



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:10 PM GMT

PDB ID : 4BQI  
Title : ARABIDOPSIS THALIANA cytosolic alpha-1,4-glucan phosphorylase (PHS2)  
in complex with maltotriose  
Authors : O'Neill, E.C.; Rashid, A.M.; Stevenson, C.E.M.; Hetru, A.C.; Gunning, A.P.;  
Rejzek, M.; Nepogodiev, S.A.; Bornemann, S.; Lawson, D.M.; Field, R.A.  
Deposited on : 2013-05-30  
Resolution : 1.90 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](mailto: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 (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

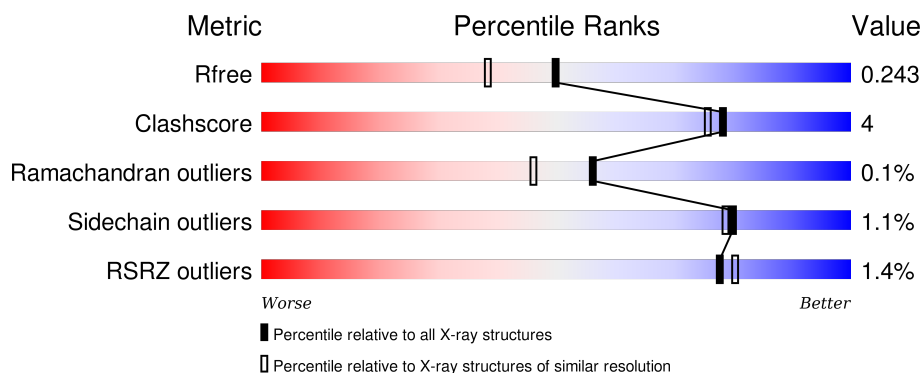
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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  $\geq 3$ , 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	874	
1	B	874	

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
3	MLR	A	951	-	-	-	X
4	PEG	A	1842	-	-	X	X
5	GOL	B	1842	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14073 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 ALPHA-GLUCAN PHOSPHORYLASE 2, CYTOSOLIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	824	Total	C	N	O	S	0	8	0
			6531	4169	1110	1229	23			
1	B	824	Total	C	N	O	S	0	7	0
			6512	4157	1109	1223	23			

There are 66 discrepancies between the modelled and reference sequences:

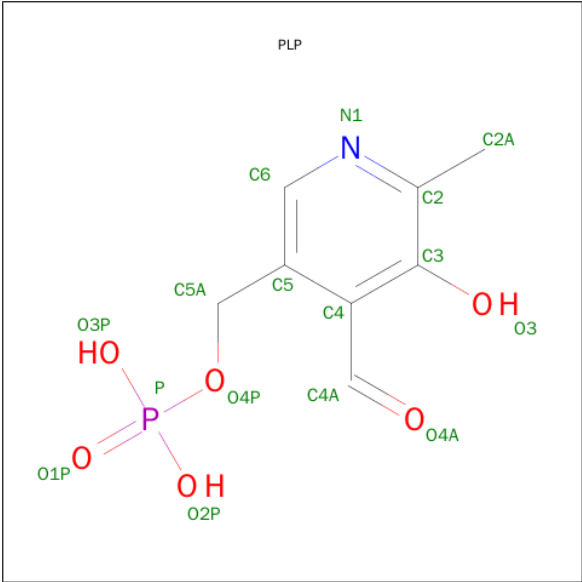
Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	EXPRESSION TAG	UNP Q9SD76
A	-31	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-30	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-29	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-28	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-27	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-26	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-25	GLY	-	EXPRESSION TAG	UNP Q9SD76
A	-24	LYS	-	EXPRESSION TAG	UNP Q9SD76
A	-23	PRO	-	EXPRESSION TAG	UNP Q9SD76
A	-22	ILE	-	EXPRESSION TAG	UNP Q9SD76
A	-21	PRO	-	EXPRESSION TAG	UNP Q9SD76
A	-20	ASN	-	EXPRESSION TAG	UNP Q9SD76
A	-19	PRO	-	EXPRESSION TAG	UNP Q9SD76
A	-18	LEU	-	EXPRESSION TAG	UNP Q9SD76
A	-17	LEU	-	EXPRESSION TAG	UNP Q9SD76
A	-16	GLY	-	EXPRESSION TAG	UNP Q9SD76
A	-15	LEU	-	EXPRESSION TAG	UNP Q9SD76
A	-14	ASP	-	EXPRESSION TAG	UNP Q9SD76
A	-13	SER	-	EXPRESSION TAG	UNP Q9SD76
A	-12	THR	-	EXPRESSION TAG	UNP Q9SD76
A	-11	GLU	-	EXPRESSION TAG	UNP Q9SD76
A	-10	ASN	-	EXPRESSION TAG	UNP Q9SD76
A	-9	LEU	-	EXPRESSION TAG	UNP Q9SD76
A	-8	TYR	-	EXPRESSION TAG	UNP Q9SD76

*Continued on next page...*

*Continued from previous page...*

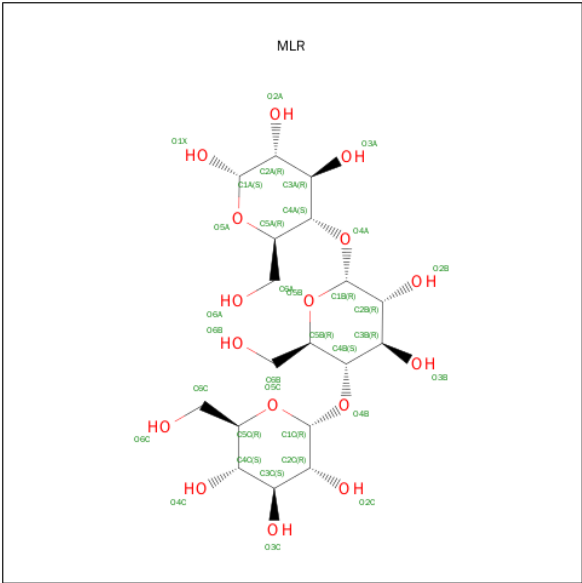
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	PHE	-	EXPRESSION TAG	UNP Q9SD76
A	-6	GLN	-	EXPRESSION TAG	UNP Q9SD76
A	-5	GLY	-	EXPRESSION TAG	UNP Q9SD76
A	-4	ILE	-	EXPRESSION TAG	UNP Q9SD76
A	-3	ASP	-	EXPRESSION TAG	UNP Q9SD76
A	-2	PRO	-	EXPRESSION TAG	UNP Q9SD76
A	-1	PHE	-	EXPRESSION TAG	UNP Q9SD76
A	0	THR	-	EXPRESSION TAG	UNP Q9SD76
B	-32	MET	-	EXPRESSION TAG	UNP Q9SD76
B	-31	HIS	-	EXPRESSION TAG	UNP Q9SD76
B	-30	HIS	-	EXPRESSION TAG	UNP Q9SD76
B	-29	HIS	-	EXPRESSION TAG	UNP Q9SD76
B	-28	HIS	-	EXPRESSION TAG	UNP Q9SD76
B	-27	HIS	-	EXPRESSION TAG	UNP Q9SD76
B	-26	HIS	-	EXPRESSION TAG	UNP Q9SD76
B	-25	GLY	-	EXPRESSION TAG	UNP Q9SD76
B	-24	LYS	-	EXPRESSION TAG	UNP Q9SD76
B	-23	PRO	-	EXPRESSION TAG	UNP Q9SD76
B	-22	ILE	-	EXPRESSION TAG	UNP Q9SD76
B	-21	PRO	-	EXPRESSION TAG	UNP Q9SD76
B	-20	ASN	-	EXPRESSION TAG	UNP Q9SD76
B	-19	PRO	-	EXPRESSION TAG	UNP Q9SD76
B	-18	LEU	-	EXPRESSION TAG	UNP Q9SD76
B	-17	LEU	-	EXPRESSION TAG	UNP Q9SD76
B	-16	GLY	-	EXPRESSION TAG	UNP Q9SD76
B	-15	LEU	-	EXPRESSION TAG	UNP Q9SD76
B	-14	ASP	-	EXPRESSION TAG	UNP Q9SD76
B	-13	SER	-	EXPRESSION TAG	UNP Q9SD76
B	-12	THR	-	EXPRESSION TAG	UNP Q9SD76
B	-11	GLU	-	EXPRESSION TAG	UNP Q9SD76
B	-10	ASN	-	EXPRESSION TAG	UNP Q9SD76
B	-9	LEU	-	EXPRESSION TAG	UNP Q9SD76
B	-8	TYR	-	EXPRESSION TAG	UNP Q9SD76
B	-7	PHE	-	EXPRESSION TAG	UNP Q9SD76
B	-6	GLN	-	EXPRESSION TAG	UNP Q9SD76
B	-5	GLY	-	EXPRESSION TAG	UNP Q9SD76
B	-4	ILE	-	EXPRESSION TAG	UNP Q9SD76
B	-3	ASP	-	EXPRESSION TAG	UNP Q9SD76
B	-2	PRO	-	EXPRESSION TAG	UNP Q9SD76
B	-1	PHE	-	EXPRESSION TAG	UNP Q9SD76
B	0	THR	-	EXPRESSION TAG	UNP Q9SD76

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



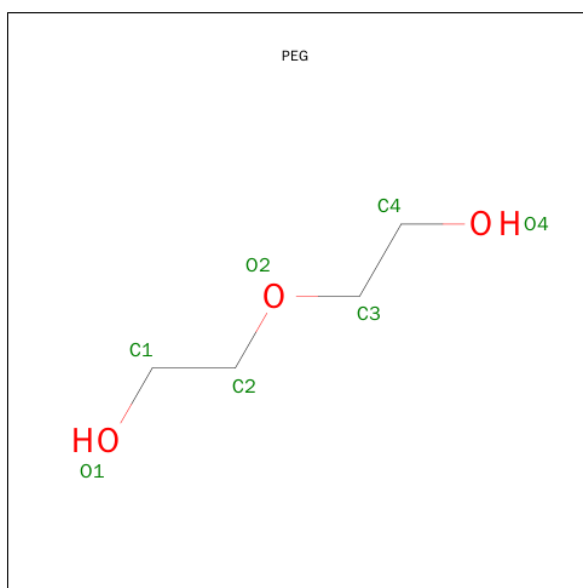
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is MALTOTRIOSE (three-letter code: MLR) (formula: C<sub>18</sub>H<sub>32</sub>O<sub>16</sub>).



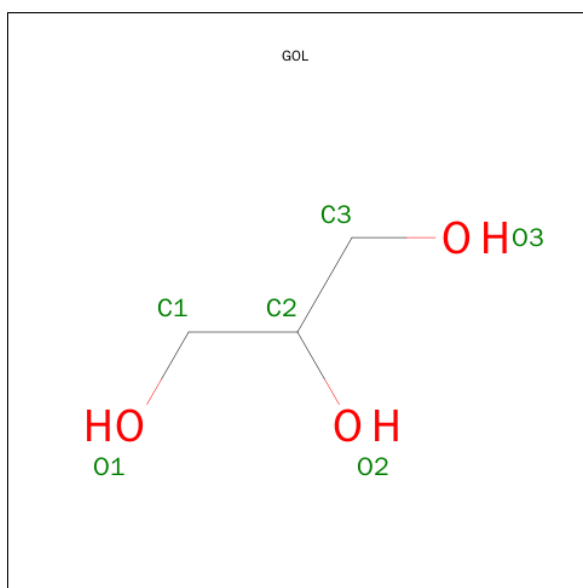
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			34	18	16		
3	B	1	Total	C	O	0	0
			34	18	16		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 6 is water.

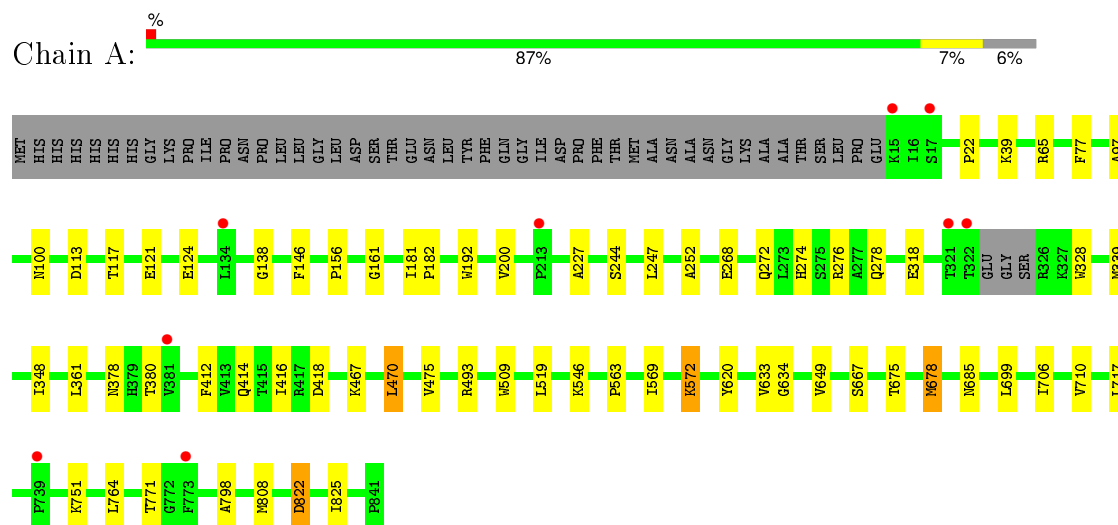
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	486	Total 486	O 486	0	0
6	B	433	Total 433	O 433	0	0



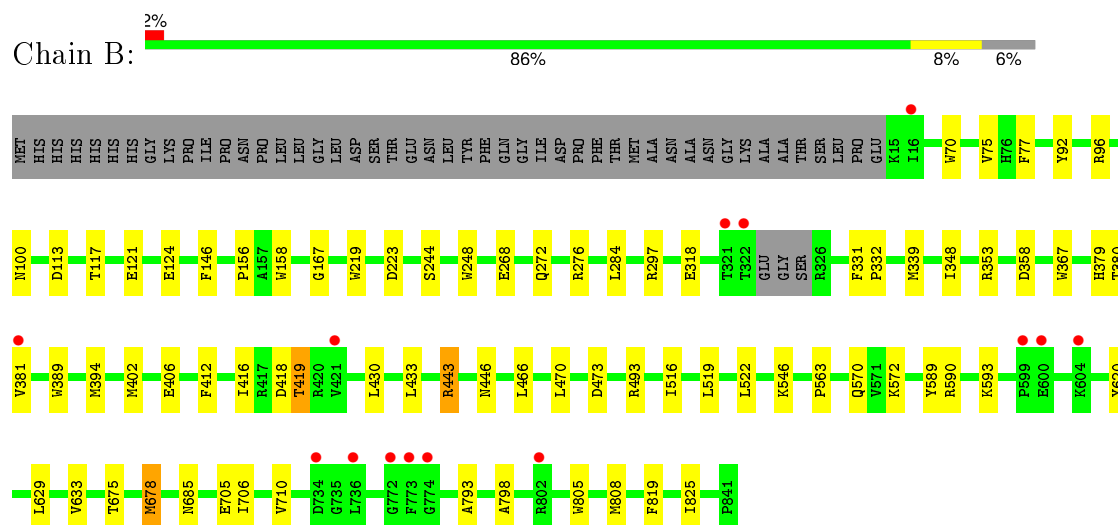
### 3 Residue-property plots [i](#)

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: ALPHA-GLUCAN PHOSPHORYLASE 2, CYTOSOLIC



#### • Molecule 1: ALPHA-GLUCAN PHOSPHORYLASE 2, CYTOSOLIC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.71Å 116.07Å 94.34Å 90.00° 107.38° 90.00°	Depositor
Resolution (Å)	52.48 – 1.90 52.48 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (52.48-1.90) 98.2 (52.48-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.196 , 0.241 0.199 , 0.243	Depositor DCC
$R_{free}$ test set	6646 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 132807 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.70 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.6338e-03.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: MLR, GOL, PEG, 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	0.78	1/6706 (0.0%)	0.80	2/9107 (0.0%)
1	B	0.76	7/6683 (0.1%)	0.79	5/9075 (0.1%)
All	All	0.77	8/13389 (0.1%)	0.79	7/18182 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	367	TRP	CD2-CE2	6.06	1.48	1.41
1	A	509	TRP	CD2-CE2	5.96	1.48	1.41
1	B	389	TRP	CD2-CE2	5.62	1.48	1.41
1	B	219	TRP	CD2-CE2	5.50	1.48	1.41
1	B	158	TRP	CD2-CE2	5.43	1.47	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	B	96[A]	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	B	96[B]	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	B	443	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	443	ARG	NE-CZ-NH2	-6.10	117.25	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	6531	0	6352	48	0
1	B	6512	0	6319	45	0
2	A	15	0	7	2	0
2	B	15	0	6	0	0
3	A	34	0	32	0	0
3	B	34	0	32	0	0
4	A	7	0	10	6	0
5	B	6	0	8	2	0
6	A	486	0	0	6	0
6	B	433	0	0	10	0
All	All	14073	0	12766	92	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 4.

The worst 5 of 92 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:418:ASP:O	1:B:419:THR:HG23	1.19	1.32
1:B:418:ASP:O	1:B:419:THR:CG2	2.02	1.07
1:A:519:LEU:H	4:A:1842:PEG:H41	1.39	0.87
1:A:822:ASP:HB2	4:A:1842:PEG:H31	1.60	0.83
1:B:705[B]:GLU:CD	1:B:819:PHE:HE1	1.87	0.76

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	828/874 (95%)	807 (98%)	21 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	827/874 (95%)	803 (97%)	23 (3%)	1 (0%)	56 46
All	All	1655/1748 (95%)	1610 (97%)	44 (3%)	1 (0%)	56 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	419	THR

### 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	687/752 (91%)	679 (99%)	8 (1%)	78 76
1	B	680/752 (90%)	673 (99%)	7 (1%)	82 81
All	All	1367/1504 (91%)	1352 (99%)	15 (1%)	80 79

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	685	ASN
1	A	771	THR
1	B	620	TYR
1	A	678	MET
1	B	572	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	278	GLN
1	A	460	GLN
1	B	100	ASN
1	B	278	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	PEG	A	1842	-	6,6,6	0.56	0	5,5,5	1.90	2 (40%)
2	PLP	A	901	1	15,15,16	0.79	1 (6%)	21,22,23	1.77	5 (23%)
3	MLR	A	951	-	36,36,36	0.53	0	53,53,53	1.35	7 (13%)
5	GOL	B	1842	-	5,5,5	0.42	0	5,5,5	0.98	0
2	PLP	B	901	1	15,15,16	1.19	0	21,22,23	1.50	3 (14%)
3	MLR	B	951	-	36,36,36	0.59	0	53,53,53	1.18	4 (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
4	PEG	A	1842	-	-	0/4/4/4	0/0/0/0
2	PLP	A	901	1	-	0/6/6/8	0/1/1/1
3	MLR	A	951	-	-	0/14/74/74	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	1842	-	-	0/4/4/4	0/0/0/0
2	PLP	B	901	1	-	0/6/6/8	0/1/1/1
3	MLR	B	951	-	-	0/14/74/74	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	PLP	O4P-C5A	-2.02	1.36	1.44

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	PLP	C4A-C4-C5	-3.61	117.12	120.88
4	A	1842	PEG	O2-C2-C1	-3.42	94.68	110.43
2	A	901	PLP	C2A-C2-C3	-2.80	117.66	121.04
2	A	901	PLP	O2P-P-O4P	-2.56	99.20	106.56
3	B	951	MLR	O3B-C3B-C4B	-2.49	103.99	109.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1842	PEG	6	0
2	A	901	PLP	2	0
5	B	1842	GOL	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	824/874 (94%)	-0.07	9 (1%) 82 84	19, 29, 47, 74	0
1	B	824/874 (94%)	0.09	14 (1%) 73 76	17, 33, 55, 88	0
All	All	1648/1748 (94%)	0.01	23 (1%) 78 80	17, 31, 51, 88	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	772	GLY	5.7
1	A	773	PHE	5.5
1	B	773	PHE	5.2
1	B	774	GLY	4.9
1	A	321	THR	4.1

### 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	PEG	A	1842	7/7	0.94	0.28	9.97	30,34,36,37	0
5	GOL	B	1842	6/6	0.89	0.13	3.14	30,36,36,37	0
3	MLR	A	951	34/34	0.85	0.16	2.32	35,42,50,52	0
3	MLR	B	951	34/34	0.90	0.12	1.06	29,35,40,49	0
2	PLP	B	901	15/16	0.95	0.13	0.41	23,26,46,50	0
2	PLP	A	901	15/16	0.96	0.12	0.15	23,25,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.