Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2021 – 02:14 PM EST

PDB ID	:	1PRC
Title	:	CRYSTALLOGRAPHIC REFINEMENT AT 2.3 ANGSTROMS RESOLUTION AND REFINED MODEL OF THE PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS
Authors	:	Deisenhofer, J.; Epp, O.; Miki, K.; Huber, R.; Michel, H.
Deposited on	:	1988-02-04
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

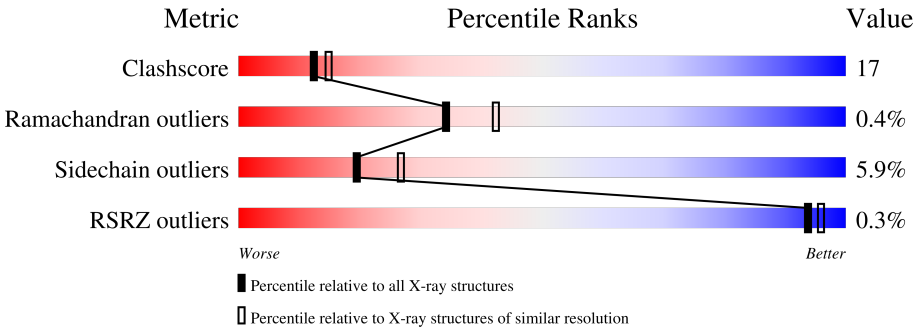
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

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 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	C	336	58% 35% 5%
2	L	273	65% 31%
3	M	323	66% 31%
4	H	258	% 61% 32% 6%

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
8	UQ1	L	614	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 10288 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	333	Total	C	N	O	S	54	0	1
			2603	1640	467	478	18			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	273	Total	C	N	O	S	13	0	0
			2171	1459	350	355	7			

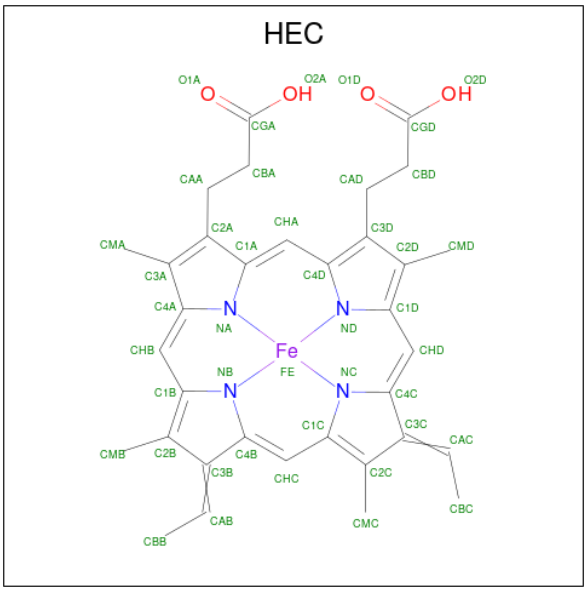
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	323	Total	C	N	O	S	26	0	0
			2555	1702	419	423	11			

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

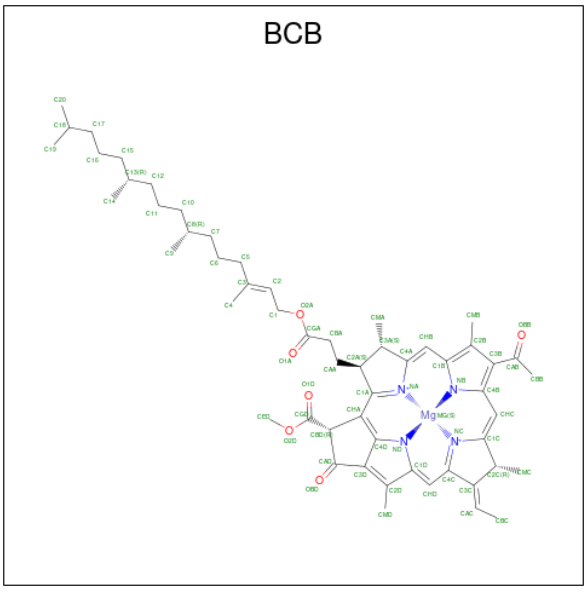
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	106	0	0
			2018	1292	344	380	2			

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



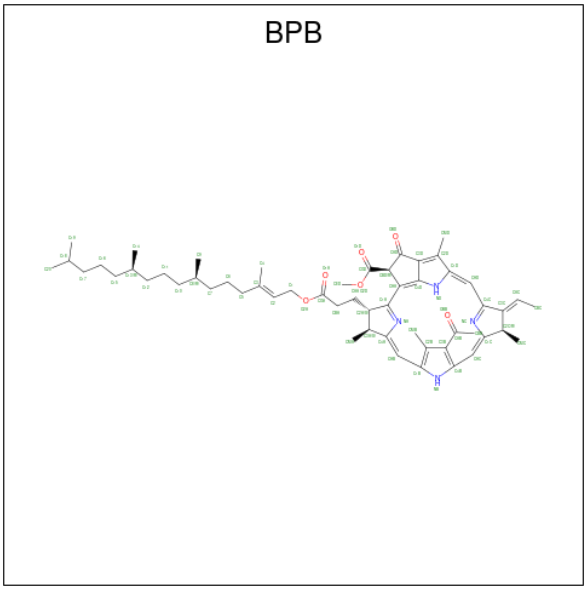
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



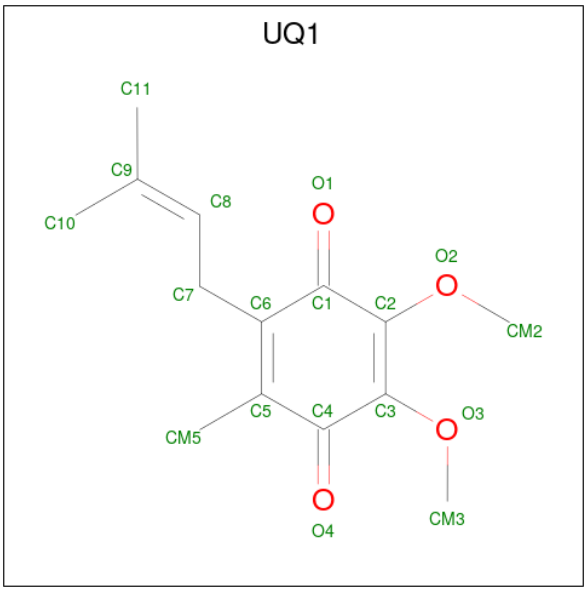
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	13	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 7 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



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

- Molecule 8 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).

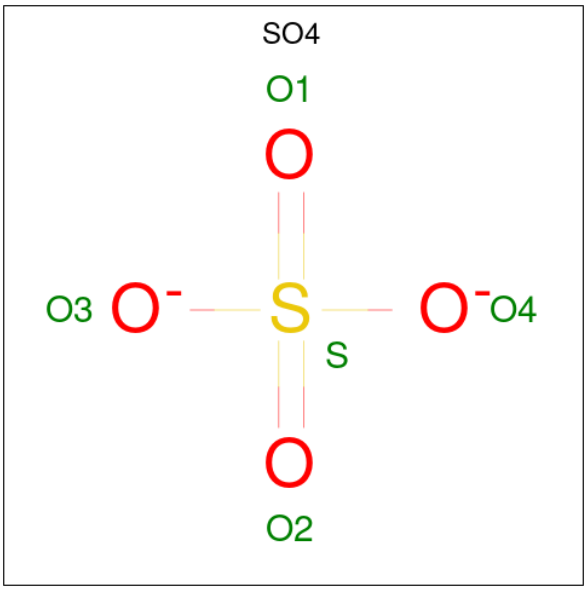


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total C O 18 14 4	0	0

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe).

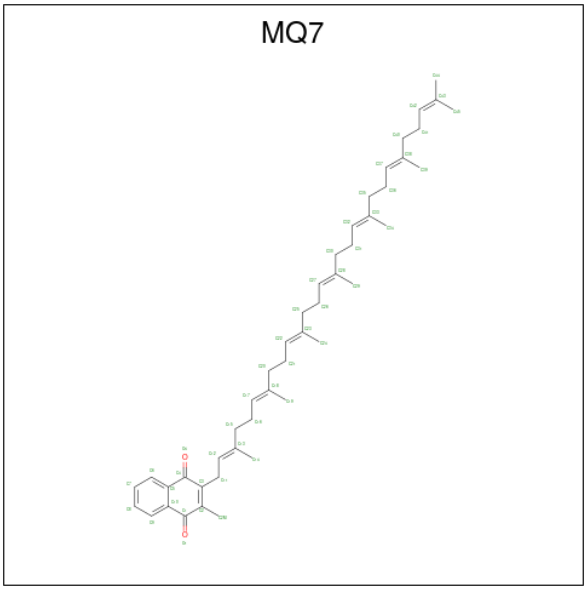
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total Fe 1 1	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



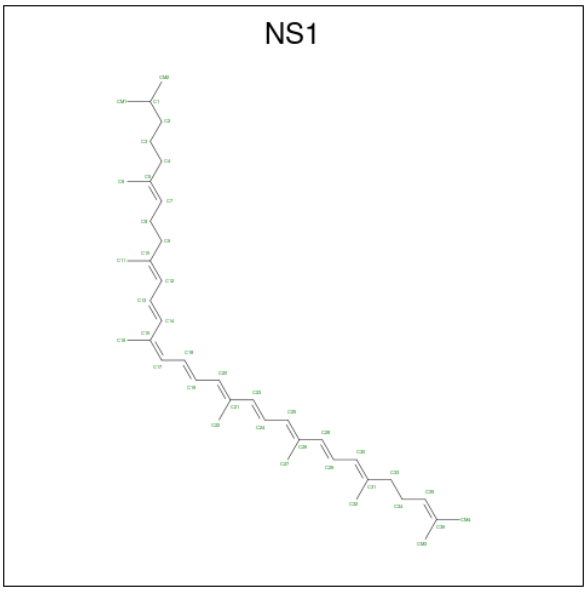
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total O S 5 4 1	0	0
10	M	1	Total O S 5 4 1	0	0
10	M	1	Total O S 5 4 1	0	0
10	M	1	Total O S 5 4 1	0	0
10	H	1	Total O S 5 4 1	0	0
10	H	1	Total O S 5 4 1	0	0
10	H	1	Total O S 5 4 1	0	0

- Molecule 11 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



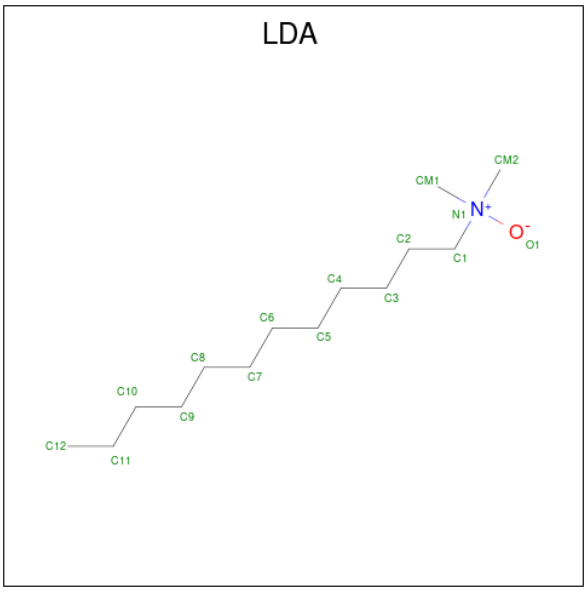
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total C O 48 46 2	4	0

- Molecule 12 is 15-trans-1,2-dihydroneurosporene (three-letter code: NS1) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C 40 40	14	0

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C N O 16 14 1 1	0	0
13	H	1	Total C N O 16 14 1 1	6	0

- Molecule 14 is water.

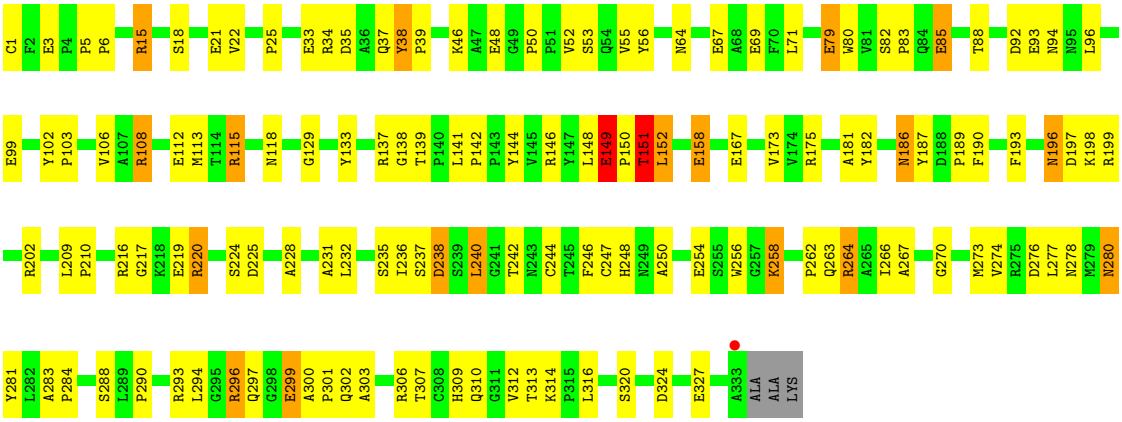
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	66	Total O 66 66	0	0
14	L	39	Total O 39 39	0	0
14	M	55	Total O 55 55	0	0
14	H	41	Total O 41 41	0	0

3 Residue-property plots (i)

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

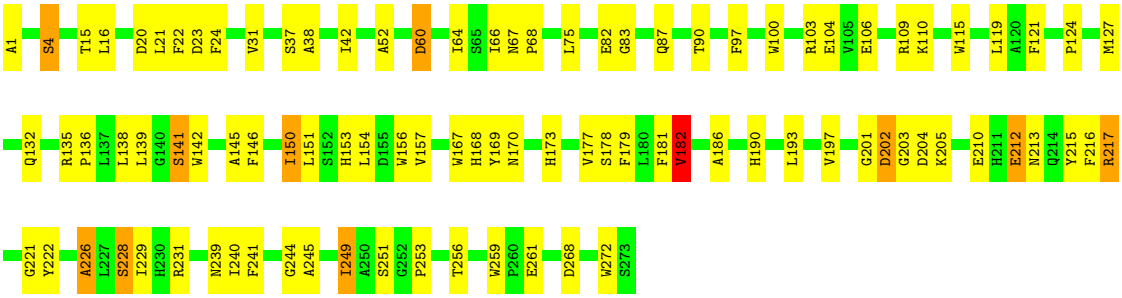
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain C:



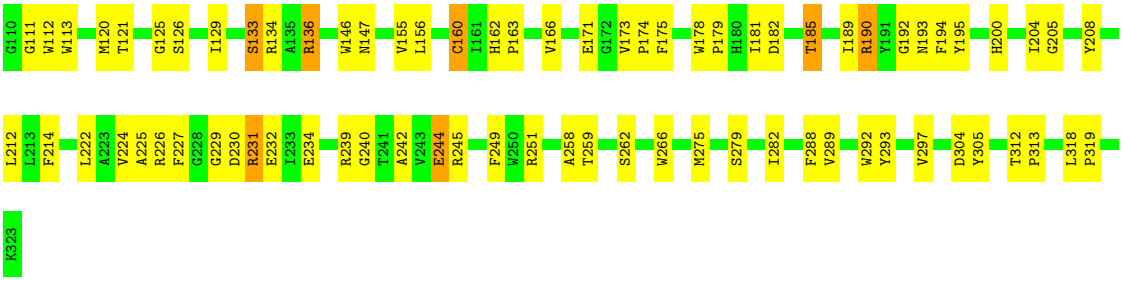
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Chain L:



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain M:



• Molecule 4: PHOTOSYNTHETIC REACTION CENTER

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	223.50Å 223.50Å 113.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.99-2.30) 75.5 (19.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.193 , (Not available) 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 64.5	EDS
L-test for twinning[1]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10288	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, BCB, UQ1, LDA, NS1, SO4, HEC, MQ7, FME, BPB

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	C	1.07	17/2670 (0.6%)	1.56	36/3639 (1.0%)
2	L	1.01	5/2259 (0.2%)	1.42	18/3084 (0.6%)
3	M	0.96	3/2659 (0.1%)	1.46	26/3637 (0.7%)
4	H	1.13	18/2055 (0.9%)	1.65	32/2807 (1.1%)
All	All	1.04	43/9643 (0.4%)	1.52	112/13167 (0.9%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	255	GLU	CD-OE2	9.06	1.35	1.25
1	C	299	GLU	CD-OE2	8.31	1.34	1.25
3	M	244	GLU	CD-OE2	8.03	1.34	1.25
2	L	261	GLU	CD-OE2	7.64	1.34	1.25
1	C	21	GLU	CD-OE2	7.48	1.33	1.25
4	H	177	GLU	CD-OE2	7.40	1.33	1.25
1	C	33	GLU	CD-OE2	7.39	1.33	1.25
1	C	158	GLU	CD-OE2	7.36	1.33	1.25
1	C	149	GLU	CD-OE2	7.18	1.33	1.25
4	H	234	GLU	CD-OE2	6.91	1.33	1.25
1	C	99	GLU	CD-OE2	6.86	1.33	1.25
4	H	122	GLU	CD-OE2	6.59	1.32	1.25
1	C	112	GLU	CD-OE2	6.56	1.32	1.25
4	H	164	GLU	CD-OE2	6.56	1.32	1.25
4	H	84	GLU	CD-OE2	6.54	1.32	1.25
1	C	167	GLU	CD-OE2	6.36	1.32	1.25
1	C	254	GLU	CD-OE1	-6.23	1.18	1.25
1	C	67	GLU	CD-OE2	6.16	1.32	1.25
4	H	119	GLU	CD-OE2	6.01	1.32	1.25
2	L	82	GLU	CD-OE2	5.94	1.32	1.25
4	H	252	GLU	CD-OE2	5.87	1.32	1.25
1	C	85	GLU	CD-OE2	5.82	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	219	GLU	CD-OE1	-5.77	1.19	1.25
1	C	79	GLU	CD-OE2	5.73	1.31	1.25
1	C	69	GLU	CD-OE2	5.71	1.31	1.25
4	H	61	GLU	CD-OE2	5.67	1.31	1.25
2	L	212	GLU	CD-OE2	5.58	1.31	1.25
1	C	3	GLU	CD-OE2	5.52	1.31	1.25
4	H	147	GLU	CD-OE2	5.48	1.31	1.25
4	H	87	GLU	CD-OE2	5.45	1.31	1.25
4	H	235	GLU	CD-OE2	5.40	1.31	1.25
2	L	104	GLU	CD-OE2	5.39	1.31	1.25
1	C	48	GLU	CD-OE2	5.37	1.31	1.25
4	H	216	GLU	CD-OE2	5.34	1.31	1.25
1	C	93	GLU	CD-OE2	5.32	1.31	1.25
3	M	22	GLU	CD-OE2	5.31	1.31	1.25
4	H	55	GLU	CD-OE2	5.22	1.31	1.25
4	H	97	GLU	CD-OE2	5.18	1.31	1.25
4	H	184	GLU	CD-OE2	5.10	1.31	1.25
3	M	232	GLU	CD-OE2	5.10	1.31	1.25
4	H	45	GLU	CD-OE2	5.04	1.31	1.25
4	H	39	GLU	CD-OE1	-5.03	1.20	1.25
2	L	210	GLU	CD-OE2	5.01	1.31	1.25

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	38	ARG	NE-CZ-NH2	-18.45	111.08	120.30
3	M	245	ARG	NE-CZ-NH2	-11.45	114.57	120.30
3	M	25	ASP	CB-CG-OD2	-10.22	109.10	118.30
4	H	153	ARG	NE-CZ-NH2	-9.86	115.37	120.30
4	H	153	ARG	NE-CZ-NH1	9.74	125.17	120.30
3	M	245	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	C	216	ARG	NE-CZ-NH1	9.51	125.05	120.30
3	M	239	ARG	NE-CZ-NH2	-9.45	115.58	120.30
3	M	27	ASP	CB-CG-OD2	-9.40	109.84	118.30
3	M	239	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	C	225	ASP	CB-CG-OD2	-9.02	110.18	118.30
2	L	231	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	C	108	ARG	NE-CZ-NH1	8.68	124.64	120.30
2	L	231	ARG	NE-CZ-NH2	-8.44	116.08	120.30
3	M	304	ASP	CB-CG-OD1	8.33	125.80	118.30
4	H	38	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	C	35	ASP	CB-CG-OD2	-8.03	111.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	236	ASP	CB-CG-OD1	7.97	125.47	118.30
2	L	215	TYR	CB-CG-CD2	-7.83	116.30	121.00
1	C	220	ARG	NE-CZ-NH2	-7.79	116.41	120.30
3	M	25	ASP	CB-CG-OD1	7.76	125.28	118.30
3	M	190	ARG	NE-CZ-NH2	-7.59	116.51	120.30
4	H	161	ASP	CB-CG-OD2	-7.58	111.48	118.30
4	H	236	ASP	CB-CG-OD2	-7.47	111.58	118.30
2	L	20	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	C	313	THR	CA-CB-CG2	-7.38	102.07	112.40
1	C	264	ARG	NE-CZ-NH2	-7.24	116.68	120.30
3	M	160	CYS	CB-CA-C	-7.06	96.28	110.40
1	C	196	ASN	CB-CA-C	-7.05	96.29	110.40
1	C	225	ASP	CB-CG-OD1	7.03	124.63	118.30
1	C	324	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	C	115	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	L	23	ASP	CB-CG-OD1	6.88	124.50	118.30
4	H	62	LEU	CB-CG-CD1	-6.78	99.48	111.00
1	C	115	ARG	NE-CZ-NH2	-6.77	116.91	120.30
3	M	251	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	C	146	ARG	NE-CZ-NH1	6.68	123.64	120.30
3	M	304	ASP	CB-CG-OD2	-6.64	112.33	118.30
3	M	43	ASP	CB-CG-OD2	-6.59	112.37	118.30
4	H	110	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	C	296	ARG	NE-CZ-NH1	6.49	123.55	120.30
3	M	85	PHE	CB-CA-C	6.39	123.18	110.40
2	L	215	TYR	CB-CG-CD1	6.35	124.81	121.00
2	L	60	ASP	CB-CG-OD2	-6.34	112.59	118.30
3	M	86	ARG	NE-CZ-NH1	6.31	123.45	120.30
3	M	230	ASP	CB-CG-OD2	-6.25	112.68	118.30
3	M	27	ASP	CB-CG-OD1	6.21	123.89	118.30
1	C	280	ASN	CB-CA-C	-6.21	97.99	110.40
1	C	197	ASP	CB-CG-OD2	-6.19	112.73	118.30
2	L	23	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	C	149	GLU	N-CA-CB	6.12	121.62	110.60
1	C	216	ARG	NE-CZ-NH2	-6.07	117.27	120.30
3	M	134	ARG	NE-CZ-NH2	-5.99	117.31	120.30
2	L	202	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	C	224	SER	CB-CA-C	-5.96	98.78	110.10
2	L	204	ASP	CB-CG-OD2	-5.92	112.97	118.30
3	M	28	ARG	NE-CZ-NH2	-5.89	117.36	120.30
3	M	231	ARG	NE-CZ-NH2	-5.87	117.36	120.30
4	H	11	ASP	CB-CG-OD1	5.87	123.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	33	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	L	217	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	151	THR	CA-CB-CG2	-5.78	104.31	112.40
3	M	43	ASP	CB-CG-OD1	5.77	123.50	118.30
4	H	34	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	C	33	GLU	CB-CA-C	-5.75	98.89	110.40
4	H	151	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	46	LYS	N-CA-CB	5.68	120.83	110.60
1	C	300	ALA	CB-CA-C	-5.68	101.58	110.10
1	C	92	ASP	CB-CG-OD1	5.65	123.38	118.30
1	C	146	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	C	199	ARG	NE-CZ-NH1	5.62	123.11	120.30
3	M	13	ARG	NE-CZ-NH1	5.62	123.11	120.30
3	M	185	THR	CA-CB-CG2	-5.59	104.57	112.40
4	H	253	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	25	PRO	N-CA-CB	5.59	110.00	103.30
4	H	129	ASP	CA-CB-CG	-5.58	101.14	113.40
2	L	186	ALA	CB-CA-C	-5.57	101.75	110.10
2	L	268	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	C	324	ASP	CB-CG-OD1	5.51	123.26	118.30
3	M	190	ARG	NE-CZ-NH1	5.48	123.04	120.30
4	H	251	PRO	N-CA-CB	5.46	109.85	103.30
4	H	11	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	C	238	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	C	152	LEU	CB-CA-C	5.43	120.52	110.20
4	H	138	ARG	CB-CA-C	-5.40	99.60	110.40
1	C	220	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	139	THR	N-CA-CB	5.34	120.44	110.30
3	M	230	ASP	CB-CG-OD1	5.31	123.08	118.30
4	H	227	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	L	182	VAL	CB-CA-C	-5.29	101.34	111.40
4	H	64	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	C	92	ASP	CB-CG-OD2	-5.27	113.56	118.30
4	H	111	ALA	CB-CA-C	5.26	117.99	110.10
4	H	129	ASP	CB-CG-OD2	-5.25	113.58	118.30
2	L	60	ASP	CB-CG-OD1	5.23	123.01	118.30
4	H	14	GLN	CB-CA-C	-5.22	99.95	110.40
2	L	150	ILE	CA-CB-CG1	-5.20	101.12	111.00
4	H	94	ASP	CB-CG-OD2	-5.18	113.64	118.30
4	H	80	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	152	LEU	N-CA-CB	-5.17	100.06	110.40
4	H	28	VAL	CG1-CB-CG2	-5.15	102.66	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	34	ARG	NE-CZ-NH2	-5.15	117.72	120.30
4	H	161	ASP	CB-CG-OD1	5.15	122.93	118.30
4	H	192	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	L	226	ALA	N-CA-CB	-5.14	102.91	110.10
4	H	66	LYS	N-CA-CB	-5.12	101.39	110.60
2	L	90	THR	CA-CB-CG2	-5.11	105.25	112.40
1	C	237	SER	CB-CA-C	-5.09	100.43	110.10
1	C	296	ARG	NE-CZ-NH2	-5.07	117.76	120.30
3	M	109	ASP	CB-CG-OD1	5.04	122.83	118.30
4	H	197	PRO	N-CA-CB	5.04	109.34	103.30
4	H	141	THR	N-CA-CB	-5.02	100.77	110.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	C	2603	0	2579	82	0
2	L	2171	0	2098	83	0
3	M	2555	0	2452	78	0
4	H	2018	0	2020	58	0
5	C	172	0	122	20	0
6	L	132	0	144	22	0
6	M	132	0	144	22	0
7	L	65	0	74	8	0
7	M	65	0	74	11	0
8	L	18	0	18	10	0
9	M	1	0	0	0	0
10	H	15	0	0	0	0
10	M	20	0	0	0	0
11	M	48	0	64	1	0
12	M	40	0	59	4	0
13	H	16	0	31	2	0
13	M	16	0	31	1	0
14	C	66	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	H	41	0	0	1	0
14	L	39	0	0	3	0
14	M	55	0	0	3	0
All	All	10288	0	9910	327	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 17.

All (327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:120:MET:HE2	6:M:603:BCB:H172	1.41	1.00
3:M:136:ARG:HE	3:M:136:ARG:HA	1.31	0.93
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.53	0.90
7:L:606:BPB:HBBB	7:L:606:BPB:HHC	1.52	0.90
6:L:602:BCB:H61	6:L:604:BCB:HBB3	1.55	0.88
4:H:152:PRO:HA	4:H:155:LEU:CD1	2.04	0.86
3:M:318:LEU:HB3	3:M:319:PRO:HD2	1.57	0.86
3:M:275:MET:HG2	7:M:605:BPB:HBCA	1.58	0.84
6:L:604:BCB:HHC	6:L:604:BCB:HBB2	1.57	0.84
2:L:139:LEU:HD21	2:L:253:PRO:HD3	1.59	0.82
6:L:604:BCB:HMB2	7:L:606:BPB:HMBA	1.62	0.82
6:M:603:BCB:HBB3	6:M:603:BCB:HMB1	1.61	0.82
1:C:202:ARG:HG2	5:C:611:HEC:CGA	2.12	0.80
1:C:270:GLY:O	1:C:274:VAL:HG12	1.81	0.79
3:M:120:MET:HE3	6:M:603:BCB:H193	1.63	0.79
2:L:190:HIS:HA	8:L:614:UQ1:O4	1.81	0.79
6:L:602:BCB:H61	6:L:604:BCB:CBB	2.13	0.79
5:C:609:HEC:HMB1	5:C:609:HEC:HBB3	1.65	0.78
4:H:82:ARG:HG2	4:H:82:ARG:HH11	1.47	0.78
7:L:606:BPB:HHC	7:L:606:BPB:CBB	2.14	0.77
4:H:152:PRO:HA	4:H:155:LEU:HD11	1.67	0.77
2:L:181:PHE:HB3	7:M:605:BPB:HBBA	1.67	0.76
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.19	0.76
1:C:196:ASN:HB3	1:C:198:LYS:H	1.49	0.76
3:M:190:ARG:HD2	3:M:190:ARG:O	1.85	0.76
2:L:202:ASP:CG	2:L:203:GLY:H	1.90	0.74
7:M:605:BPB:HMC	7:M:605:BPB:H55	1.70	0.74
4:H:133:LYS:HG3	4:H:176:SER:HB2	1.69	0.73
3:M:185:THR:O	3:M:189:ILE:HG13	1.90	0.72
2:L:212:GLU:OE1	8:L:614:UQ1:HM33	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:LEU:HG	1:C:299:GLU:HG3	1.72	0.71
1:C:141:LEU:HD12	1:C:142:PRO:HD2	1.72	0.71
4:H:45:GLU:HB3	4:H:46:PRO:HD2	1.72	0.70
4:H:152:PRO:HA	4:H:155:LEU:HD12	1.71	0.70
1:C:220:ARG:NH2	14:C:637:HOH:O	2.22	0.70
7:M:605:BPB:HBBB	7:M:605:BPB:HHC	1.73	0.70
4:H:55:GLU:HB3	4:H:58:GLN:HG3	1.73	0.70
4:H:138:ARG:NH1	4:H:228:ASP:OD1	2.25	0.70
3:M:5:THR:CG2	3:M:222:LEU:HB3	2.21	0.69
3:M:136:ARG:HA	3:M:136:ARG:NE	2.07	0.69
1:C:267:ALA:HB1	5:C:612:HEC:HMB2	1.75	0.68
6:M:603:BCB:CBD	6:M:603:BCB:HAA2	2.23	0.68
6:L:602:BCB:C6	6:L:604:BCB:HBB3	2.23	0.68
7:L:606:BPB:HBB	3:M:208:TYR:CD2	2.28	0.68
6:M:603:BCB:HAA2	6:M:603:BCB:HBD	1.75	0.67
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.30	0.67
6:M:601:BCB:CBB	12:M:613:NS1:H223	2.25	0.67
6:M:603:BCB:HMB1	6:M:603:BCB:CBB	2.24	0.67
2:L:38:ALA:O	2:L:42:ILE:HG13	1.95	0.67
3:M:288:PHE:CD1	4:H:12:ILE:HD11	2.31	0.66
2:L:151:LEU:HD21	13:H:616:LDA:H111	1.78	0.66
2:L:151:LEU:CD2	13:H:616:LDA:H111	2.26	0.65
1:C:149:GLU:OE1	1:C:296:ARG:NH1	2.27	0.65
4:H:197:PRO:HG2	4:H:200:PHE:CD1	2.32	0.65
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.31	0.65
3:M:70:LEU:HD23	3:M:73:MET:CE	2.27	0.65
3:M:160:CYS:SG	12:M:613:NS1:H322	2.36	0.64
4:H:125:ASP:HB2	4:H:232:LEU:HD21	1.78	0.64
2:L:22:PHE:HA	2:L:24:PHE:CE1	2.33	0.63
2:L:167:TRP:HE1	2:L:173:HIS:CD2	2.16	0.63
5:C:611:HEC:HBA1	5:C:611:HEC:HHA	1.80	0.63
2:L:226:ALA:HA	8:L:614:UQ1:HM32	1.80	0.62
3:M:70:LEU:HD23	3:M:73:MET:HE2	1.79	0.62
4:H:218:PHE:O	4:H:221:VAL:HG23	1.99	0.62
4:H:250:THR:HG22	4:H:252:GLU:H	1.63	0.62
1:C:248:HIS:HB3	14:C:635:HOH:O	2.00	0.62
7:L:606:BPB:HBBA	3:M:208:TYR:HB3	1.82	0.61
1:C:278:ASN:OD1	1:C:302:GLN:HB3	2.00	0.61
2:L:226:ALA:O	2:L:229:ILE:HG22	2.01	0.61
1:C:56:TYR:HB3	5:C:609:HEC:O2A	2.01	0.61
2:L:22:PHE:HA	2:L:24:PHE:HE1	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:602:BCB:CBB	6:L:602:BCB:HMB1	2.31	0.61
2:L:124:PRO:HB2	6:L:602:BCB:H93	1.83	0.61
1:C:173:VAL:HB	3:M:87:GLN:OE1	2.01	0.61
2:L:213:ASN:O	2:L:217:ARG:HG3	2.02	0.60
3:M:205:GLY:HA3	13:M:615:LDA:H121	1.84	0.60
1:C:5:PRO:CB	1:C:6:PRO:HA	2.32	0.60
6:M:601:BCB:OBB	6:M:601:BCB:HMB1	2.01	0.60
1:C:309:HIS:HE1	5:C:612:HEC:NA	1.99	0.60
1:C:102:TYR:CD1	1:C:103:PRO:HD3	2.37	0.60
2:L:178:SER:O	2:L:182:VAL:HG22	2.02	0.60
7:M:605:BPB:HMC	7:M:605:BPB:CBC	2.32	0.59
3:M:120:MET:CE	6:M:603:BCB:H193	2.32	0.59
6:M:601:BCB:HBB1	12:M:613:NS1:H223	1.83	0.59
1:C:15:ARG:HG2	14:L:629:HOH:O	2.03	0.59
1:C:108:ARG:NH1	5:C:609:HEC:O2D	2.35	0.59
1:C:244:CYS:HA	5:C:611:HEC:HHC	1.85	0.59
2:L:154:LEU:HD23	2:L:154:LEU:N	2.18	0.59
6:L:602:BCB:NA	6:M:603:BCB:HBB2	2.18	0.59
2:L:139:LEU:HD21	2:L:253:PRO:CD	2.32	0.58
4:H:4:GLY:HA2	4:H:12:ILE:HD11	1.84	0.58
5:C:609:HEC:HBB3	5:C:609:HEC:CMB	2.32	0.58
6:L:604:BCB:HHC	6:L:604:BCB:CBB	2.30	0.57
4:H:86:ARG:NH2	4:H:111:ALA:O	2.38	0.57
3:M:227:PHE:HB2	3:M:242:ALA:HB2	1.87	0.57
3:M:258:ALA:HA	4:H:36:ASP:HB3	1.85	0.57
3:M:107:LEU:HA	3:M:111:GLY:HA3	1.87	0.57
3:M:107:LEU:HD22	3:M:112:TRP:CE2	2.40	0.57
2:L:216:PHE:CE2	8:L:614:UQ1:HM53	2.40	0.56
6:L:604:BCB:HMB2	7:L:606:BPB:CMB	2.33	0.56
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.86	0.56
2:L:4:SER:HB3	4:H:40:GLY:HA2	1.85	0.56
3:M:93:LEU:HD21	3:M:113:TRP:HA	1.88	0.56
1:C:256:TRP:CH2	1:C:264:ARG:HG2	2.40	0.56
3:M:226:ARG:HG3	14:M:646:HOH:O	2.06	0.56
4:H:38:ARG:NH1	4:H:66:LYS:HB2	2.21	0.56
6:L:602:BCB:HMB1	6:L:602:BCB:HBB3	1.88	0.56
1:C:247:CYS:HB2	5:C:611:HEC:C2C	2.36	0.55
2:L:181:PHE:CD2	7:M:605:BPB:HBB	2.41	0.55
3:M:240:GLY:O	3:M:244:GLU:HG3	2.07	0.55
2:L:202:ASP:CG	2:L:203:GLY:N	2.59	0.55
4:H:137:LEU:HB2	4:H:170:ASP:OD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:179:PHE:HA	2:L:182:VAL:HG23	1.89	0.55
5:C:610:HEC:HMC1	5:C:610:HEC:HBC3	1.88	0.55
2:L:193:LEU:HD22	2:L:216:PHE:HE2	1.72	0.55
1:C:202:ARG:HG2	5:C:611:HEC:O2A	2.07	0.55
1:C:301:PRO:HG2	5:C:610:HEC:HBD1	1.87	0.55
3:M:162:HIS:O	3:M:166:VAL:HG22	2.07	0.55
1:C:244:CYS:HA	5:C:611:HEC:CHC	2.37	0.55
1:C:148:LEU:HD12	1:C:299:GLU:HB3	1.88	0.55
1:C:144:TYR:CD1	1:C:310:GLN:HG2	2.42	0.54
1:C:150:PRO:O	1:C:175:ARG:HD2	2.07	0.54
3:M:200:HIS:CE1	3:M:204:ILE:HD11	2.41	0.54
2:L:244:GLY:O	6:L:602:BCB:HED3	2.07	0.54
5:C:610:HEC:HMB1	5:C:610:HEC:HBB3	1.89	0.54
3:M:195:TYR:CZ	6:M:603:BCB:HMC2	2.42	0.54
2:L:170:ASN:HB2	2:L:259:TRP:CD1	2.43	0.53
2:L:181:PHE:CB	7:M:605:BPB:HBBA	2.38	0.53
6:L:602:BCB:C5	6:L:604:BCB:HBB3	2.38	0.53
4:H:82:ARG:HH11	4:H:82:ARG:CG	2.20	0.53
4:H:155:LEU:HB3	4:H:156:PRO:HD2	1.90	0.53
2:L:124:PRO:HB2	6:L:602:BCB:C9	2.39	0.53
2:L:193:LEU:HD22	2:L:216:PHE:CE2	2.43	0.53
4:H:70:LEU:HB3	4:H:71:PRO:HD2	1.91	0.53
3:M:318:LEU:HB3	3:M:319:PRO:CD	2.34	0.52
1:C:37:GLN:O	1:C:39:PRO:HD3	2.08	0.52
4:H:6:LEU:HD12	4:H:15:LEU:HD11	1.91	0.52
2:L:153:HIS:O	2:L:157:VAL:HG23	2.10	0.52
3:M:69:ILE:O	3:M:73:MET:HG3	2.09	0.52
3:M:29:VAL:HG23	3:M:51:LEU:HD13	1.90	0.52
3:M:195:TYR:CE2	6:M:603:BCB:HMC2	2.44	0.52
1:C:52:VAL:HA	1:C:55:VAL:HB	1.92	0.52
2:L:16:LEU:HB2	2:L:106:GLU:HG2	1.91	0.52
2:L:1:ALA:H2	4:H:43:LEU:HB3	1.74	0.52
2:L:127:MET:O	2:L:127:MET:HG3	2.10	0.52
2:L:138:LEU:HD12	2:L:249:ILE:CD1	2.40	0.52
4:H:192:ARG:NH1	4:H:221:VAL:O	2.43	0.51
1:C:80:TRP:O	1:C:138:GLY:HA2	2.10	0.51
2:L:168:HIS:CE1	6:L:602:BCB:HMC2	2.45	0.51
2:L:150:ILE:HG13	14:L:633:HOH:O	2.10	0.51
8:L:614:UQ1:C8	8:L:614:UQ1:HM51	2.39	0.51
1:C:22:VAL:HG12	2:L:256:THR:HB	1.92	0.51
1:C:290:PRO:HG2	1:C:293:ARG:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LEU:O	5:C:609:HEC:HBA1	2.11	0.51
2:L:217:ARG:NH1	14:L:647:HOH:O	2.43	0.51
4:H:90:LEU:HD23	4:H:102:GLN:C	2.32	0.50
4:H:161:ASP:OD2	4:H:161:ASP:N	2.33	0.50
2:L:21:LEU:HD23	2:L:22:PHE:CE2	2.46	0.50
3:M:155:VAL:CG2	6:M:603:BCB:H62	2.42	0.50
3:M:212:LEU:C	3:M:212:LEU:HD23	2.32	0.50
1:C:238:ASP:OD1	1:C:306:ARG:NH2	2.45	0.50
2:L:60:ASP:O	2:L:64:ILE:HG13	2.10	0.50
2:L:167:TRP:NE1	2:L:173:HIS:CD2	2.79	0.50
3:M:155:VAL:HG21	6:M:603:BCB:H8	1.94	0.49
1:C:277:LEU:O	1:C:281:TYR:HB2	2.12	0.49
3:M:70:LEU:CD2	3:M:73:MET:HE3	2.42	0.49
4:H:196:ILE:HD12	4:H:242:TYR:CE1	2.48	0.49
4:H:152:PRO:CA	4:H:155:LEU:HD12	2.41	0.49
1:C:273:MET:O	1:C:277:LEU:HG	2.12	0.49
3:M:224:VAL:O	3:M:225:ALA:C	2.50	0.49
1:C:15:ARG:NH2	14:C:667:HOH:O	2.45	0.48
3:M:51:LEU:N	3:M:51:LEU:HD12	2.28	0.48
3:M:318:LEU:CB	3:M:319:PRO:HD2	2.35	0.48
3:M:162:HIS:HD2	14:M:626:HOH:O	1.96	0.48
1:C:18:SER:HB2	2:L:156:TRP:CD1	2.48	0.48
8:L:614:UQ1:O1	8:L:614:UQ1:HM22	2.14	0.48
3:M:192:GLY:O	3:M:193:ASN:HB3	2.13	0.48
3:M:2:ASP:OD2	3:M:4:GLN:HB2	2.14	0.48
3:M:160:CYS:C	3:M:163:PRO:HD2	2.33	0.48
6:L:604:BCB:H192	6:L:604:BCB:H161	1.63	0.48
3:M:120:MET:CE	6:M:603:BCB:H172	2.28	0.48
1:C:189:PRO:CB	1:C:232:LEU:HA	2.43	0.47
3:M:5:THR:HG21	3:M:222:LEU:HB3	1.93	0.47
4:H:133:LYS:HG3	4:H:176:SER:CB	2.40	0.47
3:M:266:TRP:CH2	4:H:28:VAL:CG2	2.97	0.47
7:M:605:BPB:HHC	7:M:605:BPB:CBB	2.42	0.47
4:H:125:ASP:HB2	4:H:232:LEU:CD2	2.42	0.47
1:C:189:PRO:O	1:C:193:PHE:HB2	2.15	0.47
4:H:120:ARG:HB2	4:H:233:ARG:HA	1.97	0.47
3:M:10:ILE:O	4:H:180:PHE:HD2	1.98	0.47
3:M:234:GLU:HB2	14:H:632:HOH:O	2.14	0.47
4:H:70:LEU:HD11	4:H:76:VAL:HG23	1.96	0.47
4:H:226:SER:HB3	4:H:229:GLN:HG2	1.95	0.47
2:L:75:LEU:HD23	2:L:75:LEU:HA	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:153:HIS:CE1	2:L:154:LEU:HD21	2.50	0.47
2:L:249:ILE:O	2:L:253:PRO:HG2	2.15	0.47
4:H:138:ARG:NH1	4:H:227:ARG:NE	2.62	0.47
2:L:135:ARG:NH2	2:L:251:SER:O	2.41	0.46
6:L:602:BCB:C3	6:L:604:BCB:HBB3	2.46	0.46
3:M:129:ILE:O	3:M:133:SER:HB3	2.15	0.46
4:H:142:ASP:OD2	4:H:142:ASP:N	2.40	0.46
1:C:181:ALA:O	1:C:182:TYR:HB2	2.15	0.46
1:C:240:LEU:N	1:C:240:LEU:HD23	2.30	0.46
1:C:262:PRO:O	1:C:266:ILE:HG12	2.14	0.46
3:M:5:THR:HG22	3:M:222:LEU:HB3	1.96	0.46
4:H:45:GLU:HB3	4:H:46:PRO:CD	2.41	0.46
2:L:216:PHE:CD2	8:L:614:UQ1:H71	2.51	0.46
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.80	0.46
3:M:121:THR:HG23	3:M:156:LEU:HD21	1.98	0.46
2:L:205:LYS:HA	4:H:69:VAL:HG22	1.96	0.46
4:H:161:ASP:OD1	4:H:215:SER:OG	2.33	0.46
4:H:172:TRP:N	4:H:172:TRP:CD1	2.84	0.46
1:C:246:PHE:CE2	1:C:263:GLN:HG2	2.51	0.46
1:C:276:ASP:O	1:C:280:ASN:HB2	2.16	0.45
2:L:216:PHE:CE2	8:L:614:UQ1:CM5	2.98	0.45
1:C:38:TYR:CD2	1:C:316:LEU:HD13	2.51	0.45
2:L:245:ALA:O	2:L:249:ILE:HB	2.15	0.45
3:M:87:GLN:O	3:M:88:PHE:C	2.55	0.45
1:C:151:THR:O	1:C:152:LEU:HB2	2.17	0.45
1:C:242:THR:HA	14:C:675:HOH:O	2.17	0.45
1:C:309:HIS:O	1:C:310:GLN:C	2.54	0.45
2:L:110:LYS:HB2	2:L:110:LYS:HE2	1.73	0.45
2:L:193:LEU:HA	2:L:193:LEU:HD12	1.58	0.45
3:M:224:VAL:HG23	3:M:229:GLY:HA3	1.99	0.45
4:H:33:ARG:HD2	4:H:33:ARG:HA	1.90	0.45
1:C:309:HIS:HE1	5:C:612:HEC:C1A	2.29	0.45
4:H:197:PRO:HG2	4:H:200:PHE:HD1	1.76	0.45
2:L:228:SER:HB3	3:M:41:ILE:O	2.17	0.45
7:M:605:BPB:H55	7:M:605:BPB:CMC	2.44	0.45
1:C:137:ARG:HG3	1:C:310:GLN:HE22	1.82	0.45
7:L:606:BPB:CBB	3:M:208:TYR:CD2	2.98	0.45
2:L:240:ILE:HG22	2:L:241:PHE:CD1	2.52	0.44
3:M:70:LEU:CD2	3:M:73:MET:CE	2.94	0.44
3:M:155:VAL:HG22	6:M:603:BCB:H62	1.98	0.44
3:M:146:TRP:HA	3:M:146:TRP:CE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:605:BPB:H6A	7:M:605:BPB:H4	1.86	0.44
1:C:56:TYR:HB3	5:C:609:HEC:CGA	2.48	0.44
2:L:226:ALA:N	8:L:614:UQ1:HM21	2.32	0.44
3:M:38:LEU:CD2	3:M:46:ILE:HD11	2.47	0.44
2:L:121:PHE:O	2:L:124:PRO:HD2	2.17	0.44
2:L:132:GLN:OE1	2:L:145:ALA:HB1	2.18	0.44
6:M:601:BCB:HHC	6:M:601:BCB:HBB2	1.98	0.44
4:H:197:PRO:HG2	4:H:200:PHE:CE1	2.52	0.44
1:C:88:THR:O	1:C:88:THR:HG22	2.17	0.44
1:C:258:LYS:HD3	3:M:305:TYR:O	2.17	0.44
2:L:217:ARG:O	2:L:221:GLY:HA2	2.17	0.44
1:C:50:PRO:HG2	1:C:55:VAL:CG2	2.47	0.44
1:C:106:VAL:HG11	5:C:610:HEC:CAA	2.48	0.44
1:C:297:GLN:HE21	1:C:297:GLN:HB2	1.46	0.44
2:L:136:PRO:HB3	2:L:141:SER:O	2.18	0.44
1:C:82:SER:HB2	1:C:85:GLU:HB2	2.00	0.43
1:C:118:ASN:OD1	1:C:129:GLY:HA2	2.17	0.43
1:C:299:GLU:OE2	1:C:299:GLU:N	2.41	0.43
2:L:135:ARG:HH11	2:L:135:ARG:HD3	1.69	0.43
3:M:173:VAL:HG12	3:M:174:PRO:O	2.18	0.43
1:C:228:ALA:O	1:C:231:ALA:HB3	2.18	0.43
4:H:16:VAL:HG12	4:H:16:VAL:O	2.19	0.43
2:L:239:ASN:HD22	2:L:239:ASN:HA	1.67	0.43
3:M:178:TRP:N	3:M:179:PRO:CD	2.81	0.43
6:M:601:BCB:HBB2	12:M:613:NS1:C22	2.48	0.43
2:L:37:SER:O	2:L:38:ALA:C	2.57	0.43
3:M:69:ILE:HD13	3:M:175:PHE:CD1	2.54	0.43
4:H:230:ILE:HD13	4:H:235:GLU:HG2	2.00	0.43
1:C:186:ASN:C	1:C:187:TYR:CD1	2.91	0.43
4:H:12:ILE:H	4:H:12:ILE:HG12	1.48	0.43
6:L:602:BCB:C4A	6:M:603:BCB:HBB2	2.49	0.43
6:M:601:BCB:C4A	6:M:601:BCB:CBA	2.97	0.43
1:C:186:ASN:ND2	14:C:649:HOH:O	2.51	0.43
2:L:83:GLY:O	2:L:87:GLN:HG3	2.19	0.43
1:C:312:VAL:HG12	1:C:314:LYS:O	2.19	0.43
7:M:605:BPB:H9	7:M:605:BPB:H11A	1.78	0.43
1:C:210:PRO:HB2	4:H:3:HIS:HD2	1.84	0.42
2:L:67:ASN:HB3	2:L:68:PRO:HD2	2.00	0.42
2:L:100:TRP:O	2:L:103:ARG:HB3	2.19	0.42
3:M:12:ALA:HB2	4:H:180:PHE:CE2	2.54	0.42
3:M:67:LEU:O	3:M:68:ILE:C	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:GLY:O	1:C:220:ARG:HB2	2.19	0.42
1:C:283:ALA:N	1:C:284:PRO:HD2	2.34	0.42
2:L:52:ALA:HB3	2:L:66:ILE:CD1	2.49	0.42
1:C:71:LEU:HD23	1:C:71:LEU:HA	1.96	0.42
2:L:115:TRP:N	2:L:115:TRP:CD1	2.88	0.42
6:M:601:BCB:C4A	6:M:601:BCB:HBA1	2.50	0.42
4:H:1:FME:HE2	4:H:1:FME:HB3	1.84	0.42
1:C:102:TYR:O	1:C:103:PRO:C	2.58	0.42
3:M:259:THR:HG23	4:H:36:ASP:O	2.20	0.42
3:M:125:GLY:O	3:M:129:ILE:HG13	2.19	0.42
4:H:29:LEU:HD23	4:H:29:LEU:HA	1.82	0.42
2:L:229:ILE:O	2:L:229:ILE:HG13	2.20	0.42
3:M:289:VAL:HG21	3:M:292:TRP:CH2	2.55	0.42
1:C:79:GLU:O	1:C:83:PRO:HG3	2.19	0.41
3:M:293:TYR:O	3:M:297:VAL:HG23	2.19	0.41
2:L:156:TRP:O	2:L:157:VAL:C	2.57	0.41
2:L:146:PHE:HB3	2:L:156:TRP:CD2	2.55	0.41
2:L:201:GLY:O	2:L:202:ASP:HB3	2.20	0.41
1:C:190:PHE:HE1	1:C:303:ALA:O	2.03	0.41
2:L:139:LEU:HD23	2:L:139:LEU:HA	1.81	0.41
2:L:229:ILE:HD13	8:L:614:UQ1:H8	2.02	0.41
6:L:602:BCB:H193	11:M:608:MQ7:H292	2.02	0.41
3:M:62:GLY:O	3:M:65:ALA:HB3	2.21	0.41
3:M:282:ILE:HD13	3:M:282:ILE:HA	1.88	0.41
4:H:4:GLY:HA2	4:H:12:ILE:CD1	2.49	0.41
2:L:177:VAL:HG13	6:L:602:BCB:HMB3	2.02	0.41
3:M:95:PRO:HG2	14:M:629:HOH:O	2.20	0.41
4:H:117:TYR:HB2	4:H:236:ASP:HB3	2.02	0.41
1:C:236:ILE:O	1:C:240:LEU:HG	2.20	0.41
6:L:604:BCB:H172	6:L:604:BCB:H13	1.82	0.41
4:H:257:LEU:HD23	4:H:257:LEU:HA	1.72	0.41
1:C:102:TYR:CG	1:C:103:PRO:CD	2.96	0.41
2:L:222:TYR:HD1	3:M:45:GLN:O	2.03	0.41
3:M:231:ARG:HH22	4:H:235:GLU:CD	2.24	0.41
2:L:97:PHE:CZ	6:L:602:BCB:H112	2.55	0.41
2:L:169:TYR:OH	3:M:182:ASP:OD2	2.31	0.41
2:L:52:ALA:HB3	2:L:66:ILE:HD11	2.03	0.41
2:L:67:ASN:OD1	2:L:67:ASN:N	2.53	0.41
2:L:87:GLN:NE2	2:L:142:TRP:CD1	2.89	0.41
5:C:610:HEC:HHA	5:C:610:HEC:O1D	2.21	0.40
3:M:258:ALA:HB1	3:M:262:SER:OG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:MET:HB2	1:C:281:TYR:CD1	2.56	0.40
3:M:16:HIS:HD2	3:M:32:PRO:HG3	1.85	0.40
3:M:312:THR:HA	3:M:313:PRO:HD2	1.90	0.40
4:H:138:ARG:HG3	4:H:170:ASP:OD1	2.21	0.40
1:C:102:TYR:CE2	1:C:103:PRO:HD3	2.57	0.40
1:C:144:TYR:O	1:C:307:THR:HG23	2.22	0.40
2:L:109:ARG:HH11	2:L:109:ARG:HD2	1.77	0.40
2:L:241:PHE:CE2	7:L:606:BPB:H43	2.56	0.40
1:C:149:GLU:HB3	1:C:150:PRO:HD2	2.03	0.40
2:L:197:VAL:HG21	2:L:212:GLU:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	331/336 (98%)	306 (92%)	24 (7%)	1 (0%)	41	50
2	L	271/273 (99%)	252 (93%)	18 (7%)	1 (0%)	34	42
3	M	321/323 (99%)	300 (94%)	19 (6%)	2 (1%)	25	31
4	H	256/258 (99%)	239 (93%)	16 (6%)	1 (0%)	34	42
All	All	1179/1190 (99%)	1097 (93%)	77 (6%)	5 (0%)	34	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	22	GLU
4	H	53	ALA
3	M	88	PHE
1	C	250	ALA
2	L	31	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	281/282 (100%)	261 (93%)	20 (7%)	14	19
2	L	218/218 (100%)	210 (96%)	8 (4%)	34	48
3	M	249/249 (100%)	235 (94%)	14 (6%)	21	29
4	H	212/212 (100%)	197 (93%)	15 (7%)	14	19
All	All	960/961 (100%)	903 (94%)	57 (6%)	19	27

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	CYS
1	C	15	ARG
1	C	34	ARG
1	C	38	TYR
1	C	53	SER
1	C	64	ASN
1	C	94	ASN
1	C	115	ARG
1	C	149	GLU
1	C	151	THR
1	C	158	GLU
1	C	186	ASN
1	C	209	LEU
1	C	235	SER
1	C	240	LEU
1	C	258	LYS
1	C	288	SER
1	C	294	LEU
1	C	320	SER
1	C	327	GLU
2	L	4	SER
2	L	15	THR
2	L	119	LEU
2	L	141	SER

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Mol	Chain	Res	Type
2	L	182	VAL
2	L	228	SER
2	L	249	ILE
2	L	272	TRP
3	M	16	HIS
3	M	33	PHE
3	M	70	LEU
3	M	77	VAL
3	M	126	SER
3	M	133	SER
3	M	136	ARG
3	M	147	ASN
3	M	171	GLU
3	M	181	ILE
3	M	194	PHE
3	M	214	PHE
3	M	249	PHE
3	M	279	SER
4	H	12	ILE
4	H	28	VAL
4	H	56	ASP
4	H	82	ARG
4	H	96	PHE
4	H	142	ASP
4	H	161	ASP
4	H	169	THR
4	H	178	HIS
4	H	182	TYR
4	H	198	LEU
4	H	212	SER
4	H	217	GLN
4	H	236	ASP
4	H	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	196	ASN
1	C	297	GLN
1	C	302	GLN
1	C	310	GLN
2	L	144	HIS

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Mol	Chain	Res	Type
2	L	183	ASN
2	L	214	GLN
2	L	239	ASN
4	H	3	HIS
4	H	225	GLN
4	H	229	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FME	H	1	4	8,9,10	0.95	1 (12%)	7,9,11	2.61	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	H	1	4	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	FME	CA-N	-2.34	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	FME	CA-N-CN	-4.40	116.05	122.82
4	H	1	FME	O1-CN-N	-4.01	114.72	125.27
4	H	1	FME	C-CA-N	3.09	115.31	109.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	FME	O1-CN-N-CA
4	H	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	$\#\|Z\| > 2$
13	LDA	M	615	-	12,15,15	2.56	1 (8%)	14,17,17	1.76	5 (35%)
6	BCB	M	601	3	60,74,74	3.87	25 (41%)	48,115,115	2.62	18 (37%)
13	LDA	H	616	-	12,15,15	2.46	1 (8%)	14,17,17	0.77	0
10	SO4	M	620	-	4,4,4	0.63	0	6,6,6	0.15	0
10	SO4	M	619	-	4,4,4	0.81	0	6,6,6	0.19	0
6	BCB	M	603	3	60,74,74	4.50	30 (50%)	48,115,115	2.67	20 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	SO4	H	617	-	4,4,4	0.89	0	6,6,6	0.21	0
10	SO4	M	618	-	4,4,4	0.81	0	6,6,6	0.23	0
6	BCB	L	604	2	60,74,74	4.02	23 (38%)	48,115,115	2.50	18 (37%)
8	UQ1	L	614	-	18,18,18	0.83	1 (5%)	22,25,25	1.27	3 (13%)
5	HEC	C	612	1	26,50,50	1.10	2 (7%)	18,82,82	2.38	6 (33%)
12	NS1	M	613	-	39,39,39	2.74	12 (30%)	44,46,46	2.18	17 (38%)
10	SO4	H	622	-	4,4,4	0.92	0	6,6,6	0.28	0
6	BCB	L	602	2	60,74,74	4.21	22 (36%)	48,115,115	2.57	21 (43%)
10	SO4	H	623	-	4,4,4	0.92	0	6,6,6	0.45	0
11	MQ7	M	608	-	49,49,49	1.40	5 (10%)	60,63,63	2.33	21 (35%)
10	SO4	M	621	-	4,4,4	1.02	0	6,6,6	0.29	0
5	HEC	C	610	1	26,50,50	1.72	4 (15%)	18,82,82	1.44	2 (11%)
7	BPB	M	605	-	64,70,70	1.38	9 (14%)	64,101,101	1.31	8 (12%)
5	HEC	C	609	1	26,50,50	1.42	3 (11%)	18,82,82	1.89	6 (33%)
7	BPB	L	606	-	64,70,70	1.47	8 (12%)	64,101,101	1.67	18 (28%)
5	HEC	C	611	1	26,50,50	1.41	3 (11%)	18,82,82	1.87	5 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCB	L	602	2	-	13/41/177/177	-
6	BCB	L	604	2	-	8/41/177/177	-
6	BCB	M	603	3	-	10/41/177/177	-
11	MQ7	M	608	-	-	4/41/61/61	0/2/2/2
13	LDA	M	615	-	-	7/13/13/13	-
5	HEC	C	610	1	-	0/6/54/54	-
8	UQ1	L	614	-	-	0/9/33/33	0/1/1/1
6	BCB	M	601	3	-	5/41/177/177	-
7	BPB	M	605	-	-	12/47/105/105	0/5/6/6
13	LDA	H	616	-	-	1/13/13/13	-
5	HEC	C	609	1	-	0/6/54/54	-
5	HEC	C	612	1	-	1/6/54/54	-
12	NS1	M	613	-	-	15/43/43/43	-
7	BPB	L	606	-	-	13/47/105/105	0/5/6/6
5	HEC	C	611	1	-	2/6/54/54	-

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	603	BCB	C1A-CHA	-12.05	1.35	1.54
6	M	601	BCB	C1A-CHA	-11.70	1.35	1.54
6	M	601	BCB	CHC-C4B	-11.64	1.35	1.53
6	L	604	BCB	CHC-C4B	-11.48	1.35	1.53
6	L	602	BCB	CHD-C4C	-11.00	1.35	1.53
6	M	603	BCB	CHB-C1B	-10.70	1.36	1.53
6	L	604	BCB	CHB-C1B	-10.68	1.36	1.53
6	L	604	BCB	C1A-CHA	-10.60	1.37	1.54
6	M	603	BCB	CHC-C4B	-10.54	1.36	1.53
6	L	602	BCB	C1A-CHA	-10.50	1.37	1.54
6	L	602	BCB	CHC-C4B	-9.93	1.37	1.53
6	L	604	BCB	CHD-C4C	-9.37	1.37	1.53
6	M	601	BCB	CHD-C4C	-9.29	1.37	1.53
6	M	603	BCB	CHD-C4C	-9.06	1.38	1.53
6	L	602	BCB	CHB-C1B	-8.77	1.39	1.53
13	M	615	LDA	O1-N1	-8.71	1.21	1.42
6	L	602	BCB	CHD-C1D	-8.55	1.40	1.53
6	L	602	BCB	C2B-C1B	-8.30	1.38	1.53
13	H	616	LDA	O1-N1	-8.29	1.22	1.42
6	M	603	BCB	C3B-CAB	-8.21	1.43	1.52
6	M	601	BCB	CHB-C1B	-8.04	1.40	1.53
6	L	602	BCB	C4D-ND	-7.87	1.33	1.50
6	L	602	BCB	C3D-CAD	-7.87	1.36	1.51
6	M	603	BCB	CHD-C1D	-7.82	1.41	1.53
6	M	603	BCB	C3B-C2B	-7.80	1.34	1.55
12	M	613	NS1	C35-C36	7.78	1.54	1.32
12	M	613	NS1	C30-C31	7.70	1.42	1.34
6	M	601	BCB	C3B-C2B	-7.41	1.35	1.55
6	M	603	BCB	C2D-C1D	-7.37	1.40	1.53
6	L	604	BCB	CHD-C1D	-7.33	1.42	1.53
6	M	601	BCB	C4D-ND	-7.30	1.34	1.50
6	M	603	BCB	C2B-C1B	-7.25	1.40	1.53
6	M	603	BCB	C4B-NB	-7.14	1.35	1.50
6	M	603	BCB	C4D-ND	-7.12	1.35	1.50
6	L	604	BCB	C4D-ND	-7.11	1.35	1.50
6	L	602	BCB	C3B-C2B	-7.06	1.36	1.55
6	M	601	BCB	CHD-C1D	-6.90	1.42	1.53
6	M	603	BCB	CHB-C4A	-6.88	1.37	1.52
6	M	603	BCB	CBD-CAD	6.88	1.63	1.53
6	L	604	BCB	C2D-C1D	-6.83	1.41	1.53
6	L	602	BCB	CHB-C4A	-6.77	1.37	1.52
6	M	603	BCB	C1B-NB	-6.42	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	602	BCB	C3D-C2D	-6.26	1.38	1.55
6	L	602	BCB	C2D-C1D	-6.20	1.42	1.53
6	L	602	BCB	C1B-NB	-6.18	1.37	1.50
6	L	604	BCB	C4B-NB	-6.17	1.37	1.50
6	L	602	BCB	C4B-NB	-6.16	1.37	1.50
6	L	604	BCB	C1D-ND	-6.12	1.37	1.50
6	L	604	BCB	C3B-CAB	-5.98	1.45	1.52
6	M	601	BCB	C4B-NB	-5.97	1.37	1.50
5	C	610	HEC	C3C-C4C	-5.93	1.32	1.43
6	L	604	BCB	CHB-C4A	-5.86	1.39	1.52
6	M	601	BCB	CHB-C4A	-5.60	1.40	1.52
6	M	601	BCB	C2D-C1D	-5.30	1.43	1.53
6	M	601	BCB	C3D-C2D	-5.29	1.41	1.55
12	M	613	NS1	C25-C26	5.29	1.42	1.35
6	L	602	BCB	C1D-ND	-5.24	1.39	1.50
6	L	604	BCB	C3D-C2D	-5.18	1.41	1.55
6	M	603	BCB	C3D-C2D	-5.13	1.41	1.55
6	M	603	BCB	C1D-ND	-5.13	1.39	1.50
6	M	601	BCB	CHC-C1C	-5.13	1.41	1.52
12	M	613	NS1	C12-C10	5.01	1.39	1.34
6	M	603	BCB	C3D-CAD	-5.01	1.42	1.51
6	L	604	BCB	C2B-C1B	-4.92	1.44	1.53
6	L	604	BCB	C3B-C2B	-4.87	1.42	1.55
6	M	603	BCB	CAA-C2A	-4.85	1.44	1.53
7	M	605	BPB	C3B-C4B	4.77	1.47	1.41
6	M	601	BCB	C1D-ND	-4.74	1.40	1.50
6	L	604	BCB	CHC-C1C	-4.73	1.42	1.52
6	L	602	BCB	CHC-C1C	-4.65	1.42	1.52
6	L	604	BCB	CBD-CAD	4.50	1.59	1.53
6	M	603	BCB	CHC-C1C	-4.47	1.42	1.52
6	L	604	BCB	O1A-CGA	-4.43	1.09	1.22
12	M	613	NS1	C20-C21	4.33	1.41	1.35
6	M	601	BCB	C3D-CAD	-4.26	1.43	1.51
7	L	606	BPB	C3B-C4B	4.26	1.46	1.41
6	M	601	BCB	C1B-NB	-4.26	1.41	1.50
6	L	602	BCB	C3B-CAB	-4.25	1.47	1.52
5	C	611	HEC	CAA-C2A	-4.22	1.44	1.52
7	M	605	BPB	C1-C2	4.06	1.61	1.49
6	M	601	BCB	C1A-C2A	-4.02	1.49	1.53
7	L	606	BPB	O2D-CED	-3.99	1.35	1.45
12	M	613	NS1	C17-C15	3.81	1.40	1.35
6	M	601	BCB	O1D-CGD	-3.76	1.11	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	603	BCB	CBD-CGD	3.73	1.58	1.52
6	M	601	BCB	C2B-C1B	-3.73	1.46	1.53
11	M	608	MQ7	C10-C1	-3.72	1.41	1.48
6	L	602	BCB	O2D-CED	-3.71	1.36	1.45
6	L	604	BCB	C1B-NB	-3.69	1.42	1.50
12	M	613	NS1	C14-C15	-3.66	1.38	1.45
5	C	610	HEC	CAA-C2A	-3.65	1.45	1.52
5	C	609	HEC	C3C-C4C	-3.61	1.36	1.43
6	M	603	BCB	C2A-C3A	-3.44	1.48	1.54
5	C	609	HEC	C3B-C2B	-3.44	1.37	1.40
5	C	609	HEC	C3B-C4B	-3.42	1.36	1.43
6	L	604	BCB	C5-C3	3.40	1.58	1.51
6	M	603	BCB	O1A-CGA	-3.39	1.12	1.22
7	L	606	BPB	CAA-C2A	3.37	1.60	1.54
6	L	604	BCB	C4A-C3A	-3.37	1.49	1.53
11	M	608	MQ7	C10-C5	-3.35	1.35	1.40
6	L	604	BCB	C3D-CAD	-3.19	1.45	1.51
12	M	613	NS1	C24-C23	3.19	1.42	1.34
5	C	611	HEC	C3C-C2C	-3.07	1.37	1.40
6	L	602	BCB	CBD-CAD	3.02	1.57	1.53
5	C	611	HEC	C3B-C2B	-3.00	1.37	1.40
5	C	612	HEC	CAD-C3D	2.98	1.56	1.52
7	L	606	BPB	CBC-CAC	2.79	1.60	1.49
7	L	606	BPB	C2C-C3C	2.76	1.55	1.51
6	M	601	BCB	C5-C3	2.75	1.57	1.51
11	M	608	MQ7	C6-C5	-2.71	1.35	1.39
7	M	605	BPB	C2A-C1A	2.70	1.54	1.50
6	M	603	BCB	OBD-CAD	2.64	1.25	1.21
12	M	613	NS1	C2-C1	-2.61	1.33	1.51
6	L	604	BCB	O2A-C1	2.57	1.53	1.46
11	M	608	MQ7	C9-C10	-2.54	1.35	1.39
12	M	613	NS1	C29-C28	2.51	1.41	1.34
6	M	603	BCB	CBC-CAC	2.50	1.59	1.49
6	L	604	BCB	C2A-C3A	2.49	1.59	1.54
6	M	601	BCB	CMD-C2D	-2.49	1.48	1.53
7	M	605	BPB	C2-C3	2.49	1.38	1.33
5	C	610	HEC	C3B-C4B	-2.48	1.38	1.43
7	L	606	BPB	C4C-C3C	2.48	1.51	1.45
7	M	605	BPB	CHC-C1C	2.46	1.43	1.37
7	L	606	BPB	CMA-C3A	-2.39	1.48	1.53
8	L	614	UQ1	C7-C8	2.37	1.54	1.50
12	M	613	NS1	C22-C21	2.35	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	605	BPB	O2A-C1	2.33	1.52	1.46
7	M	605	BPB	C3B-C2B	-2.33	1.35	1.39
6	M	603	BCB	CAA-CBA	-2.30	1.45	1.52
5	C	610	HEC	C4A-C3A	-2.29	1.37	1.42
6	M	603	BCB	O1D-CGD	-2.27	1.15	1.21
6	M	601	BCB	OBD-CAD	2.26	1.25	1.21
6	M	603	BCB	C5-C3	2.26	1.56	1.51
12	M	613	NS1	C19-C18	2.25	1.41	1.36
6	M	601	BCB	CBA-CGA	2.25	1.57	1.50
6	M	603	BCB	OBB-CAB	-2.24	1.15	1.21
7	L	606	BPB	C5-C3	2.22	1.55	1.51
6	M	603	BCB	O2A-C1	2.21	1.52	1.46
6	L	602	BCB	C2A-C3A	-2.18	1.50	1.54
6	M	603	BCB	O2D-CGD	-2.18	1.27	1.33
7	M	605	BPB	CBC-CAC	2.13	1.57	1.49
6	L	602	BCB	CMD-C2D	-2.13	1.49	1.53
11	M	608	MQ7	C36-C37	2.12	1.57	1.50
6	M	601	BCB	C3B-CAB	-2.09	1.49	1.52
6	M	601	BCB	CBC-CAC	2.08	1.57	1.49
6	L	602	BCB	CBB-CAB	2.07	1.55	1.49
5	C	612	HEC	C3D-C2D	2.07	1.43	1.37
7	M	605	BPB	C6-C7	2.07	1.61	1.52
6	M	601	BCB	CBD-CAD	2.05	1.56	1.53

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	608	MQ7	C11-C3-C4	-9.24	108.61	118.50
6	M	601	BCB	CBB-CAB-C3B	8.46	125.43	116.80
5	C	612	HEC	CBD-CAD-C3D	7.18	125.73	112.49
6	L	604	BCB	C1D-CHD-C4C	7.01	127.30	112.37
6	L	604	BCB	CMD-C2D-C3D	6.94	131.53	114.29
6	M	601	BCB	C1D-CHD-C4C	6.83	126.92	112.37
6	L	602	BCB	C1D-CHD-C4C	6.69	126.62	112.37
6	M	603	BCB	CMD-C2D-C3D	6.59	130.66	114.29
6	M	603	BCB	CMB-C2B-C3B	6.23	129.75	114.29
6	L	602	BCB	CMD-C2D-C3D	6.13	129.52	114.29
6	L	602	BCB	CMB-C2B-C3B	6.07	129.35	114.29
6	M	603	BCB	C1D-CHD-C4C	6.05	125.25	112.37
6	L	604	BCB	CMB-C2B-C3B	5.98	129.15	114.29
6	M	603	BCB	CBB-CAB-C3B	5.96	122.89	116.80
6	M	601	BCB	CMD-C2D-C3D	5.81	128.72	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	602	BCB	CBB-CAB-C3B	5.55	122.46	116.80
12	M	613	NS1	C34-C35-C36	-5.18	110.04	127.75
6	L	602	BCB	C1-C2-C3	-5.05	117.31	126.04
6	M	601	BCB	OBB-CAB-CBB	-4.92	112.41	121.15
12	M	613	NS1	C19-C20-C21	4.83	134.21	127.31
5	C	609	HEC	CMC-C2C-C3C	4.54	131.15	125.82
12	M	613	NS1	CM4-C36-C35	-4.49	109.67	122.65
6	L	604	BCB	C1-C2-C3	-4.45	118.35	126.04
6	M	603	BCB	CHC-C4B-C3B	4.42	129.01	118.17
11	M	608	MQ7	C21-C22-C23	-4.40	117.06	127.66
5	C	610	HEC	CBD-CAD-C3D	4.39	120.59	112.49
6	M	601	BCB	C4-C3-C5	4.38	122.64	115.27
6	L	604	BCB	CBB-CAB-C3B	4.37	121.26	116.80
11	M	608	MQ7	C36-C37-C38	-4.36	117.17	127.66
12	M	613	NS1	CM3-C36-C35	-4.34	110.09	122.65
6	L	602	BCB	C4-C3-C5	4.27	122.45	115.27
6	M	603	BCB	C1-O2A-CGA	-4.25	105.29	116.44
11	M	608	MQ7	C39-C38-C40	4.17	122.28	115.27
11	M	608	MQ7	O1-C1-C10	-4.16	114.83	121.56
5	C	609	HEC	CBD-CAD-C3D	-3.93	105.24	112.49
11	M	608	MQ7	C34-C33-C35	3.83	121.71	115.27
6	M	603	BCB	C4-C3-C5	3.76	121.59	115.27
6	L	602	BCB	CHC-C4B-C3B	3.72	127.28	118.17
6	L	604	BCB	CHC-C4B-C3B	3.69	127.21	118.17
6	M	603	BCB	OBB-CAB-CBB	-3.69	114.60	121.15
6	M	603	BCB	O2D-CGD-O1D	-3.66	116.69	123.84
7	L	606	BPB	C1-O2A-CGA	-3.63	106.93	116.44
6	M	603	BCB	CAA-CBA-CGA	-3.59	102.75	113.25
6	M	601	BCB	CMB-C2B-C3B	3.56	123.12	114.29
6	M	603	BCB	O2A-C1-C2	3.52	117.88	108.64
5	C	611	HEC	CAA-C2A-C3A	-3.51	117.16	127.25
12	M	613	NS1	C8-C7-C5	-3.49	119.27	127.66
6	L	602	BCB	CMA-C3A-C2A	-3.46	105.87	115.73
5	C	612	HEC	CMC-C2C-C1C	-3.43	123.19	128.46
7	M	605	BPB	OBB-CAB-CBB	-3.42	112.48	120.17
13	M	615	LDA	CM2-N1-C1	3.38	117.34	110.23
11	M	608	MQ7	C9-C10-C5	3.36	123.00	119.26
6	L	604	BCB	OBB-CAB-CBB	-3.35	115.20	121.15
5	C	611	HEC	CMB-C2B-C3B	3.33	129.74	125.82
6	L	604	BCB	C16-C15-C13	-3.33	105.16	115.92
5	C	612	HEC	CMC-C2C-C3C	3.28	129.67	125.82
5	C	611	HEC	CAD-CBD-CGD	3.24	118.10	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	608	MQ7	C24-C23-C25	3.23	120.71	115.27
6	M	601	BCB	CHC-C4B-C3B	3.11	125.81	118.17
7	L	606	BPB	CAA-C2A-C1A	3.11	122.42	112.19
7	L	606	BPB	O1D-CGD-CBD	3.09	130.82	124.48
11	M	608	MQ7	C2M-C2-C1	-3.09	111.15	116.27
6	M	601	BCB	CMA-C3A-C2A	-3.03	107.09	115.73
6	L	602	BCB	C11-C10-C8	-3.01	106.19	115.92
12	M	613	NS1	C11-C10-C9	3.01	120.33	115.27
7	L	606	BPB	CED-O2D-CGD	-2.99	109.16	115.94
6	M	603	BCB	O2A-CGA-CBA	2.99	121.30	111.91
6	M	601	BCB	O2D-CGD-O1D	-2.99	118.00	123.84
6	M	601	BCB	C3B-C4B-NB	2.97	109.16	103.75
8	L	614	UQ1	CM5-C5-C6	-2.94	119.60	124.40
7	L	606	BPB	CBD-CHA-C4D	-2.90	105.27	108.54
7	L	606	BPB	C7-C6-C5	-2.90	105.49	113.36
6	M	601	BCB	CBA-CAA-C2A	-2.88	111.80	115.72
11	M	608	MQ7	O1-C1-C2	2.88	124.00	120.25
6	L	602	BCB	C14-C13-C15	-2.87	100.91	111.29
6	L	604	BCB	C4-C3-C5	2.86	120.08	115.27
11	M	608	MQ7	C30-C31-C32	-2.84	102.53	111.88
12	M	613	NS1	C18-C17-C15	-2.83	123.27	127.31
12	M	613	NS1	C13-C14-C15	-2.82	118.48	126.42
6	M	601	BCB	CAA-CBA-CGA	-2.81	105.06	113.25
5	C	611	HEC	C4B-C3B-C2B	2.79	109.36	106.35
6	M	601	BCB	C6-C7-C8	-2.76	107.00	115.92
12	M	613	NS1	C27-C26-C25	-2.76	119.06	122.92
11	M	608	MQ7	C39-C38-C37	-2.74	116.64	123.68
6	M	603	BCB	O2A-CGA-O1A	-2.72	116.73	123.59
11	M	608	MQ7	C29-C28-C30	2.71	119.84	115.27
6	M	601	BCB	C7-C6-C5	-2.70	106.03	113.36
12	M	613	NS1	C6-C5-C4	2.69	119.79	115.27
7	L	606	BPB	CMA-C3A-C2A	-2.67	103.04	113.83
6	L	604	BCB	CED-O2D-CGD	2.67	121.98	115.94
7	L	606	BPB	CHD-C1D-ND	-2.67	119.03	124.58
6	M	603	BCB	C11-C10-C8	-2.66	107.32	115.92
5	C	612	HEC	CAA-CBA-CGA	2.65	117.11	112.67
6	M	603	BCB	CHC-C1C-C2C	2.64	125.17	117.19
13	M	615	LDA	C9-C8-C7	-2.64	101.02	114.42
11	M	608	MQ7	C31-C32-C33	-2.64	121.31	127.66
11	M	608	MQ7	C14-C13-C15	2.62	119.68	115.27
7	M	605	BPB	CBC-CAC-C3C	-2.62	119.06	126.72
6	L	602	BCB	OBD-CAD-C3D	2.59	131.30	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	605	BPB	CHB-C4A-NA	-2.59	122.13	125.20
6	M	603	BCB	C7-C6-C5	-2.57	106.38	113.36
6	L	604	BCB	C11-C12-C13	-2.55	107.67	115.92
8	L	614	UQ1	C7-C8-C9	-2.54	119.30	127.26
6	L	602	BCB	C4-C3-C2	-2.52	117.21	123.68
6	L	604	BCB	CMA-C3A-C2A	-2.51	108.56	115.73
11	M	608	MQ7	O4-C4-C3	-2.51	116.53	120.56
6	L	602	BCB	CHC-C1C-C2C	2.51	124.77	117.19
7	M	605	BPB	OBB-CAB-C3B	2.49	124.41	119.99
11	M	608	MQ7	C2M-C2-C3	2.48	128.44	124.40
12	M	613	NS1	C19-C18-C17	-2.44	118.48	123.47
13	M	615	LDA	O1-N1-C1	2.44	115.25	109.27
7	M	605	BPB	CBD-CHA-C4D	-2.43	105.80	108.54
6	L	602	BCB	OBD-CAD-CBD	-2.41	121.72	127.49
7	L	606	BPB	C3D-C4D-CHA	2.39	115.95	109.49
6	L	602	BCB	CAA-CBA-CGA	-2.39	106.28	113.25
7	L	606	BPB	C4B-CHC-C1C	2.38	131.64	128.57
12	M	613	NS1	C22-C21-C20	-2.36	119.62	122.92
7	M	605	BPB	C3C-C2C-C1C	2.36	103.93	100.72
12	M	613	NS1	C14-C15-C17	2.35	122.55	118.94
7	L	606	BPB	C14-C13-C12	-2.35	102.79	111.29
6	L	604	BCB	CHC-C1C-C2C	2.34	124.25	117.19
6	L	602	BCB	CED-O2D-CGD	-2.32	110.69	115.94
5	C	609	HEC	C4C-C3C-C2C	2.29	108.82	106.35
6	L	604	BCB	C3B-C4B-NB	2.28	107.91	103.75
6	L	604	BCB	OBD-CAD-CBD	-2.28	122.02	127.49
8	L	614	UQ1	C11-C9-C10	2.26	119.60	114.60
12	M	613	NS1	CM4-C36-CM3	-2.26	109.61	114.60
5	C	610	HEC	CAD-CBD-CGD	-2.26	108.89	112.67
12	M	613	NS1	C24-C23-C21	-2.25	120.10	126.42
7	L	606	BPB	C9-C8-C10	-2.25	103.16	111.29
5	C	609	HEC	CMC-C2C-C1C	-2.23	125.03	128.46
6	M	603	BCB	C1-C2-C3	-2.23	122.18	126.04
7	L	606	BPB	O2D-CGD-O1D	-2.23	119.48	123.84
5	C	611	HEC	CMA-C3A-C2A	-2.23	120.74	124.94
7	L	606	BPB	C3A-C2A-C1A	2.22	104.67	101.34
6	M	601	BCB	C11-C10-C8	-2.22	108.74	115.92
11	M	608	MQ7	C11-C12-C13	-2.21	123.11	126.79
7	L	606	BPB	C2D-C1D-ND	2.21	113.12	109.79
11	M	608	MQ7	C45-C43-C44	2.19	119.44	114.60
7	L	606	BPB	OBD-CAD-C3D	2.19	133.79	128.52
6	L	602	BCB	O1D-CGD-CBD	2.19	128.88	124.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	602	BCB	C6-C7-C8	-2.17	108.89	115.92
7	M	605	BPB	CAA-C2A-C1A	2.15	119.24	112.19
11	M	608	MQ7	C16-C17-C18	-2.14	122.51	127.66
7	M	605	BPB	C16-C15-C13	-2.14	109.02	115.92
7	L	606	BPB	C20-C18-C19	-2.13	100.70	110.51
13	M	615	LDA	CM1-N1-C1	-2.13	105.77	110.23
6	M	603	BCB	C4-C3-C2	-2.12	118.23	123.68
6	L	604	BCB	CBA-CAA-C2A	-2.11	112.85	115.72
6	L	604	BCB	C4-C3-C2	-2.11	118.27	123.68
12	M	613	NS1	C16-C15-C17	-2.09	119.99	122.92
5	C	609	HEC	CAD-CBD-CGD	2.09	116.18	112.67
11	M	608	MQ7	C41-C42-C43	-2.09	120.61	127.75
6	M	603	BCB	C4A-C3A-C2A	-2.09	100.67	103.86
13	M	615	LDA	C6-C5-C4	-2.08	103.88	114.42
6	M	601	BCB	O2D-CGD-CBD	2.06	115.96	111.11
6	L	602	BCB	OBB-CAB-CBB	-2.06	117.50	121.15
6	M	601	BCB	C5-C3-C2	-2.05	116.97	121.12
6	M	601	BCB	OBD-CAD-CBD	-2.04	122.60	127.49
6	L	602	BCB	O2A-CGA-CBA	2.03	118.27	111.91
6	M	603	BCB	C3B-C4B-NB	2.02	107.44	103.75
7	L	606	BPB	OBB-CAB-CBB	-2.01	115.64	120.17
6	L	602	BCB	C9-C8-C7	-2.01	104.02	111.29
12	M	613	NS1	CM2-C1-CM1	2.01	119.76	110.51
6	L	604	BCB	O2A-CGA-CBA	2.01	118.20	111.91
5	C	612	HEC	CBA-CAA-C2A	2.00	116.17	112.48
5	C	609	HEC	CAD-C3D-C2D	-2.00	121.49	127.25
5	C	612	HEC	CMD-C2D-C1D	-2.00	125.39	128.46

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	611	HEC	C1A-C2A-CAA-CBA
5	C	611	HEC	C3A-C2A-CAA-CBA
6	L	602	BCB	C2B-C3B-CAB-OBB
6	L	602	BCB	C2B-C3B-CAB-CBB
6	L	602	BCB	C4-C3-C5-C6
6	M	601	BCB	C4B-C3B-CAB-OBB
6	M	601	BCB	C4B-C3B-CAB-CBB
6	M	601	BCB	C2C-C3C-CAC-CBC
6	M	603	BCB	C2B-C3B-CAB-CBB
6	M	603	BCB	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
6	M	603	BCB	CAD-CBD-CGD-O2D
6	M	603	BCB	C2-C3-C5-C6
6	M	603	BCB	C4-C3-C5-C6
7	L	606	BPB	C3A-C2A-CAA-CBA
7	M	605	BPB	C2-C3-C5-C6
7	M	605	BPB	C4-C3-C5-C6
7	M	605	BPB	C1A-C2A-CAA-CBA
7	M	605	BPB	C3A-C2A-CAA-CBA
12	M	613	NS1	C11-C10-C9-C8
12	M	613	NS1	C12-C10-C9-C8
12	M	613	NS1	C9-C10-C12-C13
12	M	613	NS1	C11-C10-C12-C13
12	M	613	NS1	C34-C35-C36-CM3
12	M	613	NS1	C3-C4-C5-C6
12	M	613	NS1	C32-C31-C33-C34
6	L	602	BCB	C2-C3-C5-C6
12	M	613	NS1	C3-C4-C5-C7
12	M	613	NS1	C30-C31-C33-C34
7	M	605	BPB	C6-C7-C8-C9
12	M	613	NS1	C22-C21-C23-C24
7	L	606	BPB	C11-C12-C13-C15
12	M	613	NS1	C16-C15-C17-C18
12	M	613	NS1	C14-C15-C17-C18
6	L	602	BCB	C14-C13-C15-C16
6	L	602	BCB	C2A-CAA-CBA-CGA
6	M	601	BCB	C5-C6-C7-C8
12	M	613	NS1	CM2-C1-C2-C3
6	L	602	BCB	C12-C13-C15-C16
7	M	605	BPB	CBA-CGA-O2A-C1
13	M	615	LDA	C1-C2-C3-C4
7	L	606	BPB	C11-C12-C13-C14
11	M	608	MQ7	C41-C42-C43-C45
7	L	606	BPB	C1A-C2A-CAA-CBA
6	L	602	BCB	C13-C15-C16-C17
6	M	603	BCB	C2A-CAA-CBA-CGA
6	L	604	BCB	C15-C16-C17-C18
6	L	604	BCB	C4B-C3B-CAB-OBB
6	L	604	BCB	C4B-C3B-CAB-CBB
13	H	616	LDA	N1-C1-C2-C3
6	L	602	BCB	CBA-CGA-O2A-C1
13	M	615	LDA	C9-C10-C11-C12
7	L	606	BPB	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	M	603	BCB	C2B-C3B-CAB-OBB
7	L	606	BPB	CAD-CBD-CGD-O2D
7	M	605	BPB	CAD-CBD-CGD-O2D
6	M	603	BCB	C3A-C2A-CAA-CBA
7	M	605	BPB	O1A-CGA-O2A-C1
13	M	615	LDA	C2-C1-N1-CM2
6	L	602	BCB	O1A-CGA-O2A-C1
12	M	613	NS1	C20-C21-C23-C24
11	M	608	MQ7	C41-C42-C43-C44
5	C	612	HEC	C2D-C3D-CAD-CBD
11	M	608	MQ7	C39-C38-C40-C41
13	M	615	LDA	C4-C5-C6-C7
6	L	602	BCB	CAD-CBD-CGD-O1D
6	L	602	BCB	CAD-CBD-CGD-O2D
7	L	606	BPB	C2-C3-C5-C6
7	L	606	BPB	CBA-CGA-O2A-C1
12	M	613	NS1	C18-C19-C20-C21
6	L	604	BCB	C14-C13-C15-C16
7	M	605	BPB	C14-C13-C15-C16
13	M	615	LDA	C6-C7-C8-C9
6	M	603	BCB	C16-C17-C18-C20
7	L	606	BPB	C13-C15-C16-C17
6	L	604	BCB	CHA-CBD-CGD-O1D
11	M	608	MQ7	C37-C38-C40-C41
13	M	615	LDA	C7-C8-C9-C10
6	L	604	BCB	C3A-C2A-CAA-CBA
6	M	601	BCB	C3A-C2A-CAA-CBA
7	M	605	BPB	CAA-CBA-CGA-O2A
6	L	604	BCB	CHA-CBD-CGD-O2D
7	L	606	BPB	C11-C10-C8-C9
13	M	615	LDA	C11-C10-C9-C8
7	L	606	BPB	CAA-CBA-CGA-O2A
7	M	605	BPB	CAA-CBA-CGA-O1A
7	L	606	BPB	C4-C3-C5-C6
6	L	602	BCB	C15-C16-C17-C18
7	M	605	BPB	C10-C11-C12-C13
6	L	604	BCB	CBA-CGA-O2A-C1
7	L	606	BPB	C11-C10-C8-C7
6	M	603	BCB	CHA-CBD-CGD-O2D

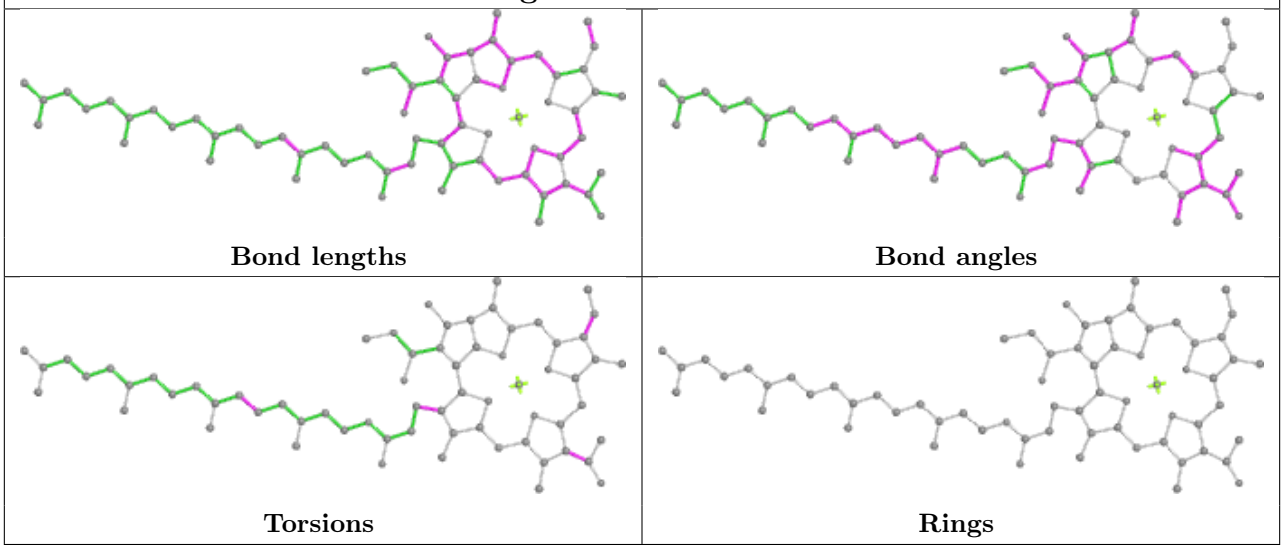
There are no ring outliers.

15 monomers are involved in 93 short contacts:

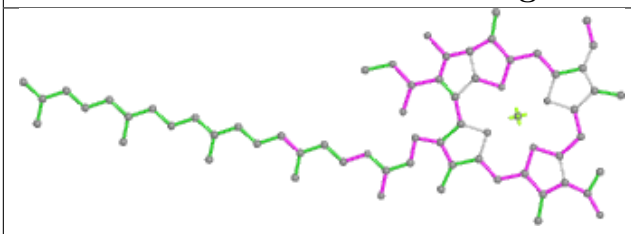
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	615	LDA	1	0
6	M	601	BCB	7	0
13	H	616	LDA	2	0
6	M	603	BCB	15	0
6	L	604	BCB	11	0
8	L	614	UQ1	10	0
5	C	612	HEC	3	0
12	M	613	NS1	4	0
6	L	602	BCB	16	0
11	M	608	MQ7	1	0
5	C	610	HEC	5	0
7	M	605	BPB	11	0
5	C	609	HEC	6	0
7	L	606	BPB	8	0
5	C	611	HEC	6	0

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 then 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.

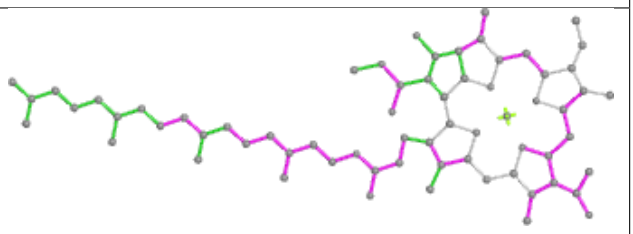
Ligand BCB M 601



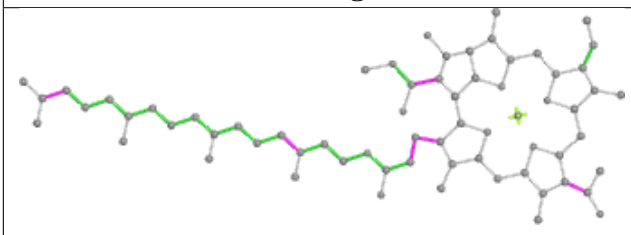
Ligand BCB M 603



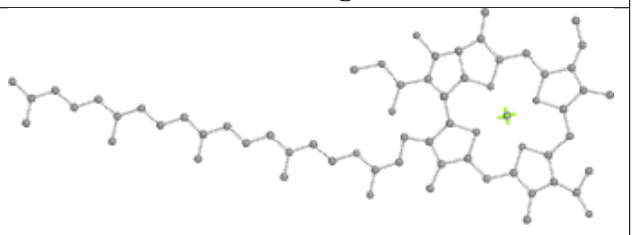
Bond lengths



Bond angles

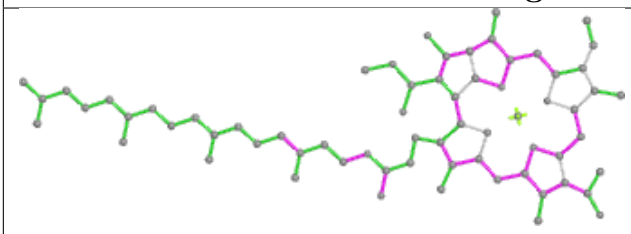


Torsions

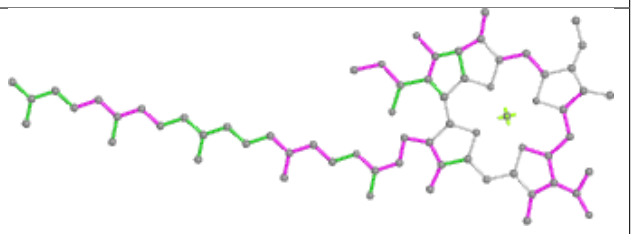


Rings

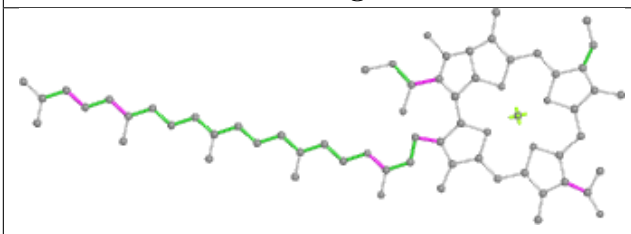
Ligand BCB L 604



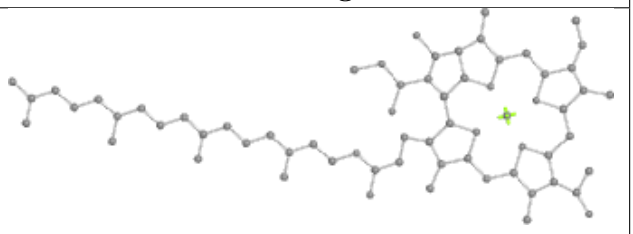
Bond lengths



Bond angles

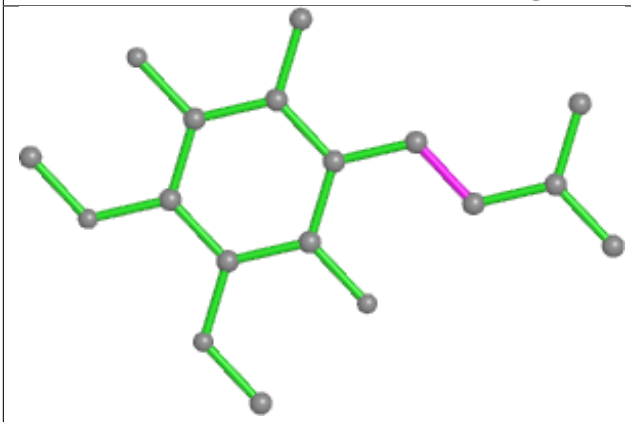


Torsions

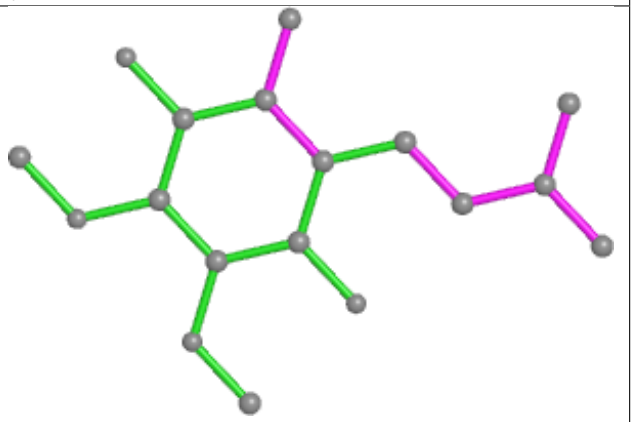


Rings

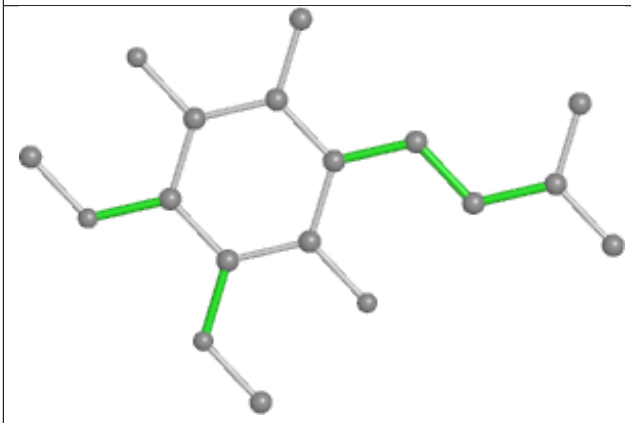
Ligand UQ1 L 614



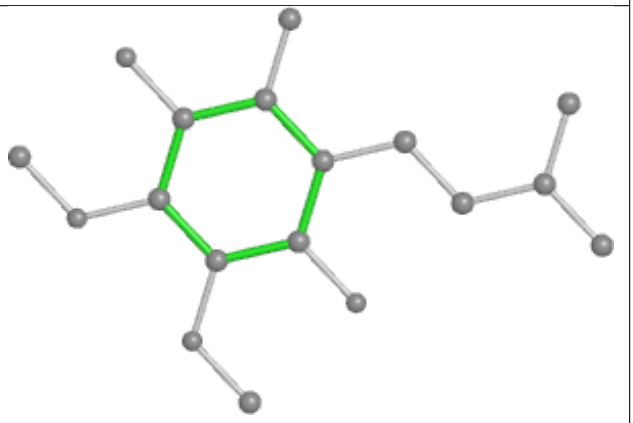
Bond lengths



Bond angles

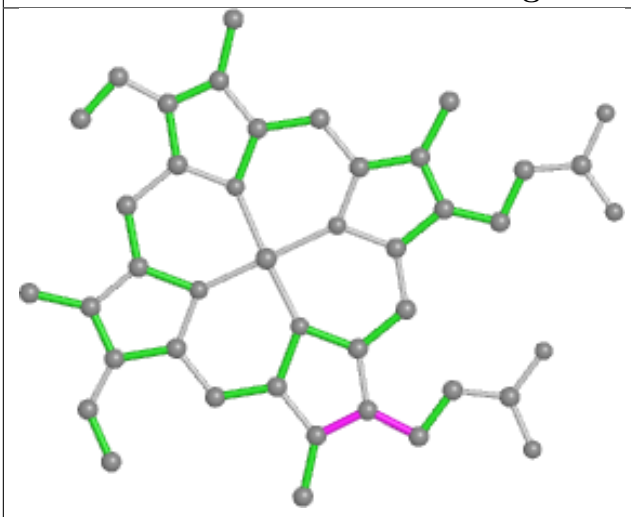


Torsions

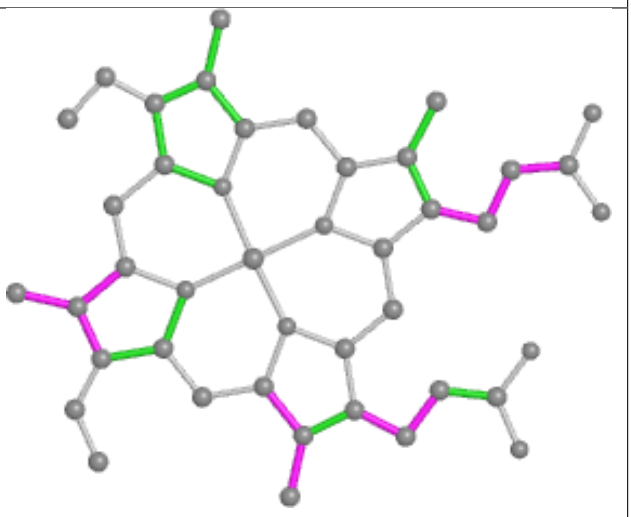


Rings

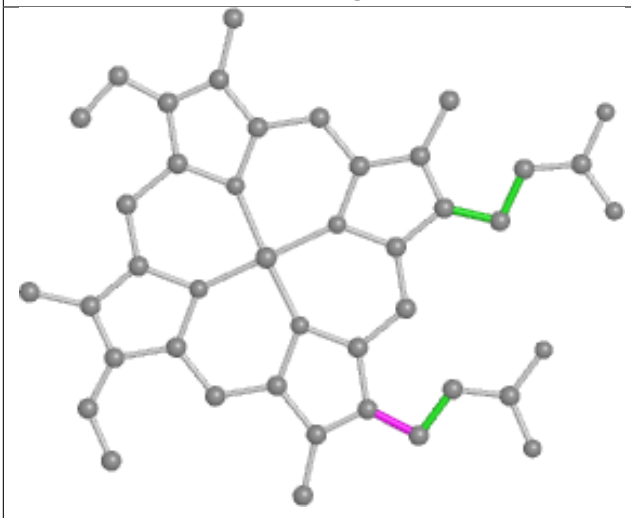
Ligand HEC C 612



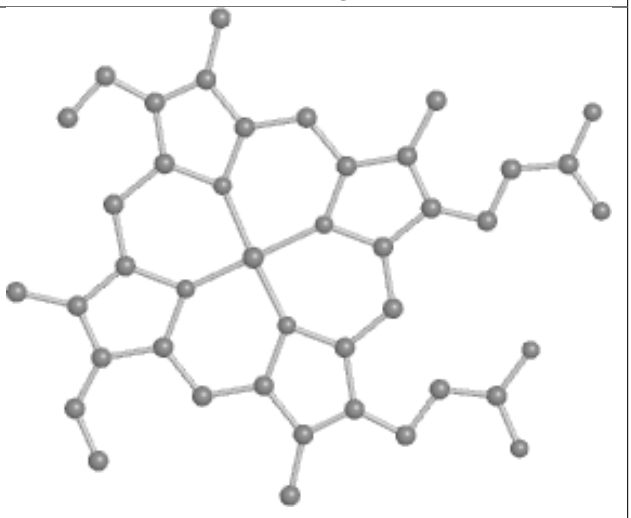
Bond lengths



Bond angles

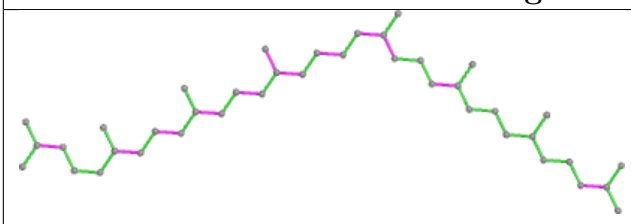


Torsions

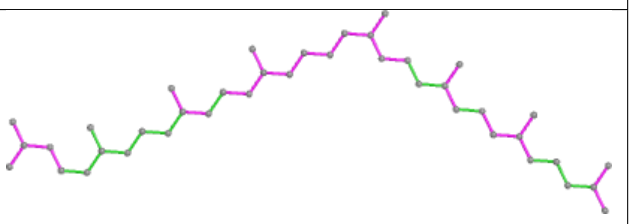


Rings

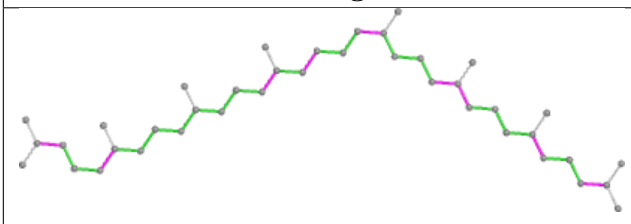
Ligand NS1 M 613



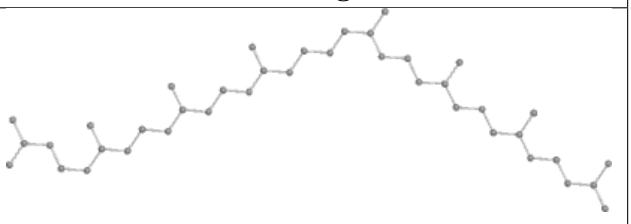
Bond lengths



Bond angles

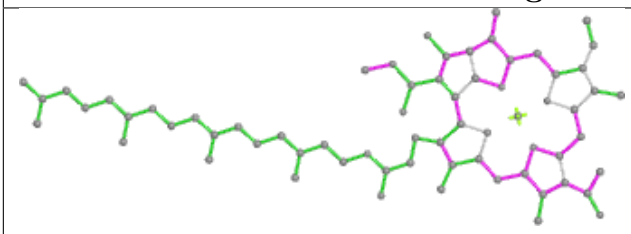


Torsions

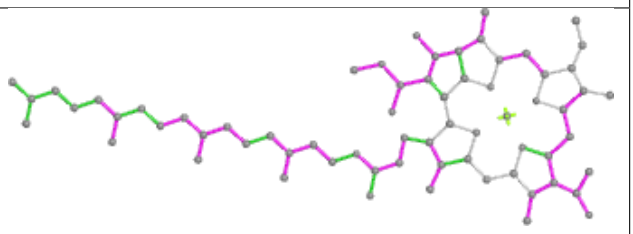


Rings

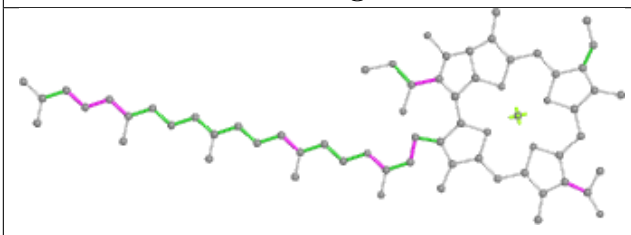
Ligand BCB L 602



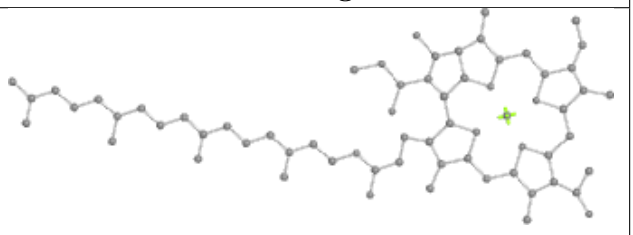
Bond lengths



Bond angles

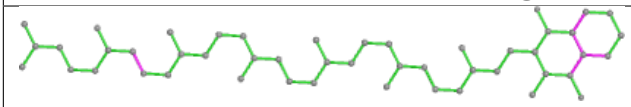


Torsions

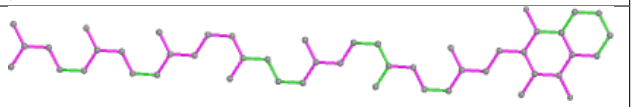


Rings

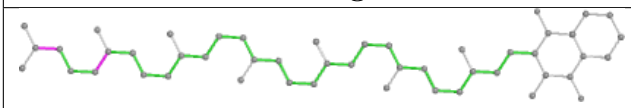
Ligand MQ7 M 608



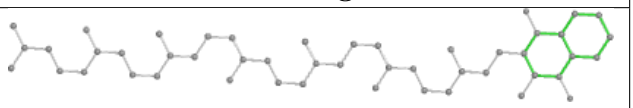
Bond lengths



Bond angles

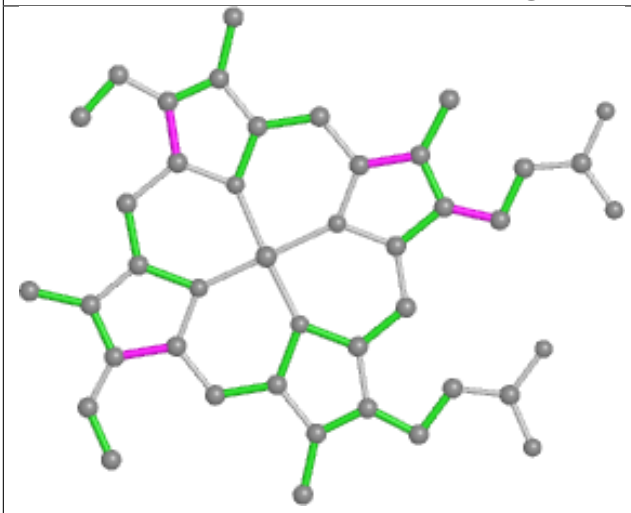


Torsions

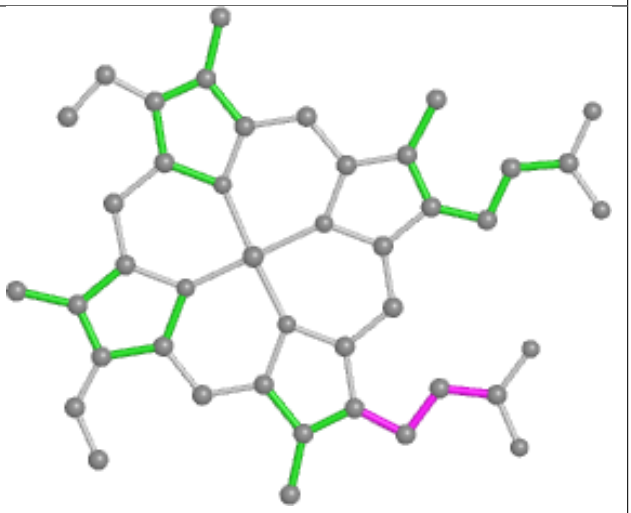


Rings

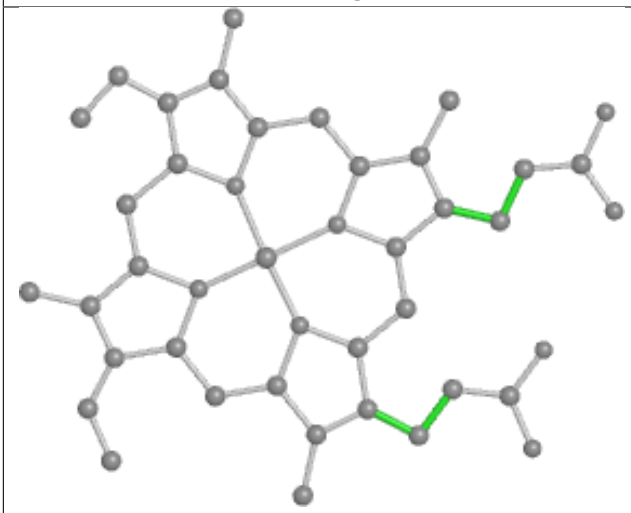
Ligand HEC C 610



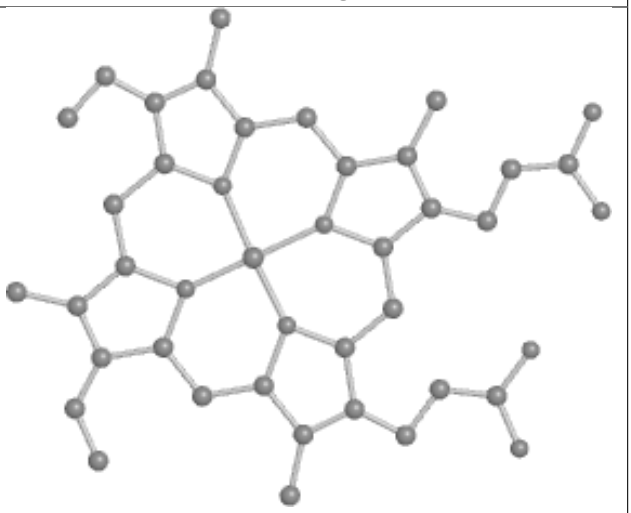
Bond lengths



Bond angles

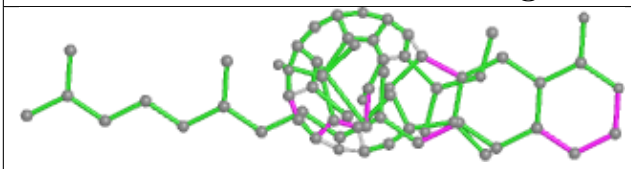


Torsions

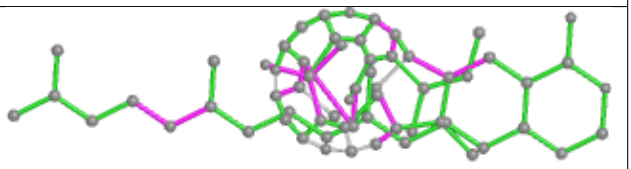


Rings

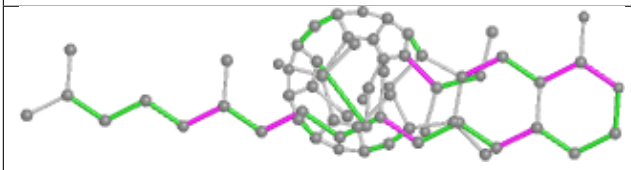
Ligand BPB M 605



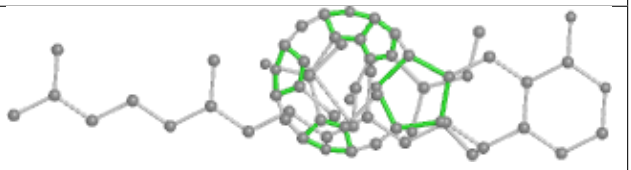
Bond lengths



Bond angles

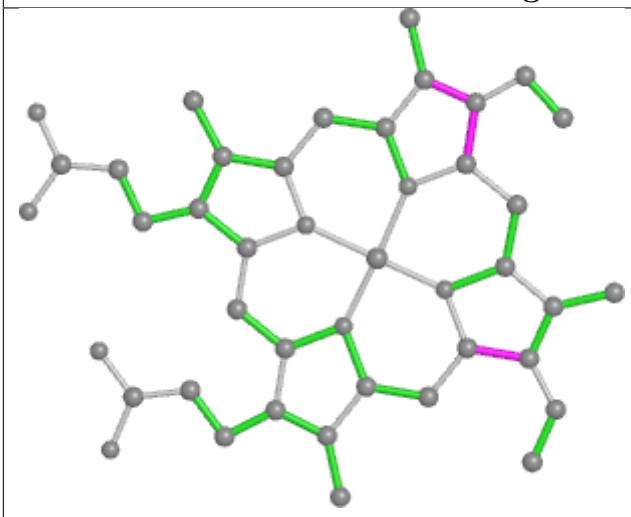


Torsions

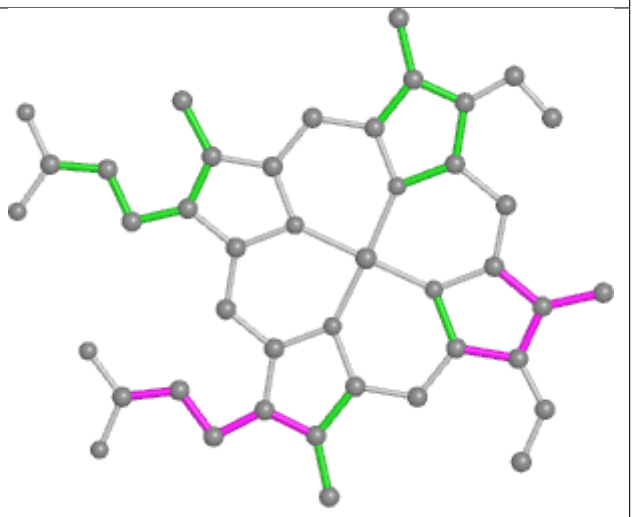


Rings

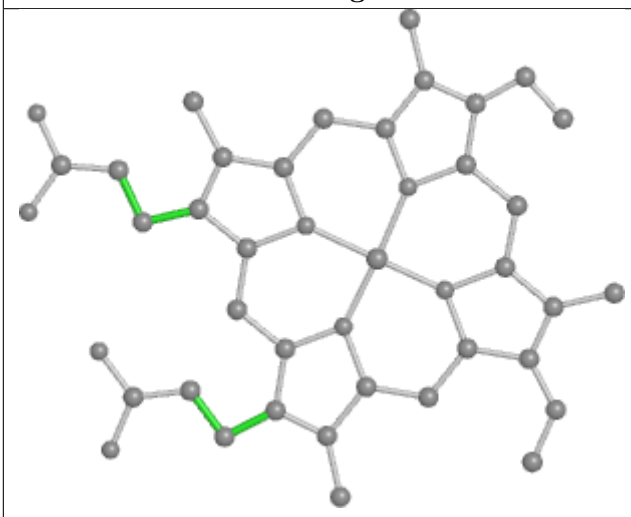
Ligand HEC C 609



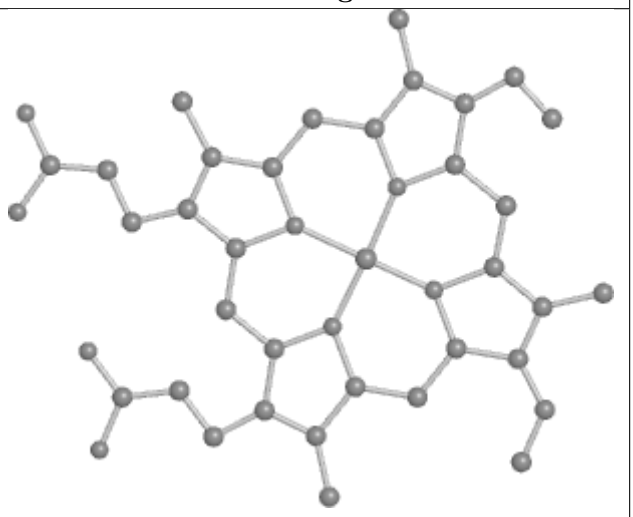
Bond lengths



Bond angles

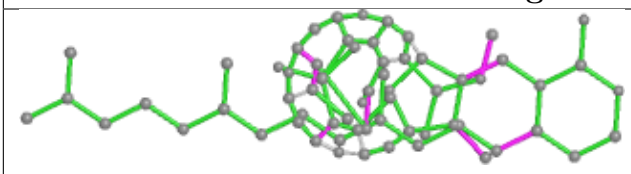


Torsions

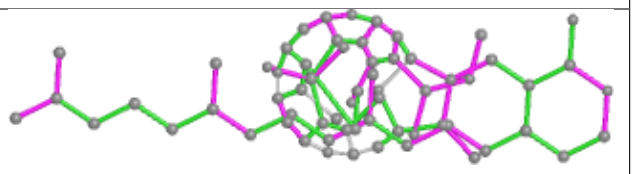


Rings

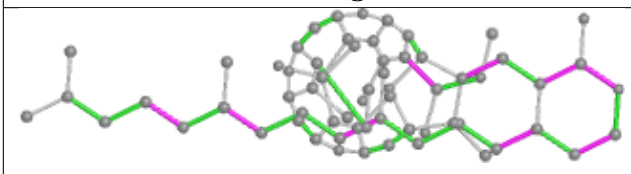
Ligand BPB L 606



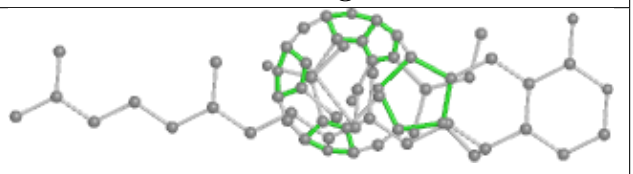
Bond lengths



Bond angles

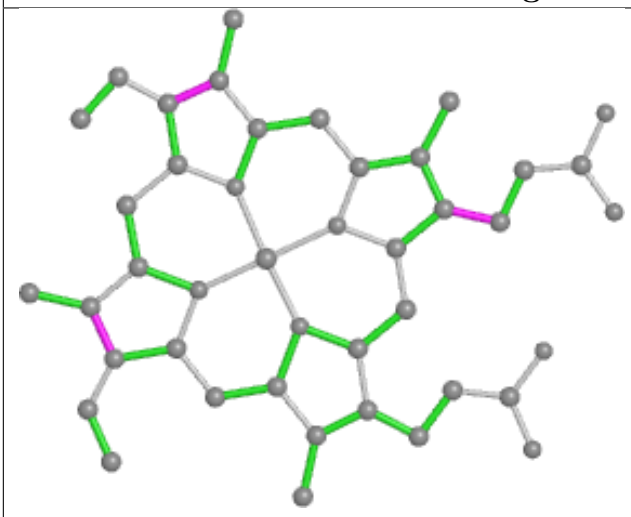


Torsions

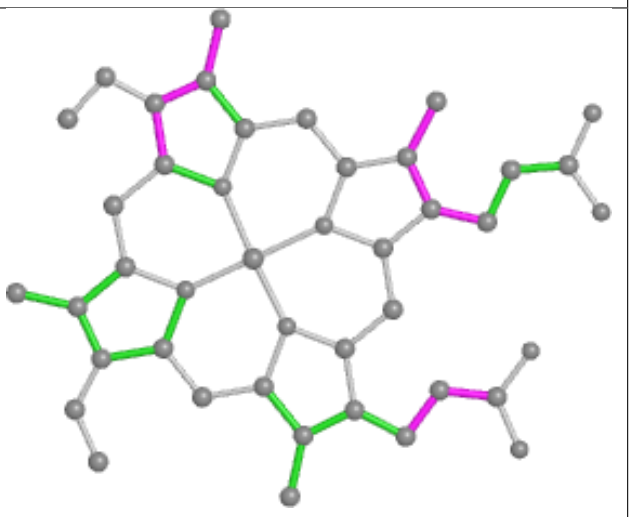


Rings

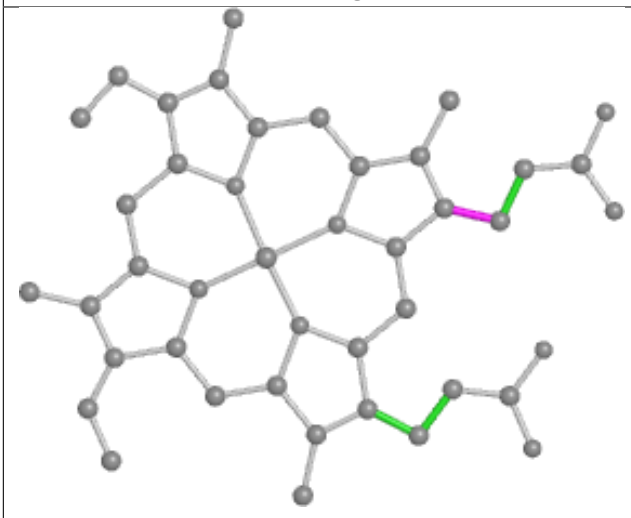
Ligand HEC C 611



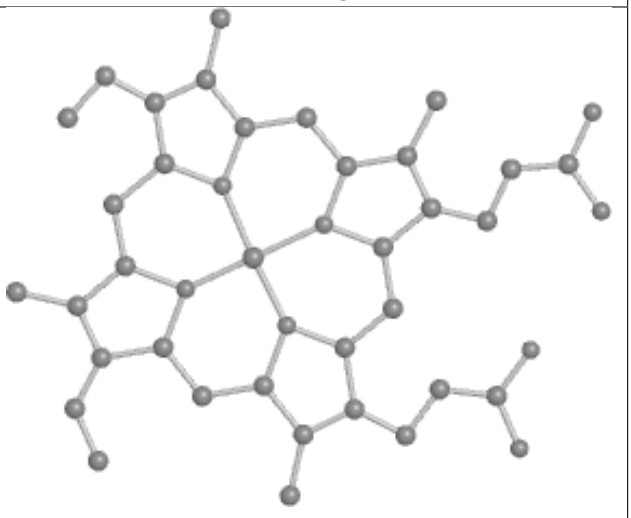
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	C	333/336 (99%)	-1.02	1 (0%) 94 96	7, 21, 46, 73	17 (5%)
2	L	273/273 (100%)	-1.15	0 100 100	6, 16, 36, 53	6 (2%)
3	M	323/323 (100%)	-1.09	0 100 100	4, 18, 41, 58	8 (2%)
4	H	250/258 (96%)	-0.95	2 (0%) 86 89	8, 23, 51, 78	17 (6%)
All	All	1179/1190 (99%)	-1.05	3 (0%) 94 96	4, 19, 44, 78	48 (4%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	46	PRO	3.6
4	H	54	PRO	3.1
1	C	333	ALA	2.9

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

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, 95^{th} 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
4	FME	H	1	10/11	0.98	0.06	21,32,41,45	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

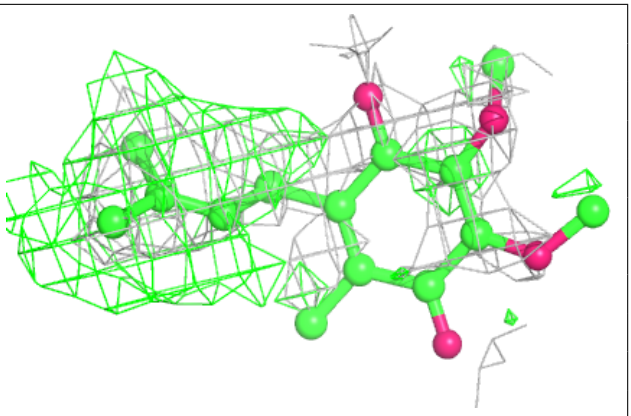
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

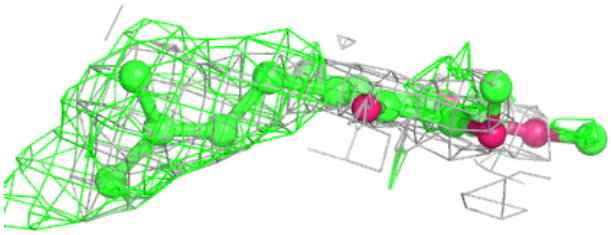
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	UQ1	L	614	18/18	0.84	0.58	19,26,29,30	18
13	LDA	H	616	16/16	0.91	0.17	0,27,42,46	6
10	SO4	H	622	5/5	0.92	0.22	73,74,85,89	0
10	SO4	H	623	5/5	0.94	0.13	58,59,62,64	5
12	NS1	M	613	40/40	0.96	0.11	0,25,39,49	14
7	BPB	M	605	65/65	0.96	0.10	0,21,62,71	7
13	LDA	M	615	16/16	0.97	0.08	17,25,36,37	0
10	SO4	M	621	5/5	0.97	0.20	68,78,81,82	0
6	BCB	L	604	66/66	0.98	0.06	3,10,27,35	0
11	MQ7	M	608	48/48	0.98	0.06	0,10,20,32	4
6	BCB	M	601	66/66	0.98	0.06	0,12,40,61	13
10	SO4	H	617	5/5	0.98	0.07	47,50,59,61	0
5	HEC	C	612	43/43	0.98	0.07	3,22,31,46	0
5	HEC	C	610	43/43	0.99	0.08	3,21,29,37	0
5	HEC	C	611	43/43	0.99	0.09	5,16,25,38	0
6	BCB	M	603	66/66	0.99	0.06	3,10,20,21	0
7	BPB	L	606	65/65	0.99	0.07	3,10,19,22	0
5	HEC	C	609	43/43	0.99	0.08	7,22,32,36	0
6	BCB	L	602	66/66	0.99	0.07	3,10,19,21	0
10	SO4	M	619	5/5	0.99	0.11	39,43,50,59	0
10	SO4	M	620	5/5	0.99	0.05	31,34,40,41	0
9	FE	M	607	1/1	1.00	0.04	19,19,19,19	0
10	SO4	M	618	5/5	1.00	0.07	22,23,35,37	0

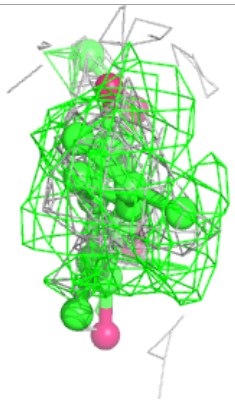
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UQ1 L 614:

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

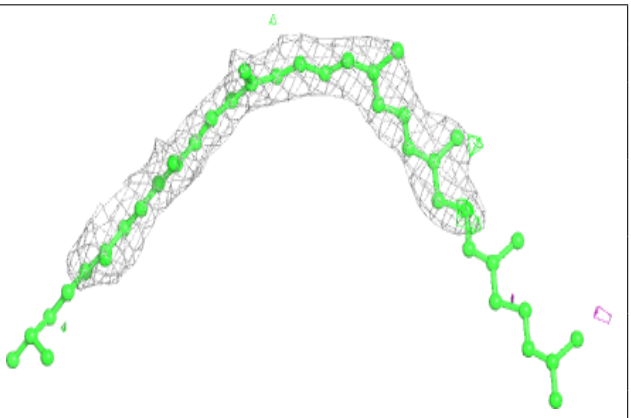


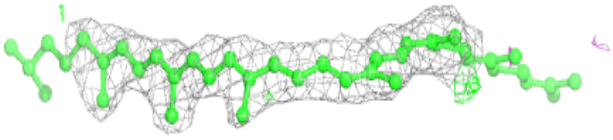


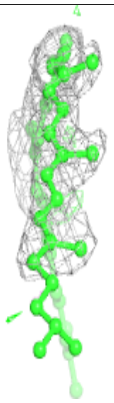


Electron density around NS1 M 613:

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

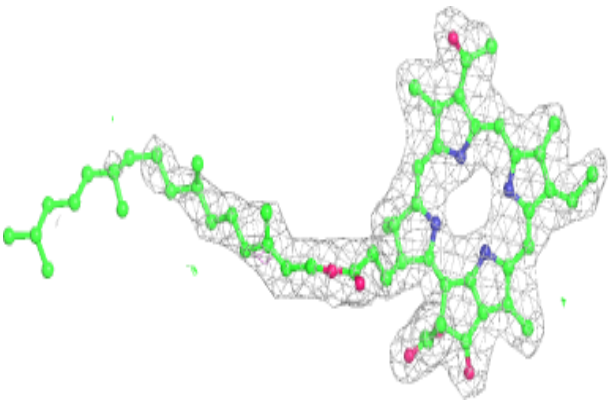


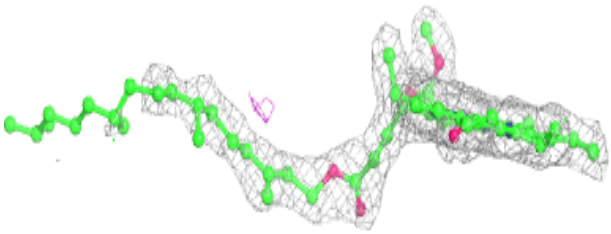


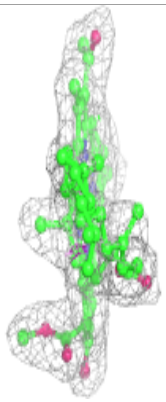


Electron density around BPB M 605:

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

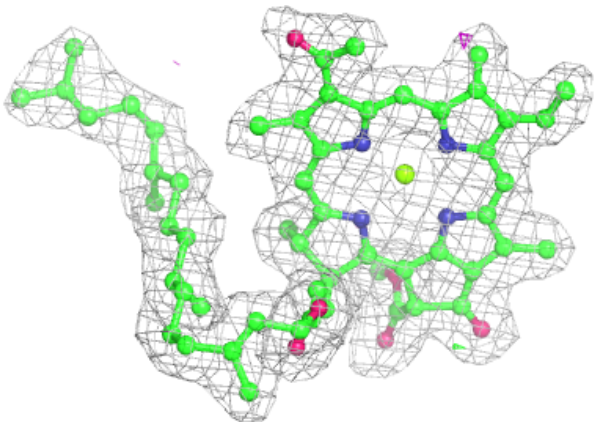


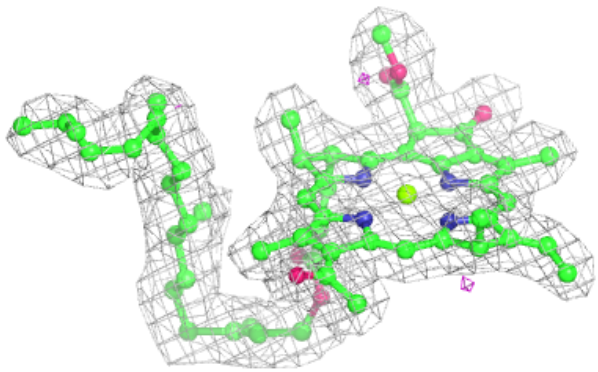


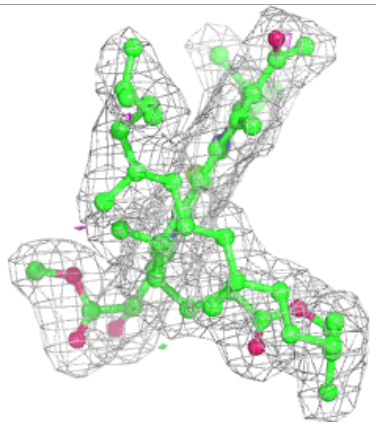


Electron density around BCB L 604:

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

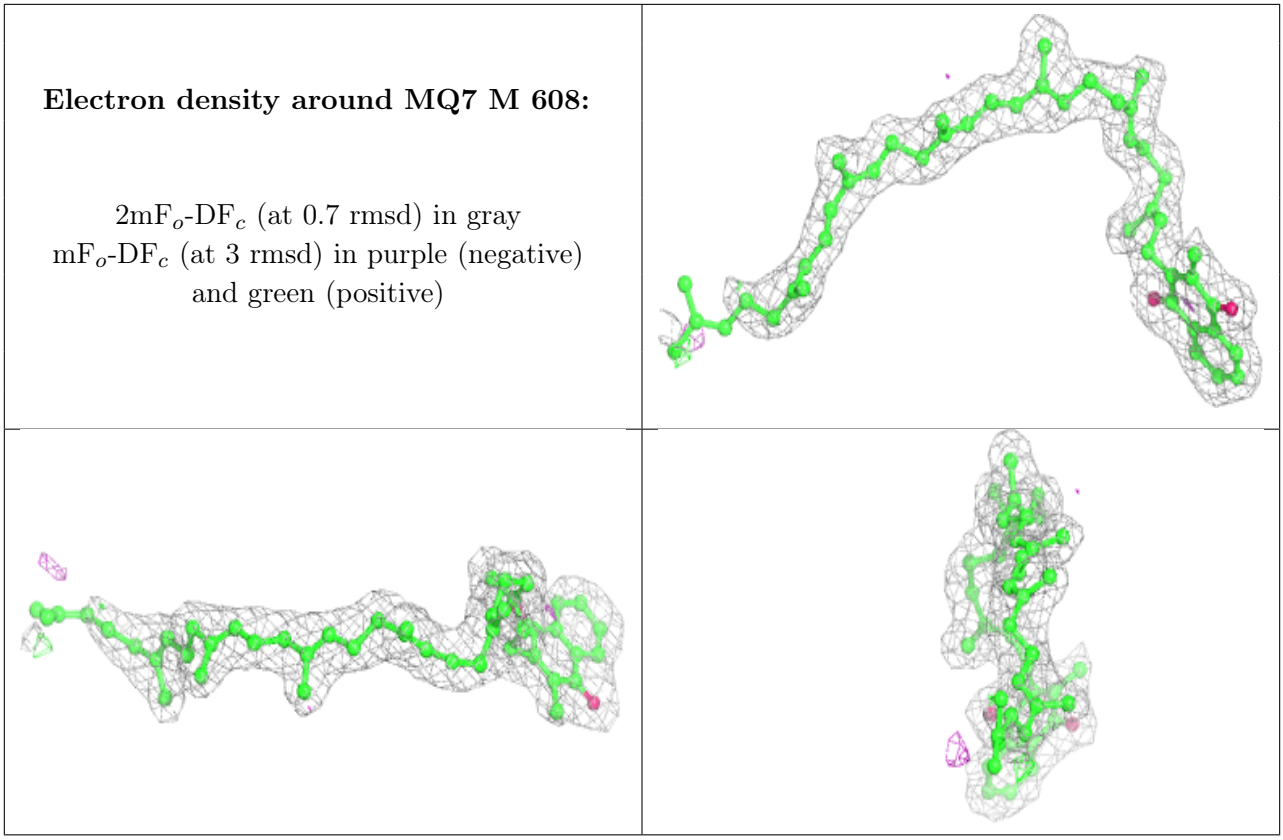






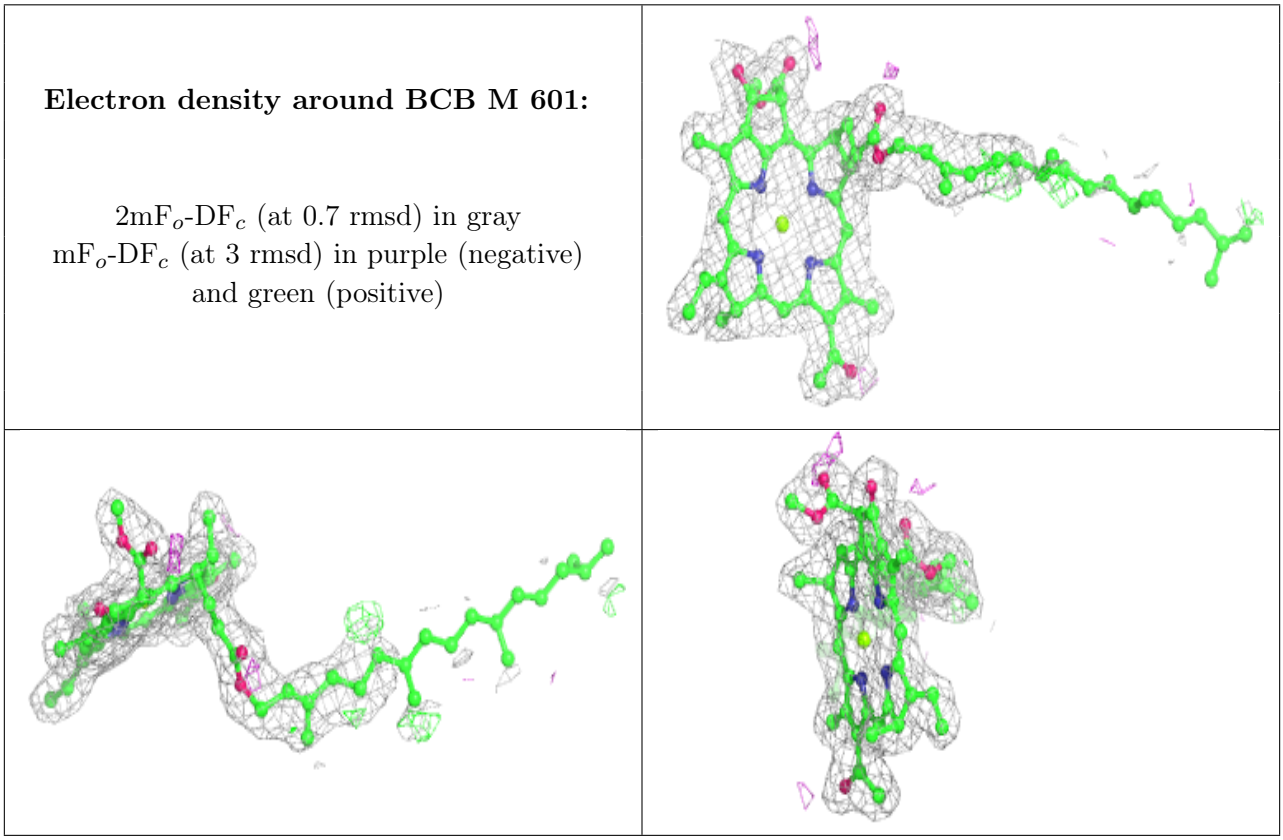
Electron density around MQ7 M 608:

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



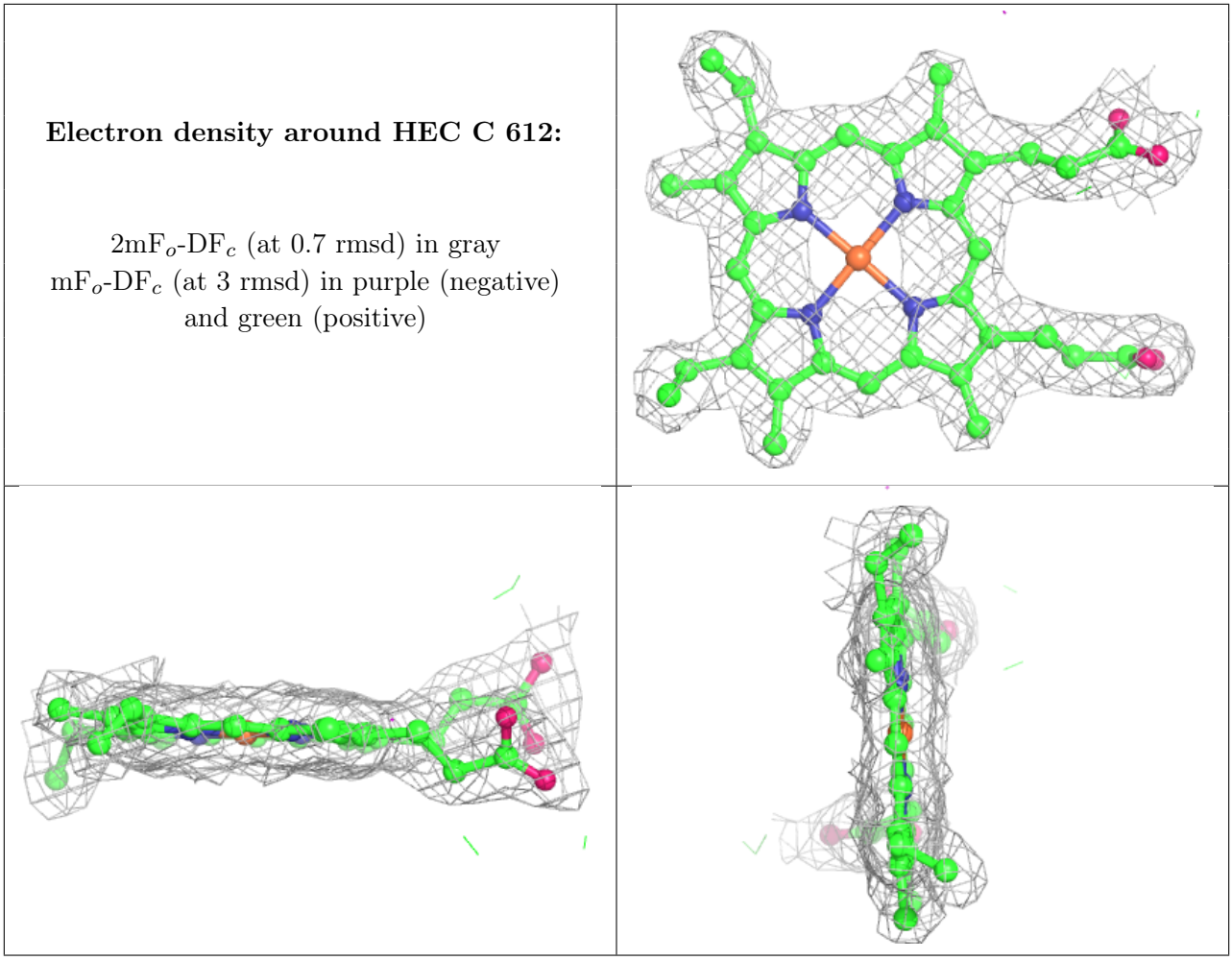
Electron density around BCB M 601:

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



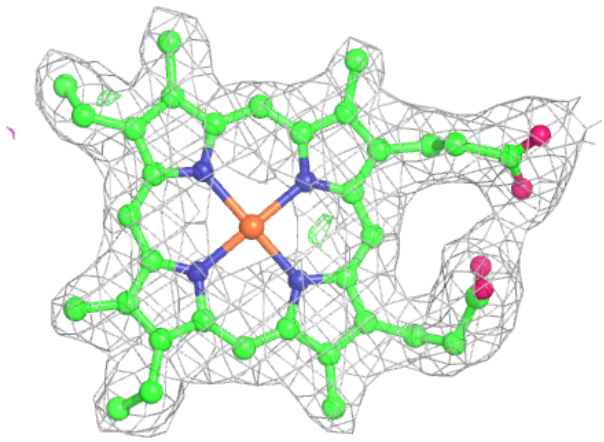
Electron density around HEC C 612:

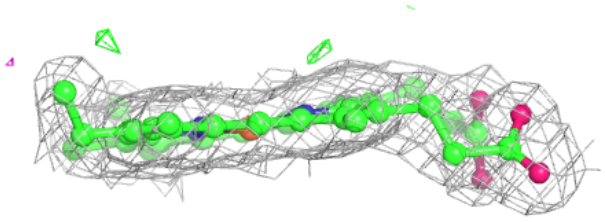
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

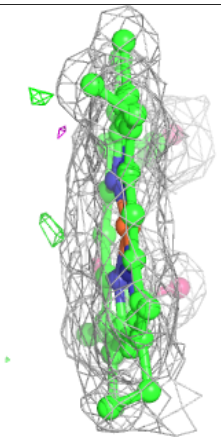


Electron density around HEC C 610:

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

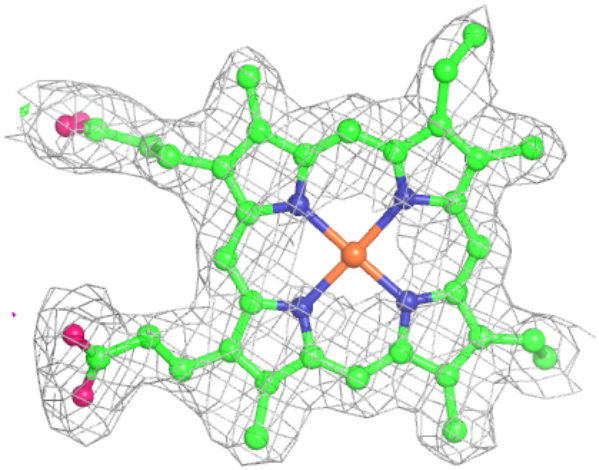


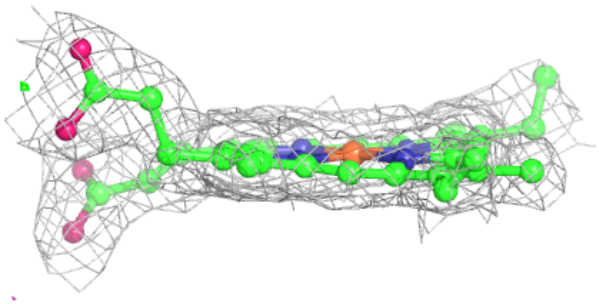




Electron density around HEC C 611:

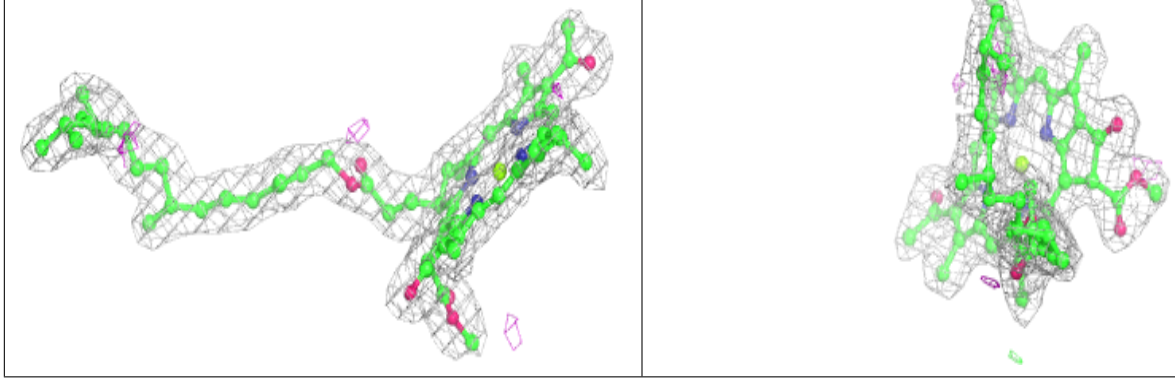
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





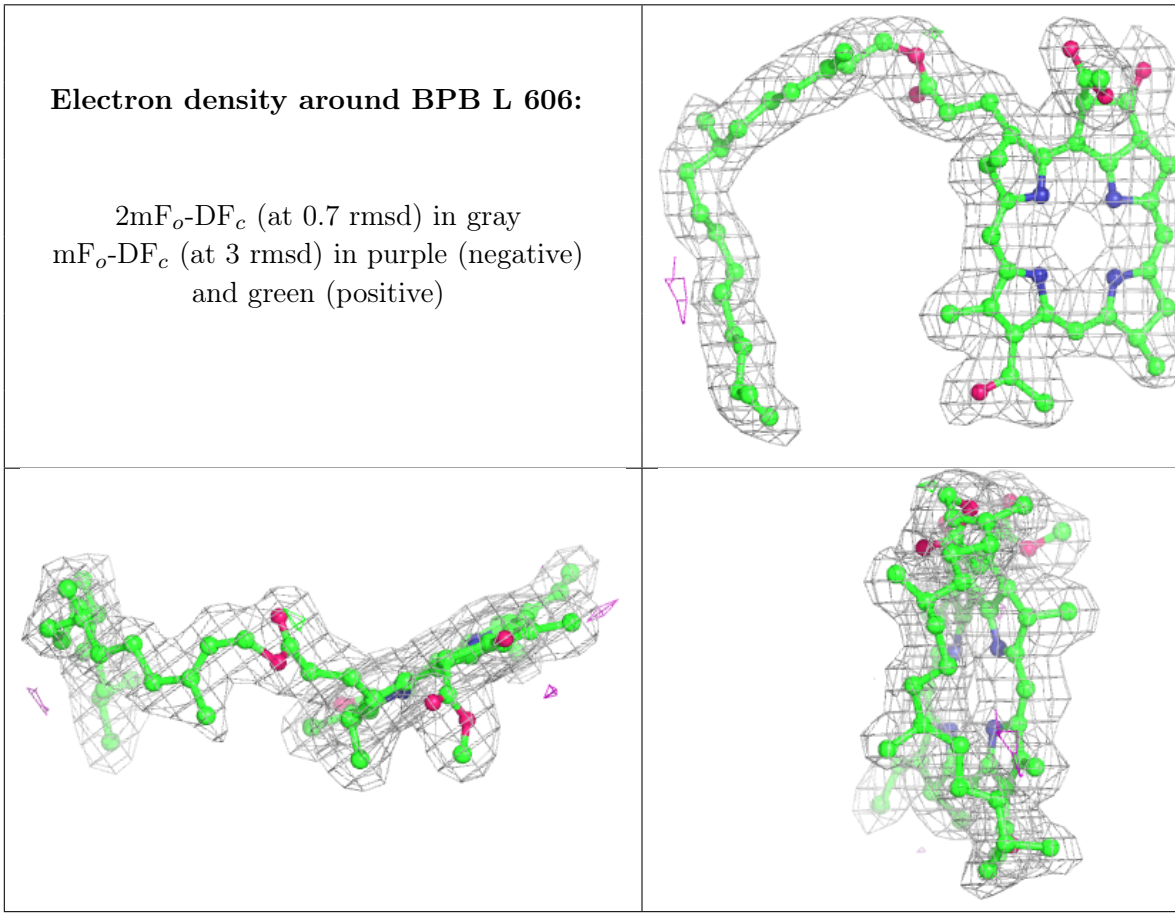
Electron density around BCB M 603:

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



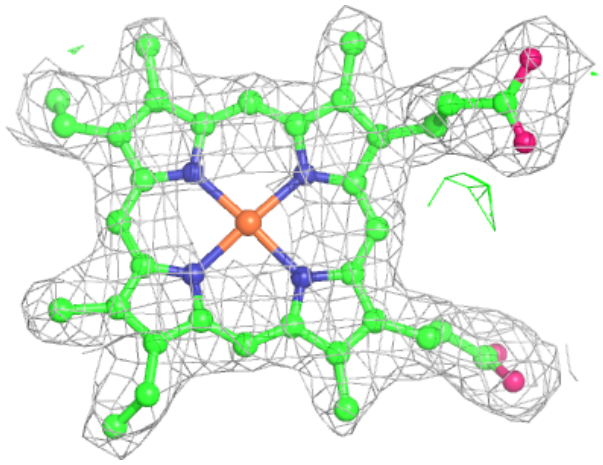
Electron density around BPB L 606:

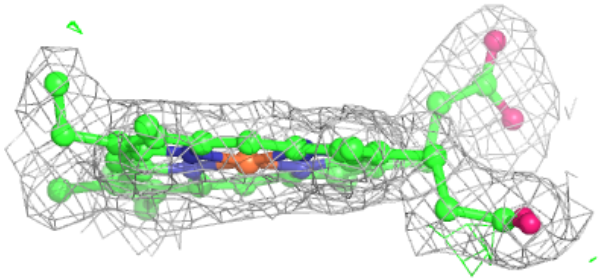
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

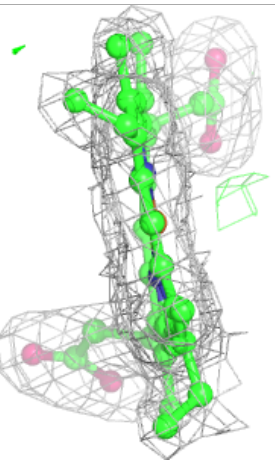


Electron density around HEC C 609:

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

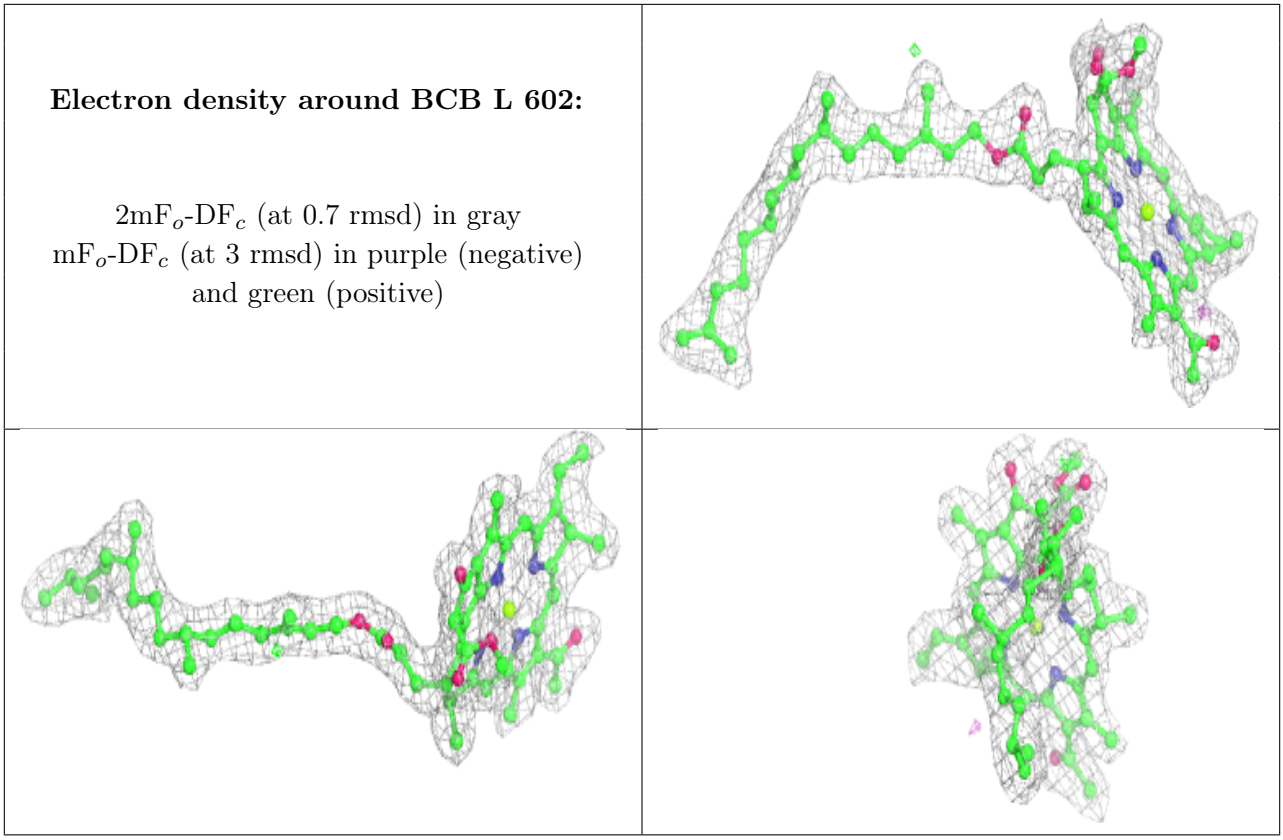






Electron density around BCB L 602:

$2mF_o$-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.