

wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 02:00 PM EDT

PDB ID : 3D38

Title : Crystal structure of new trigonal form of photosynthetic reaction center from

Blastochloris viridis. Crystals grown in microfluidics by detergent capture.

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(ATCG3D)

Deposited on : 2008-05-09

Resolution : 3.21 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.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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

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

Xtriage (Phenix) : 1.13

EDS : 2.35

buster-report : 1.1.7 (2018)

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

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

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

Validation Pipeline (wwPDB-VP) : 2.35

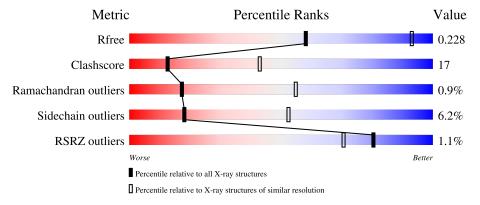


1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.21 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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	73%	24%	
2	Н	258	67%	27%	
3	L	273	72%	26%	•
4	M	323	72%	25%	•

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
11	UQ1	L	503	-	-	-	X
5	SO4	С	809	-	-	-	X
7	НТО	Н	705	-	-	-	X



2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 10311 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 cytochrome c subunit.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	C	332	Total	С	N	O	S	0	0	0
1		332	2598	1637	465	478	18	0	0	U

• Molecule 2 is a protein called Reaction center protein H chain.

\mathbf{Mol}	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace	
2	Н	250	Total 1958	C 1251	N 335	O 370	S 2	0	0	0	

• Molecule 3 is a protein called Reaction center protein L chain.

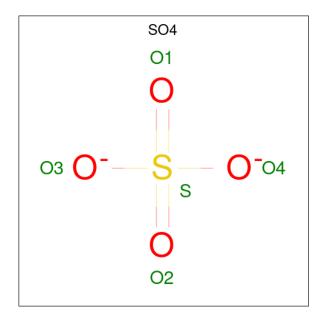
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	L	273	Total 2171	C 1459	N 350	O 355	S 7	0	0	0

• Molecule 4 is a protein called Reaction center protein M chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	M	323	Total 2555	C 1702	N 419	O 423	S 11	0	0	0

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	1	Total O S	0	0
	O	1	5 4 1		U
5	\mathbf{C}	1	Total O S	1 (1	0
		1	5 4 1		Ü
5	С	1	Total O S	1 (1	0
		_	5 4 1		Ü
5	\mathbf{C}	1	Total O S		0
			5 4 1		_
5	\mathbf{C}	1	Total O S	1 (1	0
			5 4 1		
5	\mathbf{C}	1	Total O S	1 (1	0
			5 4 1		
5	\mathbf{C}	1	Total O S	1 (1	0
			5 4 1 Total O S		
5	Н	1	$\begin{bmatrix} 10tal & 0 & 3 \\ 5 & 4 & 1 \end{bmatrix}$		0
			Total O S		
5	Η	1	$\begin{bmatrix} 10tal & 5 \\ 5 & 4 & 1 \end{bmatrix}$		0
			Total O S		
5	Н	1	$\begin{bmatrix} 5 & 4 & 1 \end{bmatrix}$	1 (1	0
			Total O S		_
5	Н	1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1 (1	0
	3.7	-	Total O S		
5	M	1	$\begin{bmatrix} 5 & 4 & 1 \end{bmatrix}$	1 (1	0
F	M	1	Total O S		0
5	M	1	5 4 1	0	0
5	M	1	Total O S	0	0
5	IVI	1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$		0

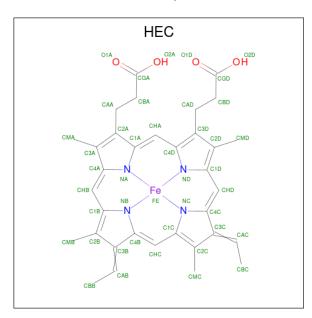
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total O S 5 4 1	0	0

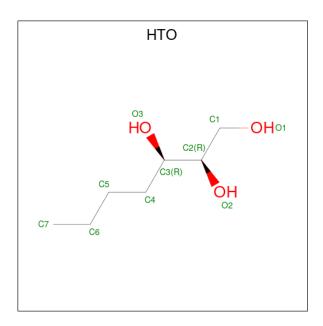
 \bullet Molecule 6 is HEME C (three-letter code: HEC) (formula: $\mathrm{C_{34}H_{34}FeN_4O_4}).$



Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	
6	С	1	Total	С	Fe	N	О	0	0	
0		1	43	34	1	4	4	0		
6	С	1	Total	С	Fe	N	О	0	0	
0		1	43	34	1	4	4	0		
6	С	1	Total	С	Fe	N	О	0	0	
0		1	43	34	1	4	4	0	U	
6	С	1	Total	С	Fe	N	О	0	0	
6	$^{\mathrm{C}}$	1	43	34	1	4	4	0	0	

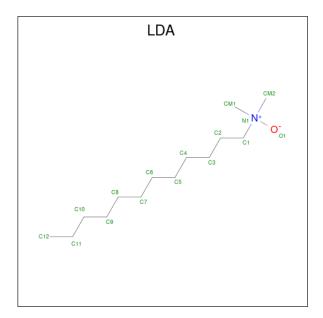
 \bullet Molecule 7 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $\mathrm{C_7H_{16}O_3}).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	С	1	Total C O		0
'		1	10 7 3	U	0
7	C	1	Total C O	0	0
'		1	10 7 3	U	0
7	П	1	Total C O	0	0
'	11	1	10 7 3	0	U

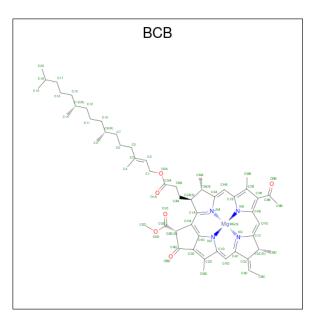
 \bullet Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Н	1	Total C N O	0	0
	11	1	16 14 1 1	U	U
Q	Н	1	Total C N O	0	0
0	11	1	16 14 1 1	U	0
0	т	1	Total C N O	0	0
0	Ъ	1	16 14 1 1	U	0
0	М	1	Total C N O	0	0
0	M	1	16 14 1 1	U	0

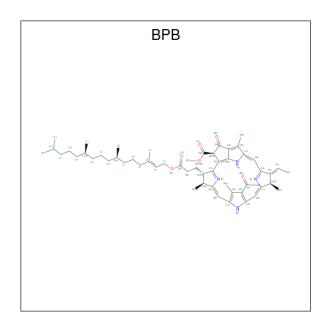
 $\bullet \ \ Molecule\ 9\ is\ BACTERIOCHLOROPHYLL\ B\ (three-letter\ code:\ BCB)\ (formula:\ C_{55}H_{72}MgN_4O_6).$



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	T	1	Total	С	Mg	N	О	0	0
9	П	1	66	55	1	4	6	U	
9	T	1	Total	С	Mg	N	О	0	0
9	ь	1	66	55	1	4	6	U	
9	М	M 1	Total	С	Mg	N	О	0	0
9	IVI		66	55	1	4	6	U	
9	M	M 1	Total	С	Mg	N	О	0	0
			66	55	1	4	6	U	

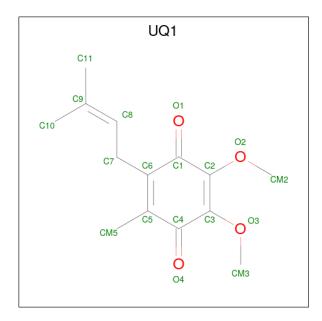
 $\bullet \ \ {\rm Molecule} \ 10 \ is \ BACTERIOPHEOPHYTIN \ B \ ({\rm three-letter} \ code: \ BPB) \ (formula: \ C_{55}H_{74}N_4O_6).$





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total 65				0	0
10	M	1	Total 65	_		_	0	0

 \bullet Molecule 11 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $\mathrm{C}_{14}\mathrm{H}_{18}\mathrm{O}_4).$



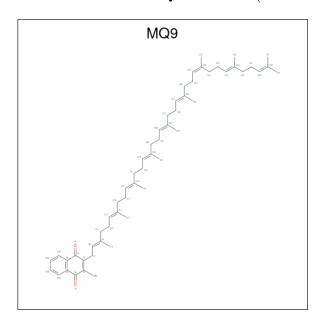
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total C O 18 14 4	0	0
11	L	1	Total C O 18 14 4	0	0



• Molecule 12 is FE (II) ION (three-letter code: FE2) (formula: Fe).

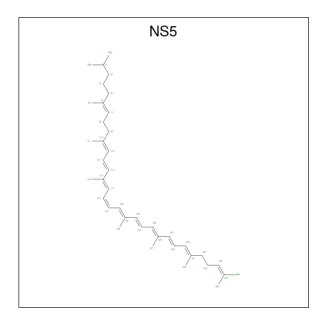
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	М	1	Total Fe 1 1	0	0

 \bullet Molecule 13 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $\mathrm{C}_{56}\mathrm{H}_{80}\mathrm{O}_2).$



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
13	M	1	Total 58	C 56	O 2	0	0

 \bullet Molecule 14 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $\mathrm{C_{40}H_{60}}).$





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

• Molecule 15 is water.

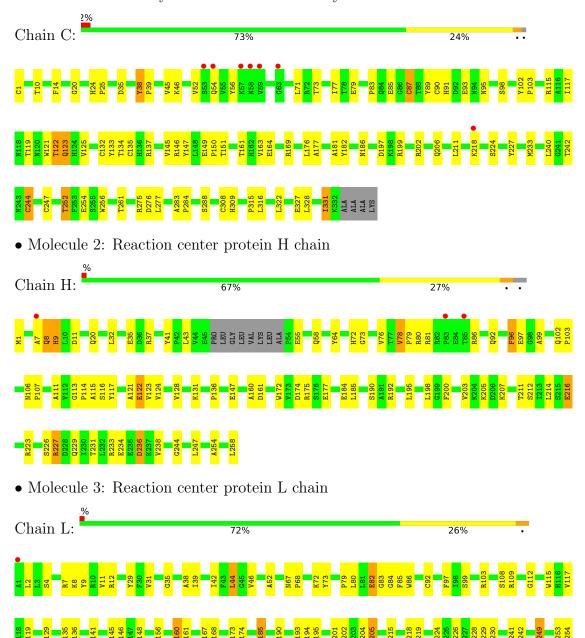
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	С	47	Total O 47 47	0	0
15	Н	28	Total O 28 28	0	0
15	L	38	Total O 38 38	0	0
15	M	46	Total O 46 46	0	0



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.

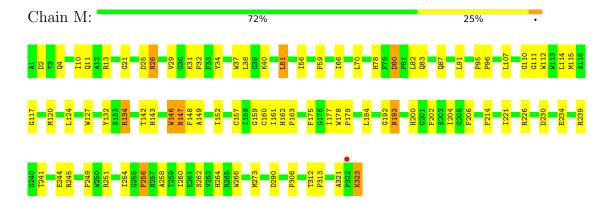
• Molecule 1: Photosynthetic reaction center cytochrome c subunit







• Molecule 4: Reaction center protein M chain





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 31 2 1	Depositor	
Cell constants	241.17Å 241.17Å 113.39Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	50.00 - 3.21	Depositor	
Resolution (A)	47.92 - 3.21	EDS	
% Data completeness	99.6 (50.00-3.21)	Depositor	
(in resolution range)	99.6 (47.92-3.21)	EDS	
R_{merge}	0.17	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.78 (at 3.19Å)	Xtriage	
Refinement program	REFMAC 5.4.0073	Depositor	
R, R_{free}	0.192 , 0.224	Depositor	
it, it free	0.196 , 0.228	DCC	
R_{free} test set	3145 reflections (5.07%)	wwPDB-VP	
Wilson B-factor (Å ²)	74.4	Xtriage	
Anisotropy	0.053	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31, 68.6	EDS	
L-test for twinning ²	$< L > = 0.47, < L^2> = 0.30$	Xtriage	
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage	
F_o, F_c correlation	0.92	EDS	
Total number of atoms	10311	wwPDB-VP	
Average B, all atoms (Å ²)	67.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.40% 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: SO4, HEC, MQ9, NS5, FE2, HTO, FME, BPB, LDA, BCB, UQ1

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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	С	0.53	1/2665~(0.0%)	0.64	0/3633	
2	Н	0.59	0/1993	0.68	0/2720	
3	L	0.60	$1/2259 \ (0.0\%)$	0.66	0/3084	
4	M	0.57	0/2659	0.65	1/3637~(0.0%)	
All	All	0.57	2/9576~(0.0%)	0.66	1/13074~(0.0%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	Ideal(Å)
1	С	87	CYS	CB-SG	-5.84	1.72	1.81
3	L	129	CYS	CB-SG	-5.38	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z} = {f Observed}(^o)$		$\mathrm{Ideal}(^{o})$
4	M	70	LEU	CA-CB-CG	7.57	132.71	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	2598	0	2573	82	0

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Mol	Chain	Non-H		H(added)	Clashes	Symm-Clashes
2	Н	1958	0	1946	65	0
3	L	2171	0	2098	64	0
4	M	2555	0	2452	76	0
5	С	35	0	0	0	0
5	Н	20	0	0	1	0
5	M	20	0	0	1	0
6	С	172	0	125	31	0
7	С	20	0	32	1	0
7	Н	10	0	16	2	0
8	Н	32	0	62	6	0
8	L	16	0	31	2	0
8	M	16	0	31	0	0
9	L	132	0	144	24	0
9	M	132	0	144	27	0
10	L	65	0	74	9	0
10	M	65	0	74	20	0
11	L	36	0	36	4	0
12	M	1	0	0	0	0
13	M	58	0	80	3	0
14	M	40	0	60	11	0
15	С	47	0	0	9	0
15	Н	28	0	0	5	0
15	L	38	0	0	3	0
15	M	46	0	0	7	0
All	All	10311	0	9978	337	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 337 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

	Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
	1:C:90:CYS:SG	6:C:401:HEC:HAC	1.31	1.69
	1:C:132:CYS:SG	6:C:402:HEC:HAB	1.48	1.52
	1:C:244:CYS:SG	6:C:403:HEC:HAB	1.54	1.47
Ī	1:C:132:CYS:SG	6:C:402:HEC:CAB	2.08	1.39
	1:C:135:CYS:SG	6:C:402:HEC:CAC	2.12	1.37

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	С	330/336 (98%)	294 (89%)	35 (11%)	1 (0%)	41 74
2	Н	246/258 (95%)	220 (89%)	22 (9%)	4 (2%)	9 42
3	L	271/273 (99%)	246 (91%)	24 (9%)	1 (0%)	34 69
4	M	321/323 (99%)	290 (90%)	26 (8%)	5 (2%)	9 42
All	All	1168/1190 (98%)	1050 (90%)	107 (9%)	11 (1%)	17 55

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Н	147	GLU
2	Н	73	GLY
4	M	32	PRO
4	M	51	LEU
4	M	193	ASN

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	F	erce	entiles
1	С	280/282 (99%)	266 (95%)	14 (5%)		24	59
2	Н	$205/212\ (97\%)$	188 (92%)	17 (8%)		11	40
3	L	218/218 (100%)	203 (93%)	15 (7%)		15	48
4	M	249/249 (100%)	236 (95%)	13 (5%)		23	58
All	All	952/961 (99%)	893 (94%)	59 (6%)		18	52



5	of 59	residues	with a	non-rotameric	sidechain	are listed	helow.
v	$o_1 o_2$	TOSIGUES	vv i ti i i ca	11011=101001110110	описсивии	anc moteri	17(/1(/)//.

Mol	Chain	Res	Type
2	Н	227	ARG
4	M	230	ASP
3	L	44	LEU
4	M	214	PHE
4	M	40	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
4	M	4	GLN
4	M	147	ASN
4	M	78	HIS
2	Н	106	ASN
3	L	239	ASN

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	Dog	Link	\mathbf{B}_{0}	ond leng	gths	В	ond ang	gles
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	Н	1	2	8,9,10	0.83	0	7,9,11	3.72	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
2	FME	Н	1	2	-	4/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
2	Н	1	FME	CA-N-CN	-9.15	108.76	122.82
2	Н	1	FME	CE-SD-CG	2.39	108.62	100.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

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 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 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).

М	1 Trms	Chain	Res	Timle	Bond lengths			Bond angles		
Mol	ol Type			Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	НТО	С	706	-	9,9,9	0.27	0	10,10,10	0.75	0
5	SO4	Н	807	-	4,4,4	0.13	0	6,6,6	0.33	0



N T 1	TD.	aı ·	ъ	т. 1	В	ond leng	$_{ m gths}$	Во	ond ang	les
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
9	BCB	M	401	4	54,74,74	2.12	8 (14%)	52,115,115	2.02	15 (28%)
9	BCB	L	401	3	54,74,74	1.93	6 (11%)	52,115,115	2.11	11 (21%)
11	UQ1	L	502	-	18,18,18	2.19	2 (11%)	22,25,25	1.37	4 (18%)
9	BCB	L	400	3	54,74,74	2.02	7 (12%)	52,115,115	1.95	14 (26%)
7	НТО	С	707	-	9,9,9	0.66	0	10,10,10	0.55	0
5	SO4	M	804	-	4,4,4	0.16	0	6,6,6	0.29	0
7	НТО	Н	705	-	9,9,9	0.69	0	10,10,10	0.83	0
5	SO4	С	809	_	4,4,4	0.14	0	6,6,6	0.10	0
13	MQ9	M	501	-	59,59,59	1.80	18 (30%)	72,75,75	1.56	20 (27%)
6	HEC	С	403	1	32,50,50	1.76	3 (9%)	24,82,82	1.28	2 (8%)
10	BPB	L	402	-	49,70,70	1.84	6 (12%)	47,101,101	1.96	15 (31%)
8	LDA	L	702	-	12,15,15	2.10	1 (8%)	14,17,17	0.63	0
8	LDA	M	704	-	12,15,15	2.16	1 (8%)	14,17,17	0.44	0
9	BCB	M	400	4	54,74,74	1.78	6 (11%)	52,115,115	2.02	13 (25%)
5	SO4	Н	806	-	4,4,4	0.17	0	6,6,6	0.26	0
5	SO4	Н	812	-	4,4,4	0.16	0	6,6,6	0.19	0
6	HEC	С	401	1	32,50,50	1.95	3 (9%)	24,82,82	1.26	1 (4%)
5	SO4	С	814	-	4,4,4	0.12	0	6,6,6	0.36	0
6	HEC	С	402	1	32,50,50	1.79	2 (6%)	24,82,82	1.47	3 (12%)
5	SO4	С	815	-	4,4,4	0.15	0	6,6,6	0.23	0
5	SO4	С	811	-	4,4,4	0.17	0	6,6,6	0.23	0
8	LDA	Н	701	-	12,15,15	2.03	1 (8%)	14,17,17	0.47	0
5	SO4	Н	803	-	4,4,4	0.17	0	6,6,6	0.24	0
14	NS5	M	600	-	39,39,39	1.57	3 (7%)	44,46,46	1.93	13 (29%)
5	SO4	M	801	-	4,4,4	0.21	0	6,6,6	0.63	0
5	SO4	С	810	-	4,4,4	0.15	0	6,6,6	0.09	0
11	UQ1	L	503	-	18,18,18	2.23	2 (11%)	22,25,25	1.23	2 (9%)
10	BPB	M	402	-	49,70,70	1.77	7 (14%)	47,101,101	1.98	10 (21%)
6	HEC	С	404	1	32,50,50	1.73	2 (6%)	24,82,82	1.46	3 (12%)
5	SO4	M	802	-	4,4,4	0.18	0	6,6,6	0.19	0
5	SO4	С	808	-	4,4,4	0.11	0	6,6,6	0.19	0
5	SO4	M	805	-	4,4,4	0.18	0	6,6,6	0.42	0
5	SO4	С	813	-	4,4,4	0.09	0	6,6,6	0.27	0
8	LDA	Н	703	-	12,15,15	1.92	1 (8%)	14,17,17	0.53	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
7	НТО	С	706	-	-	5/10/10/10	-
9	BCB	M	401	4	-	17/37/177/177	-
9	BCB	L	401	3	-	9/37/177/177	-
11	UQ1	L	502	-	-	4/9/33/33	0/1/1/1
9	BCB	L	400	3	-	16/37/177/177	-
7	НТО	С	707	-	-	8/10/10/10	-
7	НТО	Н	705	-	-	8/10/10/10	-
13	MQ9	M	501	-	-	16/53/73/73	0/2/2/2
6	HEC	С	403	1	-	4/10/54/54	-
10	BPB	L	402	-	-	15/37/105/105	0/5/6/6
8	LDA	L	702	-	-	11/13/13/13	-
9	BCB	M	400	4	-	13/37/177/177	-
8	LDA	M	704	-	-	9/13/13/13	-
6	HEC	С	402	1	-	4/10/54/54	-
6	HEC	С	401	1	-	2/10/54/54	-
8	LDA	Н	701	-	-	8/13/13/13	-
14	NS5	M	600	-	-	14/43/43/43	-
11	UQ1	L	503	-	-	0/9/33/33	0/1/1/1
10	BPB	M	402	-	-	14/37/105/105	0/5/6/6
6	HEC	С	404	1	_	4/10/54/54	-
8	LDA	Н	703	-	-	6/13/13/13	-

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
11	L	502	UQ1	C6-C5	8.12	1.50	1.35
11	L	503	UQ1	C6-C5	8.07	1.50	1.35
9	M	401	BCB	CAC-C3C	7.87	1.53	1.33
10	L	402	BPB	CAC-C3C	7.79	1.53	1.33
9	L	400	BCB	CAC-C3C	7.77	1.53	1.33

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^o)$
10	M	402	BPB	O2D-CGD-CBD	8.19	121.37	111.00
9	L	401	BCB	O2D-CGD-CBD	7.99	121.11	111.00
9	M	400	BCB	O2D-CGD-CBD	7.71	120.76	111.00
9	M	401	BCB	O2D-CGD-CBD	7.14	120.05	111.00

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\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^o)$
10	L	402	BPB	O2D-CGD-CBD	6.88	119.71	111.00

There are no chirality outliers.

5 of 187 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	С	404	HEC	C2D-C3D-CAD-CBD
6	С	404	HEC	C4D-C3D-CAD-CBD
7	С	706	НТО	C1-C2-C3-O3
7	С	706	НТО	O2-C2-C3-O3
7	С	706	НТО	O2-C2-C3-C4

There are no ring outliers.

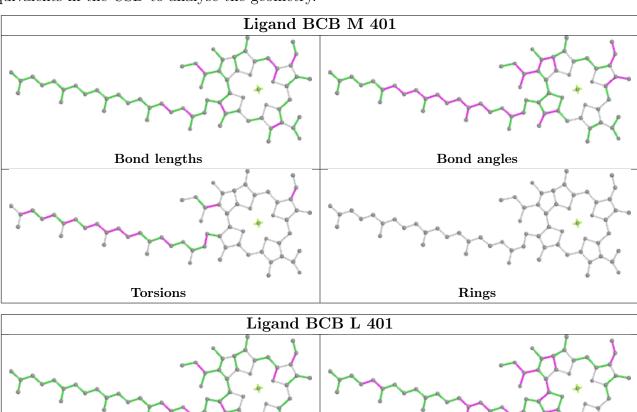
19 monomers are involved in 129 short contacts:

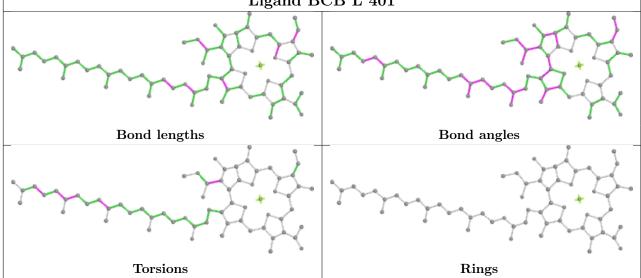
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	С	706	НТО	1	0
5	Н	807	SO4	1	0
9	M	401	BCB	17	0
9	L	401	BCB	10	0
11	L	502	UQ1	4	0
9	L	400	BCB	17	0
7	Н	705	НТО	2	0
13	M	501	MQ9	3	0
6	С	403	HEC	6	0
10	L	402	BPB	9	0
8	L	702	LDA	2	0
9	M	400	BCB	11	0
6	С	401	HEC	13	0
6	С	402	HEC	10	0
14	M	600	NS5	11	0
10	M	402	BPB	20	0
6	С	404	HEC	2	0
5	M	805	SO4	1	0
8	Н	703	LDA	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

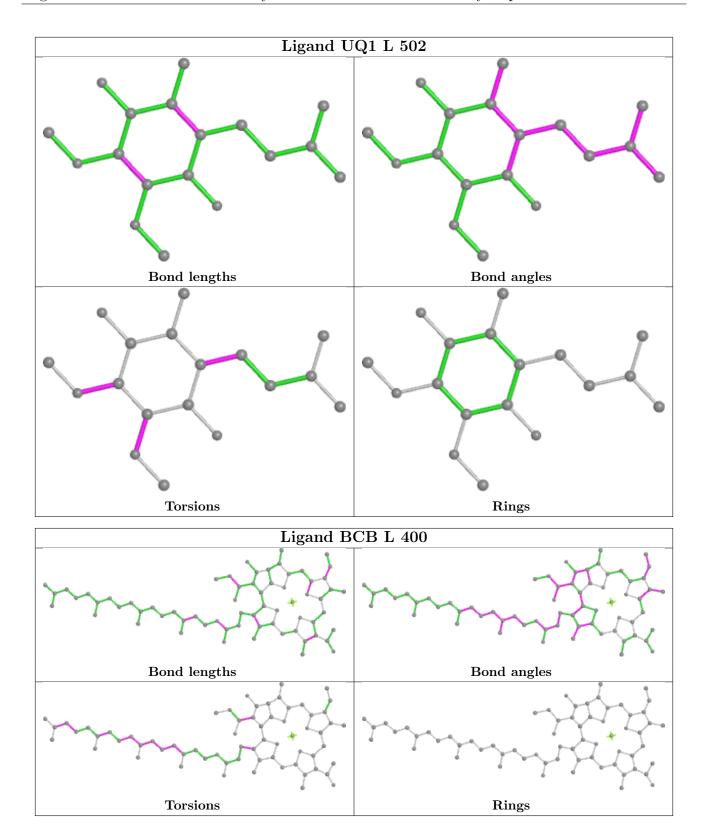


highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

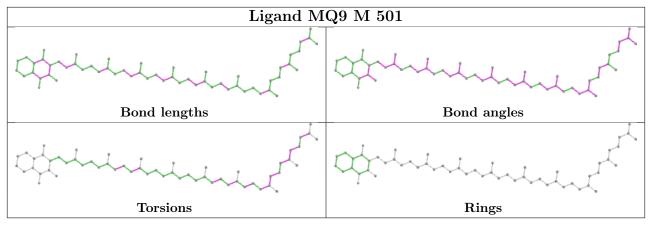


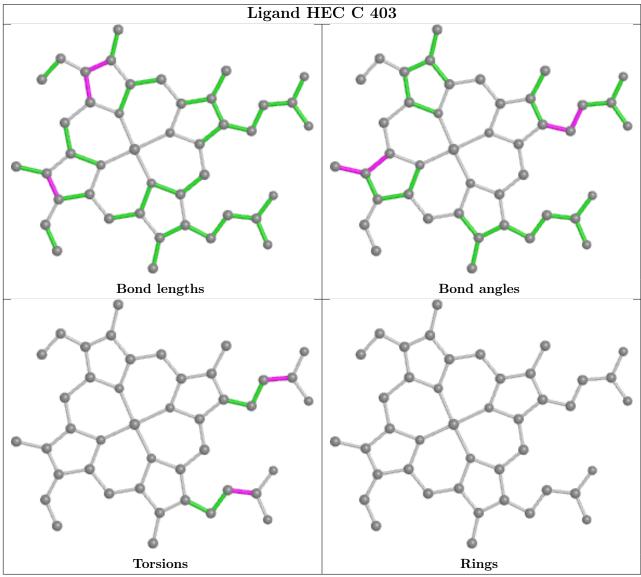




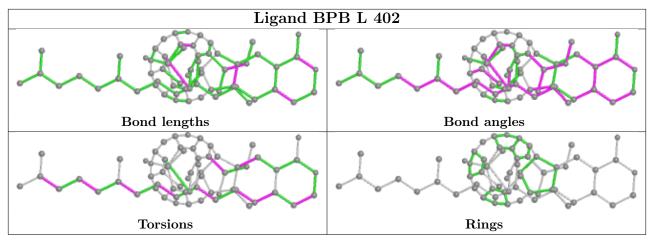


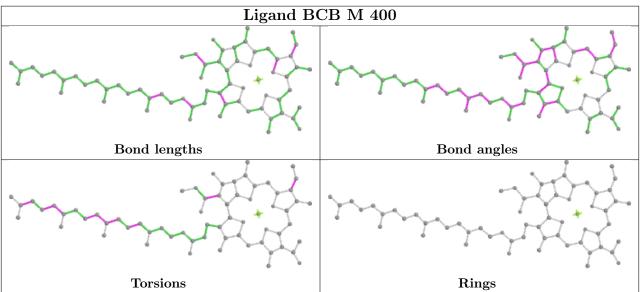




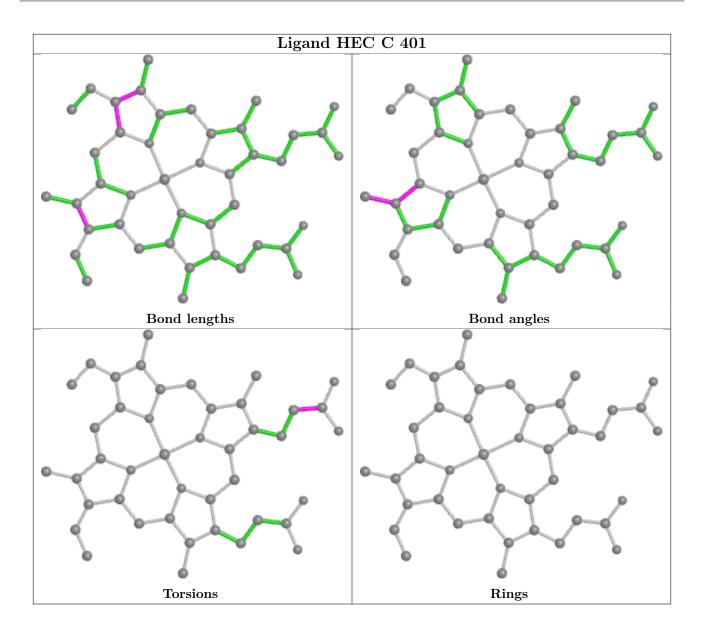




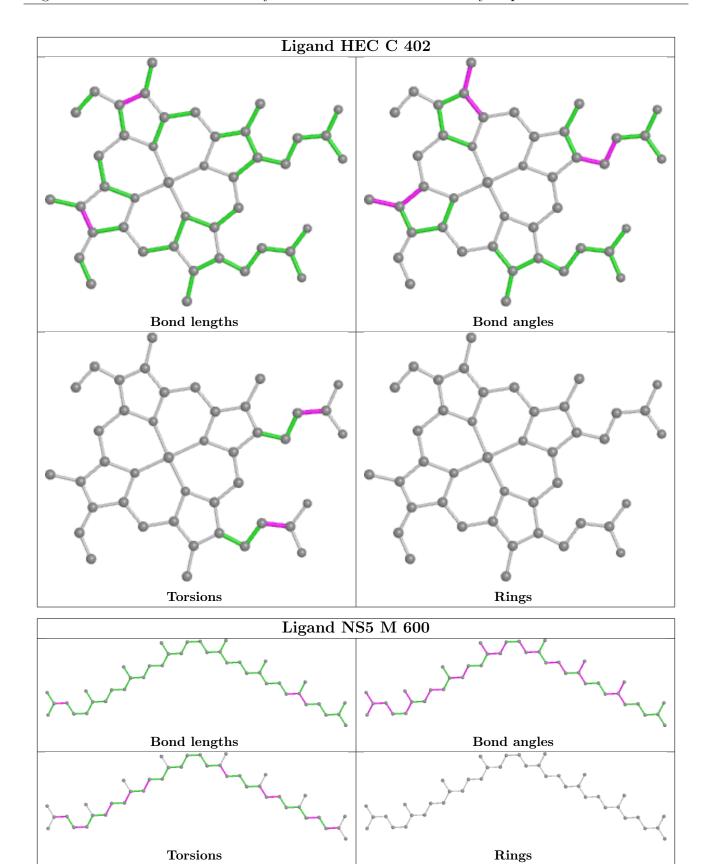




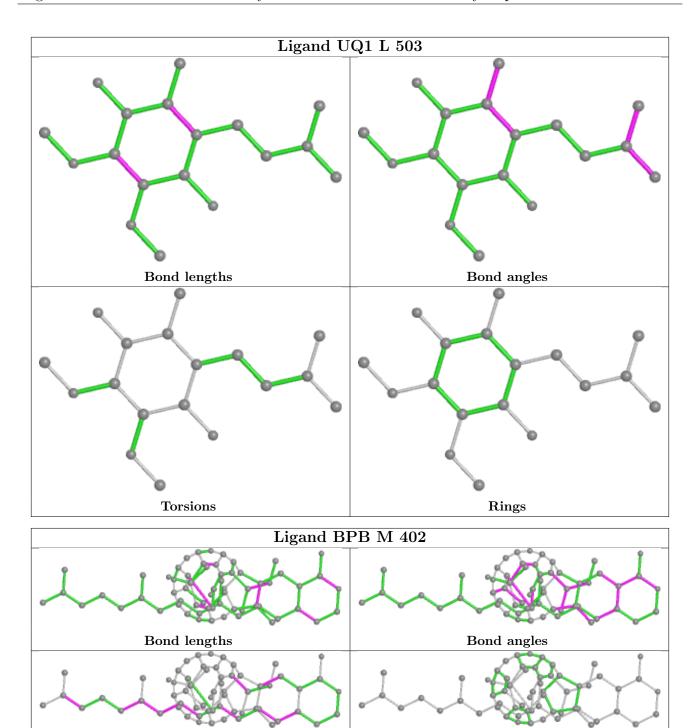








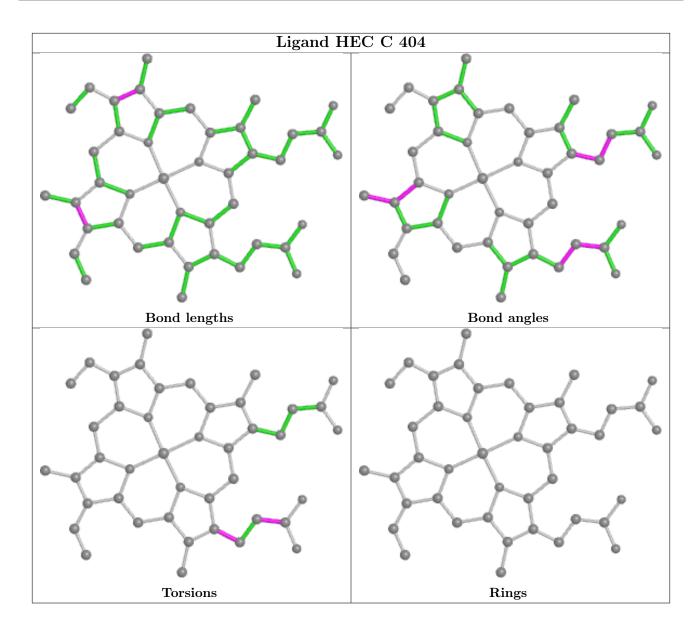






Rings

Torsions



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, 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>	# RSRZ > 2		$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9	
1	С	332/336 (98%)	-0.24	7 (2%)	63	50	46, 74, 113, 124	0
2	Н	249/258 (96%)	-0.19	3 (1%)	79	68	50, 73, 99, 105	0
3	L	273/273 (100%)	-0.58	2 (0%)	87	82	37, 54, 74, 85	0
4	M	323/323 (100%)	-0.51	1 (0%)	94	92	42, 60, 89, 117	0
All	All	1177/1190 (98%)	-0.38	13 (1%)	80	70	37, 66, 102, 124	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Н	85	THR	3.7
1	С	59	VAL	3.6
1	С	54	GLN	3.0
1	С	53	SER	2.8
2	Н	83	PRO	2.7

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
2	FME	Н	1	10/11	0.77	0.37	104,105,115,117	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



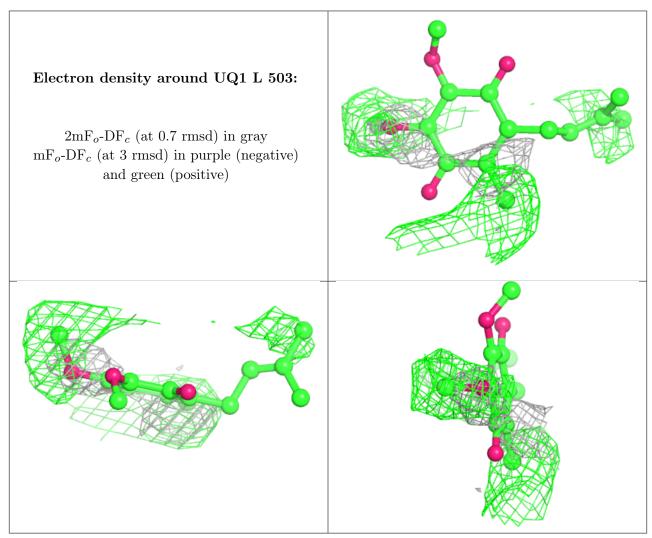
6.4 Ligands (i)

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.

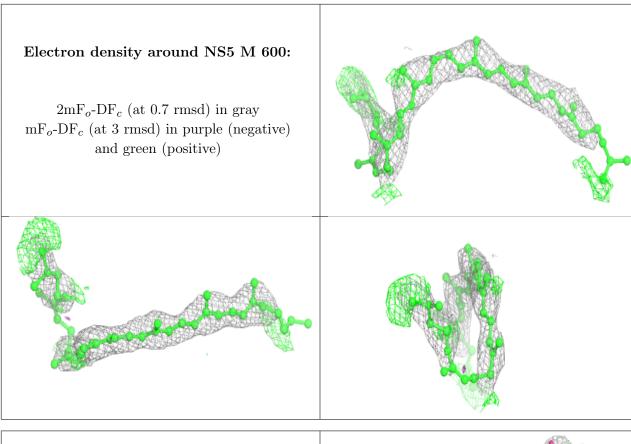
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
5	SO4	С	808	5/5	0.47	0.40	104,104,104,104	5
5	SO4	С	809	5/5	0.48	0.54	109,110,110,110	5
7	НТО	Н	705	10/10	0.55	0.59	56,59,61,61	10
11	UQ1	L	503	18/18	0.62	0.59	73,76,78,78	18
5	SO4	Н	812	5/5	0.76	0.33	92,92,93,93	5
5	SO4	Н	803	5/5	0.77	0.34	82,82,83,83	5
7	НТО	С	707	10/10	0.77	0.39	44,48,49,49	10
5	SO4	С	810	5/5	0.80	0.42	88,88,88,88	5
5	SO4	Н	807	5/5	0.81	0.42	108,108,108,109	5
5	SO4	С	813	5/5	0.82	0.43	79,79,80,80	5
5	SO4	С	811	5/5	0.85	0.60	76,76,76,77	5
14	NS5	M	600	40/40	0.87	0.28	65,71,100,101	4
7	НТО	С	706	10/10	0.88	0.71	56,57,58,58	10
10	BPB	M	402	65/65	0.89	0.28	61,67,123,124	0
11	UQ1	L	502	18/18	0.89	0.40	63,65,66,66	18
13	MQ9	M	501	58/58	0.91	0.25	40,64,102,103	0
8	LDA	M	704	16/16	0.91	0.41	68,70,73,73	16
5	SO4	С	814	5/5	0.92	0.37	48,48,49,50	5
5	SO4	С	815	5/5	0.92	0.25	40,40,41,41	5
8	LDA	Н	703	16/16	0.94	0.39	54,58,60,61	16
5	SO4	Н	806	5/5	0.95	0.14	72,72,73,73	5
5	SO4	M	804	5/5	0.95	0.18	94,95,96,96	0
8	LDA	L	702	16/16	0.95	0.36	67,73,79,80	0
8	LDA	Н	701	16/16	0.96	0.17	54,57,68,68	0
5	SO4	M	801	5/5	0.96	0.11	61,62,63,63	0
5	SO4	M	805	5/5	0.96	0.09	64,65,65,67	5
6	HEC	С	401	43/43	0.96	0.27	99,110,118,120	0
10	BPB	L	402	65/65	0.96	0.19	38,51,60,60	0
9	BCB	L	401	66/66	0.97	0.19	41,44,59,64	0
9	BCB	M	400	66/66	0.97	0.18	37,48,107,108	0
9	BCB	L	400	66/66	0.98	0.18	37,40,45,49	0
6	HEC	С	403	43/43	0.98	0.19	46,48,52,54	0
6	HEC	С	404	43/43	0.98	0.16	52,55,68,73	0
9	BCB	M	401	66/66	0.98	0.18	36,41,63,68	0
6	HEC	С	402	43/43	0.98	0.19	73,76,80,81	0
5	SO4	M	802	5/5	0.99	0.09	89,89,90,90	0
12	FE2	M	500	1/1	1.00	0.16	50,50,50,50	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.



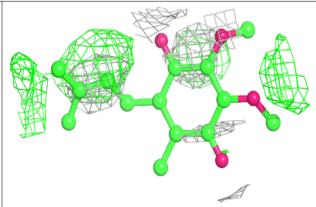


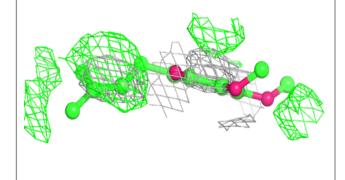


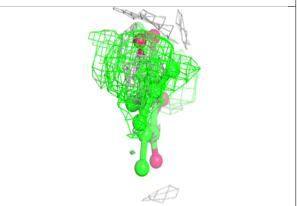


Electron density around UQ1 L 502:

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

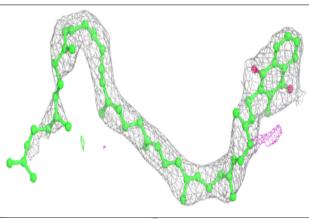


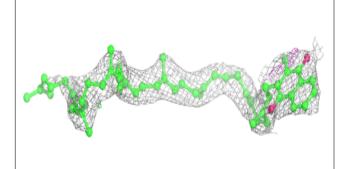


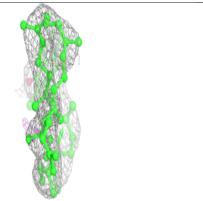


Electron density around MQ9 M 501:

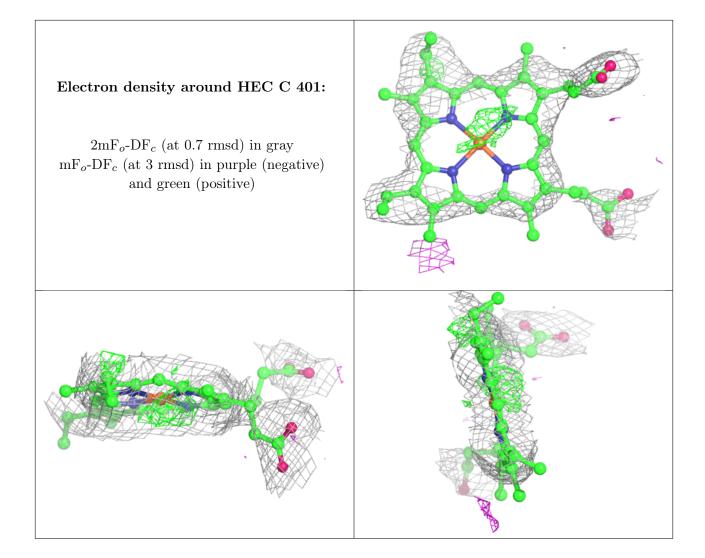
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



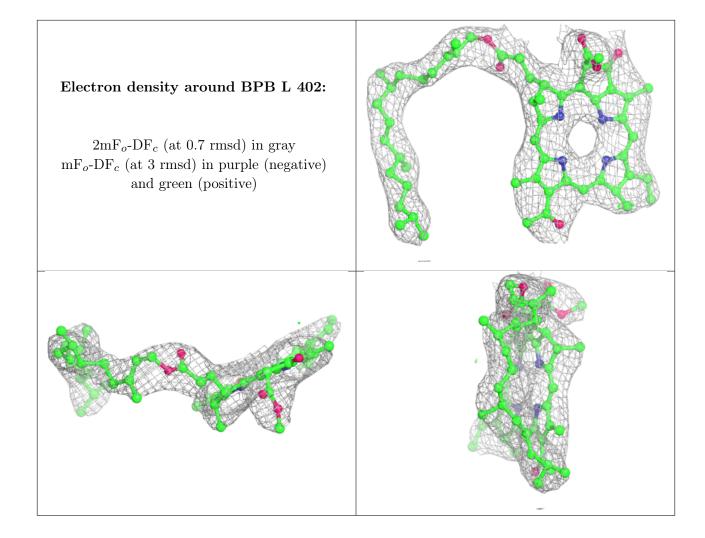








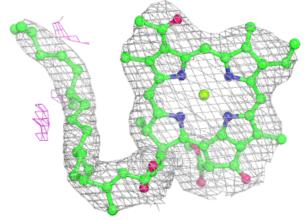


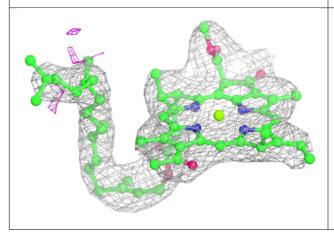


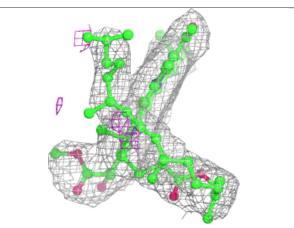


Electron density around BCB L 401:

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

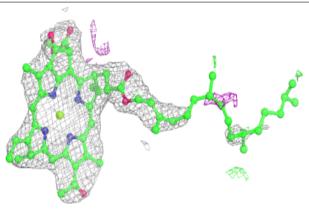


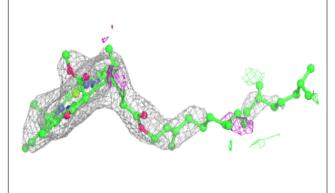


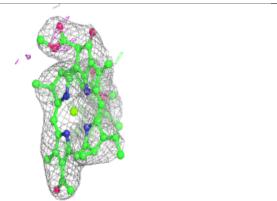


Electron density around BCB M 400:

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

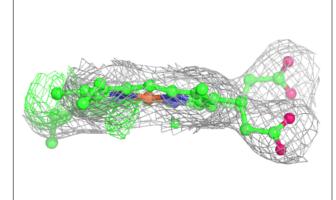


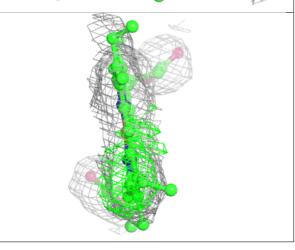




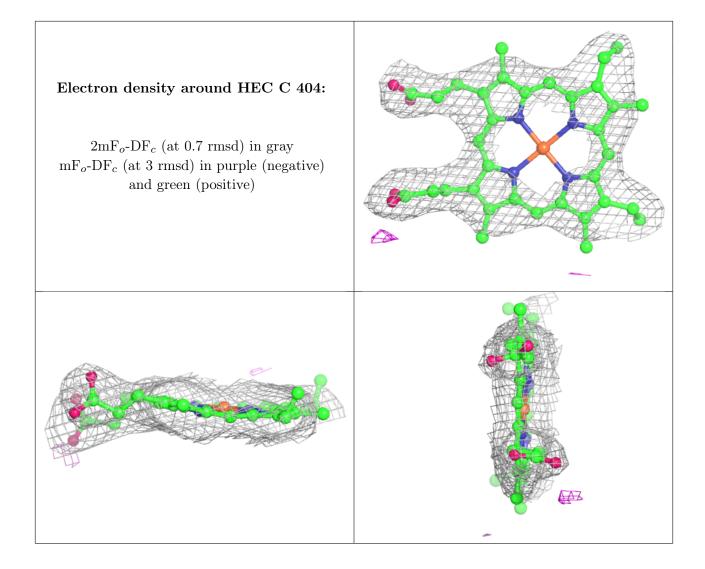


Electron density around BCB L 400: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around HEC C 403: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)











Electron density around BCB M 401: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around HEC C 402: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

