



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:30 PM UTC

PDB ID : 6V81 / pdb_00006v81
Title : The crystal structure of the outer-membrane transporter YncD
Authors : Grinter, R.
Deposited on : 2019-12-10
Resolution : 2.96 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
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

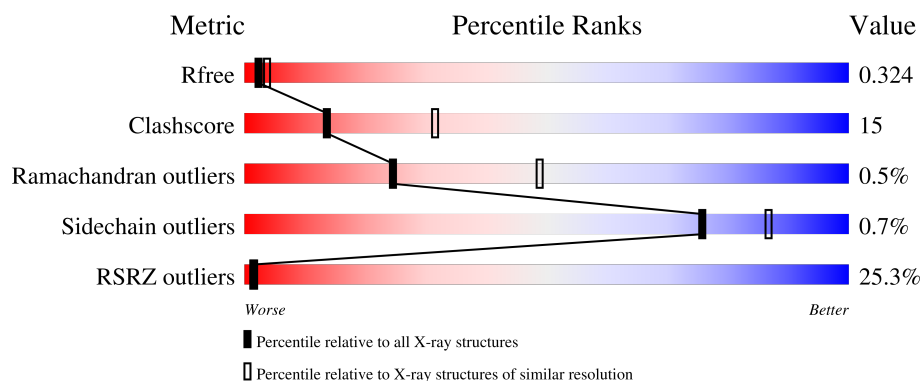
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	700	24% 65% 28% 7%

2 Entry composition [i](#)

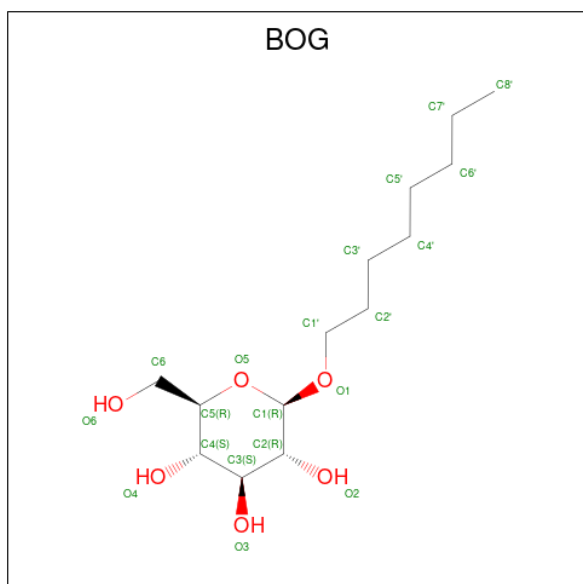
There are 3 unique types of molecules in this entry. The entry contains 5106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Probable TonB-dependent receptor YncD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	652	5085	3154	903	1010	18	0	0	0

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	87.94Å 98.64Å 124.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.97 – 2.96 43.97 – 2.96	Depositor EDS
% Data completeness (in resolution range)	75.5 (43.97-2.96) 75.5 (43.97-2.96)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.277 , 0.314 0.278 , 0.324	Depositor DCC
R_{free} test set	914 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 17.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	5106	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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: BOG, CA

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	0.26	0/5195	0.47	0/7042

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5085	0	4819	145	0
2	A	20	0	28	0	0
3	A	1	0	0	0	0
All	All	5106	0	4847	145	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 15.

All (145) 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:146:ASN:OD1	1:A:473:THR:HG23	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:HG3	1:A:286:GLU:HG3	1.65	0.76
1:A:68:LEU:H	1:A:68:LEU:HD23	1.52	0.74
1:A:135:VAL:HG22	1:A:152:MET:HG3	1.69	0.73
1:A:55:MET:HE1	1:A:133:VAL:HG23	1.70	0.72
1:A:43:THR:H	1:A:44:PRO:HD2	1.56	0.71
1:A:55:MET:HB2	1:A:67:SER:HB3	1.72	0.71
1:A:64:LEU:HB3	1:A:68:LEU:HD21	1.76	0.67
1:A:386:LEU:HD11	1:A:388:ARG:O	1.98	0.64
1:A:483:ALA:H	1:A:538:THR:HG21	1.63	0.62
1:A:146:ASN:OD1	1:A:473:THR:CG2	2.42	0.62
1:A:65:SER:OG	1:A:78:ASN:HB2	2.01	0.60
1:A:438:ASP:OD2	1:A:536:ARG:NH2	2.35	0.60
1:A:72:PRO:HB2	1:A:551:GLU:HB3	1.84	0.60
1:A:58:ALA:O	1:A:658:ARG:HD2	2.02	0.59
1:A:231:GLU:OE2	1:A:231:GLU:N	2.26	0.59
1:A:136:LEU:HB3	1:A:151:VAL:HG13	1.84	0.59
1:A:184:THR:OG1	1:A:199:THR:OG1	2.21	0.58
1:A:571:LEU:HD23	1:A:593:ILE:HB	1.86	0.58
1:A:43:THR:HG22	1:A:44:PRO:HD3	1.86	0.58
1:A:54:GLU:OE2	1:A:54:GLU:HA	2.04	0.57
1:A:248:ASP:HB3	1:A:272:THR:HG22	1.86	0.57
1:A:658:ARG:NH1	1:A:660:ASP:OD1	2.36	0.57
1:A:398:ASP:N	1:A:398:ASP:OD1	2.38	0.57
1:A:233:SER:HB2	1:A:287:ARG:HG3	1.86	0.56
1:A:342:HIS:HB3	1:A:352:PHE:CE2	2.39	0.56
1:A:46:ALA:HB2	1:A:502:GLU:OE2	2.06	0.55
1:A:115:MET:HE2	1:A:115:MET:HA	1.89	0.55
1:A:51:ASP:OD1	1:A:52:GLY:N	2.40	0.55
1:A:622:ILE:HG12	1:A:632:ALA:HB3	1.89	0.54
1:A:626:ASP:OD2	1:A:674:ASN:ND2	2.39	0.54
1:A:347:GLY:O	1:A:348:VAL:HG13	2.08	0.53
1:A:512:GLY:HA3	1:A:555:ASP:O	2.08	0.53
1:A:64:LEU:O	1:A:68:LEU:HD23	2.08	0.53
1:A:348:VAL:CG2	1:A:405:TRP:HE3	2.21	0.53
1:A:317:GLN:HB2	1:A:371:PHE:HZ	1.74	0.53
1:A:314:MET:HG3	1:A:371:PHE:CE1	2.44	0.53
1:A:331:ARG:HB3	1:A:363:GLU:HB3	1.91	0.52
1:A:371:PHE:O	1:A:372:ARG:HG2	2.09	0.52
1:A:372:ARG:HD3	1:A:380:TYR:CE2	2.45	0.52
1:A:52:GLY:HA2	1:A:55:MET:HE3	1.91	0.52
1:A:45:ALA:O	1:A:506:LYS:NZ	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD11	1:A:88:LEU:HD22	1.93	0.50
1:A:490:ASN:OD1	1:A:493:LEU:HB2	2.11	0.50
1:A:106:LEU:HB3	1:A:113:ALA:HB3	1.93	0.50
1:A:471:PHE:HE1	1:A:495:PRO:CG	2.25	0.50
1:A:224:LYS:HG3	1:A:238:ILE:CD1	2.41	0.50
1:A:580:CYS:HB2	1:A:583:GLN:O	2.13	0.49
1:A:350:VAL:HA	1:A:404:GLN:O	2.13	0.49
1:A:349:PRO:HB2	1:A:406:GLN:HB2	1.95	0.48
1:A:432:THR:HG22	1:A:435:ASN:HB3	1.94	0.48
1:A:43:THR:O	1:A:454:LYS:HD2	2.13	0.48
1:A:342:HIS:HB3	1:A:352:PHE:CZ	2.49	0.48
1:A:446:LYS:HG2	1:A:448:LEU:HD23	1.94	0.48
1:A:345:GLU:HB3	1:A:349:PRO:HA	1.97	0.47
1:A:106:LEU:HD23	1:A:107:TYR:N	2.30	0.47
1:A:398:ASP:OD2	1:A:418:ARG:NH2	2.42	0.47
1:A:136:LEU:HB3	1:A:151:VAL:CG1	2.43	0.47
1:A:187:THR:HB	1:A:196:VAL:HG22	1.97	0.47
1:A:483:ALA:N	1:A:538:THR:HG21	2.29	0.47
1:A:543:GLY:HA2	1:A:577:SER:CB	2.45	0.47
1:A:461:TRP:CD1	1:A:507:THR:HG1	2.34	0.46
1:A:342:HIS:NE2	1:A:344:GLY:HA3	2.30	0.46
1:A:124:ASN:HA	1:A:242:VAL:HG21	1.97	0.46
1:A:97:SER:OG	1:A:100:GLY:O	2.24	0.46
1:A:126:ASP:HA	1:A:220:LEU:HD13	1.97	0.46
1:A:474:PRO:CG	1:A:493:LEU:HD22	2.46	0.46
1:A:464:TYR:CZ	1:A:504:GLY:HA3	2.51	0.45
1:A:494:LYS:HB2	1:A:495:PRO:HD2	1.98	0.45
1:A:662:LEU:HD23	1:A:662:LEU:O	2.15	0.45
1:A:589:ARG:HD3	1:A:623:MET:HG3	1.99	0.45
1:A:345:GLU:HG2	1:A:350:VAL:N	2.32	0.45
1:A:166:GLU:HA	1:A:695:ILE:O	2.16	0.45
1:A:343:ARG:O	1:A:345:GLU:HG3	2.17	0.45
1:A:96:ARG:HA	1:A:673:VAL:HG11	1.99	0.45
1:A:543:GLY:CA	1:A:577:SER:HB3	2.47	0.45
1:A:56:ARG:HG3	1:A:61:ARG:HG2	1.98	0.44
1:A:73:GLY:HA3	1:A:551:GLU:OE1	2.16	0.44
1:A:389:ASP:O	1:A:390:GLU:HG3	2.18	0.44
1:A:509:ILE:HD11	1:A:554:TRP:NE1	2.32	0.44
1:A:74:LEU:HD11	1:A:88:LEU:CD2	2.47	0.44
1:A:623:MET:HE2	1:A:631:LYS:HE2	2.00	0.44
1:A:678:GLY:HA2	1:A:680:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:THR:N	1:A:44:PRO:HD2	2.30	0.44
1:A:213:HIS:CD2	1:A:247:ASP:HB3	2.52	0.44
1:A:514:LEU:C	1:A:514:LEU:HD23	2.43	0.44
1:A:252:LEU:HD22	1:A:256:GLU:HB3	2.00	0.44
1:A:482:ARG:HB3	1:A:490:ASN:HB2	2.00	0.44
1:A:656:PHE:CZ	1:A:692:GLY:HA3	2.52	0.44
1:A:523:THR:HG21	1:A:526:GLU:OE1	2.18	0.43
1:A:530:ASP:HB2	1:A:540:LYS:HB2	2.00	0.43
1:A:662:LEU:O	1:A:687:ARG:HD3	2.18	0.43
1:A:474:PRO:HG3	1:A:493:LEU:HD22	2.00	0.43
1:A:545:THR:HG22	1:A:575:TYR:HD1	1.83	0.43
1:A:125:ILE:N	1:A:125:ILE:HD12	2.33	0.43
1:A:278:GLN:HG3	1:A:304:ARG:HG3	2.01	0.43
1:A:133:VAL:HG22	1:A:154:VAL:HG13	2.01	0.43
1:A:367:GLY:O	1:A:386:LEU:HD12	2.18	0.43
1:A:75:GLN:NE2	1:A:592:GLY:O	2.52	0.43
1:A:115:MET:SD	1:A:361:MET:HG3	2.58	0.43
1:A:482:ARG:HH11	1:A:486:GLN:HB2	1.84	0.43
1:A:517:ALA:O	1:A:518:LEU:HD23	2.18	0.43
1:A:293:ASP:OD2	1:A:340:TRP:NE1	2.52	0.42
1:A:397:ILE:HG22	1:A:423:TRP:CZ3	2.54	0.42
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.91	0.42
1:A:98:THR:HG22	1:A:99:TYR:CD1	2.54	0.42
1:A:564:VAL:HG22	1:A:602:ILE:HG12	2.01	0.42
1:A:470:GLY:N	1:A:498:ASN:HB2	2.34	0.42
1:A:317:GLN:HB2	1:A:371:PHE:CZ	2.52	0.42
1:A:371:PHE:N	1:A:371:PHE:CD1	2.85	0.42
1:A:410:LYS:HG2	1:A:456:ALA:HB3	2.01	0.42
1:A:50:VAL:HG12	1:A:133:VAL:HB	2.01	0.42
1:A:647:ASN:HB3	1:A:652:THR:HG23	2.02	0.42
1:A:508:ARG:HD2	1:A:508:ARG:C	2.45	0.42
1:A:228:ARG:HH11	1:A:231:GLU:HA	1.84	0.42
1:A:345:GLU:HA	1:A:350:VAL:HG12	2.01	0.42
1:A:407:LEU:HD12	1:A:411:LEU:HD21	2.01	0.42
1:A:589:ARG:HE	1:A:595:ARG:HH21	1.68	0.42
1:A:56:ARG:NH1	1:A:130:VAL:O	2.53	0.41
1:A:61:ARG:NH2	1:A:166:GLU:OE2	2.50	0.41
1:A:514:LEU:HD23	1:A:514:LEU:O	2.19	0.41
1:A:659:VAL:HG13	1:A:689:TYR:CE1	2.55	0.41
1:A:213:HIS:NE2	1:A:272:THR:O	2.42	0.41
1:A:43:THR:H	1:A:44:PRO:CD	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:THR:HA	1:A:495:PRO:HB3	2.03	0.41
1:A:499:ASP:HB3	1:A:522:ASP:HB2	2.02	0.41
1:A:525:ASP:O	1:A:541:ASN:ND2	2.53	0.41
1:A:290:SER:HB2	1:A:293:ASP:HB3	2.00	0.41
1:A:432:THR:OG1	1:A:433:PRO:HD2	2.21	0.41
1:A:475:THR:OG1	1:A:478:GLU:HG3	2.20	0.41
1:A:502:GLU:HG2	1:A:503:ILE:N	2.35	0.41
1:A:523:THR:OG1	1:A:547:ARG:NH1	2.53	0.41
1:A:60:PRO:HB2	1:A:62:ILE:HG12	2.02	0.41
1:A:340:TRP:CD1	1:A:340:TRP:C	2.99	0.41
1:A:594:ALA:HA	1:A:622:ILE:HG22	2.03	0.41
1:A:192:GLN:O	1:A:195:ASP:HB2	2.21	0.41
1:A:50:VAL:HG13	1:A:55:MET:HE2	2.04	0.40
1:A:105:ARG:HD2	1:A:144:TYR:O	2.22	0.40
1:A:123:SER:HB3	1:A:244:ILE:HD11	2.02	0.40
1:A:248:ASP:H	1:A:273:ARG:HA	1.87	0.40
1:A:257:TRP:CD1	1:A:683:PRO:HG3	2.56	0.40
1:A:530:ASP:HB2	1:A:540:LYS:CB	2.52	0.40
1:A:87:GLN:OE1	1:A:671:VAL:O	2.39	0.40
1:A:156:THR:HG23	1:A:224:LYS:HD2	2.03	0.40
1:A:184:THR:O	1:A:184:THR:HG23	2.20	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	644/700 (92%)	607 (94%)	34 (5%)	3 (0%)	24	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	THR
1	A	687	ARG
1	A	449	PRO

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	535/577 (93%)	531 (99%)	4 (1%)	76 87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	VAL
1	A	286	GLU
1	A	557	ARG
1	A	595	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	153	ASN
1	A	310	GLN
1	A	330	GLN
1	A	486	GLN
1	A	694	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BOG	A	801	-	20,20,20	0.66	0	25,25,25	1.03	1 (4%)

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
2	BOG	A	801	-	-	4/11/31/31	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	BOG	C1-O5-C5	-2.88	108.09	113.72

There are no chirality outliers.

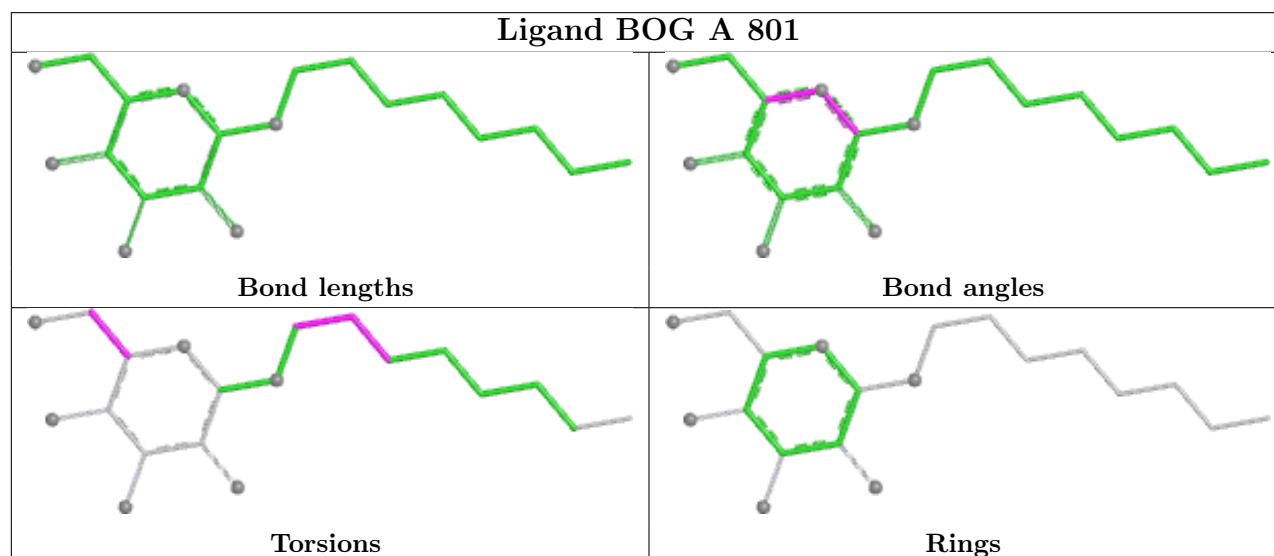
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	BOG	O5-C5-C6-O6
2	A	801	BOG	O1-C1'-C2'-C3'
2	A	801	BOG	C4-C5-C6-O6
2	A	801	BOG	C1'-C2'-C3'-C4'

There are no ring outliers.

No monomer is involved in short contacts.

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	652/700 (93%)	1.48	165 (25%) 1 1	53, 81, 113, 134	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	THR	10.9
1	A	635	TYR	10.6
1	A	54	GLU	10.6
1	A	284	ARG	10.4
1	A	617	ARG	9.8
1	A	455	TYR	9.4
1	A	286	GLU	8.7
1	A	615	GLU	8.7
1	A	599	PHE	8.5
1	A	328	THR	8.5
1	A	329	LEU	8.0
1	A	305	GLU	7.6
1	A	307	THR	7.5
1	A	124	ASN	7.5
1	A	636	THR	7.4
1	A	123	SER	7.4
1	A	125	ILE	7.2
1	A	306	THR	7.2
1	A	121	GLN	7.0
1	A	108	VAL	6.9
1	A	158	THR	6.7
1	A	327	ILE	6.3
1	A	383	LYS	6.2
1	A	456	ALA	5.8
1	A	156	THR	5.6
1	A	565	ASN	5.5
1	A	50	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	159	GLY	5.3
1	A	634	SER	5.1
1	A	269	GLN	5.1
1	A	69	THR	5.1
1	A	270	TYR	4.9
1	A	80	GLN	4.9
1	A	47	VAL	4.9
1	A	109	ASP	4.8
1	A	136	LEU	4.8
1	A	637	LEU	4.8
1	A	447	TRP	4.7
1	A	296	SER	4.7
1	A	563	ARG	4.7
1	A	135	VAL	4.7
1	A	346	LEU	4.5
1	A	368	TYR	4.5
1	A	441	ASP	4.5
1	A	138	GLY	4.5
1	A	298	MET	4.4
1	A	153	ASN	4.4
1	A	297	VAL	4.4
1	A	310	GLN	4.4
1	A	116	PRO	4.4
1	A	618	TYR	4.3
1	A	285	TYR	4.3
1	A	365	ARG	4.2
1	A	46	ALA	4.2
1	A	151	VAL	4.1
1	A	70	GLY	4.0
1	A	590	MET	4.0
1	A	152	MET	3.9
1	A	137	ARG	3.9
1	A	304	ARG	3.8
1	A	474	PRO	3.8
1	A	139	PRO	3.7
1	A	114	THR	3.7
1	A	601	SER	3.7
1	A	671	VAL	3.7
1	A	162	PRO	3.6
1	A	134	GLU	3.6
1	A	68	LEU	3.5
1	A	311	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	379	GLU	3.4
1	A	420	SER	3.4
1	A	673	VAL	3.4
1	A	57	LEU	3.4
1	A	518	LEU	3.4
1	A	234	LYS	3.4
1	A	64	LEU	3.3
1	A	386	LEU	3.3
1	A	308	GLN	3.3
1	A	395	TRP	3.3
1	A	448	LEU	3.2
1	A	96	ARG	3.2
1	A	231	GLU	3.1
1	A	155	THR	3.1
1	A	93	PHE	3.1
1	A	292	ARG	3.1
1	A	240	ASN	3.0
1	A	384	GLY	3.0
1	A	143	LEU	3.0
1	A	318	LEU	3.0
1	A	547	ARG	3.0
1	A	111	ILE	2.9
1	A	117	ASP	2.9
1	A	309	TYR	2.8
1	A	140	PHE	2.8
1	A	473	THR	2.8
1	A	79	ARG	2.8
1	A	360	ASN	2.8
1	A	475	THR	2.7
1	A	118	GLY	2.7
1	A	446	LYS	2.7
1	A	396	ASN	2.7
1	A	150	GLY	2.7
1	A	78	ASN	2.7
1	A	657	GLY	2.7
1	A	89	SER	2.7
1	A	326	VAL	2.7
1	A	88	LEU	2.7
1	A	672	ILE	2.7
1	A	555	ASP	2.7
1	A	160	GLN	2.7
1	A	391	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	578	ASN	2.6
1	A	71	VAL	2.6
1	A	127	LEU	2.6
1	A	457	MET	2.6
1	A	343	ARG	2.5
1	A	366	LYS	2.5
1	A	552	LEU	2.5
1	A	359	GLU	2.5
1	A	583	GLN	2.5
1	A	589	ARG	2.5
1	A	90	ILE	2.4
1	A	53	GLU	2.4
1	A	658	ARG	2.4
1	A	624	ALA	2.4
1	A	49	VAL	2.4
1	A	43	THR	2.4
1	A	674	ASN	2.4
1	A	120	GLY	2.4
1	A	95	SER	2.4
1	A	119	GLN	2.4
1	A	295	MET	2.4
1	A	147	ALA	2.3
1	A	548	GLN	2.3
1	A	653	VAL	2.3
1	A	643	GLY	2.3
1	A	610	TRP	2.3
1	A	230	ASP	2.3
1	A	626	ASP	2.3
1	A	110	GLY	2.3
1	A	484	ASP	2.2
1	A	454	LYS	2.2
1	A	677	ASN	2.2
1	A	410	LYS	2.2
1	A	503	ILE	2.1
1	A	557	ARG	2.1
1	A	476	ILE	2.1
1	A	580	CYS	2.1
1	A	154	VAL	2.1
1	A	609	GLY	2.1
1	A	203	THR	2.1
1	A	177	TRP	2.1
1	A	570	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	675	GLU	2.1
1	A	146	ASN	2.1
1	A	416	GLY	2.1
1	A	642	THR	2.1
1	A	267	ALA	2.1
1	A	338	SER	2.0
1	A	101	ILE	2.0
1	A	405	TRP	2.0
1	A	107	TYR	2.0
1	A	325	GLY	2.0
1	A	471	PHE	2.0
1	A	224	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](#)

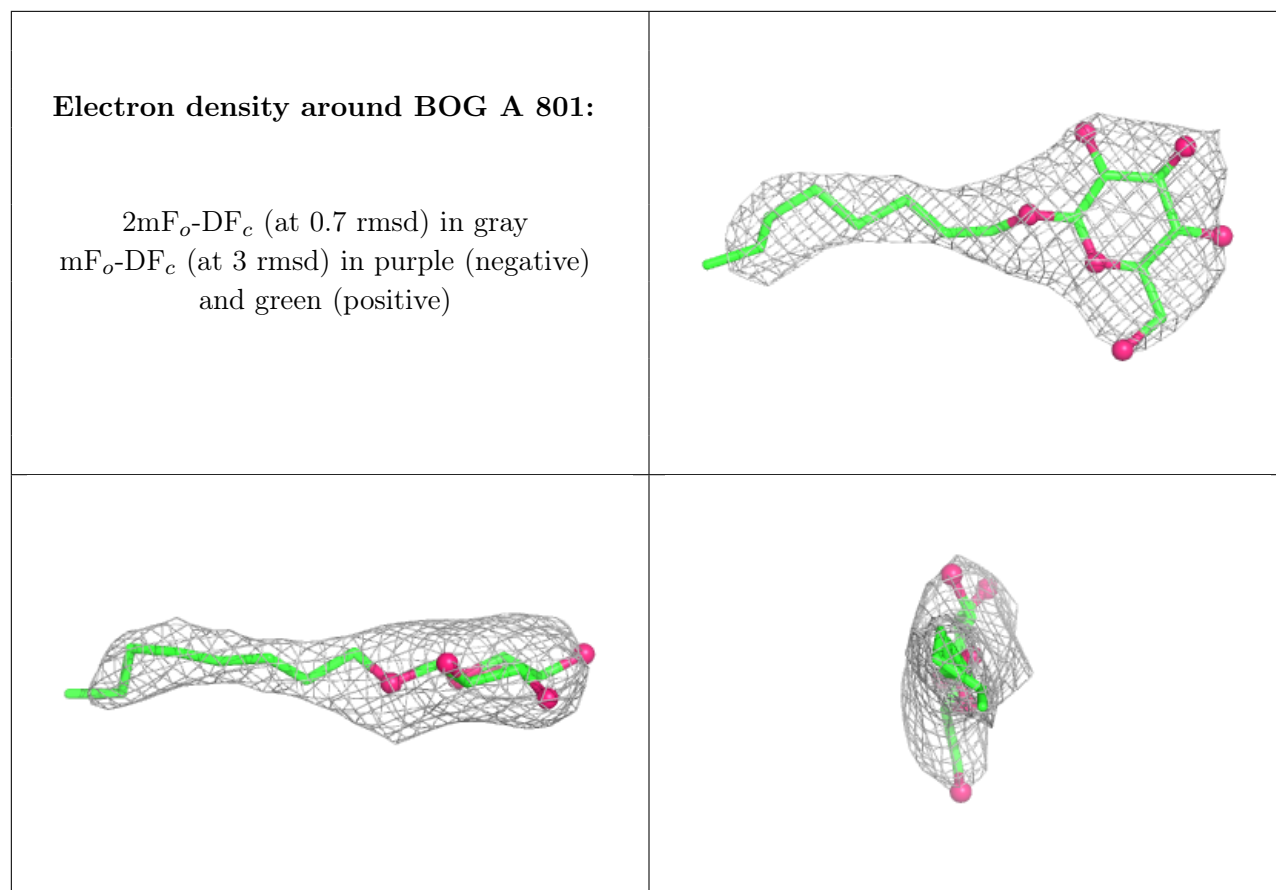
There are no oligosaccharides in this entry.

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	BOG	A	801	20/20	0.86	0.10	64,85,115,115	0
3	CA	A	802	1/1	0.99	0.09	57,57,57,57	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.