

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

Nov 14, 2023 – 01:33 pm GMT

PDB ID	:	8C5X
Title	:	Double mutant A(L37)C/S(L99)C structure of Photosynthetic Reaction Cen-
		ter From Cereibacter sphaeroides strain RV
Authors	:	Gabdulkhakov, A.; Selikhanov, G.; Fufina, T.; Vasilieva, L.; Atamas, A.;
		Uhimchuk, D.
Deposited on	:	2023-01-10
Resolution	:	2.60  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	:	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:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.60 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.



Motric	Whole archive	Similar resolution
IVIETIC	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	90%	10%	•
2	L	281	92%	8%	-
3	М	303	92%	7%	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	LDA	М	412	-	-	-	Х
5	UNL	Н	302	-	-	-	Х
5	UNL	Н	303	-	-	-	Х
5	UNL	Н	304	-	-	-	Х
5	UNL	L	307	-	-	-	Х
5	UNL	М	413	-	-	-	Х

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



# 2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 7547 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Н	240	Total 1848	C 1183	N 317	O 339	S 9	0	3	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total 2245	C 1516	N 356	O 363	S 10	0	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	37	CYS	ALA	engineered mutation	UNP P0C0Y8
L	99	CYS	SER	engineered mutation	UNP P0C0Y8
L	178	THR	SER	conflict	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	М	302	Total 2425	C 1621	N 397	O 397	S 10	0	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
М	8	THR	SER	conflict	UNP P0C0Y9

• Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf	
4	Ц	1	Total	С	Ν	0	0	0	
4	11	1	16	14	1	1	0	0	
4	4 M	1	Total	С	Ν	Ο	0	0	
4		T	16	14	1	1	0	0	
4	М	М	1	Total	С	Ν	0	0	0
4 101	1	16	14	1	1	0	0		
4	4 M	M 1	Total	С	Ν	Ο	0	0	
4	111		16	14	1	1		0	
4	М	1	Total	С	Ν	0	0	Ο	
4	111	T	16	14	1	1	0	0	
4	М	1	Total	С	Ν	Ο	0	0	
4 1/1	T	16	14	1	1	0	U		
4	М	<u>Л</u> 1	Total	С	N	0	0	0	
±	111	L	16	14	1	1		0	

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Н	4	$\begin{array}{cc} \text{Total} & \text{C} \\ 51 & 51 \end{array}$	0	0
5	L	3	$\begin{array}{cc} \text{Total} & \text{C} \\ 37 & 37 \end{array}$	0	0
5	М	3	Total C 39 39	0	0

• Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
6	L	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
6	М	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
6	М	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





8C5X	

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	L	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	L	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	L	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
7	М	1	$\begin{array}{c cc} Total & C & O \\ 4 & 2 & 2 \end{array}$	0	0
7	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

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

• Molecule 9 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		At	oms			ZeroOcc	AltConf
9	L	1	Total	С	Mg	Ν	Ο	0	0
3	Ľ	T	66	55	1	4	6	0	0
0	T	1	Total	С	Mg	Ν	Ο	0	0
3	Ľ	T	66	55	1	4	6		0
0	М	1	Total	С	Mg	Ν	Ο	0	0
3	111	T	66	55	1	4	6	0	0
0	М	1	Total	С	Mg	Ν	Ο	0	0
9	111	T	66	55	1	4	6	0	0

• Molecule 10 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
10	L	1	Total 65	C 55	N 4	0 6	0	0
10	М	1	Total 65	C 55	N 4	O 6	0	0

• Molecule 11 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
11	L	1	Total C O	0	0
		1	48 44 4	0	0
11	М	1	Total C O	0	0
	111	I	48 44 4	0	0

• Molecule 12 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula:  $C_4H_8O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0

• Molecule 13 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	L	1	Total 10	$\begin{array}{c} \mathrm{C} \\ 7 \end{array}$	O 3	0	0

• Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	М	1	Total	С	0	Р	0	0
14	111	I	81	62	17	2	0	0

• Molecule 15 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).



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

• Molecule 16 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
16	М	1	Total 43	C 41	O 2	0	0

• Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	Н	43	Total O 43 43	0	0
17	L	22	Total O 22 22	0	0
17	М	41	Total O 41 41	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 31 2 1	Depositor
Cell constants	139.85Å 139.85Å 186.56Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	29.89 - 2.60	Depositor
Resolution (A)	29.89 - 2.60	EDS
% Data completeness	100.0 (29.89-2.60)	Depositor
(in resolution range)	$100.0 \ (29.89-2.60)$	EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.67 (at 2.61 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.20.1_4487	Depositor
P.P.	0.186 , $0.207$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.189 , $0.206$	DCC
$R_{free}$ test set	3351 reflections $(5.13%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	52.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , $51.4$	EDS
L-test for $twinning^2$	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7547	wwPDB-VP
Average B, all atoms $(Å^2)$	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: U10, K, BCL, PO4, CDL, HTO, BPH, LDA, EDO, DIO, UNL, SPN, FE

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

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	Н	0.45	0/1905	0.68	0/2590	
2	L	0.48	0/2336	0.60	0/3197	
3	М	0.45	0/2524	0.58	0/3445	
All	All	0.46	0/6765	0.61	0/9232	

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	1848	0	1866	16	0
2	L	2245	0	2204	11	0
3	М	2425	0	2345	16	0
4	Н	16	0	31	2	0
4	М	96	0	186	6	0
5	Н	51	0	0	0	0
5	L	37	0	0	1	0
5	М	39	0	0	0	0
6	Н	5	0	0	0	0
6	L	5	0	0	0	0

Continued on next page...



$\begin{array}{c} \hline \begin{array}{c} \hline \end{array} \\ \hline \\ \\ \hline \end{array} \\ \hline \\ \\ \hline \end{array} \\ \hline \end{array} \\ \hline \\ \\ \hline \end{array} \\ \hline \\ \\ \hline \end{array} \\ \hline \end{array} \\ \hline \end{array} \\ \hline \\ \\ \hline \end{array} \\ \hline \end{array} \\ \hline \\ \\ \hline \end{array} \\ \hline \end{array} \\ \hline \\ \\ \hline \end{array} \\ \\ \\ \hline \end{array} \\ \\ \hline \\ \\ \\ \\$								
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
6	М	10	0	0	0 0			
7	Н	12	0	18	2	0		
7	L	12	0	18	0	0		
7	М	8	0	12	0	0		
8	Н	1	0	0	0	0		
9	L	132	0	148	1	0		
9	М	132	0	148	4	0		
10	L	65	0	76	0	0		
10	М	65	0	76	2	0		
11	L	48	0	63	3	0		
11	М	48	0	63	2	0		
12	L	6	0	8	0	0		
13	L	10	0	16	0	0		
14	М	81	0	106	6	0		
15	М	1	0	0	0	0		
16	М	43	0	70	7	0		
17	Н	43	0	0	0	0		
17	L	22	0	0	1	0		
17	М	41	0	0	0	0		
All	All	7547	0	7454	58	0		

Continued from previous page...

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 4.

The worst 5 of 58 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:301:LDA:H121	4:M:408:LDA:H91	1.63	0.78
3:M:34:PRO:HA	4:M:412:LDA:H101	1.75	0.68
2:L:62:GLN:OE1	2:L:151:TRP:NE1	2.28	0.66
3:M:161:GLY:HA3	16:M:407:SPN:H201	1.78	0.65
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.80	0.63

There are no symmetry-related clashes.



### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Н	241/242 (100%)	238~(99%)	3~(1%)	0	100 100
2	L	$281/281 \ (100\%)$	268~(95%)	12~(4%)	1 (0%)	34 57
3	М	302/303~(100%)	291 (96%)	11 (4%)	0	100 100
All	All	824/826 (100%)	797~(97%)	26 (3%)	1 (0%)	51 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	52	SER

#### 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	Percentiles		
1	Н	198/197~(100%)	195~(98%)	3~(2%)	65	83
2	L	223/221 (101%)	216~(97%)	7 (3%)	40	66
3	М	238/237~(100%)	235~(99%)	3 (1%)	69	86
All	All	659/655~(101%)	646~(98%)	13 (2%)	55	78

5 of 13 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	L	247	CYS
2	L	268	LYS

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
3	М	216	PHE
3	М	62	SER
3	М	182	HIS

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 43 ligands modelled in this entry, 10 are unknown and 2 are monoatomic - leaving 31 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).

Mal	Iol Turno Chain Bog		Dec	Tink	Bond lengths			Bond angles			
IVIOI	noi Type Chain	nes		Counts	RMSZ	=	# Z >2	Counts	RMSZ	# Z >2	
14	CDL	М	401	-	80,80,99	0.47		1 (1%)	86,92,111	0.37	0
10	BPH	М	404	-	51,70,70	0.81		1 (1%)	52,101,101	1.47	10 (19%)
11	U10	L	304	-	48,48,63	2.58		12 (25%)	58,61,79	2.10	22 (37%)
4	LDA	М	408	-	12,15,15	2.14		1 (8%)	14,17,17	0.44	0
9	BCL	М	403	-	64,74,74	1.52		8 (12%)	78,115,115	1.46	10 (12%)



Mol	Type	Chain	Bos	Link	B	ond leng	gths	Bo	ond ang	es
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
13	HTO	L	312	-	$9,\!9,\!9$	0.47	0	$10,\!10,\!10$	1.11	1 (10%)
10	BPH	L	303	-	51,70,70	1.19	4 (7%)	52,101,101	1.18	6 (11%)
4	LDA	М	412	-	12,15,15	2.01	1 (8%)	14,17,17	0.44	0
9	BCL	М	402	-	64,74,74	1.46	9 (14%)	78,115,115	1.63	15 (19%)
6	PO4	М	416	-	4,4,4	0.98	0	6,6,6	0.47	0
7	EDO	М	419	-	3,3,3	0.55	0	2,2,2	0.28	0
6	PO4	М	417	-	4,4,4	0.70	0	6,6,6	0.50	0
11	U10	М	406	-	48,48,63	2.66	13 (27%)	58,61,79	1.80	16 (27%)
7	EDO	L	309	-	3,3,3	0.52	0	2,2,2	0.30	0
7	EDO	Н	309	-	3,3,3	0.50	0	2,2,2	0.32	0
6	PO4	L	313	-	4,4,4	0.72	0	6,6,6	0.57	0
7	EDO	М	418	-	3,3,3	0.52	0	2,2,2	0.61	0
16	SPN	М	407	-	40,42,42	0.38	0	50,52,52	0.70	0
9	BCL	L	302	-	64,74,74	1.56	9 (14%)	78,115,115	1.52	12 (15%)
7	EDO	L	310	-	3,3,3	0.43	0	2,2,2	0.50	0
12	DIO	L	308	-	6,6,6	0.50	0	6,6,6	0.08	0
7	EDO	Н	308	-	3,3,3	0.60	0	2,2,2	0.13	0
4	LDA	М	410	-	12,15,15	2.11	1 (8%)	$14,\!17,\!17$	0.67	0
4	LDA	М	409	-	12,15,15	1.98	1 (8%)	14,17,17	0.48	0
4	LDA	Н	301	-	12,15,15	1.94	1 (8%)	14,17,17	0.54	0
7	EDO	L	311	-	3,3,3	0.48	0	2,2,2	0.64	0
4	LDA	М	420	-	12,15,15	2.07	1 (8%)	14,17,17	0.54	0
9	BCL	L	301	-	64,74,74	1.45	9 (14%)	78,115,115	1.46	10 (12%)
7	EDO	Н	307	-	3,3,3	0.61	0	2,2,2	0.24	0
6	PO4	Н	306	-	4,4,4	0.86	0	6,6,6	0.49	0
4	LDA	М	411	-	12,15,15	2.08	1 (8%)	14,17,17	0.50	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
14	CDL	М	401	-	-	34/91/91/110	-
10	BPH	М	404	-	-	9/37/105/105	0/5/6/6
11	U10	L	304	-	-	16/45/69/87	0/1/1/1
4	LDA	М	408	-	-	4/13/13/13	-
9	BCL	М	403	-	-	2/37/137/137	-
13	HTO	L	312	-	-	4/10/10/10	-

Continued on next page...



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BPH	L	303	-	-	3/37/105/105	0/5/6/6
4	LDA	М	412	-	-	4/13/13/13	-
9	BCL	М	402	-	-	7/37/137/137	-
7	EDO	М	419	-	-	0/1/1/1	-
11	U10	М	406	-	-	10/45/69/87	0/1/1/1
7	EDO	L	309	-	-	0/1/1/1	-
7	EDO	Н	309	-	-	0/1/1/1	-
7	EDO	М	418	-	-	0/1/1/1	-
16	SPN	М	407	-	-	13/50/51/51	-
9	BCL	L	302	-	-	1/37/137/137	-
7	EDO	L	310	-	-	0/1/1/1	-
12	DIO	L	308	-	-	-	0/1/1/1
7	EDO	Н	308	-	-	0/1/1/1	-
4	LDA	М	410	-	-	4/13/13/13	-
4	LDA	М	409	-	-	5/13/13/13	-
4	LDA	Н	301	-	-	8/13/13/13	-
7	EDO	L	311	-	-	1/1/1/1	-
4	LDA	М	420	-	-	10/13/13/13	-
9	BCL	L	301	-	-	2/37/137/137	-
7	EDO	Н	307	-	-	0/1/1/1	-
4	LDA	М	411	-	-	6/13/13/13	-

Continued from previous page...

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
4	М	410	LDA	01-N1	-7.25	1.25	1.42
4	М	408	LDA	01-N1	-7.21	1.25	1.42
4	М	411	LDA	O1-N1	-7.14	1.25	1.42
4	М	420	LDA	01-N1	-7.09	1.25	1.42
4	М	412	LDA	01-N1	-6.86	1.26	1.42

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
9	М	402	BCL	CHD-C1D-ND	-5.55	119.35	124.45
11	L	304	U10	C1M-C1-C6	-5.38	115.62	124.40
9	L	301	BCL	CHD-C1D-ND	-5.06	119.80	124.45
9	L	302	BCL	CHD-C1D-ND	-5.01	119.85	124.45
9	М	402	BCL	C4D-CHA-C1A	4.99	127.32	121.25



There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
4	Н	301	LDA	C2-C1-N1-O1
4	Н	301	LDA	C2-C1-N1-CM1
4	М	408	LDA	C2-C1-N1-CM1
4	М	409	LDA	C2-C1-N1-O1
4	М	409	LDA	C2-C1-N1-CM1

5 of 143 torsion outliers are listed below:

There are no ring outliers.

14 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	М	401	CDL	6	0
10	М	404	BPH	2	0
11	L	304	U10	3	0
4	М	408	LDA	2	0
9	М	403	BCL	2	0
4	М	412	LDA	2	0
9	М	402	BCL	2	0
11	М	406	U10	2	0
16	М	407	SPN	7	0
9	L	302	BCL	1	0
4	М	410	LDA	1	0
4	Н	301	LDA	2	0
4	М	420	LDA	1	0
7	Н	307	EDO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient 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	$OWAB(Å^2)$	Q<0.9
1	Н	240/242~(99%)	-0.56	0 100 100	40, 47, 61, 87	0
2	L	281/281 (100%)	-0.59	6 (2%) 63 58	40, 48, 75, 105	0
3	М	302/303~(99%)	-0.62	4 (1%) 77 73	37, 49, 70, 95	0
All	All	823/826~(99%)	-0.59	10 (1%) 79 76	37, 48, 70, 105	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	281	GLY	3.4
2	L	59	TRP	3.1
2	L	276	PRO	2.9
3	М	1	ALA	2.6
2	L	277	GLY	2.6

### 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	$B-factors(Å^2)$	Q<0.9
5	UNL	М	413	15/-	0.46	0.40	53,72,87,91	0
5	UNL	Н	303	12/-	0.54	0.68	85,89,96,99	0
5	UNL	Н	302	12/-	0.56	0.50	73,79,86,86	0
4	LDA	М	412	16/16	0.59	0.44	81,108,126,131	0
5	UNL	Н	304	12/-	0.61	0.44	76,81,104,105	0
5	UNL	L	306	15/-	0.66	0.36	47,64,81,85	0
11	U10	L	304	48/63	0.66	0.33	43,71,109,123	0
5	UNL	Н	305	15/-	0.74	0.30	69,73,94,96	0
5	UNL	L	307	10/-	0.77	0.55	53,74,80,82	0
5	UNL	М	414	12/-	0.78	0.38	62,71,81,83	0
4	LDA	М	410	16/16	0.79	0.23	59,69,94,107	0
4	LDA	М	420	16/16	0.83	0.28	68,77,117,120	0
5	UNL	М	415	12/-	0.85	0.39	58,84,94,94	0
7	EDO	Н	309	4/4	0.87	0.16	61,64,75,83	0
12	DIO	L	308	6/6	0.87	0.34	92,94,95,101	0
14	CDL	М	401	81/100	0.87	0.22	42,64,80,87	81
16	SPN	М	407	43/43	0.88	0.20	41,56,70,86	0
4	LDA	М	411	16/16	0.89	0.29	73,79,95,98	0
4	LDA	М	408	16/16	0.90	0.18	39,60,73,78	0
4	LDA	М	409	16/16	0.90	0.34	60,68,84,86	0
13	HTO	L	312	10/10	0.91	0.55	$63,\!75,\!86,\!89$	0
6	PO4	L	313	5/5	0.91	0.26	71,84,104,110	0
7	EDO	L	309	4/4	0.91	0.33	$61,\!65,\!70,\!73$	0
4	LDA	Н	301	16/16	0.92	0.21	66,74,80,82	0
5	UNL	L	305	12/-	0.94	0.34	61,66,73,74	0
6	PO4	М	417	5/5	0.94	0.14	47,47,61,68	5
7	EDO	Н	307	4/4	0.94	0.10	61,67,73,74	0
11	U10	М	406	48/63	0.94	0.17	33,47,68,78	0
7	EDO	L	311	4/4	0.95	0.42	53,58,62,64	0
6	PO4	Н	306	5/5	0.96	0.19	80,88,92,94	0
6	PO4	М	416	5/5	0.96	0.15	77,78,84,89	0
7	EDO	Н	308	4/4	0.96	0.35	47,48,50,65	0
7	EDO	M	418	4/4	0.96	0.28	47,48,51,54	0
9	BCL	M	402	66/66	0.96	0.15	35,48,85,95	0
10	BPH	M	404	65/65	0.96	0.12	38,49,107,122	0
9	BCL	L	302	66/66	0.97	0.15	35,43,56,69	0
7	EDO	L	310	4/4	0.97	0.21	47,48,52,56	0
9	BCL	M	403	66/66	0.97	0.17	36,46,66,80	0
7	EDO	M	419	4/4	0.97	0.12	43,46,49,50	0
8	K	H	310	1/1	0.97	0.04	50,50,50,50	0
10	BPH	L	303	65/65	0.98	0.16	33,41,53,57	0
9	BCL	L	301	66/66	0.98	0.16	36,45,52,55	0
15	FE	M	405	1/1	1.00	0.11	39, 39, 39, 39, 39	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.































### 6.5 Other polymers (i)

There are no such residues in this entry.

