Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 08:00 PM JST

PDB ID	:	7BOV
Title	:	The Structure of Bacillus subtilis glycosyltransferase,Bs-YjiC
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Deposited on	:	2020-03-20
Resolution	:	2.29 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 (i) 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 (1)) were used in the production of this report:

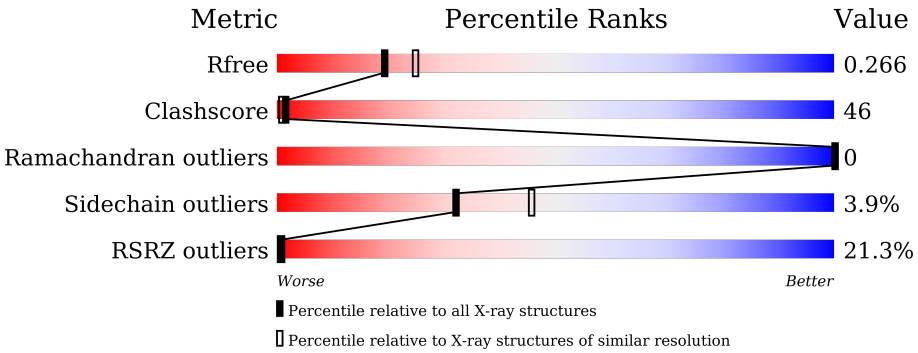
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	392	19% 51% 37% · 9%

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	NA	A	401	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2898 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.

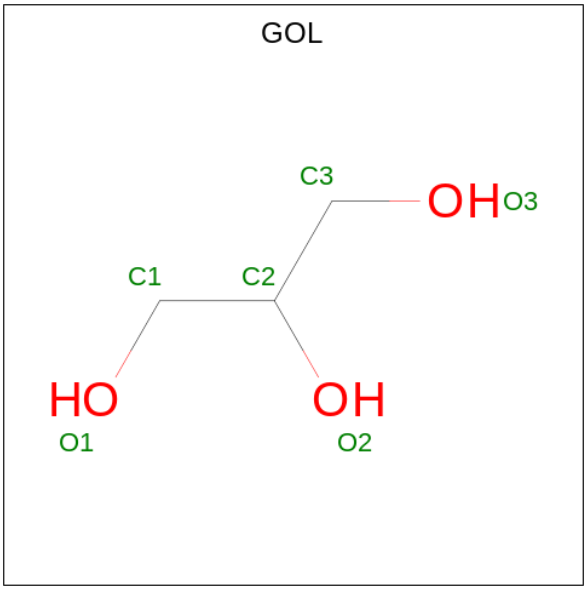
- Molecule 1 is a protein called Uncharacterized UDP-glucosyltransferase YjiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2799	1785	455	543	16			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

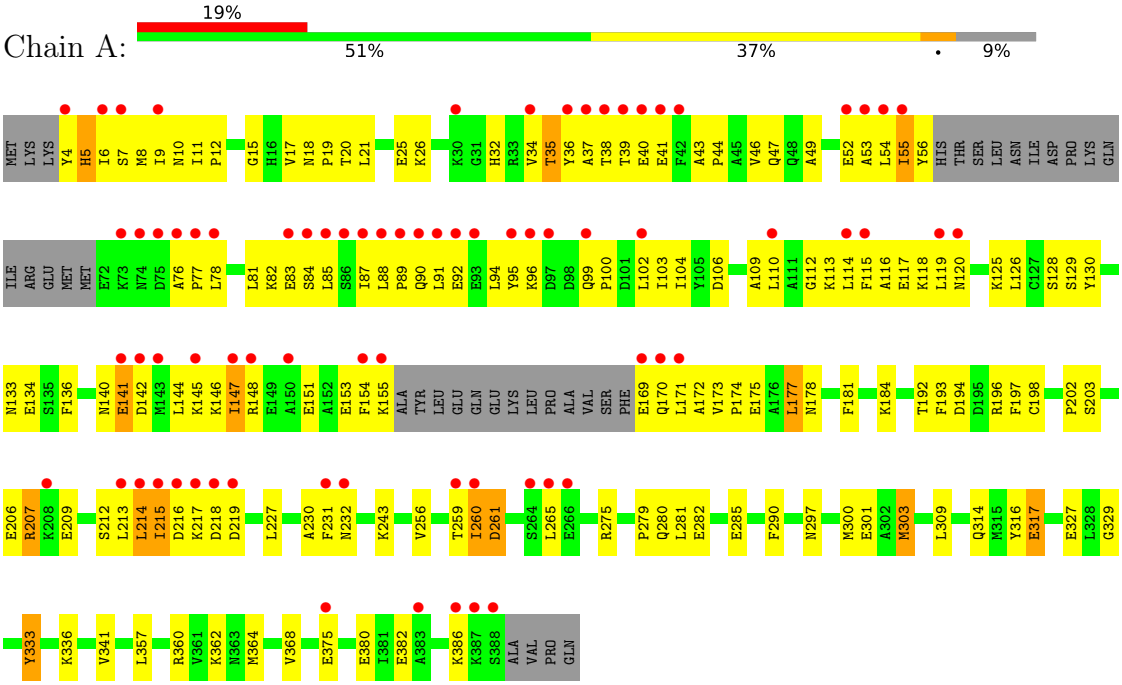
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	86	Total O 86 86	0	0

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: Uncharacterized UDP-glucosyltransferase YjiC

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	51.88Å 118.43Å 184.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.62 – 2.29 39.62 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.0 (39.62-2.29) 96.7 (39.62-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.234 , 0.266 0.234 , 0.266	Depositor DCC
R_{free} test set	1975 reflections (7.85%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 75.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2898	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: GOL, NA

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	2/2849 (0.1%)	0.80	6/3849 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	TYR	CE1-CZ	-5.57	1.31	1.38
1	A	316	TYR	CE1-CZ	-5.32	1.31	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	ILE	N-CA-C	7.27	130.63	111.00
1	A	147	ILE	N-CA-C	6.09	127.45	111.00
1	A	260	ILE	CB-CA-C	-5.74	100.12	111.60
1	A	35	THR	N-CA-C	-5.67	95.68	111.00
1	A	215	ILE	N-CA-C	-5.39	96.43	111.00
1	A	214	LEU	CA-CB-CG	-5.05	103.68	115.30

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	2799	0	2793	256	1
2	A	1	0	0	0	0
3	A	12	0	16	0	0
4	A	86	0	0	18	0
All	All	2898	0	2809	256	1

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 46.

All (256) 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:26:LYS:CE	1:A:375:GLU:HG2	1.50	1.40
1:A:173:VAL:CG1	1:A:174:PRO:HD2	1.53	1.37
1:A:78:LEU:CD1	1:A:146:LYS:HB3	1.58	1.32
1:A:40:GLU:CA	1:A:55:ILE:HG21	1.60	1.30
1:A:36:TYR:O	1:A:53:ALA:HB1	1.25	1.29
1:A:78:LEU:CD2	1:A:146:LYS:HD2	1.63	1.28
1:A:113:LYS:CE	1:A:117:GLU:OE2	1.79	1.28
1:A:92:GLU:O	1:A:95:TYR:HD2	1.10	1.26
1:A:40:GLU:CA	1:A:55:ILE:CG2	2.14	1.25
1:A:173:VAL:CG1	4:A:552:HOH:O	1.78	1.23
1:A:170:GLN:HG3	1:A:173:VAL:CG2	1.68	1.22
1:A:113:LYS:HE2	1:A:117:GLU:OE2	1.09	1.21
1:A:172:ALA:HB1	4:A:504:HOH:O	1.34	1.21
1:A:78:LEU:HD11	1:A:146:LYS:CB	1.69	1.20
1:A:173:VAL:HG11	4:A:552:HOH:O	1.30	1.20
1:A:40:GLU:HA	1:A:55:ILE:CG2	1.68	1.19
1:A:280:GLN:NE2	4:A:501:HOH:O	1.71	1.17
1:A:92:GLU:O	1:A:95:TYR:CD2	1.98	1.16
1:A:148:ARG:HD2	1:A:171:LEU:HG	1.25	1.14
1:A:173:VAL:CG1	1:A:174:PRO:CD	2.27	1.11
1:A:147:ILE:HG22	1:A:147:ILE:O	1.41	1.10
1:A:78:LEU:HD21	1:A:146:LYS:HD2	1.09	1.08
1:A:173:VAL:HG13	1:A:174:PRO:HD2	1.14	1.08
1:A:26:LYS:CE	1:A:375:GLU:CG	2.33	1.07
1:A:36:TYR:HB3	1:A:53:ALA:HB2	1.10	1.07
1:A:40:GLU:HA	1:A:55:ILE:HG21	1.21	1.07
1:A:40:GLU:N	1:A:55:ILE:CG2	2.18	1.05
1:A:173:VAL:HG12	1:A:174:PRO:HD2	1.37	1.05
1:A:26:LYS:HE3	1:A:375:GLU:CG	1.87	1.05
1:A:81:LEU:O	1:A:84:SER:N	1.91	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLU:CB	1:A:55:ILE:HG21	1.87	1.04
1:A:26:LYS:HE2	1:A:375:GLU:HG2	1.08	1.02
1:A:230:ALA:HB1	1:A:314:GLN:HE21	1.26	1.01
1:A:173:VAL:HG12	1:A:174:PRO:CD	1.89	1.01
1:A:129:SER:OG	1:A:317:GLU:OE2	1.77	1.00
1:A:173:VAL:HG13	1:A:174:PRO:CD	1.90	1.00
1:A:36:TYR:O	1:A:53:ALA:CB	2.10	0.99
1:A:36:TYR:HB3	1:A:53:ALA:CB	1.92	0.99
1:A:170:GLN:HG3	1:A:173:VAL:HG23	1.43	0.99
1:A:78:LEU:CG	1:A:146:LYS:HD2	1.94	0.97
1:A:55:ILE:O	1:A:56:TYR:HB3	1.65	0.97
1:A:78:LEU:HD21	1:A:146:LYS:CD	1.95	0.95
1:A:170:GLN:CG	1:A:173:VAL:HG23	1.97	0.93
1:A:26:LYS:HE3	1:A:375:GLU:HG2	1.42	0.92
1:A:170:GLN:CG	1:A:173:VAL:CG2	2.48	0.91
1:A:231:PHE:H	1:A:314:GLN:HE22	1.08	0.91
1:A:78:LEU:HD11	1:A:146:LYS:HB3	0.92	0.91
1:A:115:PHE:CE1	1:A:119:LEU:CD1	2.54	0.90
1:A:147:ILE:O	1:A:147:ILE:CG2	2.18	0.90
1:A:40:GLU:HB2	1:A:55:ILE:HG21	1.54	0.89
1:A:36:TYR:CB	1:A:53:ALA:HB2	2.01	0.89
1:A:38:THR:O	1:A:55:ILE:O	1.91	0.88
1:A:260:ILE:HG22	1:A:261:ASP:N	1.88	0.87
1:A:40:GLU:HA	1:A:55:ILE:HG23	1.54	0.87
1:A:230:ALA:HB1	1:A:314:GLN:NE2	1.89	0.86
1:A:170:GLN:HG3	1:A:173:VAL:HG21	1.59	0.85
1:A:173:VAL:HG12	1:A:174:PRO:N	1.91	0.85
1:A:26:LYS:HE3	1:A:375:GLU:CA	2.06	0.85
1:A:209:GLU:HG3	1:A:282:GLU:OE1	1.76	0.84
1:A:26:LYS:HE3	1:A:375:GLU:HA	1.56	0.83
1:A:115:PHE:CE1	1:A:119:LEU:HD12	2.12	0.83
1:A:209:GLU:CG	1:A:282:GLU:OE1	2.26	0.83
1:A:141:GLU:HA	1:A:144:LEU:HB2	1.60	0.82
1:A:148:ARG:HD2	1:A:171:LEU:CG	2.09	0.82
1:A:78:LEU:CG	1:A:146:LYS:CD	2.57	0.82
1:A:231:PHE:H	1:A:314:GLN:NE2	1.77	0.82
1:A:40:GLU:CA	1:A:55:ILE:HG23	2.07	0.82
1:A:213:LEU:O	1:A:214:LEU:HG	1.78	0.81
1:A:54:LEU:CD1	1:A:94:LEU:CD2	2.59	0.81
1:A:115:PHE:CE1	1:A:119:LEU:HD11	2.14	0.81
1:A:26:LYS:HE2	1:A:375:GLU:CG	2.01	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:NZ	4:A:502:HOH:O	2.12	0.80
1:A:202:PRO:HG3	1:A:300:MET:HB3	1.63	0.79
1:A:77:PRO:HB3	1:A:146:LYS:NZ	1.98	0.79
1:A:260:ILE:HG22	1:A:261:ASP:H	1.48	0.77
1:A:231:PHE:CZ	1:A:314:GLN:HB2	2.19	0.77
1:A:40:GLU:N	1:A:55:ILE:HG23	1.97	0.77
1:A:54:LEU:HD12	1:A:94:LEU:HD23	1.68	0.76
1:A:78:LEU:HD11	1:A:146:LYS:CG	2.16	0.76
1:A:78:LEU:HD11	1:A:146:LYS:CD	2.15	0.76
1:A:78:LEU:HD13	1:A:146:LYS:HB3	1.67	0.75
1:A:54:LEU:HD12	1:A:94:LEU:CD2	2.17	0.74
1:A:141:GLU:OE2	1:A:142:ASP:OD1	2.04	0.74
1:A:6:ILE:O	1:A:34:VAL:HA	1.88	0.73
1:A:40:GLU:N	1:A:55:ILE:HG22	2.03	0.73
1:A:54:LEU:HD13	1:A:94:LEU:HD21	1.71	0.73
1:A:133:ASN:ND2	1:A:192:THR:O	2.22	0.73
1:A:78:LEU:HG	1:A:146:LYS:CD	2.19	0.72
1:A:5:HIS:CD2	1:A:100:PRO:HA	2.24	0.71
1:A:77:PRO:HB3	1:A:146:LYS:HZ3	1.53	0.71
1:A:19:PRO:O	1:A:203:SER:OG	2.07	0.71
1:A:174:PRO:HG2	1:A:196:ARG:NH1	2.06	0.70
1:A:81:LEU:O	1:A:82:LYS:C	2.29	0.70
1:A:151:GLU:OE2	1:A:151:GLU:HA	1.90	0.69
1:A:231:PHE:N	1:A:314:GLN:HE22	1.85	0.69
1:A:26:LYS:CE	1:A:375:GLU:HA	2.23	0.69
1:A:115:PHE:HE1	1:A:119:LEU:HD12	1.56	0.69
1:A:265:LEU:HD12	1:A:265:LEU:H	1.58	0.68
1:A:285:GLU:HG3	4:A:555:HOH:O	1.92	0.68
1:A:36:TYR:HD1	1:A:38:THR:HG23	1.56	0.68
1:A:206:GLU:C	1:A:207:ARG:HD2	2.12	0.68
1:A:113:LYS:HE3	1:A:117:GLU:OE2	1.88	0.68
1:A:115:PHE:HE1	1:A:119:LEU:CD1	2.07	0.68
1:A:194:ASP:OD2	1:A:196:ARG:NH2	2.26	0.68
1:A:26:LYS:HE3	1:A:375:GLU:CB	2.24	0.68
1:A:54:LEU:CD1	1:A:94:LEU:HD21	2.24	0.67
1:A:170:GLN:HG2	1:A:173:VAL:HG23	1.76	0.67
1:A:11:ILE:HG23	1:A:109:ALA:HB2	1.75	0.67
1:A:303:MET:HG3	1:A:364:MET:HG3	1.77	0.67
1:A:243:LYS:HD2	1:A:341:VAL:HG21	1.76	0.66
1:A:177:LEU:HD13	1:A:177:LEU:C	2.15	0.66
1:A:78:LEU:CD1	1:A:146:LYS:CD	2.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PHE:CE2	1:A:314:GLN:HB2	2.31	0.66
1:A:113:LYS:HE2	1:A:117:GLU:CD	2.10	0.65
1:A:37:ALA:O	1:A:38:THR:HG23	1.97	0.65
1:A:327:GLU:OE1	4:A:503:HOH:O	2.14	0.64
1:A:129:SER:CB	1:A:317:GLU:OE2	2.46	0.64
1:A:95:TYR:CG	1:A:96:LYS:N	2.67	0.63
1:A:89:PRO:HA	1:A:92:GLU:HG2	1.81	0.62
1:A:95:TYR:CE1	1:A:96:LYS:HB3	2.34	0.62
1:A:141:GLU:O	1:A:145:LYS:N	2.30	0.62
1:A:95:TYR:CD1	1:A:96:LYS:N	2.67	0.62
1:A:54:LEU:HD13	1:A:94:LEU:CD2	2.28	0.61
1:A:218:ASP:O	1:A:219:ASP:HB3	2.00	0.61
1:A:78:LEU:HG	1:A:146:LYS:HD3	1.82	0.61
1:A:5:HIS:HD2	1:A:99:GLN:O	1.84	0.60
1:A:17:VAL:O	1:A:20:THR:OG1	2.14	0.60
1:A:153:GLU:HG3	1:A:153:GLU:O	2.00	0.60
1:A:39:THR:C	1:A:55:ILE:HG23	2.21	0.60
1:A:7:SER:O	1:A:103:ILE:HA	2.02	0.60
1:A:46:VAL:HG11	1:A:53:ALA:HB2	1.84	0.59
1:A:260:ILE:CG2	1:A:261:ASP:N	2.60	0.59
1:A:5:HIS:CD2	1:A:99:GLN:O	2.55	0.59
1:A:36:TYR:H	1:A:53:ALA:HA	1.67	0.59
1:A:184:LYS:HD3	4:A:558:HOH:O	2.03	0.59
1:A:362:LYS:HE3	4:A:506:HOH:O	2.03	0.59
1:A:147:ILE:O	1:A:148:ARG:C	2.41	0.58
1:A:231:PHE:N	1:A:314:GLN:NE2	2.50	0.57
1:A:32:HIS:CE1	1:A:382:GLU:OE2	2.58	0.57
1:A:43:ALA:HB2	1:A:55:ILE:HG12	1.86	0.57
1:A:78:LEU:HG	1:A:146:LYS:HD2	1.78	0.57
1:A:36:TYR:CD1	1:A:38:THR:HG23	2.39	0.57
1:A:209:GLU:N	1:A:209:GLU:OE2	2.34	0.56
1:A:329:GLY:O	1:A:360:ARG:NH1	2.39	0.56
1:A:37:ALA:O	1:A:38:THR:CG2	2.54	0.56
1:A:206:GLU:O	1:A:207:ARG:HD2	2.06	0.56
1:A:82:LYS:O	1:A:83:GLU:C	2.44	0.55
1:A:40:GLU:HB2	1:A:55:ILE:CG2	2.31	0.55
1:A:174:PRO:CG	1:A:196:ARG:NH1	2.69	0.55
1:A:25:GLU:HB2	1:A:49:ALA:HB1	1.88	0.55
1:A:113:LYS:NZ	1:A:175:GLU:OE2	2.40	0.55
1:A:141:GLU:CA	1:A:144:LEU:HB2	2.35	0.54
1:A:78:LEU:CD1	1:A:146:LYS:HD3	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PHE:CZ	1:A:119:LEU:HD11	2.42	0.54
1:A:260:ILE:CG2	1:A:261:ASP:H	2.20	0.54
1:A:174:PRO:HD2	4:A:552:HOH:O	2.07	0.54
1:A:78:LEU:CD1	1:A:146:LYS:CB	2.50	0.53
1:A:170:GLN:H	1:A:170:GLN:CD	2.12	0.53
1:A:198:CYS:SG	1:A:380:GLU:HG3	2.48	0.53
1:A:303:MET:HB3	1:A:368:VAL:HG21	1.91	0.53
1:A:336:LYS:CE	4:A:502:HOH:O	2.52	0.53
1:A:155:LYS:CB	1:A:155:LYS:NZ	2.73	0.52
1:A:78:LEU:CG	1:A:146:LYS:HD3	2.36	0.52
1:A:88:LEU:HB3	1:A:89:PRO:HD3	1.92	0.52
1:A:209:GLU:HG2	1:A:282:GLU:OE1	2.09	0.52
1:A:281:LEU:HD21	1:A:301:GLU:HG2	1.92	0.52
1:A:15:GLY:HA2	1:A:297:ASN:ND2	2.24	0.52
1:A:36:TYR:CD1	1:A:38:THR:CG2	2.91	0.52
1:A:212:SER:O	1:A:212:SER:OG	2.26	0.51
1:A:104:ILE:HG22	1:A:126:LEU:HG	1.92	0.51
1:A:5:HIS:HD2	1:A:100:PRO:HA	1.74	0.51
1:A:140:ASN:O	1:A:144:LEU:N	2.39	0.51
1:A:218:ASP:O	1:A:219:ASP:CB	2.58	0.51
1:A:35:THR:HA	1:A:52:GLU:O	2.10	0.51
1:A:170:GLN:CG	1:A:173:VAL:HG21	2.31	0.51
1:A:55:ILE:O	1:A:56:TYR:CB	2.42	0.51
1:A:82:LYS:O	1:A:85:LEU:N	2.43	0.51
1:A:55:ILE:O	1:A:55:ILE:HG22	2.11	0.50
1:A:170:GLN:HG2	1:A:170:GLN:O	2.11	0.50
1:A:102:LEU:HD12	1:A:103:ILE:N	2.27	0.50
1:A:209:GLU:HG3	1:A:282:GLU:CD	2.32	0.50
1:A:54:LEU:CD1	1:A:94:LEU:HD23	2.34	0.50
1:A:106:ASP:HA	1:A:126:LEU:HB2	1.93	0.50
1:A:78:LEU:HD11	1:A:146:LYS:HD3	1.90	0.49
1:A:303:MET:HG3	1:A:364:MET:CG	2.42	0.49
1:A:206:GLU:C	1:A:207:ARG:CD	2.81	0.49
1:A:40:GLU:O	1:A:41:GLU:C	2.49	0.49
1:A:155:LYS:NZ	1:A:155:LYS:HB2	2.28	0.49
1:A:265:LEU:HD12	1:A:265:LEU:N	2.27	0.49
1:A:17:VAL:O	1:A:21:LEU:HG	2.12	0.49
1:A:120:ASN:HA	4:A:508:HOH:O	2.11	0.49
1:A:19:PRO:HB2	1:A:181:PHE:CD2	2.48	0.49
1:A:8:MET:HA	1:A:104:ILE:O	2.13	0.48
1:A:87:ILE:HG22	1:A:91:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:HB2	1:A:155:LYS:HZ2	1.78	0.48
1:A:37:ALA:C	1:A:38:THR:HG23	2.34	0.48
1:A:56:TYR:HD2	1:A:90:GLN:HG2	1.78	0.48
1:A:9:ILE:HD12	1:A:112:GLY:HA2	1.94	0.48
1:A:19:PRO:HB2	1:A:181:PHE:CE2	2.49	0.48
1:A:56:TYR:CD2	1:A:90:GLN:HG2	2.48	0.48
1:A:77:PRO:CB	1:A:146:LYS:NZ	2.75	0.47
1:A:213:LEU:C	1:A:214:LEU:HG	2.34	0.47
1:A:78:LEU:HD21	1:A:146:LYS:CB	2.44	0.47
1:A:125:LYS:NZ	4:A:504:HOH:O	2.16	0.47
1:A:38:THR:O	1:A:55:ILE:C	2.53	0.46
1:A:134:GLU:CD	1:A:134:GLU:H	2.19	0.46
1:A:175:GLU:OE1	1:A:175:GLU:HA	2.16	0.46
1:A:46:VAL:HG11	1:A:53:ALA:CB	2.44	0.46
1:A:4:TYR:N	4:A:515:HOH:O	2.48	0.46
1:A:88:LEU:O	1:A:92:GLU:HB3	2.15	0.46
1:A:26:LYS:NZ	1:A:375:GLU:HA	2.32	0.45
1:A:78:LEU:HD21	1:A:146:LYS:CG	2.46	0.45
1:A:35:THR:HG23	1:A:35:THR:O	2.16	0.45
1:A:217:LYS:HD3	4:A:561:HOH:O	2.16	0.45
1:A:12:PRO:HB3	1:A:39:THR:OG1	2.16	0.45
1:A:18:ASN:N	1:A:19:PRO:HD2	2.31	0.45
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.43	0.45
1:A:285:GLU:CG	4:A:555:HOH:O	2.58	0.45
1:A:32:HIS:HE1	1:A:382:GLU:OE2	1.97	0.45
1:A:47:GLN:H	1:A:47:GLN:HG2	1.57	0.45
1:A:177:LEU:C	1:A:177:LEU:CD1	2.86	0.44
1:A:290:PHE:HB3	1:A:309:LEU:HD23	1.99	0.44
1:A:10:ASN:OD1	1:A:11:ILE:N	2.51	0.44
1:A:110:LEU:O	1:A:110:LEU:HG	2.13	0.44
1:A:38:THR:O	1:A:55:ILE:HA	2.17	0.43
1:A:279:PRO:HB2	1:A:282:GLU:CG	2.49	0.43
1:A:43:ALA:N	1:A:44:PRO:HD2	2.34	0.43
1:A:40:GLU:HA	1:A:55:ILE:HD13	2.01	0.42
1:A:85:LEU:O	1:A:89:PRO:HD3	2.18	0.42
1:A:214:LEU:O	1:A:215:ILE:HG12	2.18	0.42
1:A:10:ASN:HD22	1:A:20:THR:HG21	1.84	0.42
1:A:43:ALA:CB	1:A:55:ILE:CD1	2.97	0.42
1:A:194:ASP:HB3	1:A:196:ARG:H	1.83	0.42
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.87	0.42
1:A:169:GLU:HB3	1:A:170:GLN:H	1.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LYS:HB2	1:A:243:LYS:HE3	1.76	0.42
1:A:76:ALA:HA	1:A:77:PRO:HD3	1.65	0.42
1:A:173:VAL:HG12	4:A:552:HOH:O	1.77	0.42
1:A:232:ASN:O	1:A:259:THR:HG23	2.20	0.42
1:A:113:LYS:O	1:A:114:LEU:C	2.57	0.42
1:A:256:VAL:HG22	1:A:275:ARG:O	2.20	0.42
1:A:333:TYR:C	1:A:333:TYR:CD1	2.93	0.42
1:A:40:GLU:CB	1:A:55:ILE:CG2	2.70	0.41
1:A:19:PRO:HA	1:A:203:SER:OG	2.20	0.41
1:A:92:GLU:OE2	1:A:118:LYS:NZ	2.52	0.41
1:A:133:ASN:O	1:A:136:PHE:O	2.39	0.41
1:A:193:PHE:HD1	1:A:197:PHE:CD2	2.39	0.41
1:A:7:SER:HA	1:A:35:THR:HG22	2.03	0.41
1:A:113:LYS:O	1:A:116:ALA:N	2.54	0.41
1:A:5:HIS:O	1:A:5:HIS:CG	2.70	0.41
1:A:36:TYR:HB3	1:A:46:VAL:HG11	2.02	0.40
1:A:81:LEU:O	1:A:83:GLU:N	2.55	0.40
1:A:336:LYS:HE3	4:A:502:HOH:O	2.17	0.40
1:A:217:LYS:O	1:A:218:ASP:CB	2.69	0.40
1:A:329:GLY:O	1:A:357:LEU:HG	2.22	0.40
1:A:55:ILE:H	1:A:55:ILE:HG13	1.70	0.40

All (1) 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)
1:A:215:ILE:CG2	1:A:216:ASP:O[2_555]	1.46	0.74

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	351/392 (90%)	340 (97%)	11 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	307/340 (90%)	295 (96%)	12 (4%)	32 46

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	128	SER
1	A	141	GLU
1	A	154	PHE
1	A	177	LEU
1	A	178	ASN
1	A	207	ARG
1	A	261	ASP
1	A	303	MET
1	A	317	GLU
1	A	333	TYR
1	A	386	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	276	GLN
1	A	314	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	GOL	A	403	-	5,5,5	0.87	0	5,5,5	1.07	0
3	GOL	A	402	-	5,5,5	0.92	0	5,5,5	1.14	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
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	A	402	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	GOL	O1-C1-C2-C3

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, 95^{th} 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	357/392 (91%)	1.11	76 (21%) 0 1	26, 86, 189, 238	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	TYR	12.7
1	A	91	LEU	12.2
1	A	55	ILE	10.9
1	A	76	ALA	8.5
1	A	87	ILE	8.0
1	A	216	ASP	7.5
1	A	88	LEU	7.1
1	A	77	PRO	6.5
1	A	171	LEU	6.4
1	A	143	MET	6.2
1	A	170	GLN	6.1
1	A	78	LEU	5.3
1	A	115	PHE	5.1
1	A	74	ASN	5.1
1	A	97	ASP	5.0
1	A	54	LEU	5.0
1	A	86	SER	4.8
1	A	102	LEU	4.8
1	A	96	LYS	4.8
1	A	85	LEU	4.7
1	A	217	LYS	4.5
1	A	83	GLU	4.5
1	A	119	LEU	4.4
1	A	265	LEU	4.2
1	A	9	ILE	4.1
1	A	84	SER	4.0
1	A	154	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	40	GLU	3.9
1	A	120	ASN	3.8
1	A	90	GLN	3.8
1	A	4	TYR	3.8
1	A	6	ILE	3.7
1	A	213	LEU	3.7
1	A	375	GLU	3.7
1	A	218	ASP	3.6
1	A	150	ALA	3.6
1	A	214	LEU	3.6
1	A	42	PHE	3.5
1	A	93	GLU	3.3
1	A	99	GLN	3.2
1	A	266	GLU	3.2
1	A	92	GLU	3.2
1	A	260	ILE	3.2
1	A	142	ASP	3.1
1	A	231	PHE	3.1
1	A	169	GLU	3.1
1	A	208	LYS	3.0
1	A	75	ASP	2.9
1	A	38	THR	2.9
1	A	39	THR	2.8
1	A	114	LEU	2.7
1	A	147	ILE	2.7
1	A	37	ALA	2.6
1	A	34	VAL	2.6
1	A	215	ILE	2.5
1	A	110	LEU	2.5
1	A	73	LYS	2.5
1	A	36	TYR	2.5
1	A	141	GLU	2.5
1	A	53	ALA	2.5
1	A	232	ASN	2.5
1	A	155	LYS	2.5
1	A	387	LYS	2.5
1	A	145	LYS	2.4
1	A	388	SER	2.4
1	A	30	LYS	2.3
1	A	259	THR	2.3
1	A	89	PRO	2.3
1	A	7	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	41	GLU	2.2
1	A	264	SER	2.2
1	A	386	LYS	2.1
1	A	383	ALA	2.1
1	A	219	ASP	2.1
1	A	52	GLU	2.1
1	A	148	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	NA	A	401	1/1	0.67	0.69	97,97,97,97	0
3	GOL	A	403	6/6	0.72	0.14	71,73,76,77	0
3	GOL	A	402	6/6	0.85	0.18	61,63,65,66	0

6.5 Other polymers (i)

There are no such residues in this entry.