Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2017 – 12:21 PM EST

PDB ID	:	5H42
Title	:	Crystal Structure of 1,2-beta-oligoglucan phosphorylase from Lachnoclostridium phytofermentans in complex with alpha-d-glucose-1-phosphate
Authors	:	Nakajima, M.; Tanaka, N.; Furukawa, N.; Nihira, T.; Kodutsumi, Y.; Takahashi, Y.; Sugimoto, N.; Miyanaga, A.; Fushinobu, S.; Taguchi, H.; Nakai, H.
Deposited on	:	2016-10-28
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

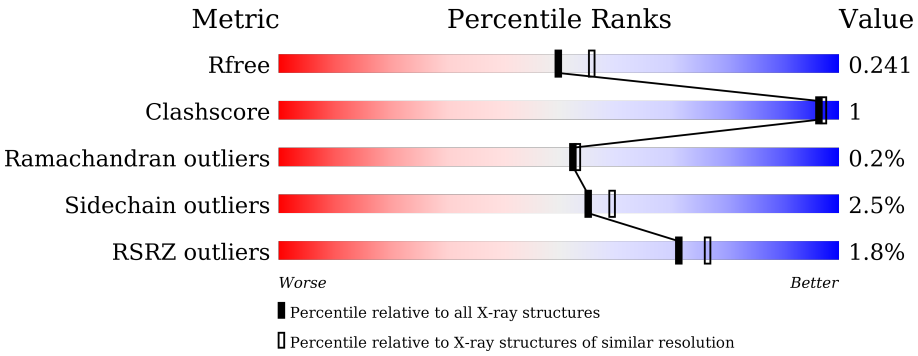
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1122	2% 92% 6%
1	B	1122	2% 93% 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	G1P	B	1202	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18512 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.

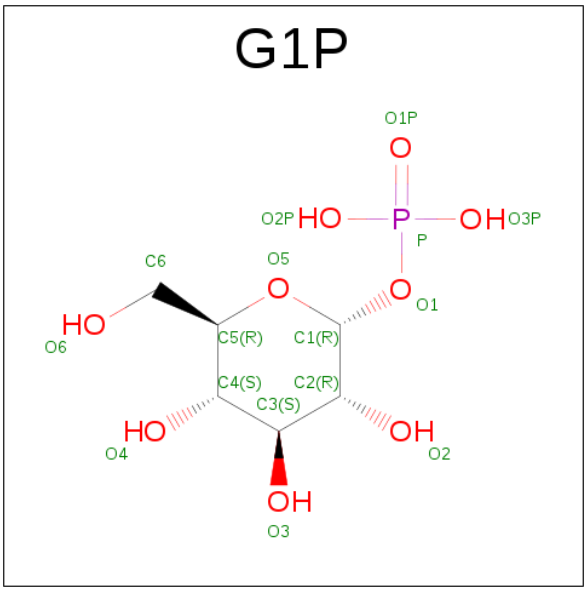
- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1108	Total	C	N	O	S	0	0	0
			8882	5689	1478	1683	32			
1	B	1113	Total	C	N	O	S	0	0	0
			8918	5712	1483	1691	32			

There are 20 discrepancies between the modelled and reference sequences:

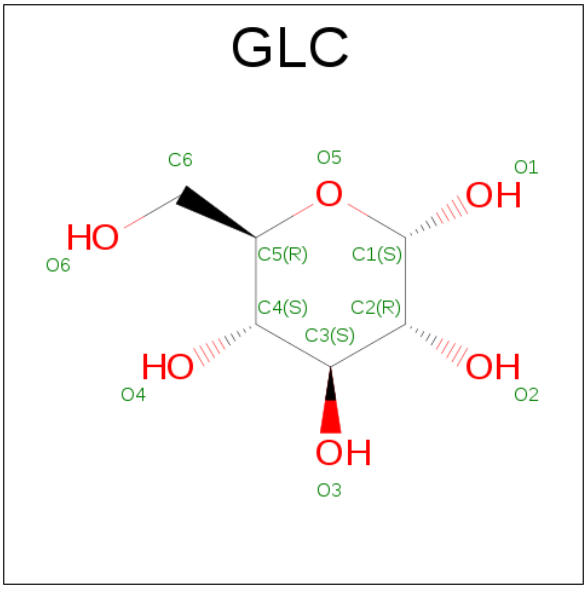
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP A9KJS6
A	1	GLY	-	expression tag	UNP A9KJS6
A	1114	LEU	-	expression tag	UNP A9KJS6
A	1115	GLU	-	expression tag	UNP A9KJS6
A	1116	HIS	-	expression tag	UNP A9KJS6
A	1117	HIS	-	expression tag	UNP A9KJS6
A	1118	HIS	-	expression tag	UNP A9KJS6
A	1119	HIS	-	expression tag	UNP A9KJS6
A	1120	HIS	-	expression tag	UNP A9KJS6
A	1121	HIS	-	expression tag	UNP A9KJS6
B	0	MET	-	expression tag	UNP A9KJS6
B	1	GLY	-	expression tag	UNP A9KJS6
B	1114	LEU	-	expression tag	UNP A9KJS6
B	1115	GLU	-	expression tag	UNP A9KJS6
B	1116	HIS	-	expression tag	UNP A9KJS6
B	1117	HIS	-	expression tag	UNP A9KJS6
B	1118	HIS	-	expression tag	UNP A9KJS6
B	1119	HIS	-	expression tag	UNP A9KJS6
B	1120	HIS	-	expression tag	UNP A9KJS6
B	1121	HIS	-	expression tag	UNP A9KJS6

- Molecule 2 is ALPHA-D-GLUCOSE-1-PHOSPHATE (three-letter code: G1P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

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



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

- Molecule 4 is water.

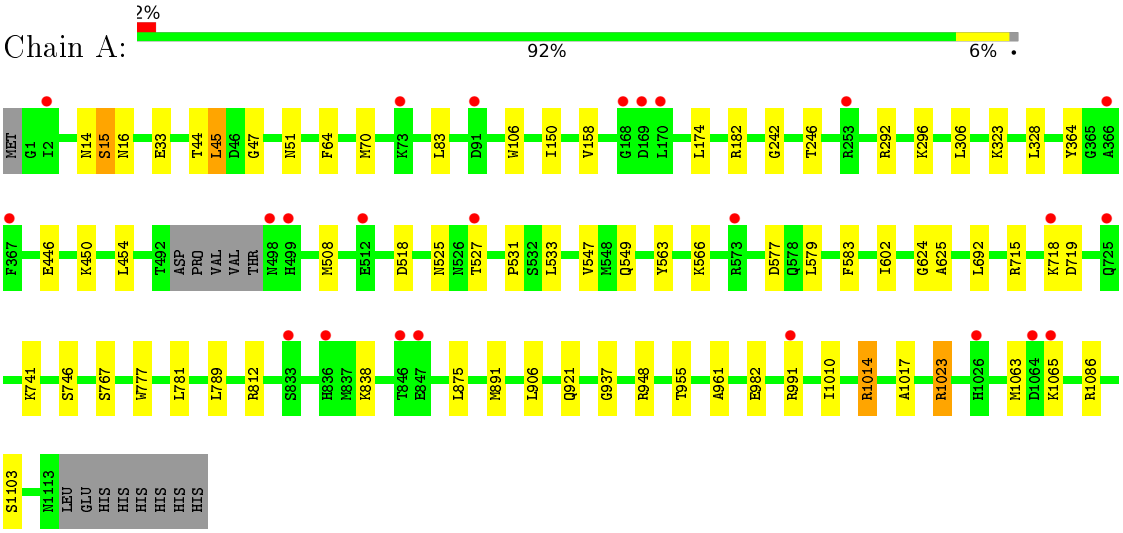
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	338	Total O 338 338	0	0
4	B	314	Total O 314 314	0	0

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.

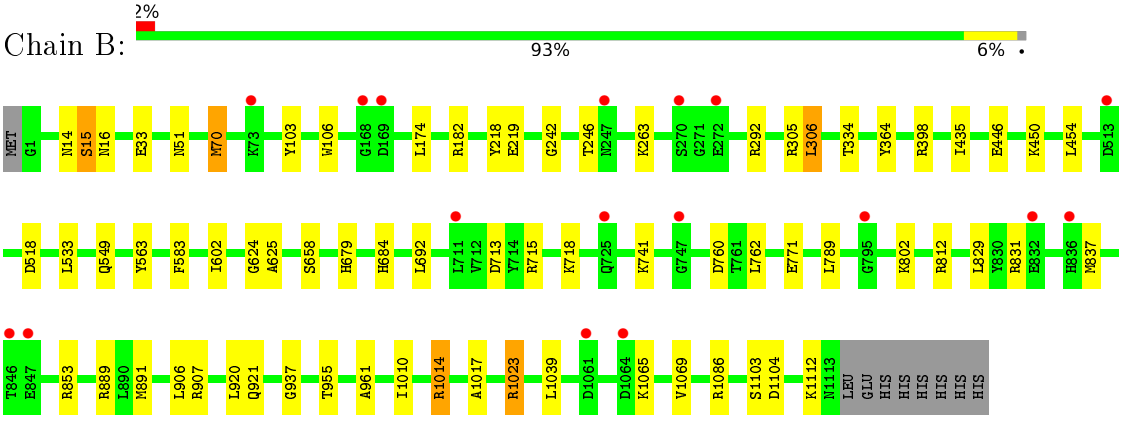
- Molecule 1: Uncharacterized protein

Chain A:



- Molecule 1: Uncharacterized protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.47Å 94.78Å 156.85Å 90.00° 93.96° 90.00°	Depositor
Resolution (Å)	48.25 – 2.10 33.03 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.7 (48.25-2.10) 95.7 (33.03-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.195 , 0.236 0.201 , 0.241	Depositor DCC
R_{free} test set	6945 reflections (5.17%)	DCC
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18512	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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, 0.333 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, G1P

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	0.76	0/9105	0.86	10/12364 (0.1%)
1	B	0.76	0/9143	0.86	14/12420 (0.1%)
All	All	0.76	0/18248	0.86	24/24784 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1063	MET	CG-SD-CE	8.97	114.56	100.20
1	A	182	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	B	1112	LYS	CB-CA-C	-7.42	95.56	110.40
1	B	891	MET	CG-SD-CE	6.96	111.34	100.20
1	B	70	MET	CG-SD-CE	-6.94	89.09	100.20
1	A	891	MET	CG-SD-CE	6.46	110.53	100.20
1	A	150	ILE	CG1-CB-CG2	-6.21	97.73	111.40
1	B	182	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	1023	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	182	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	715	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	715	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	812	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	1023	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	398	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	715	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	812	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	398	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	719	ASP	CB-CA-C	-5.22	99.96	110.40
1	A	948	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	907	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	1104	ASP	CB-CG-OD1	5.05	122.85	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	182	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	B	305	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8882	0	8638	24	0
1	B	8918	0	8675	24	0
2	A	16	0	11	1	0
2	B	32	0	22	1	0
3	B	12	0	12	2	0
4	A	338	0	0	3	0
4	B	314	0	0	1	0
All	All	18512	0	17358	50	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 1.

All (50) 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:829:LEU:HD21	1:B:837:MET:HE1	1.38	1.06
1:B:829:LEU:HD21	1:B:837:MET:CE	1.95	0.95
1:A:525:ASN:ND2	1:A:527:THR:OG1	2.19	0.76
1:A:525:ASN:CG	1:A:527:THR:OG1	2.28	0.72
1:B:33:GLU:HB2	1:B:246:THR:HG21	1.89	0.55
1:B:518:ASP:HA	1:B:533:LEU:O	2.08	0.54
1:A:518:ASP:HA	1:A:533:LEU:O	2.09	0.52
1:B:103:TYR:CE1	1:B:263:LYS:HE3	2.44	0.52
1:A:33:GLU:HB2	1:A:246:THR:HG21	1.90	0.52
1:A:44:THR:O	1:A:70:MET:HE1	2.10	0.51
1:B:306:LEU:CD2	3:B:1203:GLC:H62	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1201:G1P:P	4:A:1302:HOH:O	2.69	0.49
1:A:955:THR:HG22	1:A:961:ALA:O	2.12	0.49
1:B:955:THR:HG22	1:B:961:ALA:O	2.12	0.49
1:B:14:ASN:O	1:B:15:SER:C	2.53	0.47
1:A:937:GLY:HA3	1:A:1086:ARG:HD3	1.96	0.47
1:A:982:GLU:HG2	4:A:1542:HOH:O	2.14	0.47
1:A:16:ASN:HB3	1:A:33:GLU:HG3	1.98	0.46
1:A:47:GLY:N	1:A:70:MET:HE3	2.30	0.46
1:B:937:GLY:HA3	1:B:1086:ARG:HD3	1.98	0.46
1:A:450:LYS:NZ	1:A:563:TYR:O	2.32	0.46
1:B:450:LYS:NZ	1:B:563:TYR:O	2.30	0.46
1:A:624:GLY:O	1:A:625:ALA:HB3	2.16	0.45
1:B:624:GLY:O	1:B:625:ALA:HB3	2.16	0.45
1:A:44:THR:C	1:A:70:MET:HE1	2.37	0.44
1:B:684:HIS:HE1	1:B:760:ASP:HA	1.83	0.44
1:A:1017:ALA:HB1	1:A:1023:ARG:HG2	2.00	0.44
1:A:583:PHE:CG	1:A:602:ILE:HD13	2.53	0.44
1:A:991:ARG:HD2	4:A:1566:HOH:O	2.17	0.44
2:B:1202:G1P:O3	3:B:1203:GLC:H1	2.17	0.44
1:A:1010:ILE:O	1:A:1014:ARG:HD2	2.18	0.44
1:B:1010:ILE:O	1:B:1014:ARG:HD2	2.18	0.44
1:A:14:ASN:O	1:A:15:SER:C	2.56	0.44
1:B:435:ILE:HD11	1:B:454:LEU:HD22	2.00	0.44
1:A:777:TRP:CH2	1:A:781:LEU:HD22	2.54	0.43
1:A:106:TRP:CZ2	1:A:242:GLY:HA3	2.53	0.42
1:B:658:SER:HA	1:B:713:ASP:O	2.20	0.42
1:A:508:MET:HA	1:A:547:VAL:O	2.20	0.42
1:B:853:ARG:NH1	4:B:1321:HOH:O	2.53	0.42
1:A:446:GLU:HG2	1:A:549:GLN:HG2	2.02	0.41
1:B:16:ASN:HB3	1:B:33:GLU:HG3	2.02	0.41
1:B:1017:ALA:HB1	1:B:1023:ARG:HG2	2.01	0.41
1:B:831:ARG:HD2	1:B:837:MET:HE3	2.01	0.41
1:A:45:LEU:C	1:A:70:MET:HE1	2.41	0.41
1:A:323:LYS:NZ	1:A:577:ASP:OD1	2.53	0.41
1:B:889:ARG:HA	1:B:920:LEU:O	2.19	0.41
1:B:106:TRP:CZ2	1:B:242:GLY:HA3	2.56	0.41
1:B:446:GLU:HG2	1:B:549:GLN:HG2	2.02	0.41
1:B:583:PHE:CG	1:B:602:ILE:HD13	2.56	0.41
1:B:218:TYR:CG	1:B:219:GLU:N	2.89	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	1104/1122 (98%)	1062 (96%)	40 (4%)	2 (0%)	52	53
1	B	1111/1122 (99%)	1065 (96%)	44 (4%)	2 (0%)	52	53
All	All	2215/2244 (99%)	2127 (96%)	84 (4%)	4 (0%)	52	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	906	LEU
1	B	15	SER
1	B	906	LEU
1	A	15	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	970/984 (99%)	943 (97%)	27 (3%)	51	55
1	B	975/984 (99%)	954 (98%)	21 (2%)	60	64
All	All	1945/1968 (99%)	1897 (98%)	48 (2%)	55	59

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	51	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	64	PHE
1	A	83	LEU
1	A	158	VAL
1	A	174	LEU
1	A	292	ARG
1	A	296	LYS
1	A	306	LEU
1	A	328	LEU
1	A	364	TYR
1	A	454	LEU
1	A	531	PRO
1	A	566	LYS
1	A	579	LEU
1	A	692	LEU
1	A	718	LYS
1	A	741	LYS
1	A	746	SER
1	A	767	SER
1	A	789	LEU
1	A	838	LYS
1	A	875	LEU
1	A	921	GLN
1	A	1014	ARG
1	A	1065	LYS
1	A	1103	SER
1	B	51	ASN
1	B	70	MET
1	B	174	LEU
1	B	292	ARG
1	B	306	LEU
1	B	334	THR
1	B	364	TYR
1	B	679	HIS
1	B	692	LEU
1	B	718	LYS
1	B	741	LYS
1	B	762	LEU
1	B	771	GLU
1	B	789	LEU
1	B	802	LYS
1	B	921	GLN
1	B	1014	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1039	LEU
1	B	1065	LYS
1	B	1069	VAL
1	B	1103	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	524	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	G1P	A	1201	-	15,16,16	0.62	0	23,24,24	1.26	2 (8%)
2	G1P	B	1201	-	15,16,16	0.75	0	23,24,24	0.86	0
2	G1P	B	1202	-	15,16,16	0.67	0	23,24,24	2.23	7 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GLC	B	1203	-	12,12,12	1.19	1 (8%)	17,17,17	2.38	7 (41%)

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	G1P	A	1201	-	-	0/7/27/27	0/1/1/1
2	G1P	B	1201	-	-	0/7/27/27	0/1/1/1
2	G1P	B	1202	-	-	0/7/27/27	0/1/1/1
3	GLC	B	1203	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1203	GLC	C1-C2	2.80	1.58	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1202	G1P	O5-C1-O1	-3.57	106.66	111.36
2	B	1202	G1P	O3-C3-C4	-3.32	102.87	110.36
3	B	1203	GLC	O3-C3-C4	-2.68	104.32	110.36
2	A	1201	G1P	O2-C2-C1	-2.52	104.42	110.01
3	B	1203	GLC	C6-C5-C4	-2.42	106.92	112.99
2	B	1202	G1P	O5-C5-C4	2.06	113.59	109.67
2	B	1202	G1P	O5-C1-C2	2.07	114.58	110.28
2	B	1202	G1P	C1-C2-C3	2.24	114.43	109.98
3	B	1203	GLC	C3-C4-C5	2.29	114.31	110.23
3	B	1203	GLC	O5-C5-C6	3.11	114.45	106.38
2	A	1201	G1P	O3P-P-O2P	3.42	120.00	107.44
3	B	1203	GLC	O2-C2-C1	3.45	117.29	109.74
3	B	1203	GLC	C1-O5-C5	3.95	121.09	113.54
2	B	1202	G1P	O1-C1-C2	4.11	116.06	108.39
3	B	1203	GLC	O5-C1-C2	5.58	119.77	110.00
2	B	1202	G1P	C1-O5-C5	5.67	124.87	113.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	G1P	1	0
2	B	1202	G1P	1	0
3	B	1203	GLC	2	0

5.7 Other polymers

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	1108/1122 (98%)	-0.02	24 (2%)	65	71	14, 23, 40, 63	0
1	B	1113/1122 (99%)	0.01	17 (1%)	76	81	15, 24, 42, 61	0
All	All	2221/2244 (98%)	-0.00	41 (1%)	71	76	14, 24, 41, 63	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	711	LEU	4.6
1	B	846	THR	4.3
1	B	1064	ASP	4.1
1	A	1064	ASP	3.8
1	A	498	ASN	3.7
1	B	795	GLY	3.5
1	B	169	ASP	3.5
1	B	513	ASP	3.3
1	A	168	GLY	3.1
1	A	73	LYS	3.1
1	A	169	ASP	3.0
1	B	836	HIS	2.9
1	A	847	GLU	2.9
1	A	2	ILE	2.8
1	B	272	GLU	2.7
1	B	747	GLY	2.6
1	B	247	ASN	2.6
1	A	846	THR	2.6
1	A	718	LYS	2.5
1	B	270	SER	2.5
1	A	527	THR	2.4
1	A	836	HIS	2.4
1	A	991	ARG	2.4
1	A	91	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1061	ASP	2.3
1	B	73	LYS	2.3
1	A	573	ARG	2.3
1	A	1026	HIS	2.2
1	A	725	GLN	2.2
1	B	168	GLY	2.2
1	A	367	PHE	2.2
1	A	1065	LYS	2.2
1	A	253	ARG	2.2
1	A	499	HIS	2.1
1	A	170	LEU	2.1
1	A	833	SER	2.1
1	A	366	ALA	2.1
1	B	832	GLU	2.1
1	B	847	GLU	2.0
1	B	725	GLN	2.0
1	A	512	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
2	G1P	B	1202	16/16	0.73	0.28	2.38	36,46,74,77	0
2	G1P	B	1201	16/16	0.97	0.12	-0.77	18,21,30,30	0
2	G1P	A	1201	16/16	0.97	0.12	-1.01	21,23,34,36	0
3	GLC	B	1203	12/12	0.82	0.26	-	41,43,44,47	0

6.5 Other polymers (i)

There are no such residues in this entry.