



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 12:16 PM EDT

PDB ID : 1U7G  
Title : Crystal Structure of Ammonia Channel AmtB from E. Coli  
Authors : Khademi, S.; O'Connell III, J.; Remis, J.; Robles-Colmenares, Y.; Miercke, L.J.W.; Stroud, R.M.  
Deposited on : 2004-08-03  
Resolution : 1.40 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

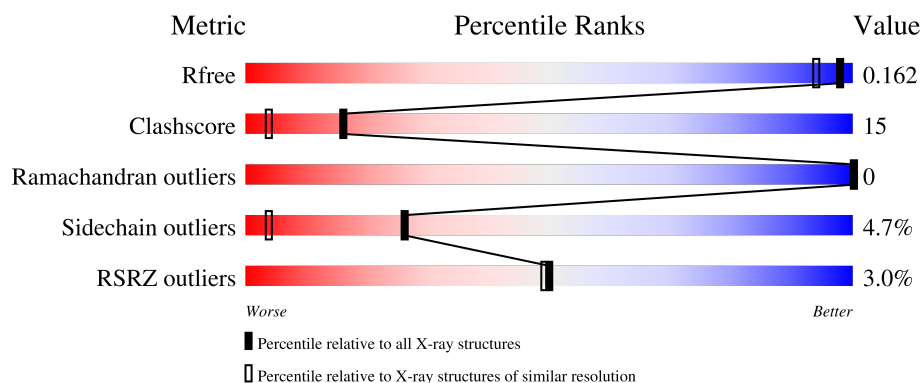
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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))
$R_{free}$	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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  $\geq 3$ , 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	385	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BOG	A	400	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3286 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.

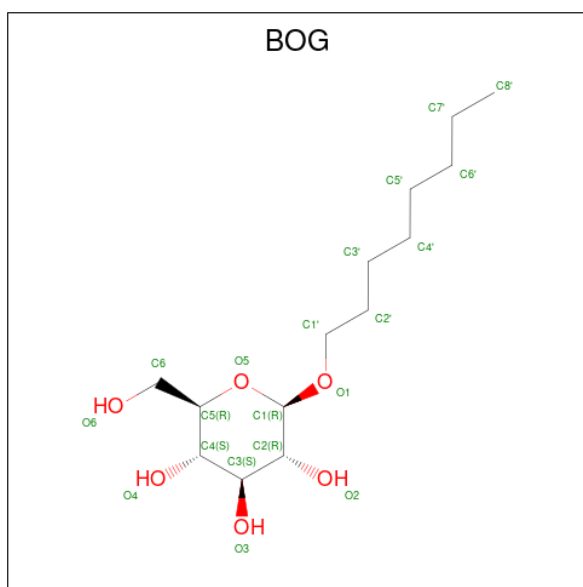
- Molecule 1 is a protein called Probable ammonium transporter.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	383	2836	1880	455	479	9	13	0	14	0

There are 14 discrepancies between the modelled and reference sequences:

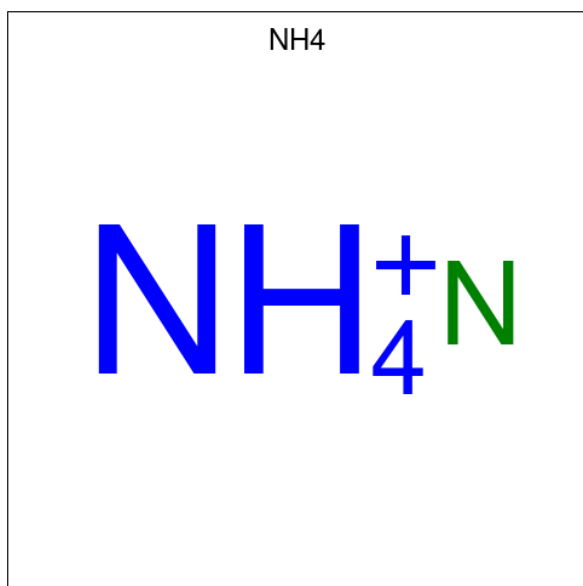
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MSE	MET	modified residue	UNP P69681
A	14	MSE	MET	modified residue	UNP P69681
A	23	MSE	MET	modified residue	UNP P69681
A	44	MSE	MET	modified residue	UNP P69681
A	68	SER	PHE	engineered mutation	UNP P69681
A	82	MSE	MET	modified residue	UNP P69681
A	92	MSE	MET	modified residue	UNP P69681
A	126	PRO	SER	engineered mutation	UNP P69681
A	146	MSE	MET	modified residue	UNP P69681
A	200	MSE	MET	modified residue	UNP P69681
A	255	LEU	LYS	engineered mutation	UNP P69681
A	301	MSE	MET	modified residue	UNP P69681
A	328	MSE	MET	modified residue	UNP P69681
A	348	MSE	MET	modified residue	UNP P69681

- Molecule 2 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



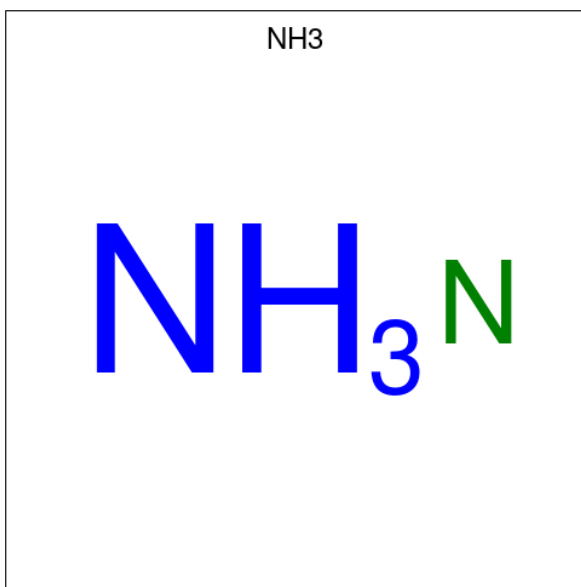
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			20	14 6		

- Molecule 3 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N).



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

- Molecule 4 is AMMONIA (three-letter code: NH3) (formula: H<sub>3</sub>N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N 1 1	0	0
4	A	1	Total N 1 1	0	0
4	A	1	Total N 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	426	Total O 426 426	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: Probable ammonium transporter



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.54Å 96.54Å 94.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.40 26.73 – 1.40	Depositor EDS
% Data completeness (in resolution range)	88.4 (30.00-1.40) 88.3 (26.73-1.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.40Å)	Xtriage
Refinement program	CNS, SHELX	Depositor
R, $R_{free}$	0.133 , 0.168 0.125 , 0.162	Depositor DCC
$R_{free}$ test set	9555 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.5	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 98.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	3286	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NH4, NH3, BOG

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	0.69	3/2949 (0.1%)	2.00	38/3999 (1.0%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88[A]	LEU	CB-CG	-6.40	1.33	1.52
1	A	88[B]	LEU	CB-CG	-6.40	1.33	1.52
1	A	341	GLY	CA-C	-5.51	1.43	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	NE-CZ-NH1	-68.10	86.25	120.30
1	A	307	ARG	NE-CZ-NH2	58.84	149.72	120.30
1	A	253	ARG	NE-CZ-NH1	-17.79	111.41	120.30
1	A	340	VAL	C-N-CA	-11.01	99.17	122.30
1	A	335[A]	SER	CB-CA-C	-8.95	93.09	110.10
1	A	335[B]	SER	CB-CA-C	-8.95	93.09	110.10
1	A	291	ALA	N-CA-CB	-8.77	97.82	110.10
1	A	291	ALA	CB-CA-C	7.94	122.01	110.10
1	A	253	ARG	NH1-CZ-NH2	7.54	127.70	119.40
1	A	62	TYR	CB-CG-CD1	7.37	125.42	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	GLY	CA-C-O	-7.34	107.38	120.60
1	A	253	ARG	CD-NE-CZ	-7.22	113.49	123.60
1	A	335[A]	SER	O-C-N	6.72	133.46	122.70
1	A	335[B]	SER	O-C-N	6.72	133.46	122.70
1	A	124	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	37	ARG	NE-CZ-NH2	6.67	123.63	120.30
1	A	307	ARG	CD-NE-CZ	-6.50	114.51	123.60
1	A	96	TYR	CG-CD1-CE1	-6.44	116.15	121.30
1	A	140	TYR	CB-CG-CD2	-6.39	117.17	121.00
1	A	140	TYR	CB-CG-CD1	5.76	124.45	121.00
1	A	307	ARG	CG-CD-NE	5.75	123.87	111.80
1	A	378	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	307	ARG	N-CA-CB	-5.64	100.44	110.60
1	A	125	PHE	CB-CG-CD1	5.61	124.73	120.80
1	A	315	PHE	CB-CG-CD1	-5.61	116.88	120.80
1	A	335[A]	SER	N-CA-CB	5.56	118.84	110.50
1	A	335[B]	SER	N-CA-CB	5.56	118.84	110.50
1	A	341	GLY	O-C-N	5.39	131.32	122.70
1	A	88[A]	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	88[B]	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	209	TYR	CG-CD1-CE1	-5.35	117.02	121.30
1	A	371	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	A	309	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	98	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	A	74	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	A	131	PHE	CB-CG-CD1	-5.19	117.17	120.80
1	A	62	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	A	374	TYR	CB-CG-CD2	-5.01	117.99	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	VAL	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	2836	0	2943	84	0
2	A	20	0	28	12	0
3	A	1	0	0	0	0
4	A	3	0	0	1	0
5	A	426	0	0	31	0
All	All	3286	0	2971	85	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 (85) 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:77:ASN:HD22	1:A:79:ASN:H	1.19	0.88
1:A:42:LEU:HA	5:A:741:HOH:O	1.75	0.86
1:A:72:ASN:HD22	1:A:74:PHE:H	1.19	0.86
1:A:329:THR:HG21	5:A:730:HOH:O	1.84	0.78
1:A:307:ARG:HG2	5:A:564:HOH:O	1.85	0.76
1:A:274:PRO:HB2	5:A:736:HOH:O	1.85	0.76
2:A:400:BOG:H1'2	5:A:527:HOH:O	1.88	0.73
1:A:72:ASN:ND2	1:A:74:PHE:H	1.86	0.72
1:A:291:ALA:HB1	5:A:746:HOH:O	1.88	0.72
1:A:77:ASN:ND2	1:A:79:ASN:H	1.90	0.69
1:A:307:ARG:HE	1:A:308[A]:VAL:HG13	1.59	0.68
1:A:45:LEU:HD12	5:A:741:HOH:O	1.94	0.67
1:A:45:LEU:HB2	5:A:741:HOH:O	1.94	0.66
1:A:199:PRO:O	1:A:203[B]:THR:HG23	1.96	0.65
1:A:200[B]:MSE:HE3	5:A:813:HOH:O	1.97	0.64
1:A:84:LYS:HD3	5:A:602:HOH:O	1.98	0.63
1:A:147:VAL:HG11	5:A:711:HOH:O	1.98	0.63
1:A:190:LYS:HD2	5:A:679:HOH:O	1.99	0.62
1:A:267:ALA:HB1	5:A:746:HOH:O	2.01	0.60
1:A:196:HIS:HB3	5:A:671:HOH:O	2.03	0.58
1:A:158:ALA:HB1	5:A:655:HOH:O	2.04	0.58
1:A:124:ARG:HD3	1:A:382:GLY:O	2.03	0.57
1:A:303:LYS:HB2	5:A:604:HOH:O	2.05	0.56
1:A:137:THR:HA	1:A:141:ILE:HD12	1.86	0.56
1:A:253:ARG:HH12	2:A:400:BOG:H4	1.70	0.56
1:A:253:ARG:NH1	2:A:400:BOG:H61	2.20	0.56
1:A:249:GLU:HG3	2:A:400:BOG:O6	2.06	0.54
1:A:183:GLY:HA2	5:A:923:HOH:O	2.07	0.53
1:A:67:ALA:O	1:A:145:HIS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:HG2	1:A:124:ARG:HH11	1.75	0.52
1:A:263:SER:OG	2:A:400:BOG:H7'2	2.09	0.52
1:A:296:LEU:HD11	2:A:400:BOG:H62	1.91	0.52
1:A:307:ARG:O	1:A:307:ARG:NE	2.42	0.51
1:A:84:LYS:HE3	5:A:747:HOH:O	2.10	0.51
1:A:350:HIS:HD2	5:A:789:HOH:O	1.93	0.51
1:A:253:ARG:CZ	2:A:400:BOG:H61	2.41	0.50
1:A:318:HIS:HE1	4:A:403:NH3:N	2.09	0.50
1:A:36:ILE:HG22	1:A:311:PRO:HG3	1.93	0.50
1:A:92:MSE:HE3	5:A:641:HOH:O	2.12	0.49
1:A:278:TYR:HD1	1:A:340:VAL:HG11	1.78	0.49
1:A:37:ARG:CD	1:A:37:ARG:H	2.26	0.49
1:A:125:PHE:O	1:A:128:VAL:HG12	2.13	0.49
1:A:72:ASN:ND2	1:A:75:PHE:H	2.11	0.49
1:A:324:VAL:O	1:A:328[A]:MSE:HG3	2.12	0.49
1:A:259[A]:LEU:CD2	2:A:400:BOG:H3'2	2.43	0.48
1:A:253:ARG:HD2	5:A:856:HOH:O	2.13	0.48
1:A:224:ASN:ND2	1:A:227:ALA:H	2.11	0.47
1:A:253:ARG:NH1	2:A:400:BOG:H4	2.28	0.47
1:A:159:LEU:HD23	5:A:848:HOH:O	2.14	0.47
1:A:32:TYR:CD2	1:A:117:GLY:HA3	2.49	0.47
1:A:326[B]:CYS:SG	1:A:359:ILE:HD11	2.55	0.46
1:A:340:VAL:HG21	5:A:642:HOH:O	2.14	0.46
1:A:340:VAL:O	1:A:340:VAL:HG22	2.15	0.46
1:A:301:MSE:HE1	1:A:304:ARG:CZ	2.46	0.46
1:A:313:ASP:HB3	2:A:400:BOG:H5'1	1.98	0.46
1:A:147:VAL:HG13	5:A:643:HOH:O	2.16	0.45
1:A:84:LYS:O	1:A:85:ASN:HB2	2.17	0.45
1:A:255:LEU:HD13	5:A:717:HOH:O	2.16	0.45
1:A:88[B]:LEU:HD21	5:A:592:HOH:O	2.17	0.45
1:A:194:LYS:HD3	5:A:671:HOH:O	2.17	0.45
1:A:92:MSE:SE	5:A:641:HOH:O	2.85	0.44
1:A:353:LEU:O	1:A:357:GLU:HG3	2.17	0.44
1:A:159:LEU:HB3	5:A:730:HOH:O	2.16	0.44
1:A:351:GLN:O	1:A:355:GLN:HG2	2.17	0.44
1:A:331:ILE:HG13	1:A:352:LEU:HD21	2.00	0.43
1:A:72:ASN:O	1:A:145:HIS:HE1	2.01	0.43
1:A:297:TRP:O	1:A:301:MSE:HG2	2.19	0.43
1:A:175:GLY:HA3	1:A:315:PHE:CE1	2.54	0.42
1:A:36:ILE:HD11	1:A:41:VAL:HA	2.02	0.42
1:A:37:ARG:NH1	1:A:121:GLU:OE1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLY:HA3	1:A:201:VAL:HG23	2.01	0.42
1:A:141:ILE:HB	1:A:142:PRO:HD3	2.02	0.42
1:A:253:ARG:HD2	1:A:253:ARG:HH11	1.19	0.42
1:A:313:ASP:CB	2:A:400:BOG:H5'1	2.49	0.42
1:A:175:GLY:HA3	1:A:315:PHE:CZ	2.56	0.41
1:A:70:GLU:O	1:A:70:GLU:HG3	2.20	0.41
1:A:259[A]:LEU:HD21	2:A:400:BOG:H3'2	2.03	0.41
1:A:307:ARG:HH11	1:A:307:ARG:HD2	0.51	0.41
1:A:84:LYS:HD2	5:A:715:HOH:O	2.20	0.41
1:A:255:LEU:N	1:A:255:LEU:HD12	2.36	0.41
1:A:60[B]:VAL:HG13	1:A:83:LEU:HG	2.03	0.41
1:A:326[B]:CYS:SG	1:A:359:ILE:HG13	2.61	0.41
1:A:307:ARG:NE	1:A:308[A]:VAL:HG13	2.30	0.40
1:A:344:GLU:HG2	5:A:844:HOH:O	2.21	0.40
1:A:191:GLU:HA	1:A:308[B]:VAL:HG23	2.04	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	395/385 (103%)	386 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	293/269 (109%)	280 (96%)	13 (4%)	28 4

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	70	GLU
1	A	72	ASN
1	A	77	ASN
1	A	84	LYS
1	A	156	HIS
1	A	185	ARG
1	A	212	TRP
1	A	224	ASN
1	A	255	LEU
1	A	306	LEU
1	A	307	ARG
1	A	384	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	72	ASN
1	A	77	ASN
1	A	79	ASN
1	A	145	HIS
1	A	197	ASN
1	A	224	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are modelled with single atom - 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	400	-	20,20,20	1.15	3 (15%)	25,25,25	1.84	6 (24%)

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	400	-	-	6/11/31/31	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	BOG	O5-C1	3.11	1.49	1.41
2	A	400	BOG	O1-C1	2.52	1.44	1.40
2	A	400	BOG	C3-C2	2.21	1.58	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	BOG	O1-C1-C2	3.97	114.51	108.30
2	A	400	BOG	C6'-C5'-C4'	-3.67	95.78	114.42
2	A	400	BOG	O5-C5-C6	3.55	115.26	106.44
2	A	400	BOG	O1-C1'-C2'	-3.37	97.74	109.56
2	A	400	BOG	O5-C5-C4	2.64	114.48	109.69

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	BOG	C4-C3-C2	-2.61	106.26	110.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

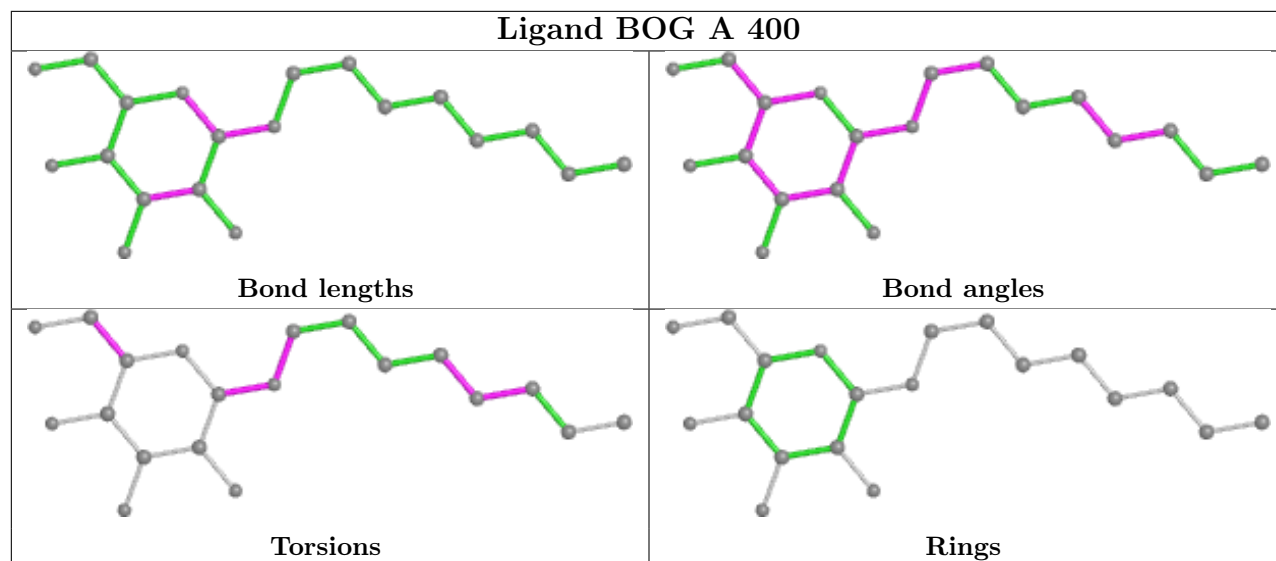
Mol	Chain	Res	Type	Atoms
2	A	400	BOG	O5-C5-C6-O6
2	A	400	BOG	C4-C5-C6-O6
2	A	400	BOG	C2'-C1'-O1-C1
2	A	400	BOG	C3'-C4'-C5'-C6'
2	A	400	BOG	C4'-C5'-C6'-C7'
2	A	400	BOG	O5-C1-O1-C1'

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	BOG	12	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	372/385 (96%)	-0.42	11 (2%) 50 49	10, 19, 42, 71	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	4.2
1	A	385	VAL	3.6
1	A	4	VAL	3.1
1	A	307	ARG	3.0
1	A	379	LEU	2.8
1	A	252	LEU	2.6
1	A	185	ARG	2.5
1	A	305	LEU	2.4
1	A	247	PHE	2.3
1	A	70	GLU	2.2
1	A	250	TRP	2.1

### 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 monosaccharides in this entry.

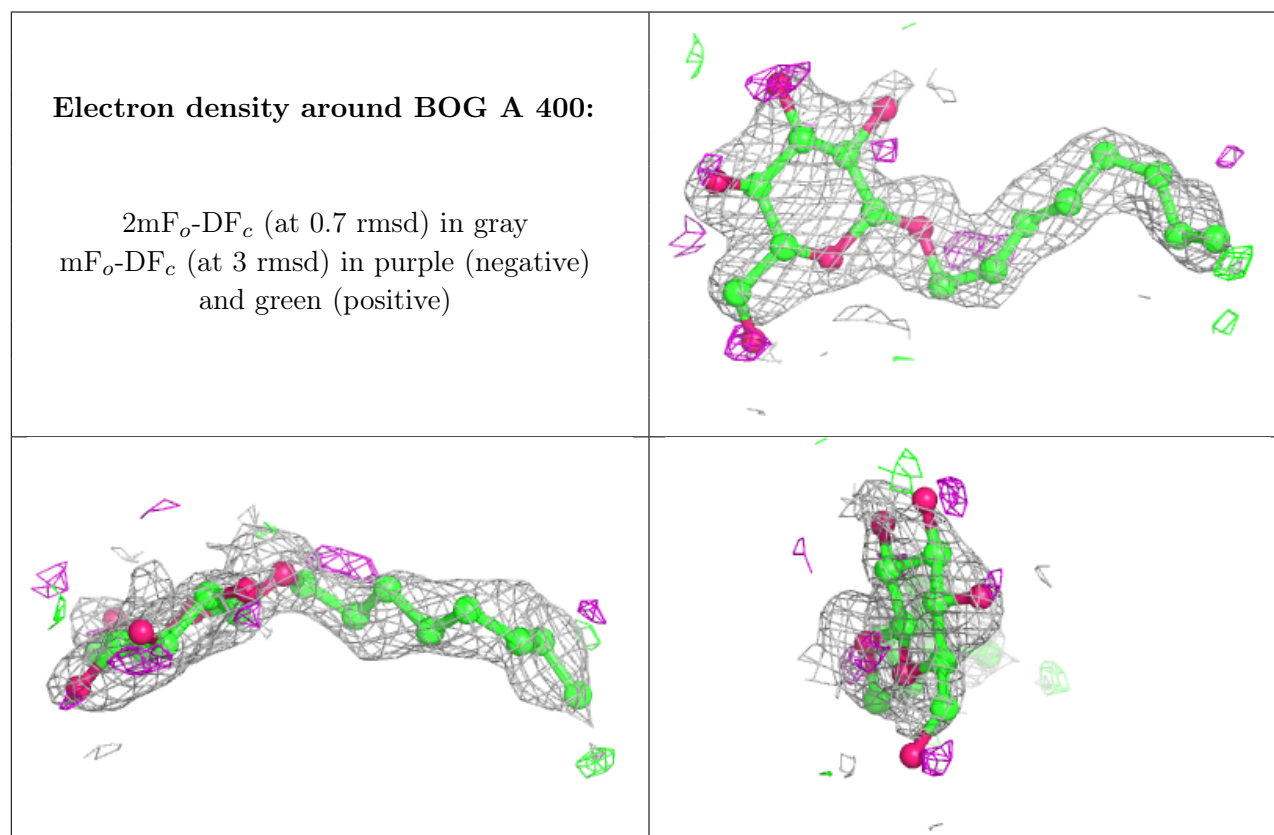
### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	BOG	A	400	20/20	0.72	0.23	45,54,68,69	0
4	NH3	A	403	1/1	0.81	0.31	53,53,53,53	0
4	NH3	A	402	1/1	0.93	0.52	45,45,45,45	1
4	NH3	A	401	1/1	0.95	0.24	36,36,36,36	1
3	NH4	A	404	1/1	0.97	0.36	30,30,30,30	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.