



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:12 AM UTC

PDB ID : 1S00 / pdb_00001s00
Title : PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG M233 REPLACED WITH CYS IN THE CHARGE-SEPARATED D+QAQB- STATE
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Deposited on : 2003-12-29
Resolution : 2.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

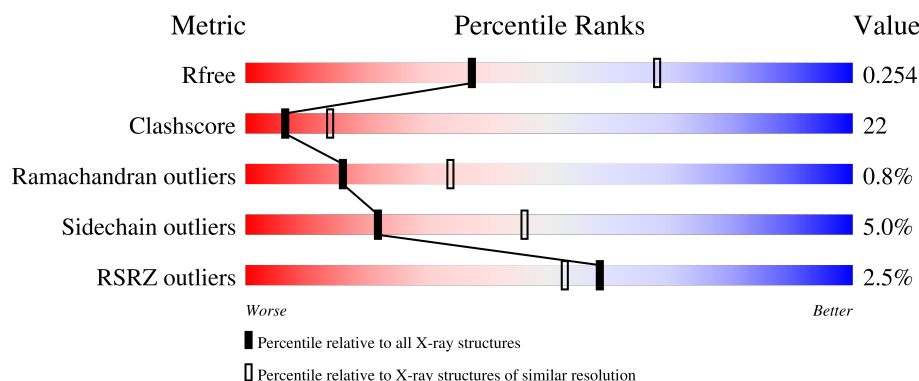
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	% 58% 37% • •
1	R	281	2% 53% 42% 5% •
2	M	307	% 66% 27% • •

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	S	307	
3	H	260	
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
4	BCL	M	1003	-	-	X	-
5	BPH	L	1006	X	-	-	-
5	BPH	M	1005	X	-	-	-
5	BPH	R	2006	X	-	-	-
6	U10	L	1009[A]	-	-	-	X
6	U10	L	1009[B]	-	-	-	X
6	U10	R	2009[A]	-	-	-	X
6	U10	R	2009[B]	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14144 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	301	Total	C	N	O	S	0	0	0
			2399	1602	390	396	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

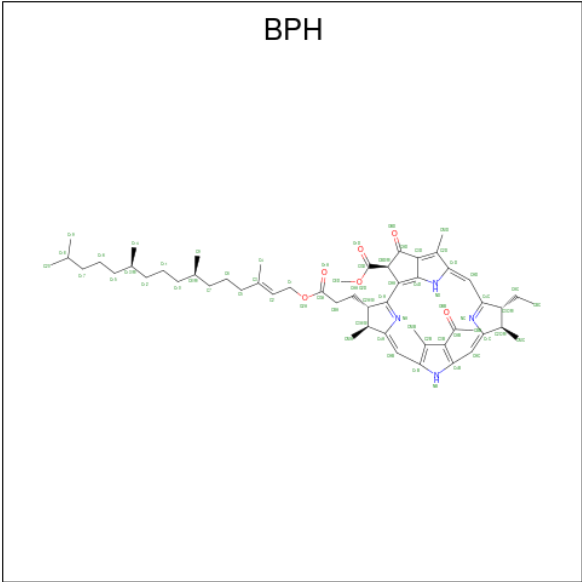
- Molecule 3 is a protein called Reaction center protein H chain.

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			

- # BCL

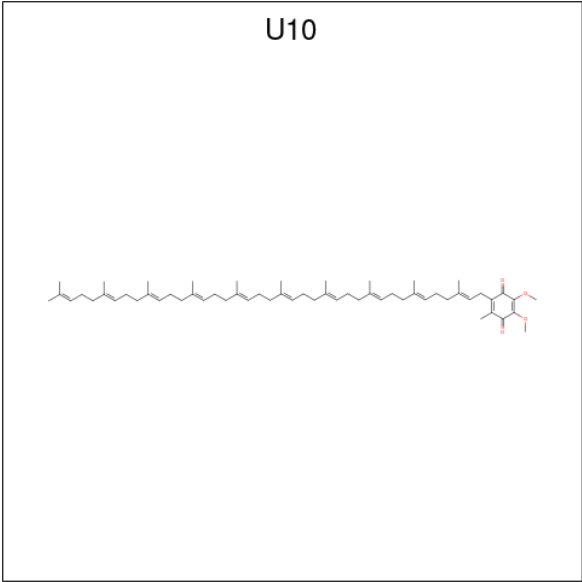
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	S	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
4	S	1	Total 66	C 55	Mg 1	N 4	O 6	0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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			55	45	4	6		
5	R	1	Total	C	N	O	0	0
			65	55	4	6		
5	S	1	Total	C	N	O	0	0
			51	41	4	6		

- Molecule 6 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).

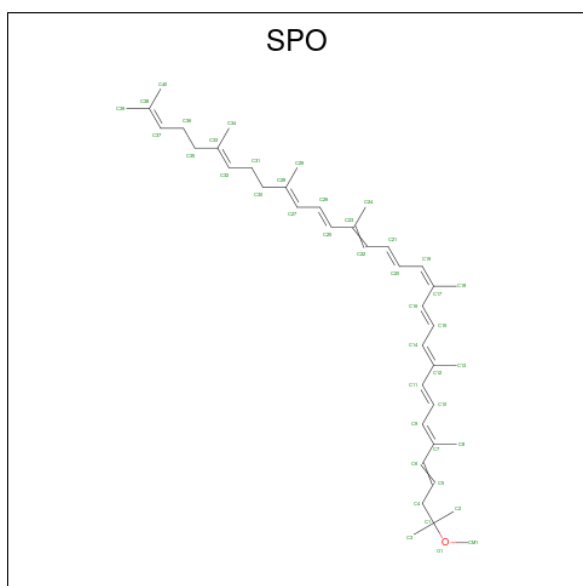


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	1
			60	52	8		
6	M	1	Total	C	O	0	0
			38	34	4		
6	R	1	Total	C	O	0	1
			36	28	8		
6	S	1	Total	C	O	0	0
			32	28	4		

- Molecule 7 is FE (II) ION (CCD ID: FE2) (formula: Fe).

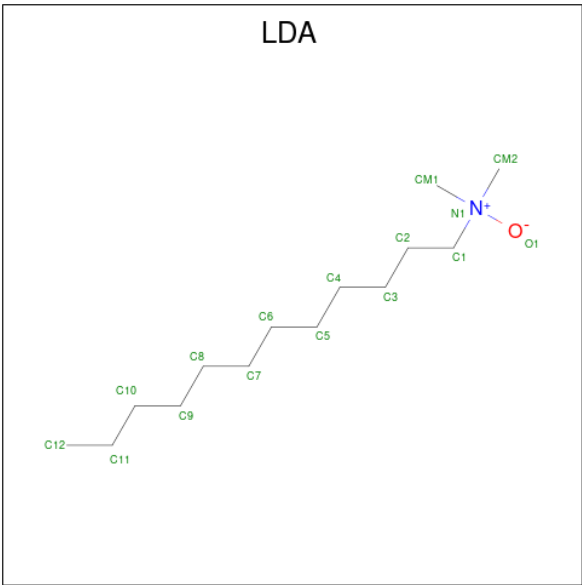
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		
7	S	1	Total	Fe	0	0
			1	1		

- Molecule 8 is SPHEROIDENE (CCD ID: 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 (CCD ID: LDA) (formula: C₁₄H₃₁NO).



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

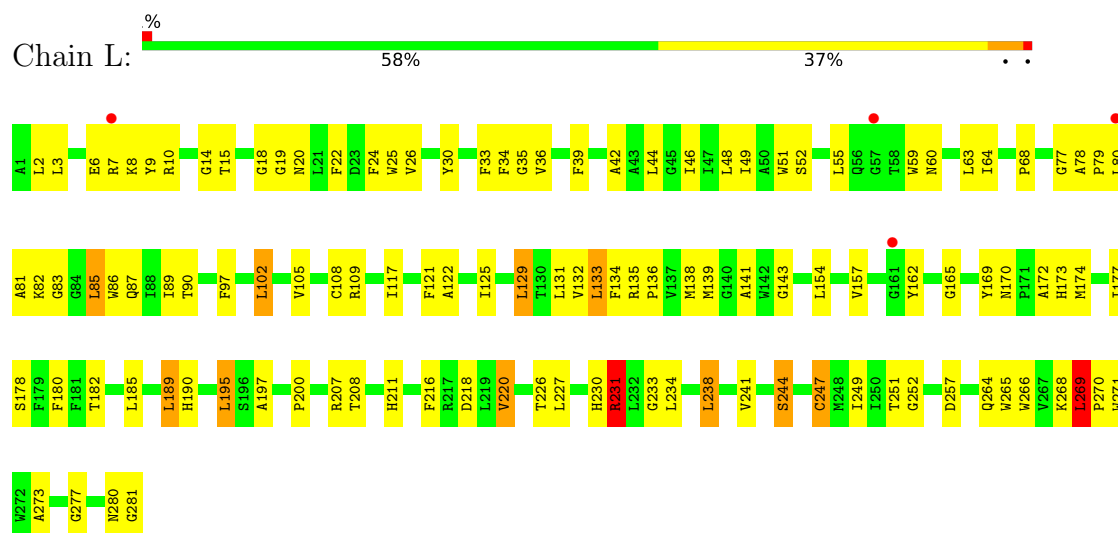
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	26	Total	O	0	0
			26	26		
10	M	42	Total	O	0	0
			42	42		
10	H	39	Total	O	0	0
			39	39		
10	R	13	Total	O	0	0
			13	13		
10	S	24	Total	O	0	0
			24	24		
10	T	12	Total	O	0	0
			12	12		

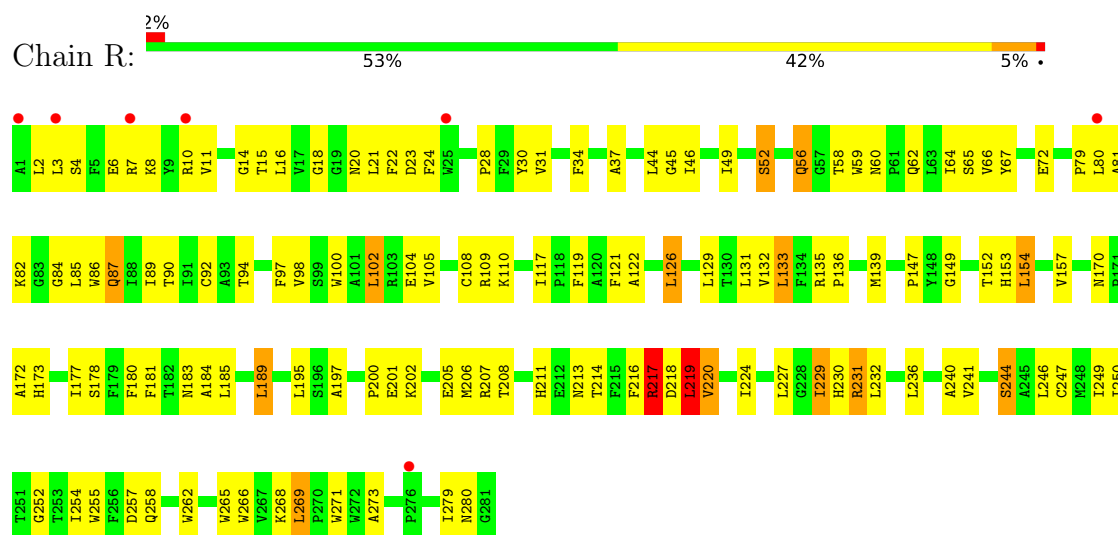
3 Residue-property plots [i](#)

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

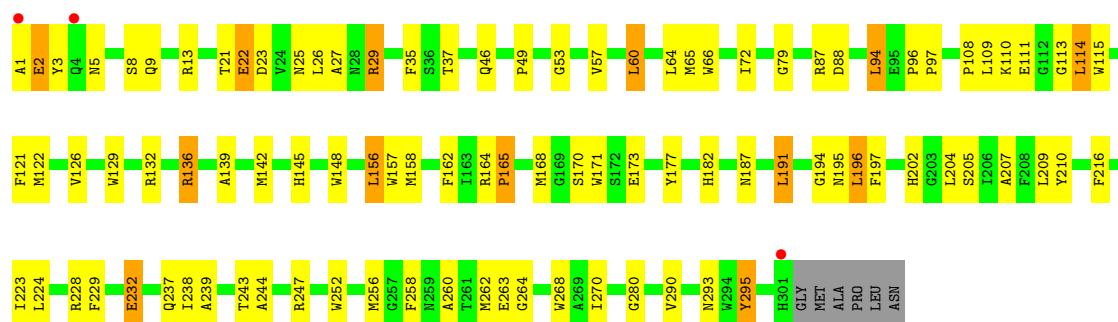


- Molecule 1: Reaction center protein L chain

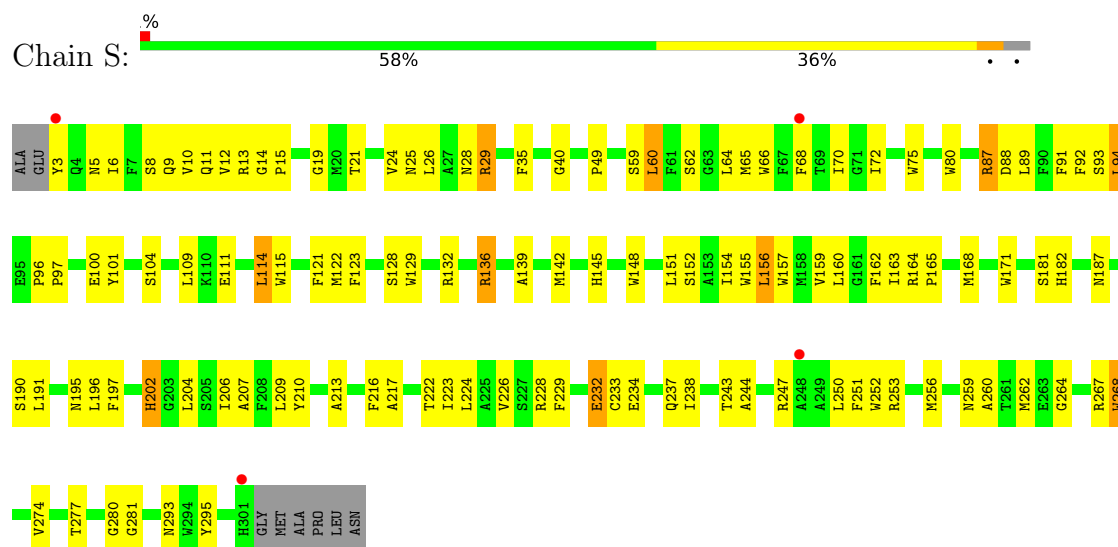


- Molecule 2: Reaction center protein M chain

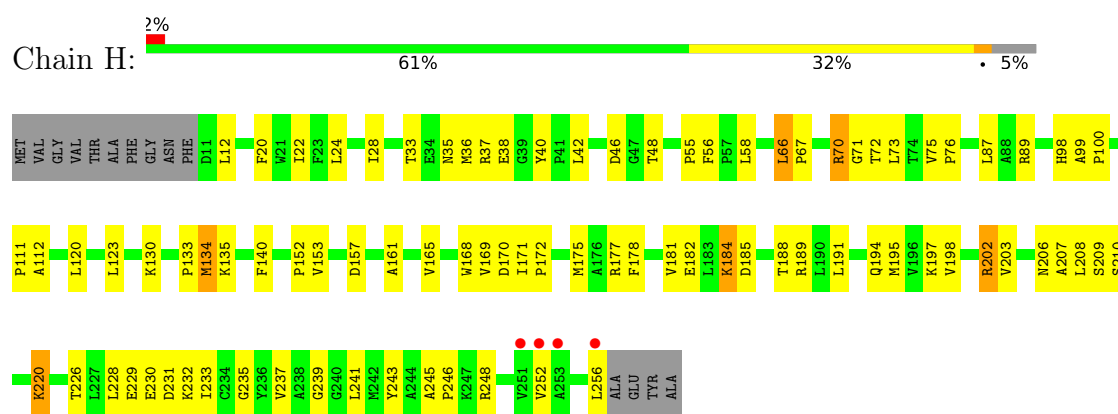




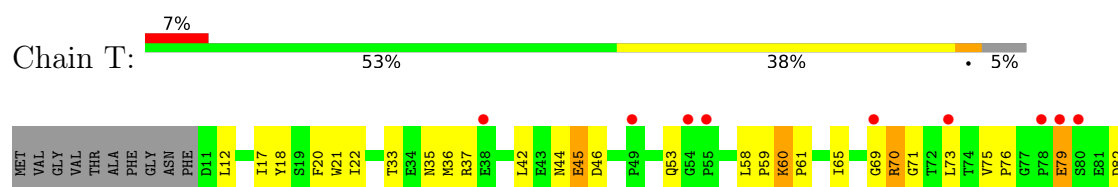
• Molecule 2: Reaction center protein M chain

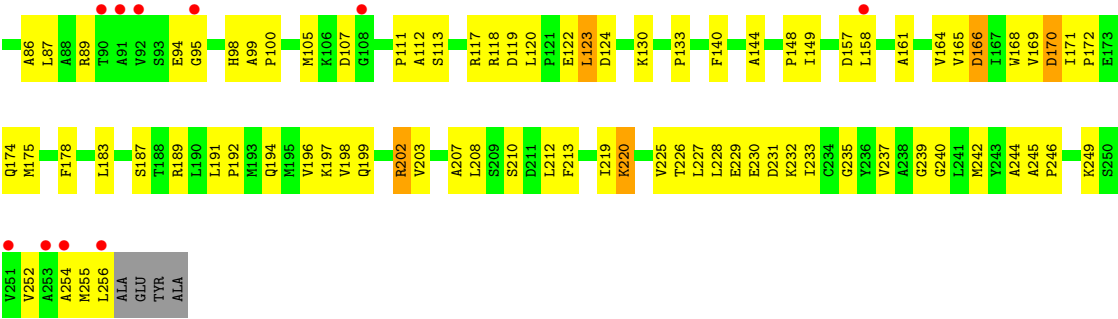


• Molecule 3: Reaction center protein H chain



• 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	137.73Å 137.73Å 277.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.84 – 2.60 39.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.84-2.60) 94.8 (39.84-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.268 0.210 , 0.254	Depositor DCC
R_{free} test set	3965 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14144	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: BCL, U10, FE2, SPO, BPH, LDA

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	0.51	0/2320	0.92	8/3175 (0.3%)
1	R	0.43	0/2320	0.96	7/3175 (0.2%)
2	M	0.51	0/2491	0.94	8/3402 (0.2%)
2	S	0.44	0/2477	0.91	6/3383 (0.2%)
3	H	0.47	0/1917	0.92	5/2608 (0.2%)
3	T	0.39	0/1917	0.90	3/2608 (0.1%)
All	All	0.46	0/13442	0.93	37/18351 (0.2%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	22	ILE	N-CA-C	-7.55	102.98	110.30
2	M	46	GLN	N-CA-C	7.31	120.43	109.25
1	R	244	SER	N-CA-C	-7.03	103.31	110.97
1	R	229	ILE	CB-CA-C	-6.77	103.15	112.02
1	R	217	ARG	N-CA-C	-6.76	103.84	111.14
2	M	210	TYR	N-CA-C	-6.75	103.85	111.14
1	L	3	LEU	N-CA-C	-6.68	101.72	110.53
2	S	217	ALA	N-CA-C	-5.93	104.89	111.36
2	S	268	TRP	N-CA-C	-5.86	104.97	111.36
3	H	66	LEU	CA-C-N	5.82	125.75	119.76
3	H	66	LEU	C-N-CA	5.82	125.75	119.76
1	R	56	GLN	N-CA-C	-5.80	106.37	113.50
3	H	133	PRO	N-CA-C	-5.69	101.60	111.32
3	T	60	LYS	N-CA-C	-5.62	102.50	109.64
2	S	267	ARG	N-CA-C	-5.59	105.18	112.23
2	M	268	TRP	N-CA-C	-5.59	105.09	111.07
2	S	160	LEU	N-CA-C	5.58	117.82	111.02
2	M	202	HIS	N-CA-C	-5.50	105.30	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	37	THR	N-CA-C	-5.50	105.83	112.54
1	L	134	PHE	N-CA-C	5.37	116.81	111.07
1	L	244	SER	N-CA-C	-5.36	105.35	111.14
3	H	243	TYR	N-CA-C	5.34	119.64	113.18
2	S	89	LEU	N-CA-C	5.33	117.51	111.11
2	S	202	HIS	N-CA-C	-5.22	105.67	111.36
2	M	295	TYR	N-CA-C	-5.21	105.50	111.07
1	L	269	LEU	CA-C-N	5.20	126.34	119.84
1	L	269	LEU	C-N-CA	5.20	126.34	119.84
1	L	26	VAL	N-CA-C	-5.19	98.52	107.24
1	R	271	TRP	N-CA-C	5.17	119.34	113.19
1	R	219	LEU	N-CA-C	5.16	116.99	111.36
3	T	170	ASP	N-CA-C	-5.16	98.92	107.99
1	L	35	GLY	N-CA-C	-5.14	106.19	112.77
2	M	22	GLU	CB-CA-C	-5.13	110.64	116.54
1	R	52	SER	N-CA-C	-5.13	105.87	111.82
2	M	79	GLY	N-CA-C	-5.12	107.01	114.90
1	L	231	ARG	N-CA-C	-5.05	105.77	111.28
3	T	169	VAL	N-CA-C	5.05	116.24	108.71

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	111	0
1	R	2232	0	2189	131	0
2	M	2399	0	2310	91	0
2	S	2385	0	2296	121	0
3	H	1869	0	1884	78	0
3	T	1869	0	1884	107	0
4	L	183	0	189	27	0
4	M	66	0	74	21	0
4	R	66	0	74	10	0
4	S	183	0	189	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	65	0	74	5	0
5	M	55	0	53	1	0
5	R	65	0	74	9	0
5	S	51	0	45	6	0
6	L	60	0	70	3	0
6	M	38	0	47	0	0
6	R	36	0	30	3	0
6	S	32	0	39	1	0
7	M	1	0	0	0	0
7	S	1	0	0	0	0
8	M	42	0	60	6	0
8	S	42	0	60	2	0
9	M	16	0	31	2	0
10	H	39	0	0	2	0
10	L	26	0	0	4	0
10	M	42	0	0	1	0
10	R	13	0	0	0	0
10	S	24	0	0	2	0
10	T	12	0	0	1	0
All	All	14144	0	13861	606	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 22.

All (606) 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:200:PRO:HB3	1:R:207:ARG:HD3	1.42	1.02
2:S:157:TRP:HB2	4:S:2003:BCL:H62	1.44	0.99
1:R:219:LEU:HD13	1:R:220:VAL:HG23	1.48	0.95
3:T:226:THR:OG1	3:T:229:GLU:HG3	1.68	0.93
3:H:33:THR:HA	3:H:36:MET:HE2	1.52	0.92
1:R:208:THR:H	1:R:211:HIS:HD2	1.18	0.92
1:R:189:LEU:HG	1:R:216:PHE:HZ	1.37	0.90
1:L:241:VAL:HG21	5:L:1006:BPH:HAC1	1.53	0.89
2:M:157:TRP:HB2	4:M:1003:BCL:H62	1.57	0.86
1:R:208:THR:H	1:R:211:HIS:CD2	1.94	0.86
2:M:239:ALA:HB1	3:H:66:LEU:HD11	1.60	0.83
1:L:55:LEU:HD13	1:L:81:ALA:HB2	1.59	0.82
1:L:77:GLY:HA2	1:L:87:GLN:HE22	1.44	0.82
2:S:21:THR:HG23	2:S:26:LEU:HD21	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:194:GLN:H	3:T:194:GLN:NE2	1.78	0.81
1:R:153:HIS:O	1:R:157:VAL:HG23	1.81	0.81
2:S:243:THR:O	2:S:247:ARG:HG3	1.81	0.81
2:M:13:ARG:HD2	2:M:35:PHE:CD2	2.16	0.80
1:L:52:SER:HB2	1:L:85:LEU:HD23	1.63	0.80
1:L:189:LEU:HG	1:L:216:PHE:HZ	1.46	0.79
3:H:70:ARG:HH11	3:H:70:ARG:HG2	1.47	0.79
3:H:228:LEU:HD11	3:H:232:LYS:HE3	1.63	0.78
2:S:197:PHE:HZ	4:S:2003:BCL:HBB2	1.47	0.78
1:L:79:PRO:HG2	1:L:82:LYS:HB2	1.66	0.77
1:L:227:LEU:HD13	2:M:232:GLU:HG2	1.65	0.77
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.66	0.77
1:L:257:ASP:HB3	10:L:1010:HOH:O	1.83	0.77
1:L:157:VAL:HG11	4:M:1003:BCL:HBB1	1.67	0.76
1:R:227:LEU:HD13	2:S:232:GLU:HG2	1.66	0.76
3:H:178:PHE:HZ	3:H:230:GLU:HG2	1.51	0.75
2:S:13:ARG:HD2	2:S:35:PHE:CD2	2.21	0.74
2:M:197:PHE:HZ	4:M:1003:BCL:HBB2	1.53	0.74
2:S:228:ARG:HA	3:T:194:GLN:CG	2.17	0.74
2:S:268:TRP:HE1	3:T:35:ASN:ND2	1.85	0.74
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.72	0.72
1:R:189:LEU:HG	1:R:216:PHE:CZ	2.24	0.72
3:T:252:VAL:O	3:T:256:LEU:HD13	1.89	0.72
1:R:241:VAL:HG21	5:R:2006:BPH:HAC1	1.70	0.72
2:S:11:GLN:HB2	3:T:144:ALA:HB3	1.70	0.72
3:T:194:GLN:H	3:T:194:GLN:CD	1.96	0.72
5:R:2006:BPH:H7C2	4:S:2004:BCL:H201	1.71	0.72
1:R:200:PRO:CB	1:R:207:ARG:HD3	2.18	0.72
1:L:190:HIS:HA	6:L:1009[B]:U10:O2	1.89	0.72
4:R:2002:BCL:HBD	4:S:2004:BCL:HBC1	1.70	0.72
1:R:79:PRO:HG2	1:R:82:LYS:HB2	1.72	0.71
2:S:101:TYR:O	2:S:104:SER:HB3	1.91	0.70
2:S:229:PHE:HB2	2:S:244:ALA:HB2	1.73	0.70
2:M:197:PHE:CZ	4:M:1003:BCL:HBB2	2.26	0.70
1:R:105:VAL:O	1:R:109:ARG:HG3	1.90	0.70
1:R:195:LEU:HB3	2:S:145:HIS:CD2	2.26	0.70
3:T:42:LEU:N	3:T:53:GLN:HE22	1.89	0.70
2:S:136:ARG:HA	2:S:136:ARG:NE	2.06	0.70
3:T:133:PRO:HG3	3:T:168:TRP:CE2	2.27	0.69
4:L:1002:BCL:HBD	4:L:1004:BCL:CBC	2.21	0.69
2:M:157:TRP:HB2	4:M:1003:BCL:C6	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:66:VAL:HG11	1:R:89:ILE:HD12	1.72	0.69
1:R:207:ARG:HG3	2:S:142:MET:HG2	1.74	0.69
3:T:171:ILE:HB	3:T:172:PRO:HD3	1.75	0.68
1:R:4:SER:HB2	3:T:79:GLU:CG	2.24	0.68
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.76	0.68
2:S:207:ALA:HA	4:S:2004:BCL:O1A	1.93	0.68
3:T:119:ASP:O	3:T:120:LEU:HD23	1.92	0.68
3:T:112:ALA:HA	3:T:235:GLY:O	1.94	0.68
3:T:87:LEU:HD23	3:T:100:PRO:HA	1.75	0.68
2:S:152:SER:HB2	2:S:274:VAL:HG13	1.75	0.67
1:L:208:THR:H	1:L:211:HIS:CD2	2.13	0.66
1:R:60:ASN:O	1:R:64:ILE:HG13	1.96	0.66
2:S:9:GLN:NE2	3:T:198:VAL:H	1.94	0.66
1:R:52:SER:HB2	1:R:85:LEU:HD23	1.76	0.66
2:S:237:GLN:HB2	2:S:262:MET:HG2	1.78	0.66
2:M:243:THR:O	2:M:247:ARG:HG3	1.96	0.66
2:M:228:ARG:HA	3:H:194:GLN:CG	2.26	0.66
4:R:2002:BCL:HBD	4:S:2004:BCL:CBC	2.25	0.66
1:R:2:LEU:HB3	1:R:6:GLU:HB3	1.77	0.66
3:T:189:ARG:HG2	3:T:189:ARG:HH11	1.60	0.65
2:M:9:GLN:NE2	3:H:198:VAL:H	1.95	0.65
3:H:202:ARG:HG2	3:H:203:VAL:N	2.10	0.65
1:L:14:GLY:O	1:L:109:ARG:HD3	1.97	0.65
2:S:268:TRP:NE1	3:T:35:ASN:HD21	1.94	0.65
3:H:37:ARG:O	3:H:38:GLU:HG2	1.97	0.65
1:R:85:LEU:O	1:R:89:ILE:HG13	1.96	0.65
3:T:165:VAL:O	3:T:166:ASP:HB2	1.94	0.65
1:L:265:TRP:O	1:L:269:LEU:HD13	1.97	0.64
2:M:2:GLU:O	2:M:3:TYR:HB3	1.98	0.64
2:M:156:LEU:HD13	4:M:1003:BCL:H43	1.79	0.64
3:H:226:THR:OG1	3:H:229:GLU:HG3	1.97	0.64
1:R:4:SER:HB2	3:T:79:GLU:HG2	1.79	0.64
3:H:170:ASP:HB2	3:H:177:ARG:HG3	1.79	0.63
1:L:218:ASP:OD1	2:M:29:ARG:HD2	1.98	0.63
2:M:53:GLY:O	2:M:57:VAL:HG23	1.97	0.63
2:M:228:ARG:HA	3:H:194:GLN:HG2	1.81	0.63
1:L:195:LEU:HB3	2:M:145:HIS:CD2	2.33	0.63
2:M:9:GLN:HE22	3:H:197:LYS:HA	1.62	0.63
2:S:25:ASN:HD22	2:S:28:ASN:ND2	1.97	0.63
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.80	0.63
4:L:1001:BCL:HBB3	4:M:1003:BCL:H41	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.33	0.62
4:L:1001:BCL:HBC1	4:M:1003:BCL:CBD	2.29	0.62
1:R:205:GLU:HG2	3:T:65:ILE:HG22	1.82	0.62
3:T:130:LYS:HE3	3:T:170:ASP:OD2	1.99	0.62
3:H:194:GLN:CD	3:H:194:GLN:H	2.08	0.62
3:H:220:LYS:HB2	3:H:220:LYS:NZ	2.15	0.62
1:R:8:LYS:HD2	3:T:113:SER:HB3	1.82	0.62
1:L:7:ARG:HH12	3:H:87:LEU:HB2	1.65	0.62
3:H:130:LYS:HE3	3:H:170:ASP:OD2	1.99	0.62
2:S:109:LEU:HD22	2:S:114:LEU:HD13	1.81	0.61
4:L:1002:BCL:HBD	4:L:1004:BCL:HBC1	1.81	0.61
1:R:20:ASN:HA	1:R:23:ASP:HB2	1.82	0.61
2:S:60:LEU:O	2:S:64:LEU:HG	2.00	0.61
1:L:189:LEU:HG	1:L:216:PHE:CZ	2.33	0.61
3:T:44:ASN:C	3:T:46:ASP:H	2.07	0.61
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.81	0.61
2:S:97:PRO:HG2	2:S:171:TRP:HB2	1.80	0.61
1:L:208:THR:H	1:L:211:HIS:HD2	1.47	0.61
2:S:229:PHE:CE2	2:S:247:ARG:HD2	2.36	0.61
4:S:2001:BCL:HBC1	4:S:2003:BCL:CAD	2.30	0.61
2:M:109:LEU:HD22	2:M:114:LEU:HD13	1.83	0.61
1:L:207:ARG:HG2	2:M:142:MET:HG2	1.83	0.60
3:H:70:ARG:HG2	3:H:70:ARG:NH1	2.14	0.60
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.01	0.60
3:H:229:GLU:O	3:H:233:ILE:HG13	2.01	0.60
1:L:200:PRO:HB3	1:L:207:ARG:HD3	1.83	0.60
2:M:280:GLY:HA2	4:M:1003:BCL:HED2	1.84	0.60
2:S:9:GLN:HE22	3:T:198:VAL:H	1.50	0.60
2:M:195:ASN:HD22	2:M:195:ASN:C	2.10	0.60
1:L:33:PHE:O	1:L:36:VAL:HG22	2.02	0.60
3:H:161:ALA:HB2	3:H:210:SER:HA	1.82	0.60
3:T:60:LYS:HG2	3:T:61:PRO:HD2	1.83	0.60
1:L:139:MET:HE3	1:L:252:GLY:HA3	1.83	0.59
1:R:86:TRP:CZ2	1:R:132:VAL:HG13	2.37	0.59
2:M:136:ARG:NE	2:M:136:ARG:HA	2.16	0.59
3:H:112:ALA:HA	3:H:235:GLY:O	2.03	0.59
2:M:1:ALA:O	2:M:2:GLU:HB2	2.02	0.59
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.82	0.59
1:R:135:ARG:HB3	1:R:136:PRO:HD3	1.85	0.59
2:M:168:MET:CB	2:M:173:GLU:HG3	2.32	0.59
3:T:33:THR:HA	3:T:36:MET:CG	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:8:SER:OG	3:T:175:MET:HE1	2.02	0.59
1:R:265:TRP:O	1:R:269:LEU:HD13	2.02	0.59
3:T:202:ARG:HG2	3:T:203:VAL:N	2.16	0.59
4:L:1001:BCL:HBC1	4:M:1003:BCL:HBD	1.85	0.59
3:H:66:LEU:HB2	3:H:71:GLY:O	2.03	0.58
3:H:152:PRO:HG2	3:H:202:ARG:HB2	1.85	0.58
2:S:62:SER:O	2:S:121:PHE:HB3	2.03	0.58
2:S:3:TYR:CZ	2:S:5:ASN:HA	2.39	0.58
2:S:25:ASN:ND2	2:S:28:ASN:ND2	2.51	0.58
3:T:105:MET:HE2	3:T:212:LEU:HD13	1.86	0.58
3:T:42:LEU:H	3:T:53:GLN:HE22	1.51	0.58
2:M:162:PHE:HB2	8:M:1010:SPO:H291	1.85	0.58
3:H:248:ARG:NH1	3:H:248:ARG:HB2	2.18	0.58
2:S:268:TRP:NE1	3:T:35:ASN:ND2	2.52	0.58
2:S:88:ASP:HB2	2:S:92:PHE:CZ	2.39	0.58
3:T:183:LEU:HD21	3:T:213:PHE:HB3	1.86	0.58
1:L:34:PHE:CE1	1:L:102:LEU:HD23	2.38	0.58
3:H:194:GLN:H	3:H:194:GLN:NE2	2.01	0.58
1:R:207:ARG:HD2	1:R:207:ARG:N	2.18	0.58
2:S:228:ARG:HA	3:T:194:GLN:HG2	1.84	0.58
2:M:9:GLN:HE22	3:H:198:VAL:H	1.52	0.57
1:R:178:SER:HA	4:S:2001:BCL:HBA2	1.86	0.57
2:S:264:GLY:HA3	3:T:35:ASN:OD1	2.04	0.57
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.39	0.57
1:L:241:VAL:CG2	5:L:1006:BPH:HAC1	2.30	0.57
2:S:152:SER:CB	2:S:274:VAL:HG13	2.33	0.57
1:R:157:VAL:HG11	4:S:2003:BCL:HBB1	1.86	0.57
2:S:9:GLN:HE22	3:T:197:LYS:HA	1.69	0.57
1:L:277:GLY:O	1:L:281:GLY:HA3	2.05	0.57
2:M:8:SER:OG	3:H:175:MET:HE1	2.05	0.57
10:L:1032:HOH:O	2:M:49:PRO:HG2	2.03	0.57
2:S:197:PHE:CZ	4:S:2003:BCL:HBB2	2.36	0.57
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.85	0.57
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.35	0.57
1:L:51:TRP:CE3	1:L:85:LEU:HD11	2.40	0.56
1:R:18:GLY:O	1:R:21:LEU:HG	2.04	0.56
1:L:44:LEU:O	1:L:48:LEU:HG	2.04	0.56
2:S:49:PRO:HG2	10:S:2019:HOH:O	2.05	0.56
3:T:44:ASN:O	3:T:46:ASP:N	2.38	0.56
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.40	0.56
2:M:182:HIS:CG	8:M:1010:SPO:H181	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:1002:BCL:HBD	4:L:1004:BCL:HBC3	1.86	0.56
1:R:230:HIS:CD2	2:S:223:ILE:HG13	2.41	0.56
2:S:209:LEU:HD22	4:S:2003:BCL:H3A	1.88	0.56
1:L:90:THR:HG23	1:L:132:VAL:HG11	1.88	0.56
3:T:12:LEU:N	3:T:12:LEU:HD22	2.21	0.56
3:T:133:PRO:HG3	3:T:168:TRP:CZ2	2.41	0.56
3:T:168:TRP:HB2	3:T:178:PHE:HB2	1.88	0.56
2:S:66:TRP:NE1	2:S:70:ILE:HD11	2.21	0.55
4:S:2001:BCL:HBB3	4:S:2003:BCL:H61	1.89	0.55
2:S:228:ARG:HA	3:T:194:GLN:HG3	1.88	0.55
2:M:195:ASN:ND2	2:M:197:PHE:H	2.04	0.55
1:L:49:ILE:HG13	1:L:89:ILE:HD13	1.88	0.55
2:S:274:VAL:HA	5:S:2005:BPH:HBC1	1.88	0.55
4:L:1002:BCL:H122	5:L:1006:BPH:H3A	1.88	0.55
2:S:24:VAL:HG22	2:S:139:ALA:HB1	1.89	0.55
2:M:290:VAL:HG11	3:H:12:LEU:HB2	1.90	0.54
2:S:210:TYR:HB2	4:S:2004:BCL:O1A	2.08	0.54
4:R:2002:BCL:H122	5:R:2006:BPH:H3A	1.89	0.54
2:S:202:HIS:CE1	2:S:206:ILE:HD11	2.42	0.54
1:R:139:MET:HE3	1:R:252:GLY:O	2.08	0.54
3:T:189:ARG:HG2	3:T:189:ARG:NH1	2.23	0.54
1:L:189:LEU:HB3	6:L:1009[A]:U10:H4M3	1.88	0.54
2:M:94:LEU:HD22	2:M:115:TRP:HB2	1.89	0.54
1:R:46:ILE:HG12	4:S:2004:BCL:H202	1.90	0.54
1:R:86:TRP:CH2	1:R:132:VAL:HG13	2.43	0.54
1:L:182:THR:HG21	6:L:1009[B]:U10:H18	1.90	0.54
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.43	0.54
3:H:182:GLU:HA	3:H:188:THR:HG22	1.89	0.53
1:L:197:ALA:HA	1:L:207:ARG:HB2	1.90	0.53
3:T:229:GLU:O	3:T:233:ILE:HG13	2.08	0.53
2:M:168:MET:HB2	2:M:173:GLU:HG3	1.89	0.53
2:S:70:ILE:HA	2:S:94:LEU:HD12	1.91	0.53
1:L:80:LEU:CD2	1:L:80:LEU:H	2.22	0.53
2:S:164:ARG:HB3	2:S:165:PRO:HD3	1.91	0.53
3:T:75:VAL:HA	3:T:76:PRO:C	2.33	0.53
3:H:40:TYR:HB3	3:H:58:LEU:HD21	1.90	0.52
1:R:11:VAL:O	1:R:110:LYS:NZ	2.35	0.52
3:T:33:THR:HA	3:T:36:MET:HG3	1.91	0.52
1:R:185:LEU:HD13	5:S:2005:BPH:ND	2.24	0.52
2:S:65:MET:HB3	2:S:121:PHE:CD2	2.44	0.52
1:R:131:LEU:HD11	4:S:2004:BCL:HBC2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:33:THR:HA	3:T:36:MET:HG2	1.91	0.52
3:T:228:LEU:O	3:T:232:LYS:HG3	2.09	0.52
2:S:10:VAL:HG21	3:T:148:PRO:HD3	1.90	0.52
3:T:86:ALA:HB3	3:T:107:ASP:HB3	1.92	0.52
3:T:44:ASN:HB2	3:T:46:ASP:OD1	2.10	0.52
3:T:178:PHE:HZ	3:T:230:GLU:HG3	1.73	0.52
2:M:237:GLN:HB2	2:M:262:MET:HG2	1.90	0.52
3:T:164:VAL:HG21	3:T:203:VAL:HG21	1.92	0.52
1:R:219:LEU:HD22	1:R:219:LEU:O	2.09	0.52
1:R:22:PHE:HA	1:R:24:PHE:CE2	2.45	0.52
1:L:15:THR:HG22	1:L:30:TYR:OH	2.10	0.51
5:R:2006:BPH:H152	4:S:2004:BCL:HBB3	1.93	0.51
2:M:232:GLU:OE1	2:M:232:GLU:N	2.39	0.51
2:S:204:LEU:HD13	3:T:20:PHE:CE2	2.45	0.51
1:L:170:ASN:HB3	1:L:173:HIS:HB2	1.91	0.51
1:R:100:TRP:O	1:R:104:GLU:HG3	2.10	0.51
1:R:246:LEU:O	1:R:250:ILE:HG12	2.10	0.51
2:S:280:GLY:HA2	4:S:2003:BCL:HED2	1.93	0.51
4:L:1002:BCL:HAA2	4:L:1004:BCL:HBC1	1.93	0.51
1:L:80:LEU:H	1:L:80:LEU:HD22	1.76	0.51
2:M:60:LEU:CD2	2:M:64:LEU:HG	2.41	0.51
4:L:1001:BCL:HBB2	8:M:1010:SPO:H243	1.92	0.51
2:S:233:CYS:O	2:S:237:GLN:HG2	2.10	0.51
1:L:117:ILE:HD13	2:M:252:TRP:CZ2	2.46	0.51
2:M:72:ILE:HD12	8:M:1010:SPO:HM11	1.93	0.51
1:L:211:HIS:HE1	2:M:22:GLU:OE1	1.93	0.51
1:R:244:SER:HB3	4:R:2002:BCL:O1A	2.10	0.51
3:T:36:MET:HB2	3:T:59:PRO:HD3	1.92	0.50
1:L:135:ARG:NH1	1:L:251:THR:O	2.45	0.50
3:H:37:ARG:C	3:H:38:GLU:HG2	2.36	0.50
1:R:200:PRO:HG3	1:R:205:GLU:O	2.10	0.50
2:S:148:TRP:HA	2:S:148:TRP:CE3	2.46	0.50
2:S:148:TRP:HA	2:S:148:TRP:HE3	1.76	0.50
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.92	0.50
2:S:64:LEU:O	2:S:68:PHE:HB2	2.11	0.50
2:S:232:GLU:O	2:S:234:GLU:HG3	2.12	0.50
3:T:45:GLU:CD	3:T:95:GLY:H	2.20	0.50
2:M:65:MET:HB3	2:M:121:PHE:CD2	2.47	0.50
3:T:122:GLU:OE1	3:T:227:LEU:HD11	2.12	0.50
2:M:209:LEU:HD22	4:M:1003:BCL:H3A	1.94	0.50
3:H:165:VAL:HG11	3:H:182:GLU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:45:GLY:O	1:R:49:ILE:HG13	2.11	0.50
1:L:233:GLY:HA3	2:M:216:PHE:CE1	2.48	0.49
1:L:180:PHE:CD2	4:L:1002:BCL:HMA3	2.47	0.49
3:H:87:LEU:HA	3:H:99:ALA:O	2.13	0.49
3:H:252:VAL:O	3:H:256:LEU:HD13	2.12	0.49
1:R:66:VAL:HG12	1:R:86:TRP:HB2	1.93	0.49
1:R:122:ALA:O	1:R:126:LEU:HD22	2.11	0.49
2:S:25:ASN:HD22	2:S:28:ASN:HD21	1.58	0.49
1:R:255:TRP:HZ2	1:R:258:GLN:O	1.96	0.49
2:S:21:THR:CG2	2:S:26:LEU:HD21	2.37	0.49
2:S:24:VAL:HG22	2:S:139:ALA:CB	2.41	0.49
1:L:226:THR:HG23	1:L:227:LEU:N	2.27	0.49
1:L:18:GLY:O	1:L:19:GLY:C	2.55	0.49
2:S:3:TYR:CE1	2:S:9:GLN:HG3	2.47	0.49
1:L:162:TYR:HA	1:L:165:GLY:O	2.13	0.49
3:T:18:TYR:O	3:T:22:ILE:HG12	2.13	0.49
1:R:72:GLU:H	1:R:72:GLU:CD	2.21	0.49
2:M:177:TYR:HE1	8:M:1010:SPO:H22	1.77	0.49
2:S:293:ASN:OD1	2:S:295:TYR:HB3	2.12	0.49
3:T:59:PRO:HG2	3:T:76:PRO:HD3	1.95	0.49
3:T:220:LYS:HG3	3:T:229:GLU:OE2	2.13	0.49
1:L:86:TRP:CH2	1:L:132:VAL:HG13	2.48	0.49
1:R:180:PHE:CD2	4:R:2002:BCL:HMA3	2.48	0.49
2:S:100:GLU:H	2:S:100:GLU:CD	2.20	0.49
2:S:222:THR:O	2:S:226:VAL:HG22	2.13	0.48
3:T:12:LEU:HD22	3:T:12:LEU:H	1.75	0.48
1:L:105:VAL:O	1:L:109:ARG:HG3	2.14	0.48
4:L:1001:BCL:HBC1	4:M:1003:BCL:CAD	2.43	0.48
3:H:55:PRO:HG2	3:H:56:PHE:CD2	2.48	0.48
3:H:220:LYS:HB2	3:H:220:LYS:HZ2	1.77	0.48
4:L:1004:BCL:O1A	2:M:207:ALA:HA	2.14	0.48
3:T:207:ALA:HB1	3:T:237:VAL:O	2.12	0.48
2:S:123:PHE:HA	2:S:157:TRP:HH2	1.79	0.48
3:T:45:GLU:HG3	3:T:94:GLU:OE1	2.13	0.48
1:L:60:ASN:ND2	1:L:63:LEU:HD23	2.28	0.48
1:L:138:MET:SD	1:L:249:ILE:HD11	2.54	0.48
1:L:170:ASN:HB3	1:L:173:HIS:CB	2.43	0.48
1:R:241:VAL:HG21	5:R:2006:BPH:CAC	2.42	0.48
1:R:241:VAL:CG2	5:R:2006:BPH:HAC1	2.43	0.48
4:L:1004:BCL:H202	5:L:1006:BPH:H7C2	1.96	0.48
1:R:44:LEU:HD23	1:R:92:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:59:SER:HB2	2:S:128:SER:OG	2.14	0.48
4:L:1001:BCL:HBB2	4:L:1001:BCL:HHC	1.96	0.48
3:H:228:LEU:CD1	3:H:232:LYS:HE3	2.39	0.48
1:R:268:LYS:HA	1:R:273:ALA:HB2	1.94	0.48
4:S:2001:BCL:HBC1	4:S:2003:BCL:CB D	2.44	0.48
1:L:42:ALA:O	1:L:46:ILE:HG13	2.13	0.47
1:R:218:ASP:OD1	2:S:29:ARG:HD2	2.13	0.47
1:R:119:PHE:O	1:R:122:ALA:HB3	2.14	0.47
1:L:172:ALA:HB3	1:L:247:CYS:HA	1.95	0.47
2:M:122:MET:O	2:M:126:VAL:HG23	2.14	0.47
2:M:256:MET:HE3	2:M:258:PHE:CE1	2.49	0.47
4:R:2002:BCL:NC	4:S:2003:BCL:HBB3	2.29	0.47
3:T:208:LEU:HD12	3:T:240:GLY:HA3	1.96	0.47
1:L:97:PHE:CE1	4:L:1002:BCL:H121	2.49	0.47
1:L:234:LEU:O	1:L:238:LEU:HB2	2.15	0.47
3:H:170:ASP:HB2	3:H:177:ARG:CG	2.44	0.47
3:H:195:MET:CE	3:H:207:ALA:HB2	2.44	0.47
1:R:246:LEU:HA	1:R:249:ILE:HG22	1.96	0.47
2:S:164:ARG:O	2:S:168:MET:HG2	2.14	0.47
1:L:60:ASN:CG	1:L:63:LEU:HD23	2.39	0.47
1:R:139:MET:HE3	1:R:252:GLY:HA3	1.96	0.47
2:S:60:LEU:O	2:S:60:LEU:HD22	2.15	0.47
2:S:65:MET:HB3	2:S:121:PHE:CE2	2.50	0.47
3:T:12:LEU:H	3:T:12:LEU:CD2	2.28	0.47
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.50	0.47
1:L:55:LEU:CD1	1:L:81:ALA:HB2	2.38	0.47
2:M:25:ASN:OD1	2:M:27:ALA:HB3	2.15	0.47
1:R:157:VAL:CG1	4:S:2003:BCL:HBB1	2.45	0.47
1:R:183:ASN:ND2	2:S:213:ALA:HA	2.30	0.47
1:R:213:ASN:O	1:R:217:ARG:HB2	2.14	0.47
1:R:250:ILE:HB	1:R:254:ILE:HD11	1.97	0.47
3:T:79:GLU:OE1	3:T:79:GLU:HA	2.15	0.47
1:R:3:LEU:HD12	2:S:250:LEU:HD21	1.96	0.47
3:T:44:ASN:C	3:T:46:ASP:N	2.72	0.47
1:L:86:TRP:CZ2	1:L:132:VAL:HG13	2.50	0.47
1:L:125:ILE:O	1:L:129:LEU:HB2	2.14	0.47
2:S:60:LEU:HA	5:S:2005:BPH:H4C2	1.97	0.47
2:S:87:ARG:HG3	2:S:88:ASP:N	2.30	0.47
1:L:227:LEU:HD11	2:M:5:ASN:HD21	1.79	0.46
3:H:111:PRO:HB2	3:H:239:GLY:HA2	1.96	0.46
4:R:2002:BCL:H2C	4:S:2003:BCL:H2C	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:LYS:HE2	1:L:9:TYR:CZ	2.50	0.46
2:M:194:GLY:O	2:M:195:ASN:HB3	2.16	0.46
5:R:2006:BPH:CMC	2:S:213:ALA:HB3	2.46	0.46
1:L:59:TRP:HA	1:L:59:TRP:CE3	2.51	0.46
1:L:80:LEU:HD22	1:L:80:LEU:N	2.30	0.46
2:S:75:TRP:HB3	2:S:80:TRP:CE3	2.49	0.46
1:L:241:VAL:HG21	5:L:1006:BPH:H2C	1.97	0.46
4:L:1001:BCL:HBB3	4:M:1003:BCL:C4	2.44	0.46
2:M:22:GLU:HB3	2:M:139:ALA:O	2.15	0.46
2:M:229:PHE:CB	2:M:244:ALA:HB2	2.40	0.46
2:S:157:TRP:HB2	4:S:2003:BCL:C6	2.32	0.46
3:T:70:ARG:NH2	3:T:123:LEU:HD13	2.31	0.46
1:L:169:TYR:HA	1:L:174:MET:HE3	1.98	0.46
1:L:268:LYS:C	1:L:273:ALA:HB2	2.41	0.46
1:L:280:ASN:ND2	2:M:88:ASP:OD1	2.40	0.46
1:R:129:LEU:O	1:R:133:LEU:HB3	2.16	0.46
2:S:162:PHE:C	2:S:165:PRO:HD2	2.40	0.46
1:L:178:SER:HA	4:L:1001:BCL:O1A	2.16	0.46
1:L:207:ARG:HA	1:L:207:ARG:HD2	1.67	0.46
1:L:220:VAL:O	1:L:220:VAL:CG1	2.62	0.46
1:L:266:TRP:HE1	2:M:87:ARG:HA	1.80	0.46
2:M:195:ASN:HD22	2:M:196:LEU:N	2.14	0.46
3:H:153:VAL:HG21	3:H:181:VAL:HG22	1.98	0.46
3:H:206:ASN:ND2	3:H:248:ARG:HD3	2.30	0.46
1:R:97:PHE:CE1	4:R:2002:BCL:H121	2.51	0.46
3:T:42:LEU:H	3:T:53:GLN:NE2	2.14	0.46
3:T:170:ASP:O	3:T:174:GLN:N	2.48	0.46
2:M:205:SER:OG	4:M:1003:BCL:HMA3	2.16	0.46
1:R:15:THR:HG22	1:R:30:TYR:OH	2.16	0.46
1:R:181:PHE:CE1	4:S:2003:BCL:O1A	2.68	0.46
1:R:2:LEU:N	1:R:2:LEU:HD12	2.30	0.45
2:M:13:ARG:O	3:H:140:PHE:HA	2.15	0.45
4:M:1003:BCL:H193	5:M:1005:BPH:HMA2	1.98	0.45
1:R:207:ARG:HB3	1:R:211:HIS:CG	2.51	0.45
4:R:2002:BCL:H52	5:R:2006:BPH:HBB2	1.97	0.45
1:R:67:TYR:CD2	1:R:147:PRO:HB3	2.52	0.45
2:S:274:VAL:HA	5:S:2005:BPH:CBC	2.47	0.45
4:L:1001:BCL:CBC	4:M:1003:BCL:CAD	2.94	0.45
2:S:3:TYR:CE2	3:T:194:GLN:HA	2.52	0.45
3:T:37:ARG:HH11	3:T:37:ARG:HG2	1.81	0.45
2:M:3:TYR:CE1	2:M:9:GLN:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:156:LEU:HD12	2:S:277:THR:HG22	1.97	0.45
3:H:24:LEU:O	3:H:28:ILE:HG13	2.16	0.45
1:R:56:GLN:NE2	1:R:58:THR:HG21	2.30	0.45
1:R:197:ALA:HA	1:R:207:ARG:HG2	1.99	0.45
1:R:214:THR:O	1:R:218:ASP:HB2	2.16	0.45
3:T:161:ALA:HB2	3:T:210:SER:HA	1.99	0.45
3:T:199:GLN:HB2	3:T:202:ARG:O	2.16	0.45
1:L:39:PHE:CD1	1:L:39:PHE:C	2.95	0.45
1:L:157:VAL:CG1	4:M:1003:BCL:HBB1	2.43	0.45
2:M:256:MET:HE3	2:M:258:PHE:CZ	2.51	0.45
3:T:245:ALA:HB3	3:T:246:PRO:HD3	1.99	0.45
3:H:46:ASP:HB3	10:H:266:HOH:O	2.16	0.45
1:L:68:PRO:HB3	1:L:86:TRP:CD2	2.52	0.45
3:H:66:LEU:HA	3:H:67:PRO:HD3	1.79	0.45
3:H:70:ARG:NH1	3:H:70:ARG:CG	2.80	0.45
3:H:140:PHE:CD2	3:H:169:VAL:HG11	2.52	0.45
1:R:6:GLU:OE2	1:R:10:ARG:NH1	2.50	0.45
1:R:14:GLY:O	1:R:109:ARG:HD3	2.17	0.45
2:S:155:TRP:NE1	2:S:281:GLY:HA3	2.32	0.45
3:H:209:SER:O	3:H:210:SER:C	2.60	0.44
1:R:3:LEU:HB2	1:R:6:GLU:HB2	1.99	0.44
1:L:7:ARG:HG2	1:L:7:ARG:HH11	1.81	0.44
3:H:40:TYR:CE2	3:H:42:LEU:HD21	2.53	0.44
3:H:184:LYS:HD3	3:H:184:LYS:N	2.33	0.44
1:R:224:ILE:HG22	6:R:2009[A]:U10:H3M3	1.99	0.44
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.99	0.44
1:R:170:ASN:HB3	1:R:173:HIS:CB	2.48	0.44
1:R:232:LEU:O	1:R:236:LEU:HG	2.18	0.44
2:S:3:TYR:CD2	3:T:194:GLN:HA	2.52	0.44
2:S:94:LEU:HD22	2:S:115:TRP:HB2	1.99	0.44
3:T:183:LEU:HD12	3:T:189:ARG:NH1	2.33	0.44
3:T:207:ALA:O	3:T:240:GLY:HA3	2.17	0.44
3:T:157:ASP:CG	3:T:210:SER:H	2.26	0.44
2:M:238:ILE:HD13	2:M:263:GLU:HB2	1.99	0.44
1:R:94:THR:O	1:R:98:VAL:HG23	2.17	0.44
1:L:60:ASN:O	1:L:64:ILE:HG13	2.18	0.44
1:L:80:LEU:HD12	1:L:85:LEU:CD1	2.48	0.44
1:L:105:VAL:O	1:L:108:CYS:HB2	2.17	0.44
1:L:139:MET:HE3	1:L:252:GLY:CA	2.47	0.44
1:R:79:PRO:C	1:R:81:ALA:H	2.25	0.44
1:R:224:ILE:N	6:R:2009[B]:U10:O5	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:279:ILE:HD12	2:S:91:PHE:C	2.42	0.44
1:L:90:THR:CG2	1:L:132:VAL:HG11	2.48	0.44
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.53	0.44
1:R:265:TRP:CG	1:R:266:TRP:N	2.85	0.44
2:S:129:TRP:O	2:S:132:ARG:HB3	2.17	0.44
1:R:173:HIS:CE1	1:R:177:ILE:HD11	2.52	0.44
3:T:111:PRO:HG2	3:T:242:MET:SD	2.58	0.44
3:T:187:SER:HB2	10:T:269:HOH:O	2.17	0.44
1:L:14:GLY:C	1:L:109:ARG:HH11	2.25	0.43
1:R:22:PHE:HA	1:R:24:PHE:HE2	1.82	0.43
1:L:231:ARG:HD2	2:M:5:ASN:O	2.17	0.43
3:H:153:VAL:HG21	3:H:181:VAL:CG2	2.47	0.43
3:H:185:ASP:OD1	3:H:185:ASP:C	2.60	0.43
1:R:213:ASN:HB3	1:R:217:ARG:NH2	2.33	0.43
1:R:268:LYS:C	1:R:273:ALA:HB2	2.44	0.43
2:S:187:ASN:HA	4:S:2003:BCL:CBC	2.49	0.43
2:S:251:PHE:CD2	2:S:251:PHE:C	2.96	0.43
2:S:253:ARG:HB2	2:S:259:ASN:OD1	2.18	0.43
3:T:255:MET:C	3:T:256:LEU:HD12	2.43	0.43
1:L:141:ALA:C	1:L:143:GLY:N	2.76	0.43
2:M:87:ARG:HG3	2:M:88:ASP:N	2.33	0.43
1:R:105:VAL:O	1:R:108:CYS:HB2	2.18	0.43
2:S:11:GLN:OE1	2:S:40:GLY:HA3	2.17	0.43
3:T:87:LEU:HD22	3:T:98:HIS:O	2.18	0.43
3:T:111:PRO:HB2	3:T:239:GLY:HA2	2.00	0.43
3:T:191:LEU:O	3:T:192:PRO:C	2.60	0.43
2:M:129:TRP:O	2:M:132:ARG:HB3	2.19	0.43
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.83	0.43
2:S:10:VAL:HG21	3:T:148:PRO:CD	2.47	0.43
3:T:117:ARG:O	3:T:118:ARG:C	2.62	0.43
3:H:40:TYR:CZ	3:H:42:LEU:HD21	2.54	0.43
1:R:184:ALA:HB3	5:S:2005:BPH:CMC	2.49	0.43
1:L:2:LEU:HB3	1:L:6:GLU:HB3	2.01	0.43
1:L:226:THR:CG2	1:L:227:LEU:N	2.81	0.43
4:L:1002:BCL:NC	4:M:1003:BCL:HBB3	2.34	0.43
2:M:204:LEU:HD13	3:H:20:PHE:CE2	2.54	0.43
1:R:231:ARG:NE	2:S:6:ILE:O	2.52	0.43
3:T:117:ARG:O	3:T:228:LEU:HB2	2.18	0.43
1:L:244:SER:HB3	4:L:1002:BCL:O1A	2.18	0.43
1:L:6:GLU:O	1:L:7:ARG:C	2.62	0.43
4:L:1002:BCL:H2C	4:M:1003:BCL:H2C	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:178:PHE:CZ	3:H:230:GLU:HG2	2.40	0.43
1:L:268:LYS:HA	1:L:268:LYS:HD3	1.71	0.43
3:H:134:MET:O	3:H:135:LYS:C	2.61	0.43
3:H:189:ARG:HG2	3:H:189:ARG:HH11	1.83	0.43
1:R:219:LEU:CD1	1:R:220:VAL:HG23	2.33	0.43
2:S:256:MET:HE1	6:S:2008:U10:H13	2.01	0.43
4:L:1004:BCL:C2	4:L:1004:BCL:H71	2.48	0.42
1:R:85:LEU:HD12	1:R:85:LEU:HA	1.89	0.42
2:S:157:TRP:HD1	4:S:2001:BCL:HBB1	1.84	0.42
3:T:36:MET:HB3	3:T:58:LEU:HD23	2.01	0.42
3:H:241:LEU:HB2	10:H:276:HOH:O	2.19	0.42
1:R:7:ARG:HH12	3:T:87:LEU:HB2	1.84	0.42
1:R:65:SER:CB	1:R:152:THR:HG21	2.49	0.42
1:R:102:LEU:O	1:R:105:VAL:HB	2.18	0.42
6:R:2009[B]:U10:H3M1	10:S:2023:HOH:O	2.18	0.42
2:M:191:LEU:HD12	2:M:191:LEU:HA	1.89	0.42
3:H:40:TYR:CB	3:H:58:LEU:HD21	2.49	0.42
1:R:97:PHE:HE1	4:R:2002:BCL:H121	1.85	0.42
1:R:172:ALA:HB3	1:R:247:CYS:HA	2.01	0.42
2:S:15:PRO:HD2	3:T:140:PHE:CE1	2.54	0.42
2:S:159:VAL:HA	2:S:163:ILE:HB	2.00	0.42
3:T:58:LEU:HD23	3:T:58:LEU:HA	1.90	0.42
1:L:269:LEU:HG	1:L:271:TRP:CH2	2.54	0.42
4:L:1001:BCL:HBC2	4:L:1001:BCL:H2C	1.79	0.42
2:M:2:GLU:O	2:M:3:TYR:CB	2.64	0.42
2:M:96:PRO:HB3	2:M:115:TRP:CE2	2.55	0.42
8:M:1010:SPO:HM12	8:M:1010:SPO:H42	1.94	0.42
3:H:157:ASP:OD1	3:H:157:ASP:N	2.53	0.42
1:R:84:GLY:HA2	1:R:87:GLN:HE21	1.84	0.42
2:S:96:PRO:HA	2:S:115:TRP:CG	2.55	0.42
3:H:89:ARG:HG2	3:H:98:HIS:CE1	2.54	0.42
3:H:168:TRP:HB2	3:H:178:PHE:HB2	2.01	0.42
1:R:16:LEU:HD11	1:R:105:VAL:HG11	2.02	0.42
2:S:196:LEU:HD12	2:S:196:LEU:HA	1.87	0.42
1:L:121:PHE:O	1:L:122:ALA:C	2.61	0.42
1:R:60:ASN:OD1	1:R:62:GLN:N	2.53	0.42
2:S:97:PRO:CG	2:S:171:TRP:HB2	2.46	0.42
3:T:37:ARG:HG2	3:T:37:ARG:NH1	2.35	0.42
1:L:131:LEU:HD11	4:L:1004:BCL:HBC2	2.01	0.42
2:M:21:THR:O	2:M:22:GLU:C	2.61	0.42
2:S:13:ARG:O	3:T:140:PHE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:66:TRP:CZ2	2:S:122:MET:HE3	2.54	0.42
2:S:260:ALA:HA	3:T:35:ASN:HB3	2.00	0.42
1:L:10:ARG:NH2	1:L:25:TRP:HB2	2.35	0.42
2:S:190:SER:HB2	4:S:2003:BCL:H3C	2.00	0.42
3:T:69:GLY:C	3:T:71:GLY:H	2.28	0.42
1:R:220:VAL:HG21	5:S:2005:BPH:HED3	2.00	0.42
1:R:280:ASN:HB2	2:S:88:ASP:OD1	2.20	0.42
2:S:14:GLY:HA3	3:T:140:PHE:CZ	2.55	0.42
1:L:180:PHE:CE2	4:L:1002:BCL:HMA3	2.54	0.42
1:L:185:LEU:CD1	1:L:189:LEU:HD22	2.49	0.42
1:R:79:PRO:O	1:R:81:ALA:N	2.53	0.42
1:R:149:GLY:HA3	1:R:152:THR:OG1	2.20	0.42
2:S:224:LEU:HD23	2:S:224:LEU:HA	1.89	0.42
2:S:232:GLU:O	2:S:234:GLU:N	2.52	0.42
3:T:219:ILE:CG2	3:T:225:VAL:HG23	2.50	0.42
1:L:208:THR:OG1	1:L:211:HIS:HD2	2.03	0.41
2:M:110:LYS:C	2:M:111:GLU:HG3	2.45	0.41
3:H:46:ASP:OD1	3:H:48:THR:OG1	2.36	0.41
1:R:28:PRO:HB3	2:S:253:ARG:HH11	1.85	0.41
1:L:280:ASN:HB2	2:M:87:ARG:HE	1.84	0.41
5:R:2006:BPH:HMC1	2:S:213:ALA:HB3	2.02	0.41
1:L:264:GLN:OE1	1:L:268:LYS:HE2	2.20	0.41
3:H:241:LEU:O	3:H:248:ARG:NH2	2.53	0.41
3:H:248:ARG:HB2	3:H:248:ARG:CZ	2.49	0.41
1:R:90:THR:HG23	1:R:132:VAL:HG11	2.02	0.41
1:R:121:PHE:O	1:R:122:ALA:C	2.61	0.41
1:R:206:MET:HE2	1:R:206:MET:HB3	1.88	0.41
3:T:17:ILE:O	3:T:21:TRP:CD1	2.73	0.41
3:T:158:LEU:HG	3:T:249:LYS:HG3	2.02	0.41
1:R:7:ARG:NH2	3:T:98:HIS:HD2	2.19	0.41
1:R:16:LEU:HD11	1:R:105:VAL:CG1	2.50	0.41
1:R:180:PHE:CD2	1:R:240:ALA:HB1	2.54	0.41
1:R:189:LEU:HD12	1:R:189:LEU:HA	1.93	0.41
1:R:268:LYS:HA	1:R:273:ALA:CB	2.49	0.41
2:S:234:GLU:O	2:S:238:ILE:HG13	2.20	0.41
2:M:5:ASN:HD22	2:M:224:LEU:HD22	1.84	0.41
3:H:66:LEU:HD23	3:H:72:THR:HA	2.02	0.41
1:R:34:PHE:HA	1:R:37:ALA:HB3	2.02	0.41
1:R:72:GLU:CD	1:R:72:GLU:N	2.78	0.41
1:R:200:PRO:O	1:R:201:GLU:C	2.64	0.41
1:L:133:LEU:HD23	1:L:133:LEU:C	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:22:GLU:HB3	2:M:23:ASP:H	1.65	0.41
2:M:109:LEU:HA	2:M:113:GLY:HA3	2.01	0.41
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.21	0.41
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.21	0.41
1:R:79:PRO:C	1:R:81:ALA:N	2.78	0.41
1:R:117:ILE:HD13	2:S:252:TRP:CZ2	2.55	0.41
1:R:246:LEU:O	1:R:249:ILE:HG22	2.21	0.41
3:T:36:MET:HE3	3:T:58:LEU:HD23	2.03	0.41
3:T:99:ALA:HA	3:T:100:PRO:HD3	1.84	0.41
1:L:85:LEU:O	1:L:89:ILE:HG13	2.21	0.41
1:L:102:LEU:HD12	1:L:102:LEU:HA	1.84	0.41
3:H:165:VAL:CG1	3:H:182:GLU:HB2	2.50	0.41
4:S:2001:BCL:HHC	4:S:2001:BCL:HBB2	2.01	0.41
3:T:212:LEU:CD1	3:T:244:ALA:HB2	2.51	0.41
1:L:51:TRP:CZ3	1:L:85:LEU:HD11	2.55	0.41
1:R:280:ASN:HB2	2:S:87:ARG:HE	1.86	0.41
2:S:151:LEU:O	2:S:155:TRP:N	2.49	0.41
4:S:2001:BCL:HBB2	8:S:2010:SPO:H243	2.03	0.41
3:T:199:GLN:OE1	3:T:202:ARG:HD2	2.21	0.41
10:L:1032:HOH:O	2:M:29:ARG:HD2	2.21	0.41
4:M:1003:BCL:H62	4:M:1003:BCL:H92	1.93	0.41
3:H:120:LEU:N	3:H:226:THR:HB	2.36	0.41
2:S:21:THR:HG23	2:S:26:LEU:CD2	2.42	0.41
2:S:93:SER:HB2	2:S:181:SER:HB3	2.03	0.41
2:S:182:HIS:CG	8:S:2010:SPO:H181	2.56	0.41
3:T:149:ILE:CD1	3:T:166:ASP:HA	2.51	0.41
1:L:78:ALA:HB1	1:L:79:PRO:HD2	2.02	0.41
1:L:83:GLY:O	1:L:87:GLN:HG3	2.21	0.41
2:M:170:SER:HB2	10:M:1041:HOH:O	2.21	0.41
2:S:151:LEU:HA	2:S:154:ILE:HB	2.02	0.41
1:L:20:ASN:HB3	10:L:1018:HOH:O	2.21	0.40
2:M:9:GLN:HE22	3:H:198:VAL:N	2.17	0.40
1:L:60:ASN:HB3	1:L:63:LEU:HB2	2.03	0.40
1:L:80:LEU:HB3	1:L:85:LEU:HD13	2.02	0.40
2:M:145:HIS:CE1	9:M:1011:LDA:HM13	2.56	0.40
1:R:3:LEU:HD12	2:S:250:LEU:CD2	2.51	0.40
1:L:129:LEU:HD12	1:L:129:LEU:HA	1.89	0.40
3:H:207:ALA:HB1	3:H:237:VAL:O	2.22	0.40
1:R:59:TRP:HA	1:R:59:TRP:CE3	2.57	0.40
1:R:133:LEU:C	1:R:136:PRO:HD2	2.46	0.40
1:R:201:GLU:O	1:R:202:LYS:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:75:TRP:HB3	2:S:80:TRP:CZ3	2.56	0.40
3:T:60:LYS:CG	3:T:61:PRO:HD2	2.50	0.40
3:T:254:ALA:C	3:T:256:LEU:H	2.29	0.40
4:L:1001:BCL:HHC	4:L:1001:BCL:CBB	2.50	0.40
4:L:1004:BCL:H161	4:L:1004:BCL:H141	1.90	0.40
2:M:108:PRO:O	2:M:109:LEU:C	2.65	0.40
2:M:187:ASN:HA	4:M:1003:BCL:CBC	2.52	0.40
2:M:195:ASN:C	2:M:195:ASN:ND2	2.77	0.40
3:H:75:VAL:HA	3:H:76:PRO:C	2.46	0.40
1:R:6:GLU:HG3	2:S:250:LEU:HD22	2.02	0.40
1:R:177:ILE:HD13	4:S:2001:BCL:HMD2	2.02	0.40
1:R:230:HIS:NE2	2:S:223:ILE:HG13	2.37	0.40
1:R:262:TRP:O	1:R:265:TRP:HD1	2.05	0.40
1:R:269:LEU:HD12	1:R:269:LEU:HA	1.91	0.40
2:M:270:ILE:HD13	9:M:1011:LDA:H32	2.04	0.40
1:R:154:LEU:O	1:R:157:VAL:HB	2.21	0.40
2:S:123:PHE:HA	2:S:157:TRP:CH2	2.57	0.40
3:T:192:PRO:CB	3:T:194:GLN:HE21	2.35	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	L	279/281 (99%)	262 (94%)	16 (6%)	1 (0%)	30	51
1	R	279/281 (99%)	264 (95%)	12 (4%)	3 (1%)	11	25
2	M	299/307 (97%)	280 (94%)	18 (6%)	1 (0%)	36	58
2	S	297/307 (97%)	284 (96%)	11 (4%)	2 (1%)	18	38
3	H	244/260 (94%)	233 (96%)	11 (4%)	0	100	100
3	T	244/260 (94%)	223 (91%)	15 (6%)	6 (2%)	4	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1642/1696 (97%)	1546 (94%)	83 (5%)	13 (1%)	16	34

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	2	GLU
3	T	45	GLU
3	T	220	LYS
1	R	80	LEU
1	R	257	ASP
2	S	195	ASN
3	T	70	ARG
3	T	124	ASP
1	L	270	PRO
3	T	89	ARG
3	T	166	ASP
1	R	31	VAL
2	S	19	GLY

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%)	208 (94%)	12 (6%)	19	41
1	R	220/220 (100%)	208 (94%)	12 (6%)	19	41
2	M	236/240 (98%)	225 (95%)	11 (5%)	23	48
2	S	235/240 (98%)	222 (94%)	13 (6%)	19	41
3	H	199/208 (96%)	189 (95%)	10 (5%)	22	46
3	T	199/208 (96%)	192 (96%)	7 (4%)	32	59
All	All	1309/1336 (98%)	1244 (95%)	65 (5%)	22	46

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	85	LEU
1	L	102	LEU
1	L	129	LEU
1	L	133	LEU
1	L	154	LEU
1	L	189	LEU
1	L	195	LEU
1	L	220	VAL
1	L	231	ARG
1	L	238	LEU
1	L	247	CYS
1	L	269	LEU
2	M	26	LEU
2	M	29	ARG
2	M	60	LEU
2	M	94	LEU
2	M	114	LEU
2	M	136	ARG
2	M	156	LEU
2	M	165	PRO
2	M	191	LEU
2	M	196	LEU
2	M	232	GLU
3	H	70	ARG
3	H	73	LEU
3	H	123	LEU
3	H	134	MET
3	H	184	LYS
3	H	191	LEU
3	H	202	ARG
3	H	208	LEU
3	H	220	LYS
3	H	231	ASP
1	R	87	GLN
1	R	102	LEU
1	R	126	LEU
1	R	133	LEU
1	R	154	LEU
1	R	189	LEU
1	R	217	ARG
1	R	219	LEU
1	R	220	VAL
1	R	229	ILE

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Mol	Chain	Res	Type
1	R	231	ARG
1	R	269	LEU
2	S	12	VAL
2	S	29	ARG
2	S	60	LEU
2	S	72	ILE
2	S	87	ARG
2	S	94	LEU
2	S	111	GLU
2	S	114	LEU
2	S	136	ARG
2	S	156	LEU
2	S	191	LEU
2	S	216	PHE
2	S	232	GLU
3	T	73	LEU
3	T	79	GLU
3	T	82	ASP
3	T	123	LEU
3	T	196	VAL
3	T	202	ARG
3	T	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	87	GLN
1	L	211	HIS
1	L	274	ASN
2	M	5	ASN
2	M	9	GLN
2	M	44	ASN
2	M	195	ASN
3	H	98	HIS
3	H	126	HIS
3	H	129	ASN
3	H	194	GLN
3	H	206	ASN
1	R	87	GLN
1	R	211	HIS
2	S	5	ASN
2	S	9	GLN

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Mol	Chain	Res	Type
2	S	28	ASN
2	S	44	ASN
2	S	195	ASN
3	T	35	ASN
3	T	44	ASN
3	T	53	GLN
3	T	174	GLN
3	T	194	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	BCL	L	1001	-	54,59,74	2.04	15 (27%)	61,97,115	2.02	15 (24%)
4	BCL	M	1003	-	69,74,74	1.74	14 (20%)	79,115,115	1.91	25 (31%)
6	U10	M	1008	-	38,38,63	2.05	13 (34%)	48,49,79	1.80	13 (27%)
6	U10	L	1009[B]	-	30,30,63	2.02	9 (30%)	37,39,79	2.01	11 (29%)
8	SPO	M	1010	-	41,41,41	3.09	21 (51%)	47,50,50	2.44	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	U10	R	2009[B]	-	18,18,63	2.14	6 (33%)	24,25,79	2.15	7 (29%)
6	U10	S	2008	-	32,32,63	1.96	10 (31%)	40,41,79	1.90	10 (25%)
9	LDA	M	1011	-	13,15,15	1.85	1 (7%)	14,17,17	1.62	4 (28%)
4	BCL	S	2004	-	69,74,74	1.83	17 (24%)	79,115,115	1.87	19 (24%)
5	BPH	M	1005	-	49,60,70	2.20	15 (30%)	47,89,101	3.06	21 (44%)
4	BCL	L	1004	-	69,74,74	1.79	13 (18%)	79,115,115	1.77	18 (22%)
8	SPO	S	2010	-	41,41,41	3.08	22 (53%)	47,50,50	2.47	17 (36%)
5	BPH	R	2006	-	59,70,70	2.11	14 (23%)	59,101,101	2.85	21 (35%)
6	U10	L	1009[A]	-	30,30,63	2.12	11 (36%)	37,39,79	2.08	11 (29%)
6	U10	R	2009[A]	-	18,18,63	2.17	6 (33%)	24,25,79	2.20	7 (29%)
5	BPH	L	1006	-	59,70,70	2.16	14 (23%)	59,101,101	2.82	22 (37%)
4	BCL	S	2003	-	69,74,74	1.79	12 (17%)	79,115,115	1.88	23 (29%)
4	BCL	L	1002	-	69,74,74	1.79	12 (17%)	79,115,115	1.90	22 (27%)
4	BCL	R	2002	-	69,74,74	1.81	11 (15%)	79,115,115	1.88	20 (25%)
4	BCL	S	2001	-	54,59,74	2.09	16 (29%)	61,97,115	1.95	17 (27%)
5	BPH	S	2005	-	45,56,70	2.32	15 (33%)	41,84,101	3.29	19 (46%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	L	1001	-	-	0/23/119/137	-
4	BCL	M	1003	-	-	9/41/137/137	-
6	U10	M	1008	-	-	4/33/57/87	0/1/1/1
6	U10	L	1009[B]	-	-	5/24/48/87	0/1/1/1
8	SPO	M	1010	-	-	13/47/47/47	-
6	U10	R	2009[B]	-	-	0/9/33/87	0/1/1/1
6	U10	S	2008	-	-	4/26/50/87	0/1/1/1
9	LDA	M	1011	-	-	7/13/13/13	-
4	BCL	S	2004	-	-	9/41/137/137	-
5	BPH	M	1005	-	1/1/16/22	6/25/93/105	0/5/6/6
4	BCL	L	1004	-	-	9/41/137/137	-
8	SPO	S	2010	-	-	12/47/47/47	-
5	BPH	R	2006	-	2/2/18/22	9/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	U10	L	1009[A]	-	-	9/24/48/87	0/1/1/1
6	U10	R	2009[A]	-	-	1/9/33/87	0/1/1/1
5	BPH	L	1006	-	2/2/18/22	8/37/105/105	0/5/6/6
4	BCL	S	2003	-	-	10/41/137/137	-
4	BCL	L	1002	-	-	4/41/137/137	-
4	BCL	R	2002	-	-	7/41/137/137	-
4	BCL	S	2001	-	-	8/23/119/137	-
5	BPH	S	2005	-	-	9/21/89/105	0/5/6/6

All (267) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	1010	SPO	C15-C16	7.96	1.55	1.34
8	S	2010	SPO	C6-C5	7.91	1.54	1.32
8	S	2010	SPO	C10-C11	7.73	1.54	1.34
8	M	1010	SPO	C6-C5	7.73	1.53	1.32
8	M	1010	SPO	C10-C11	7.58	1.54	1.34
8	S	2010	SPO	C15-C16	7.34	1.53	1.34
5	M	1005	BPH	C2C-C3C	-7.26	1.48	1.54
5	S	2005	BPH	C2C-C3C	-7.10	1.48	1.54
5	R	2006	BPH	C2C-C3C	-7.06	1.48	1.54
4	S	2003	BCL	C3B-C4B	6.97	1.54	1.41
4	R	2002	BCL	C3B-C4B	6.76	1.54	1.41
4	M	1003	BCL	C3B-C4B	6.73	1.54	1.41
4	L	1002	BCL	C3B-C4B	6.52	1.54	1.41
4	S	2001	BCL	C3B-C4B	6.41	1.53	1.41
5	L	1006	BPH	C1D-C2D	6.40	1.46	1.39
4	L	1004	BCL	C3B-C4B	6.36	1.53	1.41
9	M	1011	LDA	O1-N1	-6.24	1.26	1.42
4	S	2004	BCL	C3B-C4B	6.11	1.53	1.41
4	L	1001	BCL	C3B-C4B	5.97	1.52	1.41
5	R	2006	BPH	C1D-C2D	5.87	1.46	1.39
4	R	2002	BCL	MG-ND	5.81	2.17	2.05
4	L	1002	BCL	MG-NB	-5.77	1.94	2.05
4	S	2001	BCL	MG-NB	-5.76	1.94	2.05
4	S	2004	BCL	MG-NB	-5.75	1.94	2.05
5	S	2005	BPH	C1D-C2D	5.74	1.45	1.39
4	S	2003	BCL	MG-NB	-5.74	1.94	2.05
4	L	1001	BCL	MG-NB	-5.74	1.94	2.05
4	L	1002	BCL	MG-ND	5.63	2.16	2.05
5	L	1006	BPH	C11-C10	-5.60	1.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1005	BPH	C1B-C2B	5.59	1.45	1.39
5	M	1005	BPH	C1D-C2D	5.58	1.45	1.39
6	M	1008	U10	O4-C4	5.57	1.50	1.36
4	S	2001	BCL	MG-ND	5.55	2.16	2.05
5	L	1006	BPH	C1B-C2B	5.52	1.45	1.39
5	R	2006	BPH	C11-C10	-5.51	1.29	1.52
4	L	1004	BCL	MG-NB	-5.46	1.95	2.05
4	S	2003	BCL	MG-ND	5.34	2.16	2.05
5	L	1006	BPH	C2C-C3C	-5.33	1.50	1.54
5	S	2005	BPH	C1B-C2B	5.15	1.45	1.39
4	M	1003	BCL	MG-NB	-5.14	1.95	2.05
4	R	2002	BCL	MG-NB	-5.14	1.95	2.05
6	S	2008	U10	O4-C4	5.05	1.48	1.36
4	S	2004	BCL	MG-ND	5.01	2.15	2.05
5	R	2006	BPH	C1B-C2B	4.92	1.45	1.39
8	M	1010	SPO	C21-C20	4.92	1.49	1.36
4	M	1003	BCL	MG-ND	4.89	2.15	2.05
4	L	1004	BCL	MG-ND	4.85	2.15	2.05
6	R	2009[A]	U10	O4-C4	4.85	1.48	1.36
8	S	2010	SPO	C26-C25	4.79	1.47	1.34
6	L	1009[A]	U10	O4-C4	4.79	1.48	1.36
6	R	2009[B]	U10	O4-C4	4.79	1.48	1.36
8	S	2010	SPO	C21-C20	4.79	1.49	1.36
4	L	1001	BCL	MG-ND	4.78	2.15	2.05
8	M	1010	SPO	C26-C25	4.78	1.47	1.34
6	L	1009[B]	U10	O4-C4	4.69	1.48	1.36
6	L	1009[A]	U10	C13-C14	4.35	1.43	1.33
8	S	2010	SPO	O1-CM1	4.34	1.56	1.43
4	L	1001	BCL	C3C-C4C	-4.31	1.46	1.51
5	S	2005	BPH	O2A-CGA	4.29	1.45	1.33
5	L	1006	BPH	C3A-C2A	-4.28	1.51	1.54
6	L	1009[B]	U10	C13-C14	4.25	1.42	1.33
5	L	1006	BPH	O2D-CGD	4.24	1.43	1.33
8	M	1010	SPO	O1-CM1	4.18	1.56	1.43
5	R	2006	BPH	O2A-CGA	4.16	1.45	1.33
5	L	1006	BPH	C3B-C4B	3.99	1.47	1.41
5	L	1006	BPH	O2A-CGA	3.94	1.44	1.33
6	S	2008	U10	C13-C14	3.94	1.42	1.33
4	L	1004	BCL	C1B-C2B	3.80	1.52	1.43
5	S	2005	BPH	O2D-CGD	3.77	1.42	1.33
4	L	1001	BCL	MG-NC	-3.77	1.97	2.06
5	M	1005	BPH	O2D-CGD	3.72	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	2006	BPH	O2D-CGD	3.70	1.42	1.33
6	M	1008	U10	C13-C14	3.69	1.41	1.33
6	M	1008	U10	C7-C8	-3.67	1.44	1.50
5	S	2005	BPH	CHA-CBD	3.64	1.55	1.51
4	S	2004	BCL	C1B-C2B	3.63	1.51	1.43
4	S	2001	BCL	C3C-C4C	-3.57	1.47	1.51
6	L	1009[A]	U10	C8-C9	3.55	1.41	1.33
4	M	1003	BCL	MG-NA	3.55	2.14	2.06
4	R	2002	BCL	CBB-CAB	3.53	1.57	1.50
6	R	2009[A]	U10	O3-C3	3.52	1.45	1.36
6	L	1009[A]	U10	C6-C1	3.51	1.41	1.35
6	M	1008	U10	C23-C24	3.49	1.41	1.33
6	L	1009[A]	U10	O3-C3	3.48	1.45	1.36
4	R	2002	BCL	MG-NA	3.45	2.14	2.06
6	R	2009[B]	U10	O3-C3M	-3.42	1.37	1.45
6	L	1009[B]	U10	O3-C3M	-3.41	1.37	1.45
4	S	2001	BCL	MG-NC	-3.40	1.98	2.06
5	S	2005	BPH	C3B-C4B	3.35	1.46	1.41
5	M	1005	BPH	O2A-CGA	3.33	1.43	1.33
4	L	1002	BCL	MG-NA	3.33	2.14	2.06
8	M	1010	SPO	C4-C1	3.31	1.58	1.52
6	R	2009[B]	U10	O3-C3	3.28	1.44	1.36
6	R	2009[A]	U10	C6-C1	3.27	1.41	1.35
6	L	1009[B]	U10	C8-C9	3.23	1.40	1.33
4	S	2003	BCL	MG-NA	3.22	2.13	2.06
8	S	2010	SPO	C37-C38	3.22	1.42	1.32
4	L	1004	BCL	C3C-C4C	-3.18	1.47	1.51
4	L	1001	BCL	C1B-C2B	3.17	1.50	1.43
6	R	2009[A]	U10	C7-C8	-3.16	1.45	1.50
5	L	1006	BPH	C2-C3	3.12	1.40	1.33
4	L	1004	BCL	MG-NC	-3.12	1.98	2.06
6	S	2008	U10	O3-C3	3.10	1.44	1.36
6	L	1009[B]	U10	O3-C3	3.10	1.44	1.36
6	L	1009[A]	U10	O3-C3M	-3.10	1.38	1.45
6	S	2008	U10	O3-C3M	-3.10	1.38	1.45
6	M	1008	U10	C18-C19	3.09	1.40	1.33
5	R	2006	BPH	C1A-C2A	3.08	1.55	1.51
5	M	1005	BPH	CAA-C2A	3.07	1.60	1.54
8	M	1010	SPO	C6-C7	-3.07	1.39	1.46
6	R	2009[B]	U10	C6-C1	3.06	1.40	1.35
5	R	2006	BPH	C4D-ND	-3.04	1.34	1.38
8	M	1010	SPO	C10-C9	3.02	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	2009[A]	U10	O3-C3M	-3.01	1.38	1.45
8	S	2010	SPO	C4-C1	3.00	1.58	1.52
4	S	2004	BCL	MG-NC	-3.00	1.99	2.06
8	S	2010	SPO	C11-C12	-2.99	1.39	1.46
6	S	2008	U10	C7-C8	-2.99	1.45	1.50
5	R	2006	BPH	O2D-CED	-2.96	1.38	1.45
6	M	1008	U10	O3-C3M	-2.96	1.38	1.45
6	M	1008	U10	O3-C3	2.96	1.43	1.36
8	S	2010	SPO	C25-C23	-2.96	1.39	1.46
4	S	2001	BCL	C1B-C2B	2.95	1.50	1.43
5	R	2006	BPH	C2-C3	2.95	1.39	1.33
4	S	2004	BCL	CAA-C2A	2.95	1.59	1.54
4	S	2004	BCL	MG-NA	2.93	2.13	2.06
4	S	2001	BCL	CBB-CAB	2.92	1.55	1.50
4	L	1002	BCL	CBB-CAB	2.91	1.55	1.50
5	S	2005	BPH	C4D-ND	-2.91	1.34	1.38
4	S	2003	BCL	C3D-C4D	-2.91	1.37	1.44
6	R	2009[B]	U10	C7-C8	-2.90	1.46	1.50
6	S	2008	U10	C18-C19	2.89	1.39	1.33
8	M	1010	SPO	C32-C33	2.88	1.39	1.33
4	L	1002	BCL	C1B-C2B	2.87	1.49	1.43
8	S	2010	SPO	C10-C9	2.87	1.52	1.43
5	S	2005	BPH	C1A-C2A	2.87	1.55	1.51
4	S	2001	BCL	C3D-C4D	-2.86	1.37	1.44
8	M	1010	SPO	C25-C23	-2.86	1.39	1.46
6	L	1009[B]	U10	C18-C19	2.85	1.39	1.33
8	S	2010	SPO	O1-C1	2.85	1.57	1.41
8	M	1010	SPO	C37-C38	2.84	1.41	1.32
6	S	2008	U10	C8-C9	2.83	1.39	1.33
4	S	2004	BCL	C3C-C4C	-2.82	1.48	1.51
8	S	2010	SPO	C32-C33	2.81	1.39	1.33
8	M	1010	SPO	C11-C12	-2.81	1.39	1.46
6	S	2008	U10	C6-C1	2.80	1.40	1.35
4	S	2003	BCL	CHD-C1D	2.80	1.43	1.38
5	L	1006	BPH	O2D-CED	-2.80	1.39	1.45
6	L	1009[B]	U10	C6-C1	2.79	1.40	1.35
6	L	1009[A]	U10	C18-C19	2.79	1.39	1.33
4	S	2001	BCL	CAA-C2A	2.78	1.59	1.54
5	M	1005	BPH	O2D-CED	-2.77	1.39	1.45
4	R	2002	BCL	C1B-C2B	2.77	1.49	1.43
4	S	2001	BCL	MG-NA	2.77	2.12	2.06
4	L	1002	BCL	CHD-C1D	2.76	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1005	BPH	C3B-C4B	2.75	1.45	1.41
5	M	1005	BPH	C2-C3	2.74	1.39	1.33
5	S	2005	BPH	C2-C3	2.74	1.39	1.33
8	M	1010	SPO	C8-C7	2.73	1.56	1.50
6	R	2009[B]	U10	C8-C9	2.73	1.40	1.32
5	S	2005	BPH	CAA-C2A	2.72	1.59	1.54
4	L	1001	BCL	C3D-C4D	-2.72	1.38	1.44
4	M	1003	BCL	C1B-C2B	2.71	1.49	1.43
8	S	2010	SPO	C26-C27	2.70	1.51	1.43
4	S	2004	BCL	CBB-CAB	2.70	1.55	1.50
6	L	1009[B]	U10	C7-C8	-2.70	1.46	1.50
4	M	1003	BCL	CHD-C1D	2.69	1.43	1.38
5	S	2005	BPH	O2D-CED	-2.69	1.39	1.45
4	R	2002	BCL	CHD-C1D	2.69	1.43	1.38
5	M	1005	BPH	C3A-C2A	-2.68	1.52	1.54
8	S	2010	SPO	C6-C7	-2.68	1.40	1.46
8	M	1010	SPO	C26-C27	2.67	1.51	1.43
8	M	1010	SPO	O1-C1	2.67	1.56	1.41
6	L	1009[A]	U10	C7-C8	-2.67	1.46	1.50
4	L	1001	BCL	C1D-C2D	-2.66	1.40	1.45
5	L	1006	BPH	CHA-CBD	2.64	1.54	1.51
8	M	1010	SPO	C13-C12	2.63	1.56	1.50
6	M	1008	U10	C6-C1	2.62	1.39	1.35
8	S	2010	SPO	C8-C7	2.60	1.56	1.50
4	S	2004	BCL	C3D-C4D	-2.59	1.38	1.44
8	M	1010	SPO	C15-C14	2.54	1.51	1.43
4	L	1004	BCL	CBB-CAB	2.51	1.55	1.50
4	M	1003	BCL	C3D-C4D	-2.51	1.38	1.44
5	M	1005	BPH	CBD-CGD	-2.51	1.49	1.52
5	M	1005	BPH	C3B-C2B	-2.51	1.35	1.39
4	S	2003	BCL	CMD-C2D	2.50	1.55	1.50
4	S	2004	BCL	C4-C3	2.50	1.56	1.50
6	L	1009[A]	U10	C7-C6	2.50	1.56	1.51
6	R	2009[A]	U10	C8-C9	2.48	1.39	1.32
4	L	1001	BCL	CAA-C2A	2.48	1.58	1.54
4	S	2003	BCL	C1B-C2B	2.48	1.48	1.43
4	L	1002	BCL	C3C-C4C	-2.47	1.48	1.51
8	M	1010	SPO	C24-C23	2.46	1.55	1.50
6	L	1009[A]	U10	C15-C14	2.44	1.56	1.50
4	L	1001	BCL	CAA-CBA	2.44	1.60	1.52
4	M	1003	BCL	C4B-NB	-2.44	1.34	1.37
6	M	1008	U10	C27-C28	-2.43	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	2010	SPO	C13-C12	2.42	1.55	1.50
6	M	1008	U10	C15-C14	2.41	1.56	1.50
4	L	1002	BCL	C3D-C4D	-2.38	1.38	1.44
4	S	2004	BCL	CAA-CBA	2.38	1.60	1.52
5	R	2006	BPH	C3D-C2D	-2.38	1.35	1.39
8	S	2010	SPO	C35-C33	2.37	1.56	1.51
6	M	1008	U10	C8-C9	2.37	1.38	1.33
6	L	1009[B]	U10	C15-C14	2.37	1.56	1.50
4	R	2002	BCL	CMD-C2D	2.36	1.55	1.50
4	M	1003	BCL	C3C-C4C	-2.36	1.48	1.51
8	M	1010	SPO	C14-C12	2.36	1.41	1.35
4	L	1002	BCL	CMD-C2D	2.35	1.55	1.50
4	L	1004	BCL	C3D-C4D	-2.35	1.38	1.44
5	R	2006	BPH	CAA-C2A	2.33	1.58	1.54
5	R	2006	BPH	C3B-C4B	2.33	1.45	1.41
4	L	1004	BCL	MG-NA	2.31	2.11	2.06
4	S	2001	BCL	C1-C2	2.31	1.55	1.49
8	S	2010	SPO	C24-C23	2.30	1.55	1.50
8	S	2010	SPO	C19-C17	2.30	1.41	1.35
8	S	2010	SPO	C15-C14	2.30	1.50	1.43
5	S	2005	BPH	C3B-C2B	-2.30	1.35	1.39
4	L	1002	BCL	C4-C3	2.29	1.56	1.50
4	M	1003	BCL	OBB-CAB	-2.28	1.18	1.23
4	L	1004	BCL	C6-C5	2.27	1.60	1.52
4	L	1001	BCL	C4B-NB	-2.26	1.34	1.37
5	L	1006	BPH	C1A-C2A	2.26	1.54	1.51
5	L	1006	BPH	C4D-ND	-2.25	1.35	1.38
4	R	2002	BCL	OBB-CAB	-2.25	1.18	1.23
5	L	1006	BPH	CAA-C2A	2.24	1.58	1.54
4	S	2004	BCL	CMD-C2D	2.23	1.55	1.50
4	R	2002	BCL	C3D-C4D	-2.23	1.39	1.44
4	S	2004	BCL	C4B-NB	-2.22	1.34	1.37
4	L	1001	BCL	MG-NA	2.22	2.11	2.06
4	M	1003	BCL	CMD-C2D	2.20	1.55	1.50
6	S	2008	U10	C15-C14	2.20	1.56	1.50
4	S	2001	BCL	CAA-CBA	2.20	1.59	1.52
4	M	1003	BCL	MG-NC	-2.20	2.01	2.06
4	R	2002	BCL	C4-C3	2.20	1.56	1.50
4	S	2001	BCL	C1D-C2D	-2.19	1.41	1.45
4	S	2003	BCL	C4-C3	2.18	1.56	1.50
4	S	2003	BCL	CBB-CAB	2.18	1.54	1.50
4	L	1004	BCL	C4-C3	2.17	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1005	BPH	C4D-ND	-2.16	1.35	1.38
6	S	2008	U10	C20-C19	2.15	1.56	1.50
4	S	2003	BCL	C4B-NB	-2.15	1.35	1.37
4	S	2004	BCL	C1D-C2D	-2.14	1.41	1.45
4	L	1001	BCL	C4-C3	2.13	1.56	1.50
8	S	2010	SPO	C14-C12	2.12	1.40	1.35
4	S	2004	BCL	OBG-CAB	-2.12	1.18	1.23
6	L	1009[A]	U10	C20-C19	2.11	1.55	1.50
5	M	1005	BPH	C1A-C2A	2.10	1.54	1.51
4	S	2001	BCL	OBG-CAD	-2.10	1.18	1.22
5	R	2006	BPH	C3A-C2A	-2.08	1.52	1.54
4	S	2001	BCL	C4B-NB	-2.08	1.35	1.37
4	L	1001	BCL	OBG-CAB	-2.08	1.18	1.23
4	M	1003	BCL	CBB-CAB	2.07	1.54	1.50
4	L	1004	BCL	C1D-C2D	-2.07	1.41	1.45
4	L	1004	BCL	CMD-C2D	2.06	1.55	1.50
5	M	1005	BPH	CMB-C2B	2.05	1.55	1.51
8	M	1010	SPO	C19-C17	2.04	1.40	1.35
4	S	2003	BCL	MG-NC	-2.03	2.01	2.06
6	M	1008	U10	C30-C29	2.03	1.55	1.50
4	S	2001	BCL	C4-C3	2.03	1.55	1.50
4	L	1001	BCL	CMD-C2D	2.03	1.54	1.50
6	M	1008	U10	C20-C19	2.02	1.55	1.50
5	S	2005	BPH	C3A-C2A	-2.02	1.53	1.54
4	L	1002	BCL	OBG-CAB	-2.01	1.18	1.23
4	S	2004	BCL	CHD-C1D	2.01	1.42	1.38
5	S	2005	BPH	O1D-CGD	2.01	1.26	1.21
4	M	1003	BCL	C2-C3	-2.00	1.28	1.33

All (337) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	2005	BPH	O2D-CGD-CBD	14.28	126.64	110.95
5	R	2006	BPH	O2D-CGD-CBD	13.97	126.30	110.95
5	L	1006	BPH	O2D-CGD-CBD	13.54	125.83	110.95
5	M	1005	BPH	O2D-CGD-CBD	13.51	125.80	110.95
8	S	2010	SPO	C15-C14-C12	-6.63	117.98	127.28
6	L	1009[A]	U10	C3M-O3-C3	6.50	139.32	116.47
6	R	2009[A]	U10	C3M-O3-C3	6.48	139.25	116.47
5	R	2006	BPH	C1-C2-C3	6.40	136.69	126.20
6	R	2009[B]	U10	C3M-O3-C3	6.37	138.86	116.47
8	S	2010	SPO	C20-C21-C22	-6.32	110.59	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	2002	BCL	C4A-NA-C1A	-6.31	103.80	106.68
6	S	2008	U10	C3M-O3-C3	6.20	138.27	116.47
4	L	1002	BCL	C4A-NA-C1A	-6.19	103.85	106.68
6	L	1009[B]	U10	C3M-O3-C3	6.08	137.85	116.47
8	M	1010	SPO	C20-C21-C22	-6.06	111.12	123.52
4	L	1001	BCL	CBC-CAC-C3C	-6.00	100.68	113.41
5	L	1006	BPH	C1-C2-C3	5.95	135.95	126.20
6	M	1008	U10	C3M-O3-C3	5.85	137.03	116.47
5	S	2005	BPH	C1-C2-C3	5.81	135.72	126.20
8	M	1010	SPO	C15-C14-C12	-5.77	119.19	127.28
4	S	2001	BCL	C4A-NA-C1A	-5.61	104.12	106.68
4	S	2004	BCL	C4A-NA-C1A	-5.58	104.13	106.68
4	S	2001	BCL	CBC-CAC-C3C	-5.57	101.59	113.41
5	L	1006	BPH	CBC-CAC-C3C	5.53	124.65	113.78
5	M	1005	BPH	C1-C2-C3	5.53	135.25	126.20
4	S	2003	BCL	C4A-NA-C1A	-5.46	104.19	106.68
5	R	2006	BPH	CBC-CAC-C3C	5.34	124.27	113.78
4	M	1003	BCL	C4A-NA-C1A	-5.31	104.26	106.68
8	M	1010	SPO	C26-C27-C28	-5.30	120.23	127.69
4	L	1001	BCL	C1-C2-C3	-5.21	118.34	126.76
8	S	2010	SPO	C25-C23-C22	-5.07	111.03	119.01
5	L	1006	BPH	O1D-CGD-CBD	-5.03	117.10	124.72
8	M	1010	SPO	C25-C23-C22	-5.00	111.14	119.01
5	S	2005	BPH	O1D-CGD-CBD	-5.00	117.15	124.72
5	R	2006	BPH	O1D-CGD-CBD	-4.94	117.22	124.72
5	M	1005	BPH	O1D-CGD-CBD	-4.94	117.24	124.72
5	R	2006	BPH	C4D-CHA-CBD	-4.83	106.14	108.45
4	S	2003	BCL	C1D-ND-C4D	4.80	109.68	106.31
8	S	2010	SPO	C26-C27-C28	-4.77	120.98	127.69
4	L	1001	BCL	C4A-NA-C1A	-4.67	104.55	106.68
5	M	1005	BPH	CBC-CAC-C3C	4.65	122.93	113.78
6	M	1008	U10	C27-C28-C29	4.62	143.06	127.64
4	L	1004	BCL	C4A-NA-C1A	-4.57	104.59	106.68
4	S	2004	BCL	C1D-ND-C4D	4.55	109.50	106.31
5	L	1006	BPH	C6-C5-C3	4.54	124.53	113.47
4	M	1003	BCL	C1D-ND-C4D	4.48	109.46	106.31
5	L	1006	BPH	CED-O2D-CGD	4.48	126.07	115.92
4	L	1002	BCL	C1D-ND-C4D	4.46	109.44	106.31
5	M	1005	BPH	CED-O2D-CGD	4.40	125.90	115.92
5	S	2005	BPH	C4D-CHA-CBD	-4.39	106.35	108.45
4	L	1001	BCL	C1D-ND-C4D	4.29	109.32	106.31
8	M	1010	SPO	C24-C23-C25	4.27	124.61	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1003	BCL	C11-C12-C13	-4.27	101.78	115.97
4	S	2001	BCL	C1D-ND-C4D	4.24	109.29	106.31
4	S	2003	BCL	C11-C12-C13	-4.23	101.91	115.97
4	L	1004	BCL	C1D-ND-C4D	4.22	109.28	106.31
4	R	2002	BCL	C1D-ND-C4D	4.17	109.23	106.31
8	S	2010	SPO	C4-C5-C6	-4.15	119.09	124.91
8	S	2010	SPO	C24-C23-C25	4.08	124.33	118.09
5	R	2006	BPH	C6-C5-C3	4.06	123.35	113.47
5	S	2005	BPH	CED-O2D-CGD	4.05	125.11	115.92
4	M	1003	BCL	C4D-CHA-C1A	4.03	126.05	121.24
4	L	1004	BCL	C1-O2A-CGA	4.01	126.37	116.65
4	R	2002	BCL	C7-C6-C5	-4.01	102.57	113.26
5	R	2006	BPH	CED-O2D-CGD	3.98	124.95	115.92
5	S	2005	BPH	O2D-CGD-O1D	-3.92	116.21	123.85
4	L	1002	BCL	C7-C6-C5	-3.88	102.93	113.26
5	M	1005	BPH	C6-C5-C3	3.86	122.87	113.47
4	L	1002	BCL	C4D-CHA-C1A	3.84	125.82	121.24
4	S	2003	BCL	C4D-CHA-C1A	3.83	125.82	121.24
5	R	2006	BPH	O2D-CGD-O1D	-3.81	116.43	123.85
4	L	1001	BCL	CAC-C3C-C4C	-3.78	104.20	112.58
4	L	1002	BCL	C1-C2-C3	-3.76	120.03	126.20
5	R	2006	BPH	C11-C10-C8	3.76	128.46	115.97
8	M	1010	SPO	C3-C1-C2	3.76	117.29	110.43
6	R	2009[A]	U10	O5-C5-C6	-3.75	114.53	121.79
6	L	1009[B]	U10	O2-C2-C3	-3.74	113.11	121.03
4	S	2004	BCL	C4D-CHA-C1A	3.73	125.70	121.24
8	S	2010	SPO	C6-C7-C9	-3.73	113.14	119.01
6	L	1009[A]	U10	O5-C5-C6	-3.72	114.59	121.79
8	S	2010	SPO	C15-C16-C17	-3.71	116.18	126.36
5	S	2005	BPH	CBC-CAC-C3C	3.71	121.08	113.78
4	S	2004	BCL	CBB-CAB-C3B	3.70	128.21	120.40
4	L	1001	BCL	C4D-CHA-C1A	3.69	125.65	121.24
4	M	1003	BCL	CBB-CAB-C3B	3.67	128.14	120.40
4	S	2004	BCL	C11-C12-C13	-3.67	103.77	115.97
4	L	1004	BCL	C4D-CHA-C1A	3.65	125.60	121.24
6	S	2008	U10	O5-C5-C6	-3.63	114.76	121.79
4	S	2003	BCL	OBB-CAB-CBB	-3.63	111.64	119.77
5	L	1006	BPH	C4D-CHA-CBD	-3.62	106.72	108.45
4	L	1004	BCL	CBB-CAB-C3B	3.62	128.03	120.40
4	L	1004	BCL	OBB-CAB-CBB	-3.62	111.67	119.77
4	S	2004	BCL	CBC-CAC-C3C	-3.61	105.75	113.41
4	M	1003	BCL	CAA-CBA-CGA	-3.60	103.00	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	2009[B]	U10	O5-C5-C6	-3.60	114.83	121.79
8	M	1010	SPO	C15-C16-C17	-3.59	116.52	126.36
4	L	1004	BCL	CAC-C3C-C4C	-3.58	104.63	112.58
4	R	2002	BCL	C4D-CHA-C1A	3.57	125.50	121.24
5	S	2005	BPH	C1C-C2C-C3C	3.57	106.23	102.84
4	S	2001	BCL	C4D-CHA-C1A	3.55	125.48	121.24
5	L	1006	BPH	C11-C10-C8	3.54	127.72	115.97
5	M	1005	BPH	O2D-CGD-O1D	-3.54	116.96	123.85
6	L	1009[B]	U10	O5-C5-C6	-3.52	114.99	121.79
4	M	1003	BCL	OBb-CAB-CBB	-3.51	111.90	119.77
6	M	1008	U10	O5-C5-C6	-3.51	115.00	121.79
8	S	2010	SPO	C3-C1-C2	3.51	116.84	110.43
4	L	1001	BCL	OBb-CAB-CBB	-3.50	111.93	119.77
5	L	1006	BPH	O2D-CGD-O1D	-3.50	117.04	123.85
5	M	1005	BPH	CMA-C3A-C4A	-3.48	107.11	114.61
5	R	2006	BPH	C1C-C2C-C3C	3.48	106.15	102.84
4	M	1003	BCL	C4-C3-C5	3.47	121.26	115.23
4	S	2003	BCL	CBB-CAB-C3B	3.45	127.68	120.40
5	M	1005	BPH	C1C-C2C-C3C	3.45	106.12	102.84
4	S	2004	BCL	OBb-CAB-CBB	-3.45	112.05	119.77
8	M	1010	SPO	C4-C5-C6	-3.44	120.08	124.91
4	L	1004	BCL	CBC-CAC-C3C	-3.42	106.16	113.41
5	L	1006	BPH	C1C-C2C-C3C	3.42	106.09	102.84
4	R	2002	BCL	C11-C12-C13	-3.40	104.67	115.97
6	R	2009[B]	U10	O2-C2-C3	-3.39	113.84	121.03
4	L	1001	BCL	C2C-C3C-C4C	3.38	106.39	101.34
6	R	2009[A]	U10	O2-C2-C3	-3.37	113.89	121.03
6	L	1009[A]	U10	O2-C2-C3	-3.35	113.94	121.03
8	M	1010	SPO	C8-C7-C6	3.34	123.19	118.09
8	S	2010	SPO	C8-C7-C6	3.32	123.17	118.09
9	M	1011	LDA	CM1-N1-C1	-3.32	103.26	110.23
4	L	1001	BCL	CAA-C2A-C3A	-3.29	104.11	113.00
4	R	2002	BCL	OBb-CAB-CBB	-3.29	112.41	119.77
4	L	1002	BCL	O2D-CGD-CBD	-3.28	105.50	111.23
4	R	2002	BCL	CBB-CAB-C3B	3.28	127.31	120.40
4	S	2004	BCL	CAA-C2A-C3A	-3.27	104.16	113.00
8	M	1010	SPO	C18-C17-C19	-3.25	117.55	122.82
4	S	2001	BCL	C2C-C3C-C4C	3.25	106.20	101.34
6	L	1009[A]	U10	C1-C6-C5	-3.24	116.47	119.62
8	M	1010	SPO	C6-C7-C9	-3.24	113.92	119.01
4	S	2003	BCL	C4-C3-C5	3.23	120.83	115.23
4	S	2001	BCL	CAA-C2A-C3A	-3.21	104.32	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1001	BCL	CBB-CAB-C3B	3.19	127.12	120.40
5	S	2005	BPH	C4-C3-C5	3.18	119.87	116.13
4	L	1002	BCL	OB B-CAB-CBB	-3.17	112.66	119.77
4	L	1004	BCL	O2A-C1-C2	-3.17	95.91	108.11
4	L	1002	BCL	CBB-CAB-C3B	3.17	127.08	120.40
6	S	2008	U10	O2-C2-C3	-3.14	114.37	121.03
4	S	2001	BCL	OB B-CAB-CBB	-3.14	112.74	119.77
4	S	2004	BCL	C16-C15-C13	-3.13	105.57	115.97
5	S	2005	BPH	CMA-C3A-C4A	-3.12	107.88	114.61
4	S	2004	BCL	C1-C2-C3	-3.12	121.09	126.20
6	M	1008	U10	O2-C2-C3	-3.12	114.43	121.03
4	L	1004	BCL	C2C-C3C-C4C	3.11	106.00	101.34
4	S	2004	BCL	CAC-C3C-C4C	-3.10	105.69	112.58
6	L	1009[B]	U10	C1-C6-C5	-3.09	116.61	119.62
5	M	1005	BPH	C4D-CHA-CBD	-3.09	106.97	108.45
5	S	2005	BPH	C4C-C3C-C2C	3.09	105.78	102.84
4	S	2001	BCL	CBB-CAB-C3B	3.08	126.89	120.40
4	S	2004	BCL	CHA-C1A-NA	-3.06	119.47	126.39
4	L	1004	BCL	C11-C12-C13	-3.05	105.83	115.97
4	S	2004	BCL	C2C-C3C-C4C	3.04	105.90	101.34
5	R	2006	BPH	CMA-C3A-C4A	-3.03	108.09	114.61
4	M	1003	BCL	CHA-C1A-NA	-3.01	119.56	126.39
6	M	1008	U10	C20-C19-C21	-3.01	110.00	115.23
5	L	1006	BPH	C4C-C3C-C2C	3.01	105.70	102.84
4	M	1003	BCL	CBA-CAA-C2A	2.99	122.69	113.79
4	L	1002	BCL	O1D-CGD-CBD	2.97	130.38	124.52
4	R	2002	BCL	CHD-C1D-ND	-2.96	120.64	124.80
8	S	2010	SPO	C20-C19-C17	-2.95	123.14	127.28
4	S	2003	BCL	CAA-CBA-CGA	-2.94	104.85	113.21
5	L	1006	BPH	C7-C6-C5	-2.93	105.45	113.26
5	L	1006	BPH	CMA-C3A-C4A	-2.91	108.35	114.61
6	R	2009[A]	U10	C1-C6-C5	-2.89	116.81	119.62
8	M	1010	SPO	C10-C9-C7	-2.88	123.24	127.28
4	S	2003	BCL	CHA-C1A-NA	-2.87	119.89	126.39
4	S	2001	BCL	CHD-C1D-ND	-2.87	120.77	124.80
4	R	2002	BCL	CAA-C2A-C3A	-2.87	105.25	113.00
4	L	1002	BCL	C16-C15-C13	-2.87	106.44	115.97
6	R	2009[B]	U10	C1-C6-C5	-2.85	116.85	119.62
4	R	2002	BCL	CAC-C3C-C4C	-2.84	106.27	112.58
4	L	1001	BCL	CHA-C1A-NA	-2.84	119.95	126.39
6	L	1009[B]	U10	C20-C19-C21	-2.84	110.31	115.23
5	S	2005	BPH	C2B-C1B-NB	2.83	111.48	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1006	BPH	CMB-C2B-C3B	2.83	130.34	124.68
4	R	2002	BCL	CHA-C1A-NA	-2.83	119.98	126.39
9	M	1011	LDA	O1-N1-C1	2.82	116.20	109.27
5	R	2006	BPH	C4C-C3C-C2C	2.82	105.52	102.84
8	S	2010	SPO	C18-C17-C19	-2.82	118.25	122.82
4	S	2001	BCL	CBA-CAA-C2A	2.78	122.06	113.79
4	L	1002	BCL	CHA-C1A-NA	-2.78	120.10	126.39
5	M	1005	BPH	C1B-NB-C4B	-2.77	104.78	108.82
4	L	1002	BCL	C4D-C3D-CAD	-2.76	105.10	108.11
4	L	1001	BCL	CHD-C1D-ND	-2.76	120.92	124.80
4	L	1004	BCL	CHD-C1D-ND	-2.76	120.92	124.80
4	M	1003	BCL	CBC-CAC-C3C	-2.76	107.56	113.41
4	S	2001	BCL	CHA-C1A-NA	-2.75	120.15	126.39
6	L	1009[A]	U10	C20-C19-C21	-2.74	110.46	115.23
4	L	1002	BCL	CHD-C1D-ND	-2.74	120.94	124.80
5	M	1005	BPH	CMB-C2B-C3B	2.74	130.15	124.68
4	M	1003	BCL	CHD-C1D-ND	-2.73	120.96	124.80
6	S	2008	U10	C1-C6-C5	-2.73	116.97	119.62
5	L	1006	BPH	C2B-C1B-NB	2.72	111.40	109.43
4	L	1002	BCL	CAC-C3C-C4C	-2.72	106.54	112.58
4	S	2003	BCL	C4D-C3D-CAD	-2.72	105.15	108.11
5	M	1005	BPH	CAA-C2A-C3A	-2.71	105.68	113.00
4	L	1002	BCL	C11-C12-C13	-2.69	107.01	115.97
4	R	2002	BCL	C1-C2-C3	-2.69	121.79	126.20
6	L	1009[B]	U10	C17-C18-C19	2.68	133.76	127.62
5	M	1005	BPH	C2B-C1B-NB	2.67	111.36	109.43
6	L	1009[B]	U10	C16-C14-C13	2.67	127.15	121.17
6	L	1009[A]	U10	C16-C14-C13	2.65	127.12	121.17
6	S	2008	U10	C20-C19-C21	-2.64	110.64	115.23
4	S	2004	BCL	CHD-C1D-ND	-2.64	121.08	124.80
4	M	1003	BCL	CGD-CBD-CAD	-2.64	102.31	110.85
4	L	1004	BCL	CHA-C1A-NA	-2.64	120.42	126.39
5	M	1005	BPH	O2A-CGA-O1A	-2.63	117.04	123.63
4	S	2003	BCL	CHD-C1D-ND	-2.63	121.10	124.80
4	S	2003	BCL	CBC-CAC-C3C	-2.63	107.83	113.41
5	R	2006	BPH	CMB-C2B-C3B	2.63	129.93	124.68
4	R	2002	BCL	O1D-CGD-CBD	2.62	129.69	124.52
4	L	1002	BCL	CAA-C2A-C3A	-2.62	105.92	113.00
5	R	2006	BPH	O2A-CGA-O1A	-2.60	117.12	123.63
4	R	2002	BCL	O2D-CGD-CBD	-2.59	106.71	111.23
6	L	1009[A]	U10	C8-C7-C6	2.58	118.45	112.08
5	S	2005	BPH	CAA-C2A-C3A	-2.58	106.03	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1006	BPH	O2A-CGA-O1A	-2.58	117.18	123.63
5	S	2005	BPH	C1B-NB-C4B	-2.57	105.08	108.82
6	L	1009[A]	U10	C7-C6-C5	-2.55	115.55	118.52
4	S	2004	BCL	C4D-C3D-CAD	-2.55	105.34	108.11
5	L	1006	BPH	OBD-CAD-CBD	-2.54	122.09	125.82
6	S	2008	U10	C17-C18-C19	2.54	133.44	127.62
4	R	2002	BCL	C4D-C3D-CAD	-2.54	105.35	108.11
5	M	1005	BPH	C4C-C3C-C2C	2.54	105.25	102.84
6	M	1008	U10	C1-C6-C5	-2.52	117.17	119.62
5	M	1005	BPH	CMD-C2D-C3D	2.49	129.67	124.68
4	S	2004	BCL	C7-C6-C5	-2.49	106.64	113.26
5	S	2005	BPH	CMB-C2B-C3B	2.48	129.64	124.68
5	R	2006	BPH	C7-C6-C5	-2.48	106.65	113.26
8	M	1010	SPO	C20-C19-C17	-2.48	123.80	127.28
5	R	2006	BPH	C1B-NB-C4B	-2.48	105.21	108.82
4	S	2001	BCL	C4D-C3D-CAD	-2.47	105.42	108.11
4	S	2003	BCL	C2C-C3C-C4C	2.46	105.02	101.34
6	S	2008	U10	C16-C14-C13	2.45	126.66	121.17
6	S	2008	U10	C6-C1-C2	2.43	121.09	119.17
5	L	1006	BPH	CMA-C3A-C2A	-2.43	104.75	114.13
4	S	2001	BCL	CAC-C3C-C4C	-2.42	107.21	112.58
6	L	1009[A]	U10	C17-C18-C19	2.42	133.17	127.62
4	L	1002	BCL	C2C-C3C-C4C	2.42	104.96	101.34
6	M	1008	U10	C6-C1-C2	2.42	121.08	119.17
5	M	1005	BPH	OBD-CAD-CBD	-2.42	122.28	125.82
4	R	2002	BCL	C16-C15-C13	-2.41	107.95	115.97
5	L	1006	BPH	CAA-C2A-C3A	-2.40	106.51	113.00
4	M	1003	BCL	C2C-C3C-C4C	2.39	104.92	101.34
4	M	1003	BCL	C11-C10-C8	-2.39	108.02	115.97
4	L	1002	BCL	C12-C11-C10	-2.37	102.65	113.28
4	S	2001	BCL	C1-C2-C3	-2.36	122.94	126.76
4	S	2003	BCL	CGD-CBD-CAD	-2.36	103.21	110.85
4	R	2002	BCL	CBC-CAC-C3C	-2.35	108.43	113.41
4	M	1003	BCL	C4D-C3D-CAD	-2.34	105.56	108.11
5	S	2005	BPH	CMD-C2D-C3D	2.34	129.35	124.68
6	R	2009[A]	U10	C6-C1-C2	2.34	121.01	119.17
4	M	1003	BCL	CHD-C1D-C2D	2.33	130.34	125.49
6	R	2009[B]	U10	C6-C1-C2	2.32	121.00	119.17
4	S	2003	BCL	CAA-C2A-C3A	-2.32	106.73	113.00
4	L	1004	BCL	C4D-C3D-CAD	-2.31	105.59	108.11
4	L	1004	BCL	C12-C11-C10	-2.30	102.95	113.28
4	S	2003	BCL	CHD-C1D-C2D	2.29	130.25	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1005	BPH	C4A-C3A-C2A	2.29	105.01	102.84
5	M	1005	BPH	CMA-C3A-C2A	-2.28	105.31	114.13
5	R	2006	BPH	CAA-C2A-C3A	-2.28	106.84	113.00
4	S	2004	BCL	CMD-C2D-C3D	2.28	132.91	127.69
4	R	2002	BCL	C2C-C3C-C4C	2.27	104.74	101.34
4	L	1002	BCL	CMA-C3A-C2A	-2.26	105.22	113.98
5	S	2005	BPH	OBD-CAD-CBD	-2.25	122.53	125.82
4	R	2002	BCL	CHD-C1D-C2D	2.24	130.15	125.49
6	R	2009[A]	U10	C4-C3-C2	-2.24	116.59	120.69
5	S	2005	BPH	O2A-CGA-O1A	-2.23	118.04	123.63
4	L	1001	BCL	C4D-C3D-CAD	-2.23	105.68	108.11
4	L	1001	BCL	CMD-C2D-C3D	2.22	132.78	127.69
5	R	2006	BPH	CMD-C2D-C3D	2.22	129.12	124.68
4	M	1003	BCL	O2A-CGA-O1A	-2.21	118.11	123.63
4	R	2002	BCL	C4-C3-C5	2.21	119.06	115.23
5	L	1006	BPH	C1B-NB-C4B	-2.20	105.61	108.82
4	M	1003	BCL	C7-C6-C5	-2.20	107.41	113.26
4	S	2001	BCL	CHD-C1D-C2D	2.19	130.05	125.49
4	S	2003	BCL	CAC-C3C-C4C	-2.19	107.73	112.58
5	M	1005	BPH	C7-C6-C5	-2.18	107.45	113.26
4	M	1003	BCL	CAC-C3C-C4C	-2.18	107.75	112.58
4	L	1002	BCL	CBC-CAC-C3C	-2.18	108.80	113.41
4	S	2003	BCL	C11-C10-C8	-2.18	108.73	115.97
4	M	1003	BCL	CAA-C2A-C3A	-2.17	107.13	113.00
6	R	2009[A]	U10	C7-C6-C5	-2.17	116.00	118.52
6	L	1009[A]	U10	C4-C3-C2	-2.16	116.72	120.69
8	M	1010	SPO	C1-C4-C5	2.16	118.58	112.98
8	M	1010	SPO	C5-C6-C7	-2.16	122.63	125.89
5	L	1006	BPH	CMD-C2D-C3D	2.15	128.97	124.68
6	S	2008	U10	C4-C3-C2	-2.14	116.76	120.69
6	M	1008	U10	C16-C14-C13	2.14	125.97	121.17
4	L	1004	BCL	CMD-C2D-C3D	2.14	132.60	127.69
4	S	2003	BCL	C7-C6-C5	-2.14	107.56	113.26
6	L	1009[A]	U10	C6-C1-C2	2.14	120.86	119.17
6	L	1009[B]	U10	C3-C2-C1	2.13	122.32	118.10
4	M	1003	BCL	O1D-CGD-CBD	2.13	128.73	124.52
4	S	2001	BCL	CAA-C2A-C1A	2.13	118.96	111.97
4	S	2003	BCL	C16-C15-C13	-2.13	108.89	115.97
4	S	2003	BCL	CBA-CAA-C2A	2.13	120.13	113.79
8	S	2010	SPO	C1-C4-C5	2.13	118.51	112.98
8	S	2010	SPO	C9-C10-C11	-2.12	117.06	123.20
4	M	1003	BCL	C16-C15-C13	-2.11	108.94	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1011	LDA	C9-C8-C7	-2.11	103.72	114.37
4	L	1001	BCL	C3D-C2D-C1D	-2.10	102.96	105.83
4	L	1002	BCL	CMD-C2D-C3D	2.09	132.49	127.69
4	L	1004	BCL	C16-C15-C13	-2.09	109.01	115.97
6	L	1009[B]	U10	C6-C1-C2	2.09	120.82	119.17
4	S	2004	BCL	C12-C11-C10	-2.09	103.92	113.28
6	M	1008	U10	C17-C18-C19	2.08	132.39	127.62
5	S	2005	BPH	C6-C5-C3	2.08	123.57	113.70
4	S	2001	BCL	CMD-C2D-C3D	2.08	132.45	127.69
9	M	1011	LDA	CM2-N1-C1	2.08	114.59	110.23
6	R	2009[B]	U10	C4-C3-C2	-2.07	116.89	120.69
6	M	1008	U10	C21-C19-C18	2.07	125.81	121.17
6	M	1008	U10	C3-C2-C1	2.06	122.17	118.10
5	R	2006	BPH	C2B-C1B-NB	2.05	110.91	109.43
4	M	1003	BCL	O2A-CGA-CBA	2.05	118.07	111.83
8	S	2010	SPO	C13-C12-C11	2.04	121.20	118.09
4	S	2003	BCL	O1D-CGD-CBD	2.04	128.53	124.52
4	S	2003	BCL	C12-C11-C10	-2.03	104.17	113.28
4	L	1002	BCL	CHD-C1D-C2D	2.03	129.71	125.49
8	S	2010	SPO	C27-C26-C25	-2.03	117.31	123.20
5	L	1006	BPH	C4A-C3A-C2A	2.03	104.77	102.84
6	M	1008	U10	C4-C3-C2	-2.03	116.97	120.69
4	M	1003	BCL	C3D-C2D-C1D	-2.03	103.06	105.83
6	R	2009[B]	U10	C1M-C1-C6	-2.03	121.12	124.45
6	S	2008	U10	C21-C19-C18	2.03	125.72	121.17
6	L	1009[B]	U10	C4-C3-C2	-2.02	116.98	120.69
5	R	2006	BPH	OBD-CAD-CBD	-2.02	122.86	125.82
4	S	2004	BCL	CHD-C1D-C2D	2.02	129.68	125.49
6	M	1008	U10	C31-C29-C30	-2.02	109.95	114.59
5	R	2006	BPH	C5-C3-C2	-2.01	116.65	121.17
4	L	1004	BCL	C7-C6-C5	-2.01	107.90	113.26
8	S	2010	SPO	O1-C1-C2	2.01	122.80	108.97
6	L	1009[B]	U10	C7-C8-C9	2.00	130.28	126.83

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1006	BPH	C13
5	L	1006	BPH	C8
5	M	1005	BPH	C8
5	R	2006	BPH	C13
5	R	2006	BPH	C8

All (143) 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	S	2001	BCL	C1A-C2A-CAA-CBA
5	L	1006	BPH	C4C-C3C-CAC-CBC
5	R	2006	BPH	CBD-CGD-O2D-CED
5	S	2005	BPH	C1-C2-C3-C5
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	M	1010	SPO	C36-C37-C38-C40
8	S	2010	SPO	C3-C1-O1-CM1
8	S	2010	SPO	C4-C5-C6-C7
8	S	2010	SPO	C36-C37-C38-C39
8	S	2010	SPO	C36-C37-C38-C40
5	S	2005	BPH	CBD-CGD-O2D-CED
5	R	2006	BPH	O1D-CGD-O2D-CED
4	R	2002	BCL	C4-C3-C5-C6
4	R	2002	BCL	C2-C3-C5-C6
5	M	1005	BPH	CBD-CGD-O2D-CED
4	M	1003	BCL	C4-C3-C5-C6
4	S	2003	BCL	C4-C3-C5-C6
6	L	1009[B]	U10	C9-C11-C12-C13
6	L	1009[B]	U10	C14-C16-C17-C18
6	M	1008	U10	C24-C26-C27-C28
8	M	1010	SPO	C33-C35-C36-C37
4	M	1003	BCL	C2-C3-C5-C6
4	S	2003	BCL	C2-C3-C5-C6
4	S	2003	BCL	C15-C16-C17-C18
8	S	2010	SPO	C33-C35-C36-C37
5	L	1006	BPH	C8-C10-C11-C12
5	L	1006	BPH	C10-C11-C12-C13
5	S	2005	BPH	O1D-CGD-O2D-CED
5	R	2006	BPH	C10-C11-C12-C13
4	L	1002	BCL	C15-C16-C17-C18
5	M	1005	BPH	O1D-CGD-O2D-CED
5	S	2005	BPH	O2A-C1-C2-C3
5	R	2006	BPH	C8-C10-C11-C12
4	S	2001	BCL	C3A-C2A-CAA-CBA
4	M	1003	BCL	C3-C5-C6-C7
9	M	1011	LDA	C4-C5-C6-C7
8	M	1010	SPO	C1-C4-C5-C6
8	S	2010	SPO	C1-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	M	1005	BPH	C4-C3-C5-C6
5	L	1006	BPH	C2C-C3C-CAC-CBC
4	L	1004	BCL	C2A-CAA-CBA-CGA
4	S	2004	BCL	C1A-C2A-CAA-CBA
4	M	1003	BCL	C11-C10-C8-C7
4	S	2003	BCL	C11-C10-C8-C7
4	S	2004	BCL	C12-C13-C15-C16
5	R	2006	BPH	C12-C13-C15-C16
5	R	2006	BPH	C14-C13-C15-C16
5	M	1005	BPH	C2-C3-C5-C6
4	S	2004	BCL	C15-C16-C17-C18
5	L	1006	BPH	O2A-C1-C2-C3
5	M	1005	BPH	O2A-C1-C2-C3
5	R	2006	BPH	O2A-C1-C2-C3
4	S	2003	BCL	C13-C15-C16-C17
4	S	2003	BCL	C11-C12-C13-C14
4	S	2004	BCL	C14-C13-C15-C16
4	L	1002	BCL	C12-C13-C15-C16
4	R	2002	BCL	C12-C13-C15-C16
4	S	2003	BCL	C11-C12-C13-C15
5	L	1006	BPH	C12-C13-C15-C16
8	M	1010	SPO	C19-C20-C21-C22
6	L	1009[A]	U10	C14-C16-C17-C18
8	S	2010	SPO	C20-C21-C22-C23
9	M	1011	LDA	C2-C3-C4-C5
5	M	1005	BPH	C5-C6-C7-C8
9	M	1011	LDA	C1-C2-C3-C4
6	S	2008	U10	C5-C4-O4-C4M
6	L	1009[A]	U10	C12-C11-C9-C10
6	L	1009[A]	U10	C15-C14-C16-C17
6	L	1009[A]	U10	C5-C6-C7-C8
4	L	1004	BCL	C11-C10-C8-C9
4	R	2002	BCL	C14-C13-C15-C16
5	L	1006	BPH	C14-C13-C15-C16
9	M	1011	LDA	C2-C1-N1-CM1
9	M	1011	LDA	C2-C1-N1-CM2
6	L	1009[A]	U10	C13-C14-C16-C17
5	S	2005	BPH	C2-C3-C5-C6
4	L	1004	BCL	C11-C10-C8-C7
4	M	1003	BCL	C11-C12-C13-C15
4	S	2004	BCL	C11-C10-C8-C7
4	S	2004	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
4	S	2003	BCL	C3-C5-C6-C7
4	L	1002	BCL	C14-C13-C15-C16
4	S	2004	BCL	C11-C10-C8-C9
9	M	1011	LDA	C2-C1-N1-O1
8	S	2010	SPO	C4-C1-O1-CM1
4	L	1004	BCL	CHA-CBD-CGD-O2D
6	L	1009[A]	U10	C12-C11-C9-C8
8	M	1010	SPO	C20-C21-C22-C23
4	L	1004	BCL	C13-C15-C16-C17
4	S	2004	BCL	C11-C12-C13-C14
6	S	2008	U10	C20-C19-C21-C22
6	L	1009[B]	U10	C2-C3-O3-C3M
8	M	1010	SPO	C17-C19-C20-C21
4	M	1003	BCL	C11-C12-C13-C14
5	R	2006	BPH	C16-C17-C18-C20
6	S	2008	U10	C21-C22-C23-C24
4	S	2003	BCL	C5-C6-C7-C8
4	R	2002	BCL	C15-C16-C17-C18
6	S	2008	U10	C18-C19-C21-C22
8	M	1010	SPO	C18-C17-C19-C20
8	S	2010	SPO	C18-C17-C19-C20
9	M	1011	LDA	C6-C7-C8-C9
5	S	2005	BPH	C4-C3-C5-C6
6	L	1009[B]	U10	C15-C14-C16-C17
6	L	1009[A]	U10	C2-C3-O3-C3M
6	M	1008	U10	C5-C4-O4-C4M
4	M	1003	BCL	C11-C10-C8-C9
4	S	2003	BCL	C11-C10-C8-C9
4	S	2001	BCL	C2B-C3B-CAB-OB
4	S	2001	BCL	C2B-C3B-CAB-CB
5	S	2005	BPH	C1-C2-C3-C4
4	M	1003	BCL	C13-C15-C16-C17
8	M	1010	SPO	C16-C17-C19-C20
8	S	2010	SPO	C16-C17-C19-C20
4	M	1003	BCL	C5-C6-C7-C8
4	L	1002	BCL	C2A-CAA-CBA-CGA
6	L	1009[B]	U10	C13-C14-C16-C17
6	M	1008	U10	C20-C19-C21-C22
4	R	2002	BCL	C8-C10-C11-C12
5	R	2006	BPH	C16-C17-C18-C19
5	S	2005	BPH	CHA-CBD-CGD-O1D
6	L	1009[A]	U10	C20-C19-C21-C22

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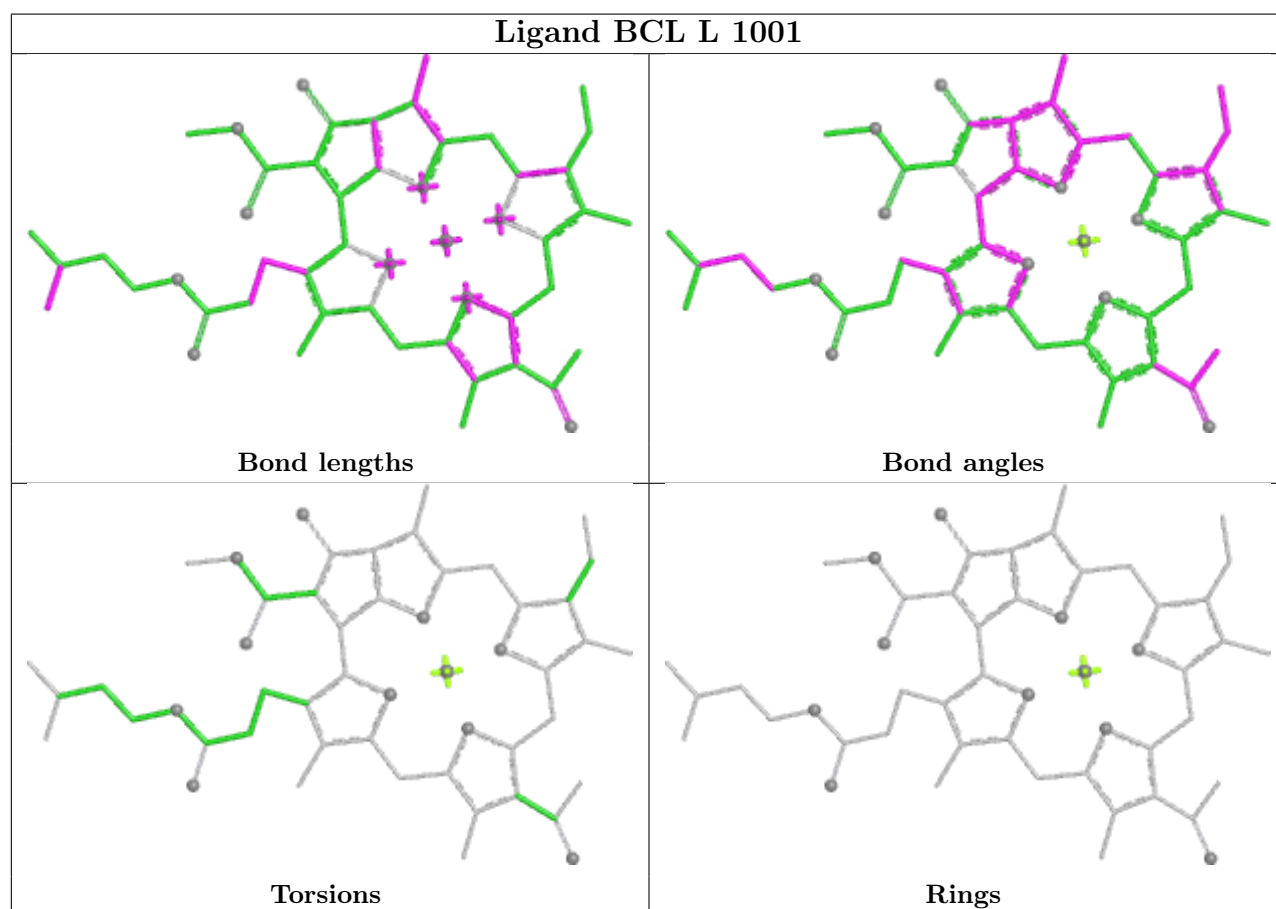
Mol	Chain	Res	Type	Atoms
8	S	2010	SPO	C17-C19-C20-C21
4	S	2001	BCL	C4B-C3B-CAB-OB
4	S	2001	BCL	C4B-C3B-CAB-CB
5	L	1006	BPH	C6-C7-C8-C9
4	S	2001	BCL	CAA-CBA-CGA-O2A
4	S	2004	BCL	C5-C6-C7-C8
5	S	2005	BPH	C2A-CAA-CBA-CGA
4	R	2002	BCL	C2A-CAA-CBA-CGA
8	S	2010	SPO	C30-C31-C32-C33
6	L	1009[A]	U10	C1-C6-C7-C8
4	S	2001	BCL	CAA-CBA-CGA-O1A
6	M	1008	U10	C14-C16-C17-C18
8	M	1010	SPO	C30-C31-C32-C33
4	L	1004	BCL	CAD-CBD-CGD-O2D
8	M	1010	SPO	C4-C1-O1-CM1
4	L	1004	BCL	C5-C6-C7-C8
6	R	2009[A]	U10	C2-C3-O3-C3M

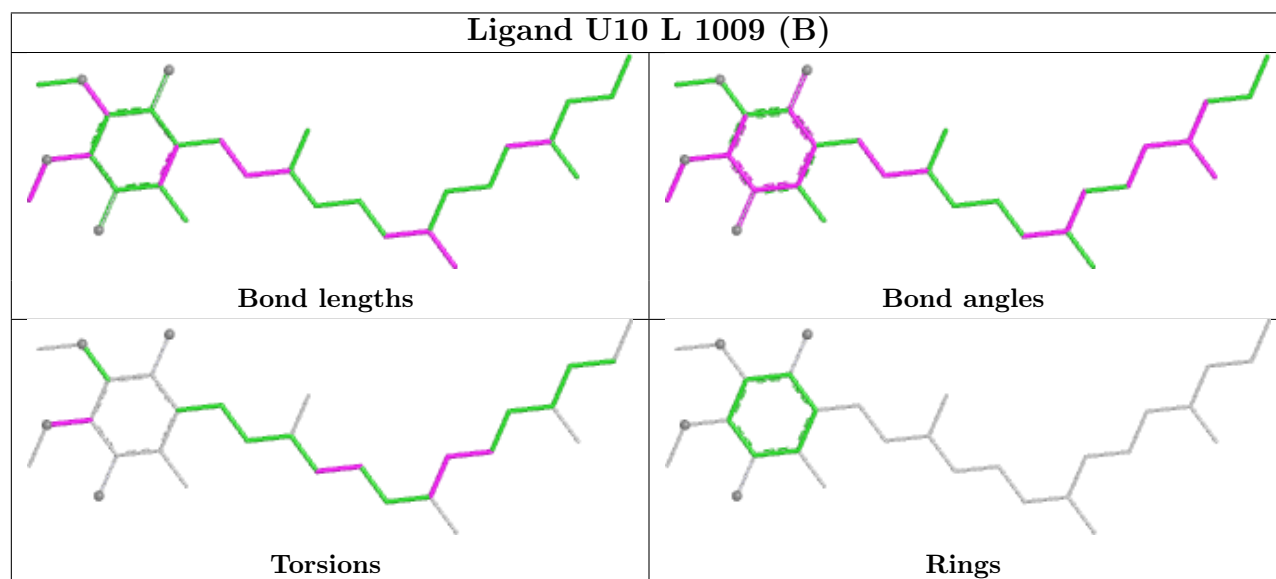
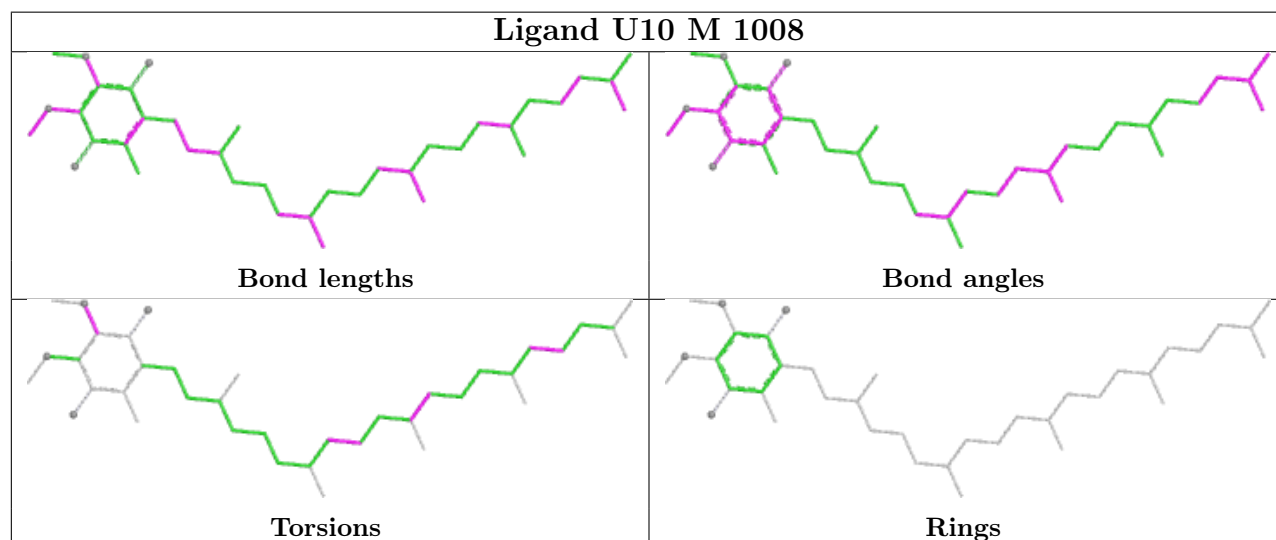
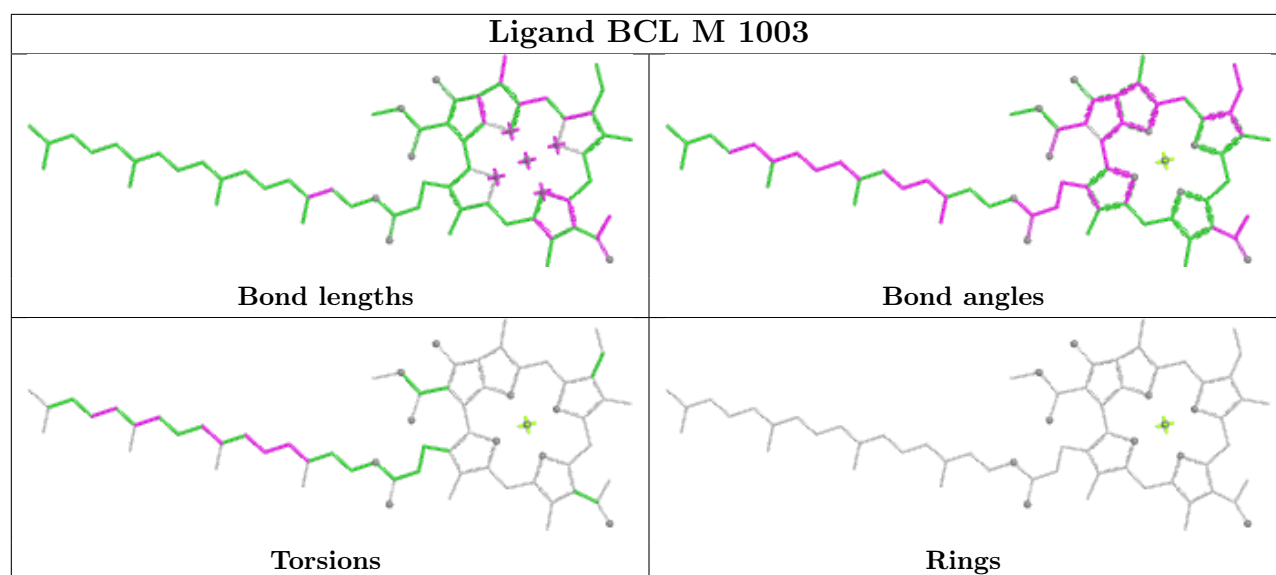
There are no ring outliers.

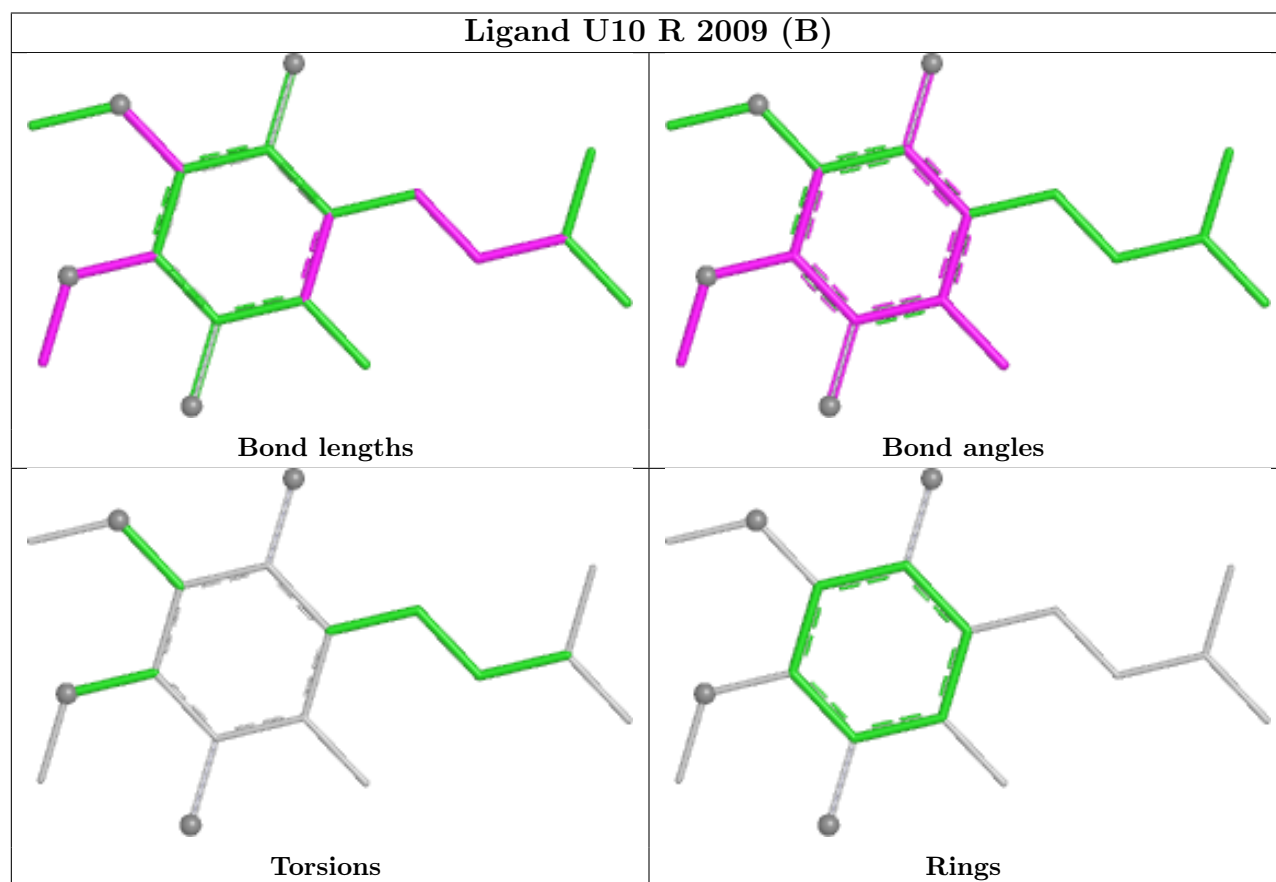
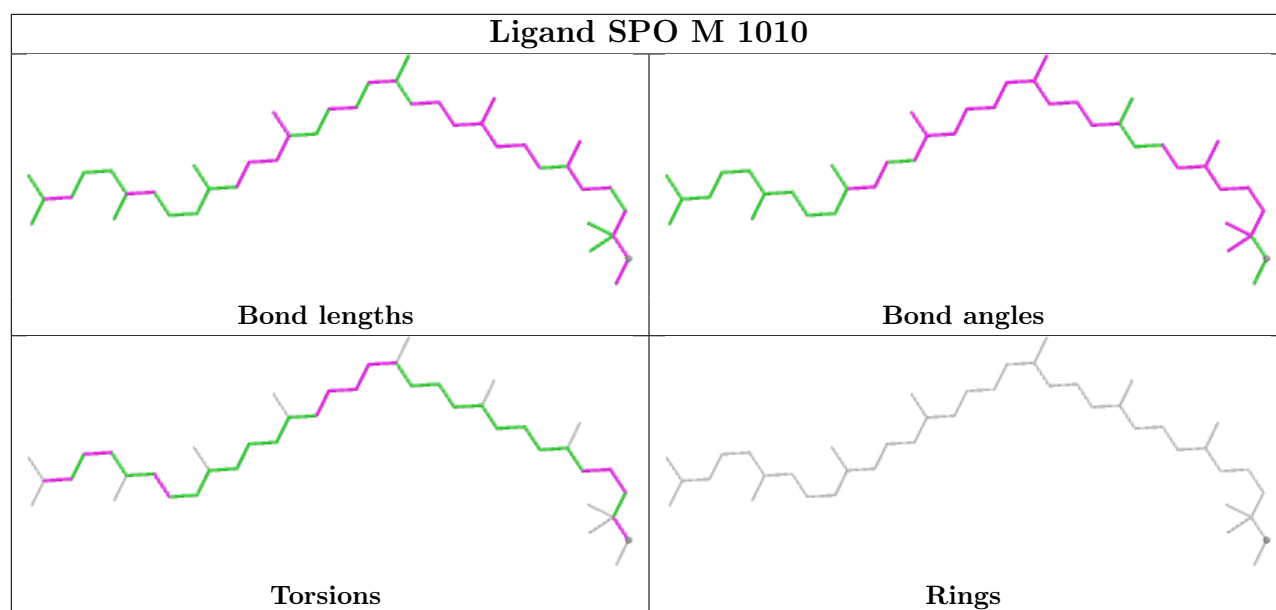
20 monomers are involved in 104 short contacts:

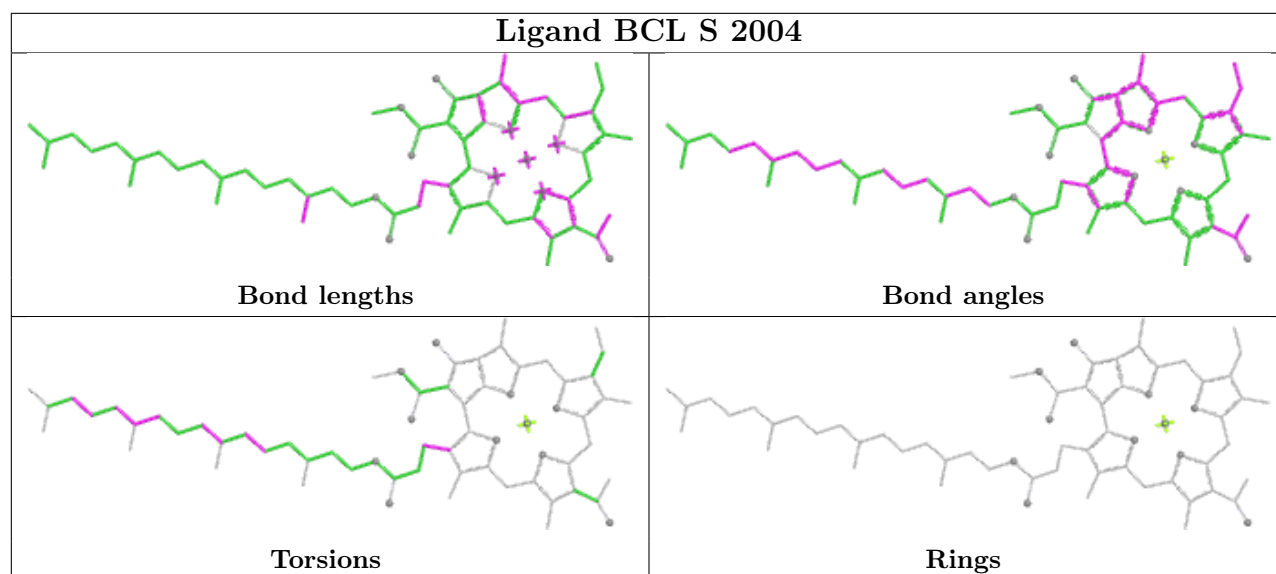
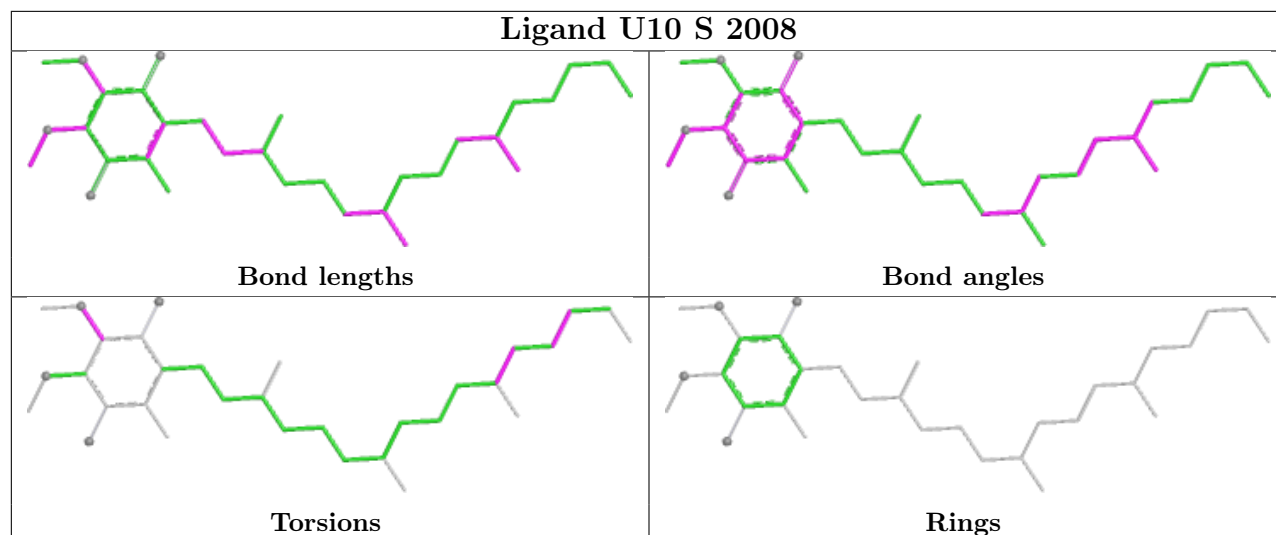
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1001	BCL	11	0
4	M	1003	BCL	21	0
6	L	1009[B]	U10	2	0
8	M	1010	SPO	6	0
6	R	2009[B]	U10	2	0
6	S	2008	U10	1	0
9	M	1011	LDA	2	0
4	S	2004	BCL	8	0
5	M	1005	BPH	1	0
4	L	1004	BCL	9	0
8	S	2010	SPO	2	0
5	R	2006	BPH	9	0
6	L	1009[A]	U10	1	0
6	R	2009[A]	U10	1	0
5	L	1006	BPH	5	0
4	S	2003	BCL	16	0
4	L	1002	BCL	11	0
4	R	2002	BCL	10	0
4	S	2001	BCL	8	0
5	S	2005	BPH	6	0

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

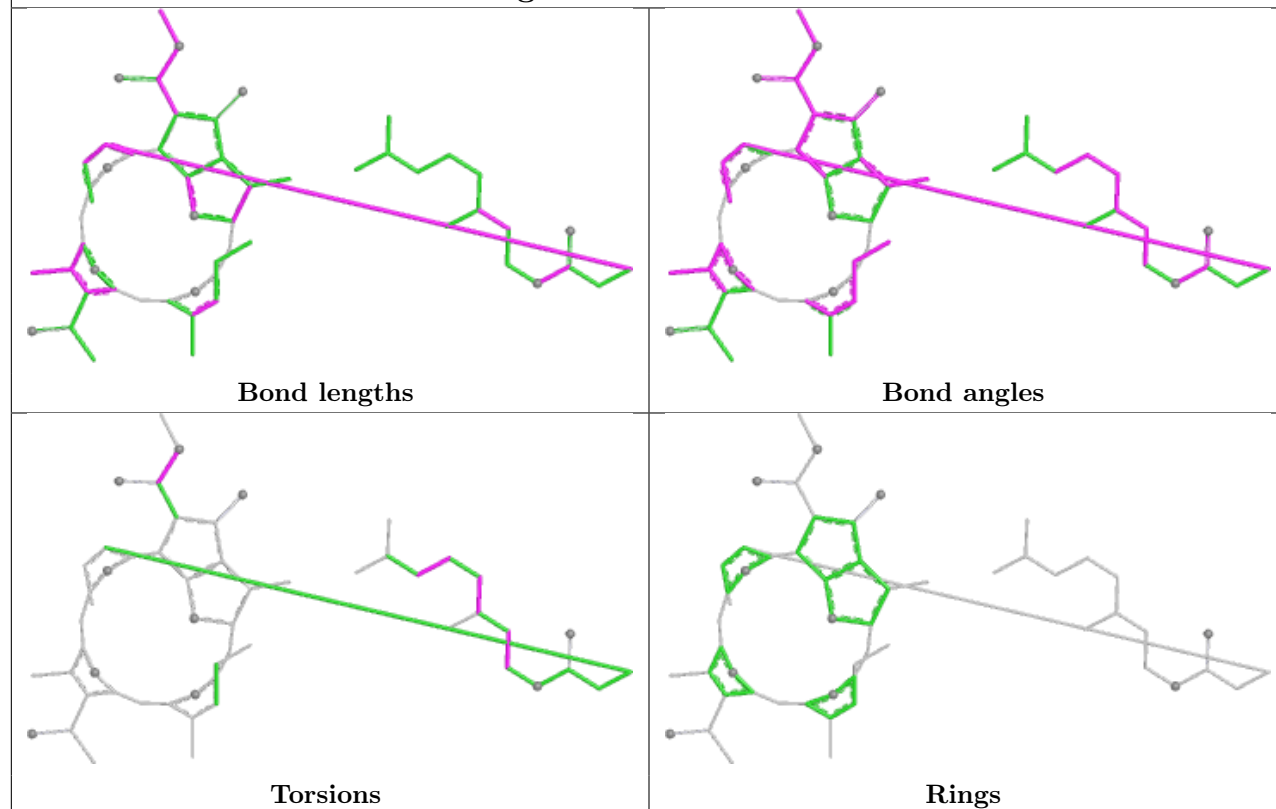




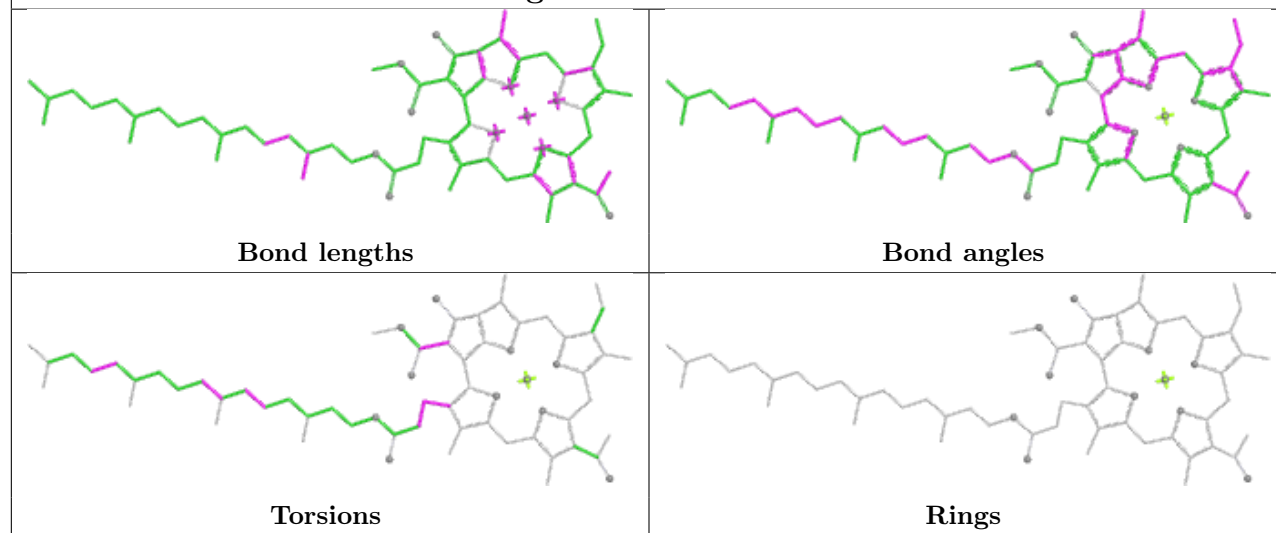


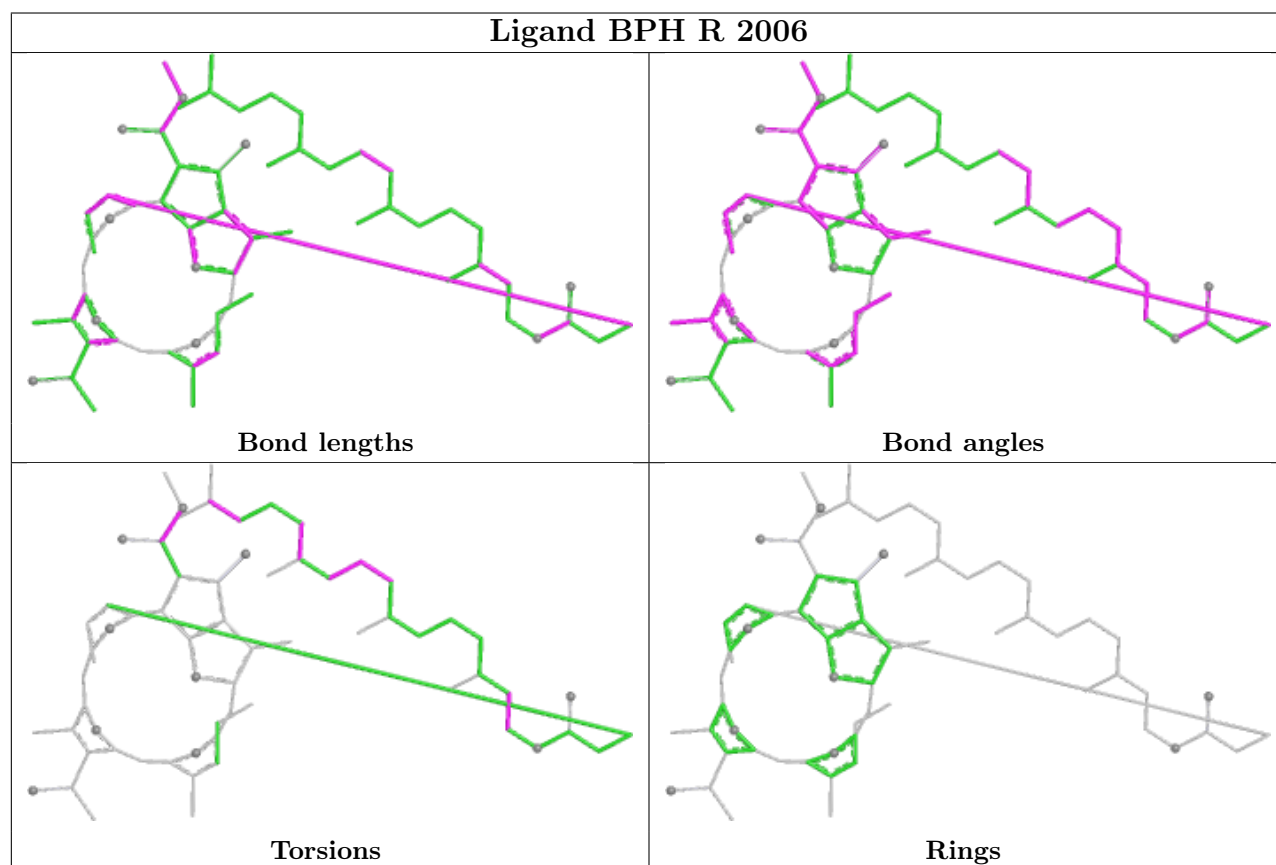
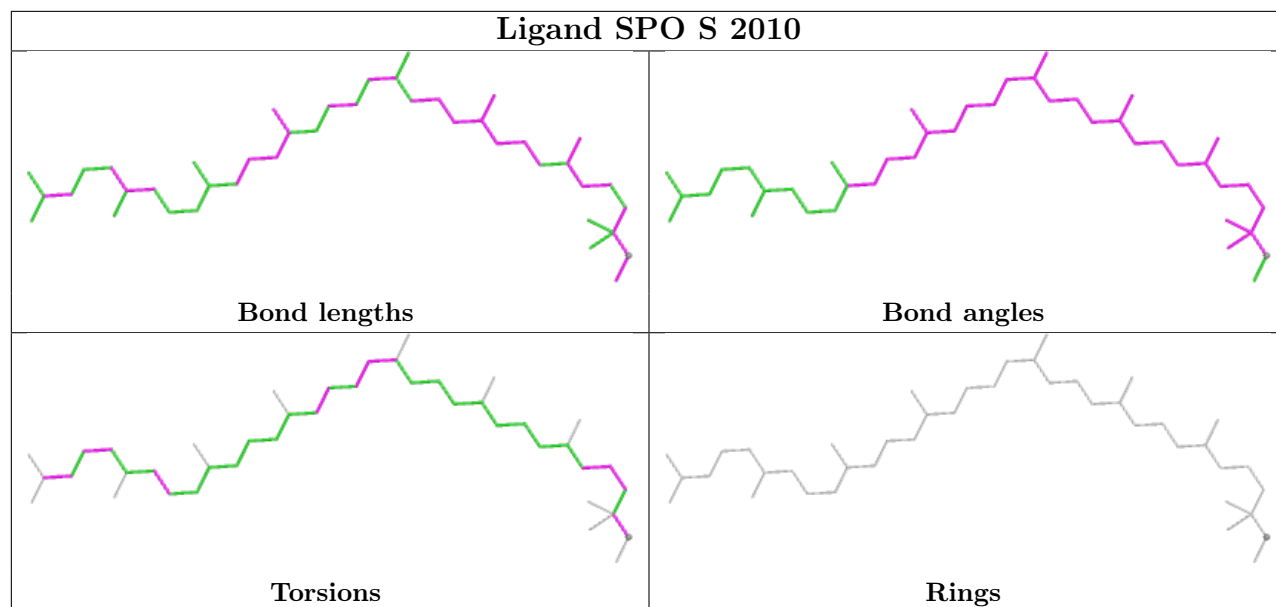


Ligand BPH M 1005

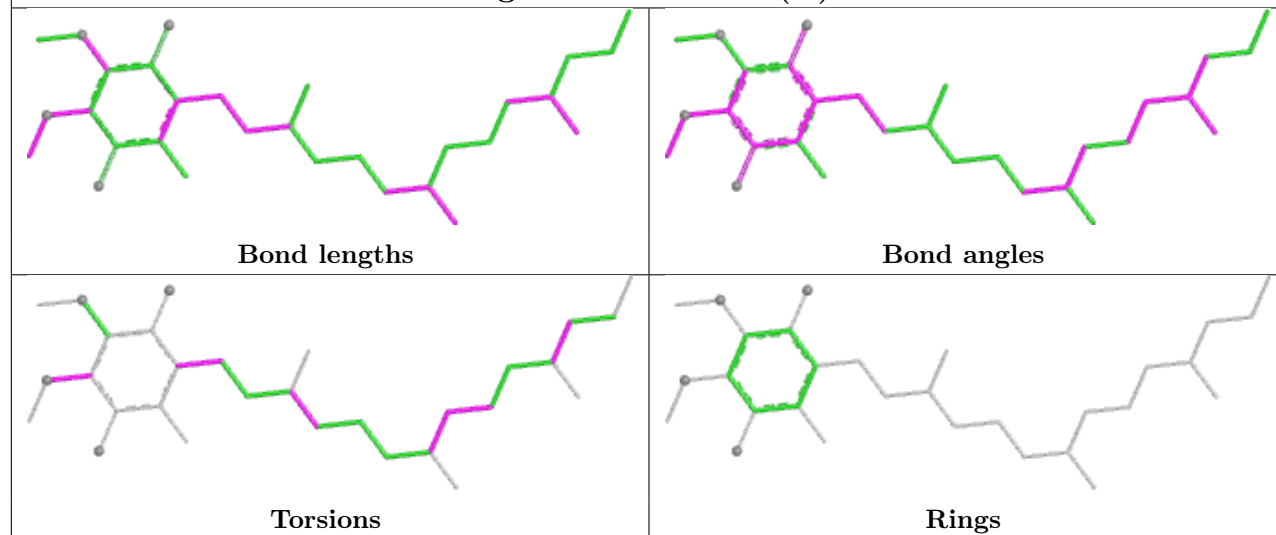


Ligand BCL L 1004

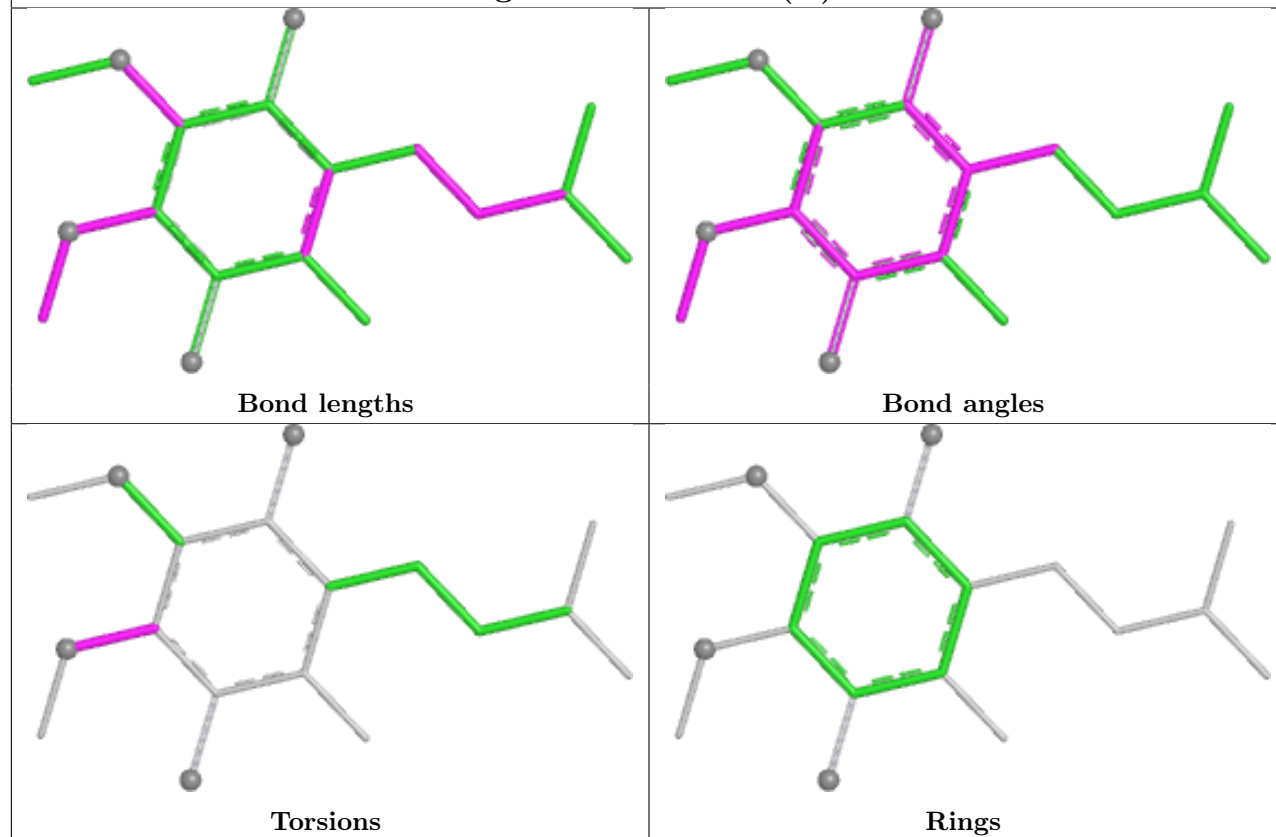


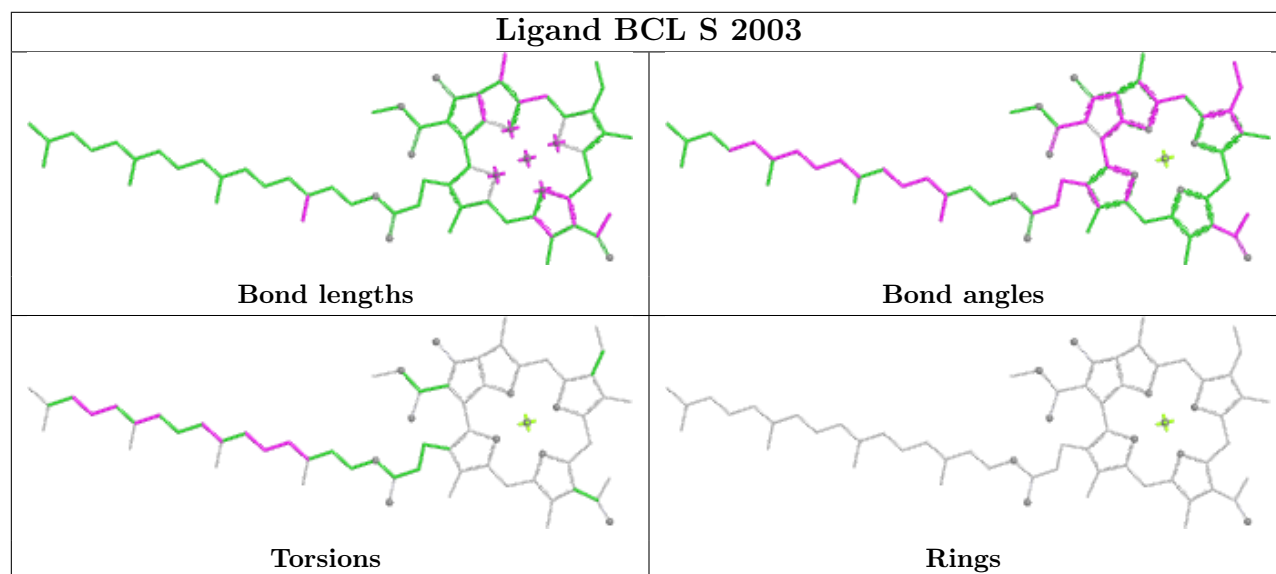
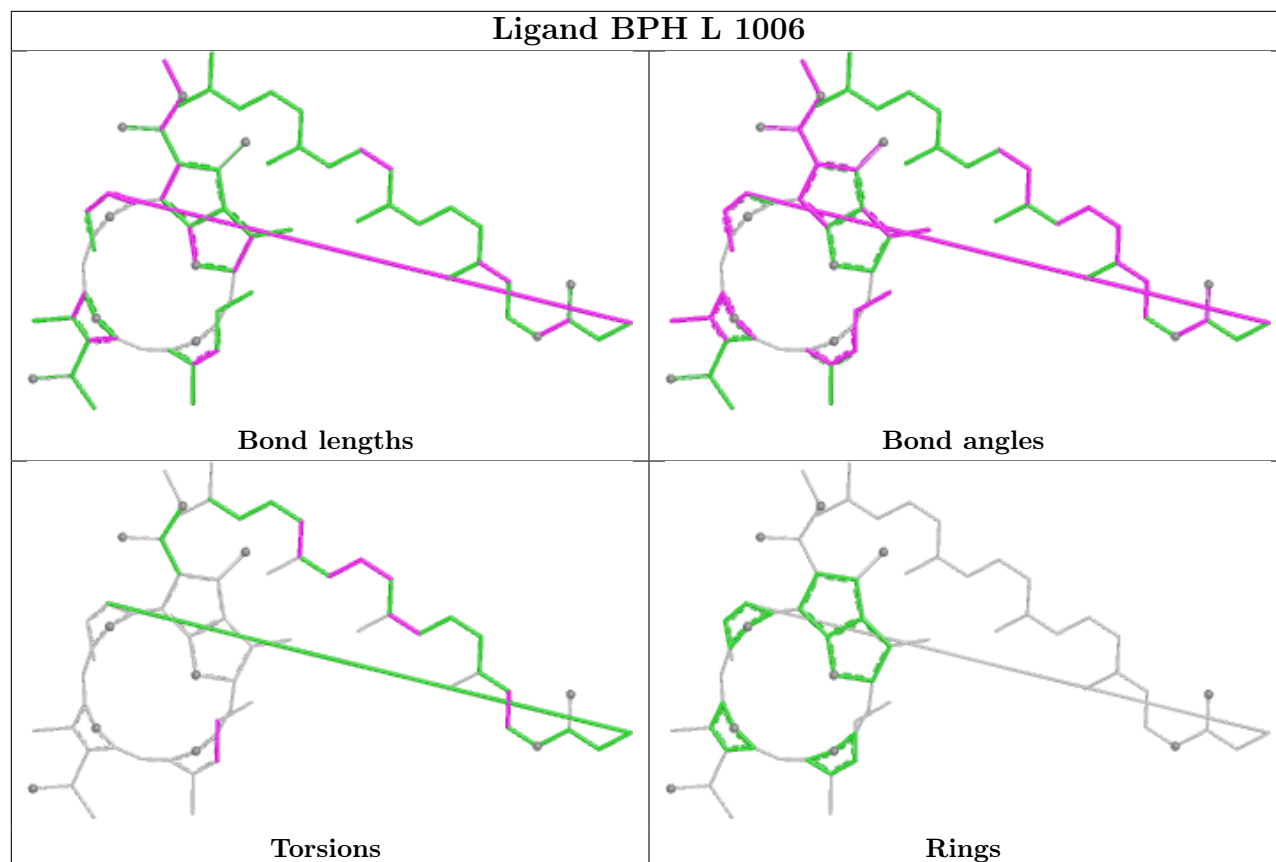


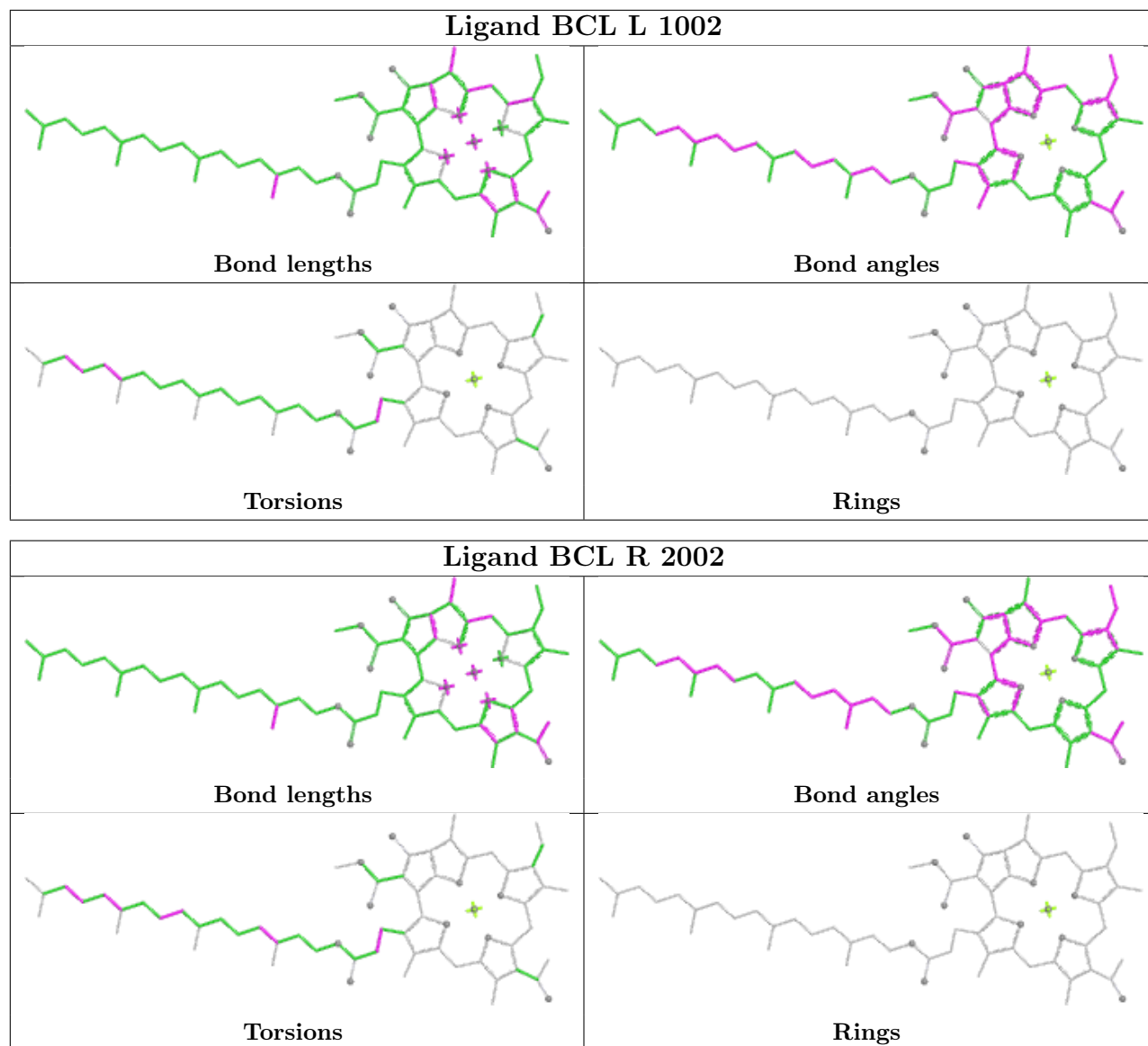
Ligand U10 L 1009 (A)

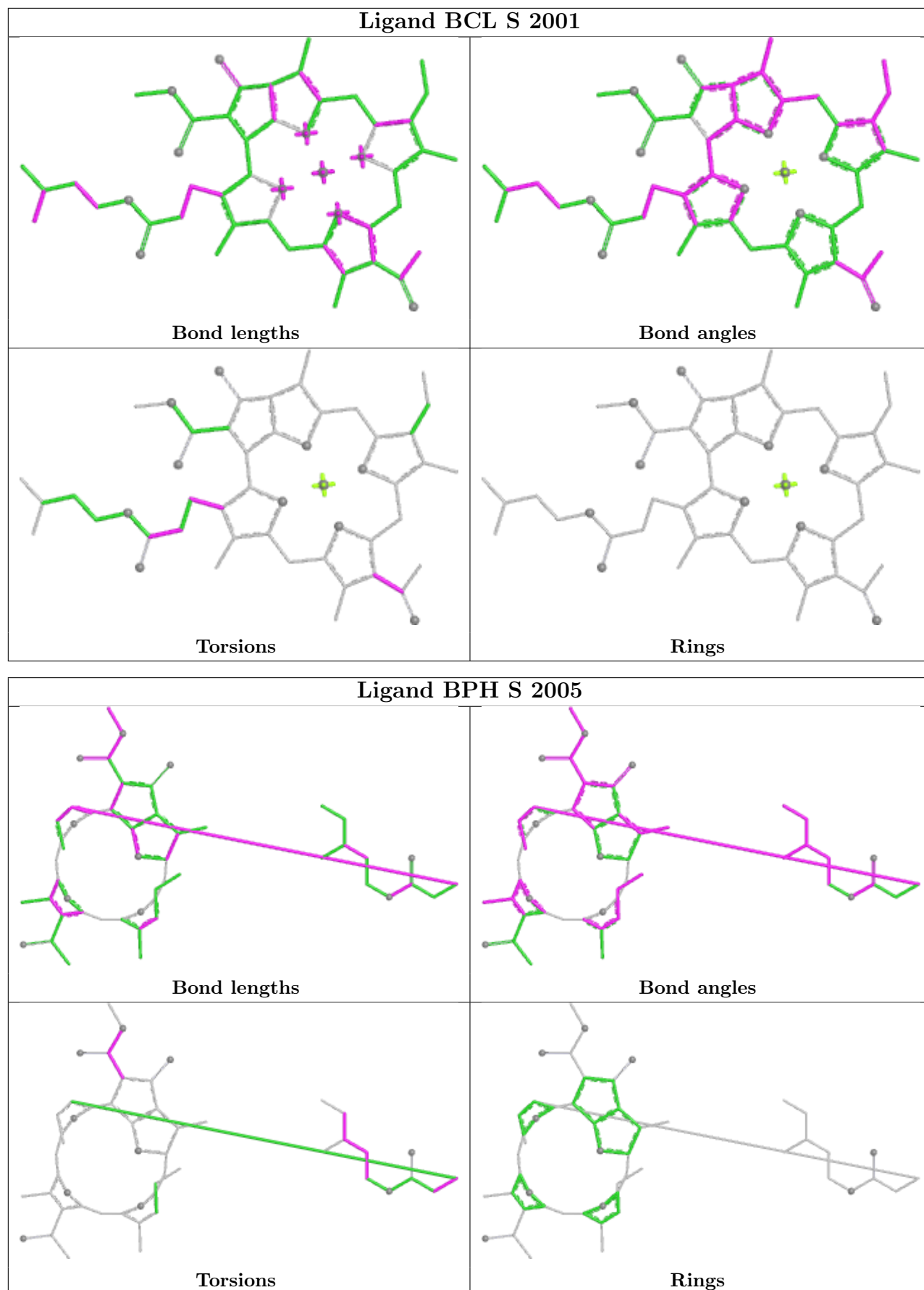


Ligand U10 R 2009 (A)









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%)	0.01	4 (1%) 73 69	23, 42, 61, 77	0
1	R	281/281 (100%)	0.42	7 (2%) 58 52	35, 56, 73, 82	0
2	M	301/307 (98%)	-0.18	3 (0%) 79 76	26, 38, 53, 85	0
2	S	299/307 (97%)	0.10	4 (1%) 75 71	37, 50, 59, 89	0
3	H	246/260 (94%)	0.02	4 (1%) 70 66	28, 44, 65, 97	0
3	T	246/260 (94%)	0.68	19 (7%) 19 15	47, 62, 84, 99	0
All	All	1654/1696 (97%)	0.16	41 (2%) 58 52	23, 49, 74, 99	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	1	ALA	5.1
2	M	1	ALA	4.0
2	M	301	HIS	3.9
3	H	256	LEU	3.6
3	T	254	ALA	3.6
3	T	256	LEU	3.4
3	T	55	PRO	3.1
3	T	78	PRO	3.1
3	T	90	THR	2.9
2	S	3	TYR	2.9
3	T	91	ALA	2.9
3	T	251	VAL	2.8
3	T	54	GLY	2.7
2	S	68	PHE	2.7
3	T	69	GLY	2.7
3	T	79	GLU	2.6
3	T	158	LEU	2.5
3	H	252	VAL	2.5
1	L	80	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	H	251	VAL	2.4
1	R	7	ARG	2.4
1	R	276	PRO	2.3
3	T	92	VAL	2.3
2	S	301	HIS	2.3
3	T	80	SER	2.3
1	L	7	ARG	2.3
2	M	4	GLN	2.3
1	R	10	ARG	2.2
1	L	161	GLY	2.2
1	R	80	LEU	2.2
3	H	253	ALA	2.2
1	R	3	LEU	2.2
3	T	38	GLU	2.2
3	T	73	LEU	2.2
2	S	248	ALA	2.1
1	R	25	TRP	2.1
3	T	49	PRO	2.1
1	L	57	GLY	2.1
3	T	253	ALA	2.1
3	T	95	GLY	2.0
3	T	108	GLY	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 oligosaccharides 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(Å ²)	Q<0.9
6	U10	L	1009[A]	30/63	0.68	0.50	54,67,69,70	30

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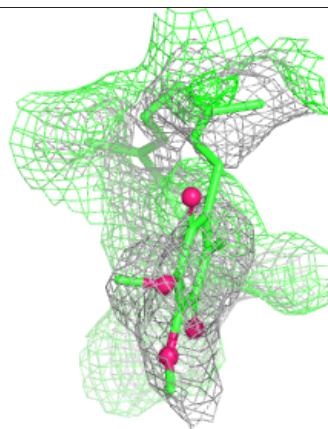
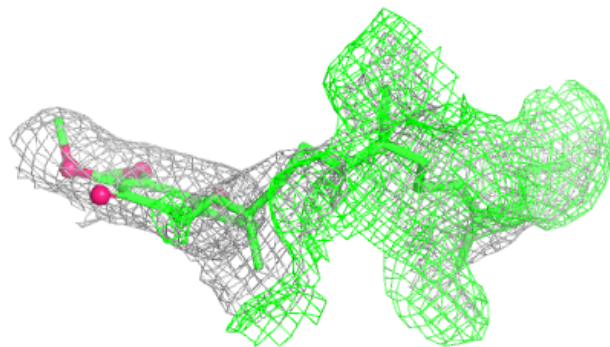
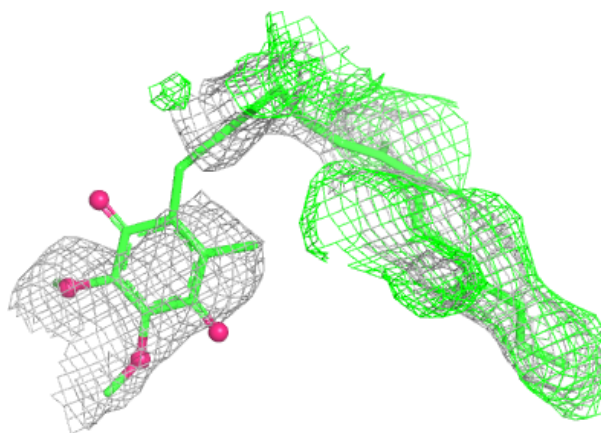
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	U10	L	1009[B]	30/63	0.68	0.50	44,54,65,66	30
6	U10	R	2009[A]	18/63	0.68	0.51	94,96,97,98	18
6	U10	R	2009[B]	18/63	0.68	0.51	95,96,97,97	18
9	LDA	M	1011	16/16	0.81	0.22	49,61,78,78	0
6	U10	S	2008	32/63	0.87	0.16	56,58,64,66	0
4	BCL	S	2001	51/66	0.87	0.15	38,45,58,61	0
4	BCL	S	2004	66/66	0.88	0.16	44,52,74,75	0
8	SPO	S	2010	42/42	0.89	0.16	38,49,64,66	0
4	BCL	R	2002	66/66	0.90	0.14	42,53,56,56	0
4	BCL	L	1001	51/66	0.90	0.12	26,32,45,48	0
4	BCL	S	2003	66/66	0.91	0.14	44,49,62,71	0
4	BCL	L	1002	66/66	0.91	0.13	31,36,44,52	0
8	SPO	M	1010	42/42	0.91	0.14	31,36,59,61	0
6	U10	M	1008	38/63	0.91	0.14	36,42,63,64	0
5	BPH	R	2006	65/65	0.91	0.13	47,56,61,62	0
4	BCL	L	1004	66/66	0.92	0.12	28,34,57,59	0
4	BCL	M	1003	66/66	0.92	0.12	24,38,47,49	0
5	BPH	M	1005	55/65	0.94	0.09	26,32,43,46	0
5	BPH	L	1006	65/65	0.94	0.10	24,35,41,43	0
5	BPH	S	2005	51/65	0.94	0.09	35,42,51,52	0
7	FE2	S	2007	1/1	0.99	0.02	51,51,51,51	0
7	FE2	M	1007	1/1	0.99	0.02	33,33,33,33	0

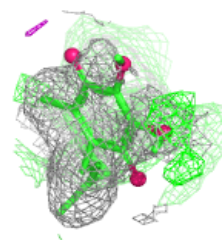
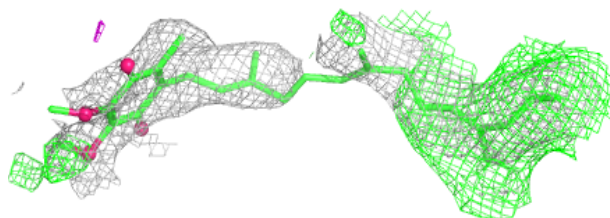
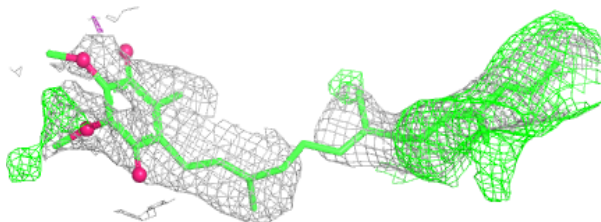
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U10 L 1009 (A):

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

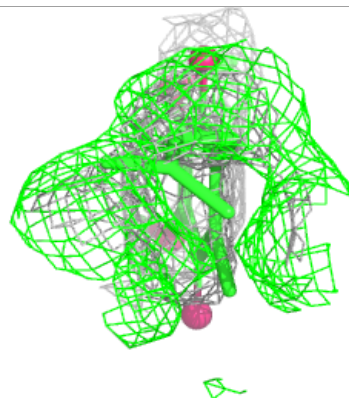
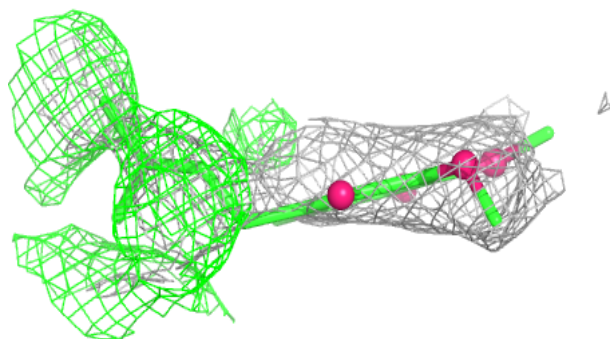
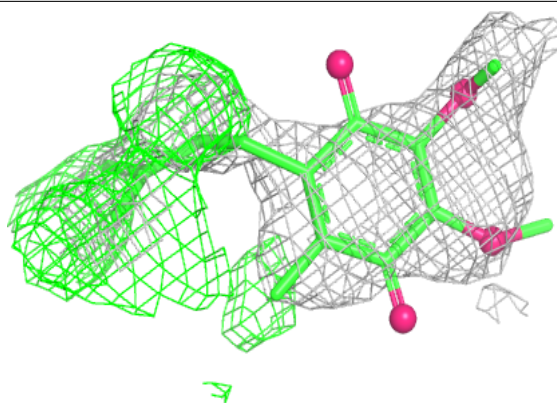
**Electron density around U10 L 1009 (B):**

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

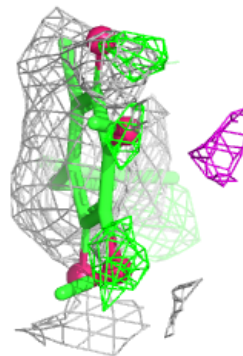
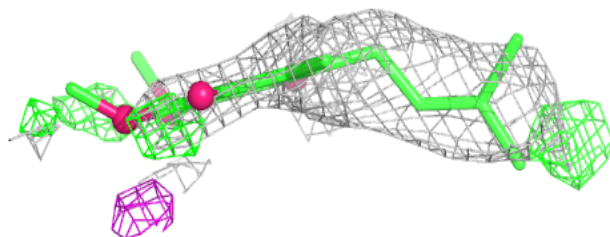
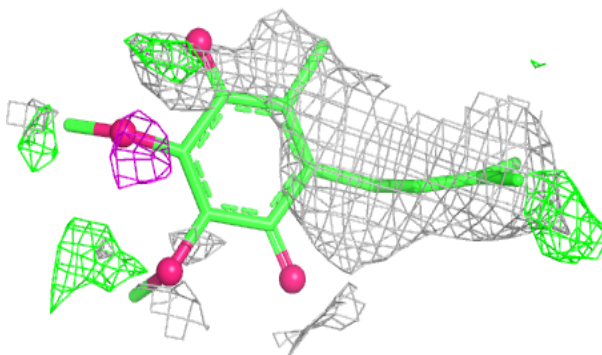


Electron density around U10 R 2009 (A):

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

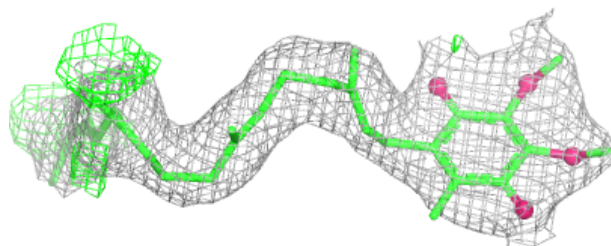
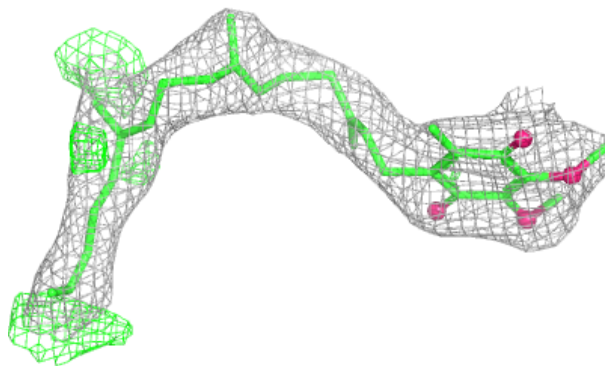
**Electron density around U10 R 2009 (B):**

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



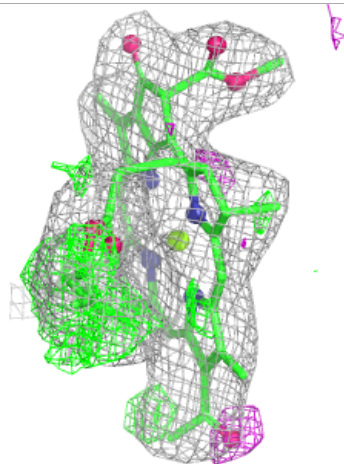
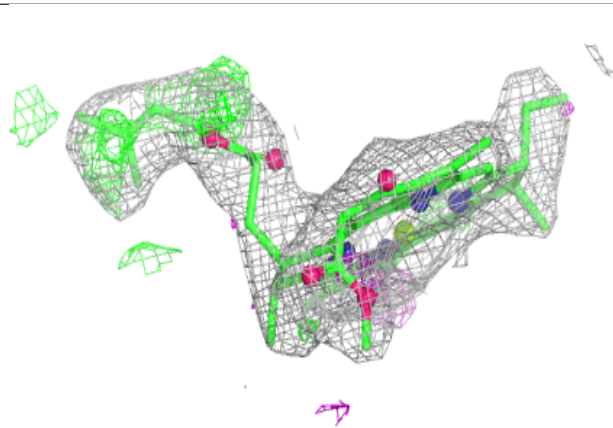
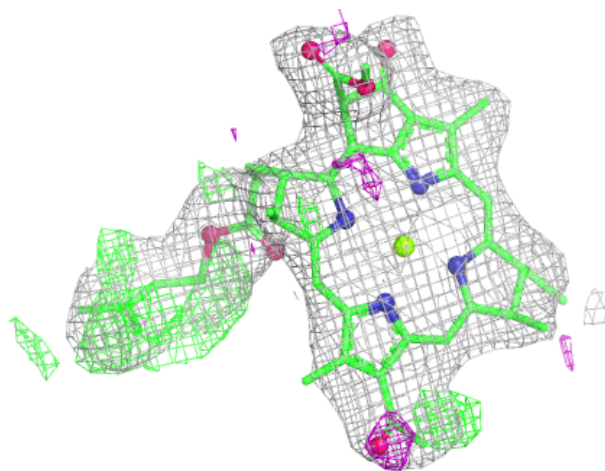
Electron density around U10 S 2008:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



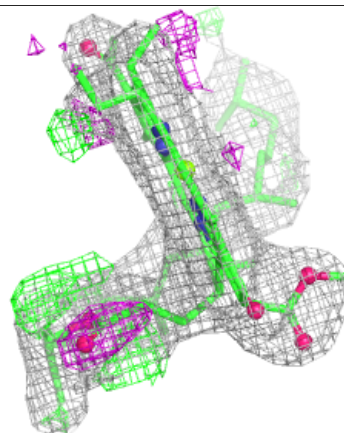
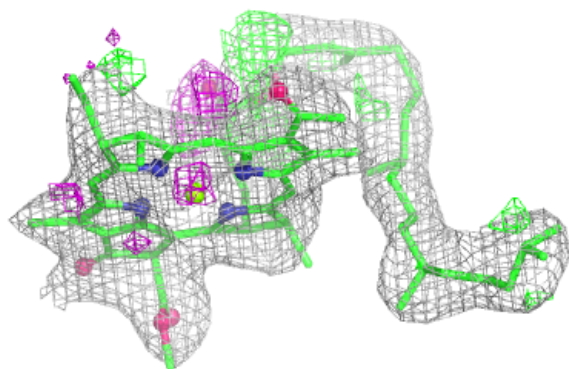
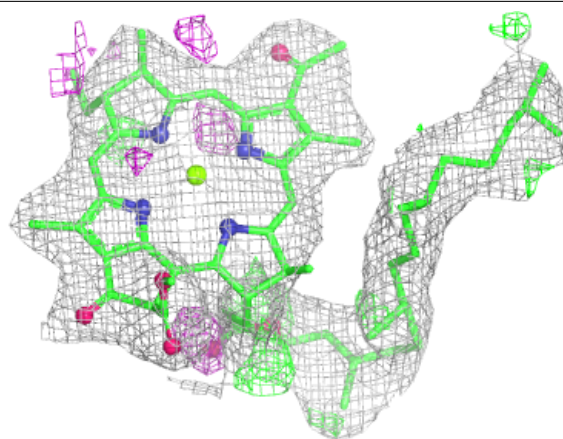
Electron density around BCL S 2001:

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

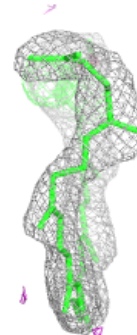
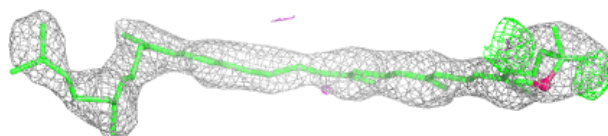
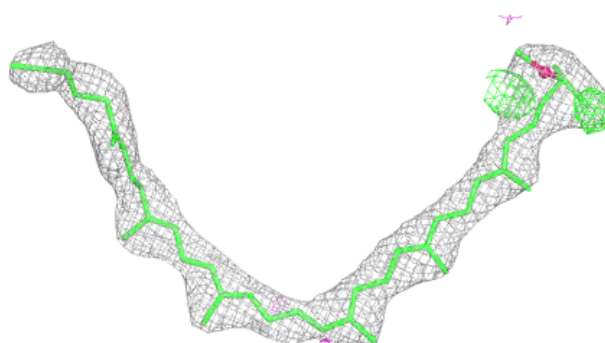


Electron density around BCL S 2004:

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

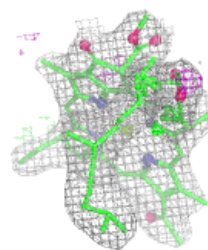
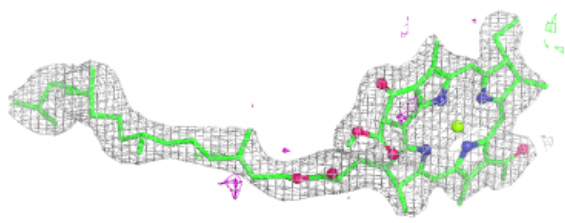
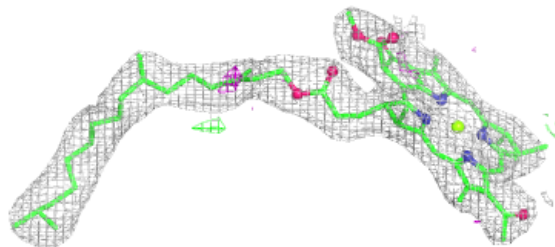
**Electron density around SPO S 2010:**

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



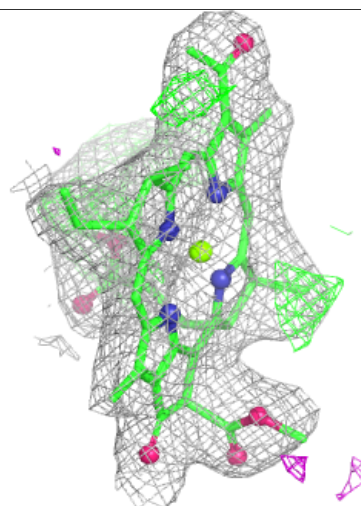
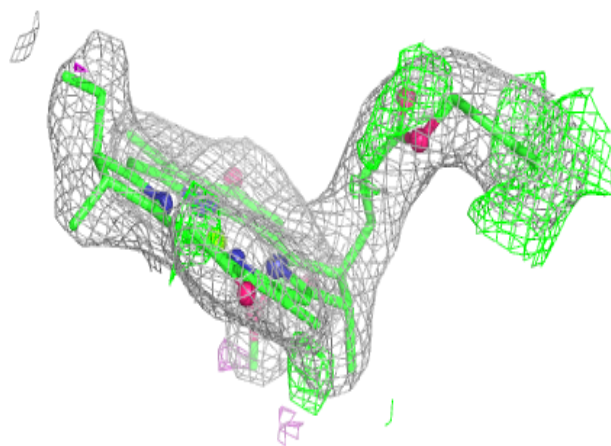
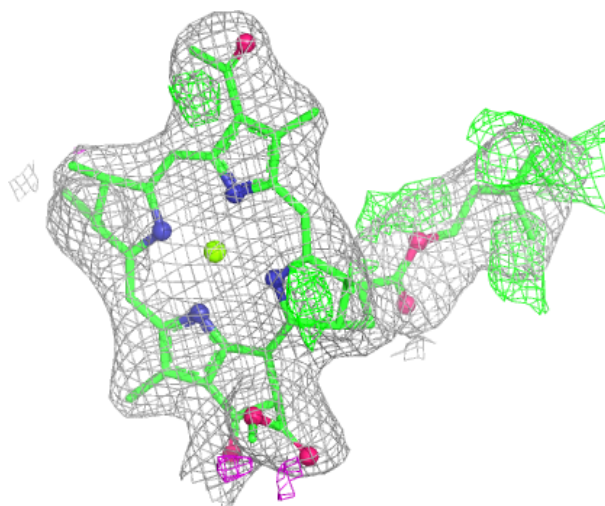
Electron density around BCL R 2002:

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



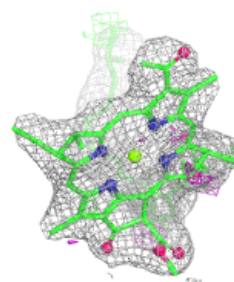
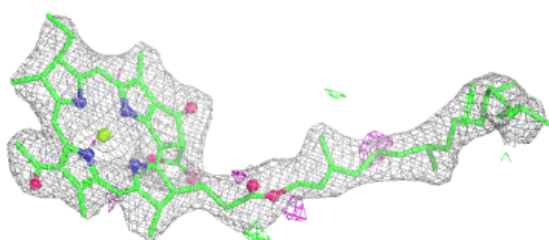
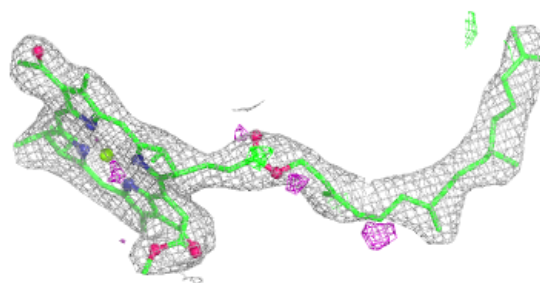
Electron density around BCL L 1001:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

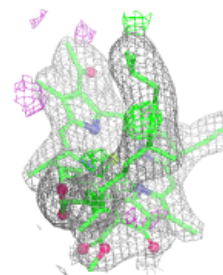
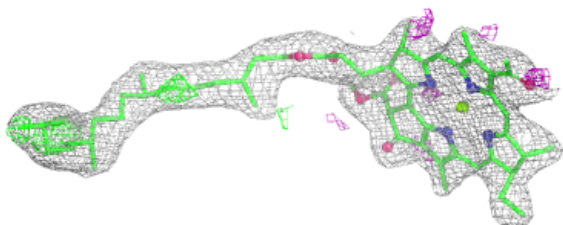
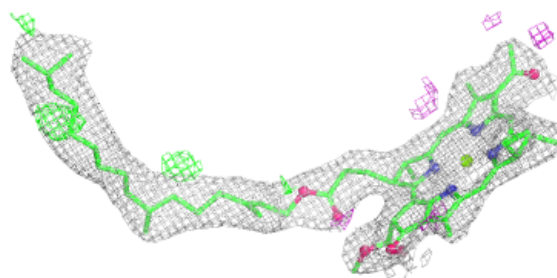


Electron density around BCL S 2003:

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

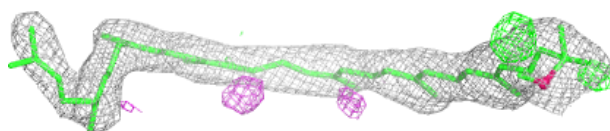
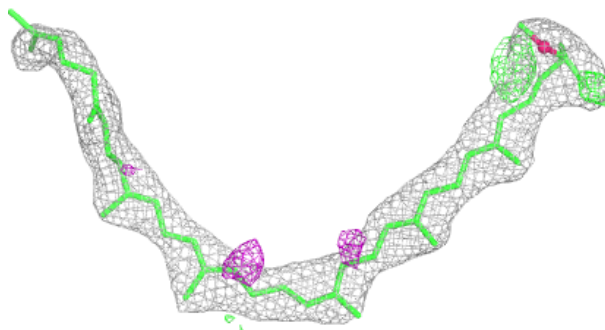
**Electron density around BCL L 1002:**

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

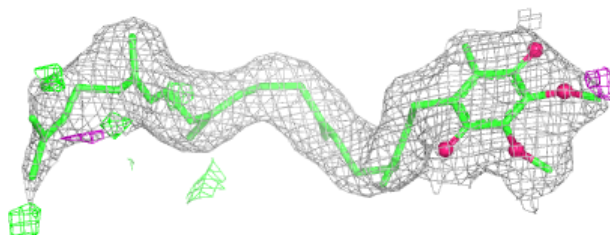
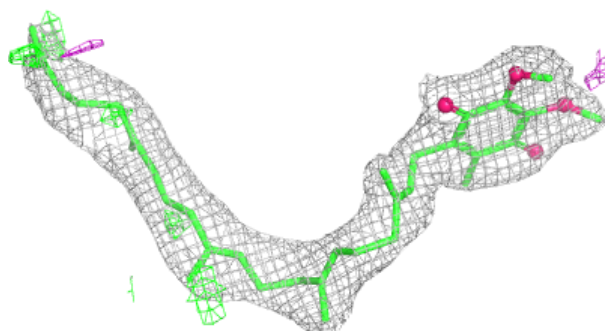


Electron density around SPO M 1010:

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

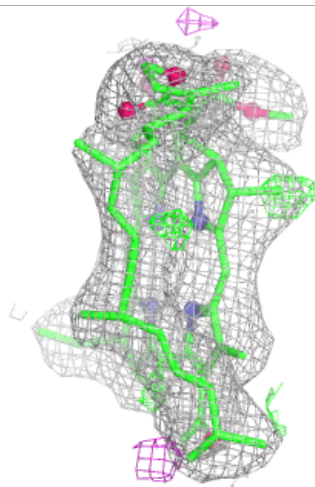
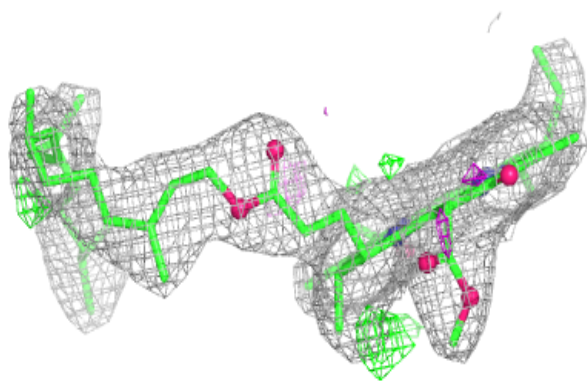
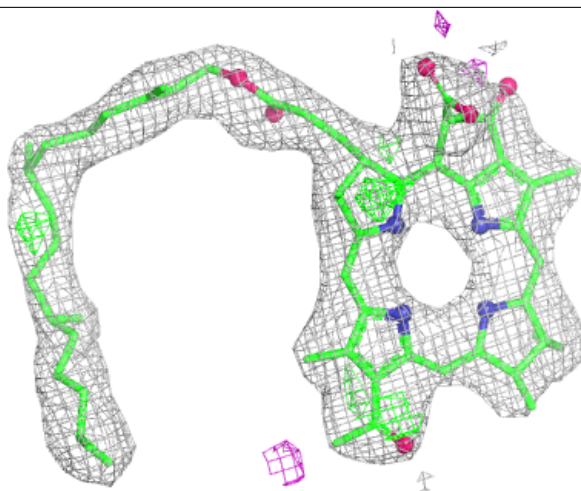
**Electron density around U10 M 1008:**

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



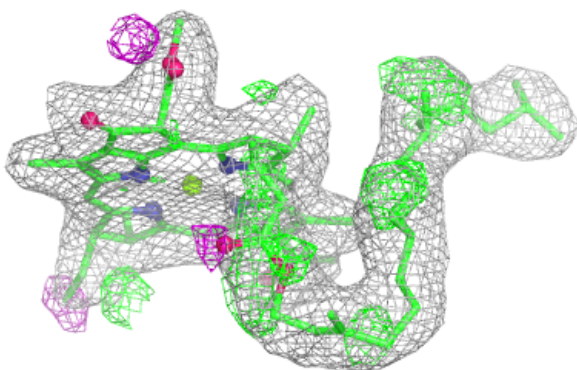
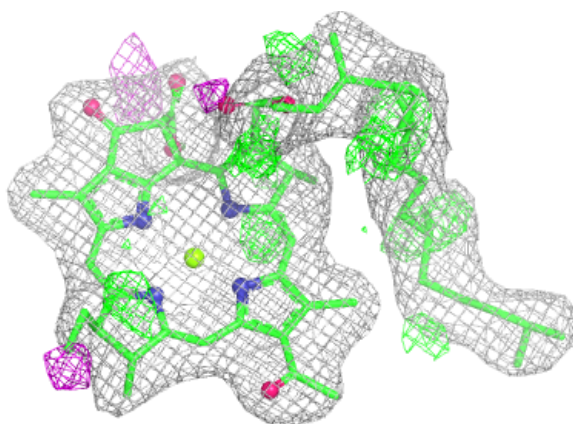
Electron density around BPH R 2006:

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and green (positive)

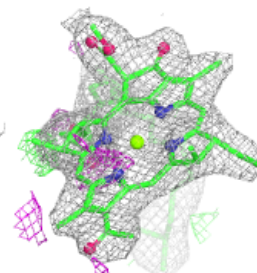
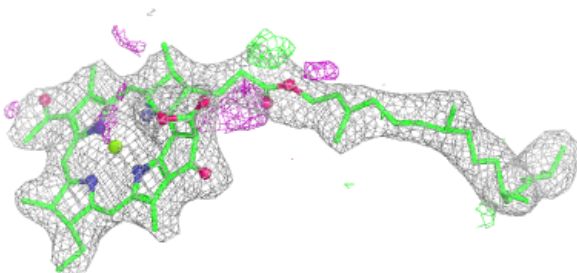
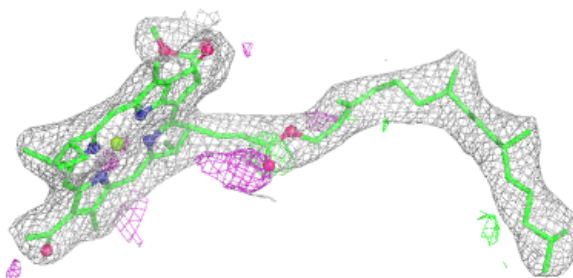


Electron density around BCL L 1004:

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and green (positive)

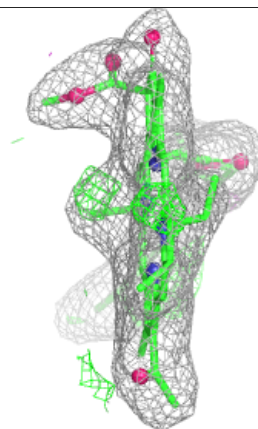
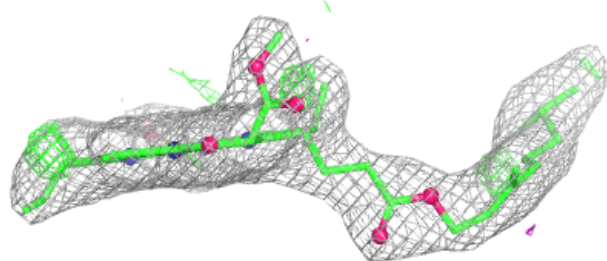
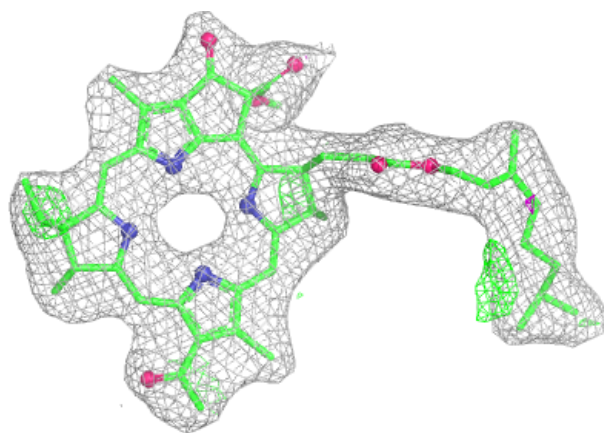
**Electron density around BCL M 1003:**

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



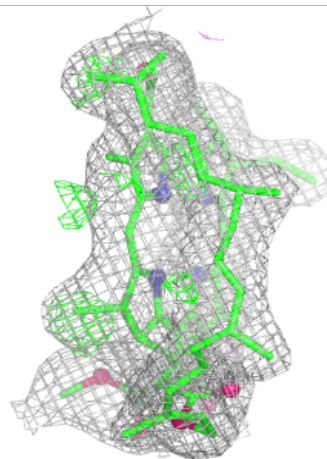
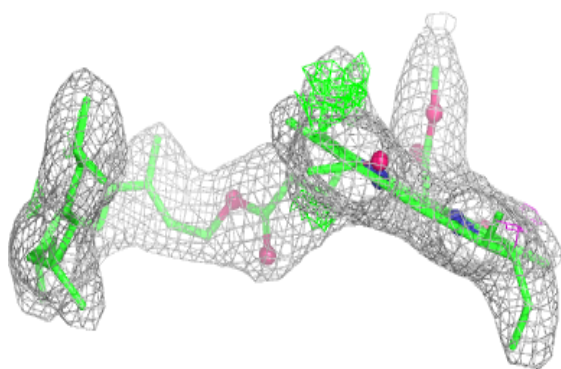
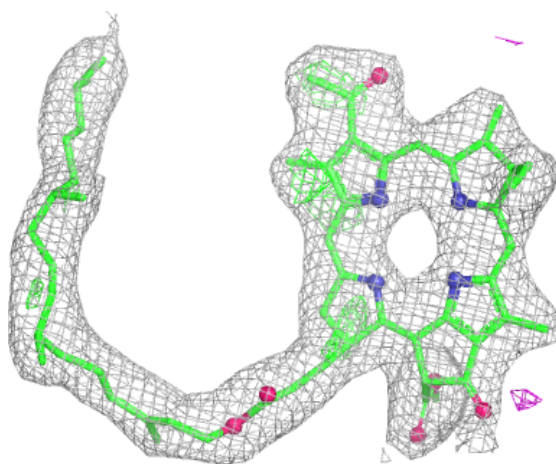
Electron density around BPH M 1005:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



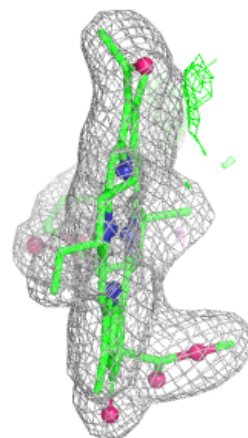
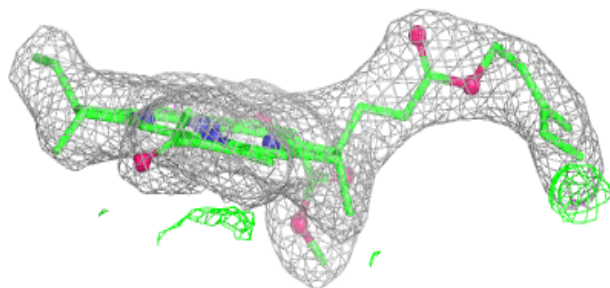
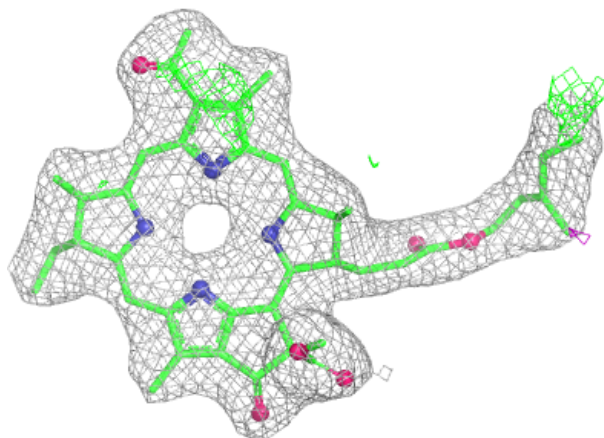
Electron density around BPH L 1006:

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



Electron density around BPH 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.