Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:51 PM GMT

PDB ID	:	1VFO
Title	:	Crystal structure of Thermoactinomyces vulgaris R-47 alpha-amylase 2/beta-cyclodextrin complex
Authors	:	Ohtaki, A.; Mizuno, M.; Tonozuka, T.; Sakano, Y.; Kamitori, S.
Deposited on	:	2004-04-16
Resolution	:	2.81 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

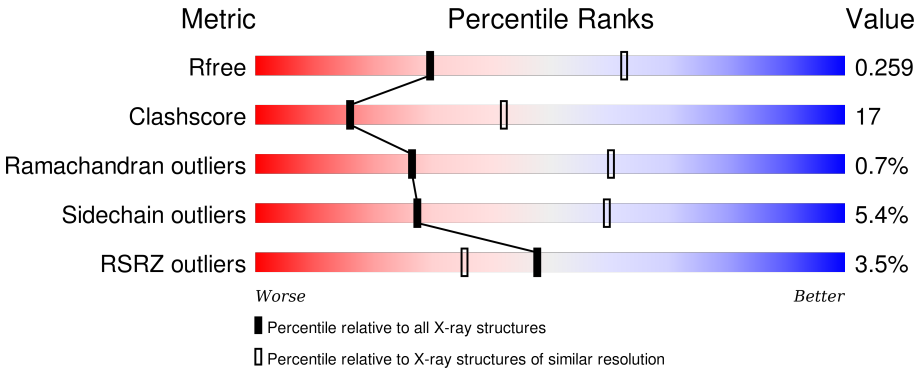
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.81 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}	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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 <=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	585	2% 69% 28%
1	B	585	5% 65% 31%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9936 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 Neopullulanase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4776	3056	833	872	15			
1	B	585	Total	C	N	O	S	0	0	0
			4776	3056	833	872	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ASN	ASP	ENGINEERED	UNP Q08751
A	421	ASN	ASP	ENGINEERED	UNP Q08751
B	325	ASN	ASP	ENGINEERED	UNP Q08751
B	421	ASN	ASP	ENGINEERED	UNP Q08751

- Molecule 2 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	7	Total	C	O	0	0
			77	42	35		

- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	7	Total	C	O	0	0
			77	42	35		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

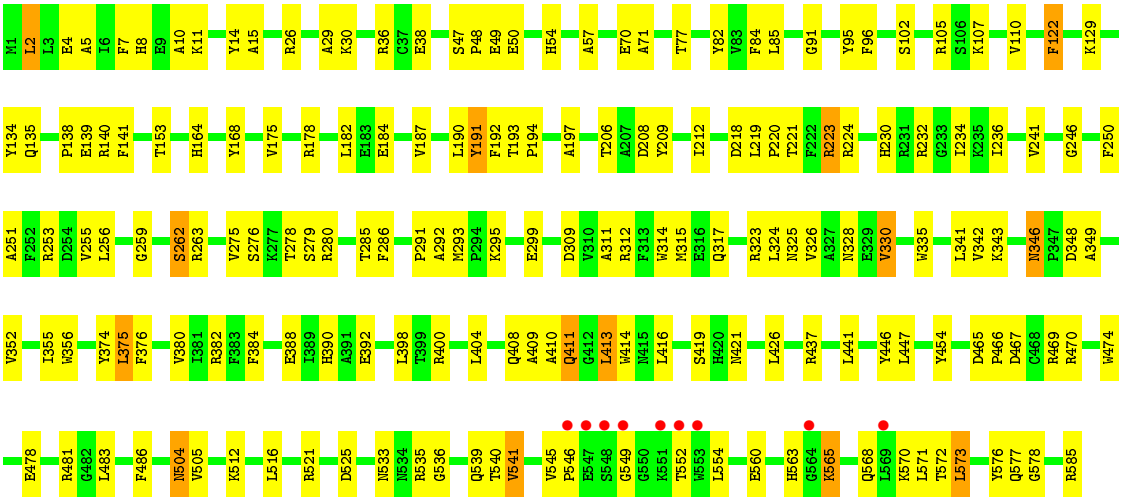
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	125	Total O 125 125	0	0
5	B	103	Total O 103 103	0	0

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 errors 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.

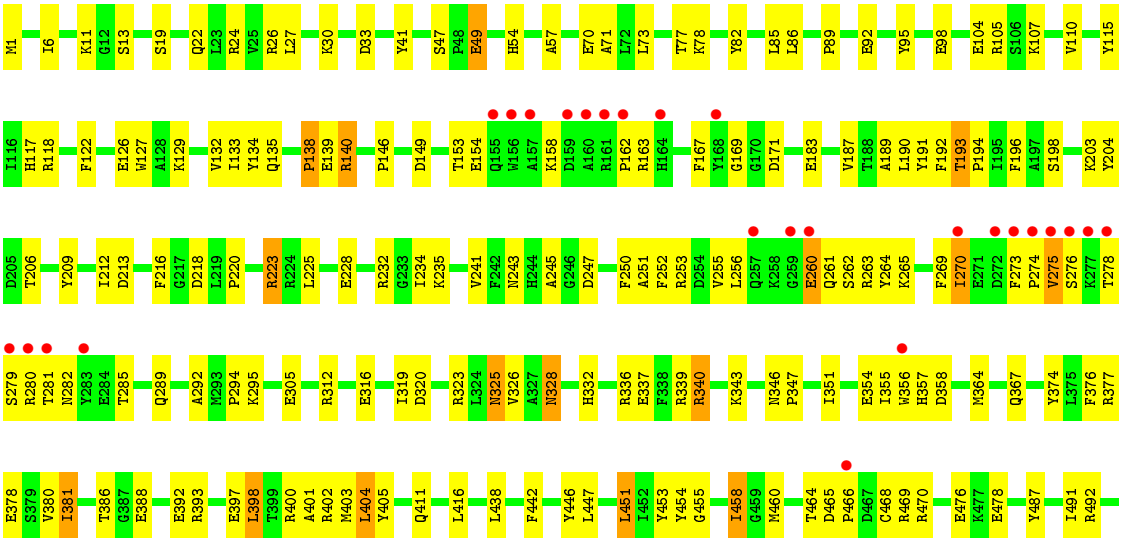
- Molecule 1: Neopullulanase 2

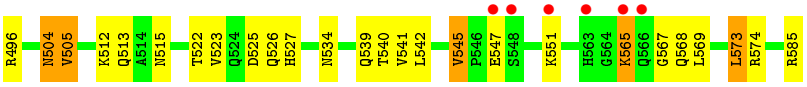
Chain A:



- Molecule 1: Neopullulanase 2

Chain B:




R496
N504
V505
K512
Q513
A514
N515
T522
V523
Q524
D525
Q526
H527
N534
Q539
T540
V541
L542
V545
P546
E547
S548
K551
H563
G564
K565
Q566
G567
Q568
L569
L573
R574
R585

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.08Å 118.81Å 114.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.87 – 2.81 38.87 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.87-2.81) 99.4 (38.87-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.256 0.208 , 0.259	Depositor DCC
R_{free} test set	3864 reflections (10.02%)	DCC
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.3	EDS
Estimated twinning fraction	0.023 for k,h,-l 0.023 for -h,-l,-k 0.023 for l,-k,h 0.009 for k,l,h 0.009 for l,h,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 38561 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9936	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CA, BGC

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	0.39	0/4906	0.64	1/6641 (0.0%)
1	B	0.38	0/4906	0.61	0/6641
All	All	0.39	0/9812	0.63	1/13282 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	323	ARG	N-CA-C	-5.06	97.34	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	TYR	Sidechain

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	4776	0	4611	129	0
1	B	4776	0	4611	195	0
2	A	77	0	63	3	0
3	B	77	0	63	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	125	0	0	9	0
5	B	103	0	0	10	0
All	All	9936	0	9348	322	0

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 17.

All (322) 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:328:ASN:HB3	1:A:355:ILE:HD12	1.37	1.02
1:B:138:PRO:HD2	1:B:193:THR:HG22	1.50	0.91
1:B:512:LYS:HE3	1:B:513:GLN:HE22	1.37	0.90
1:A:278:THR:HG23	1:A:280:ARG:H	1.36	0.89
1:B:476:GLU:HB3	5:B:1052:HOH:O	1.73	0.87
1:B:280:ARG:HA	1:B:280:ARG:HE	1.38	0.86
1:B:276:SER:HB3	1:B:278:THR:HG22	1.59	0.83
1:B:547:GLU:HG2	1:B:551:LYS:HE2	1.64	0.78
1:B:312:ARG:O	1:B:316:GLU:HG3	1.84	0.77
1:A:525:ASP:HB3	1:A:585:ARG:HD2	1.68	0.76
1:B:134:TYR:HB2	1:B:187:VAL:HG11	1.68	0.75
1:A:276:SER:OG	1:A:278:THR:HG22	1.86	0.74
1:B:285:THR:HG22	1:B:294:PRO:HA	1.69	0.74
1:B:196:PHE:HB2	5:B:1013:HOH:O	1.87	0.73
1:A:224:ARG:HA	1:A:224:ARG:HE	1.52	0.72
1:B:92:GLU:OE2	1:B:92:GLU:N	2.22	0.72
1:B:280:ARG:NE	1:B:280:ARG:HA	2.05	0.71
1:B:54:HIS:HB3	5:B:1055:HOH:O	1.90	0.71
1:B:253:ARG:HB2	1:B:253:ARG:NH1	2.06	0.70
1:B:263:ARG:HD2	5:B:1069:HOH:O	1.89	0.70
1:A:57:ALA:HA	1:A:71:ALA:HB2	1.73	0.70
1:A:410:ALA:HA	1:A:413:LEU:HD22	1.74	0.69
1:A:346:ASN:ND2	1:A:348:ASP:H	1.91	0.69
1:B:198:SER:HB3	1:B:203:LYS:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ASN:HB3	1:B:355:ILE:HG13	1.76	0.68
1:A:572:THR:C	1:A:573:LEU:HD23	2.15	0.67
1:B:241:VAL:HG23	1:B:241:VAL:O	1.95	0.67
1:B:250:PHE:CG	1:B:251:ALA:N	2.63	0.66
1:B:542:LEU:HD21	1:B:568:GLN:NE2	2.11	0.65
1:B:190:LEU:HD13	1:B:234:ILE:HG21	1.77	0.65
1:B:525:ASP:O	1:B:585:ARG:HD2	1.95	0.65
1:A:516:LEU:HD13	1:A:541:VAL:CG1	2.26	0.65
1:A:516:LEU:HD13	1:A:541:VAL:HG11	1.77	0.65
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.32	0.65
1:A:328:ASN:CB	1:A:355:ILE:HD12	2.20	0.65
1:B:256:LEU:HA	1:B:275:VAL:HB	1.80	0.64
1:B:565:LYS:O	1:B:565:LYS:HD2	1.97	0.64
1:B:253:ARG:HH11	1:B:253:ARG:HB2	1.63	0.64
1:B:253:ARG:HH11	1:B:253:ARG:CB	2.12	0.63
1:B:416:LEU:H	1:B:416:LEU:HD23	1.64	0.63
1:A:4:GLU:HG2	1:B:30:LYS:HG3	1.80	0.63
1:B:241:VAL:HG12	1:B:325:ASN:ND2	2.14	0.62
1:A:565:LYS:H	1:A:565:LYS:HD2	1.64	0.62
1:B:337:GLU:HG2	1:B:340:ARG:HH11	1.64	0.62
1:B:223:ARG:HB3	1:B:223:ARG:NH2	2.13	0.62
1:B:57:ALA:HB2	1:B:71:ALA:HB2	1.82	0.62
1:B:146:PRO:HA	1:B:149:ASP:OD2	2.00	0.62
1:B:270:ILE:HD12	1:B:270:ILE:H	1.65	0.61
1:A:36:ARG:NH2	1:A:38:GLU:OE2	2.34	0.61
1:B:526:GLN:HG3	1:B:585:ARG:OXT	2.00	0.61
1:A:309:ASP:OD2	1:A:312:ARG:NH1	2.34	0.61
1:B:245:ALA:O	1:B:294:PRO:HD2	2.01	0.61
1:B:26:ARG:HG2	1:B:70:GLU:HG3	1.83	0.60
1:A:11:LYS:N	1:A:15:ALA:HB3	2.16	0.60
1:B:212:ILE:H	1:B:212:ILE:HD12	1.65	0.60
1:B:235:LYS:HG3	1:B:320:ASP:CG	2.21	0.60
1:A:278:THR:HG23	1:A:280:ARG:N	2.14	0.60
1:A:26:ARG:HD3	1:A:70:GLU:OE2	2.02	0.60
1:B:132:VAL:HG11	1:B:491:ILE:HD12	1.84	0.59
1:A:416:LEU:HD23	1:A:416:LEU:H	1.68	0.59
1:A:504:ASN:C	1:A:504:ASN:HD22	2.06	0.59
1:A:343:LYS:HE2	1:A:349:ALA:O	2.03	0.59
1:A:447:LEU:HB2	1:A:505:VAL:CG2	2.33	0.59
1:B:163:ARG:HH11	1:B:163:ARG:HG3	1.67	0.58
1:A:138:PRO:HG2	5:A:1018:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:HG21	1:A:209:TYR:CD2	2.38	0.58
1:A:47:SER:HB3	1:A:50:GLU:HG3	1.86	0.58
1:B:402:ARG:HG2	1:B:403:MET:HE3	1.86	0.58
1:A:212:ILE:HD12	1:A:314:TRP:HH2	1.69	0.58
1:B:243:ASN:HD21	1:B:295:LYS:NZ	2.02	0.57
1:B:328:ASN:N	1:B:328:ASN:HD22	2.02	0.57
1:B:332:HIS:HD2	1:B:367:GLN:OE1	1.86	0.57
1:B:542:LEU:HD21	1:B:568:GLN:HE22	1.69	0.57
1:A:141:PHE:HB3	5:A:1112:HOH:O	2.05	0.57
1:B:319:ILE:HD12	1:B:319:ILE:C	2.25	0.57
1:B:253:ARG:HA	1:B:256:LEU:HD12	1.86	0.57
1:B:355:ILE:HD12	1:B:355:ILE:N	2.21	0.56
1:A:82:TYR:C	1:A:110:VAL:HG23	2.26	0.56
3:B:706:GLC:O5	3:B:707:GLC:H61	2.05	0.56
1:B:190:LEU:HD13	1:B:234:ILE:CG2	2.36	0.56
1:A:178:ARG:HD2	1:A:474:TRP:CH2	2.41	0.56
1:A:223:ARG:HD2	1:A:317:GLN:OE1	2.05	0.56
1:B:545:VAL:HG21	1:B:569:LEU:HB2	1.87	0.56
1:B:525:ASP:HB3	1:B:585:ARG:HD3	1.87	0.56
1:A:536:GLY:HA2	1:A:576:TYR:CE1	2.41	0.56
1:A:193:THR:HB	1:A:194:PRO:CD	2.36	0.55
1:A:392:GLU:HG3	1:A:512:LYS:HB3	1.89	0.55
1:B:133:ILE:CD1	1:B:189:ALA:HB3	2.36	0.55
1:B:465:ASP:OD2	1:B:466:PRO:HA	2.07	0.55
1:B:104:GLU:OE1	1:B:107:LYS:HE3	2.07	0.55
1:B:280:ARG:CA	1:B:280:ARG:HE	2.17	0.55
1:B:400:ARG:O	1:B:404:LEU:HD13	2.06	0.54
1:B:252:PHE:O	1:B:255:VAL:HB	2.07	0.54
1:B:243:ASN:ND2	1:B:295:LYS:NZ	2.55	0.54
1:B:171:ASP:HB2	1:B:216:PHE:O	2.08	0.54
1:B:255:VAL:HG12	1:B:275:VAL:HG21	1.90	0.54
1:B:455:GLY:HA2	1:B:458:ILE:HD11	1.90	0.54
1:B:19:SER:OG	1:B:22:GLN:HB2	2.08	0.54
1:A:573:LEU:N	1:A:573:LEU:HD23	2.22	0.54
1:B:278:THR:OG1	1:B:279:SER:N	2.41	0.53
1:B:542:LEU:HD11	1:B:568:GLN:HB3	1.90	0.53
1:A:390:HIS:HD2	1:A:392:GLU:H	1.57	0.53
1:A:311:ALA:O	1:A:315:MET:HG3	2.09	0.53
1:A:330:VAL:HG13	1:A:335:TRP:HE1	1.74	0.53
1:B:204:TYR:HD1	1:B:241:VAL:HG11	1.74	0.52
1:A:26:ARG:HG2	1:A:70:GLU:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:O	1:A:110:VAL:HG23	2.09	0.52
1:B:386:THR:OG1	1:B:388:GLU:HG3	2.09	0.52
1:B:138:PRO:CD	1:B:193:THR:HG22	2.32	0.52
1:A:400:ARG:NH1	1:B:98:GLU:O	2.42	0.52
1:A:437:ARG:HB3	1:A:486:PHE:CE1	2.44	0.52
1:B:193:THR:OG1	1:B:194:PRO:HD3	2.10	0.52
1:A:376:PHE:O	1:A:380:VAL:HG23	2.10	0.52
1:A:299:GLU:OE2	1:B:117:HIS:HB3	2.09	0.52
1:A:107:LYS:HD2	5:A:1031:HOH:O	2.10	0.52
1:B:126:GLU:O	1:B:129:LYS:HB2	2.10	0.52
1:A:190:LEU:HG	1:A:234:ILE:CG2	2.39	0.52
1:B:273:PHE:HB3	1:B:274:PRO:HA	1.91	0.52
1:B:263:ARG:HG3	1:B:263:ARG:O	2.10	0.51
1:A:278:THR:OG1	1:A:279:SER:N	2.43	0.51
1:B:250:PHE:CD1	1:B:251:ALA:N	2.78	0.51
1:B:402:ARG:HG2	1:B:403:MET:CE	2.39	0.51
1:A:478:GLU:HG3	5:A:1089:HOH:O	2.09	0.51
1:A:552:THR:HG23	1:A:563:HIS:ND1	2.26	0.51
1:B:47:SER:OG	1:B:49:GLU:HG3	2.11	0.51
1:A:95:TYR:CE2	1:A:105:ARG:HB2	2.45	0.51
1:B:192:PHE:CZ	1:B:225:LEU:HD21	2.46	0.51
1:B:468:CYS:SG	1:B:469:ARG:HG3	2.51	0.50
1:B:512:LYS:HG3	1:B:513:GLN:NE2	2.26	0.50
1:B:336:ARG:NH1	5:B:1102:HOH:O	2.43	0.50
1:B:357:HIS:O	1:B:358:ASP:C	2.49	0.50
1:A:224:ARG:NE	1:A:224:ARG:HA	2.25	0.50
1:B:212:ILE:HD12	1:B:212:ILE:N	2.27	0.50
1:A:409:ALA:O	1:A:413:LEU:HD13	2.12	0.50
1:B:278:THR:C	1:B:280:ARG:H	2.14	0.50
1:B:551:LYS:NZ	1:B:567:GLY:H	2.10	0.50
1:A:286:PHE:CZ	2:A:606:GLC:H62	2.47	0.50
1:A:2:LEU:HD12	1:A:30:LYS:CD	2.42	0.50
1:B:203:LYS:NZ	1:B:213:ASP:OD2	2.40	0.49
1:B:374:TYR:O	1:B:378:GLU:HG3	2.11	0.49
1:A:291:PRO:HG3	5:A:1036:HOH:O	2.11	0.49
1:B:33:ASP:O	1:B:89:PRO:HD3	2.12	0.49
1:B:41:TYR:HB3	1:B:82:TYR:HB3	1.93	0.49
1:A:134:TYR:HB2	1:A:187:VAL:HG11	1.94	0.49
1:A:2:LEU:HD12	1:A:30:LYS:HD2	1.93	0.49
1:A:38:GLU:OE1	1:A:54:HIS:HB3	2.12	0.49
1:B:515:ASN:HD21	1:B:534:ASN:HD22	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:LYS:HD2	5:B:1007:HOH:O	2.13	0.48
1:B:260:GLU:HG2	1:B:265:LYS:HD2	1.95	0.48
1:B:276:SER:HB2	1:B:282:ASN:OD1	2.13	0.48
1:B:416:LEU:CD2	1:B:416:LEU:H	2.25	0.48
1:B:305:GLU:OE2	1:B:305:GLU:HA	2.14	0.48
1:A:250:PHE:CG	1:A:251:ALA:N	2.81	0.48
1:B:573:LEU:N	1:B:573:LEU:HD22	2.29	0.48
1:B:487:TYR:O	1:B:491:ILE:HG12	2.14	0.48
1:B:393:ARG:O	1:B:397:GLU:HG3	2.14	0.48
1:A:256:LEU:HD23	1:A:275:VAL:HB	1.95	0.48
1:A:504:ASN:O	1:A:521:ARG:HA	2.13	0.48
1:A:206:THR:HG21	1:A:209:TYR:CG	2.49	0.48
1:A:565:LYS:HD2	1:A:568:GLN:O	2.14	0.48
1:A:577:GLN:CG	1:A:578:GLY:N	2.77	0.48
1:B:206:THR:HG21	1:B:209:TYR:CD2	2.49	0.48
1:B:351:ILE:N	1:B:351:ILE:HD12	2.29	0.48
1:A:291:PRO:HD2	5:A:1066:HOH:O	2.14	0.48
1:B:206:THR:HG21	1:B:209:TYR:CE2	2.49	0.48
1:B:343:LYS:HE2	1:B:351:ILE:HD13	1.96	0.48
1:A:504:ASN:ND2	1:A:504:ASN:C	2.67	0.47
1:A:206:THR:HG21	1:A:209:TYR:CE2	2.49	0.47
1:B:243:ASN:HD21	1:B:295:LYS:HZ3	1.61	0.47
1:B:574:ARG:HB2	1:B:574:ARG:HH11	1.79	0.47
1:B:377:ARG:HG2	1:B:381:ILE:HD13	1.96	0.47
1:A:84:PHE:HB2	1:A:96:PHE:HB3	1.96	0.47
1:B:492:ARG:HD2	1:B:496:ARG:HH12	1.79	0.47
1:A:255:VAL:HA	1:A:262:SER:OG	2.15	0.47
1:A:392:GLU:CG	1:A:512:LYS:HB3	2.45	0.47
1:B:260:GLU:HB2	1:B:273:PHE:CE2	2.50	0.47
1:B:573:LEU:N	1:B:573:LEU:CD2	2.78	0.47
1:A:140:ARG:HG2	1:A:469:ARG:O	2.14	0.47
1:A:218:ASP:OD1	1:A:220:PRO:HD2	2.14	0.47
1:A:540:THR:HG21	1:A:570:LYS:HE3	1.96	0.47
1:A:184:GLU:HB2	5:A:1056:HOH:O	2.13	0.47
1:A:341:LEU:HD23	1:A:342:VAL:N	2.30	0.47
1:A:554:LEU:HD12	1:A:560:GLU:O	2.15	0.47
1:B:458:ILE:HD13	1:B:458:ILE:N	2.30	0.46
1:B:504:ASN:ND2	1:B:504:ASN:C	2.69	0.46
1:A:346:ASN:C	1:A:346:ASN:ND2	2.68	0.46
1:A:276:SER:HG	1:A:278:THR:HG22	1.79	0.46
1:B:251:ALA:O	1:B:255:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ARG:NH2	1:A:539:GLN:OE1	2.49	0.46
1:B:447:LEU:HB2	1:B:505:VAL:CG2	2.45	0.46
1:B:133:ILE:HD13	1:B:189:ALA:HB3	1.97	0.46
1:B:256:LEU:HD23	1:B:275:VAL:HG12	1.97	0.46
1:A:26:ARG:CD	1:A:70:GLU:HG3	2.46	0.46
1:B:504:ASN:HD22	1:B:504:ASN:C	2.18	0.46
1:B:278:THR:HG23	1:B:280:ARG:H	1.80	0.46
1:A:129:LYS:HA	1:A:411:GLN:OE1	2.15	0.46
3:B:706:GLC:C1	3:B:707:GLC:H61	2.46	0.46
1:B:574:ARG:HB2	1:B:574:ARG:NH1	2.30	0.46
1:B:454:TYR:CG	1:B:454:TYR:O	2.69	0.46
1:B:6:ILE:HD13	1:B:86:LEU:CD1	2.45	0.46
1:B:339:ARG:HD2	1:B:367:GLN:O	2.16	0.46
1:B:193:THR:OG1	1:B:194:PRO:CD	2.64	0.46
1:B:354:GLU:C	1:B:355:ILE:HD12	2.36	0.46
1:B:401:ALA:HA	1:B:404:LEU:HD22	1.96	0.46
1:A:122:PHE:HB3	1:A:408:GLN:NE2	2.31	0.45
1:A:481:ARG:HG2	5:A:1060:HOH:O	2.16	0.45
1:B:243:ASN:ND2	1:B:295:LYS:HZ2	2.13	0.45
1:B:158:LYS:HD2	1:B:478:GLU:HB3	1.98	0.45
1:B:281:THR:OG1	1:B:289:GLN:HG2	2.16	0.45
1:B:85:LEU:HD13	1:B:95:TYR:CZ	2.52	0.45
1:B:6:ILE:HG23	1:B:27:LEU:HD21	1.99	0.45
1:A:325:ASN:ND2	1:A:326:VAL:HG23	2.32	0.45
1:A:7:PHE:CG	1:A:8:HIS:N	2.85	0.45
1:B:376:PHE:O	1:B:380:VAL:HG13	2.17	0.45
1:B:118:ARG:HG2	1:B:118:ARG:NH1	2.32	0.45
1:B:585:ARG:NE	5:B:1075:HOH:O	2.49	0.45
1:A:253:ARG:NE	5:A:1065:HOH:O	2.49	0.45
1:A:324:LEU:HD13	1:A:335:TRP:CH2	2.52	0.44
1:A:241:VAL:HG13	1:A:325:ASN:HD22	1.82	0.44
1:A:465:ASP:HA	1:A:466:PRO:HA	1.73	0.44
1:B:447:LEU:HB2	1:B:505:VAL:HG21	1.99	0.44
1:B:453:TYR:O	1:B:454:TYR:C	2.55	0.44
1:A:446:TYR:CG	1:A:447:LEU:N	2.85	0.44
1:A:286:PHE:CE2	2:A:606:GLC:H62	2.53	0.44
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.81	0.44
1:B:328:ASN:HB3	1:B:355:ILE:CG1	2.46	0.44
1:B:223:ARG:HB3	1:B:223:ARG:CZ	2.48	0.44
1:B:269:PHE:CE2	1:B:295:LYS:HG2	2.53	0.44
1:B:241:VAL:O	1:B:241:VAL:CG2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:GLU:HG2	1:B:340:ARG:NH1	2.33	0.44
1:A:8:HIS:HD2	1:A:26:ARG:O	2.00	0.44
1:B:404:LEU:HB3	1:B:405:TYR:CE2	2.53	0.44
1:B:118:ARG:HG2	1:B:118:ARG:HH11	1.82	0.44
1:B:525:ASP:HB3	1:B:585:ARG:CD	2.48	0.43
1:B:504:ASN:HB2	5:B:1096:HOH:O	2.18	0.43
1:B:540:THR:HG22	1:B:541:VAL:N	2.32	0.43
1:A:382:ARG:HG2	1:A:388:GLU:OE1	2.18	0.43
1:B:77:THR:O	1:B:78:LYS:HB2	2.18	0.43
1:B:241:VAL:HA	1:B:325:ASN:HD22	1.82	0.43
1:A:102:SER:OG	1:A:107:LYS:HB2	2.17	0.43
1:B:85:LEU:HD13	1:B:95:TYR:CE2	2.52	0.43
1:A:197:ALA:HB3	1:A:208:ASP:HB3	2.01	0.43
1:B:127:TRP:HD1	5:B:1023:HOH:O	2.00	0.43
1:B:325:ASN:OD1	1:B:326:VAL:HG23	2.19	0.43
1:B:133:ILE:HD12	1:B:189:ALA:HB3	2.01	0.43
1:B:270:ILE:H	1:B:270:ILE:CD1	2.27	0.43
1:B:343:LYS:HE2	1:B:351:ILE:CD1	2.49	0.43
1:B:1:MET:HE3	1:B:92:GLU:HG2	2.00	0.43
1:B:247:ASP:N	1:B:292:ALA:O	2.49	0.43
1:B:261:GLN:N	1:B:261:GLN:NE2	2.66	0.43
1:A:419:SER:C	1:A:421:ASN:H	2.21	0.43
1:A:5:ALA:O	1:A:29:ALA:HA	2.19	0.43
1:A:374:TYR:CE1	1:A:375:LEU:HD13	2.54	0.43
1:B:218:ASP:CG	1:B:220:PRO:HD2	2.38	0.43
1:A:356:TRP:CH2	2:A:601:GLC:H2	2.54	0.43
1:B:346:ASN:HA	1:B:347:PRO:HD2	1.82	0.43
1:B:398:LEU:HD21	1:B:442:PHE:HZ	1.84	0.43
1:B:262:SER:C	1:B:264:TYR:H	2.21	0.43
1:B:24:ARG:HD2	1:B:70:GLU:HG2	2.00	0.42
1:B:515:ASN:HD21	1:B:534:ASN:ND2	2.16	0.42
1:A:139:GLU:OE2	1:A:140:ARG:NH1	2.52	0.42
1:B:183:GLU:CD	1:B:232:ARG:HB3	2.39	0.42
1:B:232:ARG:NH1	5:B:1027:HOH:O	2.52	0.42
1:B:139:GLU:C	1:B:140:ARG:HG2	2.39	0.42
1:A:295:LYS:HE2	1:B:115:TYR:CZ	2.54	0.42
1:A:8:HIS:CE1	1:A:82:TYR:OH	2.73	0.42
1:A:467:ASP:O	1:A:470:ARG:HG3	2.19	0.42
1:B:460:MET:HE1	1:B:470:ARG:O	2.19	0.42
1:A:454:TYR:O	1:A:454:TYR:CG	2.72	0.42
1:A:549:GLY:HA2	1:A:585:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:VAL:O	1:B:275:VAL:HG21	2.20	0.42
1:A:47:SER:OG	1:A:48:PRO:HD2	2.19	0.42
1:B:357:HIS:HA	1:B:374:TYR:OH	2.19	0.42
1:B:247:ASP:OD2	1:B:247:ASP:C	2.58	0.42
1:A:285:THR:HB	1:A:293:MET:O	2.19	0.42
1:A:153:THR:HG23	1:A:168:TYR:HA	2.02	0.42
1:B:325:ASN:CG	1:B:326:VAL:HG23	2.39	0.42
1:B:319:ILE:HD12	1:B:320:ASP:N	2.35	0.42
1:B:522:THR:OG1	1:B:527:HIS:HD2	2.02	0.42
1:B:57:ALA:CB	1:B:71:ALA:HB2	2.47	0.42
1:A:390:HIS:HD2	1:A:392:GLU:N	2.18	0.42
1:A:380:VAL:HG13	1:A:384:PHE:HD1	1.84	0.42
1:A:374:TYR:CZ	1:A:375:LEU:HD13	2.55	0.42
1:B:392:GLU:OE1	1:B:512:LYS:HG2	2.20	0.41
1:B:135:GLN:HG3	1:B:191:TYR:CD2	2.55	0.41
1:B:340:ARG:HB3	1:B:340:ARG:HE	1.61	0.41
1:A:10:ALA:O	1:A:11:LYS:HB3	2.20	0.41
1:B:171:ASP:CB	1:B:216:PHE:HA	2.51	0.41
1:A:441:LEU:O	1:A:441:LEU:HD23	2.20	0.41
1:A:346:ASN:HD22	1:A:346:ASN:C	2.24	0.41
1:A:533:ASN:HB2	1:A:573:LEU:HD12	2.01	0.41
1:B:446:TYR:CG	1:B:447:LEU:N	2.87	0.41
1:B:228:GLU:HA	1:B:228:GLU:OE2	2.19	0.41
1:A:565:LYS:O	1:A:565:LYS:HG2	2.20	0.41
1:B:163:ARG:HG3	1:B:163:ARG:NH1	2.34	0.41
1:A:246:GLY:HA2	1:A:292:ALA:O	2.21	0.41
1:A:341:LEU:HD23	1:A:341:LEU:C	2.40	0.41
1:A:164:HIS:CE1	1:A:466:PRO:HD3	2.56	0.41
1:B:398:LEU:HA	1:B:398:LEU:HD12	1.89	0.41
1:B:250:PHE:HA	1:B:253:ARG:NH2	2.36	0.41
1:A:545:VAL:O	1:A:546:PRO:C	2.59	0.41
1:A:175:VAL:O	1:A:178:ARG:N	2.51	0.41
1:A:223:ARG:NH1	1:A:223:ARG:HB3	2.36	0.41
1:B:105:ARG:NH1	1:B:105:ARG:HG2	2.36	0.41
1:A:192:PHE:HE2	1:A:236:ILE:HD12	1.86	0.41
1:A:221:THR:O	1:A:224:ARG:HB3	2.21	0.41
1:B:149:ASP:OD1	1:B:169:GLY:HA3	2.21	0.41
1:B:465:ASP:HA	1:B:466:PRO:HA	1.85	0.40
1:B:504:ASN:HD21	1:B:522:THR:HB	1.86	0.40
1:B:398:LEU:HD21	1:B:442:PHE:CZ	2.56	0.40
1:A:352:VAL:HG21	1:A:414:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLY:O	1:A:262:SER:HB2	2.21	0.40
1:B:171:ASP:HB2	1:B:216:PHE:HA	2.02	0.40
1:B:1:MET:CE	1:B:92:GLU:HG2	2.52	0.40
1:B:241:VAL:HG12	1:B:325:ASN:CG	2.42	0.40
1:B:574:ARG:CB	1:B:574:ARG:HH11	2.35	0.40
1:A:135:GLN:HG3	1:A:191:TYR:CD2	2.56	0.40
1:A:230:HIS:C	1:A:232:ARG:H	2.25	0.40
1:B:1:MET:HB2	1:B:33:ASP:HB3	2.03	0.40
1:B:135:GLN:HB2	1:B:451:LEU:HD21	2.04	0.40
1:B:523:VAL:HG13	1:B:523:VAL:O	2.20	0.40
1:B:153:THR:HG22	1:B:154:GLU:N	2.36	0.40

There are no symmetry-related clashes.

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	583/585 (100%)	534 (92%)	47 (8%)	2 (0%)	46	78
1	B	583/585 (100%)	522 (90%)	55 (9%)	6 (1%)	19	51
All	All	1166/1170 (100%)	1056 (91%)	102 (9%)	8 (1%)	26	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	B	11	LYS
1	B	162	PRO
1	B	193	THR
1	B	464	THR
1	A	91	GLY
1	B	138	PRO

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Mol	Chain	Res	Type
1	B	275	VAL

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	493/493 (100%)	469 (95%)	24 (5%)	31	64
1	B	493/493 (100%)	464 (94%)	29 (6%)	24	55
All	All	986/986 (100%)	933 (95%)	53 (5%)	27	59

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLU
1	A	77	THR
1	A	85	LEU
1	A	122	PHE
1	A	182	LEU
1	A	191	TYR
1	A	219	LEU
1	A	223	ARG
1	A	262	SER
1	A	263	ARG
1	A	330	VAL
1	A	346	ASN
1	A	375	LEU
1	A	398	LEU
1	A	404	LEU
1	A	411	GLN
1	A	413	LEU
1	A	426	LEU
1	A	483	LEU
1	A	504	ASN
1	A	541	VAL
1	A	565	LYS

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Mol	Chain	Res	Type
1	A	571	LEU
1	A	573	LEU
1	B	13	SER
1	B	49	GLU
1	B	73	LEU
1	B	110	VAL
1	B	122	PHE
1	B	140	ARG
1	B	167	PHE
1	B	223	ARG
1	B	260	GLU
1	B	270	ILE
1	B	323	ARG
1	B	325	ASN
1	B	328	ASN
1	B	340	ARG
1	B	356	TRP
1	B	364	MET
1	B	381	ILE
1	B	398	LEU
1	B	404	LEU
1	B	411	GLN
1	B	438	LEU
1	B	451	LEU
1	B	458	ILE
1	B	504	ASN
1	B	505	VAL
1	B	539	GLN
1	B	545	VAL
1	B	565	LYS
1	B	573	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	54	HIS
1	A	90	GLN
1	A	135	GLN
1	A	155	GLN
1	A	244	HIS
1	A	261	GLN

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Mol	Chain	Res	Type
1	A	325	ASN
1	A	332	HIS
1	A	346	ASN
1	A	367	GLN
1	A	390	HIS
1	A	443	GLN
1	A	504	ASN
1	A	509	HIS
1	A	527	HIS
1	A	544	GLN
1	B	135	GLN
1	B	243	ASN
1	B	261	GLN
1	B	289	GLN
1	B	325	ASN
1	B	328	ASN
1	B	332	HIS
1	B	357	HIS
1	B	421	ASN
1	B	504	ASN
1	B	513	GLN
1	B	527	HIS
1	B	534	ASN
1	B	539	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

14 carbohydrates 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	601	2	11,11,12	0.45	0	14,15,17	0.78	1 (7%)
2	GLC	A	602	2	11,11,12	0.54	0	14,15,17	0.66	0
2	GLC	A	603	2	11,11,12	0.42	0	14,15,17	0.63	0
2	GLC	A	604	2	11,11,12	0.55	0	14,15,17	0.69	1 (7%)
2	GLC	A	605	2	11,11,12	0.58	0	14,15,17	0.68	0
2	GLC	A	606	2	11,11,12	0.77	0	14,15,17	0.76	0
2	GLC	A	607	2	11,11,12	0.57	0	14,15,17	0.78	1 (7%)
3	GLC	B	701	3	11,11,12	0.61	0	14,15,17	0.64	0
3	GLC	B	702	3	11,11,12	0.56	0	14,15,17	0.72	1 (7%)
3	BGC	B	703	3	11,11,12	0.64	0	14,15,17	0.81	0
3	GLC	B	704	3	11,11,12	0.67	0	14,15,17	1.09	1 (7%)
3	GLC	B	705	3	11,11,12	0.56	0	14,15,17	0.73	1 (7%)
3	GLC	B	706	3	11,11,12	0.54	0	14,15,17	0.60	0
3	GLC	B	707	3	11,11,12	0.57	0	14,15,17	0.74	1 (7%)

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	601	2	-	0/2/19/22	0/1/1/1
2	GLC	A	602	2	-	0/2/19/22	0/1/1/1
2	GLC	A	603	2	-	0/2/19/22	0/1/1/1
2	GLC	A	604	2	-	0/2/19/22	0/1/1/1
2	GLC	A	605	2	-	0/2/19/22	0/1/1/1
2	GLC	A	606	2	-	0/2/19/22	0/1/1/1
2	GLC	A	607	2	-	0/2/19/22	0/1/1/1
3	GLC	B	701	3	-	0/2/19/22	0/1/1/1
3	GLC	B	702	3	-	0/2/19/22	0/1/1/1
3	BGC	B	703	3	-	0/2/19/22	0/1/1/1
3	GLC	B	704	3	-	0/2/19/22	0/1/1/1
3	GLC	B	705	3	-	0/2/19/22	0/1/1/1
3	GLC	B	706	3	-	0/2/19/22	0/1/1/1
3	GLC	B	707	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	707	GLC	C1-O5-C5	2.03	114.82	112.25
3	B	702	GLC	C1-O5-C5	2.07	114.87	112.25
2	A	604	GLC	C1-O5-C5	2.08	114.89	112.25
2	A	601	GLC	C1-O5-C5	2.10	114.91	112.25
3	B	705	GLC	C1-O5-C5	2.13	114.95	112.25
2	A	607	GLC	C1-O5-C5	2.36	115.24	112.25
3	B	704	GLC	C1-O5-C5	2.78	115.77	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GLC	1	0
2	A	606	GLC	2	0
3	B	706	GLC	2	0
3	B	707	GLC	2	0

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

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	585/585 (100%)	-0.33	9 (1%) 76 68	14, 38, 69, 85	0
1	B	585/585 (100%)	-0.04	32 (5%) 29 18	18, 45, 83, 100	0
All	All	1170/1170 (100%)	-0.19	41 (3%) 48 35	14, 41, 78, 100	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	273	PHE	6.3
1	B	275	VAL	5.0
1	B	279	SER	4.4
1	B	272	ASP	4.3
1	B	155	GLN	4.3
1	B	276	SER	4.1
1	A	547	GLU	4.0
1	B	259	GLY	3.7
1	A	552	THR	3.6
1	B	157	ALA	3.4
1	B	548	SER	3.3
1	B	278	THR	3.2
1	B	281	THR	3.2
1	A	548	SER	3.2
1	A	551	LYS	3.0
1	A	553	TRP	2.9
1	B	160	ALA	2.9
1	B	260	GLU	2.9
1	B	277	LYS	2.8
1	B	162	PRO	2.7
1	B	156	TRP	2.7
1	B	547	GLU	2.7
1	B	164	HIS	2.6
1	B	566	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	270	ILE	2.6
1	B	551	LYS	2.5
1	B	565	LYS	2.5
1	B	159	ASP	2.5
1	B	168	TYR	2.4
1	A	569	LEU	2.4
1	B	161	ARG	2.3
1	A	546	PRO	2.3
1	B	466	PRO	2.3
1	A	549	GLY	2.2
1	A	564	GLY	2.2
1	B	280	ARG	2.2
1	B	283	TYR	2.1
1	B	356	TRP	2.1
1	B	257	GLN	2.0
1	B	563	HIS	2.0
1	B	274	PRO	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)

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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	GLC	B	706	11/12	0.82	0.23	1.01	91,93,94,97	0
2	GLC	A	605	11/12	0.95	0.15	0.40	37,38,39,40	0
3	GLC	B	707	11/12	0.88	0.21	0.08	90,92,93,93	0
3	GLC	B	701	11/12	0.88	0.20	-0.26	93,94,94,95	0
2	GLC	A	606	11/12	0.95	0.15	-0.40	40,45,47,49	0
2	GLC	A	607	11/12	0.94	0.17	-0.45	46,47,49,50	0
3	GLC	B	705	11/12	0.84	0.31	-	97,98,99,99	0
2	GLC	A	604	11/12	0.96	0.13	-	44,47,49,51	0
3	GLC	B	702	11/12	0.87	0.29	-	92,95,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GLC	B	704	11/12	0.76	0.31	-	96,97,98,98	0
2	GLC	A	603	11/12	0.97	0.14	-	49,49,51,51	0
2	GLC	A	602	11/12	0.93	0.17	-	44,46,48,48	0
2	GLC	A	601	11/12	0.96	0.14	-	45,46,48,50	0
3	BGC	B	703	11/12	0.84	0.29	-	95,97,98,98	0

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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	CA	A	1001	1/1	0.97	0.08	-1.73	35,35,35,35	0
4	CA	B	1002	1/1	0.98	0.07	-3.85	66,66,66,66	0

6.5 Other polymers

There are no such residues in this entry.