



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:17 am GMT

PDB ID : 1L6I
Title : Crystal Structure of the Maltodextrin Phosphorylase complexed with the products of the enzymatic reaction between glucose-1-phosphate and maltopentaose
Authors : Geremia, S.; Campagnolo, M.; Schinzel, R.; Johnson, L.N.
Deposited on : 2002-03-11
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

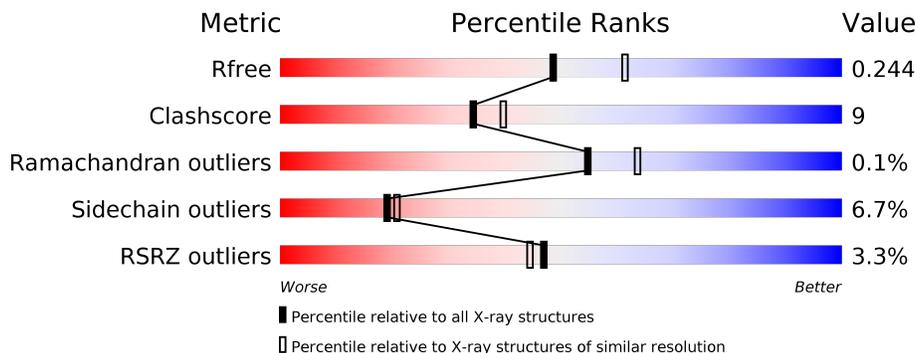
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 $\leq 5\%$. 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	796	
1	B	796	

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	B	997	-	-	-	X
2	GLC	B	998	-	-	-	X
3	PO4	A	999	-	-	X	-
3	PO4	B	999	-	-	X	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14135 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 MALTODEXTRIN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	796	6390	4079	1128	1163	20	0	0	0
1	B	796	6390	4079	1128	1163	20	0	0	0

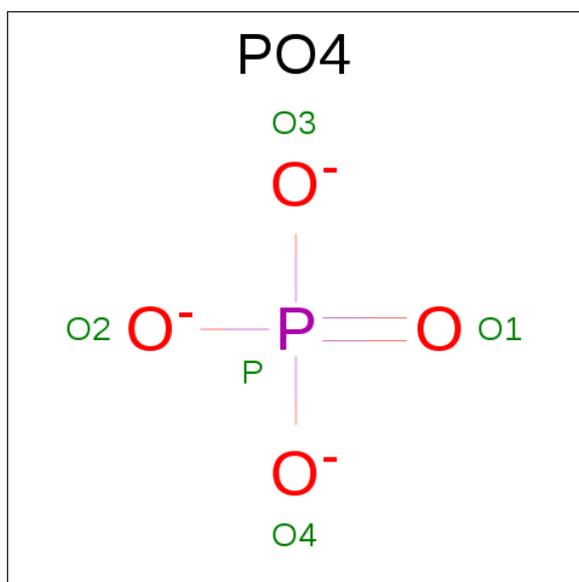
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	ALA	HIS	SEE REMARK 999	GB 606352
A	262	PHE	THR	SEE REMARK 999	GB 606352
A	263	GLU	ALA	SEE REMARK 999	GB 606352
B	261	ALA	HIS	SEE REMARK 999	GB 606352
B	262	PHE	THR	SEE REMARK 999	GB 606352
B	263	GLU	ALA	SEE REMARK 999	GB 606352

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

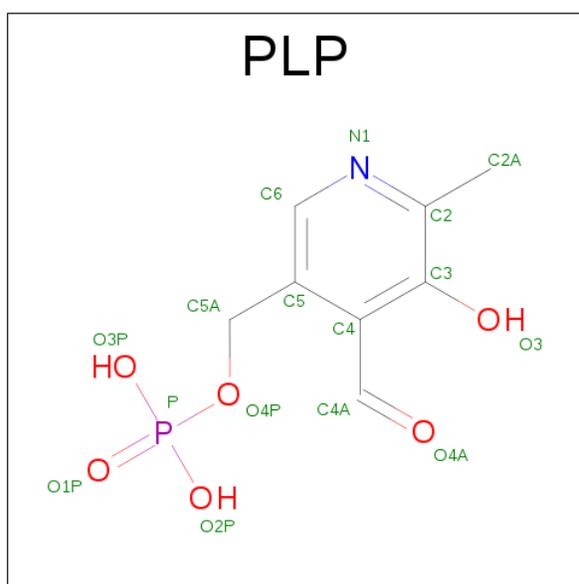
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	5	56	30	26	0	0
2	B	5	56	30	26	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	P	0	0	
			5	4	1			
3	B	1	Total	O	P	0	0	
			5	4	1			

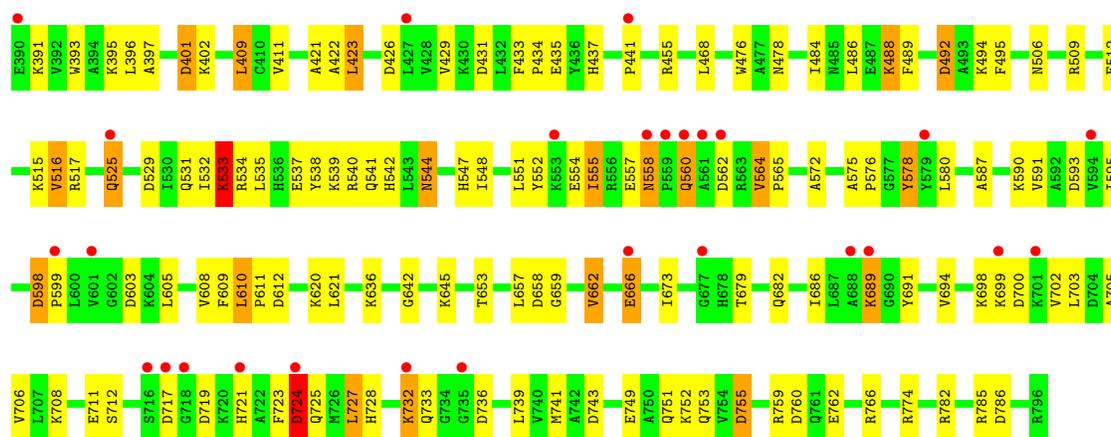
- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	606	Total 606	O 606	0	0
5	B	597	Total 597	O 597	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.33Å 105.94Å 218.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 18.54 – 2.18	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-2.20) 90.4 (18.54-2.18)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.19Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.243 0.198 , 0.244	Depositor DCC
R_{free} test set	4091 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	29.3	Xtrriage
Anisotropy	0.847	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14135	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GLC, PLP

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	1.18	10/6540 (0.2%)	1.23	52/8865 (0.6%)
1	B	1.18	5/6540 (0.1%)	1.20	50/8865 (0.6%)
All	All	1.18	15/13080 (0.1%)	1.22	102/17730 (0.6%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	723	PHE	CE2-CZ	6.05	1.48	1.37
1	A	696	TRP	CB-CG	-5.96	1.39	1.50
1	A	140	TYR	CE2-CZ	-5.67	1.31	1.38
1	B	194	GLU	CD-OE1	5.63	1.31	1.25
1	A	222	ALA	CA-CB	5.61	1.64	1.52

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ARG	NE-CZ-NH1	16.63	128.61	120.30
1	A	268	ARG	NE-CZ-NH2	-16.25	112.18	120.30
1	A	492	ASP	CB-CG-OD2	12.90	129.91	118.30
1	A	72	ARG	NE-CZ-NH1	-10.21	115.20	120.30
1	A	323	ASP	CB-CG-OD2	9.97	127.27	118.30

There are no chirality outliers.

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	6390	0	6333	109	0
1	B	6390	0	6333	143	0
2	A	56	0	48	3	0
2	B	56	0	48	3	0
3	A	5	0	0	2	0
3	B	5	0	0	3	0
4	A	15	0	7	0	0
4	B	15	0	7	0	0
5	A	606	0	0	11	0
5	B	597	0	0	16	0
All	All	14135	0	12776	244	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 9.

The worst 5 of 244 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:733:GLN:N	1:A:733:GLN:OE1	2.05	0.88
1:A:22:GLY:CA	1:B:170:ARG:HD2	2.11	0.79
1:B:733:GLN:OE1	1:B:733:GLN:N	2.14	0.79
1:A:22:GLY:HA3	1:B:170:ARG:HD2	1.65	0.79
1:A:437:HIS:CD2	1:A:441:PRO:HA	2.17	0.78

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	794/796 (100%)	766 (96%)	28 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	794/796 (100%)	759 (96%)	33 (4%)	2 (0%)	44	49
All	All	1588/1592 (100%)	1525 (96%)	61 (4%)	2 (0%)	55	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	533	LYS
1	B	558	ASN

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	667/667 (100%)	625 (94%)	42 (6%)	21	23
1	B	667/667 (100%)	620 (93%)	47 (7%)	18	19
All	All	1334/1334 (100%)	1245 (93%)	89 (7%)	19	21

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	766	ARG
1	B	177	VAL
1	B	689	LYS
1	A	785	ARG
1	B	92	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	531	GLN
1	B	97	ASN
1	B	544	ASN
1	A	544	ASN
1	B	57	ASN

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](#)

10 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	994	2	12,12,12	0.88	0	17,17,17	1.65	5 (29%)
2	GLC	A	995	2	11,11,12	1.14	1 (9%)	13,15,17	1.32	2 (15%)
2	GLC	A	996	2	11,11,12	1.10	1 (9%)	13,15,17	1.57	3 (23%)
2	GLC	A	997	2	11,11,12	1.20	2 (18%)	13,15,17	1.69	4 (30%)
2	GLC	A	998	2	11,11,12	1.19	1 (9%)	13,15,17	3.55	6 (46%)
2	GLC	B	994	2	12,12,12	0.74	0	17,17,17	1.74	4 (23%)
2	GLC	B	995	2	11,11,12	1.05	1 (9%)	13,15,17	1.07	1 (7%)
2	GLC	B	996	2	11,11,12	0.77	0	13,15,17	1.35	2 (15%)
2	GLC	B	997	2	11,11,12	0.68	0	13,15,17	1.54	3 (23%)
2	GLC	B	998	2	11,11,12	0.79	1 (9%)	13,15,17	2.57	5 (38%)

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	994	2	-	0/2/22/22	0/1/1/1
2	GLC	A	995	2	-	0/2/19/22	0/1/1/1
2	GLC	A	996	2	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	A	997	2	-	0/2/19/22	0/1/1/1
2	GLC	A	998	2	-	0/2/19/22	0/1/1/1
2	GLC	B	994	2	-	0/2/22/22	0/1/1/1
2	GLC	B	995	2	-	0/2/19/22	0/1/1/1
2	GLC	B	996	2	-	0/2/19/22	0/1/1/1
2	GLC	B	997	2	-	0/2/19/22	0/1/1/1
2	GLC	B	998	2	-	0/2/19/22	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	997	GLC	O5-C1	-2.68	1.39	1.43
2	A	996	GLC	O5-C1	-2.41	1.39	1.43
2	A	995	GLC	O5-C5	-2.32	1.38	1.43
2	B	998	GLC	C1-C2	2.02	1.57	1.52
2	A	997	GLC	C2-C3	2.28	1.55	1.52

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	997	GLC	O3-C3-C2	-3.38	103.87	110.02
2	A	998	GLC	O3-C3-C4	-3.02	103.79	110.36
2	B	994	GLC	O2-C2-C3	-2.95	103.94	110.36
2	A	996	GLC	C6-C5-C4	-2.84	106.35	113.00
2	A	998	GLC	O5-C1-C2	-2.55	106.79	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	994	GLC	1	0
2	A	997	GLC	2	0
2	B	997	GLC	3	0

5.6 Ligand geometry [i](#)

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
4	PLP	A	900	1	15,15,16	2.06	1 (6%)	20,22,23	2.03	6 (30%)
3	PO4	A	999	-	4,4,4	0.67	0	6,6,6	0.87	0
4	PLP	B	900	1	15,15,16	2.90	3 (20%)	20,22,23	3.04	8 (40%)
3	PO4	B	999	-	4,4,4	0.82	0	6,6,6	0.75	0

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
4	PLP	A	900	1	-	0/6/6/8	0/1/1/1
3	PO4	A	999	-	-	0/0/0/0	0/0/0/0
4	PLP	B	900	1	-	0/6/6/8	0/1/1/1
3	PO4	B	999	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	900	PLP	C3-C2	-9.45	1.34	1.40
4	A	900	PLP	C3-C2	-7.07	1.35	1.40
4	B	900	PLP	C5-C4	-3.84	1.36	1.40
4	B	900	PLP	C4A-C4	-2.63	1.46	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	900	PLP	C4A-C4-C5	-6.78	114.01	120.86
4	B	900	PLP	C6-C5-C4	-5.45	113.62	118.18
4	B	900	PLP	C3-C2-N1	-4.92	114.29	120.75
4	A	900	PLP	C4A-C4-C5	-3.55	117.27	120.86
4	A	900	PLP	O4P-C5A-C5	-2.99	103.30	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	PO4	2	0
3	B	999	PO4	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	796/796 (100%)	-0.13	13 (1%) 72 70	18, 32, 51, 65	0
1	B	796/796 (100%)	0.03	39 (4%) 30 29	18, 33, 52, 73	0
All	All	1592/1592 (100%)	-0.05	52 (3%) 47 44	18, 32, 52, 73	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	560	GLN	6.4
1	B	562	ASP	5.8
1	B	57	ASN	5.6
1	B	689	LYS	4.4
1	B	688	ALA	4.2

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	GLC	B	997	11/12	0.78	0.23	2.80	43,45,46,48	0
2	GLC	B	998	11/12	0.83	0.20	2.01	40,44,46,48	0
2	GLC	A	998	11/12	0.81	0.19	1.95	38,43,46,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GLC	B	995	11/12	0.78	0.21	0.93	39,45,46,46	0
2	GLC	A	995	11/12	0.80	0.15	0.87	39,45,46,46	0
2	GLC	A	997	11/12	0.89	0.13	0.64	42,45,47,47	0
2	GLC	A	996	11/12	0.89	0.14	0.43	38,40,43,45	0
2	GLC	B	994	12/12	0.86	0.21	-0.10	43,45,48,54	0
2	GLC	B	996	11/12	0.93	0.14	-0.18	39,41,43,46	0
2	GLC	A	994	12/12	0.94	0.10	-0.71	42,45,48,53	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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	B	999	5/5	0.91	0.32	4.63	58,61,62,62	0
3	PO4	A	999	5/5	0.97	0.15	0.99	59,60,61,62	0
4	PLP	A	900	15/16	0.96	0.10	-0.42	18,24,34,35	0
4	PLP	B	900	15/16	0.96	0.09	-0.64	18,26,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.