



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:33 PM UTC

PDB ID : 4AIS / pdb_00004ais
Title : A complex structure of BtGH84
Authors : He, Y.; Davies, G.J.
Deposited on : 2012-02-13
Resolution : 2.00 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

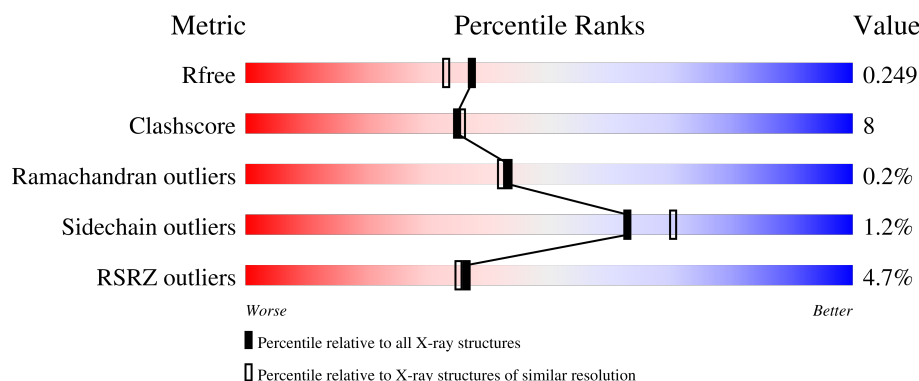
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	
1	B	737	

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	GOA	B	1716	-	X	-	-

2 Entry composition [i](#)

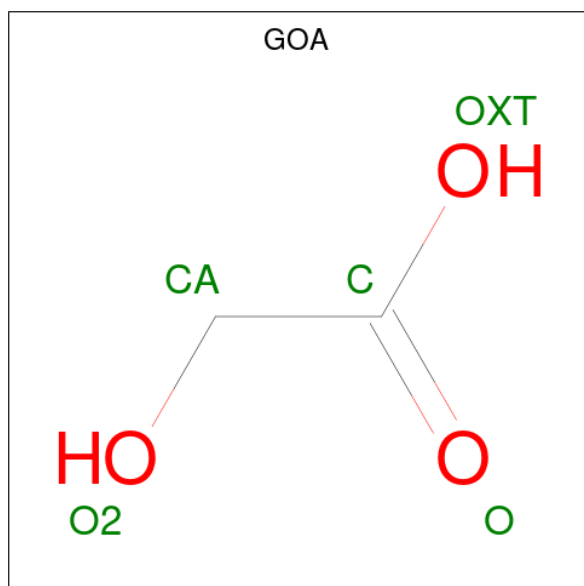
There are 4 unique types of molecules in this entry. The entry contains 11289 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	637	Total	C	N	O	S	0	3	0
			5182	3322	873	968	19			
1	B	641	Total	C	N	O	S	0	4	0
			5220	3347	880	973	20			

- Molecule 2 is GLYCOLIC ACID (CCD ID: GOA) (formula: $C_2H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			5	2	3		
2	B	1	Total	C	O	0	0
			5	2	3		

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



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

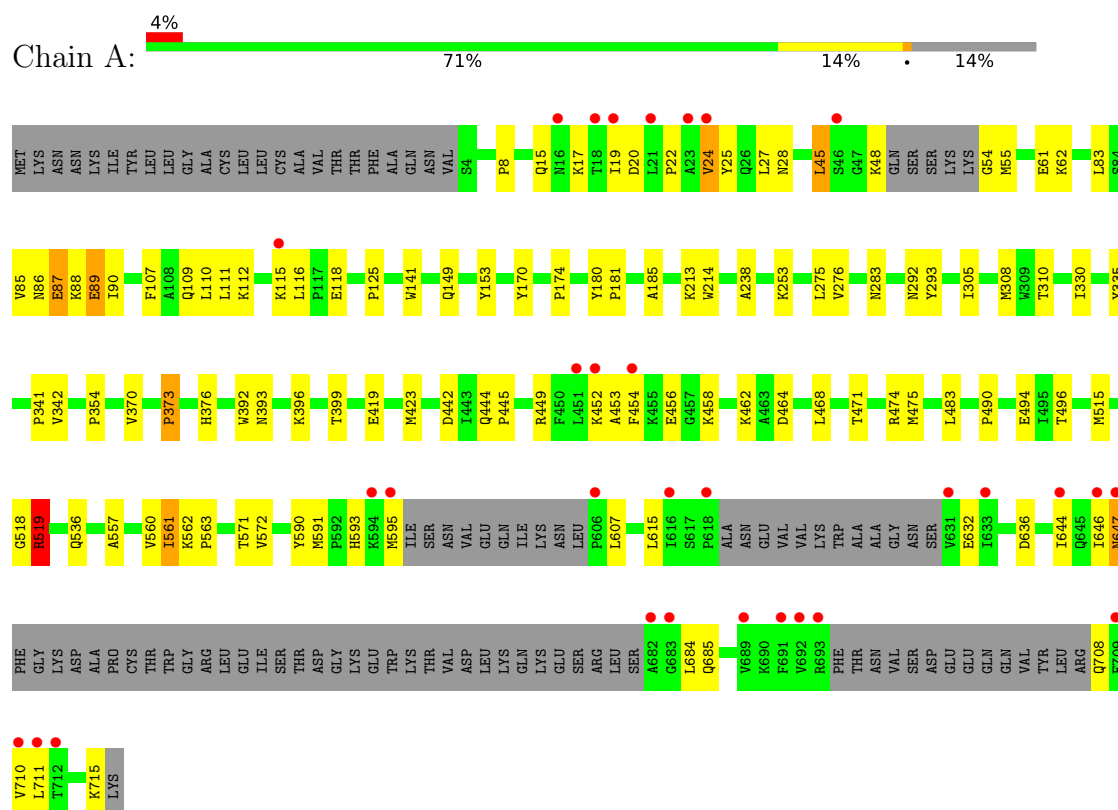
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	407	Total	O	0	0
			407	407		
4	B	452	Total	O	0	0
			452	452		

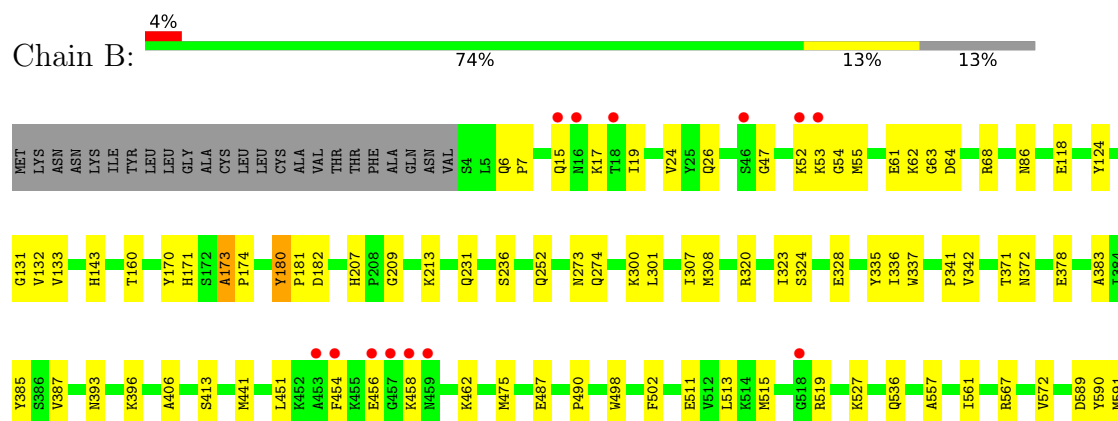
3 Residue-property plots [i](#)

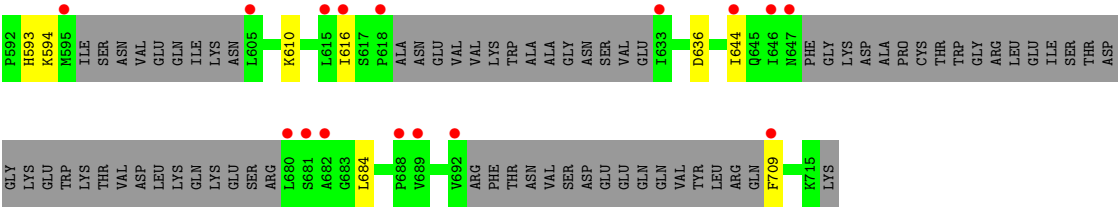
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: O-GLCNACASE BT_4395



• Molecule 1: O-GLCNACASE BT_4395





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.33Å 93.77Å 99.16Å 104.27° 94.01° 102.97°	Depositor
Resolution (Å)	33.77 – 2.00 33.77 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (33.77-2.00) 96.8 (33.77-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0086	Depositor
R, R_{free}	0.193 , 0.244 0.199 , 0.249	Depositor DCC
R_{free} test set	5687 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11289	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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: GOA, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.07	7/5320 (0.1%)	1.03	3/7207 (0.0%)
1	B	1.06	4/5359 (0.1%)	1.07	14/7259 (0.2%)
All	All	1.07	11/10679 (0.1%)	1.05	17/14466 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	ILE	C-O	-6.97	1.17	1.24
1	A	185	ALA	CA-CB	6.20	1.63	1.53
1	A	8	PRO	CA-C	5.52	1.57	1.52
1	B	143	HIS	N-CA	-5.32	1.40	1.46
1	A	560	VAL	CA-C	5.31	1.58	1.52
1	A	330	ILE	CA-CB	5.29	1.61	1.54
1	B	498	TRP	CA-C	-5.27	1.46	1.52
1	A	370	VAL	C-O	5.09	1.29	1.24
1	A	116	LEU	C-O	-5.09	1.17	1.24
1	A	24	VAL	CA-CB	5.05	1.60	1.53
1	B	173	ALA	CA-C	-5.03	1.47	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	GLU	N-CA-C	7.20	120.12	109.24
1	B	209	GLY	N-CA-C	6.88	122.25	113.24
1	A	561	ILE	N-CA-C	6.78	116.93	110.42
1	A	632	GLU	N-CA-C	6.25	119.43	108.75
1	B	180	TYR	CA-C-N	-6.09	114.36	120.21
1	B	180	TYR	C-N-CA	-6.09	114.36	120.21
1	B	62	LYS	CA-C-N	-5.86	113.91	122.46
1	B	62	LYS	C-N-CA	-5.86	113.91	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	594	LYS	N-CA-C	5.71	117.29	109.18
1	B	336	ILE	N-CA-C	5.59	116.22	108.84
1	B	132	VAL	CA-C-N	-5.33	116.19	123.12
1	B	132	VAL	C-N-CA	-5.33	116.19	123.12
1	B	393	ASN	CA-C-N	-5.26	113.61	119.19
1	B	393	ASN	C-N-CA	-5.26	113.61	119.19
1	B	182	ASP	N-CA-C	5.15	117.29	111.11
1	B	124	TYR	N-CA-C	-5.14	103.51	108.13
1	B	47	GLY	N-CA-C	-5.03	107.90	113.79

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	5182	0	5102	91	0
1	B	5220	0	5153	65	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	6	0	8	0	0
3	B	12	0	16	1	0
4	A	407	0	0	6	0
4	B	452	0	0	13	0
All	All	11289	0	10279	156	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 8.

All (156) 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:449:ARG:O	1:A:452:LYS:HG2	1.63	0.96
1:A:27:LEU:HD12	1:A:28:ASN:H	1.29	0.94
1:A:456:GLU:OE2	1:A:458:LYS:HD2	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:HIS:HD2	1:A:636:ASP:H	1.16	0.89
1:B:53:LYS:HG3	1:B:54:GLY:H	1.39	0.86
1:A:452:LYS:HG3	1:A:453:ALA:H	1.41	0.82
1:A:452:LYS:HG3	1:A:453:ALA:N	1.91	0.81
1:A:27:LEU:HD12	1:A:28:ASN:N	2.00	0.77
1:A:442:ASP:HB2	4:A:2318:HOH:O	1.84	0.77
1:A:456:GLU:HG3	1:A:458:LYS:HG3	1.69	0.75
1:A:593:HIS:CD2	1:A:636:ASP:H	2.04	0.75
1:A:646:ILE:HG22	1:A:647:ASN:H	1.52	0.75
1:A:647:ASN:C	1:A:647:ASN:OD1	2.30	0.74
1:B:593:HIS:HD2	1:B:636:ASP:H	1.36	0.73
1:B:53:LYS:CG	1:B:54:GLY:H	2.02	0.72
1:B:173:ALA:HB3	4:B:2153:HOH:O	1.89	0.72
1:A:536:GLN:HG3	1:A:590:TYR:CD1	2.25	0.71
1:A:19:ILE:CD1	1:A:118:GLU:HG2	2.21	0.71
1:B:17:LYS:HD2	1:B:118:GLU:OE1	1.91	0.71
1:A:452:LYS:CG	1:A:453:ALA:H	2.04	0.70
1:A:519:ARG:H	1:A:519:ARG:HD3	1.57	0.70
1:A:462:LYS:HE2	4:A:2323:HOH:O	1.92	0.70
1:A:444:GLN:HG3	4:A:2315:HOH:O	1.93	0.69
1:A:685:GLN:HG2	4:A:2405:HOH:O	1.91	0.68
1:B:593:HIS:CD2	1:B:636:ASP:H	2.13	0.66
1:A:19:ILE:HD12	1:A:118:GLU:HG2	1.79	0.64
1:A:449:ARG:CB	1:A:452:LYS:HE3	2.28	0.64
1:A:292:ASN:ND2	4:A:2213:HOH:O	2.31	0.63
1:A:444:GLN:HB3	1:A:445:PRO:HD3	1.81	0.63
1:B:53:LYS:HG3	1:B:54:GLY:N	2.11	0.62
1:A:24:VAL:HG22	1:A:54:GLY:HA2	1.83	0.60
1:A:615:LEU:HB3	1:A:710:VAL:HG22	1.83	0.60
1:B:593:HIS:HD2	1:B:636:ASP:N	2.00	0.59
1:B:441[A]:MET:HE3	4:B:2347:HOH:O	2.03	0.59
1:B:337:TRP:CD1	1:B:337:TRP:C	2.79	0.59
1:B:456:GLU:C	1:B:458:LYS:H	2.11	0.58
1:A:557:ALA:HB1	1:A:561:ILE:HB	1.86	0.58
1:A:449:ARG:HG2	1:A:452:LYS:HE3	1.88	0.56
1:B:173:ALA:HA	4:B:2154:HOH:O	2.05	0.56
1:A:19:ILE:HD11	1:A:118:GLU:HG2	1.88	0.55
1:A:646:ILE:HG22	1:A:647:ASN:N	2.21	0.55
1:B:324:SER:O	1:B:328:GLU:HG2	2.07	0.54
1:B:173:ALA:CA	4:B:2154:HOH:O	2.55	0.54
1:A:419:GLU:O	1:A:423[A]:MET:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:TYR:CD1	1:B:406:ALA:HB2	2.42	0.54
1:B:454:PHE:HZ	1:B:572:VAL:HG12	1.72	0.54
1:A:109:GLN:O	1:A:112:LYS:HE3	2.07	0.54
1:B:301:LEU:HD12	1:B:307:ILE:HD11	1.90	0.54
1:B:213:LYS:CE	4:B:2196:HOH:O	2.57	0.53
1:B:320:ARG:O	1:B:323:ILE:HG22	2.09	0.52
1:B:337:TRP:C	1:B:337:TRP:HD1	2.18	0.52
1:B:236:SER:HB3	1:B:274:GLN:HB2	1.91	0.51
1:A:562:LYS:HB3	1:A:563:PRO:HD3	1.92	0.51
1:B:63:GLY:HA2	1:B:68:ARG:HD3	1.93	0.51
1:B:19:ILE:HD13	1:B:55:MET:HE1	1.92	0.51
1:B:644:ILE:HD11	1:B:684:LEU:HD21	1.91	0.51
1:A:449:ARG:CG	1:A:452:LYS:HE3	2.41	0.50
1:A:647:ASN:HB3	1:A:708:GLN:HB3	1.93	0.50
1:B:591:MET:HG3	1:B:593:HIS:O	2.11	0.50
1:A:24:VAL:HG22	1:A:54:GLY:CA	2.42	0.50
1:B:308:MET:HA	1:B:335:TYR:O	2.12	0.50
1:B:341:PRO:O	1:B:342:VAL:C	2.55	0.50
1:B:511:GLU:O	1:B:515:MET:HG3	2.12	0.50
1:A:308:MET:HA	1:A:335:TYR:O	2.12	0.50
1:B:536:GLN:HG2	1:B:590:TYR:CD1	2.47	0.50
1:A:593:HIS:HD2	1:A:636:ASP:N	1.98	0.49
1:B:513:LEU:HB2	4:B:2385:HOH:O	2.12	0.49
1:B:6:GLN:HA	1:B:7:PRO:C	2.38	0.49
1:B:709:PHE:N	4:B:2447:HOH:O	2.45	0.49
1:A:17:LYS:HB2	1:A:118:GLU:HG3	1.94	0.49
1:B:396:LYS:HD2	4:B:2009:HOH:O	2.12	0.48
1:A:536:GLN:CG	1:A:590:TYR:CD1	2.96	0.48
1:A:449:ARG:O	1:A:452:LYS:CG	2.50	0.48
1:A:393:ASN:HD21	1:A:396:LYS:HD3	1.79	0.47
1:B:170:TYR:CZ	1:B:181:PRO:HD3	2.49	0.47
1:A:449:ARG:HG2	1:A:452:LYS:CE	2.43	0.47
1:A:87:GLU:H	1:A:87:GLU:CD	2.22	0.47
1:A:376:HIS:HB3	1:A:494:GLU:OE1	2.15	0.47
1:A:15:GLN:HB2	1:A:118:GLU:HB2	1.97	0.47
1:B:15:GLN:HB2	1:B:118:GLU:HB3	1.97	0.47
1:B:86:ASN:HA	1:B:118:GLU:HG3	1.97	0.47
1:A:646:ILE:O	1:A:647:ASN:CB	2.63	0.46
1:A:238:ALA:HA	1:A:276:VAL:O	2.14	0.46
1:A:464:ASP:O	1:A:468:LEU:HG	2.15	0.46
1:B:589:ASP:OD1	3:B:1718:GOL:O2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLN:NE2	4:B:2213:HOH:O	2.43	0.46
1:B:557:ALA:HB1	1:B:561:ILE:HB	1.96	0.46
1:B:131:GLY:HA3	1:B:160:THR:O	2.16	0.46
1:A:449:ARG:C	1:A:452:LYS:HG2	2.35	0.46
1:A:125:PRO:HB3	1:A:392:TRP:CE3	2.50	0.46
1:A:107:PHE:HA	1:A:110:LEU:HD12	1.98	0.45
1:A:595:MET:HB2	1:A:607:LEU:HD11	1.97	0.45
1:B:252:GLN:HE22	1:B:300:LYS:HE3	1.80	0.45
1:A:452:LYS:O	1:A:453:ALA:C	2.59	0.45
1:A:452:LYS:O	1:A:456:GLU:HG2	2.16	0.45
1:A:591:MET:HG3	1:A:593:HIS:O	2.17	0.45
1:A:141:TRP:CZ2	1:A:373:PRO:HG2	2.52	0.45
1:B:413:SER:OG	1:B:487:GLU:OE1	2.26	0.45
1:A:518:GLY:O	1:A:519:ARG:C	2.60	0.45
1:A:449:ARG:CA	1:A:452:LYS:HE3	2.47	0.44
1:B:616:ILE:HD12	1:B:709:PHE:CG	2.52	0.44
1:A:644:ILE:HD11	1:A:684:LEU:HD21	2.00	0.44
1:A:214:TRP:CD2	1:A:253:LYS:HB3	2.53	0.44
1:B:616:ILE:HD12	1:B:709:PHE:CD1	2.52	0.44
1:A:354:PRO:HB2	1:A:399:THR:HG22	1.99	0.44
1:B:170:TYR:HB2	1:B:180:TYR:CE2	2.53	0.44
1:A:45:LEU:O	1:A:48:LYS:HB2	2.16	0.43
1:A:454:PHE:CD2	1:A:571:THR:HG21	2.54	0.43
1:A:174:PRO:HD2	4:A:2124:HOH:O	2.18	0.43
1:A:293:TYR:CD1	1:A:293:TYR:C	2.97	0.43
1:A:111:LEU:HD12	1:A:111:LEU:HA	1.71	0.43
1:A:515:MET:HE2	1:A:572:VAL:HG21	2.00	0.43
1:B:567:ARG:NH1	4:B:2421:HOH:O	2.49	0.43
1:A:454:PHE:HZ	1:A:572:VAL:HG12	1.84	0.42
1:B:173:ALA:HA	1:B:174:PRO:HA	1.63	0.42
1:A:170:TYR:CZ	1:A:181:PRO:HD3	2.54	0.42
1:A:170:TYR:HB2	1:A:180:TYR:CE2	2.54	0.42
1:A:474:ARG:HA	1:A:474:ARG:HD2	1.80	0.42
1:A:515:MET:HE2	1:A:572:VAL:CG2	2.49	0.42
1:B:173:ALA:HB2	4:B:2154:HOH:O	2.18	0.42
1:B:456:GLU:C	1:B:458:LYS:N	2.73	0.42
1:B:337:TRP:NE1	1:B:372:ASN:HB2	2.35	0.42
1:B:383:ALA:O	1:B:387:VAL:HG23	2.20	0.42
1:B:396:LYS:HG3	4:B:2012:HOH:O	2.18	0.42
1:A:644:ILE:HG12	1:A:711:LEU:HD13	2.02	0.42
1:B:378:GLU:HG3	1:B:490:PRO:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PRO:HB2	1:A:25:TYR:HB3	2.02	0.42
1:A:471:THR:O	1:A:475:MET:HG3	2.19	0.42
1:A:644:ILE:CD1	1:A:684:LEU:HD21	2.49	0.42
1:B:323:ILE:HG23	1:B:324:SER:N	2.34	0.42
1:B:454:PHE:HZ	1:B:572:VAL:CG1	2.33	0.41
1:A:85:VAL:HG13	1:A:90:ILE:HG12	2.02	0.41
1:B:26:GLN:HG3	1:B:52:LYS:HA	2.02	0.41
1:B:610:LYS:NZ	4:B:2401:HOH:O	2.37	0.41
1:A:149:GLN:HB3	1:A:153:TYR:CZ	2.54	0.41
1:B:171:HIS:NE2	1:B:207:HIS:HB2	2.35	0.41
1:B:515:MET:HG2	1:B:527:LYS:HB2	2.01	0.41
1:A:490:PRO:O	1:A:494:GLU:HG3	2.21	0.41
1:A:20:ASP:OD1	1:A:115:LYS:HG2	2.20	0.41
1:A:61:GLU:O	1:A:62:LYS:C	2.62	0.41
1:B:61:GLU:O	1:B:64:ASP:HB2	2.21	0.41
1:A:283:ASN:HB3	1:A:310:THR:OG1	2.20	0.41
1:A:444:GLN:HB3	1:A:445:PRO:CD	2.50	0.41
1:A:462:LYS:HD2	1:A:462:LYS:HA	1.92	0.41
1:A:483:LEU:HA	1:A:483:LEU:HD23	1.85	0.41
1:A:55:MET:HE3	1:A:86:ASN:O	2.21	0.41
1:A:454:PHE:CE2	1:A:571:THR:HG22	2.56	0.41
1:A:275:LEU:HD23	1:A:305:ILE:HG12	2.03	0.41
1:B:454:PHE:CZ	1:B:572:VAL:CG1	3.04	0.41
1:A:83:LEU:HD23	1:A:83:LEU:C	2.46	0.40
1:B:475:MET:HG2	1:B:502:PHE:CZ	2.56	0.40
1:A:341:PRO:O	1:A:342:VAL:C	2.65	0.40
1:B:236:SER:OG	1:B:273:ASN:HB2	2.20	0.40
1:B:527:LYS:HA	1:B:527:LYS:HE2	2.04	0.40
1:A:88:LYS:HE3	1:A:89:GLU:HG2	2.03	0.40
1:B:536:GLN:HG2	1:B:590:TYR:CE1	2.56	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	628/737 (85%)	596 (95%)	30 (5%)	2 (0%)	36	35
1	B	635/737 (86%)	607 (96%)	28 (4%)	0	100	100
All	All	1263/1474 (86%)	1203 (95%)	58 (5%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	519	ARG
1	A	373	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	562/647 (87%)	555 (99%)	7 (1%)	63	70
1	B	567/647 (88%)	561 (99%)	6 (1%)	65	73
All	All	1129/1294 (87%)	1116 (99%)	13 (1%)	63	70

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

Mol	Chain	Res	Type
1	A	45	LEU
1	A	87	GLU
1	A	213	LYS
1	A	496	THR
1	A	519	ARG
1	A	647	ASN
1	A	715	LYS
1	B	24	VAL
1	B	133	VAL
1	B	371	THR
1	B	451	LEU

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Mol	Chain	Res	Type
1	B	462	LYS
1	B	519	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	189	GLN
1	A	198	ASN
1	A	292	ASN
1	A	306	GLN
1	A	401	GLN
1	A	425	ASN
1	A	537	GLN
1	A	543	GLN
1	A	583	HIS
1	A	593	HIS
1	A	643	ASN
1	A	645	GLN
1	B	26	GLN
1	B	73	GLN
1	B	189	GLN
1	B	252	GLN
1	B	254	GLN
1	B	273	ASN
1	B	274	GLN
1	B	290	ASN
1	B	292	ASN
1	B	306	GLN
1	B	425	ASN
1	B	537	GLN
1	B	543	GLN
1	B	578	GLN
1	B	583	HIS
1	B	593	HIS
1	B	608	GLN
1	B	645	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOA	B	1716	-	4,4,4	0.55	0	4,4,4	2.84	3 (75%)
3	GOL	A	1717	-	5,5,5	0.60	0	5,5,5	0.82	0
2	GOA	A	1716	-	4,4,4	0.43	0	4,4,4	1.87	1 (25%)
3	GOL	B	1717	-	5,5,5	0.68	0	5,5,5	0.52	0
3	GOL	B	1718	-	5,5,5	0.65	0	5,5,5	0.57	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
2	GOA	B	1716	-	-	2/2/2/2	-
3	GOL	A	1717	-	-	0/4/4/4	-
2	GOA	A	1716	-	-	2/2/2/2	-
3	GOL	B	1717	-	-	0/4/4/4	-
3	GOL	B	1718	-	-	0/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1716	GOA	OXT-C-CA	3.87	118.93	111.90
2	B	1716	GOA	O2-CA-C	-3.60	103.44	112.37
2	A	1716	GOA	O2-CA-C	-2.84	105.33	112.37
2	B	1716	GOA	O-C-CA	-2.08	117.45	123.48

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1716	GOA	O-C-CA-O2
2	A	1716	GOA	OXT-C-CA-O2
2	B	1716	GOA	O-C-CA-O2
2	B	1716	GOA	OXT-C-CA-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1718	GOL	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	637/737 (86%)	-0.06	31 (4%) 35 34	10, 21, 59, 74	3 (0%)
1	B	641/737 (86%)	-0.21	29 (4%) 38 37	8, 19, 53, 74	4 (0%)
All	All	1278/1474 (86%)	-0.14	60 (4%) 36 35	8, 20, 57, 74	7 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	631	VAL	5.9
1	A	24	VAL	4.5
1	B	615	LEU	4.3
1	A	682	ALA	4.1
1	A	692	VAL	3.7
1	A	644	ILE	3.7
1	A	710	VAL	3.7
1	A	606	PRO	3.6
1	A	454	PHE	3.6
1	A	646	ILE	3.6
1	B	682	ALA	3.6
1	B	647	ASN	3.6
1	B	692	VAL	3.6
1	B	595	MET	3.4
1	B	646	ILE	3.3
1	B	18	THR	3.2
1	B	457	GLY	3.2
1	A	618	PRO	3.1
1	A	633	ILE	3.1
1	A	23	ALA	3.1
1	A	451	LEU	3.0
1	B	454	PHE	3.0
1	B	680	LEU	3.0
1	A	709	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	452	LYS	2.9
1	A	683	GLY	2.9
1	A	647	ASN	2.9
1	B	458	LYS	2.8
1	A	595	MET	2.6
1	A	691	PHE	2.6
1	B	616	ILE	2.6
1	B	459	ASN	2.6
1	B	709	PHE	2.6
1	A	689	VAL	2.6
1	A	711	LEU	2.6
1	A	693	ARG	2.6
1	B	453	ALA	2.6
1	B	52	LYS	2.5
1	A	19	ILE	2.5
1	A	616	ILE	2.4
1	A	712	THR	2.4
1	B	605	LEU	2.4
1	B	681	SER	2.3
1	A	18	THR	2.3
1	A	46	SER	2.3
1	A	115	LYS	2.3
1	B	633	ILE	2.2
1	B	618	PRO	2.2
1	B	518	GLY	2.2
1	B	15	GLN	2.2
1	A	21	LEU	2.2
1	B	644	ILE	2.1
1	B	456	GLU	2.1
1	B	53	LYS	2.1
1	B	46	SER	2.1
1	A	16	ASN	2.1
1	B	688	PRO	2.1
1	A	594	LYS	2.1
1	B	689	VAL	2.0
1	B	16	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 [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	GOA	A	1716	5/5	0.91	0.12	24,24,27,29	0
3	GOL	B	1718	6/6	0.91	0.12	32,39,40,42	0
3	GOL	A	1717	6/6	0.96	0.06	17,17,19,19	0
2	GOA	B	1716	5/5	0.96	0.07	22,23,23,24	0
3	GOL	B	1717	6/6	0.97	0.05	15,16,16,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.