Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:53 am BST

PDB ID	:	6ERK
Title	:	Crystal structure of diaminopelargonic acid aminotransferase from Psychrobacter cryohalolentis
Authors	:	Boyko, K.M.; Nikolaeva, A.Y.; Bezsudnova, E.Y.; Stekhanova, T.N.; Rakitina, T.V.; Popov, V.O.
Deposited on	:	2017-10-18
Resolution	:	1.60 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

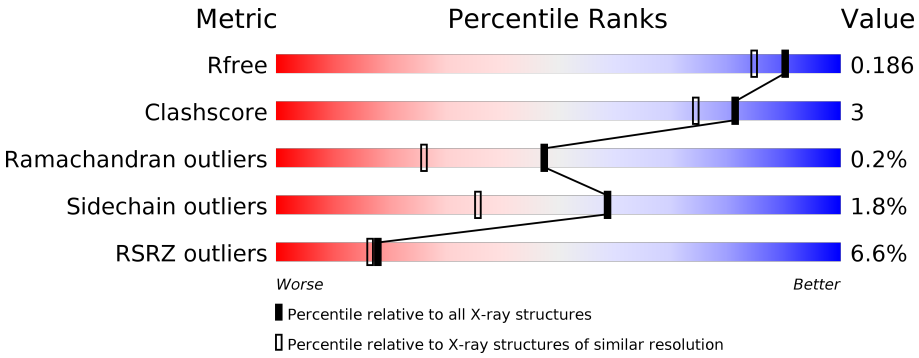
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 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 <=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	451	6% 87% 6% 7%
1	B	451	6% 84% 8% • 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7275 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 Aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	9	0
			3233	2069	528	611	25			
1	B	418	Total	C	N	O	S	0	16	0
			3255	2076	536	615	28			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q1QDV8
A	-18	GLY	-	expression tag	UNP Q1QDV8
A	-17	SER	-	expression tag	UNP Q1QDV8
A	-16	ASP	-	expression tag	UNP Q1QDV8
A	-15	LYS	-	expression tag	UNP Q1QDV8
A	-14	ILE	-	expression tag	UNP Q1QDV8
A	-13	HIS	-	expression tag	UNP Q1QDV8
A	-12	HIS	-	expression tag	UNP Q1QDV8
A	-11	HIS	-	expression tag	UNP Q1QDV8
A	-10	HIS	-	expression tag	UNP Q1QDV8
A	-9	HIS	-	expression tag	UNP Q1QDV8
A	-8	HIS	-	expression tag	UNP Q1QDV8
A	-7	GLU	-	expression tag	UNP Q1QDV8
A	-6	ASN	-	expression tag	UNP Q1QDV8
A	-5	LEU	-	expression tag	UNP Q1QDV8
A	-4	TYR	-	expression tag	UNP Q1QDV8
A	-3	PHE	-	expression tag	UNP Q1QDV8
A	-2	GLN	-	expression tag	UNP Q1QDV8
A	-1	GLY	-	expression tag	UNP Q1QDV8
A	0	HIS	-	expression tag	UNP Q1QDV8
B	-19	MET	-	initiating methionine	UNP Q1QDV8
B	-18	GLY	-	expression tag	UNP Q1QDV8
B	-17	SER	-	expression tag	UNP Q1QDV8
B	-16	ASP	-	expression tag	UNP Q1QDV8
B	-15	LYS	-	expression tag	UNP Q1QDV8

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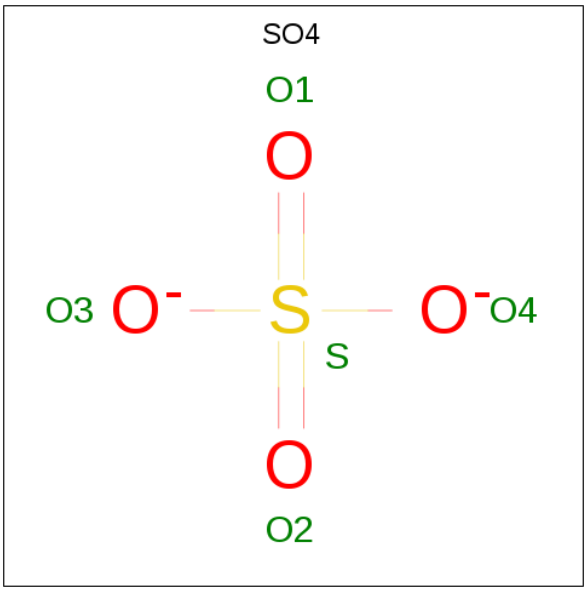
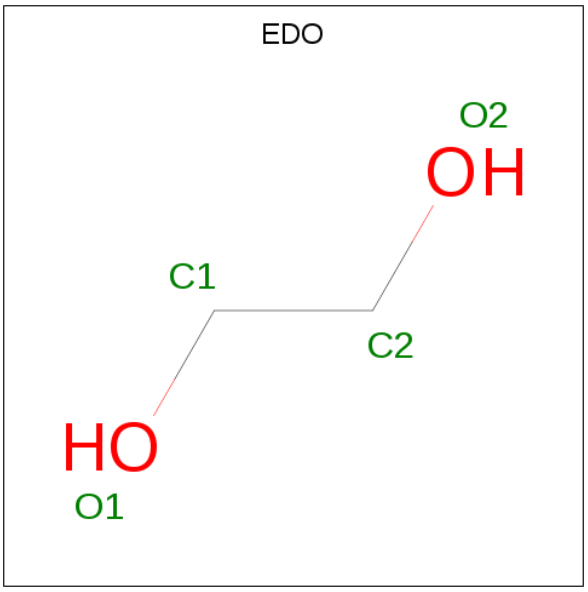
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	ILE	-	expression tag	UNP Q1QDV8
B	-13	HIS	-	expression tag	UNP Q1QDV8
B	-12	HIS	-	expression tag	UNP Q1QDV8
B	-11	HIS	-	expression tag	UNP Q1QDV8
B	-10	HIS	-	expression tag	UNP Q1QDV8
B	-9	HIS	-	expression tag	UNP Q1QDV8
B	-8	HIS	-	expression tag	UNP Q1QDV8
B	-7	GLU	-	expression tag	UNP Q1QDV8
B	-6	ASN	-	expression tag	UNP Q1QDV8
B	-5	LEU	-	expression tag	UNP Q1QDV8
B	-4	TYR	-	expression tag	UNP Q1QDV8
B	-3	PHE	-	expression tag	UNP Q1QDV8
B	-2	GLN	-	expression tag	UNP Q1QDV8
B	-1	GLY	-	expression tag	UNP Q1QDV8
B	0	HIS	-	expression tag	UNP Q1QDV8

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



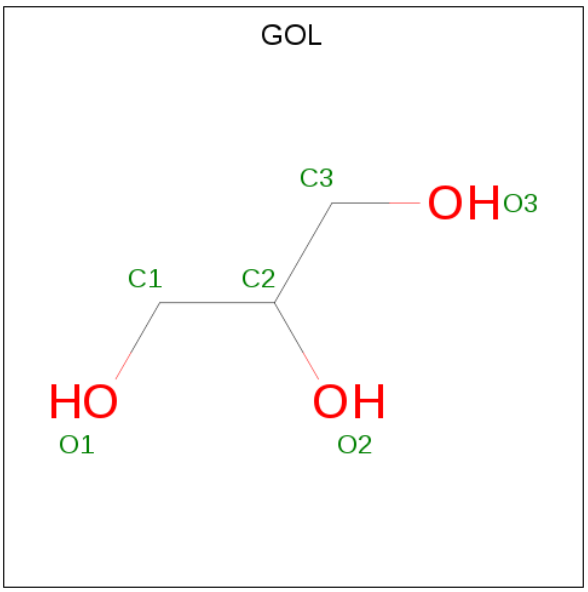
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



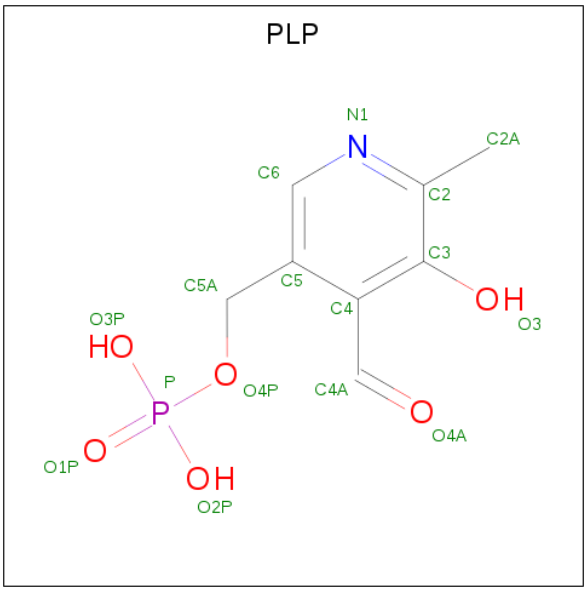
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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



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

- Molecule 6 is water.

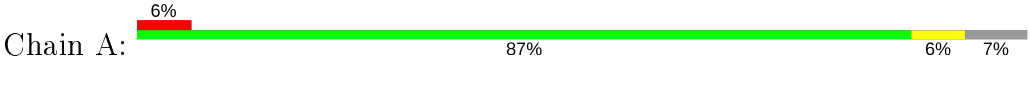
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	378	Total O 378 378	0	0
6	B	364	Total O 364 364	0	0

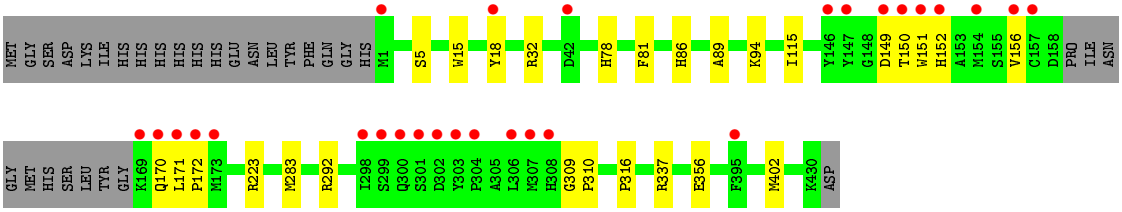
3 Residue-property plots (i)

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

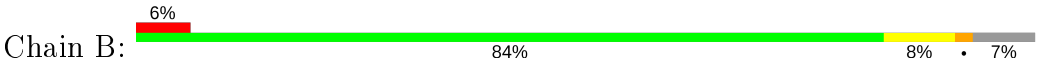
Chain A:

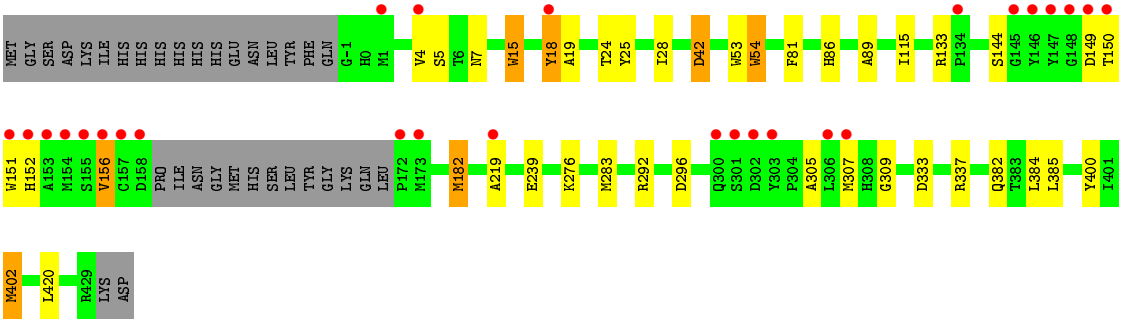




- Molecule 1: Aminotransferase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	182.07Å 67.91Å 118.07Å 90.00° 128.81° 90.00°	Depositor
Resolution (Å)	70.94 – 1.60 70.94 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (70.94-1.60) 96.8 (70.94-1.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.147 , 0.188 0.152 , 0.186	Depositor DCC
R_{free} test set	7082 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	13.9	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.106 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7275	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, PLP, EDO, SO4

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	0.95	1/3360 (0.0%)	0.98	9/4570 (0.2%)
1	B	0.98	8/3409 (0.2%)	1.01	12/4633 (0.3%)
All	All	0.96	9/6769 (0.1%)	1.00	21/9203 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	18[A]	TYR	N-CA	6.98	1.60	1.46
1	B	18[B]	TYR	N-CA	6.98	1.60	1.46
1	B	15	TRP	CG-CD1	6.89	1.46	1.36
1	B	333	ASP	N-CA	6.10	1.58	1.46
1	B	15	TRP	CG-CD2	-5.99	1.33	1.43
1	B	239	GLU	CD-OE1	-5.95	1.19	1.25
1	A	310	PRO	CA-C	5.85	1.64	1.52
1	B	144	SER	CB-OG	5.15	1.49	1.42
1	B	54	TRP	CD1-NE1	-5.09	1.29	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	402	MET	CG-SD-CE	9.86	115.98	100.20
1	B	182[A]	MET	CG-SD-CE	-9.44	85.10	100.20
1	B	182[B]	MET	CG-SD-CE	-9.44	85.10	100.20
1	A	356[A]	GLU	C-N-CA	9.32	141.88	122.30
1	A	356[B]	GLU	C-N-CA	9.32	141.88	122.30
1	A	32[A]	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	A	32[B]	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	B	333	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	B	402	MET	CG-SD-CE	6.91	111.25	100.20
1	B	133	ARG	NE-CZ-NH2	-6.42	117.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	156	VAL	CG1-CB-CG2	-6.27	100.86	110.90
1	B	337	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	402	MET	CB-CG-SD	-5.81	94.97	112.40
1	B	42[A]	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	42[B]	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	337	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	292	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	B	333	ASP	N-CA-CB	5.22	120.00	110.60
1	B	337	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	223	ARG	CD-NE-CZ	5.10	130.74	123.60
1	B	402	MET	CB-CG-SD	-5.09	97.14	112.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3233	0	3182	13	0
1	B	3255	0	3175	25	0
2	A	5	0	0	0	0
3	A	4	0	6	3	0
4	A	6	0	8	0	0
5	A	15	0	6	0	0
5	B	15	0	6	0	0
6	A	378	0	0	1	0
6	B	364	0	0	4	0
All	All	7275	0	6383	34	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 3.

All (34) 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:382:GLN:HG3	1:B:385:LEU:HD12	1.43	0.99
1:B:18[A]:TYR:HD2	6:B:708:HOH:O	1.48	0.96
1:B:18[A]:TYR:CD2	6:B:708:HOH:O	2.20	0.93
1:B:382:GLN:HA	1:B:385:LEU:HG	1.75	0.68
1:A:94:LYS:NZ	3:A:502:EDO:H12	2.09	0.67
1:B:18[A]:TYR:HE2	1:B:53:TRP:CZ2	2.14	0.66
3:A:502:EDO:H11	1:B:7:ASN:HD21	1.60	0.65
1:A:283:MET:HB3	6:B:615:HOH:O	1.96	0.64
6:A:609:HOH:O	1:B:283:MET:HB3	1.96	0.64
1:B:305:ALA:HB3	1:B:307[B]:MET:HE3	1.83	0.60
1:A:171:LEU:HD12	1:A:172:PRO:HD2	1.91	0.53
1:B:18[B]:TYR:OH	1:B:149:ASP:CG	2.46	0.52
1:A:18:TYR:OH	1:A:149:ASP:CG	2.48	0.52
1:A:150:THR:CG2	1:B:115:ILE:CD1	2.87	0.51
1:B:15:TRP:HZ3	1:B:19[B]:ALA:O	1.94	0.51
1:B:4:VAL:HG11	1:B:28:ILE:HG12	1.93	0.51
1:B:86:HIS:CE1	1:B:89:ALA:HB2	2.48	0.49
1:B:24:THR:HG1	1:B:25:TYR:HD2	1.60	0.47
1:A:86:HIS:CE1	1:A:89:ALA:HB2	2.50	0.47
1:B:219:ALA:N	6:B:612:HOH:O	2.50	0.45
1:B:54:TRP:HB2	1:B:276:LYS:HD3	1.99	0.45
1:B:292[A]:ARG:NE	1:B:296:ASP:OD1	2.51	0.44
1:B:400:TYR:CE2	1:B:402:MET:SD	3.11	0.44
1:B:18[A]:TYR:HE2	1:B:53:TRP:HZ2	1.64	0.44
1:A:94:LYS:CE	3:A:502:EDO:H12	2.47	0.43
1:A:18:TYR:OH	1:A:149:ASP:OD1	2.37	0.43
1:B:305:ALA:HB3	1:B:307[B]:MET:CE	2.47	0.43
1:A:78:HIS:HA	1:A:316:PRO:HD2	2.01	0.43
1:B:18[B]:TYR:OH	1:B:149:ASP:OD1	2.36	0.43
1:B:15:TRP:CZ3	1:B:19[B]:ALA:O	2.71	0.43
1:A:151:TRP:HB2	1:B:152:HIS:HB2	2.01	0.42
1:A:18:TYR:HH	1:A:149:ASP:CG	2.23	0.41
1:A:115[B]:ILE:CD1	1:B:150:THR:CG2	2.99	0.41
1:A:152:HIS:HB2	1:B:151:TRP:HB2	2.03	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	426/451 (94%)	409 (96%)	16 (4%)	1 (0%)	47 26
1	B	431/451 (96%)	414 (96%)	16 (4%)	1 (0%)	47 26
All	All	857/902 (95%)	823 (96%)	32 (4%)	2 (0%)	47 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	B	309	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	349/374 (93%)	344 (99%)	5 (1%)	67 47
1	B	354/374 (95%)	344 (97%)	10 (3%)	43 18
All	All	703/748 (94%)	688 (98%)	15 (2%)	59 29

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

Mol	Chain	Res	Type
1	A	5	SER
1	A	15	TRP
1	A	81	PHE
1	A	156	VAL

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Mol	Chain	Res	Type
1	A	170	GLN
1	B	5[A]	SER
1	B	5[B]	SER
1	B	42[A]	ASP
1	B	42[B]	ASP
1	B	81	PHE
1	B	156	VAL
1	B	182[A]	MET
1	B	182[B]	MET
1	B	384	LEU
1	B	420	LEU

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	346	ASN
1	A	382	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

5 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	$\#\|Z\| > 2$
3	EDO	A	502	-	3,3,3	0.93	0	2,2,2	0.95	0
4	GOL	A	503	-	5,5,5	0.57	0	5,5,5	0.74	0
5	PLP	A	504	1	15,15,16	1.86	6 (40%)	20,22,23	2.00	8 (40%)
2	SO4	A	501	-	4,4,4	0.51	0	6,6,6	0.65	0
5	PLP	B	501	1	15,15,16	2.86	6 (40%)	20,22,23	2.32	9 (45%)

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	EDO	A	502	-	-	1/1/1/1	-
4	GOL	A	503	-	-	4/4/4/4	-
5	PLP	A	504	1	-	0/6/6/8	0/1/1/1
5	PLP	B	501	1	-	0/6/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	PLP	C3-C2	6.04	1.46	1.40
5	B	501	PLP	C5-C4	6.00	1.47	1.40
5	B	501	PLP	O3-C3	-3.83	1.28	1.37
5	B	501	PLP	P-O1P	3.51	1.61	1.50
5	A	504	PLP	C5-C4	3.09	1.43	1.40
5	B	501	PLP	C3-C4	3.07	1.46	1.40
5	A	504	PLP	C3-C2	2.94	1.43	1.40
5	B	501	PLP	P-O2P	-2.84	1.43	1.54
5	A	504	PLP	C3-C4	2.42	1.45	1.40
5	A	504	PLP	P-O2P	-2.32	1.45	1.54
5	A	504	PLP	O3-C3	-2.31	1.31	1.37
5	A	504	PLP	C6-C5	2.17	1.42	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	504	PLP	O3P-P-O4P	-4.08	95.87	106.73
5	B	501	PLP	O2P-P-O4P	-3.94	96.25	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	501	PLP	C6-N1-C2	3.90	126.39	119.17
5	B	501	PLP	O3P-P-O4P	3.75	116.72	106.73
5	B	501	PLP	O4P-C5A-C5	3.48	115.97	109.35
5	B	501	PLP	C3-C2-N1	-3.42	116.34	120.77
5	B	501	PLP	C5A-C5-C6	3.41	124.98	119.37
5	B	501	PLP	C2A-C2-N1	3.26	124.03	117.67
5	A	504	PLP	C6-N1-C2	3.08	124.87	119.17
5	A	504	PLP	O4P-C5A-C5	3.01	115.08	109.35
5	A	504	PLP	C2A-C2-N1	2.78	123.10	117.67
5	A	504	PLP	C5-C6-N1	-2.35	119.91	123.82
5	A	504	PLP	O3P-P-O2P	2.34	116.58	107.64
5	B	501	PLP	O3-C3-C2	2.34	122.59	117.49
5	A	504	PLP	C5A-C5-C6	2.29	123.14	119.37
5	A	504	PLP	C2A-C2-C3	-2.28	118.07	120.89
5	B	501	PLP	O3P-P-O2P	2.20	116.06	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	GOL	C1-C2-C3-O3
4	A	503	GOL	O1-C1-C2-C3
4	A	503	GOL	O1-C1-C2-O2
3	A	502	EDO	O1-C1-C2-O2
4	A	503	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	EDO	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

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^{th} 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	420/451 (93%)	0.05	28 (6%)	17	16	7, 14, 33, 81	0
1	B	418/451 (92%)	0.09	27 (6%)	18	17	7, 16, 35, 51	0
All	All	838/902 (92%)	0.07	55 (6%)	18	17	7, 15, 35, 81	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	157	CYS	7.7
1	B	156	VAL	7.2
1	A	151	TRP	6.6
1	A	172	PRO	6.4
1	B	173	MET	6.3
1	B	172	PRO	6.2
1	B	151	TRP	6.2
1	A	171	LEU	6.1
1	A	156	VAL	6.0
1	B	4	VAL	5.8
1	A	306	LEU	5.8
1	A	170	GLN	5.6
1	A	303	TYR	4.9
1	A	173	MET	4.9
1	A	157	CYS	4.6
1	A	18	TYR	4.2
1	B	146	TYR	4.2
1	A	302	ASP	4.2
1	A	169	LYS	4.1
1	B	303	TYR	3.9
1	A	301	SER	3.8
1	B	147	TYR	3.7
1	B	1	MET	3.6
1	A	152	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	152	HIS	3.4
1	A	150	THR	3.2
1	B	302	ASP	3.2
1	A	146	TYR	3.2
1	B	158	ASP	3.1
1	B	154	MET	3.1
1	B	18[A]	TYR	3.0
1	B	306	LEU	3.0
1	B	150	THR	2.9
1	A	395	PHE	2.8
1	B	149	ASP	2.8
1	B	155	SER	2.8
1	B	307[A]	MET	2.8
1	B	153	ALA	2.8
1	A	154	MET	2.7
1	B	134	PRO	2.7
1	B	148	GLY	2.6
1	A	147	TYR	2.6
1	A	308	HIS	2.6
1	A	149	ASP	2.6
1	A	298	ILE	2.5
1	B	145	GLY	2.3
1	A	307	MET	2.3
1	A	42[A]	ASP	2.3
1	B	219	ALA	2.3
1	A	304	PRO	2.2
1	A	1	MET	2.2
1	A	300	GLN	2.2
1	A	299	SER	2.1
1	B	301	SER	2.1
1	B	300[A]	GLN	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

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^{th} 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^2)	Q<0.9
4	GOL	A	503	6/6	0.86	0.24	31,37,44,52	0
3	EDO	A	502	4/4	0.91	0.15	24,24,27,36	0
5	PLP	B	501	15/16	0.96	0.08	15,18,25,28	0
2	SO4	A	501	5/5	0.97	0.20	32,33,40,43	0
5	PLP	A	504	15/16	0.98	0.06	11,13,21,22	0

6.5 Other polymers

There are no such residues in this entry.