



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:07 pm BST

PDB ID : 1W23  
Title : Crystal structure of phosphoserine aminotransferase from *Bacillus alcalophilus*  
Authors : Dubnovitsky, A.; Kapetanidou, E.G.; Papageorgiou, A.C.  
Deposited on : 2004-06-25  
Resolution : 1.08 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

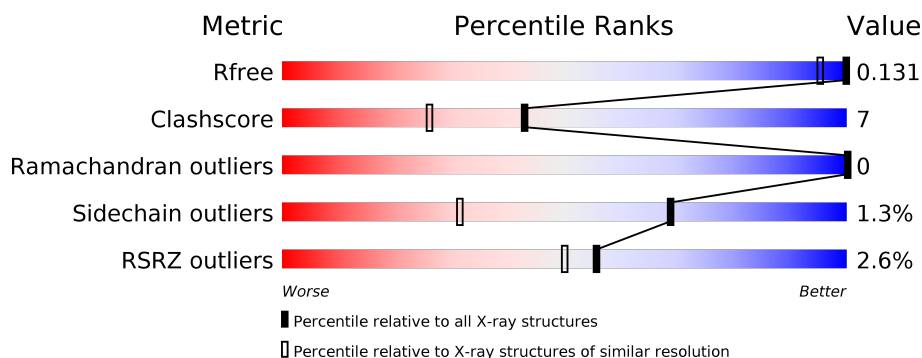
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.08 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))
$R_{free}$	130704	1386 (1.12-1.04)
Clashscore	141614	1021 (1.10-1.06)
Ramachandran outliers	138981	1381 (1.12-1.04)
Sidechain outliers	138945	1379 (1.12-1.04)
RSRZ outliers	127900	1359 (1.12-1.04)

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 respectively. 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	360	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	360	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </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
6	PLP	B	1368	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6898 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.

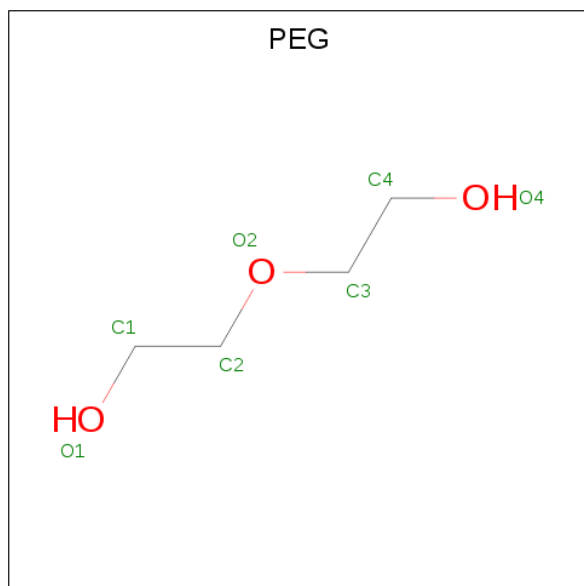
- Molecule 1 is a protein called PHOSPHOSERINE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	30	0
			2925	1869	493	548	15			
1	B	357	Total	C	N	O	S	0	28	0
			2899	1847	491	547	14			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

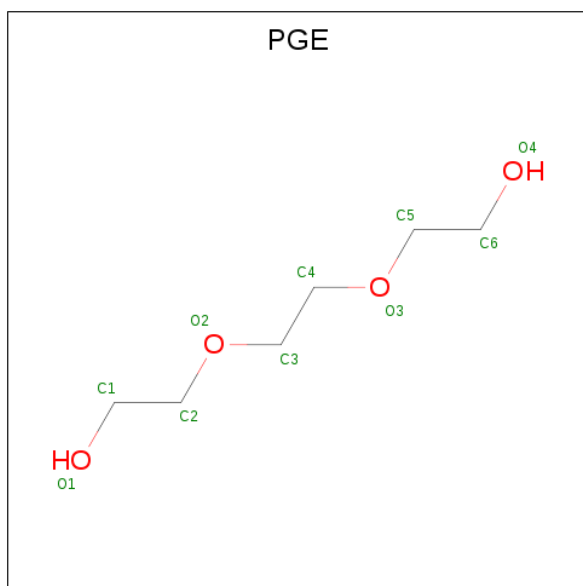
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	1
			2	2		
2	A	3	Total	Mg	0	0
			3	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).

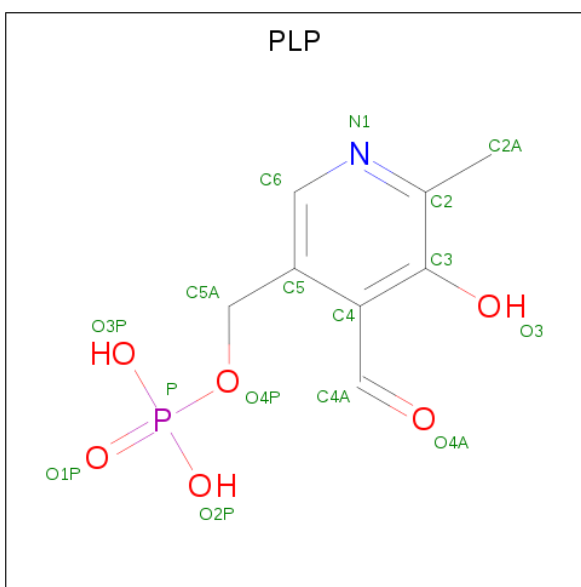


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

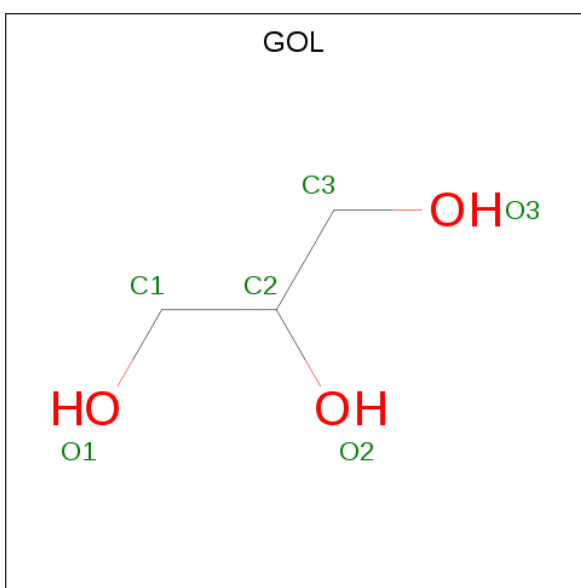
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cl	0	0
			2	2		
5	A	2	Total	Cl	0	0
			2	2		

- Molecule 6 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



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

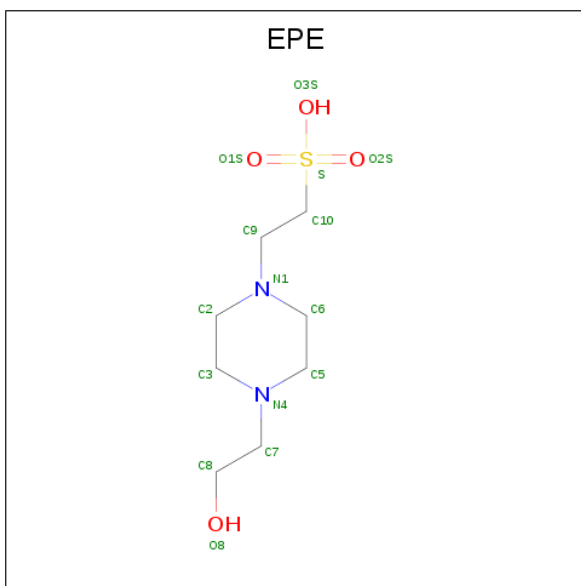
- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

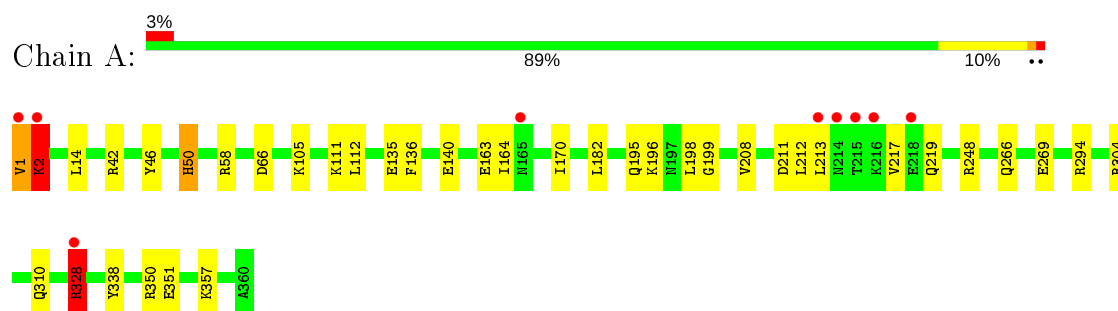
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	453	Total	O	0	0
			453	453		
9	B	524	Total	O	0	0
			524	524		

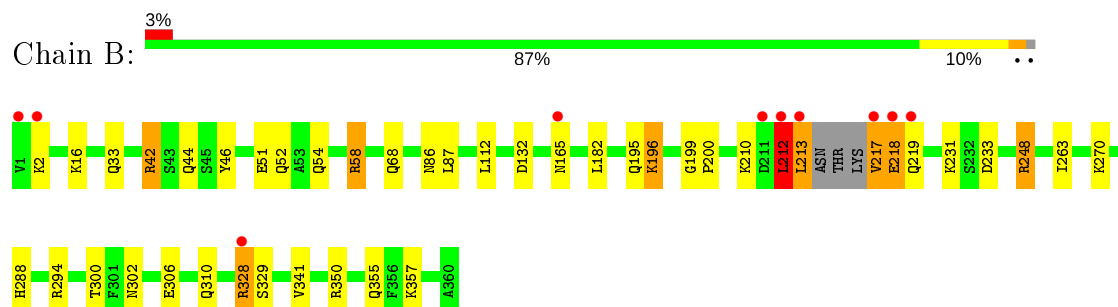
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: PHOSPHOSERINE AMINOTRANSFERASE



#### • Molecule 1: PHOSPHOSERINE AMINOTRANSFERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.47Å 84.84Å 67.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.08 19.87 – 1.08	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-1.08) 99.4 (19.87-1.08)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 1.08Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.117 , 0.139 0.126 , 0.131	Depositor DCC
$R_{free}$ test set	17505 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 66.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	6898	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, PGE, PLP, CL, PEG, EPE

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	0.77	0/3123	1.19	26/4219 (0.6%)
1	B	0.78	0/3084	1.18	26/4164 (0.6%)
All	All	0.77	0/6207	1.19	52/8383 (0.6%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	NE-CZ-NH1	14.96	127.78	120.30
1	A	328	ARG	CD-NE-CZ	12.72	141.41	123.60
1	B	42	ARG	NE-CZ-NH2	11.27	125.93	120.30
1	A	350	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	B	328	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	B	328	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	A	42	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	B	328	ARG	CD-NE-CZ	8.12	134.96	123.60
1	A	304	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	B	46	TYR	CA-CB-CG	-7.05	100.01	113.40
1	B	350	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	B	212	LEU	O-C-N	6.96	133.84	122.70
1	A	269	GLU	OE1-CD-OE2	6.96	131.65	123.30
1	B	42	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	B	350	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	B	310	GLN	CB-CG-CD	6.37	128.16	111.60
1	A	111	LYS	CD-CE-NZ	6.32	126.23	111.70
1	A	211	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	310	GLN	CG-CD-OE1	6.26	134.12	121.60
1	A	294	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	42	ARG	NH1-CZ-NH2	6.18	126.20	119.40
1	B	306	GLU	OE1-CD-OE2	6.16	130.70	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	212	LEU	CA-CB-CG	5.91	128.90	115.30
1	B	355	GLN	CG-CD-NE2	5.88	130.81	116.70
1	A	58	ARG	NH1-CZ-NH2	-5.77	113.05	119.40
1	A	310	GLN	CG-CD-OE1	5.77	133.14	121.60
1	B	196	LYS	CB-CG-CD	5.66	126.31	111.60
1	B	132	ASP	CB-CG-OD1	5.64	123.37	118.30
1	B	217	VAL	O-C-N	5.61	131.67	122.70
1	A	135	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	A	164	ILE	CA-CB-CG2	5.60	122.10	110.90
1	B	196	LYS	CD-CE-NZ	5.59	124.56	111.70
1	B	2	LYS	CA-CB-CG	5.52	125.55	113.40
1	A	217	VAL	O-C-N	5.50	131.51	122.70
1	A	66	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	198	LEU	C-N-CA	-5.46	110.83	122.30
1	A	136	PHE	CB-CG-CD1	5.45	124.61	120.80
1	A	136	PHE	CB-CG-CD2	-5.41	117.01	120.80
1	A	140	GLU	CG-CD-OE1	5.41	129.12	118.30
1	A	135	GLU	CG-CD-OE2	5.41	129.11	118.30
1	A	46	TYR	CA-CB-CG	-5.36	103.21	113.40
1	B	217	VAL	CA-CB-CG2	5.32	118.87	110.90
1	A	50[A]	HIS	CA-CB-CG	5.26	122.55	113.60
1	A	50[B]	HIS	CA-CB-CG	5.26	122.55	113.60
1	A	2	LYS	CD-CE-NZ	5.21	123.69	111.70
1	B	218	GLU	O-C-N	5.18	130.98	122.70
1	B	58	ARG	CG-CD-NE	5.17	122.67	111.80
1	B	294	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	217	VAL	CA-C-N	-5.16	105.86	117.20
1	A	248	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	217	VAL	CA-CB-CG1	-5.06	103.31	110.90

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	2925	0	2918	36	0
1	B	2899	0	2890	52	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
3	A	7	0	10	0	0
4	A	10	0	14	0	0
4	B	20	0	28	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	15	0	6	5	0
6	B	15	0	6	6	0
7	B	6	0	8	0	0
8	B	15	0	17	6	0
9	A	453	0	0	15	0
9	B	524	0	0	17	0
All	All	6898	0	5897	80	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 7.

All (80) 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:196:LYS:HZ1	6:B:1368:PLP:C4A	1.36	1.31
1:A:196:LYS:HZ1	6:A:1367:PLP:C4A	1.35	1.21
1:A:196:LYS:HZ2	6:A:1367:PLP:C4A	1.71	0.99
1:B:196:LYS:HZ2	6:B:1368:PLP:C4A	1.63	0.92
1:A:14[A]:LEU:HD23	9:A:2028:HOH:O	1.76	0.85
1:A:266[B]:GLN:NE2	9:A:2333:HOH:O	2.12	0.82
1:A:196:LYS:HZ3	6:A:1367:PLP:C4A	1.94	0.79
1:A:266[A]:GLN:NE2	9:A:2334:HOH:O	2.17	0.78
1:B:86:ASN:HB3	1:B:213:LEU:HD21	1.65	0.77
1:A:196:LYS:HD2	9:A:2274:HOH:O	1.82	0.77
1:B:44:GLN:HG3	9:B:2111:HOH:O	1.85	0.76
1:A:182[B]:LEU:HD23	9:A:2262:HOH:O	1.87	0.74
1:B:182[A]:LEU:HD23	9:B:2309:HOH:O	1.87	0.73
1:A:328:ARG:HH21	1:B:42:ARG:HH22	1.39	0.71
1:A:2:LYS:HG2	1:B:33[A]:GLN:NE2	2.05	0.70
1:A:266[B]:GLN:CD	9:A:2333:HOH:O	2.31	0.69
1:B:58:ARG:HD3	9:B:2129:HOH:O	1.92	0.68
1:B:233[B]:ASP:OD2	9:B:2345:HOH:O	2.12	0.68
1:A:328:ARG:NE	1:B:42:ARG:HH12	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LYS:NZ	6:B:1368:PLP:C4	2.58	0.66
1:B:288[B]:HIS:HE1	1:B:302[B]:ASN:HD22	1.40	0.66
1:B:210:LYS:NZ	8:B:1365:EPE:H92	2.13	0.64
1:B:51:GLU:HG2	9:B:2345:HOH:O	1.96	0.64
1:B:196:LYS:HZ3	6:B:1368:PLP:C4A	2.05	0.64
1:B:52:GLN:NE2	1:B:248:ARG:HH11	1.96	0.63
1:A:351:GLU:HG3	9:A:2426:HOH:O	1.97	0.63
1:A:266[A]:GLN:CD	9:A:2334:HOH:O	2.36	0.62
1:B:16:LYS:HE2	9:B:2051:HOH:O	2.00	0.61
1:B:288[B]:HIS:HD2	9:B:2282:HOH:O	1.84	0.59
1:B:212:LEU:O	1:B:213:LEU:HD13	2.04	0.58
1:A:105[B]:LYS:HE3	9:A:2169:HOH:O	2.02	0.57
1:A:196:LYS:NZ	6:A:1367:PLP:C4	2.60	0.57
1:B:52:GLN:HE22	1:B:248:ARG:HH11	1.54	0.55
1:B:270[B]:LYS:HE3	1:B:341:VAL:O	2.08	0.54
1:B:212:LEU:HD13	9:B:2119:HOH:O	2.07	0.54
1:A:50[A]:HIS:HE1	9:A:2294:HOH:O	1.92	0.53
1:A:328:ARG:HE	1:B:42:ARG:HH12	1.55	0.53
1:B:218:GLU:O	1:B:219:GLN:HB2	2.07	0.52
1:A:105[A]:LYS:HD2	9:A:2169:HOH:O	2.08	0.52
1:A:208[B]:VAL:CG2	1:A:213:LEU:HD12	2.41	0.51
1:B:210:LYS:HZ2	8:B:1365:EPE:H92	1.75	0.51
1:B:210:LYS:HD3	9:B:2160:HOH:O	2.11	0.50
1:A:328:ARG:NH2	1:B:42:ARG:HH22	2.10	0.50
1:A:195:GLN:HA	1:A:199:GLY:O	2.13	0.49
1:B:51:GLU:HG3	9:B:2121:HOH:O	2.11	0.49
1:B:196:LYS:HZ2	6:B:1368:PLP:C4	2.24	0.48
1:B:196:LYS:HZ3	6:B:1368:PLP:C3	2.26	0.48
1:A:219:GLN:HA	1:B:112[B]:LEU:HD11	1.93	0.48
1:B:195:GLN:HA	1:B:199:GLY:O	2.14	0.48
1:B:210:LYS:HZ3	8:B:1365:EPE:H92	1.79	0.47
1:B:288[B]:HIS:CD2	1:B:300:THR:HB	2.50	0.47
1:A:212[B]:LEU:HD12	9:A:2283:HOH:O	2.15	0.46
1:A:196:LYS:HG2	1:A:338:TYR:CZ	2.51	0.46
1:B:200:PRO:HD2	9:B:2357:HOH:O	2.14	0.46
1:B:213:LEU:HD12	1:B:213:LEU:HA	1.59	0.46
1:A:199:GLY:N	9:A:2278:HOH:O	2.48	0.46
1:B:16:LYS:NZ	9:B:2049:HOH:O	2.49	0.45
1:B:54[A]:GLN:NE2	9:B:2345:HOH:O	2.49	0.45
1:B:87[B]:LEU:HD21	1:B:213:LEU:HD22	1.97	0.45
1:B:328:ARG:HG3	1:B:329:SER:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLN:NE2	9:B:2158:HOH:O	2.49	0.45
1:A:105[B]:LYS:NZ	9:A:2173:HOH:O	2.49	0.45
1:A:112[B]:LEU:HD11	1:B:219:GLN:HA	1.99	0.45
1:A:213:LEU:HA	1:A:213:LEU:HD23	1.57	0.45
1:B:210:LYS:NZ	8:B:1365:EPE:O2S	2.50	0.45
1:B:212:LEU:HD12	1:B:212:LEU:O	2.17	0.44
8:B:1365:EPE:H22	8:B:1365:EPE:H102	1.73	0.44
1:B:357:LYS:NZ	9:B:2509:HOH:O	2.49	0.44
1:B:87[B]:LEU:HD21	1:B:212:LEU:HD12	2.00	0.43
1:A:208[B]:VAL:HG21	1:A:213:LEU:HD12	2.01	0.43
1:A:328:ARG:HE	1:B:42:ARG:NH1	2.17	0.43
1:A:196:LYS:HZ2	6:A:1367:PLP:C4	2.27	0.42
1:B:16:LYS:HD3	9:B:2049:HOH:O	2.18	0.42
1:B:165[B]:ASN:ND2	9:B:2298:HOH:O	2.52	0.42
1:B:231:LYS:HA	8:B:1365:EPE:O1S	2.19	0.41
1:B:87[B]:LEU:CD1	1:B:212:LEU:HD11	2.51	0.41
1:A:1:VAL:HG12	1:B:33[A]:GLN:NE2	2.36	0.40
1:A:357[A]:LYS:NZ	9:A:2438:HOH:O	2.53	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	388/360 (108%)	382 (98%)	6 (2%)	0	100	100
1	B	381/360 (106%)	374 (98%)	7 (2%)	0	100	100
All	All	769/720 (107%)	756 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	335/309 (108%)	330 (98%)	5 (2%)	65	26
1	B	333/309 (108%)	328 (98%)	5 (2%)	65	26
All	All	668/618 (108%)	658 (98%)	10 (2%)	69	26

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	2	LYS
1	A	170[A]	ILE
1	A	170[B]	ILE
1	A	328	ARG
1	B	212	LEU
1	B	213	LEU
1	B	217	VAL
1	B	263[A]	ILE
1	B	263[B]	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	30	ASN
1	A	68	GLN
1	A	125	ASN
1	B	52	GLN
1	B	68	GLN
1	B	125	ASN
1	B	128	GLN
1	B	139	ASN
1	B	219	GLN
1	B	359	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 ⓘ

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 for Mogul analysis.

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$
3	PEG	A	1363	-	6,6,6	1.17	1 (16%)	5,5,5	1.53	1 (20%)
6	PLP	B	1368	1	15,15,16	1.47	3 (20%)	20,22,23	1.65	5 (25%)
6	PLP	A	1367	1	15,15,16	1.34	3 (20%)	20,22,23	1.10	2 (10%)
4	PGE	A	1364	-	9,9,9	1.26	1 (11%)	8,8,8	1.12	0
4	PGE	B	1364	-	9,9,9	1.27	0	8,8,8	1.31	1 (12%)
8	EPE	B	1365	-	15,15,15	1.25	2 (13%)	18,20,20	2.12	4 (22%)
7	GOL	B	1362	-	5,5,5	0.47	0	5,5,5	0.77	0
4	PGE	B	1363	-	9,9,9	1.14	1 (11%)	8,8,8	1.19	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
3	PEG	A	1363	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PLP	B	1368	1	-	0/6/6/8	0/1/1/1
6	PLP	A	1367	1	-	0/6/6/8	0/1/1/1
4	PGE	A	1364	-	-	2/7/7/7	-
4	PGE	B	1364	-	-	1/7/7/7	-
8	EPE	B	1365	-	-	3/9/19/19	0/1/1/1
7	GOL	B	1362	-	-	0/4/4/4	-
4	PGE	B	1363	-	-	0/7/7/7	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1367	PLP	C2-N1	2.67	1.38	1.33
6	B	1368	PLP	O3-C3	-2.51	1.31	1.37
8	B	1365	EPE	C6-N1	2.47	1.53	1.46
6	B	1368	PLP	C2-N1	2.46	1.38	1.33
6	B	1368	PLP	C5A-C5	2.43	1.57	1.50
8	B	1365	EPE	C2-N1	2.24	1.53	1.46
6	A	1367	PLP	C3-C4	2.23	1.44	1.40
6	A	1367	PLP	O3-C3	-2.21	1.31	1.37
3	A	1363	PEG	O4-C4	2.18	1.53	1.42
4	B	1363	PGE	O2-C2	2.16	1.51	1.42
4	A	1364	PGE	O4-C6	2.10	1.52	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1365	EPE	O1S-S-C10	6.08	114.24	106.92
8	B	1365	EPE	O2S-S-C10	4.35	112.15	106.92
4	B	1364	PGE	O4-C6-C5	2.97	129.03	111.81
6	B	1368	PLP	C5A-C5-C6	-2.81	114.75	119.37
6	B	1368	PLP	C2A-C2-C3	2.77	124.31	120.89
8	B	1365	EPE	O8-C8-C7	2.70	122.38	111.19
6	B	1368	PLP	O4P-C5A-C5	-2.51	104.57	109.35
6	B	1368	PLP	C5-C6-N1	-2.48	119.68	123.82
3	A	1363	PEG	C3-O2-C2	2.42	123.76	113.29
8	B	1365	EPE	O3S-S-O1S	-2.36	105.50	111.27
6	B	1368	PLP	C6-C5-C4	2.26	119.94	118.16
6	A	1367	PLP	C2A-C2-C3	2.14	123.53	120.89
6	A	1367	PLP	O3P-P-O4P	-2.11	101.12	106.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1365	EPE	C8-C7-N4-C5
4	A	1364	PGE	O1-C1-C2-O2
4	A	1364	PGE	O2-C3-C4-O3
8	B	1365	EPE	N4-C7-C8-O8
3	A	1363	PEG	O2-C3-C4-O4
4	B	1364	PGE	C1-C2-O2-C3
8	B	1365	EPE	C9-C10-S-O1S

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1368	PLP	6	0
6	A	1367	PLP	5	0
8	B	1365	EPE	6	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	360/360 (100%)	-0.16	9 (2%) 57 51	9, 13, 30, 85	0
1	B	357/360 (99%)	-0.12	10 (2%) 53 47	9, 12, 34, 83	0
All	All	717/720 (99%)	-0.14	19 (2%) 56 50	9, 12, 32, 85	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	VAL	13.8
1	A	1	VAL	9.4
1	B	213	LEU	7.4
1	A	214	ASN	4.5
1	B	218	GLU	4.1
1	A	215	THR	3.7
1	B	217	VAL	3.6
1	A	216	LYS	3.4
1	A	328	ARG	3.2
1	B	211	ASP	2.7
1	B	212	LEU	2.7
1	B	328	ARG	2.7
1	A	213	LEU	2.6
1	B	219	GLN	2.6
1	B	165[A]	ASN	2.5
1	A	218	GLU	2.5
1	A	2	LYS	2.2
1	B	2	LYS	2.0
1	A	165	ASN	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	PGE	B	1364	10/10	0.61	0.21	46,54,69,81	0
8	EPE	B	1365	15/15	0.64	0.27	26,33,57,58	15
4	PGE	A	1364	10/10	0.80	0.15	35,42,57,58	0
4	PGE	B	1363	10/10	0.89	0.14	22,29,51,73	0
3	PEG	A	1363	7/7	0.90	0.09	21,23,32,55	0
7	GOL	B	1362	6/6	0.93	0.14	16,20,24,30	0
2	MG	B	1361[B]	1/1	0.97	0.07	19,19,19,19	1
2	MG	B	1361[A]	1/1	0.97	0.07	20,20,20,20	1
2	MG	A	503	1/1	0.99	0.13	16,16,16,16	1
6	PLP	A	1367	15/16	0.99	0.06	8,9,11,21	0
6	PLP	B	1368	15/16	0.99	0.05	9,10,13,22	0
5	CL	B	1366	1/1	1.00	0.04	10,10,10,10	0
2	MG	A	1362	1/1	1.00	0.13	14,14,14,14	0
2	MG	A	1361	1/1	1.00	0.12	15,15,15,15	0
5	CL	A	1365	1/1	1.00	0.05	9,9,9,9	0
5	CL	A	1366	1/1	1.00	0.05	15,15,15,15	0
5	CL	B	1367	1/1	1.00	0.05	17,17,17,17	0

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

There are no such residues in this entry.