



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:18 PM UTC

PDB ID : 2VVN / pdb_00002vvn
Title : BtGH84 in complex with NH-Butylthiazoline
Authors : He, Y.; Davies, G.J.
Deposited on : 2008-06-10
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

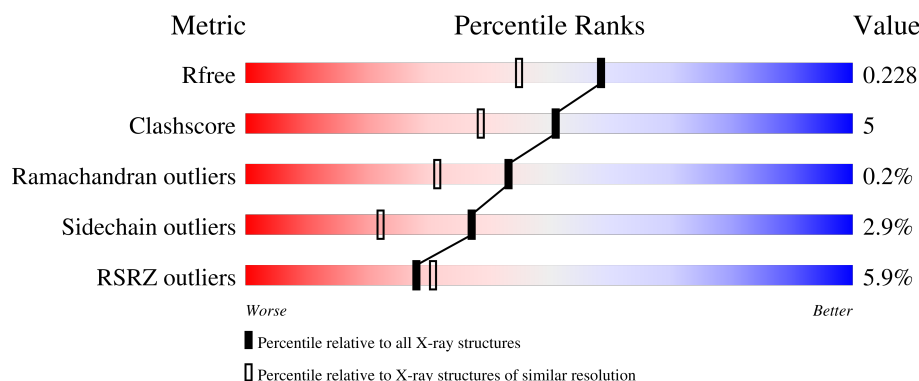
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	737	5% 76% 10% 12%
1	B	737	5% 78% 9% 12%

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
3	NH4	A	1717	-	-	X	-

2 Entry composition [i](#)

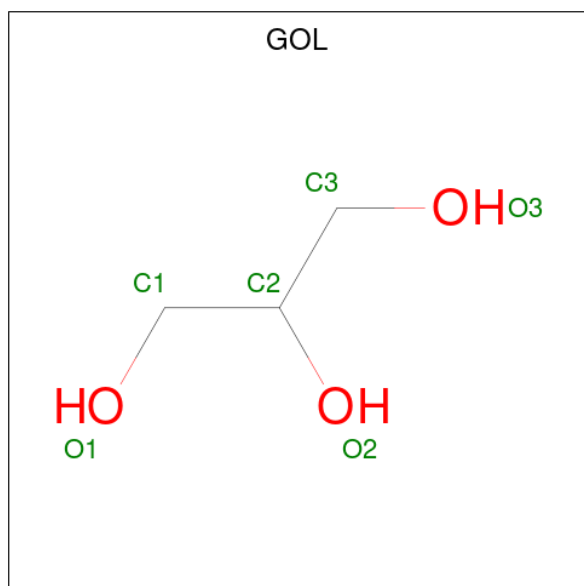
There are 5 unique types of molecules in this entry. The entry contains 11773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 O-GLCNACASE BT_4395.

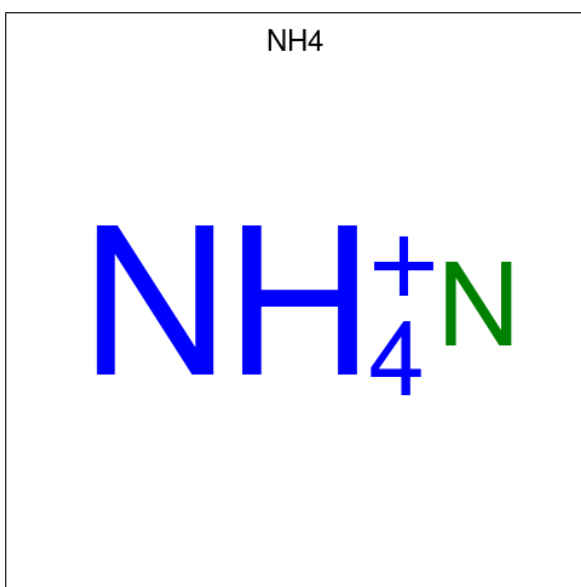
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	648	Total	C	N	O	S	0	9	0
			5307	3411	890	986	20			
1	B	648	Total	C	N	O	S	0	8	0
			5307	3408	895	984	20			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



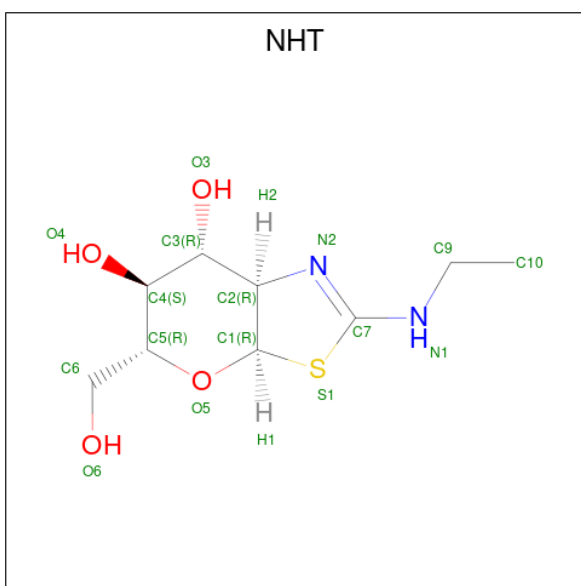
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is AMMONIUM ION (CCD ID: NH4) (formula: H_4N).



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

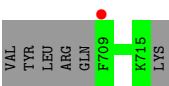
- Molecule 4 is (3AR,5R,6S,7R,7AR)-2-(ETHYLAMINO)-5-(HYDROXYMETHYL)-5,6,7,7A-TETRAHYDRO-3AH-PYRANO[3,2-D][1,3]THIAZOLE-6,7-DIOL (CCD ID: NHT) (formula: C₉H₁₆N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			16	9	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			16	9	2	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	549	Total 549	O 549	0	0
5	B	571	Total 571	O 571	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.51Å 94.50Å 99.23Å 104.53° 94.00° 102.89°	Depositor
Resolution (Å)	57.45 – 1.85 57.45 – 1.85	Depositor EDS
% Data completeness (in resolution range)	95.5 (57.45-1.85) 95.5 (57.45-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.4.0065	Depositor
R, R_{free}	0.180 , 0.224 0.186 , 0.228	Depositor DCC
R_{free} test set	7229 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11773	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NHT, GOL, NH4

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	0.84	4/5467 (0.1%)	0.94	6/7405 (0.1%)
1	B	0.82	1/5464 (0.0%)	0.92	5/7399 (0.1%)
All	All	0.83	5/10931 (0.0%)	0.93	11/14804 (0.1%)

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
1	B	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	458	LYS	CA-C	-9.64	1.41	1.52
1	B	133	VAL	CA-CB	6.13	1.61	1.54
1	A	611	ALA	C-O	-5.10	1.19	1.24
1	A	610	LYS	C-O	-5.09	1.18	1.24
1	A	164	GLY	C-O	5.00	1.30	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	LYS	N-CA-C	-10.72	92.56	109.72
1	A	518	GLY	N-CA-C	8.74	133.89	113.18
1	B	23	ALA	CA-C-N	-8.40	111.93	123.10
1	B	23	ALA	C-N-CA	-8.40	111.93	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	GLU	CB-CA-C	-6.57	100.14	111.45
1	A	457	GLY	O-C-N	-5.71	115.28	122.70
1	B	21	LEU	O-C-N	5.66	126.24	121.31
1	B	518	GLY	N-CA-C	5.38	125.92	113.18
1	A	131	GLY	N-CA-C	5.24	119.34	111.42
1	B	399	THR	CB-CA-C	-5.15	102.74	110.92
1	A	611	ALA	CB-CA-C	-5.03	110.76	116.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	457	GLY	Mainchain
1	B	4	SER	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	5307	0	5251	61	0
1	B	5307	0	5249	50	0
2	A	6	0	8	0	0
3	A	1	0	0	2	0
4	A	16	0	16	1	0
4	B	16	0	16	1	0
5	A	549	0	0	19	0
5	B	571	0	0	11	0
All	All	11773	0	10540	111	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 (111) 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:219[A]:ARG:CB	1:B:219[A]:ARG:HH11	1.63	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219[A]:ARG:HH11	1:B:219[A]:ARG:HB2	1.12	1.09
1:A:441[A]:MET:HG2	5:A:2415:HOH:O	1.52	1.08
1:A:21:LEU:HD23	1:A:48:LYS:NZ	1.73	1.02
1:B:219[A]:ARG:HH11	1:B:219[A]:ARG:CG	1.75	0.97
1:B:454:PHE:HZ	1:B:572:VAL:HG12	1.30	0.96
1:B:219[A]:ARG:HB2	1:B:219[A]:ARG:NH1	1.82	0.94
1:B:454:PHE:CZ	1:B:572:VAL:HG12	2.10	0.86
1:A:19:ILE:HD13	1:A:55:MET:HE1	1.62	0.79
1:A:21:LEU:HD23	1:A:48:LYS:HZ1	1.49	0.77
1:A:631:VAL:HG13	5:A:2254:HOH:O	1.82	0.77
1:A:581:ASN:HB3	5:A:2511:HOH:O	1.85	0.76
1:B:219[A]:ARG:NH1	1:B:219[A]:ARG:HG3	2.03	0.73
1:B:324:SER:O	1:B:328:GLU:HG2	1.89	0.73
1:A:593:HIS:HD2	1:A:636:ASP:H	1.37	0.73
1:B:219[A]:ARG:HH11	1:B:219[A]:ARG:HG3	1.55	0.72
1:B:88:LYS:HD3	1:B:89:GLU:HG2	1.72	0.71
1:B:219[A]:ARG:CG	1:B:219[A]:ARG:NH1	2.43	0.71
1:A:454:PHE:HZ	1:A:572:VAL:HG12	1.57	0.70
1:A:21:LEU:HD23	1:A:48:LYS:HZ2	1.56	0.69
1:A:72:ARG:HD2	5:A:2074:HOH:O	1.94	0.68
1:A:72:ARG:CD	5:A:2074:HOH:O	2.42	0.67
1:B:604:ASN:HA	5:B:2547:HOH:O	1.95	0.66
1:B:518:GLY:C	5:B:2487:HOH:O	2.42	0.63
1:B:536:GLN:NE2	5:B:2499:HOH:O	2.20	0.62
1:B:454:PHE:CZ	1:B:572:VAL:CG1	2.83	0.62
1:B:86:ASN:HA	1:B:118:GLU:HG3	1.84	0.60
1:A:456:GLU:OE1	1:A:458:LYS:HE3	2.01	0.60
1:A:61:GLU:OE1	3:A:1717:NH4:N	2.35	0.59
1:B:19:ILE:HG23	5:B:2125:HOH:O	2.03	0.58
1:A:456:GLU:OE1	1:A:458:LYS:CE	2.50	0.58
1:B:308:MET:HA	1:B:335:TYR:O	2.05	0.57
1:B:441[B]:MET:SD	5:B:2519:HOH:O	2.57	0.56
1:A:174:PRO:HD2	5:A:2178:HOH:O	2.05	0.56
1:A:715:LYS:HZ2	1:A:715:LYS:HB3	1.70	0.56
1:B:536:GLN:HG2	1:B:590:TYR:CD1	2.42	0.55
1:A:715:LYS:HB3	1:A:715:LYS:NZ	2.21	0.55
1:A:708:GLN:N	5:A:2543:HOH:O	2.40	0.54
1:A:679:ARG:N	5:A:2536:HOH:O	2.41	0.54
1:A:536:GLN:HG2	1:A:590:TYR:CD1	2.42	0.54
1:B:593:HIS:HD2	1:B:636:ASP:H	1.55	0.54
1:B:26:GLN:NE2	1:B:52:LYS:O	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ASP:OD2	4:B:1716:NHT:H2	2.08	0.53
1:B:21:LEU:HD12	1:B:22:PRO:HD2	1.90	0.53
1:A:452:LYS:HB3	1:A:452:LYS:NZ	2.25	0.52
1:B:355:VAL:O	1:B:399:THR:HG23	2.10	0.51
1:A:536:GLN:NE2	5:A:2479:HOH:O	2.36	0.51
1:A:32:GLU:O	3:A:1717:NH4:N	2.43	0.51
1:A:454:PHE:CZ	1:A:572:VAL:CG1	2.94	0.51
1:B:408:ARG:NE	5:B:2406:HOH:O	2.44	0.51
1:A:393:ASN:HD21	1:A:396:LYS:HD3	1.76	0.50
1:B:301:LEU:HD12	1:B:307:ILE:HD11	1.92	0.50
1:B:55:MET:HE2	1:B:90:ILE:HG13	1.93	0.50
1:A:72:ARG:HD3	5:A:2074:HOH:O	2.07	0.49
1:A:454:PHE:HZ	1:A:572:VAL:CG1	2.24	0.49
1:A:341:PRO:O	1:A:342:VAL:C	2.55	0.49
1:A:308:MET:HA	1:A:335:TYR:O	2.13	0.49
1:A:583:HIS:HB2	5:A:2513:HOH:O	2.14	0.48
1:A:442:ASP:HB2	5:A:2419:HOH:O	2.13	0.48
1:A:444:GLN:HB3	1:A:445:PRO:HD3	1.96	0.48
1:A:393:ASN:ND2	1:A:396:LYS:HD3	2.29	0.47
1:A:462:LYS:HD3	1:A:466:GLU:OE1	2.14	0.47
1:B:610:LYS:O	1:B:611:ALA:C	2.57	0.47
1:A:81:TYR:CZ	1:A:123:ASP:HB3	2.48	0.47
1:B:19:ILE:HG21	1:B:87:GLU:HA	1.96	0.47
1:A:32:GLU:HG2	5:A:2029:HOH:O	2.15	0.47
1:B:38:VAL:CG1	1:B:42:LYS:HE3	2.45	0.47
1:A:146:ARG:HD3	1:A:191:LEU:HD11	1.97	0.47
1:B:643:ASN:HA	1:B:684:LEU:HG	1.96	0.47
1:A:86:ASN:HA	1:A:118:GLU:HG2	1.96	0.47
1:A:456:GLU:O	1:A:457:GLY:C	2.57	0.46
1:A:178[A]:LEU:CD1	5:A:2174:HOH:O	2.64	0.46
1:B:341:PRO:O	1:B:342:VAL:C	2.59	0.46
1:B:238:ALA:HA	1:B:276:VAL:O	2.16	0.46
1:A:456:GLU:OE1	1:A:458:LYS:HE2	2.15	0.45
1:A:250:ASN:O	1:A:254:GLN:HG3	2.15	0.45
1:A:378:GLU:HG3	1:A:490:PRO:HB2	1.99	0.45
1:A:441[B]:MET:HG3	5:A:2415:HOH:O	2.15	0.45
1:A:243:ASP:OD2	4:A:1718:NHT:H2	2.16	0.45
1:A:562:LYS:HB3	1:A:563:PRO:HD3	1.99	0.45
1:B:269:LYS:HB2	1:B:272:ILE:HD12	1.97	0.45
1:A:32:GLU:HG3	5:A:2058:HOH:O	2.17	0.44
1:B:15:GLN:NE2	5:B:2018:HOH:O	2.39	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:GLN:HB3	1:A:708:GLN:HE22	1.82	0.44
1:A:183:LYS:HE3	5:A:2191:HOH:O	2.16	0.44
1:A:647:ASN:HB2	1:A:708:GLN:HG3	2.00	0.44
1:B:593:HIS:HE1	5:B:2544:HOH:O	2.00	0.44
1:B:647:ASN:HD22	1:B:647:ASN:C	2.25	0.44
1:A:283:ASN:HB3	1:A:310:THR:OG1	2.18	0.43
1:B:518:GLY:CA	5:B:2487:HOH:O	2.66	0.43
1:B:81:TYR:CE2	1:B:123:ASP:HB3	2.53	0.43
1:B:293:TYR:CD2	1:B:293:TYR:C	2.96	0.43
1:B:81:TYR:CZ	1:B:123:ASP:HB3	2.54	0.43
1:A:451:LEU:HD21	1:A:567:ARG:HD2	2.00	0.43
1:A:444:GLN:NE2	1:A:448:GLU:OE1	2.52	0.43
1:B:277:MET:HG2	1:B:301:LEU:HD11	2.01	0.42
1:B:408:ARG:HD2	5:B:2404:HOH:O	2.19	0.42
1:A:385:TYR:CD2	1:A:406:ALA:HB2	2.55	0.42
1:B:441[A]:MET:HE2	1:B:441[A]:MET:HB2	1.94	0.42
1:B:518:GLY:HA2	5:B:2487:HOH:O	2.20	0.42
1:A:593:HIS:HE1	5:A:2523:HOH:O	2.02	0.41
1:B:172:SER:OG	1:B:173:ALA:N	2.53	0.41
1:A:454:PHE:CZ	1:A:572:VAL:HG12	2.43	0.41
1:A:228[A]:LYS:HD2	1:A:228[A]:LYS:HA	1.84	0.41
1:A:504:LEU:HD12	1:A:541:ILE:HD12	2.03	0.41
1:A:188:LEU:HD13	1:A:229:MET:HE1	2.02	0.41
1:A:72:ARG:HB2	5:A:2069:HOH:O	2.20	0.41
1:A:214:TRP:CD2	1:A:253:LYS:HB3	2.56	0.41
1:B:562:LYS:HB3	1:B:563:PRO:HD3	2.03	0.41
1:B:644:ILE:O	1:B:681:SER:HA	2.22	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	647/737 (88%)	625 (97%)	20 (3%)	2 (0%)	36	25
1	B	646/737 (88%)	630 (98%)	16 (2%)	0	100	100
All	All	1293/1474 (88%)	1255 (97%)	36 (3%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	457	GLY
1	A	22	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	578/647 (89%)	557 (96%)	21 (4%)	31	16
1	B	577/647 (89%)	562 (97%)	15 (3%)	40	25
All	All	1155/1294 (89%)	1119 (97%)	36 (3%)	37	20

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	11	GLN
1	A	24	VAL
1	A	27	LEU
1	A	32	GLU
1	A	45	LEU
1	A	48	LYS
1	A	49	GLN
1	A	87	GLU
1	A	221	LEU
1	A	252[A]	GLN
1	A	252[B]	GLN
1	A	371	THR
1	A	408	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	416	GLU
1	A	441[A]	MET
1	A	441[B]	MET
1	A	452	LYS
1	A	642	GLU
1	A	647	ASN
1	A	715	LYS
1	B	27	LEU
1	B	45	LEU
1	B	88	LYS
1	B	213	LYS
1	B	219[A]	ARG
1	B	219[B]	ARG
1	B	221	LEU
1	B	371	THR
1	B	448	GLU
1	B	455	LYS
1	B	519	ARG
1	B	605	LEU
1	B	615	LEU
1	B	631	VAL
1	B	647	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	189	GLN
1	A	292	ASN
1	A	469	GLN
1	A	583	HIS
1	A	593	HIS
1	A	647	ASN
1	A	708	GLN
1	B	6	GLN
1	B	28	ASN
1	B	73	GLN
1	B	189	GLN
1	B	254	GLN
1	B	274	GLN
1	B	349	HIS
1	B	372	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	459	ASN
1	B	543	GLN
1	B	593	HIS
1	B	604	ASN
1	B	647	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is modelled with single atom - leaving 3 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	$\# Z > 2$
4	NHT	A	1718	-	15,17,17	0.85	0	15,24,24	1.74	3 (20%)
2	GOL	A	1716	-	5,5,5	0.33	0	5,5,5	0.46	0
4	NHT	B	1716	-	15,17,17	1.05	0	15,24,24	2.01	4 (26%)

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
4	NHT	A	1718	-	-	0/5/33/33	0/2/2/2
2	GOL	A	1716	-	-	2/4/4/4	-
4	NHT	B	1716	-	-	0/5/33/33	0/2/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1716	NHT	C3-C2-N2	-5.98	102.19	110.56
4	A	1718	NHT	C3-C2-N2	-4.89	103.71	110.56
4	B	1716	NHT	O5-C1-C2	2.97	121.82	115.27
4	A	1718	NHT	O5-C5-C4	-2.44	105.31	109.70
4	A	1718	NHT	O3-C3-C2	2.41	114.44	109.16
4	B	1716	NHT	O5-C5-C4	-2.19	105.76	109.70
4	B	1716	NHT	O3-C3-C2	2.06	113.67	109.16

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1716	GOL	C1-C2-C3-O3
2	A	1716	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1718	NHT	1	0
4	B	1716	NHT	1	0

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	648/737 (87%)	0.33	40 (6%)	26 29	11, 19, 44, 57	9 (1%)
1	B	648/737 (87%)	0.17	36 (5%)	30 33	10, 19, 44, 57	8 (1%)
All	All	1296/1474 (87%)	0.25	76 (5%)	28 31	10, 19, 44, 57	17 (1%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	631	VAL	7.3
1	A	631	VAL	6.2
1	A	518	GLY	4.7
1	A	694	PHE	4.4
1	B	689	VAL	4.1
1	A	680	LEU	3.8
1	B	127	VAL	3.8
1	A	457	GLY	3.7
1	A	540[A]	TYR	3.6
1	A	454	PHE	3.5
1	B	646	ILE	3.5
1	A	127	VAL	3.4
1	A	689	VAL	3.1
1	B	680	LEU	3.1
1	A	648	PHE	3.0
1	B	615	LEU	3.0
1	A	691	PHE	3.0
1	A	644	ILE	3.0
1	B	616	ILE	3.0
1	B	618	PRO	2.9
1	B	638	ILE	2.9
1	B	694	PHE	2.8
1	B	457	GLY	2.8
1	A	581	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	637	ALA	2.7
1	B	604	ASN	2.7
1	B	691	PHE	2.7
1	A	453	ALA	2.7
1	A	638	ILE	2.7
1	A	448	GLU	2.7
1	B	518	GLY	2.7
1	B	644	ILE	2.6
1	B	679	ARG	2.6
1	B	682	ALA	2.6
1	B	4	SER	2.6
1	A	682	ALA	2.6
1	B	286	TRP	2.6
1	A	49	GLN	2.6
1	B	693	ARG	2.5
1	A	490	PRO	2.5
1	A	126	SER	2.5
1	A	687	ALA	2.5
1	A	47	GLY	2.5
1	B	648	PHE	2.5
1	B	709	PHE	2.5
1	A	611	ALA	2.5
1	A	639	TYR	2.4
1	B	684	LEU	2.4
1	A	646	ILE	2.4
1	A	605	LEU	2.4
1	A	684	LEU	2.4
1	B	639	TYR	2.4
1	B	690	LYS	2.4
1	B	605	LEU	2.4
1	A	54	GLY	2.3
1	A	681	SER	2.3
1	A	53	LYS	2.3
1	B	640	PRO	2.3
1	A	493	VAL	2.3
1	A	499	VAL	2.3
1	A	692	VAL	2.3
1	B	453	ALA	2.2
1	B	454	PHE	2.2
1	B	637	ALA	2.2
1	B	46	SER	2.2
1	A	23	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	692	VAL	2.2
1	B	687	ALA	2.2
1	A	519	ARG	2.2
1	A	640	PRO	2.1
1	A	16	ASN	2.1
1	A	486	THR	2.1
1	B	581	ASN	2.1
1	A	124	TYR	2.0
1	B	685	GLN	2.0
1	B	470	TYR	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
3	NH4	A	1717	1/1	0.92	0.24	30,30,30,30	0
2	GOL	A	1716	6/6	0.94	0.15	29,34,36,37	0
4	NHT	B	1716	16/16	0.97	0.06	4,11,12,12	0
4	NHT	A	1718	16/16	0.98	0.06	6,9,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.