Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:20 PM GMT

PDB ID	:	4OKD
Title	:	Crystal Structure of Chlamydomonas reinhardtii Isoamylase 1 (ISA1) in complex with maltoheptaose
Authors	:	Sim, L.; Palcic, M.
Deposited on	:	2014-01-22
Resolution	:	2.40 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:

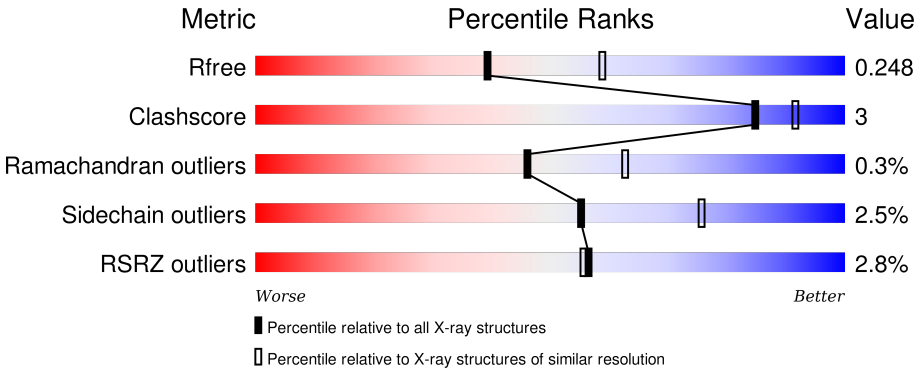
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	840	3% 88% 6% • 5%
1	B	840	2% 85% 8% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	A	1001	X	-	-	-
2	GLC	A	1007	-	-	-	X
2	GLC	B	1001	X	-	-	-
4	GLC	A	1012	-	-	-	X
4	GLC	A	1013	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13042 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 Isoamylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	0	0
			6207	3919	1090	1168	30			
1	B	792	Total	C	N	O	S	0	1	0
			6134	3878	1077	1149	30			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	MET	-	EXPRESSION TAG	UNP Q7X8Q2
A	37	GLY	-	EXPRESSION TAG	UNP Q7X8Q2
A	38	SER	-	EXPRESSION TAG	UNP Q7X8Q2
A	39	SER	-	EXPRESSION TAG	UNP Q7X8Q2
A	40	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	41	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	42	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	43	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	44	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	45	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	46	SER	-	EXPRESSION TAG	UNP Q7X8Q2
A	47	SER	-	EXPRESSION TAG	UNP Q7X8Q2
A	48	GLY	-	EXPRESSION TAG	UNP Q7X8Q2
A	49	LEU	-	EXPRESSION TAG	UNP Q7X8Q2
A	50	VAL	-	EXPRESSION TAG	UNP Q7X8Q2
A	51	PRO	-	EXPRESSION TAG	UNP Q7X8Q2
A	52	ARG	-	EXPRESSION TAG	UNP Q7X8Q2
A	53	GLY	-	EXPRESSION TAG	UNP Q7X8Q2
A	54	SER	-	EXPRESSION TAG	UNP Q7X8Q2
A	55	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	56	MET	-	EXPRESSION TAG	UNP Q7X8Q2
B	36	MET	-	EXPRESSION TAG	UNP Q7X8Q2
B	37	GLY	-	EXPRESSION TAG	UNP Q7X8Q2
B	38	SER	-	EXPRESSION TAG	UNP Q7X8Q2
B	39	SER	-	EXPRESSION TAG	UNP Q7X8Q2

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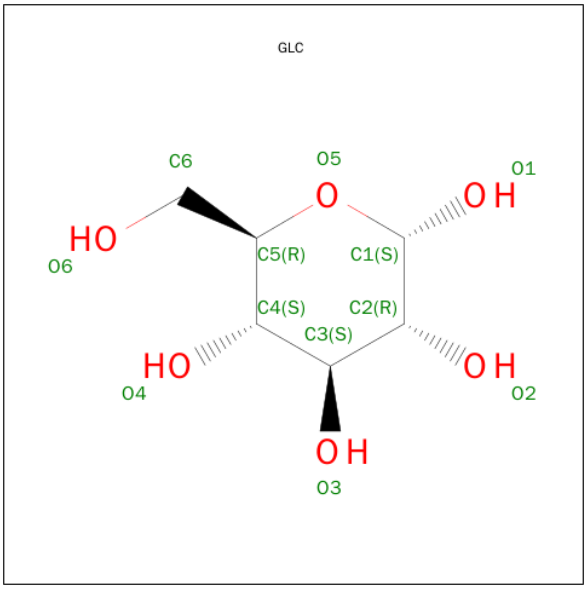
Chain	Residue	Modelled	Actual	Comment	Reference
B	40	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	41	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	42	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	43	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	44	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	45	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	46	SER	-	EXPRESSION TAG	UNP Q7X8Q2
B	47	SER	-	EXPRESSION TAG	UNP Q7X8Q2
B	48	GLY	-	EXPRESSION TAG	UNP Q7X8Q2
B	49	LEU	-	EXPRESSION TAG	UNP Q7X8Q2
B	50	VAL	-	EXPRESSION TAG	UNP Q7X8Q2
B	51	PRO	-	EXPRESSION TAG	UNP Q7X8Q2
B	52	ARG	-	EXPRESSION TAG	UNP Q7X8Q2
B	53	GLY	-	EXPRESSION TAG	UNP Q7X8Q2
B	54	SER	-	EXPRESSION TAG	UNP Q7X8Q2
B	55	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	56	MET	-	EXPRESSION TAG	UNP Q7X8Q2

- 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		
2	B	7	Total	C	O	0	0
			77	42	35		

- Molecule 3 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total C O 34 18 16	0	0
4	A	3	Total C O 34 18 16	0	0
4	B	3	Total C O 34 18 16	0	0

- Molecule 5 is water.

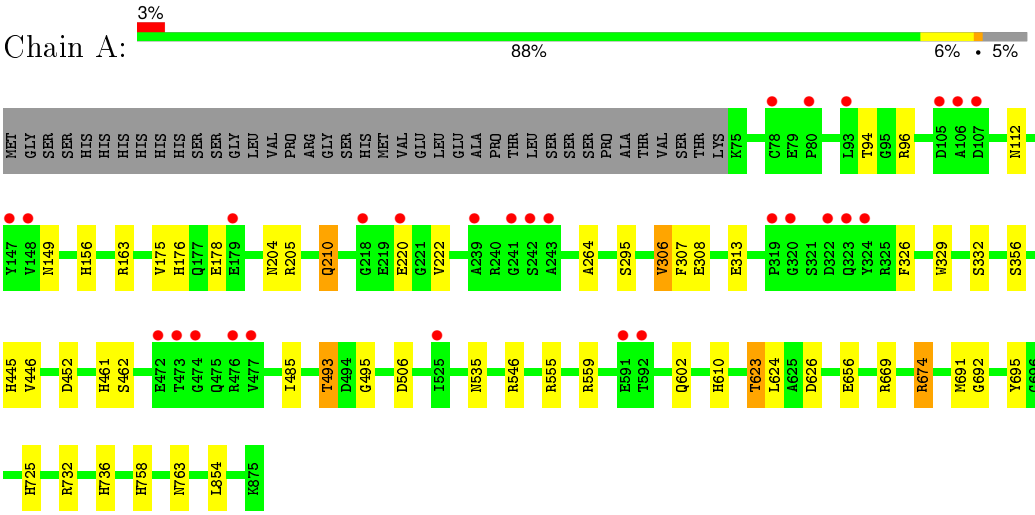
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	206	Total O 206 206	0	0
5	B	227	Total O 227 227	0	0

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.

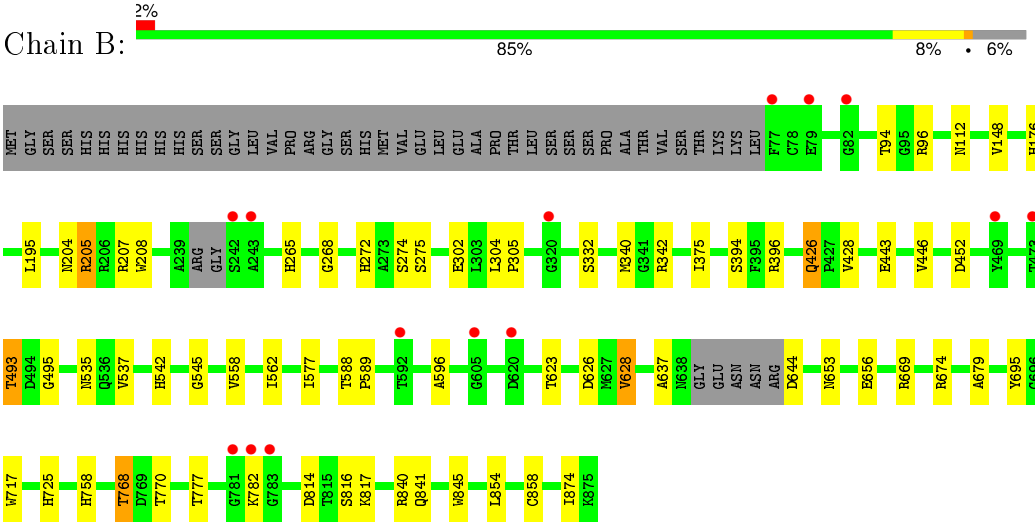
- Molecule 1: Isoamylase

Chain A:



- Molecule 1: Isoamylase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	102.75Å 102.75Å 487.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.95 – 2.40 45.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (45.95-2.40) 97.2 (45.95-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.192 , 0.227 0.223 , 0.248	Depositor DCC
R_{free} test set	5039 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 31.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	3 of 100792 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13042	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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

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	0.49	1/6390 (0.0%)	0.66	2/8723 (0.0%)
1	B	0.50	1/6319 (0.0%)	0.68	3/8629 (0.0%)
All	All	0.49	2/12709 (0.0%)	0.67	5/17352 (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
2	A	1	0
2	B	1	0
All	All	2	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	452	ASP	CG-OD1	10.73	1.50	1.25
1	A	452	ASP	CG-OD1	10.70	1.50	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	205	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	B	205	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	B	396	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	546	ARG	CG-CD-NE	-5.10	101.09	111.80
1	A	674	ARG	NE-CZ-NH1	5.07	122.83	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	GLC	C1
2	B	1001	GLC	C1

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	6207	0	5804	32	0
1	B	6134	0	5724	40	0
2	A	77	0	64	0	0
2	B	77	0	64	0	0
3	A	12	0	12	0	0
4	A	68	0	60	0	0
4	B	34	0	30	0	0
5	A	206	0	0	4	0
5	B	227	0	0	3	0
All	All	13042	0	11758	71	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 3.

All (71) 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:B:623:THR:HG21	1:B:697:HIS:O	1.74	0.86
1:B:443:GLU:HG2	5:B:1318:HOH:O	1.78	0.83
1:A:423:ASN:HD21	1:A:462:SER:H	1.39	0.70
1:A:623:THR:HG21	1:A:697:HIS:O	2.00	0.62
1:B:542:HIS:HD2	1:B:545:GLY:H	1.49	0.61
1:A:96:ARG:H	1:A:112:ASN:HD21	1.47	0.60
1:A:623:THR:HG22	1:A:626:ASP:H	1.67	0.59
1:B:768:THR:HG23	1:B:770:THR:H	1.66	0.59
1:B:628:VAL:HG13	1:B:669:ARG:HG2	1.85	0.59
1:A:758:HIS:HD2	1:A:763:ASN:H	1.52	0.58
1:B:542:HIS:CD2	1:B:545:GLY:H	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:THR:HG22	1:B:148:VAL:HG12	1.87	0.57
1:B:176:HIS:HD2	1:B:178:GLU:H	1.55	0.55
1:B:265:HIS:HD2	1:B:268:GLY:H	1.55	0.55
1:B:96:ARG:H	1:B:112:ASN:HD21	1.55	0.54
1:A:176:HIS:HD2	1:A:178:GLU:H	1.55	0.53
1:A:493:THR:HG21	5:A:1181:HOH:O	2.08	0.53
1:A:758:HIS:CD2	1:A:763:ASN:H	2.27	0.52
1:B:674:ARG:HH12	1:B:725:HIS:CD2	2.28	0.52
1:B:623:THR:CG2	1:B:697:HIS:O	2.54	0.51
1:B:558:VAL:HG13	1:B:562:ILE:HD12	1.93	0.51
1:B:94:THR:HG22	1:B:148:VAL:CG1	2.39	0.51
1:B:674:ARG:HH12	1:B:725:HIS:HD2	1.58	0.50
1:B:204:ASN:OD1	1:B:205:ARG:N	2.39	0.50
1:A:555:ARG:O	1:A:559:ARG:HG3	2.12	0.50
1:A:732:ARG:O	1:A:736:HIS:HD2	1.95	0.48
1:A:656:GLU:O	1:A:669:ARG:NH2	2.46	0.48
1:A:94:THR:O	1:A:156:HIS:HD2	1.96	0.48
1:B:426:GLN:OE1	1:B:428:VAL:N	2.42	0.48
1:B:272:HIS:HD2	1:B:274:SER:OG	1.97	0.48
1:B:588:THR:HG23	1:B:588:THR:O	2.14	0.48
1:A:485:ILE:O	1:A:493:THR:HB	2.14	0.47
1:B:485:ILE:O	1:B:493:THR:HB	2.14	0.47
1:B:814:ASP:HB3	1:B:817:LYS:HG2	1.96	0.47
1:A:692:GLY:HA2	1:A:695:TYR:CE2	2.50	0.46
1:B:709:ASP:N	5:B:1153:HOH:O	2.38	0.46
1:A:493:THR:HG22	1:A:495:GLY:H	1.81	0.46
1:A:758:HIS:HD2	1:A:763:ASN:N	2.13	0.45
1:B:304:LEU:HB3	1:B:305:PRO:HD2	1.99	0.45
1:A:854:LEU:HD13	1:B:845:TRP:CD2	2.51	0.45
1:A:204:ASN:OD1	1:A:205:ARG:N	2.43	0.44
1:A:307:PHE:O	1:A:308:GLU:C	2.56	0.44
1:B:623:THR:HG23	5:B:1103:HOH:O	2.17	0.44
1:B:623:THR:HG22	1:B:626:ASP:H	1.83	0.44
1:B:208:TRP:N	1:B:342:ARG:HG2	2.34	0.43
1:A:674:ARG:NH2	1:A:725:HIS:HD2	2.15	0.43
1:B:816:SER:HB2	1:B:854:LEU:HD22	2.01	0.43
1:A:306:VAL:HB	5:A:1122:HOH:O	2.18	0.43
1:B:562:ILE:HD11	1:B:679:ALA:HB2	2.01	0.43
1:B:589:PRO:HB3	1:B:596:ALA:HB1	2.00	0.43
1:A:493:THR:CG2	5:A:1181:HOH:O	2.66	0.42
1:A:264:ALA:HB1	1:A:691:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LEU:HB3	1:B:305:PRO:CD	2.50	0.42
1:B:653:ASN:HB2	1:B:656:GLU:O	2.19	0.42
1:A:176:HIS:CD2	1:A:178:GLU:H	2.35	0.42
1:B:275:SER:HA	1:B:717:TRP:CD1	2.55	0.42
1:B:177:GLN:NE2	1:B:185:GLY:H	2.17	0.42
1:A:295:SER:HB2	5:A:1145:HOH:O	2.20	0.42
1:A:423:ASN:ND2	1:A:461:HIS:HB2	2.35	0.41
1:B:207:ARG:C	1:B:342:ARG:HG2	2.41	0.41
1:A:610:HIS:CD2	1:A:610:HIS:H	2.37	0.41
1:A:329:TRP:CD2	1:A:706:TYR:HA	2.56	0.41
1:A:205:ARG:HD2	1:A:210:GLN:O	2.21	0.41
1:B:302:GLU:HA	1:B:375:ILE:O	2.21	0.41
1:B:758:HIS:CE1	1:B:777:THR:HG23	2.56	0.41
1:A:116:PHE:C	1:A:116:PHE:CD1	2.95	0.41
1:B:695:TYR:CE1	1:B:697:HIS:HB2	2.55	0.41
1:A:145:ASP:H	1:A:149:ASN:HD22	1.69	0.40
1:B:493:THR:CG2	1:B:495:GLY:H	2.33	0.40
1:A:326:PHE:O	1:A:707:CYS:HA	2.22	0.40
1:B:840:ARG:O	1:B:841:GLN:C	2.59	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	799/840 (95%)	757 (95%)	41 (5%)	1 (0%)	56 74
1	B	787/840 (94%)	751 (95%)	33 (4%)	3 (0%)	39 56
All	All	1586/1680 (94%)	1508 (95%)	74 (5%)	4 (0%)	46 63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	SER
1	B	394	SER
1	B	637	ALA
1	A	332	SER

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	636/686 (93%)	619 (97%)	17 (3%)	52	73
1	B	627/686 (91%)	613 (98%)	14 (2%)	60	79
All	All	1263/1372 (92%)	1232 (98%)	31 (2%)	55	76

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	ARG
1	A	175	VAL
1	A	210	GLN
1	A	220	GLU
1	A	222	VAL
1	A	306	VAL
1	A	313	GLU
1	A	356	SER
1	A	423	ASN
1	A	445	HIS
1	A	446	VAL
1	A	493	THR
1	A	506	ASP
1	A	535	ASN
1	A	602	GLN
1	A	623	THR
1	A	624	LEU
1	B	195	LEU
1	B	340	MET
1	B	426	GLN

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Mol	Chain	Res	Type
1	B	446	VAL
1	B	493	THR
1	B	535	ASN
1	B	537	VAL
1	B	577	ILE
1	B	628	VAL
1	B	644	ASP
1	B	768	THR
1	B	782	LYS
1	B	858	CYS
1	B	874	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	149	ASN
1	A	156	HIS
1	A	176	HIS
1	A	265	HIS
1	A	272	HIS
1	A	381	ASN
1	A	400	ASN
1	A	423	ASN
1	A	425	ASN
1	A	521	ASN
1	A	535	ASN
1	A	560	ASN
1	A	610	HIS
1	A	650	ASN
1	A	704	ASN
1	A	713	ASN
1	A	725	HIS
1	A	728	ASN
1	A	736	HIS
1	A	758	HIS
1	A	849	HIS
1	B	112	ASN
1	B	176	HIS
1	B	177	GLN
1	B	265	HIS
1	B	272	HIS

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Mol	Chain	Res	Type
1	B	317	GLN
1	B	381	ASN
1	B	400	ASN
1	B	425	ASN
1	B	461	HIS
1	B	542	HIS
1	B	597	ASN
1	B	638	ASN
1	B	649	ASN
1	B	713	ASN
1	B	725	HIS
1	B	728	ASN
1	B	758	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

23 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	1001	1,2	11,11,12	0.63	0	14,15,17	3.30	2 (14%)
2	GLC	A	1002	2	11,11,12	0.66	0	14,15,17	1.44	1 (7%)
2	GLC	A	1003	2	11,11,12	0.69	0	14,15,17	1.54	1 (7%)
2	GLC	A	1004	2	11,11,12	0.65	0	14,15,17	1.49	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLC	A	1005	2	11,11,12	0.57	0	14,15,17	1.30	2 (14%)
2	GLC	A	1006	2	11,11,12	0.68	0	14,15,17	0.95	1 (7%)
2	GLC	A	1007	2	11,11,12	0.50	0	14,15,17	1.15	1 (7%)
4	GLC	A	1009	4	12,12,12	0.53	0	17,17,17	0.98	1 (5%)
4	GLC	A	1010	4	11,11,12	0.65	0	14,15,17	1.28	2 (14%)
4	GLC	A	1011	4	11,11,12	0.63	0	14,15,17	1.57	3 (21%)
4	GLC	A	1012	4	12,12,12	0.50	0	17,17,17	1.10	1 (5%)
4	GLC	A	1013	4	11,11,12	0.60	0	14,15,17	0.93	1 (7%)
4	GLC	A	1014	4	11,11,12	0.45	0	14,15,17	1.37	1 (7%)
2	GLC	B	1001	1,2	11,11,12	0.85	1 (9%)	14,15,17	2.70	5 (35%)
2	GLC	B	1002	2	11,11,12	0.70	0	14,15,17	1.29	3 (21%)
2	GLC	B	1003	2	11,11,12	0.66	0	14,15,17	1.23	2 (14%)
2	GLC	B	1004	2	11,11,12	0.77	0	14,15,17	1.42	3 (21%)
2	GLC	B	1005	2	11,11,12	0.90	0	14,15,17	1.46	3 (21%)
2	GLC	B	1006	2	11,11,12	0.68	0	14,15,17	2.66	3 (21%)
2	GLC	B	1007	2	11,11,12	0.56	0	14,15,17	1.65	4 (28%)
4	GLC	B	1008	4	12,12,12	0.49	0	17,17,17	1.02	2 (11%)
4	GLC	B	1009	4	11,11,12	0.65	0	14,15,17	1.37	2 (14%)
4	GLC	B	1010	4	11,11,12	0.68	0	14,15,17	2.35	4 (28%)

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	1001	1,2	1/1/4/5	0/2/19/22	0/1/1/1
2	GLC	A	1002	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1003	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1004	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1005	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1006	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1007	2	-	0/2/19/22	0/1/1/1
4	GLC	A	1009	4	-	0/2/22/22	0/1/1/1
4	GLC	A	1010	4	-	0/2/19/22	0/1/1/1
4	GLC	A	1011	4	-	0/2/19/22	0/1/1/1
4	GLC	A	1012	4	-	0/2/22/22	0/1/1/1
4	GLC	A	1013	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLC	A	1014	4	-	0/2/19/22	0/1/1/1
2	GLC	B	1001	1,2	1/1/4/5	0/2/19/22	0/1/1/1
2	GLC	B	1002	2	-	0/2/19/22	0/1/1/1
2	GLC	B	1003	2	-	0/2/19/22	0/1/1/1
2	GLC	B	1004	2	-	0/2/19/22	0/1/1/1
2	GLC	B	1005	2	-	0/2/19/22	0/1/1/1
2	GLC	B	1006	2	-	0/2/19/22	0/1/1/1
2	GLC	B	1007	2	-	0/2/19/22	0/1/1/1
4	GLC	B	1008	4	-	0/2/22/22	0/1/1/1
4	GLC	B	1009	4	-	0/2/19/22	0/1/1/1
4	GLC	B	1010	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	GLC	C2-C3	2.00	1.55	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1006	GLC	O5-C5-C6	-4.37	97.90	107.35
2	B	1005	GLC	O5-C1-C2	-3.35	105.42	110.86
2	B	1004	GLC	O5-C1-C2	-2.35	107.05	110.86
4	A	1011	GLC	C3-C4-C5	-2.34	106.12	110.20
4	A	1011	GLC	O5-C1-C2	-2.24	107.22	110.86
2	A	1004	GLC	O5-C1-C2	-2.23	107.25	110.86
2	B	1001	GLC	O4-C4-C5	-2.20	103.41	109.24
2	B	1007	GLC	O5-C1-C2	-2.10	107.45	110.86
2	B	1002	GLC	O4-C4-C3	-2.10	105.62	110.34
2	A	1005	GLC	C6-C5-C4	-2.06	107.92	113.02
2	A	1005	GLC	C1-O5-C5	2.01	114.79	112.25
4	A	1009	GLC	C1-C2-C3	2.11	113.57	110.43
4	B	1008	GLC	O5-C5-C4	2.15	113.71	109.68
4	B	1008	GLC	C1-O5-C5	2.18	117.50	113.47
4	A	1010	GLC	C1-C2-C3	2.23	112.18	109.54
2	B	1002	GLC	C1-O5-C5	2.28	115.14	112.25
4	A	1013	GLC	C1-O5-C5	2.30	115.17	112.25
4	A	1012	GLC	C1-O5-C5	2.31	117.74	113.47
2	B	1003	GLC	O5-C5-C6	2.40	112.55	107.35
2	B	1001	GLC	O5-C5-C6	2.41	112.57	107.35
2	B	1005	GLC	O3-C3-C2	2.51	114.53	110.00
2	B	1007	GLC	C1-O5-C5	2.51	115.43	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1007	GLC	C1-O5-C5	2.52	115.45	112.25
2	B	1005	GLC	O2-C2-C3	2.60	115.34	110.12
2	B	1002	GLC	C1-C2-C3	2.62	112.64	109.54
2	B	1004	GLC	C1-C2-C3	2.63	112.65	109.54
2	B	1007	GLC	O2-C2-C1	2.64	114.49	109.21
2	B	1003	GLC	C1-O5-C5	2.65	115.61	112.25
4	A	1010	GLC	C1-O5-C5	2.69	115.66	112.25
2	B	1004	GLC	C1-O5-C5	2.73	115.71	112.25
2	B	1006	GLC	O2-C2-C1	2.82	114.86	109.21
4	B	1010	GLC	C1-O5-C5	2.92	115.95	112.25
2	B	1007	GLC	O5-C5-C6	2.94	113.70	107.35
2	A	1006	GLC	C1-C2-C3	3.01	113.10	109.54
4	B	1009	GLC	C1-C2-C3	3.02	113.12	109.54
2	A	1004	GLC	C1-O5-C5	3.27	116.39	112.25
2	B	1001	GLC	C1-C2-C3	3.31	113.46	109.54
2	A	1004	GLC	C1-C2-C3	3.39	113.55	109.54
4	B	1010	GLC	C2-C3-C4	3.40	116.81	111.04
4	B	1010	GLC	C3-C4-C5	3.42	116.17	110.20
4	B	1009	GLC	C1-O5-C5	3.61	116.82	112.25
2	A	1002	GLC	C1-C2-C3	3.70	113.91	109.54
4	A	1011	GLC	C1-O5-C5	4.15	117.51	112.25
4	A	1014	GLC	C1-O5-C5	4.18	117.55	112.25
2	A	1003	GLC	C1-O5-C5	4.70	118.21	112.25
2	A	1001	GLC	C1-C2-C3	4.96	115.41	109.54
2	B	1001	GLC	O5-C1-C2	5.30	119.45	110.86
4	B	1010	GLC	C1-C2-C3	6.23	116.91	109.54
2	B	1001	GLC	C1-O5-C5	6.71	120.76	112.25
2	B	1006	GLC	C1-O5-C5	7.89	122.27	112.25
2	A	1001	GLC	C1-O5-C5	11.05	126.27	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1001	GLC	C1
2	A	1001	GLC	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

1 ligand is 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	GLC	A	1008	-	12,12,12	0.59	0	17,17,17	1.89	6 (35%)

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	GLC	A	1008	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1008	GLC	C3-C4-C5	-2.14	106.47	110.20
3	A	1008	GLC	C4-C3-C2	-2.02	107.02	110.79
3	A	1008	GLC	O4-C4-C3	2.10	115.07	110.34
3	A	1008	GLC	C1-O5-C5	2.43	117.96	113.47
3	A	1008	GLC	C1-C2-C3	3.71	115.94	110.43
3	A	1008	GLC	O5-C1-C2	4.27	116.61	109.80

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	801/840 (95%)	0.01	29 (3%)	46	47	37, 51, 87, 113	0
1	B	792/840 (94%)	0.09	15 (1%)	70	69	35, 49, 73, 115	0
All	All	1593/1680 (94%)	0.05	44 (2%)	56	55	35, 50, 82, 115	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	PHE	5.3
1	A	474	GLY	5.0
1	A	106	ALA	4.9
1	A	320	GLY	4.4
1	B	242	SER	4.2
1	A	592	THR	4.1
1	B	79	GLU	4.1
1	B	783	GLY	3.9
1	A	322	ASP	3.6
1	A	93	LEU	3.5
1	A	591	GLU	3.5
1	A	323	GLN	3.4
1	B	82	GLY	3.3
1	A	241	GLY	3.3
1	A	319	PRO	3.2
1	A	242	SER	3.1
1	A	80	PRO	3.0
1	B	320	GLY	2.9
1	A	218	GLY	2.9
1	B	469	TYR	2.8
1	B	592	THR	2.7
1	A	243	ALA	2.7
1	B	620[A]	ASP	2.7
1	B	781	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	78	CYS	2.6
1	A	378	VAL	2.6
1	A	220	GLU	2.5
1	A	239	ALA	2.5
1	B	243	ALA	2.4
1	B	605	GLY	2.4
1	A	147	TYR	2.4
1	A	476	ARG	2.3
1	A	525	ILE	2.3
1	A	148	VAL	2.3
1	A	477	VAL	2.2
1	B	474	GLY	2.2
1	A	473	THR	2.2
1	A	324	TYR	2.2
1	A	107	ASP	2.1
1	A	179	GLU	2.1
1	A	105	ASP	2.1
1	B	473	THR	2.1
1	A	472	GLU	2.0
1	B	782	LYS	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
4	GLC	A	1013	11/12	0.94	0.30	5.84	81,84,89,91	0
4	GLC	A	1012	12/12	0.90	0.26	4.12	78,84,88,90	0
2	GLC	A	1007	11/12	0.90	0.30	2.19	76,81,84,85	0
4	GLC	A	1011	11/12	0.93	0.15	1.52	65,67,69,70	0
2	GLC	B	1007	11/12	0.90	0.18	1.01	59,65,69,71	0
2	GLC	A	1004	11/12	0.94	0.16	1.00	54,59,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GLC	B	1002	11/12	0.94	0.23	0.27	52,55,56,56	0
2	GLC	A	1005	11/12	0.95	0.12	0.26	57,60,63,63	0
4	GLC	B	1009	11/12	0.93	0.17	0.16	70,72,74,75	0
2	GLC	A	1006	11/12	0.91	0.14	0.04	62,64,68,73	0
2	GLC	B	1001	11/12	0.91	0.20	0.02	55,56,58,59	0
2	GLC	B	1003	11/12	0.92	0.18	-0.13	55,58,63,63	0
4	GLC	A	1010	11/12	0.95	0.11	-0.23	60,63,66,67	0
2	GLC	B	1006	11/12	0.90	0.17	-0.42	51,56,61,63	0
2	GLC	A	1003	11/12	0.94	0.11	-0.78	53,57,58,60	0
2	GLC	B	1004	11/12	0.91	0.14	-0.91	50,56,59,61	0
2	GLC	A	1001	11/12	0.95	0.12	-1.01	47,49,49,50	0
2	GLC	A	1002	11/12	0.97	0.09	-1.10	47,48,49,50	0
4	GLC	B	1010	11/12	0.87	0.15	-1.18	74,76,77,78	0
2	GLC	B	1005	11/12	0.94	0.10	-2.51	52,55,56,58	0
4	GLC	A	1009	12/12	0.88	0.18	-	69,76,78,79	0
4	GLC	B	1008	12/12	0.87	0.19	-	75,81,83,83	0
4	GLC	A	1014	11/12	0.89	0.21	-	79,84,87,88	0

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, 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	A	1008	12/12	0.90	0.16	1.17	64,68,75,80	0

6.5 Other polymers (i)

There are no such residues in this entry.