

# wwPDB X-ray Structure Validation Summary Report (i)

#### Nov 14, 2023 – 01:32 pm GMT

PDB ID : 8C88

Title: Double mutant G(M19)C/T(L214)C structure of Photosynthetic Reaction

Center From Cereibacter sphaeroides strain RV

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Yukhimchuk, D.

Deposited on : 2023-01-19

Resolution : 2.75 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 (i)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, 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)

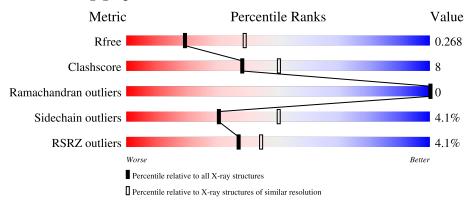
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	Н	242	79%	19%	•
2	L	281	6% 85%	15%	•
3	M	303	82%	17%	•

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
5	LDA	M	410	-	-	-	X
6	UNL	Н	303	-	-	-	X
6	UNL	Н	304	-	-	-	X
6	UNL	Н	305	-	-	-	X
6	UNL	L	506	-	-	-	X
6	UNL	M	412	-	-	-	X
7	OLC	L	501	-	-	-	X



# 2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 7341 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 H chain.

$\mathbf{Mol}$	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	Н	242	Total 1867	C 1196	N 320	O 342	S 9	0	3	0

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

$\mathbf{Mol}$	Chain	Residues		$\mathbf{At}$	oms			ZeroOcc	AltConf	Trace	
2	L	281	Total 2243	C 1515	N 356	O 363	S 9	0	2	0	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	engineered mutation	UNP P0C0Y8
L	214	CYS	THR	engineered mutation	UNP P0C0Y8

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

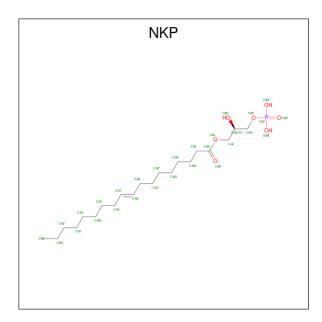
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	M	303	Total 2427	C 1619	N 398	O 398	S 12	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR SER		engineered mutation	UNP P0C0Y9
M	19	CYS	GLY	engineered mutation	UNP P0C0Y9

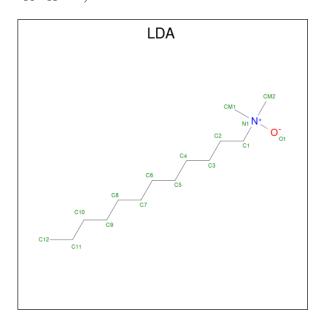
• Molecule 4 is (2R)-2-hydroxy-3-(phosphonooxy)propyl (9E)-octadec-9-enoate (three-letter code: NKP) (formula: C<sub>21</sub>H<sub>41</sub>O<sub>7</sub>P).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	Н	1	Total 29				0	0
4	M	1	Total 29	C 21	O 7	P 1	0	0

• Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



$\mathbf{Mol}$	Chain	Residues	A	Aton	$\mathbf{as}$		ZeroOcc	AltConf
5	Н	1	Total 16	C 14	N 1	O 1	0	0

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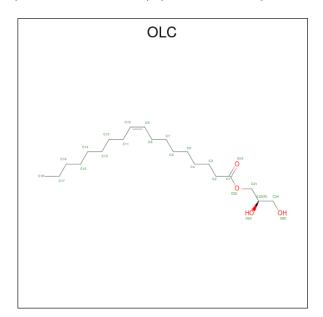
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total C N O	0	0
	1/1	1	16 14 1 1	O	U
5	M	1	Total C N O	0	0
9	1V1	1	16 14 1 1	0	U
5	M	1	Total C N O	0	0
9	1V1	1	16 14 1 1	U	0
E	М	1	Total C N O	0	0
5	M	1	16 14 1 1	U	0
E	М	1	Total C N O	0	0
5	M	1	16 14 1 1	U	U

• Molecule 6 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Н	3	Total C 39 39	0	0
6	L	3	Total C 37 37	0	0
6	M	1	Total C 12 12	0	0

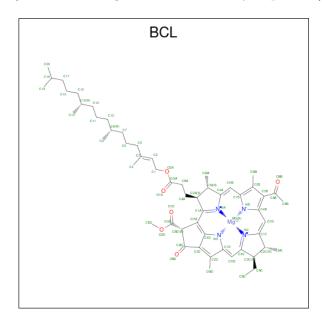
• Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula:  $C_{21}H_{40}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mo	l Cha	ain	Residues	Atoms		ZeroOcc	AltConf	
7	L	ı	1	Total 25	C 21	O 4	0	0



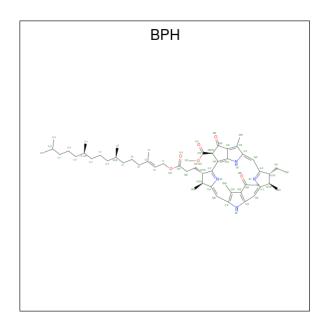
• Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	о т	1	Total	С	Mg	N	О	0	0
	1	66	55	1	4	6	U U	O	
Q	T	1	Total	С	Mg	N	О	0	0
	П	1	66	55	1	4	6		
8	M	1	Total	С	Mg	N	О	0	0
O NI	1	66	55	1	4	6	U	0	
8	M	1	Total	С	Mg	N	О	0	0
8	IVI	$oxed{1} owed{1}$	66	55	1	4	6	U	

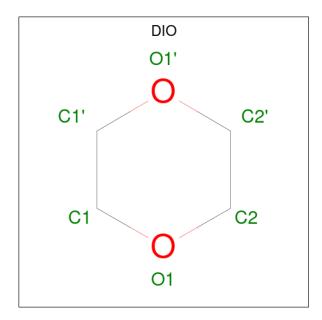
• Molecule 9 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
0	) I	1	Total				0	0
	П		65	55	4	6		
0	М	1	Total	С	N	О	0	0
9	9   M	1	65	55	4	6		

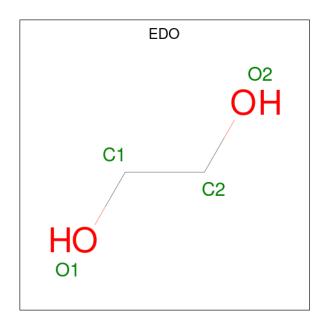
 $\bullet$  Molecule 10 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula:  $\mathrm{C_4H_8O_2}).$ 



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total C O 6 4 2	0	0

 $\bullet$  Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $\mathrm{C_2H_6O_2}).$ 





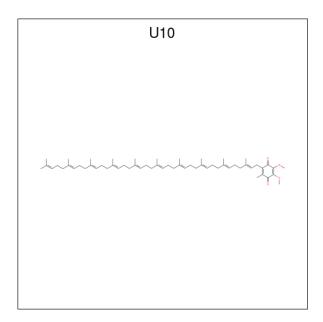
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total C O 4 2 2	0	0
11	L	1	Total C O 4 2 2	0	0
11	L	1	Total C O 4 2 2	0	0

• Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

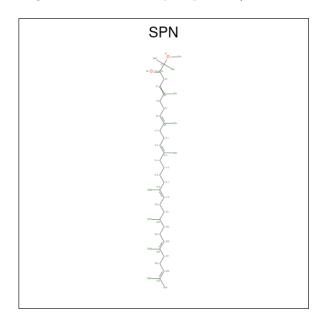
• Molecule 13 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
13	M	1	Total 48	C 44	O 4	0	0

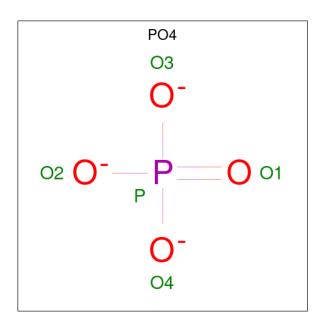
 $\bullet$  Molecule 14 is SPEROIDENONE (three-letter code: SPN) (formula:  $C_{41}H_{70}O_2)$  (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
14	M	1	Total 43	C 41	O 2	0	0

 $\bullet$  Molecule 15 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





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

## • Molecule 16 is water.

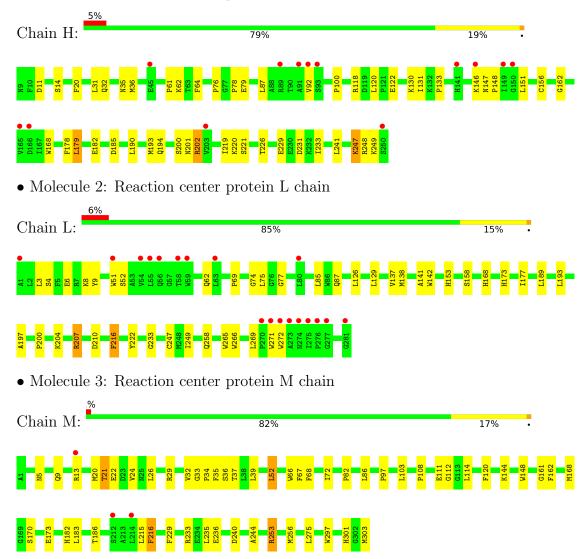
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	Н	3	Total O 3 3	0	0
16	L	8	Total O 8 8	0	0
16	M	12	Total O 12 12	0	0



# 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 H chain





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants	100.91Å 100.91Å 237.02Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.42 - 2.75	Depositor
Resolution (A)	46.42 - 2.75	EDS
% Data completeness	98.0 (46.42-2.75)	Depositor
(in resolution range)	98.1 (46.42-2.75)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.37 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0352, PHENIX 1.20.1_4487	Depositor
$R, R_{free}$	0.199 , 0.271	Depositor
it, it free	0.203 , $0.268$	DCC
$R_{free}$ test set	1285  reflections  (4.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.1	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34 , 72.0	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7341	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities 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, OLC, DIO, U10, UNL, NKP, BCL, LDA, SPN, FE, BPH, EDO

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	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	Н	0.46	0/1925	0.70	0/2617	
2	L	0.46	0/2334	0.61	0/3194	
3	M	0.47	$1/2522 \ (0.0\%)$	0.63	0/3442	
All	All	0.46	1/6781 (0.0%)	0.65	0/9253	

All (1) bond length outliers are listed below:

$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type	Atoms	${f Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
3	M	32	VAL	CB-CG1	-5.58	1.41	1.52

There are no bond angle outliers.

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	Н	1867	0	1881	38	0
2	L	2243	0	2201	27	0
3	M	2427	0	2346	42	0
4	Н	29	0	39	0	0
4	M	29	0	39	0	0
5	Н	16	0	31	2	0
5	M	80	0	155	7	0

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Mol	Chain		H(model)	H(added)	Clashes	Symm-Clashes
6	Н	39	0	0	0	0
6	L	37	0	0	0	0
6	M	12	0	0	0	0
7	L	25	0	40	2	0
8	L	132	0	148	5	0
8	M	132	0	148	5	0
9	L	65	0	76	2	0
9	M	65	0	76	3	0
10	L	6	0	8	1	0
11	L	12	0	18	2	0
12	M	1	0	0	0	0
13	M	48	0	63	4	0
14	M	43	0	70	7	0
15	M	10	0	0	0	0
16	Н	3	0	0	0	0
16	L	8	0	0	0	0
16	M	12	0	0	1	0
All	All	7341	0	7339	112	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 8.

The worst 5 of 112 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.68	0.74
2:L:189:LEU:HD13	2:L:216:PHE:HZ	1.54	0.71
1:H:11:ASP:HB3	1:H:14:SER:H	1.55	0.69
1:H:31:LEU:O	1:H:35:ASN:ND2	2.26	0.69
1:H:146:LYS:HD2	1:H:151:LEU:HD11	1.75	0.69

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 r	number of residu	ues for which	the backbone	conformation	was
analysed, and the total number of	residues.				

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Н	243/242 (100%)	235 (97%)	8 (3%)	0	100	100
2	L	281/281 (100%)	270 (96%)	11 (4%)	0	100	100
3	M	302/303 (100%)	287 (95%)	15 (5%)	0	100	100
All	All	826/826 (100%)	792 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	Н	$200/197 \; (102\%)$	191 (96%)	9 (4%)	27	46	
2	L	222/220 (101%)	211 (95%)	11 (5%)	24	42	
3	M	239/238 (100%)	231 (97%)	8 (3%)	38	58	
All	All	661/655 (101%)	633 (96%)	28 (4%)	30	49	

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	207	ARG
3	M	253[B]	ARG
2	L	247	CYS
3	M	182	HIS
2	L	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 31 ligands modelled in this entry, 7 are unknown and 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).

Mol	Trmo	Chain	Res	Link	В	ond leng	$_{ m gths}$	Во	ond angl	les
WIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
8	BCL	M	402	_	64,74,74	1.50	6 (9%)	78,115,115	1.67	14 (17%)
15	PO4	M	414	-	4,4,4	0.87	0	6,6,6	0.28	0
9	BPH	L	504	-	51,70,70	0.99	2 (3%)	52,101,101	1.37	10 (19%)
8	BCL	M	403	-	64,74,74	1.53	7 (10%)	78,115,115	1.56	10 (12%)
4	NKP	Н	301	-	28,28,28	0.32	0	31,32,32	0.61	1 (3%)
4	NKP	M	401	-	28,28,28	0.35	0	31,32,32	0.40	0
15	PO4	M	413	-	4,4,4	0.73	0	6,6,6	0.48	0
5	LDA	Н	302	-	12,15,15	2.05	1 (8%)	14,17,17	0.48	0
5	LDA	M	409	-	12,15,15	2.03	1 (8%)	14,17,17	0.58	0
5	LDA	M	415	-	12,15,15	2.03	1 (8%)	14,17,17	0.56	0
9	BPH	M	404	-	51,70,70	1.14	4 (7%)	52,101,101	1.60	9 (17%)
14	SPN	M	407	-	40,42,42	0.51	0	50,52,52	0.85	2 (4%)
10	DIO	L	508	-	6,6,6	0.48	0	6,6,6	0.10	0
11	EDO	L	510	-	3,3,3	0.47	0	2,2,2	0.47	0
7	OLC	L	501	-	24,24,24	1.03	1 (4%)	25,25,25	0.88	2 (8%)
5	LDA	M	411	-	12,15,15	2.00	1 (8%)	14,17,17	0.50	0
5	LDA	M	410	-	12,15,15	2.03	1 (8%)	14,17,17	0.74	0
11	EDO	L	511	-	3,3,3	0.55	0	2,2,2	0.17	0



Mol	Type	Chain	Res	Link	В	ond leng	$\operatorname{gths}$	Bond angles		
MIOI	туре			Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	U10	M	406	-	48,48,63	2.57	13 (27%)	58,61,79	1.76	13 (22%)
8	BCL	L	503	-	64,74,74	1.40	7 (10%)	78,115,115	1.65	14 (17%)
11	EDO	L	509	-	3,3,3	0.48	0	2,2,2	0.47	0
8	BCL	L	502	-	64,74,74	1.51	7 (10%)	78,115,115	1.51	10 (12%)
5	LDA	M	408	-	12,15,15	1.97	1 (8%)	14,17,17	0.70	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
8	BCL	M	402	-	-	5/37/137/137	-
9	BPH	L	504	-	-	6/37/105/105	0/5/6/6
8	BCL	M	403	-	-	6/37/137/137	-
4	NKP	Н	301	-	-	11/28/28/28	-
4	NKP	M	401	-	-	12/28/28/28	-
5	LDA	Н	302	-	-	4/13/13/13	-
5	LDA	M	409	-	-	7/13/13/13	-
5	LDA	M	415	-	-	9/13/13/13	-
9	BPH	M	404	-	-	4/37/105/105	0/5/6/6
14	SPN	M	407	-	-	15/50/51/51	-
10	DIO	L	508	-	-	-	0/1/1/1
11	EDO	L	510	-	-	0/1/1/1	-
7	OLC	L	501	-	-	6/24/24/24	-
5	LDA	M	411	-	-	12/13/13/13	-
5	LDA	M	410	-	-	6/13/13/13	-
11	EDO	L	511	-	-	0/1/1/1	-
13	U10	M	406	-	-	13/45/69/87	0/1/1/1
8	BCL	L	503	-	-	9/37/137/137	-
11	EDO	L	509	-	-	0/1/1/1	-
8	BCL	L	502	-	-	3/37/137/137	-
5	LDA	M	408	-	-	6/13/13/13	-

The worst 5 of 53 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
5	Н	302	LDA	O1-N1	-7.01	1.25	1.42
5	M	410	LDA	O1-N1	-6.98	1.25	1.42
5	M	415	LDA	O1-N1	-6.96	1.25	1.42
5	M	409	LDA	O1-N1	-6.92	1.26	1.42
5	M	411	LDA	O1-N1	-6.83	1.26	1.42

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
9	M	404	BPH	C1-C2-C3	-5.64	116.30	126.04
8	M	402	BCL	CHD-C1D-ND	-5.57	119.34	124.45
8	L	503	BCL	CHD-C1D-ND	-5.45	119.44	124.45
8	M	402	BCL	C4D-CHA-C1A	5.06	127.41	121.25
8	M	403	BCL	C4D-CHA-C1A	4.96	127.28	121.25

There are no chirality outliers.

5 of 134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Н	301	NKP	CAG-CAH-CAI-OAJ
4	M	401	NKP	OAF-CAG-CAH-OBC
4	M	401	NKP	OAE-CAK-OAJ-CAI
4	M	401	NKP	CAL-CAK-OAJ-CAI
5	Н	302	LDA	C2-C1-N1-O1

There are no ring outliers.

15 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	402	BCL	2	0
9	L	504	BPH	2	0
8	M	403	BCL	4	0
5	Н	302	LDA	2	0
5	M	415	LDA	3	0
9	M	404	BPH	3	0
14	M	407	SPN	7	0
10	L	508	DIO	1	0
11	L	510	EDO	1	0
7	L	501	OLC	2	0
5	M	411	LDA	4	0
11	L	511	EDO	1	0
13	M	406	U10	4	0

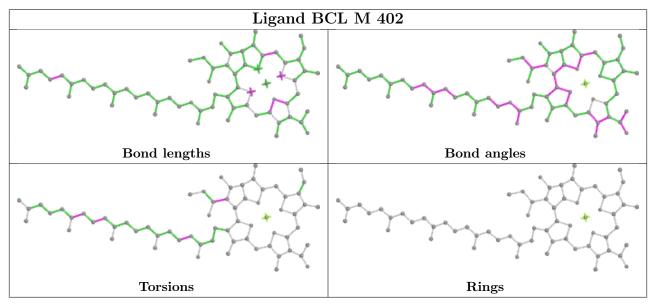
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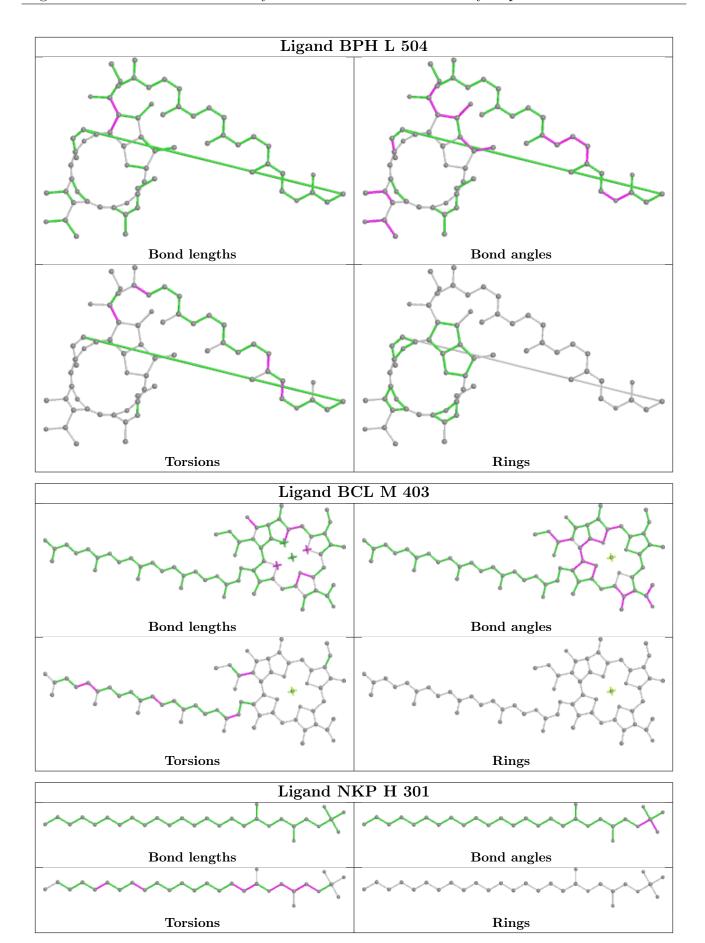
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	503	BCL	3	0
8	L	502	BCL	4	0

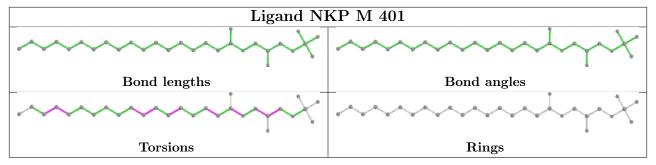
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

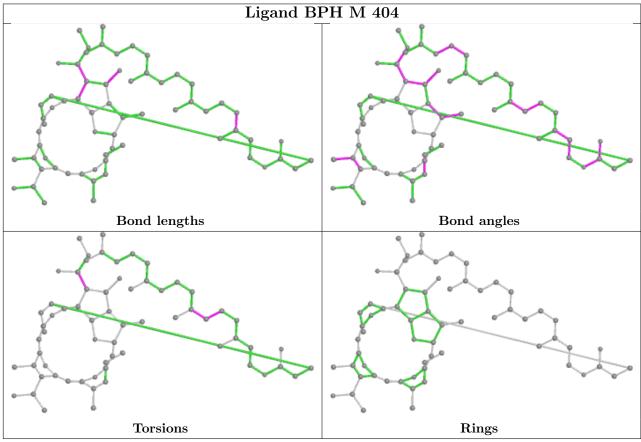


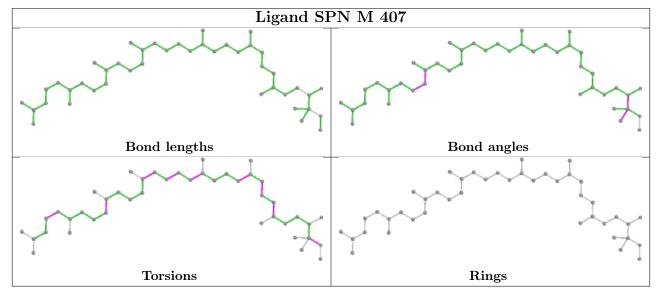




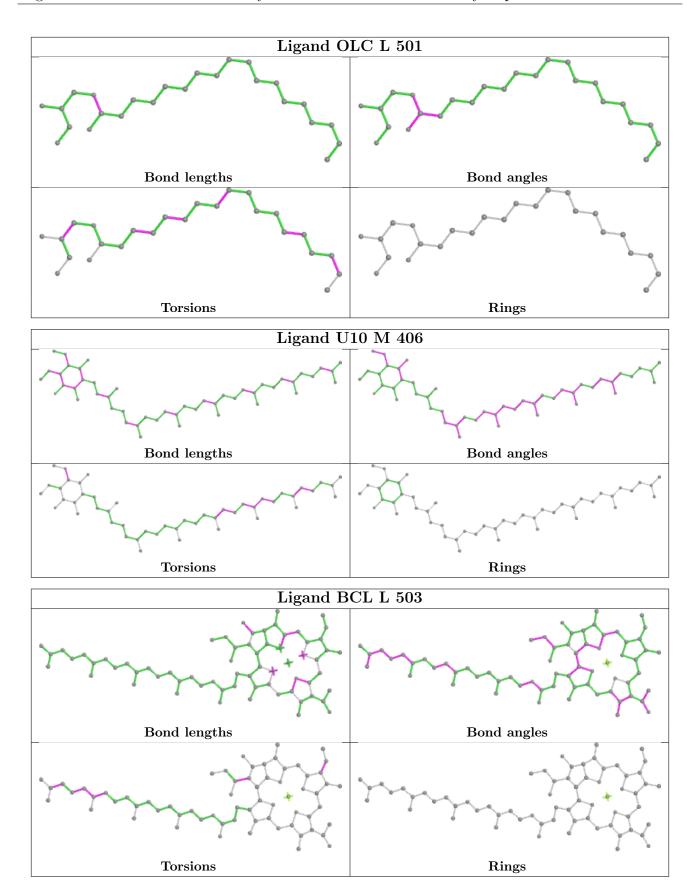




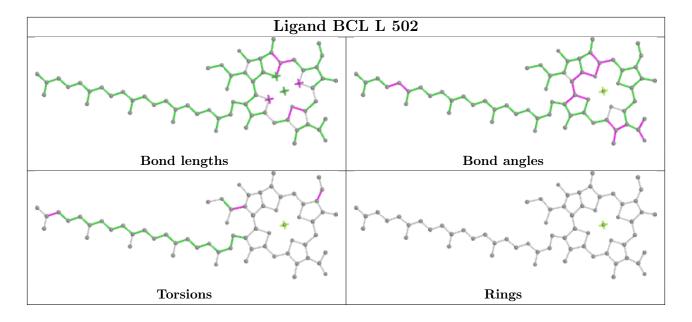












# 5.7 Other polymers (i)

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 > 2		$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	Н	$242/242 \ (100\%)$	0.09	13 (5%) 25	31	57, 73, 90, 130	0
2	L	281/281 (100%)	0.03	18 (6%) 19	23	51, 64, 108, 123	0
3	M	303/303 (100%)	-0.25	3 (0%) 82	87	48, 63, 90, 109	0
All	All	826/826 (100%)	-0.06	34 (4%) 37	44	48, 67, 94, 130	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	270	PRO	5.0
2	L	51	TRP	4.1
2	L	59	TRP	3.9
2	L	281	GLY	3.8
2	L	276	PRO	3.8

#### 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)

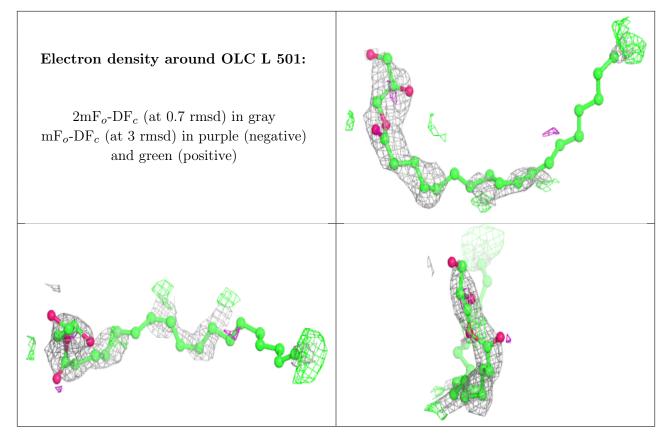
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({ ext{\AA}}^2)$	Q<0.9
6	UNL	Н	303	12/-	0.47	0.77	83,93,104,105	0
15	PO4	M	413	5/5	0.55	0.25	107,113,120,141	0
6	UNL	Н	305	15/-	0.61	0.40	82,91,99,100	0
7	OLC	L	501	25/25	0.67	0.52	68,82,89,94	0
5	LDA	M	410	16/16	0.73	0.65	72,89,124,131	0
6	UNL	L	506	15/-	0.73	0.44	72,88,108,109	0
6	UNL	M	412	12/-	0.75	0.52	70,95,109,109	0
6	UNL	Н	304	12/-	0.77	0.78	73,84,91,96	0
5	LDA	M	409	16/16	0.77	0.40	71,93,109,114	0
4	NKP	Н	301	29/29	0.81	0.33	60,85,103,107	0
4	NKP	M	401	29/29	0.82	0.30	65,77,103,112	0
5	LDA	M	411	16/16	0.84	0.32	86,95,108,109	0
6	UNL	L	507	10/-	0.85	0.36	74,80,87,91	0
5	LDA	M	408	16/16	0.86	0.26	40,73,85,86	0
9	BPH	M	404	65/65	0.86	0.27	49,60,101,108	0
5	LDA	M	415	16/16	0.86	0.53	76,89,99,105	0
11	EDO	L	509	4/4	0.87	0.41	65,69,74,79	0
14	SPN	M	407	43/43	0.88	0.35	53,73,88,96	0
6	UNL	L	505	12/-	0.88	0.47	74,76,86,94	0
10	DIO	L	508	6/6	0.89	0.47	94,99,102,109	0
11	EDO	L	511	4/4	0.92	0.58	68,73,80,82	0
13	U10	M	406	48/63	0.92	0.21	45,63,79,84	0
11	EDO	L	510	4/4	0.93	0.36	67,73,82,89	0
9	BPH	L	504	65/65	0.94	0.20	46,59,64,67	0
15	PO4	M	414	5/5	0.94	0.13	80,86,92,96	5
8	BCL	M	402	66/66	0.95	0.19	42,60,87,90	0
8	BCL	M	403	66/66	0.95	0.21	45,57,66,78	0
5	LDA	Н	302	16/16	0.95	0.25	67,72,77,78	0
8	BCL	L	502	66/66	0.97	0.18	50,61,67,74	0
8	BCL	L	503	66/66	0.97	0.19	44,55,71,81	0
12	FE	M	405	1/1	1.00	0.19	58,58,58,58	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.



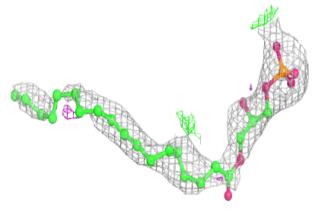


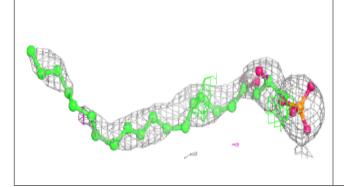
# Electron density around NKP H 301: 2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)

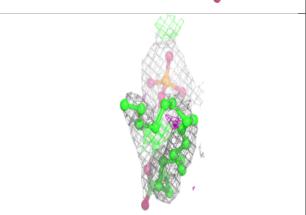


## Electron density around NKP M 401:

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

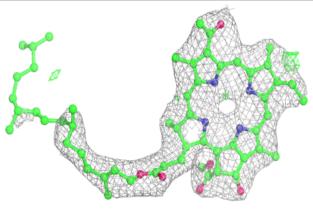


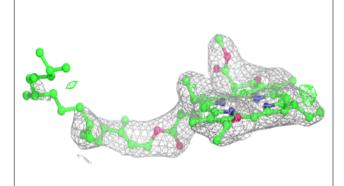


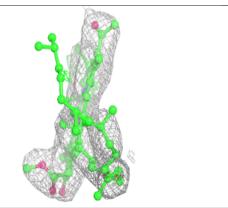


#### Electron density around BPH M 404:

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



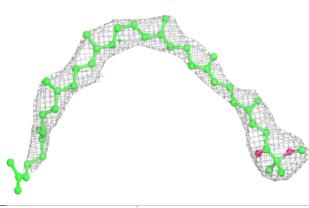


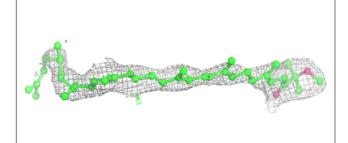




# Electron density around SPN M 407:

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

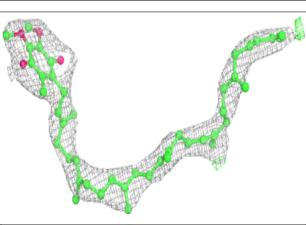


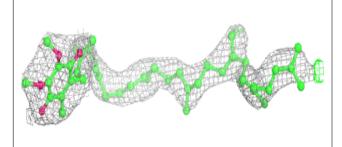


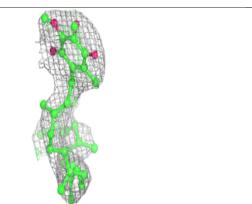


#### Electron density around U10 M 406:

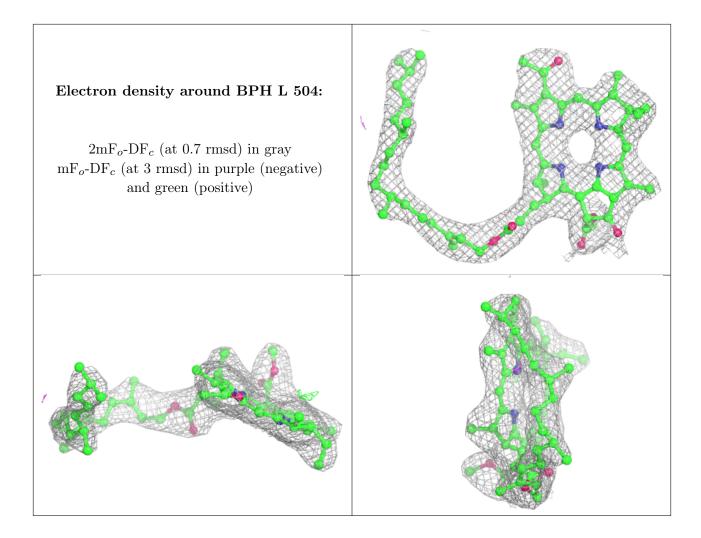
 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



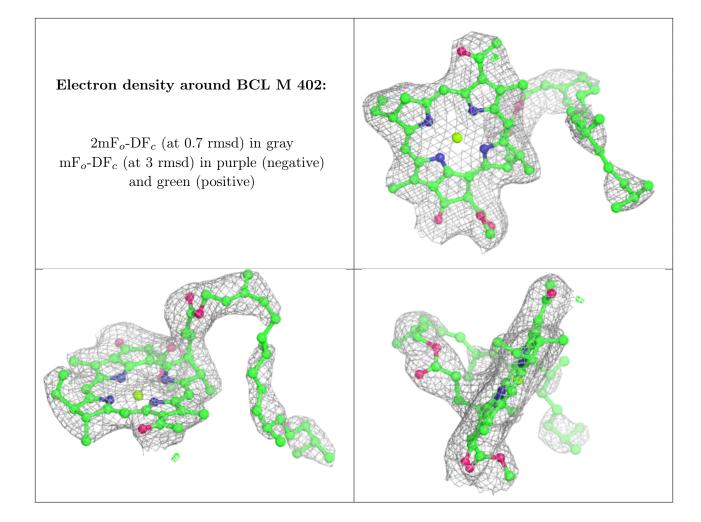




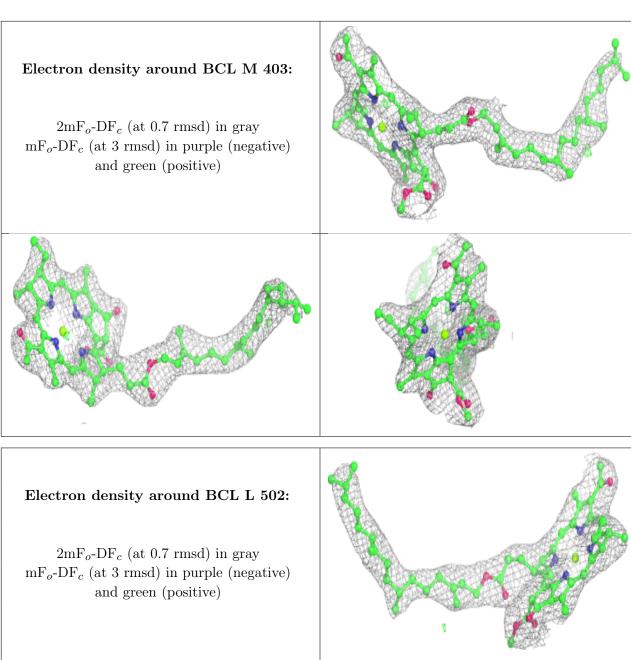


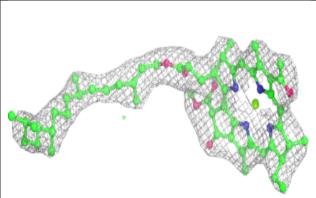


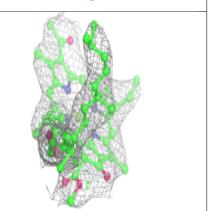




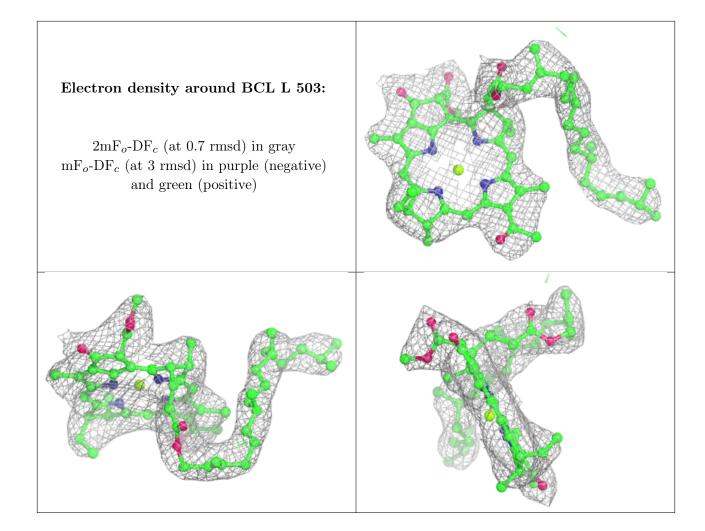




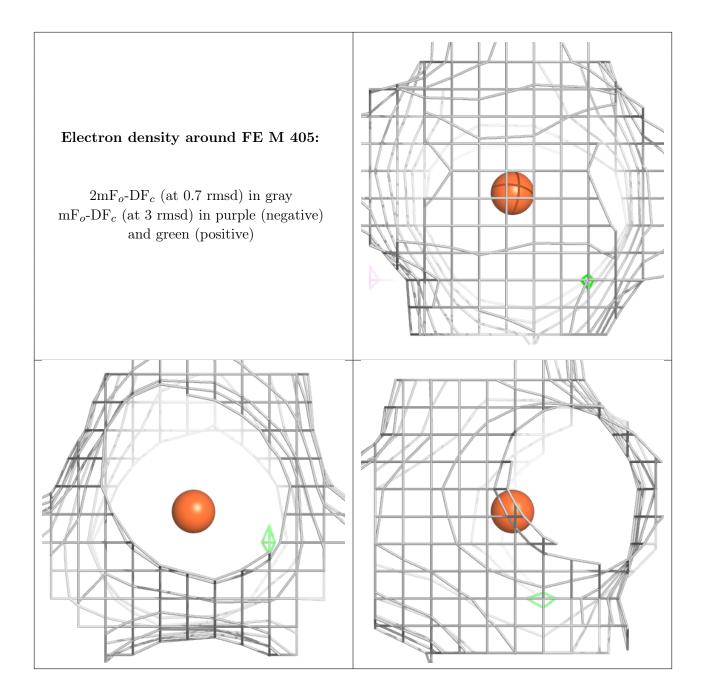












# 6.5 Other polymers (i)

There are no such residues in this entry.

