

Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 09:02 pm GMT

PDB ID : 8Q79

Title: Structure of mBaoJin at pH 6.5

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Deposited on : 2023-08-15

Resolution : 1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.orgA 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 : 1.8.4, 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)

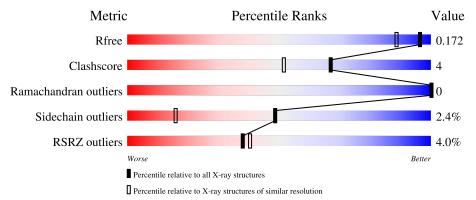
Validation Pipeline (wwPDB-VP) : 2.36

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 1.45 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \ resolution} \\ (\#{\rm Entries, \ resolution \ range(\AA)}) \end{array}$
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	A	234	83%	7% •	8%
1	В	234	86%	5% •	8%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4222 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 mBaoJin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	215	Total 1772	C 1128	N 300	O 333	S 11	0	7	0
1	В	216	Total 1771	C 1126	N 301	O 333	S 11	0	5	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	ARG	-	expression tag	UNP A0A8S0GSD4
A	-9	SER	_	expression tag	UNP A0A8S0GSD4
A	-8	MET	-	expression tag	UNP A0A8S0GSD4
A	-7	VAL	-	expression tag	UNP A0A8S0GSD4
A	-6	SER	-	expression tag	UNP A0A8S0GSD4
A	-5	LYS	-	expression tag	UNP A0A8S0GSD4
A	-4	GLY	-	expression tag	UNP A0A8S0GSD4
A	-3	GLU	-	expression tag	UNP A0A8S0GSD4
A	-2	GLU	-	expression tag	UNP A0A8S0GSD4
A	-1	GLU	-	expression tag	UNP A0A8S0GSD4
A	0	ASN	-	expression tag	UNP A0A8S0GSD4
A	55	THR	SER	engineered mutation	UNP A0A8S0GSD4
A	57	CR2	GLY	chromophore	UNP A0A8S0GSD4
A	57	CR2	TYR	chromophore	UNP A0A8S0GSD4
A	57	CR2	GLY	chromophore	UNP A0A8S0GSD4
A	75	ARG	HIS	engineered mutation	UNP A0A8S0GSD4
A	80	GLY	GLU	engineered mutation	UNP A0A8S0GSD4
A	140	PRO	GLN	engineered mutation	UNP A0A8S0GSD4
A	141	GLN	HIS	engineered mutation	UNP A0A8S0GSD4
A	165	TYR	CYS	engineered mutation	UNP A0A8S0GSD4
A	168	ALA	VAL	engineered mutation	UNP A0A8S0GSD4
A	171	TYR	ASN	engineered mutation	UNP A0A8S0GSD4
A	201	ALA	THR	engineered mutation	UNP A0A8S0GSD4
A	218	LYS	-	expression tag	UNP A0A8S0GSD4
A	219	GLY	-	expression tag	UNP A0A8S0GSD4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	220	MET	-	expression tag	UNP A0A8S0GSD4
A	221	ASP	-	expression tag	UNP A0A8S0GSD4
A	222	GLU	-	expression tag	UNP A0A8S0GSD4
A	223	LEU	-	expression tag	UNP A0A8S0GSD4
A	224	TYR	-	expression tag	UNP A0A8S0GSD4
A	225	LYS	-	expression tag	UNP A0A8S0GSD4
В	-10	ARG	-	expression tag	UNP A0A8S0GSD4
В	-9	SER	-	expression tag	UNP A0A8S0GSD4
В	-8	MET	-	expression tag	UNP A0A8S0GSD4
В	-7	VAL	-	expression tag	UNP A0A8S0GSD4
В	-6	SER	-	expression tag	UNP A0A8S0GSD4
В	-5	LYS	-	expression tag	UNP A0A8S0GSD4
В	-4	GLY	-	expression tag	UNP A0A8S0GSD4
В	-3	GLU	-	expression tag	UNP A0A8S0GSD4
В	-2	GLU	-	expression tag	UNP A0A8S0GSD4
В	-1	GLU	-	expression tag	UNP A0A8S0GSD4
В	0	ASN	-	expression tag	UNP A0A8S0GSD4
В	55	THR	SER	engineered mutation	UNP A0A8S0GSD4
В	57	CR2	GLY	chromophore	UNP A0A8S0GSD4
В	57	CR2	TYR	chromophore	UNP A0A8S0GSD4
В	57	CR2	GLY	chromophore	UNP A0A8S0GSD4
В	75	ARG	HIS	engineered mutation	UNP A0A8S0GSD4
В	80	GLY	GLU	engineered mutation	UNP A0A8S0GSD4
В	140	PRO	GLN	engineered mutation	UNP A0A8S0GSD4
В	141	GLN	HIS	engineered mutation	UNP A0A8S0GSD4
В	165	TYR	CYS	engineered mutation	UNP A0A8S0GSD4
В	168	ALA	VAL	engineered mutation	UNP A0A8S0GSD4
В	171	TYR	ASN	engineered mutation	UNP A0A8S0GSD4
В	201	ALA	THR	engineered mutation	UNP A0A8S0GSD4
В	218	LYS	-	expression tag	UNP A0A8S0GSD4
В	219	GLY	ı	expression tag	UNP A0A8S0GSD4
В	220	MET	-	expression tag	UNP A0A8S0GSD4
В	221	ASP	-	expression tag	UNP A0A8S0GSD4
В	222	GLU	ı	expression tag	UNP A0A8S0GSD4
В	223	LEU		expression tag	UNP A0A8S0GSD4
В	224	TYR	-	expression tag	UNP A0A8S0GSD4
В	225	LYS	-	expression tag	UNP A0A8S0GSD4

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	В	1	Total Cl 1 1	0	0

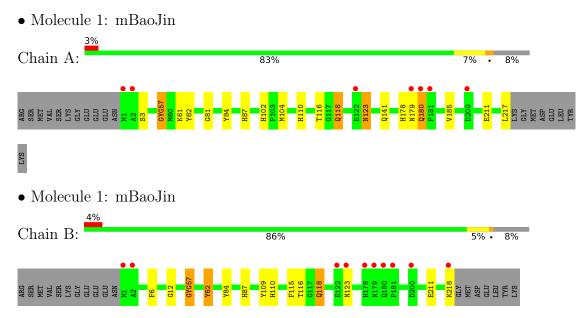
$\bullet\,$ Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	347	Total O 347 347	0	0
3	В	330	Total O 330 330	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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	45.50Å 120.31Å 52.80Å	Donositor
a, b, c, α , β , γ	90.00° 105.95° 90.00°	Depositor
Resolution (Å)	15.00 - 1.45	Depositor
Resolution (A)	14.96 - 1.45	EDS
% Data completeness	97.4 (15.00-1.45)	Depositor
(in resolution range)	97.5 (14.96-1.45)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.23 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
D D.	0.123 , 0.163	Depositor
R, R_{free}	0.127 , 0.172	DCC
R_{free} test set	4627 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 53.1	EDS
L-test for twinning ²	$ < L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4222	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.72% 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: CL, CR2

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	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.75	0/1826	0.92	2/2468 (0.1%)	
1	В	0.70	0/1819	0.91	3/2459 (0.1%)	
All	All	0.72	0/3645	0.91	5/4927 (0.1%)	

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	62	TYR	CB-CG-CD2	5.71	124.43	121.00
1	В	62	TYR	CB-CG-CD1	-5.61	117.63	121.00
1	A	84	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	В	84	TYR	CB-CG-CD2	-5.46	117.73	121.00
1	A	84	TYR	CB-CG-CD1	5.38	124.23	121.00

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	A	1772	0	1700	19	0
1	В	1771	0	1693	8	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	347	0	0	9	0
3	В	330	0	0	3	0
All	All	4222	0	3393	27	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 4.

All (27) 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)
1:A:178:HIS:CD2	1:A:180:GLN:HB2	1.94	1.02
1:A:178:HIS:HD2	1:A:180:GLN:HB2	1.32	0.88
1:A:123:ASN:OD1	1:A:123:ASN:N	2.18	0.70
1:A:110:HIS:HE1	3:A:668:HOH:O	1.76	0.68
1:A:179:ASN:HB3	3:A:653:HOH:O	1.93	0.67
1:B:110:HIS:HE1	3:B:651:HOH:O	1.78	0.67
1:A:3:SER:N	3:A:403:HOH:O	2.35	0.59
1:A:123:ASN:HB3	3:A:659:HOH:O	2.04	0.56
1:A:104[B]:MET:SD	3:A:554:HOH:O	2.58	0.55
1:B:87[A]:HIS:HD2	3:B:401:HOH:O	1.90	0.54
1:B:116:THR:HG22	1:B:118:GLN:HE22	1.72	0.54
1:A:116:THR:HG22	1:A:118:GLN:HE22	1.74	0.53
1:A:185:VAL:HG23	3:A:588:HOH:O	2.09	0.53
1:A:87[A]:HIS:HD2	3:A:401:HOH:O	1.93	0.52
1:A:116:THR:HG22	1:A:118:GLN:NE2	2.26	0.51
1:A:178:HIS:CD2	1:A:180:GLN:H	2.31	0.48
1:A:57:CR2:HA11	1:A:211:GLU:OE1	2.15	0.47
1:A:104[B]:MET:HE1	3:A:554:HOH:O	2.15	0.46
1:B:57:CR2:HA11	1:B:211:GLU:OE1	2.16	0.45
1:B:116:THR:HG22	1:B:118:GLN:NE2	2.31	0.45
1:A:178:HIS:HD2	1:A:180:GLN:H	1.68	0.42
1:B:6:PHE:HA	1:B:109:TYR:O	2.19	0.42
1:B:87[A]:HIS:HE1	3:B:615:HOH:O	2.03	0.42
1:A:61:LYS:NZ	1:A:141:GLN:HE22	2.18	0.42
1:B:12:GLY:HA2	1:B:115:PHE:O	2.20	0.41
1:A:3:SER:HB3	3:A:403:HOH:O	2.20	0.41
1:A:81:GLY:HA3	1:A:102:HIS:O	2.21	0.41

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	ntiles
1	A	217/234 (93%)	215 (99%)	2 (1%)	0	100	100
1	В	216/234 (92%)	213 (99%)	3 (1%)	0	100	100
All	All	433/468 (92%)	428 (99%)	5 (1%)	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	A	195/205~(95%)	190 (97%)	5 (3%)	46 13		
1	В	194/205 (95%)	190 (98%)	4 (2%)	53 19		
All	All	389/410 (95%)	380 (98%)	9 (2%)	49 17		

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	TYR
1	A	118	GLN
1	A	123	ASN
1	A	180	GLN
1	A	217	LEU
1	В	62	TYR
1	В	118	GLN
1	В	123	ASN

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Mol	Chain	Res	Type
1	В	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	118	GLN
1	A	141	GLN
1	A	178	HIS
1	В	110	HIS
1	В	118	GLN
1	В	141	GLN
1	В	180	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Trino	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Res	T inle	Bo	nd leng	ths	В	ond ang	les
Moi Type	Type		nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2											
1	CR2	В	57	1	20,20,21	2.87	5 (25%)	25,27,29	2.24	7 (28%)											
1	CR2	A	57	1	20,20,21	3.27	6 (30%)	25,27,29	2.02	8 (32%)											

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
1	CR2	В	57	1	-	0/6/25/26	0/2/2/2
1	CR2	A	57	1	-	0/6/25/26	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$Ideal(\AA)$
1	A	57	CR2	CB2-CA2	12.19	1.45	1.35
1	В	57	CR2	CB2-CA2	9.96	1.43	1.35
1	A	57	CR2	CA2-C2	-4.95	1.43	1.48
1	В	57	CR2	CA2-C2	-4.91	1.43	1.48
1	В	57	CR2	O2-C2	3.75	1.31	1.23
1	A	57	CR2	CA1-C1	3.56	1.53	1.49
1	В	57	CR2	C2-N3	-3.30	1.32	1.39
1	В	57	CR2	CA1-C1	2.92	1.52	1.49
1	A	57	CR2	O2-C2	2.67	1.28	1.23
1	A	57	CR2	CG2-CB2	-2.35	1.42	1.46
1	A	57	CR2	C2-N3	-2.32	1.34	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	57	CR2	CA2-C2-N3	6.62	106.50	103.37
1	В	57	CR2	O3-C3-CA3	-4.20	113.72	126.39
1	A	57	CR2	O2-C2-CA2	-4.04	128.69	130.96
1	В	57	CR2	C1-CA1-N1	-3.88	104.28	112.85
1	A	57	CR2	CA2-C2-N3	3.77	105.15	103.37
1	A	57	CR2	O3-C3-CA3	-3.73	115.14	126.39
1	В	57	CR2	O2-C2-CA2	-3.65	128.91	130.96
1	A	57	CR2	C1-CA1-N1	-3.40	105.32	112.85
1	В	57	CR2	CE1-CD1-CG2	-2.62	117.83	121.25
1	A	57	CR2	CE2-CD2-CG2	-2.54	117.94	121.25
1	A	57	CR2	CD2-CG2-CD1	2.51	121.36	117.64
1	A	57	CR2	CA1-C1-N3	2.45	125.80	122.52
1	A	57	CR2	CD1-CG2-CB2	-2.30	113.38	121.22
1	В	57	CR2	CA1-C1-N3	2.27	125.55	122.52
1	В	57	CR2	CD1-CG2-CB2	-2.17	113.84	121.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	57	CR2	1	0
1	A	57	CR2	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	214/234 (91%)	-0.33	7 (3%)	46 48	12, 17, 35, 125	0
1	В	215/234 (91%)	-0.25	10 (4%)	31 34	12, 18, 39, 128	0
All	All	429/468 (91%)	-0.29	17 (3%)	38 40	12, 18, 39, 128	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	1	MET	18.5
1	A	1	MET	15.7
1	В	181	PRO	7.2
1	A	2	ALA	5.4
1	A	179	ASN	5.4
1	A	181	PRO	4.9
1	В	218	LYS	3.7
1	В	179	ASN	3.4
1	В	200	ASP	3.2
1	A	180	GLN	3.0
1	В	180	GLN	3.0
1	В	122	GLU	2.9
1	A	200	ASP	2.9
1	В	178	HIS	2.7
1	A	122	GLU	2.6
1	В	123	ASN	2.1
1	В	2	ALA	2.0

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

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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	CR2	В	57	19/20	0.98	0.05	11,12,16,17	0
1	CR2	A	57	19/20	0.99	0.04	10,12,15,15	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

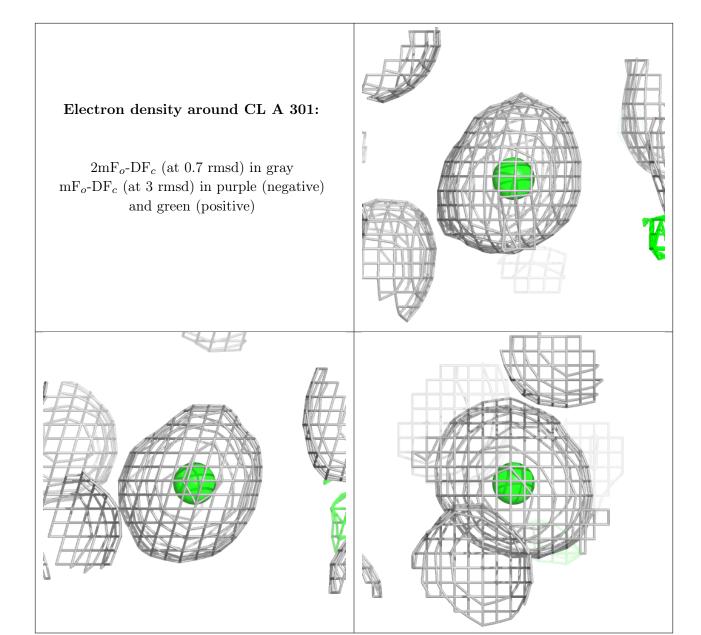
6.4 Ligands (i)

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

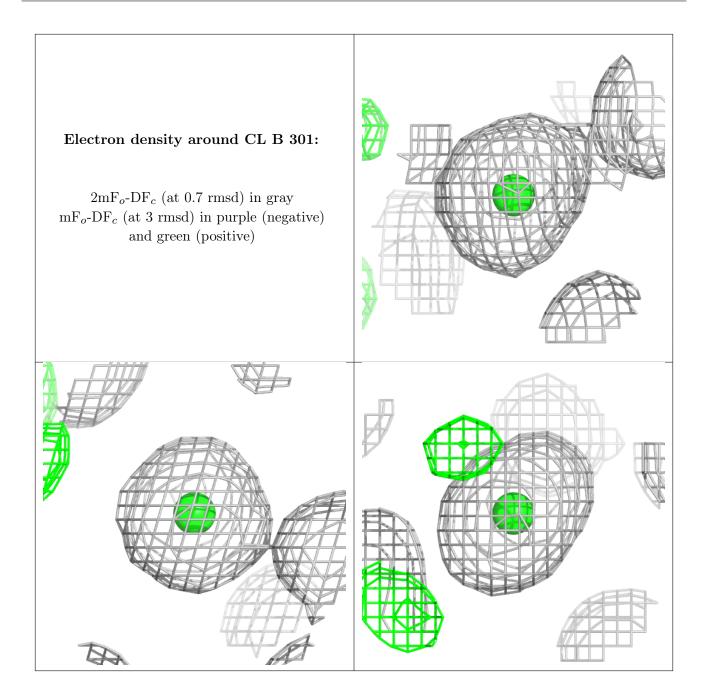
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	CL	A	301	1/1	1.00	0.04	22,22,22,22	0
2	CL	В	301	1/1	1.00	0.02	25,25,25,25	0

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.









6.5 Other polymers (i)

There are no such residues in this entry.

