

wwPDB X-ray Structure Validation Summary Report (i)

Feb 8, 2024 – 08:50 AM EST

PDB ID : 2HG9

Title: Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with

tetrabrominated phosphatidylcholine

Authors: Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.

Deposited on : 2006-06-26

Resolution : 2.45 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:

MolProbity : 4.02b-467

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

Xtriage (Phenix) : 1.13

EDS : 2.36

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)

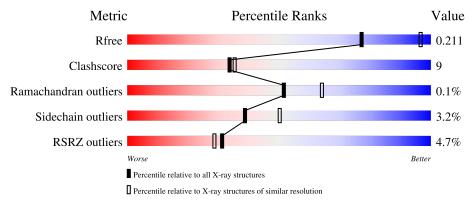
Validation Pipeline (wwPDB-VP) : 2.36

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	L	281	93%		7% •
2	M	307	7% 85%	11%	
3	Н	260	81%	0% •	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 criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CDL	M	800	-	-	-	X
11	PCK	M	802	-	-	X	X
12	LDA	Н	903	-	-	-	X
12	LDA	Н	904	-	-	-	X
12	LDA	Н	908	-	-	X	X
12	LDA	M	902	-	-	-	X
12	LDA	M	920	-	-	-	X
13	GOL	Н	708	-	-	-	X
15	PC7	Н	801	-	-	-	X
8	U10	L	502	-	-	-	X



2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 7843 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called Reaction center protein L chain.

\mathbf{Mol}	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	L	281	Total 2237	C 1511	N 356	O 362	S 8	0	3	0

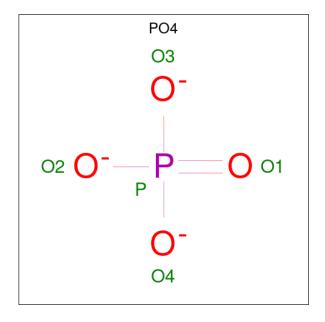
• Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	M	302	Total 2450	C 1631	N 402	O 406	S 11	0	12	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	Н	241	Total 1862	C 1189	N 323	O 339	S 11	0	9	0

• Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



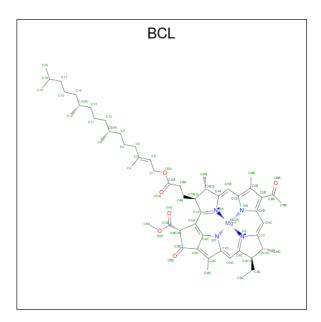


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0
4	Н	1	Total O P 5 4 1	0	0

• Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total Cl 1 1	0	0
5	M	1	Total Cl 1 1	0	0

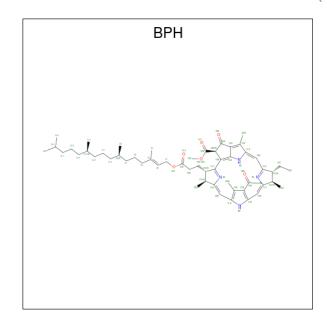
 $\bullet \ \ \mathrm{Molecule} \ 6 \ \mathrm{is} \ \mathrm{BACTERIOCHLOROPHYLL} \ \mathrm{A} \ (\mathrm{three-letter} \ \mathrm{code} \colon \ \mathrm{BCL}) \ (\mathrm{formula} \colon \ \mathrm{C}_{55} \mathrm{H}_{74} \mathrm{MgN_4O_6}).$



Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	
6	T.	1	Total	С	Mg	N	О	0	0
	L	1	66	55	1	4	6	U	U
6	T.	1	Total	С	Mg	N	О	0	0
0	П	1	66	55	1	4	6	U	
6	M	1	Total	С	Mg	N	О	0	0
0	1V1	1	66	55	1	4	6	U	
6	М	1	Total	С	Mg	N	О	0	0
0	M	1	66	55	1	4	6	U	0

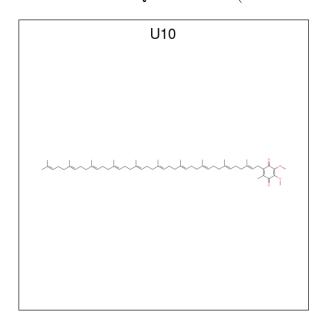


 $\bullet \ \ \mathrm{Molecule} \ 7 \ \mathrm{is} \ \mathrm{BACTERIOPHEOPHYTIN} \ \mathrm{A} \ (\mathrm{three-letter} \ \mathrm{code} \colon \ \mathrm{BPH}) \ (\mathrm{formula} \colon \ \mathrm{C}_{55}\mathrm{H}_{76}\mathrm{N}_4\mathrm{O}_6).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	T.	1	Total	_		_	0	0	
'	ם	1	65	55	4	6	O		
7	М	1	Total	С	N	O	0	0	
'	1V1	1	65	55	4	6	U	U	

 \bullet Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $\mathrm{C}_{59}\mathrm{H}_{90}\mathrm{O}_4).$



Mol	Chain	Residues	At	oms		ZeroOcc	AltConf
8	L	1	Total 48	C 44	O 4	0	0

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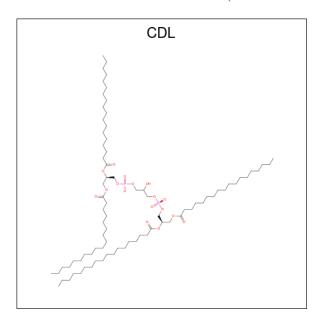
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M	ol	Chain	Residues	Ato	Atoms			AltConf
8	3	M	1	Total 48	C 44	O 4	0	0

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

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

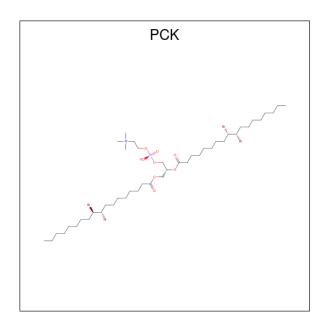
 \bullet Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	М	1	Total	С	О	Р	0	0
10	1V1	IVI I	81	62	17	2		

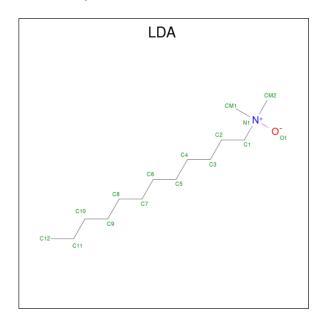
• Molecule 11 is $(7R,18S,19R)-18,19-DIBROMO-7-\{[(9S,10S)-9,10-DIBROMOOCTADECANOYL]OXY\}-4-HYDROXY-N,N,N-TRIMETHYL-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PCK) (formula: <math>C_{44}H_{85}Br_4NO_8P$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
11	М	1	Total	Br	С	N	О	Р	0	0
11	IVI	IVI I	58	4	44	1	8	1		U

 \bullet Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO).$



Mo	Cha	in	Residues	Atoms				ZeroOcc	AltConf
12	M		1	Total 16			O 1	0	0
12	M		1	Total 16	C 14	N 1	O 1	0	0

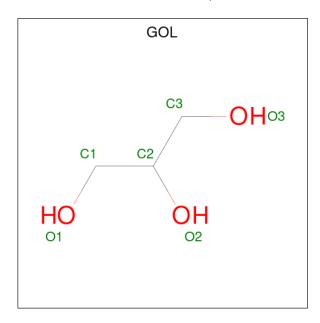
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
12	M	1	Total C N O	0	0	
12	IVI		16 14 1 1	U		
12	Н	1	Total C N O	0	0	
12	11	1	16 14 1 1	U	0	
12	Н	Н	1	Total C N O	0	0
12		1	16 14 1 1	U	U	
12	Н	1	Total C N O	0	0	
12	11	1	16 14 1 1	U	0	
12	Н	1	Total C N O	0	0	
12	П	п 1	16 14 1 1			

 \bullet Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$



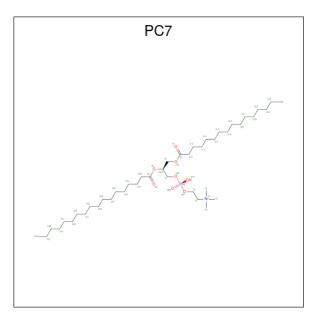
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C O 6 3 3	0	0
13	M	1	Total C O 6 3 3	0	0
13	Н	1	Total C O 6 3 3	0	0
13	Н	1	Total C O 6 3 3	0	0
13	Н	1	Total C O 6 3 3	0	0
13	Н	1	Total C O 6 3 3	0	0



• Molecule 14 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	Н	1	Total K 1 1	0	0

• Molecule 15 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)M ETHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: $C_{42}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
15	Н	1	Total	С	N	О	Р	0	0
10	11	1	52	42	1	8	1		

• Molecule 16 is water.

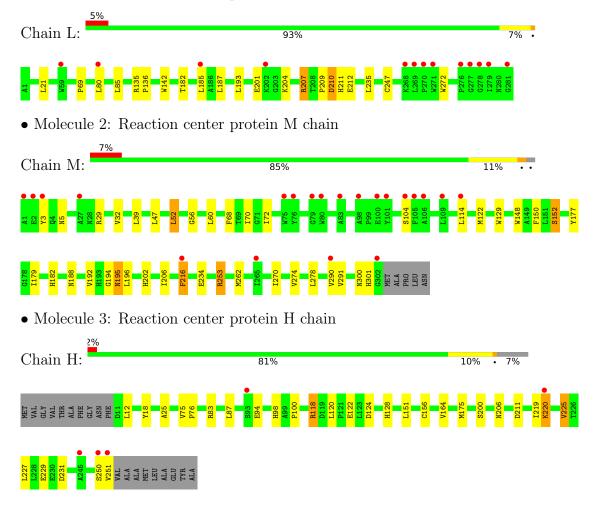
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	L	100	Total O 100 100	0	0
16	M	133	Total O 133 133	0	0
16	Н	208	Total O 208 208	0	0



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: Reaction center protein L chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	139.55Å 139.55Å 184.61Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.36 - 2.45	Depositor
resolution (A)	39.36 - 2.45	EDS
% Data completeness	98.0 (39.36-2.45)	Depositor
(in resolution range)	98.0 (39.36-2.45)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.30 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D	0.179 , 0.209	Depositor
R, R_{free}	0.183 , 0.211	DCC
R_{free} test set	3709 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 83.3	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7843	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.64% 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: PO4, CDL, U10, FE, PC7, BPH, BCL, LDA, GOL, CL, PCK, K

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		
MIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	L	0.90	0/2342	0.73	$1/3205 \ (0.0\%)$	
2	M	0.90	1/2601 (0.0%)	0.80	3/3548 (0.1%)	
3	Н	0.95	3/1961 (0.2%)	0.84	4/2663~(0.2%)	
All	All	0.92	4/6904 (0.1%)	0.79	8/9416 (0.1%)	

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
3	Н	94	GLU	CG-CD	6.20	1.61	1.51
3	Н	94	GLU	CB-CG	5.59	1.62	1.52
3	Н	94	GLU	CD-OE2	5.30	1.31	1.25
2	M	152	SER	CB-OG	5.05	1.48	1.42

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	Н	124	ASP	CB-CG-OD1	7.74	125.27	118.30
3	Н	124	ASP	CB-CG-OD2	-6.80	112.18	118.30
2	M	253[A]	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	M	253[B]	ARG	NE-CZ-NH2	6.00	123.30	120.30
3	Н	83	ARG	NE-CZ-NH2	-5.78	117.41	120.30

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	L	2237	0	2202	10	0
2	M	2450	0	2370	38	0
3	Н	1862	0	1884	21	0
4	Н	5	0	0	0	0
4	L	5	0	0	0	0
4	M	10	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	1	0
6	L	132	0	148	8	0
6	M	132	0	148	20	0
7	L	65	0	75	3	0
7	M	65	0	76	4	0
8	L	48	0	63	4	0
8	M	48	0	63	1	0
9	M	1	0	0	0	0
10	M	81	0	106	2	0
11	M	58	0	80	24	0
12	Н	64	0	124	19	0
12	M	48	0	93	9	0
13	Н	24	0	32	2	0
13	M	12	0	16	0	0
14	Н	1	0	0	0	0
15	Н	52	0	84	6	0
16	Н	208	0	0	0	0
16	L	100	0	0	0	0
16	M	133	0	0	7	0
All	All	7843	0	7564	128	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 9.

The worst 5 of 128 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
12:M:902:LDA:H121	12:H:908:LDA:H121	1.37	1.04
2:M:47[A]:LEU:HD22	11:M:802:PCK:BR4	2.11	1.04
8:L:502:U10:H351	8:L:502:U10:H38	1.41	1.03
11:M:802:PCK:H252	11:M:802:PCK:H211	1.35	1.02
2:M:122:MET:SD	12:M:920:LDA:H122	2.01	1.01



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	Perce	entiles
1	L	282/281 (100%)	275 (98%)	7 (2%)	0	100	100
2	M	312/307 (102%)	300 (96%)	11 (4%)	1 (0%)	41	49
3	Н	248/260 (95%)	245 (99%)	3 (1%)	0	100	100
All	All	842/848 (99%)	820 (97%)	21 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	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	Percentiles	
1	L	223/220 (101%)	216 (97%)	7 (3%)	40	52
2	M	248/240 (103%)	239 (96%)	9 (4%)	35	46
3	Н	205/208 (99%)	198 (97%)	7 (3%)	37	48
All	All	676/668 (101%)	653 (97%)	23 (3%)	39	48

5 of 23 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
2	M	216	PHE
3	Н	118[B]	ARG
3	Н	118[A]	ARG
3	Н	200	SER
1	L	272	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	4	GLN
2	M	28	ASN
3	Н	68	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 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		
IVIOI	Type		nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	M	701	-	4,4,4	0.88	0	6,6,6	1.24	0



Mol	Т	Clasia.	Das	Link	Во	ond leng	ths	Во	ond angl	les
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
12	LDA	Н	908	_	12,15,15	2.02	1 (8%)	14,17,17	0.97	1 (7%)
13	GOL	M	710	-	5,5,5	0.42	0	5,5,5	0.43	0
6	BCL	L	312	1	64,74,74	1.27	3 (4%)	78,115,115	1.50	15 (19%)
12	LDA	Н	901	-	12,15,15	2.02	1 (8%)	14,17,17	0.60	0
11	PCK	M	802	-	57,57,57	0.77	0	63,69,69	1.06	5 (7%)
6	BCL	M	311	2	64,74,74	1.29	3 (4%)	78,115,115	1.54	18 (23%)
6	BCL	L	314	1	64,74,74	1.12	5 (7%)	78,115,115	1.62	17 (21%)
6	BCL	M	313	2	64,74,74	1.34	3 (4%)	78,115,115	1.77	18 (23%)
13	GOL	Н	706	-	5,5,5	0.35	0	5,5,5	1.03	0
13	GOL	Н	709	-	5,5,5	0.43	0	5,5,5	0.42	0
4	PO4	M	702	-	4,4,4	0.82	0	6,6,6	1.07	0
13	GOL	Н	705	-	5,5,5	0.52	0	5,5,5	0.65	0
8	U10	L	502	-	48,48,63	1.10	3 (6%)	58,61,79	1.77	15 (25%)
4	PO4	L	703	-	4,4,4	0.90	0	6,6,6	0.86	0
12	LDA	M	902	-	12,15,15	2.00	1 (8%)	14,17,17	0.81	0
12	LDA	M	907	-	12,15,15	2.04	1 (8%)	14,17,17	0.63	0
12	LDA	Н	903	-	12,15,15	2.01	1 (8%)	14,17,17	0.50	0
12	LDA	M	920	-	12,15,15	2.03	1 (8%)	14,17,17	0.61	0
12	LDA	Н	904	-	12,15,15	1.98	1 (8%)	14,17,17	0.74	0
4	PO4	Н	704	-	4,4,4	0.79	0	6,6,6	0.84	0
8	U10	M	501	-	48,48,63	0.94	2 (4%)	58,61,79	1.58	13 (22%)
10	CDL	M	800	-	80,80,99	1.18	4 (5%)	86,92,111	1.13	6 (6%)
7	ВРН	L	402	-	51,70,70	0.92	2 (3%)	52,101,101	1.55	8 (15%)
13	GOL	M	707	-	5,5,5	0.49	0	5,5,5	0.30	0
13	GOL	Н	708	-	5,5,5	0.27	0	5,5,5	0.50	0
7	ВРН	M	401	-	51,70,70	0.77	0	52,101,101	1.66	12 (23%)
15	PC7	Н	801	-	51,51,51	0.84	1 (1%)	57,59,59	0.92	3 (5%)

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
12	LDA	Н	908	-	-	10/13/13/13	-
13	GOL	M	710	-	-	4/4/4/4	-
6	BCL	L	312	1	-	1/37/137/137	-
12	LDA	Н	901	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PCK	M	802	-	-	33/67/67/67	-
6	BCL	M	311	2	-	10/37/137/137	-
6	BCL	L	314	1	-	2/37/137/137	-
6	BCL	M	313	2	-	3/37/137/137	-
13	GOL	Н	706	-	-	2/4/4/4	-
13	GOL	Н	709	-	-	2/4/4/4	-
13	GOL	Н	705	-	-	2/4/4/4	-
8	U10	L	502	-	-	11/45/69/87	0/1/1/1
12	LDA	M	902	-	-	2/13/13/13	-
12	LDA	M	907	-	-	6/13/13/13	-
12	LDA	Н	903	-	-	9/13/13/13	-
12	LDA	Н	904	-	-	5/13/13/13	-
12	LDA	M	920	-	-	7/13/13/13	-
8	U10	M	501	-	-	5/45/69/87	0/1/1/1
10	CDL	M	800	-	-	38/91/91/110	-
7	BPH	L	402	-	-	5/37/105/105	0/5/6/6
13	GOL	M	707	-	-	3/4/4/4	-
13	GOL	Н	708	-	-	1/4/4/4	-
7	BPH	M	401	-	-	10/37/105/105	0/5/6/6
15	PC7	Н	801	_	-	23/55/55/55	-

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
12	Н	901	LDA	O1-N1	-6.96	1.25	1.42
12	Н	908	LDA	O1-N1	-6.95	1.25	1.42
12	M	907	LDA	O1-N1	-6.94	1.25	1.42
12	Н	903	LDA	O1-N1	-6.86	1.26	1.42
12	M	902	LDA	O1-N1	-6.85	1.26	1.42

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
7	M	401	BPH	O2D-CGD-CBD	5.17	117.55	111.00
7	L	402	BPH	O2D-CGD-CBD	5.05	117.39	111.00
10	M	800	CDL	OA6-CA5-C11	4.95	122.17	111.50
10	M	800	CDL	OB6-CB5-C51	4.48	121.17	111.50
7	L	402	BPH	C1-C2-C3	-4.46	118.32	126.04



There are no chirality outliers.

5 of 200 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	401	BPH	C11-C10-C8-C9
8	L	502	U10	C28-C29-C31-C32
8	L	502	U10	C30-C29-C31-C32
10	M	800	CDL	CA2-OA2-PA1-OA3
10	M	800	CDL	CA2-OA2-PA1-OA4

There are no ring outliers.

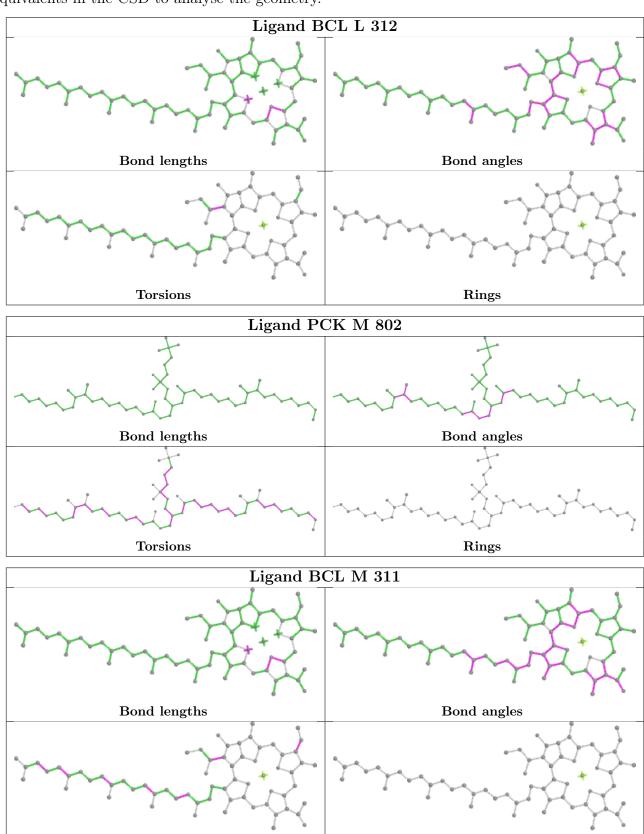
19 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	Н	908	LDA	10	0
6	L	312	BCL	4	0
12	Н	901	LDA	2	0
11	M	802	PCK	24	0
6	M	311	BCL	13	0
6	L	314	BCL	5	0
6	M	313	BCL	7	0
8	L	502	U10	4	0
12	M	902	LDA	5	0
12	M	907	LDA	1	0
12	Н	903	LDA	5	0
12	M	920	LDA	3	0
12	Н	904	LDA	7	0
8	M	501	U10	1	0
10	M	800	CDL	2	0
7	L	402	BPH	3	0
13	Н	708	GOL	2	0
7	M	401	BPH	4	0
15	Н	801	PC7	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.



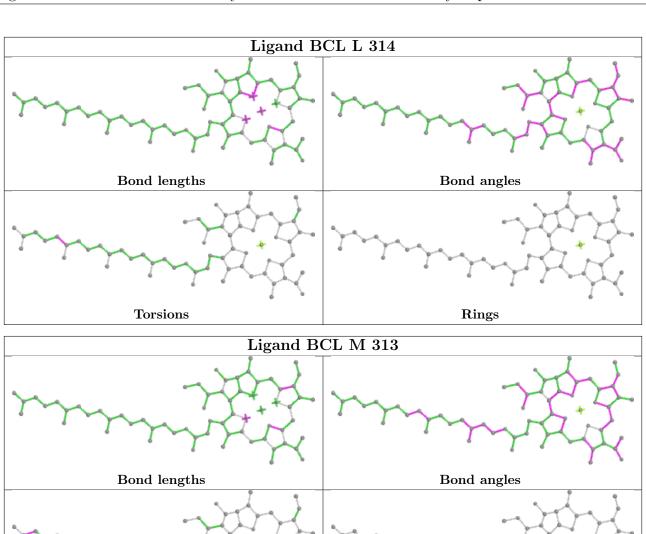
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

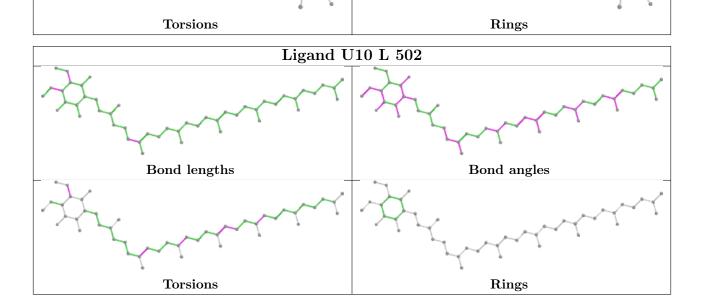




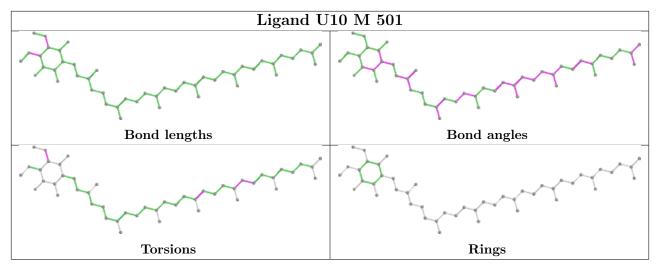
Rings

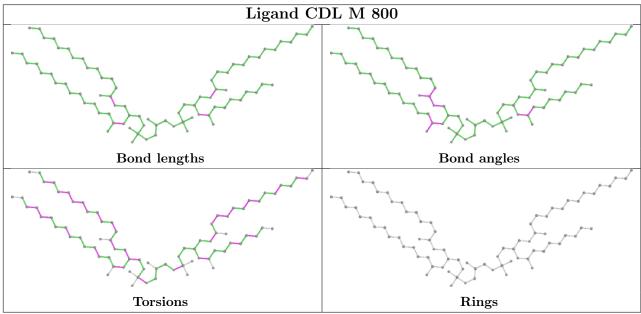
Torsions



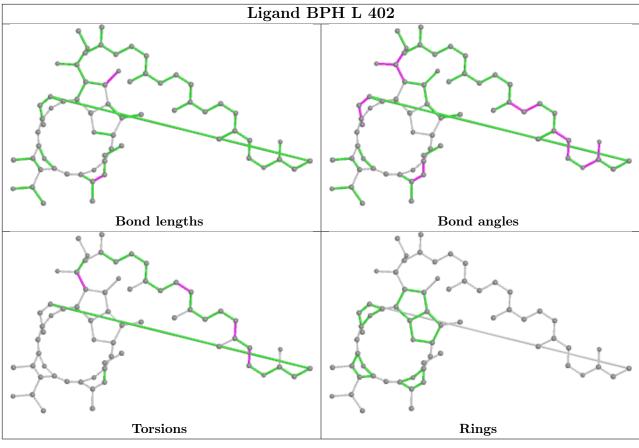


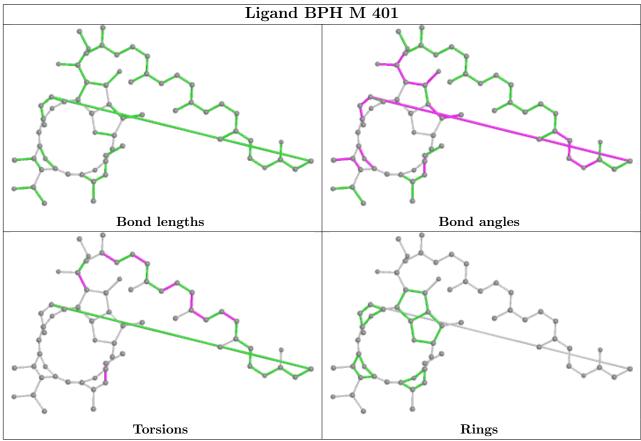




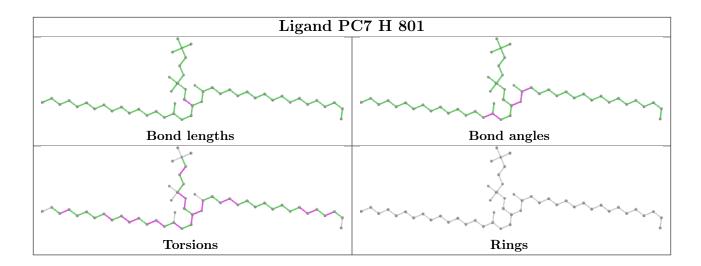












5.7 Other polymers (i)

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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	L	281/281 (100%)	-0.00	13 (4%) 32 30	43, 53, 66, 82	0
2	M	302/307 (98%)	0.18	21 (6%) 16 13	43, 53, 65, 89	0
3	Н	241/260 (92%)	-0.24	5 (2%) 63 60	44, 53, 61, 95	0
All	All	824/848 (97%)	-0.00	39 (4%) 31 29	43, 53, 65, 95	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	10.3
3	Н	251	VAL	8.6
2	M	2[A]	GLU	6.1
3	Н	250	SER	6.0
1	L	277	GLY	4.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

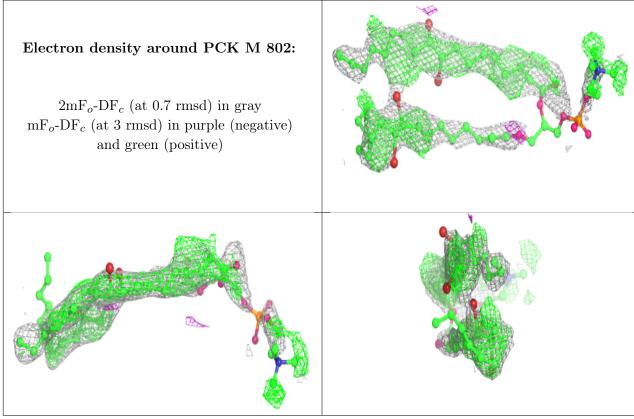
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

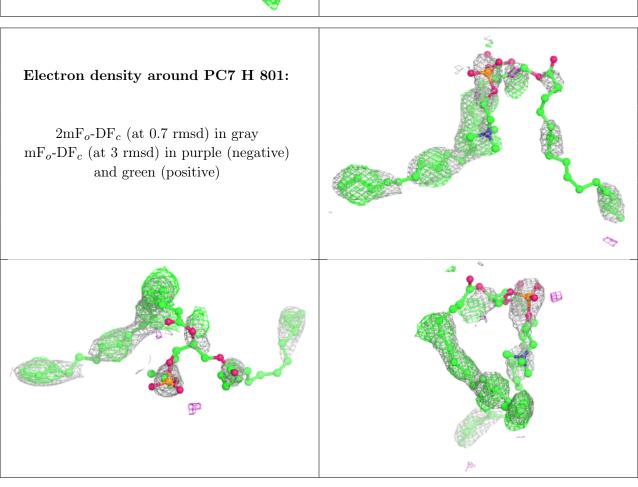


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({\rm \AA}^2)$	Q < 0.9
11	PCK	M	802	58/58	0.22	0.74	60,69,82,84	58
12	LDA	Н	904	16/16	0.37	0.63	53,54,58,58	16
15	PC7	Н	801	52/52	0.44	0.68	24,60,69,69	52
12	LDA	Н	908	16/16	0.45	0.61	45,51,61,61	16
12	LDA	Н	903	16/16	0.47	0.44	56,61,64,65	16
12	LDA	M	920	16/16	0.62	0.80	42,46,59,59	16
13	GOL	M	710	6/6	0.63	0.33	55,57,58,60	6
10	CDL	M	800	81/100	0.63	0.51	43,67,79,82	81
12	LDA	M	907	16/16	0.66	0.39	56,59,65,66	16
12	LDA	M	902	16/16	0.72	0.62	59,64,67,68	16
13	GOL	Н	708	6/6	0.72	1.10	47,49,50,52	6
5	CL	L	712	1/1	0.72	0.35	66,66,66,66	1
8	U10	L	502	48/63	0.73	0.55	40,55,73,75	48
4	PO4	L	703	5/5	0.73	0.33	61,61,62,65	5
13	GOL	M	707	6/6	0.75	0.23	49,50,52,52	6
12	LDA	Н	901	16/16	0.85	0.29	61,63,66,68	16
13	GOL	Н	706	6/6	0.87	0.26	71,72,73,74	6
4	PO4	Н	704	5/5	0.87	0.30	71,73,74,75	5
13	GOL	Н	705	6/6	0.87	0.41	48,58,59,61	6
5	CL	M	711	1/1	0.88	0.24	74,74,74,74	1
13	GOL	Н	709	6/6	0.88	0.19	55,56,57,58	6
7	BPH	M	401	65/65	0.88	0.23	45,55,106,107	0
8	U10	M	501	48/63	0.89	0.24	49,61,81,84	0
14	K	Н	700	1/1	0.93	0.11	57,57,57,57	0
4	PO4	M	702	5/5	0.94	0.12	53,53,54,55	5
6	BCL	M	311	66/66	0.94	0.22	46,54,119,120	0
6	BCL	L	312	66/66	0.96	0.16	42,50,63,67	0
4	PO4	M	701	5/5	0.96	0.14	57,58,62,62	5
6	BCL	M	313	66/66	0.96	0.19	42,50,79,87	0
7	BPH	L	402	65/65	0.96	0.15	40,52,60,61	0
6	BCL	L	314	66/66	0.97	0.15	41,48,67,71	0
9	FE	M	500	1/1	0.99	0.17	51,51,51,51	0

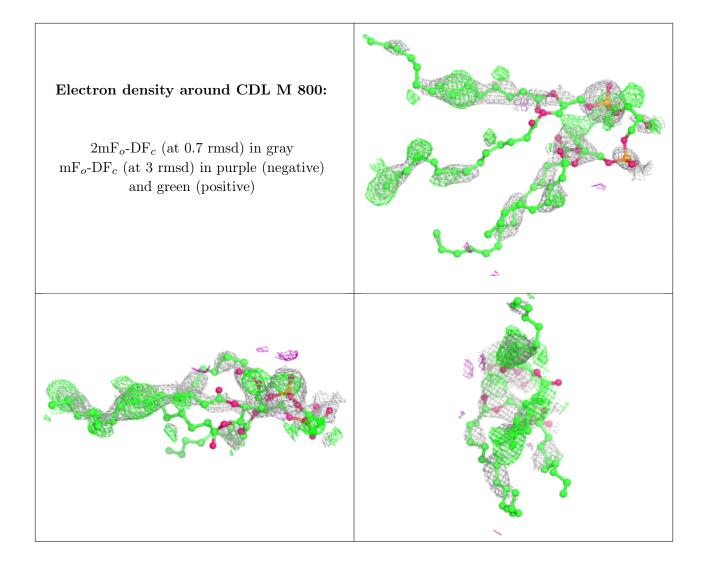
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



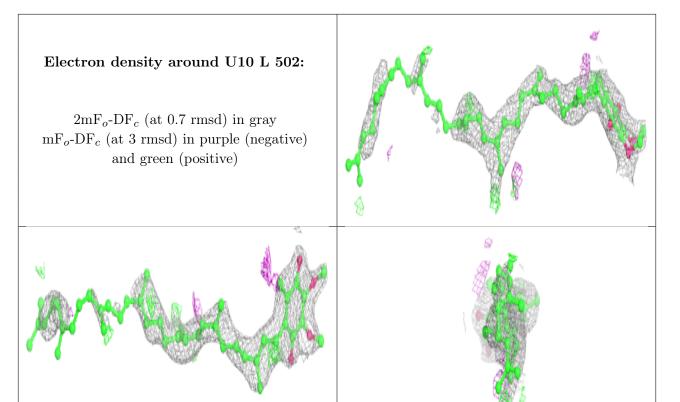








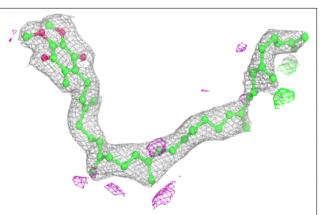


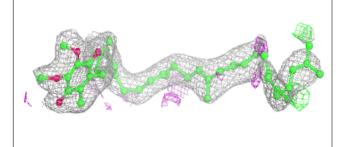


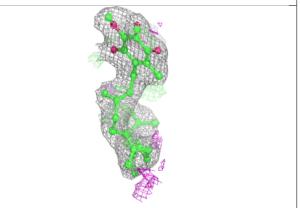


Electron density around U10 M 501:

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

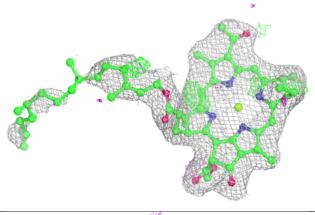


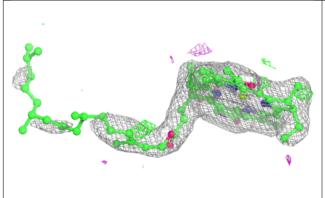


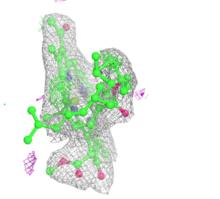


Electron density around BCL M 311:

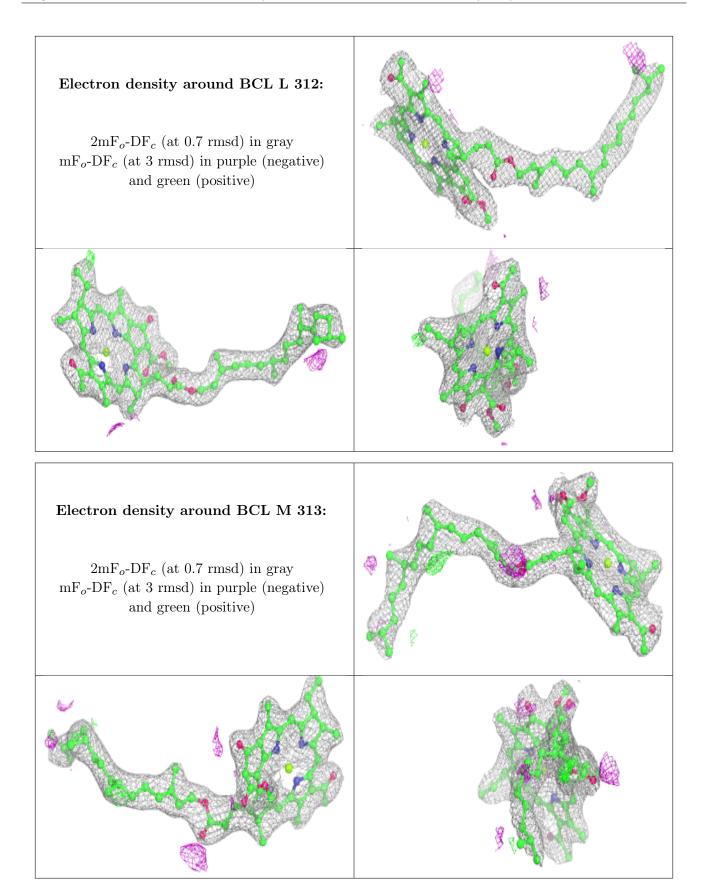
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



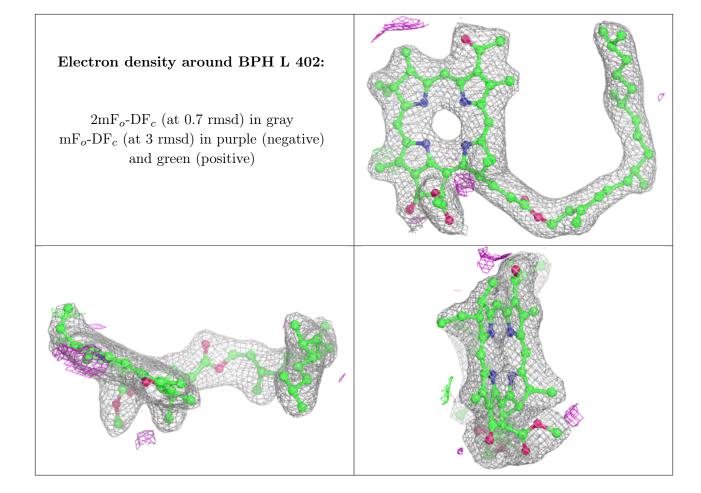




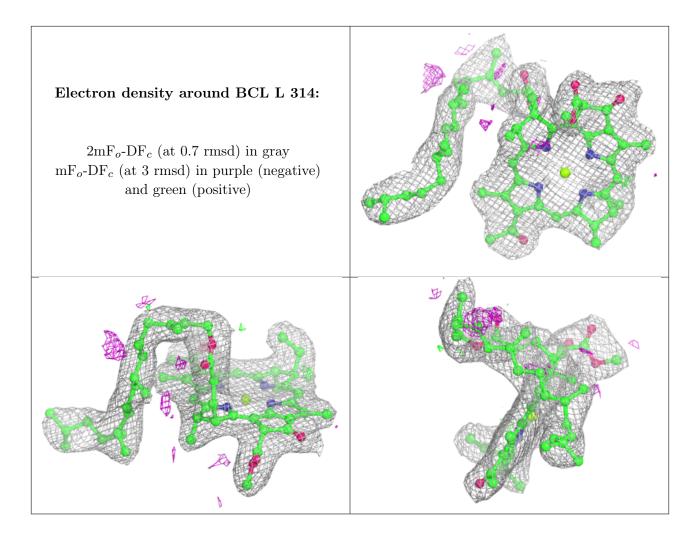












6.5 Other polymers (i)

There are no such residues in this entry.

