



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:50 AM UTC

PDB ID : 4AD2 / pdb_00004ad2
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

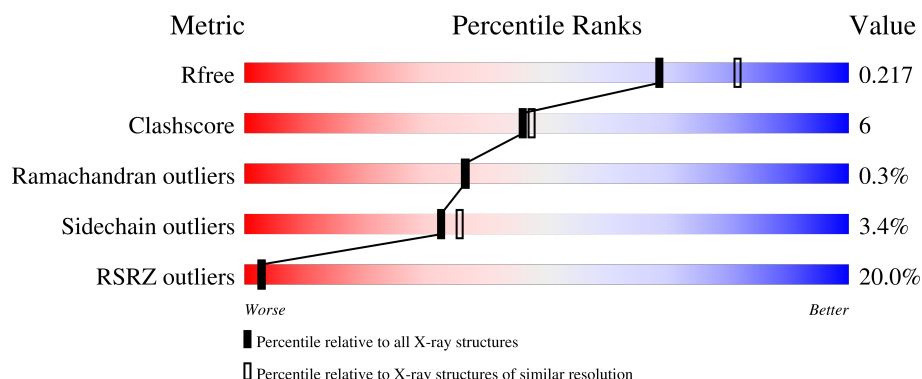
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	380	2% 84% 6% • 9%
1	B	380	% 84% 5% • 9%
1	C	380	% 80% 9% • 9%
1	D	380	69% 68% 19% • 10%

2 Entry composition [i](#)

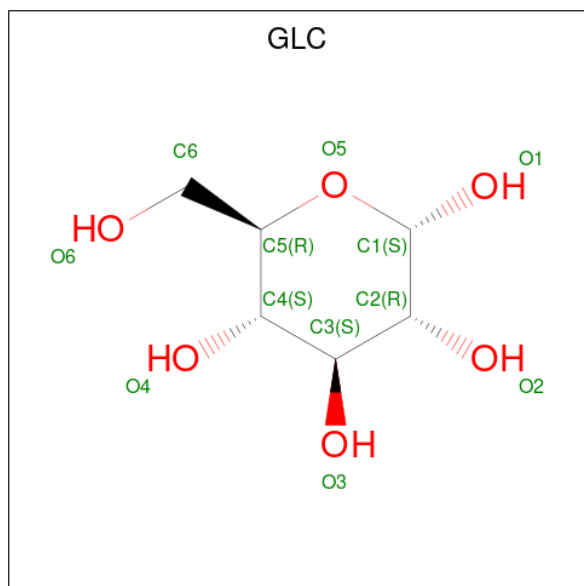
There are 4 unique types of molecules in this entry. The entry contains 12467 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



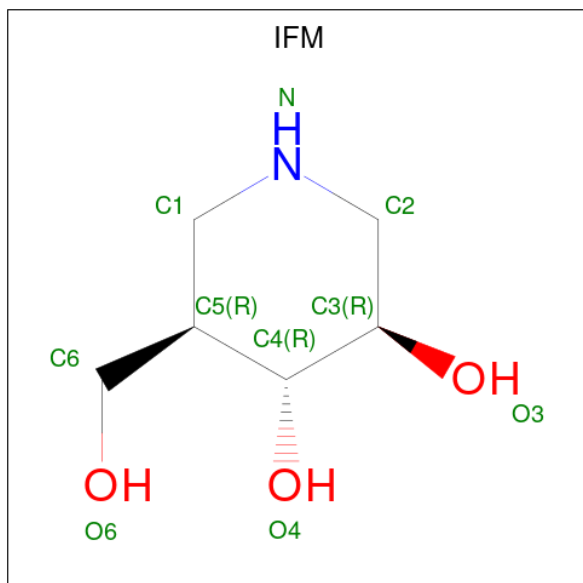
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		

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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 (CCD ID: 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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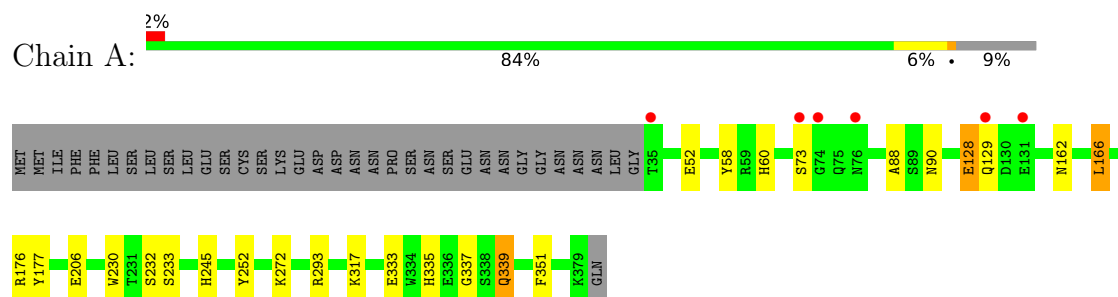
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	127	Total 127	O 127	0	0

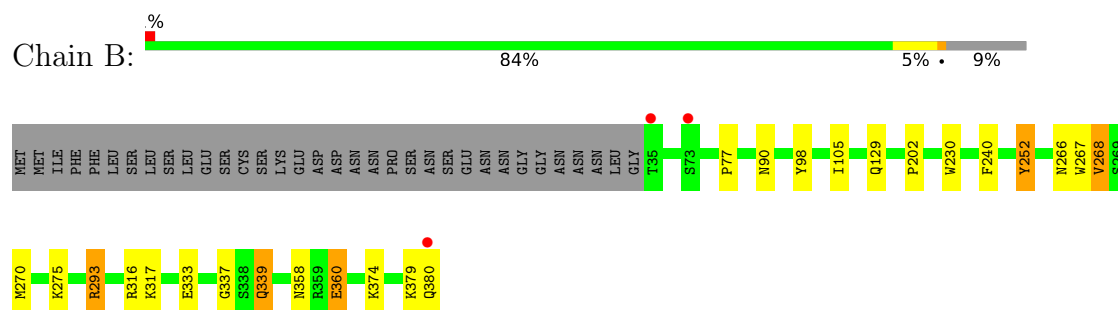
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

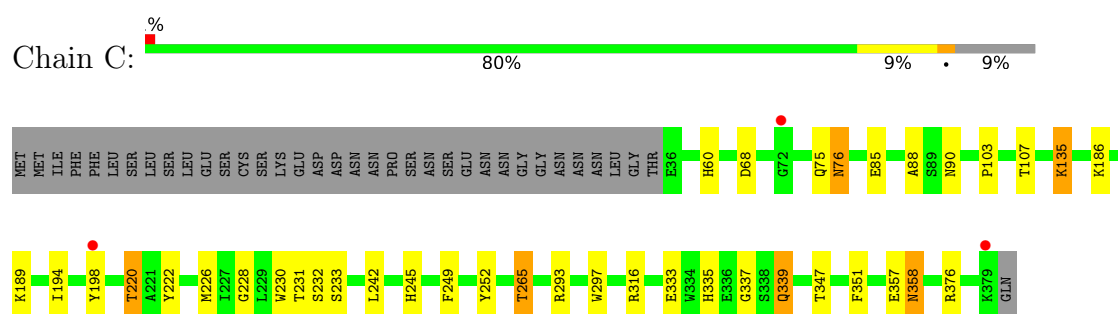
• Molecule 1: GLYCOSYL HYDROLASE FAMILY 71



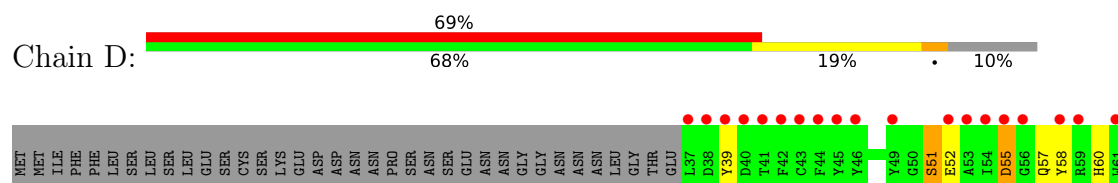
• Molecule 1: GLYCOSYL HYDROLASE FAMILY 71

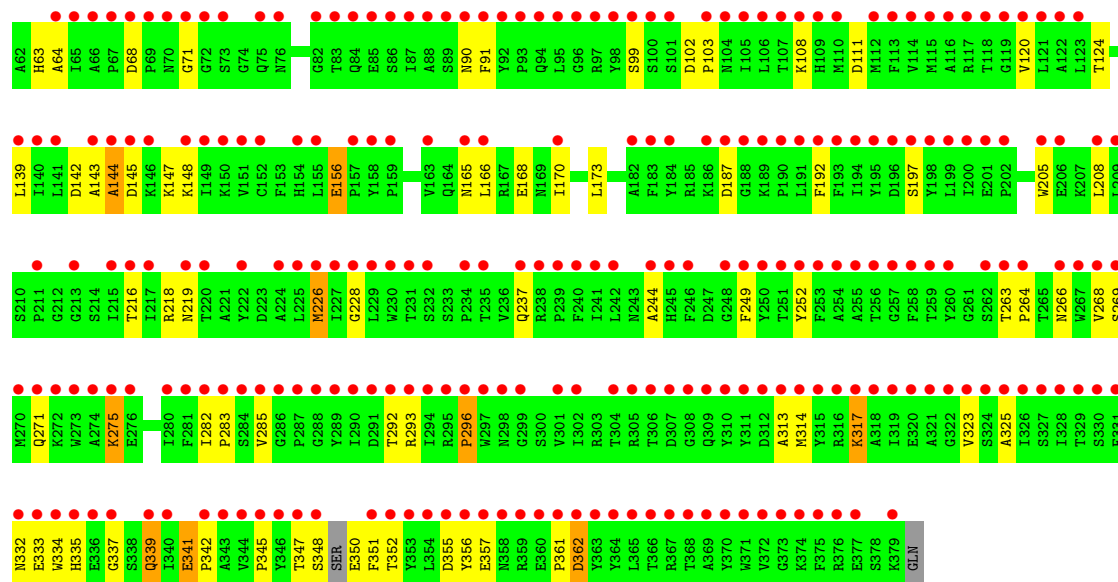


• Molecule 1: GLYCOSYL HYDROLASE FAMILY 71



• Molecule 1: GLYCOSYL HYDROLASE FAMILY 71





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 (5.00%)	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)	0.31 , 49.3	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

5.1 Standard geometry

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

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	3/2933 (0.1%)	0.84	2/3995 (0.1%)
1	B	0.76	1/2936 (0.0%)	0.84	1/3999 (0.0%)
1	C	0.82	5/2901 (0.2%)	0.83	0/3950
1	D	0.77	2/2627 (0.1%)	0.99	6/3602 (0.2%)
All	All	0.80	11/11397 (0.1%)	0.87	9/15546 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	357	GLU	C-O	-6.66	1.18	1.24
1	C	233	SER	C-O	-6.58	1.15	1.23
1	A	232	SER	C-O	-6.47	1.17	1.23
1	C	232	SER	C-O	-5.86	1.18	1.23
1	B	268	VAL	CA-CB	5.75	1.61	1.54
1	D	51	SER	CA-C	-5.46	1.45	1.52
1	D	51	SER	C-O	-5.42	1.17	1.23
1	A	128	GLU	C-O	-5.27	1.18	1.24
1	C	231	THR	C-O	-5.17	1.17	1.24
1	C	358	ASN	C-O	-5.10	1.16	1.24
1	A	233	SER	C-O	-5.03	1.17	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	296	PRO	N-CA-CB	6.42	109.99	103.25
1	D	332	ASN	N-CA-C	6.35	117.91	110.41
1	D	341	GLU	CA-C-N	6.24	127.64	119.84
1	D	341	GLU	C-N-CA	6.24	127.64	119.84
1	D	144	ALA	N-CA-C	6.22	118.15	111.36
1	A	232	SER	N-CA-C	6.19	118.10	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	VAL	N-CA-CB	6.18	118.95	110.54
1	A	73	SER	N-CA-C	5.66	117.53	111.36
1	D	237	GLN	N-CA-C	5.61	117.48	111.36

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	20	0
1	C	2806	0	2662	37	0
1	D	2545	0	2183	53	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	11	0
4	D	127	0	0	9	0
All	All	12467	0	10305	123	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 6.

All (123) 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:D:192:PHE:HB2	1:D:226:MET:HE1	1.33	1.07

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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:D:226:MET:HE2	1:D:226:MET:HA	1.37	1.03
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: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
1:C:220:THR:HG23	1:C:222:TYR:H	1.48	0.78
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:B:267:TRP:HD1	1:B:270[A]:MET:HE3	1.65	0.60
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:NE2	1:B:339:GLN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:266:ASN:CB	1:B:270[A]:MET:HE2	2.35	0.56
1:A:245:HIS:HD2	4:A:2281:HOH:O	1.89	0.56
1:B:266:ASN:HB3	1:B:270[A]:MET:HE2	1.89	0.55
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:90:ASN:HD21	1:C:293:ARG:H	1.58	0.52
1:C:135:LYS:HG2	4:C:2160:HOH:O	2.10	0.52
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:NE2	1:A:339:GLN:H	2.08	0.51
1:D:51:SER:O	1:D:55:ASP:O	2.29	0.50
1:A:230:TRP:C	1:A:230:TRP:CD1	2.89	0.50
1:B:90:ASN:HD21	1:B:293:ARG:H	1.59	0.50
1:C:339:GLN:NE2	1:C:339:GLN:H	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:194:ILE:HD11	1:C:226:MET:HE3	1.96	0.47
1:C:293:ARG:HD3	1:C:351:PHE:CZ	2.49	0.47
1:C:230:TRP:CD1	1:C:230:TRP:C	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:HIS:HD2	1:D:64:ALA:O	1.98	0.46
1:C:76:ASN:CG	1:C:76:ASN:O	2.58	0.46
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:B:266:ASN:HB2	1:B:270[A]:MET:HE2	2.00	0.44
1:D:145:ASP:C	1:D:147:LYS:N	2.75	0.44
1:D:226:MET:CE	1:D:226:MET:CA	2.91	0.44
1:B:230:TRP:C	1:B:230:TRP:CD1	2.96	0.43
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: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:C:297:TRP:CD1	1:C:297:TRP:H	2.36	0.42
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:55:ASP:C	1:D:57:GLN:H	2.27	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
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: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: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 sym-

metry 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 [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	348/380 (92%)	338 (97%)	9 (3%)	1 (0%)	36	36
1	B	348/380 (92%)	338 (97%)	9 (3%)	1 (0%)	36	36
1	C	343/380 (90%)	333 (97%)	10 (3%)	0	100	100
1	D	338/380 (89%)	316 (94%)	20 (6%)	2 (1%)	21	18
All	All	1377/1520 (91%)	1325 (96%)	48 (4%)	4 (0%)	36	36

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 [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	298/328 (91%)	293 (98%)	5 (2%)	53	62
1	B	298/328 (91%)	288 (97%)	10 (3%)	32	35
1	C	295/328 (90%)	287 (97%)	8 (3%)	39	45
1	D	228/328 (70%)	213 (93%)	15 (7%)	15	13
All	All	1119/1312 (85%)	1081 (97%)	38 (3%)	32	35

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	LEU
1	A	206	GLU
1	A	272	LYS
1	A	333	GLU
1	A	339	GLN
1	B	129	GLN
1	B	268	VAL
1	B	275	LYS
1	B	293	ARG
1	B	317	LYS
1	B	333	GLU
1	B	339	GLN
1	B	360	GLU
1	B	374	LYS
1	B	380	GLN
1	C	76	ASN
1	C	135	LYS
1	C	186	LYS
1	C	220	THR
1	C	242	LEU
1	C	265	THR
1	C	333	GLU
1	C	339	GLN
1	D	55	ASP
1	D	120	VAL
1	D	139	LEU
1	D	156	GLU
1	D	166	LEU
1	D	170	ILE
1	D	173	LEU
1	D	197	SER
1	D	226	MET
1	D	269	SER

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Mol	Chain	Res	Type
1	D	275	LYS
1	D	317	LYS
1	D	333	GLU
1	D	339	GLN
1	D	362	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	90	ASN
1	A	169	ASN
1	A	179	ASN
1	A	243	ASN
1	A	245	HIS
1	A	266	ASN
1	A	335	HIS
1	A	339	GLN
1	B	90	ASN
1	B	94	GLN
1	B	169	ASN
1	B	179	ASN
1	B	271	GLN
1	B	339	GLN
1	C	60	HIS
1	C	75	GLN
1	C	90	ASN
1	C	94	GLN
1	C	104	ASN
1	C	129	GLN
1	C	237	GLN
1	C	309	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 oligosaccharides 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	B	501	2	10,10,10	0.89	1 (10%)	9,13,13	1.33	1 (11%)
2	GLC	D	500	3	11,11,12	0.66	0	15,15,17	0.77	0
3	IFM	A	501	2	10,10,10	1.14	2 (20%)	9,13,13	1.63	1 (11%)
2	GLC	B	500	3	11,11,12	0.51	0	15,15,17	1.11	1 (6%)
3	IFM	D	501	2	10,10,10	1.07	2 (20%)	9,13,13	2.41	1 (11%)
2	GLC	A	500	3	11,11,12	0.59	0	15,15,17	1.24	1 (6%)
3	IFM	C	501	2	10,10,10	1.19	1 (10%)	9,13,13	1.77	2 (22%)
2	GLC	C	500	3	11,11,12	0.54	0	15,15,17	0.96	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	B	501	2	-	0/2/16/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	500	3	-	2/2/19/22	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	D	501	2	-	0/2/16/16	0/1/1/1
2	GLC	A	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	C	500	3	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	IFM	C2-C3	3.43	1.55	1.52
3	D	501	IFM	C2-C3	2.37	1.54	1.52
3	B	501	IFM	C2-C3	2.33	1.54	1.52
3	D	501	IFM	C1-C5	2.14	1.54	1.52
3	A	501	IFM	C2-C3	2.05	1.54	1.52
3	A	501	IFM	C1-C5	2.04	1.54	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	IFM	C1-N-C2	6.56	119.39	111.78
3	C	501	IFM	C1-N-C2	4.53	117.03	111.78
2	A	500	GLC	C1-O5-C5	4.04	117.60	112.19
3	A	501	IFM	C1-N-C2	3.68	116.05	111.78
3	B	501	IFM	C1-N-C2	3.32	115.63	111.78
2	C	500	GLC	C1-O5-C5	2.57	115.63	112.19
2	B	500	GLC	C1-O5-C5	2.48	115.51	112.19
3	C	501	IFM	C2-C3-C4	2.23	112.97	110.25

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	B	501	IFM	2	0
3	A	501	IFM	1	0
2	A	500	GLC	1	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%)	-0.46	6 (1%) 69 71	10, 19, 32, 67	5 (1%)
1	B	346/380 (91%)	-0.47	3 (0%) 81 83	9, 19, 32, 49	4 (1%)
1	C	344/380 (90%)	-0.45	3 (0%) 81 83	12, 19, 31, 51	1 (0%)
1	D	342/380 (90%)	3.17	264 (77%) 0 0	30, 56, 77, 85	0
All	All	1377/1520 (90%)	0.44	276 (20%) 3 3	9, 21, 64, 85	10 (0%)

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	363	TYR	7.7
1	D	209	LEU	7.7
1	D	370	TYR	6.7
1	D	37	LEU	6.5
1	D	150	LYS	6.3
1	D	315	TYR	6.3
1	D	360	GLU	6.2
1	D	294	ILE	6.2
1	D	196	ASP	6.2
1	D	344	VAL	6.1
1	D	42	PHE	6.0
1	D	105	ILE	6.0
1	D	240	PHE	5.9
1	D	87	ILE	5.9
1	D	112	MET	5.9
1	D	364	TYR	5.8
1	D	149	ILE	5.8
1	D	198	TYR	5.7
1	D	121	LEU	5.7
1	D	280	ILE	5.7
1	D	253	PHE	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	287	PRO	5.6
1	D	365	LEU	5.6
1	D	356	TYR	5.5
1	D	43	CYS	5.5
1	D	369	ALA	5.5
1	D	304	THR	5.4
1	D	267	TRP	5.4
1	D	88	ALA	5.4
1	D	319	ILE	5.4
1	D	116	ALA	5.3
1	D	227	ILE	5.2
1	D	41	THR	5.2
1	D	229	LEU	5.2
1	D	252	TYR	5.2
1	D	326	ILE	5.1
1	D	321	ALA	5.1
1	D	348	SER	5.1
1	D	340	ILE	5.1
1	D	283	PRO	5.1
1	D	122	ALA	5.0
1	D	254	ALA	5.0
1	D	193	PHE	5.0
1	D	274	ALA	4.9
1	D	95	LEU	4.9
1	D	246	PHE	4.9
1	D	328	ILE	4.8
1	D	91	PHE	4.8
1	D	331	PHE	4.8
1	D	84	GLN	4.8
1	D	54	ILE	4.8
1	D	191	LEU	4.8
1	D	334	TRP	4.8
1	D	70	ASN	4.7
1	D	302	ILE	4.7
1	D	353	TYR	4.7
1	D	93	PRO	4.7
1	D	290	ILE	4.6
1	D	281	PHE	4.6
1	D	351	PHE	4.6
1	D	99	SER	4.6
1	D	250	TYR	4.6
1	D	152	CYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	301	VAL	4.5
1	D	187	ASP	4.5
1	D	273	TRP	4.5
1	D	358	ASN	4.5
1	D	205	TRP	4.5
1	D	359	ARG	4.5
1	D	375	PHE	4.5
1	D	226	MET	4.4
1	D	297	TRP	4.4
1	D	217	ILE	4.4
1	D	282	ILE	4.4
1	D	368	THR	4.4
1	D	361	PRO	4.4
1	D	251	THR	4.4
1	D	288	GLY	4.4
1	D	314	MET	4.4
1	D	346	TYR	4.3
1	D	231	THR	4.3
1	D	104	ASN	4.3
1	D	354	LEU	4.3
1	D	113	PHE	4.3
1	D	313	ALA	4.3
1	D	108	LYS	4.3
1	D	120	VAL	4.3
1	D	307	ASP	4.2
1	D	228	GLY	4.2
1	D	103	PRO	4.2
1	D	242	LEU	4.2
1	D	362	ASP	4.2
1	D	325	ALA	4.1
1	D	323	VAL	4.1
1	D	255	ALA	4.1
1	D	310	TYR	4.1
1	D	249	PHE	4.1
1	D	194	ILE	4.1
1	D	53	ALA	4.1
1	D	92	TYR	4.1
1	B	35	THR	4.1
1	D	366	THR	4.1
1	D	347	THR	4.0
1	D	145	ASP	4.0
1	D	188	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	316	ARG	4.0
1	D	329	THR	4.0
1	D	308	GLY	4.0
1	D	166	LEU	3.9
1	D	184	TYR	3.9
1	D	373	GLY	3.9
1	D	285	VAL	3.9
1	D	208	LEU	3.9
1	D	151	VAL	3.8
1	D	199	LEU	3.8
1	D	296	PRO	3.8
1	D	96	GLY	3.8
1	D	86	SER	3.8
1	D	89	SER	3.8
1	D	83	THR	3.8
1	D	225	LEU	3.8
1	A	131	GLU	3.8
1	D	182	ALA	3.8
1	D	69	PRO	3.8
1	D	73	SER	3.7
1	D	241	ILE	3.7
1	D	371	TRP	3.7
1	D	202	PRO	3.7
1	D	44	PHE	3.7
1	D	215	ILE	3.7
1	D	118	THR	3.7
1	D	192	PHE	3.7
1	D	292	THR	3.7
1	D	306	THR	3.7
1	D	157	PRO	3.7
1	D	211	PRO	3.7
1	D	372	VAL	3.7
1	D	232	SER	3.6
1	D	200	ILE	3.6
1	D	332	ASN	3.6
1	D	38	ASP	3.6
1	D	143	ALA	3.6
1	D	286	GLY	3.6
1	D	268	VAL	3.6
1	D	106	LEU	3.5
1	D	258	PHE	3.5
1	D	244	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	72	GLY	3.5
1	D	109	HIS	3.5
1	D	195	TYR	3.5
1	D	339	GLN	3.5
1	D	320	GLU	3.4
1	A	35	THR	3.4
1	D	355	ASP	3.4
1	D	289	TYR	3.4
1	D	67	PRO	3.4
1	D	245	HIS	3.4
1	D	114	VAL	3.4
1	D	90	ASN	3.3
1	D	98	TYR	3.3
1	D	141	LEU	3.3
1	D	317	LYS	3.3
1	D	123	LEU	3.2
1	D	284	SER	3.2
1	D	190	PRO	3.2
1	D	318	ALA	3.2
1	D	311	TYR	3.2
1	D	345	PRO	3.2
1	D	305	ARG	3.1
1	D	144	ALA	3.1
1	D	97	ARG	3.1
1	D	163	VAL	3.1
1	D	291	ASP	3.1
1	D	357	GLU	3.1
1	D	377	GLU	3.1
1	D	115	MET	3.1
1	A	76	ASN	3.1
1	D	117	ARG	3.1
1	D	293	ARG	3.1
1	D	189	LYS	3.1
1	D	139	LEU	3.1
1	D	230	TRP	3.0
1	D	107	THR	3.0
1	D	367	ARG	3.0
1	D	262	SER	3.0
1	D	295	ARG	3.0
1	D	264	PRO	3.0
1	D	272	LYS	3.0
1	D	197	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	52	GLU	3.0
1	D	39	TYR	3.0
1	D	155	LEU	3.0
1	D	154	HIS	3.0
1	D	46	TYR	3.0
1	D	76	ASN	2.9
1	D	140	ILE	2.9
1	D	376	ARG	2.9
1	D	146	LYS	2.9
1	D	327	SER	2.9
1	D	100	SER	2.9
1	D	186	LYS	2.9
1	D	379	LYS	2.9
1	D	59	ARG	2.8
1	D	206	GLU	2.8
1	D	298	ASN	2.7
1	D	309	GLN	2.7
1	D	213	GLY	2.7
1	D	216	THR	2.7
1	D	238	ARG	2.7
1	D	56	GLY	2.7
1	C	198	TYR	2.7
1	D	94	GLN	2.7
1	D	342	PRO	2.7
1	D	45	TYR	2.7
1	D	158	TYR	2.7
1	D	65	ILE	2.7
1	D	119	GLY	2.7
1	D	235	THR	2.6
1	D	58	TYR	2.6
1	D	256	THR	2.6
1	D	269	SER	2.6
1	D	322	GLY	2.6
1	D	324	SER	2.6
1	D	312	ASP	2.6
1	D	337	GLY	2.5
1	D	266	ASN	2.5
1	D	299	GLY	2.5
1	D	335	HIS	2.5
1	D	148	LYS	2.5
1	D	183	PHE	2.5
1	A	74	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	73	SER	2.4
1	D	259	THR	2.4
1	D	330	SER	2.4
1	D	71	GLY	2.4
1	B	380	GLN	2.4
1	D	61	TRP	2.4
1	D	101	SER	2.4
1	D	110	MET	2.4
1	D	220	THR	2.4
1	D	234	PRO	2.4
1	D	270	MET	2.4
1	D	239	PRO	2.4
1	D	275	LYS	2.4
1	D	352	THR	2.4
1	D	260	TYR	2.3
1	D	64	ALA	2.3
1	D	219	ASN	2.3
1	D	237	GLN	2.3
1	D	82	GLY	2.3
1	D	55	ASP	2.3
1	D	333	GLU	2.3
1	C	72	GLY	2.3
1	D	49	TYR	2.3
1	D	40	ASP	2.3
1	D	271	GLN	2.2
1	D	224	ALA	2.2
1	D	85	GLU	2.2
1	D	170	ILE	2.2
1	D	276	GLU	2.2
1	D	159	PRO	2.2
1	A	129	GLN	2.1
1	A	73	SER	2.1
1	D	222	TYR	2.1
1	D	68	ASP	2.1
1	D	263	THR	2.1
1	D	66	ALA	2.1
1	D	248	GLY	2.1
1	C	379	LYS	2.1
1	D	343	ALA	2.1
1	D	374	LYS	2.1
1	D	336	GLU	2.0
1	D	165	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	257	GLY	2.0
1	D	201	GLU	2.0
1	D	75	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IFM	D	501	10/10	0.71	0.19	39,44,45,45	0
2	GLC	D	500	11/12	0.88	0.15	41,42,43,45	0
2	GLC	B	500	11/12	0.97	0.05	16,17,19,20	0
3	IFM	A	501	10/10	0.97	0.05	14,14,14,15	0
3	IFM	C	501	10/10	0.97	0.07	14,15,15,16	0
2	GLC	C	500	11/12	0.97	0.06	18,19,21,22	0
2	GLC	A	500	11/12	0.98	0.04	17,17,19,19	0
3	IFM	B	501	10/10	0.98	0.06	14,14,15,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.