



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:10 PM GMT

PDB ID : 4BQE
Title : Arabidopsis thaliana Cytosolic Alpha-1,4-glucan Phosphorylase (PHS2)
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 : 1.70 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 ⓘ 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

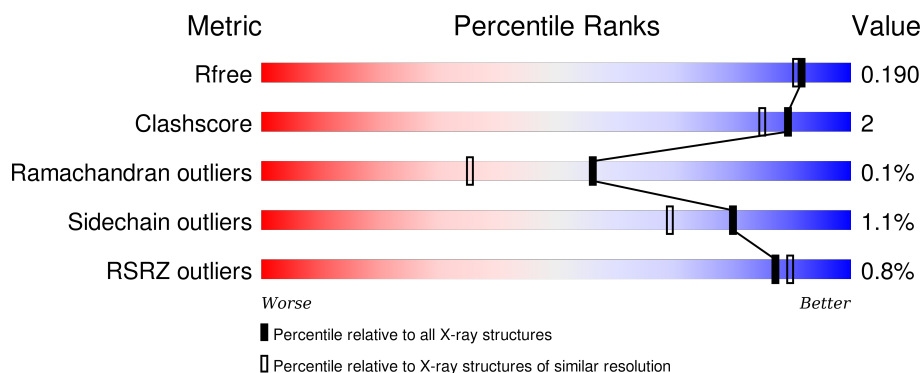
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


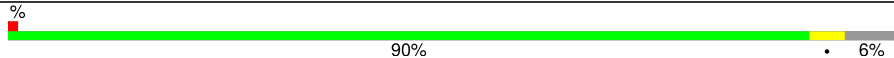
The reported resolution of this entry is 1.70 Å.

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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	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	GOL	A	1843	-	-	-	X
3	GOL	B	1843	-	-	-	X
3	GOL	B	1844	-	-	-	X
4	PEG	A	1844	-	-	X	X
4	PEG	A	1845	-	-	X	X
4	PEG	B	1845	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15207 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 2,4-GLUCAN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	824	Total	C	N	O	S	0	17	0
			6621	4231	1126	1239	25			
1	B	825	Total	C	N	O	S	0	17	0
			6631	4232	1129	1245	25			

There are 66 discrepancies between the modelled and reference sequences:

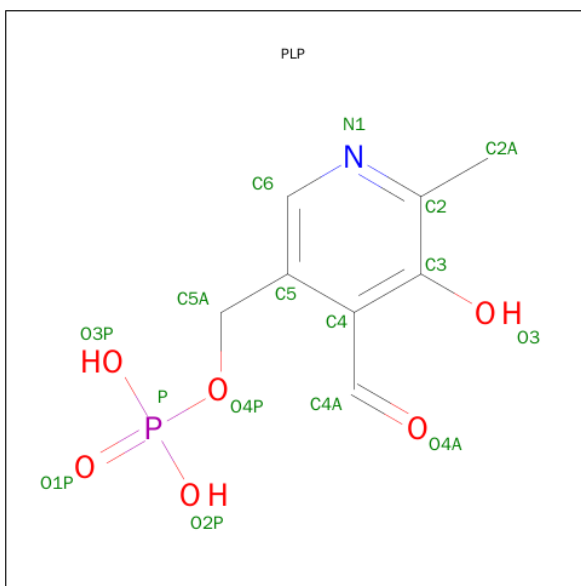
Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	EXPRESSION TAG	UNP Q9SD76
A	-31	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-30	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-29	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-28	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-27	HIS	-	EXPRESSION TAG	UNP Q9SD76
A	-26	HIS	-	EXPRESSION TAG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

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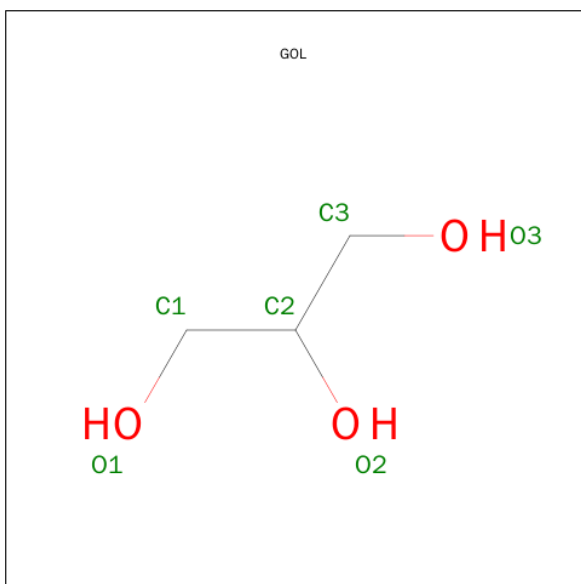
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	TYR	-	EXPRESSION TAG	UNP Q9SD76
A	-7	PHE	-	EXPRESSION TAG	UNP Q9SD76
A	-6	GLN	-	EXPRESSION TAG	UNP Q9SD76
A	-5	GLY	-	EXPRESSION TAG	UNP Q9SD76
A	-4	ILE	-	EXPRESSION TAG	UNP Q9SD76
A	-3	ASP	-	EXPRESSION TAG	UNP Q9SD76
A	-2	PRO	-	EXPRESSION TAG	UNP Q9SD76
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: $C_8H_{10}NO_6P$).



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



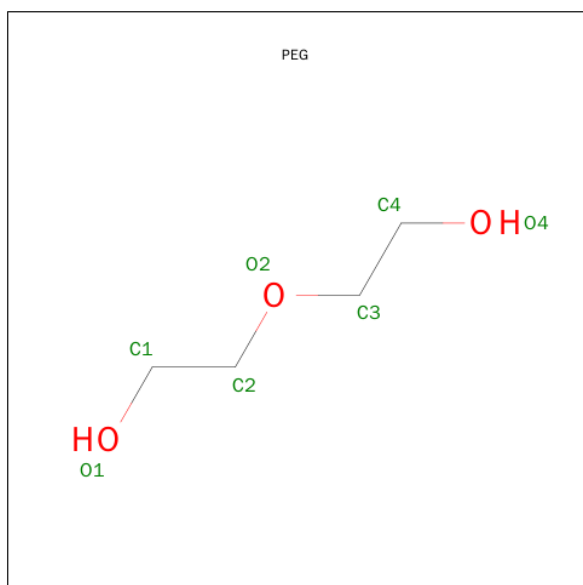
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

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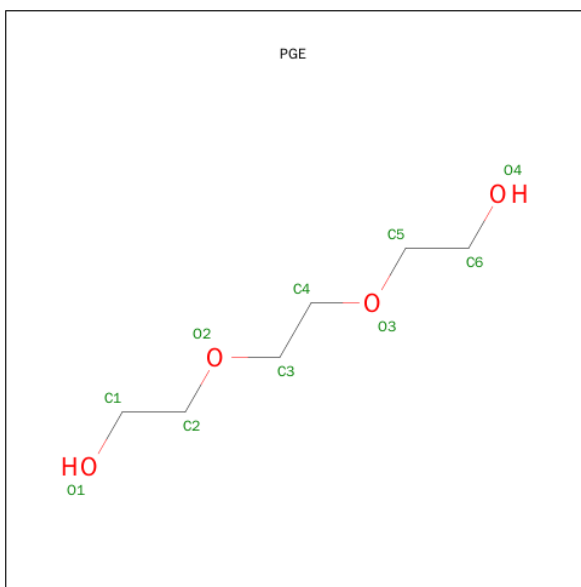
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- 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		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

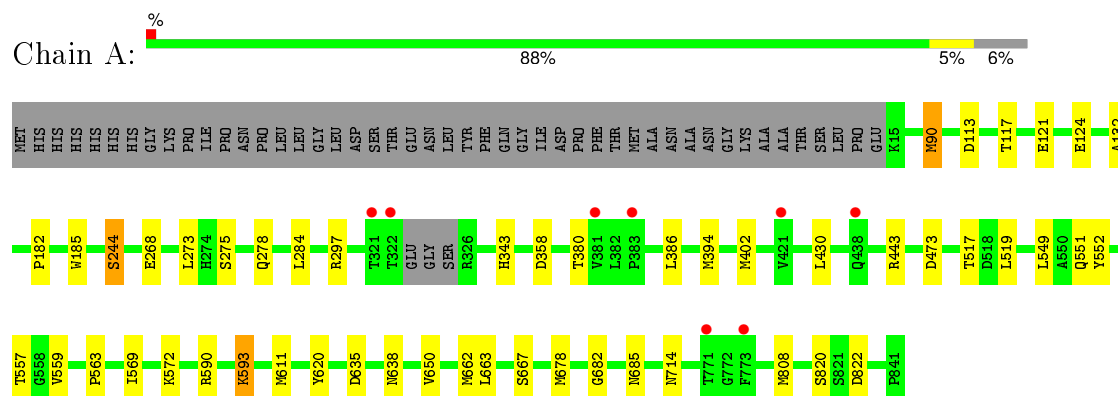
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	952	Total	O	0	15
			967	967		
6	B	892	Total	O	0	17
			909	909		

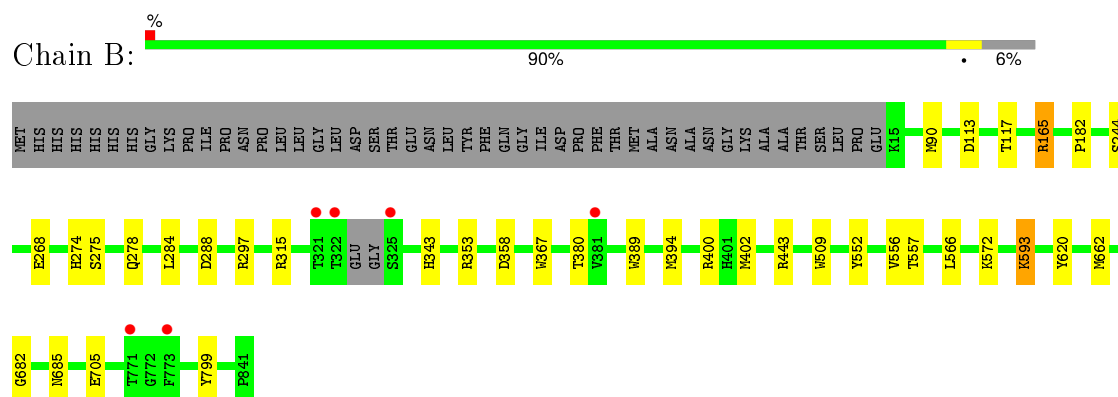
3 Residue-property plots [i](#)

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 2,4-GLUCAN PHOSPHORYLASE



- Molecule 1: ALPHA-GLUCAN PHOSPHORYLASE 2,4-GLUCAN PHOSPHORYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.67Å 117.10Å 94.18Å 90.00° 106.72° 90.00°	Depositor
Resolution (Å)	90.20 – 1.70 47.47 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (90.20-1.70) 98.9 (47.47-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.153 , 0.183 0.161 , 0.190	Depositor DCC
R_{free} test set	9587 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 190487 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15207	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 22.67 % 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 5.4375e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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, PEG, PGE, 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	0.69	0/6824	0.78	6/9257 (0.1%)
1	B	0.69	3/6833 (0.0%)	0.77	7/9265 (0.1%)
All	All	0.69	3/13657 (0.0%)	0.77	13/18522 (0.1%)

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
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	509	TRP	CD2-CE2	5.49	1.48	1.41
1	B	389	TRP	CD2-CE2	5.33	1.47	1.41
1	B	367	TRP	CD2-CE2	5.16	1.47	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	443	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	B	443	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	297	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	297	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	678	MET	CG-SD-CE	-5.77	90.96	100.20
1	B	288	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	165[A]	ARG	NE-CZ-NH2	-5.37	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165[B]	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	315	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	590[A]	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	590[B]	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	90	MET	CG-SD-CE	5.11	108.37	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	SER	Peptide

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	6621	0	6503	36	0
1	B	6631	0	6516	19	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	A	6	0	8	1	0
3	B	12	0	16	3	0
4	A	14	0	18	17	0
4	B	7	0	10	3	0
5	A	10	0	13	2	0
6	A	967	0	0	9	0
6	B	909	0	0	7	0
All	All	15207	0	13096	63	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 2.

All (63) 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:559:VAL:HG22	4:A:1845:PEG:H21	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1843:GOL:H31	6:B:3361:HOH:O	1.63	0.96
1:A:635:ASP:OD1	4:A:1845:PEG:H42	1.74	0.87
1:A:519:LEU:H	4:A:1844:PEG:H41	1.45	0.80
1:B:380:THR:HG23	6:B:3568:HOH:O	1.84	0.77
1:A:559:VAL:CG2	4:A:1845:PEG:H21	2.15	0.75
1:A:380:THR:HG21	1:A:386:LEU:HD21	1.70	0.73
1:A:559:VAL:HG22	4:A:1845:PEG:C2	2.20	0.70
4:A:1845:PEG:H12	6:A:3711:HOH:O	1.92	0.69
1:A:551[A]:GLN:HG3	6:A:2864:HOH:O	1.94	0.68
1:A:268:GLU:OE1	1:B:268:GLU:OE1	2.11	0.67
1:A:820:SER:CB	4:A:1844:PEG:H42	2.28	0.64
1:A:380:THR:HG21	1:A:386:LEU:CD2	2.31	0.60
1:A:820:SER:OG	4:A:1844:PEG:H42	2.02	0.60
1:A:394[A]:MET:HG2	1:A:402:MET:SD	2.41	0.60
1:A:121:GLU:O	1:A:124[B]:GLU:HG2	2.02	0.60
1:B:394[A]:MET:HG2	1:B:402:MET:SD	2.43	0.59
4:A:1845:PEG:C1	6:A:3711:HOH:O	2.48	0.59
1:B:165[B]:ARG:NH1	6:B:3037:HOH:O	2.37	0.57
1:B:353:ARG:HH22	3:B:1843:GOL:H2	1.69	0.56
4:B:1845:PEG:H41	6:B:2089:HOH:O	2.05	0.56
1:B:182:PRO:HA	6:B:2052:HOH:O	2.06	0.55
3:A:1843:GOL:H32	6:A:3823:HOH:O	2.04	0.55
1:A:638:ASN:HD22	4:A:1845:PEG:C3	2.20	0.54
1:A:822:ASP:HB2	4:A:1844:PEG:H31	1.90	0.54
1:B:400:ARG:HH12	4:B:1845:PEG:H21	1.76	0.50
1:A:549:LEU:HD11	1:A:663:LEU:HD23	1.94	0.50
1:B:90:MET:HG3	1:B:343:HIS:HB3	1.92	0.50
1:A:611:MET:HG2	1:A:650[B]:VAL:CG2	2.43	0.48
6:A:2294:HOH:O	1:B:274[B]:HIS:HD2	1.96	0.48
1:A:182:PRO:HA	6:A:2068:HOH:O	2.13	0.48
1:A:552:TYR:CG	1:A:662[A]:MET:HG2	2.49	0.48
1:A:517:THR:O	4:A:1844:PEG:H32	2.14	0.47
1:B:705:GLU:CD	6:B:3579:HOH:O	2.51	0.47
3:B:1843:GOL:C3	6:B:3361:HOH:O	2.41	0.46
1:B:394[A]:MET:HG3	1:B:402:MET:HG2	1.97	0.46
5:A:1846:PGE:H3	5:A:1846:PGE:H5	1.79	0.45
1:A:275:SER:HA	1:A:278[A]:GLN:HG2	1.98	0.45
1:B:275:SER:HA	1:B:278[A]:GLN:HG2	1.99	0.44
1:A:90:MET:HG3	1:A:343:HIS:HB3	1.99	0.44
1:A:394[A]:MET:HG3	1:A:402:MET:HG2	2.00	0.43
1:A:569:ILE:HD12	1:A:667:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:ASN:HD22	4:A:1845:PEG:H31	1.85	0.42
1:A:557:THR:HG21	1:A:650[A]:VAL:CG1	2.49	0.42
1:B:274[B]:HIS:CD2	1:B:278[B]:GLN:NE2	2.86	0.42
1:B:593:LYS:N	1:B:593:LYS:HD2	2.32	0.42
1:A:519:LEU:HB2	4:A:1844:PEG:H41	2.01	0.42
1:A:638:ASN:ND2	4:A:1845:PEG:H31	2.35	0.42
1:A:519:LEU:N	4:A:1844:PEG:H41	2.23	0.42
1:A:593:LYS:HD2	1:A:593:LYS:N	2.34	0.42
1:B:556:VAL:HG23	1:B:557:THR:HG23	2.02	0.42
1:A:662[B]:MET:CE	6:A:2439:HOH:O	2.68	0.42
1:A:113:ASP:O	1:A:117:THR:HG23	2.20	0.41
5:A:1846:PGE:H6	6:A:3710:HOH:O	2.20	0.41
1:B:552:TYR:CG	1:B:662[A]:MET:HG2	2.55	0.41
1:B:566:LEU:HD13	1:B:799:TYR:CD1	2.56	0.41
1:B:400:ARG:HH12	4:B:1845:PEG:C2	2.34	0.41
1:A:714:ASN:OD1	1:A:808:MET:HG2	2.21	0.41
1:B:113:ASP:O	1:B:117:THR:HG23	2.20	0.41
1:A:430:LEU:HD21	1:A:473:ASP:HB2	2.03	0.40
1:A:132:ALA:HA	1:A:185:TRP:CE3	2.57	0.40
4:A:1845:PEG:H41	6:A:3197:HOH:O	2.22	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	837/874 (96%)	815 (97%)	21 (2%)	1 (0%)	56	35
1	B	838/874 (96%)	814 (97%)	23 (3%)	1 (0%)	56	35
All	All	1675/1748 (96%)	1629 (97%)	44 (3%)	2 (0%)	56	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	682	GLY
1	A	682	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	705/752 (94%)	697 (99%)	8 (1%)	80	69
1	B	708/752 (94%)	701 (99%)	7 (1%)	82	72
All	All	1413/1504 (94%)	1398 (99%)	15 (1%)	80	69

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	SER
1	A	284	LEU
1	A	358	ASP
1	A	563	PRO
1	A	572	LYS
1	A	593	LYS
1	A	620	TYR
1	A	685	ASN
1	B	244	SER
1	B	284	LEU
1	B	358	ASP
1	B	572	LYS
1	B	593	LYS
1	B	620	TYR
1	B	685	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	B	78	ASN

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 ⓘ

9 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	1842	1	15,15,16	1.62	3 (20%)	21,22,23	1.86	6 (28%)
3	GOL	A	1843	-	5,5,5	0.30	0	5,5,5	0.52	0
4	PEG	A	1844	-	6,6,6	1.00	0	5,5,5	2.72	2 (40%)
4	PEG	A	1845	-	6,6,6	0.75	0	5,5,5	1.33	1 (20%)
5	PGE	A	1846	-	9,9,9	0.89	0	8,8,8	1.71	3 (37%)
2	PLP	B	1842	1	15,15,16	1.60	5 (33%)	21,22,23	1.92	4 (19%)
3	GOL	B	1843	-	5,5,5	0.55	0	5,5,5	1.03	0
3	GOL	B	1844	-	5,5,5	0.57	0	5,5,5	0.29	0
4	PEG	B	1845	-	6,6,6	0.92	0	5,5,5	0.70	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
2	PLP	A	1842	1	-	0/6/6/8	0/1/1/1
3	GOL	A	1843	-	-	0/4/4/4	0/0/0/0
4	PEG	A	1844	-	-	0/4/4/4	0/0/0/0
4	PEG	A	1845	-	-	0/4/4/4	0/0/0/0
5	PGE	A	1846	-	-	0/7/7/7	0/0/0/0
2	PLP	B	1842	1	-	0/6/6/8	0/1/1/1
3	GOL	B	1843	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1844	-	-	0/4/4/4	0/0/0/0
4	PEG	B	1845	-	-	0/4/4/4	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1842	PLP	O4P-C5A	-3.89	1.28	1.44
2	B	1842	PLP	O4P-C5A	-2.94	1.32	1.44
2	B	1842	PLP	C5-C4	-2.54	1.37	1.40
2	B	1842	PLP	P-O3P	-2.08	1.47	1.54
2	A	1842	PLP	C4A-C4	-2.04	1.47	1.51
2	B	1842	PLP	C3-C2	-2.02	1.39	1.40
2	A	1842	PLP	P-O4P	2.68	1.69	1.60
2	B	1842	PLP	P-O4P	2.96	1.70	1.60

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1844	PEG	O2-C3-C4	-5.06	87.13	110.43
2	B	1842	PLP	C4A-C4-C5	-4.58	116.11	120.88
2	A	1842	PLP	C4A-C4-C5	-3.50	117.23	120.88
4	A	1844	PEG	O2-C2-C1	-3.09	96.20	110.43
2	A	1842	PLP	C5-C6-N1	-3.02	118.61	123.86
2	A	1842	PLP	O4P-P-O1P	-2.85	99.88	107.14
2	A	1842	PLP	C5A-C5-C4	-2.64	118.15	121.65
2	B	1842	PLP	O4P-P-O1P	-2.57	100.60	107.14
2	A	1842	PLP	C6-C5-C4	2.06	119.90	118.15
5	A	1846	PGE	O2-C3-C4	2.16	119.97	110.36
5	A	1846	PGE	O3-C4-C3	2.17	120.03	110.36
2	B	1842	PLP	O3-C3-C2	2.22	121.52	117.66
4	A	1845	PEG	O2-C3-C4	2.70	122.85	110.43
5	A	1846	PGE	O3-C5-C6	2.96	124.05	110.43
2	A	1842	PLP	O2P-P-O4P	3.73	117.32	106.56
2	B	1842	PLP	O2P-P-O4P	4.32	118.99	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1843	GOL	1	0
4	A	1844	PEG	7	0
4	A	1845	PEG	10	0
5	A	1846	PGE	2	0
3	B	1843	GOL	3	0
4	B	1845	PEG	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	824/874 (94%)	-0.47	8 (0%) 84 87	8, 16, 32, 54	0
1	B	825/874 (94%)	-0.47	6 (0%) 89 91	8, 16, 32, 51	0
All	All	1649/1748 (94%)	-0.47	14 (0%) 87 90	8, 16, 32, 54	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	773	PHE	4.3
1	A	381	VAL	3.5
1	A	438	GLN	3.5
1	B	325	SER	3.4
1	A	773	PHE	3.1
1	A	322	THR	3.0
1	B	322	THR	3.0
1	B	321	THR	2.9
1	B	381	VAL	2.7
1	A	383	PRO	2.7
1	A	321	THR	2.7
1	A	421	VAL	2.5
1	B	771	THR	2.4
1	A	771	THR	2.1

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, 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
4	PEG	A	1844	7/7	0.93	0.27	15.30	17,19,23,25	0
3	GOL	A	1843	6/6	0.83	0.27	9.73	34,36,39,40	0
4	PEG	A	1845	7/7	0.90	0.22	8.30	32,33,37,38	0
4	PEG	B	1845	7/7	0.82	0.14	5.91	29,32,38,39	0
3	GOL	B	1843	6/6	0.90	0.13	5.34	17,21,23,27	0
3	GOL	B	1844	6/6	0.84	0.18	3.47	22,33,36,39	0
2	PLP	A	1842	15/16	0.96	0.11	0.94	11,12,24,28	0
2	PLP	B	1842	15/16	0.95	0.11	0.60	11,12,21,23	0
5	PGE	A	1846	10/10	0.76	0.12	0.56	38,42,47,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.