



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:11 PM GMT

PDB ID : 4BQF  
Title : Arabidopsis thaliana cytosolic alpha-1,4-glucan phosphorylase (PHS2) in complex with acarbose  
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 : 2.35 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](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.

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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

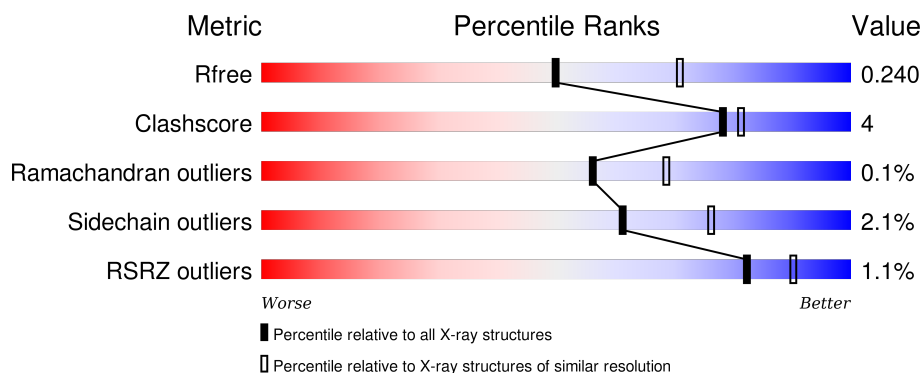
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 9%, green 85%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>9% • 6%</span> </div> </div>
1	B	874	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 9%, green 85%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>9% 5%</span> </div> </div>

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	QPS	A	951	-	-	-	X
3	QPS	B	951	-	-	-	X
4	GLC	A	953	-	-	-	X
4	GLC	B	952	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13573 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	6	0
			6552	4180	1120	1228	24			
1	B	827	Total	C	N	O	S	0	4	0
			6539	4176	1119	1220	24			

There are 66 discrepancies between the modelled and reference sequences:

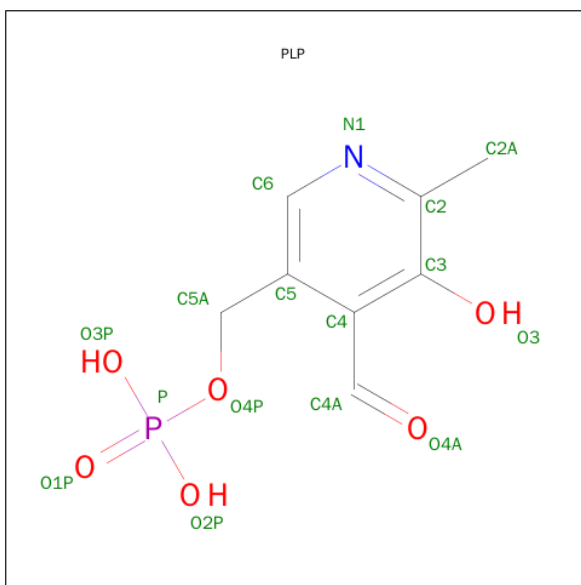
Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	EXPRESSION TAG	UNP Q9SD76
A	-31	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-30	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-29	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-28	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-27	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-26	HIS	-	EXPRESSION TAG	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

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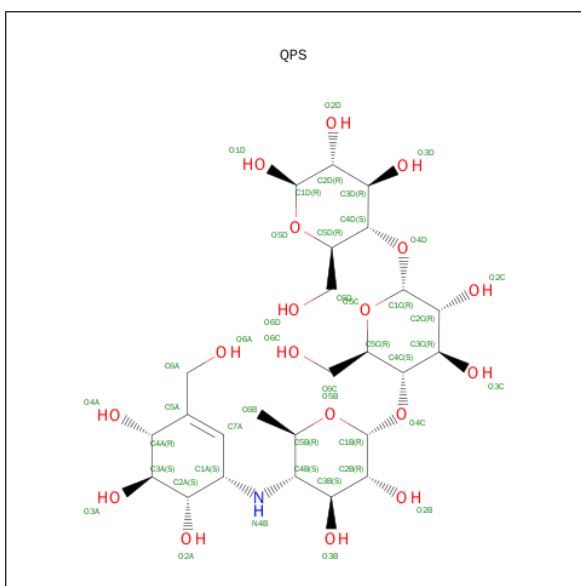
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	PHE	-	EXPRESSION TAG	UNP Q9SD76
A	-6	GLN	-	EXPRESSION TAG	UNP Q9SD76
A	-5	GLY	-	EXPRESSION TAG	UNP Q9SD76
A	-4	ILE	-	EXPRESSION TAG	UNP Q9SD76
A	-3	ASP	-	EXPRESSION TAG	UNP Q9SD76
A	-2	PRO	-	EXPRESSION TAG	UNP Q9SD76
A	-1	PHE	-	EXPRESSION TAG	UNP Q9SD76
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).



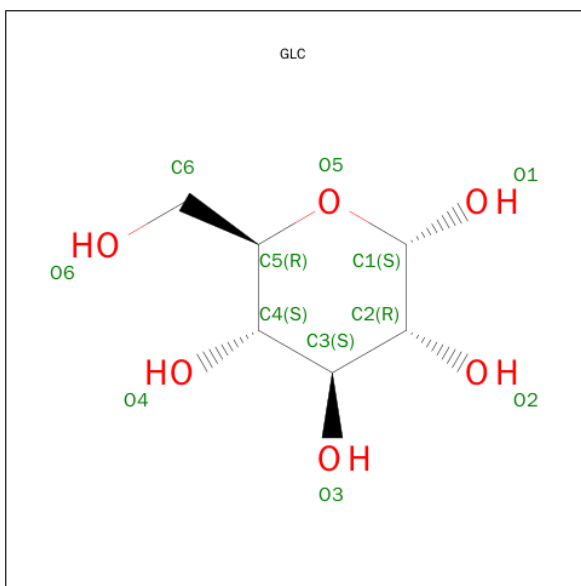
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is SUGAR (BETA-ACARBOSE) (three-letter code: QPS) (formula:  $C_{25}H_{43}NO_{18}$ ).



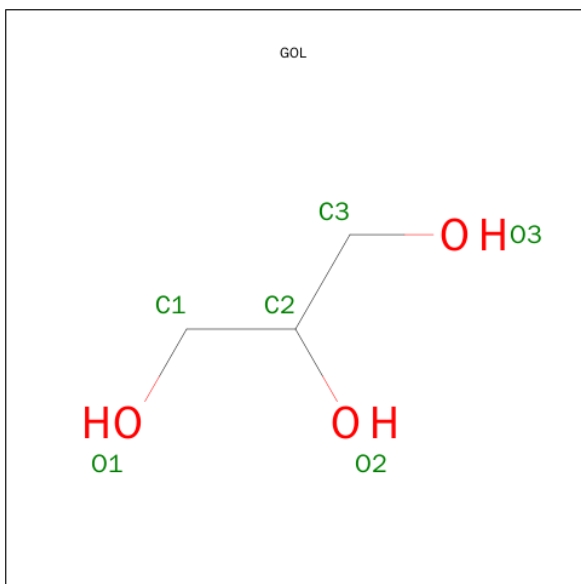
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	12	1	9		
3	B	1	Total	C	N	O	0	0
			44	25	1	18		

- Molecule 4 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula:  $C_6H_{12}O_6$ ).



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

- 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.

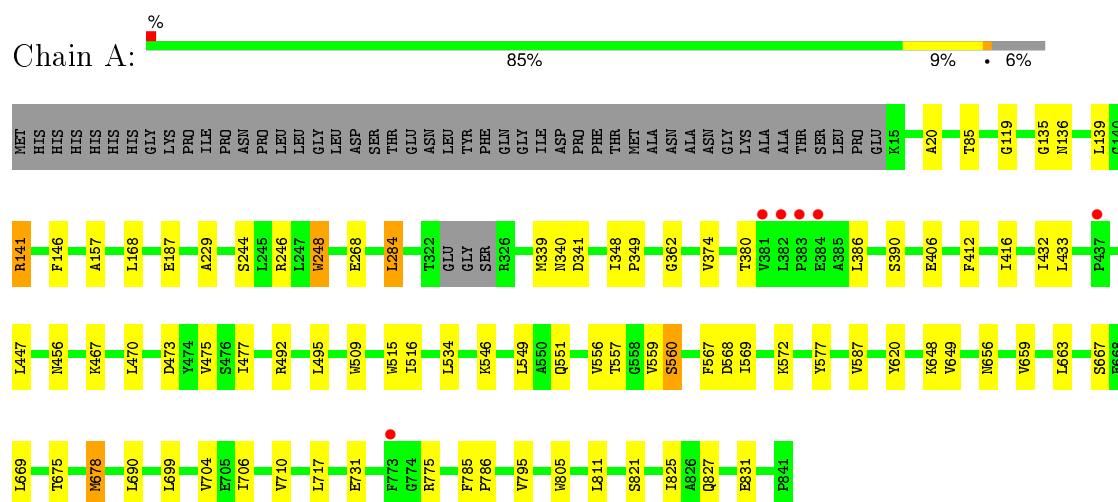
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	197	Total	O	0	0
			197	197		
6	B	147	Total	O	0	0
			147	147		



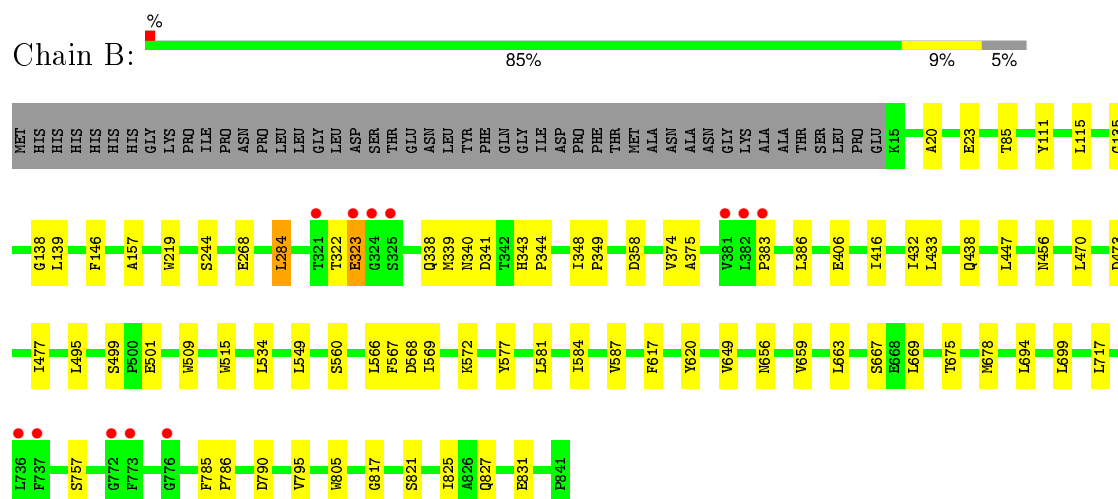
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	84.25Å 117.08Å 94.97Å 90.00° 106.79° 90.00°	Depositor
Resolution (Å)	60.99 – 2.35 53.19 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (60.99-2.35) 99.9 (53.19-2.35)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.184 , 0.240 0.186 , 0.240	Depositor DCC
$R_{free}$ test set	3671 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.7	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 73404 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	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 29.95 % 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 1.4207e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GOL, GLC, PLP, QPS

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	0.79	5/6722 (0.1%)	0.80	4/9123 (0.0%)
1	B	0.77	3/6704 (0.0%)	0.79	1/9100 (0.0%)
All	All	0.78	8/13426 (0.1%)	0.80	5/18223 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	509	TRP	CD2-CE2	6.96	1.49	1.41
1	B	219	TRP	CD2-CE2	6.11	1.48	1.41
1	A	805	TRP	CD2-CE2	5.96	1.48	1.41
1	A	187	GLU	CD-OE2	5.89	1.32	1.25
1	A	248	TRP	CD2-CE2	5.65	1.48	1.41
1	A	515	TRP	CD2-CE2	5.61	1.48	1.41
1	B	515	TRP	CD2-CE2	5.22	1.47	1.41
1	B	509	TRP	CD2-CE2	5.22	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	141	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	811	LEU	CB-CG-CD1	5.41	120.19	111.00
1	A	246	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	790	ASP	CB-CG-OD1	5.12	122.91	118.30

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	6552	0	6385	49	0
1	B	6539	0	6369	45	0
2	A	15	0	7	0	0
2	B	15	0	6	1	0
3	A	22	0	20	1	0
3	B	44	0	43	0	0
4	A	24	0	24	0	0
4	B	12	0	12	2	0
5	B	6	0	8	0	0
6	A	197	0	0	5	0
6	B	147	0	0	2	0
All	All	13573	0	12874	93	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.

All (93) 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:549:LEU:HD11	1:B:663:LEU:HD23	1.41	1.02
1:A:731:GLU:HG3	6:A:2180:HOH:O	1.68	0.93
1:B:549:LEU:HD11	1:B:663:LEU:CD2	2.06	0.85
1:B:549:LEU:CD1	1:B:663:LEU:HD23	2.12	0.79
1:B:656:ASN:OD1	1:B:659:VAL:HG23	1.86	0.76
1:A:569:ILE:HD13	1:A:663:LEU:HD22	1.74	0.69
1:A:339:MET:HE1	1:A:374:VAL:HG11	1.75	0.69
1:A:380:THR:HG21	1:A:386:LEU:CD2	2.23	0.68
1:B:383:PRO:HB3	1:B:470:LEU:HD11	1.76	0.67
1:B:473:ASP:O	1:B:477:ILE:HD12	1.95	0.66
1:B:139:LEU:HD11	1:B:340:ASN:ND2	2.13	0.64
1:A:669:LEU:HD22	1:A:795:VAL:HG11	1.79	0.64
1:A:675:THR:HB	1:A:678:MET:HG3	1.80	0.63
1:B:416:ILE:O	1:B:416:ILE:HG22	1.99	0.62
1:A:339:MET:HE1	1:A:374:VAL:CG1	2.31	0.61
1:A:569:ILE:HD12	1:A:667:SER:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:THR:HB	1:B:678:MET:HG3	1.83	0.60
1:B:581:LEU:HA	1:B:584:ILE:HG22	1.84	0.59
1:A:139:LEU:HD11	1:A:340:ASN:ND2	2.20	0.57
1:A:339:MET:CE	1:A:374:VAL:CG1	2.82	0.57
1:A:20:ALA:HB3	1:B:20:ALA:HB3	1.86	0.56
1:B:617:PHE:CZ	4:B:952:GLC:H1	2.40	0.56
1:A:699:LEU:HD12	1:A:704:VAL:HG22	1.90	0.53
1:B:146:PHE:CG	1:B:825:ILE:HD11	2.44	0.53
1:B:386:LEU:HA	6:B:2082:HOH:O	2.09	0.53
1:B:322:THR:O	1:B:323:GLU:O	2.26	0.52
1:B:432:ILE:HD13	1:B:447:LEU:HD13	1.91	0.52
1:B:416:ILE:O	1:B:416:ILE:CG2	2.58	0.51
1:A:473:ASP:O	1:A:477:ILE:HD12	2.12	0.50
1:B:135:GLY:CA	1:B:284:LEU:HD11	2.42	0.49
1:B:348:ILE:HB	1:B:349:PRO:HD3	1.94	0.48
1:B:406:GLU:HG2	1:B:433:LEU:HD11	1.95	0.48
1:A:135:GLY:CA	1:A:284:LEU:HD11	2.44	0.48
1:B:135:GLY:HA2	1:B:284:LEU:HD11	1.96	0.47
1:B:669:LEU:HD22	1:B:795:VAL:HG11	1.95	0.47
1:B:348:ILE:HB	1:B:349:PRO:CD	2.45	0.47
1:A:557:THR:O	1:A:559:VAL:HG23	2.14	0.47
1:A:135:GLY:HA2	1:A:284:LEU:HD11	1.96	0.47
1:B:339:MET:HE1	1:B:374:VAL:HG11	1.97	0.47
1:A:229:ALA:HB2	1:A:248:TRP:CZ3	2.50	0.47
1:A:516:ILE:HG22	1:A:516:ILE:O	2.15	0.46
1:A:406:GLU:HG2	1:A:433:LEU:HD11	1.97	0.46
1:B:587:VAL:HG11	1:B:649:VAL:HG21	1.96	0.46
1:B:138:GLY:HA2	2:B:901:PLP:H5A2	1.98	0.46
1:A:146:PHE:CG	1:A:825:ILE:HD11	2.51	0.46
1:B:566:LEU:HD12	1:B:567:PHE:N	2.31	0.46
1:A:556:VAL:HG23	1:A:557:THR:HG23	1.97	0.46
1:A:827:GLN:O	1:A:831:GLU:HG2	2.16	0.46
1:B:827:GLN:O	1:B:831:GLU:HG2	2.16	0.46
1:B:85:THR:O	1:B:157:ALA:HA	2.15	0.46
1:A:432:ILE:HD13	1:A:447:LEU:HD13	1.99	0.45
1:A:560:SER:O	1:A:648:LYS:NZ	2.41	0.45
1:A:546:LYS:NZ	6:A:2142:HOH:O	2.50	0.45
1:A:380:THR:CG2	1:A:386:LEU:CD2	2.93	0.45
1:A:656:ASN:OD1	1:A:659:VAL:HG23	2.17	0.45
1:A:467:LYS:HA	1:A:475:VAL:HG21	1.98	0.45
1:B:495:LEU:HD12	1:B:499:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:LEU:HD23	1:B:567:PHE:CD2	2.52	0.44
1:B:268:GLU:HG2	6:B:2072:HOH:O	2.17	0.44
1:A:699:LEU:CD1	1:A:704:VAL:HG22	2.47	0.44
1:B:694:LEU:HD12	1:B:805:TRP:CZ2	2.53	0.44
1:B:568:ASP:OD1	1:B:568:ASP:C	2.56	0.44
1:A:587:VAL:HG11	1:A:649:VAL:HG21	1.99	0.43
1:A:785:PHE:N	1:A:786:PRO:CD	2.81	0.43
1:B:146:PHE:CD2	1:B:825:ILE:HD11	2.53	0.43
1:B:569:ILE:HD12	1:B:667:SER:HB3	2.01	0.43
1:A:119:GLY:HA2	6:A:2042:HOH:O	2.18	0.43
1:A:136:ASN:OD1	1:A:168:LEU:HD22	2.18	0.43
1:A:268:GLU:HG2	6:A:2089:HOH:O	2.18	0.43
1:A:386:LEU:HA	6:A:2105:HOH:O	2.19	0.43
1:A:412:PHE:CZ	1:A:416:ILE:HD11	2.53	0.43
1:A:568:ASP:OD1	1:A:568:ASP:C	2.57	0.43
1:A:362:GLY:HA2	3:A:951:QPS:H4B	2.01	0.42
1:A:380:THR:CG2	1:A:386:LEU:HD21	2.49	0.42
1:B:534:LEU:HD12	1:B:534:LEU:O	2.20	0.42
1:A:495:LEU:HD22	1:A:690:LEU:HD11	2.02	0.42
1:B:438:GLN:HB2	1:B:438:GLN:HE21	1.65	0.42
1:B:699:LEU:HB2	1:B:717:LEU:HD11	2.02	0.42
1:A:534:LEU:O	1:A:534:LEU:HD12	2.20	0.42
1:A:85:THR:O	1:A:157:ALA:HA	2.19	0.41
1:A:348:ILE:HB	1:A:349:PRO:CD	2.50	0.41
1:A:348:ILE:HB	1:A:349:PRO:HD3	2.01	0.41
1:B:338:GLN:OE1	1:B:375:ALA:HB3	2.20	0.41
1:A:706:ILE:O	1:A:710:VAL:HG22	2.21	0.41
1:B:111:TYR:O	1:B:115:LEU:HD23	2.20	0.41
1:A:141:ARG:HD2	1:A:141:ARG:HA	1.86	0.41
1:B:584:ILE:HD12	1:B:584:ILE:HA	1.90	0.41
1:A:699:LEU:HB2	1:A:717:LEU:HD11	2.03	0.41
1:B:343:HIS:HB2	1:B:344:PRO:HD3	2.03	0.41
1:A:146:PHE:CD2	1:A:825:ILE:HD11	2.56	0.40
1:B:785:PHE:N	1:B:786:PRO:CD	2.84	0.40
1:B:617:PHE:CZ	4:B:952:GLC:C1	3.04	0.40
1:A:549:LEU:HD23	1:A:567:PHE:CD2	2.57	0.40

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	826/874 (94%)	793 (96%)	33 (4%)	0	100	100
1	B	829/874 (95%)	797 (96%)	30 (4%)	2 (0%)	52	63
All	All	1655/1748 (95%)	1590 (96%)	63 (4%)	2 (0%)	56	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	323	GLU
1	B	817	GLY

### 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	690/752 (92%)	675 (98%)	15 (2%)	60	75
1	B	684/752 (91%)	671 (98%)	13 (2%)	65	79
All	All	1374/1504 (91%)	1346 (98%)	28 (2%)	61	77

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	SER
1	A	284	LEU
1	A	341	ASP
1	A	390	SER

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Mol	Chain	Res	Type
1	A	456	ASN
1	A	470	LEU
1	A	492	ARG
1	A	551	GLN
1	A	560	SER
1	A	572	LYS
1	A	577	TYR
1	A	620	TYR
1	A	678	MET
1	A	775	ARG
1	A	821	SER
1	B	23	GLU
1	B	244	SER
1	B	284	LEU
1	B	341	ASP
1	B	358	ASP
1	B	456	ASN
1	B	501	GLU
1	B	560	SER
1	B	572	LYS
1	B	577	TYR
1	B	620	TYR
1	B	757	SER
1	B	821	SER

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	261	GLN
1	A	480	ASN
1	B	261	GLN
1	B	278	GLN
1	B	438	GLN

### 5.3.3 RNA ⓘ

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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	PLP	A	901	1	15,15,16	1.52	1 (6%)	21,22,23	2.09	5 (23%)
3	QPS	A	951	-	23,23,47	1.13	1 (4%)	32,34,70	2.11	9 (28%)
4	GLC	A	952	-	12,12,12	0.65	0	17,17,17	2.37	4 (23%)
4	GLC	A	953	-	12,12,12	0.77	0	17,17,17	1.96	6 (35%)
5	GOL	B	1842	-	5,5,5	0.39	0	5,5,5	0.33	0
2	PLP	B	901	1	15,15,16	1.70	4 (26%)	21,22,23	2.84	12 (57%)
3	QPS	B	951	-	46,47,47	0.77	0	58,70,70	1.16	5 (8%)
4	GLC	B	952	-	12,12,12	0.76	0	17,17,17	1.87	3 (17%)

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	PLP	A	901	1	-	0/6/6/8	0/1/1/1
3	QPS	A	951	-	-	0/6/46/98	0/2/2/4
4	GLC	A	952	-	-	0/2/22/22	0/1/1/1
4	GLC	A	953	-	-	0/2/22/22	0/1/1/1
5	GOL	B	1842	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	B	901	1	-	0/6/6/8	0/1/1/1
3	QPS	B	951	-	-	0/18/98/98	0/4/4/4
4	GLC	B	952	-	-	0/2/22/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	PLP	P-O3P	-2.27	1.46	1.54
3	A	951	QPS	O5B-C1B	2.13	1.47	1.41
2	B	901	PLP	P-O4P	2.34	1.68	1.60
2	B	901	PLP	C2A-C2	2.47	1.55	1.50
2	B	901	PLP	P-O1P	4.22	1.65	1.51
2	A	901	PLP	P-O1P	4.30	1.65	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	PLP	O2P-P-O1P	-5.77	92.01	110.58
2	B	901	PLP	O2P-P-O1P	-4.41	96.39	110.58
2	B	901	PLP	C6-C5-C4	-3.37	115.29	118.15
3	A	951	QPS	O2C-C2C-C1C	-3.11	102.97	109.82
3	B	951	QPS	O4D-C4D-C3D	-2.75	100.08	107.17
4	A	953	GLC	C4-C3-C2	-2.71	105.73	110.79
3	A	951	QPS	C6B-C5B-C4B	-2.45	109.35	113.62
3	B	951	QPS	O2C-C2C-C3C	-2.45	104.82	110.34
2	B	901	PLP	C4A-C4-C5	-2.23	118.56	120.88
2	B	901	PLP	C3-C2-N1	-2.22	117.55	120.61
4	A	953	GLC	O2-C2-C3	2.01	114.86	110.34
4	A	952	GLC	O2-C2-C1	2.02	114.26	109.82
3	B	951	QPS	O5D-C5D-C4D	2.05	114.08	109.75
4	A	953	GLC	O4-C4-C5	2.19	115.03	109.24
3	A	951	QPS	O5B-C5B-C6B	2.20	111.44	106.64
3	A	951	QPS	O4D-C1C-O5C	2.22	116.33	110.25
3	B	951	QPS	O2B-C2B-C1B	2.22	114.89	110.02
4	A	952	GLC	O5-C1-C2	2.23	113.36	109.80
2	B	901	PLP	C2A-C2-C3	2.29	123.80	121.04
2	B	901	PLP	O3P-P-O2P	2.34	116.30	107.38
4	A	953	GLC	O5-C1-C2	2.42	113.65	109.80
2	B	901	PLP	C6-N1-C2	2.52	124.41	119.28
2	A	901	PLP	O3-C3-C2	2.52	122.04	117.66
4	B	952	GLC	C1-C2-C3	2.54	114.21	110.43
4	A	953	GLC	O3-C3-C2	2.57	116.12	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	PLP	C5A-C5-C4	2.58	125.07	121.65
3	A	951	QPS	C3B-C4B-N4B	2.72	115.90	110.86
2	B	901	PLP	C5A-C5-C6	2.82	124.61	119.28
4	B	952	GLC	O2-C2-C3	3.08	117.27	110.34
3	B	951	QPS	O5C-C5C-C6C	3.14	114.30	106.36
2	B	901	PLP	O2P-P-O4P	3.24	115.90	106.56
2	A	901	PLP	O3P-P-O1P	3.26	121.07	110.58
3	A	951	QPS	O2C-C2C-C3C	3.51	118.23	110.34
3	A	951	QPS	O4C-C4C-C3C	3.53	116.27	107.17
2	B	901	PLP	C3-C4-C5	3.99	123.13	118.78
2	A	901	PLP	O3P-P-O4P	4.24	118.76	106.56
2	B	901	PLP	O3-C3-C2	4.76	125.93	117.66
4	A	952	GLC	C1-C2-C3	4.90	117.71	110.43
4	B	952	GLC	C1-O5-C5	4.91	122.56	113.47
4	A	953	GLC	C1-O5-C5	5.22	123.13	113.47
3	A	951	QPS	C1B-O5B-C5B	5.47	122.96	113.64
3	A	951	QPS	C1C-O5C-C5C	5.48	123.60	113.47
4	A	952	GLC	C1-O5-C5	6.23	125.00	113.47
2	B	901	PLP	O4P-C5A-C5	6.71	120.09	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	951	QPS	1	0
2	B	901	PLP	1	0
4	B	952	GLC	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 ⓘ

### 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<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%)	-0.17	6 (0%) 89 94	27, 42, 65, 96	0
1	B	827/874 (94%)	-0.08	12 (1%) 76 85	28, 46, 75, 110	0
All	All	1651/1748 (94%)	-0.13	18 (1%) 82 90	27, 44, 70, 110	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	LEU	5.0
1	B	381	VAL	4.2
1	B	773	PHE	3.7
1	B	736	LEU	3.6
1	B	383	PRO	3.5
1	A	381	VAL	3.3
1	A	383	PRO	2.7
1	B	323	GLU	2.7
1	B	776	GLY	2.6
1	A	384	GLU	2.6
1	B	325	SER	2.5
1	A	437	PRO	2.5
1	B	772	GLY	2.5
1	A	773	PHE	2.5
1	B	324	GLY	2.4
1	B	321	THR	2.1
1	B	737	PHE	2.0
1	A	382	LEU	2.0

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

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
3	QPS	A	951	22/44	0.83	0.25	4.25	45,66,82,82	0
3	QPS	B	951	44/44	0.93	0.23	4.12	43,67,106,113	0
4	GLC	B	952	12/12	0.79	0.22	3.53	65,70,73,76	0
4	GLC	A	953	12/12	0.76	0.27	2.27	70,84,90,90	0
4	GLC	A	952	12/12	0.81	0.18	1.98	69,76,81,82	0
5	GOL	B	1842	6/6	0.95	0.14	1.91	40,48,52,53	0
2	PLP	A	901	15/16	0.97	0.15	0.01	33,41,48,49	0
2	PLP	B	901	15/16	0.97	0.14	-0.92	36,46,53,57	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.