L	1004	-	-	10/37/137/137	-
4	BCL	S	2003	-	-	8/37/137/137	-
5	U10	M	1008	-	-	2/33/57/87	0/1/1/1

All (180) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	1010	SPO	C6-C5	9.15	1.55	1.32
8	S	2010	SPO	C6-C5	8.71	1.54	1.32
8	M	1010	SPO	C15-C16	8.59	1.56	1.34
8	M	1010	SPO	C10-C11	7.86	1.54	1.34
8	S	2010	SPO	C10-C11	7.82	1.54	1.34
8	S	2010	SPO	C15-C16	7.70	1.54	1.34
9	M	1012	LDA	O1-N1	-7.04	1.25	1.42
9	M	1014	LDA	O1-N1	-7.00	1.25	1.42
9	M	1013	LDA	O1-N1	-6.92	1.26	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	S	2011	LDA	O1-N1	-6.85	1.26	1.42
9	M	1011	LDA	O1-N1	-6.56	1.26	1.42
8	M	1010	SPO	C21-C20	5.41	1.50	1.36
7	M	1006	BPH	C11-C10	-5.31	1.29	1.52
7	R	2006	BPH	C11-C10	-5.30	1.29	1.52
8	S	2010	SPO	C27-C28	5.24	1.39	1.34
8	S	2010	SPO	C21-C20	5.21	1.49	1.36
8	M	1010	SPO	C14-C12	5.16	1.42	1.35
8	S	2010	SPO	C14-C12	5.07	1.42	1.35
4	L	1001	BCL	C3C-C4C	-5.03	1.45	1.51
5	R	2009	U10	O4-C4	4.91	1.48	1.36
5	S	2008	U10	O4-C4	4.90	1.48	1.36
5	L	1009	U10	O4-C4	4.84	1.48	1.36
8	S	2010	SPO	C26-C25	4.64	1.46	1.34
5	M	1008	U10	C7-C8	-4.57	1.44	1.50
5	M	1008	U10	O4-C4	4.55	1.48	1.36
8	M	1010	SPO	C27-C28	4.51	1.38	1.34
7	M	1005	BPH	O2D-CGD	4.45	1.44	1.33
8	M	1010	SPO	C26-C25	4.43	1.46	1.34
5	L	1009	U10	C13-C14	4.35	1.43	1.33
7	S	2005	BPH	O2A-CGA	4.31	1.45	1.33
8	S	2010	SPO	O1-CM1	4.26	1.56	1.43
8	M	1010	SPO	O1-CM1	4.24	1.56	1.43
7	R	2006	BPH	O2A-CGA	4.22	1.45	1.33
7	M	1006	BPH	O2D-CGD	4.19	1.43	1.33
7	R	2006	BPH	O2D-CGD	4.17	1.43	1.33
4	S	2001	BCL	C3C-C4C	-4.08	1.46	1.51
7	S	2005	BPH	O2D-CGD	3.93	1.42	1.33
7	M	1005	BPH	O2A-CGA	3.91	1.44	1.33
7	M	1006	BPH	O2A-CGA	3.83	1.44	1.33
4	S	2003	BCL	MG-NA	3.80	2.15	2.06
8	M	1010	SPO	C19-C17	3.76	1.40	1.35
4	L	1001	BCL	MG-NC	-3.65	1.97	2.06
5	M	1008	U10	C13-C14	3.65	1.41	1.33
5	L	1009	U10	C8-C9	3.64	1.41	1.33
5	S	2008	U10	C13-C14	3.63	1.41	1.33
8	M	1010	SPO	C9-C7	3.62	1.40	1.35
8	S	2010	SPO	C19-C17	3.55	1.40	1.35
4	L	1004	BCL	MG-NC	-3.51	1.97	2.06
8	S	2010	SPO	C9-C7	3.47	1.40	1.35
5	S	2008	U10	C7-C8	-3.43	1.45	1.50
5	R	2009	U10	C6-C1	3.43	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1009	U10	C6-C1	3.42	1.41	1.35
4	M	1003	BCL	C1B-NB	3.38	1.38	1.35
5	L	1009	U10	O3-C3	3.38	1.45	1.36
5	S	2008	U10	O3-C3	3.36	1.45	1.36
5	M	1008	U10	C6-C1	3.35	1.41	1.35
8	M	1010	SPO	C10-C9	3.30	1.53	1.43
5	R	2009	U10	O3-C3	3.30	1.44	1.36
5	M	1008	U10	O3-C3M	-3.25	1.37	1.45
7	M	1005	BPH	CAA-C2A	3.17	1.60	1.54
5	M	1008	U10	C23-C24	3.16	1.40	1.33
7	M	1006	BPH	CAA-C2A	3.16	1.60	1.54
4	M	1003	BCL	MG-NA	3.16	2.13	2.06
5	L	1009	U10	C23-C24	3.14	1.40	1.33
4	L	1002	BCL	MG-NA	3.12	2.13	2.06
8	S	2010	SPO	C10-C9	3.08	1.53	1.43
4	R	2002	BCL	MG-NA	3.07	2.13	2.06
4	S	2003	BCL	C1B-NB	3.06	1.37	1.35
5	S	2008	U10	C6-C1	3.06	1.40	1.35
4	L	1004	BCL	C3C-C4C	-3.05	1.47	1.51
8	M	1010	SPO	C37-C38	3.05	1.41	1.32
5	L	1009	U10	C7-C6	3.00	1.56	1.51
5	R	2009	U10	C8-C9	2.99	1.40	1.32
8	M	1010	SPO	C25-C23	-2.96	1.39	1.45
5	R	2009	U10	C7-C8	-2.96	1.46	1.50
5	R	2009	U10	O3-C3M	-2.94	1.38	1.45
7	M	1005	BPH	O2D-CED	-2.93	1.38	1.45
5	M	1008	U10	O3-C3	2.93	1.44	1.36
8	S	2010	SPO	C25-C23	-2.92	1.39	1.45
5	L	1009	U10	C7-C8	-2.92	1.46	1.50
5	R	2009	U10	C7-C6	2.91	1.56	1.51
5	S	2008	U10	O3-C3M	-2.91	1.38	1.45
5	S	2008	U10	C18-C19	2.89	1.39	1.33
7	R	2006	BPH	C2-C3	2.89	1.39	1.33
5	M	1008	U10	C18-C19	2.89	1.39	1.33
7	M	1006	BPH	O2D-CED	-2.88	1.38	1.45
4	S	2004	BCL	C3C-C4C	-2.87	1.48	1.51
4	S	2001	BCL	MG-NC	-2.87	1.99	2.06
8	M	1010	SPO	C15-C14	2.87	1.52	1.43
4	S	2004	BCL	C1B-NB	2.86	1.37	1.35
5	S	2008	U10	C8-C9	2.84	1.39	1.33
8	S	2010	SPO	C37-C38	2.82	1.40	1.32
4	R	2002	BCL	C1B-NB	2.80	1.37	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	2004	BCL	MG-NA	2.78	2.12	2.06
8	M	1010	SPO	O1-C1	2.78	1.57	1.41
7	S	2005	BPH	CAA-C2A	2.77	1.59	1.54
5	L	1009	U10	C31-C29	2.77	1.57	1.51
4	S	2004	BCL	MG-NC	-2.77	1.99	2.06
5	L	1009	U10	O3-C3M	-2.76	1.38	1.45
8	S	2010	SPO	O1-C1	2.75	1.57	1.41
8	M	1010	SPO	C11-C12	-2.73	1.40	1.45
4	S	2001	BCL	MG-NA	2.73	2.12	2.06
8	M	1010	SPO	C32-C33	2.73	1.39	1.33
5	L	1009	U10	C18-C19	2.72	1.39	1.33
8	M	1010	SPO	C22-C23	2.71	1.39	1.35
4	S	2004	BCL	CAA-C2A	2.71	1.59	1.54
8	S	2010	SPO	C8-C7	2.70	1.56	1.50
8	S	2010	SPO	C11-C12	-2.68	1.40	1.45
8	S	2010	SPO	C32-C33	2.61	1.39	1.33
4	S	2003	BCL	C4-C3	2.60	1.57	1.50
7	R	2006	BPH	CHC-C1C	2.57	1.41	1.36
7	R	2006	BPH	O2D-CED	-2.57	1.39	1.45
7	M	1005	BPH	C2-C3	2.55	1.39	1.33
7	R	2006	BPH	C2A-C1A	2.52	1.55	1.51
7	R	2006	BPH	CAA-C2A	2.51	1.58	1.54
8	S	2010	SPO	C26-C27	2.51	1.51	1.43
7	S	2005	BPH	C2-C3	2.48	1.38	1.33
4	R	2002	BCL	CBB-CAB	2.47	1.57	1.49
8	S	2010	SPO	C13-C12	2.45	1.55	1.50
5	L	1009	U10	C28-C29	2.44	1.38	1.33
8	S	2010	SPO	C6-C7	-2.43	1.40	1.45
7	M	1006	BPH	O1D-CGD	2.43	1.27	1.21
4	L	1001	BCL	C1B-NB	2.43	1.37	1.35
8	S	2010	SPO	C15-C14	2.40	1.50	1.43
7	S	2005	BPH	O2D-CED	-2.39	1.39	1.45
4	L	1001	BCL	MG-NA	2.38	2.11	2.06
7	M	1005	BPH	O1D-CGD	2.38	1.27	1.21
8	S	2010	SPO	C24-C23	2.38	1.55	1.50
4	S	2004	BCL	CAA-CBA	2.37	1.60	1.52
8	M	1010	SPO	C13-C12	2.37	1.55	1.50
4	S	2003	BCL	MG-NC	-2.37	2.00	2.06
4	L	1004	BCL	C6-C5	2.36	1.60	1.52
4	S	2004	BCL	C4-C3	2.33	1.56	1.50
4	L	1001	BCL	CAA-CBA	2.32	1.60	1.52
5	L	1009	U10	C32-C33	-2.32	1.42	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1001	BCL	C3D-CAD	-2.32	1.40	1.46
4	S	2004	BCL	C3D-CAD	-2.31	1.40	1.46
4	M	1003	BCL	C4-C3	2.31	1.56	1.50
5	M	1008	U10	C15-C14	2.31	1.56	1.50
7	S	2005	BPH	C2C-C3C	-2.31	1.48	1.54
4	S	2001	BCL	C1B-NB	2.28	1.37	1.35
4	L	1004	BCL	CBB-CAB	2.28	1.56	1.49
4	M	1003	BCL	C3D-CAD	-2.28	1.40	1.46
8	M	1010	SPO	C8-C7	2.27	1.55	1.50
8	S	2010	SPO	C35-C33	2.27	1.56	1.51
4	L	1004	BCL	MG-NA	2.27	2.11	2.06
4	R	2002	BCL	C4-C3	2.25	1.56	1.50
4	L	1001	BCL	CAA-C2A	2.22	1.58	1.54
5	L	1009	U10	C20-C19	2.21	1.56	1.50
5	L	1009	U10	C30-C29	2.21	1.56	1.50
5	M	1008	U10	C27-C28	-2.21	1.43	1.50
8	M	1010	SPO	C26-C27	2.21	1.50	1.43
5	L	1009	U10	C15-C14	2.21	1.56	1.50
4	S	2004	BCL	CBB-CAB	2.20	1.56	1.49
4	L	1002	BCL	CBB-CAB	2.17	1.56	1.49
4	M	1003	BCL	C3C-C4C	-2.16	1.48	1.51
8	S	2010	SPO	C22-C23	2.15	1.38	1.35
5	S	2008	U10	C15-C14	2.15	1.56	1.50
4	S	2001	BCL	CAA-CBA	2.15	1.59	1.52
4	L	1004	BCL	C4-C3	2.13	1.56	1.50
7	M	1006	BPH	CHC-C1C	2.13	1.40	1.36
7	M	1006	BPH	CHA-C1A	2.11	1.42	1.38
7	S	2005	BPH	CHC-C1C	2.11	1.40	1.36
5	L	1009	U10	C26-C24	2.11	1.55	1.51
8	M	1010	SPO	C40-C38	2.10	1.56	1.50
4	L	1002	BCL	C4-C3	2.09	1.56	1.50
4	S	2001	BCL	C3D-CAD	-2.09	1.40	1.46
5	S	2008	U10	C7-C6	2.09	1.54	1.51
4	M	1003	BCL	C3A-C2A	2.08	1.60	1.54
5	M	1008	U10	C8-C9	2.07	1.37	1.33
7	S	2005	BPH	C2A-C1A	2.06	1.55	1.51
7	M	1005	BPH	C2C-C3C	-2.05	1.48	1.54
7	R	2006	BPH	CHA-C1A	2.05	1.42	1.38
4	M	1003	BCL	MG-NC	-2.04	2.01	2.06
8	M	1010	SPO	C35-C33	2.03	1.55	1.51
7	R	2006	BPH	C2C-C3C	-2.03	1.48	1.54
4	L	1004	BCL	C3D-CAD	-2.03	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	2006	BPH	C3D-C2D	-2.03	1.35	1.39
4	L	1002	BCL	C1B-NB	2.02	1.37	1.35
8	M	1010	SPO	C24-C23	2.01	1.55	1.50

All (339) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	2010	SPO	C3-C1-C4	-17.48	84.02	110.86
8	M	1010	SPO	C3-C1-C4	-17.14	84.55	110.86
8	S	2010	SPO	C2-C1-C4	-16.17	86.04	110.86
8	M	1010	SPO	C2-C1-C4	-15.62	86.88	110.86
5	L	1009	U10	C32-C33-C34	14.51	162.60	127.66
7	S	2005	BPH	O2D-CGD-CBD	8.96	127.18	111.27
7	R	2006	BPH	O2D-CGD-CBD	8.42	126.24	111.27
7	M	1005	BPH	O2D-CGD-CBD	8.19	125.83	111.27
7	M	1006	BPH	O2D-CGD-CBD	8.07	125.60	111.27
5	L	1009	U10	C27-C28-C29	7.65	146.07	127.66
4	L	1002	BCL	C4A-NA-C1A	-6.59	103.74	106.71
5	R	2009	U10	C3M-O3-C3	6.49	139.47	116.47
4	S	2001	BCL	CBC-CAC-C3C	-6.44	99.14	113.47
5	L	1009	U10	C3M-O3-C3	6.39	139.10	116.47
5	S	2008	U10	C3M-O3-C3	6.32	138.85	116.47
4	R	2002	BCL	C4A-NA-C1A	-6.21	103.92	106.71
5	M	1008	U10	C3M-O3-C3	6.11	138.10	116.47
4	S	2003	BCL	C4D-C3D-CAD	-6.05	105.10	108.47
8	M	1010	SPO	C20-C21-C22	-6.03	111.12	123.47
8	S	2010	SPO	C20-C21-C22	-5.94	111.31	123.47
4	L	1001	BCL	C4D-C3D-CAD	-5.90	105.18	108.47
7	S	2005	BPH	C1-C2-C3	5.86	136.19	126.04
7	R	2006	BPH	C1-C2-C3	5.85	136.16	126.04
8	S	2010	SPO	C15-C14-C12	-5.83	118.99	127.31
4	S	2003	BCL	C4A-NA-C1A	-5.78	104.11	106.71
7	M	1006	BPH	C1-C2-C3	5.77	136.03	126.04
4	M	1003	BCL	C4D-C3D-CAD	-5.75	105.26	108.47
4	L	1001	BCL	CBC-CAC-C3C	-5.71	100.75	113.47
4	S	2001	BCL	C4A-NA-C1A	-5.60	104.19	106.71
4	R	2002	BCL	C4D-C3D-CAD	-5.51	105.40	108.47
4	L	1002	BCL	C4D-C3D-CAD	-5.46	105.43	108.47
7	M	1005	BPH	C1-C2-C3	5.43	135.44	126.04
7	R	2006	BPH	CBC-CAC-C3C	5.40	125.49	113.47
8	M	1010	SPO	C15-C14-C12	-5.37	119.64	127.31
4	S	2004	BCL	C4A-NA-C1A	-5.37	104.29	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1004	BCL	O2A-C1-C2	-5.36	94.55	108.64
4	L	1004	BCL	C4A-NA-C1A	-5.33	104.31	106.71
4	S	2001	BCL	C4D-C3D-CAD	-5.30	105.51	108.47
4	L	1004	BCL	C4D-C3D-CAD	-5.18	105.58	108.47
7	R	2006	BPH	C4A-NA-C1A	5.13	112.28	108.14
4	L	1001	BCL	C4A-NA-C1A	-5.10	104.41	106.71
8	S	2010	SPO	C25-C23-C22	-5.07	111.16	118.94
7	M	1006	BPH	C4A-NA-C1A	4.96	112.15	108.14
4	S	2003	BCL	OBD-CAD-CBD	-4.96	118.81	125.89
7	M	1005	BPH	C4A-NA-C1A	4.82	112.04	108.14
8	M	1010	SPO	C25-C23-C22	-4.74	111.67	118.94
4	S	2004	BCL	C4D-C3D-CAD	-4.73	105.83	108.47
4	M	1003	BCL	C4A-NA-C1A	-4.72	104.59	106.71
7	S	2005	BPH	C4A-NA-C1A	4.59	111.85	108.14
4	L	1004	BCL	C1-O2A-CGA	4.45	128.11	116.44
8	M	1010	SPO	C18-C17-C19	-4.38	116.78	122.92
4	S	2003	BCL	C11-C12-C13	-4.38	101.77	115.92
4	L	1001	BCL	CMD-C2D-C3D	4.34	132.80	124.68
7	M	1006	BPH	CED-O2D-CGD	4.33	125.73	115.94
4	M	1003	BCL	OBD-CAD-CBD	-4.25	119.82	125.89
7	R	2006	BPH	CED-O2D-CGD	4.17	125.37	115.94
7	M	1006	BPH	C11-C10-C8	4.17	129.39	115.92
4	M	1003	BCL	C11-C12-C13	-4.15	102.52	115.92
7	R	2006	BPH	C6-C5-C3	4.15	124.33	113.45
8	S	2010	SPO	C18-C17-C19	-4.13	117.14	122.92
5	M	1008	U10	C27-C28-C29	4.12	141.82	127.75
4	R	2002	BCL	CMD-C2D-C3D	4.11	132.37	124.68
7	S	2005	BPH	CED-O2D-CGD	4.08	125.17	115.94
7	M	1005	BPH	CED-O2D-CGD	4.08	125.17	115.94
8	S	2010	SPO	C24-C23-C25	4.06	124.47	118.08
4	L	1004	BCL	CMD-C2D-C3D	4.05	132.25	124.68
4	M	1003	BCL	CMD-C2D-C3D	4.04	132.25	124.68
7	S	2005	BPH	C6-C5-C3	4.03	124.02	113.45
4	S	2004	BCL	C11-C12-C13	-4.02	102.93	115.92
4	R	2002	BCL	OBD-CAD-CBD	-4.01	120.16	125.89
7	S	2005	BPH	O2D-CGD-O1D	-4.01	115.99	123.84
7	M	1005	BPH	C6-C5-C3	4.01	123.98	113.45
5	R	2009	U10	O5-C5-C6	-3.98	114.58	121.55
7	R	2006	BPH	C11-C10-C8	3.96	128.72	115.92
4	S	2003	BCL	CMD-C2D-C3D	3.92	132.02	124.68
5	L	1009	U10	O5-C5-C6	-3.92	114.68	121.55
4	L	1004	BCL	OBD-CAD-CBD	-3.92	120.30	125.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	2004	BCL	CMD-C2D-C3D	3.90	131.97	124.68
4	S	2001	BCL	CMD-C2D-C3D	3.89	131.95	124.68
7	S	2005	BPH	CBC-CAC-C3C	3.88	122.11	113.47
4	L	1002	BCL	OBD-CAD-CBD	-3.86	120.38	125.89
4	L	1002	BCL	CMD-C2D-C3D	3.85	131.88	124.68
5	M	1008	U10	C20-C19-C21	-3.83	108.82	115.27
4	R	2002	BCL	C7-C6-C5	-3.82	102.98	113.36
7	R	2006	BPH	O2D-CGD-O1D	-3.80	116.40	123.84
5	S	2008	U10	O5-C5-C6	-3.79	114.90	121.55
4	S	2001	BCL	C1-C2-C3	-3.78	120.64	126.75
5	M	1008	U10	O5-C5-C6	-3.77	114.94	121.55
4	L	1002	BCL	C1-C2-C3	-3.76	119.54	126.04
7	S	2005	BPH	O1D-CGD-CBD	-3.75	116.81	124.48
7	M	1006	BPH	C6-C5-C3	3.75	123.28	113.45
4	L	1004	BCL	OBB-CAB-CBB	-3.74	111.76	120.17
4	L	1002	BCL	C7-C6-C5	-3.73	103.22	113.36
8	M	1010	SPO	C24-C23-C25	3.73	123.95	118.08
7	M	1006	BPH	CBC-CAC-C3C	3.66	121.62	113.47
4	S	2004	BCL	OBB-CAB-CBB	-3.65	111.96	120.17
4	S	2003	BCL	OBB-CAB-CBB	-3.65	111.96	120.17
4	L	1001	BCL	CAC-C3C-C4C	-3.65	104.49	112.58
7	M	1005	BPH	O1D-CGD-CBD	-3.64	117.04	124.48
4	L	1004	BCL	CAC-C3C-C4C	-3.63	104.52	112.58
4	L	1001	BCL	OBD-CAD-CBD	-3.63	120.71	125.89
4	S	2001	BCL	OBD-CAD-CBD	-3.61	120.74	125.89
4	M	1003	BCL	OBB-CAB-CBB	-3.57	112.13	120.17
7	M	1006	BPH	O2D-CGD-O1D	-3.55	116.89	123.84
4	L	1001	BCL	OBB-CAB-CBB	-3.55	112.19	120.17
8	S	2010	SPO	C3-C1-C2	3.55	117.04	110.37
4	S	2001	BCL	OBB-CAB-CBB	-3.54	112.20	120.17
4	S	2003	BCL	C4-C3-C5	3.53	121.22	115.27
4	R	2002	BCL	OBB-CAB-CBB	-3.52	112.25	120.17
9	S	2011	LDA	CM1-N1-C1	-3.52	102.84	110.23
4	L	1002	BCL	OBB-CAB-CBB	-3.52	112.25	120.17
7	R	2006	BPH	O1D-CGD-CBD	-3.49	117.34	124.48
4	L	1001	BCL	C2C-C3C-C4C	3.48	106.56	101.34
5	L	1009	U10	O2-C2-C3	-3.48	113.54	120.93
8	S	2010	SPO	C15-C16-C17	-3.48	116.63	126.42
9	M	1012	LDA	CM1-N1-C1	-3.48	102.92	110.23
5	L	1009	U10	C1-C6-C5	-3.47	116.31	119.58
9	M	1013	LDA	CM1-N1-C1	-3.45	102.98	110.23
4	S	2004	BCL	OBD-CAD-CBD	-3.45	120.96	125.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1005	BPH	O2D-CGD-O1D	-3.43	117.13	123.84
7	M	1006	BPH	O1D-CGD-CBD	-3.43	117.46	124.48
9	M	1011	LDA	CM1-N1-C1	-3.42	103.06	110.23
9	M	1014	LDA	CM1-N1-C1	-3.41	103.08	110.23
4	M	1003	BCL	C4-C3-C5	3.40	121.00	115.27
5	L	1009	U10	C20-C19-C21	-3.38	109.58	115.27
8	M	1010	SPO	C3-C1-C2	3.37	116.72	110.37
8	S	2010	SPO	C6-C7-C9	-3.37	113.77	118.94
8	S	2010	SPO	C8-C7-C6	3.37	123.38	118.08
7	M	1005	BPH	CBC-CAC-C3C	3.37	120.96	113.47
4	S	2004	BCL	CBC-CAC-C3C	-3.36	105.99	113.47
5	R	2009	U10	O2-C2-C3	-3.34	113.83	120.93
5	S	2008	U10	O2-C2-C3	-3.32	113.89	120.93
8	M	1010	SPO	C15-C16-C17	-3.31	117.11	126.42
4	L	1002	BCL	CMB-C2B-C3B	3.31	130.87	124.68
5	R	2009	U10	C1-C6-C5	-3.31	116.47	119.58
4	S	2001	BCL	C2C-C3C-C4C	3.30	106.28	101.34
4	R	2002	BCL	CMB-C2B-C3B	3.28	130.81	124.68
4	S	2003	BCL	C3D-CAD-CBD	3.25	111.88	107.61
8	M	1010	SPO	C8-C7-C6	3.25	123.19	118.08
4	S	2001	BCL	CAA-C2A-C3A	-3.24	103.89	112.78
4	L	1001	BCL	CAA-C2A-C3A	-3.24	103.90	112.78
4	L	1004	BCL	CBC-CAC-C3C	-3.24	106.26	113.47
4	R	2002	BCL	C11-C12-C13	-3.21	105.53	115.92
4	L	1004	BCL	C2C-C3C-C4C	3.20	106.13	101.34
4	L	1004	BCL	C11-C12-C13	-3.19	105.61	115.92
4	S	2003	BCL	CAA-CBA-CGA	-3.15	104.04	113.25
4	S	2004	BCL	C2C-C3C-C4C	3.14	106.05	101.34
4	S	2004	BCL	CAC-C3C-C4C	-3.10	105.71	112.58
5	M	1008	U10	O2-C2-C3	-3.08	114.38	120.93
5	S	2008	U10	C20-C19-C21	-3.08	110.09	115.27
4	R	2002	BCL	O1D-CGD-CBD	3.06	130.75	124.48
7	R	2006	BPH	C2C-C3C-C4C	3.06	105.92	101.34
4	M	1003	BCL	CAA-CBA-CGA	-3.06	104.31	113.25
4	L	1002	BCL	C11-C12-C13	-3.05	106.07	115.92
4	R	2002	BCL	O2D-CGD-CBD	-3.02	105.90	111.27
4	L	1004	BCL	CMB-C2B-C3B	3.01	130.31	124.68
4	S	2004	BCL	CAA-C2A-C3A	-3.00	104.58	112.78
7	M	1006	BPH	C5-C3-C2	-2.98	115.09	121.12
5	M	1008	U10	C21-C19-C18	2.98	127.14	121.12
4	L	1002	BCL	CMB-C2B-C1B	-2.97	123.90	128.46
5	L	1009	U10	C16-C14-C13	2.96	127.11	121.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1006	BPH	C2C-C3C-C4C	2.92	105.72	101.34
4	S	2004	BCL	CMB-C2B-C3B	2.92	130.14	124.68
7	M	1005	BPH	C4D-CHA-C1A	-2.92	123.31	130.51
4	S	2003	BCL	CHA-C1A-NA	-2.91	119.73	126.40
4	S	2003	BCL	CMB-C2B-C3B	2.91	130.13	124.68
5	L	1009	U10	C21-C19-C18	2.91	127.00	121.12
7	M	1005	BPH	C2C-C3C-C4C	2.89	105.67	101.34
4	S	2004	BCL	CHA-C1A-NA	-2.89	119.79	126.40
7	S	2005	BPH	C4D-CHA-C1A	-2.88	123.42	130.51
8	M	1010	SPO	C6-C7-C9	-2.86	114.55	118.94
7	S	2005	BPH	C2C-C3C-C4C	2.86	105.62	101.34
4	L	1001	BCL	CHA-C1A-NA	-2.85	119.88	126.40
4	M	1003	BCL	CHA-C1A-NA	-2.84	119.89	126.40
4	M	1003	BCL	CMB-C2B-C3B	2.84	129.99	124.68
4	R	2002	BCL	CMB-C2B-C1B	-2.83	124.11	128.46
4	L	1002	BCL	CAC-C3C-C4C	-2.81	106.34	112.58
7	S	2005	BPH	C5-C3-C2	-2.81	115.44	121.12
4	S	2001	BCL	CHA-C1A-NA	-2.79	120.01	126.40
9	M	1013	LDA	O1-N1-C1	2.79	116.12	109.27
7	S	2005	BPH	C4-C3-C5	2.78	119.95	115.27
9	M	1014	LDA	O1-N1-C1	2.78	116.10	109.27
9	M	1012	LDA	O1-N1-C1	2.78	116.09	109.27
7	M	1006	BPH	C7-C6-C5	-2.77	105.84	113.36
9	S	2011	LDA	O1-N1-C1	2.77	116.06	109.27
7	M	1006	BPH	C4-C3-C5	2.76	119.91	115.27
4	S	2001	BCL	CMB-C2B-C3B	2.74	129.81	124.68
4	L	1002	BCL	O2D-CGD-CBD	-2.74	106.40	111.27
9	M	1011	LDA	O1-N1-C1	2.74	115.99	109.27
7	M	1005	BPH	CHD-C4C-NC	-2.74	121.95	125.20
4	L	1004	BCL	C16-C15-C13	-2.72	107.11	115.92
4	L	1002	BCL	CHA-C1A-NA	-2.71	120.19	126.40
4	M	1003	BCL	C3D-CAD-CBD	2.71	111.17	107.61
4	S	2004	BCL	CBB-CAB-C3B	2.70	128.35	120.34
4	R	2002	BCL	CHA-C1A-NA	-2.69	120.23	126.40
5	S	2008	U10	C1-C6-C5	-2.68	117.06	119.58
4	S	2004	BCL	CAC-C3C-C2C	-2.68	107.56	114.26
4	S	2004	BCL	C1-C2-C3	-2.68	121.41	126.04
4	M	1003	BCL	CBA-CAA-C2A	2.67	121.73	113.86
7	R	2006	BPH	C3C-C2C-C1C	2.66	106.16	101.87
4	R	2002	BCL	CAA-C2A-C3A	-2.66	105.50	112.78
5	M	1008	U10	C16-C14-C13	2.65	126.49	121.12
4	L	1004	BCL	CMB-C2B-C1B	-2.65	124.39	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1004	BCL	CAC-C3C-C2C	-2.64	107.65	114.26
4	L	1001	BCL	CMB-C2B-C3B	2.64	129.63	124.68
5	S	2008	U10	C16-C14-C13	2.64	126.47	121.12
5	L	1009	U10	C31-C29-C28	2.64	126.47	121.12
7	M	1006	BPH	C4D-CHA-C1A	-2.63	124.02	130.51
4	L	1004	BCL	CBB-CAB-C3B	2.63	128.14	120.34
7	S	2005	BPH	C3C-C2C-C1C	2.63	106.11	101.87
4	L	1002	BCL	C16-C15-C13	-2.63	107.43	115.92
4	L	1002	BCL	CAA-C2A-C3A	-2.62	105.59	112.78
7	S	2005	BPH	CHD-C4C-NC	-2.62	122.09	125.20
7	S	2005	BPH	CMD-C2D-C3D	2.61	129.57	124.68
7	M	1006	BPH	O2A-CGA-O1A	-2.61	116.99	123.59
9	M	1014	LDA	C6-C5-C4	-2.58	101.34	114.42
4	S	2003	BCL	CGD-CBD-CAD	-2.57	102.42	110.73
4	R	2002	BCL	CAC-C3C-C4C	-2.56	106.89	112.58
4	L	1004	BCL	CHA-C1A-NA	-2.56	120.53	126.40
7	M	1006	BPH	C3C-C2C-C1C	2.56	106.00	101.87
4	L	1004	BCL	CBA-CAA-C2A	2.56	121.41	113.86
4	L	1002	BCL	O1D-CGD-CBD	2.55	129.71	124.48
4	S	2004	BCL	O2A-C1-C2	-2.55	101.95	108.64
7	R	2006	BPH	O2A-CGA-O1A	-2.53	117.22	123.59
4	R	2002	BCL	C16-C15-C13	-2.52	107.76	115.92
7	R	2006	BPH	C4D-CHA-C1A	-2.52	124.29	130.51
7	R	2006	BPH	CHD-C4C-NC	-2.52	122.21	125.20
4	S	2003	BCL	CMB-C2B-C1B	-2.51	124.60	128.46
4	S	2003	BCL	C7-C6-C5	-2.51	106.53	113.36
5	L	1009	U10	C30-C29-C31	-2.51	111.05	115.27
7	M	1006	BPH	CMD-C2D-C3D	2.49	129.34	124.68
4	S	2003	BCL	CBA-CAA-C2A	2.49	121.21	113.86
5	R	2009	U10	C8-C7-C6	2.49	118.75	112.05
7	R	2006	BPH	C7-C6-C5	-2.48	106.63	113.36
4	M	1003	BCL	CBB-CAB-C3B	2.48	127.69	120.34
4	M	1003	BCL	CBC-CAC-C3C	-2.47	107.97	113.47
4	S	2003	BCL	CBB-CAB-C3B	2.46	127.66	120.34
8	M	1010	SPO	C10-C9-C7	-2.46	123.80	127.31
7	S	2005	BPH	CAA-C2A-C3A	-2.45	106.06	112.78
4	S	2003	BCL	C11-C10-C8	-2.45	108.01	115.92
4	S	2001	BCL	C3D-CAD-CBD	2.45	110.83	107.61
5	L	1009	U10	C22-C21-C19	2.44	121.00	112.98
4	S	2004	BCL	C3D-CAD-CBD	2.43	110.80	107.61
4	R	2002	BCL	C1-C2-C3	-2.43	121.85	126.04
7	M	1006	BPH	CHD-C4C-NC	-2.42	122.32	125.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1005	BPH	C3C-C2C-C1C	2.41	105.76	101.87
5	L	1009	U10	C8-C7-C6	2.41	118.54	112.05
4	L	1001	BCL	C3D-CAD-CBD	2.41	110.77	107.61
8	S	2010	SPO	C20-C19-C17	-2.40	123.88	127.31
7	S	2005	BPH	O2A-CGA-O1A	-2.39	117.56	123.59
4	M	1003	BCL	C7-C6-C5	-2.39	106.88	113.36
4	S	2004	BCL	CMB-C2B-C1B	-2.38	124.80	128.46
5	M	1008	U10	C1-C6-C5	-2.38	117.34	119.58
4	L	1002	BCL	CBB-CAB-C3B	2.38	127.40	120.34
4	R	2002	BCL	CBC-CAC-C3C	-2.37	108.18	113.47
4	R	2002	BCL	CBB-CAB-C3B	2.37	127.39	120.34
4	M	1003	BCL	C1-C2-C3	-2.37	121.95	126.04
9	M	1014	LDA	CM2-N1-C1	2.37	115.21	110.23
4	M	1003	BCL	C11-C10-C8	-2.36	108.30	115.92
9	S	2011	LDA	CM2-N1-C1	2.36	115.19	110.23
5	S	2008	U10	C21-C19-C18	2.35	125.88	121.12
7	S	2005	BPH	C2A-C1A-NA	-2.35	109.16	111.86
9	M	1013	LDA	C9-C8-C7	-2.35	102.51	114.42
7	M	1005	BPH	C2A-C1A-NA	-2.35	109.17	111.86
4	L	1002	BCL	C2C-C3C-C4C	2.34	104.85	101.34
5	S	2008	U10	C6-C1-C2	2.34	121.03	119.18
4	L	1004	BCL	C12-C11-C10	-2.34	102.49	113.24
4	L	1001	BCL	CHD-C4C-NC	2.33	127.66	125.08
4	M	1003	BCL	CMB-C2B-C1B	-2.32	124.90	128.46
4	L	1004	BCL	C3D-CAD-CBD	2.32	110.66	107.61
4	S	2004	BCL	C16-C15-C13	-2.32	108.43	115.92
8	M	1010	SPO	C16-C17-C19	2.31	122.49	118.94
9	M	1013	LDA	CM2-N1-C1	2.31	115.08	110.23
9	S	2011	LDA	C9-C8-C7	-2.29	102.78	114.42
9	M	1012	LDA	C9-C8-C7	-2.29	102.78	114.42
4	S	2003	BCL	CBC-CAC-C3C	-2.29	108.37	113.47
4	M	1003	BCL	C16-C15-C13	-2.29	108.53	115.92
8	S	2010	SPO	C1-C4-C5	2.29	119.11	113.06
4	S	2003	BCL	C16-C15-C13	-2.28	108.54	115.92
4	S	2003	BCL	C2C-C3C-C4C	2.28	104.75	101.34
7	M	1005	BPH	O2A-CGA-O1A	-2.28	117.84	123.59
5	M	1008	U10	C7-C6-C5	-2.28	115.74	118.48
5	R	2009	U10	C6-C1-C2	2.28	120.98	119.18
7	M	1005	BPH	CAA-C2A-C3A	-2.27	106.56	112.78
9	M	1012	LDA	CM2-N1-C1	2.26	114.98	110.23
7	R	2006	BPH	CAC-C3C-C4C	2.26	118.47	112.67
8	M	1010	SPO	C1-C4-C5	2.25	119.01	113.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1005	BPH	CMD-C2D-C3D	2.24	128.88	124.68
4	M	1003	BCL	CAC-C3C-C4C	-2.24	107.61	112.58
4	R	2002	BCL	C2C-C3C-C4C	2.23	104.68	101.34
4	S	2003	BCL	CAA-C2A-C3A	-2.23	106.67	112.78
7	R	2006	BPH	CMD-C2D-C3D	2.23	128.85	124.68
4	S	2003	BCL	C1-C2-C3	-2.22	122.20	126.04
4	L	1002	BCL	C12-C11-C10	-2.22	103.03	113.24
9	M	1011	LDA	CM2-N1-C1	2.22	114.90	110.23
7	R	2006	BPH	CAA-C2A-C1A	-2.22	106.59	112.33
4	S	2004	BCL	C7-C6-C5	-2.22	107.34	113.36
5	S	2008	U10	C17-C18-C19	2.21	132.97	127.66
4	L	1004	BCL	C7-C6-C5	-2.20	107.37	113.36
8	S	2010	SPO	C10-C9-C7	-2.20	124.17	127.31
5	R	2009	U10	C7-C6-C5	-2.20	115.83	118.48
9	M	1011	LDA	C9-C8-C7	-2.20	103.25	114.42
5	M	1008	U10	C31-C29-C30	-2.20	109.75	114.60
4	S	2003	BCL	O1D-CGD-CBD	2.20	128.98	124.48
4	S	2003	BCL	O2A-CGA-O1A	-2.19	118.06	123.59
4	R	2002	BCL	C3D-CAD-CBD	2.19	110.49	107.61
5	L	1009	U10	C6-C1-C2	2.19	120.91	119.18
5	S	2008	U10	C7-C6-C5	-2.18	115.86	118.48
4	S	2003	BCL	CAC-C3C-C2C	-2.16	108.85	114.26
4	L	1001	BCL	CBB-CAB-C3B	2.16	126.75	120.34
7	M	1006	BPH	OBD-CAD-CBD	-2.16	122.81	125.89
7	S	2005	BPH	C7-C6-C5	-2.16	107.50	113.36
7	M	1006	BPH	CAA-C2A-C1A	-2.16	106.76	112.33
4	S	2001	BCL	CMB-C2B-C1B	-2.15	125.16	128.46
7	S	2005	BPH	OBD-CAD-CBD	-2.15	122.83	125.89
7	M	1005	BPH	OBD-CAD-CBD	-2.15	122.83	125.89
7	R	2006	BPH	CAA-C2A-C3A	-2.13	106.95	112.78
7	S	2005	BPH	CAC-C3C-C2C	-2.13	108.94	114.26
4	R	2002	BCL	C4-C3-C5	2.13	118.85	115.27
4	S	2004	BCL	C11-C10-C8	-2.13	109.05	115.92
7	M	1005	BPH	O2A-C1-C2	-2.12	103.06	108.64
4	S	2001	BCL	CBB-CAB-C3B	2.11	126.62	120.34
7	R	2006	BPH	OBD-CAD-CBD	-2.11	122.88	125.89
5	L	1009	U10	C10-C9-C11	-2.10	111.73	115.27
5	L	1009	U10	C7-C6-C5	-2.10	115.96	118.48
5	M	1008	U10	C6-C1-C2	2.09	120.84	119.18
4	M	1003	BCL	O2A-CGA-O1A	-2.08	118.33	123.59
4	M	1003	BCL	O1D-CGD-CBD	2.08	128.74	124.48
4	S	2003	BCL	O2A-CGA-CBA	2.08	118.43	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	2003	BCL	CAC-C3C-C4C	-2.07	107.98	112.58
4	R	2002	BCL	C12-C11-C10	-2.07	103.74	113.24
7	M	1005	BPH	C3A-C2A-C1A	2.07	104.11	101.64
7	S	2005	BPH	C3A-C2A-C1A	2.07	104.11	101.64
4	M	1003	BCL	C2C-C3C-C4C	2.05	104.40	101.34
4	S	2004	BCL	C14-C13-C15	-2.05	103.89	111.29
4	L	1002	BCL	CBC-CAC-C3C	-2.03	108.95	113.47
9	M	1014	LDA	C9-C8-C7	-2.02	104.15	114.42
7	M	1006	BPH	C2A-C1A-NA	-2.02	109.54	111.86
7	M	1005	BPH	C7-C6-C5	-2.01	107.91	113.36

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	M	1005	BPH	C8
7	M	1006	BPH	C8
7	M	1006	BPH	C13
7	R	2006	BPH	C8
7	R	2006	BPH	C13
7	S	2005	BPH	C8

All (176) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1004	BCL	C1A-C2A-CAA-CBA
4	L	1004	BCL	C3A-C2A-CAA-CBA
4	M	1003	BCL	C4-C3-C5-C6
4	S	2003	BCL	C2-C3-C5-C6
4	S	2003	BCL	C4-C3-C5-C6
5	L	1009	U10	C24-C26-C27-C28
5	L	1009	U10	C29-C31-C32-C33
5	L	1009	U10	C31-C32-C33-C34
7	M	1005	BPH	C4B-C3B-CAB-CBB
7	M	1005	BPH	C4B-C3B-CAB-OB
7	M	1005	BPH	C2B-C3B-CAB-CBB
7	M	1006	BPH	C4C-C3C-CAC-CBC
7	M	1006	BPH	C2C-C3C-CAC-CBC
7	M	1006	BPH	C4B-C3B-CAB-CBB
7	M	1006	BPH	C1-C2-C3-C4
7	M	1006	BPH	C1-C2-C3-C5
7	R	2006	BPH	C4C-C3C-CAC-CBC
7	R	2006	BPH	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	R	2006	BPH	C4B-C3B-CAB-CBB
7	R	2006	BPH	C4B-C3B-CAB-OBB
7	R	2006	BPH	C2B-C3B-CAB-CBB
7	R	2006	BPH	O2A-C1-C2-C3
7	S	2005	BPH	C4B-C3B-CAB-CBB
7	S	2005	BPH	C4B-C3B-CAB-OBB
7	S	2005	BPH	C2B-C3B-CAB-CBB
7	S	2005	BPH	C2B-C3B-CAB-OBB
7	S	2005	BPH	C2-C3-C5-C6
7	S	2005	BPH	C4-C3-C5-C6
8	M	1010	SPO	C3-C1-O1-CM1
8	M	1010	SPO	C4-C5-C6-C7
8	M	1010	SPO	C36-C37-C38-C39
8	S	2010	SPO	C3-C1-O1-CM1
8	S	2010	SPO	C1-C4-C5-C6
8	S	2010	SPO	C4-C5-C6-C7
8	S	2010	SPO	C36-C37-C38-C40
8	S	2010	SPO	C36-C37-C38-C39
7	S	2005	BPH	CBD-CGD-O2D-CED
4	M	1003	BCL	C2-C3-C5-C6
8	M	1010	SPO	C36-C37-C38-C40
7	M	1005	BPH	CBD-CGD-O2D-CED
8	S	2010	SPO	C33-C35-C36-C37
7	R	2006	BPH	C8-C10-C11-C12
7	R	2006	BPH	C10-C11-C12-C13
7	M	1006	BPH	C10-C11-C12-C13
7	S	2005	BPH	O1D-CGD-O2D-CED
4	L	1004	BCL	C2A-CAA-CBA-CGA
7	M	1005	BPH	C2B-C3B-CAB-OBB
7	R	2006	BPH	C2B-C3B-CAB-OBB
7	S	2005	BPH	C6-C7-C8-C10
9	M	1014	LDA	C6-C7-C8-C9
7	S	2005	BPH	C6-C7-C8-C9
9	M	1012	LDA	C6-C7-C8-C9
9	M	1011	LDA	C4-C5-C6-C7
4	S	2003	BCL	C3-C5-C6-C7
9	S	2011	LDA	C1-C2-C3-C4
7	M	1005	BPH	C5-C6-C7-C8
7	R	2006	BPH	C12-C13-C15-C16
9	M	1013	LDA	C4-C5-C6-C7
7	M	1005	BPH	O1D-CGD-O2D-CED
9	M	1012	LDA	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	S	2003	BCL	C11-C10-C8-C9
4	S	2004	BCL	C1A-C2A-CAA-CBA
9	M	1014	LDA	C1-C2-C3-C4
4	R	2002	BCL	C15-C16-C17-C18
4	S	2003	BCL	C13-C15-C16-C17
8	M	1010	SPO	C33-C35-C36-C37
7	M	1006	BPH	C2B-C3B-CAB-CBB
7	R	2006	BPH	C4-C3-C5-C6
4	L	1004	BCL	C13-C15-C16-C17
7	M	1006	BPH	C8-C10-C11-C12
4	L	1002	BCL	C12-C13-C15-C16
4	S	2003	BCL	C11-C10-C8-C7
4	S	2003	BCL	C11-C12-C13-C15
4	M	1003	BCL	C11-C10-C8-C9
7	M	1006	BPH	C11-C12-C13-C14
7	R	2006	BPH	C14-C13-C15-C16
9	S	2011	LDA	C9-C10-C11-C12
7	S	2005	BPH	C5-C6-C7-C8
5	L	1009	U10	C12-C11-C9-C10
5	L	1009	U10	C25-C24-C26-C27
4	L	1002	BCL	C15-C16-C17-C18
7	M	1005	BPH	O2A-C1-C2-C3
7	M	1006	BPH	O2A-C1-C2-C3
5	L	1009	U10	C12-C11-C9-C8
7	R	2006	BPH	C2-C3-C5-C6
9	M	1012	LDA	C9-C10-C11-C12
9	M	1011	LDA	C11-C10-C9-C8
4	M	1003	BCL	C11-C10-C8-C7
4	M	1003	BCL	C11-C12-C13-C15
4	R	2002	BCL	C12-C13-C15-C16
7	M	1006	BPH	C11-C12-C13-C15
7	M	1006	BPH	C4B-C3B-CAB-OBB
8	S	2010	SPO	C20-C21-C22-C23
4	M	1003	BCL	C13-C15-C16-C17
4	S	2004	BCL	CAD-CBD-CGD-O2D
4	M	1003	BCL	C3-C5-C6-C7
5	S	2008	U10	C5-C4-O4-C4M
9	M	1011	LDA	C2-C1-N1-CM1
9	M	1011	LDA	C2-C1-N1-CM2
9	M	1012	LDA	C2-C1-N1-CM1
9	M	1012	LDA	C2-C1-N1-CM2
9	M	1013	LDA	C2-C1-N1-CM1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	M	1013	LDA	C2-C1-N1-CM2
9	M	1014	LDA	C2-C1-N1-CM1
9	M	1014	LDA	C2-C1-N1-CM2
9	S	2011	LDA	C2-C1-N1-CM1
9	S	2011	LDA	C2-C1-N1-CM2
4	L	1001	BCL	C1A-C2A-CAA-CBA
8	M	1010	SPO	C20-C21-C22-C23
7	R	2006	BPH	C16-C17-C18-C20
7	M	1006	BPH	C15-C16-C17-C18
9	M	1011	LDA	C2-C1-N1-O1
9	M	1012	LDA	C2-C1-N1-O1
9	M	1013	LDA	C2-C1-N1-O1
9	M	1014	LDA	C2-C1-N1-O1
9	S	2011	LDA	C2-C1-N1-O1
8	M	1010	SPO	C1-C4-C5-C6
4	L	1004	BCL	C11-C12-C13-C15
4	M	1003	BCL	C15-C16-C17-C18
4	L	1002	BCL	C2A-CAA-CBA-CGA
4	R	2002	BCL	C14-C13-C15-C16
5	M	1008	U10	C5-C4-O4-C4M
5	L	1009	U10	C23-C24-C26-C27
4	L	1002	BCL	C14-C13-C15-C16
4	L	1004	BCL	C11-C10-C8-C9
4	L	1004	BCL	C11-C12-C13-C14
4	S	2003	BCL	C11-C12-C13-C14
4	S	2004	BCL	C11-C10-C8-C9
7	R	2006	BPH	C16-C17-C18-C19
5	S	2008	U10	C21-C22-C23-C24
4	S	2004	BCL	C15-C16-C17-C18
8	M	1010	SPO	C17-C19-C20-C21
8	S	2010	SPO	C17-C19-C20-C21
8	M	1010	SPO	C19-C20-C21-C22
9	M	1011	LDA	C9-C10-C11-C12
7	S	2005	BPH	C2-C1-O2A-CGA
7	M	1006	BPH	C2B-C3B-CAB-OBB
8	M	1010	SPO	C18-C17-C19-C20
8	S	2010	SPO	C18-C17-C19-C20
7	S	2005	BPH	O2A-C1-C2-C3
9	S	2011	LDA	C6-C7-C8-C9
7	M	1006	BPH	C12-C13-C15-C16
9	S	2011	LDA	C11-C10-C9-C8
8	M	1010	SPO	C16-C17-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	S	2010	SPO	C16-C17-C19-C20
9	M	1014	LDA	C11-C10-C9-C8
4	R	2002	BCL	C2A-CAA-CBA-CGA
7	S	2005	BPH	C2A-CAA-CBA-CGA
5	R	2009	U10	C2-C3-O3-C3M
4	R	2002	BCL	C4-C3-C5-C6
8	M	1010	SPO	C4-C1-O1-CM1
8	S	2010	SPO	C4-C1-O1-CM1
4	S	2004	BCL	C11-C10-C8-C7
7	M	1005	BPH	C1-C2-C3-C4
4	L	1001	BCL	CAD-CBD-CGD-O2D
4	L	1002	BCL	CAD-CBD-CGD-O2D
4	S	2001	BCL	CAD-CBD-CGD-O2D
7	M	1005	BPH	CAD-CBD-CGD-O2D
7	M	1006	BPH	CAD-CBD-CGD-O2D
4	L	1002	BCL	C4-C3-C5-C6
4	L	1004	BCL	O2A-C1-C2-C3
4	S	2004	BCL	CAA-CBA-CGA-O2A
4	L	1004	BCL	CHA-CBD-CGD-O2D
7	R	2006	BPH	CHA-CBD-CGD-O2D
4	L	1004	BCL	C11-C10-C8-C7
4	M	1003	BCL	C11-C12-C13-C14
7	M	1006	BPH	C6-C7-C8-C9
7	M	1006	BPH	C14-C13-C15-C16
4	M	1003	BCL	C5-C6-C7-C8
8	S	2010	SPO	C30-C31-C32-C33
4	S	2004	BCL	CAA-CBA-CGA-O1A
8	M	1010	SPO	C30-C31-C32-C33
4	S	2001	BCL	CAA-CBA-CGA-O2A
4	S	2001	BCL	CAA-CBA-CGA-O1A
5	M	1008	U10	C3-C4-O4-C4M
7	M	1005	BPH	C2A-CAA-CBA-CGA

There are no ring outliers.

19 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	2006	BPH	5	0
4	R	2002	BCL	5	0
4	L	1002	BCL	6	0
8	S	2010	SPO	3	0
7	M	1005	BPH	2	0

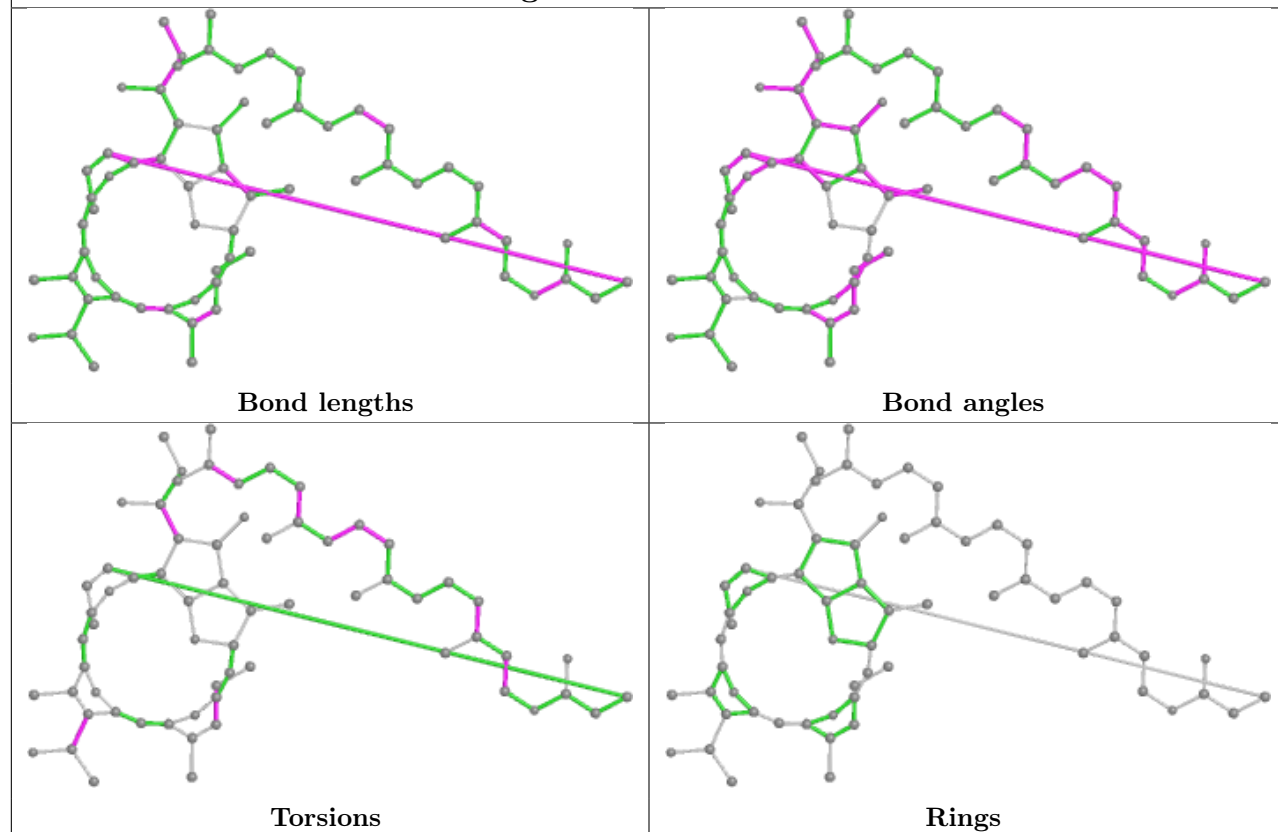
Continued on next page...

Continued from previous page...

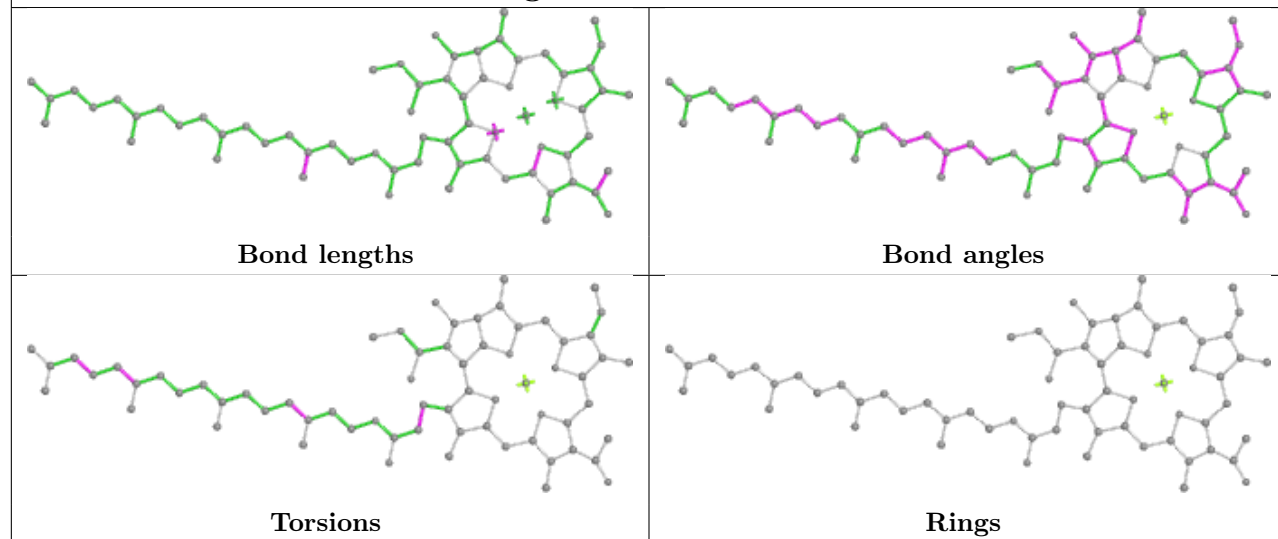
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1001	BCL	11	0
4	M	1003	BCL	13	0
9	M	1012	LDA	1	0
7	S	2005	BPH	2	0
5	L	1009	U10	3	0
7	M	1006	BPH	4	0
5	S	2008	U10	1	0
4	S	2004	BCL	5	0
9	M	1014	LDA	2	0
4	S	2001	BCL	8	0
8	M	1010	SPO	4	0
4	L	1004	BCL	9	0
4	S	2003	BCL	11	0
5	M	1008	U10	4	0

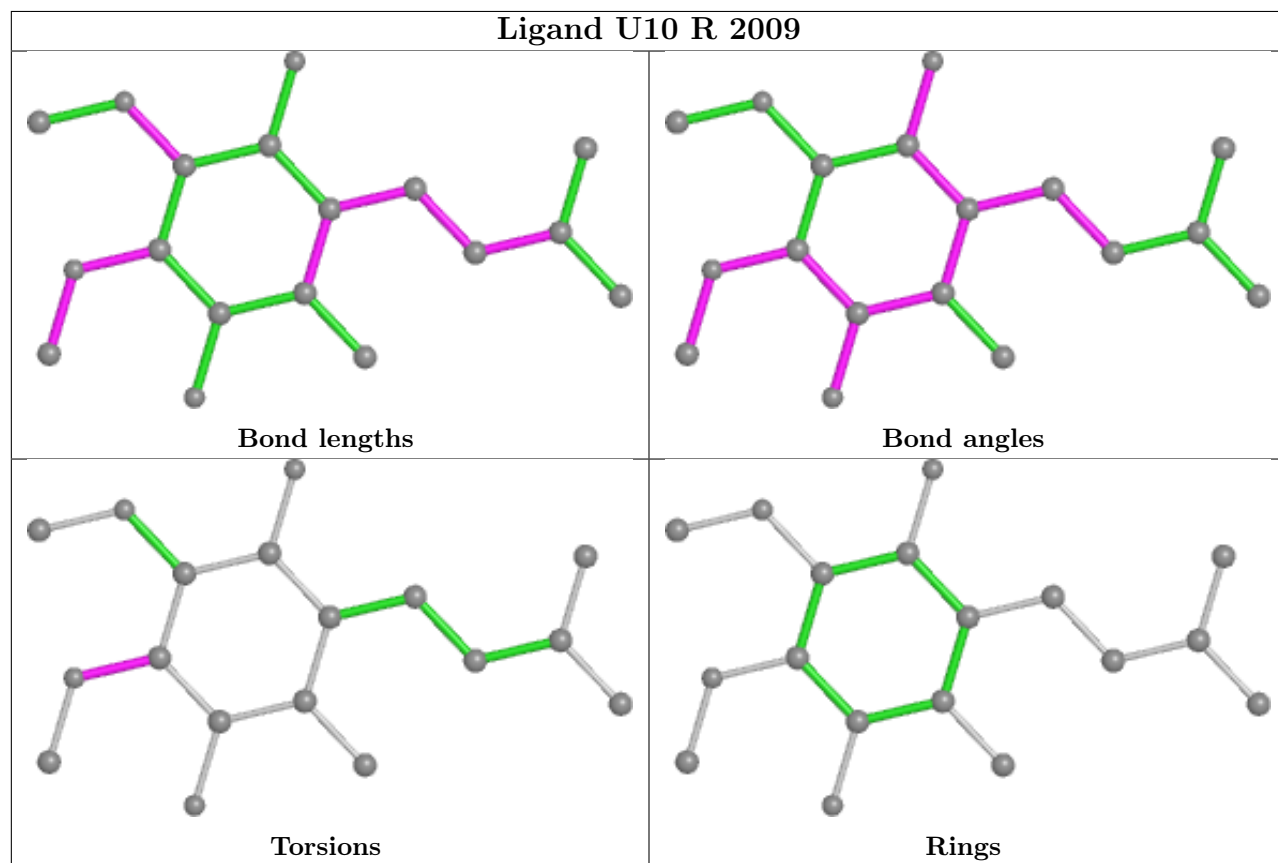
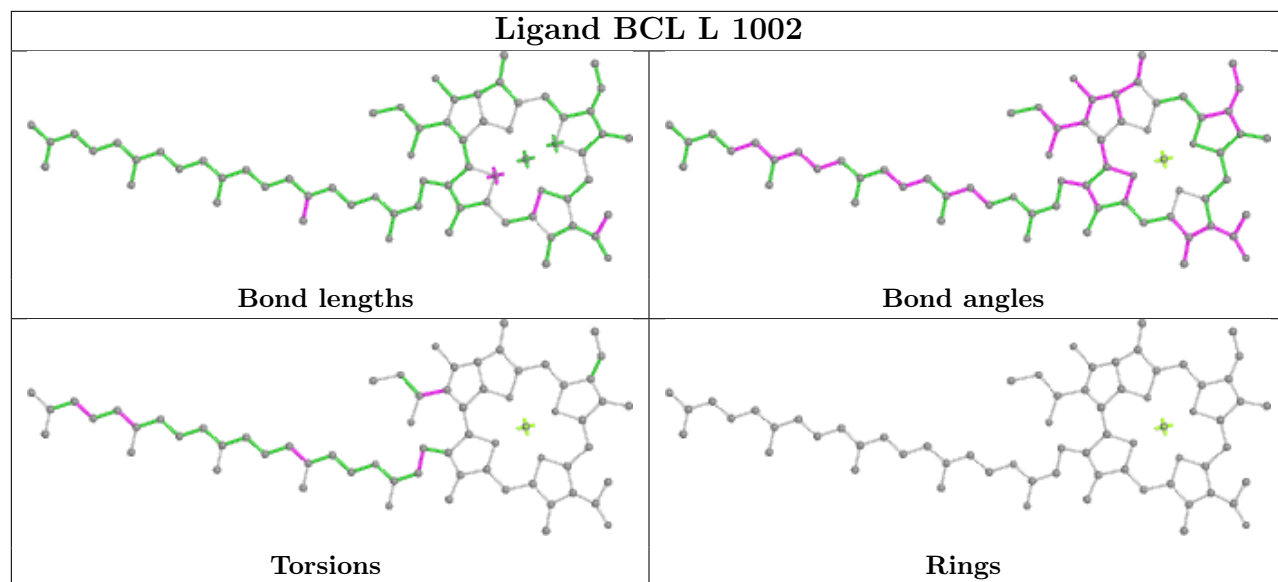
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

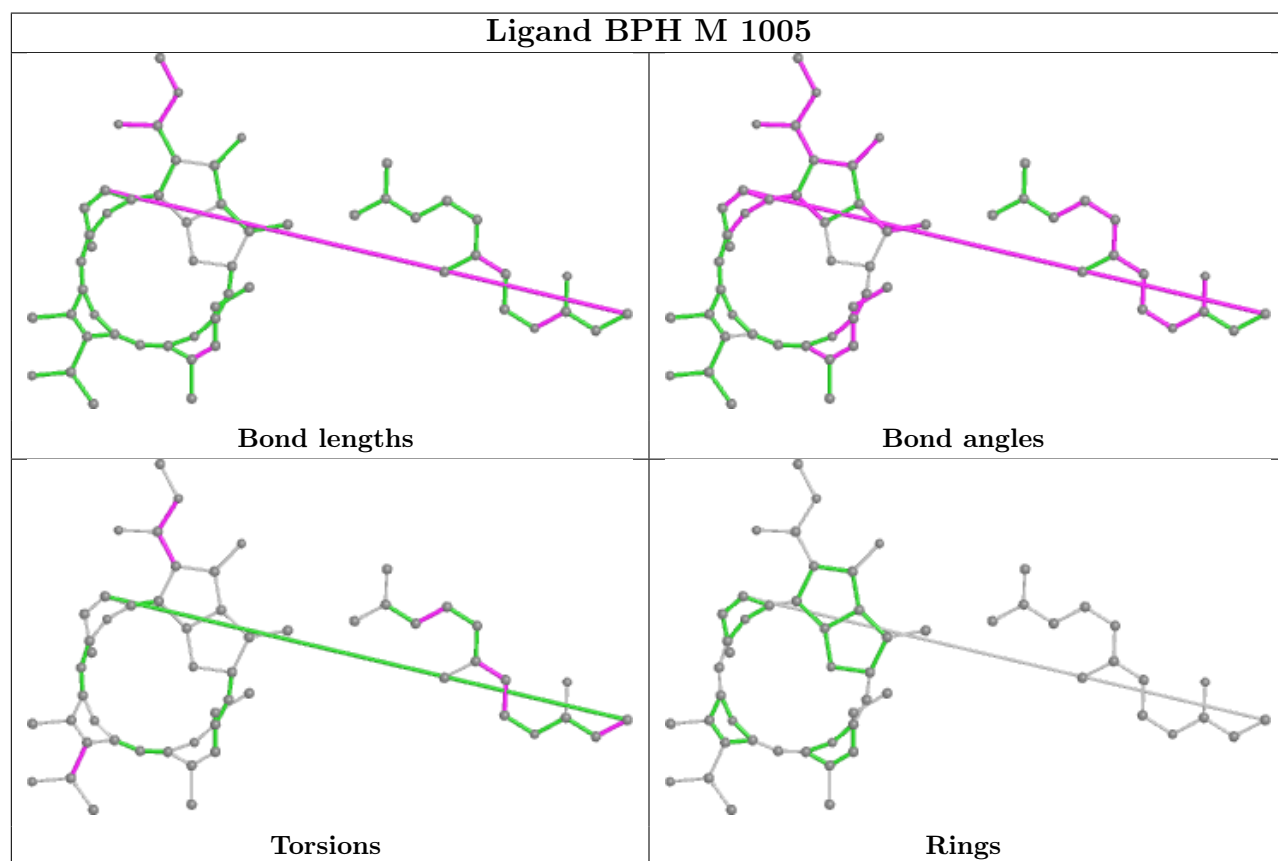
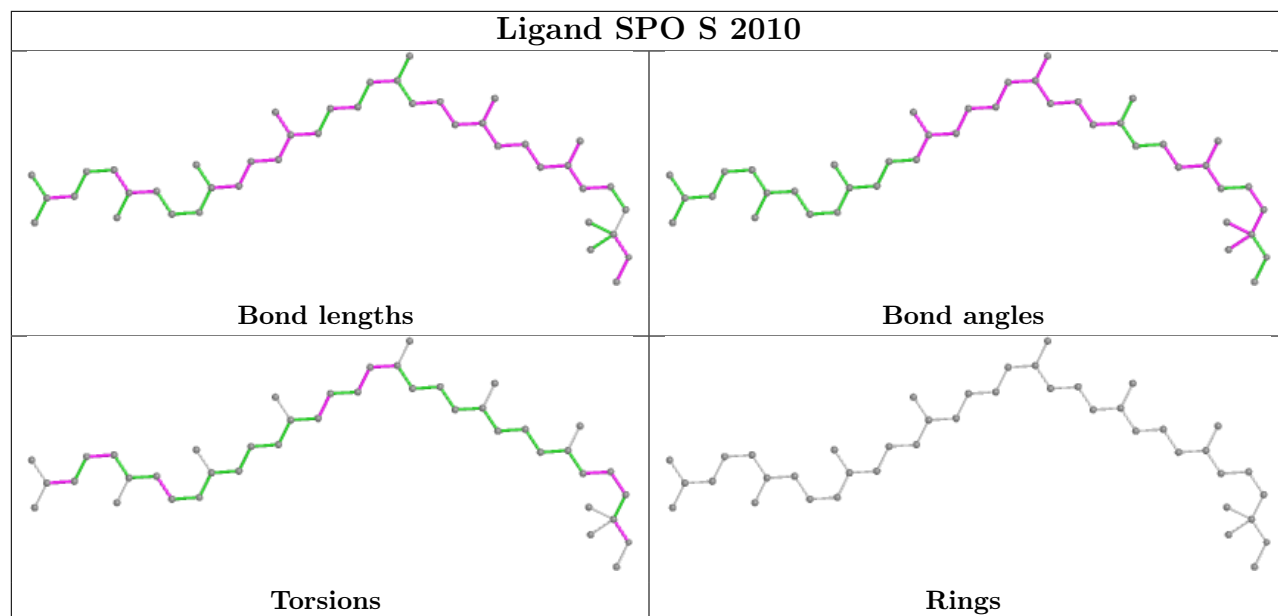
Ligand BPH R 2006

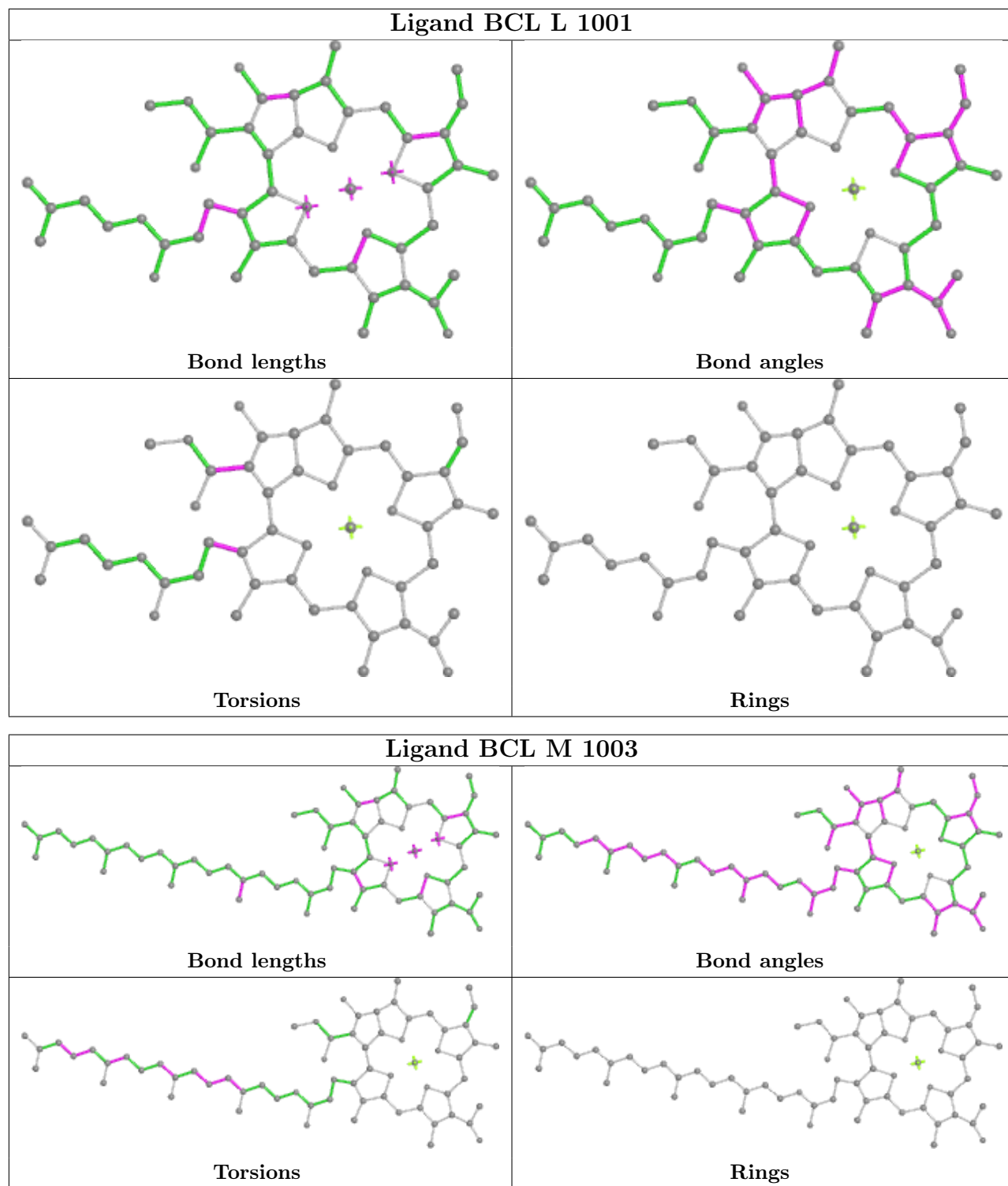


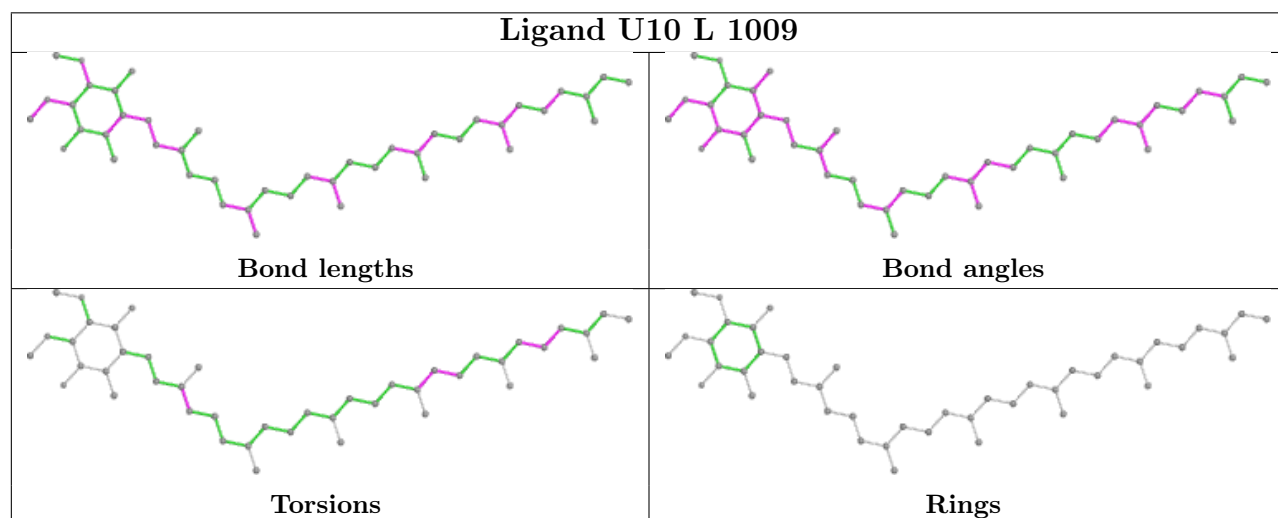
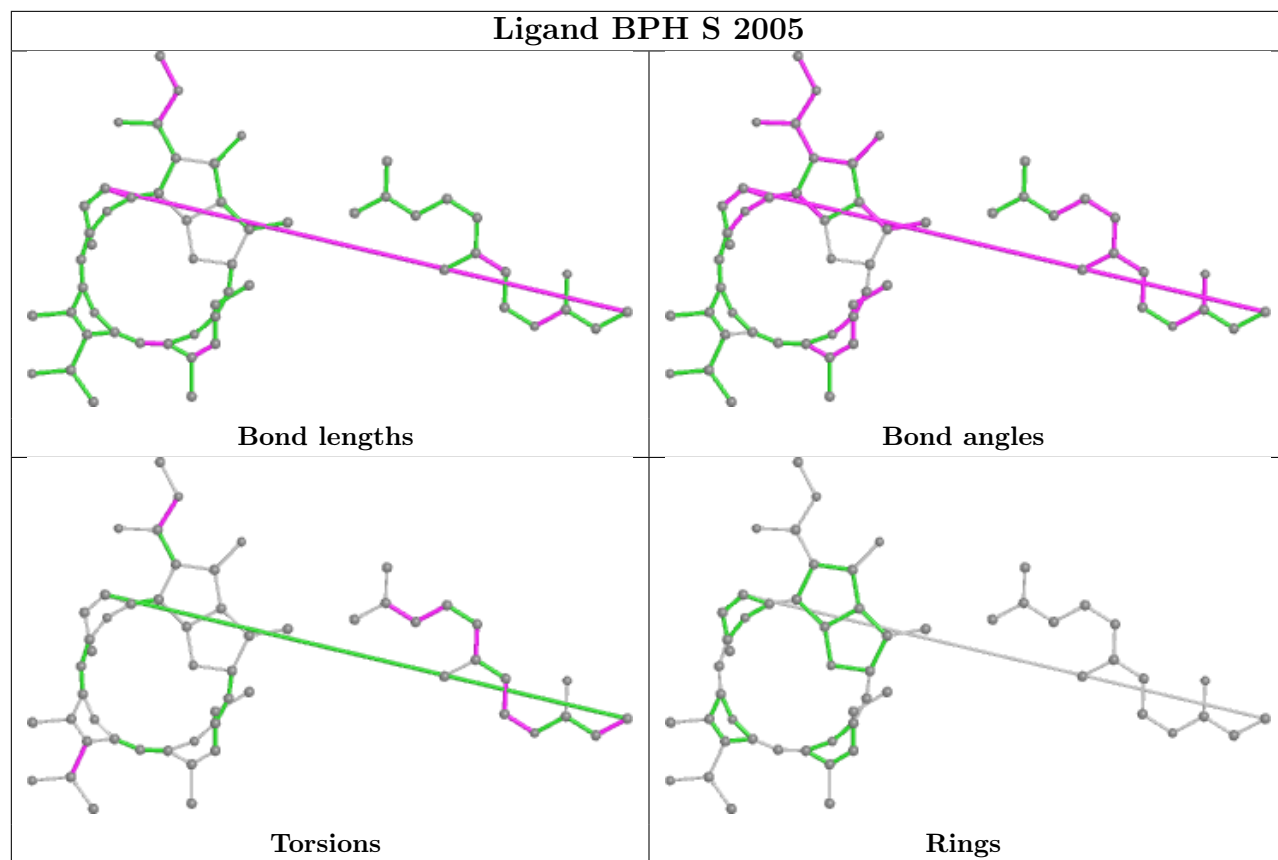
Ligand BCL R 2002



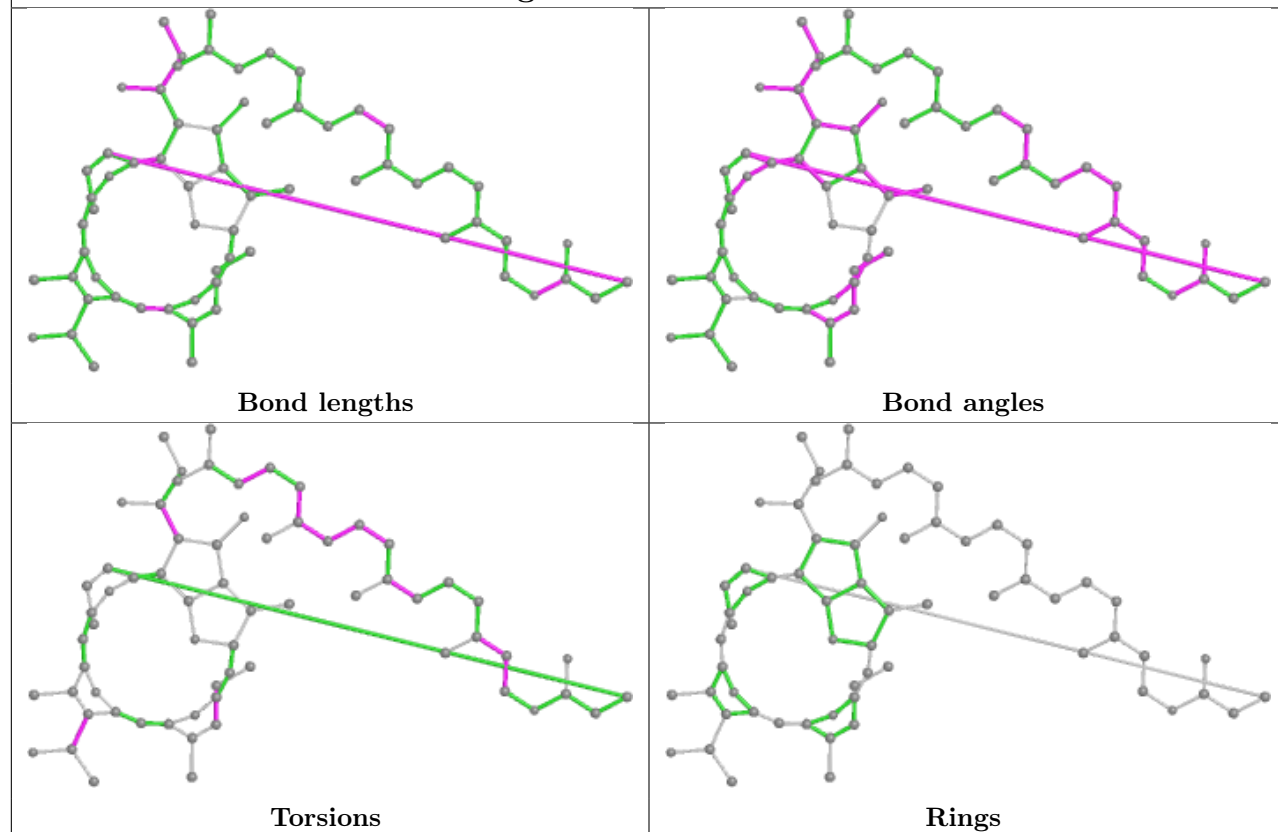




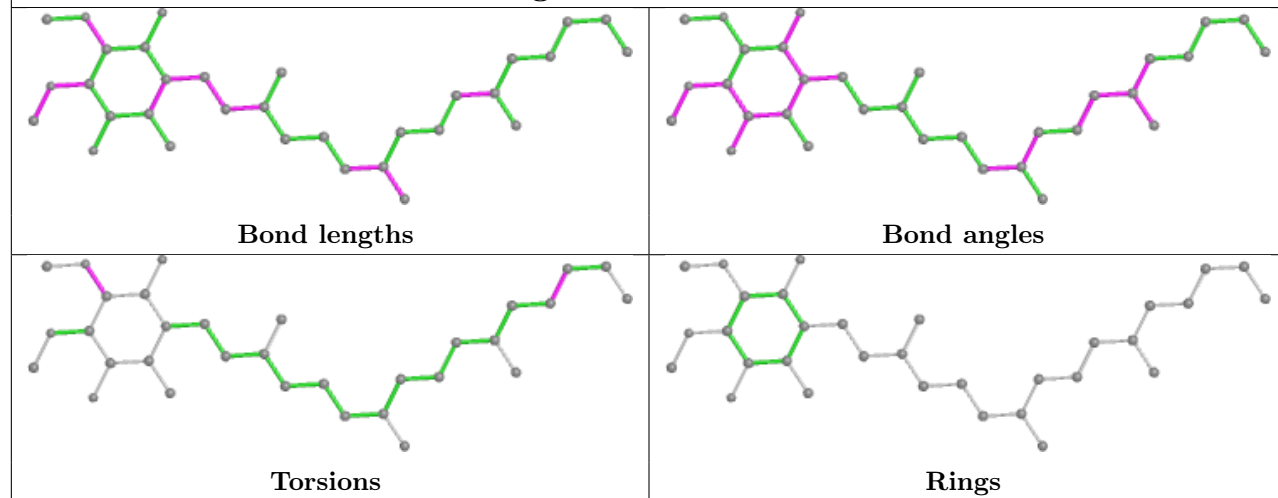


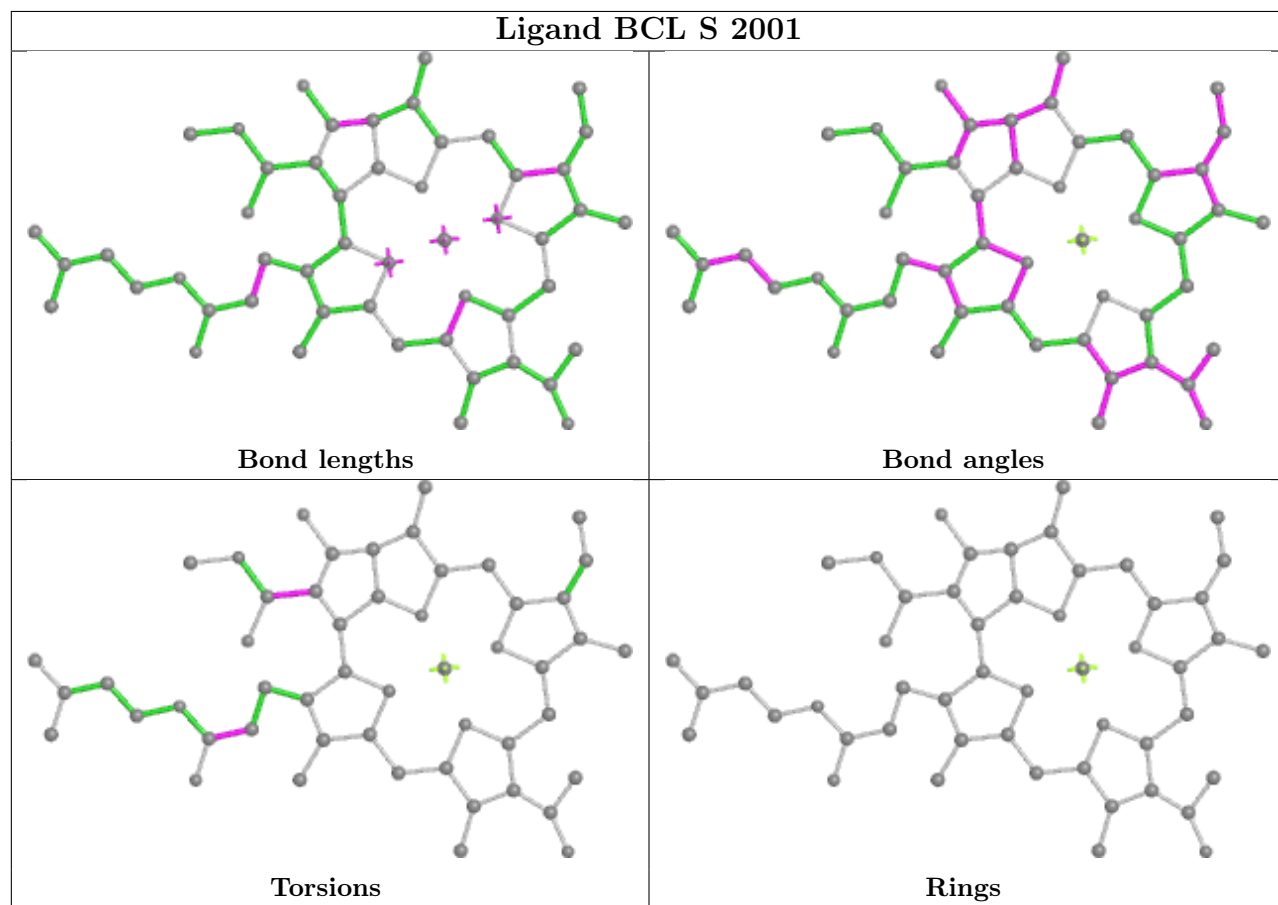
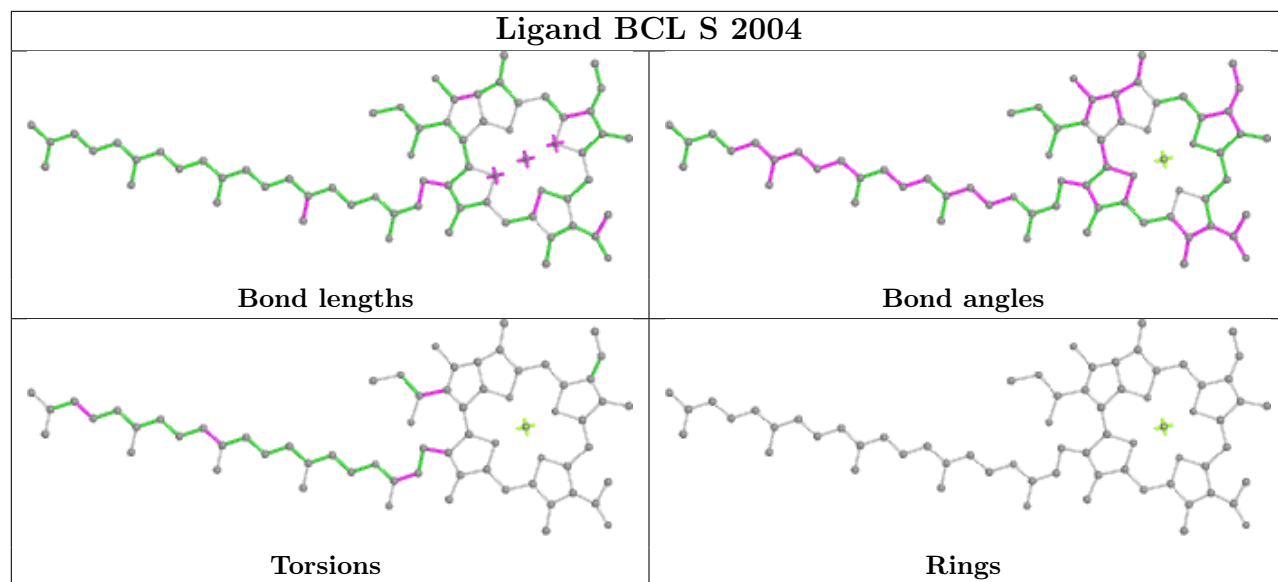


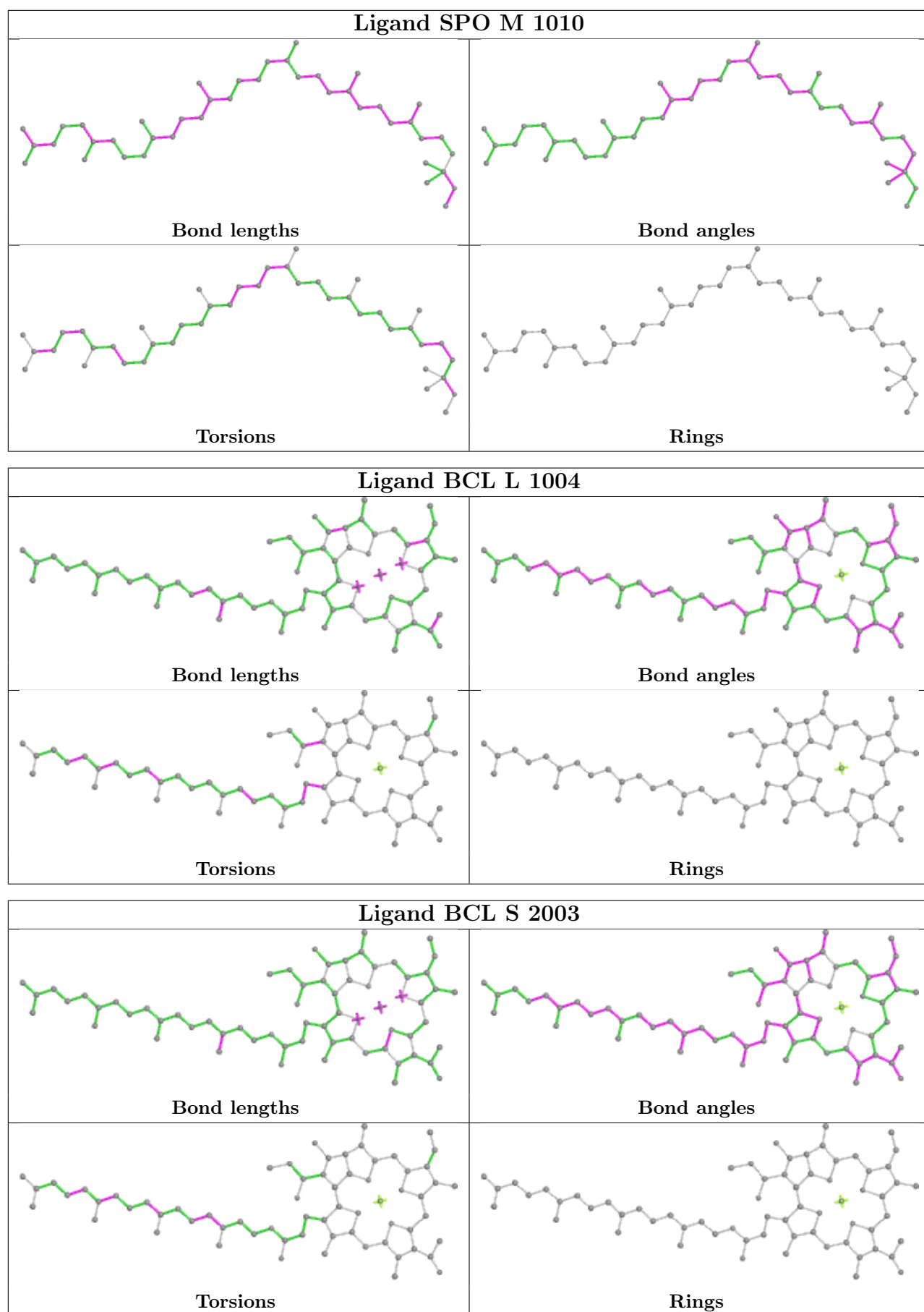
Ligand BPH M 1006

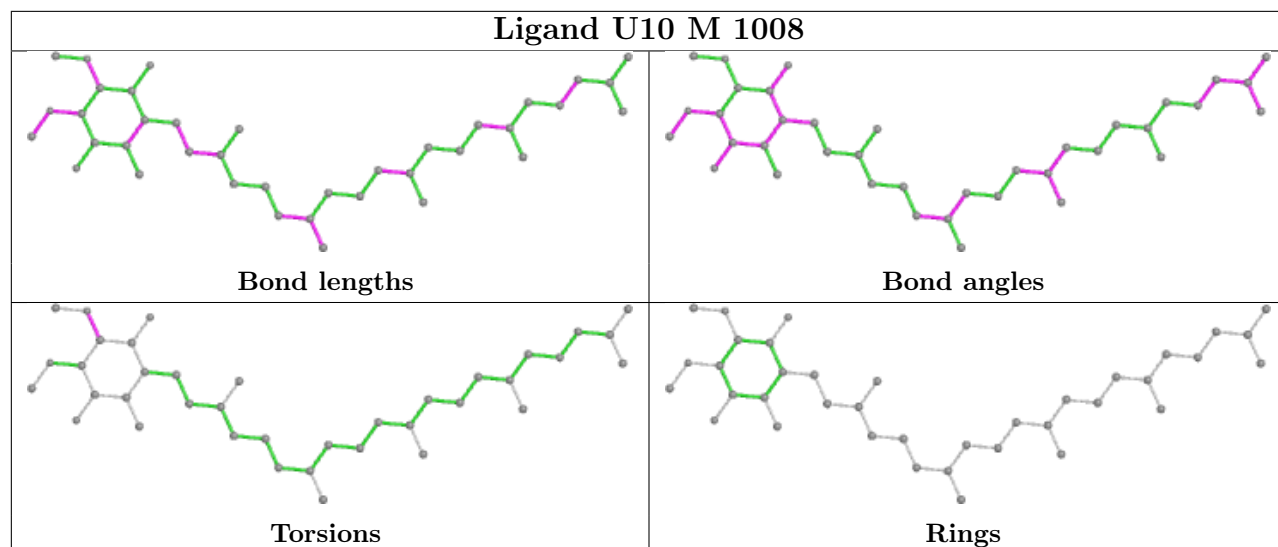


Ligand U10 S 2008









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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	281/281 (100%)	0.10	5 (1%) 68 66	17, 32, 49, 58	0
1	R	281/281 (100%)	0.29	16 (5%) 23 22	23, 41, 58, 69	0
2	M	299/307 (97%)	-0.04	12 (4%) 38 37	17, 27, 41, 67	0
2	S	299/307 (97%)	0.04	8 (2%) 54 52	24, 35, 48, 69	0
3	H	246/260 (94%)	0.08	10 (4%) 37 36	22, 34, 54, 88	0
3	T	246/260 (94%)	0.48	24 (9%) 7 7	31, 45, 70, 80	0
All	All	1652/1696 (97%)	0.15	75 (4%) 33 31	17, 36, 57, 88	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	252	VAL	6.1
3	H	254	ALA	5.6
3	H	255	MET	5.1
3	T	254	ALA	5.1
3	T	252	VAL	4.7
3	T	80	SER	4.6
3	H	251	VAL	4.6
3	T	51	ALA	4.5
3	T	92	VAL	4.5
1	R	1	ALA	4.3
3	T	54	GLY	4.1
2	S	301	HIS	4.0
3	H	256	LEU	3.9
3	H	253	ALA	3.8
1	R	140	GLY	3.8
3	T	255	MET	3.6
3	T	46	ASP	3.6
3	T	60	LYS	3.6
3	T	251	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	T	55	PRO	3.5
3	H	51	ALA	3.5
1	R	73	TYR	3.4
3	T	93	SER	3.4
3	T	79	GLU	3.4
1	R	74	GLY	3.3
3	T	18	TYR	3.3
3	H	250	SER	3.3
2	S	223	ILE	3.3
1	R	270	PRO	3.2
1	L	51	TRP	3.1
2	S	54	SER	2.9
3	T	29	TYR	2.9
2	S	226	VAL	2.9
3	T	253	ALA	2.8
3	T	58	LEU	2.8
1	R	76	GLY	2.8
1	R	75	LEU	2.8
3	T	157	ASP	2.8
1	R	51	TRP	2.7
2	M	226	VAL	2.7
2	S	3	TYR	2.7
1	R	271	TRP	2.7
2	M	225	ALA	2.7
2	M	231	GLY	2.7
1	R	281	GLY	2.5
2	M	222	THR	2.5
1	L	271	TRP	2.5
1	R	202	LYS	2.4
1	R	59	TRP	2.4
2	M	214	LEU	2.4
2	M	215	LEU	2.4
3	T	69	GLY	2.3
1	R	142	TRP	2.3
1	L	113	ILE	2.3
3	T	256	LEU	2.3
3	T	50	ALA	2.3
3	T	48	THR	2.3
1	R	269	LEU	2.3
2	M	224	LEU	2.2
2	M	221	ALA	2.2
2	M	301	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	88	ILE	2.2
3	T	56	PHE	2.2
1	R	267	VAL	2.2
2	M	211	GLY	2.2
3	T	49	PRO	2.2
1	R	256	PHE	2.1
3	H	52	ASN	2.1
3	H	18	TYR	2.1
2	M	223	ILE	2.1
2	M	227	SER	2.0
1	L	185	LEU	2.0
2	S	102	GLY	2.0
2	S	265	ILE	2.0
2	S	224	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

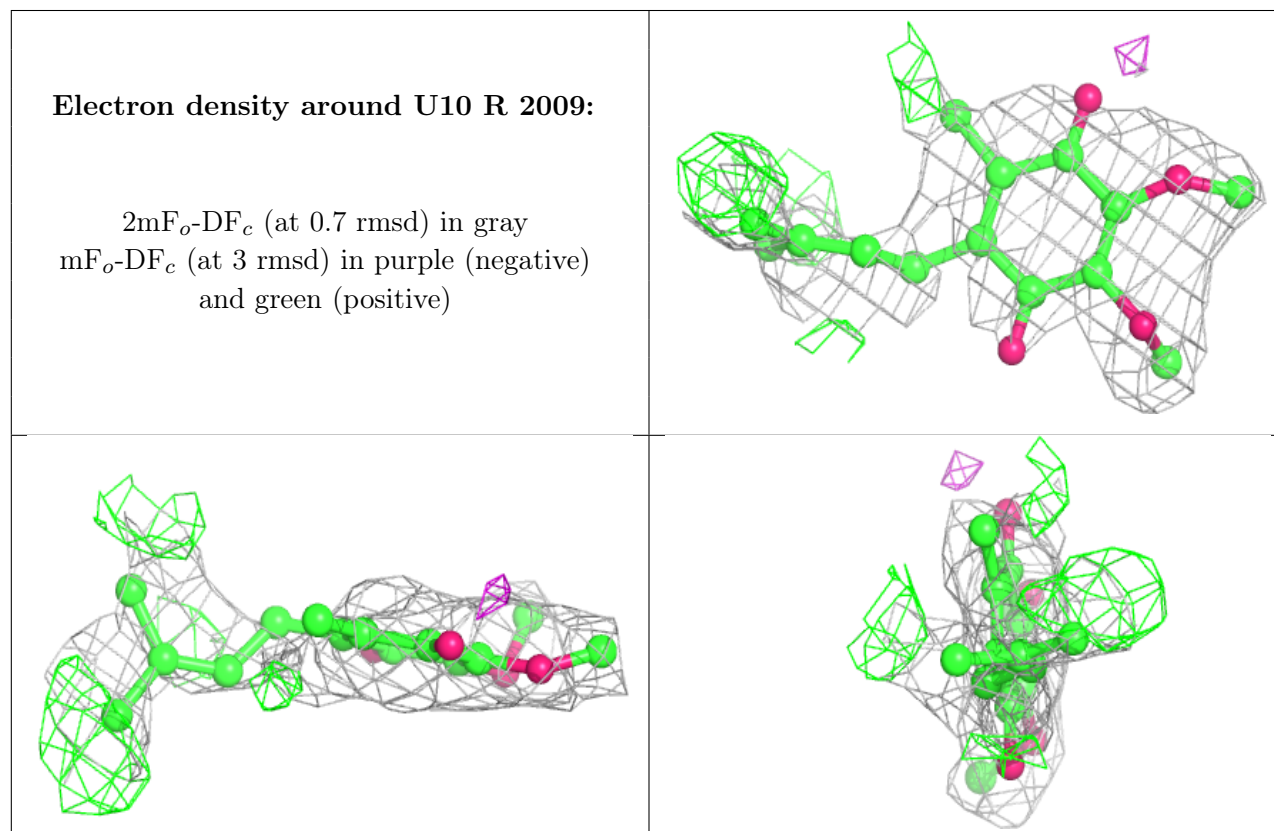
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	LDA	S	2011	16/16	0.60	0.42	74,79,85,85	0
9	LDA	M	1013	16/16	0.63	0.31	69,71,80,80	0
5	U10	R	2009	18/63	0.64	0.41	81,85,86,87	0
9	LDA	M	1011	16/16	0.64	0.26	49,57,74,74	0
5	U10	L	1009	44/63	0.66	0.34	66,72,79,79	0
9	LDA	M	1012	16/16	0.75	0.27	60,62,65,65	0
9	LDA	M	1014	16/16	0.78	0.34	50,55,59,60	0
8	SPO	S	2010	42/42	0.87	0.22	24,35,51,54	0
8	SPO	M	1010	42/42	0.87	0.21	16,28,47,51	0

Continued on next page...

Continued from previous page...

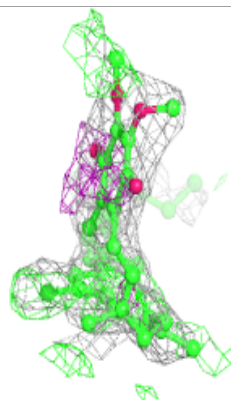
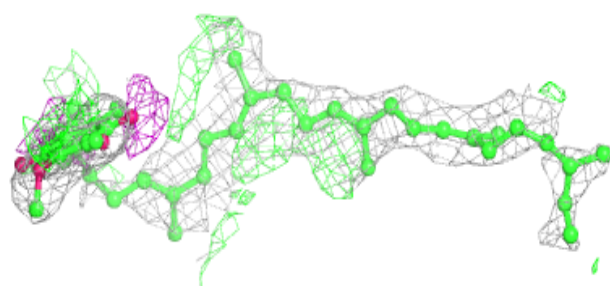
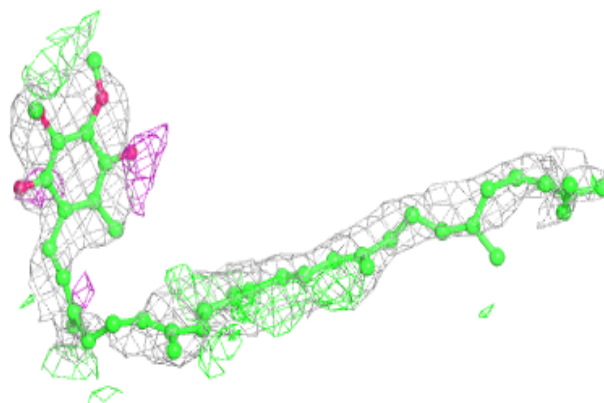
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BCL	R	2002	66/66	0.88	0.19	29,35,44,48	0
4	BCL	L	1001	51/66	0.90	0.22	17,24,51,55	0
4	BCL	S	2001	51/66	0.90	0.20	28,31,41,43	0
4	BCL	S	2003	66/66	0.90	0.21	27,33,48,55	0
4	BCL	L	1002	66/66	0.90	0.22	20,26,29,33	0
4	BCL	S	2004	66/66	0.91	0.21	26,34,58,60	0
4	BCL	L	1004	66/66	0.91	0.27	16,25,45,52	0
7	BPH	R	2006	65/65	0.92	0.19	31,38,45,46	0
5	U10	M	1008	38/63	0.92	0.30	23,30,53,53	0
4	BCL	M	1003	66/66	0.92	0.20	20,25,39,44	0
7	BPH	M	1006	65/65	0.92	0.25	23,28,37,40	0
7	BPH	M	1005	55/65	0.94	0.19	17,23,43,46	0
7	BPH	S	2005	55/65	0.94	0.17	25,30,55,58	0
5	U10	S	2008	32/63	0.94	0.34	36,42,51,54	0
6	FE2	S	2007	1/1	0.99	0.13	30,30,30,30	0
6	FE2	M	1007	1/1	0.99	0.14	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

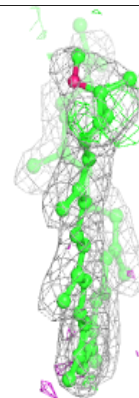
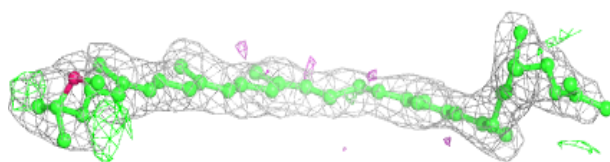
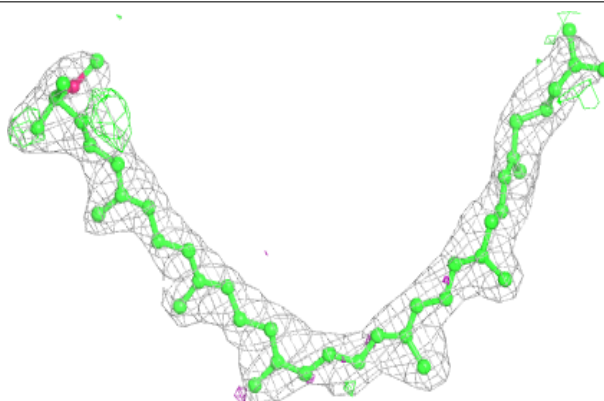


Electron density around U10 L 1009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

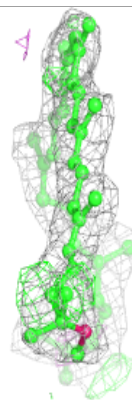
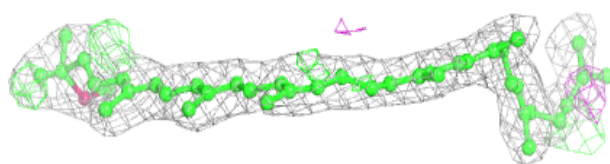
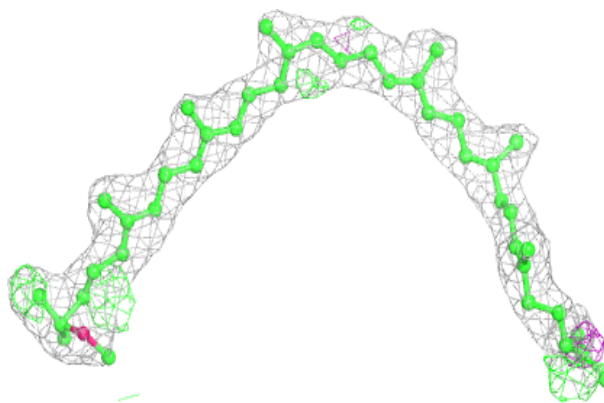
**Electron density around SPO S 2010:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

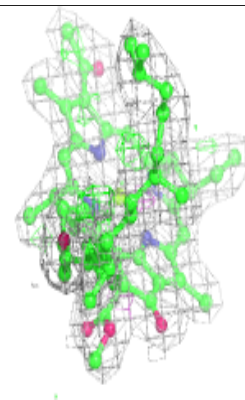
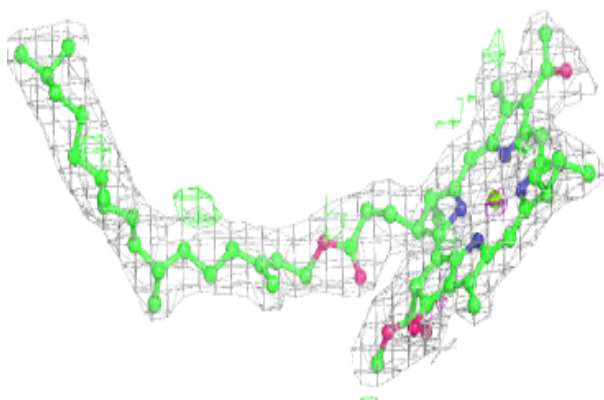


Electron density around SPO M 1010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

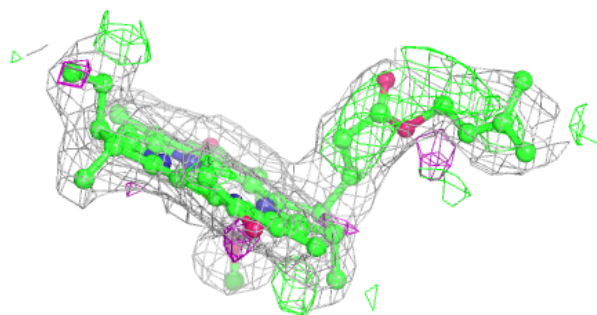
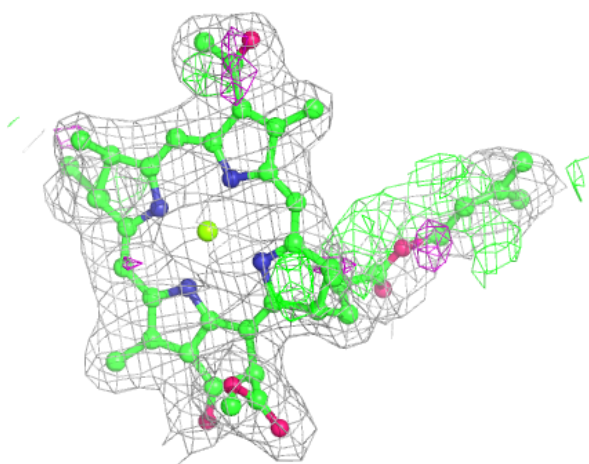
**Electron density around BCL R 2002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



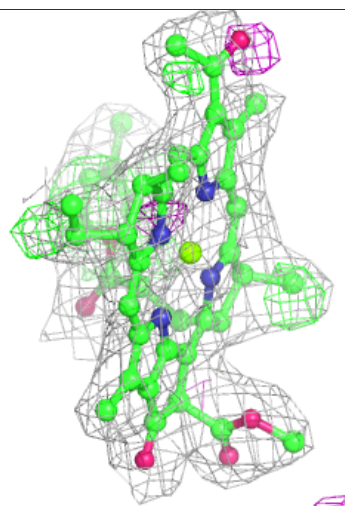
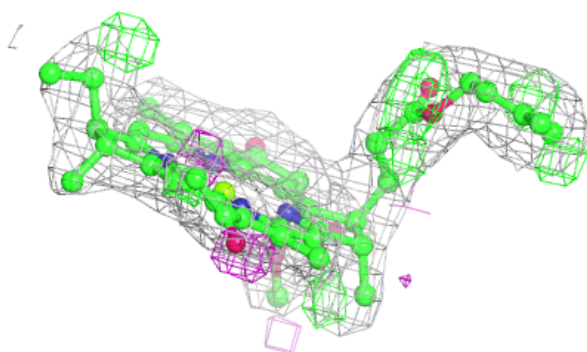
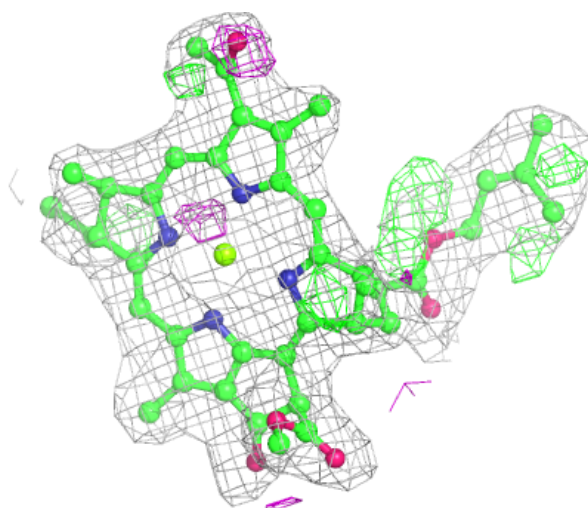
Electron density around BCL L 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



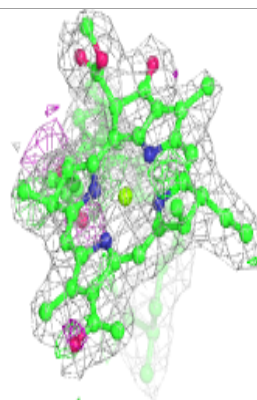
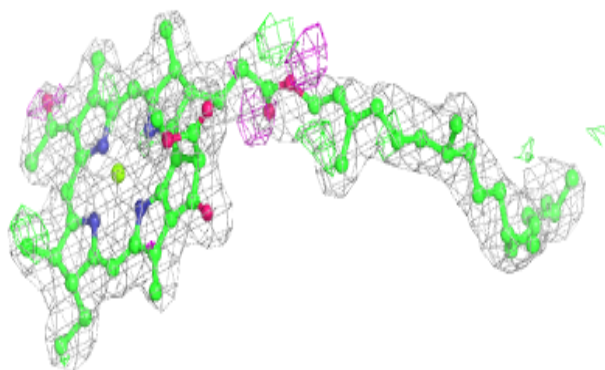
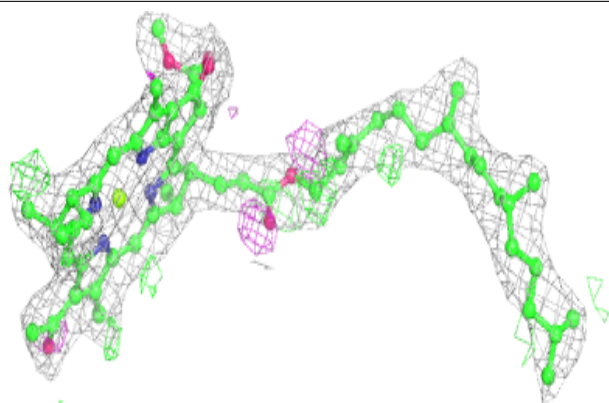
Electron density around BCL S 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

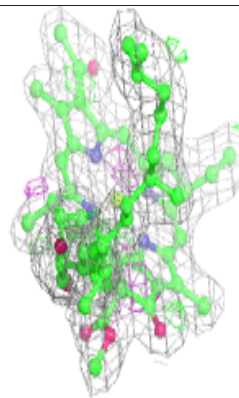
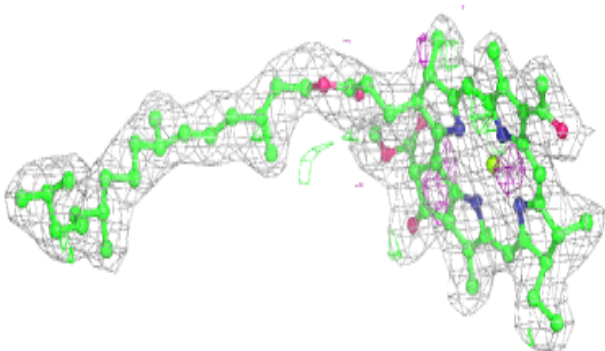
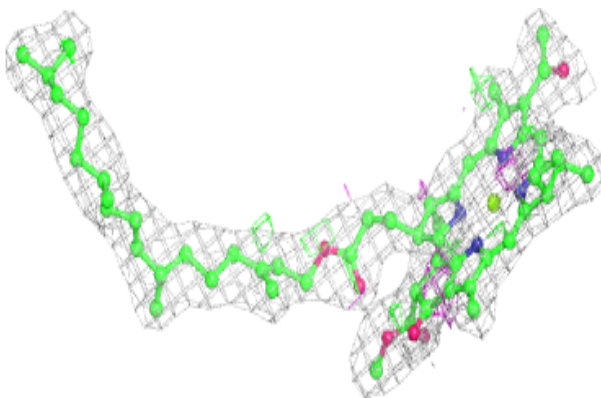


Electron density around BCL S 2003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

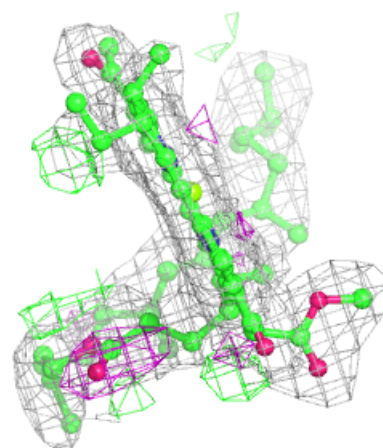
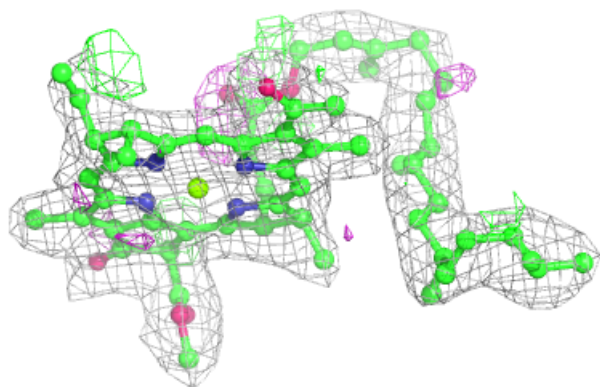
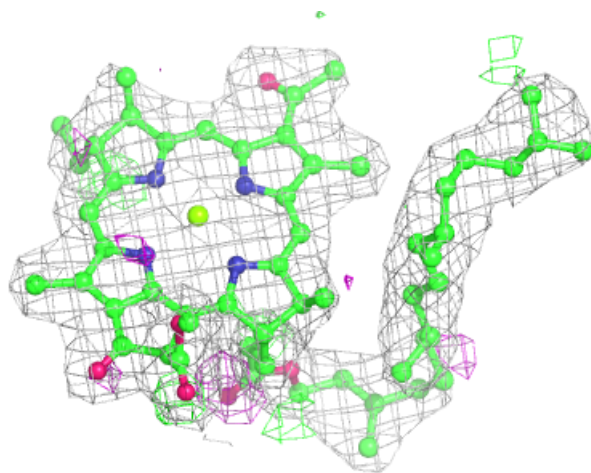
**Electron density around BCL L 1002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



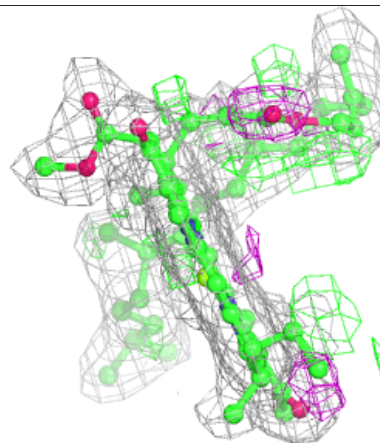
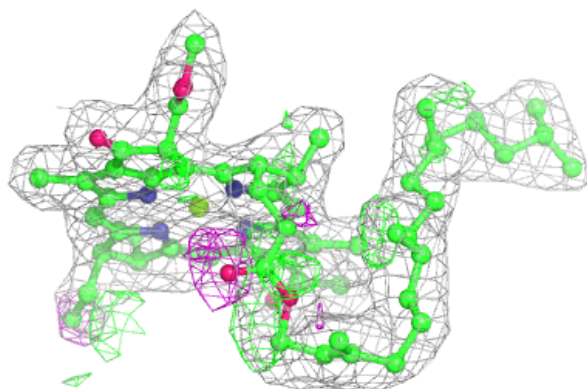
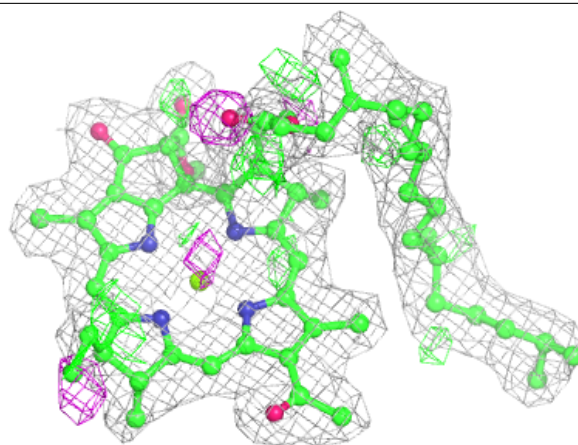
Electron density around BCL S 2004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



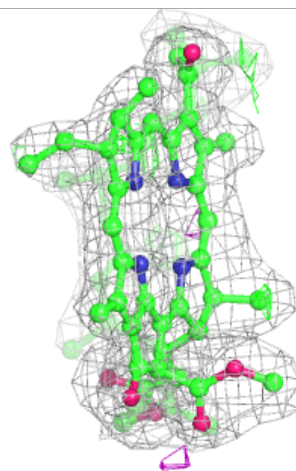
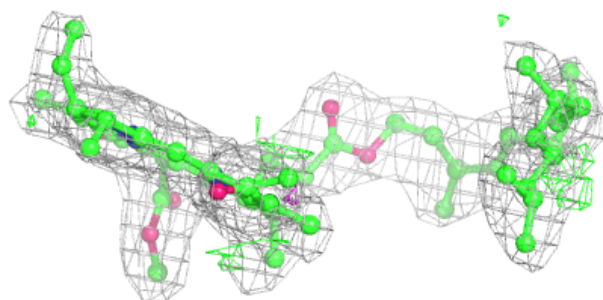
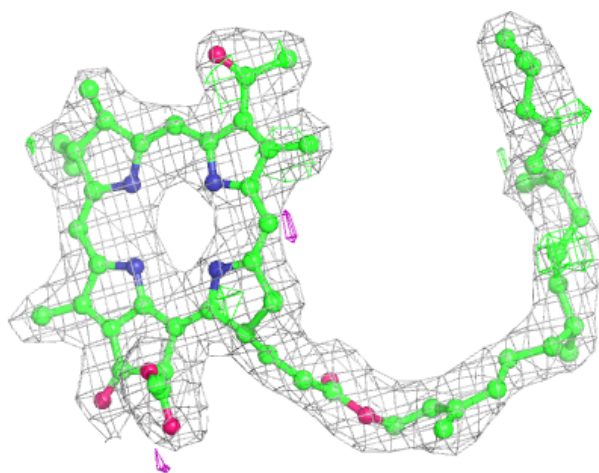
Electron density around BCL L 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



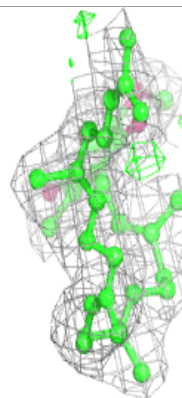
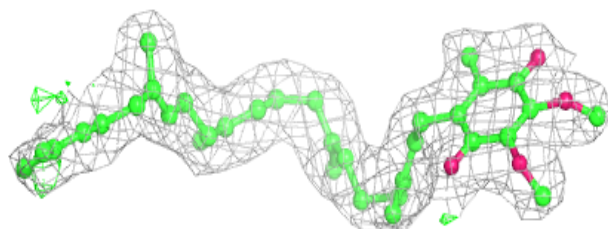
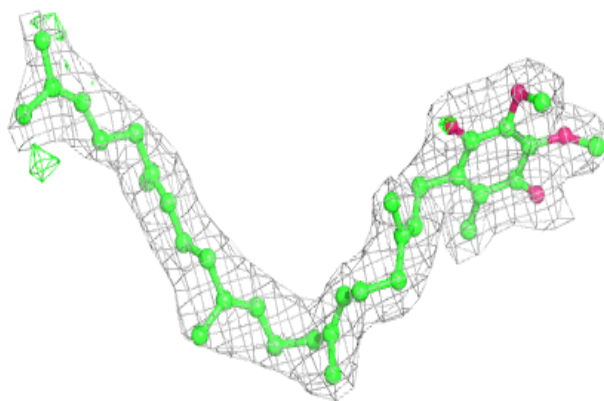
Electron density around BPH R 2006:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

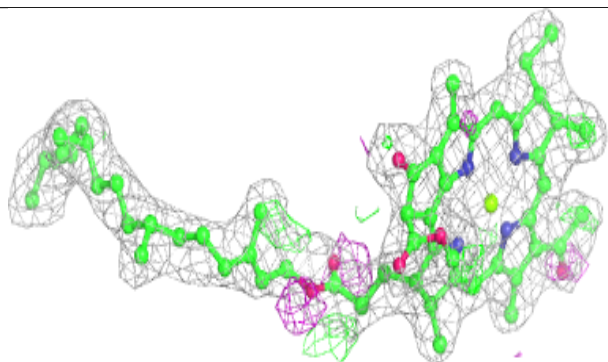
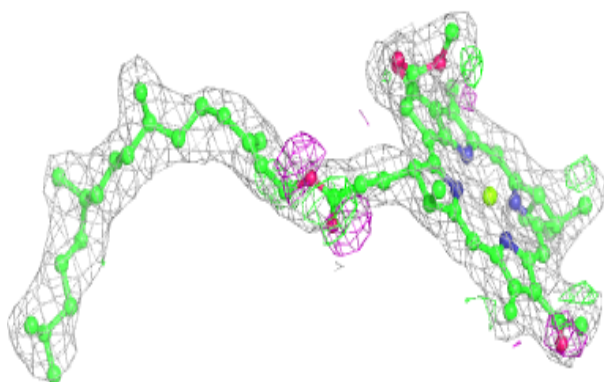


Electron density around U10 M 1008:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

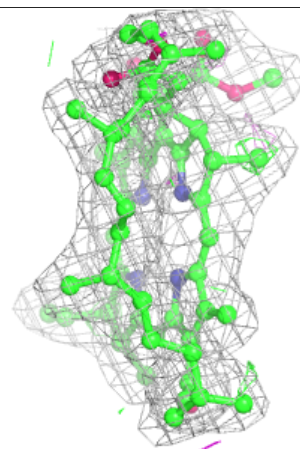
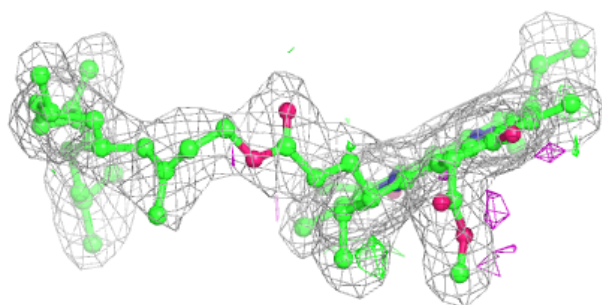
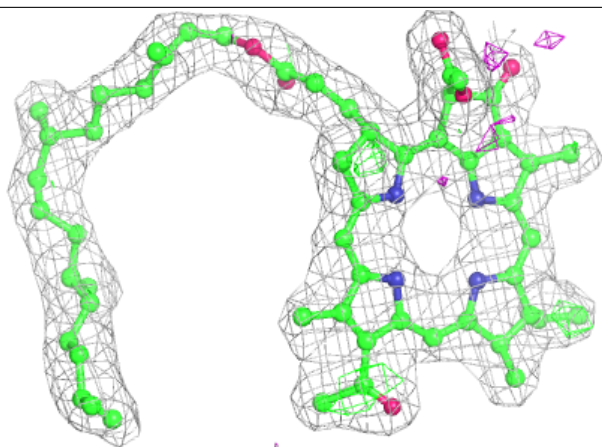
**Electron density around BCL M 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

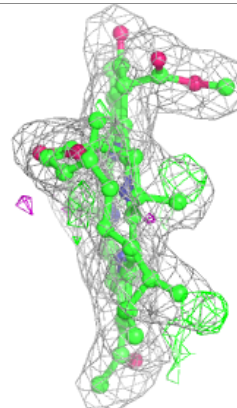
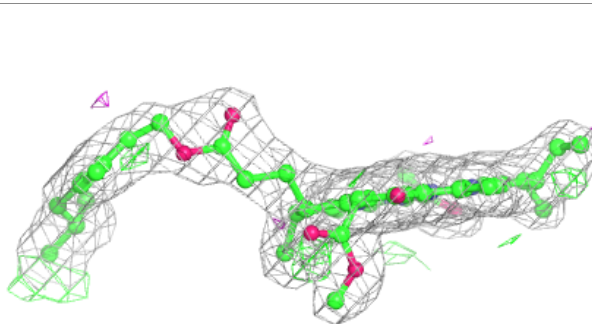
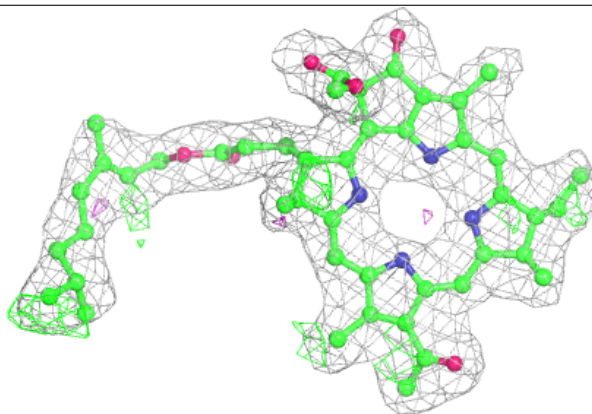


Electron density around BPH M 1006:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

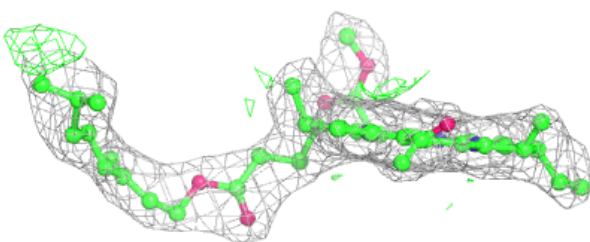
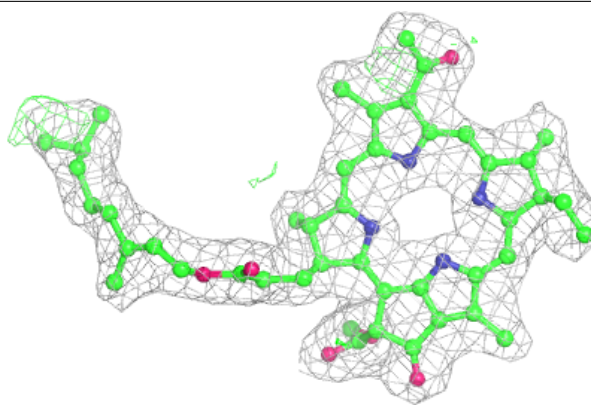
**Electron density around BPH M 1005:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

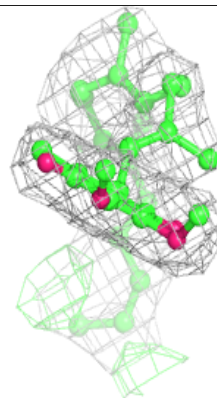
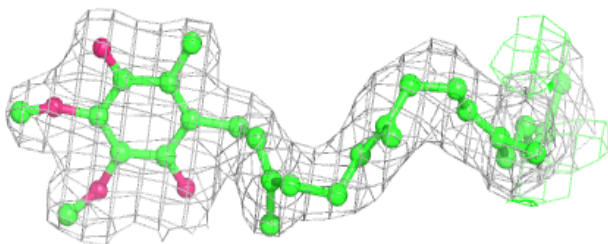


Electron density around BPH S 2005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around U10 S 2008:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.