



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:13 AM UTC

PDB ID : 1L9J / pdb_00001l9j
Title : X-Ray Structure of the Cytochrome-c(2)-Photosynthetic Reaction Center Electron Transfer Complex from Rhodobacter sphaeroides in Type I Crystals
Authors : Axelrod, H.L.; Abresch, E.C.; Okamura, M.Y.; Yeh, A.P.; Rees, D.C.; Feher, G.
Deposited on : 2002-03-24
Resolution : 3.25 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](#) ①) were used in the production of this report:

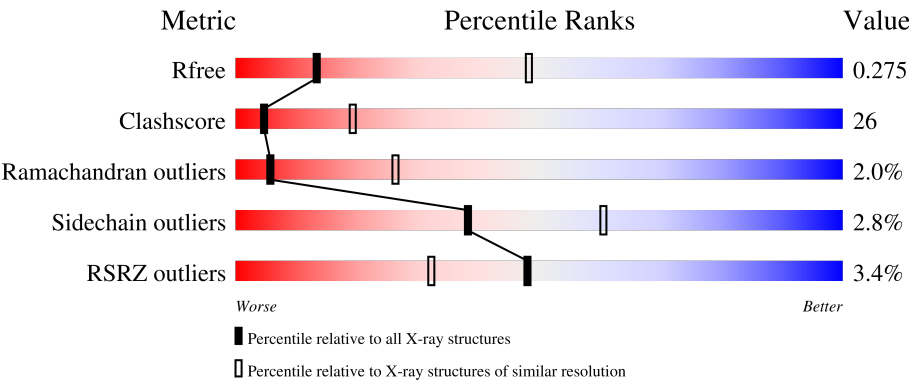
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	2% 60% 36% .
1	R	281	2% 50% 45% .
2	M	307	2% 49% 35% . 13%
2	S	307	2% 42% 41% . 13%
3	H	260	4% 49% 44% . 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	T	260	
4	C	124	
4	D	124	

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
6	BPH	L	1005	X	-	-	-
6	BPH	M	1006	X	-	-	-
6	BPH	R	2005	X	-	-	-
6	BPH	S	2006	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 15497 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	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 REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	267	Total	C	N	O	S	0	0	0
			2150	1450	347	344	9			
2	S	267	Total	C	N	O	S	0	0	0
			2150	1450	347	344	9			

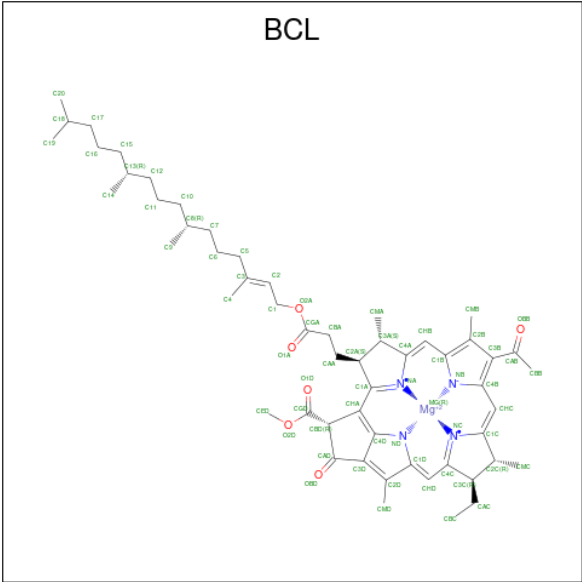
- Molecule 3 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	246	Total	C	N	O	S	0	0	0
			1871	1197	321	344	9			
3	T	246	Total	C	N	O	S	0	0	0
			1871	1197	321	344	9			

- Molecule 4 is a protein called cytochrome c-2.

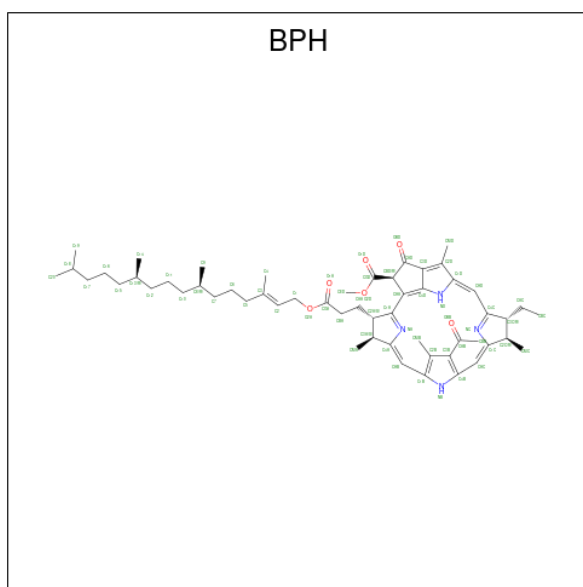
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	124	Total	C	N	O	S	0	0	0
			949	595	166	184	4			
4	D	124	Total	C	N	O	S	0	0	0
			949	595	166	184	4			

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	S	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
5	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



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

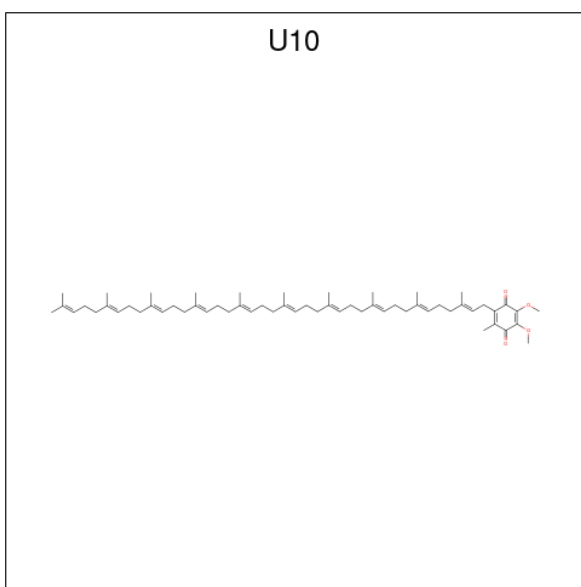
- Molecule 7 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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).

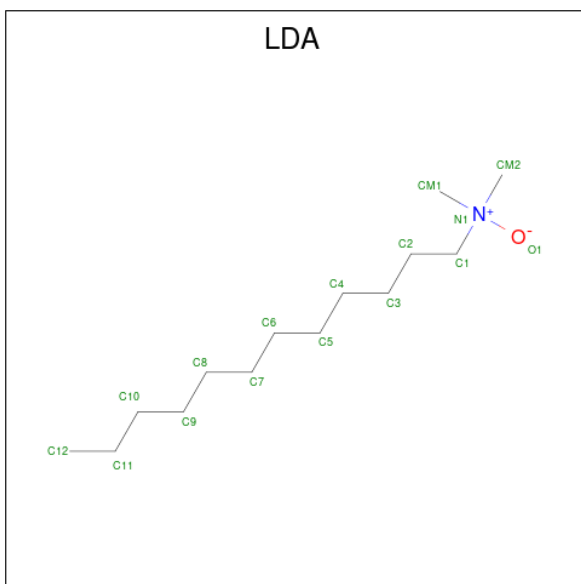
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Cl	0	0
			1	1		
8	S	1	Total	Cl	0	0
			1	1		

- Molecule 9 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			37	33	4		
9	S	1	Total	C	O	0	0
			37	33	4		

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



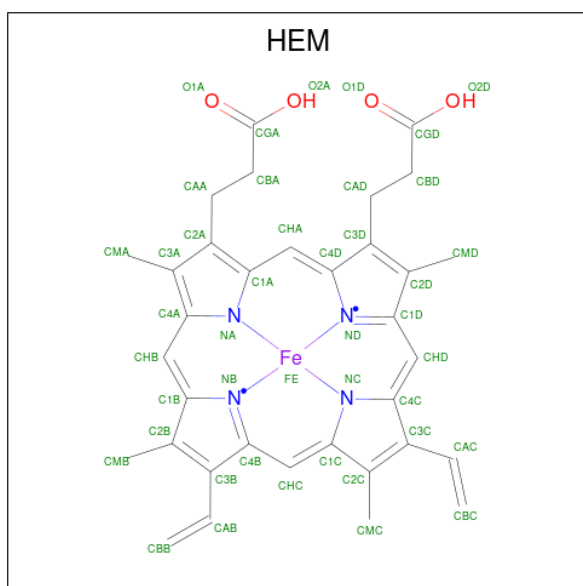
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	N	O	0	0
			16	14	1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
11	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	L	32	Total	O	0	0
			32	32		
12	M	14	Total	O	0	0
			14	14		
12	H	18	Total	O	0	0
			18	18		
12	C	10	Total	O	0	0
			10	10		

Continued on next page...

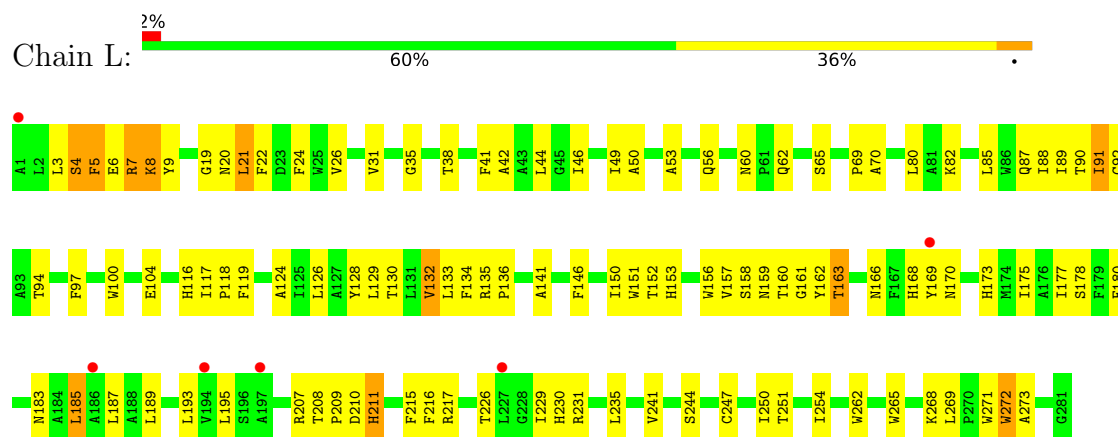
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	R	18	Total 18	O 18	0	0
12	S	15	Total 15	O 15	0	0
12	T	13	Total 13	O 13	0	0
12	D	9	Total 9	O 9	0	0

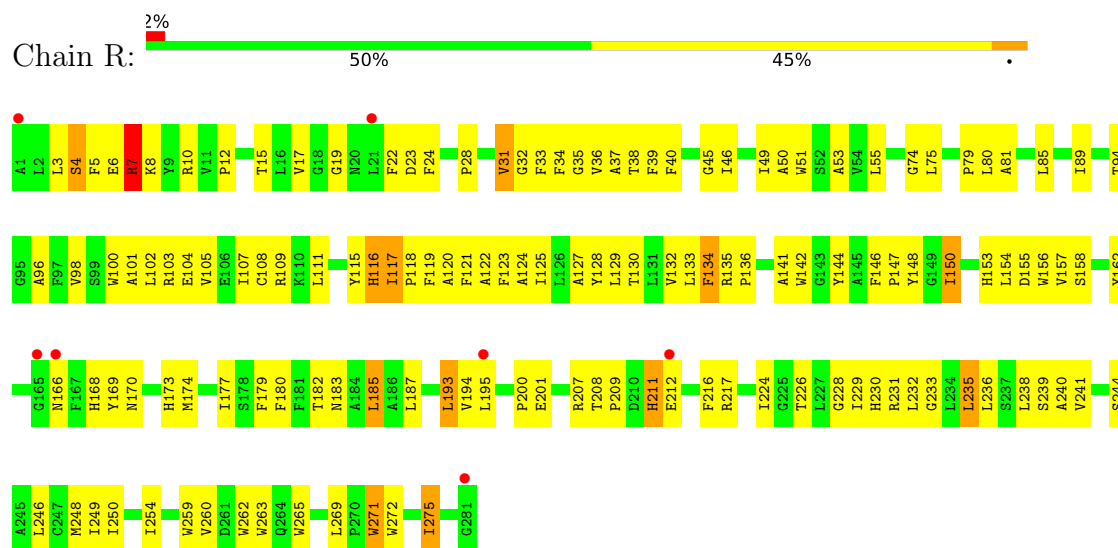
3 Residue-property plots

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

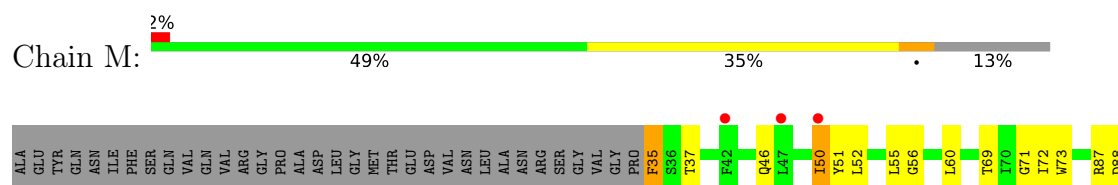
• Molecule 1: REACTION CENTER PROTEIN L CHAIN

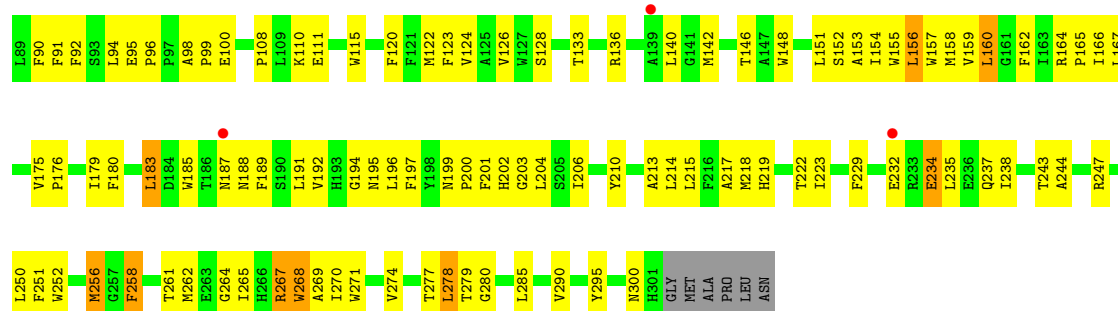


• Molecule 1: REACTION CENTER PROTEIN L CHAIN

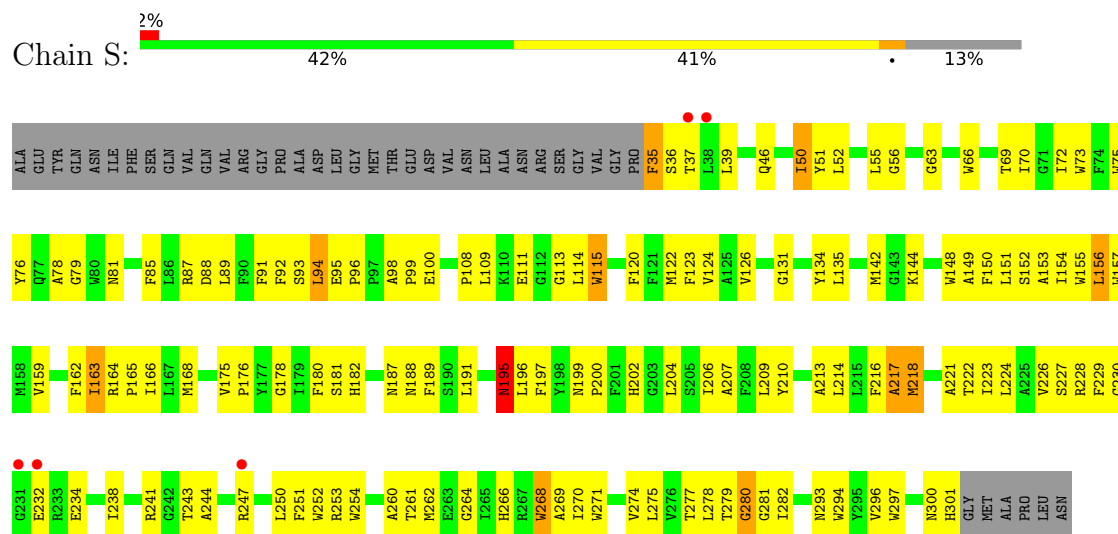


• Molecule 2: REACTION CENTER PROTEIN M CHAIN

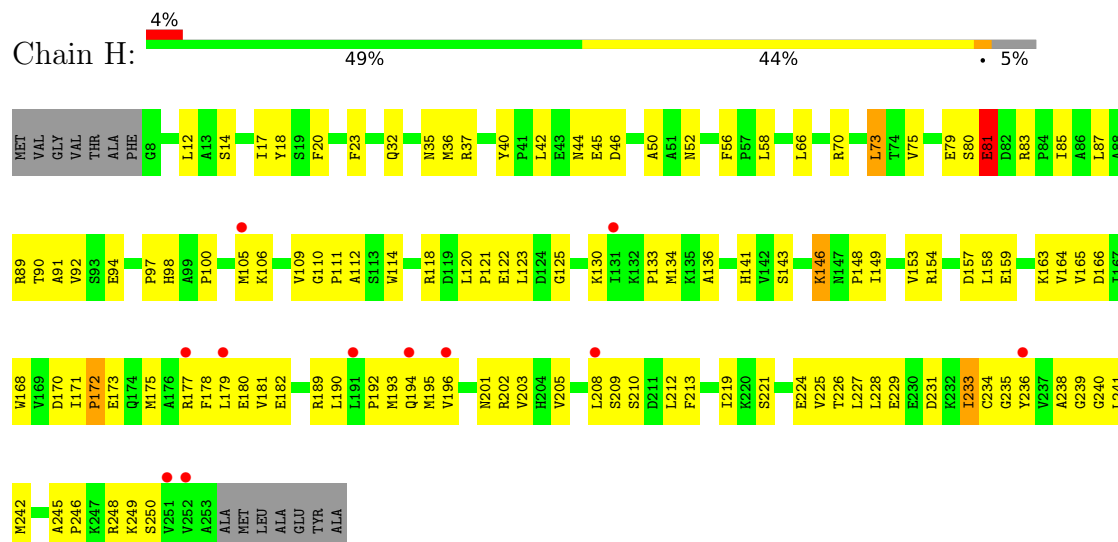




• Molecule 2: REACTION CENTER PROTEIN M CHAIN

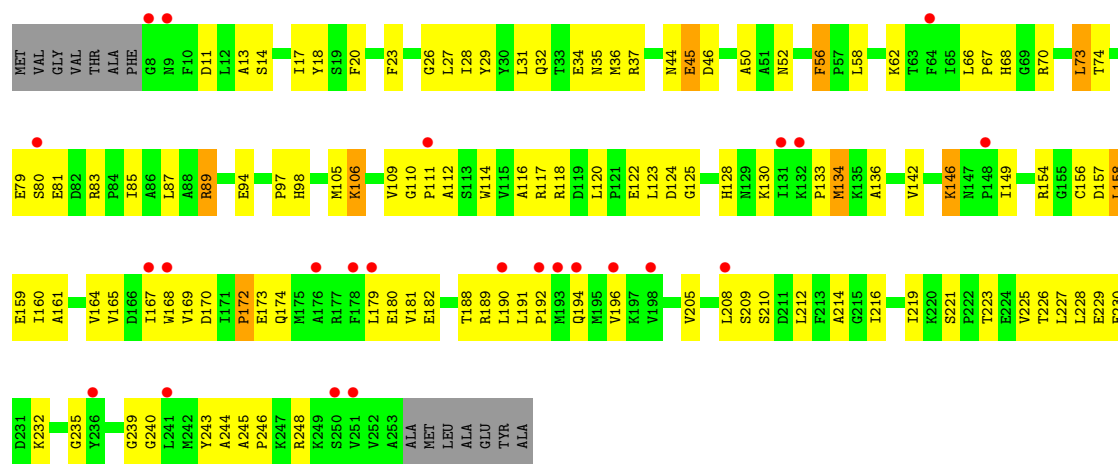


• Molecule 3: REACTION CENTER PROTEIN H CHAIN

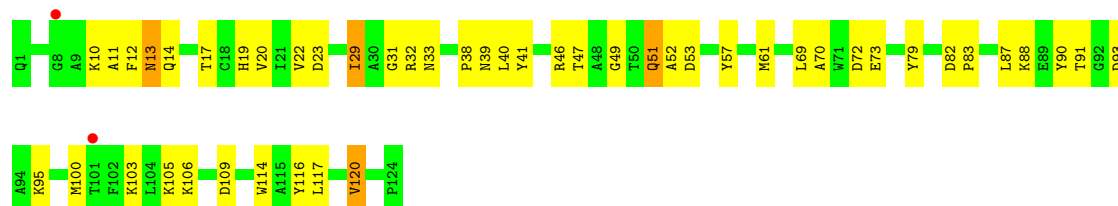


• Molecule 3: REACTION CENTER PROTEIN H CHAIN

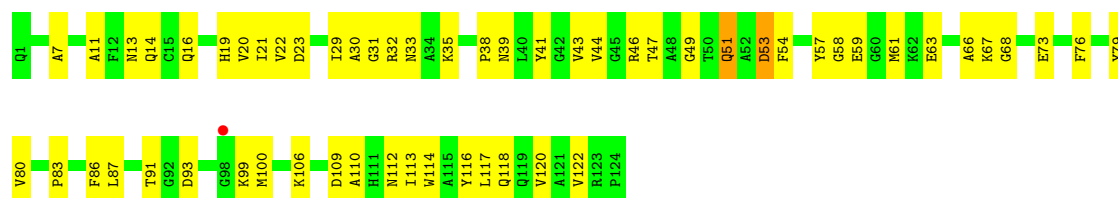




• Molecule 4: cytochrome c-2



• Molecule 4: cytochrome c-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.93Å 80.31Å 246.57Å 90.00° 92.41° 90.00°	Depositor
Resolution (Å)	49.32 – 3.25 49.32 – 3.25	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.32-3.25) 98.4 (49.32-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 3.25Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.287 0.238 , 0.275	Depositor DCC
R_{free} test set	2385 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l 0.000 for k,h,-l 0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15497	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1270e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, CL, BPH, LDA, U10, HEM, FE2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	0.39	0/2320	0.90	4/3175 (0.1%)
1	R	0.38	0/2320	0.90	5/3175 (0.2%)
2	M	0.42	0/2238	0.90	6/3057 (0.2%)
2	S	0.41	0/2238	0.90	7/3057 (0.2%)
3	H	0.35	0/1920	0.83	1/2612 (0.0%)
3	T	0.36	0/1920	0.84	3/2612 (0.1%)
4	C	0.37	0/969	0.89	3/1304 (0.2%)
4	D	0.35	0/969	0.82	1/1304 (0.1%)
All	All	0.38	0/14894	0.88	30/20296 (0.1%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	217	ALA	N-CA-C	-7.27	102.96	111.03
1	L	211	HIS	N-CA-C	-7.14	103.53	111.82
2	S	281	GLY	N-CA-C	-7.10	104.21	112.73
1	R	275	ILE	CA-C-N	6.78	127.84	119.98
1	R	275	ILE	C-N-CA	6.78	127.84	119.98
2	M	234	GLU	N-CA-C	6.25	117.76	111.07
2	S	268	TRP	N-CA-C	-6.24	103.19	111.24
2	S	115	TRP	N-CA-C	-6.07	104.36	110.97
2	S	163	ILE	N-CA-C	5.98	116.45	110.23
3	H	90	THR	N-CA-C	-5.79	106.84	114.31
1	L	132	VAL	N-CA-C	5.77	118.54	112.83
2	S	280	GLY	N-CA-C	5.77	119.65	112.73
1	R	211	HIS	N-CA-C	-5.73	105.11	111.36
2	S	210	TYR	N-CA-C	-5.65	104.50	111.40
2	M	183	LEU	N-CA-C	-5.60	105.25	111.36
2	M	128	SER	N-CA-C	-5.56	104.91	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	120	VAL	N-CA-C	5.40	118.82	113.53
3	T	56	PHE	CA-C-N	5.37	125.79	119.99
3	T	56	PHE	C-N-CA	5.37	125.79	119.99
4	C	105	LYS	N-CA-C	5.22	116.78	111.14
1	R	194	VAL	N-CA-C	5.20	115.41	110.42
2	M	160	LEU	N-CA-C	5.19	117.36	111.02
2	M	267	ARG	N-CA-C	-5.13	106.28	112.54
4	D	53	ASP	N-CA-C	5.13	119.01	112.34
2	M	268	TRP	N-CA-C	-5.12	104.63	111.24
4	C	52	ALA	N-CA-C	5.12	117.52	111.33
1	L	91	ILE	N-CA-C	-5.09	106.72	111.45
3	T	45	GLU	N-CA-C	-5.02	107.21	113.19
1	R	254	ILE	N-CA-C	-5.01	108.95	113.71
1	L	163	THR	N-CA-C	-5.00	107.01	113.01

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	100	0
1	R	2232	0	2187	132	0
2	M	2150	0	2073	126	0
2	S	2150	0	2073	156	0
3	H	1871	0	1877	116	0
3	T	1871	0	1877	115	0
4	C	949	0	916	39	0
4	D	949	0	916	49	0
5	L	132	0	148	13	0
5	M	116	0	115	14	0
5	R	132	0	148	18	0
5	S	116	0	115	14	0
6	L	55	0	53	1	0
6	M	65	0	74	3	0
6	R	55	0	53	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S	65	0	74	6	0
7	M	1	0	0	0	0
7	S	1	0	0	0	0
8	M	1	0	0	0	0
8	S	1	0	0	0	0
9	M	37	0	47	1	0
9	S	37	0	47	1	0
10	M	32	0	62	5	0
10	S	32	0	62	4	0
11	C	43	0	30	2	0
11	D	43	0	30	2	0
12	C	10	0	0	3	0
12	D	9	0	0	0	0
12	H	18	0	0	2	0
12	L	32	0	0	6	0
12	M	14	0	0	1	0
12	R	18	0	0	4	0
12	S	15	0	0	2	0
12	T	13	0	0	1	0
All	All	15497	0	15164	789	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 26.

All (789) 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)
4:C:91:THR:HG23	4:C:93:ASP:H	1.20	1.03
2:S:280:GLY:HA3	5:S:2003:BCL:CED	1.91	1.01
2:S:122:MET:HE3	2:S:157:TRP:HE1	1.28	0.97
2:S:280:GLY:HA3	5:S:2003:BCL:HED2	1.45	0.97
1:L:208:THR:HG22	1:L:210:ASP:H	1.37	0.90
1:L:208:THR:H	1:L:211:HIS:HD2	1.21	0.88
2:S:157:TRP:HB2	5:S:2003:BCL:H62	1.56	0.87
2:S:108:PRO:HG2	2:S:111:GLU:HB2	1.56	0.86
1:L:241:VAL:HG21	6:M:1006:BPH:HAC2	1.58	0.86
1:R:208:THR:H	1:R:211:HIS:HD2	1.23	0.84
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.12	0.84
3:H:130:LYS:HG3	3:H:172:PRO:HG3	1.59	0.84
1:R:193:LEU:HD11	1:R:216:PHE:HB2	1.60	0.83
2:S:195:ASN:ND2	2:S:197:PHE:H	1.77	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:42:ALA:O	1:L:46:ILE:HG12	1.80	0.82
1:R:170:ASN:HB3	1:R:173:HIS:HB3	1.60	0.82
3:T:130:LYS:HG3	3:T:172:PRO:HG3	1.64	0.80
2:M:156:LEU:HG	5:M:1003:BCL:HED1	1.62	0.80
2:S:122:MET:CE	2:S:157:TRP:HE1	1.94	0.80
2:S:195:ASN:C	2:S:195:ASN:HD22	1.91	0.79
3:H:146:LYS:HD3	3:H:146:LYS:H	1.47	0.79
3:T:245:ALA:HA	3:T:248:ARG:NH1	1.98	0.79
2:M:157:TRP:HB2	5:M:1003:BCL:H62	1.65	0.78
2:S:122:MET:HE3	2:S:157:TRP:NE1	1.99	0.77
3:H:105:MET:HE1	3:H:208:LEU:HD22	1.67	0.77
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.68	0.76
2:M:195:ASN:HD22	2:M:195:ASN:C	1.93	0.76
4:D:87:LEU:O	4:D:91:THR:HG22	1.86	0.76
2:M:187:ASN:O	2:M:191:LEU:HD23	1.85	0.75
2:S:202:HIS:CE1	2:S:206:ILE:HD11	2.22	0.75
1:R:241:VAL:HG21	6:S:2006:BPH:HAC2	1.68	0.75
3:T:157:ASP:OD2	3:T:159:GLU:HB2	1.87	0.74
3:T:133:PRO:HG3	3:T:168:TRP:CE2	2.22	0.74
1:R:135:ARG:HB3	1:R:136:PRO:HD3	1.69	0.74
2:M:234:GLU:O	2:M:238:ILE:HG13	1.87	0.74
2:M:52:LEU:HD21	2:M:60:LEU:HD12	1.67	0.74
2:M:235:LEU:HD23	2:M:238:ILE:HD12	1.69	0.73
3:T:196:VAL:HG12	3:T:205:VAL:HG22	1.69	0.73
1:R:128:TYR:HB2	5:R:2002:BCL:H62	1.68	0.73
1:R:187:LEU:HD11	2:S:269:ALA:HB1	1.70	0.73
2:M:290:VAL:HG21	3:H:12:LEU:HD23	1.70	0.73
3:H:245:ALA:HA	3:H:248:ARG:NH1	2.04	0.72
3:T:118:ARG:HD3	3:T:120:LEU:HD12	1.71	0.72
3:T:179:LEU:HD12	3:T:196:VAL:HG21	1.72	0.72
4:D:49:GLY:HA2	4:D:57:TYR:CE1	2.25	0.72
1:R:166:ASN:ND2	2:S:187:ASN:HB2	2.04	0.71
5:M:1001:BCL:HBC1	5:M:1003:BCL:CAD	2.19	0.71
3:T:11:ASP:HB3	3:T:14:SER:HG	1.56	0.71
1:L:183:ASN:ND2	2:M:213:ALA:HA	2.05	0.71
1:L:207:ARG:HG3	2:M:142:MET:HG2	1.72	0.71
4:C:51:GLN:NE2	4:C:53:ASP:H	1.88	0.71
4:D:7:ALA:HB3	4:D:112:ASN:HD22	1.56	0.71
2:M:195:ASN:ND2	2:M:197:PHE:HB2	2.05	0.71
2:S:195:ASN:HD21	2:S:197:PHE:HB2	1.54	0.71
2:M:218:MET:HE3	2:M:252:TRP:CH2	2.26	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.73	0.70
2:M:195:ASN:HD21	2:M:197:PHE:HB2	1.55	0.70
3:H:36:MET:HE3	3:H:58:LEU:HD23	1.74	0.70
4:C:51:GLN:HE22	4:C:53:ASP:H	1.36	0.70
6:R:2005:BPH:HAC1	2:S:153:ALA:HB2	1.72	0.70
4:C:20:VAL:HG23	4:C:31:GLY:HA3	1.72	0.70
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.73	0.69
1:R:115:TYR:O	1:R:118:PRO:HD2	1.92	0.69
4:D:106:LYS:HB2	4:D:109:ASP:OD2	1.92	0.69
1:L:193:LEU:HD11	1:L:216:PHE:HB2	1.73	0.69
2:S:260:ALA:HB2	9:S:2008:U10:H103	1.74	0.69
1:L:208:THR:HG21	3:H:125:GLY:HA2	1.73	0.69
2:M:52:LEU:O	2:M:56:GLY:HA3	1.92	0.69
2:M:243:THR:O	2:M:247:ARG:HG3	1.93	0.68
1:R:35:GLY:HA2	1:R:103:ARG:HD2	1.73	0.68
6:R:2005:BPH:H5C2	2:S:63:GLY:HA3	1.74	0.68
2:S:123:PHE:HA	2:S:157:TRP:HH2	1.58	0.68
1:R:208:THR:H	1:R:211:HIS:CD2	2.09	0.68
1:R:170:ASN:HB3	1:R:173:HIS:CB	2.23	0.68
2:M:195:ASN:ND2	2:M:197:PHE:H	1.92	0.67
2:M:122:MET:HE3	2:M:157:TRP:HE1	1.59	0.67
5:L:1004:BCL:HAA2	10:M:1010:LDA:H31	1.76	0.67
3:T:11:ASP:HB3	3:T:14:SER:OG	1.94	0.67
2:S:35:PHE:CE1	2:S:37:THR:HB	2.30	0.67
3:H:154:ARG:NH1	3:H:158:LEU:HD22	2.10	0.67
4:C:11:ALA:O	4:C:14:GLN:HG2	1.94	0.67
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.30	0.67
1:L:208:THR:HG23	1:L:209:PRO:HD2	1.76	0.66
1:R:162:TYR:OH	2:S:191:LEU:HD21	1.94	0.66
4:D:118:GLN:HA	4:D:122:VAL:HG23	1.78	0.66
3:H:165:VAL:HG21	3:H:182:GLU:HB2	1.77	0.66
1:L:128:TYR:HB2	5:L:1002:BCL:H62	1.78	0.66
12:R:2008:HOH:O	3:T:81:GLU:HB2	1.96	0.66
2:M:136:ARG:HD3	12:M:1017:HOH:O	1.95	0.65
1:L:208:THR:H	1:L:211:HIS:CD2	2.11	0.65
4:C:29:ILE:HD12	4:C:29:ILE:N	2.11	0.65
1:R:111:LEU:HD21	2:S:254:TRP:CH2	2.31	0.65
2:M:195:ASN:HD22	2:M:197:PHE:H	1.43	0.65
2:S:280:GLY:HA3	5:S:2003:BCL:HED3	1.74	0.65
2:M:46:GLN:HG2	2:M:51:TYR:HA	1.78	0.65
1:R:244:SER:HB3	5:R:2002:BCL:HBA2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:122:MET:O	2:M:126:VAL:HG23	1.97	0.65
5:R:2004:BCL:H203	6:S:2006:BPH:H111	1.78	0.65
3:H:89:ARG:HH21	3:H:92:VAL:HA	1.61	0.64
4:C:49:GLY:HA2	4:C:57:TYR:CZ	2.31	0.64
1:R:116:HIS:O	1:R:119:PHE:HB3	1.97	0.64
1:R:226:THR:O	1:R:229:ILE:HG22	1.96	0.64
2:M:188:ASN:O	2:M:192:VAL:HG23	1.98	0.64
1:R:37:ALA:O	1:R:40:PHE:HB3	1.97	0.64
3:T:146:LYS:H	3:T:146:LYS:HD3	1.63	0.64
2:M:162:PHE:C	2:M:165:PRO:HD2	2.23	0.64
2:S:78:ALA:HB2	2:S:92:PHE:CZ	2.33	0.64
2:M:90:PHE:HD1	2:M:179:ILE:HG13	1.63	0.64
1:L:175:ILE:O	1:L:178:SER:HB3	1.98	0.64
2:M:122:MET:HE1	10:M:1011:LDA:HM22	1.80	0.64
2:S:52:LEU:HG	2:S:56:GLY:HA3	1.79	0.64
2:S:155:TRP:O	2:S:159:VAL:HG23	1.97	0.63
5:L:1002:BCL:HBD	5:L:1004:BCL:CBC	2.28	0.63
4:C:106:LYS:HB2	4:C:109:ASP:OD2	1.98	0.63
3:H:91:ALA:HB1	12:H:262:HOH:O	1.99	0.63
2:S:187:ASN:O	2:S:191:LEU:HD23	1.98	0.63
3:H:225:VAL:HG23	3:H:229:GLU:HB2	1.80	0.63
1:R:246:LEU:O	1:R:249:ILE:HG22	1.98	0.63
5:R:2004:BCL:O1A	2:S:207:ALA:HA	1.99	0.62
2:M:162:PHE:O	2:M:165:PRO:HD2	1.99	0.62
2:M:194:GLY:HA2	12:C:1011:HOH:O	1.97	0.62
3:H:70:ARG:HH22	3:H:123:LEU:HD13	1.63	0.62
2:S:98:ALA:HB1	2:S:99:PRO:HD2	1.82	0.62
2:S:264:GLY:HA3	3:T:35:ASN:OD1	1.99	0.62
3:T:45:GLU:HG3	3:T:94:GLU:OE1	1.99	0.62
1:R:5:PHE:HB2	1:R:8:LYS:NZ	2.14	0.62
2:M:87:ARG:HG3	2:M:88:ASP:OD1	1.99	0.62
2:M:122:MET:HE1	10:M:1011:LDA:CM2	2.30	0.62
3:H:201:ASN:OD1	3:H:202:ARG:HG2	1.99	0.62
5:R:2004:BCL:HAA2	10:S:2010:LDA:H31	1.81	0.62
3:T:170:ASP:OD2	3:T:173:GLU:HB2	2.00	0.62
4:D:73:GLU:HB2	4:D:114:TRP:NE1	2.15	0.62
4:D:38:PRO:HB3	4:D:54:PHE:CG	2.35	0.62
1:R:135:ARG:HD3	12:R:2007:HOH:O	1.98	0.61
1:R:248:MET:HG2	5:R:2002:BCL:O1D	2.00	0.61
4:C:91:THR:HG23	4:C:93:ASP:N	2.03	0.61
3:H:36:MET:CE	3:H:58:LEU:HD23	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:49:GLY:HA2	4:C:57:TYR:CE1	2.35	0.61
3:T:122:GLU:HB2	3:T:227:LEU:HD21	1.80	0.61
2:M:72:ILE:HG23	2:M:73:TRP:N	2.16	0.61
2:M:90:PHE:CD1	2:M:179:ILE:HG13	2.36	0.61
2:M:156:LEU:HD13	5:M:1003:BCL:H43	1.82	0.61
3:T:133:PRO:HA	3:T:168:TRP:HA	1.83	0.61
1:L:183:ASN:HD21	2:M:213:ALA:HA	1.65	0.61
1:L:166:ASN:ND2	2:M:187:ASN:HB2	2.16	0.60
1:R:207:ARG:HG3	2:S:142:MET:HG2	1.83	0.60
2:S:109:LEU:HA	2:S:113:GLY:HA3	1.81	0.60
1:L:244:SER:O	1:L:247:CYS:HB3	2.01	0.60
2:S:202:HIS:HE1	2:S:206:ILE:HD11	1.66	0.60
1:R:173:HIS:CE1	1:R:177:ILE:HD11	2.37	0.60
3:H:79:GLU:HG3	3:H:81:GLU:HG2	1.84	0.60
1:L:262:TRP:O	1:L:265:TRP:HD1	1.85	0.60
2:M:122:MET:CE	2:M:157:TRP:HE1	2.15	0.60
2:S:123:PHE:HA	2:S:157:TRP:CH2	2.36	0.60
2:S:195:ASN:HD22	2:S:197:PHE:H	1.49	0.60
2:S:199:ASN:ND2	2:S:294:TRP:CE2	2.70	0.60
3:T:245:ALA:HA	3:T:248:ARG:HH12	1.65	0.60
3:H:157:ASP:OD2	3:H:159:GLU:HB2	2.02	0.60
3:H:179:LEU:HD12	3:H:196:VAL:HG21	1.82	0.60
1:L:94:THR:HG23	1:L:129:LEU:HD21	1.84	0.60
2:M:200:PRO:HB2	3:H:17:ILE:HD13	1.84	0.59
2:M:256:MET:HE2	2:M:258:PHE:HE2	1.66	0.59
1:R:4:SER:HB2	3:T:79:GLU:HG2	1.84	0.59
3:T:225:VAL:HG23	3:T:229:GLU:HB2	1.84	0.59
1:R:166:ASN:HD21	2:S:187:ASN:HB2	1.68	0.59
1:L:250:ILE:HB	1:L:254:ILE:HD11	1.84	0.59
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.83	0.59
3:T:149:ILE:HA	3:T:164:VAL:CG1	2.32	0.59
1:L:56:GLN:HE22	1:L:65:SER:H	1.50	0.58
2:S:297:TRP:HE1	3:T:13:ALA:HB3	1.67	0.58
1:L:269:LEU:HD13	1:L:271:TRP:CZ2	2.38	0.58
2:S:96:PRO:HD3	2:S:176:PRO:HB3	1.85	0.58
3:T:120:LEU:N	3:T:226:THR:HB	2.18	0.58
1:L:4:SER:HB2	3:H:79:GLU:HG2	1.86	0.58
1:R:6:GLU:HG2	1:R:10:ARG:HD2	1.84	0.58
5:S:2001:BCL:HBC1	5:S:2003:BCL:HBD	1.85	0.58
2:M:235:LEU:HA	2:M:238:ILE:HD12	1.85	0.58
2:M:270:ILE:HG23	2:M:271:TRP:N	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:190:LEU:C	3:T:191:LEU:HD22	2.28	0.58
1:L:187:LEU:HD11	2:M:269:ALA:HB1	1.86	0.58
3:H:66:LEU:N	3:H:66:LEU:HD12	2.17	0.58
1:R:128:TYR:O	1:R:132:VAL:HG22	2.02	0.58
4:D:20:VAL:HG23	4:D:31:GLY:HA3	1.86	0.57
3:H:40:TYR:HB3	3:H:58:LEU:HD21	1.86	0.57
2:S:162:PHE:C	2:S:165:PRO:HD2	2.29	0.57
3:H:83:ARG:HH21	3:H:114:TRP:NE1	2.03	0.57
2:M:271:TRP:HA	2:M:274:VAL:HG22	1.86	0.57
3:H:134:MET:C	3:H:136:ALA:H	2.13	0.57
2:S:301:HIS:CD2	3:T:14:SER:HB3	2.40	0.57
5:M:1001:BCL:HBB3	5:M:1003:BCL:H61	1.86	0.57
3:H:111:PRO:HG3	3:H:242:MET:SD	2.44	0.57
5:R:2002:BCL:HBD	5:R:2004:BCL:CBC	2.35	0.57
2:S:222:THR:O	2:S:226:VAL:HG22	2.04	0.57
3:H:80:SER:O	3:H:81:GLU:C	2.48	0.57
1:R:7:ARG:HG3	1:R:7:ARG:HH11	1.70	0.57
4:D:22:VAL:HB	4:D:39:ASN:ND2	2.19	0.57
4:D:51:GLN:HE22	4:D:53:ASP:N	2.03	0.57
5:R:2002:BCL:H2C	5:S:2003:BCL:H2C	1.87	0.56
2:S:134:TYR:HE1	2:S:144:LYS:HG3	1.70	0.56
2:M:295:TYR:CZ	4:C:32:ARG:HD3	2.40	0.56
2:M:175:VAL:HB	10:M:1011:LDA:HM13	1.87	0.56
2:M:290:VAL:CG2	3:H:12:LEU:HD23	2.34	0.56
3:H:14:SER:HA	3:H:17:ILE:HG22	1.87	0.56
2:S:95:GLU:HA	2:S:176:PRO:HB3	1.88	0.56
3:T:133:PRO:HG3	3:T:168:TRP:CD2	2.41	0.56
2:M:156:LEU:CG	5:M:1003:BCL:HED1	2.33	0.56
2:S:229:PHE:CZ	2:S:247:ARG:NH1	2.73	0.56
1:L:6:GLU:HG3	2:M:250:LEU:HD22	1.86	0.56
3:T:228:LEU:O	3:T:232:LYS:HG2	2.06	0.56
3:H:225:VAL:CG2	3:H:229:GLU:HB2	2.36	0.56
1:R:115:TYR:O	1:R:117:ILE:N	2.39	0.56
1:R:231:ARG:O	1:R:235:LEU:HB2	2.06	0.56
3:T:161:ALA:HB2	3:T:210:SER:HB2	1.88	0.56
4:D:61:MET:HE1	4:D:79:TYR:CZ	2.41	0.56
3:H:219:ILE:O	3:H:219:ILE:HG13	2.05	0.56
4:C:19:HIS:HA	12:C:1018:HOH:O	2.06	0.56
4:D:29:ILE:HD12	4:D:29:ILE:N	2.21	0.56
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.88	0.56
2:S:55:LEU:N	2:S:55:LEU:HD22	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:79:GLY:C	2:S:81:ASN:H	2.14	0.56
2:S:280:GLY:CA	5:S:2003:BCL:HED2	2.29	0.56
3:H:121:PRO:HD3	3:H:226:THR:HG22	1.88	0.55
1:R:229:ILE:HG23	1:R:230:HIS:N	2.21	0.55
3:H:50:ALA:C	3:H:52:ASN:H	2.13	0.55
3:H:130:LYS:HG3	3:H:172:PRO:CG	2.36	0.55
4:C:12:PHE:CE1	4:C:40:LEU:HD12	2.41	0.55
4:C:87:LEU:O	4:C:91:THR:HB	2.07	0.55
4:C:88:LYS:O	4:C:91:THR:HG22	2.07	0.55
4:D:22:VAL:HB	4:D:39:ASN:HD21	1.72	0.55
2:M:300:ASN:N	2:M:300:ASN:HD22	2.04	0.55
1:L:117:ILE:HD13	2:M:251:PHE:CE2	2.41	0.55
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.88	0.55
3:T:45:GLU:OE1	3:T:94:GLU:HA	2.07	0.55
2:M:72:ILE:HG23	2:M:73:TRP:H	1.70	0.55
3:H:163:LYS:C	3:H:181:VAL:HG23	2.31	0.55
1:R:174:MET:HE2	5:S:2001:BCL:HED3	1.89	0.55
2:S:96:PRO:HG3	2:S:115:TRP:NE1	2.22	0.55
1:L:85:LEU:O	1:L:89:ILE:HG13	2.08	0.54
1:L:170:ASN:HB3	1:L:173:HIS:CB	2.37	0.54
1:R:85:LEU:O	1:R:89:ILE:HG13	2.07	0.54
2:S:195:ASN:ND2	2:S:197:PHE:HB2	2.21	0.54
4:D:66:ALA:C	4:D:68:GLY:H	2.16	0.54
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.42	0.54
5:L:1002:BCL:HBD	5:L:1004:BCL:HBC3	1.88	0.54
2:S:122:MET:HE1	10:S:2011:LDA:CM2	2.37	0.54
2:S:159:VAL:HA	2:S:163:ILE:HB	1.89	0.54
2:S:164:ARG:NH2	2:S:168:MET:HE2	2.22	0.54
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.90	0.54
2:M:218:MET:HE3	2:M:252:TRP:CZ3	2.41	0.54
4:C:12:PHE:HE1	4:C:40:LEU:HD12	1.72	0.54
3:T:112:ALA:HB2	3:T:239:GLY:HA3	1.88	0.54
4:D:38:PRO:HD3	4:D:54:PHE:CE2	2.43	0.54
2:M:96:PRO:HA	2:M:115:TRP:CG	2.43	0.54
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.07	0.54
1:L:88:ILE:O	1:L:91:ILE:HB	2.08	0.54
1:R:28:PRO:HB3	2:S:253:ARG:NH1	2.23	0.54
1:R:180:PHE:CE2	5:R:2002:BCL:HMA2	2.43	0.54
3:T:245:ALA:HB3	3:T:246:PRO:HD3	1.88	0.54
2:S:195:ASN:ND2	2:S:195:ASN:C	2.58	0.54
2:S:271:TRP:HA	2:S:274:VAL:HG22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:ASP:HA	4:D:41:TYR:CD2	2.43	0.54
1:R:269:LEU:HD13	1:R:271:TRP:CZ2	2.43	0.53
4:C:116:TYR:O	4:C:120:VAL:HG22	2.07	0.53
4:C:22:VAL:HB	4:C:39:ASN:HD21	1.73	0.53
5:R:2002:BCL:HBD	5:R:2004:BCL:HBC1	1.90	0.53
3:H:105:MET:HE1	3:H:208:LEU:CD2	2.37	0.53
1:R:122:ALA:HA	1:R:125:ILE:HD12	1.90	0.53
3:T:44:ASN:C	3:T:46:ASP:H	2.16	0.53
3:T:165:VAL:CG2	3:T:182:GLU:H	2.22	0.53
4:D:49:GLY:HA2	4:D:57:TYR:CZ	2.44	0.53
4:D:7:ALA:CB	4:D:112:ASN:HD22	2.21	0.53
1:L:22:PHE:HA	1:L:24:PHE:HE2	1.74	0.53
1:L:162:TYR:OH	2:M:191:LEU:HD21	2.09	0.53
3:H:45:GLU:HG3	3:H:94:GLU:OE1	2.09	0.53
3:T:83:ARG:HG3	3:T:83:ARG:HH11	1.74	0.53
3:T:66:LEU:HD12	3:T:66:LEU:H	1.74	0.53
3:T:70:ARG:HH22	3:T:123:LEU:HD13	1.73	0.53
3:T:110:GLY:C	3:T:112:ALA:H	2.16	0.53
2:S:50:ILE:C	2:S:50:ILE:HD12	2.34	0.53
4:D:51:GLN:NE2	4:D:54:PHE:H	2.07	0.53
1:R:6:GLU:HG3	2:S:250:LEU:CD2	2.38	0.52
1:R:6:GLU:OE2	1:R:10:ARG:NH1	2.42	0.52
2:S:148:TRP:O	2:S:151:LEU:HB3	2.10	0.52
2:S:195:ASN:HD22	2:S:196:LEU:N	2.07	0.52
3:T:114:TRP:CE3	3:T:232:LYS:HD3	2.43	0.52
1:L:135:ARG:NH1	1:L:251:THR:O	2.38	0.52
6:L:1005:BPH:HAC1	2:M:153:ALA:HB2	1.91	0.52
2:M:122:MET:HE3	2:M:157:TRP:NE1	2.24	0.52
3:H:133:PRO:HB3	3:H:166:ASP:OD2	2.10	0.52
2:S:94:LEU:HA	12:S:2016:HOH:O	2.09	0.52
5:L:1002:BCL:HBD	5:L:1004:BCL:HBC1	1.90	0.52
3:H:105:MET:CE	3:H:212:LEU:HD13	2.39	0.52
3:T:226:THR:OG1	3:T:229:GLU:HG3	2.09	0.52
4:C:69:LEU:HB2	4:C:90:TYR:CE2	2.45	0.52
1:L:31:VAL:O	1:L:35:GLY:HA3	2.09	0.52
1:L:208:THR:HG21	3:H:125:GLY:CA	2.39	0.52
1:R:75:LEU:HA	1:R:142:TRP:NE1	2.25	0.52
4:D:46:ARG:HG2	4:D:47:THR:N	2.23	0.52
1:L:229:ILE:HG23	1:L:230:HIS:N	2.24	0.52
1:L:146:PHE:HB3	1:L:156:TRP:CD2	2.45	0.52
1:L:3:LEU:C	1:L:5:PHE:H	2.18	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:97:PRO:O	3:H:98:HIS:HD2	1.93	0.52
3:H:118:ARG:HD3	3:H:120:LEU:HD12	1.91	0.52
1:R:101:ALA:O	1:R:104:GLU:HB2	2.10	0.52
2:S:152:SER:O	2:S:155:TRP:HB3	2.11	0.52
2:S:268:TRP:HE1	3:T:35:ASN:ND2	2.08	0.52
3:H:195:MET:HE2	3:H:238:ALA:HA	1.91	0.51
4:C:100:MET:HG3	11:C:1009:HEM:C4C	2.45	0.51
1:R:182:THR:O	1:R:183:ASN:C	2.53	0.51
2:M:55:LEU:H	2:M:55:LEU:HD22	1.75	0.51
1:R:49:ILE:HG13	1:R:89:ILE:HD13	1.93	0.51
1:R:150:ILE:O	5:R:2004:BCL:HED1	2.09	0.51
3:T:189:ARG:HG2	3:T:189:ARG:HH11	1.74	0.51
3:H:114:TRP:HZ3	3:H:228:LEU:HD11	1.75	0.51
1:R:50:ALA:O	1:R:53:ALA:HB3	2.10	0.51
1:R:262:TRP:O	1:R:265:TRP:HD1	1.92	0.51
2:S:214:LEU:O	2:S:217:ALA:HB3	2.11	0.51
4:D:46:ARG:NH1	4:D:51:GLN:HB2	2.25	0.51
1:L:226:THR:O	1:L:229:ILE:HG22	2.09	0.51
1:R:187:LEU:CD1	2:S:269:ALA:HB1	2.40	0.51
2:S:300:ASN:N	2:S:300:ASN:HD22	2.09	0.51
3:T:112:ALA:HA	3:T:235:GLY:O	2.11	0.51
1:R:157:VAL:O	1:R:158:SER:C	2.52	0.51
4:D:51:GLN:NE2	4:D:51:GLN:C	2.68	0.51
2:M:160:LEU:HD22	2:M:185:TRP:CH2	2.46	0.51
2:M:278:LEU:O	2:M:279:THR:C	2.53	0.51
1:R:141:ALA:HB3	1:R:144:TYR:CD2	2.46	0.51
1:R:244:SER:CB	5:R:2002:BCL:HBA2	2.41	0.51
1:R:246:LEU:O	1:R:250:ILE:HG23	2.10	0.51
2:S:293:ASN:HD22	4:D:13:ASN:HB3	1.76	0.51
12:S:2027:HOH:O	3:T:34:GLU:HG3	2.10	0.51
2:M:148:TRP:O	2:M:151:LEU:HB3	2.09	0.51
1:R:124:ALA:O	1:R:127:ALA:HB3	2.11	0.51
1:R:183:ASN:ND2	2:S:213:ALA:HA	2.26	0.51
1:R:193:LEU:HD22	1:R:212:GLU:HG3	1.92	0.51
4:D:11:ALA:O	4:D:14:GLN:HG2	2.11	0.51
5:L:1004:BCL:HBB3	6:M:1006:BPH:H152	1.92	0.51
3:H:112:ALA:HA	3:H:235:GLY:O	2.11	0.51
3:T:36:MET:HE2	3:T:58:LEU:HD23	1.93	0.51
1:L:82:LYS:HA	12:L:1027:HOH:O	2.11	0.50
3:H:168:TRP:CE2	3:H:190:LEU:HD21	2.46	0.50
3:T:157:ASP:C	3:T:159:GLU:H	2.19	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:128:TYR:CZ	1:L:132:VAL:HG21	2.46	0.50
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.11	0.50
3:T:106:LYS:HE2	3:T:106:LYS:HA	1.92	0.50
3:H:245:ALA:N	3:H:246:PRO:CD	2.74	0.50
5:S:2001:BCL:HBC1	5:S:2003:BCL:CBD	2.41	0.50
3:T:146:LYS:HD3	3:T:146:LYS:N	2.27	0.50
1:L:80:LEU:O	1:L:85:LEU:HG	2.11	0.50
3:H:114:TRP:CZ3	3:H:228:LEU:HD11	2.46	0.50
1:R:74:GLY:O	1:R:141:ALA:HA	2.11	0.50
1:R:115:TYR:O	1:R:116:HIS:C	2.54	0.50
2:M:88:ASP:HB2	2:M:92:PHE:CZ	2.46	0.50
3:T:165:VAL:HG23	3:T:182:GLU:H	1.76	0.50
3:T:225:VAL:CG2	3:T:229:GLU:HB2	2.42	0.50
3:H:32:GLN:HG2	3:H:56:PHE:CD2	2.47	0.50
3:T:189:ARG:HD2	3:T:216:ILE:CG2	2.41	0.50
1:L:153:HIS:O	1:L:157:VAL:HG23	2.12	0.50
1:L:180:PHE:CD2	5:L:1002:BCL:HMA3	2.47	0.50
3:H:73:LEU:CD2	3:H:75:VAL:HG13	2.42	0.50
3:H:157:ASP:CG	3:H:210:SER:HG	2.20	0.50
2:S:72:ILE:CG2	2:S:73:TRP:N	2.75	0.50
3:T:83:ARG:HG3	3:T:83:ARG:O	2.10	0.50
2:M:265:ILE:O	2:M:268:TRP:HB2	2.12	0.50
1:R:31:VAL:HG12	1:R:32:GLY:N	2.26	0.50
3:T:50:ALA:C	3:T:52:ASN:H	2.19	0.50
1:L:170:ASN:HB3	1:L:173:HIS:HB3	1.93	0.49
2:S:55:LEU:HD22	2:S:55:LEU:H	1.75	0.49
2:S:274:VAL:HG23	2:S:275:LEU:N	2.26	0.49
3:T:180:GLU:HG3	3:T:188:THR:OG1	2.12	0.49
2:S:202:HIS:O	2:S:206:ILE:HG13	2.12	0.49
3:T:209:SER:H	3:T:212:LEU:HD12	1.76	0.49
2:M:35:PHE:CE1	2:M:37:THR:HB	2.47	0.49
2:S:66:TRP:NE1	2:S:70:ILE:HD11	2.28	0.49
1:L:169:TYR:HE1	2:M:180:PHE:CD2	2.30	0.49
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.94	0.49
1:R:105:VAL:O	1:R:109:ARG:HD3	2.12	0.49
3:T:133:PRO:O	3:T:136:ALA:N	2.46	0.49
4:D:21:ILE:HD12	4:D:30:ALA:HB3	1.94	0.49
2:M:280:GLY:CA	5:M:1003:BCL:HED3	2.43	0.49
1:R:28:PRO:O	2:S:254:TRP:HA	2.11	0.49
1:R:180:PHE:HE2	5:R:2002:BCL:HMA2	1.78	0.49
4:C:46:ARG:HG2	4:C:47:THR:N	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:241:VAL:HG21	6:M:1006:BPH:CAC	2.37	0.49
2:M:155:TRP:O	2:M:159:VAL:HG23	2.11	0.49
3:H:73:LEU:HD22	3:H:75:VAL:HG13	1.93	0.49
2:S:275:LEU:HD23	2:S:278:LEU:HD12	1.95	0.49
4:D:118:GLN:HA	4:D:122:VAL:CG2	2.43	0.49
3:H:120:LEU:N	3:H:226:THR:HB	2.28	0.49
1:R:46:ILE:HD13	5:R:2004:BCL:H201	1.95	0.49
2:S:191:LEU:N	2:S:191:LEU:HD22	2.28	0.49
2:S:228:ARG:C	2:S:230:GLY:H	2.21	0.49
2:S:300:ASN:C	2:S:301:HIS:ND1	2.71	0.49
1:L:130:THR:HA	1:L:134:PHE:HD2	1.77	0.49
1:R:117:ILE:HD13	2:S:251:PHE:CE2	2.48	0.49
1:R:169:TYR:CE2	1:R:260:VAL:HG23	2.48	0.49
2:S:46:GLN:HG2	2:S:51:TYR:HA	1.95	0.49
2:S:164:ARG:HH22	2:S:168:MET:HE2	1.78	0.49
1:R:263:TRP:CD2	2:S:180:PHE:HZ	2.31	0.49
2:S:271:TRP:O	2:S:275:LEU:HG	2.12	0.49
3:T:44:ASN:C	3:T:46:ASP:N	2.71	0.49
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.47	0.48
1:L:65:SER:HB2	1:L:152:THR:HG21	1.94	0.48
1:R:179:PHE:HB3	1:R:240:ALA:HB2	1.95	0.48
3:T:124:ASP:OD1	3:T:125:GLY:N	2.46	0.48
3:H:105:MET:HE2	3:H:212:LEU:HD13	1.94	0.48
1:R:117:ILE:HB	1:R:118:PRO:CD	2.43	0.48
4:D:91:THR:HG23	4:D:93:ASP:N	2.28	0.48
1:L:87:GLN:O	1:L:91:ILE:HG12	2.13	0.48
2:M:120:PHE:O	2:M:124:VAL:HG23	2.12	0.48
12:L:1007:HOH:O	3:H:81:GLU:HB2	2.14	0.48
2:M:152:SER:OG	2:M:278:LEU:HG	2.13	0.48
2:M:280:GLY:C	5:M:1003:BCL:CED	2.86	0.48
3:T:181:VAL:O	3:T:181:VAL:HG13	2.14	0.48
4:D:76:PHE:O	4:D:80:VAL:HG22	2.14	0.48
5:R:2002:BCL:H142	5:R:2004:BCL:HBB2	1.96	0.48
2:S:241:ARG:NH2	3:T:79:GLU:OE2	2.44	0.48
3:T:219:ILE:HG13	3:T:219:ILE:O	2.13	0.48
1:R:177:ILE:HD13	5:S:2001:BCL:HMD2	1.96	0.48
3:T:73:LEU:HD22	3:T:74:THR:N	2.28	0.48
1:L:124:ALA:O	5:L:1002:BCL:H51	2.13	0.48
1:L:6:GLU:HG3	2:M:250:LEU:CD2	2.44	0.48
3:H:17:ILE:HG23	3:H:18:TYR:N	2.29	0.48
3:H:32:GLN:HG2	3:H:56:PHE:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:70:ARG:NH2	3:T:123:LEU:HD13	2.29	0.48
4:D:83:PRO:O	4:D:86:PHE:HB3	2.13	0.48
1:R:272:TRP:HA	1:R:275:ILE:HG13	1.95	0.47
2:S:191:LEU:CD2	2:S:191:LEU:H	2.26	0.47
2:S:232:GLU:N	2:S:232:GLU:OE1	2.47	0.47
3:T:161:ALA:HB2	3:T:210:SER:CB	2.43	0.47
1:L:117:ILE:HB	1:L:118:PRO:CD	2.44	0.47
2:M:199:ASN:OD1	2:M:201:PHE:N	2.48	0.47
1:R:132:VAL:HG13	1:R:146:PHE:CE1	2.49	0.47
1:R:166:ASN:OD1	1:R:168:HIS:HB2	2.14	0.47
2:S:122:MET:O	2:S:126:VAL:HG23	2.15	0.47
3:T:83:ARG:O	3:T:85:ILE:HD12	2.15	0.47
4:D:109:ASP:O	4:D:110:ALA:C	2.58	0.47
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.80	0.47
3:H:219:ILE:HA	3:H:229:GLU:OE2	2.15	0.47
2:S:91:PHE:CD1	2:S:91:PHE:N	2.83	0.47
2:S:209:LEU:HD22	5:S:2003:BCL:H3A	1.97	0.47
3:T:36:MET:CE	3:T:58:LEU:HD23	2.44	0.47
3:H:170:ASP:OD2	3:H:172:PRO:HG2	2.13	0.47
1:R:187:LEU:HD11	2:S:269:ALA:CB	2.42	0.47
1:R:238:LEU:O	1:R:239:SER:C	2.58	0.47
4:D:100:MET:HG3	11:D:2009:HEM:C4C	2.49	0.47
3:H:180:GLU:HA	3:H:189:ARG:O	2.15	0.47
2:S:156:LEU:HD13	5:S:2003:BCL:H43	1.97	0.47
1:L:3:LEU:HD23	3:H:42:LEU:HD21	1.96	0.47
3:H:87:LEU:HD21	3:H:109:VAL:HG21	1.96	0.47
2:S:134:TYR:CE1	2:S:144:LYS:HG3	2.50	0.47
3:T:165:VAL:HB	3:T:180:GLU:HG2	1.97	0.47
3:H:50:ALA:O	3:H:52:ASN:N	2.44	0.47
2:S:75:TRP:O	2:S:76:TYR:C	2.58	0.47
2:S:218:MET:HE3	2:S:252:TRP:CZ3	2.49	0.47
3:T:32:GLN:HG2	3:T:56:PHE:CE2	2.50	0.47
3:T:243:TYR:O	3:T:246:PRO:HD2	2.15	0.47
1:L:41:PHE:O	1:L:42:ALA:C	2.58	0.46
4:C:46:ARG:O	4:C:70:ALA:HA	2.15	0.46
1:R:75:LEU:HA	1:R:142:TRP:CD1	2.50	0.46
2:S:175:VAL:HB	10:S:2011:LDA:O1	2.15	0.46
3:T:154:ARG:HB3	3:T:160:ILE:HA	1.98	0.46
1:L:3:LEU:HD23	3:H:42:LEU:CD2	2.45	0.46
2:M:69:THR:O	2:M:72:ILE:HG22	2.16	0.46
4:C:17:THR:HA	4:C:32:ARG:HH12	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:79:PRO:O	1:R:80:LEU:C	2.57	0.46
1:R:135:ARG:NH1	1:R:248:MET:O	2.48	0.46
4:D:38:PRO:HB3	4:D:54:PHE:CD2	2.50	0.46
4:D:57:TYR:HA	11:D:2009:HEM:O1D	2.15	0.46
1:L:8:LYS:O	3:H:110:GLY:N	2.43	0.46
1:L:50:ALA:O	1:L:53:ALA:HB3	2.15	0.46
3:H:83:ARG:O	3:H:85:ILE:HD12	2.15	0.46
1:L:69:PRO:O	1:L:70:ALA:C	2.59	0.46
1:L:244:SER:HB3	5:L:1002:BCL:HED3	1.97	0.46
2:M:280:GLY:C	5:M:1003:BCL:HED3	2.41	0.46
3:H:122:GLU:OE2	3:H:130:LYS:HD3	2.16	0.46
3:H:181:VAL:HG13	3:H:181:VAL:O	2.16	0.46
4:C:29:ILE:N	4:C:29:ILE:CD1	2.79	0.46
1:R:185:LEU:C	1:R:185:LEU:HD12	2.41	0.46
2:S:229:PHE:O	2:S:244:ALA:HB2	2.16	0.46
3:T:17:ILE:HG23	3:T:18:TYR:N	2.31	0.46
2:M:300:ASN:N	2:M:300:ASN:ND2	2.64	0.46
1:R:207:ARG:HD2	1:R:207:ARG:N	2.30	0.46
3:T:32:GLN:HG2	3:T:56:PHE:CD2	2.51	0.46
3:T:154:ARG:NH1	3:T:158:LEU:HB3	2.31	0.46
2:M:50:ILE:HD12	2:M:50:ILE:C	2.41	0.46
1:R:5:PHE:HB2	1:R:8:LYS:HZ1	1.81	0.46
1:R:185:LEU:HD12	1:R:185:LEU:O	2.16	0.46
5:R:2004:BCL:H3A	5:R:2004:BCL:HBA2	1.66	0.46
2:S:204:LEU:O	2:S:207:ALA:HB3	2.16	0.46
4:D:33:ASN:HD21	4:D:35:LYS:NZ	2.14	0.46
1:R:7:ARG:HG3	1:R:7:ARG:NH1	2.30	0.45
1:R:200:PRO:HB3	1:R:207:ARG:HD3	1.98	0.45
2:S:79:GLY:C	2:S:81:ASN:N	2.74	0.45
2:S:218:MET:HE3	2:S:252:TRP:CH2	2.51	0.45
2:S:266:HIS:O	2:S:270:ILE:HG22	2.14	0.45
1:L:135:ARG:HD3	12:L:1006:HOH:O	2.16	0.45
2:M:261:THR:O	2:M:262:MET:C	2.59	0.45
4:C:10:LYS:O	4:C:13:ASN:HB2	2.16	0.45
3:T:105:MET:HE1	3:T:208:LEU:HD21	1.98	0.45
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.97	0.45
1:L:217:ARG:HD3	12:L:1021:HOH:O	2.16	0.45
1:R:135:ARG:HG3	1:R:135:ARG:HH11	1.80	0.45
1:R:162:TYR:OH	2:S:191:LEU:CD2	2.65	0.45
2:S:296:VAL:O	2:S:297:TRP:C	2.57	0.45
1:L:268:LYS:HA	1:L:273:ALA:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:83:ARG:HH21	3:H:114:TRP:HE1	1.65	0.45
3:H:221:SER:OG	3:H:224:GLU:HG2	2.16	0.45
1:R:166:ASN:ND2	2:S:187:ASN:CB	2.77	0.45
3:T:134:MET:HE1	3:T:142:VAL:CG2	2.46	0.45
1:L:208:THR:C	1:L:210:ASP:H	2.24	0.45
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.51	0.45
2:M:206:ILE:HG22	2:M:210:TYR:CE2	2.52	0.45
4:C:93:ASP:OD1	4:C:95:LYS:HG2	2.16	0.45
1:R:55:LEU:HD13	1:R:81:ALA:HB2	1.99	0.45
2:S:178:GLY:HA3	2:S:181:SER:OG	2.17	0.45
3:T:165:VAL:HG21	3:T:182:GLU:HB2	1.98	0.45
3:T:149:ILE:HA	3:T:164:VAL:HG12	1.99	0.45
4:D:61:MET:HE1	4:D:79:TYR:CE1	2.52	0.45
4:D:116:TYR:O	4:D:120:VAL:HG22	2.16	0.45
3:H:229:GLU:O	3:H:233:ILE:HG13	2.17	0.45
4:C:87:LEU:O	4:C:91:THR:CG2	2.65	0.45
1:L:7:ARG:O	1:L:9:TYR:N	2.50	0.45
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.47	0.45
2:M:153:ALA:HA	2:M:277:THR:HG21	1.99	0.45
3:H:201:ASN:OD1	3:H:202:ARG:NH1	2.49	0.45
4:C:19:HIS:HE1	4:C:38:PRO:HD2	1.82	0.45
1:R:6:GLU:HG3	2:S:250:LEU:HD21	1.97	0.45
2:S:149:ALA:O	2:S:152:SER:HB3	2.17	0.45
3:T:181:VAL:HG12	3:T:191:LEU:HD23	1.99	0.45
3:H:173:GLU:HG2	12:H:276:HOH:O	2.17	0.45
4:C:61:MET:HE1	4:C:79:TYR:CZ	2.51	0.45
1:R:233:GLY:HA3	2:S:216:PHE:CZ	2.52	0.45
2:M:55:LEU:HD22	2:M:55:LEU:N	2.32	0.44
3:H:20:PHE:O	3:H:23:PHE:HB3	2.16	0.44
2:S:221:ALA:O	2:S:222:THR:C	2.60	0.44
3:T:227:LEU:O	3:T:228:LEU:C	2.60	0.44
1:L:193:LEU:CD1	1:L:216:PHE:HB2	2.45	0.44
3:H:163:LYS:O	3:H:181:VAL:HG23	2.17	0.44
3:H:192:PRO:O	3:H:193:MET:C	2.60	0.44
1:R:216:PHE:HE2	1:R:224:ILE:HG22	1.82	0.44
1:L:44:LEU:HD23	1:L:92:CYS:SG	2.58	0.44
1:L:195:LEU:HD21	2:M:267:ARG:HG3	1.99	0.44
1:L:208:THR:C	1:L:210:ASP:N	2.71	0.44
2:M:154:ILE:HG23	2:M:157:TRP:HE3	1.83	0.44
3:H:79:GLU:CG	3:H:81:GLU:HG2	2.47	0.44
3:H:81:GLU:O	3:H:81:GLU:HG3	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:148:PRO:O	3:H:164:VAL:HB	2.17	0.44
4:C:114:TRP:HA	4:C:117:LEU:HD12	1.98	0.44
1:R:94:THR:HG23	1:R:129:LEU:HD21	1.98	0.44
2:S:36:SER:O	2:S:39:LEU:HB3	2.18	0.44
2:S:204:LEU:HD13	3:T:20:PHE:CE2	2.53	0.44
3:T:106:LYS:HA	3:T:106:LYS:CE	2.46	0.44
3:T:240:GLY:O	3:T:244:ALA:N	2.44	0.44
4:D:58:GLY:HA2	4:D:99:LYS:HE2	1.99	0.44
3:H:225:VAL:HG23	3:H:229:GLU:CB	2.46	0.44
3:T:169:VAL:HG12	3:T:170:ASP:N	2.32	0.44
5:L:1004:BCL:H3A	5:L:1004:BCL:HBA2	1.67	0.44
2:M:162:PHE:O	2:M:166:ILE:HG13	2.18	0.44
2:M:219:HIS:HA	9:M:1008:U10:O2	2.17	0.44
4:D:38:PRO:HD3	4:D:54:PHE:CZ	2.53	0.44
4:D:51:GLN:C	4:D:51:GLN:HE21	2.25	0.44
2:M:189:PHE:CD1	2:M:189:PHE:C	2.95	0.44
1:R:130:THR:HA	1:R:134:PHE:HD2	1.82	0.44
2:S:73:TRP:HE3	2:S:114:LEU:HD12	1.83	0.44
2:S:131:GLY:O	2:S:135:LEU:HG	2.17	0.44
2:M:237:GLN:HB2	2:M:262:MET:HG2	1.99	0.44
3:H:146:LYS:H	3:H:146:LYS:CD	2.23	0.44
3:H:170:ASP:OD2	3:H:173:GLU:HB2	2.18	0.44
2:S:73:TRP:CE3	2:S:114:LEU:HD12	2.53	0.44
2:S:293:ASN:OD1	2:S:293:ASN:C	2.61	0.44
3:T:154:ARG:HD2	3:T:158:LEU:O	2.18	0.44
1:L:150:ILE:HG22	1:L:151:TRP:N	2.32	0.44
4:C:23:ASP:HA	4:C:41:TYR:CD2	2.53	0.44
1:R:224:ILE:HG12	1:R:228:GLY:HA3	2.00	0.44
2:S:89:LEU:HA	2:S:92:PHE:CD2	2.53	0.44
2:S:204:LEU:HG	10:S:2010:LDA:HM11	2.00	0.44
1:L:159:ASN:O	1:L:160:THR:C	2.60	0.44
1:L:170:ASN:HB3	1:L:173:HIS:HB2	2.00	0.44
3:H:14:SER:O	3:H:17:ILE:HG22	2.18	0.44
3:H:165:VAL:HG23	3:H:182:GLU:H	1.83	0.44
1:R:111:LEU:HD21	2:S:254:TRP:CZ3	2.52	0.44
5:R:2002:BCL:HBA1	5:R:2004:BCL:HBC1	2.00	0.44
2:M:164:ARG:HG2	2:M:164:ARG:HH11	1.83	0.43
2:M:290:VAL:HG11	3:H:12:LEU:HB3	1.99	0.43
1:R:49:ILE:CG1	1:R:89:ILE:HD13	2.48	0.43
1:R:94:THR:CG2	1:R:129:LEU:HD21	2.48	0.43
1:R:230:HIS:CD2	2:S:223:ILE:HG13	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:221:SER:C	3:T:223:THR:H	2.26	0.43
1:L:100:TRP:O	1:L:104:GLU:HG3	2.19	0.43
3:H:66:LEU:HD12	3:H:66:LEU:H	1.83	0.43
3:H:133:PRO:HG3	3:H:168:TRP:CE2	2.54	0.43
1:R:148:TYR:HB3	6:S:2006:BPH:H161	2.00	0.43
2:S:293:ASN:ND2	4:D:13:ASN:HB3	2.32	0.43
1:L:133:LEU:C	1:L:136:PRO:HD2	2.43	0.43
2:S:243:THR:HG23	2:S:244:ALA:N	2.33	0.43
2:M:200:PRO:HB2	3:H:17:ILE:CD1	2.49	0.43
3:H:233:ILE:O	3:H:234:CYS:C	2.60	0.43
4:C:33:ASN:HA	12:C:1010:HOH:O	2.17	0.43
1:R:209:PRO:O	1:R:212:GLU:HB3	2.17	0.43
2:S:52:LEU:O	2:S:56:GLY:HA3	2.18	0.43
2:S:96:PRO:HG3	2:S:115:TRP:CE2	2.53	0.43
2:S:162:PHE:O	2:S:165:PRO:HD2	2.18	0.43
3:T:20:PHE:O	3:T:23:PHE:HB3	2.18	0.43
1:L:128:TYR:CE2	1:L:132:VAL:HG21	2.54	0.43
2:M:222:THR:O	2:M:223:ILE:C	2.61	0.43
1:R:153:HIS:O	1:R:156:TRP:HB3	2.18	0.43
1:R:200:PRO:O	1:R:201:GLU:C	2.61	0.43
3:T:85:ILE:HD12	3:T:85:ILE:N	2.33	0.43
1:L:7:ARG:HH11	1:L:7:ARG:HG3	1.84	0.43
1:L:97:PHE:CE1	5:L:1002:BCL:H121	2.53	0.43
2:M:71:GLY:O	2:M:72:ILE:C	2.62	0.43
2:S:120:PHE:O	2:S:124:VAL:HG23	2.18	0.43
2:M:110:LYS:C	2:M:111:GLU:HG3	2.43	0.43
2:M:256:MET:HE2	2:M:258:PHE:CE2	2.50	0.43
1:R:49:ILE:HD11	6:S:2006:BPH:H122	2.01	0.43
1:R:130:THR:HA	1:R:134:PHE:CD2	2.53	0.43
2:S:93:SER:HB2	2:S:181:SER:HB3	2.00	0.43
3:T:154:ARG:HD2	3:T:158:LEU:C	2.44	0.43
2:M:268:TRP:HE1	3:H:35:ASN:ND2	2.17	0.43
1:L:19:GLY:C	1:L:21:LEU:H	2.27	0.43
1:L:161:GLY:C	1:L:163:THR:H	2.27	0.43
1:R:170:ASN:O	1:R:174:MET:HG3	2.18	0.43
2:S:150:PHE:CE2	2:S:154:ILE:HD11	2.54	0.43
2:S:199:ASN:ND2	2:S:294:TRP:CZ2	2.87	0.43
2:S:300:ASN:N	2:S:300:ASN:ND2	2.64	0.43
3:T:67:PRO:O	3:T:68:HIS:HB2	2.18	0.43
3:T:227:LEU:O	3:T:230:GLU:N	2.51	0.43
1:R:217:ARG:HD3	12:R:2011:HOH:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:195:ASN:ND2	2:S:197:PHE:N	2.55	0.43
2:M:258:PHE:H	2:M:258:PHE:HD2	1.67	0.42
3:H:37:ARG:HB3	3:H:75:VAL:HB	2.01	0.42
1:R:107:ILE:HG23	2:S:254:TRP:HE3	1.84	0.42
2:S:200:PRO:HB2	3:T:17:ILE:HD13	2.01	0.42
2:S:268:TRP:CE3	3:T:31:LEU:HD13	2.54	0.42
2:S:297:TRP:NE1	3:T:13:ALA:HB3	2.33	0.42
2:M:157:TRP:HD1	5:M:1001:BCL:HBB1	1.84	0.42
3:T:79:GLU:HG3	3:T:81:GLU:HG2	2.01	0.42
3:T:188:THR:O	3:T:189:ARG:HG2	2.18	0.42
4:D:59:GLU:O	4:D:63:GLU:HG3	2.19	0.42
1:L:117:ILE:HB	12:L:1016:HOH:O	2.18	0.42
1:L:185:LEU:CD2	1:L:189:LEU:HD12	2.49	0.42
2:M:214:LEU:HG	2:M:215:LEU:N	2.34	0.42
5:M:1003:BCL:HAA2	5:M:1003:BCL:HBD	2.01	0.42
1:R:33:PHE:O	1:R:36:VAL:HG22	2.19	0.42
1:R:111:LEU:HD21	2:S:254:TRP:HH2	1.83	0.42
1:R:122:ALA:O	1:R:123:PHE:C	2.62	0.42
2:S:206:ILE:HG23	5:S:2003:BCL:HMB2	2.01	0.42
3:T:134:MET:HB2	3:T:167:ILE:O	2.19	0.42
3:T:173:GLU:O	3:T:174:GLN:HB3	2.19	0.42
1:L:90:THR:O	1:L:90:THR:HG22	2.18	0.42
1:L:161:GLY:C	1:L:163:THR:N	2.77	0.42
2:M:195:ASN:HD21	2:M:197:PHE:CB	2.27	0.42
2:M:270:ILE:HG23	2:M:271:TRP:H	1.83	0.42
2:M:271:TRP:HA	2:M:274:VAL:CG2	2.49	0.42
3:H:44:ASN:C	3:H:46:ASP:N	2.77	0.42
3:H:83:ARG:HG3	3:H:83:ARG:HH11	1.84	0.42
3:H:170:ASP:O	3:H:171:ILE:C	2.63	0.42
4:C:12:PHE:O	4:C:13:ASN:C	2.62	0.42
2:S:162:PHE:O	2:S:166:ILE:HG13	2.19	0.42
3:T:130:LYS:HG3	3:T:172:PRO:CG	2.41	0.42
1:R:169:TYR:HE1	2:S:180:PHE:CD2	2.38	0.42
1:R:173:HIS:HE1	1:R:177:ILE:HD11	1.80	0.42
3:T:26:GLY:O	3:T:29:TYR:HB3	2.20	0.42
2:M:133:THR:HG21	2:M:146:THR:HG22	2.01	0.42
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.84	0.42
4:C:41:TYR:O	4:C:46:ARG:NH2	2.53	0.42
3:T:154:ARG:HD2	3:T:158:LEU:HA	2.00	0.42
3:H:157:ASP:HA	3:H:249:LYS:HG2	2.01	0.42
2:S:150:PHE:O	2:S:154:ILE:HG13	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:261:THR:O	2:S:262:MET:C	2.63	0.42
3:T:66:LEU:HD12	3:T:66:LEU:N	2.34	0.42
1:L:269:LEU:HD12	1:L:272:TRP:CZ2	2.55	0.42
2:M:55:LEU:H	2:M:55:LEU:CD2	2.33	0.42
3:H:233:ILE:O	3:H:236:TYR:N	2.53	0.42
4:C:57:TYR:HA	11:C:1009:HEM:O1D	2.20	0.42
1:R:34:PHE:CZ	1:R:102:LEU:HD13	2.55	0.42
1:R:125:ILE:O	1:R:128:TYR:HB3	2.20	0.42
2:S:195:ASN:HD21	2:S:197:PHE:CB	2.28	0.42
3:T:191:LEU:HA	3:T:192:PRO:HD3	1.83	0.42
4:D:91:THR:HG23	4:D:93:ASP:H	1.84	0.42
3:H:209:SER:O	3:H:213:PHE:HD1	2.02	0.42
2:S:279:THR:O	2:S:282:ILE:HB	2.20	0.42
1:L:229:ILE:CG2	1:L:230:HIS:N	2.82	0.42
3:H:149:ILE:HA	3:H:164:VAL:HG12	2.01	0.42
4:C:51:GLN:NE2	4:C:53:ASP:N	2.64	0.42
1:L:116:HIS:O	1:L:119:PHE:HB3	2.19	0.41
1:L:141:ALA:HB1	12:L:1018:HOH:O	2.20	0.41
1:L:215:PHE:HD1	2:M:140:LEU:HD12	1.85	0.41
2:M:91:PHE:N	2:M:91:PHE:CD1	2.88	0.41
2:M:95:GLU:OE1	2:M:176:PRO:HB3	2.19	0.41
3:H:149:ILE:HA	3:H:164:VAL:CG1	2.50	0.41
3:H:175:MET:HE2	3:H:177:ARG:HG2	2.02	0.41
1:R:6:GLU:HG3	2:S:250:LEU:HD22	2.01	0.41
2:S:199:ASN:HB3	2:S:202:HIS:HB3	2.02	0.41
2:M:195:ASN:C	2:M:195:ASN:ND2	2.63	0.41
3:H:66:LEU:N	3:H:66:LEU:CD1	2.83	0.41
1:R:80:LEU:O	1:R:85:LEU:HG	2.21	0.41
1:R:120:ALA:O	1:R:121:PHE:C	2.63	0.41
2:S:88:ASP:O	2:S:89:LEU:C	2.64	0.41
2:S:191:LEU:N	2:S:191:LEU:CD2	2.83	0.41
4:D:32:ARG:O	4:D:33:ASN:HB3	2.19	0.41
2:M:204:LEU:HG	10:M:1010:LDA:HM11	2.03	0.41
1:L:268:LYS:C	1:L:273:ALA:HB2	2.45	0.41
2:M:156:LEU:HD12	2:M:277:THR:HG22	2.02	0.41
3:H:141:HIS:CD2	3:H:143:SER:HB3	2.56	0.41
3:H:225:VAL:HA	3:H:229:GLU:OE1	2.20	0.41
1:R:147:PRO:HD2	1:R:156:TRP:HB2	2.02	0.41
2:S:50:ILE:HD12	2:S:50:ILE:O	2.21	0.41
3:T:117:ARG:O	3:T:228:LEU:HB2	2.20	0.41
3:T:157:ASP:C	3:T:159:GLU:N	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:232:GLU:N	2:M:232:GLU:OE1	2.54	0.41
2:M:235:LEU:O	2:M:238:ILE:HB	2.21	0.41
1:R:94:THR:O	1:R:98:VAL:HG23	2.21	0.41
1:R:238:LEU:HD23	6:S:2006:BPH:CBC	2.51	0.41
2:S:69:THR:O	2:S:72:ILE:HG22	2.19	0.41
3:T:156:CYS:C	3:T:158:LEU:H	2.27	0.41
3:T:212:LEU:C	3:T:214:ALA:H	2.27	0.41
4:D:49:GLY:HA2	4:D:57:TYR:CD1	2.56	0.41
2:M:123:PHE:HA	2:M:157:TRP:HH2	1.85	0.41
2:M:167:LEU:HD12	2:M:285:LEU:HD11	2.01	0.41
3:H:153:VAL:HG22	3:H:203:VAL:HB	2.03	0.41
5:R:2002:BCL:HBD	5:R:2004:BCL:HBC3	2.01	0.41
4:D:16:GLN:HE21	4:D:32:ARG:HG3	1.86	0.41
4:D:43:VAL:HG13	4:D:44:VAL:N	2.36	0.41
5:L:1002:BCL:H2C	5:M:1003:BCL:H2C	2.02	0.41
2:M:110:LYS:O	2:M:111:GLU:HG3	2.20	0.41
3:H:146:LYS:HD3	3:H:146:LYS:N	2.25	0.41
3:H:171:ILE:N	3:H:172:PRO:HD2	2.36	0.41
2:S:191:LEU:HD22	2:S:191:LEU:H	1.86	0.41
3:T:87:LEU:HD21	3:T:109:VAL:HG21	2.03	0.41
4:D:116:TYR:CZ	4:D:120:VAL:HG21	2.55	0.41
3:H:50:ALA:C	3:H:52:ASN:N	2.78	0.41
1:R:96:ALA:HB1	6:S:2006:BPH:H2	2.02	0.41
1:R:133:LEU:C	1:R:136:PRO:HD2	2.46	0.41
2:S:234:GLU:O	2:S:238:ILE:HG13	2.21	0.41
3:T:37:ARG:NE	3:T:62:LYS:HD2	2.36	0.41
1:L:157:VAL:O	1:L:158:SER:C	2.63	0.41
1:L:166:ASN:HD21	2:M:187:ASN:HB2	1.83	0.41
2:M:98:ALA:HB1	2:M:99:PRO:HD2	2.03	0.41
2:M:278:LEU:HD23	2:M:278:LEU:HA	1.94	0.41
2:S:224:LEU:HA	2:S:227:SER:HB3	2.02	0.41
5:S:2001:BCL:HBB2	5:S:2001:BCL:HHC	2.03	0.41
3:T:70:ARG:HH22	3:T:123:LEU:CD1	2.34	0.41
3:T:109:VAL:O	3:T:110:GLY:C	2.63	0.41
3:T:159:GLU:HG3	12:T:268:HOH:O	2.21	0.41
3:T:212:LEU:C	3:T:214:ALA:N	2.79	0.41
1:L:26:VAL:HG23	1:L:31:VAL:CG2	2.50	0.41
1:L:60:ASN:C	1:L:62:GLN:H	2.29	0.41
4:C:82:ASP:OD2	4:C:103:LYS:HE2	2.21	0.41
3:T:110:GLY:O	3:T:112:ALA:N	2.53	0.41
5:L:1002:BCL:HBC2	5:M:1003:BCL:HBC2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:154:ILE:HG22	2:M:158:MET:HG2	2.03	0.40
1:R:17:VAL:HB	1:R:33:PHE:CD2	2.56	0.40
2:S:148:TRP:CE3	2:S:148:TRP:HA	2.56	0.40
2:S:156:LEU:HD12	2:S:277:THR:HG22	2.03	0.40
3:T:89:ARG:HA	3:T:98:HIS:CD2	2.56	0.40
1:L:231:ARG:O	1:L:235:LEU:HB2	2.21	0.40
2:M:214:LEU:O	2:M:217:ALA:HB3	2.21	0.40
4:C:17:THR:O	4:C:17:THR:HG22	2.21	0.40
4:C:72:ASP:O	4:C:73:GLU:C	2.64	0.40
1:R:12:PRO:HD3	3:T:97:PRO:HB3	2.02	0.40
1:R:38:THR:O	1:R:39:PHE:C	2.64	0.40
1:R:117:ILE:HG21	2:S:251:PHE:CZ	2.56	0.40
1:R:155:ASP:HA	12:R:2018:HOH:O	2.21	0.40
2:S:154:ILE:HG23	2:S:157:TRP:HE3	1.85	0.40
2:S:188:ASN:O	2:S:189:PHE:C	2.63	0.40
3:H:81:GLU:O	3:H:81:GLU:CG	2.69	0.40
3:H:240:GLY:O	3:H:241:LEU:C	2.63	0.40
1:R:3:LEU:O	1:R:5:PHE:N	2.55	0.40
1:R:22:PHE:O	1:R:24:PHE:N	2.55	0.40
1:R:45:GLY:O	1:R:46:ILE:C	2.64	0.40
1:R:128:TYR:CE2	1:R:132:VAL:HG21	2.56	0.40
1:R:232:LEU:O	1:R:236:LEU:HG	2.21	0.40
2:S:95:GLU:HA	2:S:96:PRO:HD3	1.91	0.40
2:S:196:LEU:HD23	2:S:196:LEU:HA	1.94	0.40
1:L:268:LYS:HA	1:L:273:ALA:CB	2.51	0.40
3:H:134:MET:C	3:H:136:ALA:N	2.79	0.40
1:R:100:TRP:O	1:R:104:GLU:HG3	2.22	0.40
2:S:55:LEU:H	2:S:55:LEU:CD2	2.34	0.40
3:T:27:LEU:O	3:T:28:ILE:C	2.65	0.40
3:T:70:ARG:NH2	3:T:123:LEU:CD1	2.85	0.40
4:D:113:ILE:O	4:D:117:LEU:HG	2.21	0.40
1:L:168:HIS:HB3	2:M:183:LEU:HD13	2.04	0.40
2:M:203:GLY:O	2:M:204:LEU:C	2.65	0.40
2:M:206:ILE:HG12	5:M:1003:BCL:CHB	2.52	0.40
2:M:213:ALA:O	2:M:214:LEU:C	2.64	0.40
1:R:51:TRP:CD1	1:R:51:TRP:C	2.99	0.40
4:D:19:HIS:HE1	4:D:38:PRO:HD2	1.86	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%)	227 (81%)	46 (16%)	6 (2%)	5	25
1	R	279/281 (99%)	231 (83%)	36 (13%)	12 (4%)	2	13
2	M	265/307 (86%)	228 (86%)	36 (14%)	1 (0%)	30	59
2	S	265/307 (86%)	220 (83%)	42 (16%)	3 (1%)	11	38
3	H	244/260 (94%)	198 (81%)	42 (17%)	4 (2%)	7	30
3	T	244/260 (94%)	199 (82%)	37 (15%)	8 (3%)	3	18
4	C	122/124 (98%)	109 (89%)	12 (10%)	1 (1%)	16	44
4	D	122/124 (98%)	105 (86%)	16 (13%)	1 (1%)	16	44
All	All	1820/1944 (94%)	1517 (83%)	267 (15%)	36 (2%)	6	26

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	7	ARG
1	R	23	ASP
1	R	116	HIS
3	T	80	SER
3	T	89	ARG
1	L	5	PHE
1	L	7	ARG
1	L	8	LYS
3	H	81	GLU
3	H	233	ILE
3	H	250	SER
1	R	4	SER
1	R	259	TRP
3	T	116	ALA
3	T	128	HIS
3	T	172	PRO
1	L	4	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	20	ASN
1	L	272	TRP
2	M	278	LEU
3	H	172	PRO
1	R	15	THR
1	R	271	TRP
2	S	195	ASN
2	S	218	MET
1	R	31	VAL
1	R	117	ILE
1	R	134	PHE
2	S	85	PHE
3	T	134	MET
3	T	158	LEU
4	D	67	LYS
4	C	83	PRO
3	T	111	PRO
1	R	150	ILE
1	R	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%)	217 (99%)	3 (1%)	59	72
1	R	220/220 (100%)	213 (97%)	7 (3%)	34	58
2	M	209/240 (87%)	201 (96%)	8 (4%)	29	55
2	S	209/240 (87%)	201 (96%)	8 (4%)	29	55
3	H	199/208 (96%)	193 (97%)	6 (3%)	36	59
3	T	199/208 (96%)	195 (98%)	4 (2%)	48	66
4	C	93/93 (100%)	90 (97%)	3 (3%)	34	58
4	D	93/93 (100%)	92 (99%)	1 (1%)	65	75
All	All	1442/1522 (95%)	1402 (97%)	40 (3%)	38	60

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	126	LEU
1	L	185	LEU
2	M	35	PHE
2	M	50	ILE
2	M	94	LEU
2	M	100	GLU
2	M	156	LEU
2	M	196	LEU
2	M	256	MET
2	M	258	PHE
3	H	73	LEU
3	H	81	GLU
3	H	106	LYS
3	H	146	LYS
3	H	194	GLN
3	H	231	ASP
4	C	13	ASN
4	C	29	ILE
4	C	51	GLN
1	R	7	ARG
1	R	108	CYS
1	R	154	LEU
1	R	185	LEU
1	R	193	LEU
1	R	195	LEU
1	R	235	LEU
2	S	35	PHE
2	S	50	ILE
2	S	87	ARG
2	S	94	LEU
2	S	100	GLU
2	S	156	LEU
2	S	182	HIS
2	S	195	ASN
3	T	73	LEU
3	T	106	LYS
3	T	146	LYS
3	T	194	GLN
4	D	51	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39)

such sidechains are listed below:

Mol	Chain	Res	Type
1	L	56	GLN
1	L	87	GLN
1	L	173	HIS
1	L	183	ASN
1	L	211	HIS
1	L	258	GLN
2	M	195	ASN
2	M	300	ASN
3	H	32	GLN
3	H	52	ASN
3	H	98	HIS
3	H	194	GLN
3	H	199	GLN
4	C	13	ASN
4	C	16	GLN
4	C	33	ASN
4	C	51	GLN
4	C	81	GLN
4	C	119	GLN
1	R	56	GLN
1	R	87	GLN
1	R	159	ASN
1	R	173	HIS
1	R	211	HIS
2	S	46	GLN
2	S	77	GLN
2	S	188	ASN
2	S	195	ASN
2	S	202	HIS
2	S	300	ASN
3	T	52	ASN
3	T	68	HIS
3	T	194	GLN
3	T	199	GLN
4	D	13	ASN
4	D	16	GLN
4	D	33	ASN
4	D	51	GLN
4	D	112	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 4 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$
10	LDA	S	2010	-	13,15,15	1.81	1 (7%)	14,17,17	1.78	3 (21%)
5	BCL	M	1003	2	69,74,74	1.88	15 (21%)	79,115,115	1.93	24 (30%)
11	HEM	C	1009	4	50,50,50	1.81	11 (22%)	67,82,82	1.30	10 (14%)
6	BPH	S	2006	-	59,70,70	2.24	15 (25%)	59,101,101	2.92	21 (35%)
10	LDA	S	2011	-	13,15,15	1.99	1 (7%)	14,17,17	1.55	4 (28%)
6	BPH	R	2005	-	49,60,70	2.35	15 (30%)	47,89,101	3.09	21 (44%)
5	BCL	S	2003	2	69,74,74	1.82	13 (18%)	79,115,115	1.89	19 (24%)
6	BPH	M	1006	-	59,70,70	2.29	16 (27%)	59,101,101	2.83	22 (37%)
5	BCL	S	2001	2	53,58,74	2.05	14 (26%)	58,95,115	2.04	16 (27%)
5	BCL	R	2004	1	69,74,74	1.81	13 (18%)	79,115,115	1.80	20 (25%)
9	U10	M	1008	-	37,37,63	1.93	10 (27%)	46,47,79	1.84	11 (23%)
9	U10	S	2008	-	37,37,63	2.01	12 (32%)	46,47,79	1.87	11 (23%)
5	BCL	R	2002	1	69,74,74	1.77	11 (15%)	79,115,115	1.84	20 (25%)
10	LDA	M	1011	-	13,15,15	1.95	1 (7%)	14,17,17	1.74	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	LDA	M	1010	-	13,15,15	1.92	1 (7%)	14,17,17	1.77	3 (21%)
5	BCL	L	1002	1	69,74,74	1.74	11 (15%)	79,115,115	1.81	21 (26%)
6	BPH	L	1005	-	49,60,70	2.36	15 (30%)	47,89,101	3.07	20 (42%)
5	BCL	M	1001	2	53,58,74	2.06	13 (24%)	58,95,115	1.94	14 (24%)
11	HEM	D	2009	4	50,50,50	1.80	14 (28%)	67,82,82	1.27	9 (13%)
5	BCL	L	1004	1	69,74,74	1.82	14 (20%)	79,115,115	1.83	19 (24%)

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
10	LDA	S	2010	-	-	4/13/13/13	-
5	BCL	M	1003	2	-	9/41/137/137	-
11	HEM	C	1009	4	-	4/14/54/54	-
6	BPH	S	2006	-	2/2/18/22	17/37/105/105	0/5/6/6
10	LDA	S	2011	-	-	6/13/13/13	-
6	BPH	R	2005	-	1/1/16/22	7/25/93/105	0/5/6/6
5	BCL	S	2003	2	-	8/41/137/137	-
6	BPH	M	1006	-	2/2/18/22	16/37/105/105	0/5/6/6
5	BCL	S	2001	2	-	5/22/118/137	-
5	BCL	R	2004	1	-	13/41/137/137	-
9	U10	M	1008	-	-	3/32/56/87	0/1/1/1
9	U10	S	2008	-	-	3/32/56/87	0/1/1/1
5	BCL	R	2002	1	-	11/41/137/137	-
10	LDA	M	1011	-	-	6/13/13/13	-
10	LDA	M	1010	-	-	6/13/13/13	-
5	BCL	L	1002	1	-	10/41/137/137	-
6	BPH	L	1005	-	1/1/16/22	9/25/93/105	0/5/6/6
5	BCL	M	1001	2	-	7/22/118/137	-
11	HEM	D	2009	4	-	4/14/54/54	-
5	BCL	L	1004	1	-	9/41/137/137	-

All (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1006	BPH	C2C-C3C	-8.51	1.47	1.54
6	L	1005	BPH	C2C-C3C	-8.26	1.47	1.54
6	R	2005	BPH	C2C-C3C	-7.71	1.48	1.54
6	S	2006	BPH	C2C-C3C	-7.58	1.48	1.54
10	S	2011	LDA	O1-N1	-6.83	1.25	1.42
5	R	2004	BCL	C3B-C4B	6.72	1.54	1.41
6	L	1005	BPH	C1D-C2D	6.70	1.46	1.39
10	M	1011	LDA	O1-N1	-6.69	1.25	1.42
5	S	2001	BCL	MG-NB	-6.65	1.92	2.05
6	S	2006	BPH	C1D-C2D	6.58	1.46	1.39
10	M	1010	LDA	O1-N1	-6.50	1.26	1.42
5	M	1003	BCL	MG-NB	-6.48	1.92	2.05
5	M	1001	BCL	C3B-C4B	6.48	1.53	1.41
5	R	2002	BCL	C3B-C4B	6.44	1.53	1.41
5	L	1004	BCL	C3B-C4B	6.42	1.53	1.41
6	R	2005	BPH	C1D-C2D	6.33	1.46	1.39
5	L	1002	BCL	C3B-C4B	6.31	1.53	1.41
5	S	2003	BCL	C3B-C4B	6.27	1.53	1.41
5	L	1002	BCL	MG-NB	-6.14	1.93	2.05
10	S	2010	LDA	O1-N1	-6.01	1.27	1.42
6	M	1006	BPH	C1D-C2D	6.00	1.46	1.39
5	S	2003	BCL	MG-NB	-5.99	1.93	2.05
5	M	1003	BCL	C3B-C4B	5.95	1.52	1.41
6	S	2006	BPH	C1B-C2B	5.89	1.46	1.39
11	D	2009	HEM	CBB-CAB	5.86	1.58	1.30
11	C	1009	HEM	CBB-CAB	5.74	1.58	1.30
5	R	2002	BCL	MG-NB	-5.74	1.94	2.05
5	M	1001	BCL	MG-NB	-5.60	1.94	2.05
5	S	2001	BCL	C3B-C4B	5.59	1.52	1.41
6	M	1006	BPH	C11-C10	-5.55	1.29	1.52
6	M	1006	BPH	C1B-C2B	5.54	1.45	1.39
6	S	2006	BPH	C11-C10	-5.49	1.29	1.52
6	R	2005	BPH	C1B-C2B	5.40	1.45	1.39
5	M	1001	BCL	MG-ND	5.40	2.16	2.05
5	L	1004	BCL	MG-NB	-5.27	1.95	2.05
11	C	1009	HEM	CBC-CAC	5.16	1.55	1.30
6	L	1005	BPH	C1B-C2B	5.13	1.45	1.39
11	D	2009	HEM	CBC-CAC	5.13	1.55	1.30
5	R	2004	BCL	MG-NB	-5.10	1.95	2.05
5	R	2002	BCL	MG-ND	5.04	2.15	2.05
5	M	1003	BCL	MG-ND	5.04	2.15	2.05
5	S	2003	BCL	MG-ND	4.97	2.15	2.05
9	S	2008	U10	O4-C4	4.93	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1002	BCL	MG-ND	4.71	2.15	2.05
5	R	2004	BCL	MG-ND	4.63	2.15	2.05
5	S	2001	BCL	MG-ND	4.53	2.14	2.05
5	L	1004	BCL	MG-ND	4.49	2.14	2.05
6	M	1006	BPH	O2A-CGA	4.39	1.46	1.33
6	R	2005	BPH	O2A-CGA	4.37	1.46	1.33
6	S	2006	BPH	O2A-CGA	4.37	1.46	1.33
9	M	1008	U10	O4-C4	4.28	1.47	1.36
6	R	2005	BPH	O2D-CGD	4.15	1.43	1.33
6	L	1005	BPH	O2A-CGA	4.13	1.45	1.33
6	L	1005	BPH	O2D-CGD	4.08	1.43	1.33
5	M	1001	BCL	C3C-C4C	-4.00	1.46	1.51
6	M	1006	BPH	O2D-CGD	3.96	1.43	1.33
9	M	1008	U10	C13-C14	3.90	1.42	1.33
6	S	2006	BPH	O2D-CGD	3.86	1.42	1.33
9	S	2008	U10	C13-C14	3.85	1.41	1.33
9	S	2008	U10	C6-C1	3.75	1.41	1.35
5	M	1003	BCL	MG-NA	3.64	2.14	2.06
9	M	1008	U10	C23-C24	3.58	1.41	1.33
5	S	2003	BCL	MG-NA	3.56	2.14	2.06
6	M	1006	BPH	CHA-CBD	3.44	1.55	1.51
6	S	2006	BPH	CHA-CBD	3.44	1.55	1.51
9	S	2008	U10	C23-C24	3.43	1.41	1.33
11	D	2009	HEM	CMD-C2D	3.42	1.57	1.50
5	S	2001	BCL	CBB-CAB	3.38	1.56	1.50
6	R	2005	BPH	C3B-C4B	3.37	1.46	1.41
5	M	1003	BCL	CBB-CAB	3.30	1.56	1.50
9	S	2008	U10	O3-C3	3.29	1.44	1.36
9	M	1008	U10	O3-C3M	-3.29	1.38	1.45
9	S	2008	U10	O3-C3M	-3.28	1.38	1.45
11	C	1009	HEM	CMD-C2D	3.25	1.57	1.50
6	R	2005	BPH	C1A-C2A	3.23	1.55	1.51
9	M	1008	U10	C8-C9	3.22	1.40	1.33
5	R	2004	BCL	MG-NA	3.22	2.13	2.06
5	L	1004	BCL	C1B-C2B	3.16	1.50	1.43
9	S	2008	U10	C8-C9	3.16	1.40	1.33
9	M	1008	U10	O3-C3	3.16	1.44	1.36
5	R	2002	BCL	CBB-CAB	3.14	1.56	1.50
5	S	2001	BCL	C3D-C4D	-3.14	1.37	1.44
5	R	2002	BCL	C1B-C2B	3.14	1.50	1.43
6	L	1005	BPH	CHA-CBD	3.12	1.55	1.51
5	S	2003	BCL	C1B-C2B	3.12	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1004	BCL	CBB-CAB	3.11	1.56	1.50
5	L	1002	BCL	C1B-C2B	3.10	1.50	1.43
5	S	2001	BCL	C3C-C4C	-3.10	1.47	1.51
6	L	1005	BPH	C4D-ND	-3.10	1.33	1.38
5	L	1004	BCL	MG-NA	3.09	2.13	2.06
5	S	2001	BCL	C4B-NB	-3.08	1.33	1.37
5	M	1001	BCL	MG-NC	-3.06	1.99	2.06
5	M	1001	BCL	CBB-CAB	3.06	1.56	1.50
5	S	2003	BCL	CBB-CAB	3.04	1.56	1.50
6	R	2005	BPH	CHA-CBD	3.04	1.55	1.51
5	R	2004	BCL	C1B-C2B	3.02	1.50	1.43
6	S	2006	BPH	C1A-C2A	3.00	1.55	1.51
5	R	2002	BCL	MG-NA	3.00	2.13	2.06
9	M	1008	U10	C7-C8	-2.98	1.45	1.50
5	M	1003	BCL	C3D-C4D	-2.97	1.37	1.44
6	M	1006	BPH	C3B-C4B	2.97	1.46	1.41
5	M	1003	BCL	C1B-C2B	2.96	1.50	1.43
6	L	1005	BPH	C2-C3	2.96	1.39	1.33
6	M	1006	BPH	O2D-CED	-2.95	1.38	1.45
6	M	1006	BPH	C1A-C2A	2.95	1.55	1.51
9	M	1008	U10	C18-C19	2.94	1.39	1.33
9	M	1008	U10	C6-C1	2.91	1.40	1.35
11	C	1009	HEM	CAB-C3B	2.91	1.55	1.47
5	L	1002	BCL	CBB-CAB	2.91	1.55	1.50
6	R	2005	BPH	O2D-CED	-2.90	1.38	1.45
6	S	2006	BPH	O2D-CED	-2.89	1.38	1.45
6	R	2005	BPH	C4D-ND	-2.86	1.34	1.38
9	S	2008	U10	C7-C8	-2.86	1.46	1.50
5	L	1004	BCL	C3D-C4D	-2.85	1.37	1.44
5	M	1001	BCL	MG-NA	2.85	2.13	2.06
5	S	2001	BCL	MG-NC	-2.85	1.99	2.06
6	M	1006	BPH	C2-C3	2.84	1.39	1.33
6	L	1005	BPH	CAA-C2A	2.83	1.59	1.54
5	L	1004	BCL	C3C-C4C	-2.83	1.48	1.51
5	R	2004	BCL	C3D-C4D	-2.83	1.37	1.44
11	C	1009	HEM	C4D-ND	-2.82	1.35	1.40
6	M	1006	BPH	C4D-ND	-2.82	1.34	1.38
6	L	1005	BPH	C3B-C2B	-2.81	1.34	1.39
5	R	2004	BCL	CBB-CAB	2.81	1.55	1.50
9	S	2008	U10	C18-C19	2.80	1.39	1.33
5	R	2004	BCL	C3C-C4C	-2.79	1.48	1.51
5	S	2001	BCL	MG-NA	2.79	2.12	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1006	BPH	CAA-C2A	2.78	1.59	1.54
5	M	1001	BCL	C3D-C4D	-2.78	1.37	1.44
11	D	2009	HEM	CAB-C3B	2.77	1.54	1.47
5	M	1001	BCL	C1B-C2B	2.75	1.49	1.43
6	R	2005	BPH	CAA-C2A	2.74	1.59	1.54
5	R	2004	BCL	MG-NC	-2.73	1.99	2.06
5	L	1002	BCL	MG-NA	2.73	2.12	2.06
6	M	1006	BPH	C3B-C2B	-2.72	1.35	1.39
5	S	2003	BCL	C3D-C4D	-2.71	1.38	1.44
5	L	1004	BCL	MG-NC	-2.71	1.99	2.06
6	L	1005	BPH	C1A-C2A	2.70	1.55	1.51
6	L	1005	BPH	O2D-CED	-2.69	1.39	1.45
5	L	1004	BCL	CHD-C1D	2.65	1.43	1.38
11	D	2009	HEM	C4A-C3A	2.61	1.49	1.43
5	S	2001	BCL	C1B-C2B	2.61	1.49	1.43
6	R	2005	BPH	C2-C3	2.60	1.39	1.33
6	S	2006	BPH	CAA-C2A	2.60	1.59	1.54
6	S	2006	BPH	C3D-C2D	-2.59	1.35	1.39
11	C	1009	HEM	CAC-C3C	2.59	1.54	1.47
5	S	2001	BCL	OBG-CAB	-2.59	1.17	1.23
6	L	1005	BPH	C3B-C4B	2.58	1.45	1.41
6	R	2005	BPH	C3B-C2B	-2.57	1.35	1.39
6	S	2006	BPH	C3B-C4B	2.57	1.45	1.41
6	S	2006	BPH	C2-C3	2.56	1.39	1.33
11	D	2009	HEM	C4D-ND	-2.56	1.35	1.40
11	C	1009	HEM	C4A-C3A	2.54	1.49	1.43
5	S	2001	BCL	CHD-C1D	2.53	1.43	1.38
5	R	2002	BCL	C3D-C4D	-2.50	1.38	1.44
5	R	2004	BCL	C4-C3	2.48	1.56	1.50
9	S	2008	U10	C15-C14	2.46	1.56	1.50
5	R	2002	BCL	CHD-C1D	2.45	1.43	1.38
11	C	1009	HEM	FE-NC	2.44	2.03	1.95
5	M	1003	BCL	C4B-NB	-2.44	1.34	1.37
5	M	1003	BCL	CMD-C2D	2.43	1.55	1.50
5	M	1003	BCL	C1D-C2D	-2.42	1.40	1.45
5	S	2003	BCL	CMD-C2D	2.42	1.55	1.50
11	D	2009	HEM	C1C-NC	-2.42	1.35	1.39
11	D	2009	HEM	C4D-C3D	2.41	1.49	1.45
6	L	1005	BPH	C3D-C2D	-2.40	1.35	1.39
6	S	2006	BPH	C4D-ND	-2.38	1.35	1.38
5	L	1002	BCL	C3D-C4D	-2.37	1.38	1.44
5	S	2001	BCL	CAA-C2A	2.36	1.58	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1009	HEM	C4D-C3D	2.34	1.49	1.45
11	D	2009	HEM	FE-ND	2.34	2.02	1.94
11	C	1009	HEM	C1C-NC	-2.33	1.35	1.39
5	M	1003	BCL	C4-C3	2.33	1.56	1.50
5	L	1002	BCL	CHD-C1D	2.31	1.42	1.38
5	L	1004	BCL	C4-C3	2.29	1.56	1.50
5	M	1001	BCL	CAA-C2A	2.28	1.58	1.54
9	M	1008	U10	C15-C14	2.27	1.56	1.50
5	L	1004	BCL	C6-C5	2.27	1.60	1.52
11	D	2009	HEM	CAC-C3C	2.27	1.53	1.47
5	M	1001	BCL	CAA-CBA	2.25	1.59	1.52
5	R	2004	BCL	CHD-C1D	2.24	1.42	1.38
6	S	2006	BPH	C3B-C2B	-2.24	1.35	1.39
5	R	2004	BCL	CMD-C2D	2.23	1.55	1.50
5	R	2002	BCL	C4-C3	2.22	1.56	1.50
11	C	1009	HEM	C1D-C2D	2.22	1.49	1.44
5	S	2003	BCL	OBB-CAB	-2.21	1.18	1.23
5	L	1002	BCL	C3C-C4C	-2.21	1.48	1.51
6	R	2005	BPH	O1D-CGD	2.21	1.26	1.21
5	R	2002	BCL	CMD-C2D	2.20	1.55	1.50
5	M	1001	BCL	OBB-CAB	-2.18	1.18	1.23
5	L	1002	BCL	C4-C3	2.17	1.56	1.50
5	M	1001	BCL	CHD-C1D	2.16	1.42	1.38
5	M	1003	BCL	C5-C3	2.16	1.55	1.51
5	L	1004	BCL	C3B-CAB	2.15	1.53	1.46
5	S	2003	BCL	C4-C3	2.15	1.55	1.50
11	D	2009	HEM	FE-NC	2.13	2.02	1.95
6	M	1006	BPH	C3D-C2D	-2.12	1.36	1.39
6	L	1005	BPH	O1D-CGD	2.12	1.26	1.21
11	D	2009	HEM	CHD-C1D	-2.11	1.34	1.39
6	M	1006	BPH	O1D-CGD	2.10	1.26	1.21
9	S	2008	U10	C7-C6	2.10	1.55	1.51
9	S	2008	U10	C20-C19	2.09	1.55	1.50
6	R	2005	BPH	C3D-C2D	-2.09	1.36	1.39
11	D	2009	HEM	C1D-C2D	2.09	1.48	1.44
5	R	2004	BCL	C6-C5	2.08	1.59	1.52
5	S	2003	BCL	C1D-C2D	-2.08	1.41	1.45
5	L	1004	BCL	C1A-CHA	-2.06	1.34	1.43
5	M	1003	BCL	OBB-CAB	-2.05	1.18	1.23
5	L	1002	BCL	MG-NC	-2.05	2.01	2.06
5	S	2001	BCL	CMD-C2D	2.05	1.55	1.50
5	R	2002	BCL	C1D-C2D	-2.04	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1003	BCL	MG-NC	-2.03	2.01	2.06
11	D	2009	HEM	CBD-CAD	2.02	1.58	1.51
5	S	2003	BCL	OBD-CAD	-2.01	1.19	1.22
5	S	2003	BCL	C4B-NB	-2.01	1.35	1.37
5	M	1003	BCL	C3C-C4C	-2.01	1.49	1.51

All (292) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	2006	BPH	O2D-CGD-CBD	14.63	127.02	110.95
6	M	1006	BPH	O2D-CGD-CBD	13.97	126.30	110.95
6	R	2005	BPH	O2D-CGD-CBD	13.82	126.13	110.95
6	L	1005	BPH	O2D-CGD-CBD	13.79	126.09	110.95
6	M	1006	BPH	C1-C2-C3	6.90	137.50	126.20
6	S	2006	BPH	C1-C2-C3	6.52	136.88	126.20
9	S	2008	U10	C3M-O3-C3	6.50	139.33	116.47
9	M	1008	U10	C3M-O3-C3	6.50	139.30	116.47
5	S	2001	BCL	C4A-NA-C1A	-6.32	103.79	106.68
6	L	1005	BPH	C1-C2-C3	6.19	136.34	126.20
6	R	2005	BPH	C1-C2-C3	6.18	136.31	126.20
5	R	2002	BCL	C4A-NA-C1A	-6.06	103.91	106.68
5	M	1001	BCL	CBC-CAC-C3C	-5.89	100.92	113.41
5	L	1002	BCL	C4A-NA-C1A	-5.85	104.01	106.68
5	L	1004	BCL	C4A-NA-C1A	-5.72	104.07	106.68
5	R	2004	BCL	C4A-NA-C1A	-5.45	104.19	106.68
5	M	1001	BCL	C4A-NA-C1A	-5.41	104.21	106.68
5	M	1003	BCL	C4A-NA-C1A	-5.32	104.25	106.68
5	S	2003	BCL	C4A-NA-C1A	-5.31	104.26	106.68
6	S	2006	BPH	C4D-CHA-CBD	-5.26	105.93	108.45
6	S	2006	BPH	O1D-CGD-CBD	-5.10	116.99	124.72
6	L	1005	BPH	C4D-CHA-CBD	-4.97	106.07	108.45
6	R	2005	BPH	C4D-CHA-CBD	-4.95	106.08	108.45
6	R	2005	BPH	O1D-CGD-CBD	-4.88	117.33	124.72
5	S	2001	BCL	C1D-ND-C4D	4.78	109.66	106.31
5	L	1004	BCL	C1D-ND-C4D	4.72	109.63	106.31
6	L	1005	BPH	O1D-CGD-CBD	-4.61	117.73	124.72
5	R	2004	BCL	C1D-ND-C4D	4.56	109.51	106.31
5	S	2001	BCL	CBC-CAC-C3C	-4.54	103.79	113.41
6	M	1006	BPH	O1D-CGD-CBD	-4.48	117.94	124.72
6	M	1006	BPH	C4D-CHA-CBD	-4.47	106.31	108.45
5	M	1003	BCL	C1D-ND-C4D	4.44	109.42	106.31
5	M	1001	BCL	C1D-ND-C4D	4.36	109.37	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	2006	BPH	C6-C5-C3	4.34	124.04	113.47
5	M	1003	BCL	C4D-CHA-C1A	4.32	126.40	121.24
6	R	2005	BPH	CED-O2D-CGD	4.25	125.55	115.92
5	L	1002	BCL	C1D-ND-C4D	4.24	109.29	106.31
6	L	1005	BPH	CED-O2D-CGD	4.23	125.52	115.92
5	S	2003	BCL	C1D-ND-C4D	4.20	109.26	106.31
5	S	2003	BCL	C4D-CHA-C1A	4.19	126.24	121.24
5	R	2002	BCL	C1D-ND-C4D	4.18	109.25	106.31
6	M	1006	BPH	O2D-CGD-O1D	-4.15	115.76	123.85
6	M	1006	BPH	CED-O2D-CGD	4.10	125.23	115.92
6	S	2006	BPH	O2D-CGD-O1D	-4.04	115.99	123.85
6	M	1006	BPH	C6-C5-C3	4.03	123.28	113.47
5	S	2001	BCL	CBB-CAB-C3B	4.00	128.84	120.40
6	S	2006	BPH	CBC-CAC-C3C	3.95	121.55	113.78
6	L	1005	BPH	O2D-CGD-O1D	-3.95	116.16	123.85
5	S	2003	BCL	O2D-CGD-CBD	-3.94	104.35	111.23
6	R	2005	BPH	CBC-CAC-C3C	3.92	121.49	113.78
5	S	2003	BCL	C11-C12-C13	-3.92	102.94	115.97
5	L	1004	BCL	C1-O2A-CGA	3.92	126.13	116.65
6	S	2006	BPH	CED-O2D-CGD	3.90	124.77	115.92
5	M	1003	BCL	O2D-CGD-CBD	-3.85	104.49	111.23
6	L	1005	BPH	CBC-CAC-C3C	3.84	121.32	113.78
10	M	1010	LDA	CM1-N1-C1	-3.82	102.20	110.23
10	S	2010	LDA	CM1-N1-C1	-3.80	102.25	110.23
6	R	2005	BPH	C6-C5-C3	3.77	122.64	113.47
6	R	2005	BPH	O2D-CGD-O1D	-3.76	116.54	123.85
5	L	1004	BCL	CBC-CAC-C3C	-3.74	105.48	113.41
5	M	1003	BCL	CBB-CAB-C3B	3.70	128.20	120.40
6	M	1006	BPH	CBC-CAC-C3C	3.70	121.05	113.78
5	R	2002	BCL	C11-C12-C13	-3.69	103.68	115.97
6	S	2006	BPH	C11-C10-C8	3.69	128.23	115.97
5	L	1002	BCL	C4D-CHA-C1A	3.67	125.62	121.24
5	S	2003	BCL	CBB-CAB-C3B	3.67	128.13	120.40
6	L	1005	BPH	C6-C5-C3	3.64	122.34	113.47
6	M	1006	BPH	C11-C10-C8	3.62	128.01	115.97
5	S	2003	BCL	OBB-CAB-CBB	-3.61	111.67	119.77
10	M	1011	LDA	CM1-N1-C1	-3.61	102.65	110.23
9	S	2008	U10	O5-C5-C6	-3.61	114.81	121.79
6	R	2005	BPH	C1C-C2C-C3C	3.59	106.25	102.84
5	R	2002	BCL	C4D-CHA-C1A	3.58	125.52	121.24
5	S	2001	BCL	OBB-CAB-CBB	-3.58	111.75	119.77
5	R	2004	BCL	CBC-CAC-C3C	-3.58	105.82	113.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	2004	BCL	C11-C12-C13	-3.57	104.08	115.97
9	M	1008	U10	O5-C5-C6	-3.57	114.89	121.79
5	L	1004	BCL	OBB-CAB-CBB	-3.56	111.79	119.77
5	L	1004	BCL	C4D-CHA-C1A	3.55	125.48	121.24
5	S	2001	BCL	C4D-CHA-C1A	3.52	125.44	121.24
5	R	2002	BCL	OBB-CAB-CBB	-3.51	111.90	119.77
5	R	2004	BCL	CBB-CAB-C3B	3.51	127.81	120.40
6	M	1006	BPH	C4C-C3C-C2C	3.51	106.18	102.84
5	M	1003	BCL	C11-C12-C13	-3.50	104.32	115.97
5	R	2002	BCL	CBB-CAB-C3B	3.49	127.77	120.40
6	R	2005	BPH	C4C-C3C-C2C	3.49	106.16	102.84
5	L	1004	BCL	CBB-CAB-C3B	3.48	127.73	120.40
5	M	1001	BCL	C4D-CHA-C1A	3.47	125.39	121.24
5	R	2004	BCL	OBB-CAB-CBB	-3.47	112.00	119.77
5	S	2001	BCL	CAC-C3C-C4C	-3.45	104.93	112.58
6	S	2006	BPH	C4C-C3C-C2C	3.43	106.10	102.84
5	S	2003	BCL	O1D-CGD-CBD	3.42	131.27	124.52
5	M	1003	BCL	OBB-CAB-CBB	-3.41	112.14	119.77
6	L	1005	BPH	C4C-C3C-C2C	3.36	106.03	102.84
6	M	1006	BPH	C1C-C2C-C3C	3.35	106.03	102.84
5	L	1004	BCL	C11-C12-C13	-3.35	104.84	115.97
5	R	2004	BCL	C1-O2A-CGA	3.34	124.74	116.65
6	S	2006	BPH	C1C-C2C-C3C	3.34	106.02	102.84
5	R	2004	BCL	C4D-CHA-C1A	3.33	125.22	121.24
6	L	1005	BPH	C1C-C2C-C3C	3.32	106.00	102.84
10	S	2010	LDA	O1-N1-C1	3.31	117.40	109.27
5	M	1001	BCL	CBB-CAB-C3B	3.28	127.32	120.40
11	C	1009	HEM	C2D-C1D-ND	-3.27	106.13	109.90
5	M	1001	BCL	C2C-C3C-C4C	3.25	106.20	101.34
9	S	2008	U10	O2-C2-C3	-3.24	114.17	121.03
10	M	1010	LDA	O1-N1-C1	3.21	117.16	109.27
11	D	2009	HEM	C1D-C2D-C3D	3.21	110.36	106.98
5	R	2004	BCL	C16-C15-C13	-3.21	105.29	115.97
5	M	1003	BCL	O1D-CGD-CBD	3.21	130.85	124.52
5	L	1004	BCL	C16-C15-C13	-3.20	105.32	115.97
5	L	1002	BCL	C11-C12-C13	-3.18	105.39	115.97
5	M	1001	BCL	OBB-CAB-CBB	-3.17	112.68	119.77
5	M	1003	BCL	CHA-C1A-NA	-3.14	119.28	126.39
11	D	2009	HEM	C2D-C1D-ND	-3.13	106.29	109.90
5	S	2003	BCL	CHA-C1A-NA	-3.12	119.32	126.39
9	M	1008	U10	O2-C2-C3	-3.10	114.46	121.03
5	R	2002	BCL	O1D-CGD-CBD	3.09	130.61	124.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	2002	BCL	O2D-CGD-CBD	-3.08	105.84	111.23
11	C	1009	HEM	CBD-CAD-C3D	-3.07	104.03	112.53
5	L	1002	BCL	CBB-CAB-C3B	3.07	126.87	120.40
5	S	2003	BCL	C16-C15-C13	-3.06	105.80	115.97
9	S	2008	U10	C1-C6-C5	-3.06	116.65	119.62
5	M	1001	BCL	CAA-C2A-C3A	-3.05	104.75	113.00
5	R	2002	BCL	C16-C15-C13	-3.04	105.86	115.97
6	S	2006	BPH	CMA-C3A-C4A	-3.01	108.12	114.61
5	L	1002	BCL	OBG-CAB-CBB	-3.01	113.02	119.77
9	M	1008	U10	C1-C6-C5	-3.01	116.69	119.62
6	L	1005	BPH	CMA-C3A-C4A	-3.01	108.13	114.61
11	C	1009	HEM	C1D-C2D-C3D	3.01	110.14	106.98
5	M	1003	BCL	C4-C3-C5	3.00	120.44	115.23
5	M	1003	BCL	C4D-C3D-CAD	-3.00	104.85	108.11
5	L	1004	BCL	C2C-C3C-C4C	2.99	105.81	101.34
6	M	1006	BPH	CMA-C3A-C4A	-2.96	108.24	114.61
6	S	2006	BPH	O2A-CGA-O1A	-2.96	116.23	123.63
5	S	2001	BCL	CAA-C2A-C3A	-2.95	105.02	113.00
5	M	1001	BCL	CHD-C1D-ND	-2.95	120.65	124.80
10	M	1011	LDA	O1-N1-C1	2.94	116.48	109.27
5	R	2002	BCL	CHA-C1A-NA	-2.91	119.79	126.39
9	S	2008	U10	C20-C19-C21	-2.91	110.18	115.23
5	L	1002	BCL	CHA-C1A-NA	-2.89	119.85	126.39
5	R	2004	BCL	C2C-C3C-C4C	2.87	105.64	101.34
5	L	1002	BCL	O2D-CGD-CBD	-2.86	106.23	111.23
9	M	1008	U10	C20-C19-C21	-2.85	110.28	115.23
6	S	2006	BPH	C7-C6-C5	-2.82	105.75	113.26
5	M	1003	BCL	C16-C15-C13	-2.80	106.66	115.97
5	S	2001	BCL	CHD-C1D-ND	-2.79	120.88	124.80
5	R	2004	BCL	CAC-C3C-C4C	-2.78	106.41	112.58
5	M	1001	BCL	CHA-C1A-NA	-2.77	120.11	126.39
5	L	1002	BCL	O1D-CGD-CBD	2.77	129.98	124.52
11	D	2009	HEM	CBB-CAB-C3B	-2.76	113.75	127.53
6	M	1006	BPH	O2A-CGA-O1A	-2.75	116.74	123.63
11	C	1009	HEM	CBB-CAB-C3B	-2.73	113.88	127.53
5	L	1002	BCL	CHD-C1D-ND	-2.73	120.96	124.80
5	S	2003	BCL	C4-C3-C5	2.73	119.96	115.23
5	S	2003	BCL	CBC-CAC-C3C	-2.71	107.66	113.41
5	S	2003	BCL	C4D-C3D-CAD	-2.70	105.17	108.11
5	L	1002	BCL	CAC-C3C-C4C	-2.69	106.62	112.58
5	S	2001	BCL	CGD-CBD-CAD	-2.67	102.20	110.85
9	S	2008	U10	C7-C8-C9	2.67	131.43	126.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1005	BPH	C1B-NB-C4B	-2.67	104.93	108.82
5	L	1004	BCL	CHA-C1A-NA	-2.66	120.36	126.39
5	S	2001	BCL	CHA-C1A-NA	-2.66	120.37	126.39
5	M	1003	BCL	CAA-CBA-CGA	-2.66	105.65	113.21
5	R	2004	BCL	CHA-C1A-NA	-2.64	120.41	126.39
5	M	1001	BCL	C4D-C3D-CAD	-2.64	105.24	108.11
5	L	1002	BCL	C16-C15-C13	-2.64	107.20	115.97
6	M	1006	BPH	C1B-NB-C4B	-2.64	104.97	108.82
5	L	1004	BCL	O2A-C1-C2	-2.63	97.99	108.11
10	S	2011	LDA	CM1-N1-C1	-2.63	104.71	110.23
11	D	2009	HEM	CAD-CBD-CGD	2.62	120.61	113.67
9	M	1008	U10	C17-C18-C19	2.62	133.62	127.62
6	S	2006	BPH	C1B-NB-C4B	-2.62	105.00	108.82
5	L	1004	BCL	CHD-C1D-ND	-2.60	121.14	124.80
5	S	2001	BCL	C2C-C3C-C4C	2.59	105.22	101.34
11	D	2009	HEM	CMD-C2D-C1D	-2.58	121.00	125.03
11	D	2009	HEM	CBC-CAC-C3C	-2.58	114.62	127.53
5	R	2004	BCL	CHD-C1D-ND	-2.58	121.17	124.80
5	R	2002	BCL	CBC-CAC-C3C	-2.57	107.96	113.41
5	M	1003	BCL	CGD-CBD-CAD	-2.57	102.53	110.85
6	M	1006	BPH	C7-C6-C5	-2.56	106.44	113.26
5	R	2004	BCL	C1-C2-C3	-2.55	122.02	126.20
5	S	2003	BCL	C7-C6-C5	-2.55	106.46	113.26
6	R	2005	BPH	CMA-C3A-C4A	-2.54	109.13	114.61
11	D	2009	HEM	CBD-CAD-C3D	-2.53	105.55	112.53
9	M	1008	U10	C6-C1-C2	2.50	121.14	119.17
5	L	1002	BCL	C4D-C3D-CAD	-2.49	105.40	108.11
5	R	2004	BCL	C7-C6-C5	-2.48	106.66	113.26
5	S	2003	BCL	CHD-C1D-ND	-2.47	121.33	124.80
5	R	2002	BCL	CHD-C1D-ND	-2.47	121.33	124.80
5	M	1003	BCL	CHD-C1D-ND	-2.46	121.33	124.80
5	L	1004	BCL	C4D-C3D-CAD	-2.46	105.43	108.11
5	R	2002	BCL	CAC-C3C-C4C	-2.46	107.12	112.58
5	L	1002	BCL	C2C-C3C-C4C	2.46	105.02	101.34
11	C	1009	HEM	CMD-C2D-C1D	-2.45	121.20	125.03
5	R	2002	BCL	C4D-C3D-CAD	-2.45	105.44	108.11
5	L	1002	BCL	CAA-CBA-CGA	-2.44	106.28	113.21
6	R	2005	BPH	C1B-NB-C4B	-2.44	105.26	108.82
11	C	1009	HEM	CBC-CAC-C3C	-2.44	115.35	127.53
5	R	2002	BCL	C2C-C3C-C4C	2.43	104.98	101.34
10	M	1010	LDA	CM2-N1-C1	2.43	115.33	110.23
6	R	2005	BPH	OBD-CAD-CBD	-2.43	122.26	125.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1009	HEM	CAD-CBD-CGD	2.42	120.09	113.67
5	M	1003	BCL	CBC-CAC-C3C	-2.42	108.28	113.41
9	S	2008	U10	C17-C18-C19	2.42	133.15	127.62
11	C	1009	HEM	C4D-ND-C1D	2.41	108.07	105.21
9	S	2008	U10	C6-C1-C2	2.40	121.06	119.17
6	L	1005	BPH	O2A-CGA-O1A	-2.39	117.64	123.63
9	S	2008	U10	C7-C6-C5	-2.39	115.74	118.52
9	M	1008	U10	C7-C8-C9	2.39	130.94	126.83
6	R	2005	BPH	O2A-CGA-O1A	-2.37	117.70	123.63
5	S	2001	BCL	CHD-C1D-C2D	2.36	130.39	125.49
10	M	1011	LDA	CM2-N1-C1	2.36	115.18	110.23
10	S	2011	LDA	CM2-N1-C1	2.34	115.15	110.23
6	R	2005	BPH	C5-C3-C2	-2.34	115.92	121.17
9	S	2008	U10	C16-C14-C13	2.33	126.40	121.17
11	D	2009	HEM	C4D-ND-C1D	2.33	107.96	105.21
5	L	1002	BCL	CBC-CAC-C3C	-2.32	108.50	113.41
10	S	2011	LDA	C6-C5-C4	-2.31	102.67	114.37
10	S	2010	LDA	CM2-N1-C1	2.31	115.09	110.23
6	L	1005	BPH	CAA-C2A-C3A	-2.31	106.76	113.00
5	L	1004	BCL	CAC-C3C-C4C	-2.31	107.47	112.58
6	L	1005	BPH	C5-C3-C2	-2.30	116.00	121.17
9	M	1008	U10	C7-C6-C5	-2.29	115.85	118.52
6	L	1005	BPH	CMB-C2B-C3B	2.28	129.24	124.68
5	M	1003	BCL	CAC-C3C-C4C	-2.28	107.53	112.58
5	R	2004	BCL	O2A-C1-C2	-2.28	99.35	108.11
5	L	1002	BCL	CAA-C2A-C3A	-2.27	106.86	113.00
5	R	2002	BCL	CAA-C2A-C3A	-2.27	106.87	113.00
5	S	2001	BCL	O1D-CGD-CBD	2.27	128.99	124.52
9	M	1008	U10	C16-C14-C13	2.27	126.26	121.17
5	R	2004	BCL	C4D-C3D-CAD	-2.25	105.66	108.11
6	R	2005	BPH	C2B-C1B-NB	2.25	111.06	109.43
5	L	1004	BCL	CHD-C1D-C2D	2.25	130.16	125.49
9	M	1008	U10	C4-C3-C2	-2.24	116.57	120.69
5	M	1003	BCL	CBA-CAA-C2A	2.24	120.46	113.79
5	M	1001	BCL	CHD-C1D-C2D	2.24	130.15	125.49
6	S	2006	BPH	CMB-C2B-C3B	2.24	129.16	124.68
5	S	2003	BCL	C2C-C3C-C4C	2.24	104.69	101.34
6	R	2005	BPH	C7-C6-C5	-2.23	107.31	113.26
6	R	2005	BPH	CAA-C2A-C3A	-2.22	107.00	113.00
6	M	1006	BPH	C2B-C1B-NB	2.22	111.03	109.43
10	S	2011	LDA	O1-N1-C1	2.20	114.68	109.27
6	S	2006	BPH	O2A-CGA-CBA	2.20	118.55	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1002	BCL	C7-C6-C5	-2.20	107.41	113.26
5	M	1001	BCL	CGD-CBD-CAD	-2.19	103.77	110.85
6	S	2006	BPH	CAA-C2A-C3A	-2.18	107.10	113.00
6	M	1006	BPH	CMD-C2D-C3D	2.18	129.04	124.68
10	M	1011	LDA	C9-C8-C7	-2.17	103.38	114.37
6	R	2005	BPH	CMD-C2D-C3D	2.17	129.01	124.68
9	S	2008	U10	C4-C3-C2	-2.16	116.72	120.69
6	S	2006	BPH	C4A-C3A-C2A	2.16	104.89	102.84
6	M	1006	BPH	CAA-C2A-C3A	-2.16	107.17	113.00
5	M	1003	BCL	C3D-C2D-C1D	-2.14	102.91	105.83
5	S	2001	BCL	CMA-C3A-C2A	-2.13	105.75	113.98
6	L	1005	BPH	C7-C6-C5	-2.13	107.59	113.26
5	R	2004	BCL	C12-C11-C10	-2.13	103.74	113.28
5	L	1004	BCL	C7-C6-C5	-2.13	107.59	113.26
6	R	2005	BPH	C4-C3-C5	2.12	118.91	115.23
5	R	2002	BCL	C11-C10-C8	-2.10	108.97	115.97
5	L	1002	BCL	CHD-C1D-C2D	2.10	129.85	125.49
6	M	1006	BPH	CMB-C2B-C3B	2.10	128.87	124.68
5	M	1003	BCL	C12-C11-C10	-2.10	103.89	113.28
6	R	2005	BPH	CMB-C2B-C3B	2.10	128.87	124.68
5	R	2004	BCL	CHD-C1D-C2D	2.09	129.84	125.49
5	R	2002	BCL	CAA-CBA-CGA	-2.09	107.27	113.21
5	R	2004	BCL	CBA-CAA-C2A	2.09	120.01	113.79
5	L	1004	BCL	CBA-CAA-C2A	2.09	120.00	113.79
5	R	2002	BCL	CMD-C2D-C3D	2.09	132.47	127.69
5	M	1003	BCL	C7-C6-C5	-2.08	107.71	113.26
5	S	2003	BCL	C3D-C2D-C1D	-2.08	102.99	105.83
5	M	1003	BCL	C2C-C3C-C4C	2.07	104.44	101.34
11	C	1009	HEM	CAD-C3D-C4D	2.07	128.30	124.70
5	M	1003	BCL	CAA-C2A-C3A	-2.06	107.43	113.00
5	L	1004	BCL	C12-C11-C10	-2.06	104.05	113.28
5	M	1003	BCL	CMD-C2D-C3D	2.06	132.41	127.69
5	S	2003	BCL	CAA-C2A-C3A	-2.05	107.46	113.00
5	S	2003	BCL	CMD-C2D-C3D	2.05	132.39	127.69
6	L	1005	BPH	CMD-C2D-C3D	2.05	128.78	124.68
6	M	1006	BPH	C5-C3-C2	-2.05	116.57	121.17
6	L	1005	BPH	C2B-C1B-NB	2.04	110.91	109.43
6	S	2006	BPH	CMD-C2D-C3D	2.04	128.77	124.68
5	S	2001	BCL	C4D-C3D-CAD	-2.04	105.89	108.11
5	R	2002	BCL	C14-C13-C15	-2.04	104.01	111.27
5	M	1001	BCL	CMD-C2D-C3D	2.04	132.36	127.69
5	L	1002	BCL	C4-C3-C5	2.03	118.75	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1006	BPH	OBD-CAD-CBD	-2.03	122.85	125.82
6	M	1006	BPH	O2A-CGA-CBA	2.03	118.01	111.83
11	C	1009	HEM	C2A-C1A-NA	2.03	112.40	110.15
11	D	2009	HEM	CAD-C3D-C4D	2.02	128.22	124.70
6	S	2006	BPH	OBD-CAD-CBD	-2.02	122.86	125.82
5	L	1002	BCL	C12-C11-C10	-2.01	104.27	113.28
6	L	1005	BPH	OBD-CAD-CBD	-2.00	122.89	125.82

All (6) chirality outliers are listed below:

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

All (157) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	1004	BCL	C1A-C2A-CAA-CBA
5	L	1004	BCL	C3A-C2A-CAA-CBA
5	R	2004	BCL	C1A-C2A-CAA-CBA
5	R	2004	BCL	C3A-C2A-CAA-CBA
5	S	2001	BCL	CHA-CBD-CGD-O1D
5	S	2001	BCL	CHA-CBD-CGD-O2D
6	L	1005	BPH	C4C-C3C-CAC-CBC
6	M	1006	BPH	C4C-C3C-CAC-CBC
6	M	1006	BPH	O2A-C1-C2-C3
6	M	1006	BPH	C1-C2-C3-C5
6	R	2005	BPH	C4C-C3C-CAC-CBC
6	S	2006	BPH	C4C-C3C-CAC-CBC
6	S	2006	BPH	O2A-C1-C2-C3
6	S	2006	BPH	C1-C2-C3-C5
10	M	1010	LDA	C2-C1-N1-CM2
10	S	2010	LDA	C2-C1-N1-CM2
11	D	2009	HEM	C2C-C3C-CAC-CBC
6	S	2006	BPH	O1D-CGD-O2D-CED
6	M	1006	BPH	CBD-CGD-O2D-CED
6	S	2006	BPH	CBD-CGD-O2D-CED
6	M	1006	BPH	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	R	2005	BPH	CBD-CGD-O2D-CED
5	L	1002	BCL	C3-C5-C6-C7
9	M	1008	U10	C24-C26-C27-C28
9	S	2008	U10	C24-C26-C27-C28
6	R	2005	BPH	O1D-CGD-O2D-CED
5	M	1003	BCL	C3-C5-C6-C7
5	R	2002	BCL	C5-C6-C7-C8
6	L	1005	BPH	C5-C6-C7-C8
6	S	2006	BPH	C10-C11-C12-C13
5	L	1002	BCL	C5-C6-C7-C8
6	M	1006	BPH	C8-C10-C11-C12
5	R	2004	BCL	C2A-CAA-CBA-CGA
6	M	1006	BPH	C10-C11-C12-C13
6	S	2006	BPH	C8-C10-C11-C12
5	M	1001	BCL	C4B-C3B-CAB-CBB
6	L	1005	BPH	C2A-CAA-CBA-CGA
5	R	2002	BCL	C8-C10-C11-C12
6	L	1005	BPH	O2A-C1-C2-C3
6	M	1006	BPH	C16-C17-C18-C19
6	M	1006	BPH	C16-C17-C18-C20
10	M	1011	LDA	C2-C3-C4-C5
5	L	1002	BCL	C3A-C2A-CAA-CBA
5	R	2002	BCL	C3A-C2A-CAA-CBA
5	R	2002	BCL	C3-C5-C6-C7
5	S	2003	BCL	C3-C5-C6-C7
5	L	1004	BCL	C2A-CAA-CBA-CGA
5	M	1003	BCL	C4-C3-C5-C6
5	S	2003	BCL	C5-C6-C7-C8
10	M	1010	LDA	C1-C2-C3-C4
6	R	2005	BPH	C2A-CAA-CBA-CGA
11	C	1009	HEM	C2B-C3B-CAB-CBB
11	C	1009	HEM	C2C-C3C-CAC-CBC
5	M	1003	BCL	C5-C6-C7-C8
6	S	2006	BPH	C5-C6-C7-C8
6	M	1006	BPH	C5-C6-C7-C8
10	S	2010	LDA	C1-C2-C3-C4
11	D	2009	HEM	C4C-C3C-CAC-CBC
6	S	2006	BPH	C15-C16-C17-C18
6	L	1005	BPH	C2C-C3C-CAC-CBC
6	M	1006	BPH	C2C-C3C-CAC-CBC
6	R	2005	BPH	C2C-C3C-CAC-CBC
6	S	2006	BPH	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	L	1002	BCL	C1A-C2A-CAA-CBA
5	R	2002	BCL	C1A-C2A-CAA-CBA
5	R	2004	BCL	C12-C13-C15-C16
6	S	2006	BPH	C16-C17-C18-C20
5	L	1002	BCL	O2A-C1-C2-C3
5	M	1001	BCL	C2B-C3B-CAB-CBB
5	R	2002	BCL	O2A-C1-C2-C3
6	S	2006	BPH	C16-C17-C18-C19
5	R	2004	BCL	C14-C13-C15-C16
10	M	1010	LDA	C9-C10-C11-C12
5	S	2003	BCL	C11-C12-C13-C15
5	M	1003	BCL	C13-C15-C16-C17
5	M	1003	BCL	C2-C3-C5-C6
5	R	2002	BCL	C15-C16-C17-C18
6	M	1006	BPH	C1-C2-C3-C4
6	S	2006	BPH	C1-C2-C3-C4
10	S	2011	LDA	C4-C5-C6-C7
10	M	1011	LDA	C4-C5-C6-C7
5	S	2003	BCL	C15-C16-C17-C18
5	M	1001	BCL	C4B-C3B-CAB-OB
5	S	2003	BCL	C11-C12-C13-C14
5	R	2004	BCL	C5-C6-C7-C8
5	L	1002	BCL	C12-C13-C15-C16
5	L	1004	BCL	C11-C12-C13-C15
5	M	1003	BCL	C11-C12-C13-C15
10	S	2011	LDA	C2-C3-C4-C5
11	D	2009	HEM	C2B-C3B-CAB-CBB
5	M	1001	BCL	C2B-C3B-CAB-OB
5	L	1002	BCL	C15-C16-C17-C18
5	L	1002	BCL	C8-C10-C11-C12
10	M	1010	LDA	C2-C1-N1-CM1
10	M	1011	LDA	C2-C1-N1-CM1
10	M	1011	LDA	C2-C1-N1-CM2
10	S	2010	LDA	C2-C1-N1-CM1
10	S	2011	LDA	C2-C1-N1-CM1
10	S	2011	LDA	C2-C1-N1-CM2
6	L	1005	BPH	O1D-CGD-O2D-CED
5	S	2003	BCL	C1A-C2A-CAA-CBA
5	M	1003	BCL	C12-C13-C15-C16
5	R	2002	BCL	C12-C13-C15-C16
5	L	1002	BCL	C14-C13-C15-C16
5	M	1003	BCL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	M	1011	LDA	C1-C2-C3-C4
5	M	1001	BCL	C1-C2-C3-C4
5	S	2001	BCL	C1-C2-C3-C4
10	M	1010	LDA	C2-C1-N1-O1
10	M	1011	LDA	C2-C1-N1-O1
10	S	2010	LDA	C2-C1-N1-O1
10	S	2011	LDA	C2-C1-N1-O1
9	S	2008	U10	C5-C4-O4-C4M
5	R	2004	BCL	CHA-CBD-CGD-O1D
5	R	2004	BCL	CHA-CBD-CGD-O2D
6	M	1006	BPH	C15-C16-C17-C18
6	S	2006	BPH	C14-C13-C15-C16
5	R	2004	BCL	C11-C12-C13-C15
6	L	1005	BPH	CBD-CGD-O2D-CED
5	L	1004	BCL	C14-C13-C15-C16
5	M	1003	BCL	C14-C13-C15-C16
11	C	1009	HEM	C4B-C3B-CAB-CBB
11	C	1009	HEM	C4C-C3C-CAC-CBC
11	D	2009	HEM	C4B-C3B-CAB-CBB
5	R	2002	BCL	C13-C15-C16-C17
5	L	1004	BCL	C5-C6-C7-C8
9	M	1008	U10	C20-C19-C21-C22
9	M	1008	U10	C18-C19-C21-C22
5	L	1004	BCL	C12-C13-C15-C16
6	S	2006	BPH	C12-C13-C15-C16
6	M	1006	BPH	C4-C3-C5-C6
6	M	1006	BPH	C14-C13-C15-C16
6	S	2006	BPH	C4-C3-C5-C6
5	S	2003	BCL	C4-C3-C5-C6
6	L	1005	BPH	CHA-CBD-CGD-O2D
6	S	2006	BPH	C2-C3-C5-C6
5	R	2002	BCL	C14-C13-C15-C16
5	R	2004	BCL	C11-C10-C8-C9
5	S	2003	BCL	C3A-C2A-CAA-CBA
5	R	2002	BCL	C2A-CAA-CBA-CGA
5	L	1004	BCL	C11-C10-C8-C9
5	L	1004	BCL	C11-C12-C13-C14
5	S	2001	BCL	CAA-CBA-CGA-O2A
6	M	1006	BPH	C12-C13-C15-C16
6	R	2005	BPH	C2-C1-O2A-CGA
10	S	2011	LDA	C1-C2-C3-C4
9	S	2008	U10	C14-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	L	1002	BCL	C2A-CAA-CBA-CGA
5	R	2004	BCL	C11-C12-C13-C14
5	M	1001	BCL	CAA-CBA-CGA-O2A
10	M	1010	LDA	C4-C5-C6-C7
6	L	1005	BPH	C2-C1-O2A-CGA
5	R	2004	BCL	C11-C10-C8-C7
6	R	2005	BPH	O2A-C1-C2-C3
5	M	1001	BCL	CAA-CBA-CGA-O1A
5	S	2001	BCL	CAA-CBA-CGA-O1A
5	R	2004	BCL	CAD-CBD-CGD-O2D

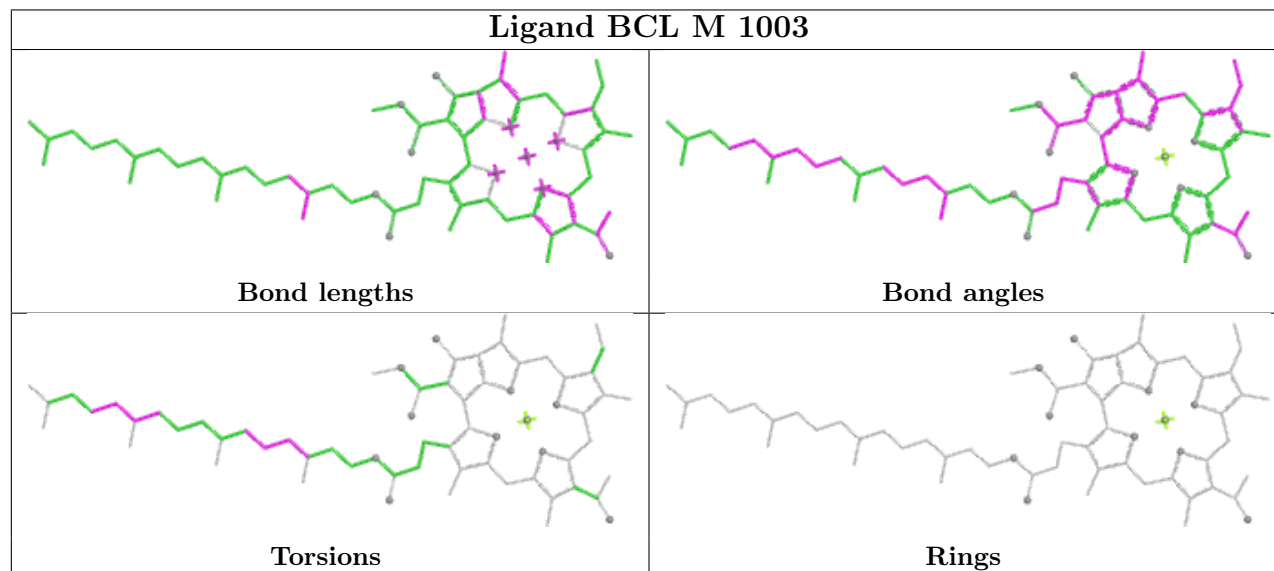
There are no ring outliers.

20 monomers are involved in 79 short contacts:

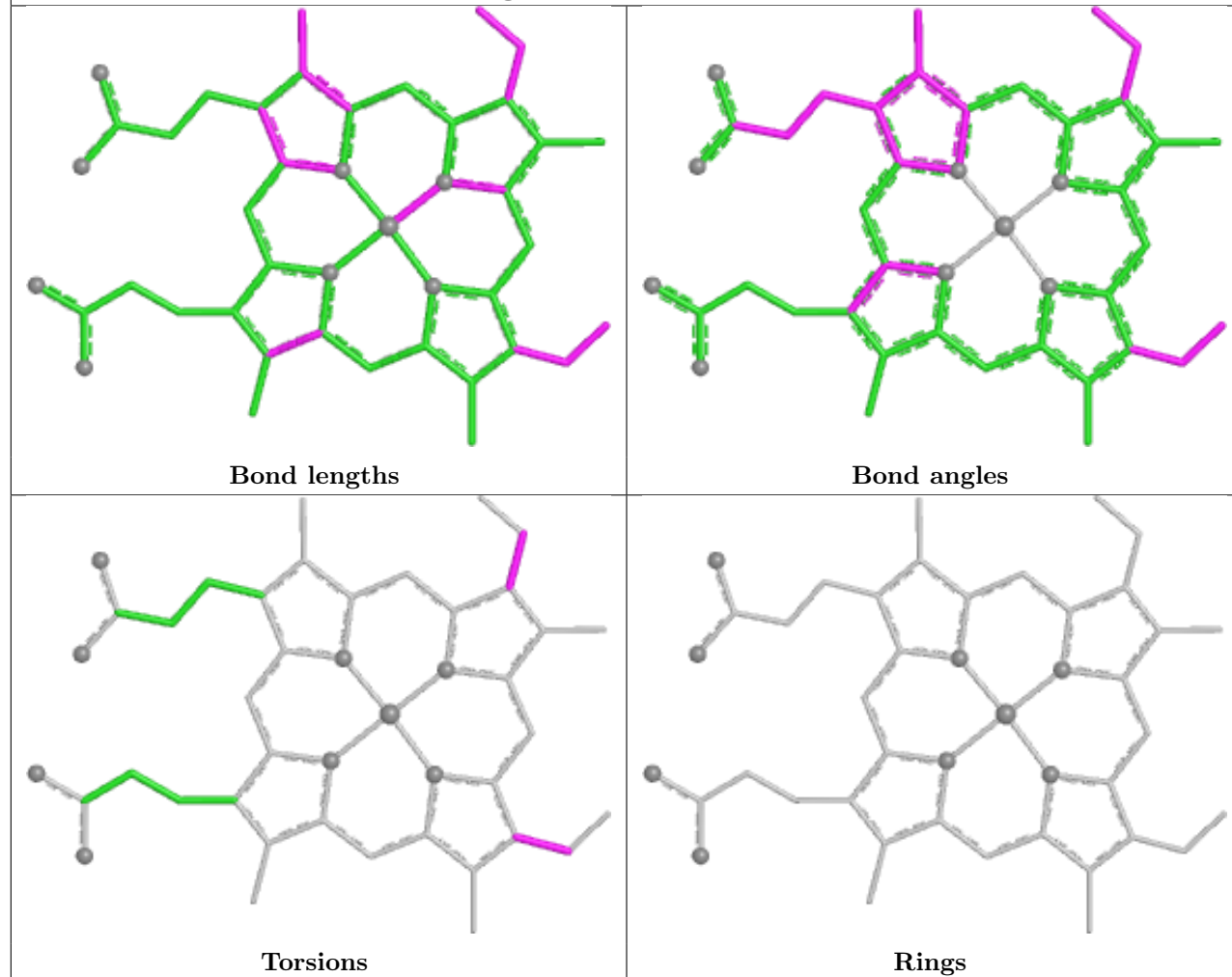
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	S	2010	LDA	2	0
5	M	1003	BCL	13	0
11	C	1009	HEM	2	0
6	S	2006	BPH	6	0
10	S	2011	LDA	2	0
6	R	2005	BPH	2	0
5	S	2003	BCL	11	0
6	M	1006	BPH	3	0
5	S	2001	BCL	5	0
5	R	2004	BCL	11	0
9	M	1008	U10	1	0
9	S	2008	U10	1	0
5	R	2002	BCL	12	0
10	M	1011	LDA	3	0
10	M	1010	LDA	2	0
5	L	1002	BCL	10	0
6	L	1005	BPH	1	0
5	M	1001	BCL	3	0
11	D	2009	HEM	2	0
5	L	1004	BCL	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

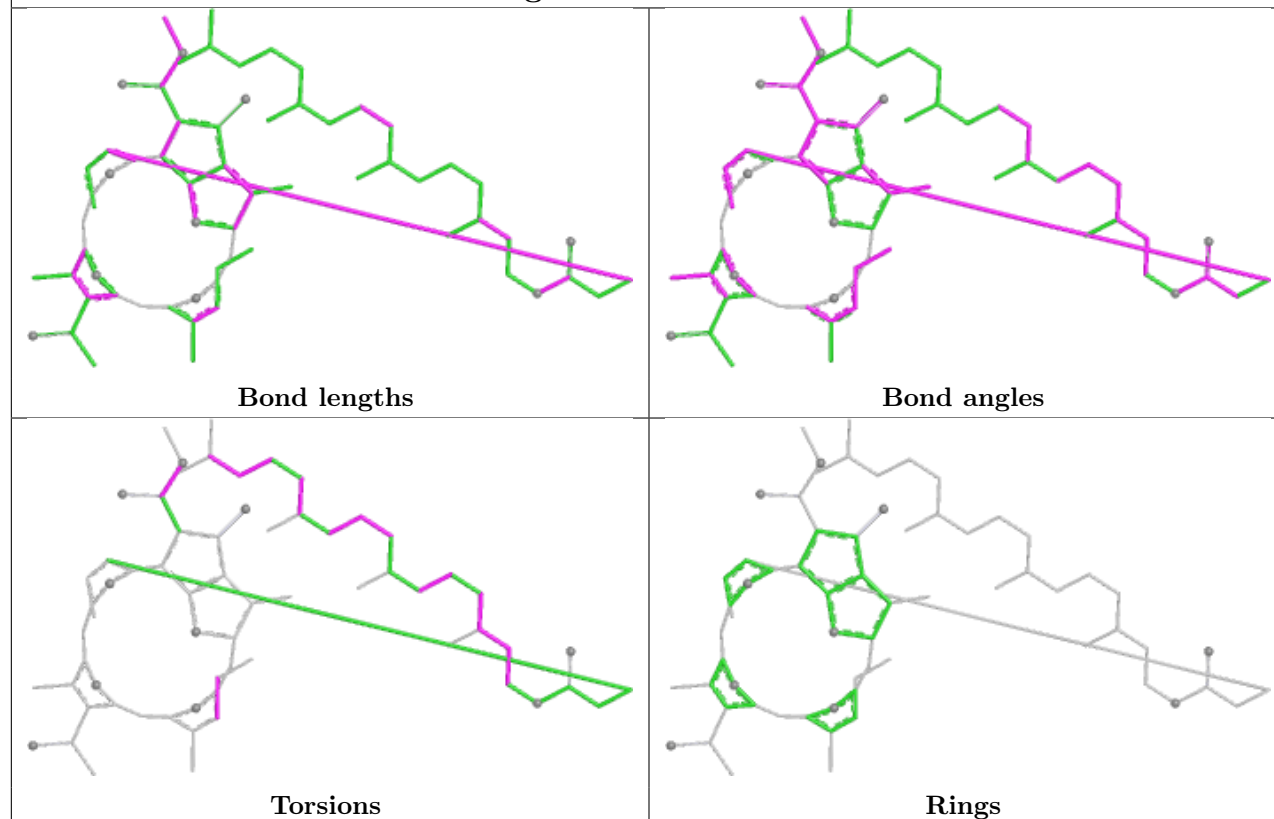
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



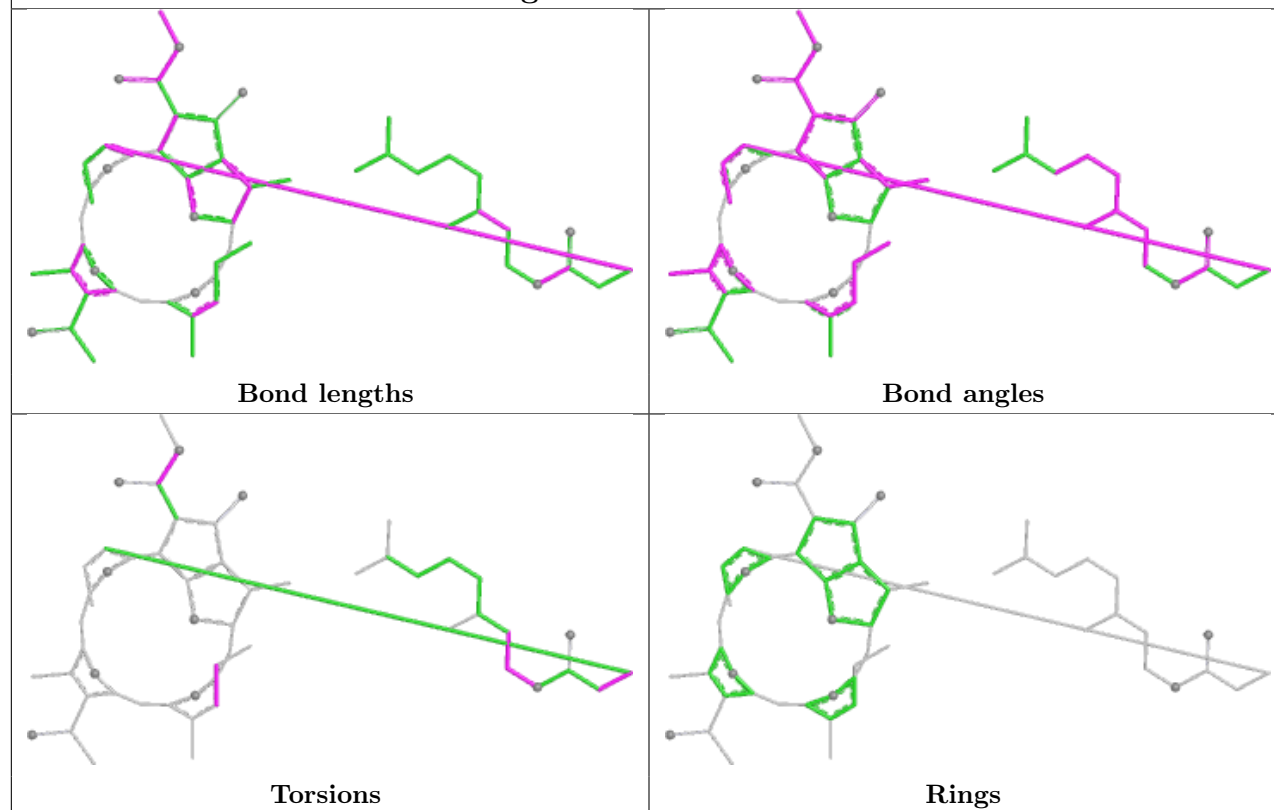
Ligand HEM C 1009

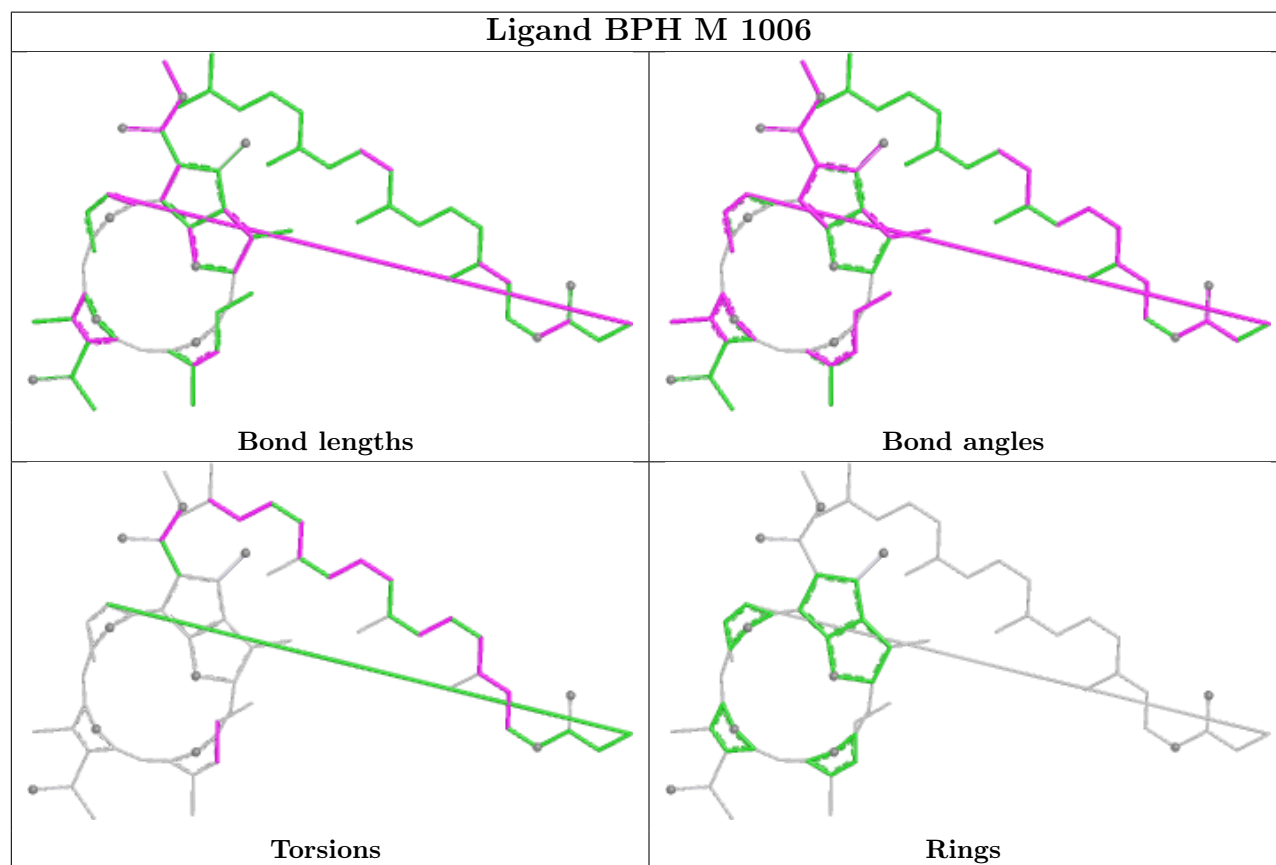
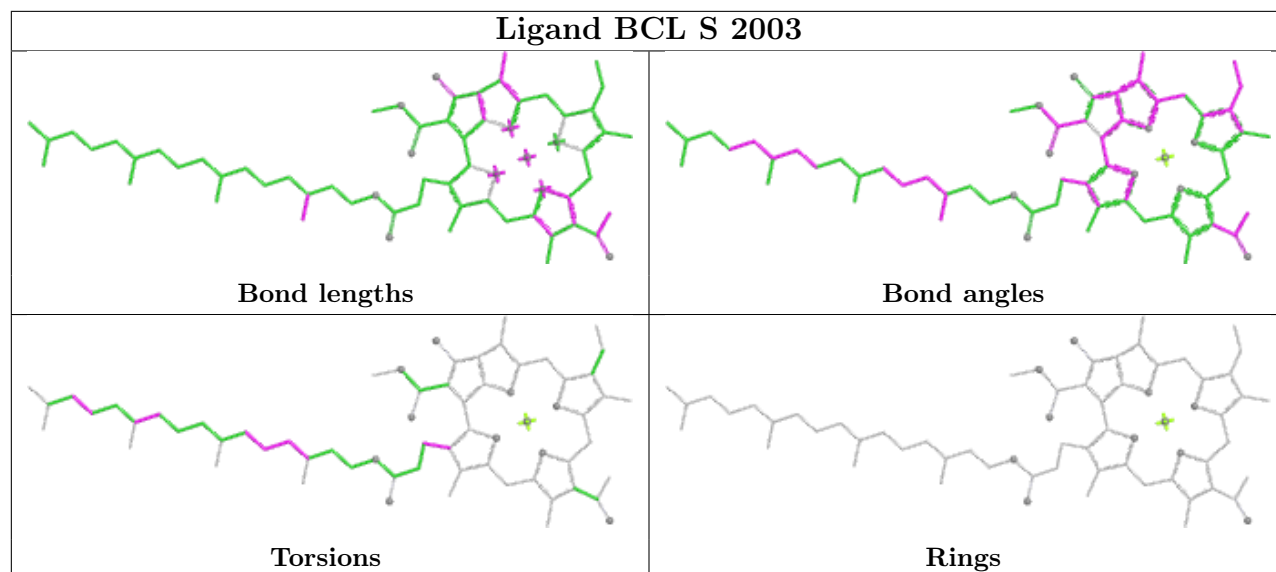


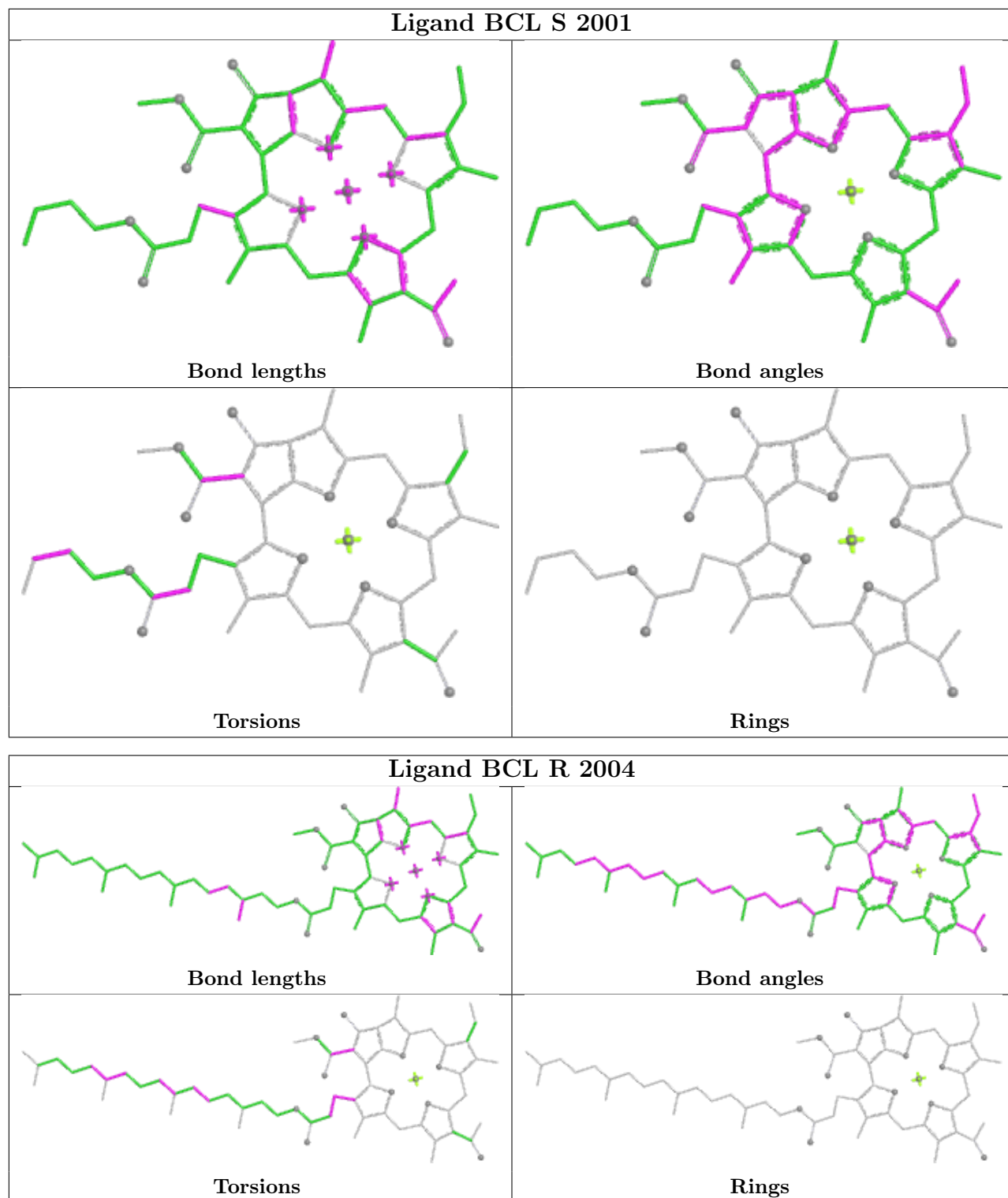
Ligand BPH S 2006

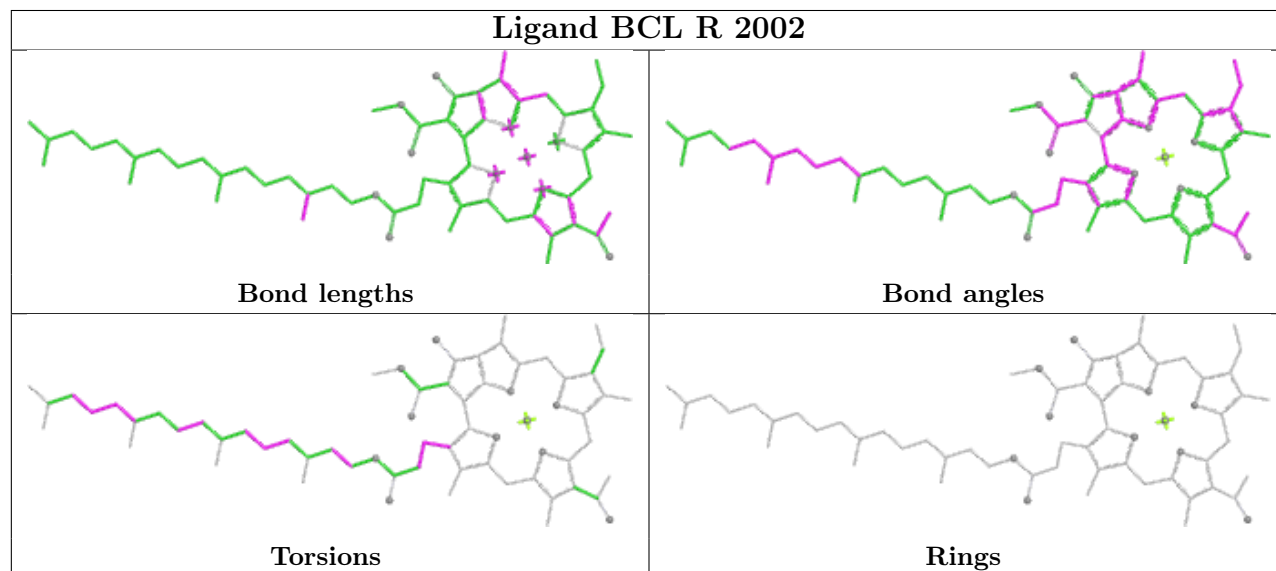
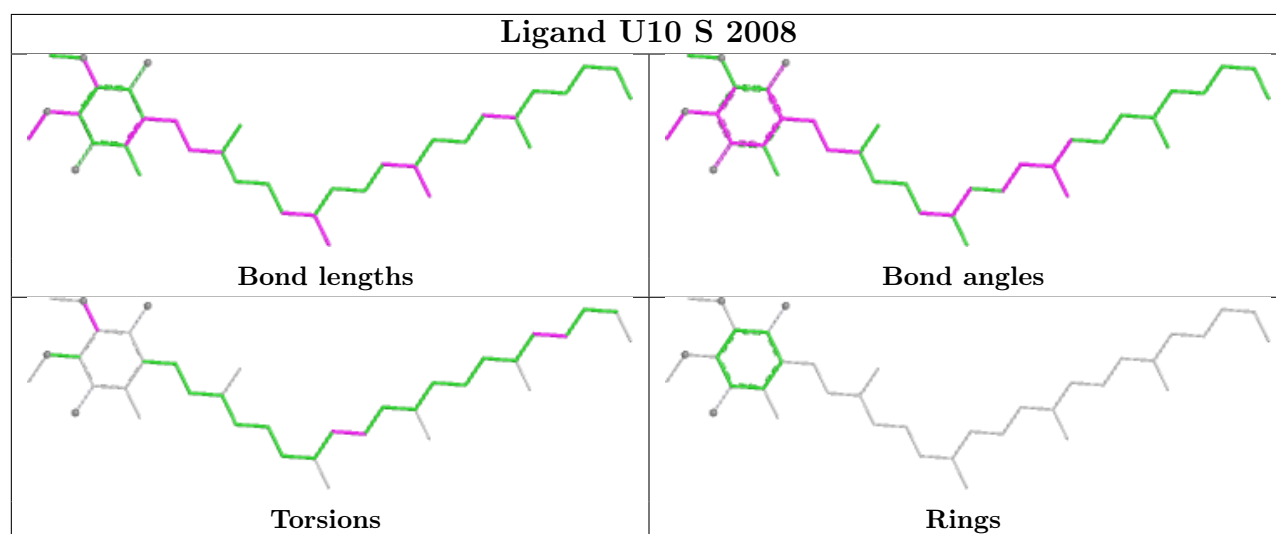
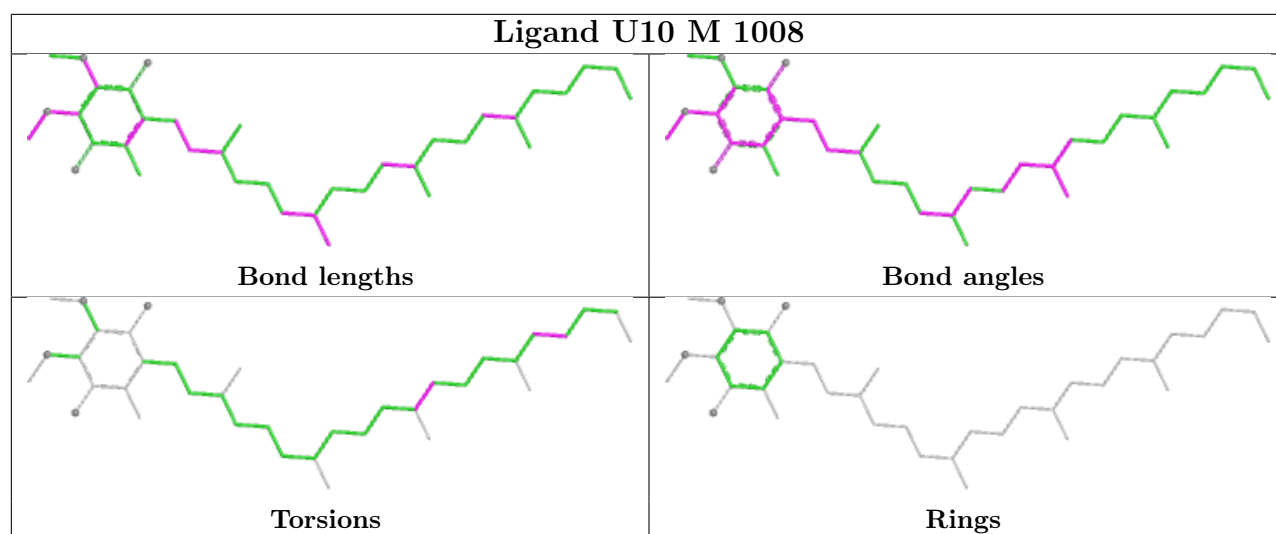


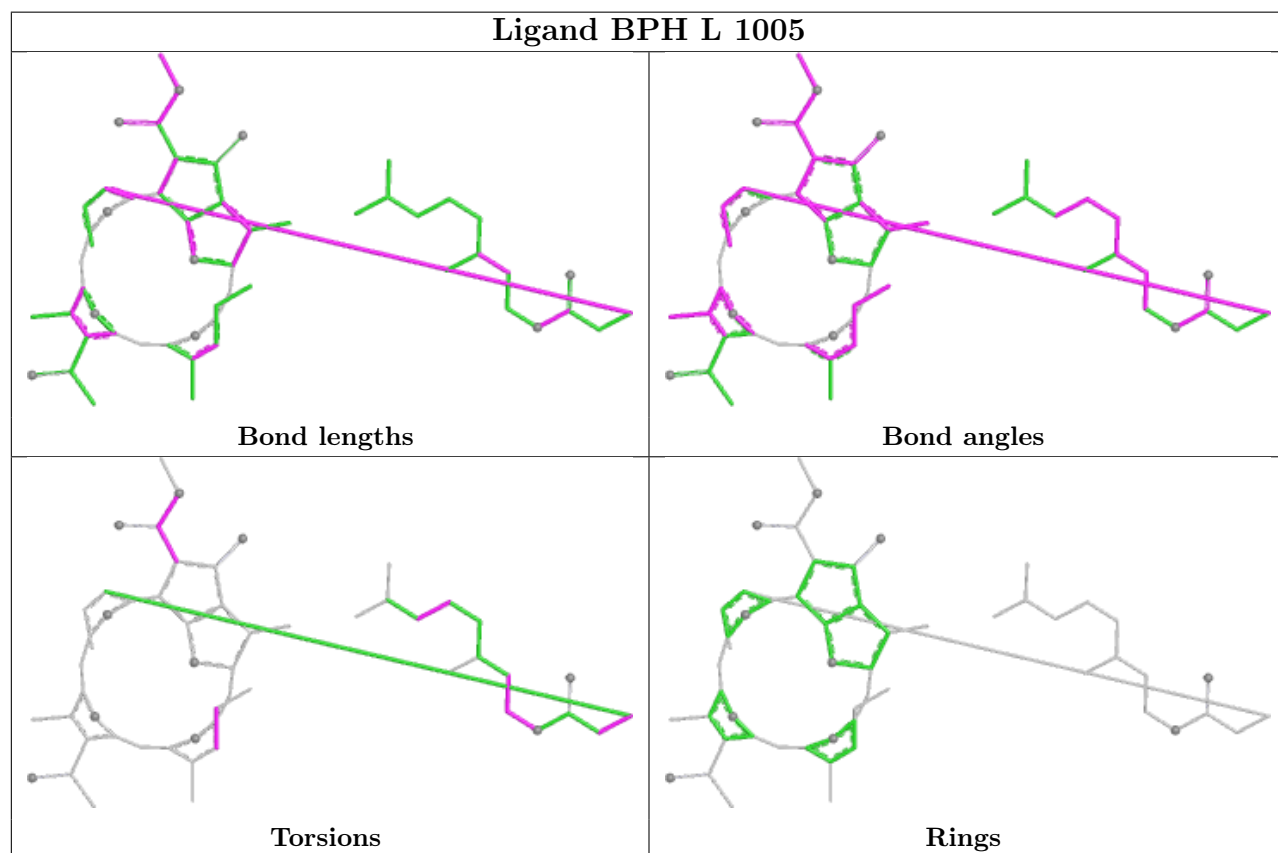
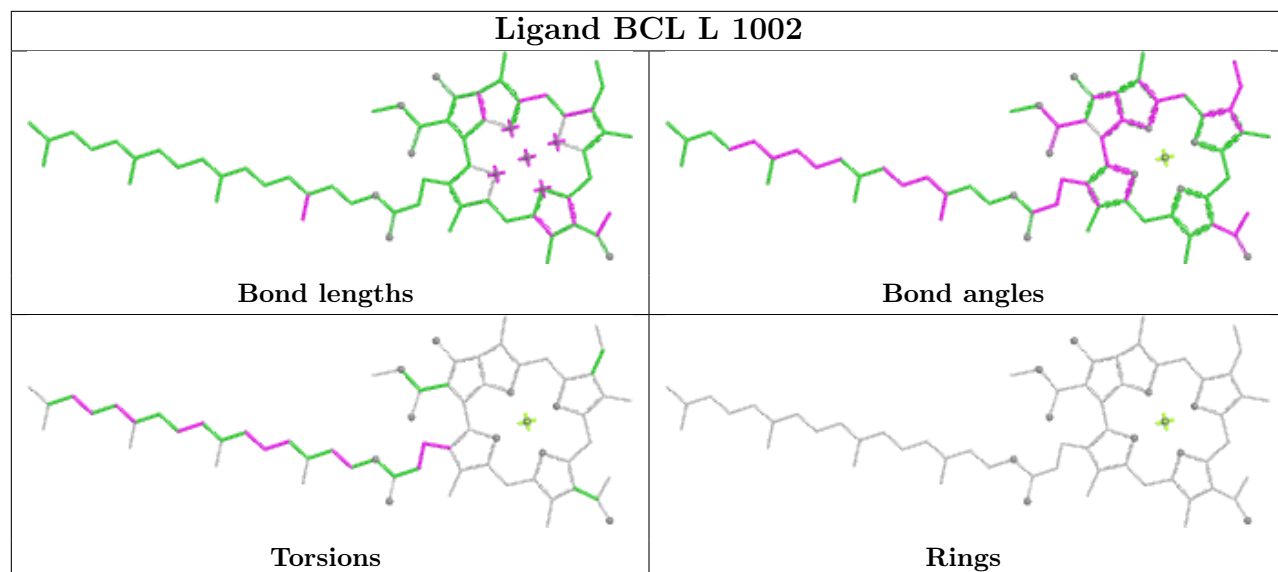
Ligand BPH R 2005

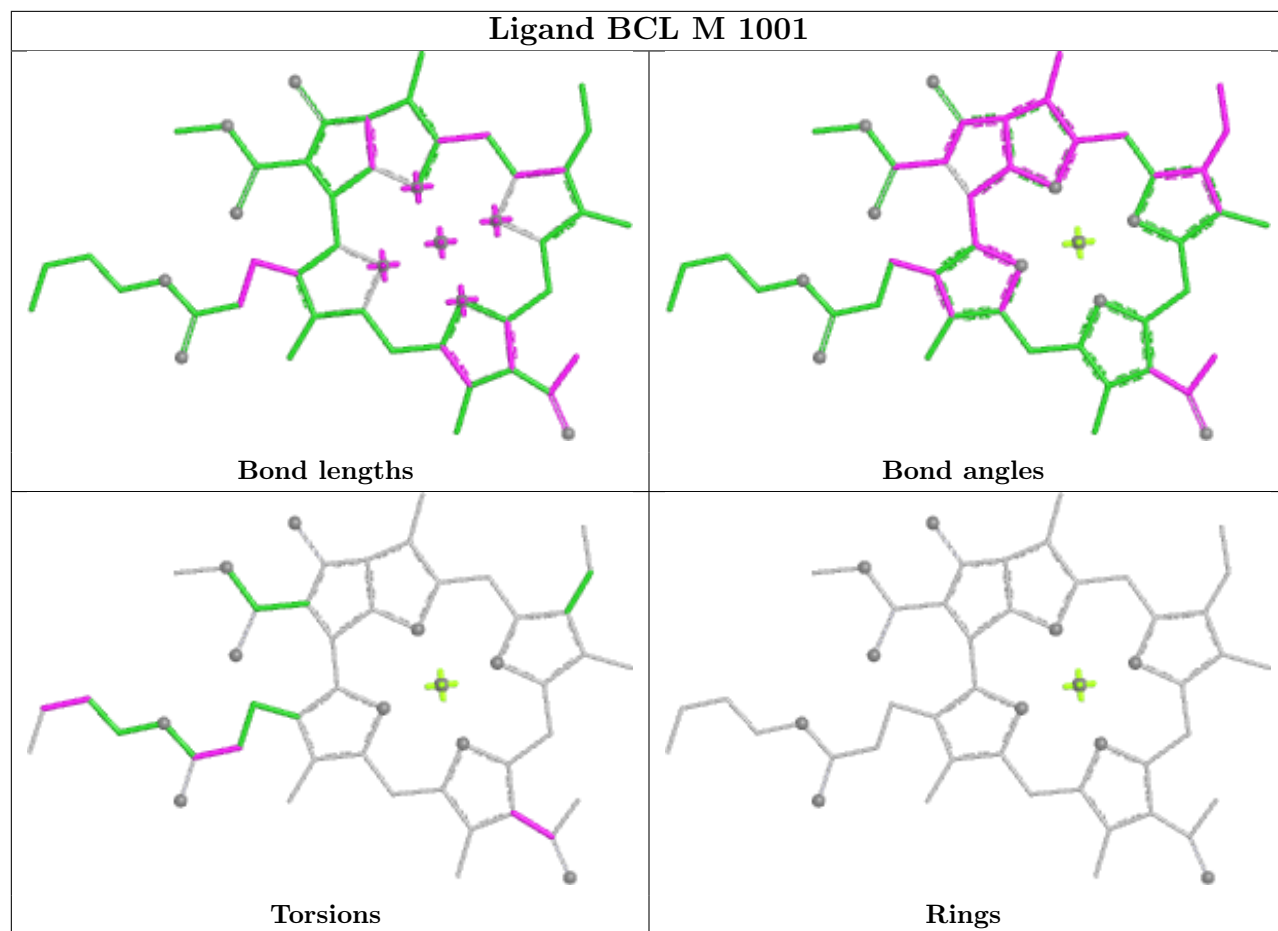




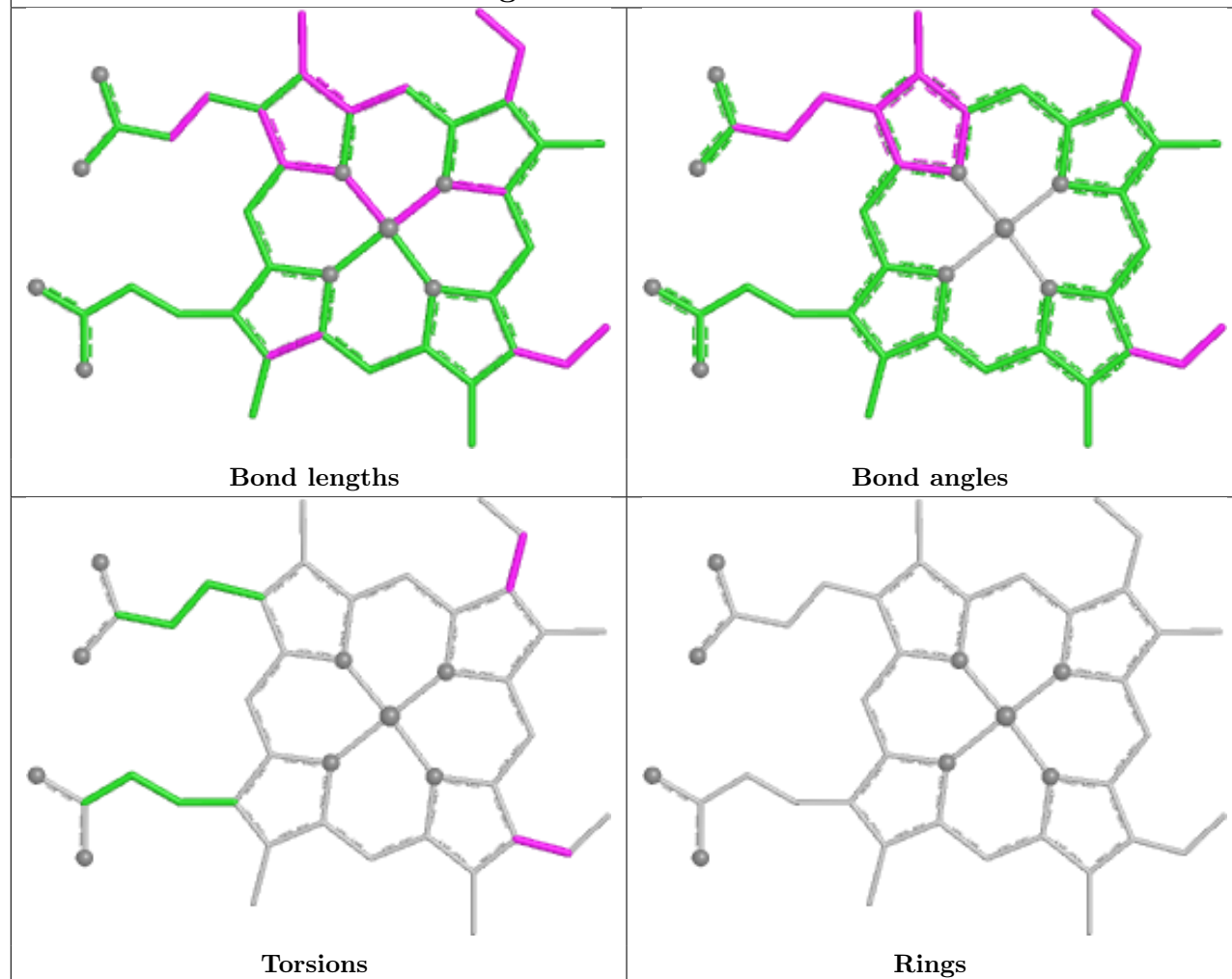




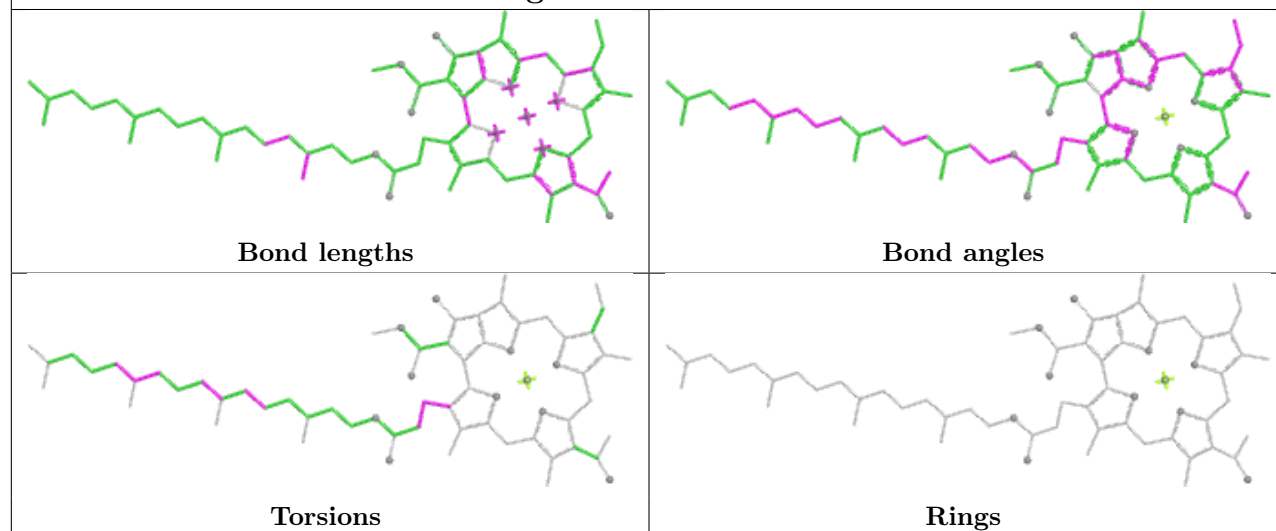




Ligand HEM D 2009



Ligand BCL L 1004



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%)	-0.25	6 (2%) 63 44	34, 59, 84, 103	0
1	R	281/281 (100%)	0.08	7 (2%) 58 39	38, 72, 106, 122	0
2	M	267/307 (86%)	-0.18	6 (2%) 62 43	25, 52, 109, 134	0
2	S	267/307 (86%)	-0.14	5 (1%) 66 48	33, 61, 110, 139	0
3	H	246/260 (94%)	0.31	11 (4%) 38 25	44, 98, 148, 167	0
3	T	246/260 (94%)	0.65	24 (9%) 13 10	42, 121, 157, 172	0
4	C	124/124 (100%)	-0.03	2 (1%) 70 52	40, 70, 95, 140	0
4	D	124/124 (100%)	0.01	1 (0%) 82 68	50, 82, 105, 146	0
All	All	1836/1944 (94%)	0.05	62 (3%) 48 32	25, 71, 131, 172	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	179	LEU	5.2
3	H	196	VAL	4.9
2	S	37	THR	4.6
3	T	196	VAL	4.6
3	H	251	VAL	4.5
3	T	111	PRO	4.4
3	T	178	PHE	4.3
3	T	251	VAL	4.1
3	T	194	GLN	4.0
3	T	167	ILE	3.8
4	C	101	THR	3.6
3	H	131	ILE	3.4
1	L	194	VAL	3.3
1	L	1	ALA	3.2
3	T	208	LEU	3.1
3	H	194	GLN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	R	166	ASN	3.1
3	T	198	VAL	3.0
3	H	179	LEU	3.0
3	T	193	MET	2.9
1	R	165	GLY	2.9
3	T	192	PRO	2.8
2	S	232	GLU	2.8
3	H	208	LEU	2.8
3	T	64	PHE	2.8
3	T	241	LEU	2.7
1	L	186	ALA	2.7
3	H	252	VAL	2.7
3	T	168	TRP	2.7
1	L	197	ALA	2.7
3	T	250	SER	2.6
2	M	232	GLU	2.6
3	T	131	ILE	2.6
3	T	132	LYS	2.6
1	R	281	GLY	2.5
3	T	9	ASN	2.5
3	H	236	TYR	2.4
1	R	1	ALA	2.4
2	M	139	ALA	2.4
3	T	148	PRO	2.3
3	T	176	ALA	2.3
2	M	42	PHE	2.3
3	T	8	GLY	2.3
3	T	190	LEU	2.3
2	S	231	GLY	2.2
2	M	187	ASN	2.2
4	D	98	GLY	2.2
1	R	21	LEU	2.2
3	T	236	TYR	2.2
3	H	191	LEU	2.2
2	S	247	ARG	2.2
3	T	80	SER	2.1
4	C	8	GLY	2.1
1	L	169	TYR	2.1
3	H	177	ARG	2.1
1	R	212	GLU	2.1
1	L	227	LEU	2.1
2	M	47	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	105	MET	2.0
2	M	50	ILE	2.0
1	R	195	LEU	2.0
2	S	38	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.

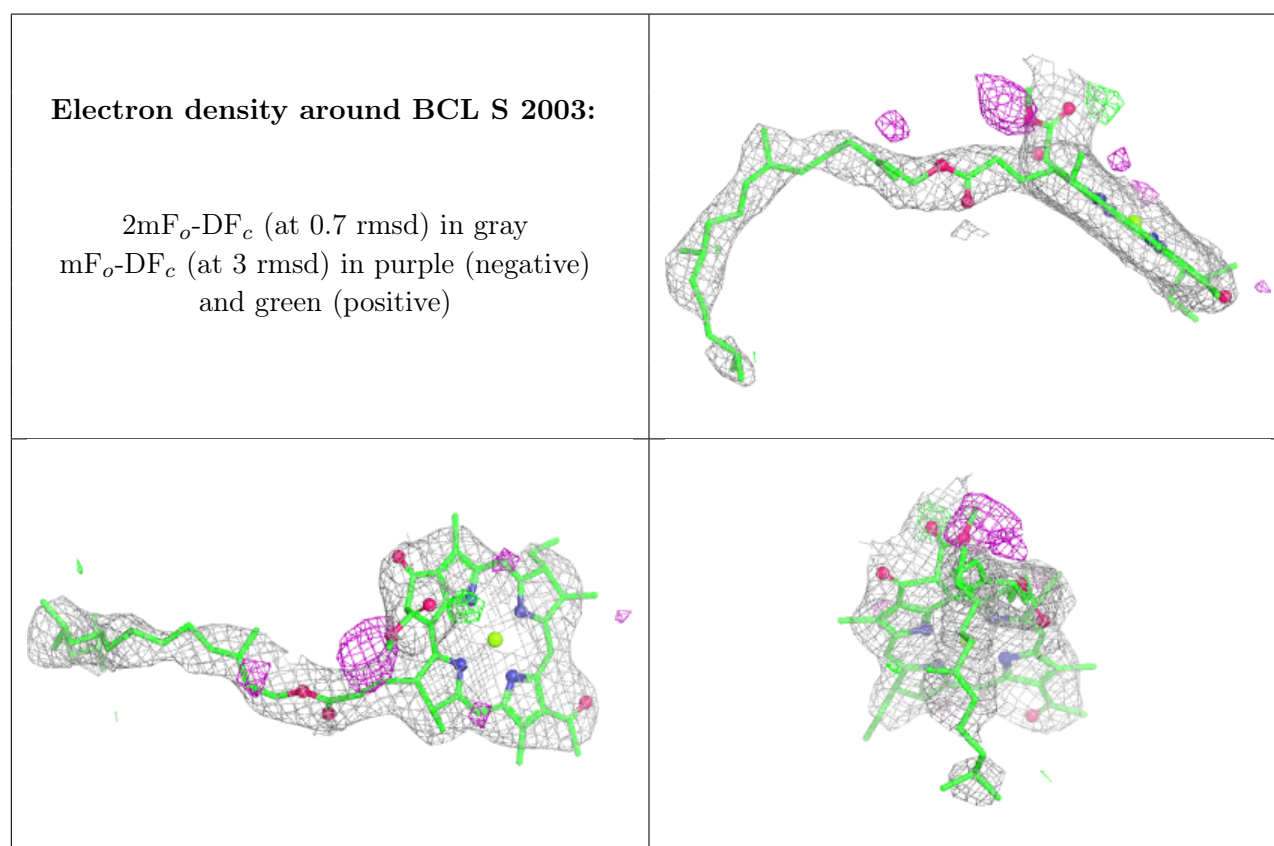
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	LDA	S	2011	16/16	0.86	0.38	91,98,110,111	0
10	LDA	M	1011	16/16	0.88	0.31	86,89,95,95	0
8	CL	S	2012	1/1	0.88	0.07	71,71,71,71	0
10	LDA	M	1010	16/16	0.89	0.18	50,54,57,59	0
5	BCL	S	2003	66/66	0.91	0.15	36,42,73,75	0
9	U10	M	1008	37/63	0.91	0.19	44,54,68,69	0
10	LDA	S	2010	16/16	0.91	0.23	59,82,94,94	0
9	U10	S	2008	37/63	0.91	0.18	52,62,87,87	0
6	BPH	R	2005	55/65	0.92	0.15	63,70,94,96	0
8	CL	M	1012	1/1	0.93	0.10	66,66,66,66	0
5	BCL	S	2001	50/66	0.93	0.13	51,60,71,76	0
5	BCL	M	1003	66/66	0.93	0.13	33,40,55,59	0
5	BCL	R	2002	66/66	0.93	0.12	38,43,56,58	0
6	BPH	L	1005	55/65	0.94	0.13	43,52,91,93	0
5	BCL	L	1004	66/66	0.94	0.13	42,48,67,71	0
5	BCL	R	2004	66/66	0.94	0.14	46,52,69,74	0
5	BCL	M	1001	50/66	0.94	0.11	37,46,58,61	0
5	BCL	L	1002	66/66	0.94	0.12	29,40,50,55	0
6	BPH	M	1006	65/65	0.95	0.11	48,56,67,69	0

Continued on next page...

Continued from previous page...

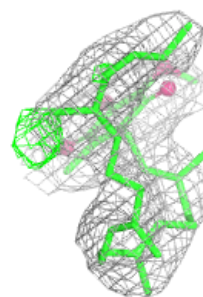
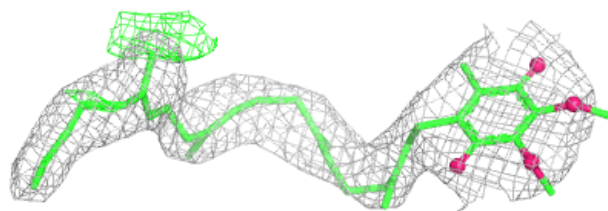
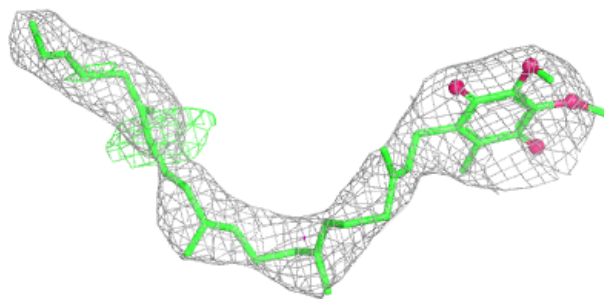
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BPH	S	2006	65/65	0.95	0.11	50,57,67,70	0
11	HEM	C	1009	43/43	0.97	0.09	35,42,52,55	0
11	HEM	D	2009	43/43	0.97	0.11	49,52,64,70	0
7	FE2	M	1007	1/1	1.00	0.01	45,45,45,45	0
7	FE2	S	2007	1/1	1.00	0.02	54,54,54,54	0

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.

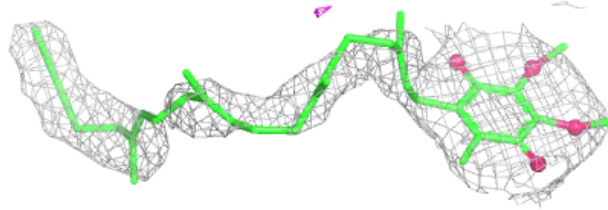
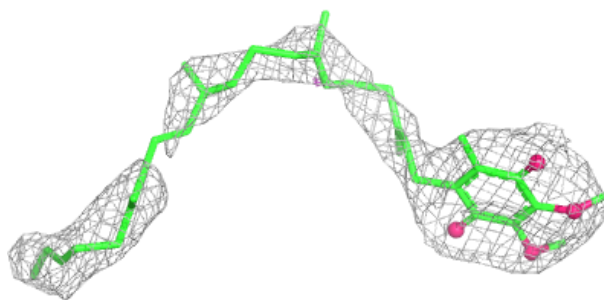


Electron density around U10 M 1008:

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

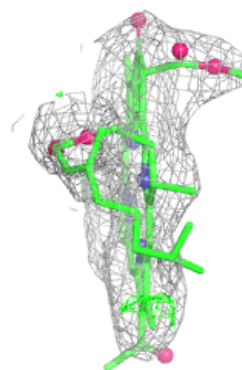
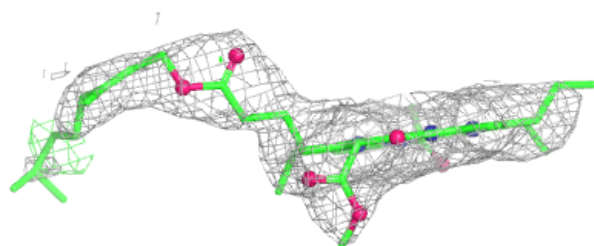
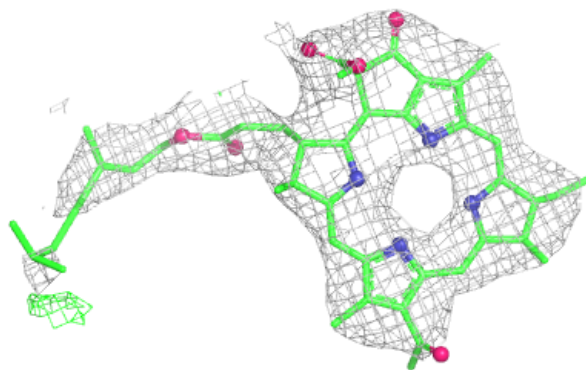
**Electron density around U10 S 2008:**

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



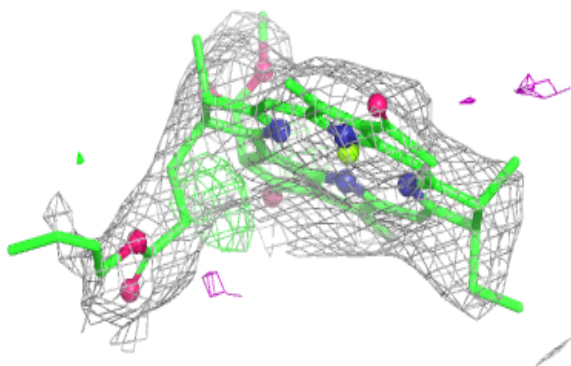
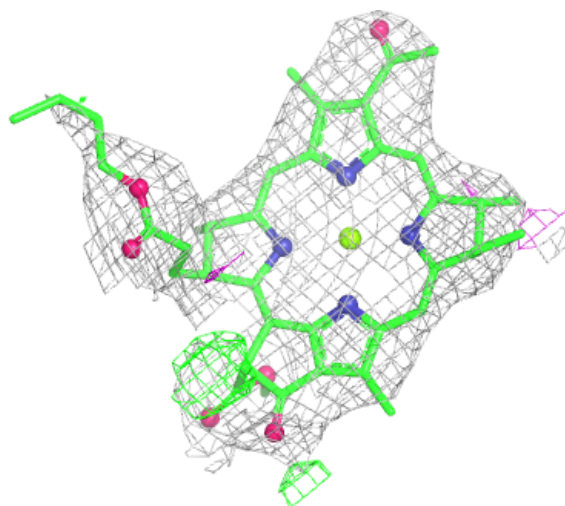
Electron density around BPH R 2005:

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



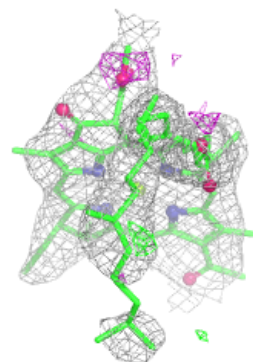
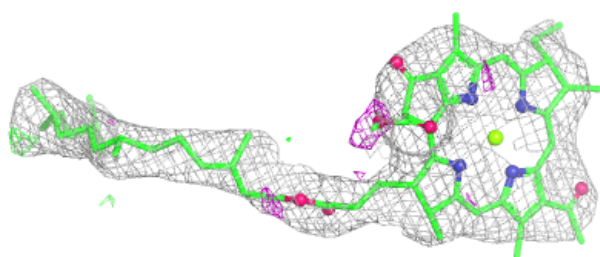
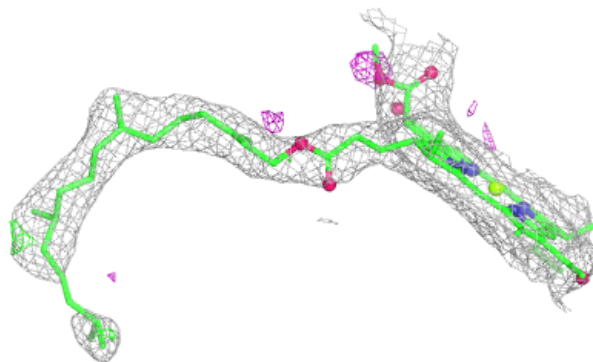
Electron density around BCL S 2001:

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

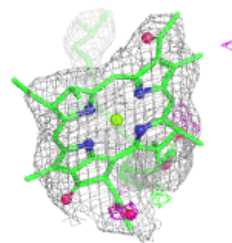
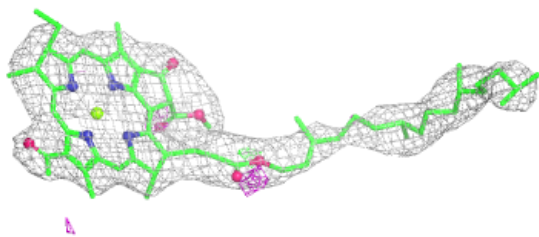
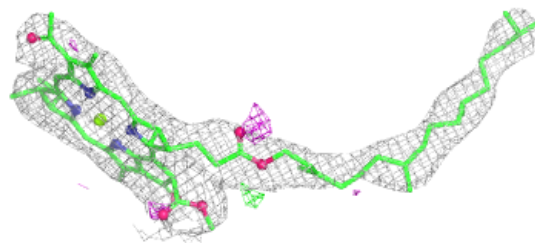


Electron density around BCL M 1003:

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

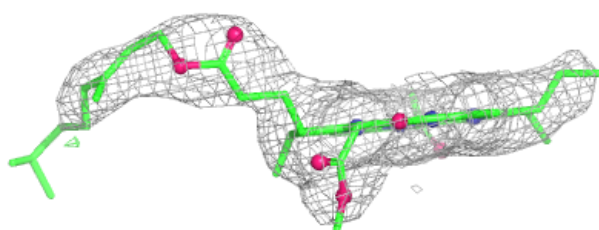
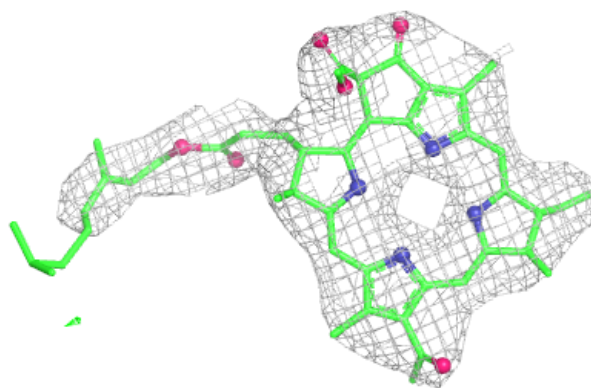
**Electron density around BCL R 2002:**

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

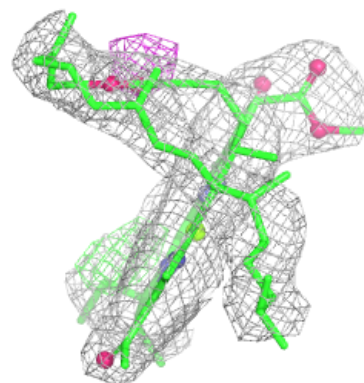
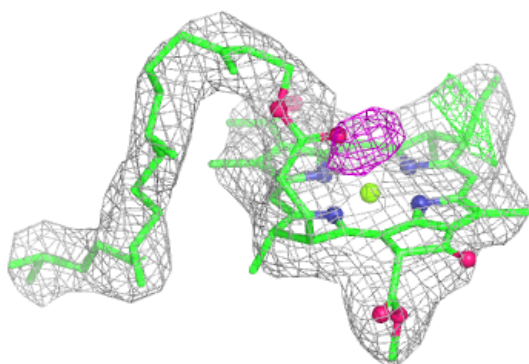
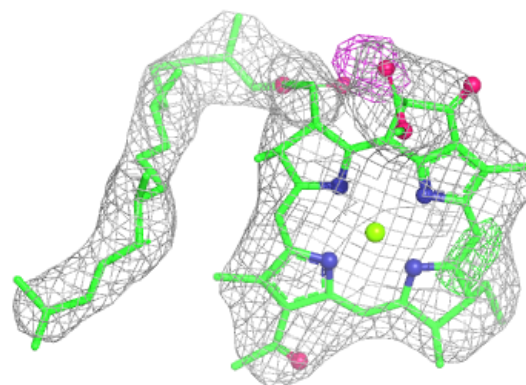


Electron density around BPH L 1005:

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

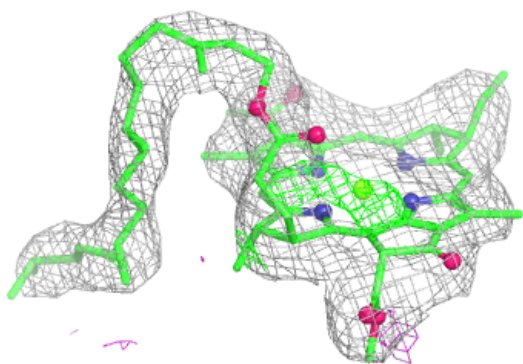
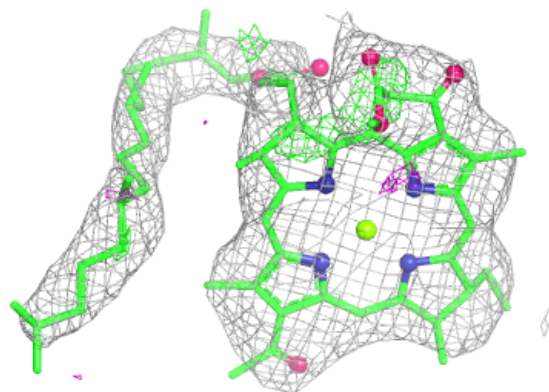
**Electron density around BCL L 1004:**

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



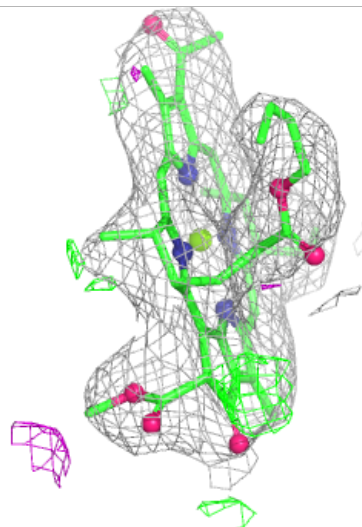
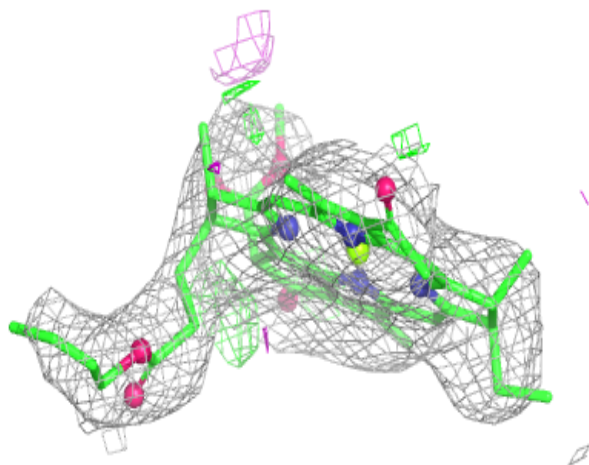
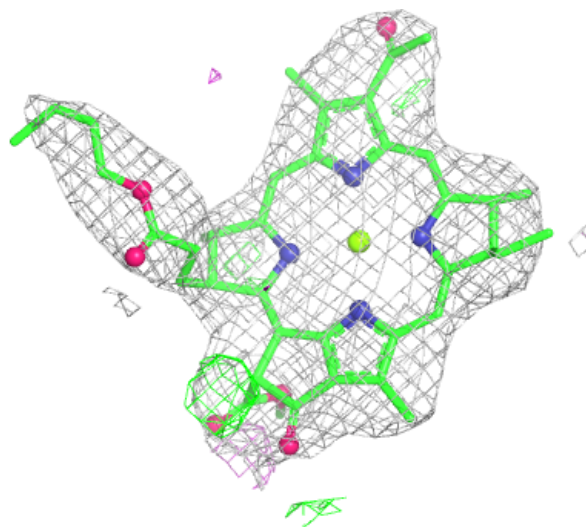
Electron density around BCL R 2004:

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



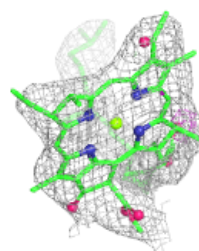
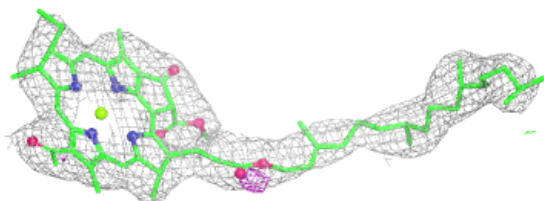
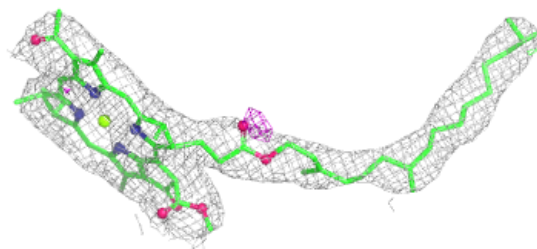
Electron density around BCL M 1001:

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

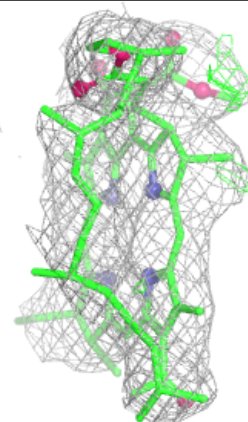
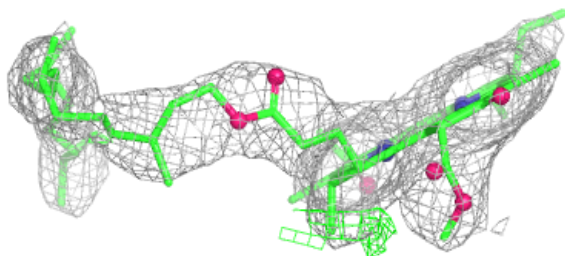
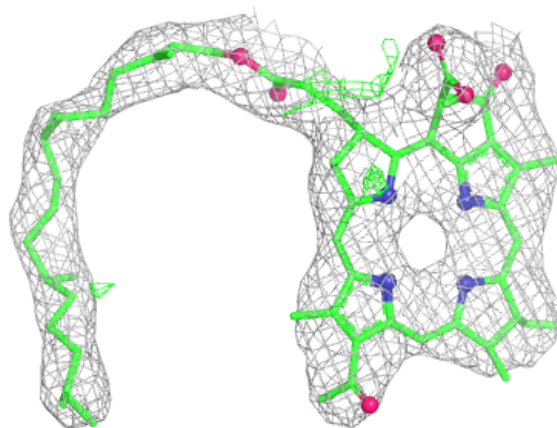


Electron density around BCL L 1002:

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

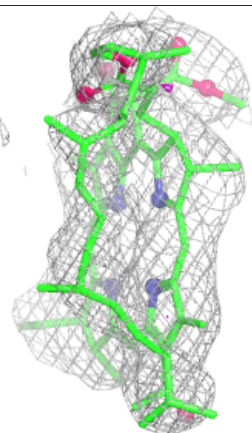
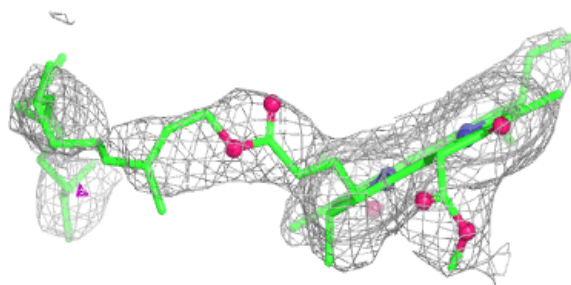
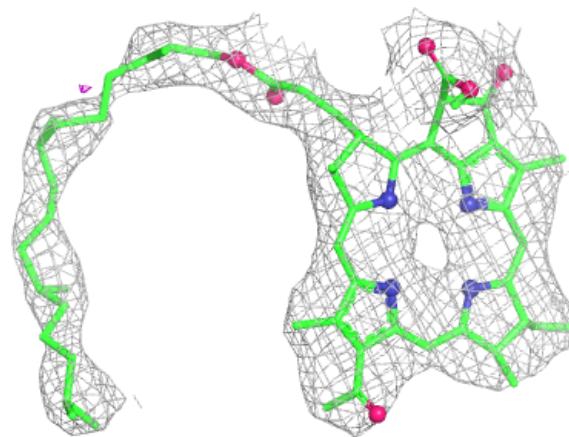
**Electron density around BPH M 1006:**

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



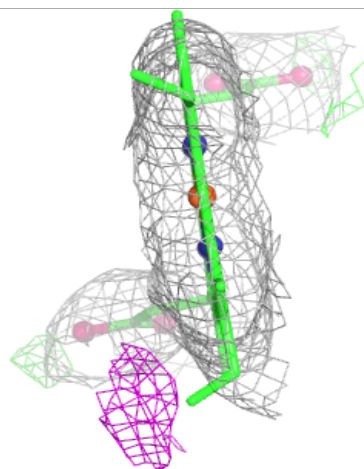
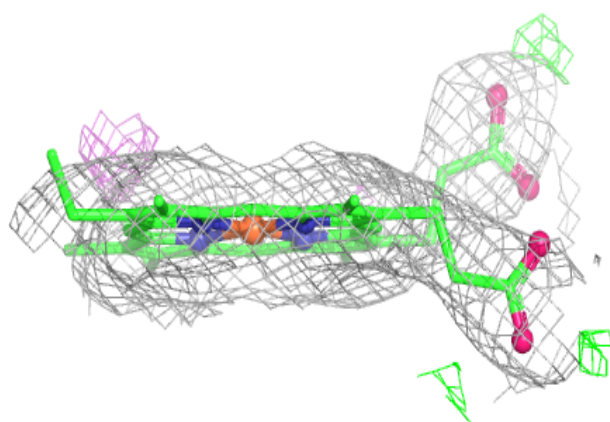
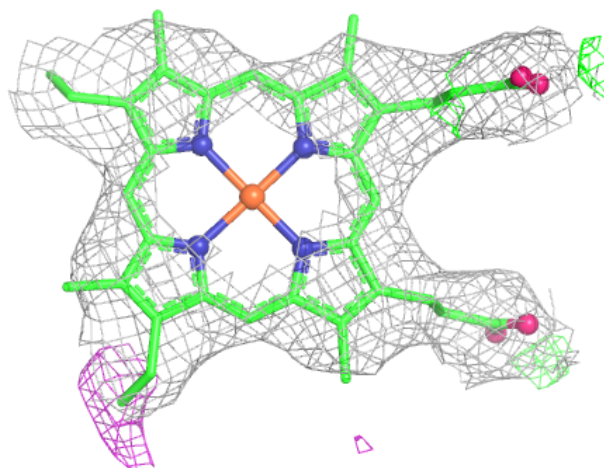
Electron density around BPH S 2006:

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



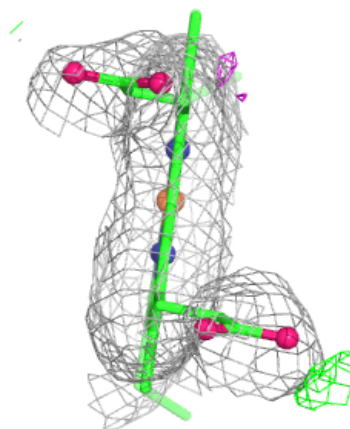
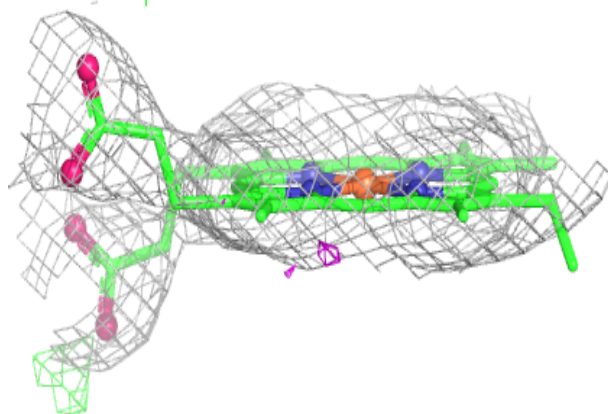
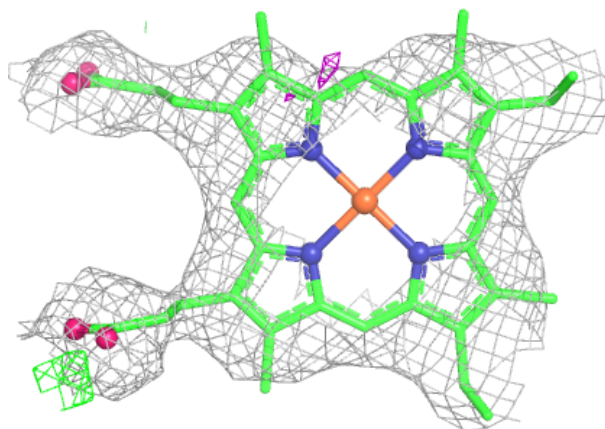
Electron density around HEM C 1009:

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



Electron density around HEM D 2009:

$2mF_o-DF_c$ (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.