



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 24, 2023 – 05:02 AM EDT

PDB ID : 5KQU
Title : Directed Evolution of Transaminases By Ancestral Reconstruction. Using Old Proteins for New Chemistries
Authors : Wilding, M.; Newman, J.; Peat, T.S.; Scott, C.
Deposited on : 2016-07-06
Resolution : 2.62 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.35.1
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) : 2.35.1

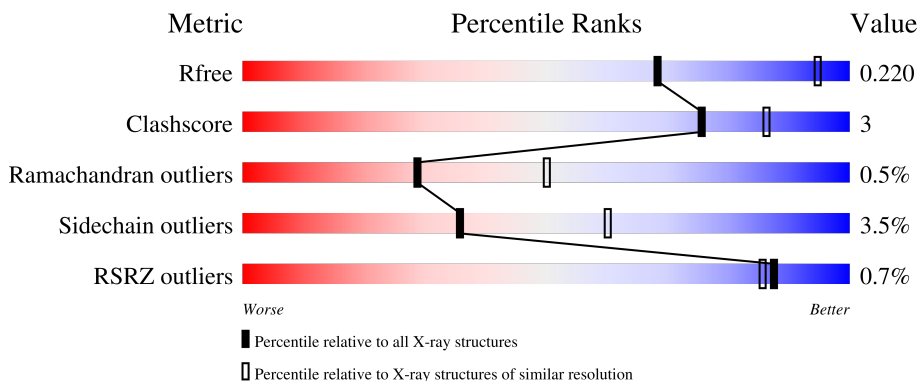
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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.



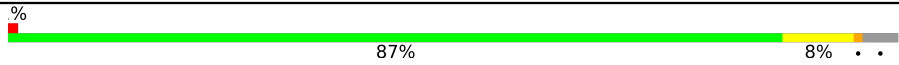
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 of 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 $\leq 5\%$. 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	479	88% 6% • 5%
1	B	479	87% 8% •
1	C	479	% 87% 8% • •
1	D	479	% 86% 8% • 5%
1	E	479	% 87% 8% • 5%

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Mol	Chain	Length	Quality of chain
1	F	479	 A horizontal bar chart representing the quality of chain. The bar is primarily green, indicating a high quality score of 87%. A small yellow segment at the end indicates a lower quality score of 8%. The bar is labeled with a '%' sign at the start and '87%' and '8%' at the corresponding positions along the bar.

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
2	PLP	A	501	-	-	X	-
2	PLP	D	501	-	-	X	-
2	PLP	E	501	-	-	X	-

2 Entry composition [i](#)

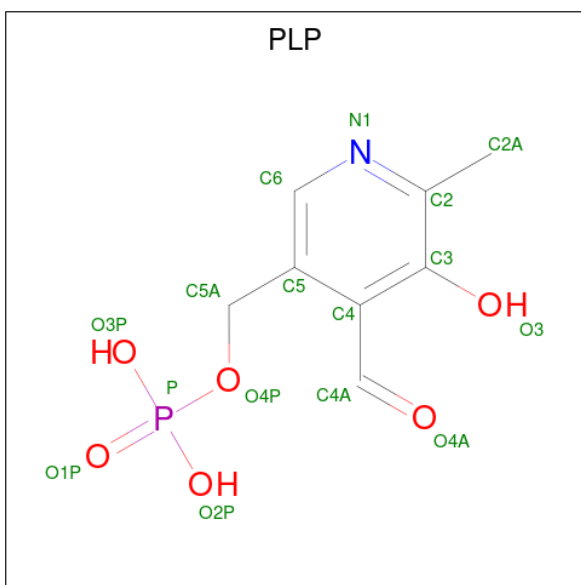
There are 3 unique types of molecules in this entry. The entry contains 21243 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-aminobutyrate transaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	457	Total 3493	C 2216	N 610	O 648	S 19	0	1	0
1	B	458	Total 3503	C 2221	N 611	O 652	S 19	0	1	0
1	C	459	Total 3508	C 2224	N 612	O 653	S 19	0	1	0
1	D	457	Total 3496	C 2217	N 610	O 650	S 19	0	1	0
1	E	457	Total 3496	C 2217	N 610	O 650	S 19	0	1	0
1	F	459	Total 3511	C 2226	N 612	O 653	S 20	0	1	0

- 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
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		


- Molecule 3 is water.

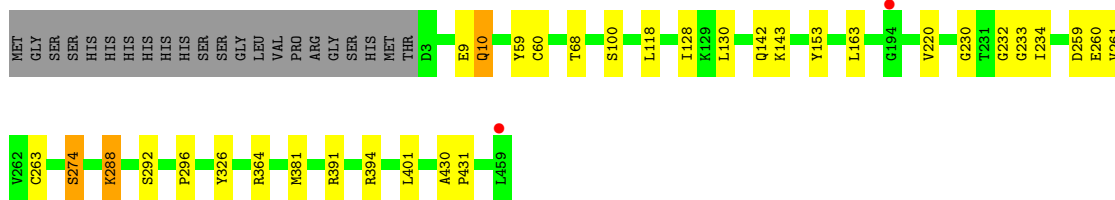
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	31	Total	O	0	0
			31	31		
3	C	28	Total	O	0	0
			28	28		
3	D	20	Total	O	0	0
			20	20		
3	E	11	Total	O	0	0
			11	11		
3	F	23	Total	O	0	0
			23	23		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

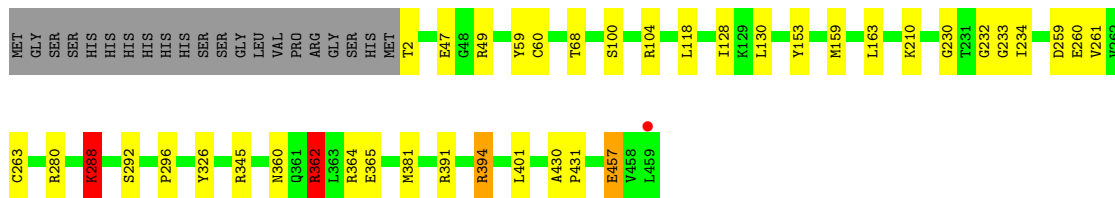
- Molecule 1: 4-aminobutyrate transaminase

Chain A: 




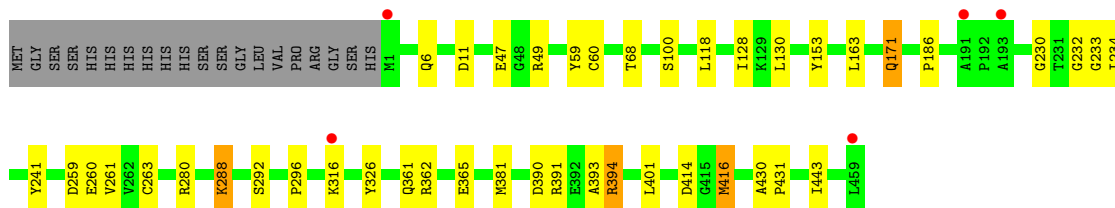
- Molecule 1: 4-aminobutyrate transaminase

Chain B: 




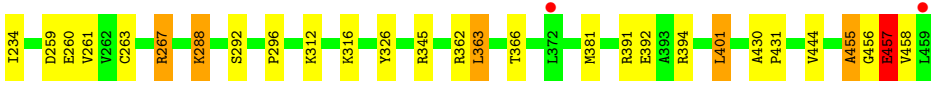
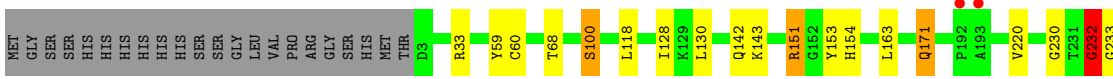
- Molecule 1: 4-aminobutyrate transaminase

Chain C: 

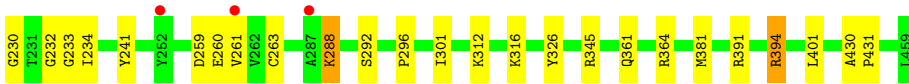
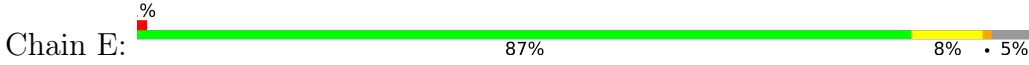


- Molecule 1: 4-aminobutyrate transaminase

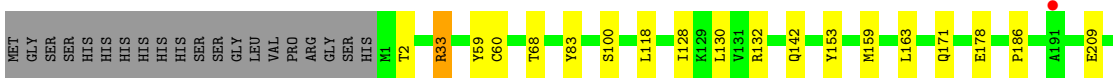
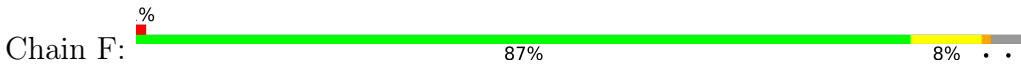
Chain D: 



• Molecule 1: 4-aminobutyrate transaminase



• Molecule 1: 4-aminobutyrate transaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.10Å 146.89Å 131.78Å 90.00° 97.68° 90.00°	Depositor
Resolution (Å)	48.90 – 2.62 43.77 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.90-2.62) 99.7 (43.77-2.62)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.188 , 0.220 0.191 , 0.220	Depositor DCC
R_{free} test set	4128 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtrriage
Anisotropy	0.015	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21243	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.55	1/3573 (0.0%)	0.76	1/4842 (0.0%)
1	B	0.54	0/3583	0.77	7/4856 (0.1%)
1	C	0.54	0/3588	0.78	6/4863 (0.1%)
1	D	0.55	0/3576	0.82	7/4846 (0.1%)
1	E	0.51	0/3576	0.77	6/4846 (0.1%)
1	F	0.54	1/3591 (0.0%)	0.79	6/4866 (0.1%)
All	All	0.54	2/21487 (0.0%)	0.78	33/29119 (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
1	B	0	2
1	C	0	1
1	D	0	3
1	E	0	1
1	F	0	2
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	274	SER	CB-OG	-7.37	1.32	1.42
1	A	274	SER	CB-OG	-6.14	1.34	1.42

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	267	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	C	394	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	C	391	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	D	33	ARG	NE-CZ-NH2	6.85	123.72	120.30
1	F	391	ARG	NE-CZ-NH1	6.74	123.67	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	GLY	Peptide
1	B	2	THR	Peptide
1	B	232	GLY	Peptide
1	C	232	GLY	Peptide
1	D	232	GLY	Mainchain

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	3493	0	3445	21	0
1	B	3503	0	3454	20	0
1	C	3508	0	3459	24	0
1	D	3496	0	3447	32	0
1	E	3496	0	3447	26	0
1	F	3511	0	3467	14	0
2	A	15	0	6	8	0
2	B	15	0	6	4	0
2	C	15	0	7	4	0
2	D	15	0	6	11	0
2	E	15	0	6	9	0
2	F	15	0	6	2	0
3	A	33	0	0	1	0
3	B	31	0	0	1	0
3	C	28	0	0	1	0
3	D	20	0	0	0	0
3	E	11	0	0	0	0
3	F	23	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21243	0	20756	131	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.

The worst 5 of 131 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:D:259:ASP:CG	2:D:501:PLP:H2A2	1.38	1.42
1:D:259:ASP:OD2	2:D:501:PLP:C2A	1.69	1.38
1:E:259:ASP:CG	2:E:501:PLP:H2A2	1.55	1.27
1:D:259:ASP:OD2	2:D:501:PLP:H2A2	1.01	1.17
1:C:416:MET:HE1	1:C:443:ILE:HA	1.25	1.16

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	456/479 (95%)	435 (95%)	19 (4%)	2 (0%)	34 55
1	B	457/479 (95%)	436 (95%)	19 (4%)	2 (0%)	34 55
1	C	458/479 (96%)	437 (95%)	19 (4%)	2 (0%)	34 55
1	D	456/479 (95%)	434 (95%)	19 (4%)	3 (1%)	22 41
1	E	456/479 (95%)	435 (95%)	19 (4%)	2 (0%)	34 55
1	F	458/479 (96%)	434 (95%)	22 (5%)	2 (0%)	34 55
All	All	2741/2874 (95%)	2611 (95%)	117 (4%)	13 (0%)	29 50

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	457	GLU
1	A	288	LYS
1	D	288	LYS
1	E	288	LYS
1	F	288	LYS

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	352/371 (95%)	342 (97%)	10 (3%)	43	68
1	B	354/371 (95%)	344 (97%)	10 (3%)	43	68
1	C	354/371 (95%)	344 (97%)	10 (3%)	43	68
1	D	353/371 (95%)	339 (96%)	14 (4%)	31	55
1	E	353/371 (95%)	341 (97%)	12 (3%)	37	61
1	F	355/371 (96%)	338 (95%)	17 (5%)	25	47
All	All	2121/2226 (95%)	2048 (97%)	73 (3%)	36	61

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	33	ARG
1	F	394	ARG
1	F	68	THR
1	F	209	GLU
1	C	130	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	C	6	GLN
1	C	10	GLN
1	E	25	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	E	501	1	15,15,16	3.56	4 (26%)	20,22,23	2.69	8 (40%)
2	PLP	F	501	1	15,15,16	3.57	3 (20%)	20,22,23	2.19	7 (35%)
2	PLP	A	501	1	15,15,16	3.68	3 (20%)	20,22,23	3.09	8 (40%)
2	PLP	B	501	1	15,15,16	2.93	3 (20%)	20,22,23	1.70	5 (25%)
2	PLP	D	501	1	15,15,16	3.99	6 (40%)	20,22,23	3.56	8 (40%)
2	PLP	C	501	1	15,15,16	3.29	3 (20%)	20,22,23	2.35	7 (35%)

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	E	501	1	-	3/6/6/8	0/1/1/1
2	PLP	F	501	1	-	0/6/6/8	0/1/1/1
2	PLP	A	501	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	B	501	1	-	1/6/6/8	0/1/1/1
2	PLP	D	501	1	-	1/6/6/8	0/1/1/1
2	PLP	C	501	1	-	3/6/6/8	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	PLP	C5-C4	10.46	1.52	1.40
2	D	501	PLP	C5-C4	10.24	1.51	1.40
2	A	501	PLP	C5-C4	9.21	1.50	1.40
2	A	501	PLP	C3-C2	8.79	1.49	1.40
2	C	501	PLP	C5-C4	8.70	1.50	1.40

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLP	C2A-C2-C3	-7.55	111.56	120.89
2	D	501	PLP	C6-C5-C4	7.51	124.07	118.16
2	D	501	PLP	C4A-C4-C3	7.32	132.91	120.50
2	D	501	PLP	C3-C4-C5	-7.28	110.88	118.74
2	C	501	PLP	C2A-C2-C3	-6.49	112.87	120.89

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PLP	C5A-O4P-P-O2P
2	C	501	PLP	C5A-O4P-P-O1P
2	C	501	PLP	C5A-O4P-P-O2P
2	C	501	PLP	C5A-O4P-P-O3P
2	E	501	PLP	C5A-O4P-P-O2P

There are no ring outliers.

6 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	PLP	9	0
2	F	501	PLP	2	0
2	A	501	PLP	8	0
2	B	501	PLP	4	0
2	D	501	PLP	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	PLP	4	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	457/479 (95%)	-0.45	2 (0%) 92 91	21, 35, 55, 73	0
1	B	458/479 (95%)	-0.25	1 (0%) 95 95	19, 36, 58, 83	0
1	C	459/479 (95%)	-0.26	5 (1%) 80 78	21, 35, 61, 72	0
1	D	457/479 (95%)	-0.15	4 (0%) 84 82	22, 42, 72, 87	0
1	E	457/479 (95%)	-0.02	5 (1%) 80 78	23, 46, 71, 84	0
1	F	459/479 (95%)	-0.34	3 (0%) 87 85	22, 39, 63, 83	0
All	All	2747/2874 (95%)	-0.25	20 (0%) 87 85	19, 38, 64, 87	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	459	LEU	3.9
1	B	459	LEU	3.4
1	F	191	ALA	2.9
1	E	261	VAL	2.8
1	C	459	LEU	2.6

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 monosaccharides 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, 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	B-factors(Å ²)	Q<0.9
2	PLP	D	501	15/16	0.91	0.27	41,62,69,73	0
2	PLP	E	501	15/16	0.92	0.27	46,59,63,66	0
2	PLP	C	501	15/16	0.94	0.22	43,51,56,58	0
2	PLP	F	501	15/16	0.94	0.23	42,44,48,51	0
2	PLP	A	501	15/16	0.96	0.15	37,44,47,47	0
2	PLP	B	501	15/16	0.96	0.23	39,42,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.