



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 08:28 PM GMT

PDB ID : 3WWJ  
Title : Crystal structure of an engineered sitagliptin-producing transaminase, ATA-117-Rd11  
Authors : Guan, L.J.; Ohtsuka, J.; Okai, M.; Miyakawa, T.; Mase, T.; Zhi, Y.; Hou, F.; Ito, N.; Yasohara, Y.; Tanokura, M.  
Deposited on : 2014-06-18  
Resolution : 2.20 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](mailto: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.

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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

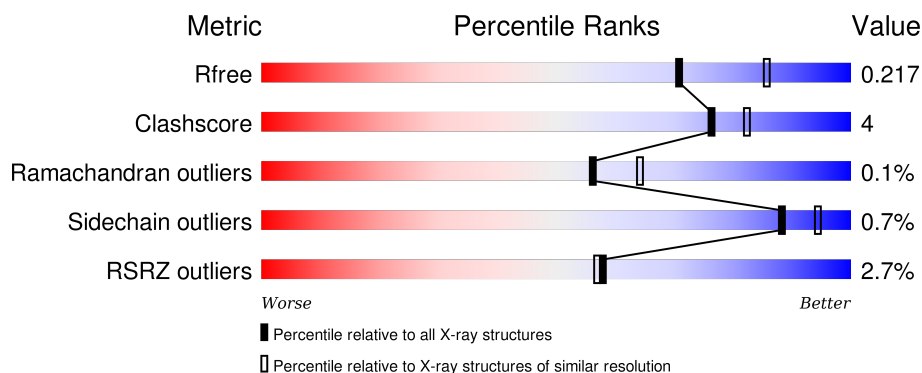
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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  $\geq 3$ , 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>%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	330	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>.</div> </div> </div>
1	C	330	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>.</div> </div> </div>
1	D	330	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>.</div> </div> </div>
1	E	330	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	330	<div><div></div><div>3%</div><div>89%</div><div>8%</div><div></div><div></div></div>
1	G	330	<div><div></div><div>2%</div><div>87%</div><div>10%</div><div></div><div></div></div>
1	H	330	<div><div></div><div>2%</div><div>88%</div><div>9%</div><div></div><div></div></div>
1	I	330	<div><div></div><div>3%</div><div>88%</div><div>8%</div><div></div><div></div></div>
1	J	330	<div><div></div><div>2%</div><div>87%</div><div>9%</div><div></div><div></div></div>
1	K	330	<div><div></div><div>4%</div><div>91%</div><div>6%</div><div></div><div></div></div>
1	L	330	<div><div></div><div>9%</div><div>85%</div><div>11%</div><div></div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32226 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	320	Total	C	N	O	S	0	2	0
			2521	1603	426	485	7			
1	B	323	Total	C	N	O	S	0	1	0
			2536	1614	428	487	7			
1	C	321	Total	C	N	O	S	0	1	0
			2523	1605	427	484	7			
1	D	322	Total	C	N	O	S	0	2	0
			2536	1613	431	485	7			
1	E	321	Total	C	N	O	S	0	0	0
			2514	1599	426	483	6			
1	F	322	Total	C	N	O	S	0	1	0
			2529	1609	427	486	7			
1	G	321	Total	C	N	O	S	0	2	0
			2531	1610	430	484	7			
1	H	321	Total	C	N	O	S	0	1	0
			2520	1604	426	483	7			
1	I	320	Total	C	N	O	S	0	1	0
			2512	1598	425	482	7			
1	J	319	Total	C	N	O	S	0	1	0
			2508	1594	425	483	6			
1	K	320	Total	C	N	O	S	0	1	0
			2512	1598	425	482	7			
1	L	318	Total	C	N	O	S	0	0	0
			2490	1582	423	479	6			

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	PRO	SER	ENGINEERED MUTATION	UNP F7J696
A	60	PHE	TYR	ENGINEERED MUTATION	UNP F7J696
A	61	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
A	62	THR	HIS	ENGINEERED MUTATION	UNP F7J696
A	65	ALA	VAL	ENGINEERED MUTATION	UNP F7J696

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Chain	Residue	Modelled	Actual	Comment	Reference
A	69	THR	VAL	ENGINEERED MUTATION	UNP F7J696
A	81	GLY	ASP	ENGINEERED MUTATION	UNP F7J696
A	94	ILE	MET	ENGINEERED MUTATION	UNP F7J696
A	96	LEU	ILE	ENGINEERED MUTATION	UNP F7J696
A	122	MET	PHE	ENGINEERED MUTATION	UNP F7J696
A	124	THR	SER	ENGINEERED MUTATION	UNP F7J696
A	126	THR	SER	ENGINEERED MUTATION	UNP F7J696
A	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
A	150	SER	TYR	ENGINEERED MUTATION	UNP F7J696
A	152	CSO	VAL	ENGINEERED MUTATION	UNP F7J696
A	169	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
A	199	ILE	VAL	ENGINEERED MUTATION	UNP F7J696
A	209	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
A	215	CYS	GLY	ENGINEERED MUTATION	UNP F7J696
A	217	ASN	GLY	ENGINEERED MUTATION	UNP F7J696
A	223	PRO	SER	ENGINEERED MUTATION	UNP F7J696
A	269	PRO	LEU	ENGINEERED MUTATION	UNP F7J696
A	273	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
A	282	SER	THR	ENGINEERED MUTATION	UNP F7J696
A	284	GLY	ALA	ENGINEERED MUTATION	UNP F7J696
A	297	SER	PRO	ENGINEERED MUTATION	UNP F7J696
A	306	VAL	ILE	ENGINEERED MUTATION	UNP F7J696
A	321	PRO	SER	ENGINEERED MUTATION	UNP F7J696
B	8	PRO	SER	ENGINEERED MUTATION	UNP F7J696
B	60	PHE	TYR	ENGINEERED MUTATION	UNP F7J696
B	61	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
B	62	THR	HIS	ENGINEERED MUTATION	UNP F7J696
B	65	ALA	VAL	ENGINEERED MUTATION	UNP F7J696
B	69	THR	VAL	ENGINEERED MUTATION	UNP F7J696
B	81	GLY	ASP	ENGINEERED MUTATION	UNP F7J696
B	94	ILE	MET	ENGINEERED MUTATION	UNP F7J696
B	96	LEU	ILE	ENGINEERED MUTATION	UNP F7J696
B	122	MET	PHE	ENGINEERED MUTATION	UNP F7J696
B	124	THR	SER	ENGINEERED MUTATION	UNP F7J696
B	126	THR	SER	ENGINEERED MUTATION	UNP F7J696
B	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
B	150	SER	TYR	ENGINEERED MUTATION	UNP F7J696
B	152	CSO	VAL	ENGINEERED MUTATION	UNP F7J696
B	169	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
B	199	ILE	VAL	ENGINEERED MUTATION	UNP F7J696
B	209	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
B	215	CYS	GLY	ENGINEERED MUTATION	UNP F7J696

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Chain	Residue	Modelled	Actual	Comment	Reference
B	217	ASN	GLY	ENGINEERED MUTATION	UNP F7J696
B	223	PRO	SER	ENGINEERED MUTATION	UNP F7J696
B	269	PRO	LEU	ENGINEERED MUTATION	UNP F7J696
B	273	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
B	282	SER	THR	ENGINEERED MUTATION	UNP F7J696
B	284	GLY	ALA	ENGINEERED MUTATION	UNP F7J696
B	297	SER	PRO	ENGINEERED MUTATION	UNP F7J696
B	306	VAL	ILE	ENGINEERED MUTATION	UNP F7J696
B	321	PRO	SER	ENGINEERED MUTATION	UNP F7J696
C	8	PRO	SER	ENGINEERED MUTATION	UNP F7J696
C	60	PHE	TYR	ENGINEERED MUTATION	UNP F7J696
C	61	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
C	62	THR	HIS	ENGINEERED MUTATION	UNP F7J696
C	65	ALA	VAL	ENGINEERED MUTATION	UNP F7J696
C	69	THR	VAL	ENGINEERED MUTATION	UNP F7J696
C	81	GLY	ASP	ENGINEERED MUTATION	UNP F7J696
C	94	ILE	MET	ENGINEERED MUTATION	UNP F7J696
C	96	LEU	ILE	ENGINEERED MUTATION	UNP F7J696
C	122	MET	PHE	ENGINEERED MUTATION	UNP F7J696
C	124	THR	SER	ENGINEERED MUTATION	UNP F7J696
C	126	THR	SER	ENGINEERED MUTATION	UNP F7J696
C	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
C	150	SER	TYR	ENGINEERED MUTATION	UNP F7J696
C	152	CSO	VAL	ENGINEERED MUTATION	UNP F7J696
C	169	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
C	199	ILE	VAL	ENGINEERED MUTATION	UNP F7J696
C	209	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
C	215	CYS	GLY	ENGINEERED MUTATION	UNP F7J696
C	217	ASN	GLY	ENGINEERED MUTATION	UNP F7J696
C	223	PRO	SER	ENGINEERED MUTATION	UNP F7J696
C	269	PRO	LEU	ENGINEERED MUTATION	UNP F7J696
C	273	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
C	282	SER	THR	ENGINEERED MUTATION	UNP F7J696
C	284	GLY	ALA	ENGINEERED MUTATION	UNP F7J696
C	297	SER	PRO	ENGINEERED MUTATION	UNP F7J696
C	306	VAL	ILE	ENGINEERED MUTATION	UNP F7J696
C	321	PRO	SER	ENGINEERED MUTATION	UNP F7J696
D	8	PRO	SER	ENGINEERED MUTATION	UNP F7J696
D	60	PHE	TYR	ENGINEERED MUTATION	UNP F7J696
D	61	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
D	62	THR	HIS	ENGINEERED MUTATION	UNP F7J696
D	65	ALA	VAL	ENGINEERED MUTATION	UNP F7J696

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Chain	Residue	Modelled	Actual	Comment	Reference
D	69	THR	VAL	ENGINEERED MUTATION	UNP F7J696
D	81	GLY	ASP	ENGINEERED MUTATION	UNP F7J696
D	94	ILE	MET	ENGINEERED MUTATION	UNP F7J696
D	96	LEU	ILE	ENGINEERED MUTATION	UNP F7J696
D	122	MET	PHE	ENGINEERED MUTATION	UNP F7J696
D	124	THR	SER	ENGINEERED MUTATION	UNP F7J696
D	126	THR	SER	ENGINEERED MUTATION	UNP F7J696
D	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
D	150	SER	TYR	ENGINEERED MUTATION	UNP F7J696
D	152	CSO	VAL	ENGINEERED MUTATION	UNP F7J696
D	169	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
D	199	ILE	VAL	ENGINEERED MUTATION	UNP F7J696
D	209	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
D	215	CYS	GLY	ENGINEERED MUTATION	UNP F7J696
D	217	ASN	GLY	ENGINEERED MUTATION	UNP F7J696
D	223	PRO	SER	ENGINEERED MUTATION	UNP F7J696
D	269	PRO	LEU	ENGINEERED MUTATION	UNP F7J696
D	273	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
D	282	SER	THR	ENGINEERED MUTATION	UNP F7J696
D	284	GLY	ALA	ENGINEERED MUTATION	UNP F7J696
D	297	SER	PRO	ENGINEERED MUTATION	UNP F7J696
D	306	VAL	ILE	ENGINEERED MUTATION	UNP F7J696
D	321	PRO	SER	ENGINEERED MUTATION	UNP F7J696
E	8	PRO	SER	ENGINEERED MUTATION	UNP F7J696
E	60	PHE	TYR	ENGINEERED MUTATION	UNP F7J696
E	61	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
E	62	THR	HIS	ENGINEERED MUTATION	UNP F7J696
E	65	ALA	VAL	ENGINEERED MUTATION	UNP F7J696
E	69	THR	VAL	ENGINEERED MUTATION	UNP F7J696
E	81	GLY	ASP	ENGINEERED MUTATION	UNP F7J696
E	94	ILE	MET	ENGINEERED MUTATION	UNP F7J696
E	96	LEU	ILE	ENGINEERED MUTATION	UNP F7J696
E	122	MET	PHE	ENGINEERED MUTATION	UNP F7J696
E	124	THR	SER	ENGINEERED MUTATION	UNP F7J696
E	126	THR	SER	ENGINEERED MUTATION	UNP F7J696
E	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
E	150	SER	TYR	ENGINEERED MUTATION	UNP F7J696
E	152	CSO	VAL	ENGINEERED MUTATION	UNP F7J696
E	169	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
E	199	ILE	VAL	ENGINEERED MUTATION	UNP F7J696
E	209	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
E	215	CYS	GLY	ENGINEERED MUTATION	UNP F7J696

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Chain	Residue	Modelled	Actual	Comment	Reference
E	217	ASN	GLY	ENGINEERED MUTATION	UNP F7J696
E	223	PRO	SER	ENGINEERED MUTATION	UNP F7J696
E	269	PRO	LEU	ENGINEERED MUTATION	UNP F7J696
E	273	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
E	282	SER	THR	ENGINEERED MUTATION	UNP F7J696
E	284	GLY	ALA	ENGINEERED MUTATION	UNP F7J696
E	297	SER	PRO	ENGINEERED MUTATION	UNP F7J696
E	306	VAL	ILE	ENGINEERED MUTATION	UNP F7J696
E	321	PRO	SER	ENGINEERED MUTATION	UNP F7J696
F	8	PRO	SER	ENGINEERED MUTATION	UNP F7J696
F	60	PHE	TYR	ENGINEERED MUTATION	UNP F7J696
F	61	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
F	62	THR	HIS	ENGINEERED MUTATION	UNP F7J696
F	65	ALA	VAL	ENGINEERED MUTATION	UNP F7J696
F	69	THR	VAL	ENGINEERED MUTATION	UNP F7J696
F	81	GLY	ASP	ENGINEERED MUTATION	UNP F7J696
F	94	ILE	MET	ENGINEERED MUTATION	UNP F7J696
F	96	LEU	ILE	ENGINEERED MUTATION	UNP F7J696
F	122	MET	PHE	ENGINEERED MUTATION	UNP F7J696
F	124	THR	SER	ENGINEERED MUTATION	UNP F7J696
F	126	THR	SER	ENGINEERED MUTATION	UNP F7J696
F	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
F	150	SER	TYR	ENGINEERED MUTATION	UNP F7J696
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F	273	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
F	282	SER	THR	ENGINEERED MUTATION	UNP F7J696
F	284	GLY	ALA	ENGINEERED MUTATION	UNP F7J696
F	297	SER	PRO	ENGINEERED MUTATION	UNP F7J696
F	306	VAL	ILE	ENGINEERED MUTATION	UNP F7J696
F	321	PRO	SER	ENGINEERED MUTATION	UNP F7J696
G	8	PRO	SER	ENGINEERED MUTATION	UNP F7J696
G	60	PHE	TYR	ENGINEERED MUTATION	UNP F7J696
G	61	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
G	62	THR	HIS	ENGINEERED MUTATION	UNP F7J696
G	65	ALA	VAL	ENGINEERED MUTATION	UNP F7J696

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Chain	Residue	Modelled	Actual	Comment	Reference
G	69	THR	VAL	ENGINEERED MUTATION	UNP F7J696
G	81	GLY	ASP	ENGINEERED MUTATION	UNP F7J696
G	94	ILE	MET	ENGINEERED MUTATION	UNP F7J696
G	96	LEU	ILE	ENGINEERED MUTATION	UNP F7J696
G	122	MET	PHE	ENGINEERED MUTATION	UNP F7J696
G	124	THR	SER	ENGINEERED MUTATION	UNP F7J696
G	126	THR	SER	ENGINEERED MUTATION	UNP F7J696
G	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
G	150	SER	TYR	ENGINEERED MUTATION	UNP F7J696
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G	297	SER	PRO	ENGINEERED MUTATION	UNP F7J696
G	306	VAL	ILE	ENGINEERED MUTATION	UNP F7J696
G	321	PRO	SER	ENGINEERED MUTATION	UNP F7J696
H	8	PRO	SER	ENGINEERED MUTATION	UNP F7J696
H	60	PHE	TYR	ENGINEERED MUTATION	UNP F7J696
H	61	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
H	62	THR	HIS	ENGINEERED MUTATION	UNP F7J696
H	65	ALA	VAL	ENGINEERED MUTATION	UNP F7J696
H	69	THR	VAL	ENGINEERED MUTATION	UNP F7J696
H	81	GLY	ASP	ENGINEERED MUTATION	UNP F7J696
H	94	ILE	MET	ENGINEERED MUTATION	UNP F7J696
H	96	LEU	ILE	ENGINEERED MUTATION	UNP F7J696
H	122	MET	PHE	ENGINEERED MUTATION	UNP F7J696
H	124	THR	SER	ENGINEERED MUTATION	UNP F7J696
H	126	THR	SER	ENGINEERED MUTATION	UNP F7J696
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H	150	SER	TYR	ENGINEERED MUTATION	UNP F7J696
H	152	CSO	VAL	ENGINEERED MUTATION	UNP F7J696
H	169	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
H	199	ILE	VAL	ENGINEERED MUTATION	UNP F7J696
H	209	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
H	215	CYS	GLY	ENGINEERED MUTATION	UNP F7J696

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Chain	Residue	Modelled	Actual	Comment	Reference
H	217	ASN	GLY	ENGINEERED MUTATION	UNP F7J696
H	223	PRO	SER	ENGINEERED MUTATION	UNP F7J696
H	269	PRO	LEU	ENGINEERED MUTATION	UNP F7J696
H	273	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
H	282	SER	THR	ENGINEERED MUTATION	UNP F7J696
H	284	GLY	ALA	ENGINEERED MUTATION	UNP F7J696
H	297	SER	PRO	ENGINEERED MUTATION	UNP F7J696
H	306	VAL	ILE	ENGINEERED MUTATION	UNP F7J696
H	321	PRO	SER	ENGINEERED MUTATION	UNP F7J696
I	8	PRO	SER	ENGINEERED MUTATION	UNP F7J696
I	60	PHE	TYR	ENGINEERED MUTATION	UNP F7J696
I	61	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
I	62	THR	HIS	ENGINEERED MUTATION	UNP F7J696
I	65	ALA	VAL	ENGINEERED MUTATION	UNP F7J696
I	69	THR	VAL	ENGINEERED MUTATION	UNP F7J696
I	81	GLY	ASP	ENGINEERED MUTATION	UNP F7J696
I	94	ILE	MET	ENGINEERED MUTATION	UNP F7J696
I	96	LEU	ILE	ENGINEERED MUTATION	UNP F7J696
I	122	MET	PHE	ENGINEERED MUTATION	UNP F7J696
I	124	THR	SER	ENGINEERED MUTATION	UNP F7J696
I	126	THR	SER	ENGINEERED MUTATION	UNP F7J696
I	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
I	150	SER	TYR	ENGINEERED MUTATION	UNP F7J696
I	152	CSO	VAL	ENGINEERED MUTATION	UNP F7J696
I	169	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
I	199	ILE	VAL	ENGINEERED MUTATION	UNP F7J696
I	209	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
I	215	CYS	GLY	ENGINEERED MUTATION	UNP F7J696
I	217	ASN	GLY	ENGINEERED MUTATION	UNP F7J696
I	223	PRO	SER	ENGINEERED MUTATION	UNP F7J696
I	269	PRO	LEU	ENGINEERED MUTATION	UNP F7J696
I	273	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
I	282	SER	THR	ENGINEERED MUTATION	UNP F7J696
I	284	GLY	ALA	ENGINEERED MUTATION	UNP F7J696
I	297	SER	PRO	ENGINEERED MUTATION	UNP F7J696
I	306	VAL	ILE	ENGINEERED MUTATION	UNP F7J696
I	321	PRO	SER	ENGINEERED MUTATION	UNP F7J696
J	8	PRO	SER	ENGINEERED MUTATION	UNP F7J696
J	60	PHE	TYR	ENGINEERED MUTATION	UNP F7J696
J	61	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
J	62	THR	HIS	ENGINEERED MUTATION	UNP F7J696
J	65	ALA	VAL	ENGINEERED MUTATION	UNP F7J696

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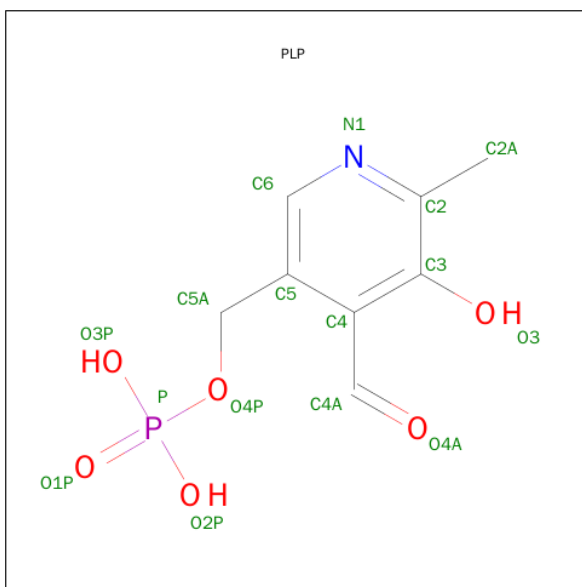
Chain	Residue	Modelled	Actual	Comment	Reference
J	69	THR	VAL	ENGINEERED MUTATION	UNP F7J696
J	81	GLY	ASP	ENGINEERED MUTATION	UNP F7J696
J	94	ILE	MET	ENGINEERED MUTATION	UNP F7J696
J	96	LEU	ILE	ENGINEERED MUTATION	UNP F7J696
J	122	MET	PHE	ENGINEERED MUTATION	UNP F7J696
J	124	THR	SER	ENGINEERED MUTATION	UNP F7J696
J	126	THR	SER	ENGINEERED MUTATION	UNP F7J696
J	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
J	150	SER	TYR	ENGINEERED MUTATION	UNP F7J696
J	152	CSO	VAL	ENGINEERED MUTATION	UNP F7J696
J	169	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
J	199	ILE	VAL	ENGINEERED MUTATION	UNP F7J696
J	209	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
J	215	CYS	GLY	ENGINEERED MUTATION	UNP F7J696
J	217	ASN	GLY	ENGINEERED MUTATION	UNP F7J696
J	223	PRO	SER	ENGINEERED MUTATION	UNP F7J696
J	269	PRO	LEU	ENGINEERED MUTATION	UNP F7J696
J	273	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
J	282	SER	THR	ENGINEERED MUTATION	UNP F7J696
J	284	GLY	ALA	ENGINEERED MUTATION	UNP F7J696
J	297	SER	PRO	ENGINEERED MUTATION	UNP F7J696
J	306	VAL	ILE	ENGINEERED MUTATION	UNP F7J696
J	321	PRO	SER	ENGINEERED MUTATION	UNP F7J696
K	8	PRO	SER	ENGINEERED MUTATION	UNP F7J696
K	60	PHE	TYR	ENGINEERED MUTATION	UNP F7J696
K	61	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
K	62	THR	HIS	ENGINEERED MUTATION	UNP F7J696
K	65	ALA	VAL	ENGINEERED MUTATION	UNP F7J696
K	69	THR	VAL	ENGINEERED MUTATION	UNP F7J696
K	81	GLY	ASP	ENGINEERED MUTATION	UNP F7J696
K	94	ILE	MET	ENGINEERED MUTATION	UNP F7J696
K	96	LEU	ILE	ENGINEERED MUTATION	UNP F7J696
K	122	MET	PHE	ENGINEERED MUTATION	UNP F7J696
K	124	THR	SER	ENGINEERED MUTATION	UNP F7J696
K	126	THR	SER	ENGINEERED MUTATION	UNP F7J696
K	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
K	150	SER	TYR	ENGINEERED MUTATION	UNP F7J696
K	152	CSO	VAL	ENGINEERED MUTATION	UNP F7J696
K	169	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
K	199	ILE	VAL	ENGINEERED MUTATION	UNP F7J696
K	209	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
K	215	CYS	GLY	ENGINEERED MUTATION	UNP F7J696

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Chain	Residue	Modelled	Actual	Comment	Reference
K	217	ASN	GLY	ENGINEERED MUTATION	UNP F7J696
K	223	PRO	SER	ENGINEERED MUTATION	UNP F7J696
K	269	PRO	LEU	ENGINEERED MUTATION	UNP F7J696
K	273	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
K	282	SER	THR	ENGINEERED MUTATION	UNP F7J696
K	284	GLY	ALA	ENGINEERED MUTATION	UNP F7J696
K	297	SER	PRO	ENGINEERED MUTATION	UNP F7J696
K	306	VAL	ILE	ENGINEERED MUTATION	UNP F7J696
K	321	PRO	SER	ENGINEERED MUTATION	UNP F7J696
L	8	PRO	SER	ENGINEERED MUTATION	UNP F7J696
L	60	PHE	TYR	ENGINEERED MUTATION	UNP F7J696
L	61	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
L	62	THR	HIS	ENGINEERED MUTATION	UNP F7J696
L	65	ALA	VAL	ENGINEERED MUTATION	UNP F7J696
L	69	THR	VAL	ENGINEERED MUTATION	UNP F7J696
L	81	GLY	ASP	ENGINEERED MUTATION	UNP F7J696
L	94	ILE	MET	ENGINEERED MUTATION	UNP F7J696
L	96	LEU	ILE	ENGINEERED MUTATION	UNP F7J696
L	122	MET	PHE	ENGINEERED MUTATION	UNP F7J696
L	124	THR	SER	ENGINEERED MUTATION	UNP F7J696
L	126	THR	SER	ENGINEERED MUTATION	UNP F7J696
L	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
L	150	SER	TYR	ENGINEERED MUTATION	UNP F7J696
L	152	CSO	VAL	ENGINEERED MUTATION	UNP F7J696
L	169	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
L	199	ILE	VAL	ENGINEERED MUTATION	UNP F7J696
L	209	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
L	215	CYS	GLY	ENGINEERED MUTATION	UNP F7J696
L	217	ASN	GLY	ENGINEERED MUTATION	UNP F7J696
L	223	PRO	SER	ENGINEERED MUTATION	UNP F7J696
L	269	PRO	LEU	ENGINEERED MUTATION	UNP F7J696
L	273	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
L	282	SER	THR	ENGINEERED MUTATION	UNP F7J696
L	284	GLY	ALA	ENGINEERED MUTATION	UNP F7J696
L	297	SER	PRO	ENGINEERED MUTATION	UNP F7J696
L	306	VAL	ILE	ENGINEERED MUTATION	UNP F7J696
L	321	PRO	SER	ENGINEERED MUTATION	UNP F7J696

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	E	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	F	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	G	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	H	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	I	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	J	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	K	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	L	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

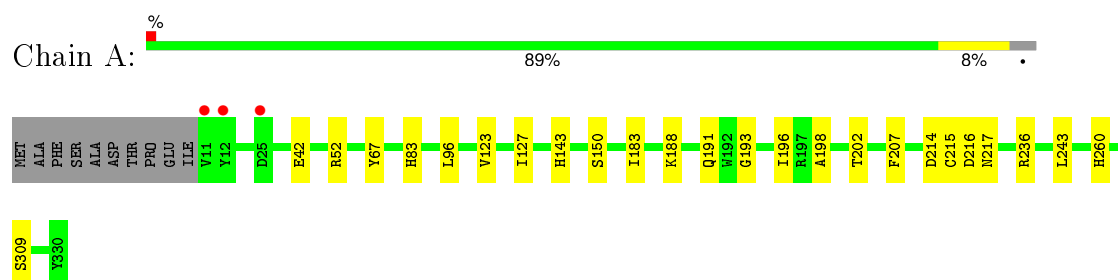
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total 174	O 174	0	0
3	B	182	Total 182	O 182	0	0
3	C	161	Total 161	O 161	0	0
3	D	179	Total 179	O 179	0	0
3	E	124	Total 124	O 124	0	0
3	F	144	Total 144	O 144	0	0
3	G	199	Total 199	O 199	0	0
3	H	183	Total 183	O 183	0	0
3	I	119	Total 119	O 119	0	0
3	J	137	Total 137	O 137	0	0
3	K	115	Total 115	O 115	0	0
3	L	85	Total 85	O 85	0	0

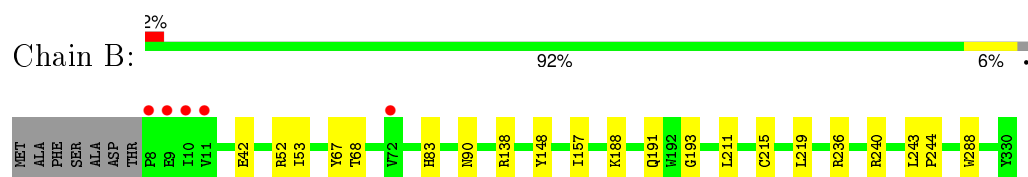
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

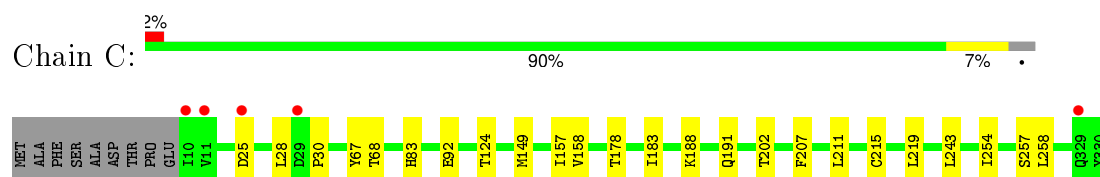
- Molecule 1: (R)-amine transaminase



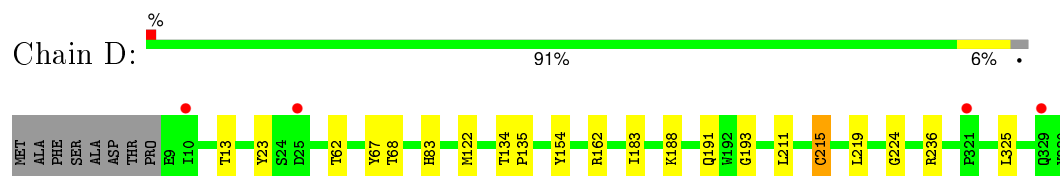
- Molecule 1: (R)-amine transaminase



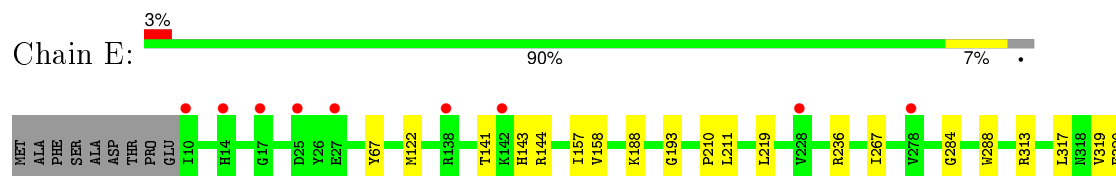
- Molecule 1: (R)-amine transaminase

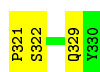


- Molecule 1: (R)-amine transaminase

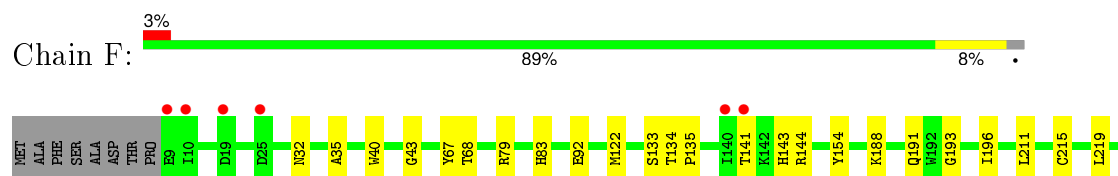


- Molecule 1: (R)-amine transaminase

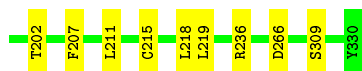
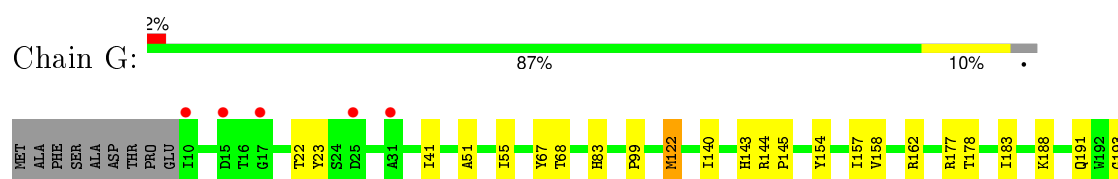




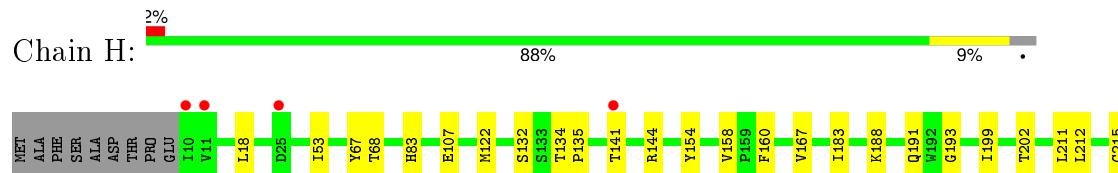
- Molecule 1: (R)-amine transaminase



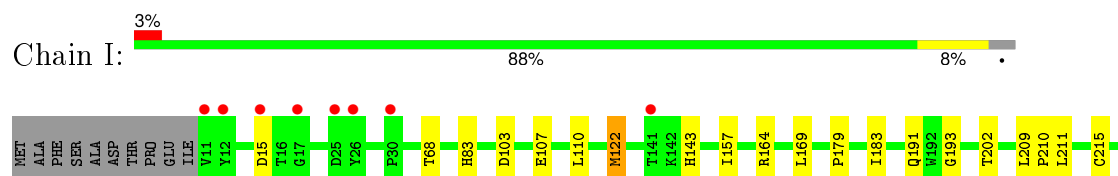
- Molecule 1: (R)-amine transaminase



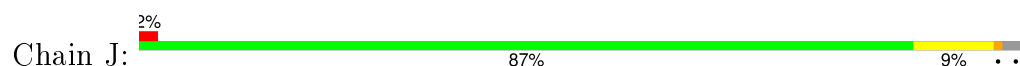
- Molecule 1: (R)-amine transaminase



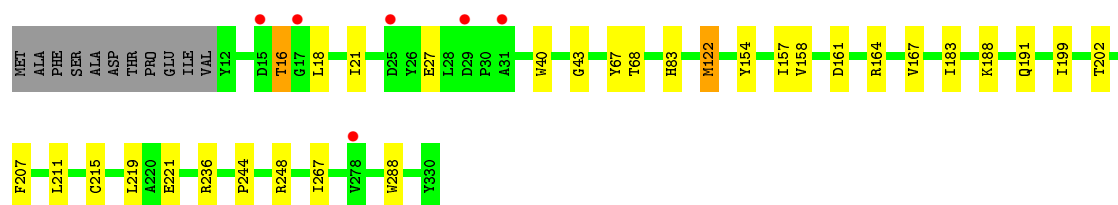
- Molecule 1: (R)-amine transaminase



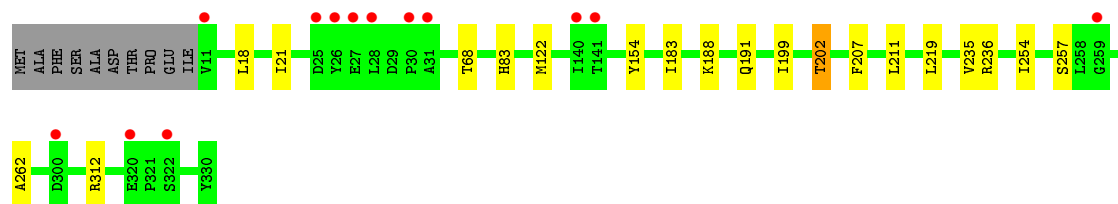
- Molecule 1: (R)-amine transaminase



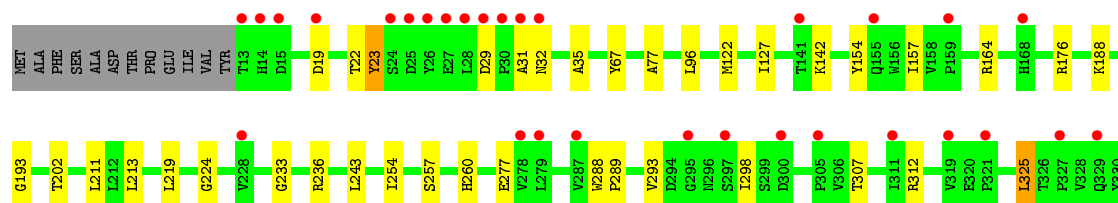
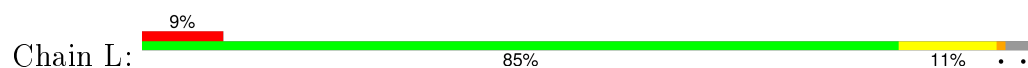




- Molecule 1: (R)-amine transaminase



- 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, $\alpha$ , $\beta$ , $\gamma$	82.01Å 133.54Å 195.54Å 90.00° 100.41° 90.00°	Depositor
Resolution (Å)	19.96 – 2.20 19.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.3 (19.96-2.20) 96.4 (19.96-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2519.40 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.168 , 0.213 0.174 , 0.217	Depositor DCC
$R_{free}$ test set	10186 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.4	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 201958 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32226	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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 35.63 % 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 5.6637e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, 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	0.48	0/2580	0.66	1/3522 (0.0%)
1	B	0.49	0/2596	0.67	1/3544 (0.0%)
1	C	0.45	0/2579	0.63	0/3521
1	D	0.49	0/2595	0.66	0/3542
1	E	0.42	0/2570	0.62	0/3509
1	F	0.45	0/2588	0.63	0/3533
1	G	0.50	0/2590	0.68	1/3535 (0.0%)
1	H	0.48	0/2579	0.65	0/3521
1	I	0.41	0/2571	0.60	0/3510
1	J	0.45	0/2564	0.63	0/3500
1	K	0.41	0/2571	0.58	0/3510
1	L	0.39	0/2545	0.58	0/3474
All	All	0.45	0/30928	0.63	3/42221 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	177	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	236	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	214	ASP	CB-CG-OD1	5.26	123.03	118.30

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	2521	0	2454	21	0
1	B	2536	0	2473	19	0
1	C	2523	0	2459	17	0
1	D	2536	0	2474	18	0
1	E	2514	0	2446	18	0
1	F	2529	0	2466	20	0
1	G	2531	0	2471	28	0
1	H	2520	0	2460	27	0
1	I	2512	0	2449	19	0
1	J	2508	0	2439	24	0
1	K	2512	0	2449	13	0
1	L	2490	0	2426	22	0
2	A	16	0	7	0	0
2	B	16	0	7	1	0
2	C	16	0	7	0	0
2	D	16	0	8	3	0
2	E	16	0	7	2	0
2	F	16	0	7	1	0
2	G	16	0	8	2	0
2	H	16	0	7	3	0
2	I	16	0	7	0	0
2	J	16	0	8	2	0
2	K	16	0	7	1	0
2	L	16	0	7	1	0
3	A	174	0	0	6	0
3	B	182	0	0	2	0
3	C	161	0	0	2	0
3	D	179	0	0	2	0
3	E	124	0	0	4	0
3	F	144	0	0	2	0
3	G	199	0	0	6	0
3	H	183	0	0	4	0
3	I	119	0	0	3	0
3	J	137	0	0	3	0
3	K	115	0	0	1	0
3	L	85	0	0	3	0
All	All	32226	0	29553	225	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 4.

The worst 5 of 225 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:E:122:MET:HE2	1:E:284:GLY:HA2	1.56	0.85
1:F:215[A]:CYS:SG	3:L:534:HOH:O	2.38	0.80
1:G:215[B]:CYS:SG	3:G:595:HOH:O	2.39	0.80
1:H:122:MET:HE1	1:H:284:GLY:HA2	1.64	0.79
1:E:267:ILE:HG23	3:E:571:HOH:O	1.81	0.78

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	319/330 (97%)	308 (97%)	11 (3%)	0	100	100
1	B	321/330 (97%)	310 (97%)	11 (3%)	0	100	100
1	C	319/330 (97%)	310 (97%)	9 (3%)	0	100	100
1	D	321/330 (97%)	311 (97%)	10 (3%)	0	100	100
1	E	318/330 (96%)	308 (97%)	8 (2%)	2 (1%)	30	29
1	F	320/330 (97%)	308 (96%)	11 (3%)	1 (0%)	46	50
1	G	320/330 (97%)	310 (97%)	10 (3%)	0	100	100
1	H	319/330 (97%)	307 (96%)	12 (4%)	0	100	100
1	I	318/330 (96%)	306 (96%)	12 (4%)	0	100	100
1	J	317/330 (96%)	306 (96%)	11 (4%)	0	100	100
1	K	318/330 (96%)	307 (96%)	11 (4%)	0	100	100
1	L	315/330 (96%)	303 (96%)	11 (4%)	1 (0%)	46	50
All	All	3825/3960 (97%)	3694 (97%)	127 (3%)	4 (0%)	56	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	321	PRO
1	L	23	TYR
1	F	321	PRO
1	E	210	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	274/280 (98%)	273 (100%)	1 (0%)	93	97
1	B	276/280 (99%)	276 (100%)	0	100	100
1	C	274/280 (98%)	272 (99%)	2 (1%)	88	94
1	D	275/280 (98%)	271 (98%)	4 (2%)	72	84
1	E	272/280 (97%)	272 (100%)	0	100	100
1	F	275/280 (98%)	274 (100%)	1 (0%)	93	97
1	G	275/280 (98%)	271 (98%)	4 (2%)	72	84
1	H	274/280 (98%)	274 (100%)	0	100	100
1	I	273/280 (98%)	271 (99%)	2 (1%)	88	94
1	J	272/280 (97%)	268 (98%)	4 (2%)	72	84
1	K	273/280 (98%)	271 (99%)	2 (1%)	88	94
1	L	270/280 (96%)	266 (98%)	4 (2%)	72	84
All	All	3283/3360 (98%)	3259 (99%)	24 (1%)	88	94

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	144	ARG
1	I	122	MET
1	L	202	THR
1	G	309	SER
1	I	15	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such

sidechains are listed below:

Mol	Chain	Res	Type
1	F	74	ASN
1	F	318	ASN
1	K	191	GLN
1	F	90	ASN
1	G	74	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CSO	A	152	1	3,6,7	2.16	1 (33%)	2,6,8	1.48	1 (50%)
1	CSO	B	152	1	3,6,7	1.74	1 (33%)	2,6,8	1.52	1 (50%)
1	CSO	C	152	1	3,6,7	1.79	1 (33%)	2,6,8	1.34	0
1	CSO	D	152	1	3,6,7	1.60	1 (33%)	2,6,8	1.50	1 (50%)
1	CSO	E	152	1	3,6,7	1.59	1 (33%)	2,6,8	1.51	1 (50%)
1	CSO	F	152	1	3,6,7	2.08	1 (33%)	2,6,8	1.60	1 (50%)
1	CSO	G	152	1	3,6,7	2.10	1 (33%)	2,6,8	1.40	0
1	CSO	H	152	1	3,6,7	1.81	1 (33%)	2,6,8	1.32	0
1	CSO	I	152	1	3,6,7	1.75	1 (33%)	2,6,8	1.48	1 (50%)
1	CSO	J	152	1	3,6,7	2.24	1 (33%)	2,6,8	1.59	1 (50%)
1	CSO	K	152	1	3,6,7	1.27	0	2,6,8	1.50	1 (50%)
1	CSO	L	152	1	3,6,7	2.05	1 (33%)	2,6,8	1.59	1 (50%)

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
1	CSO	A	152	1	-	0/1/5/7	0/0/0/0
1	CSO	B	152	1	-	0/1/5/7	0/0/0/0
1	CSO	C	152	1	-	0/1/5/7	0/0/0/0
1	CSO	D	152	1	-	0/1/5/7	0/0/0/0
1	CSO	E	152	1	-	0/1/5/7	0/0/0/0
1	CSO	F	152	1	-	0/1/5/7	0/0/0/0
1	CSO	G	152	1	-	0/1/5/7	0/0/0/0
1	CSO	H	152	1	-	0/1/5/7	0/0/0/0
1	CSO	I	152	1	-	0/1/5/7	0/0/0/0
1	CSO	J	152	1	-	0/1/5/7	0/0/0/0
1	CSO	K	152	1	-	0/1/5/7	0/0/0/0
1	CSO	L	152	1	-	0/1/5/7	0/0/0/0

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	152	CSO	CB-SG	-3.75	1.77	1.82
1	A	152	CSO	CB-SG	-3.61	1.77	1.82
1	G	152	CSO	CB-SG	-3.53	1.77	1.82
1	F	152	CSO	CB-SG	-3.48	1.77	1.82
1	L	152	CSO	CB-SG	-3.44	1.77	1.82

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	152	CSO	O-C-CA	-2.25	119.69	125.72
1	F	152	CSO	O-C-CA	-2.24	119.71	125.72
1	J	152	CSO	O-C-CA	-2.16	119.92	125.72
1	E	152	CSO	O-C-CA	-2.13	120.00	125.72
1	K	152	CSO	O-C-CA	-2.10	120.08	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 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	-	16,16,16	3.60	3 (18%)	21,23,23	1.38	2 (9%)
2	PLP	B	401	-	16,16,16	3.72	3 (18%)	21,23,23	1.48	4 (19%)
2	PLP	C	401	-	16,16,16	3.53	3 (18%)	21,23,23	1.27	2 (9%)
2	PLP	D	401	-	16,16,16	3.16	3 (18%)	21,23,23	1.27	2 (9%)
2	PLP	E	401	-	16,16,16	3.71	3 (18%)	21,23,23	1.40	4 (19%)
2	PLP	F	401	-	16,16,16	3.48	3 (18%)	21,23,23	1.44	5 (23%)
2	PLP	G	401	-	16,16,16	3.56	3 (18%)	21,23,23	1.41	5 (23%)
2	PLP	H	401	-	16,16,16	3.13	3 (18%)	21,23,23	1.57	4 (19%)
2	PLP	I	401	-	16,16,16	3.62	3 (18%)	21,23,23	1.29	3 (14%)
2	PLP	J	401	-	16,16,16	3.65	3 (18%)	21,23,23	1.43	2 (9%)
2	PLP	K	401	-	16,16,16	4.05	3 (18%)	21,23,23	1.48	2 (9%)
2	PLP	L	401	-	16,16,16	3.72	3 (18%)	21,23,23	1.22	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	-	-	0/8/8/8	0/1/1/1
2	PLP	B	401	-	-	0/8/8/8	0/1/1/1
2	PLP	C	401	-	-	0/8/8/8	0/1/1/1
2	PLP	D	401	-	-	0/8/8/8	0/1/1/1
2	PLP	E	401	-	-	0/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	F	401	-	-	0/8/8/8	0/1/1/1
2	PLP	G	401	-	-	0/8/8/8	0/1/1/1
2	PLP	H	401	-	-	0/8/8/8	0/1/1/1
2	PLP	I	401	-	-	0/8/8/8	0/1/1/1
2	PLP	J	401	-	-	0/8/8/8	0/1/1/1
2	PLP	K	401	-	-	0/8/8/8	0/1/1/1
2	PLP	L	401	-	-	0/8/8/8	0/1/1/1

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	C4-C5	4.71	1.48	1.42
2	E	401	PLP	C4-C5	5.06	1.48	1.42
2	B	401	PLP	C4-C5	5.27	1.48	1.42
2	H	401	PLP	C4-C5	5.33	1.49	1.42
2	J	401	PLP	C4-C5	5.45	1.49	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	401	PLP	C3-C4-C5	-4.37	115.09	118.26
2	H	401	PLP	O4A-C4A-C4	-4.05	115.75	125.03
2	J	401	PLP	C2A-C2-C3	-3.41	117.44	120.90
2	B	401	PLP	C2A-C2-C3	-3.19	117.67	120.90
2	C	401	PLP	C3-C4-C5	-3.03	116.06	118.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	PLP	1	0
2	D	401	PLP	3	0
2	E	401	PLP	2	0
2	F	401	PLP	1	0
2	G	401	PLP	2	0
2	H	401	PLP	3	0
2	J	401	PLP	2	0
2	K	401	PLP	1	0
2	L	401	PLP	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	319/330 (96%)	-0.19	3 (0%) 85 85	22, 29, 45, 63	0
1	B	322/330 (97%)	-0.23	5 (1%) 74 73	21, 28, 42, 74	0
1	C	320/330 (96%)	-0.20	5 (1%) 74 73	22, 31, 45, 61	0
1	D	321/330 (97%)	-0.23	4 (1%) 81 80	19, 27, 41, 60	0
1	E	320/330 (96%)	0.06	9 (2%) 56 55	24, 37, 55, 69	0
1	F	321/330 (97%)	-0.07	9 (2%) 56 55	20, 32, 49, 68	0
1	G	320/330 (96%)	-0.14	5 (1%) 74 73	19, 29, 47, 60	0
1	H	320/330 (96%)	-0.21	5 (1%) 74 73	19, 29, 44, 61	0
1	I	319/330 (96%)	-0.01	11 (3%) 49 47	25, 36, 52, 69	0
1	J	318/330 (96%)	-0.06	6 (1%) 70 68	22, 33, 54, 67	0
1	K	319/330 (96%)	0.13	13 (4%) 41 39	25, 38, 53, 69	0
1	L	317/330 (96%)	0.57	30 (9%) 10 9	31, 55, 73, 84	0
All	All	3836/3960 (96%)	-0.05	105 (2%) 58 57	19, 33, 58, 84	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	28	LEU	5.3
1	A	11	VAL	5.1
1	L	15	ASP	4.8
1	G	10	ILE	4.6
1	F	141	THR	4.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CSO	A	152	7/8	0.93	0.10	-	28,29,31,33	0
1	CSO	K	152	7/8	0.80	0.15	-	39,41,47,47	0
1	CSO	H	152	7/8	0.96	0.08	-	24,25,28,30	0
1	CSO	J	152	7/8	0.93	0.10	-	35,37,44,44	0
1	CSO	I	152	7/8	0.92	0.09	-	39,40,41,43	0
1	CSO	G	152	7/8	0.95	0.09	-	25,27,30,30	0
1	CSO	D	152	7/8	0.92	0.11	-	24,25,28,29	0
1	CSO	F	152	7/8	0.92	0.11	-	27,29,34,35	0
1	CSO	C	152	7/8	0.88	0.12	-	30,32,35,36	0
1	CSO	E	152	7/8	0.91	0.12	-	30,31,35,36	0
1	CSO	B	152	7/8	0.95	0.09	-	28,28,31,34	0
1	CSO	L	152	7/8	0.86	0.14	-	51,51,53,53	0

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PLP	B	401	16/16	0.95	0.14	1.97	22,27,30,31	0
2	PLP	K	401	16/16	0.94	0.15	1.76	29,36,42,47	0
2	PLP	H	401	16/16	0.96	0.13	1.28	24,25,31,35	0
2	PLP	C	401	16/16	0.96	0.13	1.08	25,30,36,38	0
2	PLP	I	401	16/16	0.95	0.12	0.93	22,34,41,43	0
2	PLP	G	401	16/16	0.96	0.12	0.86	22,25,31,35	0
2	PLP	A	401	16/16	0.96	0.12	0.72	24,28,36,38	0
2	PLP	J	401	16/16	0.95	0.12	0.71	22,27,36,39	0
2	PLP	D	401	16/16	0.96	0.11	0.37	20,23,32,32	0
2	PLP	F	401	16/16	0.97	0.10	-0.21	24,29,33,33	0
2	PLP	E	401	16/16	0.97	0.10	-0.23	28,38,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PLP	L	401	16/16	0.93	0.12	-0.26	34,43,51,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.