



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 06:59 PM GMT

PDB ID : 3WWI
Title : Crystal structure of the G136F mutant of the first R-stereoselective -
transaminase identified from *Arthrobacter* sp. KNK168 (FERM-BP-5228)
Authors : Guan, L.J.; Ohtsuka, J.; Miyakawa, T.; Zhi, Y.; Ito, N.; Yasohara, Y.;
Tanokura, M.
Deposited on : 2014-06-18
Resolution : 2.27 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

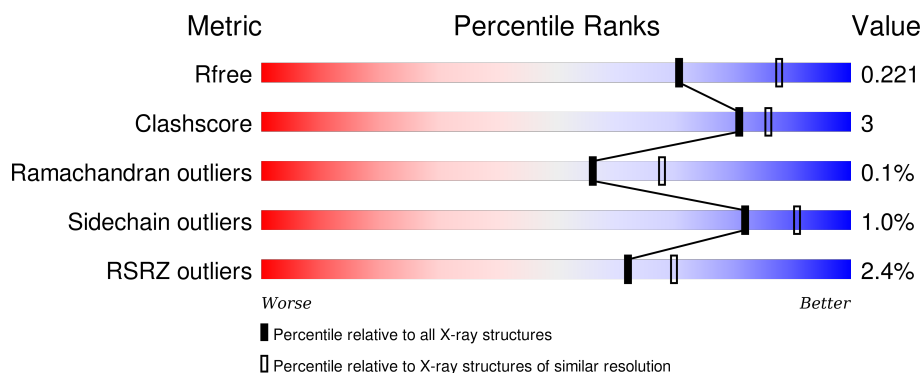
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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}	91344	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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. 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	330	<div> <div>5%</div> <div>93%</div> <div>• •</div> </div>
1	B	330	<div> <div>5%</div> <div>92%</div> <div>5% •</div> </div>
1	C	330	<div> <div>5%</div> <div>90%</div> <div>7% • •</div> </div>
1	D	330	<div> <div>5%</div> <div>92%</div> <div>6% •</div> </div>
1	E	330	<div> <div>5%</div> <div>91%</div> <div>6% • •</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	330	<div><div></div><div>89%</div><div>7% ..</div></div>
1	G	330	<div><div>2%</div><div></div><div>91%</div><div>7% .</div></div>
1	H	330	<div><div>2%</div><div></div><div>92%</div><div>5% .</div></div>
1	I	330	<div><div>%</div><div></div><div>93%</div><div>. .</div></div>
1	J	330	<div><div>4%</div><div></div><div>90%</div><div>7% ..</div></div>
1	K	330	<div><div>3%</div><div></div><div>90%</div><div>8% .</div></div>
1	L	330	<div><div>9%</div><div></div><div>85%</div><div>12% ..</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32328 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 (R)-amine transaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2525	1609	428	484	4			
1	B	322	Total	C	N	O	S	0	0	0
			2525	1609	428	484	4			
1	C	322	Total	C	N	O	S	0	0	0
			2525	1609	428	484	4			
1	D	322	Total	C	N	O	S	0	0	0
			2525	1609	428	484	4			
1	E	322	Total	C	N	O	S	0	0	0
			2525	1609	428	484	4			
1	F	322	Total	C	N	O	S	0	0	0
			2521	1606	427	484	4			
1	G	322	Total	C	N	O	S	0	0	0
			2525	1609	428	484	4			
1	H	322	Total	C	N	O	S	0	0	0
			2521	1606	427	484	4			
1	I	322	Total	C	N	O	S	0	0	0
			2525	1609	428	484	4			
1	J	322	Total	C	N	O	S	0	0	0
			2525	1609	428	484	4			
1	K	322	Total	C	N	O	S	0	0	0
			2525	1609	428	484	4			
1	L	322	Total	C	N	O	S	0	0	0
			2525	1609	428	484	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
B	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
C	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
D	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
E	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
G	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
H	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
I	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
J	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
K	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
L	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	I	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	J	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	K	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	L	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

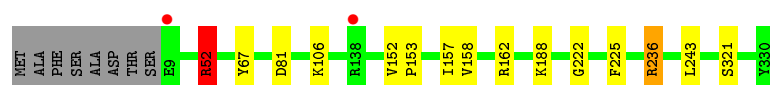
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	182	Total	O	0	0
			182	182		
3	B	187	Total	O	0	0
			187	187		
3	C	185	Total	O	0	0
			185	185		
3	D	211	Total	O	0	0
			211	211		
3	E	101	Total	O	0	0
			101	101		
3	F	197	Total	O	0	0
			197	197		
3	G	139	Total	O	0	0
			139	139		
3	H	229	Total	O	0	0
			229	229		
3	I	176	Total	O	0	0
			176	176		
3	J	82	Total	O	0	0
			82	82		
3	K	115	Total	O	0	0
			115	115		
3	L	52	Total	O	0	0
			52	52		

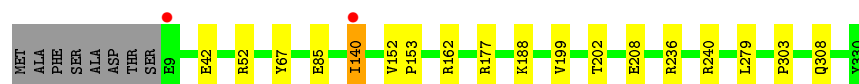
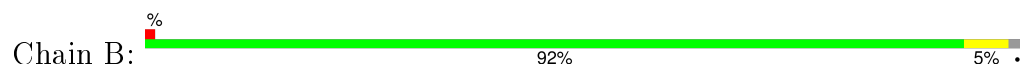
3 Residue-property plots [i](#)

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

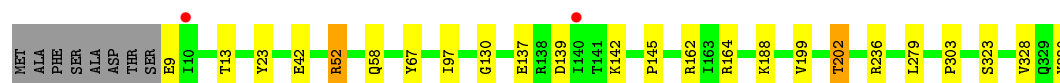
- Molecule 1: (R)-amine transaminase



- Molecule 1: (R)-amine transaminase



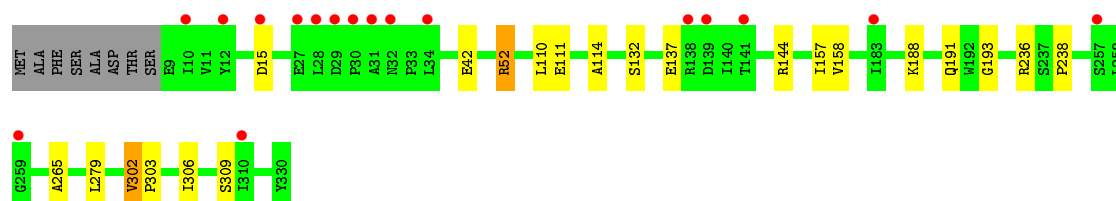
- Molecule 1: (R)-amine transaminase



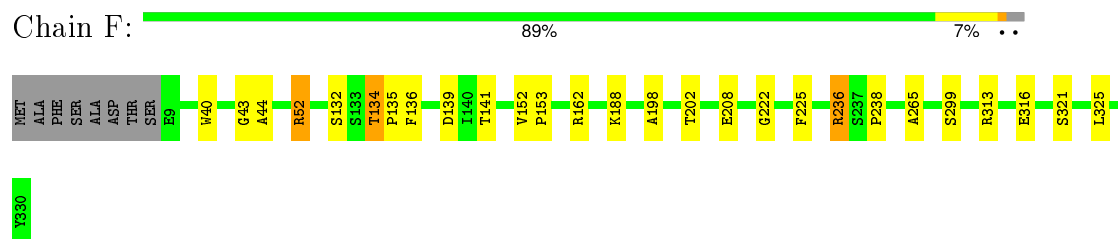
- Molecule 1: (R)-amine transaminase



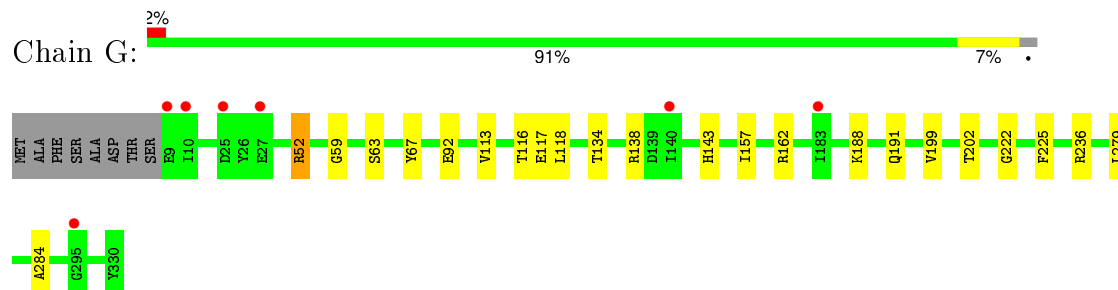
- Molecule 1: (R)-amine transaminase



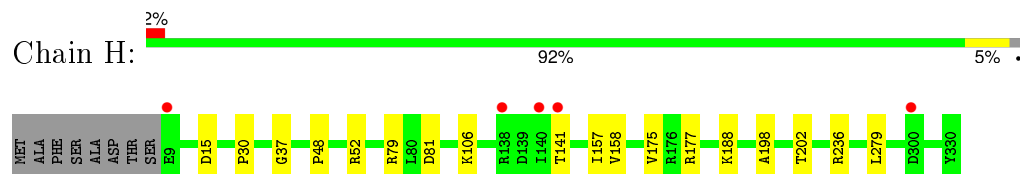
• Molecule 1: (R)-amine transaminase



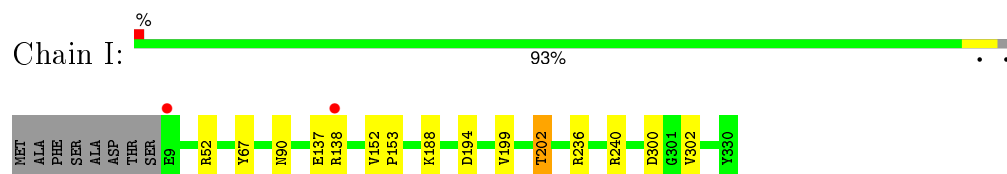
• Molecule 1: (R)-amine transaminase



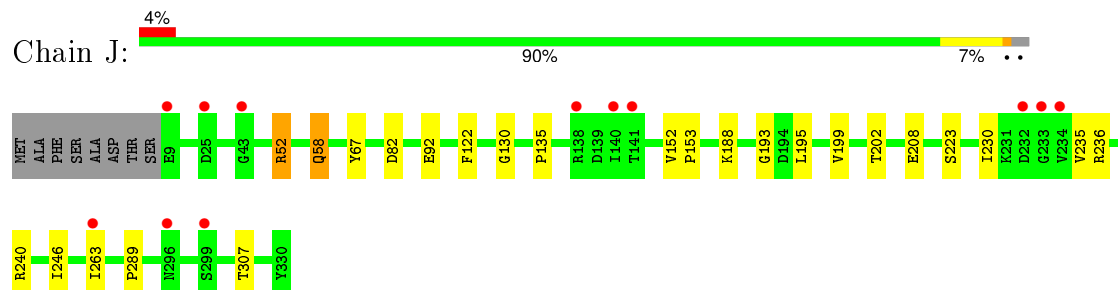
• Molecule 1: (R)-amine transaminase



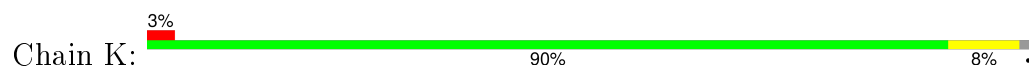
• Molecule 1: (R)-amine transaminase

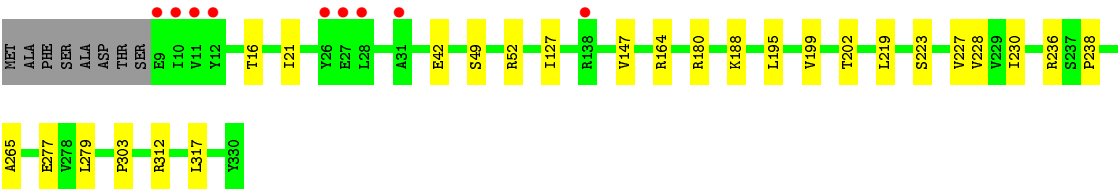


• Molecule 1: (R)-amine transaminase

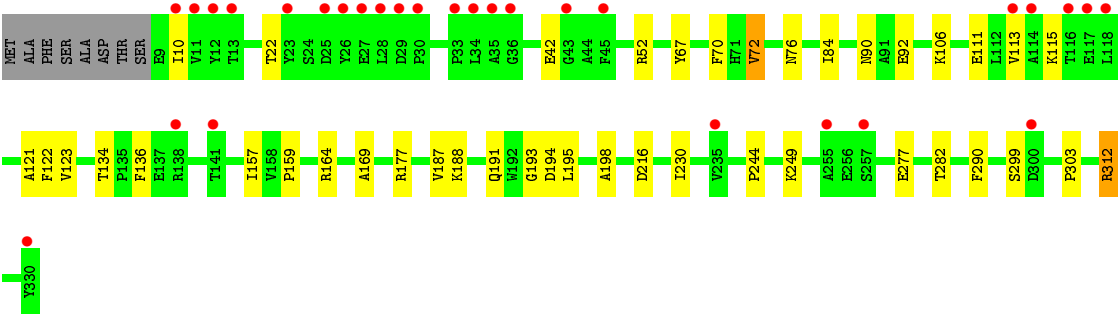
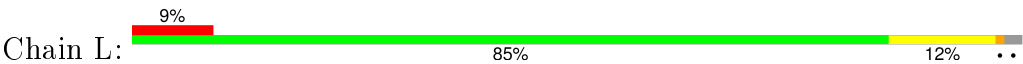


• Molecule 1: (R)-amine transaminase





• Molecule 1: (R)-amine transaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.96Å 134.28Å 196.04Å 90.00° 100.34° 90.00°	Depositor
Resolution (Å)	40.00 – 2.27 39.13 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.00-2.27) 98.8 (39.13-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.171 , 0.218 0.178 , 0.221	Depositor DCC
R_{free} test set	9592 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.5	EDS
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 190851 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32328	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.47 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.2659e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.69	0/2588	0.82	5/3534 (0.1%)
1	B	0.69	0/2588	0.78	5/3534 (0.1%)
1	C	0.66	0/2588	0.81	4/3534 (0.1%)
1	D	0.68	0/2588	0.81	2/3534 (0.1%)
1	E	0.57	0/2588	0.71	2/3534 (0.1%)
1	F	0.65	0/2584	0.77	3/3530 (0.1%)
1	G	0.58	0/2588	0.73	2/3534 (0.1%)
1	H	0.73	0/2584	0.84	6/3530 (0.2%)
1	I	0.67	0/2588	0.80	6/3534 (0.2%)
1	J	0.57	0/2588	0.73	1/3534 (0.0%)
1	K	0.58	0/2588	0.72	1/3534 (0.0%)
1	L	0.52	0/2588	0.67	0/3534
All	All	0.64	0/31048	0.77	37/42400 (0.1%)

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	D	236	ARG	NE-CZ-NH1	9.27	124.93	120.30
1	B	52	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	I	52	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	C	236	ARG	NE-CZ-NH1	8.34	124.47	120.30

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	2525	0	2464	14	0
1	B	2525	0	2464	15	0
1	C	2525	0	2464	21	0
1	D	2525	0	2464	16	0
1	E	2525	0	2464	16	0
1	F	2521	0	2453	18	0
1	G	2525	0	2464	18	0
1	H	2521	0	2453	10	0
1	I	2525	0	2464	11	0
1	J	2525	0	2464	20	0
1	K	2525	0	2464	24	0
1	L	2525	0	2464	28	0
2	A	15	0	6	5	0
2	B	15	0	7	5	0
2	C	15	0	6	3	0
2	D	15	0	6	4	0
2	E	15	0	6	3	0
2	F	15	0	7	3	0
2	G	15	0	6	3	0
2	H	15	0	6	4	0
2	I	15	0	6	3	0
2	J	15	0	6	4	0
2	K	15	0	6	4	0
2	L	15	0	6	3	0
3	A	182	0	0	2	0
3	B	187	0	0	1	0
3	C	185	0	0	4	0
3	D	211	0	0	1	0
3	E	101	0	0	0	0
3	F	197	0	0	2	0
3	G	139	0	0	3	0
3	H	229	0	0	1	0
3	I	176	0	0	1	0
3	J	82	0	0	0	0
3	K	115	0	0	3	0
3	L	52	0	0	1	0
All	All	32328	0	29620	196	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 196 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:F:188:LYS:NZ	2:F:401:PLP:C4A	1.94	1.29
1:B:188:LYS:HZ1	2:B:401:PLP:C4A	1.47	1.27
1:D:188:LYS:NZ	2:D:401:PLP:C4A	1.98	1.25
1:H:188:LYS:NZ	2:H:401:PLP:C4A	2.01	1.22
1:B:188:LYS:NZ	2:B:401:PLP:C4A	2.01	1.20

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	320/330 (97%)	308 (96%)	12 (4%)	0	100	100
1	B	320/330 (97%)	310 (97%)	10 (3%)	0	100	100
1	C	320/330 (97%)	311 (97%)	9 (3%)	0	100	100
1	D	320/330 (97%)	311 (97%)	9 (3%)	0	100	100
1	E	320/330 (97%)	314 (98%)	6 (2%)	0	100	100
1	F	320/330 (97%)	316 (99%)	3 (1%)	1 (0%)	46	55
1	G	320/330 (97%)	309 (97%)	11 (3%)	0	100	100
1	H	320/330 (97%)	309 (97%)	11 (3%)	0	100	100
1	I	320/330 (97%)	307 (96%)	13 (4%)	0	100	100
1	J	320/330 (97%)	307 (96%)	13 (4%)	0	100	100
1	K	320/330 (97%)	311 (97%)	9 (3%)	0	100	100
1	L	320/330 (97%)	308 (96%)	10 (3%)	2 (1%)	30	34
All	All	3840/3960 (97%)	3721 (97%)	116 (3%)	3 (0%)	56	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	299	SER
1	F	299	SER
1	L	244	PRO

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	273/279 (98%)	272 (100%)	1 (0%)	93	97
1	B	273/279 (98%)	272 (100%)	1 (0%)	93	97
1	C	273/279 (98%)	272 (100%)	1 (0%)	93	97
1	D	273/279 (98%)	270 (99%)	3 (1%)	80	89
1	E	273/279 (98%)	269 (98%)	4 (2%)	72	84
1	F	272/279 (98%)	269 (99%)	3 (1%)	80	89
1	G	273/279 (98%)	271 (99%)	2 (1%)	88	94
1	H	272/279 (98%)	269 (99%)	3 (1%)	80	89
1	I	273/279 (98%)	271 (99%)	2 (1%)	88	94
1	J	273/279 (98%)	270 (99%)	3 (1%)	80	89
1	K	273/279 (98%)	271 (99%)	2 (1%)	88	94
1	L	273/279 (98%)	266 (97%)	7 (3%)	54	69
All	All	3274/3348 (98%)	3242 (99%)	32 (1%)	82	91

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	162	ARG
1	H	175	VAL
1	L	122	PHE
1	H	141	THR
1	I	137	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	74	ASN
1	I	90	ASN
1	L	58	GLN
1	G	191	GLN
1	L	74	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 ⓘ

12 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	401	-	15,15,16	2.47	4 (26%)	21,22,23	1.55	4 (19%)
2	PLP	B	401	-	15,15,16	2.98	3 (20%)	21,22,23	1.44	4 (19%)
2	PLP	C	401	-	15,15,16	2.50	4 (26%)	21,22,23	1.43	3 (14%)
2	PLP	D	401	-	15,15,16	3.08	3 (20%)	21,22,23	1.67	5 (23%)
2	PLP	E	401	-	15,15,16	3.33	4 (26%)	21,22,23	1.78	6 (28%)
2	PLP	F	401	-	15,15,16	2.76	4 (26%)	21,22,23	1.55	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	G	401	-	15,15,16	2.97	3 (20%)	21,22,23	1.09	0
2	PLP	H	401	-	15,15,16	1.97	4 (26%)	21,22,23	1.57	5 (23%)
2	PLP	I	401	-	15,15,16	2.61	3 (20%)	21,22,23	1.49	4 (19%)
2	PLP	J	401	-	15,15,16	3.06	3 (20%)	21,22,23	1.83	6 (28%)
2	PLP	K	401	-	15,15,16	3.17	4 (26%)	21,22,23	1.47	3 (14%)
2	PLP	L	401	-	15,15,16	2.85	3 (20%)	21,22,23	1.50	4 (19%)

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	401	-	-	0/6/6/8	0/1/1/1
2	PLP	B	401	-	-	0/6/6/8	0/1/1/1
2	PLP	C	401	-	-	0/6/6/8	0/1/1/1
2	PLP	D	401	-	-	0/6/6/8	0/1/1/1
2	PLP	E	401	-	-	0/6/6/8	0/1/1/1
2	PLP	F	401	-	-	0/6/6/8	0/1/1/1
2	PLP	G	401	-	-	0/6/6/8	0/1/1/1
2	PLP	H	401	-	-	0/6/6/8	0/1/1/1
2	PLP	I	401	-	-	0/6/6/8	0/1/1/1
2	PLP	J	401	-	-	0/6/6/8	0/1/1/1
2	PLP	K	401	-	-	0/6/6/8	0/1/1/1
2	PLP	L	401	-	-	0/6/6/8	0/1/1/1

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	401	PLP	C4A-C4	-2.41	1.46	1.51
2	H	401	PLP	C4A-C4	-2.34	1.46	1.51
2	F	401	PLP	C4A-C4	-2.28	1.47	1.51
2	C	401	PLP	C4A-C4	-2.16	1.47	1.51
2	E	401	PLP	C4A-C4	-2.11	1.47	1.51

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	401	PLP	C2A-C2-C3	-3.58	117.28	120.90
2	J	401	PLP	O4P-P-O1P	-3.53	98.22	107.08
2	A	401	PLP	C2A-C2-C3	-3.32	117.54	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	PLP	O2P-P-O4P	-2.96	98.08	106.72
2	K	401	PLP	O2P-P-O4P	-2.77	98.63	106.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	5	0
2	B	401	PLP	5	0
2	C	401	PLP	3	0
2	D	401	PLP	4	0
2	E	401	PLP	3	0
2	F	401	PLP	3	0
2	G	401	PLP	3	0
2	H	401	PLP	4	0
2	I	401	PLP	3	0
2	J	401	PLP	4	0
2	K	401	PLP	4	0
2	L	401	PLP	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, 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	322/330 (97%)	-0.36	2 (0%) 90 93	24, 34, 52, 105	0
1	B	322/330 (97%)	-0.34	2 (0%) 90 93	26, 34, 57, 94	0
1	C	322/330 (97%)	-0.34	2 (0%) 90 93	26, 36, 57, 90	0
1	D	322/330 (97%)	-0.37	4 (1%) 81 85	25, 34, 55, 88	0
1	E	322/330 (97%)	0.14	17 (5%) 30 38	35, 53, 78, 115	0
1	F	322/330 (97%)	-0.37	0 100 100	26, 35, 55, 95	0
1	G	322/330 (97%)	-0.21	7 (2%) 65 72	31, 44, 69, 103	0
1	H	322/330 (97%)	-0.44	5 (1%) 74 80	24, 31, 48, 105	0
1	I	322/330 (97%)	-0.32	2 (0%) 90 93	23, 38, 58, 93	0
1	J	322/330 (97%)	0.18	12 (3%) 45 53	33, 52, 75, 96	0
1	K	322/330 (97%)	-0.06	9 (2%) 56 65	29, 48, 74, 105	0
1	L	322/330 (97%)	0.52	29 (9%) 12 16	40, 68, 91, 114	0
All	All	3864/3960 (97%)	-0.16	91 (2%) 62 70	23, 40, 75, 115	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	35	ALA	6.1
1	L	138	ARG	5.5
1	L	11	VAL	5.2
1	L	10	ILE	4.8
1	L	26	TYR	4.6

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 [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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PLP	I	401	15/16	0.97	0.18	1.24	25,37,46,48	0
2	PLP	C	401	15/16	0.98	0.18	0.98	26,32,37,43	0
2	PLP	G	401	15/16	0.98	0.16	0.84	28,39,47,48	0
2	PLP	J	401	15/16	0.97	0.17	0.83	37,52,56,60	0
2	PLP	F	401	15/16	0.99	0.15	0.74	22,28,34,36	0
2	PLP	H	401	15/16	0.98	0.14	0.63	20,28,34,36	0
2	PLP	K	401	15/16	0.98	0.15	0.53	33,40,47,48	0
2	PLP	L	401	15/16	0.95	0.14	0.30	49,62,66,71	0
2	PLP	A	401	15/16	0.98	0.14	0.25	26,29,30,30	0
2	PLP	D	401	15/16	0.99	0.16	0.24	22,28,37,42	0
2	PLP	B	401	15/16	0.99	0.14	0.08	25,29,36,37	0
2	PLP	E	401	15/16	0.98	0.13	0.03	35,44,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.