

wwPDB X-ray Structure Validation Summary Report (i)

Jul 4, 2022 – 08:29 pm BST

PDB ID : 7P0Q

Title: F(M197)H mutant structure of Photosynthetic Reaction Center From

Rhodobacter Sphaeroides strain RV by fixed-target serial synchrotron crys-

tallography (100K, 26keV)

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Deposited on : 2021-06-30

Resolution : 1.73 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 : 2.29

buster-report : 1.1.7 (2018)

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

Refmac : 5.8.0267

CCP4 : 7.1.010 (Gargrove)

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

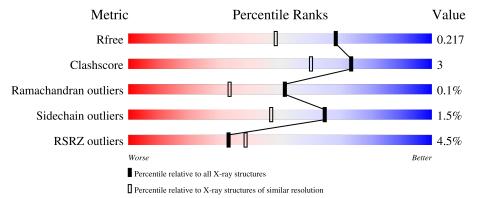
Validation Pipeline (wwPDB-VP) : 2.29

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 1.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	241	90%	10%
2	L	281	96%	
3	M	303	92%	7%



2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 7717 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.

M	[ol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
]	1	Н	241	Total 1897	C 1212	N 325	O 350	S 10	0	8	0

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

Mol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
2	T.	281	Total	С	N	О	S	0	2	0
2	ш	201	2247	1519	356	364	8		2	

There is a discrepancy between the modelled and reference sequences:

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

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

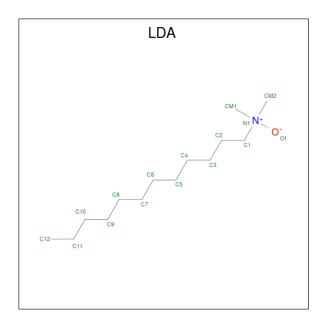
\mathbf{Mol}	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
3	M	302	Total 2432	C 1622	N 399	O 400	S 11	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Μ	8	THR	SER	engineered mutation	UNP P0C0Y9
M	197	HIS	PHE	engineered mutation	UNP P0C0Y9

• Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).





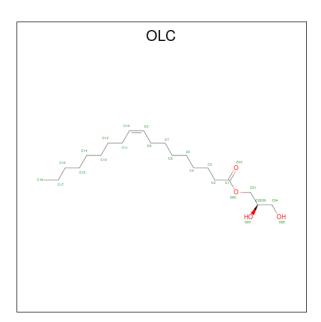
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
1	Н	1	Total C N O	0	0	
4	11	1	16 14 1 1	U		
1	Н	1	Total C N O	0	0	
4	11	1	16 14 1 1	U	U	
1	M	1	Total C N O	0	0	
4	IVI	1	16 14 1 1	U	0	
1	М	1	Total C N O	0	0	
4	M	1	16 14 1 1	U	0	

• Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Н	1	Total C 15 15	0	0
5	L	2	Total C 30 30	0	0
5	M	4	Total C 60 60	0	0

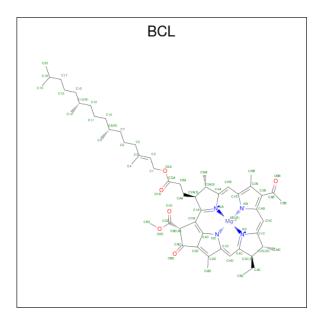
 \bullet Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4).$





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total 25	C 21	O 4	0	0

 \bullet Molecule 7 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	
7	Т	1	Total	С	Mg	N	О	0	0	
'	ь	1	66	55	1	4	6	U		
7	т	1	Total	С	Mg	N	О	0	0	
′	ь	1	66	55	1	4	6	U	U	

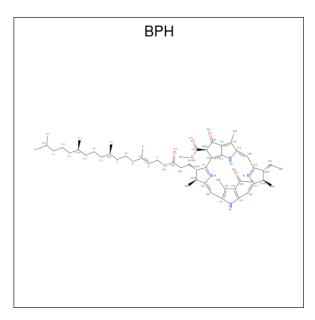
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
7	М	1	Total	С	Mg	N	О	0	0	
'	IVI	1	66	55	1	4	6	U	U	
7	М	1	Total	С	Mg	N	О	0	0	
'	IVI	1	66	55	1	4	6	U	U	

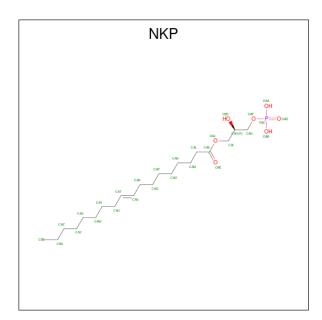
• Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

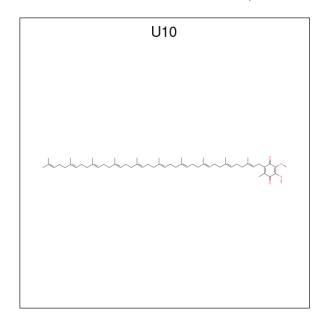
• Molecule 9 is (2R)-2-hydroxy-3-(phosphonooxy) propyl (9E)-octadec-9-enoate (three-letter code: NKP) (formula: $C_{21}H_{41}O_7P$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
O)	М	1	Total	С	О	Р	0	0	
	1/1	1	29	21	7	1	0		
0	М	1	Total	С	Ο	Р	0	0	
9	1V1	1	29	21	7	1	0	U	

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



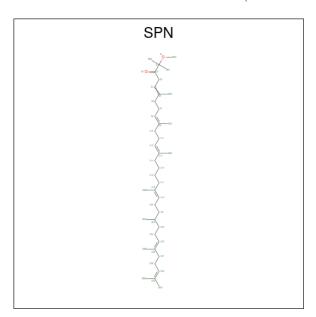
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	М	1	Total C O	0	0
	111	1	63 59 4		

 \bullet Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).



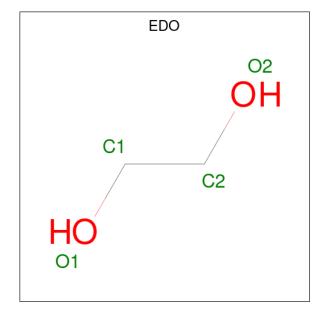
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total Fe 1 1	0	0

 \bullet Molecule 12 is SPEROIDENONE (three-letter code: SPN) (formula: $\mathrm{C_{41}H_{70}O_2}).$



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

 \bullet Molecule 13 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total 4	C 2	O 2	0	0

• Molecule 14 is water.

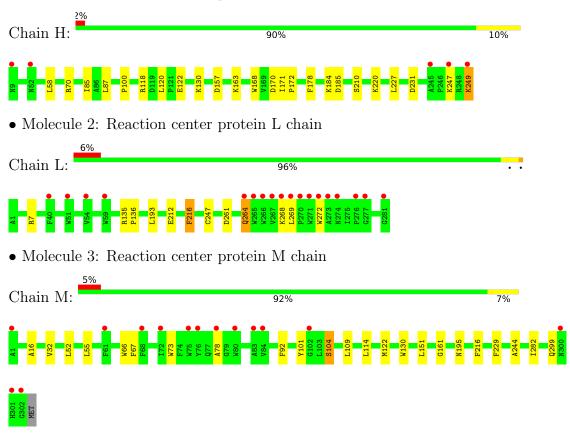
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	Н	186	Total O 186 186	0	0
14	L	96	Total O 96 96	0	0
14	M	102	Total O 102 102	0	0



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	99.97Å 99.97Å 239.22Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 - 1.73	Depositor
rtesolution (A)	48.93 - 1.73	EDS
% Data completeness	99.3 (48.93-1.73)	Depositor
(in resolution range)	100.0 (48.93-1.73)	EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.25 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.203	Depositor
it, it free	0.191 , 0.217	DCC
R_{free} test set	6292 reflections $(4.96%)$	wwPDB-VP
Wilson B-factor (\mathring{A}^2)	30.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7717	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.43% 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: LDA, NKP, OLC, EDO, UNL, FE, SPN, U10, BCL, BPH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bond angles		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Н	0.53	0/1949	0.69	0/2652	
2	L	0.60	0/2339	0.65	0/3201	
3	M	0.59	0/2524	0.62	0/3446	
All	All	0.58	0/6812	0.65	0/9299	

There are no bond length outliers.

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	1897	0	1898	13	0
2	L	2247	0	2202	9	0
3	M	2432	0	2349	15	0
4	Н	32	0	62	1	0
4	M	32	0	62	0	0
5	Н	15	0	0	0	0
5	L	30	0	0	0	0
5	M	60	0	0	0	0
6	L	25	0	40	1	0
7	L	132	0	148	3	0

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Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	132	0	148	5	0
8	L	65	0	76	0	0
8	M	65	0	76	1	0
9	M	58	0	78	1	0
10	M	63	0	90	1	0
11	M	1	0	0	0	0
12	M	43	0	70	5	0
13	M	4	0	6	0	0
14	Н	186	0	0	1	0
14	L	96	0	0	2	0
14	M	102	0	0	1	0
All	All	7717	0	7305	49	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 3.

The worst 5 of 49 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ (\rm \mathring{A}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:H:118[A]:ARG:HD3	1:H:120:LEU:HD12	1.52	0.92
1:H:70:ARG:O	1:H:118[A]:ARG:NH2	2.29	0.66
3:M:161:GLY:HA3	12:M:411:SPN:H201	1.76	0.66
7:M:407:BCL:CAB	12:M:411:SPN:H162	2.27	0.64
3:M:109:LEU:HG	3:M:114[B]:LEU:HG	1.78	0.64

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 Allowe				
1	Н	247/241 (102%)	243 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
2	L	281/281 (100%)	276 (98%)	5 (2%)	0	100	100
3	M	303/303 (100%)	295 (97%)	7 (2%)	1 (0%)	41	23
All	All	831/825 (101%)	814 (98%)	16 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	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	Perce	ntiles
1	Н	203/196~(104%)	199 (98%)	4 (2%)	55	33
2	L	222/220 (101%)	217 (98%)	5 (2%)	50	27
3	M	239/237 (101%)	237 (99%)	2 (1%)	81	72
All	All	664/653 (102%)	653 (98%)	11 (2%)	65	41

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	264	GLN
2	L	272	TRP
3	M	216	PHE
3	M	104	SER
2	L	216[A]	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 24 ligands modelled in this entry, 7 are unknown and 1 is monoatomic - leaving 16 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	В	ond leng	$_{ m gths}$	Во	ond angl	es
WIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	U10	M	405	-	63,63,63	2.59	18 (28%)	76,79,79	1.75	21 (27%)
4	LDA	M	412	-	12,15,15	1.96	1 (8%)	14,17,17	0.62	0
4	LDA	M	413	-	12,15,15	2.08	1 (8%)	14,17,17	0.61	0
7	BCL	M	408	-	58,74,74	1.43	8 (13%)	69,115,115	1.51	11 (15%)
8	BPH	L	505	-	51,70,70	1.15	4 (7%)	52,101,101	1.04	4 (7%)
9	NKP	M	401	-	28,28,28	0.38	0	31,32,32	0.61	1 (3%)
13	EDO	M	415	-	3,3,3	0.44	0	2,2,2	1.26	0
9	NKP	M	403	-	28,28,28	0.53	0	31,32,32	0.47	0
6	OLC	L	501	-	24,24,24	0.90	1 (4%)	25,25,25	1.11	2 (8%)
7	BCL	L	503	-	58,74,74	1.54	6 (10%)	69,115,115	1.34	9 (13%)
7	BCL	M	407	-	58,74,74	1.43	6 (10%)	69,115,115	1.54	13 (18%)
4	LDA	Н	401	-	12,15,15	2.02	1 (8%)	14,17,17	0.77	0
7	BCL	L	504	-	58,74,74	1.33	4 (6%)	69,115,115	1.35	8 (11%)
12	SPN	M	411	-	40,42,42	0.60	0	50,52,52	1.60	10 (20%)
8	BPH	M	409	-	51,70,70	1.04	4 (7%)	52,101,101	2.11	11 (21%)
4	LDA	Н	403	-	12,15,15	2.06	1 (8%)	14,17,17	0.58	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
10	U10	M	405	-	-	19/63/87/87	0/1/1/1
4	LDA	M	412	-	-	7/13/13/13	-
4	LDA	M	413	-	-	8/13/13/13	-
7	BCL	M	408	-	-	3/37/137/137	-
8	BPH	L	505	-	-	4/37/105/105	0/5/6/6
9	NKP	M	401	-	-	9/28/28/28	-
13	EDO	M	415	-	-	1/1/1/1	-
9	NKP	M	403	-	-	10/28/28/28	-
6	OLC	L	501	-	-	7/24/24/24	-
7	BCL	L	503	-	-	1/37/137/137	-
7	BCL	M	407	-	-	2/37/137/137	-
4	LDA	Н	401	-	-	10/13/13/13	-
7	BCL	L	504	-	-	5/37/137/137	-
12	SPN	M	411	-	-	17/50/51/51	-
8	ВРН	M	409	-	-	9/37/105/105	0/5/6/6
4	LDA	Н	403	-	-	4/13/13/13	-

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
4	M	413	LDA	O1-N1	-7.11	1.25	1.42
4	Н	403	LDA	O1-N1	-7.05	1.25	1.42
4	Н	401	LDA	O1-N1	-6.90	1.26	1.42
4	M	412	LDA	O1-N1	-6.65	1.26	1.42
10	M	405	U10	C43-C44	6.56	1.48	1.33

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
8	M	409	BPH	C16-C15-C13	8.29	142.70	115.92
8	M	409	BPH	C11-C10-C8	8.06	141.98	115.92
7	M	408	BCL	C4A-NA-C1A	5.61	109.23	106.71
12	M	411	SPN	CM6-C18-C17	4.81	123.36	115.27
7	M	407	BCL	CMB-C2B-C1B	-4.66	121.30	128.46

There are no chirality outliers.



5 of 116 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Н	401	LDA	C2-C1-N1-O1
4	Н	401	LDA	C2-C1-N1-CM1
4	Н	401	LDA	C2-C1-N1-CM2
4	M	412	LDA	C2-C1-N1-O1
4	M	412	LDA	C2-C1-N1-CM1

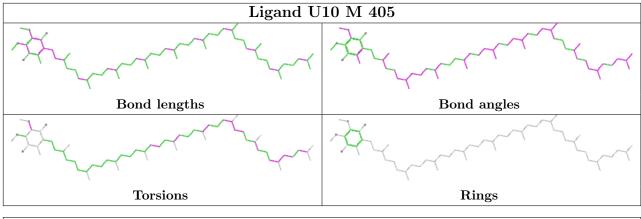
There are no ring outliers.

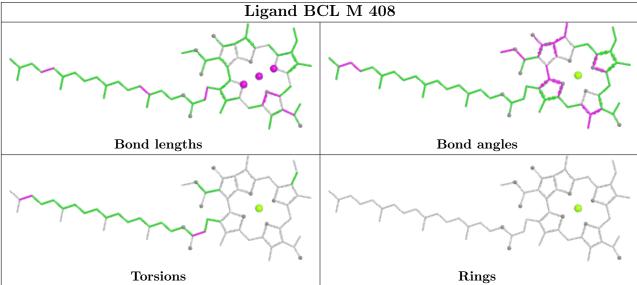
10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	405	U10	1	0
7	M	408	BCL	3	0
9	M	401	NKP	1	0
6	L	501	OLC	1	0
7	L	503	BCL	2	0
7	M	407	BCL	2	0
4	Н	401	LDA	1	0
7	L	504	BCL	1	0
12	M	411	SPN	5	0
8	M	409	BPH	1	0

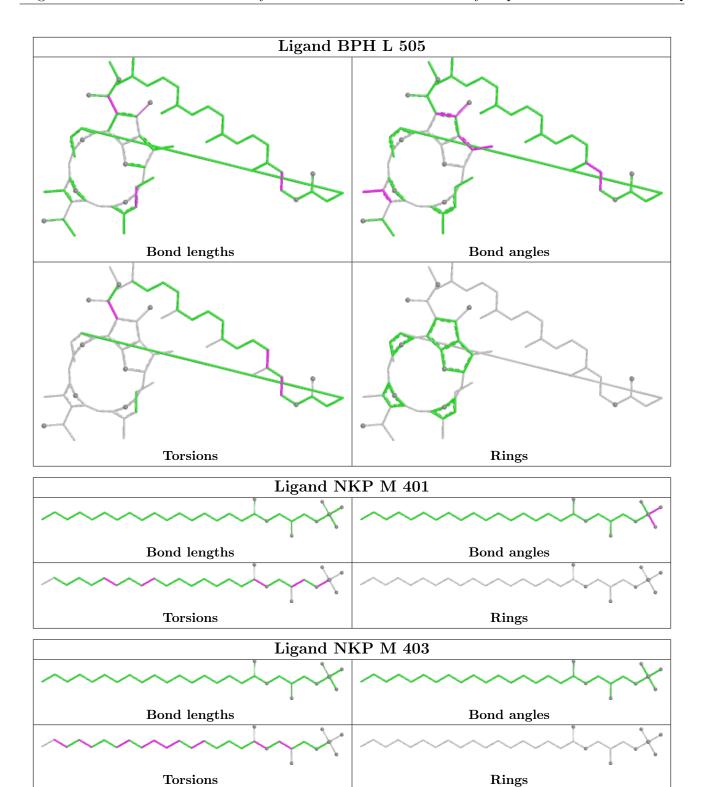
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



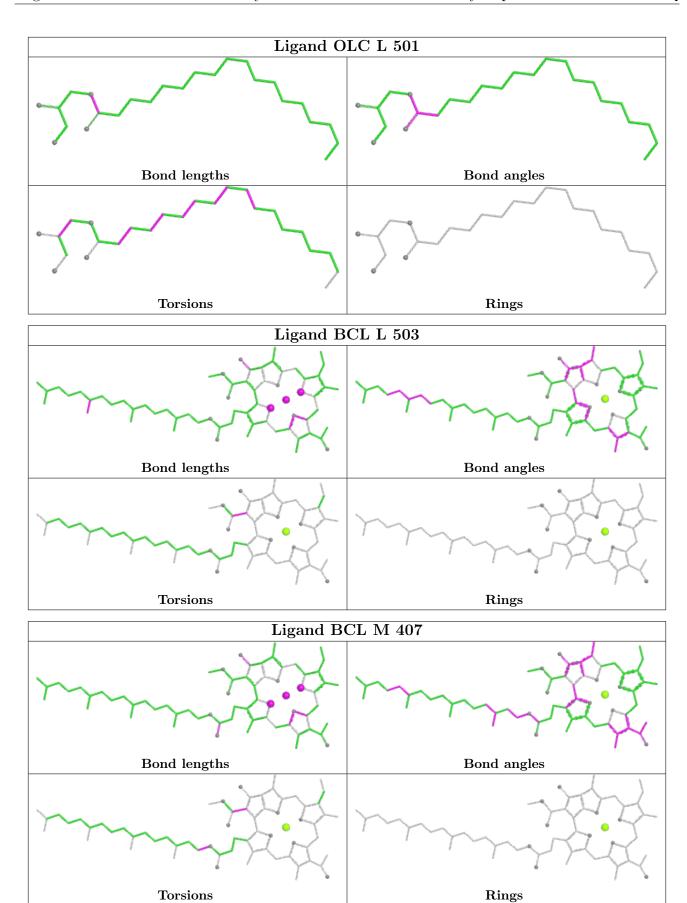




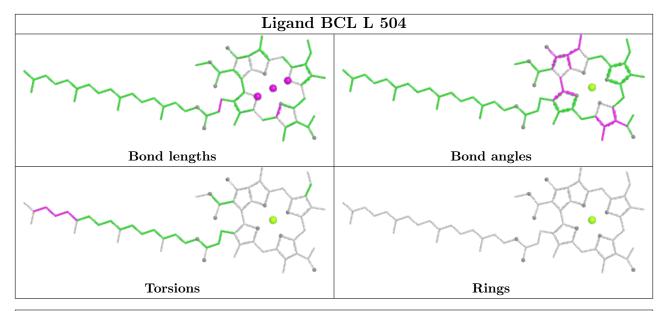


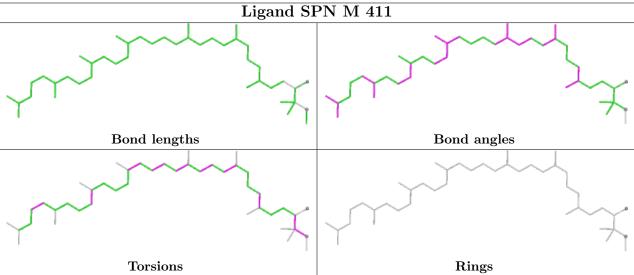




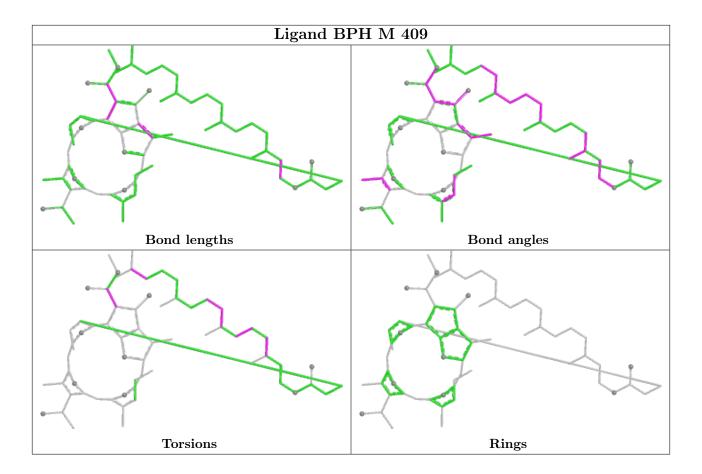












5.7 Other polymers (i)

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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	Н	241/241 (100%)	-0.16	5 (2%) 63 70	25, 34, 49, 76	0
2	L	281/281 (100%)	0.06	18 (6%) 19 23	24, 31, 56, 74	0
3	M	302/303~(99%)	0.18	14 (4%) 32 38	22, 32, 54, 80	0
All	All	824/825 (99%)	0.04	37 (4%) 33 38	22, 32, 54, 80	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	9.5
2	L	59	TRP	8.7
2	L	270	PRO	7.6
3	M	301	HIS	7.0
3	M	302	GLY	5.8

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
5	UNL	L	502	15/-	0.66	0.19	41,48,60,64	0
5	UNL	Н	402	15/-	0.68	0.23	49,60,67,67	0
4	LDA	M	412	16/16	0.68	0.33	52,57,70,73	0
5	UNL	M	402	15/-	0.70	0.20	51,62,67,67	0
4	LDA	M	413	16/16	0.72	0.32	53,62,82,85	0
5	UNL	M	404	15/-	0.75	0.27	31,46,56,57	0
4	LDA	Н	403	16/16	0.79	0.20	36,44,52,56	0
5	UNL	M	414	15/-	0.82	0.13	45,52,61,65	0
4	LDA	Н	401	16/16	0.84	0.15	49,57,65,66	0
5	UNL	L	506	15/-	0.85	0.13	42,47,54,57	0
6	OLC	L	501	25/25	0.85	0.13	30,43,54,56	0
12	SPN	M	411	43/43	0.85	0.15	30,43,58,61	0
9	NKP	M	403	29/29	0.86	0.17	33,55,69,72	0
10	U10	M	405	63/63	0.87	0.19	20,33,64,67	0
5	UNL	M	406	15/-	0.90	0.23	42,47,58,59	0
9	NKP	M	401	29/29	0.91	0.17	32,51,73,78	0
13	EDO	M	415	4/4	0.92	0.09	44,45,56,58	0
8	BPH	M	409	65/65	0.94	0.11	23,30,72,75	0
7	BCL	L	503	66/66	0.94	0.11	23,26,33,39	0
7	BCL	M	408	66/66	0.96	0.08	21,26,47,61	0
8	BPH	L	505	65/65	0.96	0.12	22,25,31,32	0
7	BCL	L	504	66/66	0.96	0.14	22,26,38,48	0
7	BCL	M	407	66/66	0.96	0.09	23,30,60,63	0
11	FE	M	410	1/1	1.00	0.09	25,25,25,25	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.

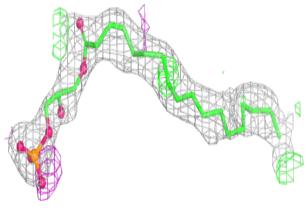


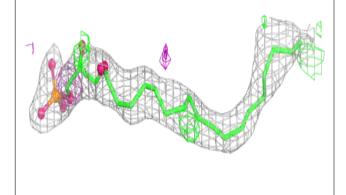
Electron density around OLC L 501: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around SPN M 411: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)

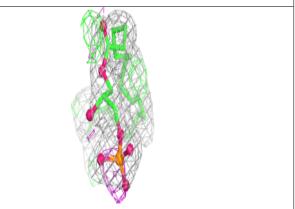


Electron density around NKP M 403:

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

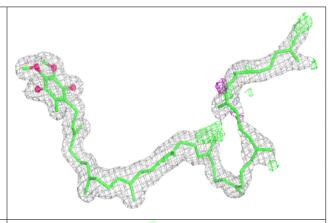


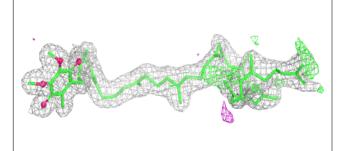


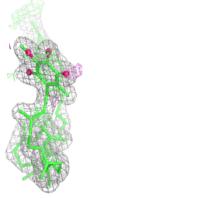


Electron density around U10 M 405:

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



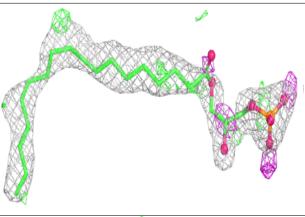


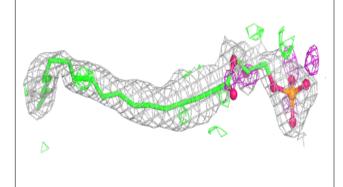


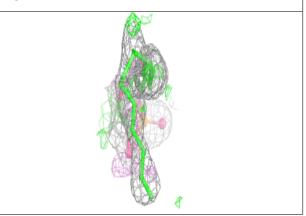


Electron density around NKP M 401:

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

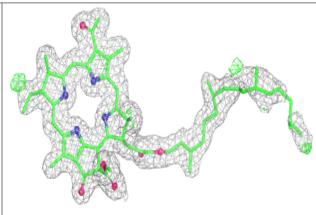


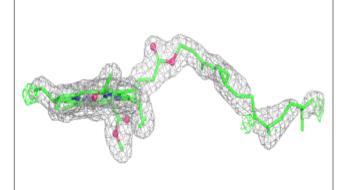


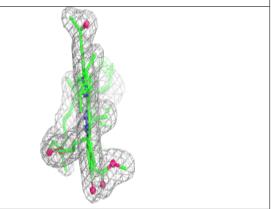


Electron density around BPH M 409:

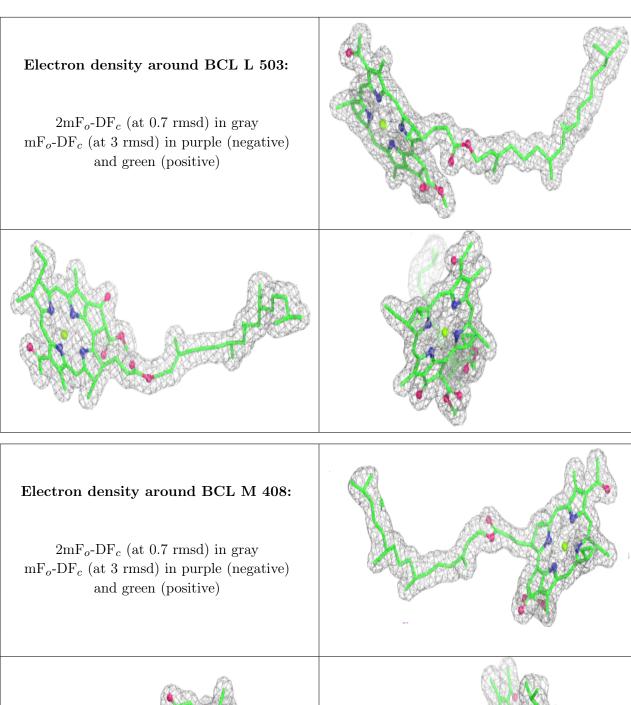
 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

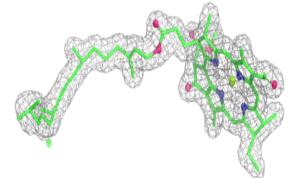


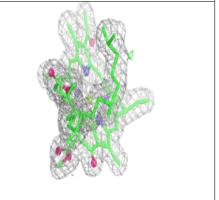




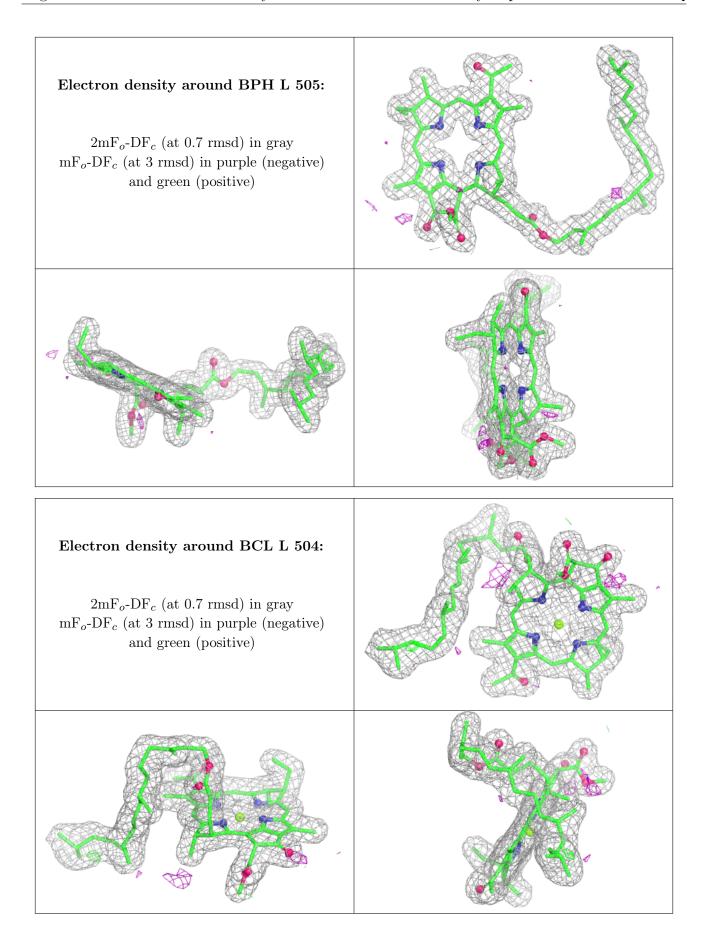




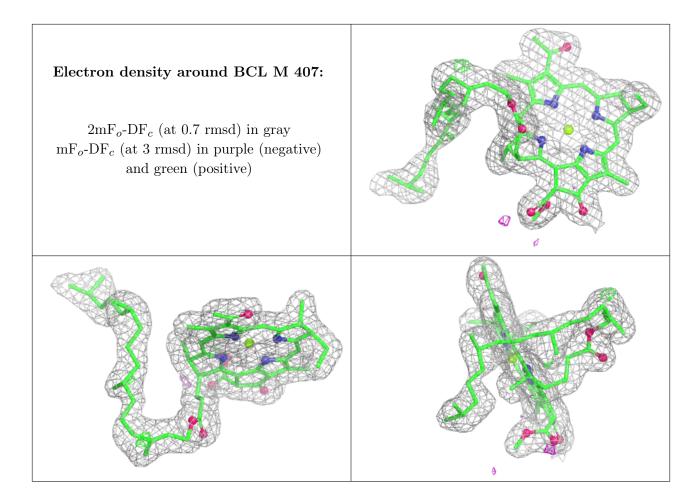












6.5 Other polymers (i)

There are no such residues in this entry.

