



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:10 AM UTC

PDB ID : 1DV6 / pdb_00001dv6
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES IN THE CHARGE-NEUTRAL DQAQB STATE WITH THE PROTON TRANSFER INHIBITOR ZN2+
Authors : Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.
Deposited on : 2000-01-19
Resolution : 2.50 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

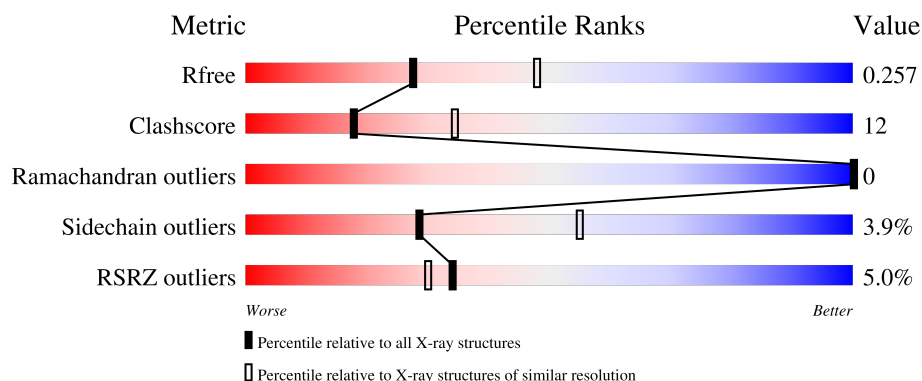
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	9% 75% 22% .
1	R	281	5% 74% 24% .
2	M	307	3% 75% 21% ..
2	S	307	2% 72% 24% ..

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Mol	Chain	Length	Quality of chain
3	H	260	7% 72% 22% • 5%
3	T	260	4% 70% 23% • 5%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 14349 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 PHOTOSYNTHETIC REACTION CENTER.

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

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	299	Total	C	N	O	S	0	0	0
			2390	1597	391	392	10			
2	S	299	Total	C	N	O	S	0	0	0
			2390	1597	391	392	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	307	ALA	ASN	conflict	UNP P02953
S	307	ALA	ASN	conflict	UNP P02953

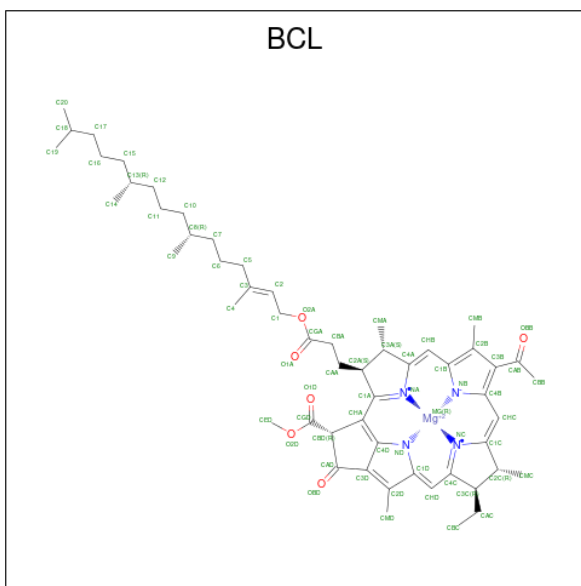
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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			

There are 2 discrepancies between the modelled and reference sequences:

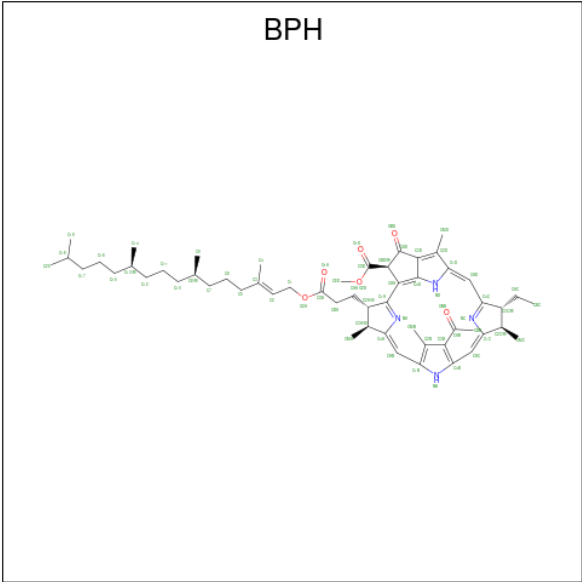
Chain	Residue	Modelled	Actual	Comment	Reference
H	8	GLN	GLY	conflict	UNP P11846
T	8	GLN	GLY	conflict	UNP P11846

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



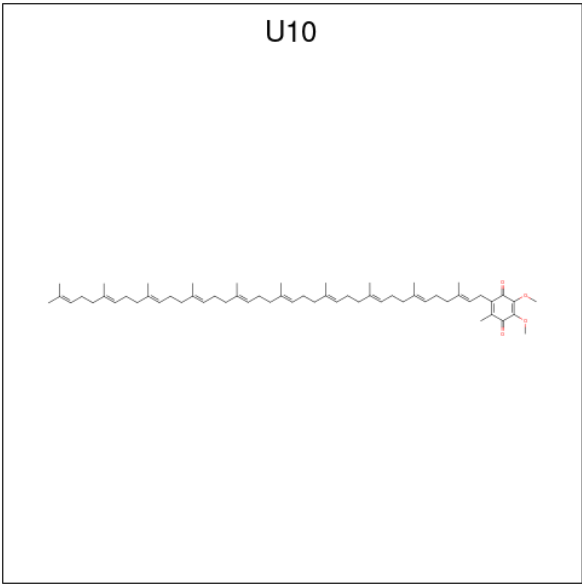
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	S	1	Total 51	C 40	Mg 1	N 4	O 6	0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

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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
			51	41	4	6		
5	R	1	Total	C	N	O	0	0
			65	55	4	6		
5	S	1	Total	C	N	O	0	0
			52	42	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	0
			44	40	4		
6	M	1	Total	C	O	0	0
			38	34	4		
6	R	1	Total	C	O	0	0
			18	14	4		
6	S	1	Total	C	O	0	0
			32	28	4		

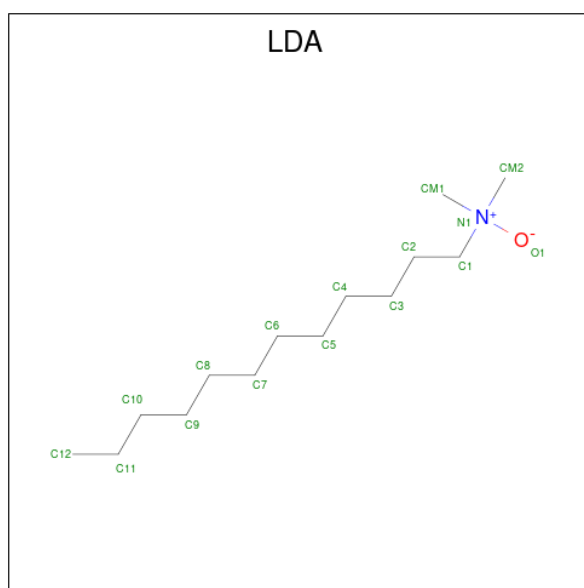
- Molecule 7 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Cl	0	0
			1	1		
8	S	1	Total	Cl	0	0
			1	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		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			10	8	1	1		
9	S	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	1	Total	Zn	0	0
			1	1		
10	T	1	Total	Zn	0	0
			1	1		

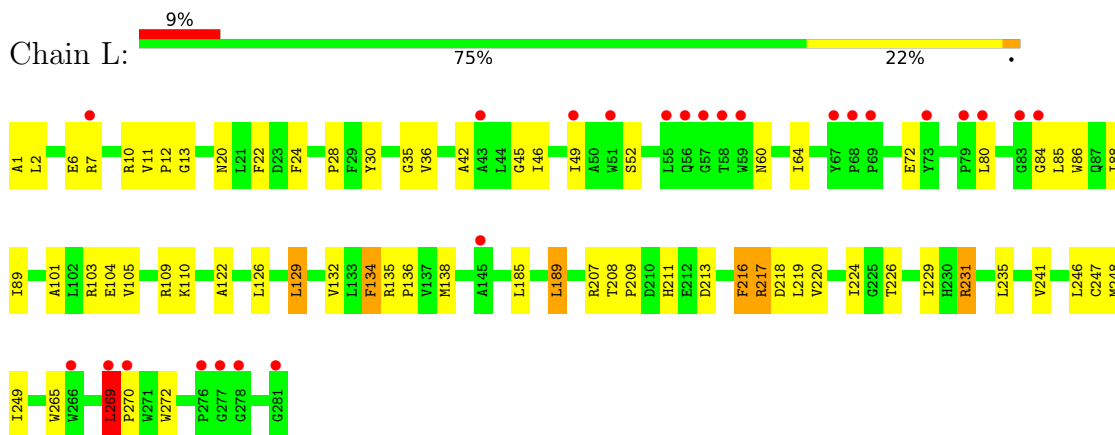
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	75	Total	O	0	0
			75	75		
11	M	92	Total	O	0	0
			92	92		
11	H	82	Total	O	0	0
			82	82		
11	R	55	Total	O	0	0
			55	55		
11	S	75	Total	O	0	0
			75	75		
11	T	61	Total	O	0	0
			61	61		

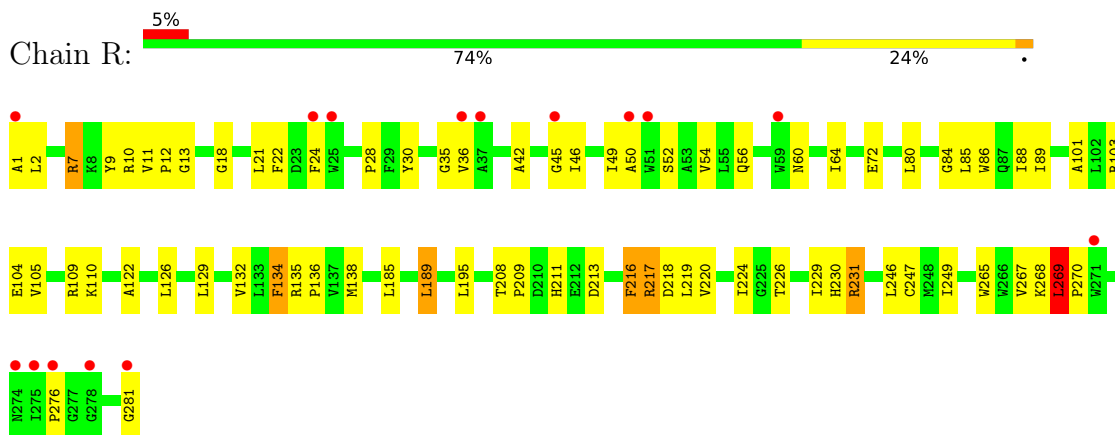
3 Residue-property plots

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

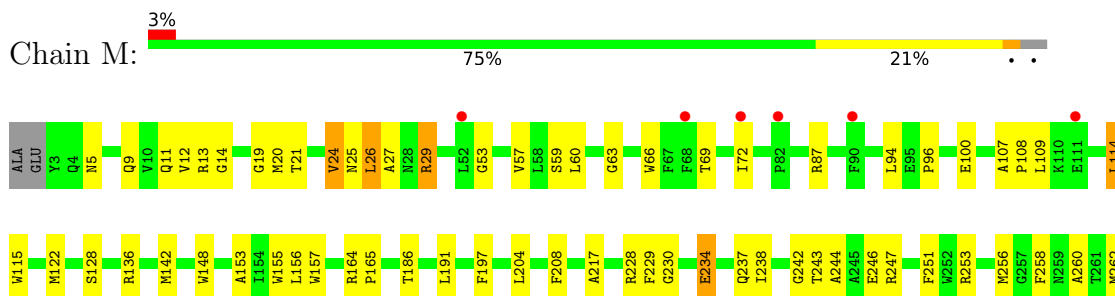
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

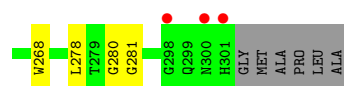


• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

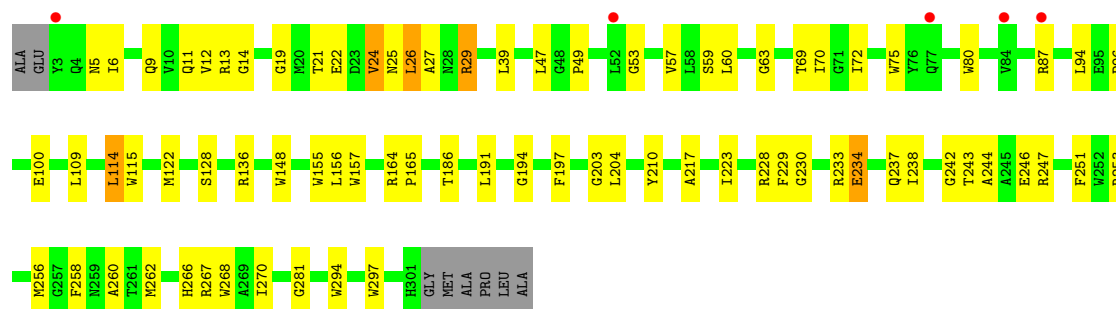


• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

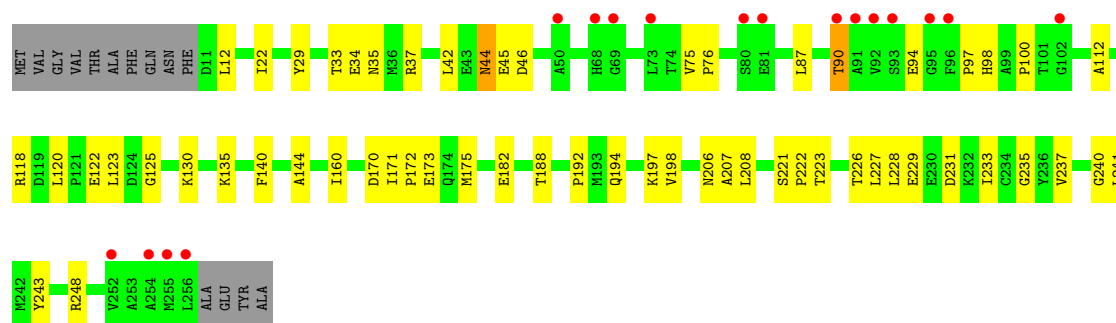
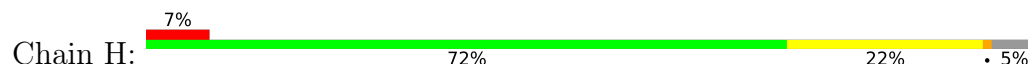




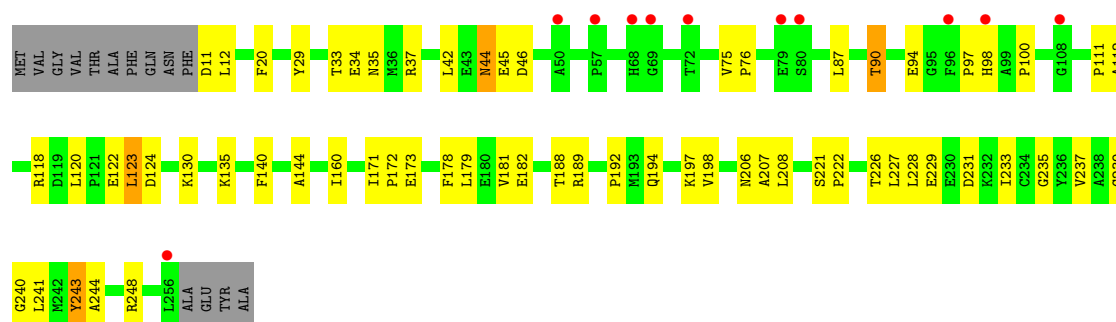
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	141.52Å 141.52Å 278.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.52 – 2.50 27.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (27.52-2.50) 96.7 (27.52-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.265 0.229 , 0.257	Depositor DCC
R_{free} test set	4424 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14349	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: LDA, BPH, ZN, CL, FE2, U10, BCL

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	0.48	0/2320	0.89	6/3175 (0.2%)
1	R	0.45	0/2320	0.89	5/3175 (0.2%)
2	M	0.48	0/2482	0.88	4/3389 (0.1%)
2	S	0.46	0/2482	0.88	7/3389 (0.2%)
3	H	0.44	0/1917	0.90	4/2608 (0.2%)
3	T	0.43	0/1917	0.90	2/2608 (0.1%)
All	All	0.46	0/13438	0.89	28/18344 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	19	GLY	N-CA-C	6.65	121.06	112.68
2	M	19	GLY	N-CA-C	6.60	120.99	112.68
1	R	269	LEU	CA-C-N	6.57	128.05	119.84
1	R	269	LEU	C-N-CA	6.57	128.05	119.84
3	H	243	TYR	N-CA-C	6.35	120.63	113.01
3	T	243	TYR	N-CA-C	6.33	120.61	113.01
1	L	269	LEU	CA-C-N	6.32	127.74	119.84
1	L	269	LEU	C-N-CA	6.32	127.74	119.84
3	T	44	ASN	N-CA-C	-6.07	102.70	110.53
3	H	44	ASN	N-CA-C	-5.88	102.61	110.55
2	S	217	ALA	N-CA-C	-5.83	105.01	111.36
1	L	134	PHE	N-CA-C	5.55	118.05	111.33
2	S	6	ILE	N-CA-C	-5.50	105.75	111.58
2	M	217	ALA	N-CA-C	-5.41	105.47	111.36
1	L	219	LEU	N-CA-C	5.40	116.84	111.07
1	R	134	PHE	N-CA-C	5.33	117.78	111.33
1	R	219	LEU	N-CA-C	5.31	116.75	111.07
1	R	30	TYR	N-CA-C	-5.29	101.91	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	268	TRP	N-CA-C	-5.24	105.65	111.36
1	L	30	TYR	N-CA-C	-5.22	102.03	110.32
2	S	22	GLU	CB-CA-C	-5.21	110.55	116.54
3	H	22	ILE	N-CA-C	-5.19	105.44	110.42
3	H	170	ASP	N-CA-C	-5.18	100.07	108.41
2	S	234	GLU	N-CA-C	5.18	116.92	111.28
2	M	268	TRP	N-CA-C	-5.18	105.72	111.36
2	M	234	GLU	N-CA-C	5.11	116.85	111.28
1	L	6	GLU	N-CA-C	5.03	117.88	111.69
2	S	233	ARG	N-CA-C	-5.01	103.71	110.68

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	2187	55	0
1	R	2232	0	2187	60	0
2	M	2390	0	2304	56	0
2	S	2390	0	2304	65	0
3	H	1869	0	1884	40	0
3	T	1869	0	1884	59	0
4	L	66	0	74	8	0
4	M	183	0	188	20	0
4	R	132	0	148	8	0
4	S	117	0	115	10	0
5	L	65	0	76	8	0
5	M	51	0	45	3	0
5	R	65	0	76	6	0
5	S	52	0	47	3	0
6	L	44	0	57	2	0
6	M	38	0	47	0	0
6	R	18	0	15	2	0
6	S	32	0	39	2	0
7	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	S	1	0	0	0	0
8	M	1	0	0	1	0
8	S	1	0	0	0	0
9	M	42	0	78	7	0
9	S	16	0	31	1	0
10	H	1	0	0	0	0
10	T	1	0	0	0	0
11	H	82	0	0	2	0
11	L	75	0	0	5	0
11	M	92	0	0	4	0
11	R	55	0	0	7	0
11	S	75	0	0	15	0
11	T	61	0	0	18	0
All	All	14349	0	13786	340	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (340) 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)
3:T:239:GLY:HA2	11:T:2042:HOH:O	1.54	1.05
2:S:267:ARG:HA	11:S:2068:HOH:O	1.66	0.94
1:R:195:LEU:HD11	11:S:2068:HOH:O	1.70	0.91
1:L:217:ARG:HD2	11:M:1077:HOH:O	1.77	0.83
3:T:178:PHE:HB3	11:T:2036:HOH:O	1.78	0.82
2:M:122:MET:HE1	9:M:1014:LDA:HM22	1.58	0.82
4:M:1001:BCL:HBB3	4:M:1003:BCL:H41	1.61	0.81
3:T:118:ARG:HD3	3:T:120:LEU:HD12	1.63	0.80
4:R:2004:BCL:HED2	2:S:203:GLY:HA3	1.64	0.80
3:H:118:ARG:HD3	3:H:120:LEU:HD12	1.64	0.78
2:S:11:GLN:HB2	3:T:144:ALA:HB3	1.67	0.76
5:L:1006:BPH:H102	4:M:1004:BCL:C19	2.15	0.76
2:S:228:ARG:HA	3:T:194:GLN:CG	2.16	0.74
2:M:13:ARG:O	3:H:140:PHE:HA	1.90	0.72
2:S:21:THR:O	2:S:24:VAL:HG13	1.88	0.72
1:L:11:VAL:HG13	1:L:12:PRO:HD2	1.71	0.72
3:T:130:LYS:HB2	11:T:2044:HOH:O	1.88	0.72
2:S:53:GLY:O	2:S:57:VAL:HG23	1.89	0.72
2:S:63:GLY:HA3	5:S:2005:BPH:H5C1	1.71	0.71
1:R:11:VAL:HG13	1:R:12:PRO:HD2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:21:THR:O	2:M:24:VAL:HG13	1.91	0.71
1:R:189:LEU:HG	1:R:216:PHE:HZ	1.56	0.71
4:R:2004:BCL:HED2	2:S:203:GLY:CA	2.21	0.70
2:M:53:GLY:O	2:M:57:VAL:HG23	1.92	0.70
2:M:197:PHE:HZ	4:M:1003:BCL:HBB2	1.57	0.69
2:S:294:TRP:N	11:S:2052:HOH:O	2.26	0.68
2:S:197:PHE:HZ	4:S:2003:BCL:HBB2	1.58	0.68
4:M:1001:BCL:HHC	4:M:1001:BCL:HBB2	1.76	0.68
6:S:2008:U10:H4M2	6:S:2008:U10:H3M3	1.76	0.68
1:L:80:LEU:O	1:L:85:LEU:HB2	1.95	0.67
1:R:7:ARG:HG3	11:R:2049:HOH:O	1.93	0.67
5:R:2006:BPH:HHC	5:R:2006:BPH:HBB3	1.75	0.67
1:L:52:SER:HB2	1:L:85:LEU:HD23	1.77	0.67
1:R:80:LEU:O	1:R:85:LEU:HB2	1.95	0.67
3:T:111:PRO:HG2	11:T:2042:HOH:O	1.95	0.66
2:M:9:GLN:NE2	3:H:198:VAL:H	1.93	0.66
1:L:189:LEU:HG	1:L:216:PHE:HZ	1.59	0.66
2:S:228:ARG:HA	3:T:194:GLN:HG3	1.78	0.65
3:T:123:LEU:C	11:T:2044:HOH:O	2.39	0.65
1:R:9:TYR:HD1	11:T:2061:HOH:O	1.80	0.65
1:R:276:PRO:HA	11:R:2046:HOH:O	1.97	0.65
3:H:173:GLU:HG3	11:H:1081:HOH:O	1.96	0.65
3:T:173:GLU:HG3	11:T:2045:HOH:O	1.97	0.65
3:T:111:PRO:C	11:T:2042:HOH:O	2.39	0.64
1:R:52:SER:HB2	1:R:85:LEU:HD23	1.79	0.64
1:R:1:ALA:HB1	3:T:42:LEU:HB3	1.80	0.63
4:R:2004:BCL:CED	2:S:203:GLY:HA3	2.28	0.63
4:S:2001:BCL:CBB	4:S:2001:BCL:HHC	2.29	0.62
1:L:208:THR:H	1:L:211:HIS:CD2	2.17	0.62
2:S:109:LEU:HD22	2:S:114:LEU:HD13	1.80	0.62
1:R:224:ILE:HG22	6:R:2009:U10:H3M3	1.81	0.62
11:L:1029:HOH:O	2:M:253:ARG:HD3	1.98	0.62
2:M:109:LEU:HD22	2:M:114:LEU:HD13	1.81	0.62
1:R:208:THR:H	1:R:211:HIS:CD2	2.16	0.61
2:M:9:GLN:HE22	3:H:198:VAL:H	1.46	0.61
2:S:297:TRP:NE1	3:T:11:ASP:OD1	2.26	0.61
3:T:112:ALA:N	11:T:2042:HOH:O	2.33	0.61
5:R:2006:BPH:HBB2	2:S:210:TYR:HB3	1.81	0.61
2:S:122:MET:HE3	2:S:157:TRP:HE1	1.66	0.61
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.83	0.60
3:T:37:ARG:HH11	3:T:76:PRO:HD3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:197:PHE:CZ	4:S:2003:BCL:HBB2	2.37	0.60
4:M:1003:BCL:HBB2	4:M:1003:BCL:HHC	1.83	0.60
2:M:197:PHE:CZ	4:M:1003:BCL:HBB2	2.35	0.60
11:S:2045:HOH:O	3:T:34:GLU:HG3	2.02	0.60
1:L:1:ALA:HB1	3:H:42:LEU:HB3	1.83	0.60
3:T:189:ARG:HB2	11:T:2051:HOH:O	2.01	0.59
1:L:28:PRO:HB3	2:M:253:ARG:NH1	2.18	0.59
3:T:181:VAL:HB	11:T:2051:HOH:O	2.01	0.58
1:L:60:ASN:O	1:L:64:ILE:HG13	2.04	0.58
3:H:37:ARG:HH11	3:H:76:PRO:HD3	1.68	0.58
2:S:21:THR:HG23	2:S:26:LEU:HD11	1.85	0.58
3:T:87:LEU:HD23	3:T:100:PRO:HA	1.85	0.58
4:M:1001:BCL:HHC	4:M:1001:BCL:CBB	2.34	0.57
4:M:1003:BCL:HHC	4:M:1003:BCL:CBB	2.34	0.57
2:S:243:THR:O	2:S:247:ARG:HG3	2.04	0.57
1:R:60:ASN:O	1:R:64:ILE:HG13	2.03	0.57
1:R:218:ASP:OD1	2:S:29:ARG:HD2	2.04	0.57
1:L:52:SER:CB	1:L:85:LEU:HD23	2.34	0.57
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.85	0.57
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.86	0.57
3:T:37:ARG:NH1	3:T:76:PRO:HD3	2.20	0.57
2:S:253:ARG:HD3	11:S:2061:HOH:O	2.03	0.57
1:R:28:PRO:HB3	2:S:253:ARG:NH1	2.19	0.56
1:R:105:VAL:HG12	1:R:109:ARG:HD2	1.85	0.56
1:R:231:ARG:HD2	2:S:5:ASN:O	2.06	0.56
2:M:204:LEU:HG	9:M:1013:LDA:HM11	1.86	0.56
1:L:241:VAL:HG21	5:L:1006:BPH:HAC1	1.86	0.56
2:M:122:MET:HE3	2:M:157:TRP:HE1	1.71	0.56
2:M:228:ARG:HA	3:H:194:GLN:CG	2.35	0.56
1:R:49:ILE:HG12	1:R:89:ILE:HD13	1.88	0.56
3:H:194:GLN:CD	3:H:194:GLN:H	2.14	0.56
3:T:182:GLU:HA	3:T:188:THR:HG22	1.87	0.56
3:T:239:GLY:CA	11:T:2042:HOH:O	2.30	0.56
1:L:224:ILE:HG22	6:L:1009:U10:H3M3	1.87	0.56
3:T:194:GLN:CD	3:T:194:GLN:H	2.13	0.55
1:L:105:VAL:HG12	1:L:109:ARG:HD2	1.88	0.55
3:H:37:ARG:NH1	3:H:76:PRO:HD3	2.21	0.55
3:T:226:THR:OG1	3:T:229:GLU:HG3	2.06	0.55
1:L:218:ASP:OD1	2:M:29:ARG:HD2	2.06	0.55
3:H:241:LEU:O	3:H:248:ARG:NH2	2.39	0.55
2:M:243:THR:O	2:M:247:ARG:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:2001:BCL:HBB3	4:S:2003:BCL:H41	1.88	0.55
2:S:9:GLN:HE22	3:T:198:VAL:H	1.54	0.55
2:S:228:ARG:HA	3:T:194:GLN:HG2	1.88	0.55
1:R:208:THR:H	1:R:211:HIS:HD2	1.53	0.55
4:S:2003:BCL:CBB	4:S:2003:BCL:HHC	2.36	0.55
1:R:52:SER:CB	1:R:85:LEU:HD23	2.36	0.55
2:S:164:ARG:HB3	2:S:165:PRO:HD3	1.89	0.55
1:L:226:THR:HG23	11:L:1051:HOH:O	2.08	0.54
1:R:217:ARG:HD2	11:S:2017:HOH:O	2.08	0.54
1:L:208:THR:H	1:L:211:HIS:HD2	1.54	0.54
4:M:1001:BCL:HBB2	9:M:1014:LDA:HM11	1.90	0.54
3:T:90:THR:HB	3:T:97:PRO:O	2.07	0.54
1:L:20:ASN:HB3	11:L:1072:HOH:O	2.06	0.54
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.07	0.54
1:R:195:LEU:CD1	11:S:2068:HOH:O	2.43	0.54
2:S:256:MET:HE3	2:S:258:PHE:CE1	2.43	0.54
2:M:13:ARG:NH2	11:M:1100:HOH:O	2.38	0.54
2:S:13:ARG:HG2	2:S:14:GLY:N	2.23	0.53
1:L:2:LEU:HG	1:L:10:ARG:NH1	2.24	0.53
3:T:34:GLU:O	3:T:37:ARG:HD3	2.09	0.53
3:T:241:LEU:O	3:T:248:ARG:NH2	2.41	0.53
1:L:213:ASP:O	1:L:217:ARG:HB2	2.09	0.53
1:R:213:ASP:O	1:R:217:ARG:HB2	2.09	0.53
5:L:1006:BPH:H7C2	4:M:1004:BCL:H193	1.91	0.53
1:R:220:VAL:HG22	1:R:220:VAL:O	2.08	0.53
1:R:189:LEU:HG	1:R:216:PHE:CZ	2.41	0.53
1:R:281:GLY:C	11:R:2046:HOH:O	2.50	0.53
1:R:2:LEU:HG	1:R:10:ARG:NH1	2.23	0.53
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.90	0.53
2:M:13:ARG:HG2	2:M:14:GLY:N	2.24	0.53
5:R:2006:BPH:HHC	5:R:2006:BPH:CBB	2.38	0.53
3:H:90:THR:HB	3:H:97:PRO:O	2.08	0.52
3:H:207:ALA:O	3:H:240:GLY:HA3	2.09	0.52
5:S:2005:BPH:HBB3	5:S:2005:BPH:HMB1	1.91	0.52
2:M:208:PHE:HE1	9:M:1013:LDA:H112	1.73	0.52
1:R:22:PHE:HA	1:R:24:PHE:HE1	1.74	0.52
4:R:2004:BCL:H193	5:R:2006:BPH:C10	2.39	0.52
3:T:207:ALA:O	3:T:240:GLY:HA3	2.10	0.52
1:L:72:GLU:CD	1:L:72:GLU:H	2.17	0.52
3:H:233:ILE:O	3:H:237:VAL:HG23	2.09	0.52
1:R:72:GLU:H	1:R:72:GLU:CD	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:34:GLU:O	3:H:37:ARG:HD3	2.10	0.52
3:H:182:GLU:HA	3:H:188:THR:HG22	1.91	0.52
1:L:189:LEU:HG	1:L:216:PHE:CZ	2.43	0.52
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.90	0.52
1:R:22:PHE:HA	1:R:24:PHE:CE1	2.45	0.52
5:M:1005:BPH:HBB3	5:M:1005:BPH:HMB1	1.91	0.51
1:L:22:PHE:HA	1:L:24:PHE:HE1	1.74	0.51
11:M:1070:HOH:O	3:H:175:MET:HE1	2.09	0.51
4:R:2004:BCL:H193	5:R:2006:BPH:H102	1.92	0.51
1:L:22:PHE:HA	1:L:24:PHE:CE1	2.45	0.51
3:T:233:ILE:O	3:T:237:VAL:HG23	2.11	0.51
3:H:75:VAL:HA	3:H:76:PRO:C	2.36	0.51
1:R:135:ARG:HB3	1:R:136:PRO:HD3	1.93	0.51
1:L:265:TRP:O	1:L:269:LEU:HD13	2.11	0.51
2:M:256:MET:HE3	2:M:258:PHE:CE1	2.45	0.50
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.94	0.50
1:R:230:HIS:CD2	2:S:223:ILE:HG13	2.47	0.50
3:T:75:VAL:HA	3:T:76:PRO:C	2.36	0.50
2:M:9:GLN:HE22	3:H:197:LYS:HA	1.75	0.50
1:L:272:TRP:CD2	2:M:87:ARG:HB3	2.47	0.50
4:L:1002:BCL:HAA2	4:L:1002:BCL:HBD	1.93	0.50
2:M:230:GLY:HA2	11:M:1058:HOH:O	2.10	0.50
1:L:28:PRO:HB3	2:M:253:ARG:HH11	1.76	0.49
1:R:56:GLN:HA	11:R:2059:HOH:O	2.12	0.49
5:S:2005:BPH:HBB3	5:S:2005:BPH:CMB	2.42	0.49
11:S:2022:HOH:O	3:T:173:GLU:HG2	2.10	0.49
3:H:87:LEU:HD22	3:H:98:HIS:O	2.13	0.49
1:L:220:VAL:O	1:L:220:VAL:HG22	2.12	0.49
2:M:59:SER:HB2	2:M:128:SER:OG	2.12	0.49
2:S:59:SER:HB2	2:S:128:SER:OG	2.13	0.49
2:S:260:ALA:HB1	3:T:35:ASN:OD1	2.13	0.49
4:L:1002:BCL:HMB3	4:L:1002:BCL:CBB	2.42	0.48
2:S:270:ILE:CG2	11:S:2068:HOH:O	2.61	0.48
4:S:2003:BCL:HBB2	4:S:2003:BCL:HHC	1.94	0.48
3:T:29:TYR:O	3:T:33:THR:HG23	2.13	0.48
2:S:49:PRO:HG2	11:S:2025:HOH:O	2.13	0.48
1:L:185:LEU:HD12	1:L:189:LEU:HD22	1.96	0.48
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.13	0.48
1:R:267:VAL:HG13	2:S:87:ARG:HD2	1.95	0.48
11:R:2017:HOH:O	3:T:130:LYS:HE2	2.14	0.48
2:S:21:THR:HG22	11:S:2049:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:265:TRP:O	1:R:269:LEU:HD13	2.13	0.48
6:S:2008:U10:H4M2	6:S:2008:U10:C3M	2.42	0.48
2:S:204:LEU:HD13	3:T:20:PHE:CE2	2.48	0.48
1:R:28:PRO:HB3	2:S:253:ARG:HH11	1.77	0.47
1:L:86:TRP:CH2	1:L:132:VAL:HG13	2.49	0.47
2:M:242:GLY:O	2:M:246:GLU:HG3	2.14	0.47
1:R:86:TRP:CH2	1:R:132:VAL:HG13	2.50	0.47
11:L:1018:HOH:O	3:H:130:LYS:HE2	2.13	0.47
5:R:2006:BPH:H151	5:R:2006:BPH:H192	1.95	0.47
1:L:231:ARG:HD2	2:M:5:ASN:O	2.14	0.47
2:S:242:GLY:O	2:S:246:GLU:HG3	2.14	0.47
3:T:87:LEU:HD22	3:T:98:HIS:O	2.14	0.47
8:M:1011:CL:CL	9:M:1012:LDA:CM2	3.00	0.47
1:L:11:VAL:CG1	11:L:1055:HOH:O	2.63	0.47
2:M:155:TRP:NE1	2:M:281:GLY:HA3	2.29	0.47
3:H:29:TYR:O	3:H:33:THR:HG23	2.15	0.47
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.96	0.47
2:S:9:GLN:NE2	3:T:198:VAL:H	2.12	0.47
3:T:130:LYS:CB	11:T:2044:HOH:O	2.54	0.47
1:L:208:THR:HB	1:L:209:PRO:HD2	1.97	0.47
3:T:45:GLU:HG3	3:T:94:GLU:OE1	2.15	0.47
1:L:35:GLY:HA2	1:L:103:ARG:HD2	1.97	0.47
2:M:114:LEU:HD12	2:M:114:LEU:HA	1.76	0.47
1:R:45:GLY:O	1:R:49:ILE:HG13	2.14	0.46
2:S:234:GLU:O	2:S:238:ILE:HG13	2.15	0.46
1:L:208:THR:HB	1:L:209:PRO:CD	2.46	0.46
1:R:42:ALA:O	1:R:46:ILE:HG13	2.16	0.46
1:R:85:LEU:O	1:R:89:ILE:HG13	2.15	0.46
3:T:192:PRO:HB3	3:T:194:GLN:HE21	1.80	0.46
1:R:35:GLY:HA2	1:R:103:ARG:HD2	1.96	0.46
4:M:1001:BCL:OBB	9:M:1014:LDA:H12	2.16	0.46
4:M:1004:BCL:HMB1	4:M:1004:BCL:HBB2	1.97	0.46
2:S:155:TRP:NE1	2:S:281:GLY:HA3	2.31	0.46
1:L:42:ALA:O	1:L:46:ILE:HG13	2.16	0.46
1:L:45:GLY:O	1:L:49:ILE:HG13	2.15	0.46
1:R:189:LEU:HB3	6:R:2009:U10:H4M3	1.97	0.46
1:L:101:ALA:O	1:L:104:GLU:HB2	2.16	0.46
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.45	0.45
2:M:25:ASN:OD1	2:M:27:ALA:HB3	2.16	0.45
2:M:153:ALA:HB2	5:M:1005:BPH:HAC1	1.99	0.45
2:S:25:ASN:OD1	2:S:27:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:248:MET:CG	4:L:1002:BCL:HED2	2.47	0.45
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.52	0.45
3:T:122:GLU:HB2	3:T:227:LEU:HD21	1.99	0.45
2:S:229:PHE:HB2	2:S:244:ALA:HB2	1.97	0.45
3:T:112:ALA:HB2	11:T:2042:HOH:O	2.15	0.45
2:S:69:THR:O	2:S:72:ILE:HG22	2.16	0.45
1:R:185:LEU:HD12	1:R:189:LEU:HD22	1.98	0.45
4:S:2003:BCL:HBC2	4:S:2003:BCL:H2C	1.82	0.45
2:M:280:GLY:HA2	4:M:1003:BCL:HED2	1.97	0.45
3:H:192:PRO:HB3	3:H:194:GLN:HE21	1.82	0.45
4:R:2004:BCL:CBB	4:R:2004:BCL:HMB1	2.46	0.45
1:L:84:GLY:O	1:L:88:ILE:HG12	2.17	0.45
2:S:148:TRP:HA	2:S:148:TRP:CE3	2.52	0.45
2:M:69:THR:O	2:M:72:ILE:HG22	2.17	0.45
1:R:122:ALA:O	1:R:126:LEU:HD13	2.17	0.45
2:S:148:TRP:HA	2:S:148:TRP:HE3	1.82	0.45
3:H:223:THR:HB	11:H:1067:HOH:O	2.16	0.44
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.82	0.44
3:H:44:ASN:HB2	3:H:46:ASP:OD1	2.17	0.44
1:R:208:THR:HB	1:R:209:PRO:CD	2.47	0.44
1:R:208:THR:HB	1:R:209:PRO:HD2	1.98	0.44
1:L:220:VAL:HG21	6:L:1009:U10:C15	2.47	0.44
1:R:1:ALA:C	1:R:2:LEU:HD12	2.41	0.44
2:S:100:GLU:H	2:S:100:GLU:CD	2.26	0.44
1:L:246:LEU:HA	1:L:249:ILE:HG22	2.00	0.44
2:S:21:THR:HG23	2:S:26:LEU:CD1	2.48	0.44
3:T:124:ASP:N	11:T:2044:HOH:O	2.51	0.44
1:L:1:ALA:C	1:L:2:LEU:HD12	2.42	0.44
4:L:1002:BCL:H192	5:L:1006:BPH:HMA2	2.00	0.44
4:M:1001:BCL:CBB	9:M:1014:LDA:HM11	2.47	0.44
4:L:1002:BCL:CGA	4:M:1004:BCL:HBC1	2.48	0.44
4:M:1004:BCL:HMB1	4:M:1004:BCL:CBB	2.47	0.44
3:H:122:GLU:HB2	3:H:227:LEU:HD21	2.00	0.44
1:R:84:GLY:O	1:R:88:ILE:HG12	2.18	0.44
3:H:45:GLU:HG3	3:H:94:GLU:OE1	2.17	0.44
1:R:11:VAL:HG11	3:T:243:TYR:OH	2.17	0.44
4:S:2001:BCL:HHC	4:S:2001:BCL:HBB2	1.98	0.44
1:R:269:LEU:HA	1:R:270:PRO:HD3	1.88	0.43
3:T:44:ASN:HB2	3:T:46:ASP:OD1	2.18	0.43
1:L:122:ALA:O	1:L:126:LEU:HD13	2.18	0.43
1:L:134:PHE:O	1:L:138:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:246:LEU:HA	1:R:249:ILE:HG22	1.99	0.43
2:M:251:PHE:CD2	2:M:251:PHE:C	2.96	0.43
2:S:194:GLY:C	11:S:2052:HOH:O	2.62	0.43
3:T:112:ALA:HA	3:T:235:GLY:O	2.17	0.43
1:R:110:LYS:NZ	11:R:2051:HOH:O	2.52	0.43
1:L:85:LEU:O	1:L:89:ILE:HG13	2.18	0.43
5:L:1006:BPH:CBB	5:L:1006:BPH:HMB3	2.49	0.43
2:M:228:ARG:HA	3:H:194:GLN:HG2	2.01	0.43
1:L:248:MET:HG3	4:L:1002:BCL:HED2	2.01	0.43
1:R:18:GLY:O	1:R:21:LEU:HG	2.18	0.43
2:S:13:ARG:HG2	2:S:14:GLY:H	1.83	0.43
1:L:207:ARG:HG2	2:M:142:MET:HG2	2.01	0.43
1:R:101:ALA:O	1:R:104:GLU:HB2	2.19	0.43
2:S:186:THR:OG1	4:S:2001:BCL:H3C	2.18	0.43
2:S:251:PHE:CD2	2:S:251:PHE:C	2.97	0.43
1:R:49:ILE:CG1	1:R:89:ILE:HD13	2.49	0.42
3:T:240:GLY:O	3:T:244:ALA:HB3	2.19	0.42
2:M:100:GLU:CD	2:M:100:GLU:H	2.26	0.42
3:H:221:SER:HA	3:H:222:PRO:HD3	1.80	0.42
2:S:26:LEU:HB2	11:S:2077:HOH:O	2.19	0.42
2:S:70:ILE:HG21	9:S:2012:LDA:H22	2.01	0.42
4:L:1002:BCL:CBA	4:M:1004:BCL:HBC1	2.49	0.42
2:M:63:GLY:HA3	5:M:1005:BPH:H5C2	2.00	0.42
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.55	0.42
2:M:237:GLN:HB2	2:M:262:MET:HG2	2.01	0.42
2:M:234:GLU:O	2:M:238:ILE:HG13	2.19	0.42
2:S:237:GLN:HB2	2:S:262:MET:HG2	2.02	0.42
1:L:13:GLY:O	1:L:110:LYS:HE2	2.20	0.42
4:R:2002:BCL:CGA	4:R:2004:BCL:HBC1	2.49	0.42
3:H:171:ILE:HB	3:H:172:PRO:HD3	2.02	0.42
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.84	0.42
1:R:134:PHE:O	1:R:138:MET:HG3	2.20	0.42
3:T:171:ILE:HB	3:T:172:PRO:HD3	2.01	0.42
3:T:206:ASN:HD21	3:T:248:ARG:HD2	1.85	0.42
2:M:21:THR:HG23	2:M:26:LEU:CD1	2.49	0.41
2:S:230:GLY:HA2	11:S:2019:HOH:O	2.20	0.41
3:T:160:ILE:N	3:T:160:ILE:HD12	2.34	0.41
1:L:226:THR:O	1:L:229:ILE:HG22	2.19	0.41
2:S:39:LEU:HD12	2:S:47:LEU:HD11	2.02	0.41
2:S:96:PRO:HB3	2:S:115:TRP:CE2	2.55	0.41
2:S:266:HIS:O	11:S:2068:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:45:GLU:HG3	3:T:94:GLU:CD	2.44	0.41
3:T:179:LEU:C	11:T:2036:HOH:O	2.63	0.41
5:L:1006:BPH:H102	4:M:1004:BCL:H192	1.96	0.41
3:T:241:LEU:HB2	11:T:2035:HOH:O	2.19	0.41
1:L:129:LEU:HD12	1:L:129:LEU:HA	1.90	0.41
3:H:112:ALA:HA	3:H:235:GLY:O	2.20	0.41
4:R:2002:BCL:HMB3	4:R:2002:BCL:CBB	2.51	0.41
3:T:197:LYS:NZ	11:T:2059:HOH:O	2.53	0.41
4:L:1002:BCL:H122	5:L:1006:BPH:H3A	2.03	0.41
2:M:136:ARG:NE	2:M:136:ARG:HA	2.35	0.41
1:R:50:ALA:O	1:R:54:VAL:HG23	2.21	0.41
3:T:221:SER:HA	3:T:222:PRO:HD3	1.80	0.41
2:M:186:THR:HG23	4:M:1003:BCL:HMD1	2.03	0.41
2:S:13:ARG:O	3:T:140:PHE:HA	2.21	0.41
1:L:269:LEU:HA	1:L:270:PRO:HD3	1.89	0.41
2:M:278:LEU:HD12	2:M:278:LEU:HA	1.92	0.41
3:H:45:GLU:HG3	3:H:94:GLU:CD	2.46	0.41
1:R:185:LEU:HD23	4:S:2001:BCL:H43	2.02	0.41
2:S:136:ARG:HA	2:S:136:ARG:NE	2.35	0.41
5:L:1006:BPH:H102	4:M:1004:BCL:H191	1.98	0.41
2:M:107:ALA:HA	2:M:108:PRO:HD3	1.94	0.41
3:H:160:ILE:N	3:H:160:ILE:HD12	2.36	0.41
2:M:228:ARG:HA	3:H:194:GLN:HG3	2.03	0.40
2:M:96:PRO:HB3	2:M:115:TRP:CE2	2.56	0.40
1:R:268:LYS:HG3	11:R:2048:HOH:O	2.20	0.40
2:S:228:ARG:CA	3:T:194:GLN:HG3	2.50	0.40
2:M:20:MET:SD	3:H:125:GLY:HA3	2.62	0.40
2:S:24:VAL:O	2:S:26:LEU:HD13	2.21	0.40
2:S:75:TRP:HB3	2:S:80:TRP:CZ3	2.56	0.40
1:R:226:THR:O	1:R:229:ILE:HG22	2.20	0.40
2:S:256:MET:HE3	2:S:258:PHE:CZ	2.57	0.40
1:L:85:LEU:HA	1:L:85:LEU:HD12	1.88	0.40
1:R:13:GLY:O	1:R:110:LYS:HE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	262 (94%)	17 (6%)	0	100	100
1	R	279/281 (99%)	262 (94%)	17 (6%)	0	100	100
2	M	297/307 (97%)	288 (97%)	9 (3%)	0	100	100
2	S	297/307 (97%)	288 (97%)	9 (3%)	0	100	100
3	H	244/260 (94%)	234 (96%)	10 (4%)	0	100	100
3	T	244/260 (94%)	234 (96%)	10 (4%)	0	100	100
All	All	1640/1696 (97%)	1568 (96%)	72 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	210 (96%)	10 (4%)	24	49
1	R	220/220 (100%)	211 (96%)	9 (4%)	27	53
2	M	235/239 (98%)	226 (96%)	9 (4%)	29	56
2	S	235/239 (98%)	226 (96%)	9 (4%)	29	56
3	H	199/209 (95%)	192 (96%)	7 (4%)	32	58
3	T	199/209 (95%)	192 (96%)	7 (4%)	32	58
All	All	1308/1336 (98%)	1257 (96%)	51 (4%)	28	55

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	36	VAL
1	L	129	LEU
1	L	189	LEU
1	L	216	PHE
1	L	217	ARG
1	L	231	ARG
1	L	235	LEU
1	L	247	CYS
1	L	269	LEU
2	M	12	VAL
2	M	24	VAL
2	M	26	LEU
2	M	29	ARG
2	M	60	LEU
2	M	94	LEU
2	M	114	LEU
2	M	156	LEU
2	M	191	LEU
3	H	12	LEU
3	H	90	THR
3	H	123	LEU
3	H	135	LYS
3	H	208	LEU
3	H	228	LEU
3	H	231	ASP
1	R	7	ARG
1	R	36	VAL
1	R	129	LEU
1	R	189	LEU
1	R	216	PHE
1	R	217	ARG
1	R	231	ARG
1	R	247	CYS
1	R	269	LEU
2	S	12	VAL
2	S	24	VAL
2	S	26	LEU
2	S	29	ARG
2	S	60	LEU
2	S	94	LEU
2	S	114	LEU

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Mol	Chain	Res	Type
2	S	156	LEU
2	S	191	LEU
3	T	12	LEU
3	T	90	THR
3	T	123	LEU
3	T	135	LYS
3	T	208	LEU
3	T	228	LEU
3	T	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	87	GLN
1	L	211	HIS
1	L	258	GLN
1	L	274	ASN
2	M	9	GLN
2	M	188	ASN
2	M	300	ASN
3	H	194	GLN
3	H	199	GLN
3	H	206	ASN
1	R	87	GLN
1	R	211	HIS
1	R	258	GLN
1	R	274	ASN
2	S	9	GLN
2	S	187	ASN
2	S	300	ASN
3	T	194	GLN
3	T	199	GLN
3	T	206	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [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 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 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	S	2003	2	69,74,74	1.05	5 (7%)	79,115,115	1.87	15 (18%)
4	BCL	S	2001	2	54,59,74	1.20	6 (11%)	61,97,115	1.93	18 (29%)
6	U10	R	2009	-	18,18,63	2.01	4 (22%)	24,25,79	1.28	4 (16%)
9	LDA	M	1013	-	13,15,15	2.35	1 (7%)	14,17,17	1.40	3 (21%)
9	LDA	M	1014	-	7,9,15	3.22	2 (28%)	8,11,17	1.47	1 (12%)
5	BPH	M	1005	-	45,56,70	1.32	6 (13%)	41,84,101	2.83	21 (51%)
6	U10	M	1008	-	38,38,63	1.93	9 (23%)	48,49,79	1.11	4 (8%)
4	BCL	M	1004	1	69,74,74	1.07	7 (10%)	79,115,115	2.05	23 (29%)
4	BCL	M	1001	2	54,59,74	1.20	7 (12%)	61,97,115	2.10	18 (29%)
5	BPH	L	1006	-	59,70,70	1.26	6 (10%)	59,101,101	2.33	15 (25%)
9	LDA	M	1012	-	13,15,15	2.18	1 (7%)	14,17,17	1.46	2 (14%)
4	BCL	M	1003	2	69,74,74	0.98	5 (7%)	79,115,115	1.66	16 (20%)
5	BPH	R	2006	-	59,70,70	1.11	5 (8%)	59,101,101	2.34	19 (32%)
6	U10	L	1009	-	44,44,63	1.80	9 (20%)	54,56,79	1.30	5 (9%)
6	U10	S	2008	-	32,32,63	1.78	6 (18%)	40,41,79	1.10	4 (10%)
4	BCL	L	1002	1	69,74,74	1.06	6 (8%)	79,115,115	1.69	15 (18%)
4	BCL	R	2002	1	69,74,74	1.12	4 (5%)	79,115,115	1.73	18 (22%)
5	BPH	S	2005	-	46,57,70	1.31	6 (13%)	42,85,101	2.77	18 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	LDA	S	2012	-	13,15,15	2.32	1 (7%)	14,17,17	1.35	1 (7%)
4	BCL	R	2004	1	69,74,74	1.04	6 (8%)	79,115,115	1.82	17 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	S	2003	2	-	7/41/137/137	-
4	BCL	S	2001	2	-	2/23/119/137	-
6	U10	R	2009	-	-	4/9/33/87	0/1/1/1
9	LDA	M	1013	-	-	5/13/13/13	-
9	LDA	M	1014	-	-	2/7/7/13	-
5	BPH	M	1005	-	-	6/21/89/105	0/5/6/6
6	U10	M	1008	-	-	3/33/57/87	0/1/1/1
4	BCL	M	1004	1	-	7/41/137/137	-
4	BCL	M	1001	2	-	4/23/119/137	-
5	BPH	L	1006	-	-	9/37/105/105	0/5/6/6
9	LDA	M	1012	-	-	8/13/13/13	-
4	BCL	M	1003	2	-	1/41/137/137	-
5	BPH	R	2006	-	-	6/37/105/105	0/5/6/6
6	U10	L	1009	-	-	14/41/65/87	0/1/1/1
6	U10	S	2008	-	-	5/26/50/87	0/1/1/1
4	BCL	L	1002	1	-	3/41/137/137	-
4	BCL	R	2002	1	-	5/41/137/137	-
5	BPH	S	2005	-	-	7/22/90/105	0/5/6/6
9	LDA	S	2012	-	-	5/13/13/13	-
4	BCL	R	2004	1	-	5/41/137/137	-

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1014	LDA	O1-N1	-8.17	1.22	1.42
9	M	1013	LDA	O1-N1	-8.06	1.22	1.42
9	S	2012	LDA	O1-N1	-7.91	1.22	1.42
9	M	1012	LDA	O1-N1	-7.43	1.24	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1008	U10	C6-C1	6.78	1.47	1.35
6	S	2008	U10	C6-C1	6.24	1.46	1.35
6	R	2009	U10	C6-C1	5.95	1.45	1.35
6	L	1009	U10	C6-C1	5.63	1.45	1.35
4	R	2002	BCL	C2-C3	4.15	1.42	1.33
5	L	1006	BPH	C3D-CAD	-3.82	1.40	1.47
6	M	1008	U10	C8-C9	3.79	1.41	1.33
6	L	1009	U10	C7-C8	-3.78	1.44	1.50
5	L	1006	BPH	C2-C3	3.70	1.41	1.33
5	S	2005	BPH	C3D-CAD	-3.70	1.40	1.47
5	R	2006	BPH	C3D-CAD	-3.67	1.40	1.47
6	L	1009	U10	C28-C29	3.62	1.41	1.33
4	S	2001	BCL	C1D-C2D	-3.53	1.38	1.45
5	M	1005	BPH	C3D-CAD	-3.51	1.41	1.47
6	S	2008	U10	C13-C14	3.42	1.40	1.33
5	S	2005	BPH	C3B-CAB	-3.36	1.40	1.49
5	M	1005	BPH	C3A-C2A	-3.36	1.51	1.54
4	M	1004	BCL	O2D-CGD	-3.24	1.25	1.33
4	R	2004	BCL	O2D-CGD	-3.23	1.25	1.33
4	M	1004	BCL	C1B-NB	-3.23	1.33	1.37
4	S	2001	BCL	O2D-CGD	-3.22	1.25	1.33
6	S	2008	U10	C18-C19	3.22	1.40	1.33
4	R	2002	BCL	C1D-C2D	-3.20	1.39	1.45
6	M	1008	U10	C23-C24	3.20	1.40	1.33
5	S	2005	BPH	O2D-CGD	-3.17	1.25	1.33
6	M	1008	U10	C18-C19	3.16	1.40	1.33
4	L	1002	BCL	C2-C3	3.15	1.40	1.33
6	L	1009	U10	C8-C9	3.10	1.40	1.33
4	R	2002	BCL	O2D-CGD	-3.09	1.25	1.33
4	L	1002	BCL	O2D-CGD	-3.09	1.25	1.33
5	M	1005	BPH	O2D-CGD	-3.08	1.25	1.33
4	M	1001	BCL	O2D-CGD	-3.08	1.25	1.33
6	M	1008	U10	C7-C8	-3.07	1.45	1.50
4	S	2003	BCL	C1D-C2D	-3.04	1.39	1.45
5	R	2006	BPH	O2D-CGD	-2.99	1.25	1.33
4	S	2003	BCL	O2D-CGD	-2.95	1.26	1.33
4	M	1003	BCL	C1D-C2D	-2.92	1.39	1.45
4	S	2003	BCL	C2-C3	2.91	1.39	1.33
6	L	1009	U10	C18-C19	2.90	1.39	1.33
5	R	2006	BPH	O2A-CGA	-2.89	1.24	1.33
6	L	1009	U10	C33-C34	2.88	1.39	1.33
4	M	1001	BCL	C1D-C2D	-2.87	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1006	BPH	O2A-CGA	-2.87	1.25	1.33
6	R	2009	U10	C8-C9	2.86	1.41	1.32
4	M	1003	BCL	O2D-CGD	-2.86	1.26	1.33
4	R	2004	BCL	C2-C3	2.84	1.39	1.33
6	M	1008	U10	C13-C14	2.83	1.39	1.33
5	L	1006	BPH	O2D-CGD	-2.80	1.26	1.33
6	M	1008	U10	C28-C29	2.80	1.40	1.32
6	S	2008	U10	C8-C9	2.80	1.39	1.33
5	M	1005	BPH	C2-C3	2.76	1.39	1.33
4	S	2001	BCL	C1D-ND	-2.76	1.34	1.37
6	R	2009	U10	C7-C6	2.75	1.56	1.51
5	M	1005	BPH	O2A-CGA	-2.71	1.25	1.33
4	M	1004	BCL	C1D-C2D	-2.67	1.40	1.45
4	M	1003	BCL	O2A-CGA	-2.67	1.25	1.33
6	L	1009	U10	C13-C14	2.63	1.39	1.33
4	M	1004	BCL	O2A-CGA	-2.60	1.25	1.33
5	S	2005	BPH	O2A-CGA	-2.59	1.25	1.33
4	M	1001	BCL	O2A-CGA	-2.59	1.25	1.33
6	L	1009	U10	C23-C24	2.55	1.38	1.33
5	R	2006	BPH	C3B-CAB	-2.51	1.42	1.49
4	M	1001	BCL	C1D-ND	-2.51	1.34	1.37
4	M	1004	BCL	C2-C3	2.50	1.38	1.33
4	S	2003	BCL	O2A-CGA	-2.49	1.26	1.33
4	L	1002	BCL	C1D-C2D	-2.47	1.40	1.45
4	L	1002	BCL	O2A-CGA	-2.45	1.26	1.33
4	R	2002	BCL	O2A-CGA	-2.44	1.26	1.33
4	S	2001	BCL	O2A-CGA	-2.44	1.26	1.33
5	S	2005	BPH	C2C-C3C	-2.43	1.52	1.54
4	M	1003	BCL	C2-C3	2.41	1.38	1.33
4	R	2004	BCL	O2A-CGA	-2.41	1.26	1.33
5	L	1006	BPH	C1C-C2C	2.40	1.56	1.51
4	L	1002	BCL	C1B-NB	-2.36	1.34	1.37
4	S	2003	BCL	C1D-ND	-2.35	1.34	1.37
5	R	2006	BPH	C2-C3	2.34	1.38	1.33
5	S	2005	BPH	C2-C3	2.31	1.38	1.33
6	M	1008	U10	C30-C29	2.30	1.56	1.50
6	L	1009	U10	C4-C3	2.29	1.44	1.36
5	M	1005	BPH	C3B-CAB	-2.27	1.43	1.49
5	L	1006	BPH	C3B-CAB	-2.24	1.43	1.49
4	M	1001	BCL	CMD-C2D	2.22	1.55	1.50
4	S	2001	BCL	C3C-C4C	2.21	1.54	1.51
6	S	2008	U10	C4-C3	2.21	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1001	BCL	CMB-C2B	2.20	1.55	1.50
4	M	1004	BCL	C3D-CAD	-2.20	1.37	1.45
4	M	1001	BCL	C2-C3	2.14	1.38	1.32
4	R	2004	BCL	C3D-CAD	-2.14	1.38	1.45
4	S	2001	BCL	C2-C3	2.13	1.38	1.32
6	S	2008	U10	C7-C6	2.10	1.55	1.51
4	M	1004	BCL	CBB-CAB	2.09	1.54	1.50
6	R	2009	U10	C4-C3	2.08	1.43	1.36
4	L	1002	BCL	C4-C3	2.06	1.55	1.50
4	R	2004	BCL	C1D-C2D	-2.06	1.41	1.45
4	M	1003	BCL	C3D-CAD	-2.04	1.38	1.45
9	M	1014	LDA	C1-N1	-2.04	1.49	1.51
4	R	2004	BCL	CMD-C2D	2.02	1.54	1.50
6	M	1008	U10	C7-C6	2.01	1.55	1.51

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1006	BPH	C4D-CHA-CBD	-7.86	104.69	108.45
4	M	1001	BCL	C1C-NC-C4C	7.26	109.99	106.68
5	R	2006	BPH	C4D-CHA-CBD	-7.26	104.97	108.45
4	M	1004	BCL	C1C-NC-C4C	7.22	109.97	106.68
5	S	2005	BPH	C4D-CHA-CBD	-7.07	105.07	108.45
5	S	2005	BPH	C3D-C4D-ND	6.89	116.54	107.71
5	L	1006	BPH	O2D-CGD-CBD	6.72	118.33	110.95
5	M	1005	BPH	O2D-CGD-CBD	6.58	118.18	110.95
4	S	2003	BCL	C1C-NC-C4C	6.46	109.62	106.68
5	R	2006	BPH	C3D-C4D-ND	6.39	115.90	107.71
5	S	2005	BPH	O2D-CGD-CBD	6.33	117.90	110.95
5	L	1006	BPH	C2B-C1B-NB	6.26	113.96	109.43
5	M	1005	BPH	C4D-CHA-CBD	-6.05	105.55	108.45
5	S	2005	BPH	C4D-ND-C1D	-5.96	101.73	108.87
5	L	1006	BPH	C3D-C4D-ND	5.80	115.15	107.71
5	M	1005	BPH	C3D-C4D-ND	5.74	115.07	107.71
4	R	2002	BCL	C1C-NC-C4C	5.66	109.26	106.68
4	M	1004	BCL	C4A-NA-C1A	5.64	109.25	106.68
4	M	1001	BCL	C4A-NA-C1A	5.60	109.23	106.68
5	R	2006	BPH	O2D-CGD-CBD	5.59	117.09	110.95
4	R	2004	BCL	C1C-NC-C4C	5.55	109.21	106.68
4	L	1002	BCL	C1C-NC-C4C	5.50	109.19	106.68
5	R	2006	BPH	C4D-ND-C1D	-5.49	102.29	108.87
4	S	2003	BCL	C1D-ND-C4D	-5.41	102.52	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1004	BCL	C1D-ND-C4D	-5.23	102.64	106.31
4	M	1004	BCL	C4D-CHA-C1A	5.15	127.38	121.24
4	S	2001	BCL	C1C-NC-C4C	5.07	108.99	106.68
5	M	1005	BPH	C4A-C3A-C2A	5.02	107.61	102.84
4	M	1003	BCL	C4A-NA-C1A	5.00	108.96	106.68
4	M	1003	BCL	C4D-CHA-C1A	4.94	127.14	121.24
5	M	1005	BPH	C4D-ND-C1D	-4.84	103.08	108.87
5	M	1005	BPH	C4-C3-C5	4.76	121.73	116.13
4	R	2004	BCL	C4D-CHA-C1A	4.76	126.92	121.24
4	S	2003	BCL	C4D-CHA-C1A	4.75	126.91	121.24
4	R	2004	BCL	C1D-ND-C4D	-4.71	103.00	106.31
4	L	1002	BCL	C4D-CHA-C1A	4.68	126.82	121.24
4	L	1002	BCL	C1D-ND-C4D	-4.64	103.06	106.31
4	S	2003	BCL	C3D-C4D-ND	4.60	117.46	109.99
4	S	2001	BCL	C4D-CHA-C1A	4.48	126.59	121.24
5	R	2006	BPH	C3D-CAD-CBD	4.46	113.48	107.61
4	M	1001	BCL	C4D-CHA-C1A	4.44	126.54	121.24
5	R	2006	BPH	C7-C6-C5	-4.39	101.56	113.26
4	S	2003	BCL	C4A-NA-C1A	4.34	108.66	106.68
6	L	1009	U10	C25-C24-C26	4.33	122.75	115.23
4	R	2004	BCL	C3D-C4D-ND	4.33	117.02	109.99
5	L	1006	BPH	C4D-ND-C1D	-4.30	103.72	108.87
4	M	1004	BCL	C3D-C4D-ND	4.26	116.92	109.99
5	M	1005	BPH	C1-O2A-CGA	4.26	126.97	116.65
5	L	1006	BPH	CMA-C3A-C4A	-4.24	105.48	114.61
5	M	1005	BPH	C3D-CAD-CBD	4.23	113.18	107.61
4	R	2004	BCL	C4A-NA-C1A	4.15	108.57	106.68
4	L	1002	BCL	C3D-C4D-ND	4.11	116.66	109.99
4	M	1001	BCL	C4D-C3D-CAD	-4.09	103.66	108.11
5	L	1006	BPH	C3D-CAD-CBD	4.08	112.97	107.61
5	S	2005	BPH	C3D-CAD-CBD	4.03	112.91	107.61
4	M	1003	BCL	C1D-ND-C4D	-3.99	103.52	106.31
5	M	1005	BPH	OBD-CAD-C3D	-3.98	121.69	127.89
4	R	2002	BCL	C4D-CHA-C1A	3.97	125.98	121.24
4	R	2004	BCL	C1-C2-C3	-3.95	119.72	126.20
4	S	2001	BCL	C1D-ND-C4D	-3.90	103.58	106.31
5	R	2006	BPH	CMA-C3A-C4A	-3.88	106.24	114.61
4	S	2001	BCL	C3D-C2D-C1D	3.87	111.11	105.83
4	R	2002	BCL	CED-O2D-CGD	3.85	124.66	115.92
4	S	2001	BCL	C4D-C3D-CAD	-3.84	103.94	108.11
4	S	2001	BCL	C3D-C4D-ND	3.80	116.17	109.99
5	S	2005	BPH	C1-O2A-CGA	3.77	125.79	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1003	BCL	C3D-C4D-ND	3.76	116.09	109.99
5	M	1005	BPH	CMA-C3A-C4A	-3.75	106.53	114.61
4	S	2001	BCL	C4A-NA-C1A	3.67	108.35	106.68
4	R	2004	BCL	C4D-C3D-CAD	-3.67	104.12	108.11
4	M	1003	BCL	C4D-C3D-CAD	-3.65	104.15	108.11
5	S	2005	BPH	C2B-C1B-NB	3.64	112.06	109.43
5	S	2005	BPH	C2D-C1D-ND	3.59	112.03	109.43
4	M	1004	BCL	C4-C3-C5	3.57	121.43	115.23
4	S	2003	BCL	C4D-C3D-CAD	-3.55	104.25	108.11
4	R	2002	BCL	C4D-C3D-CAD	-3.53	104.27	108.11
4	M	1001	BCL	C1-O2A-CGA	3.46	125.03	116.65
4	M	1001	BCL	C3D-C4D-ND	3.41	115.53	109.99
4	R	2002	BCL	C1D-ND-C4D	-3.39	103.93	106.31
5	R	2006	BPH	C1-O2A-CGA	3.39	124.86	116.65
5	S	2005	BPH	OBD-CAD-C3D	-3.37	122.63	127.89
5	R	2006	BPH	C2D-C1D-ND	3.37	111.86	109.43
5	L	1006	BPH	OBD-CAD-C3D	-3.31	122.73	127.89
4	M	1004	BCL	C4D-C3D-CAD	-3.27	104.56	108.11
4	M	1001	BCL	C1D-ND-C4D	-3.26	104.03	106.31
4	L	1002	BCL	C4D-C3D-CAD	-3.24	104.58	108.11
4	M	1001	BCL	C2A-C3A-C4A	3.24	107.10	101.87
4	M	1003	BCL	O2D-CGD-CBD	3.23	116.88	111.23
5	L	1006	BPH	C1B-NB-C4B	-3.22	104.12	108.82
4	L	1002	BCL	C4-C3-C5	3.21	120.81	115.23
4	R	2002	BCL	OBD-CAD-C3D	-3.21	120.92	128.42
4	S	2001	BCL	C1-O2A-CGA	3.20	124.41	116.65
4	S	2003	BCL	C3A-C2A-C1A	3.17	106.09	101.34
5	R	2006	BPH	O1D-CGD-CBD	-3.15	119.94	124.72
4	R	2002	BCL	C3D-C4D-ND	3.15	115.11	109.99
4	R	2004	BCL	CHA-C4D-ND	-3.14	126.07	132.55
4	S	2003	BCL	CHA-C4D-ND	-3.13	126.10	132.55
5	S	2005	BPH	C1B-NB-C4B	-3.10	104.30	108.82
5	R	2006	BPH	C4A-C3A-C2A	3.06	105.75	102.84
4	M	1004	BCL	CHA-C4D-ND	-3.03	126.30	132.55
4	S	2003	BCL	C3D-C2D-C1D	3.01	109.94	105.83
5	R	2006	BPH	CMC-C2C-C1C	-3.01	108.14	114.61
4	M	1003	BCL	C15-C13-C12	2.98	127.17	112.07
4	R	2002	BCL	CHA-C1A-NA	-2.98	119.64	126.39
5	S	2005	BPH	O1D-CGD-CBD	-2.95	120.25	124.72
4	M	1001	BCL	OBD-CAD-C3D	-2.94	121.55	128.42
4	M	1004	BCL	CMD-C2D-C3D	-2.93	120.97	127.69
9	M	1012	LDA	O1-N1-C1	2.91	116.42	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1004	BCL	CAC-C3C-C4C	-2.90	106.15	112.58
4	M	1004	BCL	C2A-C3A-C4A	2.87	106.50	101.87
4	R	2004	BCL	O2D-CGD-CBD	2.85	116.22	111.23
4	R	2004	BCL	OBD-CAD-C3D	-2.85	121.76	128.42
5	L	1006	BPH	C7-C6-C5	-2.84	105.68	113.26
4	S	2001	BCL	CHA-C4D-ND	-2.82	126.73	132.55
4	S	2001	BCL	O2D-CGD-CBD	2.81	116.15	111.23
4	R	2002	BCL	CMA-C3A-C4A	-2.80	104.24	111.77
5	M	1005	BPH	C4C-C3C-C2C	2.77	105.48	102.84
4	L	1002	BCL	C4A-NA-C1A	2.77	107.94	106.68
4	M	1003	BCL	C1C-NC-C4C	2.77	107.94	106.68
4	R	2002	BCL	C2A-C3A-C4A	2.76	106.33	101.87
4	M	1003	BCL	C3D-C2D-C1D	2.76	109.59	105.83
5	L	1006	BPH	O1D-CGD-CBD	-2.75	120.55	124.72
5	M	1005	BPH	O2A-C1-C2	-2.75	97.52	108.11
4	M	1001	BCL	C3D-C2D-C1D	2.75	109.58	105.83
4	R	2002	BCL	C3D-C2D-C1D	2.74	109.58	105.83
4	S	2001	BCL	C2A-C3A-C4A	2.74	106.29	101.87
5	S	2005	BPH	C4A-C3A-C2A	2.72	105.42	102.84
6	S	2008	U10	C10-C9-C11	2.69	119.90	115.23
5	M	1005	BPH	O1D-CGD-CBD	-2.69	120.64	124.72
4	M	1001	BCL	O2D-CGD-CBD	2.69	115.93	111.23
6	M	1008	U10	C4M-O4-C4	2.67	125.86	116.47
5	M	1005	BPH	CMD-C2D-C3D	-2.66	119.36	124.68
4	M	1003	BCL	C1-O2A-CGA	2.66	123.09	116.65
5	S	2005	BPH	C3B-C4B-NB	2.66	111.92	108.05
5	S	2005	BPH	C4C-C3C-C2C	2.66	105.37	102.84
5	R	2006	BPH	OBD-CAD-C3D	-2.65	123.76	127.89
5	L	1006	BPH	CMB-C2B-C3B	2.65	129.98	124.68
4	M	1004	BCL	C3D-C2D-C1D	2.63	109.42	105.83
5	R	2006	BPH	CMB-C2B-C3B	2.62	129.92	124.68
4	M	1004	BCL	C3B-C4B-NB	2.62	113.21	109.76
4	L	1002	BCL	CHA-C4D-ND	-2.61	127.16	132.55
4	M	1003	BCL	CHA-C4D-ND	-2.60	127.17	132.55
4	M	1004	BCL	CHA-C1A-NA	-2.56	120.60	126.39
4	R	2002	BCL	O2D-CGD-CBD	2.55	115.69	111.23
5	M	1005	BPH	CMB-C2B-C3B	2.54	129.76	124.68
4	M	1003	BCL	OBD-CAD-C3D	-2.54	122.48	128.42
4	R	2002	BCL	CAC-C3C-C4C	-2.54	106.96	112.58
4	R	2004	BCL	CAC-C3C-C4C	-2.54	106.96	112.58
5	R	2006	BPH	CED-O2D-CGD	2.53	121.66	115.92
5	M	1005	BPH	CED-O2D-CGD	2.51	121.61	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1008	U10	C3M-O3-C3	2.50	125.26	116.47
4	M	1001	BCL	CHA-C1A-NA	-2.50	120.74	126.39
4	R	2002	BCL	C4A-NA-C1A	2.50	107.82	106.68
5	L	1006	BPH	CMC-C2C-C1C	-2.49	109.25	114.61
4	S	2003	BCL	O2D-CGD-CBD	2.48	115.57	111.23
4	S	2003	BCL	C1-O2A-CGA	2.48	122.66	116.65
4	M	1004	BCL	C1-C2-C3	-2.47	122.14	126.20
5	R	2006	BPH	C2B-C1B-NB	2.47	111.22	109.43
5	S	2005	BPH	O2A-C1-C2	-2.46	98.64	108.11
4	M	1001	BCL	CHA-C4D-ND	-2.46	127.48	132.55
4	S	2001	BCL	CMA-C3A-C4A	-2.45	105.18	111.77
6	R	2009	U10	C1-C6-C5	-2.45	117.24	119.62
4	M	1004	BCL	CHD-C1D-ND	-2.44	121.36	124.80
4	L	1002	BCL	C3D-C2D-C1D	2.44	109.17	105.83
4	M	1004	BCL	C15-C13-C12	-2.43	99.74	112.07
4	M	1004	BCL	CMD-C2D-C1D	2.41	128.97	124.73
9	S	2012	LDA	O1-N1-C1	2.41	115.18	109.27
4	S	2003	BCL	CAC-C3C-C4C	-2.40	107.25	112.58
6	L	1009	U10	C1M-C1-C6	-2.40	120.50	124.45
4	S	2001	BCL	CHA-C1A-NA	-2.39	120.98	126.39
6	L	1009	U10	C30-C29-C31	2.38	119.36	115.23
4	R	2004	BCL	C6-C5-C3	-2.38	107.67	113.47
5	S	2005	BPH	CMA-C3A-C4A	-2.37	109.51	114.61
4	M	1001	BCL	CMC-C2C-C1C	-2.36	105.43	111.77
4	L	1002	BCL	C2A-C3A-C4A	2.36	105.68	101.87
4	M	1004	BCL	C2C-C3C-C4C	2.35	104.87	101.34
6	L	1009	U10	C35-C34-C36	2.35	118.89	116.13
4	R	2004	BCL	C2A-C3A-C4A	2.35	105.66	101.87
4	L	1002	BCL	CHA-C1A-NA	-2.35	121.07	126.39
4	M	1004	BCL	O1D-CGD-CBD	-2.34	119.90	124.52
6	S	2008	U10	C1M-C1-C6	-2.32	120.64	124.45
4	M	1004	BCL	OBD-CAD-C3D	-2.31	123.03	128.42
6	L	1009	U10	C4M-O4-C4	2.30	124.57	116.47
4	M	1003	BCL	C7-C6-C5	-2.29	107.15	113.26
4	L	1002	BCL	CMA-C3A-C4A	-2.29	105.62	111.77
6	R	2009	U10	C3M-O3-C3	2.28	124.48	116.47
4	M	1001	BCL	CMA-C3A-C4A	-2.27	105.68	111.77
4	R	2002	BCL	C1-O2A-CGA	2.26	122.13	116.65
6	R	2009	U10	C3-C2-C1	2.26	122.57	118.10
9	M	1013	LDA	O1-N1-C1	2.26	114.81	109.27
6	S	2008	U10	C21-C22-C23	-2.25	107.69	112.57
4	R	2002	BCL	C2B-C1B-NB	2.24	112.65	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	2004	BCL	C2B-C1B-NB	2.24	112.64	110.33
4	M	1001	BCL	OBB-CAB-CBB	-2.23	114.77	119.77
4	M	1001	BCL	CHB-C4A-NA	2.22	127.61	124.40
4	S	2001	BCL	OBD-CAD-C3D	-2.22	123.22	128.42
4	R	2002	BCL	CHA-C4D-ND	-2.22	127.97	132.55
4	S	2001	BCL	CHC-C4B-NB	-2.21	120.73	124.05
6	M	1008	U10	C31-C29-C30	2.20	119.66	114.59
4	M	1003	BCL	C2B-C1B-NB	2.19	112.60	110.33
4	S	2001	BCL	C1-C2-C3	2.19	130.30	126.76
9	M	1014	LDA	O1-N1-C1	2.19	114.64	109.27
4	M	1003	BCL	C3A-C2A-C1A	2.19	104.61	101.34
9	M	1012	LDA	C6-C5-C4	-2.18	103.32	114.37
6	M	1008	U10	C25-C24-C26	2.18	119.01	115.23
5	M	1005	BPH	C2B-C1B-NB	2.17	111.00	109.43
4	R	2004	BCL	C3D-C2D-C1D	2.16	108.78	105.83
4	M	1004	BCL	O2D-CGD-CBD	2.16	115.00	111.23
4	M	1003	BCL	O2A-CGA-CBA	2.15	118.40	111.83
4	R	2004	BCL	CHB-C4A-NA	2.15	127.50	124.40
5	M	1005	BPH	C1A-C2A-C3A	-2.15	100.80	102.84
9	M	1013	LDA	C6-C5-C4	-2.14	103.54	114.37
5	R	2006	BPH	C1B-NB-C4B	-2.12	105.72	108.82
4	R	2004	BCL	CHA-C1A-NA	-2.10	121.63	126.39
4	S	2003	BCL	O2A-CGA-CBA	2.10	118.24	111.83
6	R	2009	U10	C8-C7-C6	2.09	117.24	112.08
5	M	1005	BPH	CMC-C2C-C1C	-2.09	110.10	114.61
4	L	1002	BCL	OBB-CAB-CBB	-2.09	115.08	119.77
4	S	2003	BCL	CAB-C3B-C2B	-2.09	123.40	127.74
4	R	2002	BCL	C6-C5-C3	2.09	118.56	113.47
5	M	1005	BPH	C3B-C4B-NB	2.09	111.09	108.05
5	R	2006	BPH	OBD-CAD-CBD	-2.09	122.76	125.82
4	S	2003	BCL	CHC-C4B-NB	-2.08	120.92	124.05
5	R	2006	BPH	C3B-C4B-NB	2.08	111.08	108.05
5	S	2005	BPH	CMB-C2B-C3B	2.07	128.82	124.68
4	L	1002	BCL	CAA-C2A-C1A	-2.07	105.20	111.97
5	L	1006	BPH	O2A-CGA-CBA	2.06	118.13	111.83
4	M	1001	BCL	C2C-C3C-C4C	2.06	104.42	101.34
5	S	2005	BPH	CED-O2D-CGD	2.05	120.57	115.92
9	M	1013	LDA	C4-C3-C2	-2.05	104.00	114.37
5	L	1006	BPH	C1-O2A-CGA	2.04	121.59	116.65
4	S	2001	BCL	C2C-C3C-C4C	2.04	104.39	101.34
4	L	1002	BCL	C6-C5-C3	2.03	118.42	113.47
4	S	2001	BCL	C2A-C1A-CHA	2.03	127.39	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	2008	U10	C3M-O3-C3	2.03	123.59	116.47
4	M	1004	BCL	CMC-C2C-C3C	-2.01	106.19	113.98
5	M	1005	BPH	C1B-NB-C4B	-2.01	105.89	108.82

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1001	BCL	C2C-C3C-CAC-CBC
4	R	2004	BCL	C2C-C3C-CAC-CBC
4	R	2004	BCL	CBD-CGD-O2D-CED
5	M	1005	BPH	C2C-C3C-CAC-CBC
5	R	2006	BPH	C4C-C3C-CAC-CBC
5	R	2006	BPH	C2C-C3C-CAC-CBC
5	S	2005	BPH	C4C-C3C-CAC-CBC
5	S	2005	BPH	C2C-C3C-CAC-CBC
9	M	1012	LDA	C2-C1-N1-CM1
9	M	1012	LDA	C2-C1-N1-CM2
9	M	1013	LDA	C2-C1-N1-CM2
9	M	1014	LDA	N1-C1-C2-C3
4	R	2004	BCL	O1D-CGD-O2D-CED
6	L	1009	U10	C25-C24-C26-C27
6	L	1009	U10	C23-C24-C26-C27
5	S	2005	BPH	CBD-CGD-O2D-CED
6	L	1009	U10	C24-C26-C27-C28
6	M	1008	U10	C24-C26-C27-C28
4	R	2002	BCL	CBD-CGD-O2D-CED
6	L	1009	U10	C19-C21-C22-C23
4	R	2002	BCL	C15-C16-C17-C18
5	S	2005	BPH	O1D-CGD-O2D-CED
4	M	1001	BCL	C1-C2-C3-C5
6	L	1009	U10	C28-C29-C31-C32
4	L	1002	BCL	CBD-CGD-O2D-CED
9	S	2012	LDA	C11-C10-C9-C8
9	M	1012	LDA	C2-C3-C4-C5
6	L	1009	U10	C30-C29-C31-C32
4	R	2002	BCL	O1D-CGD-O2D-CED
9	S	2012	LDA	C1-C2-C3-C4
4	L	1002	BCL	C15-C16-C17-C18
9	S	2012	LDA	C6-C7-C8-C9
9	M	1012	LDA	C7-C8-C9-C10
4	S	2003	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	M	1013	LDA	C11-C10-C9-C8
5	R	2006	BPH	C10-C11-C12-C13
6	L	1009	U10	C29-C31-C32-C33
5	S	2005	BPH	C3-C5-C6-C7
9	M	1013	LDA	C1-C2-C3-C4
4	S	2003	BCL	C2C-C3C-CAC-CBC
5	R	2006	BPH	C4-C3-C5-C6
6	L	1009	U10	C12-C11-C9-C10
5	R	2006	BPH	C2-C3-C5-C6
6	L	1009	U10	C12-C11-C9-C8
5	L	1006	BPH	C10-C11-C12-C13
6	L	1009	U10	C15-C14-C16-C17
6	L	1009	U10	C13-C14-C16-C17
9	M	1012	LDA	C1-C2-C3-C4
5	L	1006	BPH	C15-C16-C17-C18
9	M	1013	LDA	C4-C5-C6-C7
9	M	1012	LDA	C4-C5-C6-C7
4	L	1002	BCL	O1D-CGD-O2D-CED
4	S	2003	BCL	C12-C13-C15-C16
5	L	1006	BPH	C11-C10-C8-C7
9	M	1014	LDA	C2-C3-C4-C5
9	M	1012	LDA	C6-C7-C8-C9
4	M	1001	BCL	C1-C2-C3-C4
4	S	2003	BCL	C14-C13-C15-C16
6	L	1009	U10	C9-C11-C12-C13
4	S	2003	BCL	C4C-C3C-CAC-CBC
4	R	2004	BCL	C12-C13-C15-C16
4	S	2003	BCL	C13-C15-C16-C17
6	R	2009	U10	C5-C6-C7-C8
4	S	2001	BCL	C2-C1-O2A-CGA
4	S	2003	BCL	O1D-CGD-O2D-CED
6	S	2008	U10	C20-C19-C21-C22
5	R	2006	BPH	C15-C16-C17-C18
9	S	2012	LDA	C2-C3-C4-C5
5	M	1005	BPH	C2-C3-C5-C6
4	M	1004	BCL	C12-C13-C15-C16
4	R	2004	BCL	C14-C13-C15-C16
9	M	1012	LDA	C2-C1-N1-O1
5	M	1005	BPH	C4C-C3C-CAC-CBC
4	M	1004	BCL	C3-C5-C6-C7
6	L	1009	U10	C2-C3-O3-C3M
6	R	2009	U10	C2-C3-O3-C3M

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Mol	Chain	Res	Type	Atoms
6	S	2008	U10	C5-C4-O4-C4M
4	M	1004	BCL	CHA-CBD-CGD-O1D
4	M	1004	BCL	CHA-CBD-CGD-O2D
4	M	1004	BCL	C14-C13-C15-C16
9	S	2012	LDA	N1-C1-C2-C3
6	S	2008	U10	C14-C16-C17-C18
4	R	2002	BCL	C2A-CAA-CBA-CGA
5	S	2005	BPH	C4-C3-C5-C6
9	M	1013	LDA	C2-C3-C4-C5
5	M	1005	BPH	O1A-CGA-O2A-C1
5	L	1006	BPH	C8-C10-C11-C12
5	M	1005	BPH	CBA-CGA-O2A-C1
5	S	2005	BPH	C2-C3-C5-C6
4	M	1004	BCL	C13-C15-C16-C17
5	M	1005	BPH	C4-C3-C5-C6
6	M	1008	U10	C5-C4-O4-C4M
6	R	2009	U10	C4-C3-O3-C3M
6	S	2008	U10	C18-C19-C21-C22
4	M	1003	BCL	C14-C13-C15-C16
5	L	1006	BPH	O2A-C1-C2-C3
6	S	2008	U10	C21-C22-C23-C24
5	L	1006	BPH	C11-C10-C8-C9
5	L	1006	BPH	C2-C3-C5-C6
6	L	1009	U10	C18-C19-C21-C22
5	L	1006	BPH	C4-C3-C5-C6
4	R	2002	BCL	C4-C3-C5-C6
4	S	2001	BCL	O1A-CGA-O2A-C1
6	R	2009	U10	C1-C6-C7-C8
6	M	1008	U10	C21-C22-C23-C24
4	M	1004	BCL	CAD-CBD-CGD-O2D
5	L	1006	BPH	CAD-CBD-CGD-O2D
4	M	1001	BCL	C2-C1-O2A-CGA

There are no ring outliers.

19 monomers are involved in 67 short contacts:

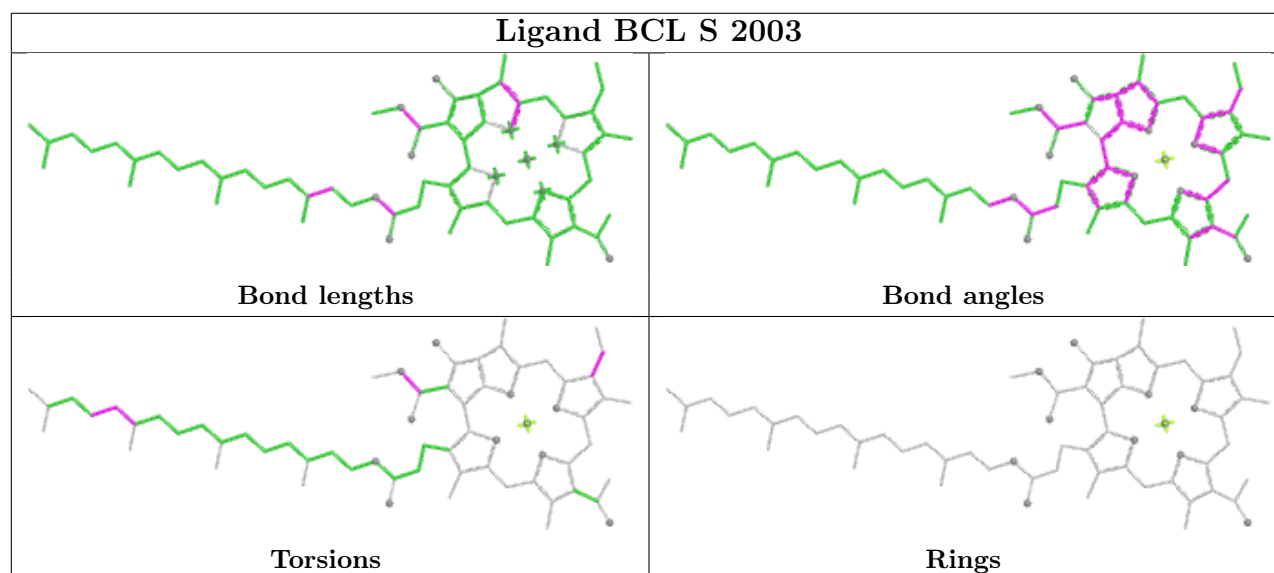
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	2003	BCL	6	0
4	S	2001	BCL	5	0
6	R	2009	U10	2	0
9	M	1013	LDA	2	0
9	M	1014	LDA	4	0

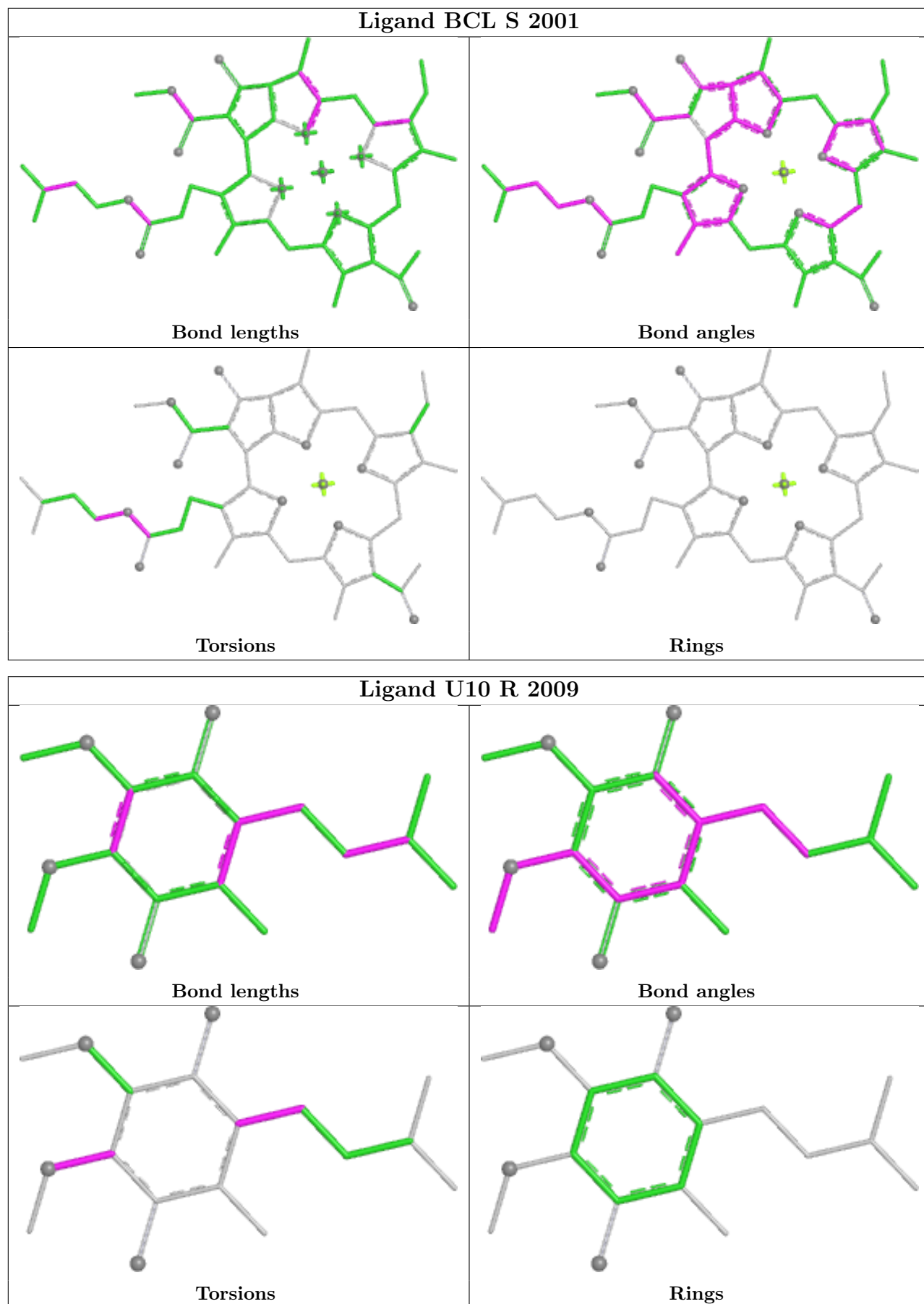
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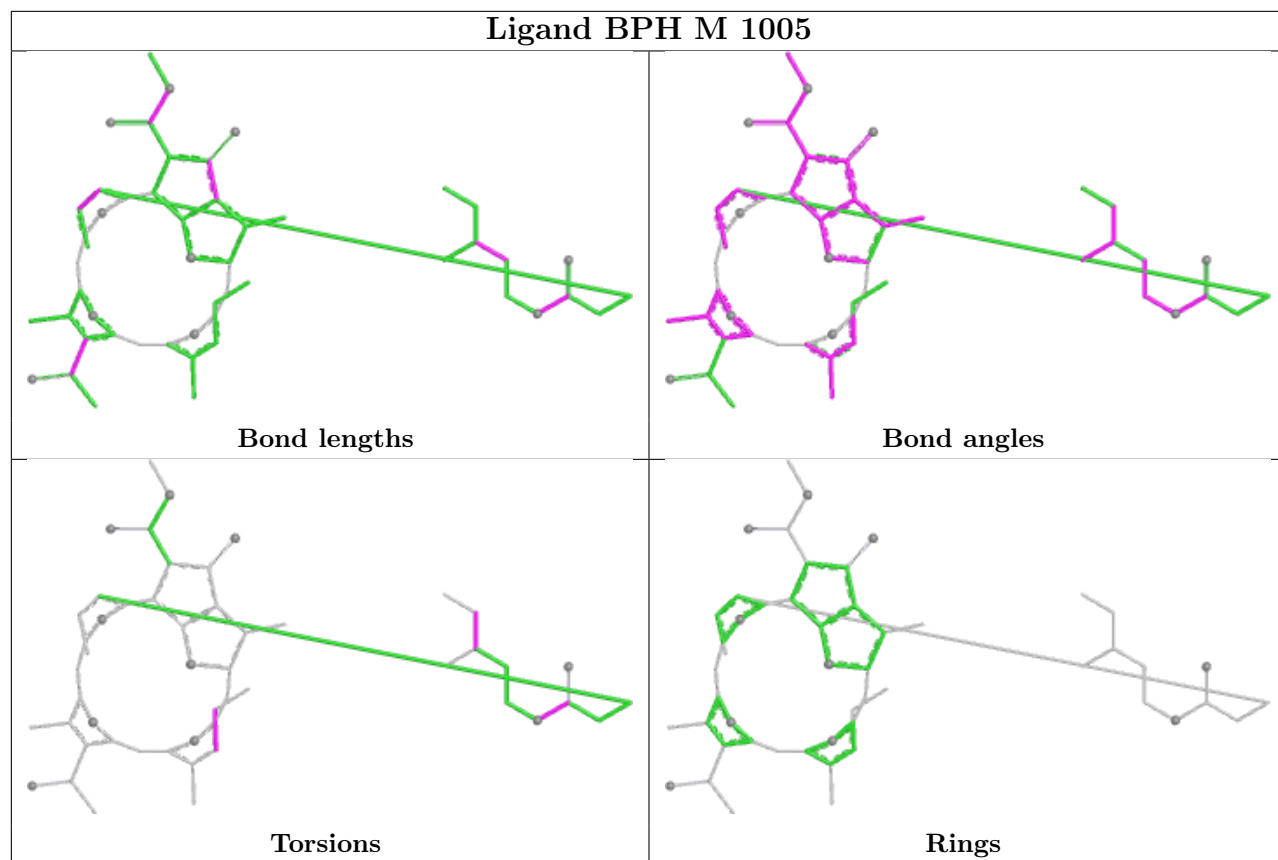
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1005	BPH	3	0
4	M	1004	BCL	8	0
4	M	1001	BCL	6	0
5	L	1006	BPH	8	0
9	M	1012	LDA	1	0
4	M	1003	BCL	7	0
5	R	2006	BPH	6	0
6	L	1009	U10	2	0
6	S	2008	U10	2	0
4	L	1002	BCL	8	0
4	R	2002	BCL	2	0
5	S	2005	BPH	3	0
9	S	2012	LDA	1	0
4	R	2004	BCL	7	0

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.

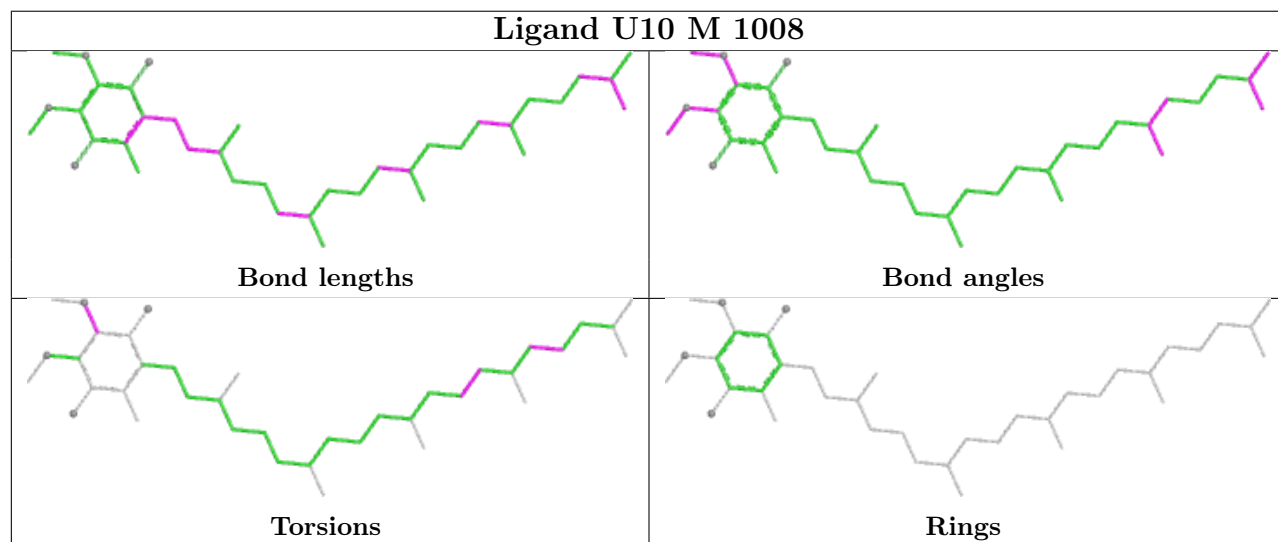


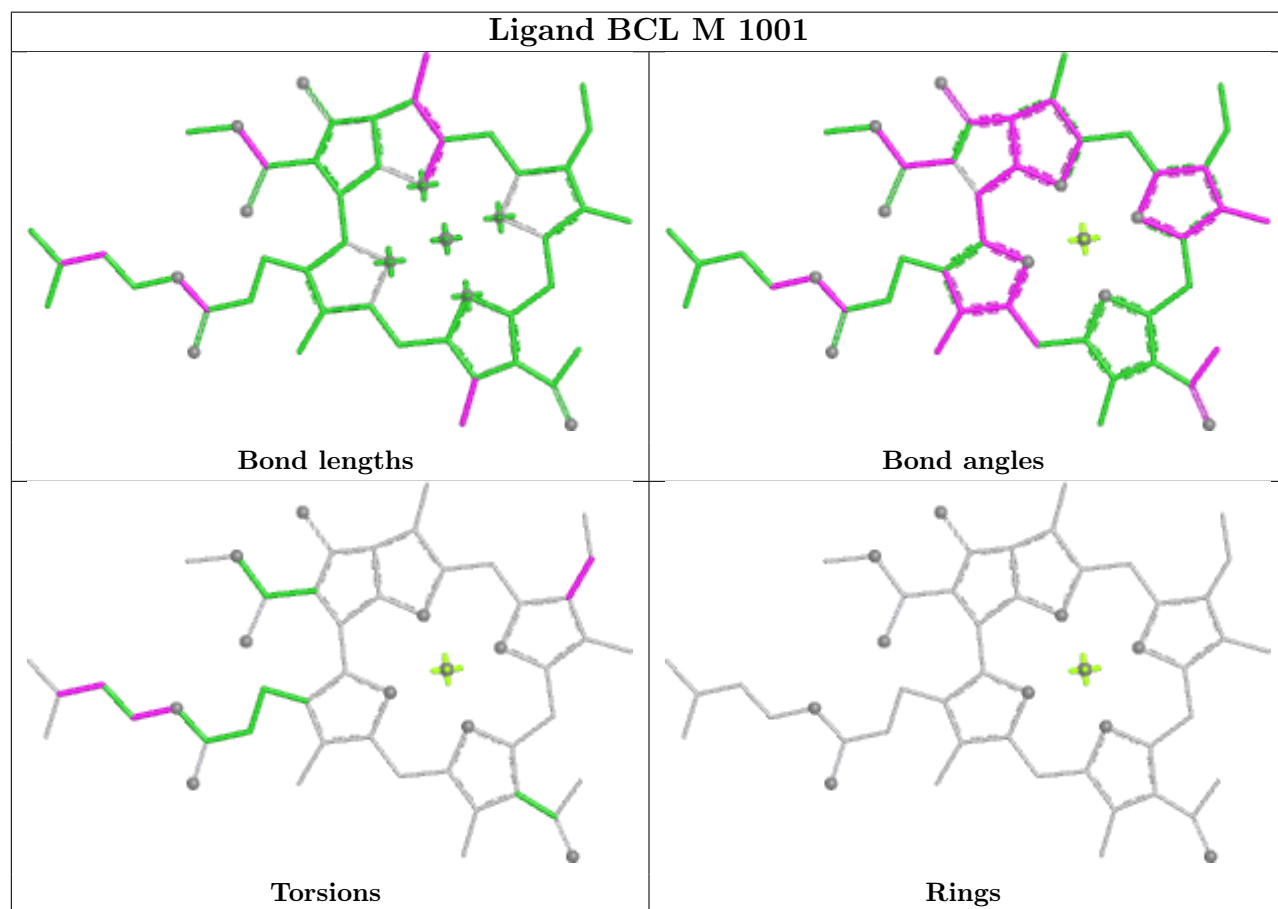
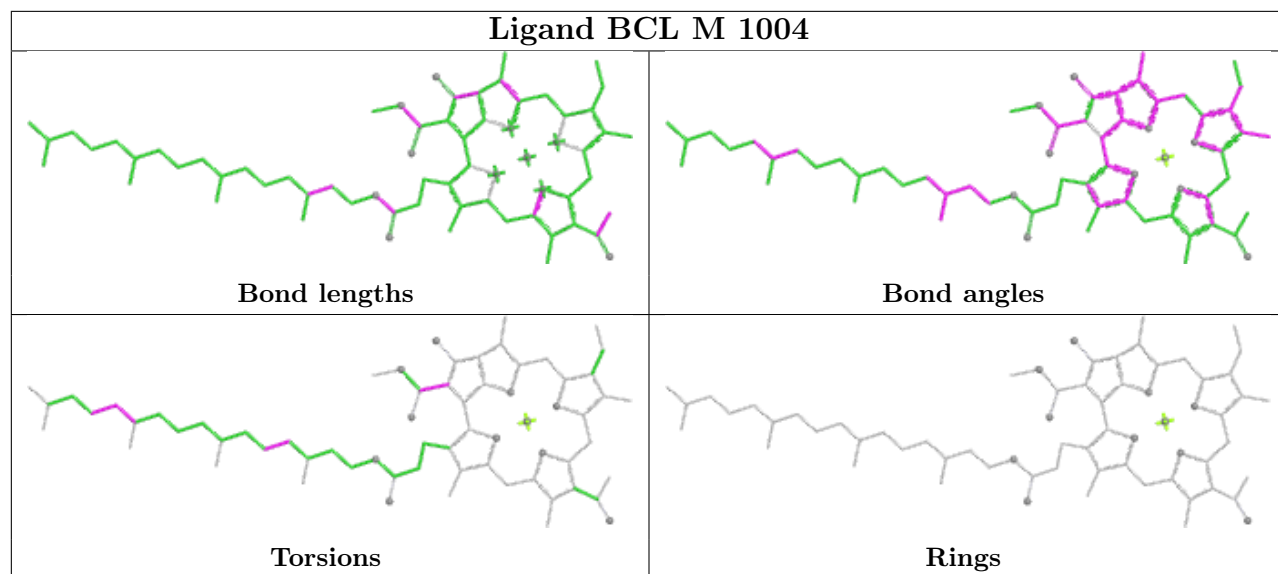


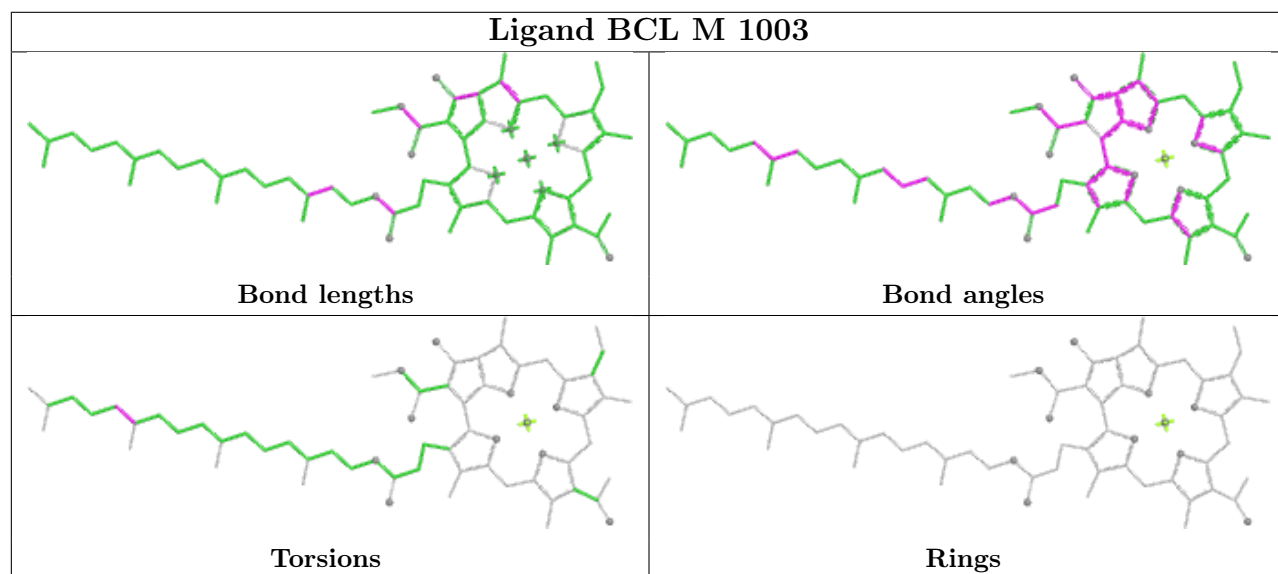
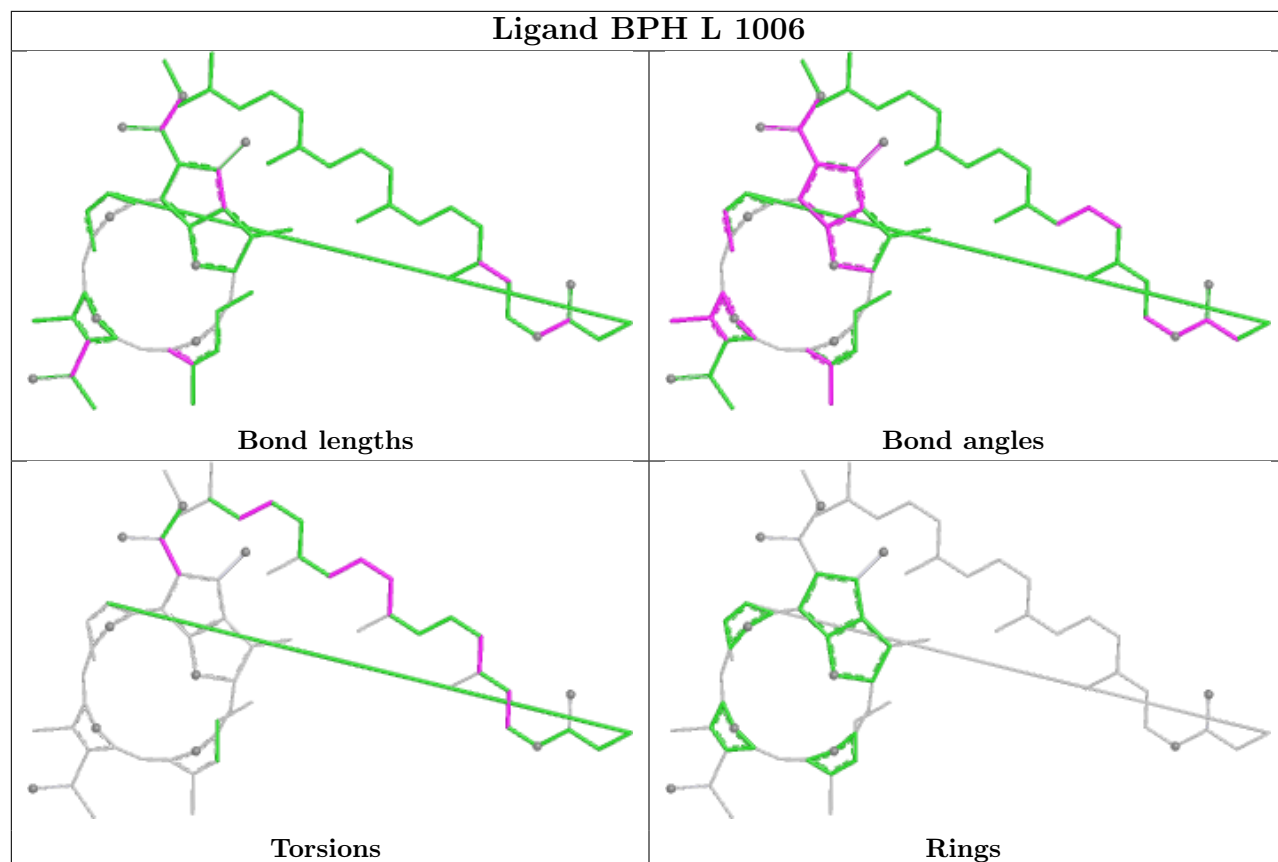
Ligand BPH M 1005



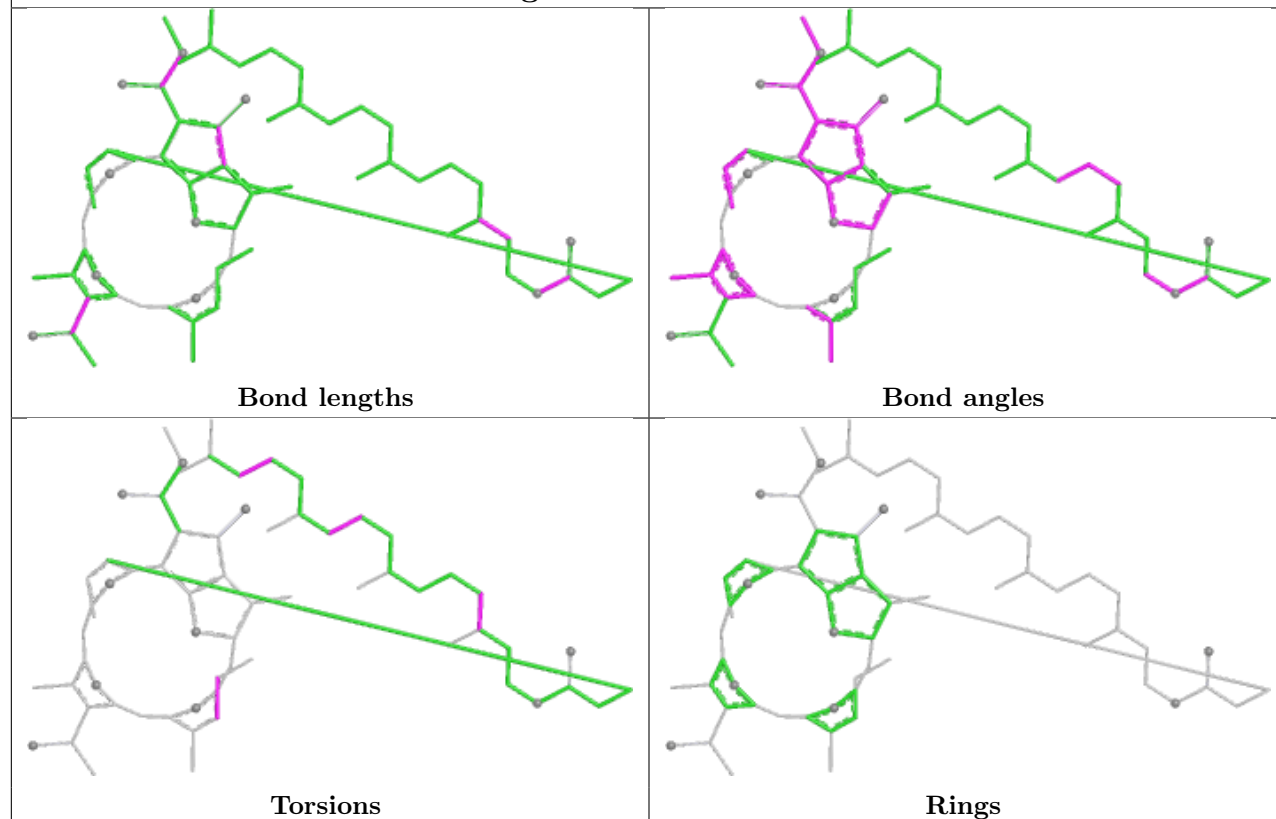
Ligand U10 M 1008



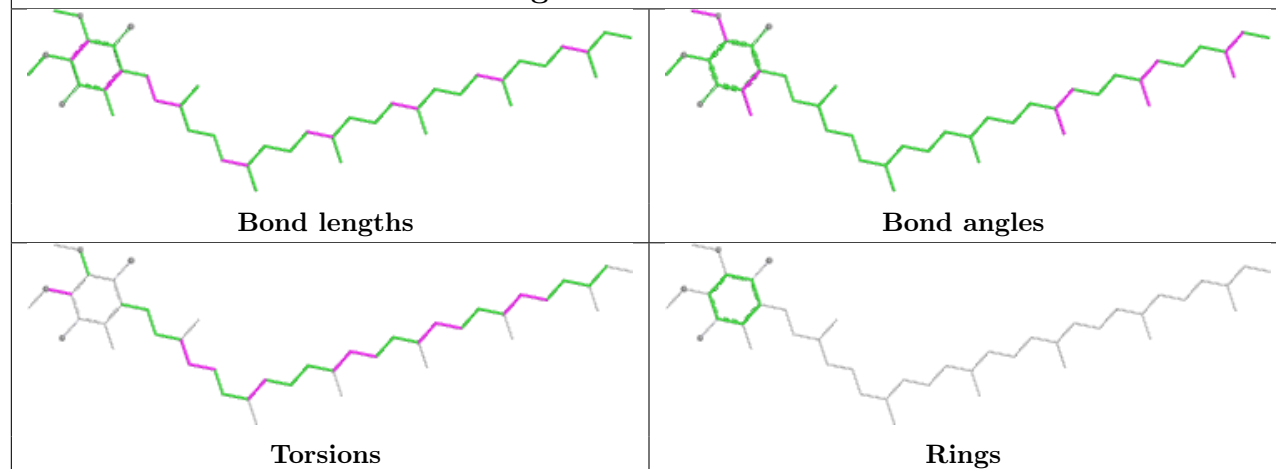


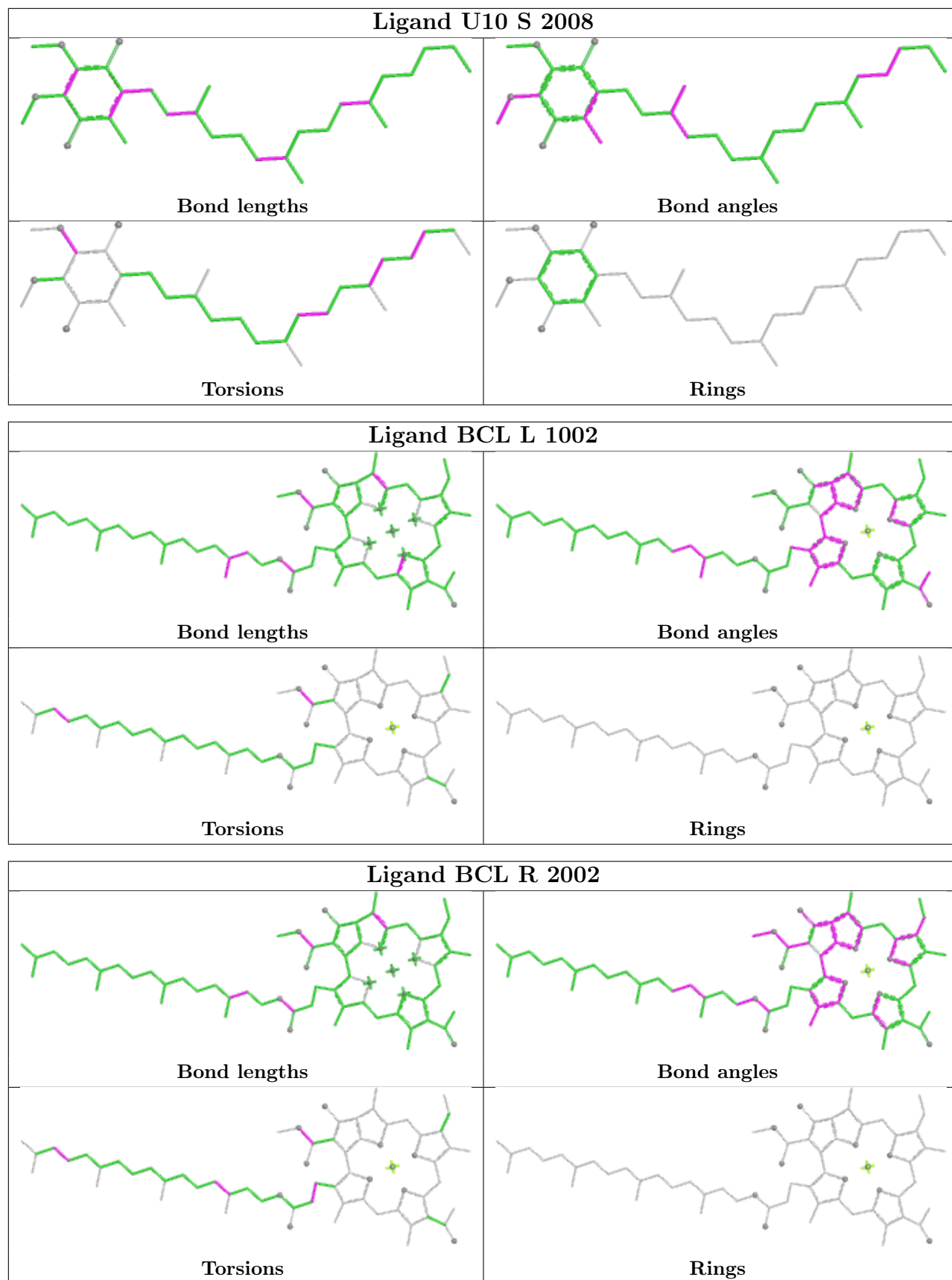


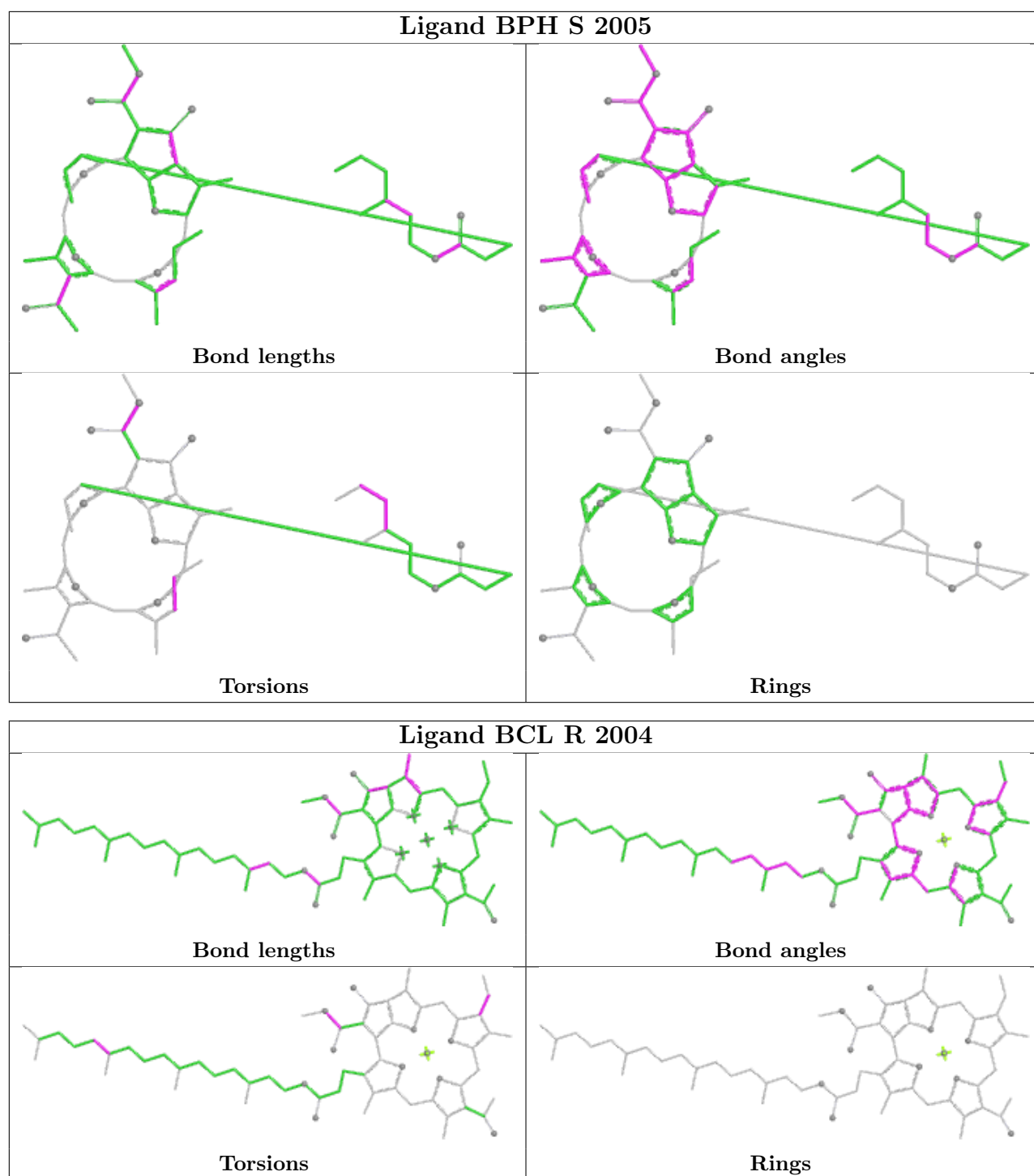
Ligand BPH R 2006



Ligand U10 L 1009







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%)	0.59	25 (8%)	15 13	30, 49, 74, 85	0
1	R	281/281 (100%)	0.59	15 (5%)	32 28	33, 50, 73, 85	0
2	M	299/307 (97%)	0.28	9 (3%)	52 48	34, 44, 59, 76	0
2	S	299/307 (97%)	0.40	5 (1%)	69 65	36, 46, 59, 75	0
3	H	246/260 (94%)	0.59	17 (6%)	23 20	40, 52, 73, 90	0
3	T	246/260 (94%)	0.57	11 (4%)	38 33	42, 53, 74, 90	0
All	All	1652/1696 (97%)	0.50	82 (4%)	34 30	30, 48, 71, 90	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	93	SER	5.3
3	H	68	HIS	5.2
3	H	80	SER	5.0
3	T	256	LEU	4.2
1	R	281	GLY	3.8
1	L	84	GLY	3.6
3	H	255	MET	3.6
1	L	51	TRP	3.5
1	L	80	LEU	3.4
3	H	252	VAL	3.4
2	S	77	GLN	3.3
1	R	271	TRP	3.1
2	S	84	VAL	3.1
3	H	254	ALA	3.1
2	M	298	GLY	3.1
2	M	82	PRO	3.0
1	L	83	GLY	2.9
3	H	95	GLY	2.9
1	L	278	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
3	T	69	GLY	2.8
3	H	92	VAL	2.8
3	H	256	LEU	2.8
2	M	301	HIS	2.8
1	R	276	PRO	2.7
1	L	69	PRO	2.7
3	H	50	ALA	2.7
3	H	91	ALA	2.7
3	T	79	GLU	2.6
3	T	80	SER	2.6
1	R	275	ILE	2.6
1	R	1	ALA	2.6
1	L	269	LEU	2.5
3	T	108	GLY	2.5
1	R	36	VAL	2.5
1	L	57	GLY	2.5
3	H	69	GLY	2.5
1	L	49	ILE	2.5
1	L	56	GLN	2.5
1	R	51	TRP	2.5
1	L	67	TYR	2.4
1	L	145	ALA	2.4
2	M	68	PHE	2.4
1	R	50	ALA	2.4
1	L	58	THR	2.4
1	L	55	LEU	2.4
1	L	73	TYR	2.4
1	L	59	TRP	2.4
3	H	90	THR	2.3
3	T	72	THR	2.3
1	R	278	GLY	2.3
3	H	102	GLY	2.3
1	L	79	PRO	2.3
1	L	277	GLY	2.3
3	T	96	PHE	2.2
1	L	270	PRO	2.2
3	T	98	HIS	2.2
2	M	111	GLU	2.2
1	L	276	PRO	2.2
1	R	25	TRP	2.2
2	S	87	ARG	2.1
1	L	68	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	T	68	HIS	2.1
1	L	43	ALA	2.1
3	T	50	ALA	2.1
2	M	90	PHE	2.1
2	S	3	TYR	2.1
3	H	96	PHE	2.1
1	R	37	ALA	2.1
1	R	59	TRP	2.1
1	L	7	ARG	2.1
2	S	52	LEU	2.1
3	T	57	PRO	2.1
1	R	24	PHE	2.0
1	R	274	ASN	2.0
2	M	52	LEU	2.0
1	R	45	GLY	2.0
2	M	72	ILE	2.0
3	H	73	LEU	2.0
3	H	81	GLU	2.0
1	L	281	GLY	2.0
2	M	300	ASN	2.0
1	L	266	TRP	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($\text{\AA}^2$)	Q<0.9
6	U10	L	1009	44/63	0.78	0.23	70,83,97,97	0
9	LDA	M	1014	10/16	0.78	0.27	51,53,57,58	0

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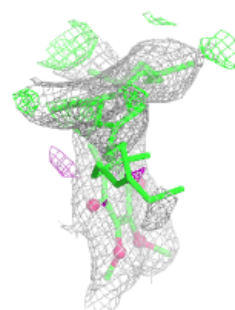
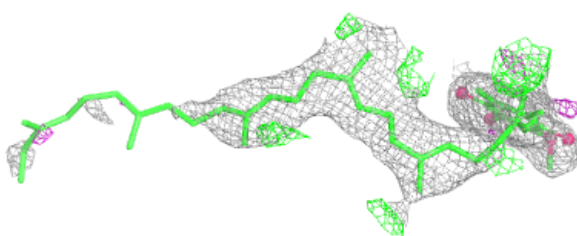
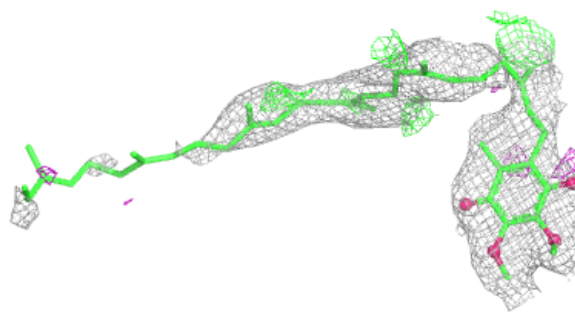
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	LDA	S	2012	16/16	0.79	0.22	51,61,69,70	0
9	LDA	M	1012	16/16	0.82	0.17	57,61,69,69	0
9	LDA	M	1013	16/16	0.82	0.13	53,56,58,58	0
6	U10	R	2009	18/63	0.83	0.17	73,75,76,76	0
6	U10	S	2008	32/63	0.90	0.11	52,54,56,56	0
4	BCL	R	2002	66/66	0.91	0.11	40,44,51,54	0
5	BPH	R	2006	65/65	0.92	0.12	50,56,60,62	0
4	BCL	R	2004	66/66	0.92	0.10	35,42,66,68	0
4	BCL	S	2001	51/66	0.92	0.09	38,42,49,51	0
5	BPH	L	1006	65/65	0.92	0.10	31,40,43,44	0
4	BCL	S	2003	66/66	0.93	0.10	41,42,55,56	0
6	U10	M	1008	38/63	0.93	0.09	31,37,54,54	0
5	BPH	S	2005	52/65	0.94	0.09	41,44,59,62	0
4	BCL	L	1002	66/66	0.94	0.09	34,38,41,43	0
4	BCL	M	1004	66/66	0.94	0.09	29,33,53,57	0
5	BPH	M	1005	51/65	0.95	0.07	31,33,40,42	0
8	CL	M	1011	1/1	0.95	0.09	45,45,45,45	0
4	BCL	M	1001	51/66	0.95	0.07	33,35,45,47	0
4	BCL	M	1003	66/66	0.96	0.08	29,35,44,49	0
8	CL	S	2011	1/1	0.96	0.17	66,66,66,66	0
10	ZN	T	2010	1/1	0.96	0.05	60,60,60,60	0
10	ZN	H	1010	1/1	0.99	0.03	57,57,57,57	0
7	FE2	M	1007	1/1	1.00	0.03	35,35,35,35	0
7	FE2	S	2007	1/1	1.00	0.02	42,42,42,42	0

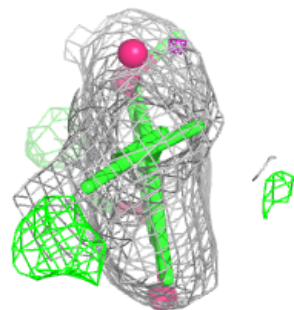
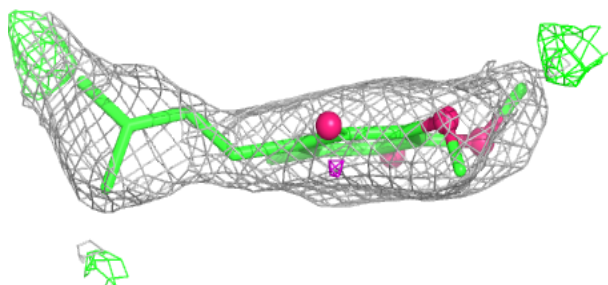
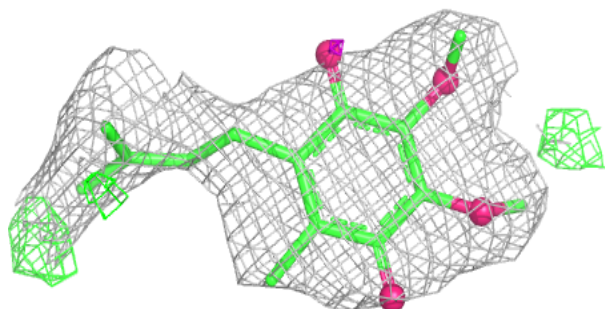
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U10 L 1009:

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

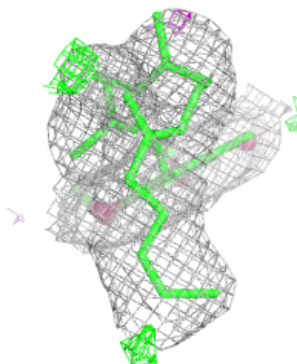
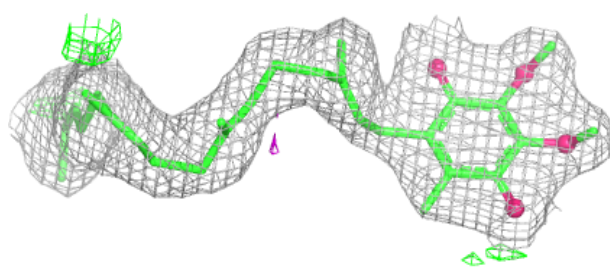
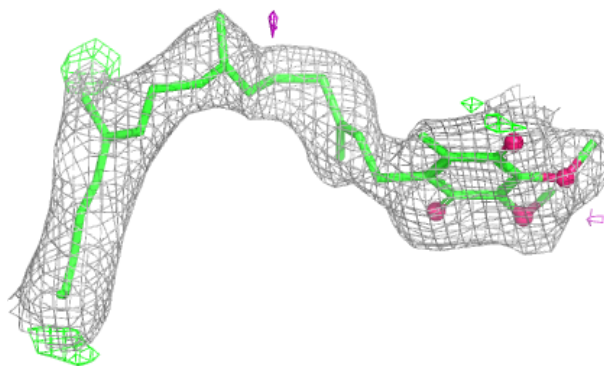
**Electron density around U10 R 2009:**

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

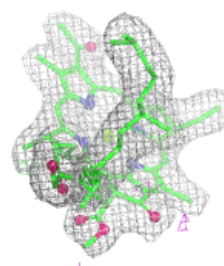
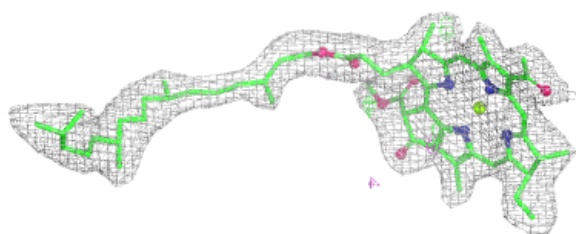
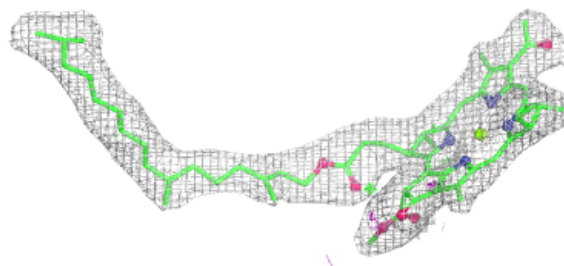


Electron density around U10 S 2008:

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

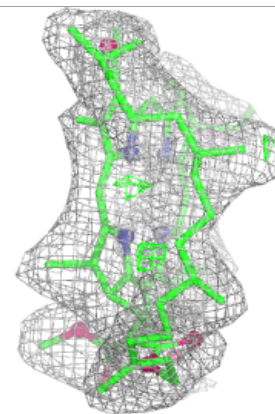
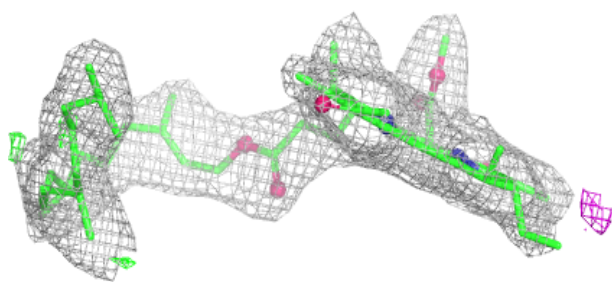
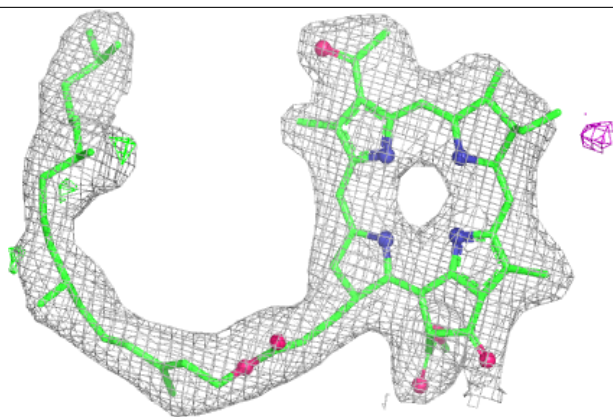
**Electron density around BCL R 2002:**

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

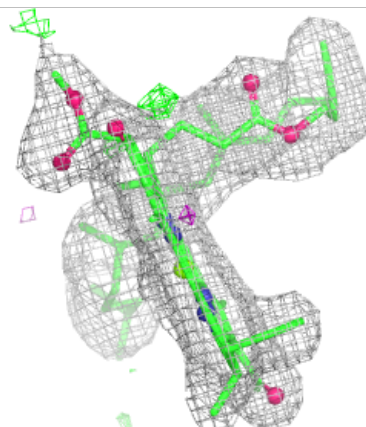
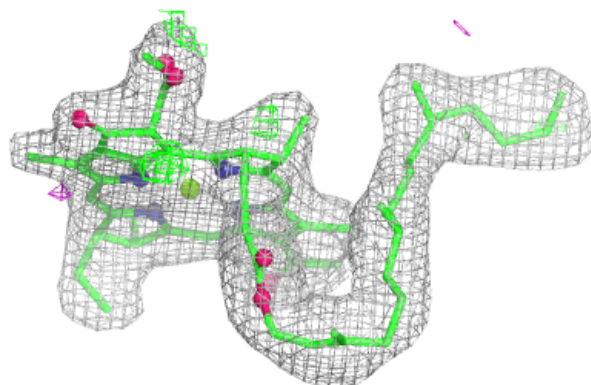
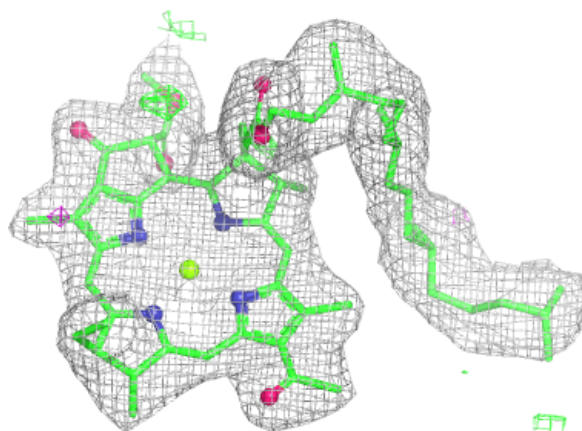


Electron density around BPH R 2006:

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

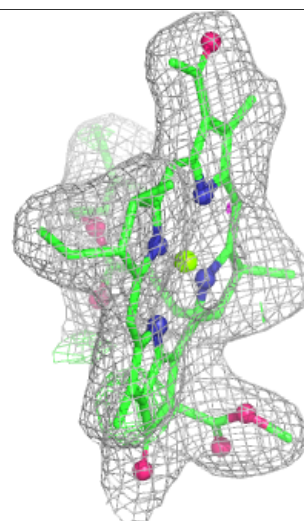
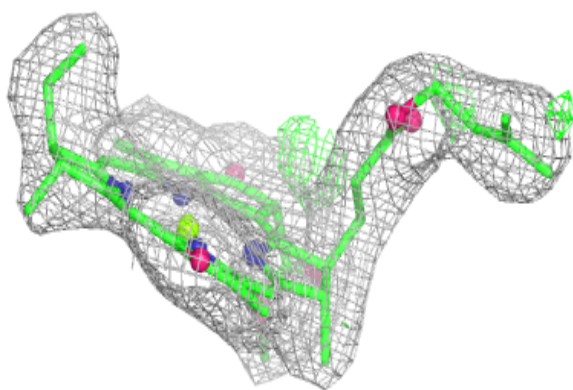
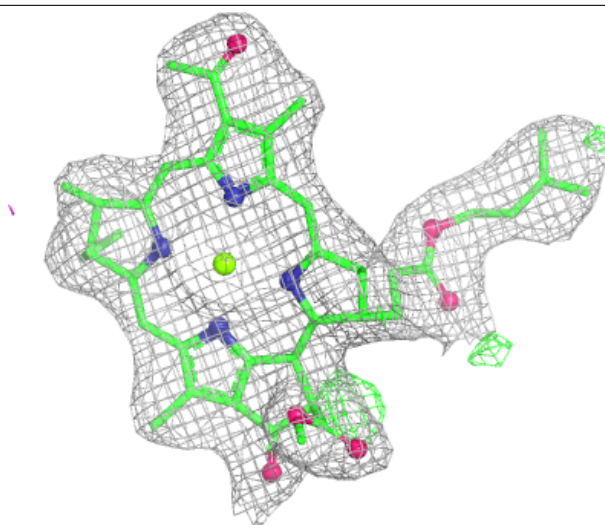
**Electron density around BCL R 2004:**

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



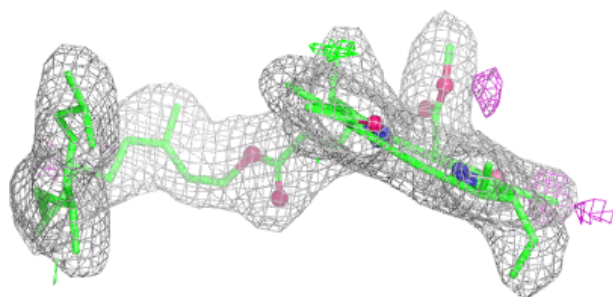
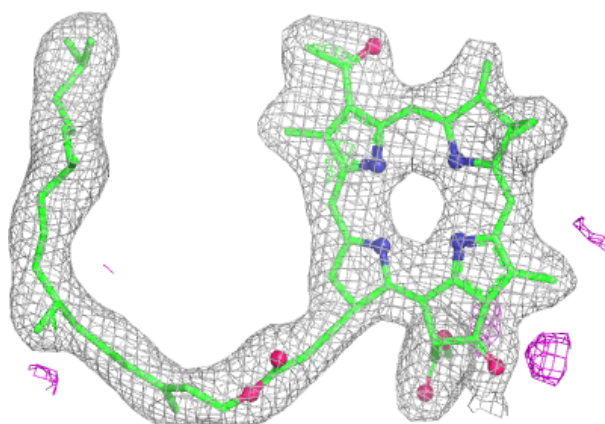
Electron density around BCL S 2001:

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

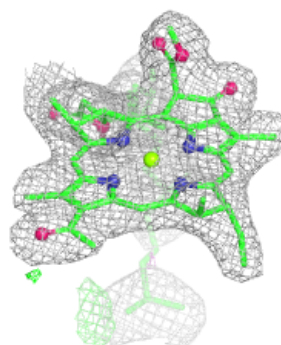
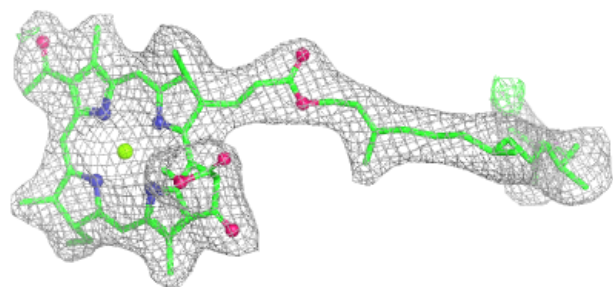
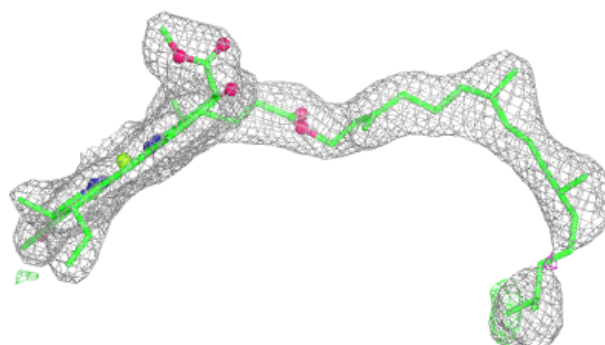


Electron density around BPH L 1006:

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

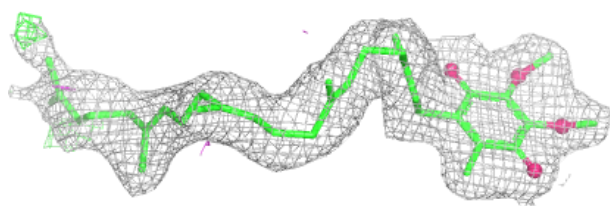
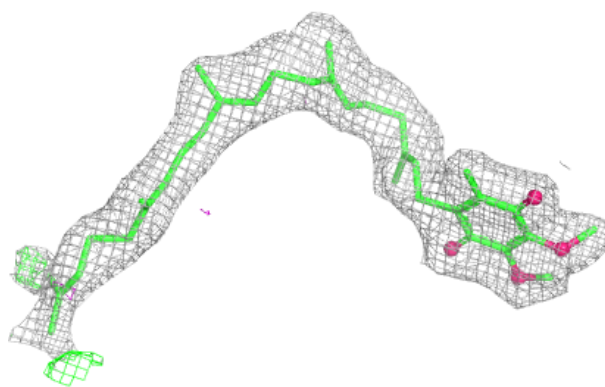
**Electron density around BCL S 2003:**

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

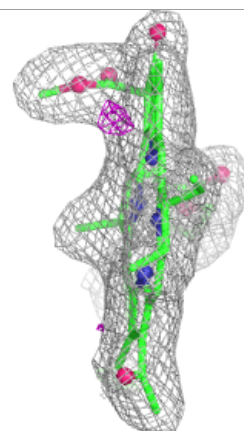
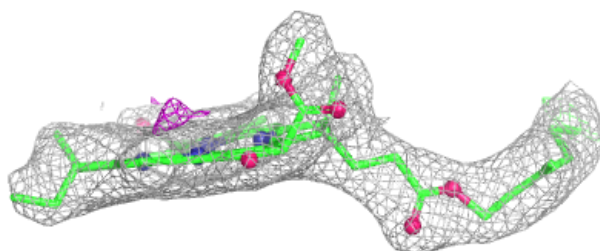
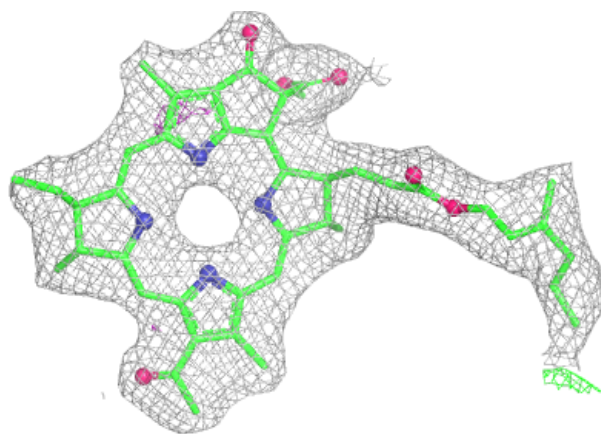


Electron density around U10 M 1008:

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

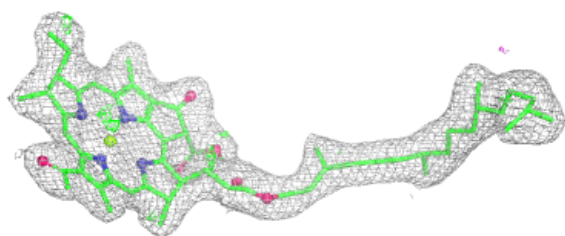
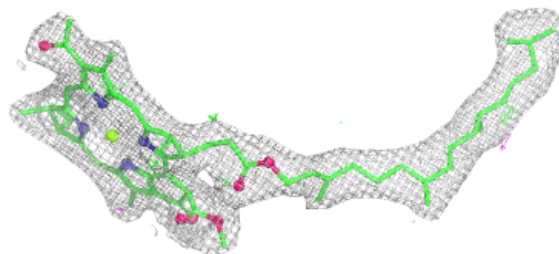
**Electron density around BPH S 2005:**

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



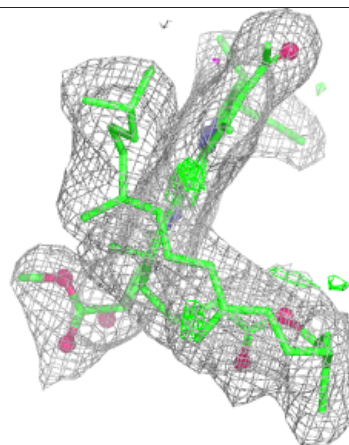
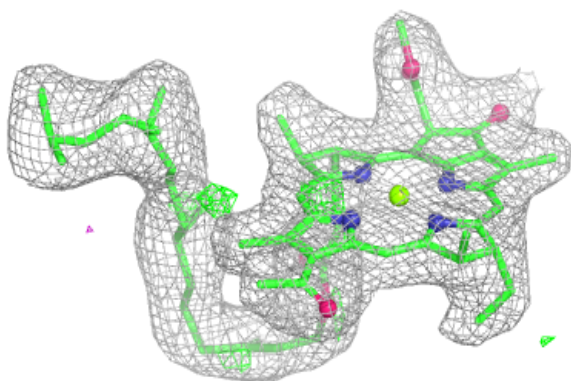
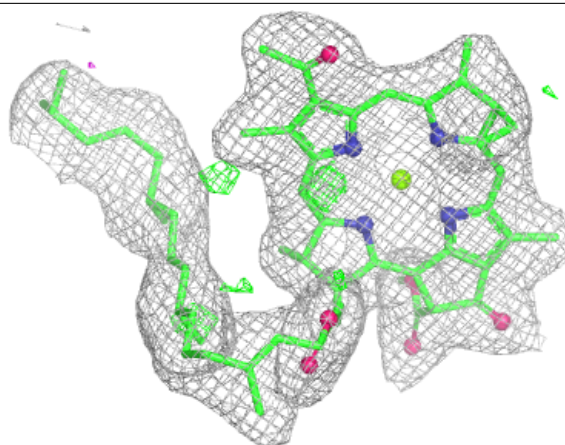
Electron density around BCL L 1002:

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



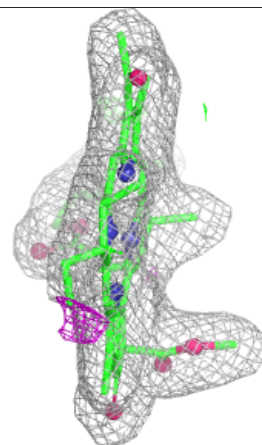
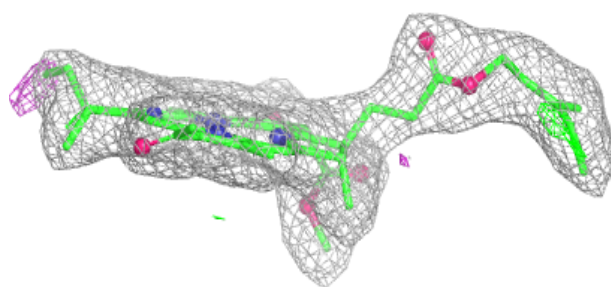
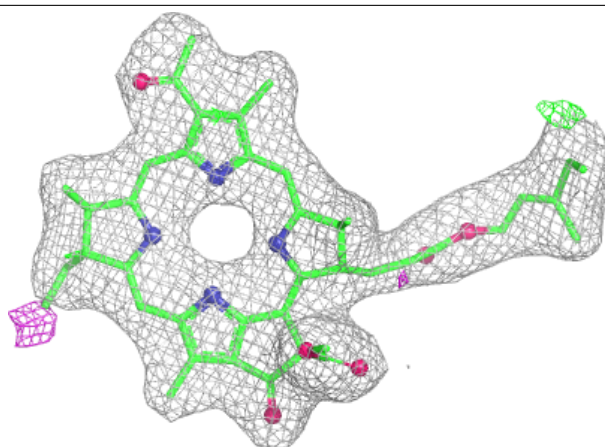
Electron density around BCL M 1004:

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



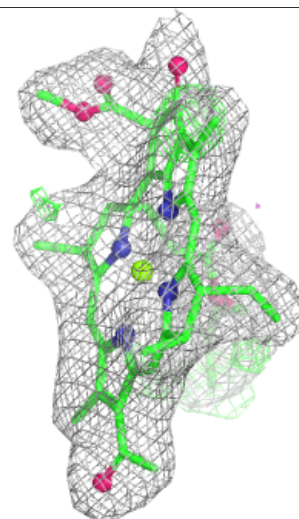
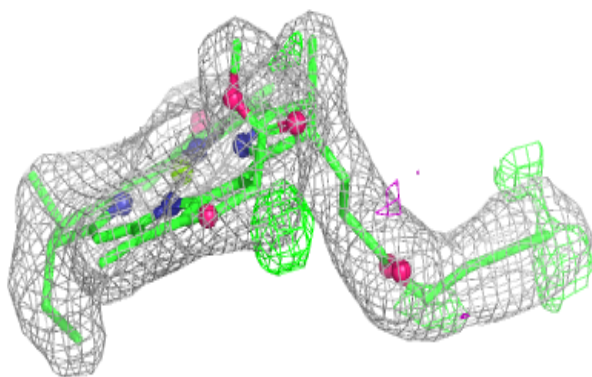
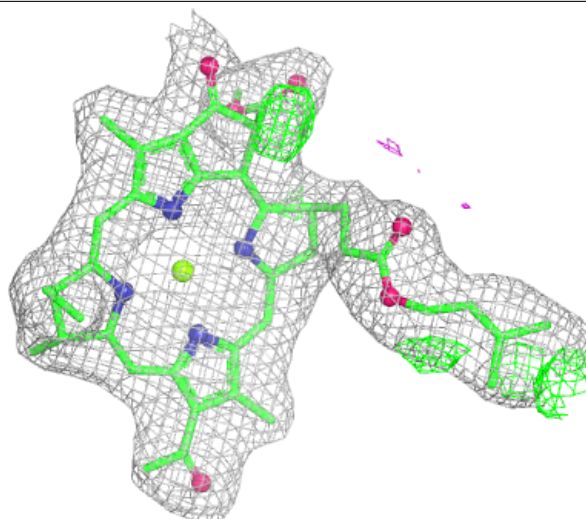
Electron density around BPH M 1005:

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



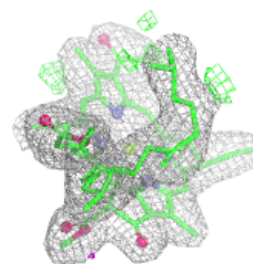
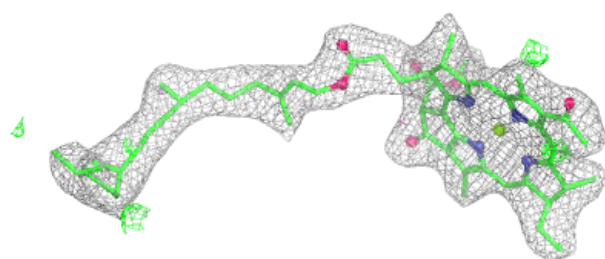
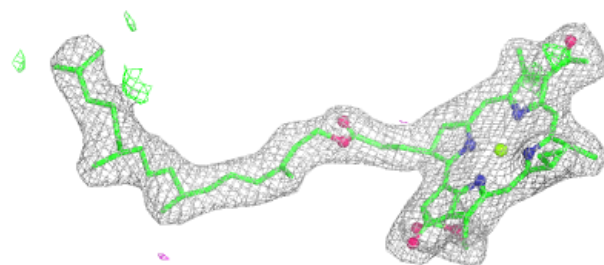
Electron density around BCL M 1001:

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



Electron density around BCL 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.