WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 5, 2023 – 03:23 am GMT

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

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

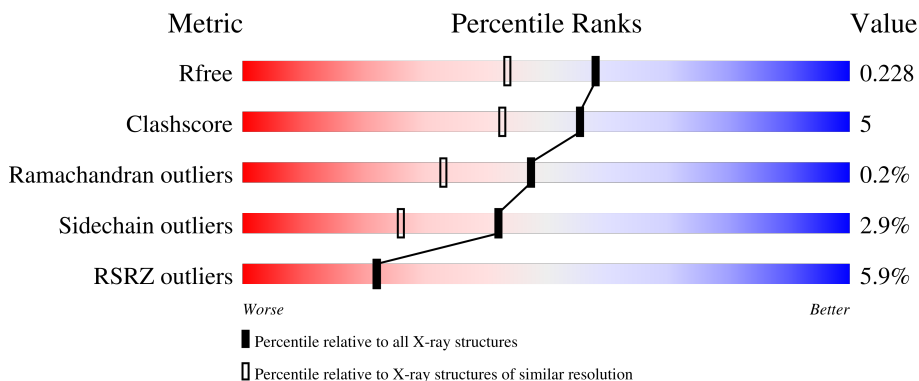|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.228
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		2.9%
RSRZ outliers		5.9%

Worse *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (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 <=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% / 77% / 9% · 12%
1	B	737	5% / 79% / 8% · 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:

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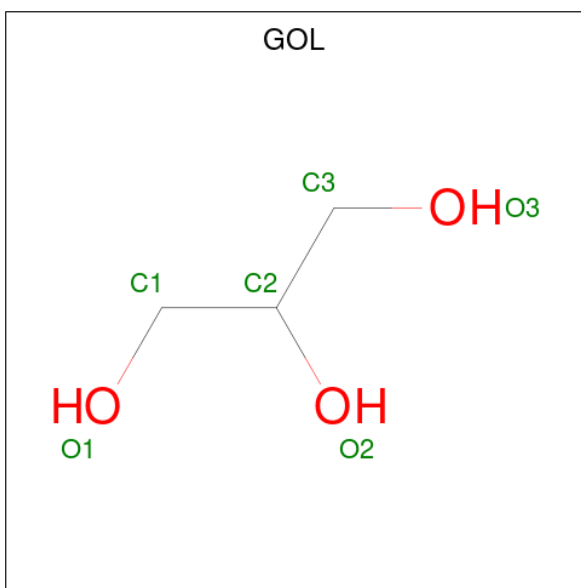| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NH4	A	1717	-	-	X	-

2 Entry composition ⓘ

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 5307	C 3411	N 890	O 986	S 20	0	9	0
1	B	648	Total 5307	C 3408	N 895	O 984	S 20	0	8	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

- Molecule 3 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).

NH4
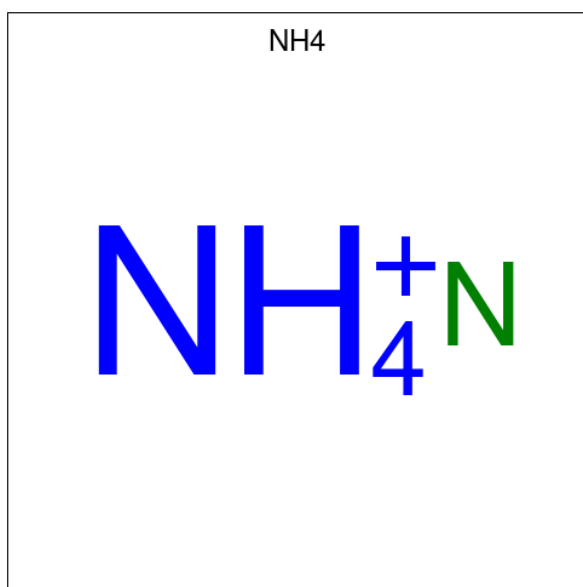
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	N 1	0	0

- 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 (three-letter code: NHT) (formula: $C_9H_{16}N_2O_4S$).

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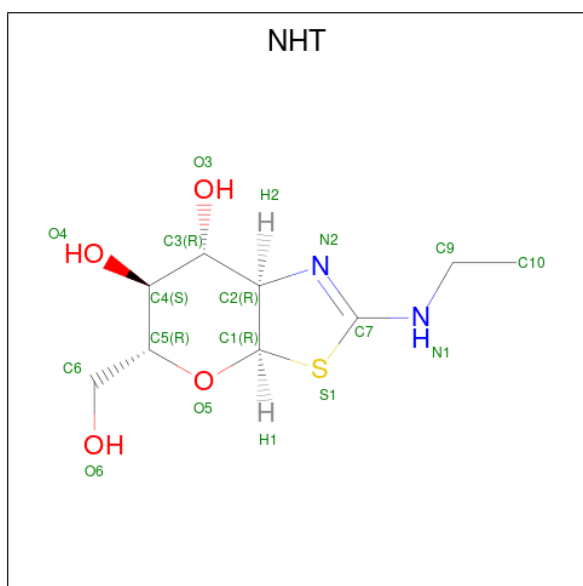
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 16	C 9	N 2	O 4	S 1	0	0
4	B	1	Total 16	C 9	N 2	O 4	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	549	Total O 549 549	0	0
5	B	571	Total O 571 571	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: O-GLCNACASE BT_4395
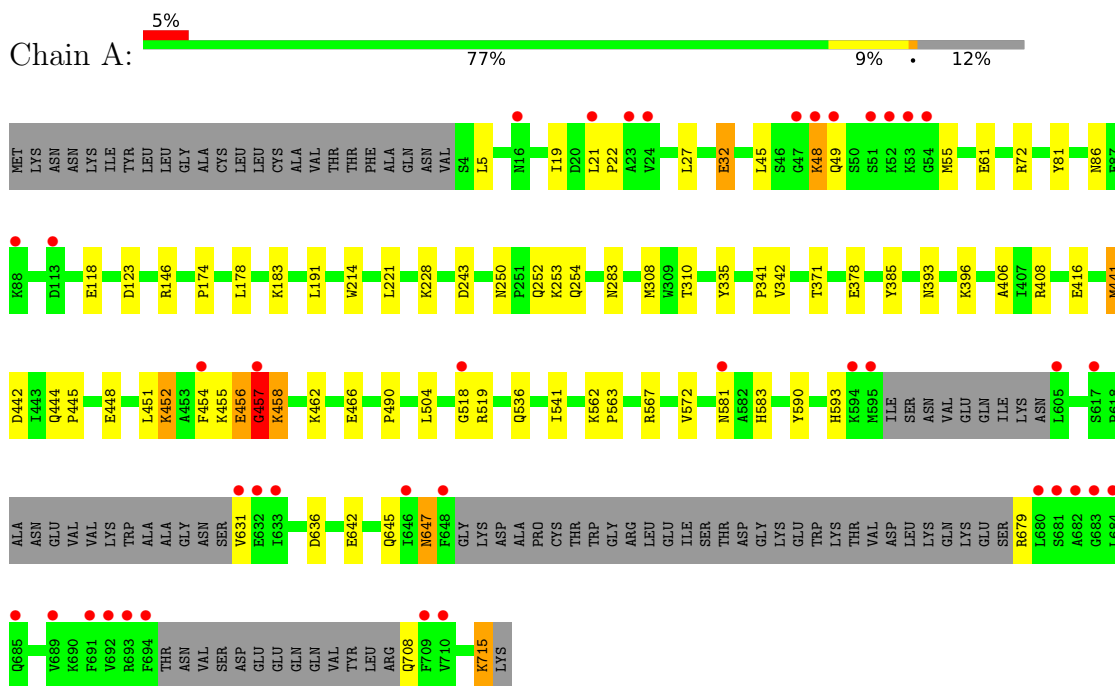
- Molecule 1: O-GLCNACASE BT_4395
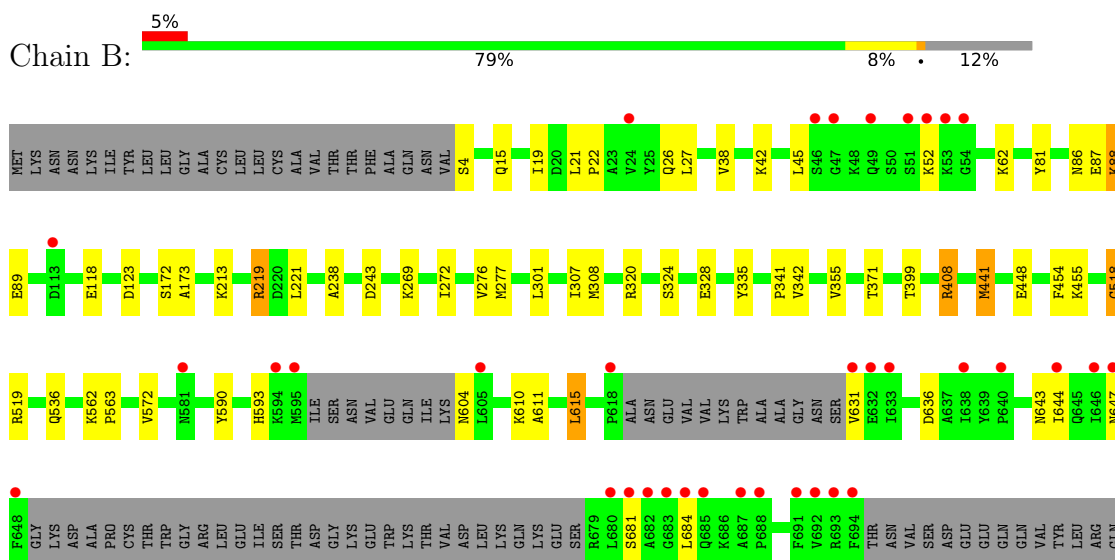
4 Data and refinement statistics (i)

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 57.47 – 1.85	Depositor EDS
% Data completeness (in resolution range)	95.5 (57.45-1.85) 95.5 (57.47-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (Å²)	22.1	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.36 , 51.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11773	wwPDB-VP
Average B, all atoms (Å²)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.70	0/5467	0.70	3/7405 (0.0%)
1	B	0.68	0/5464	0.68	2/7399 (0.0%)
All	All	0.69	0/10931	0.69	5/14804 (0.0%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	GLY	N-CA-C	8.31	133.89	113.10
1	B	615	LEU	CA-CB-CG	7.90	133.47	115.30
1	A	458	LYS	N-CA-C	-6.83	92.56	111.00
1	A	456	GLU	CB-CA-C	-5.13	100.14	110.40
1	B	518	GLY	N-CA-C	5.13	125.92	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	457	GLY	Mainchain

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Mol	Chain	Res	Type	Group
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	47	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	108	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 (108) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:518:GLY:C	5:B:2487:HOH:O	2.42	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:B:536:GLN:HG2	1:B:590:TYR:CD1	2.42	0.55
1:A:715:LYS:NZ	1:A:715:LYS:HB3	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:178[A]:LEU:CD1	5:A:2174:HOH:O	2.64	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:A:341:PRO:O	1:A:342:VAL:C	2.55	0.44
1:B:15:GLN:NE2	5:B:2018:HOH:O	2.39	0.44
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:320:ARG:O	1:B:324:SER:OG	2.31	0.44
1:B:593:HIS:HE1	5:B:2544:HOH:O	2.00	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: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:B:610:LYS:O	1:B:611:ALA:C	2.57	0.43
1:A:444:GLN:NE2	1:A:448:GLU:OE1	2.52	0.43
1:A:452:LYS:HB3	1:A:452:LYS:HZ2	1.83	0.42
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:456:GLU:O	1:A:457:GLY:C	2.57	0.42
1:A:385:TYR:CD2	1:A:406:ALA:HB2	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:SER:OG	1:B:173:ALA:N	2.53	0.41
1:A:715:LYS:HB3	1:A:715:LYS:HZ2	1.83	0.41
1:B:341:PRO:O	1:B:342:VAL:C	2.59	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:19:ILE:HD13	1:A:55: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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	41	26
1	B	646/737 (88%)	630 (98%)	16 (2%)	0	100	100
All	All	1293/1474 (88%)	1255 (97%)	36 (3%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	457	GLY
1	A	22	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	578/647 (89%)	558 (96%)	20 (4%)	36	18
1	B	577/647 (89%)	560 (97%)	17 (3%)	42	26
All	All	1155/1294 (89%)	1118 (97%)	37 (3%)	42	22

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	27	LEU
1	A	32	GLU
1	A	45	LEU
1	A	48	LYS
1	A	49	GLN
1	A	221	LEU
1	A	252[A]	GLN
1	A	252[B]	GLN
1	A	371	THR
1	A	408	ARG
1	A	416	GLU
1	A	441[A]	MET
1	A	441[B]	MET
1	A	452	LYS
1	A	455	LYS
1	A	519	ARG
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

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Mol	Chain	Res	Type
1	B	371	THR
1	B	408	ARG
1	B	441[A]	MET
1	B	441[B]	MET
1	B	448	GLU
1	B	455	LYS
1	B	519	ARG
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 (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	273	ASN
1	A	425	ASN
1	A	593	HIS
1	A	647	ASN
1	A	708	GLN
1	B	6	GLN
1	B	189	GLN
1	B	254	GLN
1	B	274	GLN
1	B	306	GLN
1	B	349	HIS
1	B	459	ASN
1	B	543	GLN
1	B	593	HIS
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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	1716	-	15,17,17	1.01	0	14,24,24	1.32	2 (14%)
4	NHT	A	1718	-	15,17,17	0.83	0	14,24,24	1.23	2 (14%)
2	GOL	A	1716	-	5,5,5	0.33	0	5,5,5	0.44	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
4	NHT	B	1716	-	-	0/5/33/33	0/2/2/2
4	NHT	A	1718	-	-	0/5/33/33	0/2/2/2
2	GOL	A	1716	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1716	NHT	O5-C1-C2	2.97	121.82	115.27
4	A	1718	NHT	O5-C5-C4	-2.41	105.31	109.69
4	A	1718	NHT	O3-C3-C2	2.32	114.44	109.14
4	B	1716	NHT	O5-C5-C4	-2.17	105.76	109.69

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	B	1716	NHT	1	0
4	A	1718	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%)	0.07	39 (6%)	21	21	13, 19, 44, 57	0
1	B	648/737 (87%)	0.02	37 (5%)	23	23	11, 19, 44, 57	0
All	All	1296/1474 (87%)	0.04	76 (5%)	22	22	11, 19, 44, 57	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	631	VAL	8.8
1	A	680	LEU	8.6
1	A	694	PHE	6.8
1	B	646	ILE	6.4
1	B	631	VAL	5.1
1	B	693	ARG	4.8
1	A	53	LYS	4.7
1	A	682	ALA	4.6
1	B	680	LEU	4.5
1	A	633	ILE	4.5
1	B	647	ASN	4.4
1	A	47	GLY	4.4
1	A	691	PHE	4.3
1	A	49	GLN	4.2
1	B	694	PHE	4.2
1	A	457	GLY	4.1
1	A	595	MET	4.1
1	A	693	ARG	4.1
1	B	633	ILE	4.1
1	B	49	GLN	3.9
1	A	692	VAL	3.9
1	A	21	LEU	3.8
1	B	648	PHE	3.8
1	A	681	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	687	ALA	3.7
1	A	709	PHE	3.6
1	A	594	LYS	3.6
1	B	47	GLY	3.5
1	B	605	LEU	3.5
1	A	52	LYS	3.5
1	B	684	LEU	3.5
1	A	689	VAL	3.4
1	B	24	VAL	3.3
1	A	454	PHE	3.3
1	A	648	PHE	3.2
1	A	16	ASN	3.1
1	A	54	GLY	3.1
1	B	46	SER	3.1
1	B	52	LYS	3.0
1	B	688	PRO	3.0
1	B	685	GLN	2.9
1	B	53	LYS	2.9
1	A	632	GLU	2.9
1	A	24	VAL	2.9
1	B	682	ALA	2.9
1	A	518	GLY	2.8
1	B	691	PHE	2.8
1	B	51	SER	2.8
1	A	605	LEU	2.6
1	A	88	LYS	2.6
1	B	594	LYS	2.6
1	A	683	GLY	2.6
1	A	685	GLN	2.5
1	A	113	ASP	2.5
1	B	709	PHE	2.5
1	B	54	GLY	2.5
1	B	692	VAL	2.5
1	B	640	PRO	2.4
1	A	23	ALA	2.4
1	A	51	SER	2.4
1	B	644	ILE	2.4
1	B	710	VAL	2.3
1	A	48	LYS	2.3
1	B	618	PRO	2.3
1	B	683	GLY	2.2
1	A	646	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	113	ASP	2.2
1	B	632	GLU	2.2
1	A	581	ASN	2.2
1	A	684	LEU	2.1
1	B	681	SER	2.1
1	A	710	VAL	2.1
1	B	638	ILE	2.1
1	B	595	MET	2.1
1	A	617	SER	2.1
1	B	581	ASN	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	GOL	A	1716	6/6	0.95	0.17	29,34,36,37	0
3	NH4	A	1717	1/1	0.96	0.34	30,30,30,30	0
4	NHT	A	1718	16/16	0.99	0.05	6,9,13,13	0
4	NHT	B	1716	16/16	0.99	0.06	4,11,12,12	0

6.5 Other polymers ⓘ

There are no such residues in this entry.