



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:28 pm BST

PDB ID : 5WAB
Title : Crystal Structure of Bifidobacterium adolescentis GH3 beta-glucosidase
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Deposited on : 2017-06-26
Resolution : 2.45 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 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 : 2.11
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) : 2.11

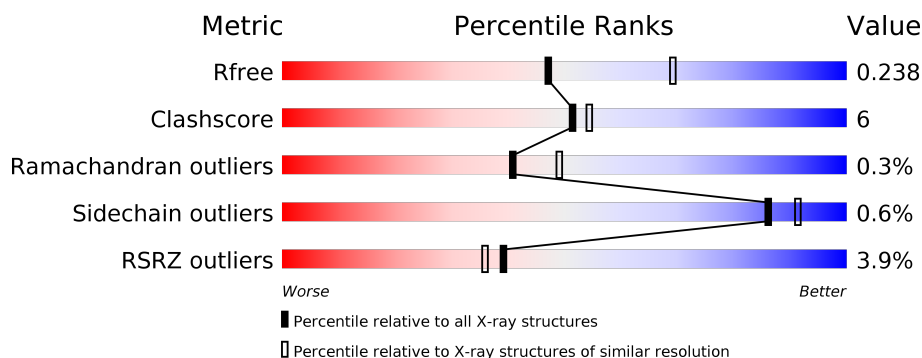
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 on 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	751	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>10%</div> </div> </div>
1	B	751	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>12%</div> </div> </div>
1	C	751	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>13%</div> </div> </div>
1	D	751	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>7%</div> </div> </div>

2 Entry composition [i](#)

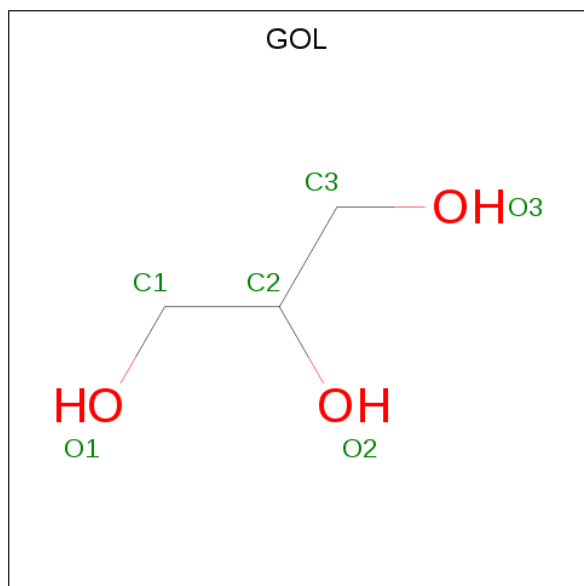
There are 3 unique types of molecules in this entry. The entry contains 21767 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	0	0
			5089	3219	864	989	17			
1	B	659	Total	C	N	O	S	0	0	0
			4997	3153	850	977	17			
1	C	654	Total	C	N	O	S	0	0	0
			4959	3131	838	973	17			
1	D	701	Total	C	N	O	S	0	0	0
			5314	3357	897	1039	21			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).




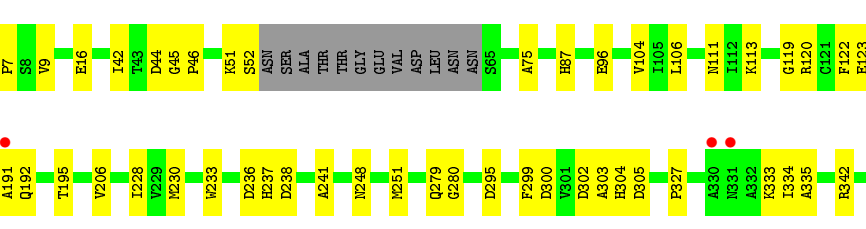
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	363	Total 363	O 363	0	0
3	B	337	Total 337	O 337	0	0
3	C	289	Total 289	O 289	0	0
3	D	413	Total 413	O 413	0	0

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

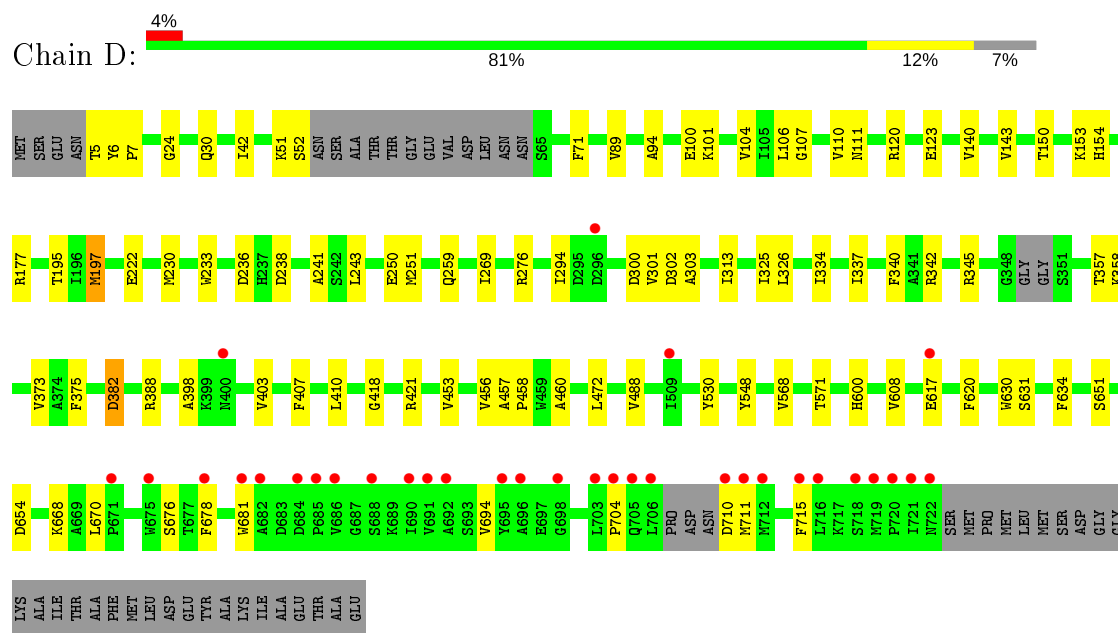
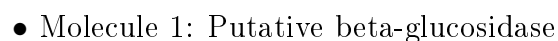
- Chain A: 



Position	Amino Acid	Information Content (bits)
1	Met	0.02
2	Ser	0.01
3	Asn	0.38
4	Thr	0.01
5	Leu	0.01
6	Val	0.01
7	Met	0.01
8	Met	0.01
9	Met	0.01
10	Met	0.01
11	Met	0.01
12	Met	0.01
13	Met	0.01
14	Met	0.01
15	Met	0.01
16	Met	0.01
17	Met	0.01
18	Met	0.01
19	Met	0.01
20	Met	0.01
21	Met	0.01
22	Met	0.01
23	Met	0.01
24	Met	0.01
25	Met	0.01
26	Met	0.01
27	Met	0.01
28	Met	0.01
29	Met	0.01
30	Met	0.01
31	Met	0.01
32	Met	0.01
33	Lys	0.38
34	Gln	0.38
35	Met	0.01
36	Met	0.01
37	Met	0.01
38	Met	0.01
39	Met	0.01
40	Met	0.01
41	Met	0.01
42	Met	0.01
43	Met	0.01
44	Met	0.01
45	Met	0.01
46	Met	0.01
47	Met	0.01
48	Met	0.01
49	Met	0.01
50	Met	0.01
51	Met	0.01
52	Met	0.01
53	Met	0.01
54	Met	0.01
55	Met	0.01
56	Met	0.01
57	Met	0.01
58	Met	0.01
59	Met	0.01
60	Met	0.01
61	Met	0.01
62	Met	0.01
63	Met	0.01
64	Met	0.01
65	Met	0.01
66	Met	0.01
67	Met	0.01
68	Met	0.01
69	Met	0.01
70	Met	0.01
71	Met	0.01
72	Met	0.01
73	Met	0.01
74	Met	0.01
75	Met	0.01
76	Met	0.01
77	Met	0.01
78	Met	0.01
79	Met	0.01
80	Met	0.01
81	Met	0.01
82	Met	0.01
83	Met	0.01
84	Met	0.01
85	Met	0.01
86	Met	0.01
87	Met	0.01
88	Met	0.01
89	Met	0.01
90	Met	0.01
91	Met	0.01
92	Met	0.01
93	Met	0.01
94	Gly	0.38
95	Met	0.01
96	Met	0.01
97	Met	0.01
98	Met	0.01
99	Met	0.01
100	Met	0.01

- Chain B:
-
- 2% 79% 8% 12%
- MET SER GLU ASN TS Y6 P7 S8 V9 K17 W27 E33 A34 K35 I42 G45 S52 ASN SER ALA THR THR GLY GLU VAL ASP LEU ASN ASN S65 A92 N93 A94 E95 E96 K101 V104 G107 P108 G109 V110 N111 R120 V140 V143 T150

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	94.61Å 96.43Å 106.77Å 87.76° 89.11° 61.00°	Depositor
Resolution (Å)	44.51 – 2.45 44.51 – 2.45	Depositor EDS
% Data completeness (in resolution range)	85.5 (44.51-2.45) 85.5 (44.51-2.45)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.195 , 0.234 0.203 , 0.238	Depositor DCC
R_{free} test set	5227 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.034 for k,-h+k,l 0.034 for h-k,h,l 0.034 for -h+k,-h,l 0.034 for -k,h-k,l 0.039 for h,h-k,-l 0.036 for -h+k,k,-l 0.035 for -h,-k,l 0.058 for k,h,-l 0.038 for -k,-h,-l 0.036 for -h,-h+k,-l 0.039 for h-k,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21767	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: 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	0.29	0/5206	0.48	0/7100
1	B	0.28	0/5108	0.48	0/6959
1	C	0.28	0/5070	0.49	0/6909
1	D	0.29	0/5435	0.49	0/7404
All	All	0.28	0/20819	0.49	0/28372

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5089	0	4881	59	0
1	B	4997	0	4816	41	0
1	C	4959	0	4769	61	0
1	D	5314	0	5094	67	0
2	A	6	0	8	0	0
3	A	363	0	0	14	4
3	B	337	0	0	14	1
3	C	289	0	0	24	0
3	D	413	0	0	17	3
All	All	21767	0	19568	225	4

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 6.

All (225) 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:101:LYS:O	3:B:801:HOH:O	1.81	0.97
1:B:500:MET:SD	3:B:984:HOH:O	2.24	0.92
1:C:222:GLU:OE2	3:C:801:HOH:O	1.88	0.91
1:A:237:HIS:ND1	3:A:906:HOH:O	2.10	0.85
1:A:651:SER:HB3	1:A:654:ASP:HB2	1.58	0.84
1:B:426:ILE:O	3:B:802:HOH:O	1.99	0.81
1:C:486:GLY:O	3:C:802:HOH:O	2.00	0.80
1:A:16:GLU:OE2	3:A:902:HOH:O	2.00	0.78
1:B:581:ALA:O	3:B:803:HOH:O	2.01	0.78
1:C:348:GLY:O	3:C:803:HOH:O	2.01	0.77
1:B:651:SER:HB3	1:B:654:ASP:HB2	1.67	0.77
1:C:9:VAL:O	3:C:804:HOH:O	2.02	0.77
1:A:96:GLU:OE1	3:A:903:HOH:O	2.03	0.76
1:D:24:GLY:O	3:D:801:HOH:O	2.04	0.76
1:D:42:ILE:HG13	1:D:104:VAL:HB	1.70	0.74
1:C:670:LEU:O	3:C:805:HOH:O	2.04	0.74
1:B:173:GLN:OE1	3:B:804:HOH:O	2.06	0.74
1:D:651:SER:HB3	1:D:654:ASP:HB2	1.69	0.73
1:A:302:ASP:OD1	1:A:358:LYS:NZ	2.20	0.72
1:A:236:ASP:O	3:A:904:HOH:O	2.08	0.72
1:D:52:SER:O	3:D:804:HOH:O	2.07	0.72
1:D:668:LYS:O	3:D:803:HOH:O	2.07	0.72
1:D:382:ASP:O	3:D:802:HOH:O	2.06	0.71
1:A:119:GLY:O	3:A:905:HOH:O	2.09	0.70
1:C:651:SER:HB3	1:C:654:ASP:HB2	1.72	0.70
1:D:301:VAL:HG13	1:D:357:THR:HG21	1.72	0.70
1:D:30:GLN:O	3:D:805:HOH:O	2.10	0.69
1:C:267:GLY:O	3:C:808:HOH:O	2.10	0.69
1:D:300:ASP:OD2	3:D:807:HOH:O	2.10	0.69
1:C:265:ARG:NE	3:C:822:HOH:O	2.23	0.68
1:D:472:LEU:O	3:D:806:HOH:O	2.10	0.68
1:C:360:THR:O	3:C:810:HOH:O	2.12	0.67
1:A:42:ILE:HG13	1:A:104:VAL:HB	1.76	0.67
1:D:110:VAL:O	3:D:808:HOH:O	2.13	0.66
1:A:342:ARG:O	3:A:908:HOH:O	2.13	0.66
1:C:241:ALA:O	3:C:811:HOH:O	2.14	0.65
1:C:84:GLU:OE2	3:C:812:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:THR:OG1	1:D:617:GLU:OE1	2.13	0.65
1:D:694:VAL:HG21	1:D:715:PHE:CE1	2.30	0.65
1:A:632:GLU:O	3:A:907:HOH:O	2.13	0.65
1:D:302:ASP:OD1	1:D:358:LYS:NZ	2.30	0.65
1:D:388:ARG:NH1	3:D:824:HOH:O	2.30	0.65
1:B:660:VAL:O	3:B:806:HOH:O	2.15	0.64
1:A:228:ILE:HD11	1:A:280:GLY:HA3	1.80	0.64
1:B:294:ILE:O	3:B:805:HOH:O	2.15	0.64
1:C:283:ASP:OD1	3:C:813:HOH:O	2.15	0.64
1:A:676:SER:HB2	1:A:681:TRP:HE1	1.62	0.64
1:D:259:GLN:OE1	3:D:809:HOH:O	2.15	0.63
1:A:571:THR:OG1	1:A:617:GLU:OE1	2.11	0.63
1:C:12:LEU:N	3:C:804:HOH:O	2.33	0.62
1:C:153:LYS:NZ	3:C:820:HOH:O	2.22	0.62
1:A:206:VAL:O	3:A:909:HOH:O	2.16	0.62
1:C:237:HIS:N	3:C:806:HOH:O	2.05	0.62
1:C:325:ILE:HD13	1:C:464:LYS:HB2	1.81	0.61
1:A:51:LYS:HG2	1:A:52:SER:H	1.65	0.61
1:B:443:ASN:OD1	3:B:807:HOH:O	2.16	0.61
1:A:402:ASP:OD1	3:A:910:HOH:O	2.17	0.60
1:C:230:MET:HE3	1:C:251:MET:HG3	1.82	0.60
1:C:637:TRP:O	1:C:668:LYS:NZ	2.31	0.60
1:A:509:ILE:HD11	1:C:525:PHE:HB2	1.84	0.59
1:A:228:ILE:HG23	1:A:248:ASN:HB2	1.85	0.59
1:C:333:LYS:HG3	1:C:402:ASP:H	1.68	0.59
1:B:572:VAL:HG11	1:B:608:VAL:HG21	1.85	0.59
1:D:120:ARG:NE	1:D:123:GLU:OE1	2.35	0.58
1:A:305:ASP:OD2	3:A:911:HOH:O	2.17	0.58
1:B:42:ILE:HG13	1:B:104:VAL:HB	1.84	0.57
1:A:333:LYS:NZ	1:A:400:ASN:O	2.23	0.57
1:D:388:ARG:NH1	3:D:820:HOH:O	2.37	0.57
1:B:150:THR:O	1:B:195:THR:HB	2.05	0.57
1:C:9:VAL:HB	1:C:17:LYS:HD3	1.86	0.57
1:C:42:ILE:HG13	1:C:104:VAL:HB	1.87	0.57
1:D:140:VAL:HA	1:D:150:THR:HG21	1.86	0.57
1:A:581:ALA:N	3:A:929:HOH:O	2.32	0.56
1:A:238:ASP:HB3	1:A:241:ALA:HB3	1.87	0.55
1:C:443:ASN:ND2	3:C:847:HOH:O	2.38	0.55
1:D:222:GLU:OE2	3:D:811:HOH:O	2.18	0.55
1:A:230:MET:HE3	1:A:251:MET:HG3	1.88	0.54
1:D:313:ILE:HD13	1:D:488:VAL:HG21	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LYS:HG2	1:C:52:SER:H	1.72	0.54
1:C:334:ILE:HB	1:C:373:VAL:HG12	1.90	0.54
1:A:9:VAL:HG22	1:A:279:GLN:OE1	2.08	0.54
1:A:580:ALA:HA	3:A:929:HOH:O	2.06	0.54
1:B:9:VAL:HG22	1:B:17:LYS:HE2	1.90	0.53
1:D:694:VAL:HG21	1:D:715:PHE:HE1	1.72	0.53
1:C:606:ARG:NH1	1:C:619:THR:O	2.42	0.53
1:C:168:SER:HA	1:C:202:ARG:HB2	1.91	0.53
1:A:335:ALA:HB1	1:A:397:THR:HG22	1.91	0.53
1:A:482:ASP:HB3	1:A:488:VAL:HG12	1.90	0.53
1:D:111:ASN:OD1	1:D:154:HIS:HB2	2.09	0.52
1:C:51:LYS:O	1:C:65:SER:N	2.41	0.52
1:B:238:ASP:HB3	1:B:241:ALA:HB3	1.90	0.52
1:D:5:THR:N	3:D:840:HOH:O	2.40	0.52
1:A:153:LYS:HE3	1:A:154:HIS:CE1	2.45	0.52
1:A:44:ASP:HA	1:A:106:LEU:HB2	1.91	0.52
1:D:704:PRO:HB2	1:D:711:MET:HE2	1.92	0.51
1:C:490:PRO:O	3:C:815:HOH:O	2.19	0.51
1:A:589:ALA:HB3	1:A:645:THR:HB	1.92	0.51
1:C:268:ARG:NH1	3:C:826:HOH:O	2.25	0.51
1:C:32:VAL:HB	1:C:37:ILE:HB	1.92	0.51
1:C:333:LYS:NZ	3:C:848:HOH:O	2.38	0.51
1:B:377:PRO:HG2	1:B:390:LEU:HD22	1.92	0.51
1:C:200:TYR:OH	1:C:233:TRP:O	2.18	0.51
1:B:539:ASP:HA	3:B:984:HOH:O	2.10	0.50
1:C:325:ILE:HD11	1:C:465:GLY:N	2.26	0.50
1:C:482:ASP:OD2	3:C:816:HOH:O	2.20	0.50
1:D:153:LYS:HG3	1:D:197:MET:HE3	1.93	0.50
1:D:230:MET:HE3	1:D:251:MET:HG3	1.93	0.50
1:A:421:ARG:NH2	1:A:453:VAL:O	2.37	0.49
1:B:177:ARG:HG3	1:B:630:TRP:CD2	2.47	0.49
1:A:120:ARG:NH2	1:A:154:HIS:HE1	2.09	0.49
1:B:344:PRO:HB2	1:B:359:MET:HE1	1.94	0.49
1:D:337:ILE:HD11	1:D:398:ALA:HB2	1.93	0.49
1:A:191:ALA:O	1:A:192:GLN:HG2	2.12	0.49
1:B:111:ASN:OD1	1:B:154:HIS:HB2	2.13	0.49
1:B:326:LEU:HB3	1:B:548:TYR:OH	2.12	0.49
1:D:276:ARG:NH2	3:D:848:HOH:O	2.45	0.49
1:C:188:VAL:O	1:C:192:GLN:NE2	2.46	0.48
1:D:676:SER:HB2	1:D:681:TRP:HE1	1.78	0.48
1:C:140:VAL:HA	1:C:150:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:TRP:N	1:C:233:TRP:CD1	2.80	0.48
1:A:342:ARG:HB2	1:A:363:LEU:HD12	1.96	0.48
1:B:363:LEU:HD11	1:B:375:PHE:CD1	2.49	0.48
1:C:150:THR:O	1:C:195:THR:HB	2.14	0.48
1:B:382:ASP:OD1	1:B:384:GLU:HB2	2.14	0.47
1:C:469:SER:HB2	1:C:472:LEU:HD11	1.96	0.47
1:D:107:GLY:O	1:D:150:THR:HB	2.14	0.47
1:C:22:SER:O	3:C:818:HOH:O	2.20	0.47
1:C:217:ASP:O	1:C:221:ASP:HB2	2.14	0.47
1:A:568:VAL:HB	1:A:620:PHE:HB2	1.97	0.47
1:D:421:ARG:NH2	1:D:453:VAL:O	2.41	0.46
1:A:228:ILE:HD11	1:A:280:GLY:CA	2.44	0.46
1:A:327:PRO:HG3	1:A:548:TYR:CE2	2.49	0.46
1:D:153:LYS:HG2	1:D:154:HIS:CD2	2.50	0.46
1:D:418:GLY:N	3:D:857:HOH:O	2.49	0.46
1:A:6:TYR:HA	1:A:7:PRO:HA	1.77	0.46
1:B:581:ALA:HB2	1:B:609:PHE:CD2	2.51	0.46
1:A:150:THR:O	1:A:195:THR:HB	2.15	0.45
1:B:177:ARG:HG3	1:B:630:TRP:CE2	2.51	0.45
1:D:710:ASP:N	3:D:856:HOH:O	2.49	0.45
1:A:75:ALA:HB2	1:A:122:PHE:HA	1.98	0.45
1:C:325:ILE:HD12	1:C:445:VAL:HG22	1.99	0.45
1:D:238:ASP:HB3	1:D:241:ALA:HB3	1.97	0.45
1:C:152:LEU:HB3	1:C:196:ILE:HG12	1.99	0.45
1:B:109:GLY:HA2	1:B:153:LYS:HG3	1.99	0.45
1:C:233:TRP:HA	1:C:251:MET:O	2.16	0.45
1:C:386:ALA:HB3	1:C:388:ARG:HH12	1.81	0.45
1:C:541:PRO:HG2	1:C:544:PHE:HB2	1.99	0.45
1:A:120:ARG:HH22	1:A:154:HIS:HE1	1.65	0.45
1:D:101:LYS:NZ	1:D:294:ILE:O	2.50	0.44
1:D:456:VAL:HG12	1:D:460:ALA:HB2	2.00	0.44
1:B:7:PRO:HG3	1:B:35:LYS:O	2.16	0.44
1:D:457:ALA:N	1:D:458:PRO:HD2	2.33	0.44
1:D:568:VAL:HB	1:D:620:PHE:HB2	2.00	0.44
1:C:95:GLU:OE1	1:C:304:HIS:NE2	2.42	0.43
1:D:177:ARG:HG3	1:D:630:TRP:CD2	2.52	0.43
1:A:87:HIS:HA	1:A:138:GLY:O	2.18	0.43
1:D:153:LYS:HG2	1:D:154:HIS:NE2	2.33	0.43
1:D:631:SER:HB3	1:D:634:PHE:HB2	1.99	0.43
1:C:300:ASP:HB3	1:C:303:ALA:HB3	2.00	0.43
1:A:113:LYS:HE2	1:A:124:TYR:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:SER:O	3:B:808:HOH:O	2.21	0.43
1:D:42:ILE:HG23	1:D:106:LEU:HD21	2.01	0.43
1:D:325:ILE:HD11	1:D:403:VAL:HG23	1.99	0.43
1:D:6:TYR:HA	1:D:7:PRO:HA	1.84	0.43
1:B:140:VAL:HA	1:B:150:THR:HG21	2.01	0.43
1:D:345:ARG:HD3	1:D:410:LEU:O	2.18	0.43
1:B:94:ALA:HB2	1:B:143:VAL:HA	2.01	0.43
1:B:345:ARG:NH2	3:B:851:HOH:O	2.51	0.43
1:D:236:ASP:HB3	1:D:250:GLU:HG3	2.01	0.43
1:D:340:PHE:HB2	1:D:407:PHE:HB3	2.01	0.43
1:D:634:PHE:CE1	1:D:670:LEU:HG	2.53	0.42
1:D:94:ALA:HB2	1:D:143:VAL:HG13	2.01	0.42
1:B:627:PHE:HA	3:B:857:HOH:O	2.19	0.42
1:B:92:ALA:O	1:B:96:GLU:HG3	2.19	0.42
1:C:29:LEU:HG	1:C:42:ILE:HD13	2.02	0.42
1:D:51:LYS:HG2	1:D:52:SER:H	1.84	0.42
1:A:334:ILE:HB	1:A:373:VAL:HG12	2.01	0.42
1:A:396:GLU:HG2	3:A:1071:HOH:O	2.18	0.42
1:A:404:VAL:CG1	1:A:444:ILE:HG12	2.50	0.42
1:A:457:ALA:N	1:A:458:PRO:HD2	2.34	0.42
1:A:672:LEU:HD13	1:A:681:TRP:CD2	2.54	0.42
1:A:404:VAL:HG13	1:A:444:ILE:HA	2.01	0.42
1:C:30:GLN:N	3:C:817:HOH:O	2.20	0.42
1:C:511:TRP:HA	1:C:512:PRO:HA	1.79	0.42
1:A:111:ASN:OD1	1:A:154:HIS:HB2	2.20	0.42
1:B:564:ASN:HB3	1:B:639:VAL:HG11	2.02	0.42
1:A:228:ILE:HD12	1:A:248:ASN:ND2	2.34	0.42
1:A:300:ASP:HB3	1:A:303:ALA:HB3	2.00	0.42
1:C:412:GLU:N	3:C:853:HOH:O	2.40	0.42
1:D:71:PHE:CD1	1:D:89:VAL:HG13	2.54	0.42
1:A:369:ARG:NH2	3:A:940:HOH:O	2.44	0.42
1:C:276:ARG:HD3	3:C:839:HOH:O	2.18	0.42
1:A:530:TYR:CD1	1:C:509:ILE:HD11	2.54	0.42
1:C:177:ARG:HG3	1:C:630:TRP:CE2	2.55	0.42
1:A:299:PHE:HB2	1:A:304:HIS:CE1	2.55	0.41
1:B:120:ARG:NE	3:B:855:HOH:O	2.52	0.41
1:B:638:HIS:HA	1:B:666:ASP:OD2	2.20	0.41
1:C:337:ILE:HD11	1:C:398:ALA:HB2	2.01	0.41
1:C:75:ALA:HB2	1:C:122:PHE:HA	2.02	0.41
1:D:678:PHE:HE2	1:D:715:PHE:HZ	1.68	0.41
1:D:326:LEU:HB3	1:D:548:TYR:OH	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ARG:NH2	1:D:375:PHE:HE2	2.18	0.41
1:D:676:SER:HB2	1:D:681:TRP:NE1	2.34	0.41
1:D:678:PHE:CE2	1:D:715:PHE:HZ	2.38	0.41
1:B:509:ILE:HD11	1:D:530:TYR:CE1	2.55	0.41
1:B:670:LEU:HD12	1:B:670:LEU:HA	1.91	0.41
1:B:107:GLY:O	1:B:150:THR:HB	2.20	0.41
1:B:230:MET:HE3	1:B:251:MET:HG3	2.01	0.41
1:B:427:PRO:HA	3:B:870:HOH:O	2.20	0.41
1:A:46:PRO:HG2	1:A:123:GLU:OE2	2.20	0.41
1:D:230:MET:CE	1:D:251:MET:HG3	2.51	0.41
1:D:51:LYS:HD2	1:D:100:GLU:HB3	2.01	0.41
1:D:243:LEU:HD22	1:D:269:ILE:HD13	2.02	0.41
1:B:394:ALA:HB3	1:B:433:LEU:HD11	2.03	0.41
1:D:334:ILE:HB	1:D:373:VAL:HG12	2.02	0.41
1:A:155:PHE:CD1	1:A:156:ALA:HB2	2.56	0.41
1:C:44:ASP:HA	1:C:106:LEU:HB2	2.02	0.41
1:A:177:ARG:HG3	1:A:630:TRP:CE2	2.56	0.41
1:D:300:ASP:HB3	1:D:303:ALA:HB3	2.03	0.41
1:C:111:ASN:OD1	1:C:154:HIS:HB2	2.21	0.41
1:C:133:GLY:HA3	3:C:961:HOH:O	2.21	0.41
1:D:358:LYS:HG3	3:D:838:HOH:O	2.22	0.40
1:A:363:LEU:HD11	1:A:375:PHE:CD1	2.56	0.40
1:D:94:ALA:HB2	1:D:143:VAL:HA	2.03	0.40
1:D:150:THR:O	1:D:195:THR:HB	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1028:HOH:O	3:D:906:HOH:O[1_545]	2.00	0.20
3:A:1172:HOH:O	3:D:1172:HOH:O[1_545]	2.10	0.10
3:A:1181:HOH:O	3:B:1037:HOH:O[1_545]	2.16	0.04
3:A:1208:HOH:O	3:D:1036:HOH:O[1_545]	2.18	0.02

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	668/751 (89%)	647 (97%)	20 (3%)	1 (0%)	51	64
1	B	653/751 (87%)	632 (97%)	20 (3%)	1 (0%)	47	57
1	C	648/751 (86%)	624 (96%)	19 (3%)	5 (1%)	19	22
1	D	693/751 (92%)	675 (97%)	18 (3%)	0	100	100
All	All	2662/3004 (89%)	2578 (97%)	77 (3%)	7 (0%)	41	49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	330	ALA
1	A	45	GLY
1	C	45	GLY
1	C	398	ALA
1	B	45	GLY
1	C	397	THR
1	C	192	GLN

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	521/598 (87%)	518 (99%)	3 (1%)	86	91
1	B	518/598 (87%)	517 (100%)	1 (0%)	93	96
1	C	514/598 (86%)	510 (99%)	4 (1%)	81	88
1	D	549/598 (92%)	544 (99%)	5 (1%)	78	86
All	All	2102/2392 (88%)	2089 (99%)	13 (1%)	86	91

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

Mol	Chain	Res	Type
1	A	233	TRP
1	A	295	ASP
1	A	600	HIS
1	B	233	TRP
1	C	509	ILE
1	C	600	HIS
1	C	606	ARG
1	C	670	LEU
1	D	197	MET
1	D	233	TRP
1	D	382	ASP
1	D	600	HIS
1	D	608	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	173	GLN

5.3.3 RNA [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	GOL	A	801	-	5,5,5	0.99	0	5,5,5	0.91	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	GOL	A	801	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O1-C1-C2-C3
2	A	801	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	674/751 (89%)	0.12	33 (4%) 29 27	13, 28, 57, 88	0
1	B	659/751 (87%)	0.01	16 (2%) 59 54	15, 29, 53, 71	0
1	C	654/751 (87%)	0.12	22 (3%) 45 41	18, 34, 58, 78	0
1	D	701/751 (93%)	0.02	33 (4%) 31 29	14, 27, 50, 66	0
All	All	2688/3004 (89%)	0.07	104 (3%) 39 36	13, 30, 55, 88	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	687	GLY	6.8
1	A	685	PRO	6.4
1	A	675	TRP	6.2
1	A	681	TRP	6.0
1	A	686	VAL	5.6
1	B	34	ALA	5.3
1	B	7	PRO	4.9
1	A	678	PHE	4.9
1	C	672	LEU	4.8
1	A	677	THR	4.7
1	A	684	ASP	4.6
1	A	688	SER	4.3
1	D	711	MET	4.3
1	D	720	PRO	4.1
1	A	689	LYS	4.1
1	D	715	PHE	4.0
1	A	683	ASP	4.0
1	A	691	VAL	4.0
1	B	672	LEU	4.0
1	D	400	ASN	3.8
1	A	676	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	684	ASP	3.8
1	A	671	PRO	3.8
1	A	690	ILE	3.7
1	D	675	TRP	3.7
1	D	681	TRP	3.7
1	B	671	PRO	3.5
1	D	704	PRO	3.5
1	D	682	ALA	3.4
1	C	389	THR	3.4
1	D	685	PRO	3.4
1	A	402	ASP	3.4
1	D	721	ILE	3.4
1	A	400	ASN	3.4
1	A	672	LEU	3.4
1	A	330	ALA	3.3
1	A	692	ALA	3.3
1	D	692	ALA	3.3
1	A	679	GLY	3.2
1	C	33	GLU	3.2
1	A	669	ALA	3.1
1	D	712	MET	3.1
1	D	718	SER	3.1
1	D	722	ASN	3.0
1	B	392	ALA	3.0
1	A	682	ALA	3.0
1	C	388	ARG	3.0
1	B	674	GLU	3.0
1	B	670	LEU	2.9
1	D	703	LEU	2.9
1	B	675	TRP	2.9
1	D	716	LEU	2.9
1	D	706	LEU	2.9
1	B	5	THR	2.8
1	D	691	VAL	2.8
1	A	371	VAL	2.8
1	A	439	ALA	2.8
1	D	698	GLY	2.7
1	C	331	ASN	2.7
1	D	686	VAL	2.7
1	B	676	SER	2.7
1	A	670	LEU	2.7
1	A	680	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	398	ALA	2.6
1	D	719	MET	2.6
1	A	674	GLU	2.5
1	C	34	ALA	2.5
1	D	695	TYR	2.5
1	D	690	ILE	2.4
1	C	671	PRO	2.4
1	D	671	PRO	2.4
1	A	413	ALA	2.4
1	A	191	ALA	2.4
1	C	13	THR	2.4
1	C	27	TRP	2.4
1	B	33	GLU	2.4
1	C	233	TRP	2.4
1	D	617	GLU	2.3
1	B	554	ASP	2.3
1	D	509	ILE	2.3
1	B	388	ARG	2.3
1	C	387	ASP	2.2
1	C	35	LYS	2.2
1	D	688	SER	2.2
1	C	384	GLU	2.2
1	B	179	ILE	2.1
1	C	392	ALA	2.1
1	D	678	PHE	2.1
1	C	7	PRO	2.1
1	C	613	GLY	2.1
1	A	673	ASP	2.1
1	D	296	ASP	2.1
1	C	400	ASN	2.1
1	D	705	GLN	2.1
1	D	696	ALA	2.1
1	C	674	GLU	2.1
1	A	331	ASN	2.1
1	D	710	ASP	2.1
1	C	24	GLY	2.1
1	B	35	LYS	2.1
1	C	372	ASP	2.0
1	C	395	VAL	2.0
1	C	255	TYR	2.0
1	B	27	TRP	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 carbohydrates 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(\AA^2)	Q<0.9
2	GOL	A	801	6/6	0.91	0.19	46,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.