



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:25 AM UTC

PDB ID : 1LSP / pdb_00001lsp
Title : THE CRYSTAL STRUCTURE OF A BULGECIN-INHIBITED G-TYPE
LYSOZYME FROM THE EGG-WHITE OF THE AUSTRALIAN BLACK
SWAN. A COMPARISON OF THE BINDING OF BULGECIN TO THREE
MURAMIDASES
Authors : Karlsen, S.; Rao, Z.H.; Hough, E.; Isaacs, N.W.
Deposited on : 1995-02-09
Resolution : 2.45 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.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](#) ①) 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

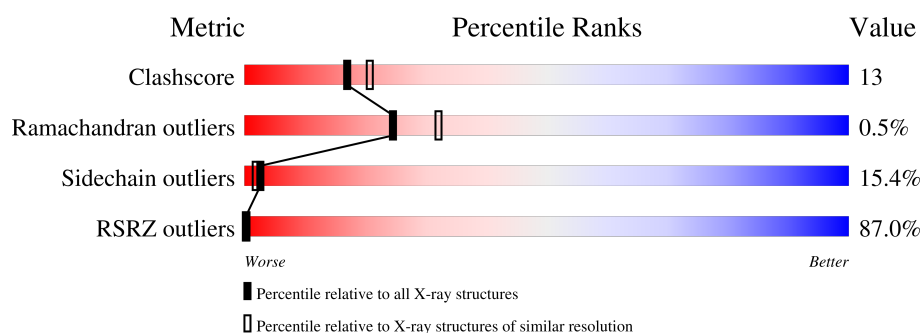
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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 $\leq 5\%$. 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	185	87% 37% 41% 18% .

2 Entry composition [i](#)

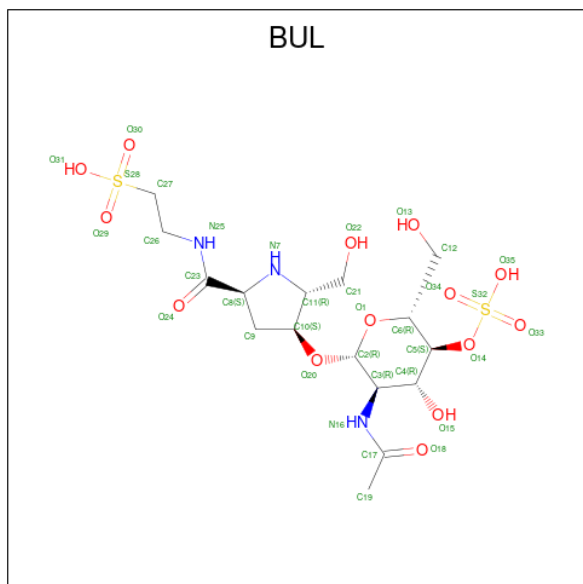
There are 3 unique types of molecules in this entry. The entry contains 1578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1434	892	265	270	7			

- Molecule 2 is BULGECIN A (CCD ID: BUL) (formula: $C_{16}H_{29}N_3O_{14}S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	16	3	14	2		

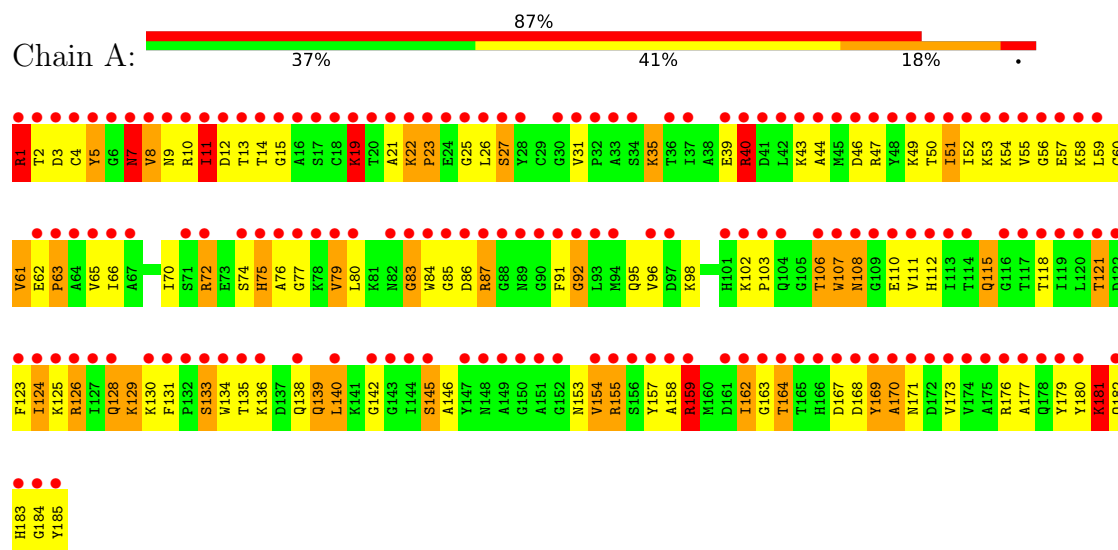
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		

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: LYSOZYME



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.69Å 65.33Å 38.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.45 8.00 – 2.46	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.45) 75.6 (8.00-2.46)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.45Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.175 , (Not available) 0.486 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.41	EDS
Total number of atoms	1578	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.28% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BUL

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	1.15	1/1461 (0.1%)	2.77	161/1965 (8.2%)

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	A	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	HIS	CA-CB	5.64	1.60	1.53

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	VAL	O-C-N	12.37	128.34	120.42
1	A	11	ILE	CA-C-O	12.14	136.35	121.54
1	A	86	ASP	CA-CB-CG	11.85	124.45	112.60
1	A	176	ARG	NE-CZ-NH1	-11.78	109.72	121.50
1	A	176	ARG	NE-CZ-NH2	11.41	129.47	119.20
1	A	31	VAL	CA-C-O	-10.94	111.36	118.69
1	A	40	ARG	NE-CZ-NH2	-10.48	109.77	119.20
1	A	79	VAL	N-CA-CB	-9.62	95.36	111.23
1	A	181	LYS	N-CA-CB	9.28	123.90	110.16
1	A	181	LYS	CB-CA-C	-9.06	95.44	110.85
1	A	44	ALA	CA-C-O	8.40	129.33	120.42
1	A	158	ALA	CA-C-O	-8.37	110.65	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	SER	CA-C-O	8.19	129.47	119.31
1	A	139	GLN	CA-C-O	-8.04	111.89	120.42
1	A	184	GLY	N-CA-C	8.02	126.58	115.27
1	A	135	THR	CA-CB-OG1	-7.99	97.61	109.60
1	A	155	ARG	CD-NE-CZ	-7.98	113.22	124.40
1	A	9	ASN	CA-CB-CG	7.78	120.38	112.60
1	A	51	ILE	N-CA-C	-7.72	103.27	110.53
1	A	181	LYS	CA-C-O	7.64	128.51	120.42
1	A	11	ILE	O-C-N	-7.54	113.32	122.59
1	A	75	HIS	CA-CB-CG	-7.45	106.36	113.80
1	A	136	LYS	CB-CA-C	7.39	122.48	110.88
1	A	167	ASP	CA-CB-CG	7.37	119.97	112.60
1	A	46	ASP	CA-C-N	7.32	132.95	120.72
1	A	46	ASP	C-N-CA	7.32	132.95	120.72
1	A	121	THR	CA-CB-OG1	-7.21	98.79	109.60
1	A	180	TYR	CA-C-O	-7.08	110.53	119.31
1	A	154	VAL	CA-C-O	6.99	129.28	120.75
1	A	123	PHE	CA-C-O	-6.98	111.94	119.97
1	A	95	GLN	CA-C-N	6.97	131.64	121.18
1	A	95	GLN	C-N-CA	6.97	131.64	121.18
1	A	124	ILE	CB-CA-C	-6.94	102.64	112.22
1	A	106	THR	CB-CA-C	6.94	121.37	109.51
1	A	86	ASP	CA-C-O	-6.88	112.33	120.10
1	A	145	SER	O-C-N	-6.86	112.99	122.46
1	A	40	ARG	NH1-CZ-NH2	6.84	128.19	119.30
1	A	169	TYR	CA-C-O	-6.82	113.04	121.02
1	A	91	PHE	CA-C-O	-6.81	112.83	120.66
1	A	106	THR	N-CA-CB	-6.76	99.38	110.41
1	A	173	VAL	CA-C-O	-6.70	114.08	121.05
1	A	72	ARG	NH1-CZ-NH2	6.70	128.00	119.30
1	A	168	ASP	O-C-N	6.69	129.73	121.84
1	A	170	ALA	CA-C-N	6.67	129.46	120.65
1	A	170	ALA	C-N-CA	6.67	129.46	120.65
1	A	96	VAL	CA-C-O	-6.67	112.89	120.95
1	A	106	THR	CA-CB-OG1	-6.63	99.65	109.60
1	A	61	VAL	CB-CA-C	6.58	120.95	110.82
1	A	79	VAL	CB-CA-C	6.55	122.04	111.29
1	A	125	LYS	CA-C-O	6.53	127.48	119.97
1	A	112	HIS	CA-CB-CG	-6.49	107.31	113.80
1	A	136	LYS	N-CA-C	-6.48	104.14	111.07
1	A	142	GLY	CA-C-O	6.46	127.70	121.05
1	A	158	ALA	N-CA-C	6.45	119.12	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	GLY	N-CA-C	-6.37	104.03	112.82
1	A	128	GLN	CA-C-N	6.36	129.32	120.29
1	A	128	GLN	C-N-CA	6.36	129.32	120.29
1	A	46	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	21	ALA	CA-C-O	-6.16	113.40	120.24
1	A	23	PRO	CA-C-N	6.16	133.60	121.58
1	A	23	PRO	C-N-CA	6.16	133.60	121.58
1	A	107	TRP	N-CA-C	6.16	119.89	112.38
1	A	25	GLY	CA-C-O	-6.12	112.03	119.68
1	A	65	VAL	CA-C-N	6.09	129.07	120.42
1	A	65	VAL	C-N-CA	6.09	129.07	120.42
1	A	66	ILE	CA-C-N	6.09	128.94	120.29
1	A	66	ILE	C-N-CA	6.09	128.94	120.29
1	A	56	GLY	N-CA-C	-6.05	105.02	112.77
1	A	134	TRP	N-CA-C	-6.04	102.98	110.41
1	A	153	ASN	CA-C-N	-6.04	114.83	122.43
1	A	153	ASN	C-N-CA	-6.04	114.83	122.43
1	A	168	ASP	CA-C-O	-6.03	112.20	118.65
1	A	53	LYS	CA-CB-CG	-6.00	102.10	114.10
1	A	77	GLY	O-C-N	-6.00	114.90	122.70
1	A	91	PHE	N-CA-C	6.00	119.26	109.24
1	A	162	ILE	CB-CA-C	5.96	120.21	111.33
1	A	10	ARG	CD-NE-CZ	-5.88	116.16	124.40
1	A	154	VAL	CB-CA-C	5.88	118.72	111.25
1	A	139	GLN	N-CA-C	-5.88	104.95	111.36
1	A	57	GLU	N-CA-C	-5.86	104.97	111.36
1	A	155	ARG	O-C-N	5.80	129.21	122.25
1	A	133	SER	O-C-N	5.79	130.19	122.43
1	A	115	GLN	O-C-N	-5.78	115.89	122.08
1	A	77	GLY	CA-C-N	5.78	132.57	121.54
1	A	77	GLY	C-N-CA	5.78	132.57	121.54
1	A	111	VAL	O-C-N	5.76	127.76	121.83
1	A	155	ARG	NE-CZ-NH2	-5.74	114.03	119.20
1	A	15	GLY	CA-C-N	5.74	128.91	120.82
1	A	15	GLY	C-N-CA	5.74	128.91	120.82
1	A	4	CYS	CA-C-O	-5.71	113.40	119.97
1	A	134	TRP	CA-CB-CG	5.69	124.41	113.60
1	A	50	THR	CA-CB-OG1	-5.68	101.08	109.60
1	A	72	ARG	NE-CZ-NH2	-5.67	114.09	119.20
1	A	35	LYS	CA-CB-CG	-5.67	102.76	114.10
1	A	163	GLY	O-C-N	5.65	129.32	122.60
1	A	138	GLN	CB-CG-CD	-5.64	103.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	GLN	OE1-CD-NE2	5.62	128.22	122.60
1	A	106	THR	CA-C-O	-5.62	114.62	121.36
1	A	171	ASN	N-CA-C	-5.61	104.85	110.97
1	A	164	THR	N-CA-CB	5.61	118.12	110.38
1	A	51	ILE	N-CA-CB	5.61	117.75	110.57
1	A	177	ALA	CA-C-N	5.61	127.79	120.28
1	A	177	ALA	C-N-CA	5.61	127.79	120.28
1	A	13	THR	CA-CB-OG1	-5.57	101.25	109.60
1	A	80	LEU	N-CA-C	5.57	119.14	110.17
1	A	153	ASN	N-CA-C	-5.56	105.99	112.89
1	A	146	ALA	CA-C-N	5.55	127.98	120.38
1	A	146	ALA	C-N-CA	5.55	127.98	120.38
1	A	146	ALA	N-CA-C	-5.51	105.35	111.36
1	A	76	ALA	CB-CA-C	5.50	119.23	111.86
1	A	129	LYS	CA-C-O	5.50	126.25	120.42
1	A	5	TYR	N-CA-C	5.49	119.96	112.88
1	A	83	GLY	CA-C-O	-5.45	112.27	119.25
1	A	54	LYS	N-CA-C	5.45	117.65	111.11
1	A	7	ASN	CA-C-N	5.45	129.08	120.47
1	A	7	ASN	C-N-CA	5.45	129.08	120.47
1	A	19	LYS	N-CA-CB	5.44	118.71	110.28
1	A	13	THR	N-CA-C	5.44	117.66	109.23
1	A	126	ARG	O-C-N	5.44	128.35	122.15
1	A	140	LEU	CA-C-N	5.43	127.50	120.44
1	A	140	LEU	C-N-CA	5.43	127.50	120.44
1	A	159	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	A	159	ARG	N-CA-C	-5.39	104.12	111.56
1	A	98	LYS	CG-CD-CE	-5.38	98.92	111.30
1	A	14	THR	O-C-N	5.35	129.03	122.34
1	A	92	GLY	CA-C-N	5.33	127.42	120.28
1	A	92	GLY	C-N-CA	5.33	127.42	120.28
1	A	133	SER	CA-C-O	-5.33	112.83	119.38
1	A	162	ILE	N-CA-C	-5.28	102.70	109.30
1	A	49	LYS	CA-C-O	-5.28	114.93	120.63
1	A	2	THR	CA-C-N	-5.25	114.23	122.79
1	A	2	THR	C-N-CA	-5.25	114.23	122.79
1	A	110	GLU	CB-CG-CD	5.25	121.52	112.60
1	A	103	PRO	N-CA-CB	5.23	108.21	103.34
1	A	118	THR	CA-C-O	-5.23	115.33	120.82
1	A	126	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	72	ARG	CA-CB-CG	5.22	124.54	114.10
1	A	12	ASP	CB-CA-C	5.21	118.93	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	GLY	O-C-N	-5.20	116.98	122.13
1	A	44	ALA	N-CA-CB	-5.19	102.48	110.16
1	A	158	ALA	CB-CA-C	-5.17	101.06	110.63
1	A	79	VAL	CA-C-N	5.17	131.43	122.64
1	A	79	VAL	C-N-CA	5.17	131.43	122.64
1	A	19	LYS	N-CA-C	-5.17	105.83	111.82
1	A	27	SER	CA-C-O	5.14	125.36	119.35
1	A	146	ALA	CB-CA-C	5.14	119.58	110.85
1	A	123	PHE	CA-C-N	5.13	127.70	120.42
1	A	123	PHE	C-N-CA	5.13	127.70	120.42
1	A	173	VAL	CA-C-N	5.12	128.70	120.30
1	A	173	VAL	C-N-CA	5.12	128.70	120.30
1	A	115	GLN	CA-C-N	5.12	125.77	120.03
1	A	115	GLN	C-N-CA	5.12	125.77	120.03
1	A	51	ILE	CA-C-O	-5.11	115.38	121.05
1	A	84	TRP	CA-CB-CG	-5.10	103.91	113.60
1	A	35	LYS	CA-C-N	5.08	127.05	120.44
1	A	35	LYS	C-N-CA	5.08	127.05	120.44
1	A	7	ASN	CB-CA-C	5.08	118.90	109.70
1	A	3	ASP	N-CA-C	5.06	119.01	111.87
1	A	55	VAL	CA-CB-CG2	5.04	118.96	110.40
1	A	157	TYR	N-CA-CB	5.04	117.28	109.98
1	A	39	GLU	CB-CG-CD	5.03	121.14	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ARG	Sidechain
1	A	126	ARG	Sidechain
1	A	159	ARG	Sidechain
1	A	40	ARG	Sidechain
1	A	72	ARG	Sidechain
1	A	87	ARG	Sidechain

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	1434	0	1426	36	0
2	A	35	0	26	2	0
3	A	109	0	0	6	0
All	All	1578	0	1452	36	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 13.

All (36) 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:7:ASN:HB2	3:A:203:HOH:O	1.27	1.24
1:A:19:LYS:HB3	3:A:218:HOH:O	1.77	0.84
1:A:87:ARG:HB2	2:A:295:BUL:O29	1.93	0.68
1:A:159:ARG:HB3	1:A:162:ILE:HD12	1.76	0.65
1:A:130:LYS:HG2	1:A:131:PHE:CE2	2.33	0.64
1:A:130:LYS:HG2	1:A:131:PHE:CD2	2.32	0.64
1:A:5:TYR:O	1:A:140:LEU:HB2	1.98	0.63
1:A:35:LYS:HG2	1:A:179:TYR:HB2	1.80	0.63
1:A:145:SER:HB2	1:A:170:ALA:HB2	1.80	0.62
1:A:22:LYS:N	1:A:22:LYS:HD2	2.14	0.62
1:A:62:GLU:HG3	3:A:229:HOH:O	2.00	0.61
1:A:22:LYS:HE2	1:A:26:LEU:O	2.02	0.59
1:A:74:SER:O	1:A:75:HIS:HB2	2.03	0.59
1:A:40:ARG:NE	3:A:209:HOH:O	2.35	0.58
1:A:145:SER:HB2	1:A:170:ALA:CB	2.36	0.54
1:A:19:LYS:N	1:A:19:LYS:HD2	2.22	0.53
1:A:63:PRO:HB2	1:A:185:TYR:O	2.07	0.53
1:A:164:THR:HB	1:A:169:TYR:HB2	1.93	0.51
1:A:155:ARG:HB2	3:A:198:HOH:O	2.11	0.49
1:A:52:ILE:HD11	1:A:70:ILE:HD12	1.94	0.49
1:A:130:LYS:HE2	1:A:154:VAL:O	2.13	0.48
1:A:22:LYS:HD2	1:A:22:LYS:H	1.80	0.47
1:A:19:LYS:HD3	3:A:265:HOH:O	2.14	0.47
1:A:128:GLN:HG2	1:A:139:GLN:OE1	2.16	0.46
1:A:124:ILE:O	1:A:128:GLN:HG3	2.16	0.46
1:A:8:VAL:HG12	1:A:181:LYS:HD3	1.97	0.45
1:A:61:VAL:O	1:A:63:PRO:HD3	2.18	0.44
1:A:108:ASN:HD22	1:A:108:ASN:H	1.65	0.44
1:A:1:ARG:O	1:A:60:CYS:HA	2.18	0.43
1:A:1:ARG:HG2	1:A:1:ARG:HH11	1.84	0.43
1:A:52:ILE:CD1	1:A:70:ILE:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:NH1	2:A:295:BUL:O29	2.53	0.41
1:A:11:ILE:HD11	1:A:140:LEU:HD23	2.01	0.41
1:A:83:GLY:HA3	1:A:107:TRP:HB2	2.02	0.41
1:A:92:GLY:HA2	1:A:107:TRP:O	2.21	0.41
1:A:145:SER:CB	1:A:170:ALA:HB2	2.49	0.40

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	A	183/185 (99%)	174 (95%)	8 (4%)	1 (0%)	24	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	PRO

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	149/149 (100%)	126 (85%)	23 (15%)	2	2

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	7	ASN
1	A	8	VAL
1	A	11	ILE
1	A	19	LYS
1	A	22	LYS
1	A	23	PRO
1	A	27	SER
1	A	43	LYS
1	A	47	ARG
1	A	51	ILE
1	A	58	LYS
1	A	59	LEU
1	A	79	VAL
1	A	102	LYS
1	A	106	THR
1	A	108	ASN
1	A	115	GLN
1	A	121	THR
1	A	129	LYS
1	A	133	SER
1	A	181	LYS
1	A	182	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	166	HIS
1	A	171	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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$
2	BUL	A	295	-	36,36,36	1.48	7 (19%)	43,53,53	3.29	22 (51%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BUL	A	295	-	-	5/28/60/60	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	295	BUL	C8-N7	4.01	1.55	1.46
2	A	295	BUL	O1-C6	-3.16	1.36	1.44
2	A	295	BUL	C10-C11	3.07	1.59	1.53
2	A	295	BUL	C2-C3	-2.92	1.48	1.53
2	A	295	BUL	C11-N7	2.70	1.52	1.48
2	A	295	BUL	O20-C2	-2.38	1.35	1.41
2	A	295	BUL	O20-C10	-2.12	1.40	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	295	BUL	O15-C4-C3	-9.09	91.49	109.58
2	A	295	BUL	C9-C8-C23	6.66	121.70	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	295	BUL	O1-C6-C5	6.62	123.41	109.72
2	A	295	BUL	C5-O14-S32	-5.37	106.15	119.04
2	A	295	BUL	C4-C3-N16	5.10	120.01	110.62
2	A	295	BUL	O35-S32-O33	5.03	126.16	108.56
2	A	295	BUL	C23-C8-N7	-4.67	101.75	111.04
2	A	295	BUL	C2-O20-C10	4.61	122.98	115.27
2	A	295	BUL	O34-S32-O33	-4.05	96.61	112.24
2	A	295	BUL	O20-C2-O1	-3.89	100.45	110.69
2	A	295	BUL	C2-O1-C6	3.60	120.75	113.72
2	A	295	BUL	O31-S28-O29	3.53	120.24	111.40
2	A	295	BUL	O15-C4-C5	-3.52	100.92	109.94
2	A	295	BUL	O35-S32-O14	3.40	114.19	106.37
2	A	295	BUL	O31-S28-C27	3.37	112.60	106.00
2	A	295	BUL	C9-C10-C11	3.13	108.41	103.88
2	A	295	BUL	O22-C21-C11	-2.86	104.17	111.10
2	A	295	BUL	O1-C2-C3	2.69	115.68	110.59
2	A	295	BUL	O30-S28-O29	-2.66	105.17	113.82
2	A	295	BUL	C12-C6-C5	2.59	120.66	113.38
2	A	295	BUL	O20-C2-C3	2.14	111.55	108.07
2	A	295	BUL	O18-C17-N16	-2.08	118.31	121.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	295	BUL	N7-C11-C21-O22
2	A	295	BUL	C5-O14-S32-O35
2	A	295	BUL	O13-C12-C6-C5
2	A	295	BUL	C26-C27-S28-O29
2	A	295	BUL	O18-C17-N16-C3

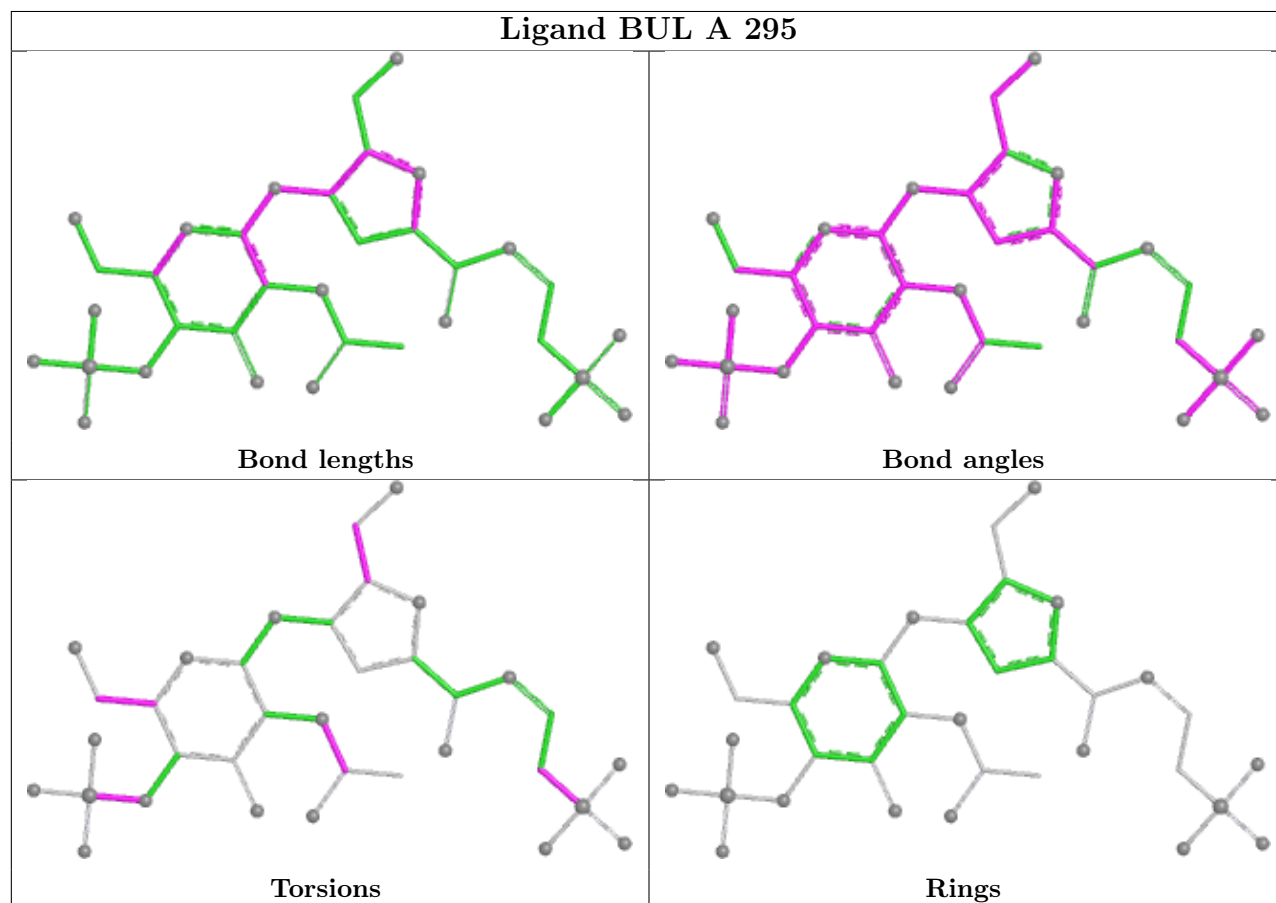
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	295	BUL	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 than 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

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	185/185 (100%)	3.61	161 (87%) 0 0	3, 11, 25, 39	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	LYS	8.6
1	A	132	PRO	7.3
1	A	172	ASP	7.0
1	A	3	ASP	6.8
1	A	87	ARG	6.6
1	A	149	ALA	6.4
1	A	122	ASP	6.3
1	A	111	VAL	6.1
1	A	120	LEU	6.0
1	A	56	GLY	5.9
1	A	171	ASN	5.8
1	A	57	GLU	5.7
1	A	12	ASP	5.6
1	A	52	ILE	5.5
1	A	156	SER	5.4
1	A	123	PHE	5.4
1	A	117	THR	5.4
1	A	169	TYR	5.3
1	A	133	SER	5.2
1	A	124	ILE	5.2
1	A	9	ASN	5.2
1	A	82	ASN	5.2
1	A	4	CYS	5.2
1	A	22	LYS	5.2
1	A	110	GLU	5.2
1	A	93	LEU	5.2
1	A	31	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	44	ALA	5.1
1	A	127	ILE	5.1
1	A	54	LYS	5.0
1	A	182	GLN	5.0
1	A	116	GLY	5.0
1	A	174	VAL	5.0
1	A	113	ILE	4.9
1	A	42	LEU	4.9
1	A	165	THR	4.9
1	A	62	GLU	4.8
1	A	1	ARG	4.8
1	A	150	GLY	4.7
1	A	50	THR	4.7
1	A	63	PRO	4.7
1	A	152	GLY	4.7
1	A	19	LYS	4.7
1	A	27	SER	4.6
1	A	77	GLY	4.6
1	A	175	ALA	4.6
1	A	180	TYR	4.6
1	A	59	LEU	4.6
1	A	158	ALA	4.6
1	A	104	GLN	4.6
1	A	28	TYR	4.6
1	A	48	TYR	4.6
1	A	39	GLU	4.5
1	A	7	ASN	4.5
1	A	15	GLY	4.5
1	A	108	ASN	4.5
1	A	47	ARG	4.4
1	A	185	TYR	4.4
1	A	10	ARG	4.4
1	A	40	ARG	4.4
1	A	20	THR	4.4
1	A	114	THR	4.3
1	A	51	ILE	4.3
1	A	140	LEU	4.2
1	A	177	ALA	4.2
1	A	147	TYR	4.2
1	A	97	ASP	4.2
1	A	112	HIS	4.2
1	A	79	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	43	LYS	4.1
1	A	78	LYS	4.1
1	A	23	PRO	4.1
1	A	157	TYR	4.1
1	A	64	ALA	4.0
1	A	109	GLY	4.0
1	A	142	GLY	4.0
1	A	26	LEU	4.0
1	A	36	THR	4.0
1	A	84	TRP	3.9
1	A	32	PRO	3.9
1	A	155	ARG	3.9
1	A	126	ARG	3.9
1	A	134	TRP	3.8
1	A	83	GLY	3.8
1	A	179	TYR	3.8
1	A	107	TRP	3.8
1	A	144	ILE	3.8
1	A	130	LYS	3.7
1	A	162	ILE	3.7
1	A	161	ASP	3.7
1	A	148	ASN	3.7
1	A	166	HIS	3.6
1	A	128	GLN	3.6
1	A	91	PHE	3.6
1	A	34	SER	3.5
1	A	138	GLN	3.5
1	A	65	VAL	3.5
1	A	173	VAL	3.5
1	A	102	LYS	3.4
1	A	14	THR	3.4
1	A	170	ALA	3.4
1	A	13	THR	3.3
1	A	92	GLY	3.3
1	A	167	ASP	3.3
1	A	85	GLY	3.2
1	A	72	ARG	3.1
1	A	121	THR	3.0
1	A	53	LYS	3.0
1	A	55	VAL	3.0
1	A	151	ALA	3.0
1	A	18	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	86	ASP	3.0
1	A	30	GLY	2.9
1	A	8	VAL	2.9
1	A	106	THR	2.9
1	A	71	SER	2.9
1	A	118	THR	2.9
1	A	178	GLN	2.9
1	A	154	VAL	2.9
1	A	67	ALA	2.9
1	A	103	PRO	2.9
1	A	75	HIS	2.8
1	A	96	VAL	2.8
1	A	163	GLY	2.8
1	A	74	SER	2.8
1	A	164	THR	2.8
1	A	6	GLY	2.8
1	A	11	ILE	2.8
1	A	2	THR	2.8
1	A	21	ALA	2.8
1	A	25	GLY	2.7
1	A	24	GLU	2.7
1	A	45	MET	2.7
1	A	41	ASP	2.6
1	A	89	ASN	2.6
1	A	90	GLY	2.6
1	A	119	ILE	2.6
1	A	176	ARG	2.5
1	A	46	ASP	2.5
1	A	183	HIS	2.5
1	A	184	GLY	2.4
1	A	76	ALA	2.4
1	A	168	ASP	2.4
1	A	80	LEU	2.4
1	A	17	SER	2.4
1	A	88	GLY	2.4
1	A	135	THR	2.3
1	A	33	ALA	2.3
1	A	145	SER	2.3
1	A	136	LYS	2.3
1	A	131	PHE	2.3
1	A	16	ALA	2.2
1	A	58	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	94	MET	2.1
1	A	5	TYR	2.1
1	A	143	GLY	2.1
1	A	37	ILE	2.1
1	A	66	ILE	2.1
1	A	159	ARG	2.1
1	A	101	HIS	2.1
1	A	49	LYS	2.0

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](#)

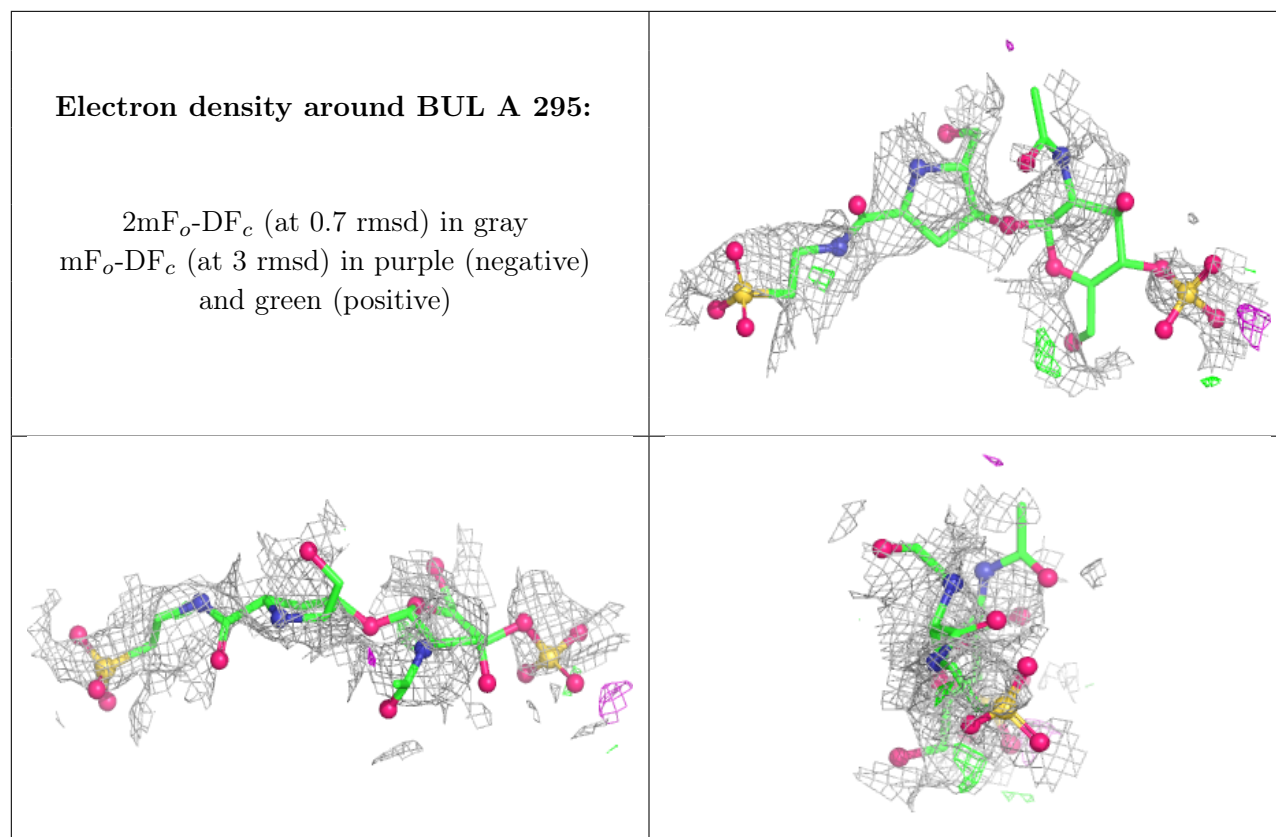
There are no oligosaccharides in this entry.

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, 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($\text{\AA}^2$)	Q<0.9
2	BUL	A	295	35/35	0.76	0.20	1,16,37,59	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.