



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2026 – 01:32 pm BST

PDB ID : 9RVQ / pdb_00009rvq
Title : Structure of CrtA with betaOG
Authors : Hachmi, M.; Jacob-Dubuisson, F.; Arnoux, P.
Deposited on : 2025-07-08
Resolution : 2.08 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 : 1.8.4, CSD as541be (2020)
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

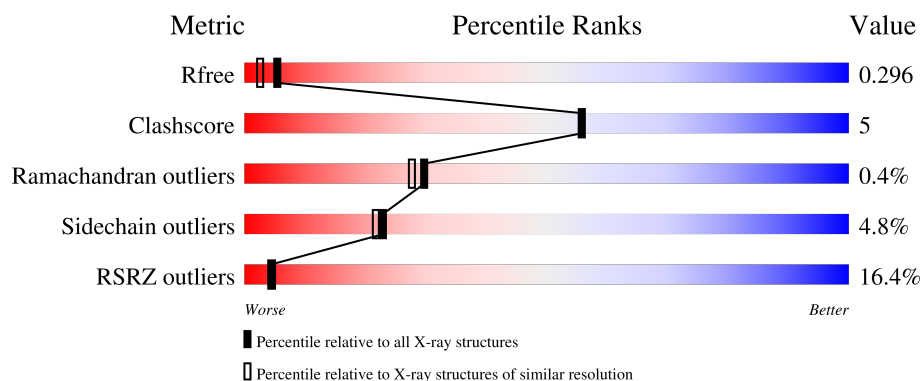
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	732	<div> <div>16%</div> <div>81% 12% • 6%</div> </div>
1	B	732	<div> <div>15%</div> <div>80% 13% • 6%</div> </div>

2 Entry composition [i](#)

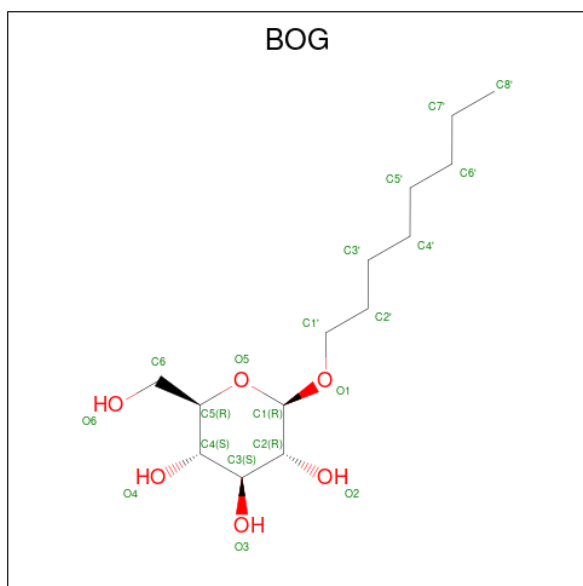
There are 4 unique types of molecules in this entry. The entry contains 11296 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TonB-dependent receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	6	0
			5387	3355	1003	1025	4			
1	B	691	Total	C	N	O	S	0	9	0
			5396	3362	999	1031	4			

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

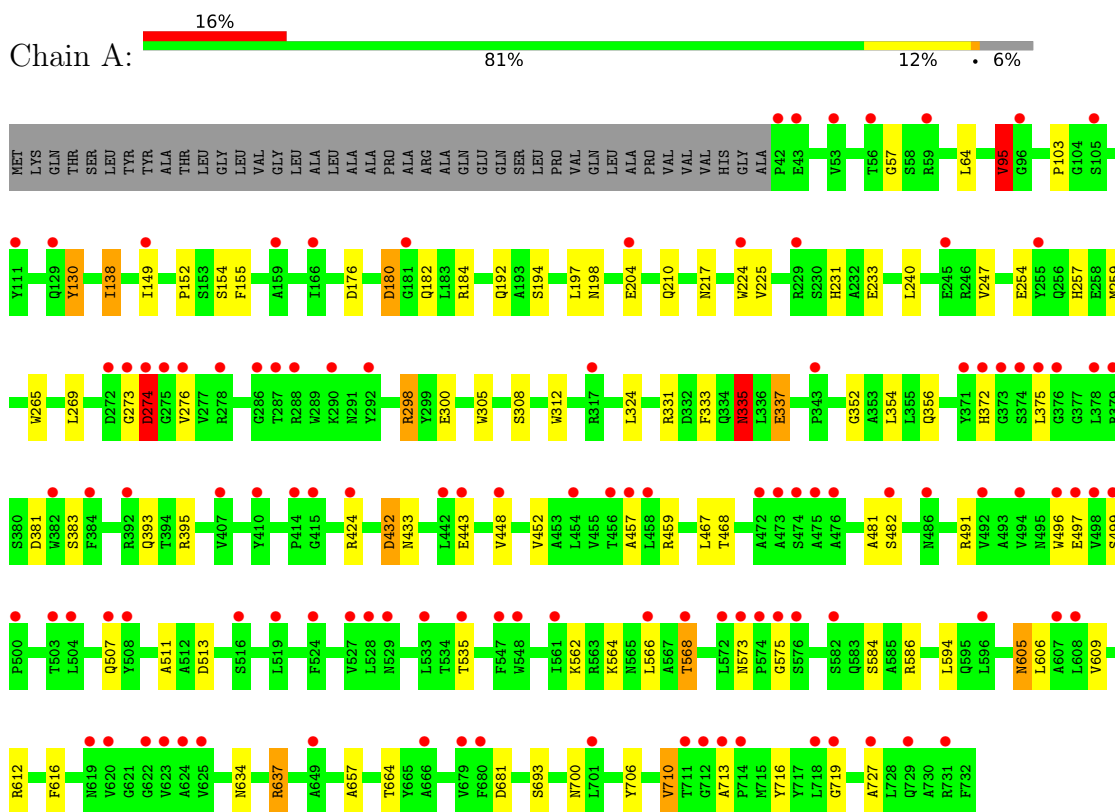
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	274	Total	O	0	0
			274	274		

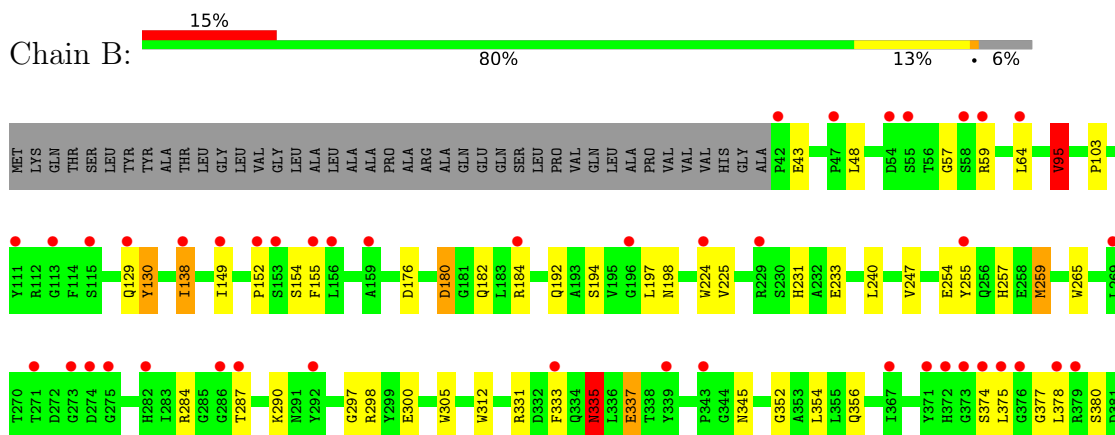
3 Residue-property plots [i](#)

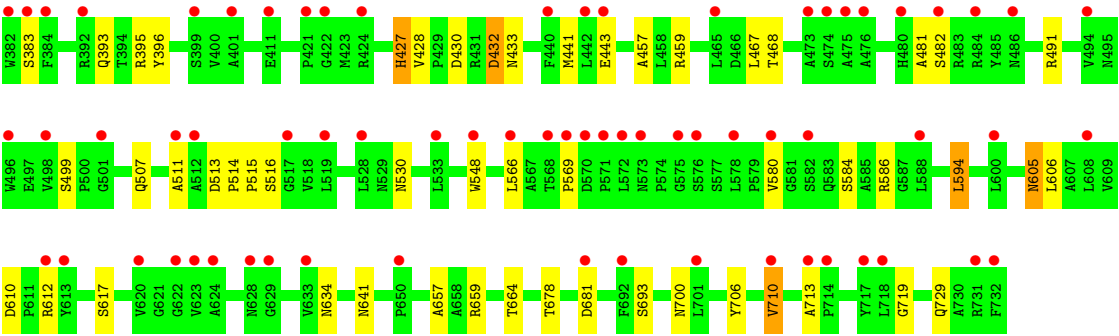
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: TonB-dependent receptor



• Molecule 1: TonB-dependent receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.10Å 120.08Å 119.55Å 90.00° 102.24° 90.00°	Depositor
Resolution (Å)	116.83 – 2.08 116.83 – 2.08	Depositor EDS
% Data completeness (in resolution range)	48.4 (116.83-2.08) 48.3 (116.83-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.07Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.247 , 0.303 0.242 , 0.296	Depositor DCC
R_{free} test set	2828 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11296	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5618e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BOG, GOL

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	0.72	1/5511 (0.0%)	1.05	18/7502 (0.2%)
1	B	0.73	2/5520 (0.0%)	1.05	21/7519 (0.3%)
All	All	0.72	3/11031 (0.0%)	1.05	39/15021 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	ILE	CG1-CD1	-7.87	1.21	1.51
1	A	138	ILE	CG1-CD1	-7.54	1.22	1.51
1	B	378	LEU	CA-C	5.41	1.55	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	513	ASP	CA-CB-CG	6.93	119.53	112.60
1	B	430	ASP	CA-CB-CG	6.88	119.48	112.60
1	A	700	ASN	CA-C-N	6.78	129.69	120.54
1	A	700	ASN	C-N-CA	6.78	129.69	120.54
1	B	700	ASN	CA-C-N	6.73	129.62	120.54
1	B	700	ASN	C-N-CA	6.73	129.62	120.54
1	A	180	ASP	CA-CB-CG	6.72	119.32	112.60
1	B	513	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	713	ALA	N-CA-C	-6.50	95.45	109.81
1	B	95	VAL	N-CA-CB	6.49	118.30	110.31
1	B	713	ALA	N-CA-C	-6.44	95.58	109.81
1	A	130	TYR	CA-C-N	6.37	129.68	120.38
1	A	130	TYR	C-N-CA	6.37	129.68	120.38
1	B	335	ASN	N-CA-C	6.35	118.83	109.24
1	B	432	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	274	ASP	CA-CB-CG	6.26	118.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	TYR	CA-C-N	6.25	129.28	120.28
1	B	130	TYR	C-N-CA	6.25	129.28	120.28
1	B	610	ASP	CA-CB-CG	6.22	118.82	112.60
1	B	180	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	335	ASN	N-CA-C	6.14	118.50	109.24
1	B	64	LEU	CA-C-N	6.02	128.34	120.28
1	B	64	LEU	C-N-CA	6.02	128.34	120.28
1	A	64	LEU	CA-C-N	6.00	128.32	120.28
1	A	64	LEU	C-N-CA	6.00	128.32	120.28
1	A	95	VAL	N-CA-CB	5.95	118.11	110.13
1	B	176	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	605	ASN	CA-CB-CG	5.53	118.12	112.60
1	A	432	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	427[A]	HIS	CA-C-N	5.31	131.96	122.13
1	B	427[A]	HIS	C-N-CA	5.31	131.96	122.13
1	B	427[B]	HIS	CA-C-N	5.31	131.96	122.13
1	B	427[B]	HIS	C-N-CA	5.31	131.96	122.13
1	A	176	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	605	ASN	CA-CB-CG	5.21	117.81	112.60
1	B	337	GLU	N-CA-C	5.20	121.40	113.61
1	A	337	GLU	N-CA-C	5.18	121.38	113.61
1	A	497	GLU	CA-C-N	5.05	127.38	120.46
1	A	497	GLU	C-N-CA	5.05	127.38	120.46

There are no chirality outliers.

There are no planarity outliers.

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	5387	0	5195	46	0
1	B	5396	0	5198	54	0
2	A	20	0	27	1	0
2	B	20	0	26	0	0
3	B	6	0	8	1	0
4	A	193	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	274	0	0	5	0
All	All	11296	0	10454	99	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 5.

All (99) 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:B:182:GLN:HE21	1:B:729:GLN:HE21	1.22	0.86
1:A:204:GLU:OE1	2:A:801:BOG:O3	1.96	0.83
1:B:259:MET:HE3	1:B:300:GLU:HB2	1.61	0.83
1:A:432:ASP:HB2	1:A:468:THR:HB	1.73	0.70
1:B:634:ASN:HA	1:B:664:THR:HG23	1.74	0.69
1:A:634:ASN:HA	1:A:664:THR:HG23	1.74	0.69
1:A:95:VAL:HG13	1:A:605:ASN:HB2	1.73	0.69
1:B:95:VAL:HG13	1:B:605:ASN:HB2	1.75	0.68
1:B:432:ASP:HB2	1:B:468:THR:HB	1.74	0.67
1:A:254:GLU:HB2	1:A:305:TRP:HB2	1.77	0.66
1:B:182:GLN:HE21	1:B:729:GLN:NE2	1.91	0.66
1:B:634:ASN:HD21	1:B:710:VAL:H	1.45	0.65
1:A:634:ASN:HD21	1:A:710:VAL:H	1.45	0.64
1:B:254:GLU:HB2	1:B:305:TRP:HB2	1.78	0.64
1:A:335:ASN:HB3	4:A:912:HOH:O	1.98	0.64
1:A:259:MET:HE1	1:A:298[A]:ARG:HG3	1.79	0.62
1:A:634:ASN:HA	1:A:664:THR:CG2	2.31	0.61
1:A:231:HIS:HD2	1:A:233:GLU:OE1	1.84	0.61
1:B:516:SER:HB3	1:B:530:ASN:HD21	1.66	0.61
1:A:383:SER:HB3	1:A:443:GLU:HB3	1.83	0.60
1:B:383:SER:HB3	1:B:443:GLU:HB3	1.83	0.59
1:B:375:LEU:HB2	1:B:380:SER:HB2	1.83	0.59
1:B:634:ASN:HA	1:B:664:THR:CG2	2.31	0.59
1:B:335:ASN:HB3	4:B:932:HOH:O	2.01	0.59
1:B:231:HIS:HD2	1:B:233:GLU:OE1	1.86	0.59
1:B:396:TYR:HB3	1:B:427[B]:HIS:HB3	1.85	0.58
1:A:609:VAL:O	1:A:637:ARG:HB3	2.05	0.57
1:B:657:ALA:HB3	1:B:681:ASP:HB2	1.87	0.57
1:A:184[B]:ARG:HE	1:A:192:GLN:HE21	1.52	0.57
1:A:657:ALA:HB3	1:A:681:ASP:HB2	1.87	0.56
1:A:154:SER:HB2	1:A:511:ALA:HA	1.86	0.56
1:B:154:SER:HB2	1:B:511:ALA:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:HA	1:A:459:ARG:HB3	1.88	0.55
1:B:331:ARG:HH12	1:B:393:GLN:HE22	1.54	0.55
1:B:155:PHE:HA	1:B:459:ARG:HB3	1.88	0.55
1:A:331:ARG:HH12	1:A:393:GLN:HE22	1.56	0.54
1:B:129:GLN:HB3	4:B:1023:HOH:O	2.07	0.54
1:B:59:ARG:NH2	1:B:441:MET:SD	2.81	0.54
1:B:331:ARG:HH12	1:B:393:GLN:NE2	2.06	0.53
1:B:569:PRO:HD2	1:B:617:SER:HB2	1.90	0.53
1:B:259:MET:HG2	1:B:300:GLU:HG3	1.91	0.52
1:B:584:SER:CB	1:B:586:ARG:HH12	2.22	0.52
1:A:331:ARG:HH12	1:A:393:GLN:NE2	2.08	0.51
1:A:259:MET:HE1	1:A:298[A]:ARG:CG	2.41	0.51
1:B:584:SER:OG	1:B:586:ARG:NH1	2.27	0.51
1:A:233:GLU:OE2	1:A:257:HIS:HD2	1.94	0.50
1:B:427[B]:HIS:HE1	4:B:945:HOH:O	1.95	0.50
1:B:233:GLU:OE2	1:B:257:HIS:HD2	1.95	0.50
1:A:259:MET:CE	1:A:298[A]:ARG:HG3	2.40	0.50
1:B:224:TRP:CD1	4:B:972:HOH:O	2.66	0.49
1:A:265:TRP:CE3	1:A:337:GLU:HB2	2.47	0.49
1:B:265:TRP:CE3	1:B:337:GLU:HB2	2.47	0.49
1:A:182:GLN:HB3	1:A:194:SER:HB2	1.94	0.49
1:A:184[A]:ARG:HG3	1:A:727:ALA:HB2	1.95	0.48
1:B:182:GLN:HB3	1:B:194:SER:HB2	1.94	0.47
1:B:182:GLN:NE2	1:B:729:GLN:HE21	2.03	0.47
1:A:337:GLU:HG2	1:A:352:GLY:O	2.15	0.47
1:B:152:PRO:HB3	1:B:511:ALA:HB2	1.98	0.46
1:A:372:HIS:ND1	1:A:381:ASP:OD2	2.44	0.46
1:A:152:PRO:HB3	1:A:511:ALA:HB2	1.97	0.45
1:A:467:LEU:HB2	1:A:481:ALA:HB3	1.99	0.45
1:A:568:THR:CG2	1:A:616:PHE:HA	2.47	0.45
1:B:257:HIS:HE1	1:B:300:GLU:OE1	1.98	0.45
1:B:184:ARG:HB3	1:B:192:GLN:HG2	1.98	0.45
1:A:257:HIS:HE1	1:A:300:GLU:OE1	1.99	0.45
1:B:337:GLU:HG2	1:B:352:GLY:O	2.16	0.45
1:B:284:ARG:NH1	1:B:345:ASN:O	2.49	0.44
1:B:457:ALA:HB3	1:B:491:ARG:HG2	1.99	0.44
1:A:103:PRO:HG2	1:A:265:TRP:CD2	2.53	0.44
1:A:57:GLY:HA2	1:A:149:ILE:HD12	1.99	0.44
1:B:333:PHE:HB2	1:B:356:GLN:HB3	2.00	0.44
1:B:57:GLY:HA2	1:B:149:ILE:HD12	1.99	0.44
1:B:103:PRO:HG2	1:B:265:TRP:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:LEU:HB2	1:B:481:ALA:HB3	2.00	0.43
1:A:457:ALA:HB3	1:A:491:ARG:HG2	2.00	0.43
1:A:333:PHE:HB2	1:A:356:GLN:HB3	1.99	0.43
1:A:584:SER:OG	1:A:586:ARG:NH2	2.51	0.43
1:A:562:LYS:HB3	1:A:564:LYS:HE2	1.98	0.43
1:A:240:LEU:C	1:A:240:LEU:HD23	2.44	0.43
1:B:247:VAL:HG22	1:B:312:TRP:CD1	2.54	0.43
1:B:48:LEU:HD21	3:B:802:GOL:H12	2.01	0.43
1:A:194:SER:OG	1:A:217:ASN:OD1	2.29	0.42
1:B:706:TYR:CZ	1:B:719:GLY:HA3	2.55	0.42
1:B:240:LEU:C	1:B:240:LEU:HD23	2.45	0.42
1:B:287:THR:HA	1:B:290:LYS:HG2	2.02	0.42
1:A:706:TYR:CZ	1:A:719:GLY:HA3	2.55	0.41
1:B:641:ASN:OD1	4:B:901:HOH:O	2.21	0.41
1:B:375:LEU:HB2	1:B:380:SER:CB	2.51	0.41
1:B:659:ARG:O	1:B:678:THR:HA	2.20	0.41
1:A:247:VAL:HG22	1:A:312:TRP:CD1	2.56	0.41
1:A:269:LEU:HD21	1:A:716:TYR:CG	2.56	0.41
1:B:514:PRO:HA	1:B:515:PRO:HD3	1.94	0.41
1:A:210:GLN:OE1	1:B:255:TYR:OH	2.31	0.41
1:A:259:MET:HA	1:A:259:MET:HE3	2.03	0.41
1:B:548[B]:TRP:HZ3	1:B:594:LEU:HD21	1.86	0.40
1:B:297:GLY:O	1:B:298:ARG:HG3	2.20	0.40
1:A:308:SER:HB3	1:A:324:LEU:HB3	2.04	0.40
1:A:274:ASP:OD1	1:A:276:VAL:HG23	2.22	0.40
1:A:452:VAL:HG23	1:A:496:TRP:CD1	2.56	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	695/732 (95%)	672 (97%)	20 (3%)	3 (0%)	30	28
1	B	698/732 (95%)	670 (96%)	25 (4%)	3 (0%)	30	28
All	All	1393/1464 (95%)	1342 (96%)	45 (3%)	6 (0%)	30	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	TYR
1	A	273	GLY
1	B	130	TYR
1	B	377	GLY
1	B	428	VAL
1	A	575	GLY

5.3.2 Protein sidechains ⓘ

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	549/573 (96%)	519 (94%)	30 (6%)	19	17
1	B	552/573 (96%)	527 (96%)	25 (4%)	24	24
All	All	1101/1146 (96%)	1046 (95%)	55 (5%)	23	20

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	VAL
1	A	138	ILE
1	A	180	ASP
1	A	197	LEU
1	A	198	ASN
1	A	224	TRP
1	A	225	VAL
1	A	274	ASP
1	A	298[A]	ARG
1	A	298[B]	ARG

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Mol	Chain	Res	Type
1	A	335	ASN
1	A	354	LEU
1	A	375	LEU
1	A	395	ARG
1	A	424	ARG
1	A	433	ASN
1	A	448	VAL
1	A	482	SER
1	A	499	SER
1	A	507	GLN
1	A	535	THR
1	A	566	LEU
1	A	568	THR
1	A	573	ASN
1	A	594	LEU
1	A	606	LEU
1	A	612	ARG
1	A	637	ARG
1	A	693	SER
1	A	710	VAL
1	B	43[A]	GLU
1	B	43[B]	GLU
1	B	95	VAL
1	B	138	ILE
1	B	180	ASP
1	B	197	LEU
1	B	198	ASN
1	B	225[A]	VAL
1	B	225[B]	VAL
1	B	259	MET
1	B	335	ASN
1	B	354	LEU
1	B	374	SER
1	B	395	ARG
1	B	433	ASN
1	B	482	SER
1	B	499	SER
1	B	507	GLN
1	B	566	LEU
1	B	580	VAL
1	B	594	LEU
1	B	606	LEU

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Mol	Chain	Res	Type
1	B	612	ARG
1	B	693	SER
1	B	710	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	219	ASN
1	A	231	HIS
1	A	257	HIS
1	A	393	GLN
1	A	495	ASN
1	A	583	GLN
1	A	619	ASN
1	A	634	ASN
1	A	729	GLN
1	B	118	GLN
1	B	174	GLN
1	B	192	GLN
1	B	219	ASN
1	B	231	HIS
1	B	256	GLN
1	B	257	HIS
1	B	393	GLN
1	B	486	ASN
1	B	530	ASN
1	B	583	GLN
1	B	634	ASN
1	B	729	GLN

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](#)

3 ligands 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	$\# Z > 2$
3	GOL	B	802	-	5,5,5	0.15	0	5,5,5	0.40	0
2	BOG	A	801	-	20,20,20	0.25	0	25,25,25	0.50	0
2	BOG	B	801	-	20,20,20	0.18	0	25,25,25	0.36	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
3	GOL	B	802	-	-	2/4/4/4	-
2	BOG	A	801	-	-	3/11/31/31	0/1/1/1
2	BOG	B	801	-	-	1/11/31/31	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	GOL	O1-C1-C2-C3
2	A	801	BOG	C3'-C4'-C5'-C6'
3	B	802	GOL	O1-C1-C2-O2
2	A	801	BOG	C5'-C6'-C7'-C8'

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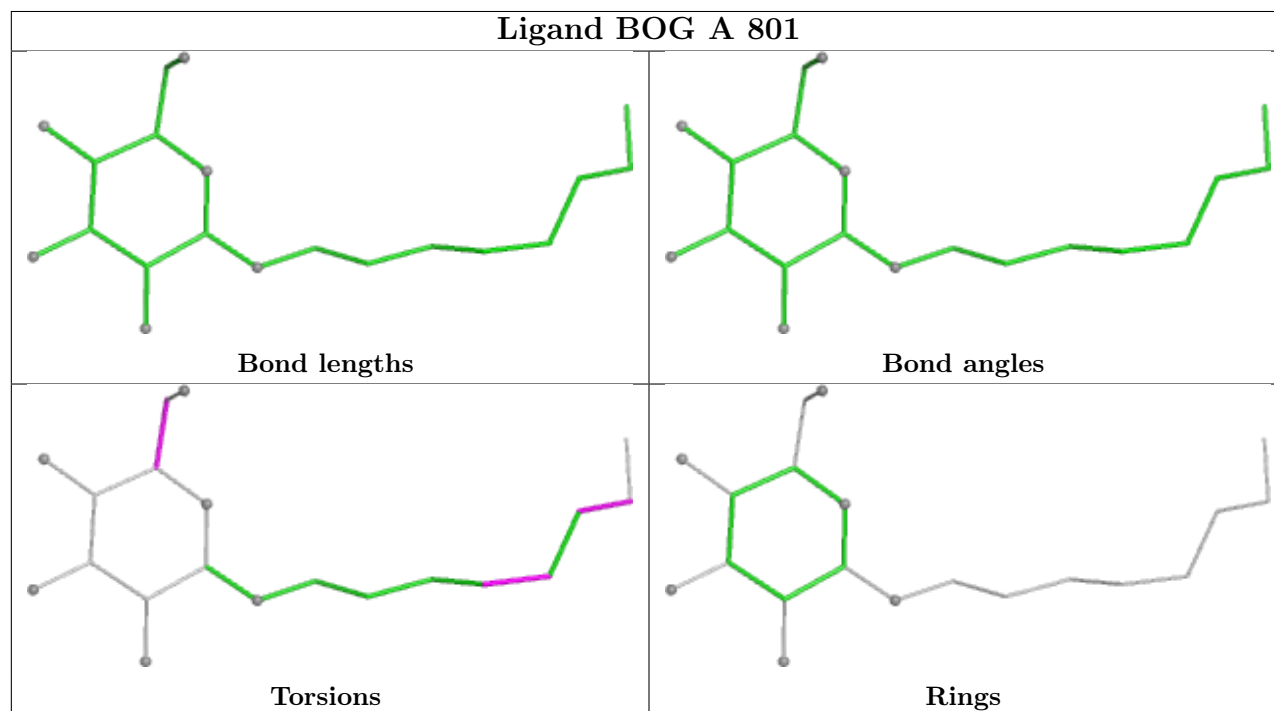
Mol	Chain	Res	Type	Atoms
2	B	801	BOG	C3'-C4'-C5'-C6'
2	A	801	BOG	C4-C5-C6-O6

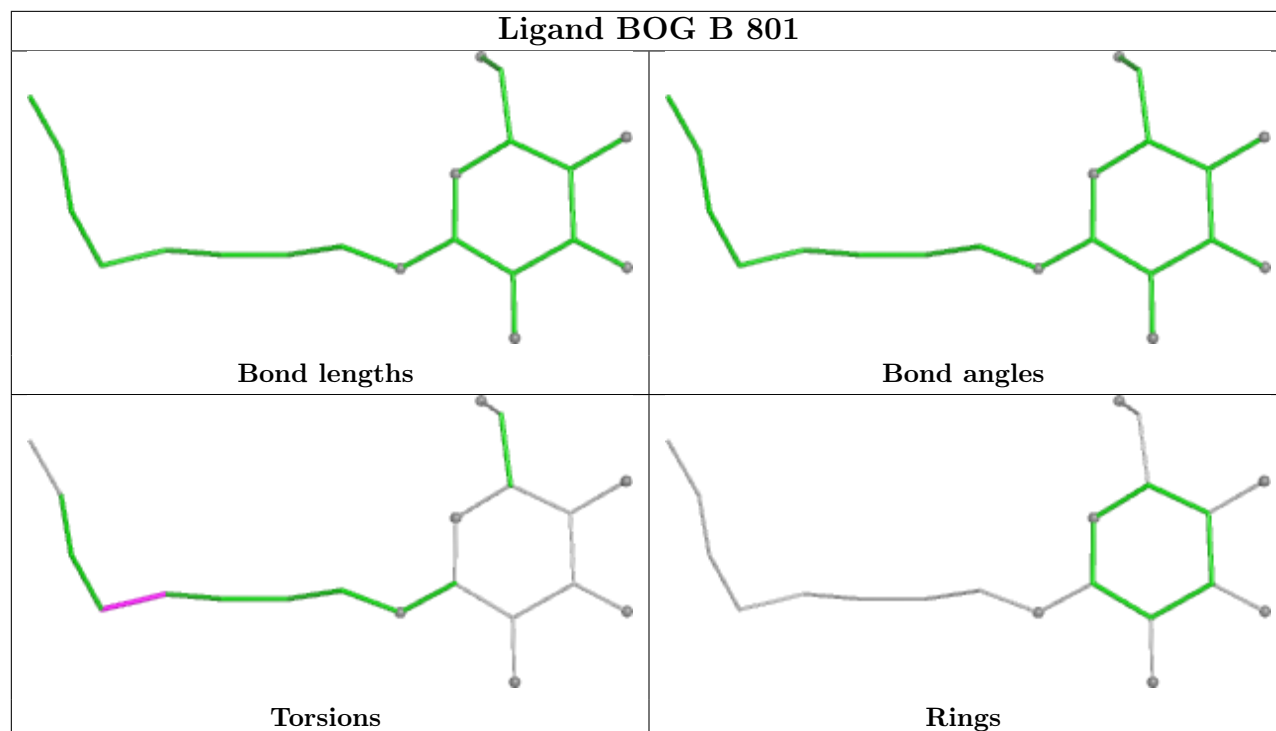
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	GOL	1	0
2	A	801	BOG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	691/732 (94%)	1.02	114 (16%)  	11, 45, 71, 93	6 (0%)
1	B	691/732 (94%)	1.00	112 (16%)  	11, 42, 68, 87	9 (1%)
All	All	1382/1464 (94%)	1.01	226 (16%)  	11, 44, 70, 93	15 (1%)

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	375	LEU	7.8
1	A	528	LEU	7.7
1	A	476	ALA	5.8
1	A	713	ALA	5.8
1	A	712	GLY	5.7
1	B	375	LEU	5.4
1	B	713	ALA	5.3
1	B	184	ARG	5.1
1	B	528	LEU	5.0
1	B	422	GLY	4.9
1	B	224	TRP	4.9
1	B	42	PRO	4.8
1	A	548[A]	TRP	4.7
1	B	373	GLY	4.6
1	B	484[A]	ARG	4.4
1	B	275	GLY	4.4
1	A	472	ALA	4.4
1	A	498	VAL	4.4
1	A	274	ASP	4.3
1	A	317[A]	ARG	4.3
1	B	401	ALA	4.3
1	A	574	PRO	4.2
1	A	519	LEU	4.2
1	A	224	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	476	ALA	4.0
1	B	286	GLY	4.0
1	A	272	ASP	4.0
1	A	701	LEU	3.9
1	A	620	VAL	3.9
1	B	155	PHE	3.9
1	B	149	ILE	3.9
1	A	275	GLY	3.8
1	A	287	THR	3.8
1	B	374	SER	3.8
1	A	718	LEU	3.8
1	B	152	PRO	3.8
1	B	731	ARG	3.8
1	B	287	THR	3.7
1	B	378	LEU	3.7
1	B	156	LEU	3.6
1	A	575	GLY	3.6
1	A	535	THR	3.5
1	A	59	ARG	3.5
1	B	372	HIS	3.5
1	B	718	LEU	3.5
1	B	475	ALA	3.5
1	A	376	GLY	3.5
1	A	384	PHE	3.4
1	B	273	GLY	3.4
1	B	494	VAL	3.4
1	A	500	PRO	3.4
1	A	378	LEU	3.4
1	A	288	ARG	3.4
1	A	729	GLN	3.3
1	A	624	ALA	3.3
1	B	548[A]	TRP	3.3
1	A	292	TYR	3.2
1	A	474	SER	3.2
1	A	473	ALA	3.2
1	B	480	HIS	3.2
1	A	373	GLY	3.2
1	A	149	ILE	3.1
1	B	572	LEU	3.1
1	B	371	TYR	3.1
1	B	274	ASP	3.1
1	A	572	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	474	SER	3.1
1	B	482	SER	3.1
1	A	286	GLY	3.1
1	A	622	GLY	3.1
1	B	424	ARG	3.0
1	A	245	GLU	3.0
1	B	111	TYR	3.0
1	A	159	ALA	3.0
1	A	255[A]	TYR	3.0
1	B	570	ASP	3.0
1	B	620	VAL	3.0
1	A	503	THR	3.0
1	A	111	TYR	3.0
1	A	607	ALA	2.9
1	B	384	PHE	2.9
1	B	399	SER	2.9
1	A	727	ALA	2.9
1	B	271	THR	2.9
1	A	392[A]	ARG	2.9
1	B	292	TYR	2.9
1	B	576	SER	2.9
1	B	376	GLY	2.9
1	A	527	VAL	2.9
1	A	166	ILE	2.9
1	B	568	THR	2.9
1	A	204	GLU	2.9
1	A	374	SER	2.9
1	B	255	TYR	2.8
1	B	613	TYR	2.8
1	B	512	ALA	2.8
1	B	575	GLY	2.8
1	B	588	LEU	2.8
1	A	494	VAL	2.8
1	A	625	VAL	2.8
1	A	516	SER	2.8
1	B	379	ARG	2.8
1	B	339	TYR	2.8
1	A	475	ALA	2.8
1	A	608	LEU	2.8
1	A	456	THR	2.8
1	B	333	PHE	2.8
1	B	64	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	496	TRP	2.8
1	B	443	GLU	2.7
1	A	504	LEU	2.7
1	B	442	LEU	2.7
1	A	371	TYR	2.7
1	B	159	ALA	2.7
1	B	566	LEU	2.7
1	B	701	LEU	2.7
1	B	571	PRO	2.7
1	B	383	SER	2.7
1	B	580	VAL	2.7
1	A	343	PRO	2.6
1	A	372	HIS	2.6
1	B	582	SER	2.6
1	A	596	LEU	2.6
1	B	55	SER	2.6
1	A	276	VAL	2.6
1	A	42	PRO	2.6
1	B	54	ASP	2.6
1	B	129	GLN	2.6
1	A	181	GLY	2.6
1	B	282	HIS	2.6
1	A	711	THR	2.6
1	A	458	LEU	2.6
1	A	499	SER	2.6
1	B	533	LEU	2.6
1	B	732	PHE	2.5
1	A	407	VAL	2.5
1	B	573	ASN	2.5
1	A	229	ARG	2.5
1	B	367	ILE	2.5
1	A	573	ASN	2.5
1	A	619	ASN	2.5
1	A	105	SER	2.5
1	A	507	GLN	2.5
1	A	714	PRO	2.5
1	B	624	ALA	2.5
1	A	566	LEU	2.5
1	B	578	LEU	2.5
1	B	608	LEU	2.5
1	A	273	GLY	2.5
1	B	517	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	486	ASN	2.5
1	A	568	THR	2.5
1	A	442	LEU	2.5
1	B	59	ARG	2.5
1	B	714	PRO	2.4
1	A	457	ALA	2.4
1	B	486	ASN	2.4
1	A	497	GLU	2.4
1	B	382	TRP	2.4
1	A	410	TYR	2.4
1	A	424	ARG	2.4
1	A	454	LEU	2.4
1	A	533	LEU	2.4
1	B	600	LEU	2.4
1	B	440	PHE	2.4
1	A	492	VAL	2.4
1	A	679	VAL	2.4
1	B	138	ILE	2.4
1	B	633	VAL	2.4
1	A	379	ARG	2.4
1	B	421	PRO	2.4
1	B	343	PRO	2.4
1	B	473	ALA	2.3
1	B	269	LEU	2.3
1	B	629	GLY	2.3
1	B	229	ARG	2.3
1	A	649	ALA	2.3
1	A	731	ARG	2.3
1	A	415	GLY	2.3
1	B	519	LEU	2.3
1	A	576	SER	2.3
1	A	561	ILE	2.3
1	A	623	VAL	2.3
1	B	622	GLY	2.3
1	B	692	PHE	2.2
1	A	56	THR	2.2
1	A	666	ALA	2.2
1	B	115	SER	2.2
1	A	529	ASN	2.2
1	A	53	VAL	2.2
1	A	448	VAL	2.2
1	A	719	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	465	LEU	2.2
1	A	508	TYR	2.2
1	B	153	SER	2.2
1	B	392	ARG	2.2
1	B	612	ARG	2.2
1	A	414	PRO	2.2
1	A	524	PHE	2.2
1	A	43	GLU	2.2
1	B	511	ALA	2.2
1	A	382	TRP	2.2
1	B	496	TRP	2.2
1	B	498	VAL	2.1
1	B	113	GLY	2.1
1	A	443	GLU	2.1
1	B	681	ASP	2.1
1	A	680	PHE	2.1
1	B	623	VAL	2.1
1	A	547	PHE	2.1
1	A	482	SER	2.1
1	A	582	SER	2.1
1	B	569	PRO	2.1
1	B	196	GLY	2.1
1	B	710	VAL	2.1
1	B	58	SER	2.1
1	B	411	GLU	2.0
1	B	628	ASN	2.0
1	A	129	GLN	2.0
1	A	278	ARG	2.0
1	B	650	PRO	2.0
1	A	96	GLY	2.0
1	B	717	TYR	2.0
1	A	290	LYS	2.0
1	B	47	PRO	2.0
1	B	501	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

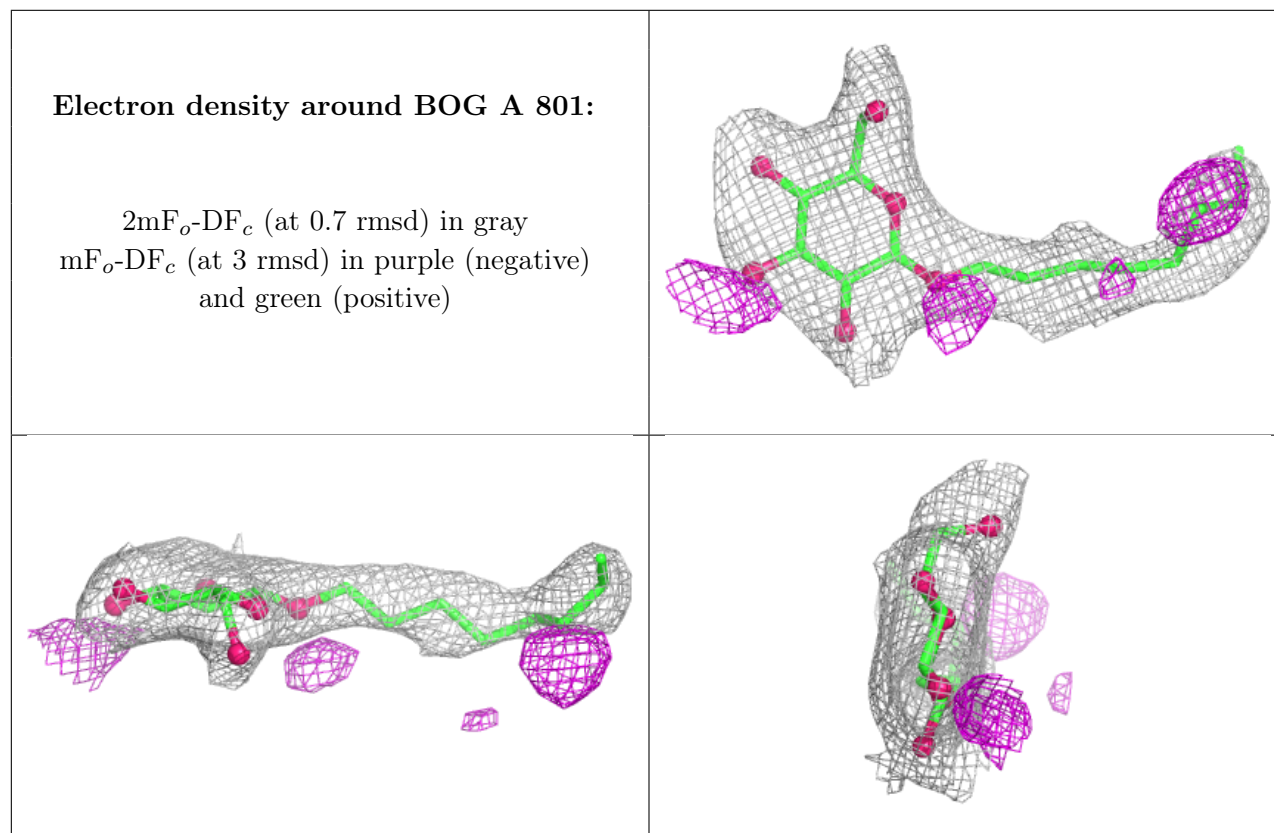
There are no oligosaccharides in this entry.

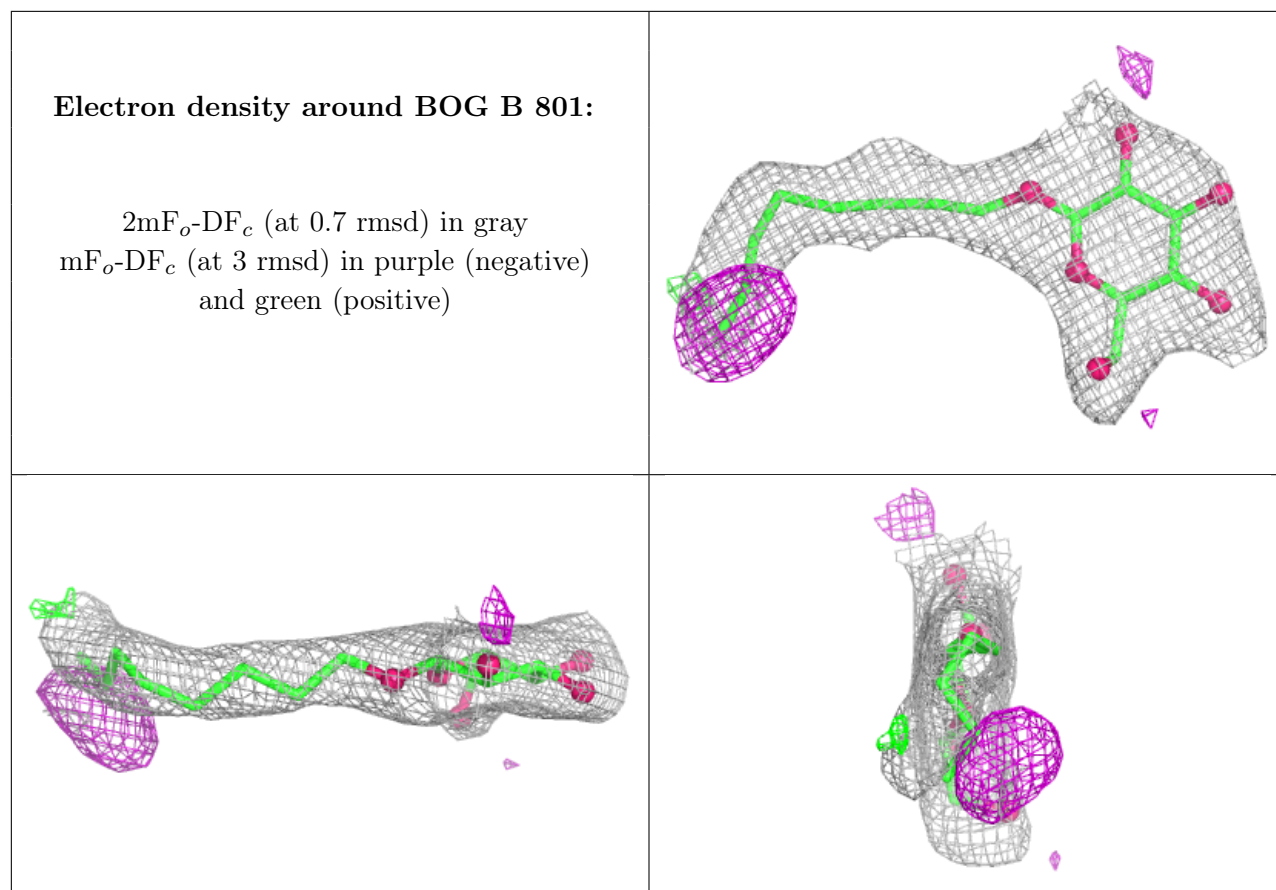
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
3	GOL	B	802	6/6	0.77	0.19	50,52,52,52	0
2	BOG	A	801	20/20	0.87	0.15	39,44,47,48	0
2	BOG	B	801	20/20	0.88	0.12	37,44,45,46	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 ⓘ

There are no such residues in this entry.