



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:07 PM UTC

PDB ID : 8QBJ / pdb_00008qbj
Title : Structure of mBaoJin at pH 4.6
Authors : Samygina, V.R.; Vlaskina, A.V.; Gabdulkhakov, A.; Subach, O.M.; Subach, F.V.
Deposited on : 2023-08-24
Resolution : 1.80 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.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

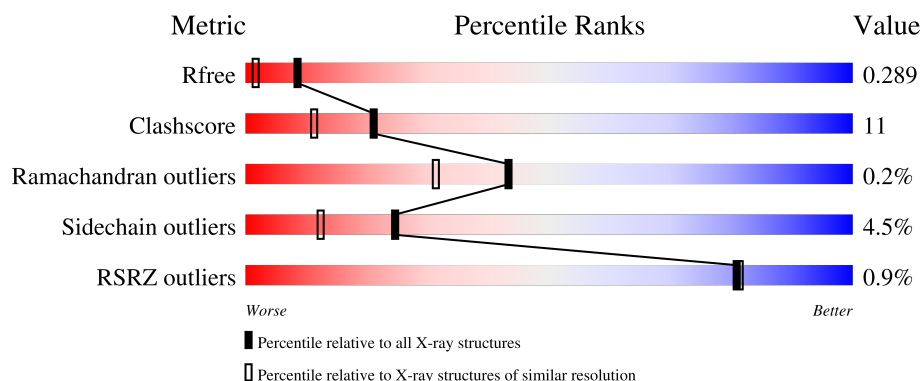
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	 71% 20% • 7%
1	C	234	 % 65% 24% •• 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4187 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	217	Total	C	N	O	S	0	4	0
			1772	1124	306	332	10			
1	C	215	Total	C	N	O	S	0	3	0
			1758	1118	300	330	10			

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	73	ARG	HIS	engineered mutation	UNP A0A8S0GSD4
A	78	GLY	GLU	engineered mutation	UNP A0A8S0GSD4
A	138	PRO	GLN	engineered mutation	UNP A0A8S0GSD4
A	139	GLN	HIS	engineered mutation	UNP A0A8S0GSD4
A	163	TYR	CYS	engineered mutation	UNP A0A8S0GSD4
A	166	ALA	VAL	engineered mutation	UNP A0A8S0GSD4
A	169	TYR	ASN	engineered mutation	UNP A0A8S0GSD4
A	199	ALA	THR	engineered mutation	UNP A0A8S0GSD4
A	216	LYS	-	expression tag	UNP A0A8S0GSD4
A	217	GLY	-	expression tag	UNP A0A8S0GSD4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	218	MET	-	expression tag	UNP A0A8S0GSD4
A	219	ASP	-	expression tag	UNP A0A8S0GSD4
A	220	GLU	-	expression tag	UNP A0A8S0GSD4
A	221	LEU	-	expression tag	UNP A0A8S0GSD4
A	222	TYR	-	expression tag	UNP A0A8S0GSD4
A	223	LYS	-	expression tag	UNP A0A8S0GSD4
C	-10	ARG	-	expression tag	UNP A0A8S0GSD4
C	-9	SER	-	expression tag	UNP A0A8S0GSD4
C	-8	MET	-	expression tag	UNP A0A8S0GSD4
C	-7	VAL	-	expression tag	UNP A0A8S0GSD4
C	-6	SER	-	expression tag	UNP A0A8S0GSD4
C	-5	LYS	-	expression tag	UNP A0A8S0GSD4
C	-4	GLY	-	expression tag	UNP A0A8S0GSD4
C	-3	GLU	-	expression tag	UNP A0A8S0GSD4
C	-2	GLU	-	expression tag	UNP A0A8S0GSD4
C	-1	GLU	-	expression tag	UNP A0A8S0GSD4
C	0	ASN	-	expression tag	UNP A0A8S0GSD4
C	55	THR	SER	engineered mutation	UNP A0A8S0GSD4
C	57	CR2	GLY	chromophore	UNP A0A8S0GSD4
C	57	CR2	TYR	chromophore	UNP A0A8S0GSD4
C	57	CR2	GLY	chromophore	UNP A0A8S0GSD4
C	73	ARG	HIS	engineered mutation	UNP A0A8S0GSD4
C	78	GLY	GLU	engineered mutation	UNP A0A8S0GSD4
C	138	PRO	GLN	engineered mutation	UNP A0A8S0GSD4
C	139	GLN	HIS	engineered mutation	UNP A0A8S0GSD4
C	163	TYR	CYS	engineered mutation	UNP A0A8S0GSD4
C	166	ALA	VAL	engineered mutation	UNP A0A8S0GSD4
C	169	TYR	ASN	engineered mutation	UNP A0A8S0GSD4
C	199	ALA	THR	engineered mutation	UNP A0A8S0GSD4
C	216	LYS	-	expression tag	UNP A0A8S0GSD4
C	217	GLY	-	expression tag	UNP A0A8S0GSD4
C	218	MET	-	expression tag	UNP A0A8S0GSD4
C	219	ASP	-	expression tag	UNP A0A8S0GSD4
C	220	GLU	-	expression tag	UNP A0A8S0GSD4
C	221	LEU	-	expression tag	UNP A0A8S0GSD4
C	222	TYR	-	expression tag	UNP A0A8S0GSD4
C	223	LYS	-	expression tag	UNP A0A8S0GSD4

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is water.

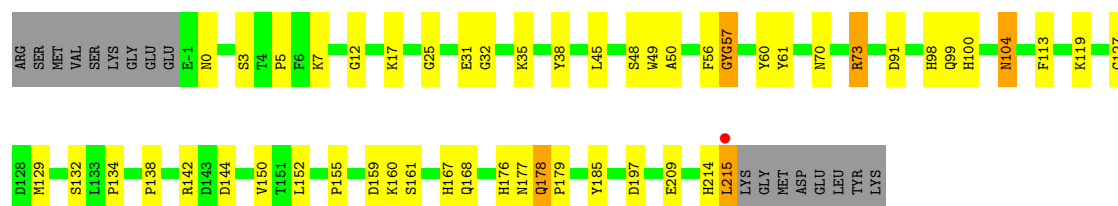
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	343	Total 343	O 343	0	0
3	C	312	Total 312	O 312	0	0

3 Residue-property plots

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.

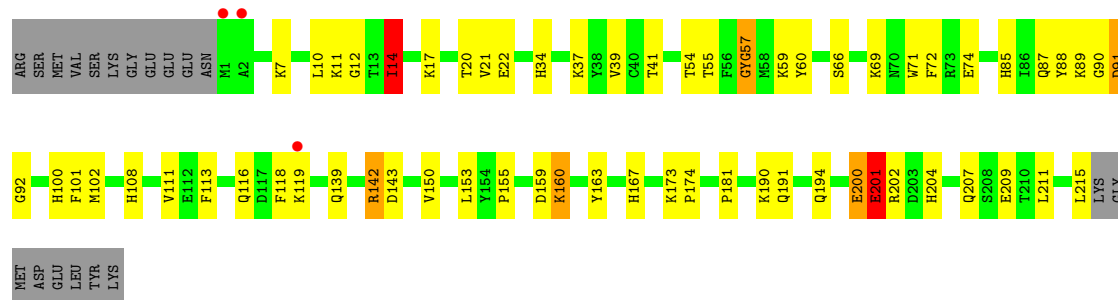
• Molecule 1: mBaoJin

Chain A: 



• Molecule 1: mBaoJin

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.45Å 78.92Å 84.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.80 15.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	87.0 (15.00-1.80) 87.0 (15.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.199 , 0.284 0.209 , 0.289	Depositor DCC
R_{free} test set	1822 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4187	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.41	12/1815 (0.7%)	1.49	8/2454 (0.3%)
1	C	1.41	13/1798 (0.7%)	1.56	11/2433 (0.5%)
All	All	1.41	25/3613 (0.7%)	1.52	19/4887 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	VAL	C-O	8.97	1.32	1.24
1	A	129	MET	C-O	8.72	1.34	1.23
1	A	5	PRO	C-O	8.39	1.33	1.23
1	C	34	HIS	CE1-NE2	7.72	1.40	1.32
1	C	101	PHE	C-O	7.21	1.31	1.23
1	C	102	MET	C-O	-6.90	1.15	1.24
1	C	91	ASP	C-O	6.53	1.32	1.24
1	A	168	GLN	C-O	6.20	1.31	1.24
1	A	138	PRO	C-O	6.10	1.31	1.23
1	C	194	GLN	C-O	6.02	1.31	1.23
1	C	207	GLN	C-O	-5.94	1.16	1.23
1	A	185	TYR	C-O	5.72	1.30	1.23
1	A	25	GLY	C-O	5.71	1.31	1.23
1	A	152	LEU	C-O	5.69	1.30	1.23
1	A	38	TYR	C-O	-5.62	1.17	1.24
1	A	132	SER	C-O	5.61	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	191	GLN	C-O	5.50	1.30	1.23
1	A	70	ASN	C-O	5.46	1.31	1.23
1	C	14	ILE	C-O	5.42	1.30	1.24
1	C	55	THR	N-CA	5.40	1.52	1.46
1	C	204	HIS	CE1-NE2	5.27	1.37	1.32
1	A	155	PRO	C-O	5.26	1.29	1.23
1	A	56	PHE	C-O	5.10	1.33	1.23
1	C	21	VAL	C-O	5.09	1.29	1.24
1	C	11	LYS	C-O	5.03	1.29	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	ALA	N-CA-C	-7.31	103.34	111.82
1	C	91	ASP	CA-CB-CG	7.24	119.84	112.60
1	C	201	GLU	CB-CG-CD	7.04	124.57	112.60
1	A	91	ASP	CA-CB-CG	6.95	119.55	112.60
1	C	159	ASP	CA-CB-CG	6.36	118.96	112.60
1	C	201	GLU	CB-CA-C	5.88	122.56	112.44
1	C	174	PRO	CA-C-O	-5.84	114.68	121.34
1	A	91	ASP	CA-C-O	-5.67	114.85	120.80
1	C	20	THR	CA-CB-OG1	-5.55	101.27	109.60
1	C	88	TYR	CA-C-O	-5.48	114.44	120.69
1	C	200	GLU	CA-C-N	-5.47	111.85	122.62
1	C	200	GLU	C-N-CA	-5.47	111.85	122.62
1	C	54	THR	N-CA-C	-5.46	105.49	111.82
1	A	134	PRO	N-CA-CB	5.44	108.08	103.35
1	A	177	ASN	CB-CA-C	-5.27	103.11	111.48
1	C	155	PRO	CA-C-O	-5.25	115.47	121.56
1	A	0	ASN	CB-CA-C	-5.16	100.50	109.64
1	A	98	HIS	CA-CB-CG	5.10	118.90	113.80
1	A	104	ASN	N-CA-C	-5.04	105.79	112.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	201	GLU	Peptide

5.2 Too-close contacts ⓘ

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	1686	36	0
1	C	1758	0	1668	45	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	343	0	0	16	2
3	C	312	0	0	11	1
All	All	4187	0	3354	76	3

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 11.

All (76) 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:C:200:GLU:C	1:C:201:GLU:HG2	1.79	1.04
1:A:142[B]:ARG:NH1	1:C:163[B]:TYR:CE2	2.27	1.00
1:C:200:GLU:O	1:C:201:GLU:HG2	1.65	0.94
1:C:72:PHE:CE2	3:C:635:HOH:O	2.23	0.90
1:C:200:GLU:O	1:C:201:GLU:CG	2.22	0.87
1:C:17:LYS:HD3	3:C:590:HOH:O	1.76	0.84
1:A:142[B]:ARG:NH1	1:C:163[B]:TYR:CD2	2.45	0.83
1:C:201:GLU:HB2	3:C:412:HOH:O	1.80	0.81
1:A:150:VAL:HG23	3:A:549:HOH:O	1.82	0.79
1:C:85[B]:HIS:NE2	1:C:87:GLN:HB2	1.98	0.79
1:C:71:TRP:HB3	3:C:635:HOH:O	1.82	0.78
1:A:7:LYS:NZ	3:A:404:HOH:O	2.17	0.76
1:A:161:SER:O	1:C:142:ARG:NH2	2.19	0.75
1:C:69:LYS:HD2	3:C:429:HOH:O	1.85	0.75
1:A:176:HIS:H	1:A:178:GLN:HE22	1.32	0.75
1:A:178:GLN:HE21	1:A:178:GLN:H	1.35	0.75
1:A:17:LYS:HD2	3:A:661:HOH:O	1.87	0.73
1:A:31:GLU:OE2	3:A:402:HOH:O	2.12	0.68
1:C:72:PHE:CZ	3:C:635:HOH:O	2.44	0.67
1:A:3[A]:SER:HB3	3:A:401:HOH:O	1.95	0.67
1:A:176:HIS:H	1:A:178:GLN:NE2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:CG2	3:A:549:HOH:O	2.42	0.64
1:A:7:LYS:CE	3:A:468:HOH:O	2.46	0.63
1:C:74:GLU:HG3	3:C:675:HOH:O	1.99	0.62
1:A:178:GLN:HG3	3:A:501:HOH:O	2.01	0.61
1:A:104:ASN:OD1	3:A:403:HOH:O	2.15	0.58
1:C:143:ASP:O	1:C:173:LYS:NZ	2.37	0.58
1:C:59:LYS:NZ	1:C:139:GLN:HE22	2.03	0.56
1:A:73:ARG:HD3	3:A:496:HOH:O	2.06	0.56
1:C:181:PRO:CB	3:C:675:HOH:O	2.53	0.55
1:C:91:ASP:OD1	1:C:119:LYS:HG2	2.06	0.54
1:C:71:TRP:CD1	1:C:181:PRO:HG2	2.43	0.54
1:C:90:GLY:O	1:C:119:LYS:NZ	2.38	0.52
1:A:167:HIS:CE1	1:C:167:HIS:ND1	2.79	0.51
1:C:190:LYS:HG2	1:C:211:LEU:HD23	1.92	0.50
1:A:7:LYS:HE3	3:A:468:HOH:O	2.10	0.50
1:C:59:LYS:HZ3	1:C:139:GLN:HE22	1.58	0.49
1:C:190:LYS:HG2	1:C:211:LEU:CD2	2.43	0.49
1:A:45:LEU:HD22	1:A:49:TRP:CE2	2.48	0.48
1:C:7:LYS:CE	3:C:405:HOH:O	2.61	0.47
1:C:7:LYS:HE3	3:C:405:HOH:O	2.14	0.47
1:C:92:GLY:HA3	1:C:118:PHE:CD1	2.49	0.47
1:A:57:CR2:O3	1:A:100:HIS:HE1	1.97	0.47
1:C:200:GLU:O	1:C:201:GLU:CD	2.58	0.47
1:A:32:GLY:HA2	1:A:61:TYR:O	2.14	0.47
1:A:45:LEU:HD22	1:A:49:TRP:CD2	2.50	0.46
1:C:14:ILE:HD11	1:C:118:PHE:CD2	2.50	0.46
1:A:144:ASP:HB2	3:A:685:HOH:O	2.15	0.46
1:C:17:LYS:CD	3:C:590:HOH:O	2.50	0.46
1:A:160[B]:LYS:HB3	1:A:160[B]:LYS:HE3	1.59	0.46
1:C:39:VAL:HG13	1:C:202:ARG:HB2	1.98	0.46
1:A:179:PRO:O	3:A:405:HOH:O	2.20	0.46
1:A:197:ASP:OD1	1:A:197:ASP:C	2.59	0.46
1:A:57:CR2:HA11	1:A:209:GLU:OE1	2.17	0.45
1:A:215:LEU:O	1:A:215:LEU:HD12	2.17	0.45
1:A:167:HIS:ND1	1:C:167:HIS:CE1	2.86	0.43
1:A:159:ASP:OD1	1:A:159:ASP:C	2.61	0.43
1:C:200:GLU:O	1:C:201:GLU:OE1	2.37	0.43
1:C:37:LYS:HB3	1:C:37:LYS:HE2	1.90	0.43
1:C:12:GLY:HA2	1:C:113:PHE:O	2.19	0.42
1:C:39:VAL:HG11	1:C:202:ARG:NE	2.34	0.42
1:A:12:GLY:HA2	1:A:113:PHE:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:VAL:CG1	1:C:202:ARG:HB2	2.49	0.42
1:C:100:HIS:HA	1:C:108:HIS:O	2.20	0.42
1:C:39:VAL:HG11	1:C:202:ARG:CD	2.48	0.42
1:C:57:CR2:HA11	1:C:209:GLU:OE1	2.21	0.41
1:C:91:ASP:CG	1:C:92:GLY:H	2.28	0.41
1:A:215:LEU:HD12	1:A:215:LEU:C	2.45	0.41
1:A:178:GLN:CG	3:A:501:HOH:O	2.67	0.41
1:A:48:SER:HB2	1:A:127:GLY:HA2	2.03	0.41
1:A:99:GLN:NE2	3:A:438:HOH:O	2.53	0.41
1:C:10:LEU:HD23	1:C:10:LEU:C	2.46	0.41
1:C:22:GLU:HG3	1:C:41:THR:HG21	2.03	0.40
1:C:39:VAL:HG11	1:C:202:ARG:HD2	2.03	0.40
1:A:214:HIS:ND1	3:A:411:HOH:O	2.36	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:405:HOH:O	3:A:617:HOH:O[2_454]	1.82	0.38
3:A:409:HOH:O	3:A:557:HOH:O[2_454]	1.98	0.22
3:C:599:HOH:O	3:C:664:HOH:O[2_554]	2.04	0.16

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	A	216/234 (92%)	211 (98%)	5 (2%)	0	100	100
1	C	213/234 (91%)	207 (97%)	5 (2%)	1 (0%)	24	14
All	All	429/468 (92%)	418 (97%)	10 (2%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	160	LYS

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	193/205 (94%)	187 (97%)	6 (3%)	35	23
1	C	191/205 (93%)	180 (94%)	11 (6%)	18	7
All	All	384/410 (94%)	367 (96%)	17 (4%)	24	13

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	60	TYR
1	A	73	ARG
1	A	119	LYS
1	A	178	GLN
1	A	215	LEU
1	C	14	ILE
1	C	60	TYR
1	C	66	SER
1	C	89	LYS
1	C	116	GLN
1	C	142	ARG
1	C	150	VAL
1	C	153	LEU
1	C	160	LYS
1	C	201	GLU
1	C	215	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN

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Mol	Chain	Res	Type
1	A	100	HIS
1	A	168	GLN
1	A	178	GLN
1	C	139	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	CR2	C	57	1	20,20,21	3.82	8 (40%)	25,27,29	3.69	8 (32%)
1	CR2	A	57	1	20,20,21	3.58	5 (25%)	25,27,29	2.24	11 (44%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	CR2	CB2-CA2	13.28	1.47	1.35
1	C	57	CR2	CB2-CA2	12.19	1.46	1.35
1	C	57	CR2	CA2-C2	-8.21	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	CR2	C2-N3	-5.08	1.28	1.40
1	A	57	CR2	O2-C2	5.06	1.33	1.23
1	C	57	CR2	C2-N3	-5.00	1.28	1.40
1	C	57	CR2	O2-C2	3.86	1.30	1.23
1	C	57	CR2	C1-N2	2.95	1.37	1.32
1	A	57	CR2	OH-CZ	-2.48	1.31	1.37
1	C	57	CR2	CA1-C1	-2.43	1.46	1.49
1	C	57	CR2	CA2-N2	-2.28	1.33	1.38
1	C	57	CR2	CE2-CD2	2.13	1.42	1.38
1	A	57	CR2	CD1-CG2	-2.05	1.35	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	CR2	O2-C2-CA2	-15.21	121.31	131.02
1	C	57	CR2	CA2-C2-N3	5.95	108.49	103.50
1	A	57	CR2	CG2-CB2-CA2	-4.07	125.03	129.87
1	C	57	CR2	O3-C3-CA3	-4.04	107.29	125.47
1	A	57	CR2	C3-CA3-N3	4.01	121.55	112.43
1	A	57	CR2	C2-N3-C1	-3.65	106.44	108.08
1	A	57	CR2	CD1-CG2-CB2	-3.26	110.01	121.22
1	A	57	CR2	N3-C1-N2	3.12	115.36	111.75
1	A	57	CR2	O3-C3-CA3	-3.04	111.80	125.47
1	A	57	CR2	CD2-CG2-CD1	2.99	122.08	117.65
1	C	57	CR2	CA1-C1-N3	2.82	126.30	122.52
1	C	57	CR2	O2-C2-N3	2.80	130.16	124.31
1	A	57	CR2	CD1-CE1-CZ	-2.78	116.94	119.88
1	A	57	CR2	CE2-CD2-CG2	-2.62	117.84	121.22
1	C	57	CR2	CB2-CA2-N2	-2.60	125.23	128.76
1	A	57	CR2	O2-C2-CA2	-2.26	129.58	131.02
1	C	57	CR2	CD1-CE1-CZ	2.19	122.19	119.88
1	C	57	CR2	CD2-CG2-CB2	2.18	128.71	121.22
1	A	57	CR2	CA2-C2-N3	2.07	105.24	103.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	57	CR2	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	57	CR2	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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

6.1 Protein, DNA and RNA chains

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, 95th 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	216/234 (92%)	-0.20	1 (0%) 87 88	7, 16, 32, 46	4 (1%)
1	C	214/234 (91%)	0.01	3 (1%) 73 73	10, 20, 37, 75	3 (1%)
All	All	430/468 (91%)	-0.09	4 (0%) 81 81	7, 18, 34, 75	7 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	5.8
1	C	1	MET	3.9
1	C	119	LYS	2.2
1	A	215	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95th 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
1	CR2	A	57	19/20	0.96	0.05	9,11,14,16	0
1	CR2	C	57	19/20	0.97	0.04	11,12,14,17	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

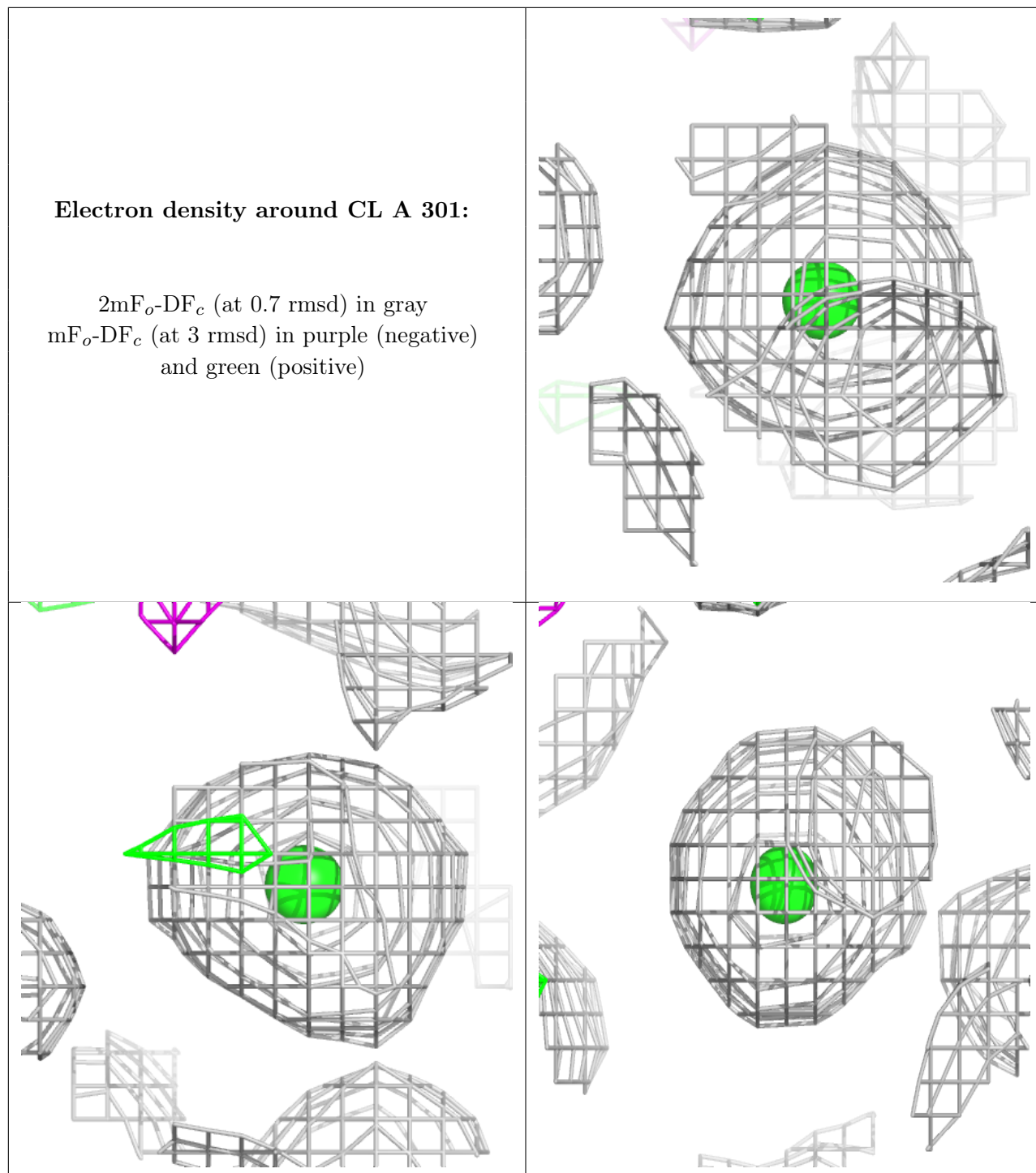
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	A	301	1/1	0.99	0.04	15,15,15,15	0
2	CL	C	301	1/1	1.00	0.03	17,17,17,17	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.

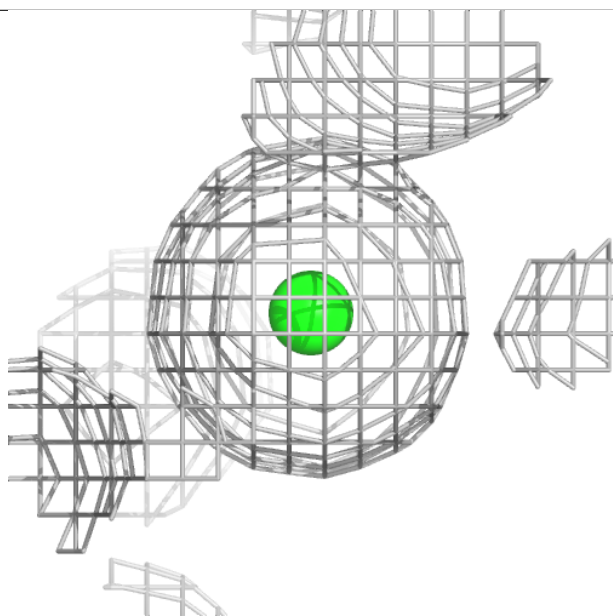
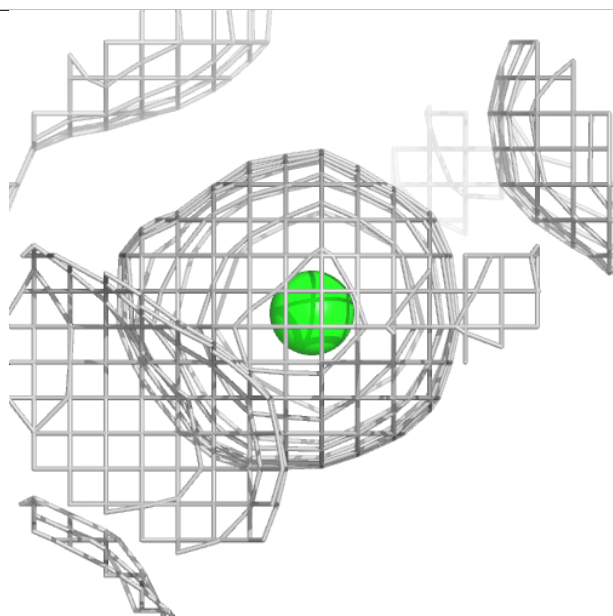
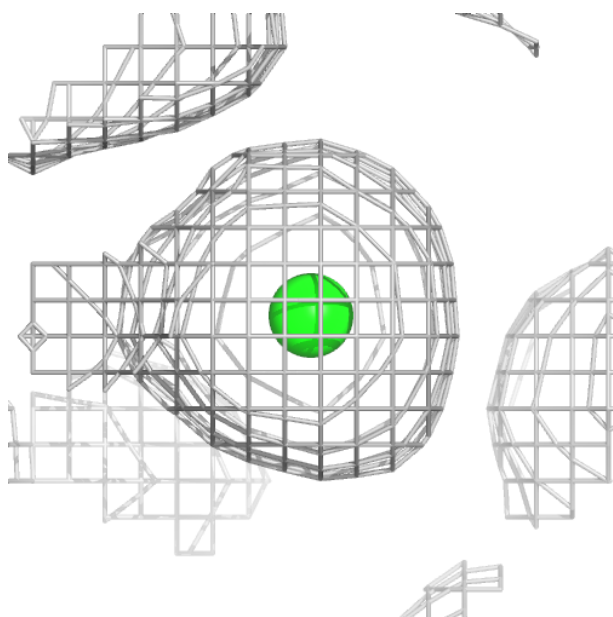
Electron density around CL A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.