



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:16 PM GMT

PDB ID : 3E5P
Title : Crystal structure of alanine racemase from E.faecalis
Authors : Hwang, K.Y.; Priyadarshi, A.; Lee, E.H.; Sung, M.W.
Deposited on : 2008-08-14
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

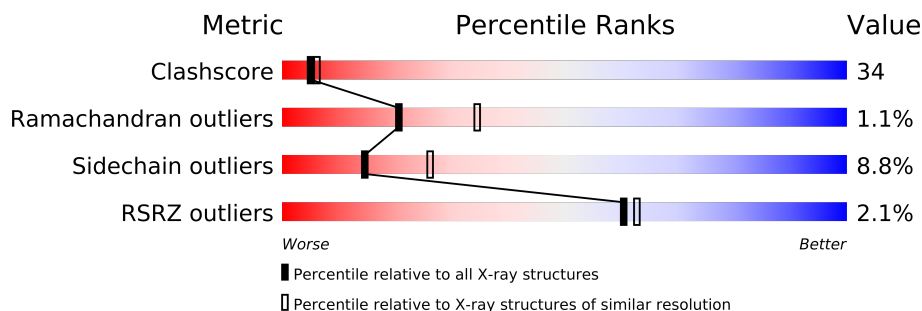
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	371	
1	B	371	
1	C	371	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	PPI	A	400	-	X
3	PPI	B	400	-	X
3	PPI	C	400	-	X
4	EPE	A	430	-	X
5	2PE	C	401	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8905 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

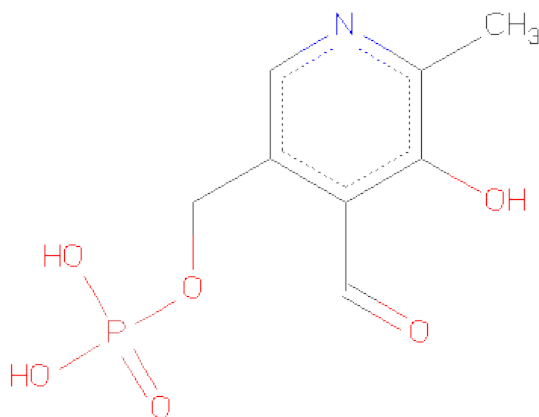
- Molecule 1 is a protein called Alanine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2879	1835	494	538	12			
1	B	371	Total	C	N	O	S	0	0	0
			2887	1840	495	539	13			
1	C	371	Total	C	N	O	S	0	0	0
			2887	1840	495	539	13			

There are 3 discrepancies between the modelled and reference sequences:

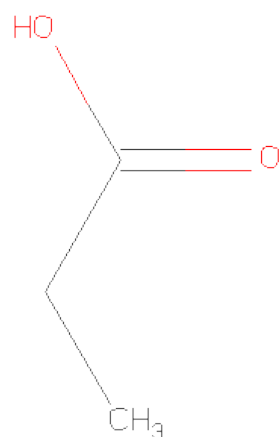
Chain	Residue	Modelled	Actual	Comment	Reference
A	329	PRO	SER	ENGINEERED	UNP Q837J0
B	329	PRO	SER	ENGINEERED	UNP Q837J0
C	329	PRO	SER	ENGINEERED	UNP Q837J0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



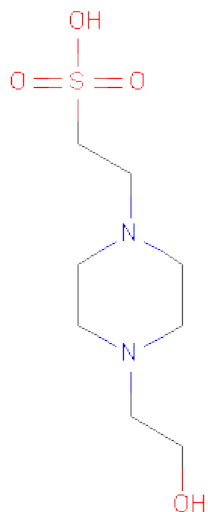
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is PROPANOIC ACID (three-letter code: PPI) (formula: C₃H₆O₂).



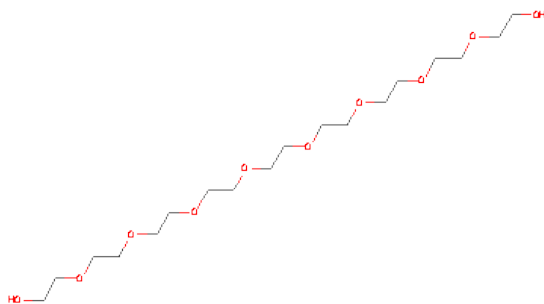
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	C	1	Total	C	O	0	0
			5	3	2		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 5 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	C	1	28	18	10	0	0

- Molecule 6 is water.

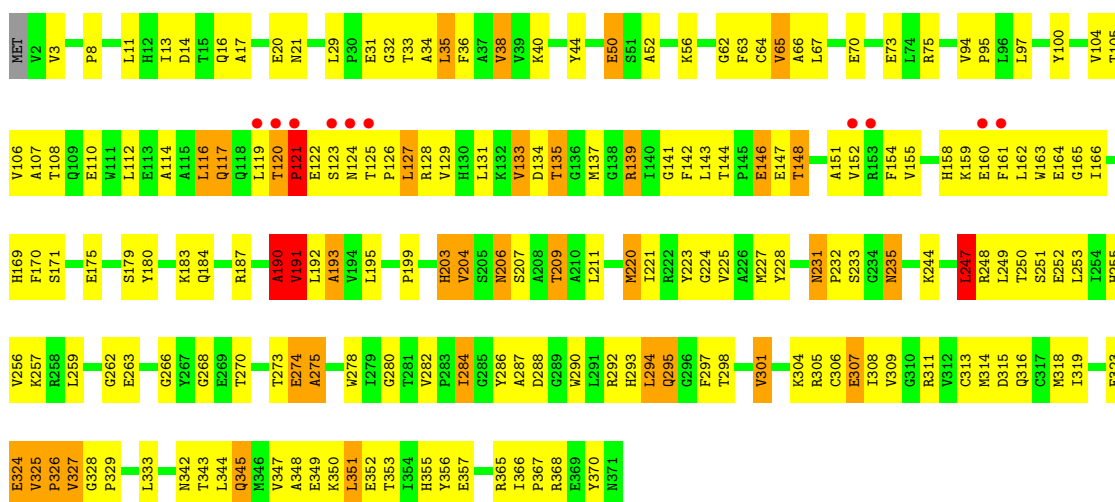
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	57	Total 57	O 57	0	0
6	B	48	Total 48	O 48	0	0
6	C	41	Total 41	O 41	0	0

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.

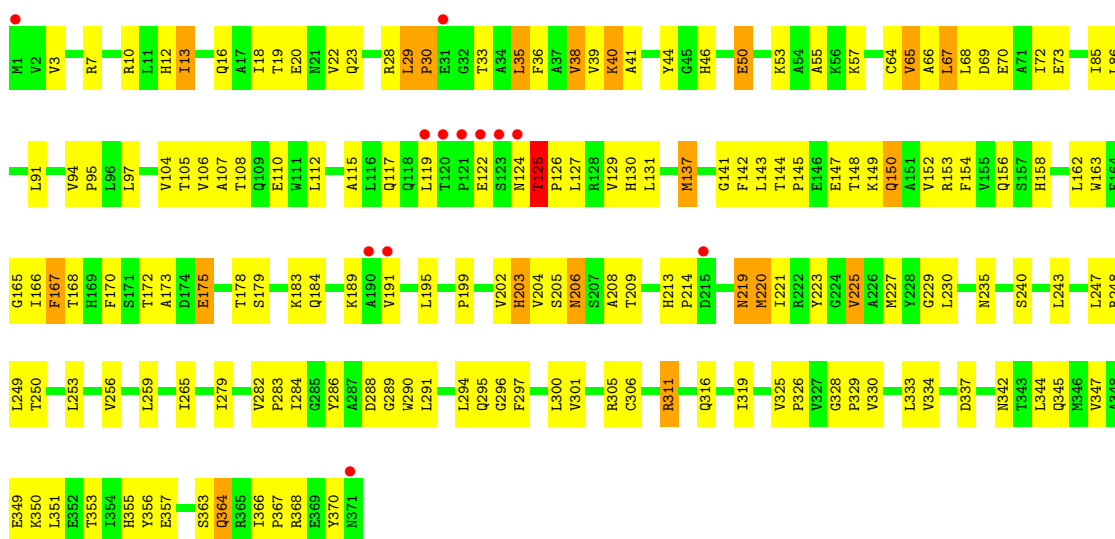
• Molecule 1: Alanine racemase

Chain A:



• Molecule 1: Alanine racemase

Chain B:



• Molecule 1: Alanine racemase

	K350	R258	E164	I98	M1
	L351	L259	G165	Q99	V2
	E352	A261	I167	Y100	G4
	T353	G262	T168	V104	H6
	I354	E263		T105	R7
	H355	G264	T172	V106	
	Y356	I265	E175	A107	L11
	E357	G266	I176	T108	H12
		Y267	Q184	E110	I13
	T361	G268	Q187	F111	I14
	F362	E269	I187	L112	T15
S363	T270	Y271	F188	A115	Q16
Q364			K189	L116	A17
	Y370	A275	I190	Q117	E20
N371		I279	V191	Q118	
			L192	L119	K24
	I284		A193	T120	E25
	G285		V194	P121	
	Y286		L195	E122	R28
	G287		E196	S123	L29
	D288		P199	H124	P30
				T125	
	R292		H203	P126	T33
	H293		V204	L127	A34
	L294		G205	R128	L35
	Q295		N206	V129	
				H130	R38
	V299		T209	L131	V39
	V301		H213	K132	K40
				V133	
	R305			D134	Y44
	C306		N219	T135	
	E307		M220	G136	E50
	I308		I221	M137	
	V309		R222	G138	C64
	G310		Y223	R139	V65
	R311		G224	I140	A66
				G141	L67
					L68
	Q316		M227	T144	D69
	I319		N231	P145	E70
			P232	E146	A71
	V325		S233	E147	
	V326		K244	T148	R75
	V327			K149	
	G328		L247	Q150	Q80
	P329		R248	A151	L84
	V330		L249	V152	R85
	T332		T250	I153	I85
	L333		S251	F154	L86
			E252	V155	
	N342		L253	K159	L91
	T343		V256	E160	V94
	L344		V257	F161	P95
				L162	L96
				Y163	L97

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	94.63Å 156.52Å 147.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 39.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-2.50) 98.0 (39.05-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.281 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 26.5	EDS
Estimated twinning fraction	0.020 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.032 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 37447 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8905	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PPI, EPE, 2PE, 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	1.01	23/2942 (0.8%)	0.89	17/4001 (0.4%)
1	B	0.38	1/2950 (0.0%)	0.71	3/4011 (0.1%)
1	C	0.55	5/2950 (0.2%)	0.73	3/4011 (0.1%)
All	All	0.70	29/8842 (0.3%)	0.78	23/12023 (0.2%)

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	2
1	B	0	1
1	C	0	2
All	All	0	5

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	VAL	CB-CG2	-17.91	1.15	1.52
1	A	327	VAL	CB-CG1	-17.09	1.17	1.52
1	A	325	VAL	CA-CB	-16.88	1.19	1.54
1	A	324	GLU	CB-CG	-12.02	1.29	1.52
1	A	325	VAL	CB-CG2	-10.51	1.30	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ASP	CB-CA-C	-18.61	73.18	110.40
1	B	124	ASN	CB-CA-C	15.35	141.10	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	PRO	N-CA-C	11.26	141.38	112.10
1	C	135	THR	N-CA-CB	-10.04	91.23	110.30
1	A	135	THR	N-CA-CB	-9.54	92.17	110.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	ALA	Peptide
1	A	323	GLU	Mainchain
1	B	29	LEU	Peptide
1	C	144	THR	Peptide
1	C	190	ALA	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2879	0	2868	226	0
1	B	2887	0	2879	163	0
1	C	2887	0	2880	212	0
2	A	16	0	7	3	0
2	B	16	0	7	0	0
2	C	16	0	6	0	0
3	A	5	0	5	0	0
3	B	5	0	5	0	0
3	C	5	0	5	5	0
4	A	15	0	16	11	0
5	C	28	0	38	9	0
6	A	57	0	0	4	0
6	B	48	0	0	6	0
6	C	41	0	0	3	0
All	All	8905	0	8716	586	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 34.

The worst 5 of 586 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:190:ALA:CA	1:A:191:VAL:HG23	1.45	1.43
1:B:145:PRO:HG3	1:B:191:VAL:CG2	1.47	1.41
1:B:145:PRO:CG	1:B:191:VAL:HG22	1.51	1.41
1:A:325:VAL:CG2	1:A:326:PRO:HD2	1.65	1.26
1:A:190:ALA:N	1:A:191:VAL:HG23	1.56	1.19

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	368/371 (99%)	320 (87%)	43 (12%)	5 (1%)	16	27
1	B	369/371 (100%)	328 (89%)	38 (10%)	3 (1%)	27	46
1	C	369/371 (100%)	332 (90%)	33 (9%)	4 (1%)	21	34
All	All	1106/1113 (99%)	980 (89%)	114 (10%)	12 (1%)	21	34

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	PRO
1	B	125	THR
1	B	30	PRO
1	C	4	GLY
1	C	190	ALA

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	305/306 (100%)	278 (91%)	27 (9%)	14	26
1	B	306/306 (100%)	278 (91%)	28 (9%)	13	24
1	C	306/306 (100%)	280 (92%)	26 (8%)	15	28
All	All	917/918 (100%)	836 (91%)	81 (9%)	14	26

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	137	MET
1	B	223	TYR
1	C	252	GLU
1	B	143	LEU
1	B	203	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	117	GLN
1	B	203	HIS
1	C	316	GLN
1	B	158	HIS
1	B	206	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	390	1	16,16,16	2.28	5 (31%)	23,23,23	3.07	10 (43%)
3	PPI	A	400	-	4,4,4	0.68	0	4,4,4	0.94	0
4	EPE	A	430	-	15,15,15	2.20	8 (53%)	20,20,20	6.10	12 (60%)
2	PLP	B	390	1	16,16,16	2.61	7 (43%)	23,23,23	2.08	9 (39%)
3	PPI	B	400	-	4,4,4	0.76	0	4,4,4	0.59	0
2	PLP	C	390	1	16,16,16	1.71	5 (31%)	23,23,23	2.28	8 (34%)
3	PPI	C	400	-	4,4,4	0.91	0	4,4,4	0.66	0
5	2PE	C	401	-	27,27,27	1.05	1 (3%)	26,26,26	0.57	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	390	1	-	0/8/8/8	0/1/1/1
3	PPI	A	400	-	-	0/2/2/2	0/0/0/0
4	EPE	A	430	-	-	0/9/19/19	0/1/1/1
2	PLP	B	390	1	-	0/8/8/8	0/1/1/1
3	PPI	B	400	-	-	0/2/2/2	0/0/0/0
2	PLP	C	390	1	-	0/8/8/8	0/1/1/1
3	PPI	C	400	-	-	0/2/2/2	0/0/0/0
5	2PE	C	401	-	-	0/25/25/25	0/0/0/0

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	390	PLP	C3-C2	-7.78	1.35	1.40
2	A	390	PLP	C3-C2	-5.13	1.37	1.40
4	A	430	EPE	C5-N4	-4.57	1.34	1.47
2	A	390	PLP	P-O2P	-3.34	1.42	1.54
2	B	390	PLP	P-O1P	-3.24	1.40	1.51

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	430	EPE	O2S-S-C10	20.62	124.48	106.81
4	A	430	EPE	O3S-S-C10	-12.50	90.10	105.93
2	A	390	PLP	C5A-C5-C6	-10.02	100.31	119.28
4	A	430	EPE	C5-C6-N1	-7.90	95.04	110.61
2	C	390	PLP	C3-C4-C5	-6.01	113.39	118.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	370/371 (99%)	0.07	10 (2%) 52 54	15, 33, 57, 80	0
1	B	371/371 (100%)	0.04	12 (3%) 45 47	16, 36, 59, 79	0
1	C	371/371 (100%)	0.03	2 (0%) 88 90	18, 33, 57, 66	0
All	All	1112/1113 (99%)	0.05	24 (2%) 60 61	15, 34, 58, 80	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	123	SER	6.9
1	B	120	THR	6.8
1	A	121	PRO	6.7
1	B	121	PRO	6.0
1	B	124	ASN	4.2

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 ⓘ

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. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PPI	B	400	5/5	0.36	13.28	65,66,66,69	0
4	EPE	A	430	15/15	0.41	8.48	41,47,59,61	0
3	PPI	C	400	5/5	0.38	7.68	53,55,57,59	0
3	PPI	A	400	5/5	0.40	4.98	64,65,66,67	0
5	2PE	C	401	28/28	0.29	4.67	57,61,65,65	0
2	PLP	A	390	16/16	0.14	0.05	20,20,20,20	0
2	PLP	C	390	16/16	0.15	-0.79	20,20,20,20	0
2	PLP	B	390	16/16	0.12	-0.82	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.