

wwPDB X-ray Structure Validation Summary Report (i)

Jul 31, 2023 – 09:35 PM EDT

PDB ID : 7PRC

Title: PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEU-

DOMONAS VIRIDIS (DG-420315 (TRIAZINE) COMPLEX)

Authors : Lancaster, C.R.D.; Michel, H.

Deposited on : 1997-08-01

Resolution : 2.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.orgA 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 : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.34

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

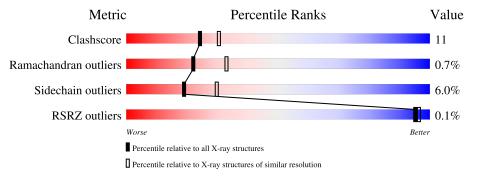
Validation Pipeline (wwPDB-VP) : 2.34

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 2.65 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	С	336	76%	20%	
2	L	273	78%	21%	•
3	M	323	76%	22%	-
4	Н	258	70%	26%	•

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	BPB	L	402	X	-	_	-



2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 10476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	C	332	Total	С	N	О	S	51	1	0
1		332	2607	1642	467	480	18	91	1	

• Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol Chain Re	Residues	Atoms				ZeroOcc	AltConf	Trace	
2 L	273	Total 2171	C 1459	N 350	O 355	S 7	14	0	0

• Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

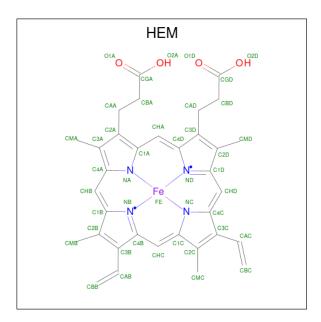
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	M	323	Total 2577	C 1720	N 421	O 425	S 11	19	2	0

• Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	П	258	Total	С	N	O	S	122	0	0
4	11	236	2018	1292	344	380	2	122	U	U

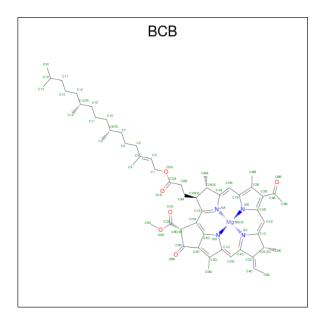
• Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	
5	С	1	Total	С	Fe	N	О	0	0	
9		1	43	34	1	4	4	0	U	
5	С	1	Total	С	Fe	N	О	0	0	
9		1	43	34	1	4	4	0	0	
5	С	1	Total	С	Fe	N	О	0	0	
9		1	43	34	1	4	4	0	U	
5	С	1	Total	С	Fe	N	О	0	0	
9	5 C	1	43	34	1	4	4	0		

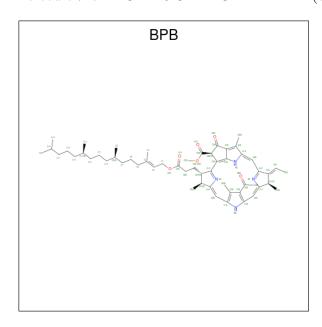
 $\bullet \ \ \mathrm{Molecule} \ 6 \ \mathrm{is} \ \mathrm{BACTERIOCHLOROPHYLL} \ \mathrm{B} \ (\mathrm{three-letter} \ \mathrm{code} \colon \ \mathrm{BCB}) \ (\mathrm{formula} \colon \ \mathrm{C}_{55}\mathrm{H}_{72}\mathrm{MgN}_4\mathrm{O}_6).$





Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	
6	Т	1	Total	С	Mg	N	О	0	0	
	ш	1	66	55	1	4	6	0		
6	Т	1	Total	С	Mg	N	О	0	0	
0		1	66	55	1	4	6	0		
6	М	1	Total	С	Mg	N	О	0	0	
0	IVI	1	66	55	1	4	6	U	0	
6	М	1	Total	С	Mg	N	О	0	0	
	M	1	66	55	1	4	6	U		

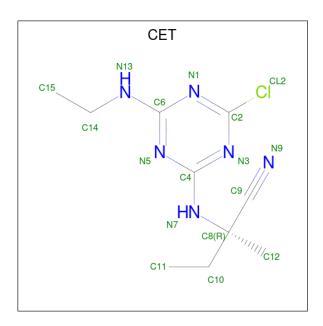
 $\bullet \ \ Molecule\ 7\ is\ BACTERIOPHEOPHYTIN\ B\ (three-letter\ code:\ BPB)\ (formula:\ C_{55}H_{74}N_4O_6).$



Ι	Mol	Chain	Residues	A	Aton	ns	ZeroOcc	AltConf
	7	L	1	Total 65			7	0
	7	L	1	Total 65			0	0

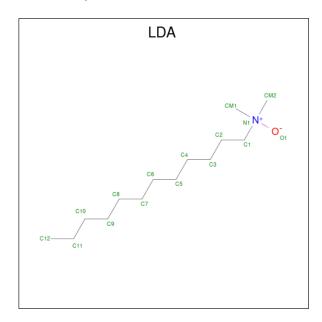
• Molecule 8 is 2-CHLORO-4-ETHYLAMINO-6-(R(+)-2'-CYANO-4-BUTYLAMINO)-1,3,5-TRIAZINE (three-letter code: CET) (formula: $C_{10}H_{15}ClN_6$).





Mo	Chain	Residues	Atoms				ZeroOcc	AltConf	
0	т	1	Total	С	Cl	N	0	0	
0	L	1	17	10	1	6	U		

 \bullet Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO).$



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

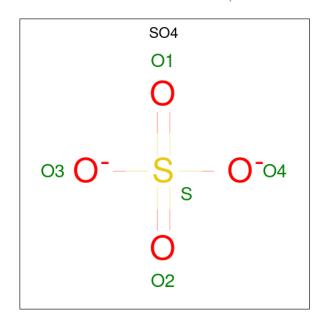


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total C N O	0	0
9	1V1	1	16 14 1 1	U	U
9	M	1	Total C N O	5	0
9	1V1	1	16 14 1 1		U
0	M	1	Total C N O	4	0
9	1V1	1	16 14 1 1	4	U
0	H	1	Total C N O	0	0
9	11	1	16 14 1 1	U	U

• Molecule 10 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

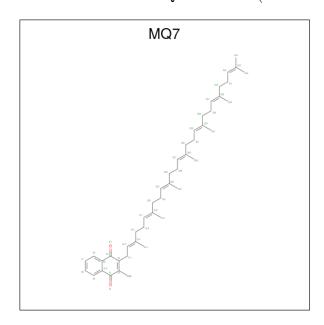
 \bullet Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total O S 5 4 1	0	0
11	M	1	Total O S 5 4 1	0	0
11	M	1	Total O S 5 4 1	0	0
11	Н	1	Total O S 5 4 1	0	0

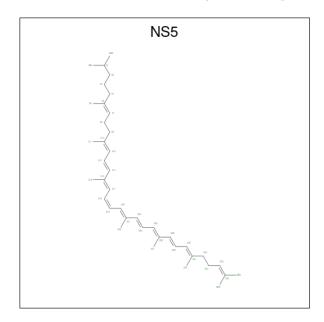


 \bullet Molecule 12 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $\rm C_{46}H_{64}O_2).$



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

 \bullet Molecule 13 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $\mathrm{C}_{40}\mathrm{H}_{60}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C 40 40	4	0

• Molecule 14 is water.



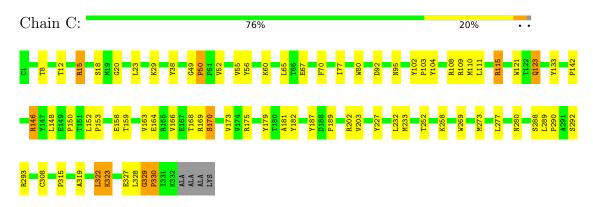
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	С	118	Total O 118 118	0	0
14	L	55	Total O 55 55	0	0
14	M	78	Total O 78 78	0	0
14	Н	64	Total O 64 64	0	0



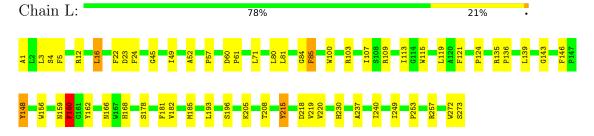
3 Residue-property plots (i)

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.

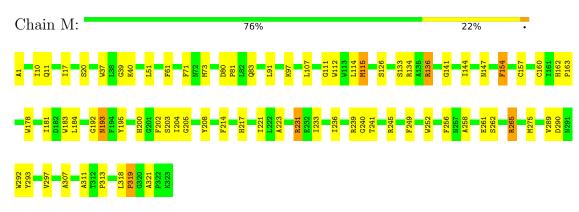
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER



• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

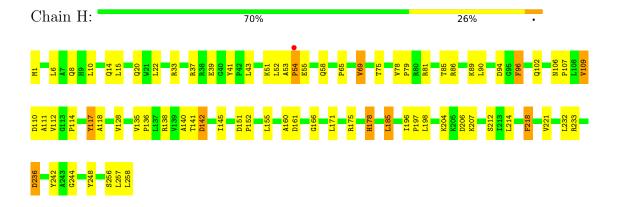


• Molecule 3: PHOTOSYNTHETIC REACTION CENTER



• Molecule 4: PHOTOSYNTHETIC REACTION CENTER







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	223.50Å 223.50Å 113.60Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 - 2.65	Depositor
rtesolution (A)	29.74 - 2.60	EDS
% Data completeness	88.3 (10.00-2.65)	Depositor
(in resolution range)	87.0 (29.74-2.60)	EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	3.59 (at 2.61Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
D D.	0.184 , 0.231	Depositor
R, R_{free}	0.180 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 90.4	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10476	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: FE2, LDA, CET, BCB, NS5, HEM, MQ7, FME, BPB, SO4

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).

Mal	Mol Chain	Bo	nd lengths	Bond angles		
MIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	С	0.55	0/2674	0.67	2/3645~(0.1%)	
2	L	0.58	0/2259	0.62	0/3084	
3	M	0.58	0/2683	0.62	0/3669	
4	Н	0.67	2/2055 $(0.1%)$	0.86	4/2807 (0.1%)	
All	All	0.59	$2/9671 \ (0.0\%)$	0.69	$6/13205 \; (0.0\%)$	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	С	0	4
2	L	0	7
3	M	0	5
4	Н	0	2
All	All	0	18

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	Ideal(Å)
4	Н	54	PRO	C-N	14.77	1.68	1.34
4	Н	52	LEU	C-N	-6.29	1.19	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
4	Н	52	LEU	O-C-N	-18.31	93.41	122.70
4	Н	52	LEU	CA-C-N	13.07	145.95	117.20
4	Н	52	LEU	C-N-CA	8.96	144.09	121.70



Mol	Chain	Res	Type	Atoms	${f Z}$	$Observed(^o)$	$\mathbf{Ideal}(^o)$
4	Н	53	ALA	CB-CA-C	-6.78	99.92	110.10
1	С	50	PRO	CB-CA-C	-5.63	97.93	112.00

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	С	15	ARG	Sidechain
1	С	187	TYR	Sidechain
1	С	202	ARG	Sidechain
1	С	227	TYR	Sidechain
2	L	85	PHE	Sidechain

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	С	2607	0	2575	54	0
2	L	2171	0	2098	46	0
3	M	2577	0	2468	60	0
4	Н	2018	0	2019	51	0
5	С	172	0	120	6	0
6	L	132	0	144	10	0
6	M	132	0	144	14	0
7	L	130	0	148	18	0
8	L	17	0	15	1	0
9	Н	16	0	31	1	0
9	L	16	0	31	0	0
9	M	64	0	124	5	0
10	M	1	0	0	0	0
11	Н	5	0	0	0	0
11	M	15	0	0	2	0
12	M	48	0	64	1	0
13	M	40	0	60	7	0
14	С	118	0	0	3	0
14	Н	64	0	0	0	0
14	L	55	0	0	1	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	M	78	0	0	2	0
All	All	10476	0	10041	216	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 11.

The worst 5 of 216 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
1100111 1	1100111 2	$\operatorname{distance}\ (ext{\AA})$	overlap (Å)
4:H:54:PRO:C	4:H:55:GLU:N	1.68	1.44
7:L:402:BPB:HHC	7:L:402:BPB:HBBB	1.54	0.90
6:M:805:BCB:HBB2	6:M:805:BCB:HHC	1.57	0.85
7:L:402:BPB:HHC	7:L:402:BPB:CBB	2.09	0.83
2:L:181:PHE:HB3	7:L:401:BPB:CBB	2.10	0.81

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	Percent	iles
1	C	331/336 (98%)	314 (95%)	14 (4%)	3 (1%)	17 2	26
2	L	271/273 (99%)	255 (94%)	14 (5%)	2 (1%)	22 3	33
3	M	323/323 (100%)	308 (95%)	12 (4%)	3 (1%)	17 2	26
4	Н	256/258~(99%)	241 (94%)	15 (6%)	0	100 1	.00
All	All	1181/1190 (99%)	1118 (95%)	55 (5%)	8 (1%)	22 3	33

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type	
3	M	51	LEU	



Mol	Chain	Res	Type
3	M	193	ASN
2	L	57	PRO
1	С	67	GLU
2	L	23	ASP

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	С	281/282 (100%)	263 (94%)	18 (6%)	17	27	
2	L	218/218 (100%)	212 (97%)	6 (3%)	43	61	
3	M	251/249 (101%)	238 (95%)	13 (5%)	23	36	
4	Н	212/212 (100%)	190 (90%)	22 (10%)	7	10	
All	All	962/961 (100%)	903 (94%)	59 (6%)	19	29	

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	97	LYS
4	Н	236	ASP
3	M	214	PHE
4	Н	212	SER
4	Н	142	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	183	ASN
2	L	214	GLN
2	L	239	ASN
3	M 14		ASN
4	Н	102	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	В	ond leng	gths	В	ond ang	gles
WIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	FME	Н	1	4	8,9,10	0.61	0	7,9,11	2.81	2 (28%)

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	Н	1	4	-	3/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
4	Н	1	FME	O1-CN-N	-5.63	110.45	125.27
4	Н	1	FME	CA-N-CN	-4.04	116.60	122.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

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



There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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).

N / 1	TD.	aı ·	ъ	т. 1	В	ond leng	$_{ m gths}$	Вс	ond angl	les
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEM	С	338	1	41,50,50	1.34	3 (7%)	45,82,82	1.09	3 (6%)
9	LDA	Н	703	-	12,15,15	2.27	1 (8%)	14,17,17	0.68	0
12	MQ7	M	501	-	49,49,49	1.49	12 (24%)	60,63,63	1.74	12 (20%)
9	LDA	M	706	-	12,15,15	2.19	1 (8%)	14,17,17	0.50	0
13	NS5	M	600	-	39,39,39	0.81	1 (2%)	44,46,46	1.20	6 (13%)
6	BCB	L	302	2	54,74,74	1.56	5 (9%)	52,115,115	2.03	10 (19%)
6	BCB	M	806	3	54,74,74	1.50	8 (14%)	52,115,115	2.45	12 (23%)
8	CET	L	502	-	16,17,17	1.34	2 (12%)	21,23,23	0.89	1 (4%)
11	SO4	M	804	-	4,4,4	0.90	0	6,6,6	0.70	0
5	HEM	С	339	1	41,50,50	1.50	5 (12%)	45,82,82	1.15	3 (6%)
9	LDA	L	702	-	12,15,15	2.27	1 (8%)	14,17,17	0.54	0
11	SO4	Н	801	-	4,4,4	0.55	0	6,6,6	0.33	0
9	LDA	M	704	-	12,15,15	1.93	1 (8%)	14,17,17	0.54	0
5	HEM	С	340	1	41,50,50	1.56	8 (19%)	45,82,82	1.48	10 (22%)
6	BCB	L	304	2	54,74,74	1.41	7 (12%)	52,115,115	2.47	15 (28%)
9	LDA	M	705	-	12,15,15	2.19	1 (8%)	14,17,17	0.50	0
7	BPB	L	402	-	49,70,70	1.41	7 (14%)	47,101,101	2.24	10 (21%)
11	SO4	M	802	-	4,4,4	0.57	0	6,6,6	0.83	0
11	SO4	M	803	-	4,4,4	0.67	0	6,6,6	0.78	0



Mol	Type	Chain	Res	Link	В	Bond lengths				Bond angles		
MIOI					Counts	RMSZ		# Z > 2	Counts	RMSZ	# Z > 2	
6	BCB	M	805	3	54,74,74	1.58		9 (16%)	52,115,115	2.35	13 (25%)	
7	BPB	L	401	-	49,70,70	1.32		7 (14%)	47,101,101	2.29	8 (17%)	
5	HEM	С	337	1	41,50,50	1.52		4 (9%)	45,82,82	1.31	6 (13%)	
9	LDA	M	701	-	12,15,15	2.49		1 (8%)	14,17,17	0.71	0	

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	HEM	С	338	1	-	6/12/54/54	-
9	LDA	Н	703	-	-	3/13/13/13	-
12	MQ7	M	501	-	-	2/41/61/61	0/2/2/2
9	LDA	M	706	-	-	4/13/13/13	-
13	NS5	M	600	-	-	14/43/43/43	-
6	BCB	L	302	2	-	7/37/177/177	-
6	BCB	M	806	3	-	12/37/177/177	-
8	CET	L	502	-	-	0/11/14/14	0/1/1/1
5	HEM	С	339	1	-	2/12/54/54	-
9	LDA	L	702	-	-	4/13/13/13	-
9	LDA	M	704	-	-	6/13/13/13	-
5	HEM	С	340	1	-	4/12/54/54	-
6	BCB	L	304	2	-	6/37/177/177	-
9	LDA	M	705	-	-	1/13/13/13	-
7	BPB	L	402	-	1/1/18/23	5/37/105/105	0/5/6/6
6	BCB	M	805	3	-	12/37/177/177	-
7	BPB	L	401	-	-	8/37/105/105	0/5/6/6
5	HEM	С	337	1	-	4/12/54/54	-
9	LDA	M	701	-	-	5/13/13/13	-

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\mathring{A})$	Ideal(Å)
9	M	701	LDA	O1-N1	-8.57	1.22	1.42
9	Н	703	LDA	O1-N1	-7.82	1.23	1.42
9	L	702	LDA	O1-N1	-7.79	1.23	1.42



N	/Iol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
	9	M	705	LDA	O1-N1	-7.56	1.24	1.42
	9	M	706	LDA	O1-N1	-7.53	1.24	1.42

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
7	L	401	BPB	O2D-CGD-CBD	10.76	124.63	111.00
6	L	304	BCB	O2D-CGD-CBD	10.33	124.09	111.00
7	L	402	BPB	O2D-CGD-CBD	9.29	122.77	111.00
6	M	806	BCB	O2D-CGD-CBD	8.68	121.99	111.00
6	M	805	BCB	O2D-CGD-CBD	7.75	120.82	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	L	402	BPB	C13

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	302	BCB	C4-C3-C5-C6
6	M	805	BCB	C3A-C2A-CAA-CBA
6	M	805	BCB	C2-C3-C5-C6
6	M	806	BCB	CAD-CBD-CGD-O1D
6	M	806	BCB	CAD-CBD-CGD-O2D

There are no ring outliers.

19 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	С	338	HEM	2	0
9	Н	703	LDA	1	0
12	M	501	MQ7	1	0
9	M	706	LDA	1	0
13	M	600	NS5	7	0
6	L	302	BCB	6	0
6	M	806	BCB	7	0
8	L	502	CET	1	0
11	M	804	SO4	1	0
5	С	339	HEM	1	0
9	M	704	LDA	2	0

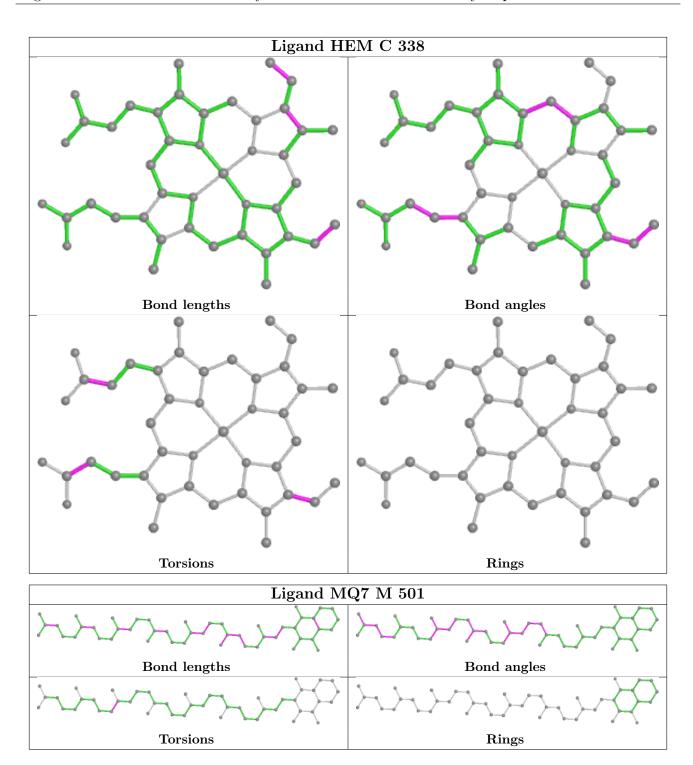


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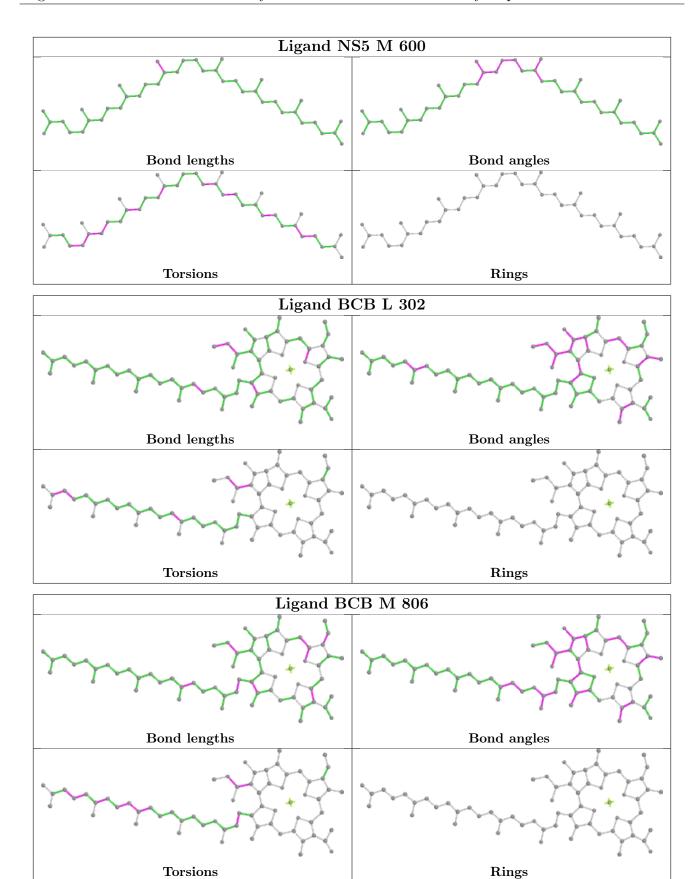
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	304	BCB	4	0
9	M	705	LDA	1	0
7	L	402	BPB	5	0
11	M	803	SO4	1	0
6	M	805	BCB	8	0
7	L	401	BPB	13	0
5	С	337	HEM	3	0
9	M	701	LDA	2	0

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.

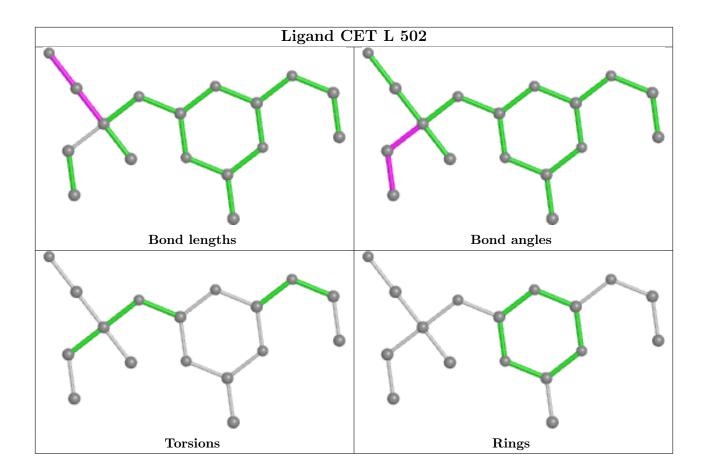




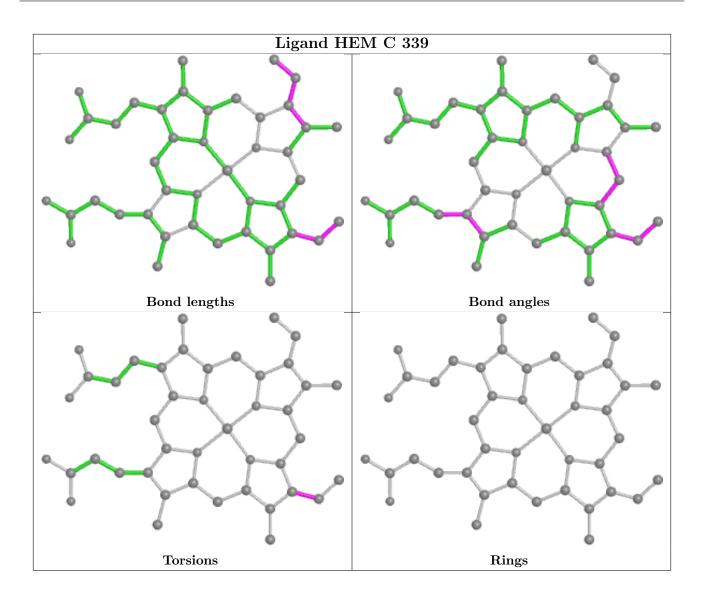




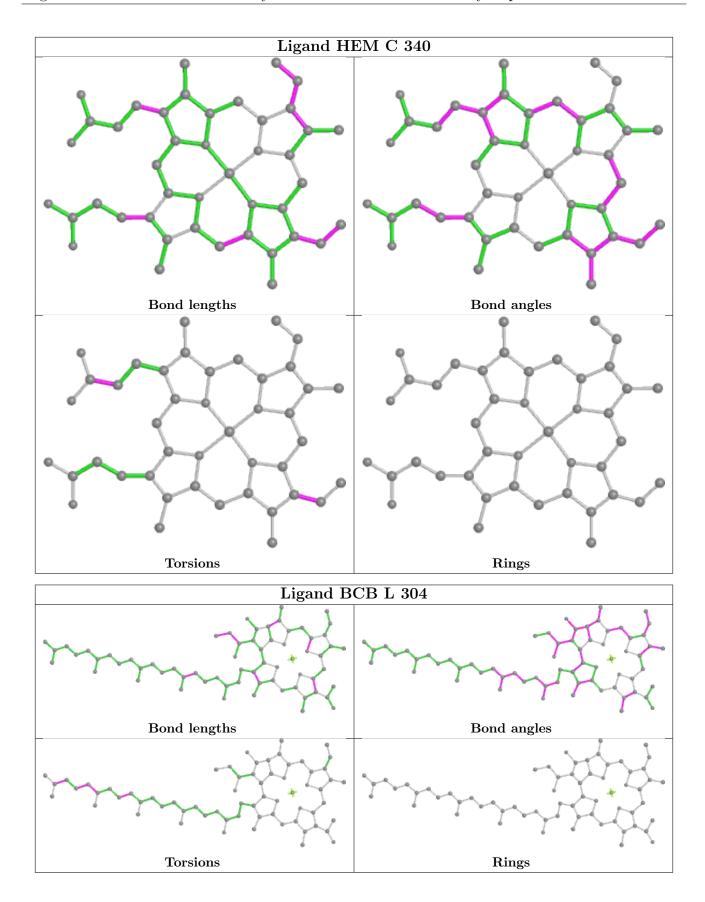




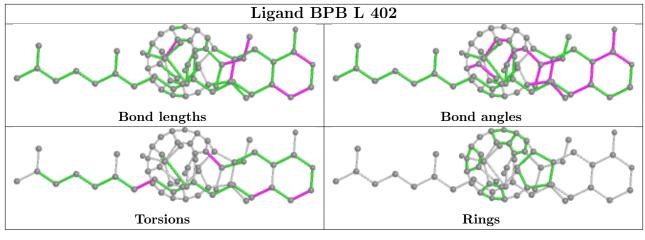


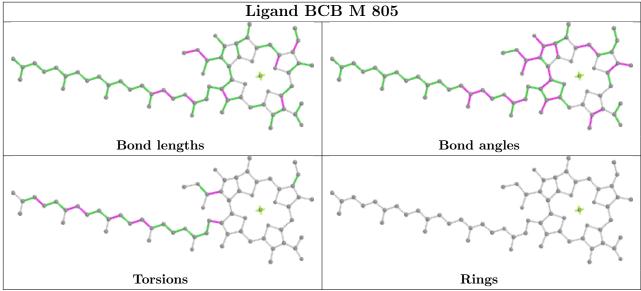


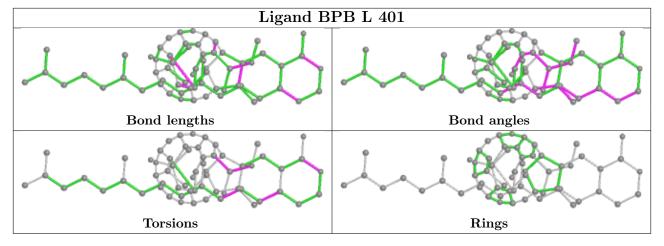




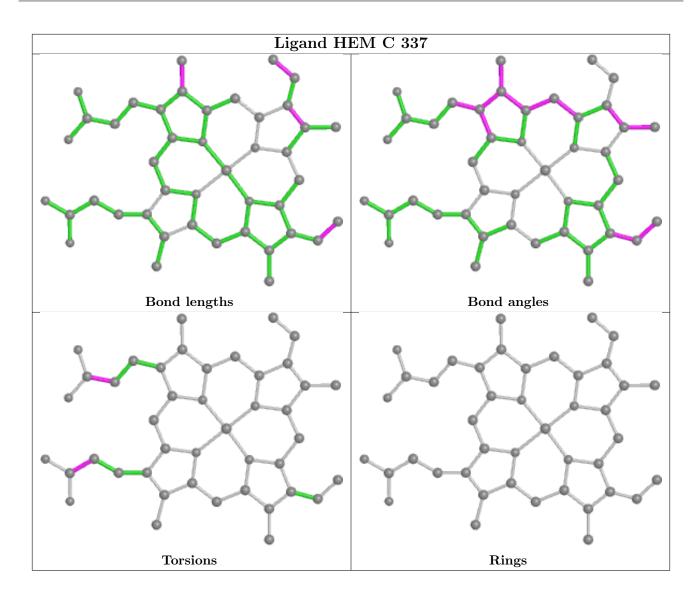












5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	Н	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Н	54:PRO	С	55:GLU	N	1.68



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Н	52:LEU	С	53:ALA	N	1.19



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<rsrz></rsrz>	$\#\mathrm{RSRZ}{>}2$	$egin{array}{ c c c c c c c c c c c c c c c c c c c$	9
1	С	332/336~(98%)	-0.77	0 100 100	4, 20, 44, 66 18 (5%	(c)
2	L	$273/273\ (100\%)$	-0.91	0 100 100	4, 16, 41, 61 6 (2%))
3	M	$323/323\ (100\%)$	-0.78	0 100 100	4, 18, 48, 60 10 (3%	(c)
4	Н	$249/258 \ (96\%)$	-0.65	1 (0%) 92 93	6, 27, 58, 76 19 (7%	(c)
All	All	1177/1190 (98%)	-0.78	1 (0%) 95 96	4, 20, 48, 76 53 (4%)	(c)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Н	54	PRO	3.3

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	FME	Н	1	10/11	0.96	0.10	23,30,40,42	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

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

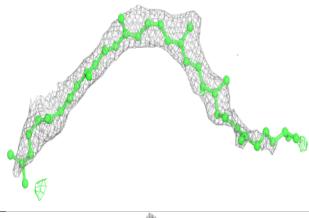
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathrm{A}}^2)$	Q<0.9
9	LDA	L	702	16/16	0.73	0.38	17,45,71,72	0
9	LDA	M	706	16/16	0.77	0.36	68,71,72,73	4
9	LDA	M	705	16/16	0.80	0.23	53,58,69,69	5
9	LDA	M	704	16/16	0.80	0.34	55,59,79,81	0
13	NS5	M	600	40/40	0.84	0.23	23,40,76,76	4
9	LDA	Н	703	16/16	0.93	0.22	27,38,57,58	0
12	MQ7	M	501	48/48	0.94	0.13	3,15,34,38	0
11	SO4	M	803	5/5	0.95	0.18	73,74,76,77	0
7	BPB	L	401	65/65	0.95	0.13	2,21,70,70	7
6	BCB	M	805	66/66	0.95	0.12	2,15,44,46	0
9	LDA	M	701	16/16	0.96	0.11	11,21,24,27	0
6	BCB	M	806	66/66	0.97	0.12	2,10,25,29	0
5	HEM	С	338	43/43	0.97	0.14	11,22,28,33	0
7	BPB	L	402	65/65	0.97	0.10	2,6,13,17	0
5	HEM	С	340	43/43	0.97	0.11	5,13,30,44	0
6	BCB	L	302	66/66	0.97	0.11	2,8,15,19	0
5	HEM	С	337	43/43	0.97	0.10	8,21,30,39	0
5	HEM	С	339	43/43	0.98	0.10	2,10,15,23	0
11	SO4	M	804	5/5	0.98	0.12	39,39,44,44	0
11	SO4	Н	801	5/5	0.98	0.09	56,56,57,57	0
6	BCB	L	304	66/66	0.98	0.12	2,6,21,27	0
8	CET	L	502	17/17	0.98	0.11	10,18,21,25	0
11	SO4	M	802	5/5	0.99	0.09	21,24,27,28	0
10	FE2	M	500	1/1	0.99	0.04	16,16,16,16	0

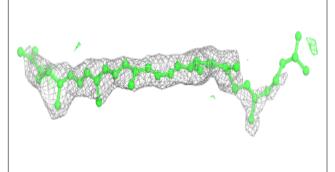
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

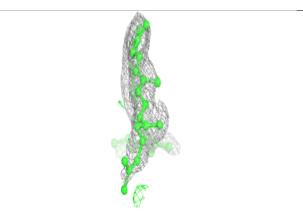


Electron density around NS5 M 600:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

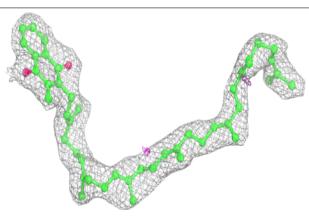


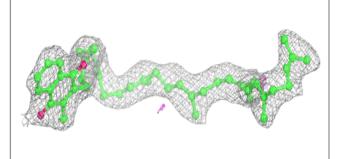


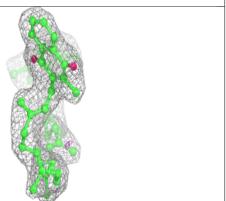


Electron density around MQ7 M 501:

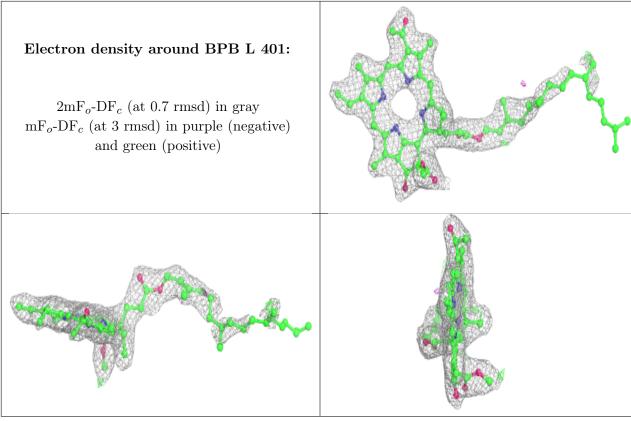
 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



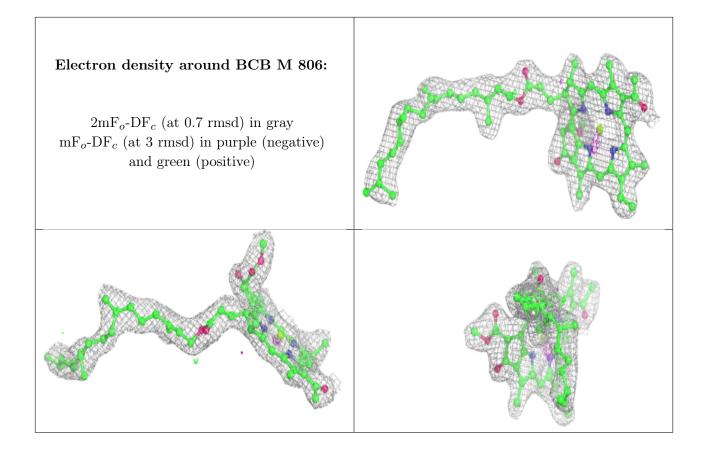




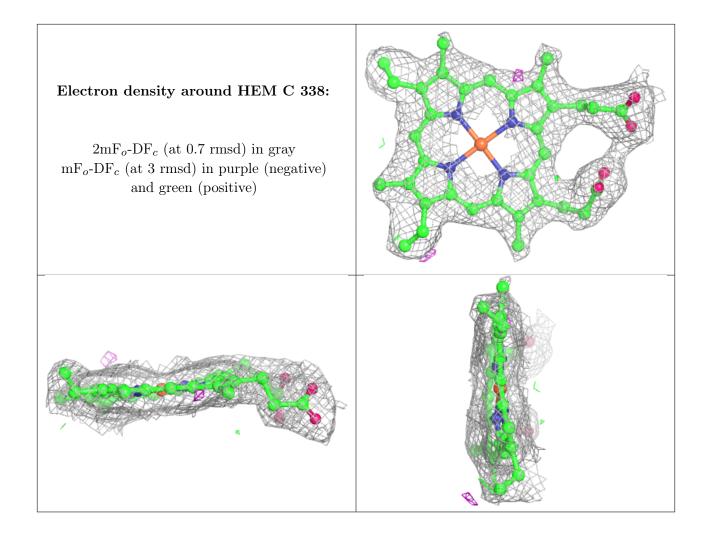




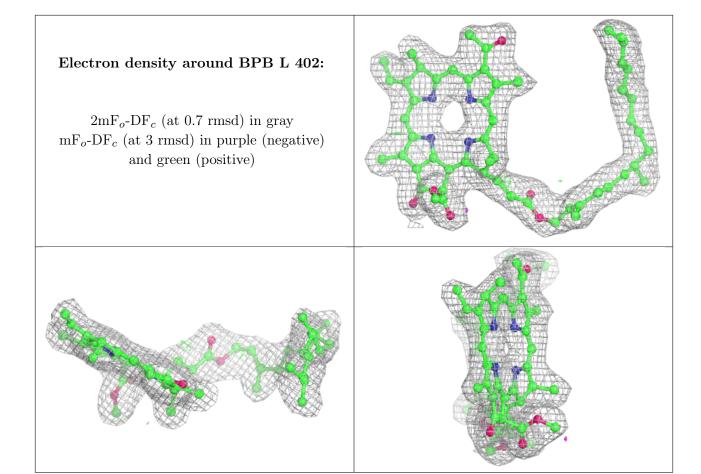






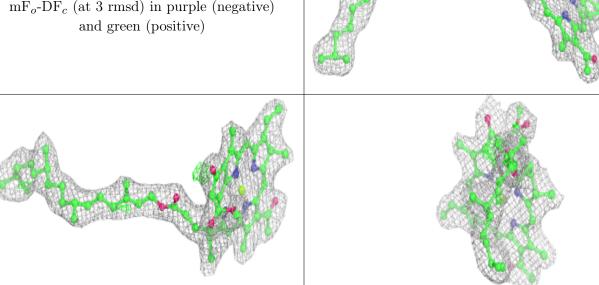




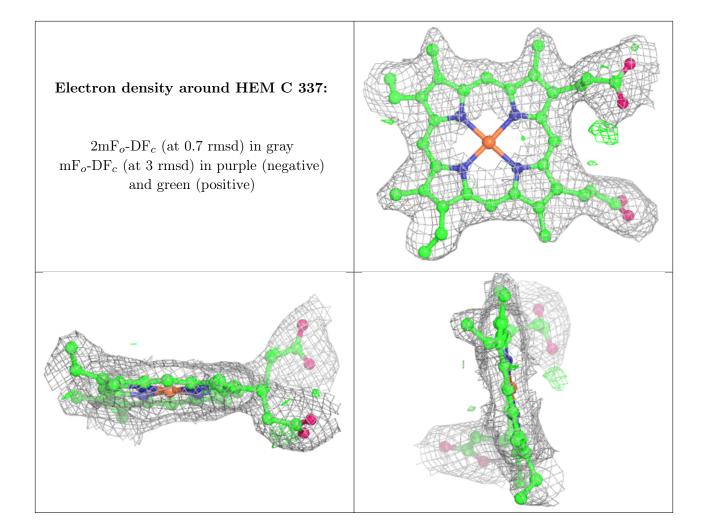




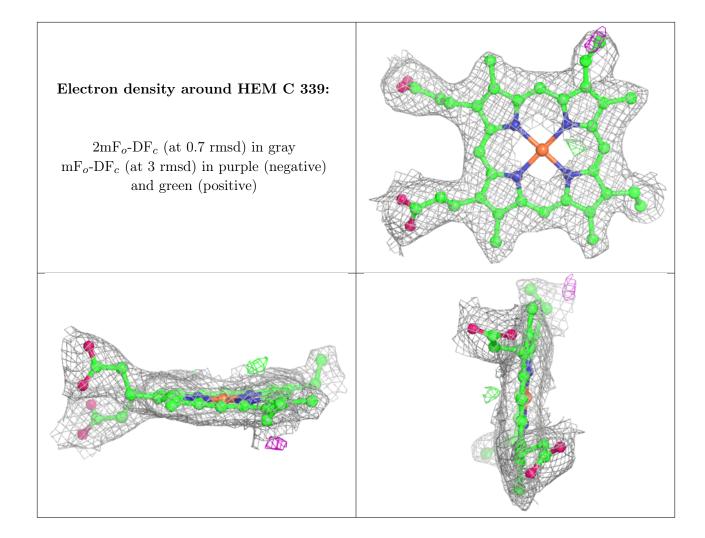
Electron density around HEM C 340: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around BCB L 302: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative)







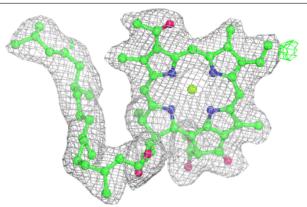


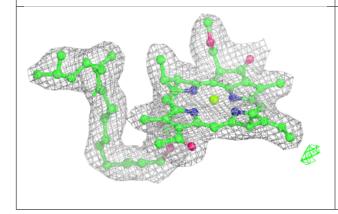


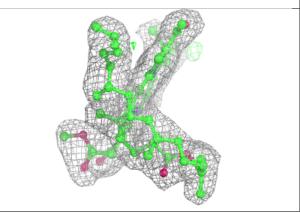


Electron density around BCB L 304:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

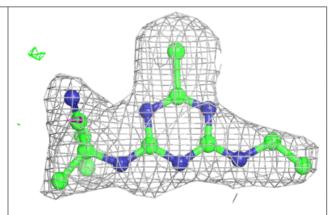


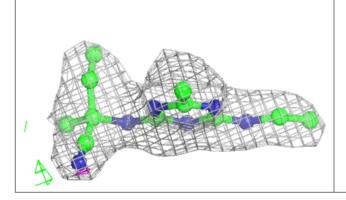


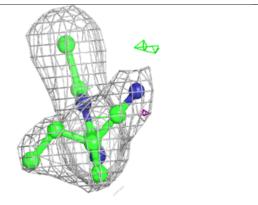


Electron density around CET L 502:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

