Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 09:06 AM EDT

PDB ID	:	1PRC / pdb_00001prc
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 (i) 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:

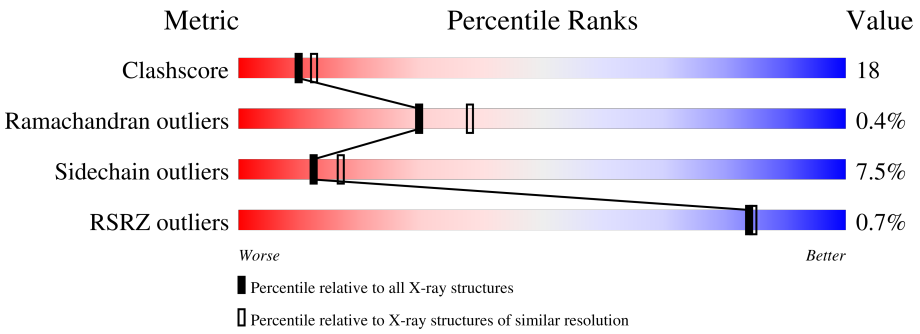
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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	51% 40% 7% ••
2	L	273	63% 32% 5% •
3	M	323	58% 34% 8%
4	H	258	3% 59% 32% 7% •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	HEC	C	609	X	-	-	-
5	HEC	C	610	X	-	-	-
5	HEC	C	611	X	-	-	-
5	HEC	C	612	X	-	-	-
6	BCB	L	602	X	-	-	-
6	BCB	L	604	X	-	-	-
6	BCB	M	601	X	-	-	-
6	BCB	M	603	X	-	-	-
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
			Total	C	N	O	S			
1	C	333	2603	1640	467	478	18	54	0	1

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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

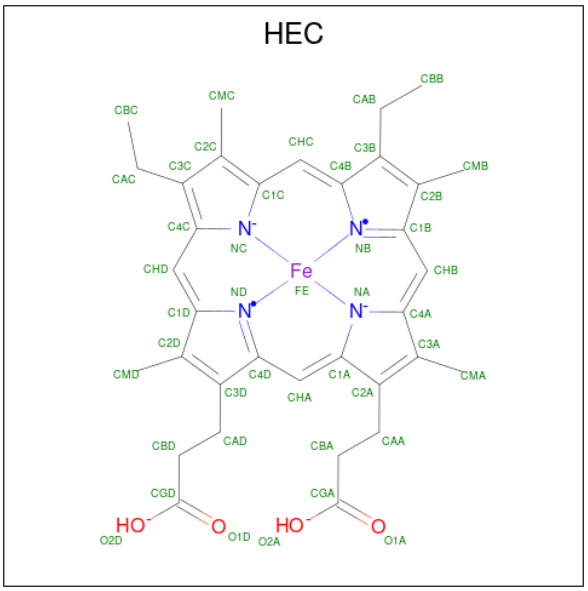
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

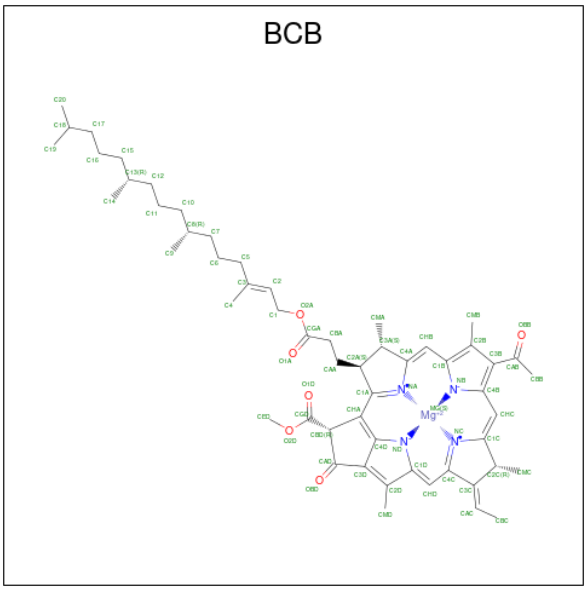
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	258	2018	1292	344	380	2	106	0	0

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



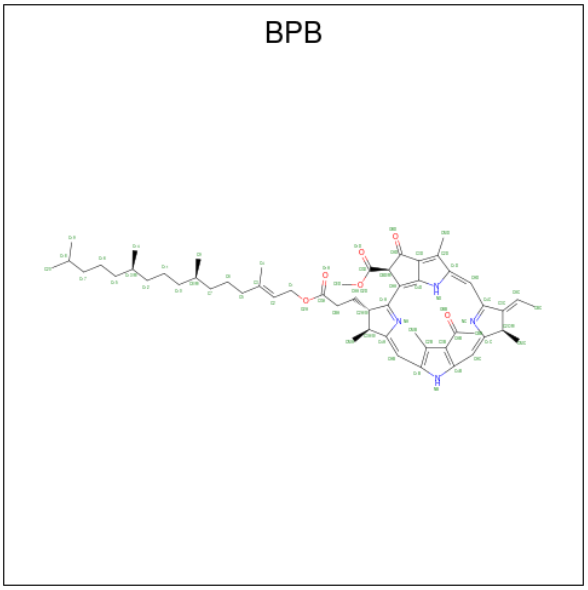
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0

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



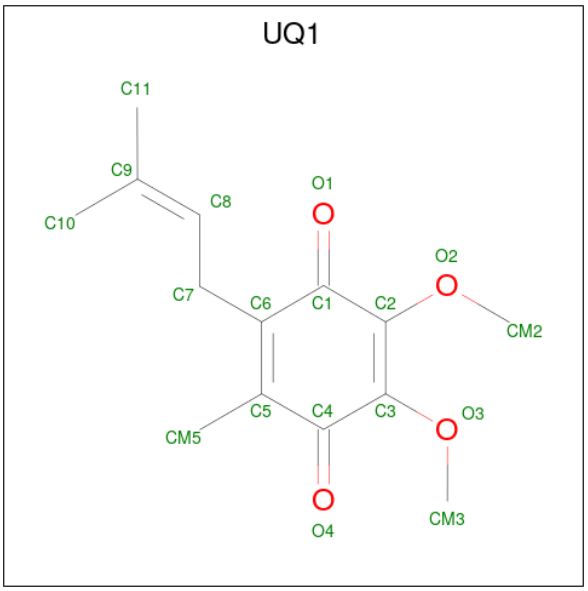
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
6	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
6	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
6	M	1	66	55	1	4	6	13	0
			Total	C	Mg	N	O		
6	M	1	66	55	1	4	6	0	0

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



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

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

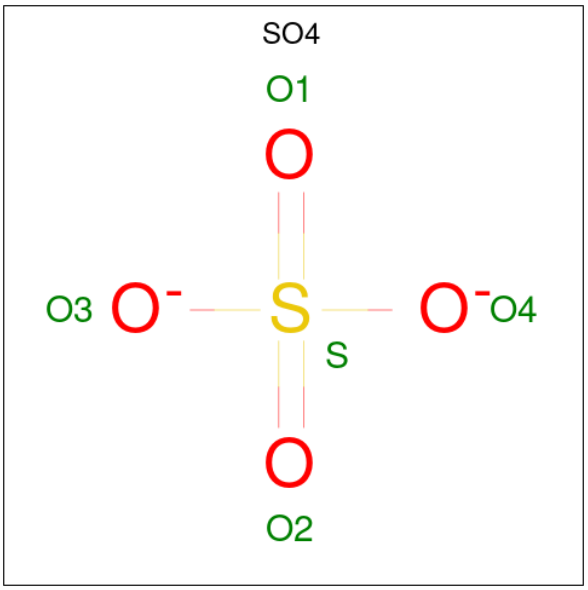


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	L	1	18	14	4	0	0

- Molecule 9 is FE (III) ION (CCD ID: FE) (formula: Fe).

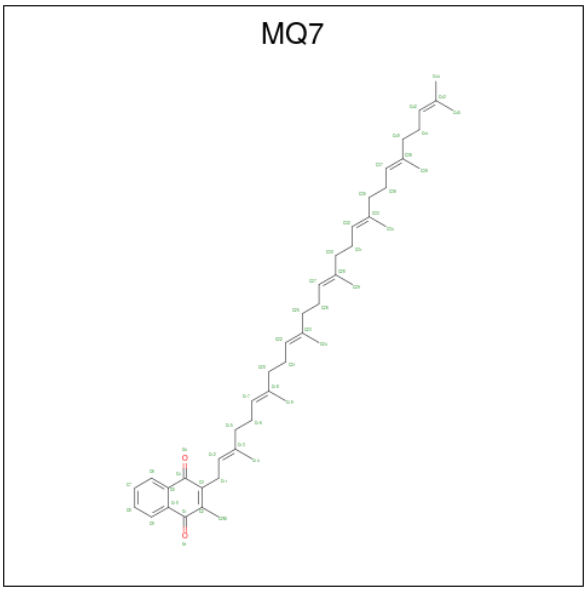
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
9	M	1	1	1	0	0

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



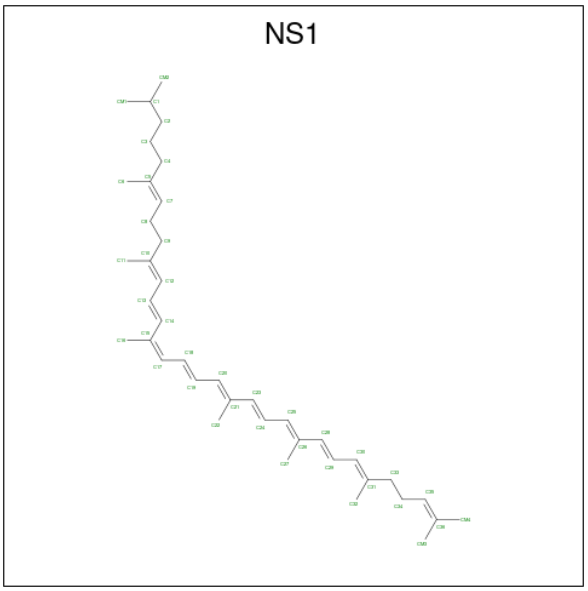
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
10	M	1	5	4	1	0	0
			Total	O	S		
10	M	1	5	4	1	0	0
			Total	O	S		
10	M	1	5	4	1	0	0
			Total	O	S		
10	M	1	5	4	1	0	0
			Total	O	S		
10	H	1	5	4	1	0	0
			Total	O	S		
10	H	1	5	4	1	0	0
			Total	O	S		
10	H	1	5	4	1	0	0

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



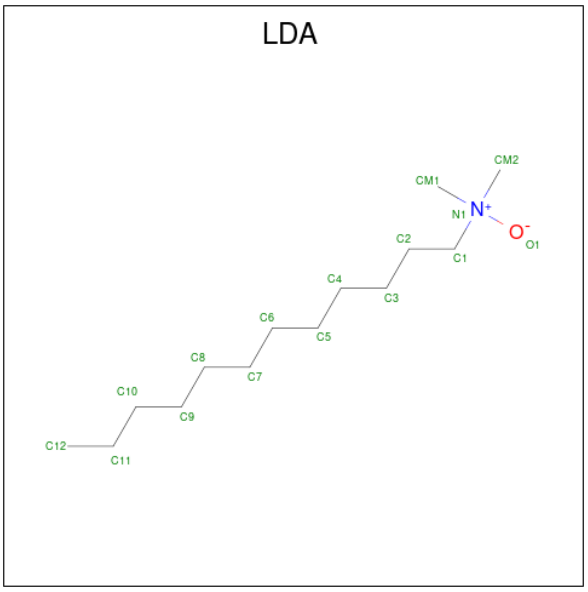
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	M	1	48	46	2	4	0

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



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

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



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

- Molecule 14 is water.

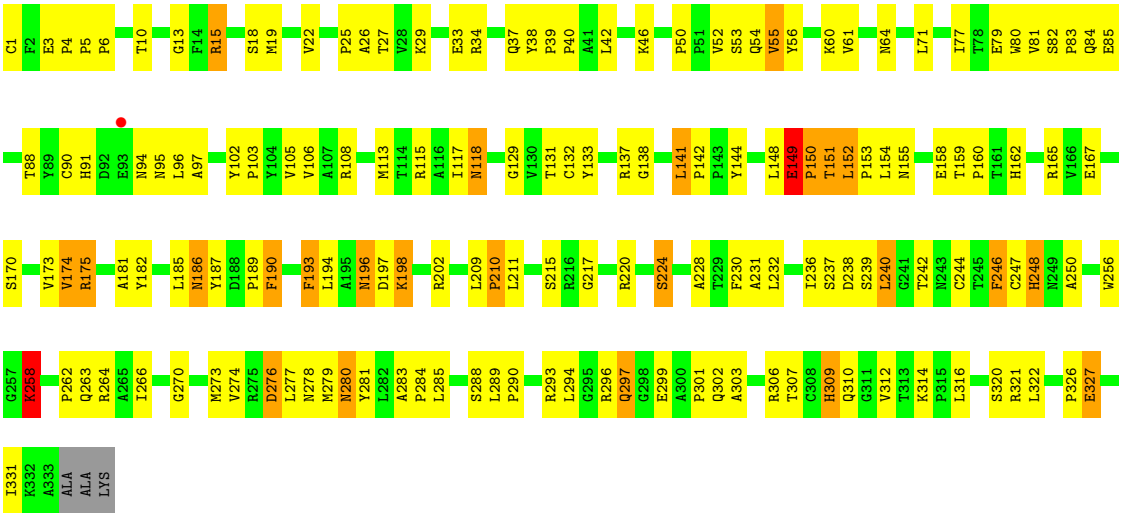
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	C	66	66	66	0	0
			Total	O		
14	L	39	39	39	0	0
			Total	O		
14	M	55	55	55	0	0
			Total	O		
14	H	41	41	41	0	0

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.

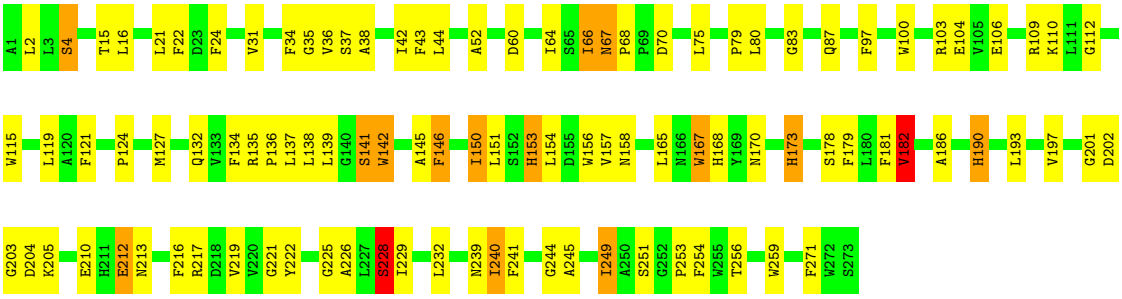
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain C: 51% 40% 7% ••



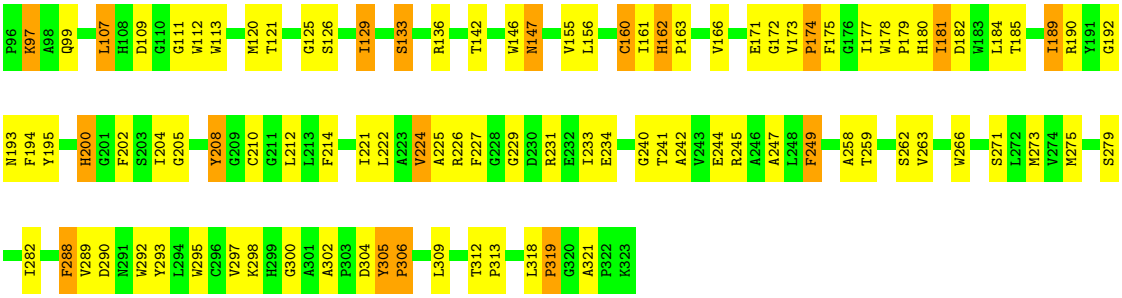
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Chain L: 63% 32% 5% •



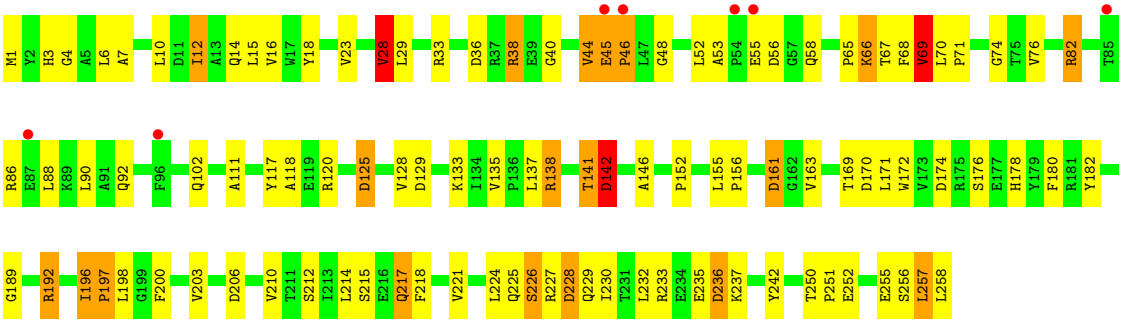
• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain M: 58% 34% 8%



• 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) 75.3 (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 , 60.8	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, UQ1, MQ7, BCB, LDA, NS1, BPB, FME, SO4, HEC

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	1.28	3/2670 (0.1%)	1.91	67/3639 (1.8%)
2	L	1.32	2/2259 (0.1%)	1.77	36/3084 (1.2%)
3	M	1.28	2/2659 (0.1%)	1.82	65/3637 (1.8%)
4	H	1.32	3/2055 (0.1%)	1.97	59/2807 (2.1%)
All	All	1.30	10/9643 (0.1%)	1.87	227/13167 (1.7%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	167	TRP	N-CA	-6.09	1.38	1.46
3	M	208	TYR	N-CA	-5.79	1.39	1.46
3	M	180	HIS	CE1-NE2	5.55	1.38	1.32
4	H	118	ALA	N-CA	-5.50	1.39	1.45
4	H	255	GLU	CD-OE2	5.40	1.35	1.25
1	C	117	ILE	CA-CB	-5.12	1.48	1.54
4	H	174	ASP	CG-OD2	5.11	1.35	1.25
1	C	174	VAL	C-N	-5.09	1.27	1.34
2	L	104	GLU	C-N	-5.00	1.27	1.33
1	C	196	ASN	CA-C	-5.00	1.46	1.52

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	129	ASP	CA-CB-CG	-11.46	101.14	112.60
1	C	81	VAL	N-CA-C	10.65	120.44	110.74
3	M	161	ILE	N-CA-C	10.20	121.07	110.36
2	L	254	PHE	CA-CB-CG	-9.98	103.82	113.80
3	M	290	ASP	CA-CB-CG	9.95	122.55	112.60
3	M	160	CYS	CB-CA-C	-9.21	96.28	110.83
4	H	38	ARG	NE-CZ-NH2	-9.03	111.08	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	331	ILE	N-CA-C	8.94	122.82	108.97
1	C	61	VAL	N-CA-C	8.82	119.66	111.45
4	H	68	PHE	CA-C-N	-8.75	111.44	122.37
4	H	68	PHE	C-N-CA	-8.75	111.44	122.37
3	M	200	HIS	N-CA-C	-8.68	101.76	111.14
1	C	55	VAL	N-CA-C	8.40	118.96	110.23
2	L	190	HIS	CA-CB-CG	-8.26	105.54	113.80
1	C	40	PRO	CB-CA-C	-8.01	100.79	111.12
2	L	182	VAL	CB-CA-C	-8.00	101.34	112.14
3	M	321	ALA	N-CA-C	-7.92	99.37	110.31
1	C	152	LEU	CB-CA-C	7.80	120.52	109.92
3	M	85	PHE	CB-CA-C	7.73	123.18	110.81
1	C	152	LEU	N-CA-CB	-7.71	100.06	110.77
1	C	162	HIS	CA-C-N	7.65	131.31	120.53
1	C	162	HIS	C-N-CA	7.65	131.31	120.53
1	C	198	LYS	N-CA-C	7.62	119.38	111.14
1	C	194	LEU	N-CA-C	7.55	122.78	113.50
1	C	224	SER	CB-CA-C	-7.52	98.78	110.81
1	C	196	ASN	CB-CA-C	-7.42	96.29	110.24
4	H	174	ASP	CA-CB-CG	7.32	119.92	112.60
2	L	271	PHE	CA-CB-CG	7.28	121.08	113.80
1	C	246	PHE	N-CA-C	-7.22	103.94	112.89
4	H	7	ALA	N-CA-C	-7.22	98.56	109.96
1	C	3	GLU	N-CA-C	-7.17	101.07	110.39
4	H	206	ASP	CA-CB-CG	7.14	119.74	112.60
1	C	196	ASN	CA-CB-CG	-7.05	105.55	112.60
4	H	14	GLN	CB-CA-C	-6.93	99.95	110.90
1	C	193	PHE	N-CA-C	6.85	121.68	113.12
4	H	228	ASP	CA-CB-CG	6.81	119.41	112.60
4	H	197	PRO	N-CA-CB	6.78	109.34	103.31
1	C	280	ASN	CB-CA-C	-6.68	97.99	110.01
3	M	224	VAL	CA-C-O	6.68	126.52	119.91
1	C	237	SER	CB-CA-C	-6.63	100.43	110.90
2	L	34	PHE	CA-CB-CG	-6.58	107.22	113.80
1	C	279	MET	N-CA-C	6.58	118.11	111.07
4	H	163	VAL	N-CA-CB	-6.55	101.52	110.56
1	C	46	LYS	N-CA-CB	6.54	120.83	110.23
4	H	48	GLY	N-CA-C	-6.54	101.03	112.55
3	M	295	TRP	N-CA-C	-6.49	104.05	112.23
1	C	197	ASP	CA-C-N	6.47	129.24	120.44
1	C	197	ASP	C-N-CA	6.47	129.24	120.44
4	H	65	PRO	CA-C-N	6.41	132.02	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	65	PRO	C-N-CA	6.41	132.02	122.99
3	M	86	ARG	N-CA-C	6.38	117.92	110.97
4	H	251	PRO	N-CA-CB	6.37	109.85	103.48
2	L	112	GLY	CA-C-N	-6.36	115.30	122.48
2	L	112	GLY	C-N-CA	-6.36	115.30	122.48
1	C	248	HIS	CA-CB-CG	6.34	120.14	113.80
2	L	79	PRO	N-CA-CB	6.32	108.63	103.32
4	H	163	VAL	N-CA-C	6.30	118.45	108.87
1	C	185	LEU	N-CA-CB	6.30	119.33	109.69
3	M	214	PHE	CA-CB-CG	-6.30	107.50	113.80
2	L	44	LEU	N-CA-CB	6.27	119.28	109.94
1	C	155	ASN	CA-CB-CG	-6.26	106.34	112.60
4	H	128	VAL	CA-C-N	6.25	129.81	120.31
4	H	128	VAL	C-N-CA	6.25	129.81	120.31
4	H	203	VAL	CB-CA-C	-6.25	104.54	111.35
4	H	226	SER	N-CA-C	-6.22	100.43	110.32
4	H	74	GLY	N-CA-C	-6.21	103.75	111.70
1	C	289	LEU	N-CA-C	6.21	118.46	110.39
4	H	67	THR	CA-C-N	-6.14	114.60	122.77
4	H	67	THR	C-N-CA	-6.14	114.60	122.77
2	L	67	ASN	N-CA-C	6.13	119.17	110.40
2	L	66	ILE	CB-CA-C	-6.13	102.67	111.19
3	M	305	TYR	CA-C-N	6.12	126.08	120.03
3	M	305	TYR	C-N-CA	6.12	126.08	120.03
2	L	219	VAL	N-CA-C	6.12	116.31	110.74
1	C	25	PRO	N-CA-CB	6.07	110.00	103.33
3	M	99	GLN	CA-C-N	-6.03	113.15	122.49
3	M	99	GLN	C-N-CA	-6.03	113.15	122.49
2	L	137	LEU	N-CA-C	-6.02	104.63	111.07
1	C	40	PRO	N-CA-CB	6.01	109.04	103.39
2	L	153	HIS	CA-CB-CG	6.01	119.81	113.80
1	C	150	PRO	N-CA-CB	5.99	108.63	103.36
2	L	134	PHE	N-CA-C	5.99	117.48	111.07
3	M	233	ILE	N-CA-C	5.98	116.45	110.23
2	L	240	ILE	N-CA-C	-5.98	104.52	110.62
4	H	192	ARG	N-CA-C	5.96	117.58	110.19
1	C	197	ASP	N-CA-C	-5.96	105.32	112.59
2	L	35	GLY	N-CA-C	-5.95	104.94	113.86
3	M	181	ILE	CB-CA-C	5.93	119.80	112.04
3	M	189	ILE	CA-C-N	5.91	128.79	120.28
3	M	189	ILE	C-N-CA	5.91	128.79	120.28
3	M	221	ILE	N-CA-C	5.89	116.63	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	182	VAL	N-CA-CB	5.89	118.55	110.54
3	M	182	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	60	LYS	N-CA-C	5.85	118.88	111.69
1	C	258	LYS	N-CA-CB	5.84	119.38	110.44
3	M	67	LEU	CA-C-N	-5.84	113.07	120.60
3	M	67	LEU	C-N-CA	-5.84	113.07	120.60
2	L	142	TRP	N-CA-C	-5.82	106.14	113.18
3	M	88	PHE	CA-CB-CG	-5.80	108.00	113.80
1	C	149	GLU	N-CA-CB	5.80	121.62	111.19
3	M	304	ASP	CA-CB-CG	5.77	118.37	112.60
3	M	300	GLY	N-CA-C	5.76	123.30	115.30
3	M	85	PHE	CA-CB-CG	5.75	119.55	113.80
4	H	210	VAL	CB-CA-C	-5.74	103.90	110.73
2	L	212	GLU	CB-CA-C	-5.72	101.29	110.79
1	C	84	GLN	CA-CB-CG	-5.72	102.67	114.10
4	H	146	ALA	N-CA-C	5.71	117.67	110.24
1	C	276	ASP	CB-CA-C	-5.71	102.17	110.96
3	M	180	HIS	CA-CB-CG	5.69	119.49	113.80
3	M	94	TYR	N-CA-C	5.66	118.88	110.39
4	H	256	SER	CB-CA-C	5.65	119.10	109.72
3	M	271	SER	CB-CA-C	-5.64	101.96	110.92
4	H	171	LEU	CA-C-N	-5.63	115.16	123.05
4	H	171	LEU	C-N-CA	-5.63	115.16	123.05
4	H	28	VAL	N-CA-C	5.63	115.82	110.42
4	H	225	GLN	CB-CA-C	5.63	118.91	110.08
1	C	193	PHE	CA-CB-CG	-5.62	108.18	113.80
4	H	92	GLN	N-CA-CB	5.62	118.66	109.95
4	H	141	THR	N-CA-CB	-5.62	100.77	110.32
2	L	225	GLY	CA-C-O	5.62	126.60	121.77
3	M	210	CYS	CA-C-N	5.61	126.17	119.94
3	M	210	CYS	C-N-CA	5.61	126.17	119.94
4	H	174	ASP	N-CA-C	-5.58	98.67	108.20
3	M	306	PRO	CB-CA-C	-5.57	103.66	110.95
4	H	125	ASP	CA-CB-CG	5.56	118.16	112.60
3	M	81	PRO	CB-CA-C	-5.55	103.46	112.62
2	L	146	PHE	CB-CA-C	5.54	116.84	108.86
3	M	309	LEU	N-CA-CB	5.54	117.43	109.78
4	H	66	LYS	N-CA-CB	-5.53	101.39	110.68
2	L	158	ASN	CB-CA-C	-5.53	102.45	110.96
1	C	4	PRO	N-CA-C	5.52	117.44	110.70
3	M	147	ASN	CA-C-O	5.52	126.37	120.24
4	H	224	LEU	CA-C-N	-5.52	113.40	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	224	LEU	C-N-CA	-5.52	113.40	122.79
1	C	54	GLN	CA-C-N	5.52	128.00	120.77
1	C	54	GLN	C-N-CA	5.52	128.00	120.77
1	C	159	THR	CB-CA-C	5.49	117.26	109.08
3	M	66	ILE	N-CA-C	5.49	115.62	110.30
4	H	255	GLU	N-CA-C	5.49	117.61	110.53
4	H	178	HIS	CA-CB-CG	5.48	119.28	113.80
3	M	177	ILE	N-CA-C	5.48	115.57	110.42
4	H	237	LYS	CA-C-N	5.47	127.96	120.46
4	H	237	LYS	C-N-CA	5.47	127.96	120.46
4	H	135	VAL	N-CA-CB	-5.47	105.85	111.87
3	M	174	PRO	CA-C-O	-5.46	114.61	122.31
2	L	150	ILE	CA-CB-CG1	-5.46	101.12	110.40
2	L	228	SER	N-CA-C	5.46	117.99	111.71
3	M	172	GLY	O-C-N	5.45	128.21	122.59
2	L	186	ALA	CB-CA-C	-5.45	101.75	110.79
1	C	10	THR	CA-C-O	-5.45	115.07	121.44
2	L	70	ASP	CA-CB-CG	5.44	118.04	112.60
3	M	298	LYS	N-CA-CB	5.44	118.22	110.06
4	H	138	ARG	CB-CA-C	-5.44	99.60	110.42
3	M	97	LYS	N-CA-CB	5.43	118.19	110.16
1	C	170	SER	N-CA-C	5.43	119.07	112.23
3	M	109	ASP	CB-CA-C	-5.42	104.32	111.74
2	L	204	ASP	N-CA-CB	5.39	118.65	110.45
4	H	46	PRO	N-CA-C	5.38	123.54	112.47
1	C	77	ILE	CB-CA-C	-5.37	105.00	112.04
2	L	104	GLU	CA-C-O	5.37	126.15	119.97
4	H	217	GLN	N-CA-CB	5.36	119.11	110.42
3	M	202	PHE	CA-CB-CG	-5.32	108.48	113.80
4	H	52	LEU	N-CA-C	-5.32	106.47	113.12
1	C	141	LEU	CB-CA-C	-5.32	104.91	110.17
3	M	162	HIS	N-CA-CB	5.32	118.22	110.30
1	C	230	PHE	CA-C-N	5.31	127.35	120.44
1	C	230	PHE	C-N-CA	5.31	127.35	120.44
3	M	78	HIS	CA-C-N	5.31	129.89	122.08
3	M	78	HIS	C-N-CA	5.31	129.89	122.08
3	M	60	ALA	CA-C-O	-5.31	115.42	121.00
1	C	33	GLU	CB-CA-C	-5.31	98.89	109.99
1	C	327	GLU	CA-CB-CG	-5.30	103.49	114.10
3	M	184	LEU	O-C-N	5.30	127.74	122.12
1	C	190	PHE	CA-CB-CG	-5.29	108.51	113.80
3	M	29	VAL	N-CA-C	5.29	117.17	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	34	PHE	CA-C-N	-5.26	113.71	120.34
2	L	34	PHE	C-N-CA	-5.26	113.71	120.34
3	M	247	ALA	N-CA-C	5.26	117.09	111.36
3	M	302	ALA	N-CA-C	5.26	116.32	109.64
1	C	321	ARG	N-CA-C	-5.26	105.19	113.02
3	M	288	PHE	CA-C-N	-5.25	115.69	122.99
3	M	288	PHE	C-N-CA	-5.25	115.69	122.99
1	C	309	HIS	N-CA-CB	5.25	117.84	110.12
4	H	189	GLY	O-C-N	5.24	126.75	122.51
1	C	160	PRO	CB-CA-C	-5.23	104.13	110.98
4	H	18	TYR	CB-CA-C	-5.23	100.63	110.67
1	C	280	ASN	N-CA-C	5.22	119.63	113.16
1	C	91	HIS	N-CA-C	5.22	118.51	110.42
3	M	273	MET	O-C-N	5.19	128.66	122.27
2	L	43	PHE	CA-CB-CG	-5.18	108.61	113.80
4	H	88	LEU	CB-CA-C	-5.18	101.69	110.19
1	C	42	LEU	N-CA-CB	5.18	117.63	110.17
3	M	319	PRO	CB-CA-C	-5.18	105.91	111.56
4	H	69	VAL	N-CA-CB	5.17	116.90	111.00
1	C	118	ASN	CA-CB-CG	-5.16	107.44	112.60
2	L	254	PHE	N-CA-C	5.15	119.72	113.38
3	M	245	ARG	NE-CZ-NH2	-5.14	114.57	119.20
3	M	208	TYR	N-CA-C	-5.14	105.76	111.36
1	C	326	PRO	N-CA-CB	5.13	108.64	103.25
3	M	263	VAL	CA-C-N	5.11	128.08	120.31
3	M	263	VAL	C-N-CA	5.11	128.08	120.31
4	H	18	TYR	CA-C-N	-5.11	113.03	120.29
4	H	18	TYR	C-N-CA	-5.11	113.03	120.29
3	M	107	LEU	CB-CA-C	-5.11	101.99	110.68
1	C	285	LEU	CA-C-N	-5.10	112.20	120.72
1	C	285	LEU	C-N-CA	-5.10	112.20	120.72
2	L	80	LEU	N-CA-C	5.09	117.23	111.02
1	C	175	ARG	O-C-N	5.08	128.16	122.22
2	L	173	HIS	CA-C-N	-5.07	113.48	120.28
2	L	173	HIS	C-N-CA	-5.07	113.48	120.28
4	H	203	VAL	N-CA-C	5.07	114.91	108.12
4	H	45	GLU	CA-C-N	5.07	126.17	119.84
4	H	45	GLU	C-N-CA	5.07	126.17	119.84
4	H	44	VAL	CA-C-N	5.06	134.15	121.80
4	H	44	VAL	C-N-CA	5.06	134.15	121.80
4	H	142	ASP	CA-CB-CG	5.06	117.66	112.60
3	M	60	ALA	N-CA-C	5.05	116.48	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	210	PRO	N-CA-CB	5.04	108.54	103.25
3	M	83	GLN	N-CA-C	-5.04	106.65	112.89
1	C	29	LYS	CA-C-N	-5.03	113.60	120.44
1	C	29	LYS	C-N-CA	-5.03	113.60	120.44
1	C	215	SER	CA-C-N	-5.01	114.94	122.81
1	C	215	SER	C-N-CA	-5.01	114.94	122.81
3	M	109	ASP	CA-C-N	-5.01	116.31	123.08
3	M	109	ASP	C-N-CA	-5.01	116.31	123.08
1	C	309	HIS	N-CA-C	5.01	116.74	111.28
3	M	95	PRO	N-CA-C	-5.00	104.59	110.70

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	92	0
2	L	2171	0	2098	82	0
3	M	2555	0	2452	88	0
4	H	2018	0	2020	58	0
5	C	172	0	122	19	0
6	L	132	0	144	22	0
6	M	132	0	144	21	0
7	L	65	0	74	8	0
7	M	65	0	74	11	0
8	L	18	0	18	8	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
14	H	41	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	L	39	0	0	3	0
14	M	55	0	0	3	0
All	All	10288	0	9910	340	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (340) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:120:MET:HE2	6:M:603:BCB:H172	1.40	1.02
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
3:M:70:LEU:HD23	3:M:73:MET:HE3	1.56	0.87
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
3:M:69:ILE:HG22	3:M:73:MET:HE2	1.63	0.80
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
2:L:190:HIS:HA	8:L:614:UQ1:O4	1.81	0.79
2:L:202:ASP:CG	2:L:203:GLY:H	1.90	0.79
6:L:602:BCB:H61	6:L:604:BCB:CBB	2.13	0.79
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
3:M:120:MET:HE3	6:M:603:BCB:H193	1.66	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
3:M:70:LEU:CD2	3:M:73:MET:HE3	2.15	0.75
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
1:C:148:LEU:HG	1:C:299:GLU:HG3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:M:603:BCB:HMB3	6:M:603:BCB:CBB	2.23	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
6:M:603:BCB:HMB3	6:M:603:BCB:HBB3	1.76	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
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	0.64
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
1:C:13:GLY:HA3	1:C:19:MET:HE3	1.81	0.62
2:L:226:ALA:HA	8:L:614:UQ1:HM32	1.80	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
3:M:142:THR:HG1	3:M:146:TRP:CD1	2.19	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)
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
5:C:609:HEC:CMB	5:C:609:HEC:HBB3	2.32	0.60
2:L:202:ASP:CG	2:L:203:GLY:N	2.59	0.60
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
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
2:L:127:MET:HE2	6:L:602:BCB:O1A	2.04	0.57
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
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
6:L:604:BCB:HMB1	7:L:606:BPB:HMBA	1.88	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
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
4:H:137:LEU:HB2	4:H:170:ASP:OD2	2.06	0.55
2:L:179:PHE:HA	2:L:182:VAL:HG23	1.89	0.55
2:L:193:LEU:HD22	2:L:216:PHE:HE2	1.72	0.55
4:H:90:LEU:HD23	4:H:102:GLN:C	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:M:212:LEU:C	3:M:212:LEU:HD23	2.32	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
6:L:602:BCB:HBB3	6:L:602:BCB:HMB1	1.90	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:160:CYS:C	3:M:163:PRO:HD2	2.33	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: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
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
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
3:M:224:VAL:O	3:M:225:ALA:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:309:HIS:O	1:C:310:GLN:C	2.54	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
3:M:87:GLN:O	3:M:88:PHE:C	2.55	0.49
1:C:277:LEU:O	1:C:281:TYR:HB2	2.12	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
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
3:M:2:ASP:OD2	3:M:4:GLN:HB2	2.14	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
3:M:192:GLY:O	3:M:193:ASN:HB3	2.13	0.48
1:C:186:ASN:C	1:C:187:TYR:CD1	2.91	0.47
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
2:L:216:PHE:CE2	8:L:614:UQ1:HM51	2.48	0.47
3:M:69:ILE:CG2	3:M:73:MET:HE2	2.39	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
2:L:153:HIS:CE1	2:L:154:LEU:HD21	2.50	0.47
3:M:67:LEU:O	3:M:68:ILE:C	2.53	0.47
2:L:249:ILE:O	2:L:253:PRO:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:M:231:ARG:HH22	4:H:235:GLU:CD	2.24	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
1:C:151:THR:O	1:C:152:LEU:HB2	2.17	0.45
2:L:37:SER:O	2:L:38:ALA:C	2.57	0.45
1:C:242:THR:HA	14:C:675:HOH:O	2.17	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:90:CYS:SG	5:C:609:HEC:HMC1	2.57	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
6:L:604:BCB:HMB1	7:L:606:BPB:CMB	2.48	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
2:L:156:TRP:O	2:L:157:VAL:C	2.57	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:L:602:BCB:HMB1	6:L:602:BCB:CBB	2.48	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
3:M:249:PHE:CD2	3:M:249:PHE:C	2.95	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:102:TYR:O	1:C:103:PRO:C	2.58	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
3:M:241:THR:O	3:M:242:ALA:C	2.61	0.43
1:C:228:ALA:O	1:C:231:ALA:HB3	2.18	0.43
1:C:152:LEU:HA	1:C:153:PRO:C	2.44	0.43
4:H:16:VAL:HG12	4:H:16:VAL:O	2.19	0.43
2:L:210:GLU:CD	4:H:176:SER:HG	2.26	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
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
4:H:12:ILE:H	4:H:12:ILE:HG12	1.48	0.43
1:C:165:ARG:C	1:C:167:GLU:H	2.26	0.43
1:C:239:SER:C	1:C:240:LEU:HD23	2.44	0.43
6:L:602:BCB:C4A	6:M:603:BCB:HBB2	2.49	0.43
3:M:84:PHE:O	3:M:85:PHE:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:120:MET:HE3	3:M:175:PHE:HE1	1.84	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:21:GLY:C	3:M:23:TRP:N	2.77	0.42
1:C:95:ASN:C	1:C:97:ALA:H	2.26	0.42
1:C:174:VAL:HG23	3:M:87:GLN:CD	2.44	0.42
3:M:12:ALA:HB2	4:H:180:PHE:CE2	2.54	0.42
4:H:214:LEU:O	4:H:215:SER:C	2.61	0.42
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:113:MET:HE3	5:C:610:HEC:HBC2	2.02	0.42
1:C:71:LEU:HD23	1:C:71:LEU:HA	1.96	0.42
1:C:131:THR:O	1:C:132:CYS:C	2.62	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
5:C:611:HEC:HMA3	5:C:611:HEC:HAA1	1.66	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: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:190:ARG:HD2	3:M:190:ARG:C	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:26:ALA:O	1:C:27:THR:C	2.63	0.41
2:L:97:PHE:CZ	6:L:602:BCB:H112	2.55	0.41
1:C:224:SER:OG	3:M:97:LYS:O	2.39	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
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:275:MET:HE2	3:M:275:MET:HA	2.03	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%)	36 46
2	L	271/273 (99%)	252 (93%)	18 (7%)	1 (0%)	30 38
3	M	321/323 (99%)	300 (94%)	19 (6%)	2 (1%)	21 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	256/258 (99%)	239 (93%)	16 (6%)	1 (0%)	30	38
All	All	1179/1190 (99%)	1097 (93%)	77 (6%)	5 (0%)	30	38

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%)	258 (92%)	23 (8%)	10	14
2	L	218/218 (100%)	207 (95%)	11 (5%)	22	33
3	M	249/249 (100%)	231 (93%)	18 (7%)	13	18
4	H	212/212 (100%)	192 (91%)	20 (9%)	8	11
All	All	960/961 (100%)	888 (92%)	72 (8%)	12	17

All (72) 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	53	SER
1	C	64	ASN
1	C	94	ASN
1	C	105	VAL
1	C	115	ARG
1	C	149	GLU

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Mol	Chain	Res	Type
1	C	151	THR
1	C	154	LEU
1	C	158	GLU
1	C	186	ASN
1	C	209	LEU
1	C	211	LEU
1	C	240	LEU
1	C	258	LYS
1	C	288	SER
1	C	294	LEU
1	C	297	GLN
1	C	320	SER
1	C	322	LEU
1	C	327	GLU
2	L	2	LEU
2	L	4	SER
2	L	15	THR
2	L	36	VAL
2	L	119	LEU
2	L	141	SER
2	L	165	LEU
2	L	182	VAL
2	L	228	SER
2	L	232	LEU
2	L	249	ILE
3	M	10	ILE
3	M	11	GLN
3	M	16	HIS
3	M	33	PHE
3	M	56	ILE
3	M	66	ILE
3	M	70	LEU
3	M	77	VAL
3	M	126	SER
3	M	129	ILE
3	M	133	SER
3	M	147	ASN
3	M	171	GLU
3	M	181	ILE
3	M	194	PHE
3	M	249	PHE
3	M	279	SER

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Mol	Chain	Res	Type
3	M	306	PRO
4	H	10	LEU
4	H	12	ILE
4	H	23	VAL
4	H	28	VAL
4	H	44	VAL
4	H	56	ASP
4	H	69	VAL
4	H	82	ARG
4	H	141	THR
4	H	142	ASP
4	H	161	ASP
4	H	169	THR
4	H	182	TYR
4	H	196	ILE
4	H	198	LEU
4	H	212	SER
4	H	217	GLN
4	H	236	ASP
4	H	257	LEU
4	H	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	196	ASN
1	C	297	GLN
1	C	302	GLN
2	L	144	HIS
2	L	158	ASN
2	L	183	ASN
2	L	213	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 (i)

There are no RNA molecules in this entry.

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

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	0.96	1 (12%)	8,9,11	2.54	3 (37%)

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	-2.45	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	-4.10	114.72	125.32
4	H	1	FME	C-CA-N	3.01	115.31	109.50

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.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides 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	$\#\|Z\| > 2$
5	HEC	C	611	1	50,50,50	1.65	15 (30%)	68,82,82	1.67	10 (14%)
5	HEC	C	610	1	50,50,50	2.01	15 (30%)	68,82,82	1.43	12 (17%)
6	BCB	L	602	2	68,74,74	1.36	7 (10%)	77,115,115	1.84	24 (31%)
6	BCB	M	603	3	68,74,74	1.72	15 (22%)	77,115,115	1.91	19 (24%)
5	HEC	C	609	1	50,50,50	1.90	12 (24%)	68,82,82	1.52	16 (23%)
7	BPB	M	605	-	57,70,70	1.81	15 (26%)	55,101,101	1.68	8 (14%)
10	SO4	M	621	-	4,4,4	1.06	0	6,6,6	0.20	0
10	SO4	H	617	-	4,4,4	0.94	0	6,6,6	0.18	0
10	SO4	M	619	-	4,4,4	0.87	0	6,6,6	0.21	0
13	LDA	M	615	-	13,15,15	2.61	2 (15%)	14,17,17	1.77	5 (35%)
10	SO4	M	620	-	4,4,4	0.71	0	6,6,6	0.17	0
8	UQ1	L	614	-	18,18,18	0.80	1 (5%)	24,25,25	1.33	3 (12%)
6	BCB	M	601	3	68,74,74	1.50	11 (16%)	77,115,115	1.54	15 (19%)
10	SO4	H	622	-	4,4,4	0.97	0	6,6,6	0.25	0
11	MQ7	M	608	-	49,49,49	1.44	5 (10%)	61,63,63	2.37	21 (34%)
7	BPB	L	606	-	57,70,70	1.91	13 (22%)	55,101,101	2.32	19 (34%)
10	SO4	M	618	-	4,4,4	0.87	0	6,6,6	0.24	0
13	LDA	H	616	-	13,15,15	2.84	2 (15%)	14,17,17	0.77	0
6	BCB	L	604	2	68,74,74	1.73	12 (17%)	77,115,115	1.59	14 (18%)
5	HEC	C	612	1	50,50,50	1.76	13 (26%)	68,82,82	1.47	10 (14%)
10	SO4	H	623	-	4,4,4	0.97	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	NS1	M	613	-	39,39,39	2.09	11 (28%)	46,46,46	2.27	17 (36%)

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
5	HEC	C	611	1	1/1/3/7	7/14/54/54	-
5	HEC	C	610	1	1/1/3/7	6/14/54/54	-
13	LDA	M	615	-	-	7/13/13/13	-
6	BCB	L	602	2	3/3/21/26	11/41/137/137	-
8	UQ1	L	614	-	-	0/9/33/33	0/1/1/1
13	LDA	H	616	-	-	1/13/13/13	-
6	BCB	M	601	3	1/1/21/26	2/41/137/137	-
6	BCB	L	604	2	3/3/21/26	6/41/137/137	-
5	HEC	C	609	1	1/1/3/7	8/14/54/54	-
5	HEC	C	612	1	1/1/3/7	4/14/54/54	-
6	BCB	M	603	3	3/3/21/26	7/41/137/137	-
7	BPB	M	605	-	-	10/37/105/105	0/5/6/6
7	BPB	L	606	-	-	9/37/105/105	0/5/6/6
11	MQ7	M	608	-	-	4/41/61/61	0/2/2/2
12	NS1	M	613	-	-	15/43/43/43	-

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	615	LDA	O1-N1	-8.31	1.21	1.42
13	H	616	LDA	O1-N1	-7.91	1.22	1.42
12	M	613	NS1	C35-C36	7.46	1.54	1.32
5	C	610	HEC	C4C-C3C	-6.15	1.32	1.44
13	H	616	LDA	C1-N1	-6.11	1.45	1.51
6	L	604	BCB	MG-NA	6.06	2.20	2.06
7	L	606	BPB	C3A-C2A	-6.06	1.49	1.54
6	M	601	BCB	C3B-C4B	5.22	1.51	1.41
6	M	603	BCB	CAA-C2A	-5.05	1.44	1.54
7	M	605	BPB	C1B-C2B	4.97	1.45	1.39
5	C	609	HEC	C4B-C3B	-4.83	1.36	1.45
6	L	604	BCB	C3B-C4B	4.77	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	605	BPB	CHA-CBD	4.58	1.57	1.51
5	C	612	HEC	C4D-C3D	-4.55	1.37	1.45
6	L	604	BCB	O1A-CGA	-4.40	1.09	1.22
5	C	610	HEC	FE-NB	4.26	2.08	1.94
7	M	605	BPB	C1-C2	4.25	1.61	1.49
6	M	603	BCB	MG-ND	-4.25	1.97	2.05
5	C	610	HEC	C4D-C3D	-4.24	1.37	1.45
7	L	606	BPB	O2D-CED	-4.20	1.35	1.45
7	M	605	BPB	CBD-CGD	-4.19	1.47	1.52
7	L	606	BPB	C3D-C4D	4.11	1.46	1.41
5	C	609	HEC	C4C-C3C	-4.05	1.36	1.44
5	C	610	HEC	C4A-C3A	-4.02	1.37	1.45
13	M	615	LDA	C1-N1	-4.01	1.47	1.51
6	L	602	BCB	O2D-CED	-3.91	1.36	1.45
5	C	610	HEC	C4B-C3B	-3.82	1.38	1.45
5	C	609	HEC	C1D-ND	-3.82	1.33	1.40
5	C	611	HEC	FE-NC	3.80	2.07	1.95
6	M	601	BCB	O1D-CGD	-3.76	1.11	1.21
5	C	609	HEC	FE-ND	3.75	2.06	1.94
12	M	613	NS1	C14-C15	-3.68	1.38	1.46
7	M	605	BPB	C1D-C2D	3.67	1.43	1.39
7	M	605	BPB	C3B-C4B	3.67	1.47	1.41
11	M	608	MQ7	C10-C1	-3.63	1.41	1.48
6	L	602	BCB	C4C-C3C	3.59	1.51	1.44
6	M	603	BCB	MG-NA	-3.52	1.97	2.06
5	C	612	HEC	FE-NA	3.51	2.06	1.95
6	L	604	BCB	C1B-NB	3.47	1.42	1.37
11	M	608	MQ7	C10-C5	-3.44	1.35	1.40
6	L	604	BCB	C5-C3	3.43	1.58	1.51
5	C	609	HEC	C4C-NC	-3.40	1.33	1.39
6	M	603	BCB	O1A-CGA	-3.36	1.12	1.22
7	L	606	BPB	C3B-C4B	3.27	1.46	1.41
7	L	606	BPB	C1D-C2D	3.27	1.43	1.39
5	C	612	HEC	C3D-C2D	3.26	1.43	1.36
5	C	609	HEC	C1C-C2C	-3.25	1.35	1.43
6	M	603	BCB	OBB-CAB	-3.25	1.15	1.23
6	L	604	BCB	C2C-C3C	-3.23	1.47	1.51
5	C	612	HEC	CBD-CGD	3.23	1.58	1.50
5	C	612	HEC	FE-NC	3.17	2.05	1.95
7	L	606	BPB	CMA-C3A	-3.13	1.48	1.53
7	L	606	BPB	CAA-C2A	3.13	1.60	1.54
6	L	602	BCB	MG-ND	-3.12	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	613	NS1	C24-C23	3.11	1.42	1.34
6	L	604	BCB	MG-NC	-3.10	1.98	2.06
5	C	610	HEC	CBA-CGA	3.07	1.57	1.50
7	L	606	BPB	C1B-C2B	3.04	1.42	1.39
12	M	613	NS1	C25-C26	3.03	1.42	1.35
5	C	610	HEC	C1A-C2A	-3.01	1.39	1.45
5	C	612	HEC	FE-NB	3.00	2.04	1.94
5	C	611	HEC	C4D-C3D	-2.99	1.40	1.45
5	C	612	HEC	C4B-NB	-2.96	1.35	1.40
5	C	611	HEC	FE-ND	2.95	2.04	1.94
5	C	610	HEC	C1D-C2D	-2.94	1.38	1.44
11	M	608	MQ7	C6-C5	-2.89	1.35	1.39
7	L	606	BPB	CBC-CAC	2.85	1.60	1.49
5	C	611	HEC	C4B-C3B	-2.85	1.40	1.45
12	M	613	NS1	C2-C1	-2.84	1.33	1.51
5	C	612	HEC	C1A-C2A	-2.83	1.40	1.45
6	L	604	BCB	C3D-C4D	-2.83	1.37	1.44
6	M	603	BCB	C3B-C4B	2.80	1.46	1.41
5	C	609	HEC	C4B-NB	-2.77	1.35	1.40
6	M	601	BCB	C5-C3	2.77	1.57	1.51
11	M	608	MQ7	C9-C10	-2.71	1.35	1.39
6	L	604	BCB	O2A-C1	2.70	1.53	1.46
5	C	609	HEC	C1A-NA	-2.69	1.34	1.39
5	C	611	HEC	O2A-CGA	2.66	1.39	1.30
6	M	603	BCB	C1D-C2D	-2.66	1.40	1.45
5	C	611	HEC	C4B-NB	-2.62	1.35	1.40
5	C	611	HEC	C4C-NC	-2.60	1.34	1.39
7	L	606	BPB	C3D-CAD	-2.59	1.42	1.47
7	M	605	BPB	C3B-C2B	-2.57	1.35	1.39
5	C	612	HEC	C1C-NC	-2.57	1.34	1.39
6	M	601	BCB	C1B-NB	2.57	1.41	1.37
6	M	603	BCB	CBC-CAC	2.56	1.59	1.49
7	M	605	BPB	C1A-C2A	2.56	1.54	1.51
7	M	605	BPB	C2-C3	2.55	1.38	1.33
6	L	604	BCB	MG-NB	-2.55	2.00	2.05
5	C	611	HEC	CAA-C2A	-2.53	1.44	1.51
6	L	602	BCB	CBB-CAB	2.50	1.55	1.50
6	L	602	BCB	C3D-CAD	-2.50	1.36	1.45
12	M	613	NS1	C20-C21	2.47	1.41	1.35
7	L	606	BPB	C4D-ND	-2.46	1.34	1.38
5	C	611	HEC	C1D-ND	-2.46	1.36	1.40
7	M	605	BPB	O2A-C1	2.45	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	613	NS1	C29-C28	2.44	1.41	1.34
6	M	601	BCB	C2C-C3C	2.43	1.55	1.51
6	M	603	BCB	CAA-CBA	-2.43	1.45	1.52
5	C	611	HEC	CBD-CAD	2.42	1.60	1.51
12	M	613	NS1	C22-C21	2.42	1.55	1.50
5	C	610	HEC	C1C-NC	-2.41	1.35	1.39
7	L	606	BPB	CBD-CAD	2.38	1.61	1.53
5	C	610	HEC	FE-ND	2.38	2.02	1.94
6	L	604	BCB	MG-ND	2.36	2.10	2.05
5	C	609	HEC	FE-NC	2.36	2.02	1.95
5	C	610	HEC	C1C-C2C	-2.34	1.37	1.43
5	C	609	HEC	C4A-NA	-2.34	1.35	1.39
6	L	602	BCB	OBB-CAB	-2.33	1.17	1.23
6	M	603	BCB	O2A-C1	2.33	1.52	1.46
5	C	611	HEC	C4A-C3A	-2.32	1.40	1.45
5	C	612	HEC	C1D-C2D	-2.32	1.39	1.44
6	M	603	BCB	C5-C3	2.27	1.56	1.51
6	M	601	BCB	C4C-C3C	2.27	1.49	1.44
6	M	603	BCB	O1D-CGD	-2.27	1.15	1.21
5	C	610	HEC	C1A-NA	-2.27	1.35	1.39
6	M	603	BCB	C3B-C2B	-2.27	1.34	1.42
11	M	608	MQ7	C36-C37	2.27	1.57	1.50
6	M	601	BCB	CBA-CGA	2.26	1.57	1.50
5	C	612	HEC	FE-ND	2.25	2.01	1.94
8	L	614	UQ1	C7-C8	2.24	1.54	1.50
7	L	606	BPB	C5-C3	2.24	1.55	1.51
6	M	601	BCB	CHD-C1D	2.23	1.42	1.38
6	M	601	BCB	MG-ND	-2.20	2.01	2.05
12	M	613	NS1	C30-C31	2.19	1.42	1.35
7	M	605	BPB	CBC-CAC	2.19	1.57	1.49
5	C	612	HEC	CAC-C3C	2.18	1.56	1.51
6	L	604	BCB	C1D-C2D	-2.18	1.41	1.45
12	M	613	NS1	C17-C15	2.18	1.40	1.35
6	M	603	BCB	C3A-C2A	-2.17	1.48	1.54
6	M	603	BCB	O2D-CGD	-2.17	1.27	1.33
5	C	612	HEC	C1D-ND	-2.17	1.36	1.40
5	C	611	HEC	C2A-C3A	-2.15	1.32	1.36
5	C	611	HEC	C1A-C2A	-2.14	1.41	1.45
5	C	610	HEC	CAA-C2A	-2.14	1.45	1.51
6	M	601	BCB	CBC-CAC	2.14	1.57	1.49
5	C	611	HEC	CBD-CGD	2.14	1.55	1.50
7	M	605	BPB	CMD-C2D	-2.13	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	605	BPB	C6-C7	2.12	1.61	1.52
5	C	610	HEC	C3B-C2B	2.06	1.41	1.36
12	M	613	NS1	C19-C18	2.06	1.41	1.36
5	C	609	HEC	O2A-CGA	2.05	1.37	1.30
5	C	609	HEC	C4A-C3A	-2.05	1.41	1.45
6	M	601	BCB	MG-NB	2.05	2.09	2.05
5	C	610	HEC	C1B-C2B	-2.05	1.40	1.44
6	L	602	BCB	MG-NB	-2.02	2.01	2.05
7	M	605	BPB	C3A-C2A	2.02	1.56	1.54
5	C	611	HEC	O1A-CGA	2.00	1.28	1.22
7	M	605	BPB	C1D-ND	2.00	1.42	1.38

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	608	MQ7	C11-C3-C4	-9.46	108.61	118.58
7	L	606	BPB	C4D-CHA-CBD	-6.64	105.27	108.45
7	L	606	BPB	OBD-CAD-CBD	-5.90	117.17	125.82
5	C	611	HEC	CAA-C2A-C3A	-5.72	117.16	127.87
6	M	603	BCB	CAA-C2A-C1A	-5.69	93.32	111.97
7	M	605	BPB	C4D-CHA-CBD	-5.53	105.80	108.45
6	L	602	BCB	C1-C2-C3	-5.43	117.31	126.20
12	M	613	NS1	C34-C35-C36	-5.28	110.04	127.64
7	L	606	BPB	C2D-C1D-ND	5.11	113.12	109.43
6	M	603	BCB	C1C-NC-C4C	5.06	108.99	106.68
6	M	603	BCB	C4A-NA-C1A	-5.05	104.38	106.68
12	M	613	NS1	C19-C20-C21	4.94	134.21	127.28
6	L	604	BCB	C1-C2-C3	-4.79	118.35	126.20
5	C	612	HEC	CBD-CAD-C3D	4.77	125.73	112.53
6	M	603	BCB	C1-O2A-CGA	-4.69	105.29	116.65
11	M	608	MQ7	C21-C22-C23	-4.62	117.06	127.62
11	M	608	MQ7	C36-C37-C38	-4.57	117.17	127.62
5	C	611	HEC	CAA-C2A-C1A	4.52	134.04	124.85
11	M	608	MQ7	C11-C3-C2	4.41	132.45	124.89
12	M	613	NS1	C29-C30-C31	-4.37	121.54	127.69
12	M	613	NS1	CM4-C36-C35	-4.33	109.67	122.66
6	L	602	BCB	C4D-CHA-C1A	4.31	126.38	121.24
6	M	601	BCB	C4-C3-C5	4.27	122.64	115.23
11	M	608	MQ7	O1-C1-C10	-4.22	114.83	121.57
12	M	613	NS1	CM3-C36-C35	-4.19	110.09	122.66
6	L	602	BCB	C4-C3-C5	4.16	122.45	115.23
11	M	608	MQ7	C39-C38-C40	4.06	122.28	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	606	BPB	O1D-CGD-CBD	4.02	130.82	124.72
7	L	606	BPB	C1-O2A-CGA	-4.01	106.93	116.65
5	C	612	HEC	C1D-ND-C4D	3.91	109.84	105.21
7	M	605	BPB	C4D-ND-C1D	-3.88	104.22	108.87
12	M	613	NS1	C13-C12-C10	-3.81	122.33	127.69
5	C	611	HEC	CBC-CAC-C3C	3.80	122.73	112.42
7	L	606	BPB	OBD-CAD-C3D	3.78	133.79	127.89
6	L	604	BCB	CHD-C1D-ND	-3.78	119.48	124.80
6	L	604	BCB	C4A-NA-C1A	3.77	108.40	106.68
5	C	611	HEC	CMA-C3A-C4A	3.74	131.31	124.73
6	L	602	BCB	CBC-CAC-C3C	-3.74	116.56	126.70
11	M	608	MQ7	C34-C33-C35	3.73	121.71	115.23
6	M	603	BCB	CAA-CBA-CGA	-3.68	102.75	113.21
6	M	603	BCB	O2D-CGD-O1D	-3.68	116.69	123.85
7	L	606	BPB	CMA-C3A-C4A	-3.67	106.71	114.61
6	M	603	BCB	C4-C3-C5	3.66	121.59	115.23
12	M	613	NS1	C8-C7-C5	-3.65	119.27	127.62
7	L	606	BPB	CMD-C2D-C3D	3.64	131.97	124.68
7	M	605	BPB	OBB-CAB-CBB	-3.62	112.48	120.19
5	C	612	HEC	CBC-CAC-C3C	3.61	122.21	112.42
5	C	609	HEC	CAD-C3D-C4D	3.57	130.93	124.70
6	L	604	BCB	C1C-NC-C4C	3.56	108.30	106.68
7	L	606	BPB	C4D-ND-C1D	-3.47	104.71	108.87
6	L	602	BCB	CHD-C4C-C3C	-3.43	121.60	125.91
7	M	605	BPB	C2D-C1D-ND	3.43	111.91	109.43
5	C	609	HEC	CAD-C3D-C2D	-3.40	121.49	127.87
13	M	615	LDA	CM2-N1-C1	3.38	117.34	110.23
5	C	611	HEC	C2A-C1A-NA	-3.35	107.09	110.32
11	M	608	MQ7	C9-C10-C5	3.33	123.00	119.26
6	M	601	BCB	OBB-CAB-CBB	-3.29	112.41	119.77
6	M	601	BCB	C4A-NA-C1A	3.27	108.17	106.68
5	C	612	HEC	CHA-C4D-ND	3.26	127.93	124.42
6	L	604	BCB	C16-C15-C13	-3.25	105.16	115.97
6	L	604	BCB	C4D-CHA-C1A	3.24	125.11	121.24
7	M	605	BPB	C3D-C4D-ND	3.21	111.83	107.71
5	C	609	HEC	CMD-C2D-C1D	3.17	129.99	125.03
5	C	610	HEC	CHC-C1C-NC	3.17	129.61	123.86
6	M	603	BCB	CHD-C4C-C3C	-3.16	121.95	125.91
11	M	608	MQ7	C24-C23-C25	3.16	120.71	115.23
6	L	602	BCB	CHD-C1D-ND	-3.15	120.37	124.80
7	L	606	BPB	C2B-C1B-NB	-3.14	107.16	109.43
6	M	603	BCB	O2A-CGA-CBA	3.11	121.30	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	611	HEC	CHB-C1B-NB	3.08	127.74	124.42
6	M	601	BCB	O2D-CGD-O1D	-3.01	118.00	123.85
11	M	608	MQ7	C2M-C2-C1	-3.00	111.15	116.68
7	L	606	BPB	CED-O2D-CGD	-2.98	109.16	115.92
5	C	610	HEC	CHB-C4A-NA	2.97	127.69	124.45
5	C	612	HEC	CHB-C1B-NB	2.96	127.61	124.42
6	L	602	BCB	C3B-C4B-NB	-2.96	105.85	109.76
8	L	614	UQ1	CM5-C5-C6	-2.95	119.60	124.45
6	L	602	BCB	C11-C10-C8	-2.94	106.19	115.97
12	M	613	NS1	C11-C10-C9	2.94	120.33	115.23
5	C	610	HEC	CHA-C1A-NA	2.93	127.64	124.45
7	L	606	BPB	C7-C6-C5	-2.91	105.49	113.26
5	C	610	HEC	CBD-CAD-C3D	2.91	120.59	112.53
6	L	602	BCB	C14-C13-C15	-2.91	100.91	111.27
5	C	610	HEC	CAB-C3B-C4B	2.89	128.55	124.79
6	M	601	BCB	CHD-C1D-ND	-2.88	120.75	124.80
5	C	610	HEC	C2C-C1C-NC	-2.88	105.53	110.14
12	M	613	NS1	C13-C14-C15	-2.87	118.48	126.36
6	M	601	BCB	CAA-CBA-CGA	-2.87	105.06	113.21
7	L	606	BPB	CMA-C3A-C2A	-2.87	103.04	114.13
5	C	611	HEC	CAD-C3D-C4D	2.87	129.69	124.70
5	C	612	HEC	CMA-C3A-C4A	2.87	129.78	124.73
12	M	613	NS1	C18-C17-C15	-2.86	123.27	127.28
6	M	603	BCB	CHD-C1D-ND	-2.82	120.84	124.80
8	L	614	UQ1	C7-C8-C9	-2.81	119.30	127.25
6	L	604	BCB	C4-C3-C5	2.79	120.08	115.23
5	C	609	HEC	CAB-C3B-C4B	2.77	128.40	124.79
11	M	608	MQ7	C31-C32-C33	-2.76	121.31	127.62
6	M	603	BCB	O2A-CGA-O1A	-2.76	116.73	123.63
7	L	606	BPB	C3D-C4D-ND	2.72	111.20	107.71
11	M	608	MQ7	C39-C38-C37	-2.72	116.64	123.63
5	C	612	HEC	C2D-C1D-ND	-2.72	106.72	109.84
6	M	601	BCB	C7-C6-C5	-2.71	106.03	113.26
6	M	601	BCB	O2D-CGD-CBD	2.70	115.96	111.23
6	M	601	BCB	C6-C7-C8	-2.70	107.00	115.97
11	M	608	MQ7	O1-C1-C2	2.70	124.00	120.45
6	L	602	BCB	C4A-NA-C1A	2.70	107.91	106.68
5	C	609	HEC	C1C-C2C-C3C	-2.69	103.73	106.82
6	L	604	BCB	CED-O2D-CGD	2.67	121.98	115.92
11	M	608	MQ7	C29-C28-C30	2.65	119.84	115.23
7	M	605	BPB	OBB-CAB-C3B	2.64	124.41	119.99
13	M	615	LDA	C9-C8-C7	-2.64	101.02	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	609	HEC	CBD-CAD-C3D	-2.64	105.24	112.53
12	M	613	NS1	C6-C5-C4	2.63	119.79	115.23
5	C	610	HEC	CHD-C4C-NC	2.61	128.59	123.86
5	C	609	HEC	CMC-C2C-C3C	2.61	131.15	125.62
6	M	603	BCB	C11-C10-C8	-2.60	107.32	115.97
5	C	609	HEC	C2B-C1B-NB	-2.59	106.91	109.90
11	M	608	MQ7	O4-C4-C3	-2.58	116.53	120.67
6	M	603	BCB	C7-C6-C5	-2.58	106.38	113.26
6	M	601	BCB	CAA-C2A-C1A	-2.57	103.56	111.97
11	M	608	MQ7	C14-C13-C15	2.56	119.68	115.23
7	M	605	BPB	OBD-CAD-CBD	-2.55	122.08	125.82
6	M	603	BCB	O2A-C1-C2	2.54	117.88	108.11
5	C	610	HEC	C4C-NC-C1C	2.54	109.95	105.82
6	L	602	BCB	C4-C3-C2	-2.50	117.21	123.63
6	L	604	BCB	C11-C12-C13	-2.49	107.67	115.97
5	C	609	HEC	O1A-CGA-CBA	-2.48	115.23	123.09
12	M	613	NS1	C19-C18-C17	-2.46	118.48	123.52
6	M	603	BCB	C1-C2-C3	-2.45	122.18	126.20
6	L	602	BCB	CAA-C2A-C1A	2.44	119.99	111.97
6	L	602	BCB	CAA-CBA-CGA	-2.44	106.28	113.21
13	M	615	LDA	O1-N1-C1	2.44	115.25	109.27
6	M	601	BCB	C4D-CHA-C1A	2.43	124.14	121.24
11	M	608	MQ7	C2M-C2-C3	2.42	128.44	124.45
5	C	609	HEC	C4B-NB-C1B	2.40	108.05	105.21
6	L	602	BCB	CHA-C1A-NA	-2.39	120.98	126.39
6	M	601	BCB	CBB-CAB-C3B	2.39	125.43	120.40
5	C	610	HEC	CHA-C4D-ND	2.38	126.98	124.42
7	L	606	BPB	C14-C13-C12	-2.38	102.79	111.27
5	C	612	HEC	C4B-NB-C1B	2.36	108.01	105.21
5	C	611	HEC	CHD-C1D-ND	2.35	127.28	124.37
6	L	602	BCB	C1C-NC-C4C	2.34	107.75	106.68
6	L	604	BCB	CMB-C2B-C1B	-2.32	121.88	125.42
12	M	613	NS1	C27-C26-C25	-2.32	119.06	122.82
6	M	603	BCB	OBB-CAB-CBB	-2.31	114.60	119.77
6	L	602	BCB	CED-O2D-CGD	-2.30	110.69	115.92
12	M	613	NS1	C24-C23-C21	-2.28	120.10	126.36
7	L	606	BPB	C9-C8-C10	-2.28	103.16	111.27
6	L	604	BCB	CHD-C4C-C3C	-2.27	123.06	125.91
5	C	611	HEC	CAD-C3D-C2D	-2.27	123.62	127.87
12	M	613	NS1	C14-C15-C17	2.25	122.55	119.01
5	C	609	HEC	CHC-C1C-C2C	-2.24	120.91	127.43
5	C	609	HEC	O2A-CGA-CBA	2.24	121.09	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	606	BPB	O2D-CGD-O1D	-2.24	119.48	123.85
11	M	608	MQ7	C16-C17-C18	-2.23	122.51	127.62
6	M	601	BCB	CGD-CBD-CAD	-2.21	103.68	110.85
6	L	602	BCB	O1D-CGD-CBD	2.21	128.88	124.52
7	L	606	BPB	C20-C18-C19	-2.20	100.70	110.53
6	M	603	BCB	CAA-C2A-C3A	-2.20	107.06	113.00
5	C	610	HEC	C3C-C4C-NC	-2.18	107.73	110.15
8	L	614	UQ1	C11-C9-C10	2.18	119.60	114.59
6	M	601	BCB	C11-C10-C8	-2.17	108.74	115.97
12	M	613	NS1	CM4-C36-CM3	-2.16	109.61	114.59
11	M	608	MQ7	C11-C12-C13	-2.16	123.11	126.83
5	C	612	HEC	CAB-C3B-C4B	2.15	127.58	124.79
5	C	611	HEC	C1B-C2B-C3B	-2.14	104.73	106.98
7	L	606	BPB	OBB-CAB-CBB	-2.14	115.64	120.19
6	L	602	BCB	C6-C7-C8	-2.13	108.89	115.97
6	L	602	BCB	C2A-C1A-CHA	2.13	127.56	123.87
13	M	615	LDA	CM1-N1-C1	-2.13	105.77	110.23
11	M	608	MQ7	C41-C42-C43	-2.11	120.61	127.64
11	M	608	MQ7	C45-C43-C44	2.11	119.44	114.59
6	L	602	BCB	O2A-CGA-CBA	2.11	118.27	111.83
6	M	603	BCB	C4-C3-C2	-2.10	118.23	123.63
5	C	609	HEC	CHC-C1C-NC	2.10	127.67	123.86
6	L	602	BCB	CMA-C3A-C2A	-2.10	105.87	113.98
5	C	609	HEC	C4A-NA-C1A	2.09	109.23	105.82
7	M	605	BPB	C16-C15-C13	-2.09	109.02	115.97
6	L	604	BCB	O2A-CGA-CBA	2.09	118.20	111.83
6	L	604	BCB	C4-C3-C2	-2.09	118.27	123.63
5	C	610	HEC	CHD-C1D-ND	2.08	126.94	124.37
13	M	615	LDA	C6-C5-C4	-2.08	103.88	114.37
12	M	613	NS1	CM2-C1-CM1	2.07	119.76	110.53
6	L	602	BCB	CMB-C2B-C1B	-2.06	122.28	125.42
5	C	609	HEC	CAA-C2A-C1A	2.06	129.05	124.85
6	M	603	BCB	C2B-C1B-NB	2.05	112.46	110.33
5	C	610	HEC	CAD-C3D-C2D	-2.05	124.02	127.87
5	C	609	HEC	CAA-C2A-C3A	-2.05	124.02	127.87
6	L	604	BCB	OBB-CAB-CBB	-2.04	115.20	119.77
5	C	612	HEC	CHA-C4D-C3D	-2.04	121.80	124.77
6	L	602	BCB	C9-C8-C7	-2.04	104.02	111.27
6	M	601	BCB	C1C-NC-C4C	2.02	107.60	106.68
6	L	602	BCB	CGD-CBD-CAD	-2.01	104.33	110.85

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	609	HEC	NA
5	C	610	HEC	NA
5	C	611	HEC	NA
5	C	612	HEC	NA
6	L	602	BCB	NC
6	L	602	BCB	NA
6	L	602	BCB	ND
6	L	604	BCB	NC
6	L	604	BCB	NA
6	L	604	BCB	ND
6	M	601	BCB	NA
6	M	603	BCB	NC
6	M	603	BCB	NA
6	M	603	BCB	ND

All (97) 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	M	601	BCB	C2C-C3C-CAC-CBC
6	M	603	BCB	CAD-CBD-CGD-O1D
6	M	603	BCB	CAD-CBD-CGD-O2D
7	L	606	BPB	C1A-C2A-CAA-CBA
7	L	606	BPB	C3A-C2A-CAA-CBA
7	M	605	BPB	C4-C3-C5-C6
7	M	605	BPB	C3A-C2A-CAA-CBA
12	M	613	NS1	C9-C10-C12-C13
12	M	613	NS1	C11-C10-C12-C13
12	M	613	NS1	C34-C35-C36-CM3
5	C	609	HEC	C2B-C3B-CAB-CBB
6	L	602	BCB	C4-C3-C5-C6
6	M	603	BCB	C4-C3-C5-C6
12	M	613	NS1	C11-C10-C9-C8
6	M	603	BCB	C2-C3-C5-C6
7	M	605	BPB	C2-C3-C5-C6
12	M	613	NS1	C12-C10-C9-C8
12	M	613	NS1	C3-C4-C5-C6
12	M	613	NS1	C32-C31-C33-C34
12	M	613	NS1	C3-C4-C5-C7
12	M	613	NS1	C30-C31-C33-C34
6	L	602	BCB	C2-C3-C5-C6
7	M	605	BPB	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
5	C	611	HEC	C4C-C3C-CAC-CBC
7	L	606	BPB	C11-C12-C13-C15
12	M	613	NS1	C16-C15-C17-C18
12	M	613	NS1	C22-C21-C23-C24
6	L	602	BCB	C2A-CAA-CBA-CGA
12	M	613	NS1	C14-C15-C17-C18
6	M	601	BCB	C5-C6-C7-C8
12	M	613	NS1	CM2-C1-C2-C3
7	M	605	BPB	CBA-CGA-O2A-C1
5	C	610	HEC	C2B-C3B-CAB-CBB
5	C	610	HEC	C4C-C3C-CAC-CBC
5	C	609	HEC	C4C-C3C-CAC-CBC
5	C	611	HEC	C2C-C3C-CAC-CBC
13	M	615	LDA	C1-C2-C3-C4
6	L	602	BCB	C13-C15-C16-C17
6	M	603	BCB	C2A-CAA-CBA-CGA
5	C	609	HEC	C2C-C3C-CAC-CBC
11	M	608	MQ7	C41-C42-C43-C45
6	L	604	BCB	C15-C16-C17-C18
6	L	602	BCB	CBA-CGA-O2A-C1
6	M	603	BCB	C3A-C2A-CAA-CBA
5	C	610	HEC	C2C-C3C-CAC-CBC
13	M	615	LDA	C9-C10-C11-C12
5	C	612	HEC	C2B-C3B-CAB-CBB
7	M	605	BPB	O1A-CGA-O2A-C1
6	L	604	BCB	C2B-C3B-CAB-OBB
6	L	604	BCB	C2B-C3B-CAB-CBB
7	L	606	BPB	O2A-C1-C2-C3
6	L	602	BCB	O1A-CGA-O2A-C1
13	M	615	LDA	C2-C1-N1-CM2
5	C	610	HEC	C4B-C3B-CAB-CBB
12	M	613	NS1	C20-C21-C23-C24
11	M	608	MQ7	C39-C38-C40-C41
6	L	602	BCB	CAD-CBD-CGD-O2D
11	M	608	MQ7	C41-C42-C43-C44
6	L	602	BCB	CAD-CBD-CGD-O1D
6	L	604	BCB	CHA-CBD-CGD-O2D
12	M	613	NS1	C18-C19-C20-C21
5	C	609	HEC	C4B-C3B-CAB-CBB
6	L	602	BCB	C12-C13-C15-C16
13	H	616	LDA	N1-C1-C2-C3
13	M	615	LDA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
7	L	606	BPB	CBA-CGA-O2A-C1
11	M	608	MQ7	C37-C38-C40-C41
6	L	604	BCB	C3A-C2A-CAA-CBA
5	C	612	HEC	C2D-C3D-CAD-CBD
6	L	602	BCB	C14-C13-C15-C16
7	L	606	BPB	C11-C12-C13-C14
7	M	605	BPB	C14-C13-C15-C16
5	C	612	HEC	C2C-C3C-CAC-CBC
5	C	609	HEC	CAA-CBA-CGA-O2A
6	M	603	BCB	C16-C17-C18-C20
13	M	615	LDA	C6-C7-C8-C9
7	L	606	BPB	C13-C15-C16-C17
5	C	611	HEC	CAD-CBD-CGD-O2D
13	M	615	LDA	C7-C8-C9-C10
5	C	611	HEC	C2B-C3B-CAB-CBB
5	C	609	HEC	CAD-CBD-CGD-O1D
5	C	612	HEC	C4C-C3C-CAC-CBC
5	C	610	HEC	CAD-CBD-CGD-O2D
7	L	606	BPB	C2-C3-C5-C6
5	C	609	HEC	CAA-CBA-CGA-O1A
5	C	611	HEC	CAD-CBD-CGD-O1D
7	M	605	BPB	CAA-CBA-CGA-O2A
5	C	610	HEC	CAA-CBA-CGA-O1A
13	M	615	LDA	C11-C10-C9-C8
6	L	602	BCB	C15-C16-C17-C18
7	M	605	BPB	C10-C11-C12-C13
7	L	606	BPB	CAA-CBA-CGA-O2A
7	M	605	BPB	CAA-CBA-CGA-O1A
5	C	609	HEC	CAD-CBD-CGD-O2D
6	L	604	BCB	CBA-CGA-O2A-C1

There are no ring outliers.

15 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	611	HEC	7	0
5	C	610	HEC	4	0
6	L	602	BCB	16	0
6	M	603	BCB	15	0
5	C	609	HEC	6	0
7	M	605	BPB	11	0
13	M	615	LDA	1	0

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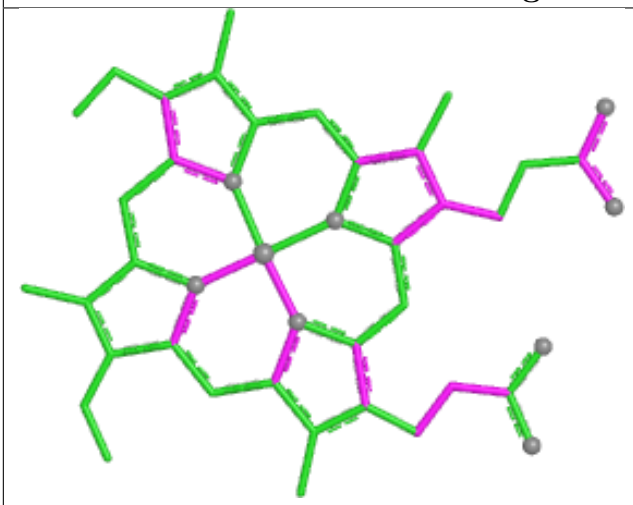
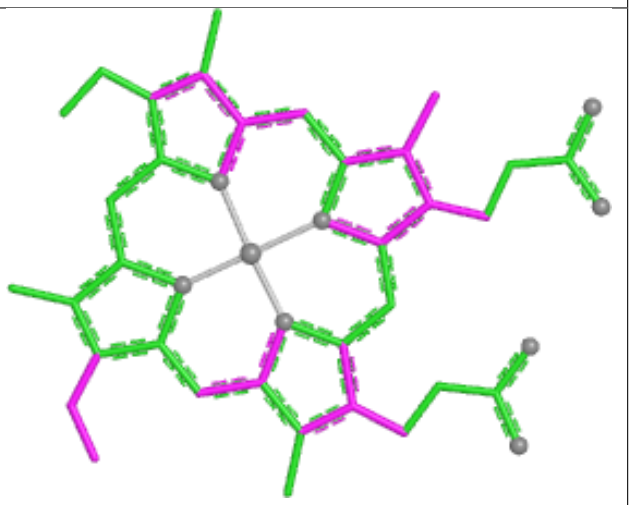
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	614	UQ1	8	0
6	M	601	BCB	6	0
11	M	608	MQ7	1	0
7	L	606	BPB	8	0
13	H	616	LDA	2	0
6	L	604	BCB	11	0
5	C	612	HEC	2	0
12	M	613	NS1	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

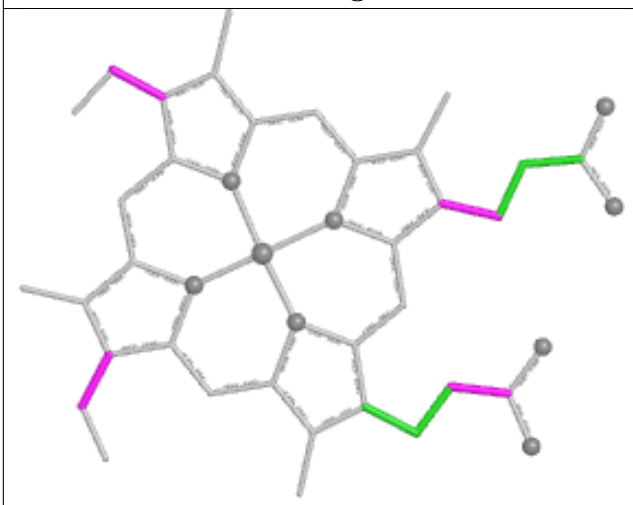
Ligand HEC C 611



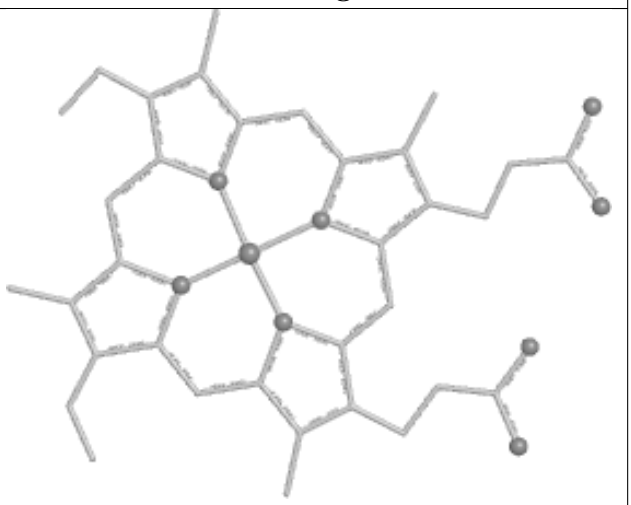
Bond lengths



Bond angles

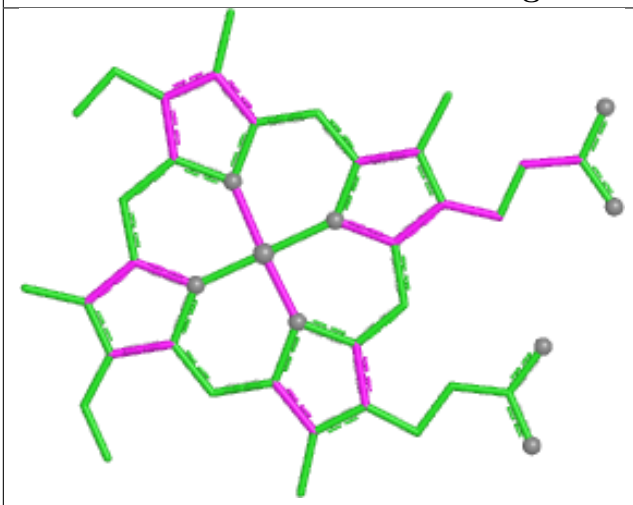


Torsions



Rings

Ligand HEC C 610



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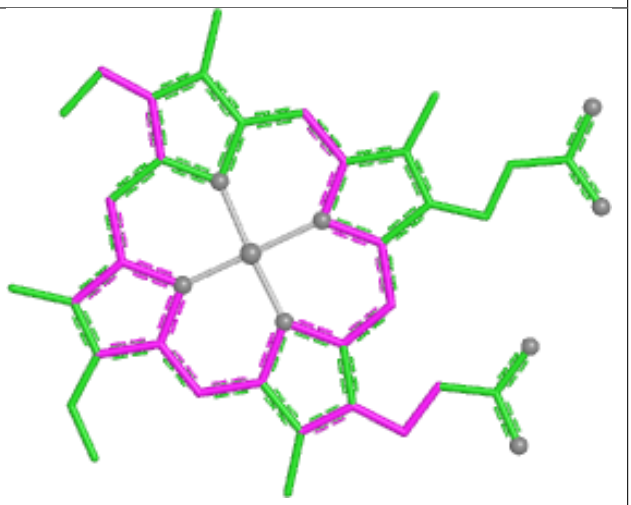
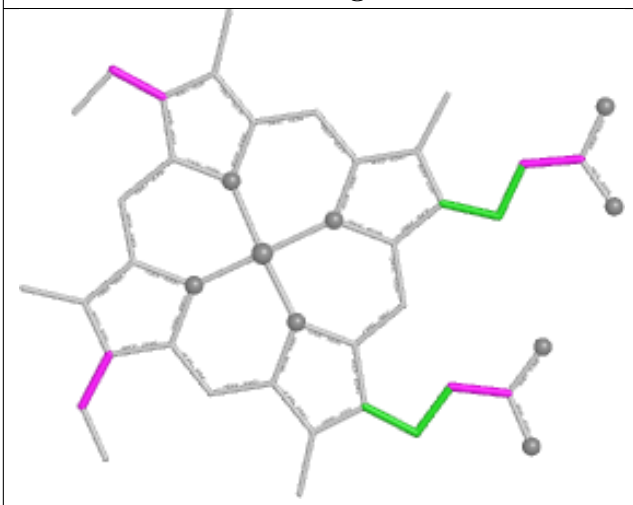


Bond angles



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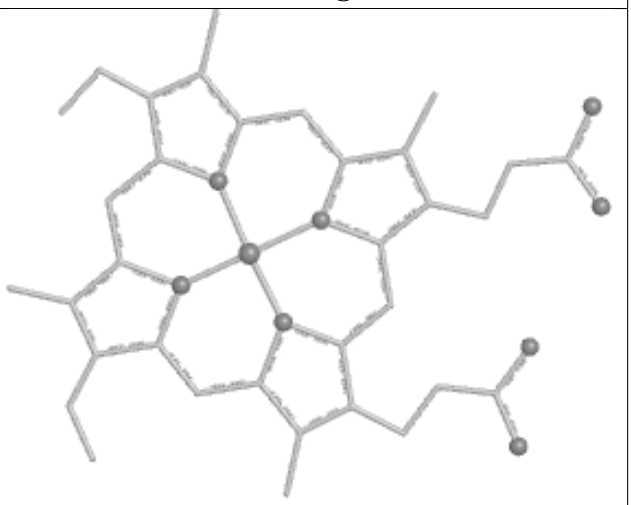
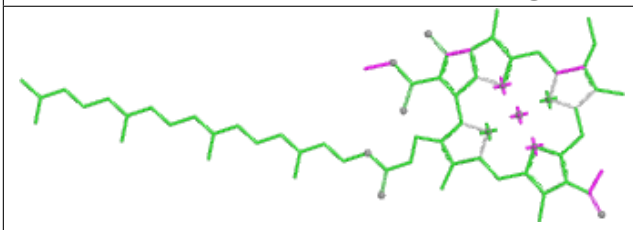


Rings

Ligand BCB L 602



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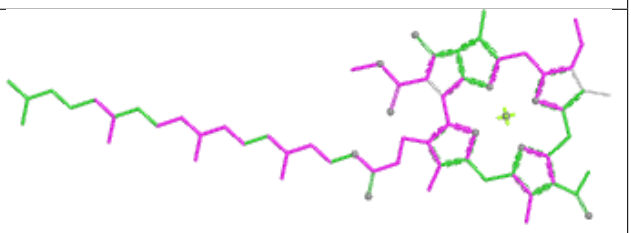
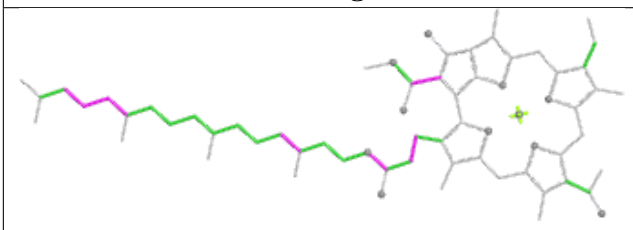
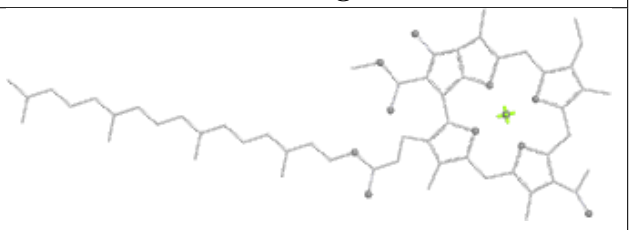


Bond angles

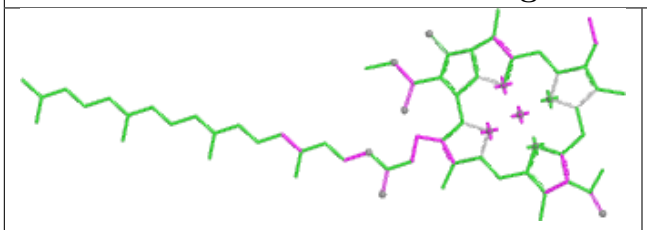


Torsions



Rings

Ligand BCB M 603



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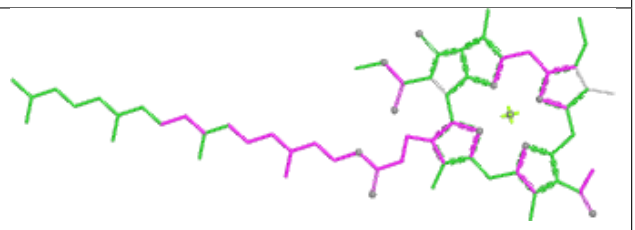
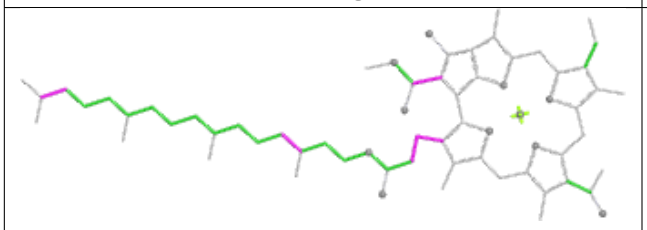


Bond angles



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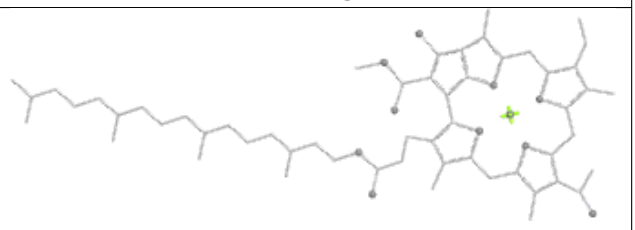
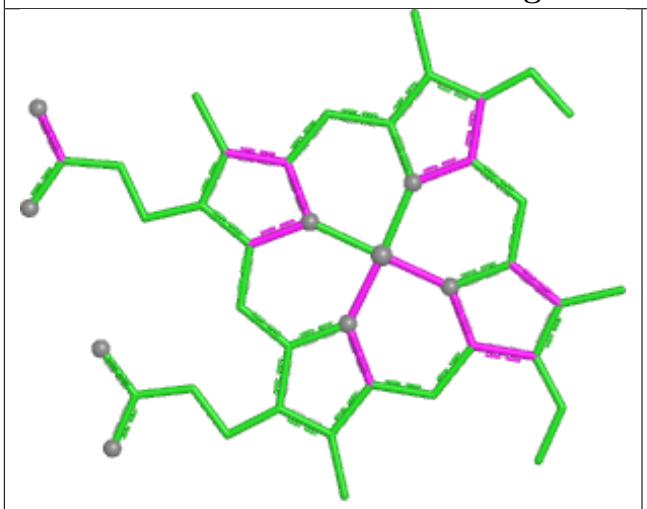


Rings

Ligand HEC C 609



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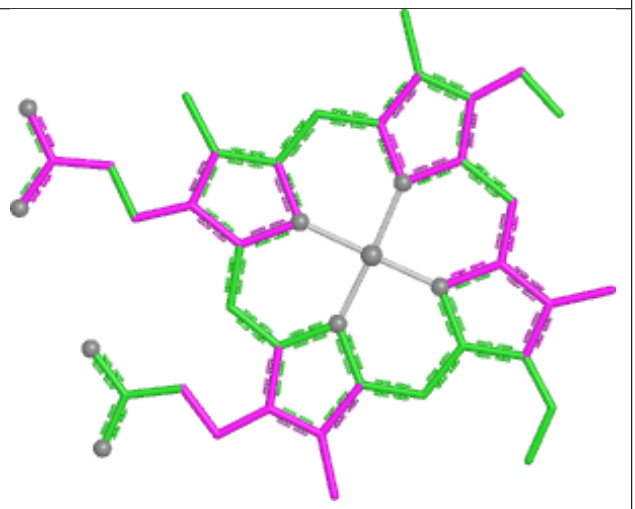

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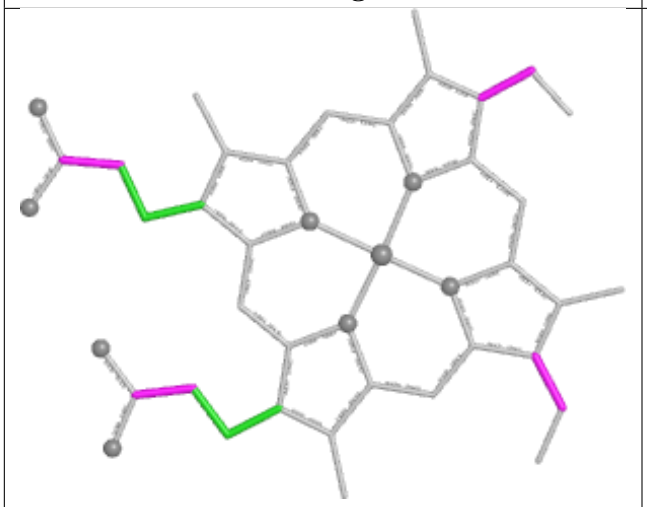

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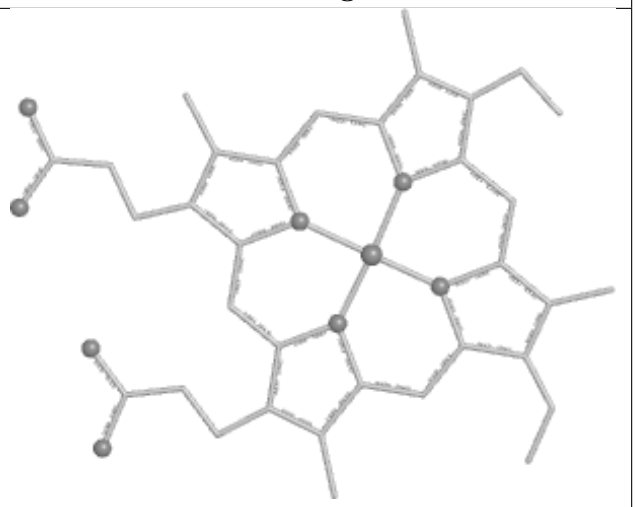
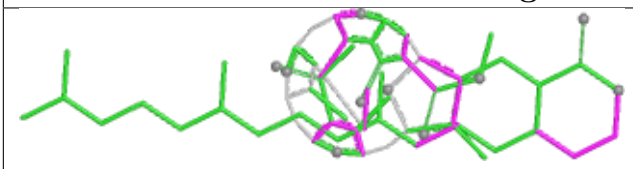


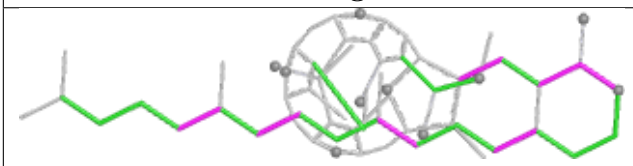
Rings

Ligand BPB M 605



Bond lengths

Bond angles



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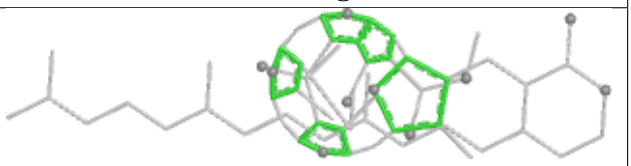
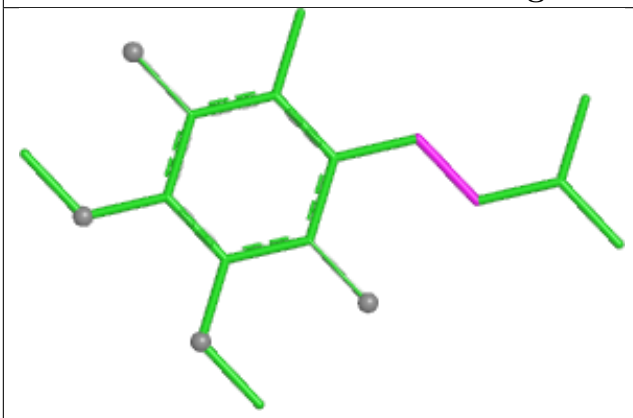


Rings

Ligand UQ1 L 614



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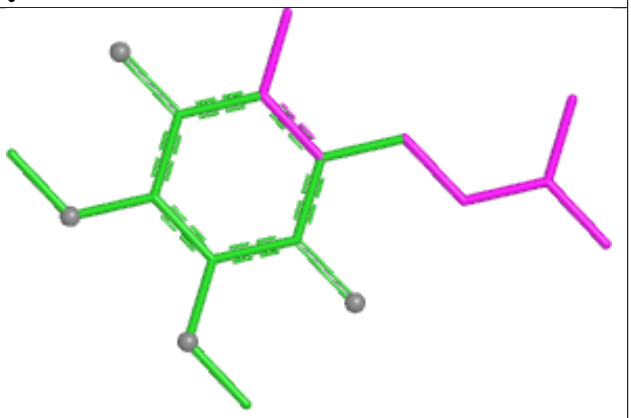
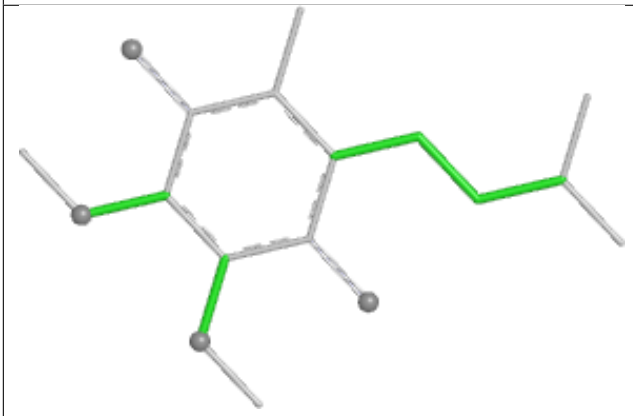


Bond angles



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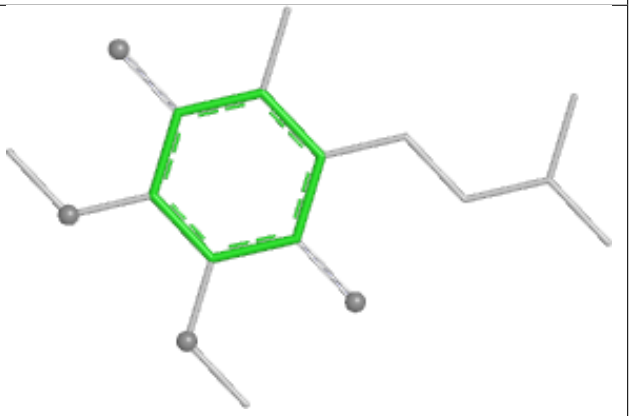
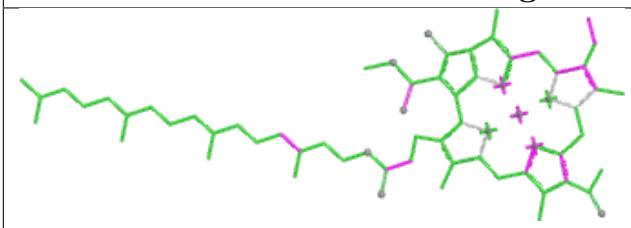


Rings

Ligand BCB M 601



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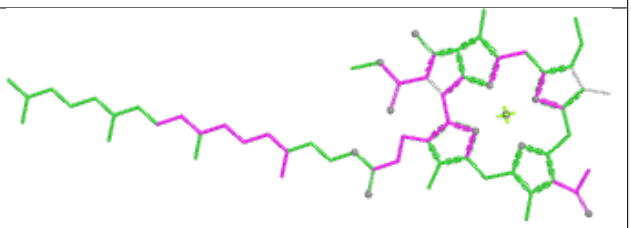
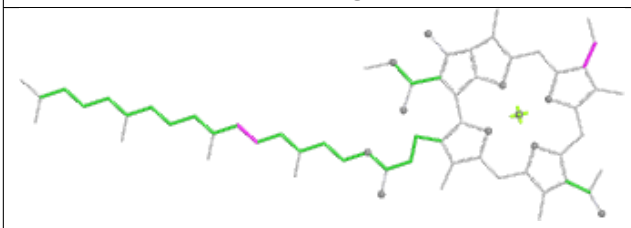


Bond angles



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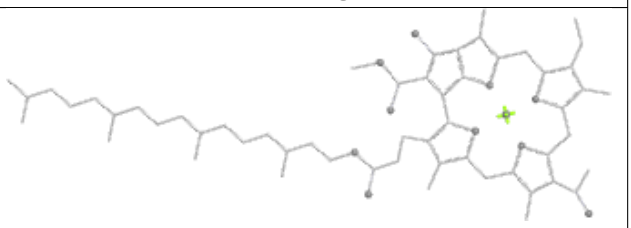
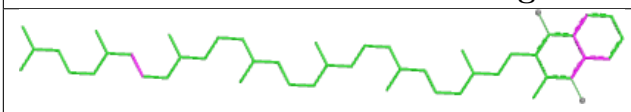
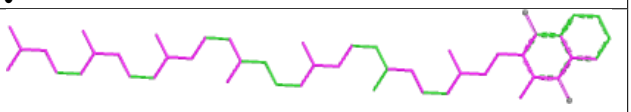


Rings

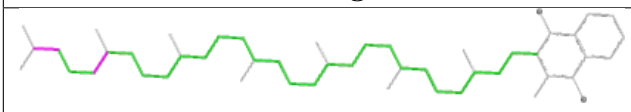
Ligand MQ7 M 608



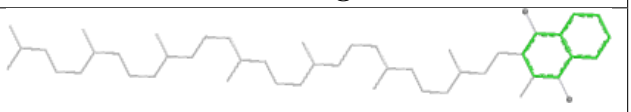
Bond lengths



Bond angles

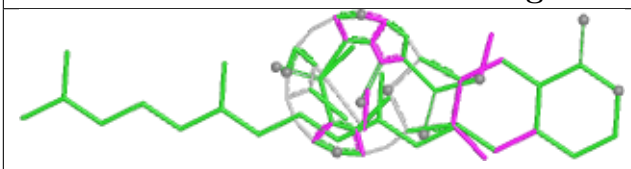


Torsions



Rings

Ligand BPB L 606



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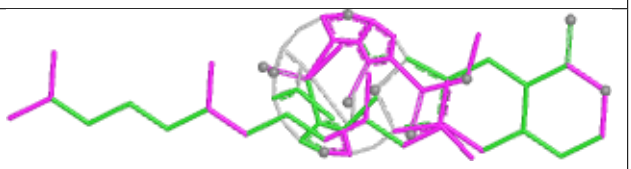
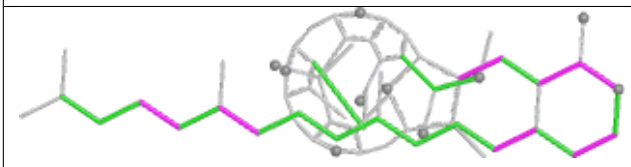
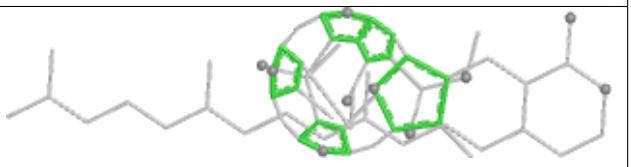


Bond angles



Torsions



Rings

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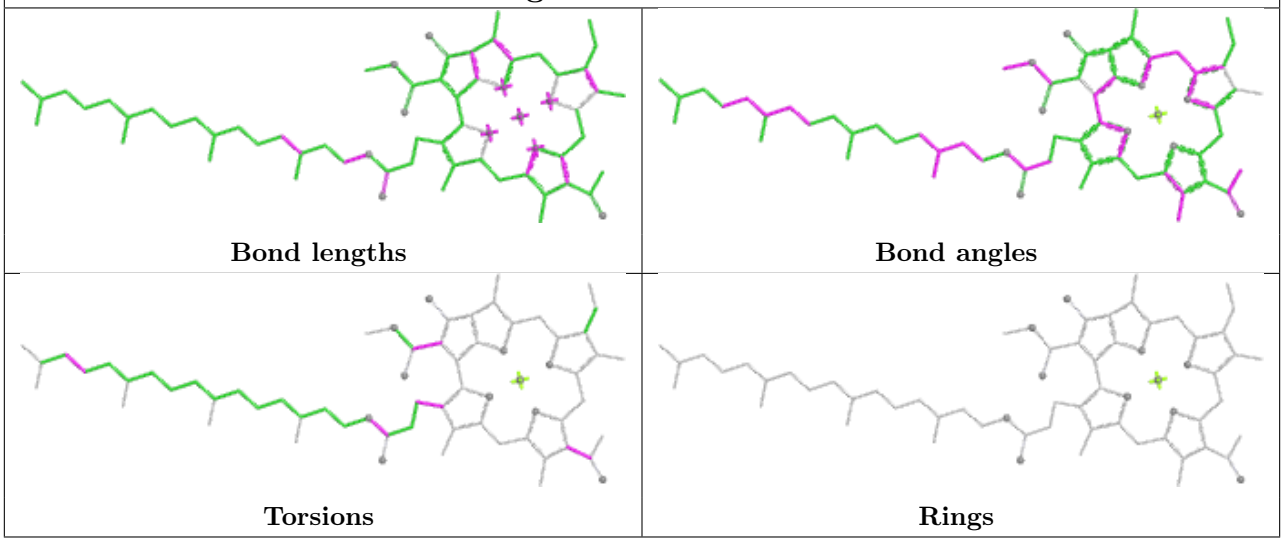
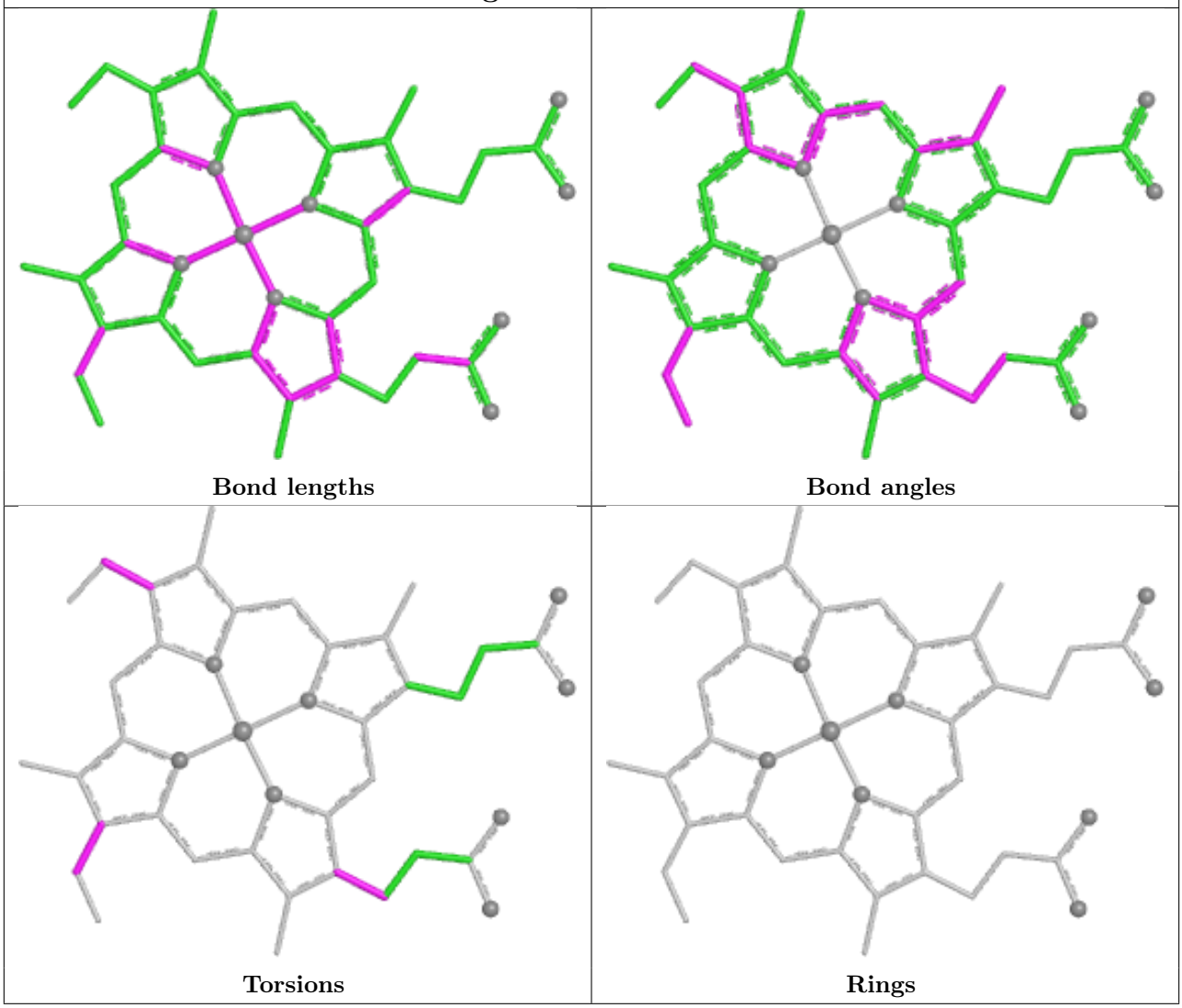
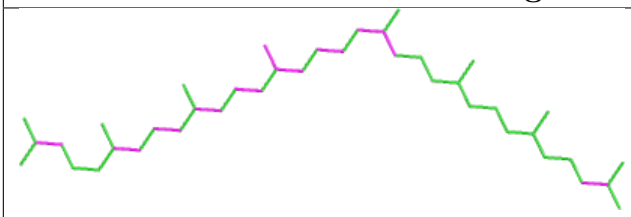
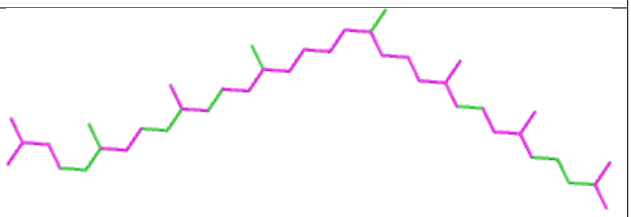
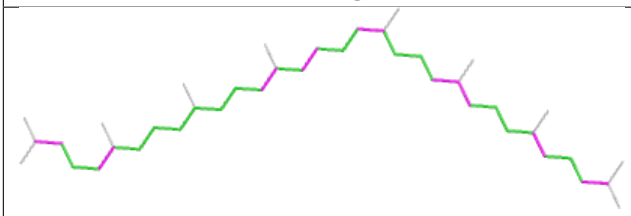
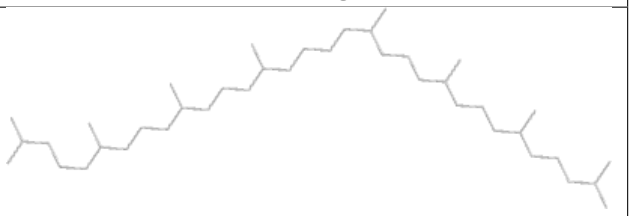


Ligand HEC C 612



Ligand NS1 M 613	
 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	C	333/336 (99%)	-0.68	1 (0%)	90	90	7, 21, 42, 73	17 (5%)
2	L	273/273 (100%)	-0.86	0	100	100	6, 16, 35, 47	6 (2%)
3	M	323/323 (100%)	-0.77	0	100	100	4, 18, 41, 58	8 (2%)
4	H	250/258 (96%)	-0.56	7 (2%)	55	57	8, 23, 46, 78	17 (6%)
All	All	1179/1190 (99%)	-0.72	8 (0%)	84	85	4, 19, 42, 78	48 (4%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	54	PRO	3.2
4	H	45	GLU	2.8
4	H	55	GLU	2.8
4	H	46	PRO	2.8
4	H	96	PHE	2.5
4	H	85	THR	2.5
4	H	87	GLU	2.1
1	C	93	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
4	FME	H	1	10/11	0.96	0.07	21,32,41,45	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

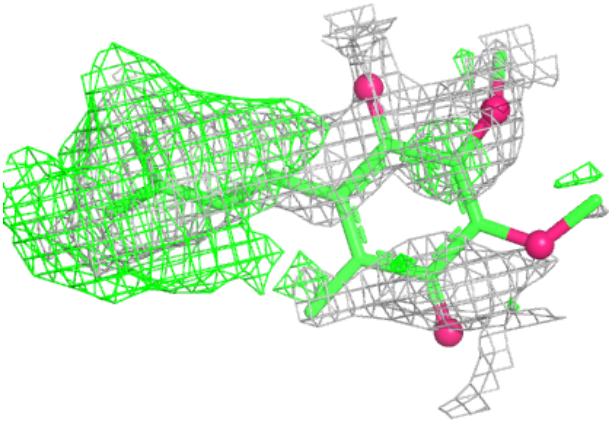
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

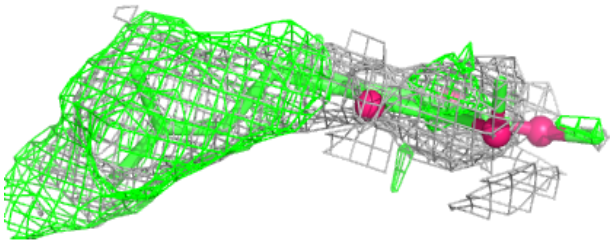
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	UQ1	L	614	18/18	0.81	0.37	19,26,29,30	18
10	SO4	H	622	5/5	0.84	0.17	73,74,85,89	0
13	LDA	H	616	16/16	0.85	0.14	0,27,42,46	6
10	SO4	H	623	5/5	0.89	0.12	58,59,62,64	5
10	SO4	M	621	5/5	0.89	0.15	68,78,81,82	0
12	NS1	M	613	40/40	0.92	0.10	0,25,39,49	14
13	LDA	M	615	16/16	0.94	0.07	17,25,36,37	0
10	SO4	H	617	5/5	0.94	0.09	47,50,59,61	0
11	MQ7	M	608	48/48	0.97	0.05	0,10,20,32	4
6	BCB	M	601	66/66	0.97	0.06	0,12,40,61	13
10	SO4	M	619	5/5	0.97	0.10	39,43,50,59	0
7	BPB	M	605	65/65	0.97	0.07	0,21,62,71	7
7	BPB	L	606	65/65	0.98	0.04	3,10,19,22	0
6	BCB	L	604	66/66	0.98	0.04	3,10,27,35	0
6	BCB	L	602	66/66	0.98	0.04	3,10,19,21	0
6	BCB	M	603	66/66	0.98	0.05	3,10,20,21	0
5	HEC	C	611	43/43	0.99	0.04	5,16,25,38	0
10	SO4	M	618	5/5	0.99	0.04	22,23,35,37	0
5	HEC	C	612	43/43	0.99	0.05	3,22,31,46	0
10	SO4	M	620	5/5	0.99	0.04	31,34,40,41	0
5	HEC	C	609	43/43	0.99	0.06	7,22,32,36	0
5	HEC	C	610	43/43	0.99	0.05	3,21,29,37	0
9	FE	M	607	1/1	1.00	0.01	19,19,19,19	0

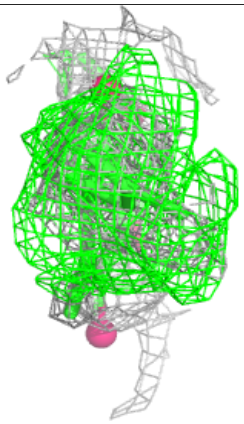
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

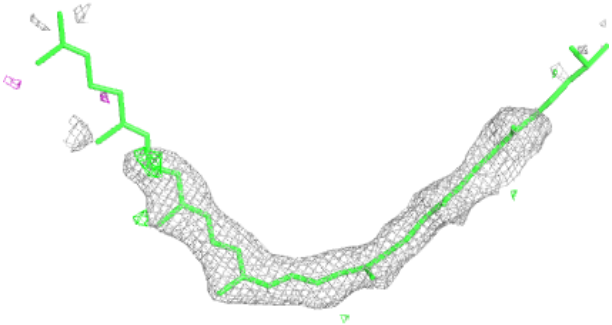


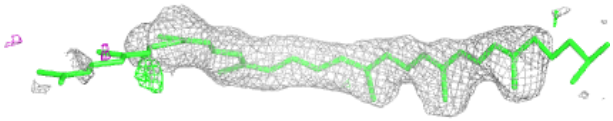


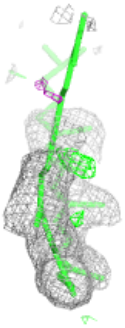


Electron density around NS1 M 613:

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

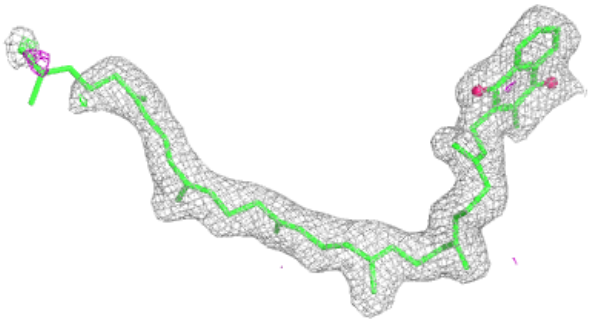


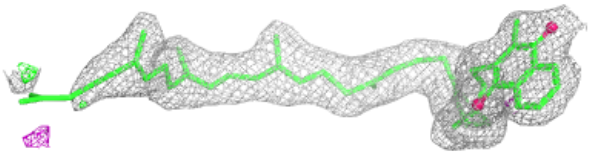


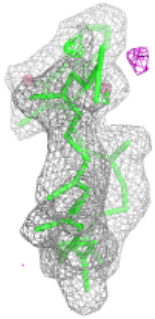


Electron density around MQ7 M 608:

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

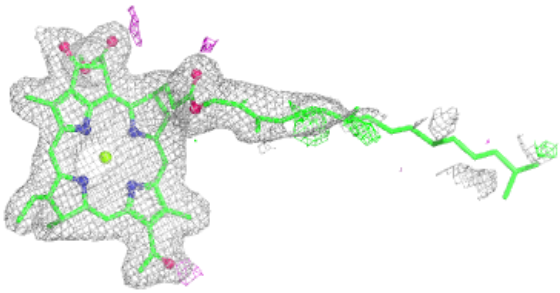


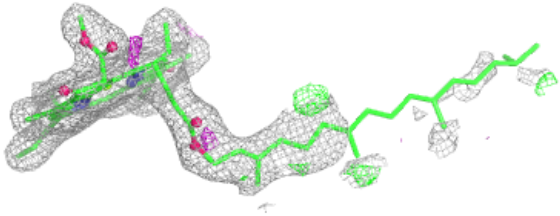




Electron density around BCB M 601:

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





Electron density around BPB M 605:

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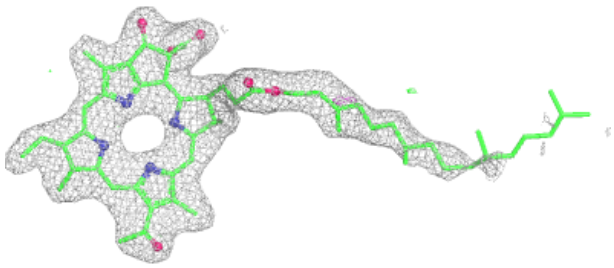
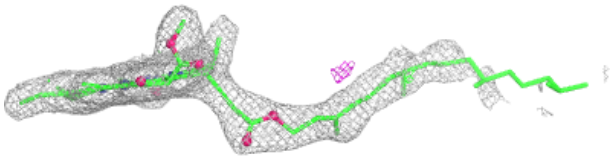
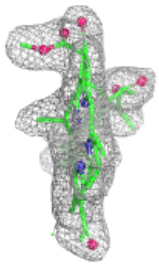
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

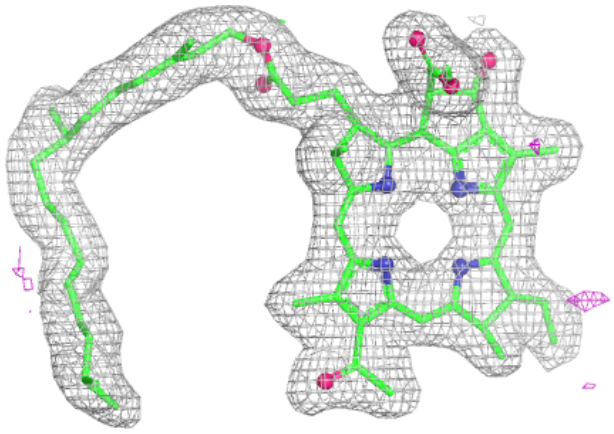


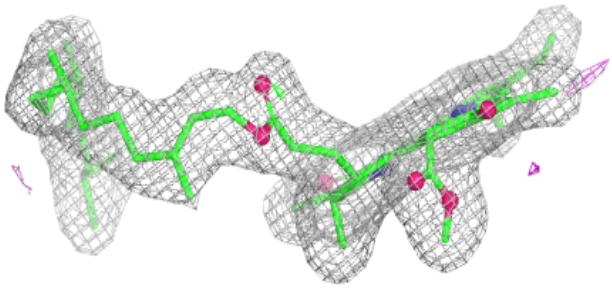




Electron density around BPB L 606:

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





Electron density around BCB L 604:

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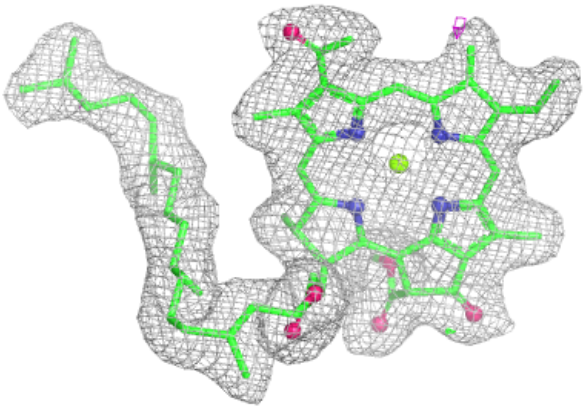
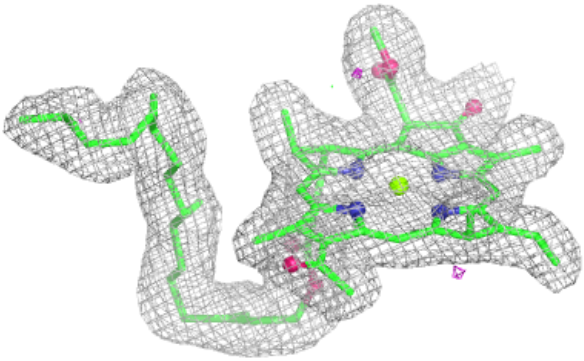
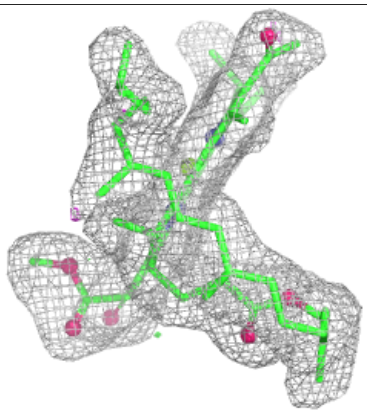
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BCB L 602:

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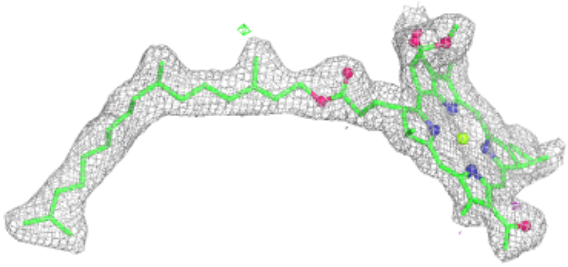
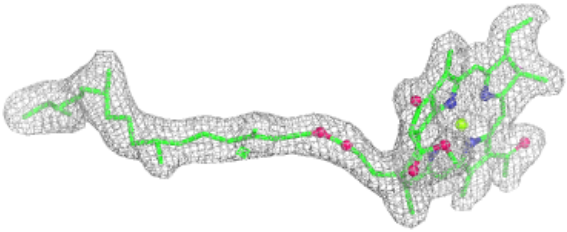
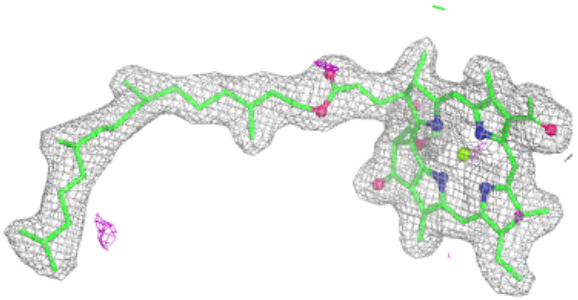
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

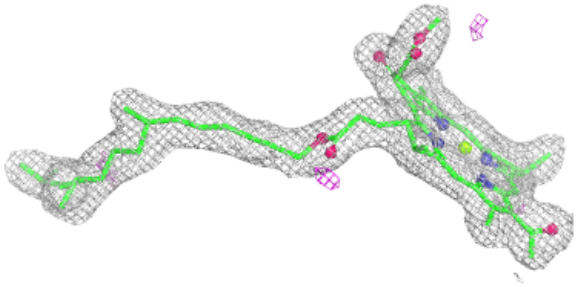


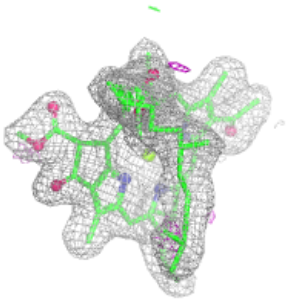


Electron density around BCB M 603:

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

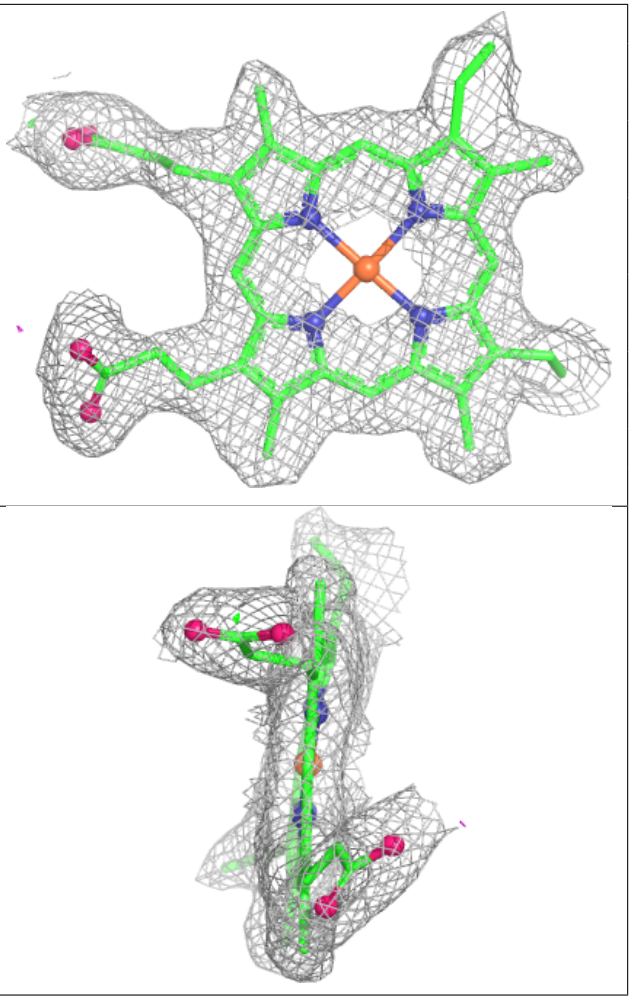






Electron density around HEC C 611:

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



Electron density around HEC C 612:

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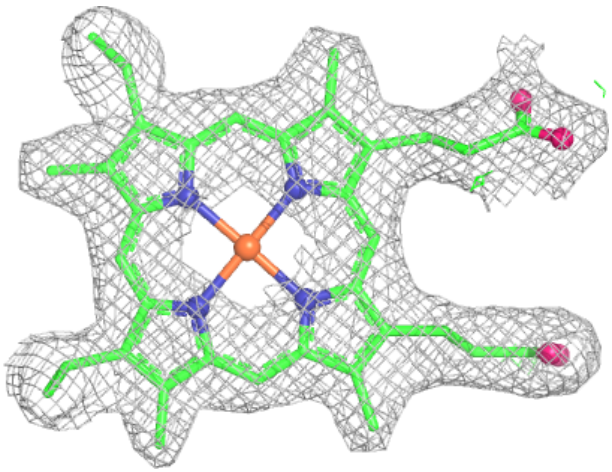
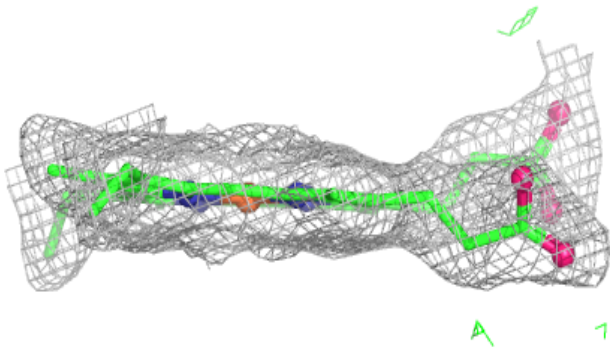
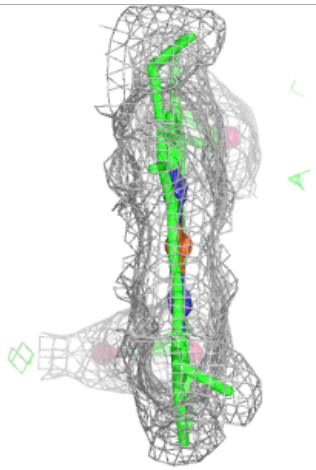
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEC C 609:

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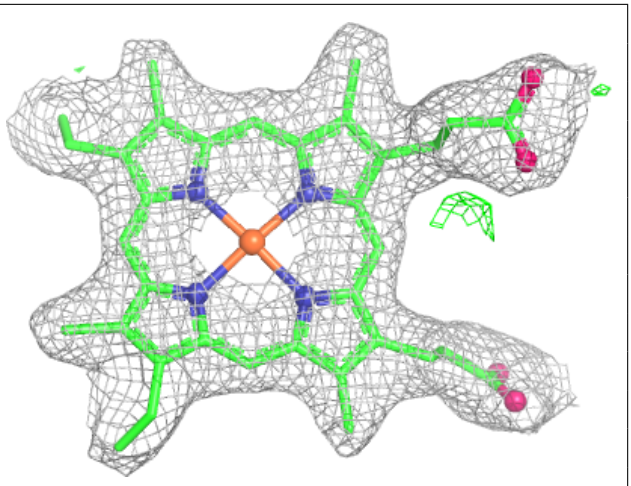
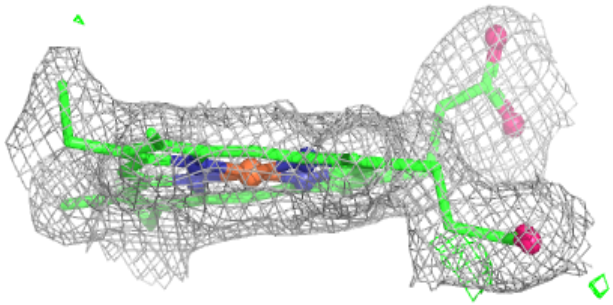
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEC C 610:

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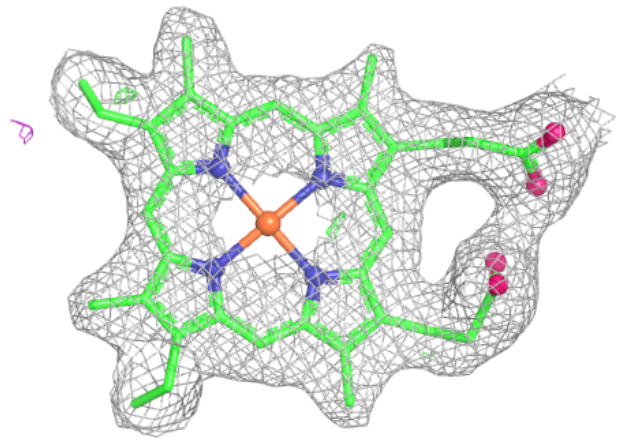
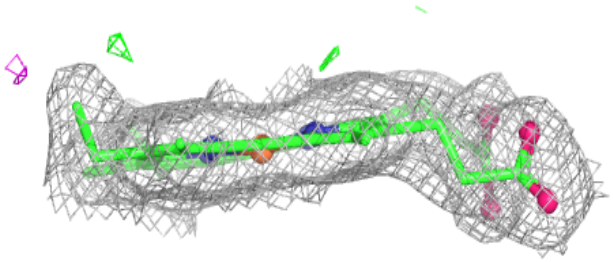
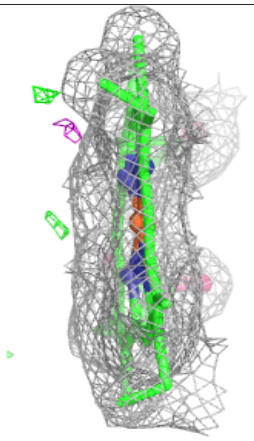
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.