



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:57 am GMT

PDB ID : 4AD2
Title : Structure of the GH99 endo-alpha-mannosidase from Bacteroides xylanisolvens in complex with glucose-1,3-isofagomine
Authors : Thompson, A.J.; Williams, R.J.; Hakki, Z.; Alonzi, D.S.; Wennekes, T.; Gloster, T.M.; Songsrirote, K.; Thomas-Oates, J.E.; Wrodnigg, T.M.; Spreitz, J.; Stuetz, A.E.; Butters, T.D.; Williams, S.J.; Davies, G.J.
Deposited on : 2011-12-21
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

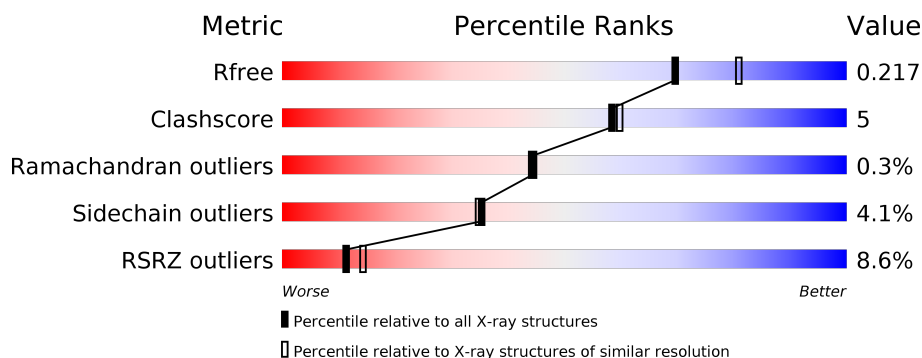
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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. 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	380	<div> <div>84%</div> <div>6% • 9%</div> </div>
1	B	380	<div> <div>84%</div> <div>6% • 9%</div> </div>
1	C	380	<div> <div>80%</div> <div>8% • 9%</div> </div>
1	D	380	<div> <div>29%</div> <div>69%</div> <div>19% • 10%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IFM	C	501	-	-	-	X

2 Entry composition [i](#)

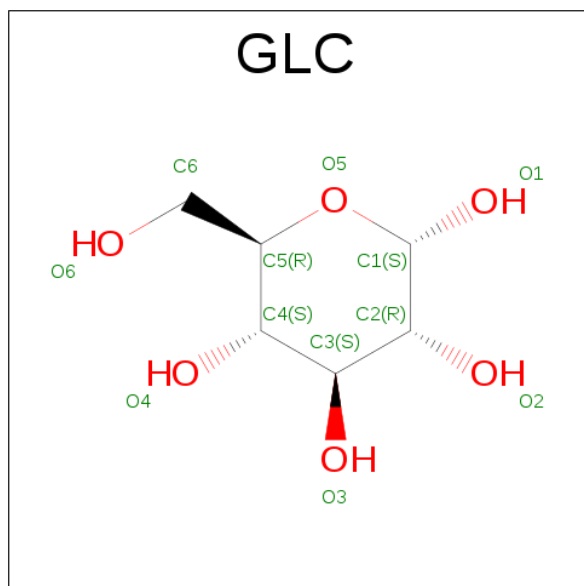
There are 4 unique types of molecules in this entry. The entry contains 12467 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLYCOSYL HYDROLASE FAMILY 71.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	5	0
			2826	1822	468	528	8			
1	B	346	Total	C	N	O	S	0	4	0
			2832	1827	470	526	9			
1	C	344	Total	C	N	O	S	0	1	0
			2806	1808	467	523	8			
1	D	342	Total	C	N	O	S	0	0	0
			2545	1628	432	478	7			

- Molecule 2 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: C₆H₁₂O₆).



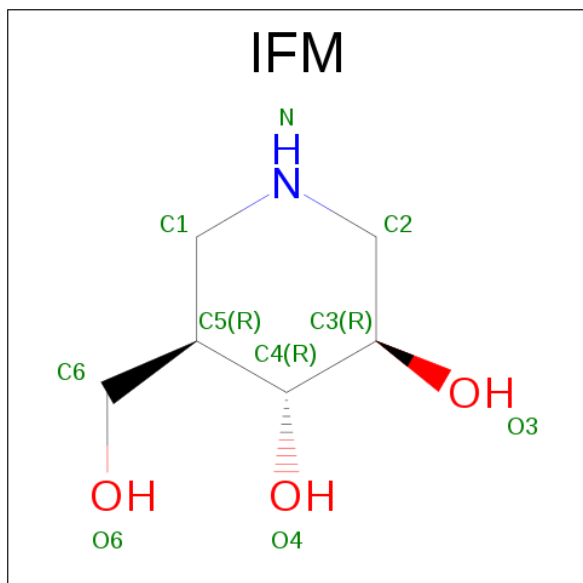
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (three-letter code: IFM) (formula: $C_6H_{13}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	1	3		
3	B	1	Total	C	N	O	0	0
			10	6	1	3		
3	C	1	Total	C	N	O	0	0
			10	6	1	3		
3	D	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	416	Total	O	0	0
			416	416		
4	B	444	Total	O	0	0
			444	444		
4	C	387	Total	O	0	0
			387	387		

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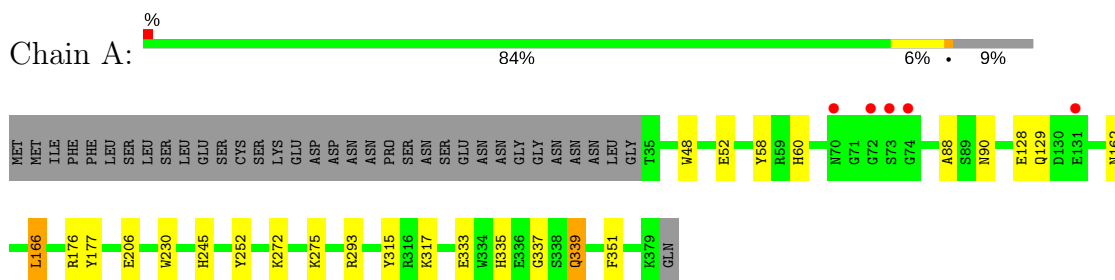
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	127	Total 127	O 127	0	0

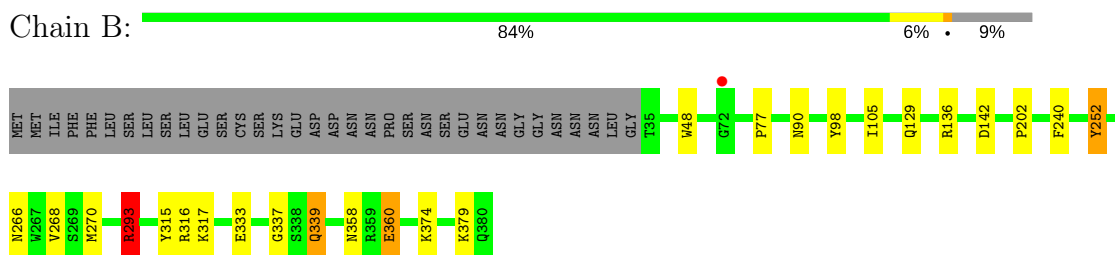
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

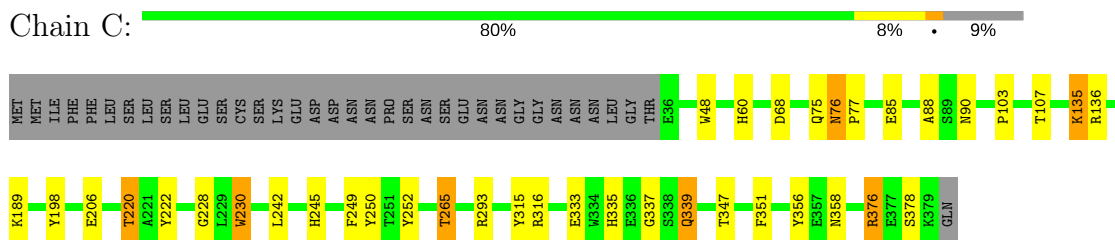
• Molecule 1: GLYCOSYL HYDROLASE FAMILY 71



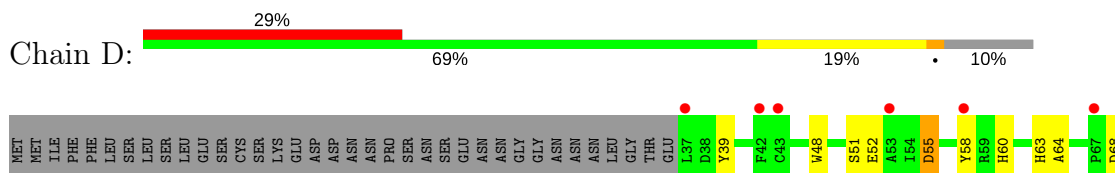
• Molecule 1: GLYCOSYL HYDROLASE FAMILY 71

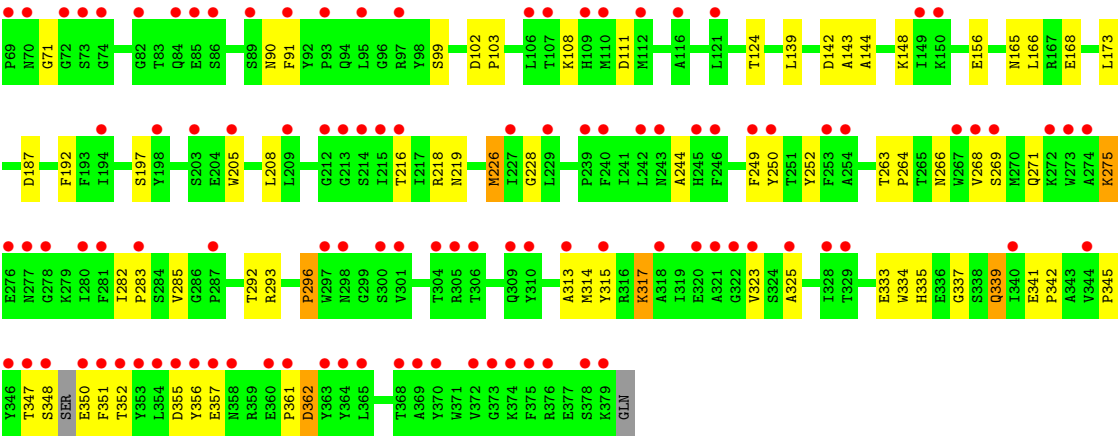


• Molecule 1: GLYCOSYL HYDROLASE FAMILY 71



• Molecule 1: GLYCOSYL HYDROLASE FAMILY 71





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.30Å 223.30Å 84.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.36 – 2.10 44.36 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.36-2.10) 99.9 (44.36-2.10)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0086	Depositor
R, R_{free}	0.186 , 0.217 0.186 , 0.217	Depositor DCC
R_{free} test set	7043 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12467	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: IFM, GLC

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	0.75	0/2933	0.68	0/3995
1	B	0.67	0/2936	0.68	4/3999 (0.1%)
1	C	0.74	1/2901 (0.0%)	0.68	2/3950 (0.1%)
1	D	0.59	0/2627	0.63	1/3602 (0.0%)
All	All	0.69	1/11397 (0.0%)	0.67	7/15546 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	356	TYR	CD1-CE1	-5.94	1.30	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	B	293	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	136	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	D	296	PRO	N-CA-CB	5.58	109.99	103.30
1	C	376	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	136	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	142	ASP	CB-CG-OD1	5.01	122.81	118.30

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	2826	0	2681	17	0
1	B	2832	0	2691	16	0
1	C	2806	0	2662	36	0
1	D	2545	0	2183	52	1
2	A	11	0	10	1	0
2	B	11	0	10	0	0
2	C	11	0	10	0	0
2	D	11	0	10	0	0
3	A	10	0	12	1	0
3	B	10	0	12	2	0
3	C	10	0	12	1	0
3	D	10	0	12	0	0
4	A	416	0	0	4	1
4	B	444	0	0	3	0
4	C	387	0	0	12	0
4	D	127	0	0	9	0
All	All	12467	0	10305	117	2

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 (117) 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:C:85:GLU:HG2	4:C:2355:HOH:O	1.53	1.06
1:B:316:ARG:HH21	1:C:358:ASN:ND2	1.55	1.04
1:C:347:THR:HG22	4:C:2350:HOH:O	1.63	0.98
1:B:316:ARG:HH21	1:C:358:ASN:HD21	0.98	0.97
1:B:316:ARG:NH2	1:C:358:ASN:HD21	1.63	0.95
1:D:192:PHE:HB2	1:D:226:MET:HE1	1.48	0.92
1:C:60:HIS:HD2	1:C:335:HIS:HE1	1.06	0.92
1:C:60:HIS:HD2	1:C:335:HIS:CE1	1.88	0.92
1:C:68:ASP:H	1:C:75:GLN:HE22	1.20	0.90
1:C:265:THR:HG23	4:C:2281:HOH:O	1.70	0.89
1:B:379:LYS:HD3	4:B:2389:HOH:O	1.77	0.85
1:C:265:THR:CG2	4:C:2281:HOH:O	2.23	0.84
1:C:60:HIS:CD2	1:C:335:HIS:HE1	1.95	0.82
1:D:192:PHE:HB2	1:D:226:MET:CE	2.11	0.81
1:D:313:ALA:O	1:D:317:LYS:HG3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:THR:HG23	1:C:222:TYR:H	1.48	0.78
1:D:226:MET:HE2	1:D:226:MET:HA	1.67	0.77
1:D:226:MET:HA	1:D:226:MET:CE	2.16	0.75
1:B:358:ASN:OD1	1:C:316[A]:ARG:NH2	2.20	0.75
1:D:91:PHE:HE1	4:D:2106:HOH:O	1.72	0.72
1:C:107:THR:HG22	4:C:2058:HOH:O	1.92	0.69
1:C:220:THR:CG2	1:C:222:TYR:H	2.05	0.69
1:A:60:HIS:ND1	1:A:335:HIS:HE1	1.92	0.68
1:D:264:PRO:HB2	1:D:317:LYS:HD3	1.75	0.67
1:D:341:GLU:HG2	1:D:342:PRO:HD2	1.77	0.67
1:A:337:GLY:HA2	1:A:339:GLN:HE22	1.59	0.66
1:D:337:GLY:HA2	1:D:339:GLN:HE22	1.62	0.64
1:D:124:THR:OG1	1:D:156:GLU:OE1	2.17	0.63
1:C:245:HIS:HD2	4:C:2134:HOH:O	1.81	0.62
1:C:189:LYS:HD2	4:C:2223:HOH:O	1.99	0.62
1:A:90:ASN:HD21	1:A:293:ARG:H	1.49	0.61
1:D:334:TRP:CZ3	1:D:339:GLN:HG3	2.36	0.61
1:D:313:ALA:O	1:D:317:LYS:CG	2.50	0.60
1:C:293:ARG:HD3	1:C:351:PHE:CE1	2.37	0.59
1:D:52:GLU:HA	1:D:55:ASP:O	2.01	0.59
1:A:162:ASN:O	1:A:166:LEU:HB2	2.02	0.58
1:B:339:GLN:H	1:B:339:GLN:NE2	2.02	0.58
1:C:60:HIS:CD2	1:C:335:HIS:CE1	2.78	0.58
1:A:176:ARG:HD3	1:A:177:TYR:CZ	2.39	0.57
1:D:165:ASN:HA	1:D:168:GLU:HG2	1.86	0.57
1:A:60:HIS:ND1	1:A:335:HIS:CE1	2.74	0.56
1:C:198:TYR:HD1	4:C:2229:HOH:O	1.87	0.56
1:D:263:THR:HB	1:D:266:ASN:ND2	2.20	0.56
1:A:245:HIS:HD2	4:A:2281:HOH:O	1.89	0.56
1:C:68:ASP:N	1:C:75:GLN:HE22	1.99	0.55
1:D:271:GLN:HE21	1:D:275:LYS:HD2	1.70	0.55
1:A:245:HIS:HE1	4:A:2279:HOH:O	1.89	0.55
1:A:293:ARG:HD3	1:A:351:PHE:CE1	2.42	0.54
1:C:337:GLY:HA2	1:C:339:GLN:HE22	1.72	0.54
1:D:51:SER:HB3	1:D:99:SER:HB2	1.88	0.54
1:A:293:ARG:HD2	4:A:2331:HOH:O	2.08	0.53
1:D:283:PRO:HD2	1:D:325:ALA:O	2.08	0.53
1:D:356:TYR:O	1:D:357:GLU:CB	2.53	0.53
1:C:88:ALA:O	1:C:335:HIS:HD2	1.92	0.53
1:C:135:LYS:HG2	4:C:2160:HOH:O	2.10	0.52
1:C:90:ASN:HD21	1:C:293:ARG:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:HIS:ND1	1:D:335:HIS:HE1	2.08	0.52
1:A:88:ALA:O	1:A:335:HIS:HD2	1.93	0.51
1:D:348:SER:CB	1:D:350:GLU:HB3	2.39	0.51
1:A:339:GLN:H	1:A:339:GLN:NE2	2.08	0.51
1:D:51:SER:O	1:D:55:ASP:O	2.29	0.50
1:B:90:ASN:HD21	1:B:293:ARG:H	1.59	0.50
1:C:339:GLN:H	1:C:339:GLN:NE2	2.10	0.49
1:B:360:GLU:HG2	4:B:2423:HOH:O	2.11	0.49
1:D:144:ALA:HB1	4:D:2054:HOH:O	2.12	0.49
1:D:165:ASN:O	1:D:168:GLU:HG2	2.12	0.49
1:B:337:GLY:HA2	1:B:339:GLN:HE22	1.78	0.48
1:C:293:ARG:HD2	4:C:2306:HOH:O	2.13	0.48
1:B:77:PRO:HD2	4:B:2074:HOH:O	2.12	0.48
1:D:334:TRP:CH2	1:D:339:GLN:HG3	2.49	0.48
1:D:208:LEU:O	1:D:216:THR:HA	2.14	0.48
1:B:252:TYR:CZ	3:B:501:IFM:H1C1	2.48	0.48
1:C:293:ARG:HD3	1:C:351:PHE:CZ	2.49	0.47
1:D:285:VAL:HG13	1:D:314:MET:HB3	1.97	0.47
1:D:347:THR:HA	1:D:351:PHE:O	2.15	0.46
1:D:293:ARG:HB2	4:D:2024:HOH:O	2.16	0.46
1:B:316:ARG:NH2	1:C:358:ASN:ND2	2.33	0.46
1:D:63:HIS:HD2	1:D:64:ALA:O	1.98	0.46
1:A:230:TRP:C	1:A:230:TRP:CD1	2.89	0.45
1:D:263:THR:HB	1:D:266:ASN:HD22	1.81	0.45
1:D:143:ALA:HB1	4:D:2030:HOH:O	2.16	0.45
1:A:52:GLU:HB2	1:A:58:TYR:CE2	2.52	0.45
1:C:103:PRO:O	1:C:107:THR:HG23	2.16	0.45
1:D:347:THR:HB	1:D:352:THR:HG22	1.98	0.45
1:D:226:MET:CA	1:D:226:MET:CE	2.91	0.44
1:D:228:GLY:O	1:D:249:PHE:HA	2.18	0.43
1:D:268:VAL:HG23	4:D:2112:HOH:O	2.18	0.43
1:C:378:SER:OG	4:C:2381:HOH:O	2.14	0.43
1:C:252:TYR:CZ	3:C:501:IFM:H1C1	2.54	0.43
1:D:218:ARG:HD2	4:D:2073:HOH:O	2.17	0.43
1:D:282:ILE:HG12	1:D:325:ALA:HB3	2.00	0.43
1:D:90:ASN:ND2	4:D:2024:HOH:O	2.52	0.43
1:A:128:GLU:O	1:A:129:GLN:HB2	2.19	0.42
1:C:376:ARG:HD3	4:C:2133:HOH:O	2.20	0.42
1:D:362:ASP:HA	4:D:2114:HOH:O	2.19	0.42
1:B:252:TYR:CE2	3:B:501:IFM:H1C1	2.55	0.42
1:D:283:PRO:CG	1:D:323:VAL:HG21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:TRP:C	1:C:230:TRP:CD1	2.93	0.42
1:A:293:ARG:HB2	4:A:2078:HOH:O	2.18	0.42
1:B:202:PRO:HD3	1:B:240:PHE:CE2	2.54	0.42
1:D:108:LYS:O	1:D:111:ASP:HB2	2.19	0.42
1:D:192:PHE:CD2	1:D:226:MET:HE1	2.55	0.42
1:A:317:LYS:HD3	1:A:317:LYS:HA	1.92	0.41
1:D:102:ASP:HA	1:D:103:PRO:HD2	1.87	0.41
1:D:39:TYR:OH	1:D:148:LYS:O	2.32	0.41
1:D:51:SER:HA	1:D:58:TYR:CD2	2.55	0.41
1:B:98:TYR:HB2	1:B:105:ILE:HG13	2.02	0.41
1:D:292:THR:O	1:D:296:PRO:HA	2.21	0.41
1:B:266:ASN:CB	1:B:270[A]:MET:HE2	2.50	0.41
1:C:76:ASN:O	1:C:76:ASN:CG	2.58	0.41
1:D:142:ASP:HB2	4:D:2053:HOH:O	2.21	0.40
1:D:205:TRP:CB	1:D:244:ALA:HB1	2.51	0.40
1:C:228:GLY:O	1:C:249:PHE:HA	2.22	0.40
1:D:68:ASP:HB3	1:D:71:GLY:HA3	2.03	0.40
2:A:500:GLC:O5	3:A:501:IFM:H2C1	2.21	0.40
1:D:90:ASN:OD1	1:D:293:ARG:HG2	2.21	0.40
1:D:345:PRO:HA	1:D:355:ASP:HB3	2.02	0.40

All (2) 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)
4:A:2185:HOH:O	4:A:2185:HOH:O[6_555]	0.77	1.43
1:D:187:ASP:O	1:D:219:ASN:ND2[6_554]	1.98	0.22

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	348/380 (92%)	338 (97%)	9 (3%)	1 (0%)	44	44
1	B	348/380 (92%)	338 (97%)	9 (3%)	1 (0%)	44	44
1	C	343/380 (90%)	333 (97%)	10 (3%)	0	100	100
1	D	338/380 (89%)	316 (94%)	20 (6%)	2 (1%)	28	24
All	All	1377/1520 (91%)	1325 (96%)	48 (4%)	4 (0%)	44	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	TYR
1	D	252	TYR
1	B	252	TYR
1	D	361	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	298/328 (91%)	290 (97%)	8 (3%)	50	54
1	B	298/328 (91%)	288 (97%)	10 (3%)	42	43
1	C	295/328 (90%)	282 (96%)	13 (4%)	33	31
1	D	228/328 (70%)	213 (93%)	15 (7%)	19	16
All	All	1119/1312 (85%)	1073 (96%)	46 (4%)	35	35

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	TRP
1	A	166	LEU
1	A	206	GLU
1	A	272	LYS
1	A	275	LYS
1	A	315	TYR
1	A	333	GLU

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Mol	Chain	Res	Type
1	A	339	GLN
1	B	48	TRP
1	B	129	GLN
1	B	268	VAL
1	B	293	ARG
1	B	315	TYR
1	B	317	LYS
1	B	333	GLU
1	B	339	GLN
1	B	360	GLU
1	B	374	LYS
1	C	48	TRP
1	C	76	ASN
1	C	77	PRO
1	C	135	LYS
1	C	206	GLU
1	C	220	THR
1	C	230	TRP
1	C	242	LEU
1	C	250	TYR
1	C	265	THR
1	C	315	TYR
1	C	333	GLU
1	C	339	GLN
1	D	48	TRP
1	D	55	ASP
1	D	139	LEU
1	D	166	LEU
1	D	173	LEU
1	D	197	SER
1	D	226	MET
1	D	250	TYR
1	D	269	SER
1	D	275	LYS
1	D	315	TYR
1	D	317	LYS
1	D	333	GLU
1	D	339	GLN
1	D	362	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	90	ASN
1	A	94	GLN
1	A	169	ASN
1	A	245	HIS
1	A	266	ASN
1	A	335	HIS
1	A	339	GLN
1	B	90	ASN
1	B	169	ASN
1	B	179	ASN
1	B	339	GLN
1	B	380	GLN
1	C	60	HIS
1	C	75	GLN
1	C	90	ASN
1	C	237	GLN
1	C	335	HIS
1	C	339	GLN
1	C	358	ASN
1	D	63	HIS
1	D	219	ASN
1	D	237	GLN
1	D	266	ASN
1	D	271	GLN
1	D	335	HIS
1	D	339	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 carbohydrates in this entry.

5.6 Ligand geometry

8 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	GLC	A	500	3	11,11,12	0.60	0	13,15,17	1.30	1 (7%)
3	IFM	A	501	2	9,10,10	0.97	0	9,13,13	1.52	1 (11%)
2	GLC	B	500	3	11,11,12	0.52	0	13,15,17	1.15	2 (15%)
3	IFM	B	501	2	9,10,10	0.77	0	9,13,13	1.52	2 (22%)
2	GLC	C	500	3	11,11,12	0.55	0	13,15,17	1.11	2 (15%)
3	IFM	C	501	2	9,10,10	1.10	1 (11%)	9,13,13	1.75	2 (22%)
2	GLC	D	500	3	11,11,12	0.68	0	13,15,17	0.87	0
3	IFM	D	501	2	9,10,10	0.82	0	9,13,13	2.27	1 (11%)

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	GLC	A	500	3	-	0/2/19/22	0/1/1/1
3	IFM	A	501	2	-	0/2/16/16	0/1/1/1
2	GLC	B	500	3	-	0/2/19/22	0/1/1/1
3	IFM	B	501	2	-	0/2/16/16	0/1/1/1
2	GLC	C	500	3	-	0/2/19/22	0/1/1/1
3	IFM	C	501	2	-	0/2/16/16	0/1/1/1
2	GLC	D	500	3	-	0/2/19/22	0/1/1/1
3	IFM	D	501	2	-	0/2/16/16	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	IFM	C2-C3	2.87	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	IFM	C5-C1-N	-2.53	106.30	112.48
2	C	500	GLC	O5-C1-C2	-2.29	107.20	110.79
2	B	500	GLC	O2-C2-C3	-2.02	106.21	110.17
3	C	501	IFM	C2-C3-C4	2.26	112.97	110.30
2	B	500	GLC	C1-O5-C5	2.43	115.51	112.17
2	C	500	GLC	C1-O5-C5	2.51	115.63	112.17
3	B	501	IFM	C1-N-C2	3.06	115.63	111.86
3	A	501	IFM	C1-N-C2	3.41	116.05	111.86
2	A	500	GLC	C1-O5-C5	3.94	117.60	112.17
3	C	501	IFM	C1-N-C2	4.20	117.03	111.86
3	D	501	IFM	C1-N-C2	6.12	119.39	111.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	GLC	1	0
3	A	501	IFM	1	0
3	B	501	IFM	2	0
3	C	501	IFM	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	345/380 (90%)	-0.58	5 (1%) 75 79	13, 19, 32, 67	0
1	B	346/380 (91%)	-0.52	1 (0%) 93 94	12, 19, 32, 49	0
1	C	344/380 (90%)	-0.63	0 100 100	12, 19, 31, 51	0
1	D	342/380 (90%)	1.58	112 (32%) 0 0	30, 56, 77, 85	0
All	All	1377/1520 (90%)	-0.04	118 (8%) 11 14	12, 22, 64, 85	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	363	TYR	11.2
1	D	347	THR	6.4
1	D	353	TYR	6.2
1	D	378	SER	6.1
1	D	352	THR	5.5
1	D	112	MET	5.4
1	D	370	TYR	5.3
1	D	212	GLY	5.1
1	D	73	SER	5.0
1	D	351	PHE	5.0
1	D	346	TYR	4.8
1	D	70	ASN	4.8
1	D	209	LEU	4.4
1	D	358	ASN	4.4
1	D	242	LEU	4.3
1	D	355	ASP	4.3
1	D	313	ALA	4.2
1	D	376	ARG	4.1
1	D	280	ILE	4.1
1	D	91	PHE	3.9
1	D	360	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	86	SER	3.8
1	D	116	ALA	3.8
1	A	73	SER	3.8
1	D	67	PRO	3.8
1	D	240	PHE	3.7
1	D	216	THR	3.7
1	D	84	GLN	3.6
1	D	344	VAL	3.6
1	D	273	TRP	3.6
1	D	215	ILE	3.6
1	D	213	GLY	3.6
1	D	53	ALA	3.5
1	D	340	ILE	3.5
1	D	214	SER	3.4
1	D	350	GLU	3.4
1	D	356	TYR	3.3
1	D	95	LEU	3.3
1	D	379	LYS	3.3
1	D	43	CYS	3.3
1	D	42	PHE	3.3
1	D	106	LEU	3.3
1	A	72	GLY	3.2
1	D	267	TRP	3.2
1	D	297	TRP	3.2
1	D	69	PRO	3.2
1	D	74	GLY	3.2
1	D	365	LEU	3.1
1	D	268	VAL	3.1
1	D	315	TYR	3.1
1	D	372	VAL	3.1
1	D	274	ALA	3.0
1	D	109	HIS	3.0
1	D	245	HIS	3.0
1	D	300	SER	3.0
1	D	283	PRO	2.9
1	D	281	PHE	2.9
1	D	250	TYR	2.9
1	D	306	THR	2.8
1	D	323	VAL	2.8
1	D	97	ARG	2.8
1	D	203	SER	2.8
1	D	304	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	72	GLY	2.7
1	D	246	PHE	2.7
1	D	272	LYS	2.7
1	D	375	PHE	2.7
1	A	74	GLY	2.7
1	D	82	GLY	2.7
1	D	89	SER	2.7
1	D	369	ALA	2.7
1	D	364	TYR	2.7
1	D	287	PRO	2.7
1	D	58	TYR	2.6
1	D	361	PRO	2.6
1	D	310	TYR	2.6
1	D	278	GLY	2.6
1	D	85	GLU	2.6
1	D	269	SER	2.6
1	A	70	ASN	2.6
1	D	93	PRO	2.6
1	D	121	LEU	2.5
1	D	150	LYS	2.5
1	D	227	ILE	2.5
1	D	325	ALA	2.5
1	D	320	GLU	2.5
1	D	354	LEU	2.4
1	D	373	GLY	2.4
1	D	374	LYS	2.4
1	D	329	THR	2.4
1	D	205	TRP	2.4
1	D	309	GLN	2.3
1	D	243	ASN	2.3
1	D	328	ILE	2.3
1	D	239	PRO	2.3
1	D	110	MET	2.3
1	D	318	ALA	2.3
1	D	253	PHE	2.3
1	D	198	TYR	2.2
1	D	276	GLU	2.2
1	D	321	ALA	2.2
1	D	298	ASN	2.2
1	D	72	GLY	2.2
1	D	249	PHE	2.1
1	D	301	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	348	SER	2.1
1	D	107	THR	2.1
1	D	277	ASN	2.1
1	A	131	GLU	2.1
1	D	37	LEU	2.1
1	D	368	THR	2.1
1	D	305	ARG	2.0
1	D	254	ALA	2.0
1	D	322	GLY	2.0
1	D	357	GLU	2.0
1	D	149	ILE	2.0
1	D	194	ILE	2.0
1	D	229	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	IFM	C	501	10/10	0.97	0.11	2.21	14,15,15,16	0
3	IFM	B	501	10/10	0.98	0.17	1.86	14,14,15,16	0
2	GLC	B	500	11/12	0.98	0.12	1.12	16,17,19,20	0
3	IFM	D	501	10/10	0.76	0.21	0.84	39,44,45,45	0
2	GLC	D	500	11/12	0.94	0.15	0.51	41,42,43,45	0
2	GLC	C	500	11/12	0.98	0.08	0.20	18,19,21,22	0
3	IFM	A	501	10/10	0.97	0.08	0.04	14,14,14,15	0
2	GLC	A	500	11/12	0.98	0.05	-3.15	17,17,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.