



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 8, 2021 – 06:10 PM BST

PDB ID : 6S8W
Title : Aromatic aminotransferase AroH (Aro8) form *Aspergillus fumigatus* in complex with PLP (internal aldimine)
Authors : Giardina, G.; Mirco, D.; Spizzichino, S.; Zelante, T.; Cutruzzola, F.; Romani, L.; Cellini, B.
Deposited on : 2019-07-10
Resolution : 2.40 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 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 : 2.23.1
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) : 2.23.1

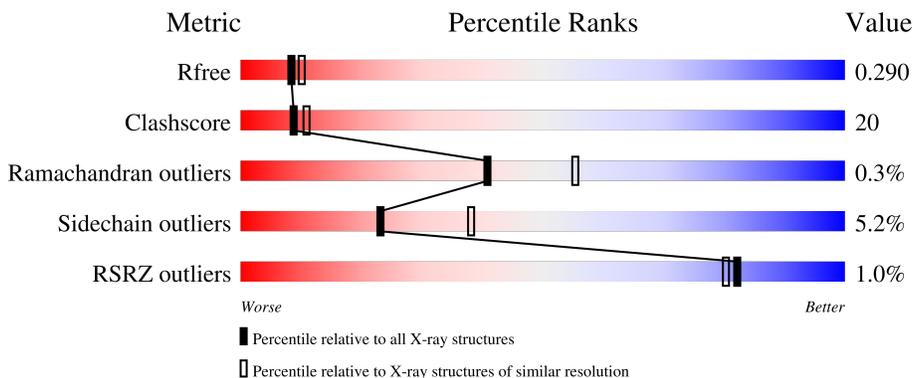
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	534	 64% 27% 8%
1	B	534	 64% 25% 8%
1	C	534	 60% 25% 12%
1	D	534	 58% 31% 8%

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	C	601	-	-	X	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 14737 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 Aromatic aminotransferase Aro8, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	489	Total 3689	C 2360	N 629	O 686	S 14	0	0	0
1	B	491	Total 3721	C 2379	N 640	O 689	S 13	0	0	0
1	C	470	Total 3475	C 2219	N 604	O 638	S 14	0	0	0
1	D	490	Total 3620	C 2322	N 624	O 661	S 13	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

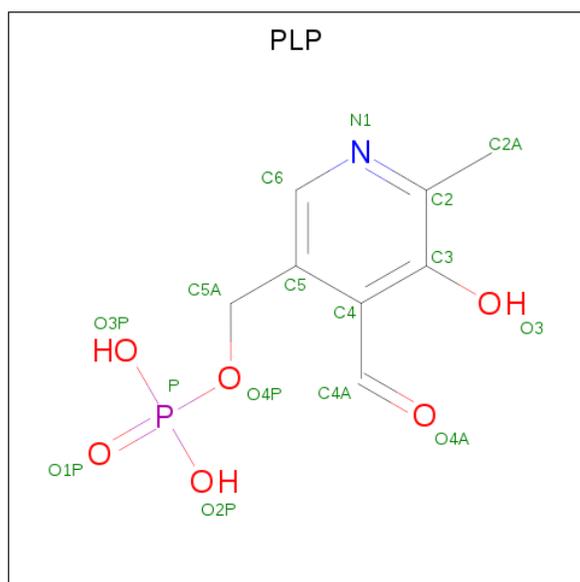
Chain	Residue	Modelled	Actual	Comment	Reference
A	527	LEU	-	expression tag	UNP Q4X0F7
A	528	GLU	-	expression tag	UNP Q4X0F7
A	529	HIS	-	expression tag	UNP Q4X0F7
A	530	HIS	-	expression tag	UNP Q4X0F7
A	531	HIS	-	expression tag	UNP Q4X0F7
A	532	HIS	-	expression tag	UNP Q4X0F7
A	533	HIS	-	expression tag	UNP Q4X0F7
A	534	HIS	-	expression tag	UNP Q4X0F7
B	527	LEU	-	expression tag	UNP Q4X0F7
B	528	GLU	-	expression tag	UNP Q4X0F7
B	529	HIS	-	expression tag	UNP Q4X0F7
B	530	HIS	-	expression tag	UNP Q4X0F7
B	531	HIS	-	expression tag	UNP Q4X0F7
B	532	HIS	-	expression tag	UNP Q4X0F7
B	533	HIS	-	expression tag	UNP Q4X0F7
B	534	HIS	-	expression tag	UNP Q4X0F7
C	527	LEU	-	expression tag	UNP Q4X0F7
C	528	GLU	-	expression tag	UNP Q4X0F7
C	529	HIS	-	expression tag	UNP Q4X0F7
C	530	HIS	-	expression tag	UNP Q4X0F7
C	531	HIS	-	expression tag	UNP Q4X0F7

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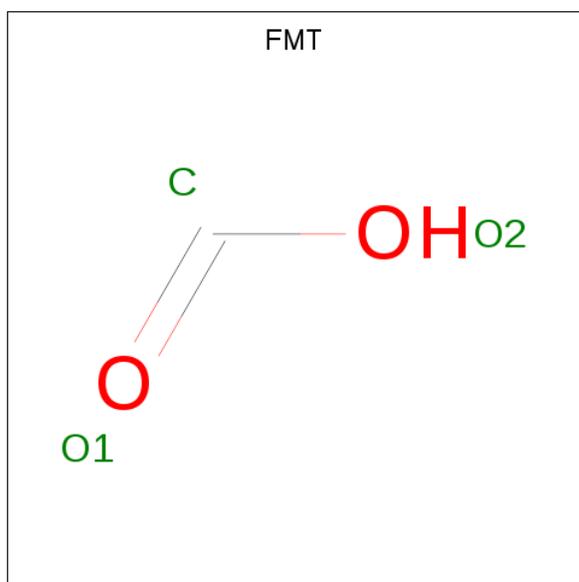
Chain	Residue	Modelled	Actual	Comment	Reference
C	532	HIS	-	expression tag	UNP Q4X0F7
C	533	HIS	-	expression tag	UNP Q4X0F7
C	534	HIS	-	expression tag	UNP Q4X0F7
D	527	LEU	-	expression tag	UNP Q4X0F7
D	528	GLU	-	expression tag	UNP Q4X0F7
D	529	HIS	-	expression tag	UNP Q4X0F7
D	530	HIS	-	expression tag	UNP Q4X0F7
D	531	HIS	-	expression tag	UNP Q4X0F7
D	532	HIS	-	expression tag	UNP Q4X0F7
D	533	HIS	-	expression tag	UNP Q4X0F7
D	534	HIS	-	expression tag	UNP Q4X0F7

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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					

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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

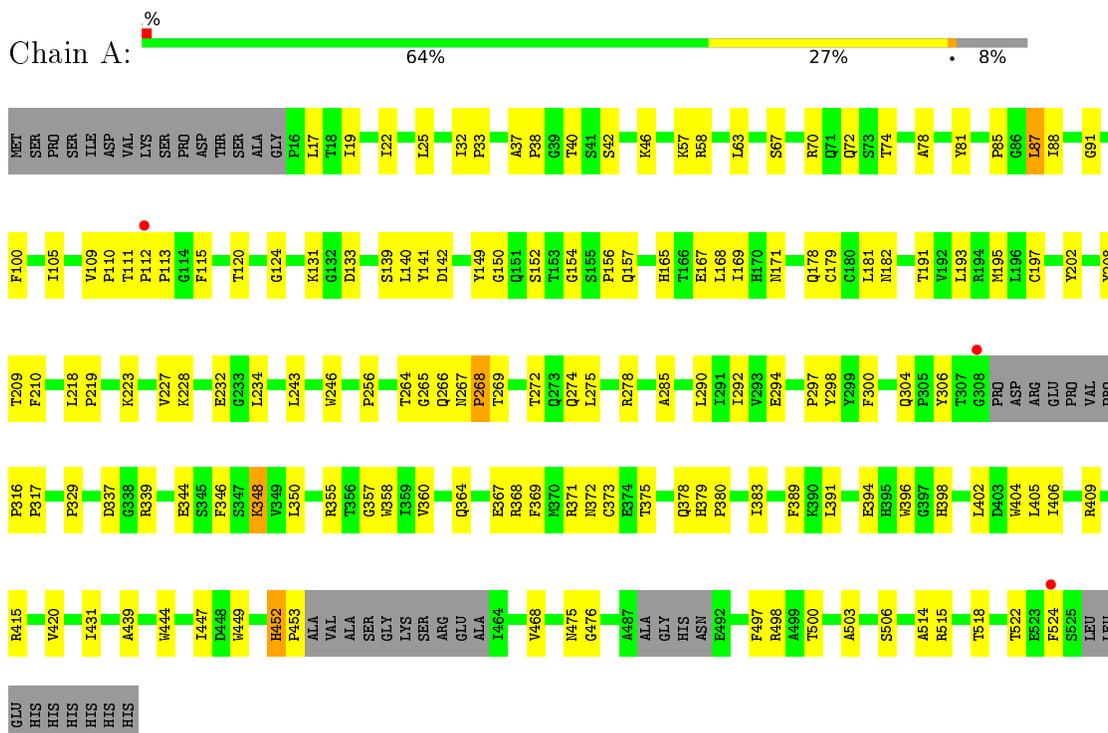
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	55	Total O 55 55	0	0
4	B	58	Total O 58 58	0	0
4	C	28	Total O 28 28	0	0
4	D	25	Total O 25 25	0	0

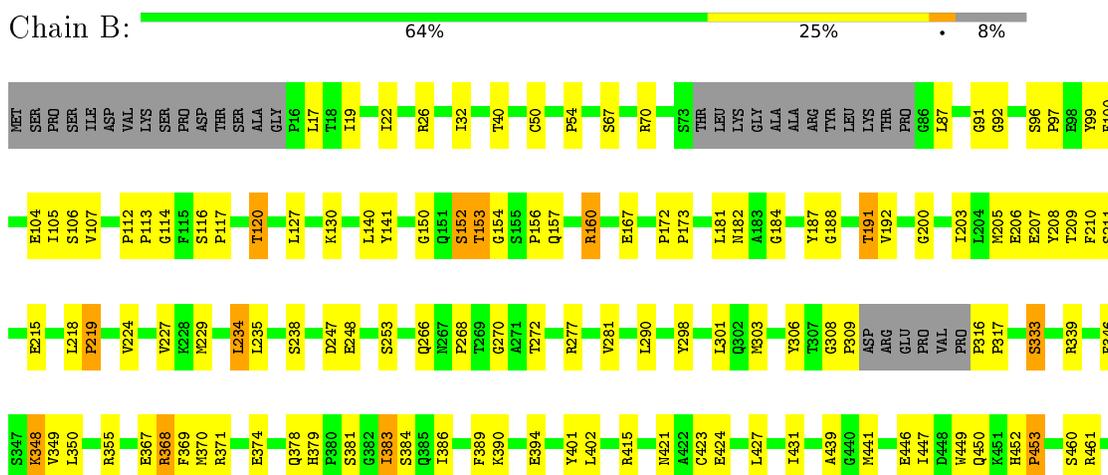
3 Residue-property plots [i](#)

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: Aromatic aminotransferase Aro8, putative

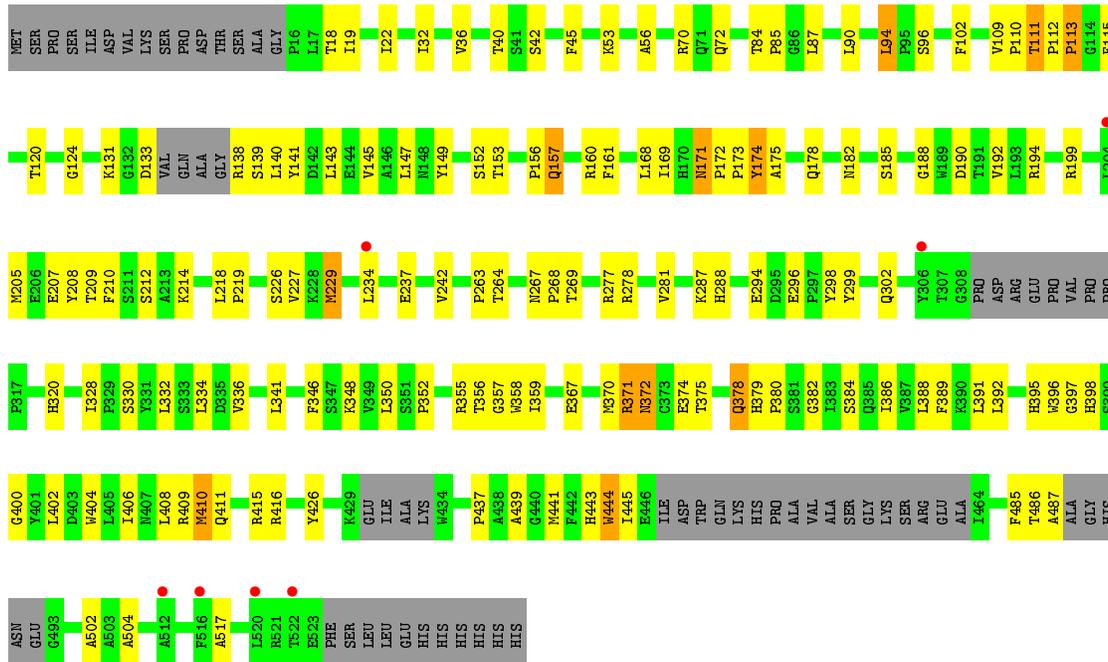


- Molecule 1: Aromatic aminotransferase Aro8, putative

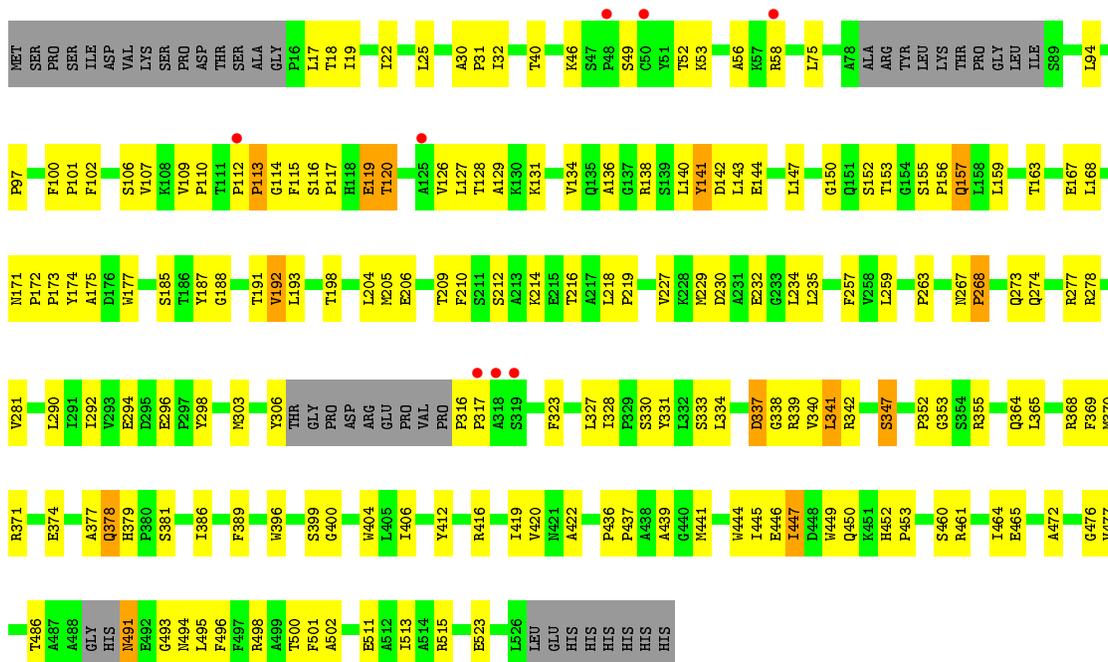




● Molecule 1: Aromatic aminotransferase Aro8, putative



● Molecule 1: Aromatic aminotransferase Aro8, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.21Å 75.26Å 121.63Å 84.77° 87.51° 65.37°	Depositor
Resolution (Å)	47.20 – 2.40 47.21 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.20-2.40) 97.2 (47.21-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.245 , 0.293 0.246 , 0.290	Depositor DCC
R_{free} test set	3871 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtrriage
Anisotropy	0.555	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.029 for h,h-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14737	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.50% 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: FMT, 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	0.63	0/3791	0.70	0/5171
1	B	0.64	0/3823	0.70	1/5212 (0.0%)
1	C	0.64	0/3566	0.72	1/4863 (0.0%)
1	D	0.64	0/3720	0.71	0/5082
All	All	0.64	0/14900	0.71	2/20328 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ARG	CG-CD-NE	6.42	125.28	111.80
1	C	444	TRP	CA-CB-CG	5.10	123.39	113.70

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	3689	0	3455	128	0
1	B	3721	0	3520	128	0
1	C	3475	0	3215	173	0
1	D	3620	0	3357	182	0
2	A	15	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	6	1	0
2	C	15	0	6	6	0
2	D	15	0	6	3	0
3	A	3	0	1	0	0
3	D	3	0	1	0	0
4	A	55	0	0	3	0
4	B	58	0	0	4	0
4	C	28	0	0	2	0
4	D	25	0	0	1	0
All	All	14737	0	13573	577	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 20.

The worst 5 of 577 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:C:208:TYR:H	1:C:229:MET:CE	1.42	1.31
1:B:306:TYR:OH	1:B:421:ASN:ND2	1.72	1.22
1:C:109:VAL:HG21	1:C:391:LEU:CD1	1.68	1.22
1:C:207:GLU:HB3	1:C:229:MET:HE2	1.21	1.19
1:D:22:ILE:HD11	1:D:168:LEU:HD11	1.20	1.17

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	481/534 (90%)	455 (95%)	26 (5%)	0	100 100
1	B	483/534 (90%)	457 (95%)	25 (5%)	1 (0%)	47 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	458/534 (86%)	432 (94%)	23 (5%)	3 (1%)	22	32
1	D	482/534 (90%)	455 (94%)	25 (5%)	2 (0%)	34	48
All	All	1904/2136 (89%)	1799 (94%)	99 (5%)	6 (0%)	41	55

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	378	GLN
1	B	453	PRO
1	D	113	PRO
1	C	111	THR
1	C	378	GLN

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	368/449 (82%)	356 (97%)	12 (3%)	38	57
1	B	376/449 (84%)	355 (94%)	21 (6%)	21	34
1	C	334/449 (74%)	316 (95%)	18 (5%)	22	36
1	D	349/449 (78%)	326 (93%)	23 (7%)	16	26
All	All	1427/1796 (80%)	1353 (95%)	74 (5%)	23	38

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	167	GLU
1	D	486	THR
1	D	192	VAL
1	D	347	SER
1	B	368	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	171	ASN
1	D	165	HIS
1	D	157	GLN
1	D	378	GLN
1	A	475	ASN

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	B	601	1	15,15,16	0.78	1 (6%)	20,22,23	0.58	0
3	FMT	A	602	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	601	-	0,2,2	0.00	-	0,1,1	0.00	-
2	PLP	D	602	1	15,15,16	0.85	1 (6%)	20,22,23	0.60	0
2	PLP	A	601	1	15,15,16	0.91	1 (6%)	20,22,23	0.57	0
2	PLP	C	601	1	15,15,16	0.78	1 (6%)	20,22,23	0.84	1 (5%)

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	C	601	1	-	2/6/6/8	0/1/1/1
2	PLP	B	601	1	-	3/6/6/8	0/1/1/1
2	PLP	A	601	1	-	3/6/6/8	0/1/1/1
2	PLP	D	602	1	-	3/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	PLP	C4A-C4	-2.55	1.46	1.51
2	C	601	PLP	C4A-C4	-2.54	1.46	1.51
2	A	601	PLP	C4A-C4	-2.49	1.46	1.51
2	D	602	PLP	C4A-C4	-2.40	1.46	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	PLP	O4P-C5A-C5	2.60	114.31	109.35

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PLP	C5A-O4P-P-O1P
2	A	601	PLP	C5A-O4P-P-O2P
2	B	601	PLP	C5A-O4P-P-O2P
2	B	601	PLP	C5A-O4P-P-O3P
2	D	602	PLP	C5A-O4P-P-O2P

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	PLP	1	0
2	D	602	PLP	3	0
2	A	601	PLP	2	0
2	C	601	PLP	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, 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	489/534 (91%)	-0.31	3 (0%) 89 88	32, 48, 77, 102	0
1	B	491/534 (91%)	-0.33	1 (0%) 95 94	30, 50, 71, 96	0
1	C	470/534 (88%)	-0.09	7 (1%) 73 72	40, 62, 95, 105	0
1	D	490/534 (91%)	-0.05	8 (1%) 72 70	39, 68, 91, 119	0
All	All	1940/2136 (90%)	-0.20	19 (0%) 82 80	30, 57, 89, 119	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	520	LEU	6.3
1	D	50	CYS	4.9
1	D	319	SER	3.9
1	C	234	LEU	3.3
1	B	524	PHE	3.2

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(\AA^2)	Q<0.9
2	PLP	C	601	15/16	0.91	0.19	69,71,73,73	0
3	FMT	D	601	3/3	0.93	0.15	47,47,47,48	0
3	FMT	A	602	3/3	0.96	0.13	53,53,53,53	0
2	PLP	D	602	15/16	0.97	0.13	57,60,60,61	0
2	PLP	B	601	15/16	0.97	0.13	45,48,49,49	0
2	PLP	A	601	15/16	0.97	0.12	44,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.