Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:05 PM BST

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)

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

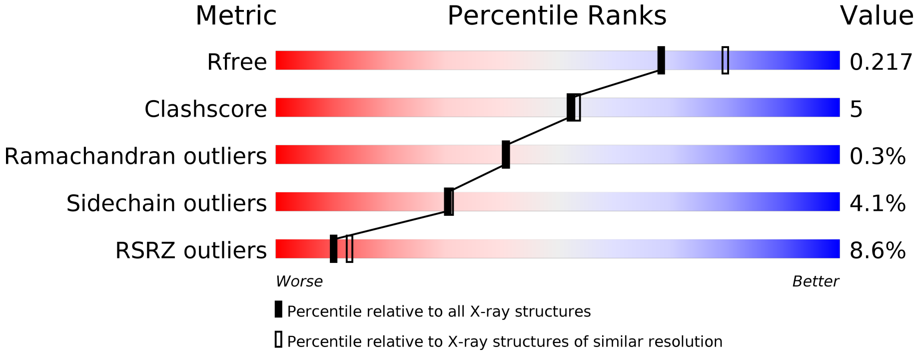
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance ⓘ

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

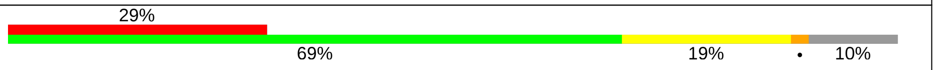
The reported resolution of this entry is 2.10 Å.

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 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	380	
1	B	380	
1	C	380	
1	D	380	

2 Entry composition ⓘ

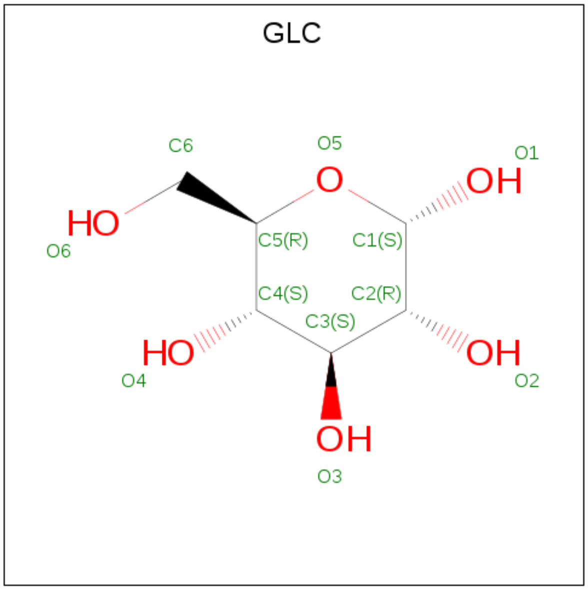
There are 4 unique types of molecules in this entry. The entry contains 12467 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2826	C 1822	N 468	O 528	S 8	0	5	0
1	B	346	Total 2832	C 1827	N 470	O 526	S 9	0	4	0
1	C	344	Total 2806	C 1808	N 467	O 523	S 8	0	1	0
1	D	342	Total 2545	C 1628	N 432	O 478	S 7	0	0	0

- Molecule 2 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



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

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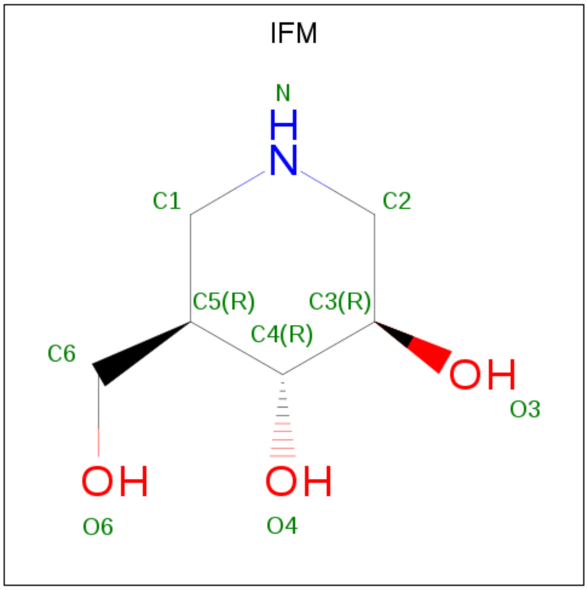
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 11 6 5	0	0
2	D	1	Total C O 11 6 5	0	0

- 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 10 6 1 3	0	0
3	B	1	Total C N O 10 6 1 3	0	0
3	C	1	Total C N O 10 6 1 3	0	0
3	D	1	Total C N O 10 6 1 3	0	0

- Molecule 4 is water.

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

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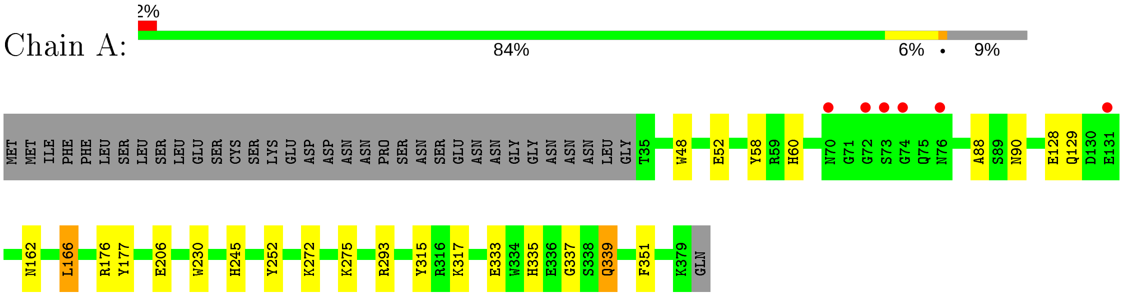
Mol	**Chain**	**Residues**	**Atoms**		**ZeroOcc**	**AltConf**
			Total	O		
4	D	127	127	127	0	0

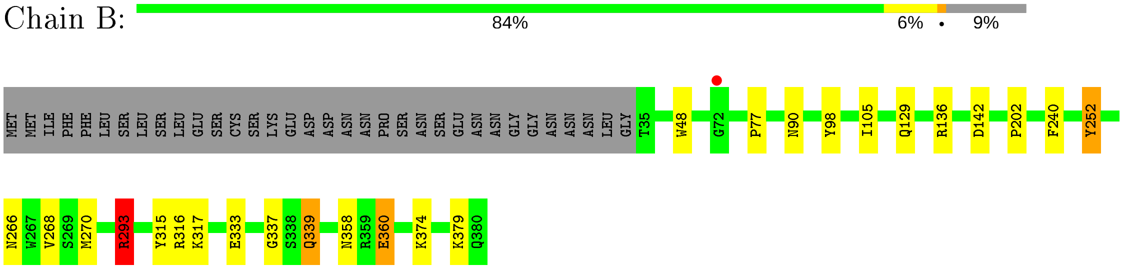
3 Residue-property plots ⓘ

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

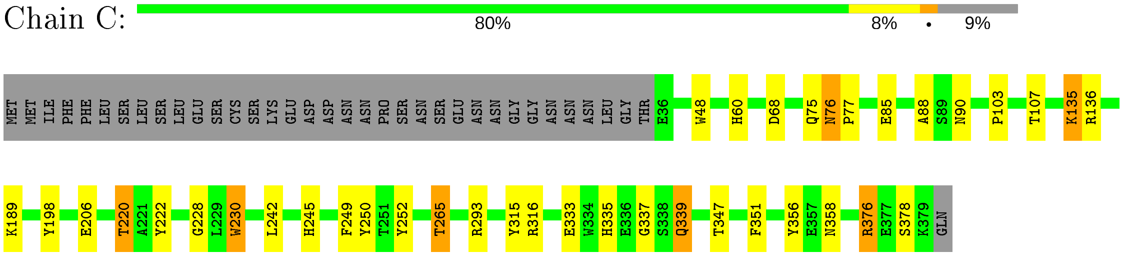
- Molecule 1: GLYCOSYL HYDROLASE FAMILY 71



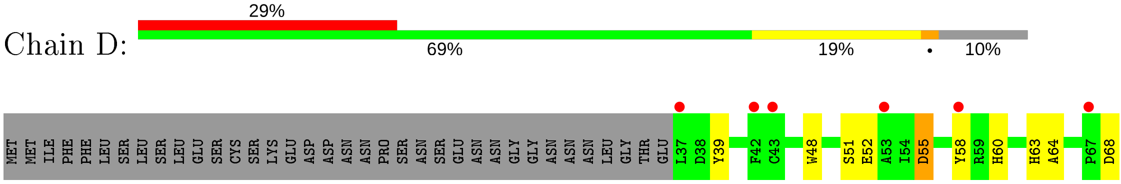
- Molecule 1: GLYCOSYL HYDROLASE FAMILY 71

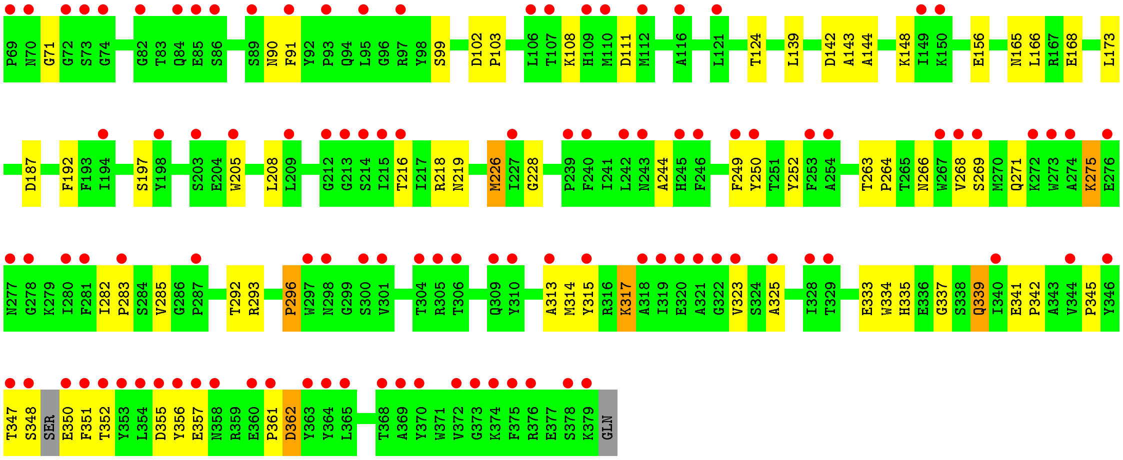


- Molecule 1: GLYCOSYL HYDROLASE FAMILY 71



- Molecule 1: GLYCOSYL HYDROLASE FAMILY 71




P69
N70
G71
G72
S73
G74
G82
T83
Q84
E85
S86
S89
N90
F91
Y92
P93
Q94
L95
G96
R97
Y98
S99
D102
P103
L106
T107
K108
H109
M110
D111
M112
A116
L121
T124
L139
D142
A143
A144
K148
I149
K150
E156
N165
L166
R167
E168
L173
D187
F192
F193
I194
S197
Y198
S203
E204
W205
L208
L209
G212
G213
S214
I215
T216
I217
R218
N219
M226
I227
G228
P239
F240
I241
L242
N243
A244
H245
F246
F249
Y250
T251
Y252
F253
A254
T263
P264
T265
N266
W267
V268
S269
M270
Q271
K272
W273
A274
K275
E276
N277
G278
K279
I280
F281
I282
P283
S284
V285
G286
P287
T292
R293
P296
W297
N298
G299
S300
V301
T304
R305
T306
Q309
Y310
A313
M314
Y315
R316
K317
A318
I319
E320
A321
G322
V323
S324
A325
I328
T329
E333
W334
H335
E336
G337
S338
Q339
I340
E341
P342
A343
V344
P345
Y346
T347
S348
SER
E350
F351
T352
Y353
L354
D355
Y356
E357
N358
R359
E360
P361
D362
Y363
Y364
L365
T368
A369
Y370
W371
V372
G373
K374
F375
R376
E377
S378
K379
GLN

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
$< I/\sigma(I) >$ [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 (5.00%)	wwPDB-VP
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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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 ⓘ

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%)	41	41
1	B	348/380 (92%)	338 (97%)	9 (3%)	1 (0%)	41	41
1	C	343/380 (90%)	333 (97%)	10 (3%)	0	100	100
1	D	338/380 (89%)	316 (94%)	20 (6%)	2 (1%)	25	21
All	All	1377/1520 (91%)	1325 (96%)	48 (4%)	4 (0%)	41	41

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%)	44	48
1	B	298/328 (91%)	288 (97%)	10 (3%)	37	39
1	C	295/328 (90%)	282 (96%)	13 (4%)	28	28
1	D	228/328 (70%)	213 (93%)	15 (7%)	16	14
All	All	1119/1312 (85%)	1073 (96%)	46 (4%)	30	31

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 monosaccharides 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	$\#\|Z\| > 2$
3	IFM	A	501	2	9,10,10	0.99	0	9,13,13	1.69	1 (11%)
3	IFM	C	501	2	9,10,10	1.18	1 (11%)	9,13,13	1.87	2 (22%)
3	IFM	D	501	2	9,10,10	0.88	1 (11%)	9,13,13	2.55	1 (11%)
2	GLC	B	500	3	11,11,12	0.53	0	15,15,17	1.20	2 (13%)
3	IFM	B	501	2	9,10,10	0.83	1 (11%)	9,13,13	1.41	1 (11%)
2	GLC	D	500	3	11,11,12	0.68	0	15,15,17	0.84	0
2	GLC	C	500	3	11,11,12	0.56	0	15,15,17	1.06	2 (13%)
2	GLC	A	500	3	11,11,12	0.61	0	15,15,17	1.26	1 (6%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	IFM	C2-C3	3.20	1.55	1.52
3	D	501	IFM	C2-C3	2.18	1.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	IFM	C2-C3	2.14	1.54	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	IFM	C1-N-C2	7.00	119.39	111.70
3	C	501	IFM	C1-N-C2	4.86	117.03	111.70
2	A	500	GLC	C1-O5-C5	3.99	117.60	112.19
3	A	501	IFM	C1-N-C2	3.96	116.05	111.70
3	B	501	IFM	C1-N-C2	3.58	115.63	111.70
2	C	500	GLC	C1-O5-C5	2.54	115.63	112.19
2	B	500	GLC	C1-O5-C5	2.45	115.51	112.19
2	C	500	GLC	O5-C1-C2	-2.32	107.20	110.77
3	C	501	IFM	C2-C3-C4	2.25	112.97	110.33
2	B	500	GLC	O5-C5-C6	2.17	110.60	107.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	500	GLC	O5-C5-C6-O6
2	D	500	GLC	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	IFM	1	0
3	C	501	IFM	1	0
3	B	501	IFM	2	0
2	A	500	GLC	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%)	-0.59	6 (1%)	70	74	13, 19, 32, 67	0
1	B	346/380 (91%)	-0.52	1 (0%)	94	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	119 (8%)	10	13	12, 22, 64, 85	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	363	TYR	11.4
1	D	347	THR	6.3
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	4.9
1	D	346	TYR	4.8
1	D	70	ASN	4.8
1	D	358	ASN	4.5
1	D	209	LEU	4.4
1	D	242	LEU	4.4
1	D	355	ASP	4.3
1	D	313	ALA	4.2
1	D	280	ILE	4.2
1	D	376	ARG	4.1
1	A	73	SER	3.8
1	D	91	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	360	GLU	3.8
1	D	86	SER	3.7
1	D	116	ALA	3.7
1	D	240	PHE	3.7
1	D	67	PRO	3.7
1	D	84	GLN	3.7
1	D	273	TRP	3.7
1	D	216	THR	3.7
1	D	215	ILE	3.6
1	D	53	ALA	3.6
1	D	344	VAL	3.5
1	D	213	GLY	3.5
1	D	214	SER	3.5
1	D	340	ILE	3.4
1	D	350	GLU	3.4
1	D	356	TYR	3.3
1	D	43	CYS	3.3
1	D	42	PHE	3.3
1	D	95	LEU	3.3
1	D	379	LYS	3.3
1	A	72	GLY	3.3
1	D	297	TRP	3.2
1	D	267	TRP	3.2
1	D	69	PRO	3.2
1	D	106	LEU	3.2
1	D	74	GLY	3.2
1	D	268	VAL	3.1
1	D	365	LEU	3.1
1	D	372	VAL	3.1
1	D	315	TYR	3.1
1	D	274	ALA	3.0
1	D	109	HIS	3.0
1	D	245	HIS	3.0
1	D	300	SER	2.9
1	D	283	PRO	2.8
1	D	281	PHE	2.8
1	D	250	TYR	2.8
1	D	306	THR	2.8
1	D	272	LYS	2.8
1	D	246	PHE	2.8
1	D	375	PHE	2.8
1	D	97	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	203	SER	2.8
1	D	369	ALA	2.7
1	B	72	GLY	2.7
1	D	304	THR	2.7
1	D	89	SER	2.7
1	D	364	TYR	2.7
1	D	323	VAL	2.6
1	D	278	GLY	2.6
1	D	361	PRO	2.6
1	D	82	GLY	2.6
1	A	74	GLY	2.6
1	D	227	ILE	2.6
1	D	58	TYR	2.6
1	D	93	PRO	2.6
1	D	287	PRO	2.6
1	D	310	TYR	2.6
1	D	269	SER	2.6
1	D	85	GLU	2.6
1	A	70	ASN	2.5
1	D	373	GLY	2.5
1	D	121	LEU	2.5
1	D	354	LEU	2.5
1	D	320	GLU	2.5
1	D	150	LYS	2.5
1	D	325	ALA	2.4
1	D	328	ILE	2.4
1	D	239	PRO	2.4
1	D	329	THR	2.4
1	D	243	ASN	2.3
1	D	309	GLN	2.3
1	D	205	TRP	2.3
1	D	318	ALA	2.3
1	D	374	LYS	2.3
1	D	198	TYR	2.3
1	D	110	MET	2.2
1	D	253	PHE	2.2
1	D	276	GLU	2.2
1	D	298	ASN	2.2
1	D	321	ALA	2.2
1	D	249	PHE	2.2
1	D	301	VAL	2.1
1	D	107	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	72	GLY	2.1
1	D	368	THR	2.1
1	D	277	ASN	2.1
1	D	348	SER	2.1
1	D	305	ARG	2.1
1	D	322	GLY	2.1
1	A	76	ASN	2.0
1	D	37	LEU	2.0
1	D	254	ALA	2.0
1	A	131	GLU	2.0
1	D	357	GLU	2.0
1	D	149	ILE	2.0
1	D	194	ILE	2.0
1	D	319	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled '$Q < 0.9$' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IFM	D	501	10/10	0.77	0.21	39,44,45,45	0
2	GLC	D	500	11/12	0.94	0.15	41,42,43,45	0
3	IFM	A	501	10/10	0.97	0.08	14,14,14,15	0
3	IFM	C	501	10/10	0.97	0.11	14,15,15,16	0
3	IFM	B	501	10/10	0.98	0.16	14,14,15,16	0
2	GLC	B	500	11/12	0.98	0.12	16,17,19,20	0
2	GLC	C	500	11/12	0.98	0.08	18,19,21,22	0
2	GLC	A	500	11/12	0.98	0.05	17,17,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.