Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 07:47 PM BST

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 Full wwPDB X-ray Structure Validation 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:

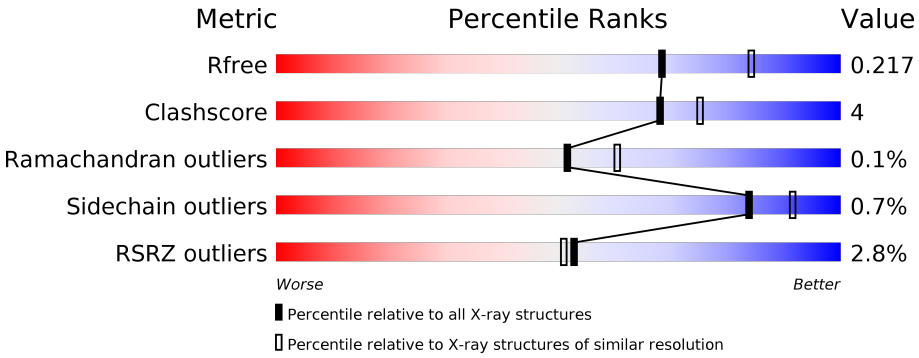
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 >=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 <=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	89% 8%
1	B	330	2% 92% 6%
1	C	330	2% 90% 7%
1	D	330	91% 6%
1	E	330	3% 90% 7%
1	F	330	3% 89% 8%

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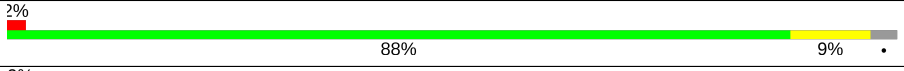
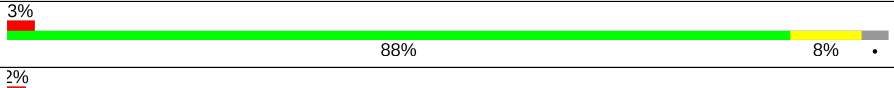
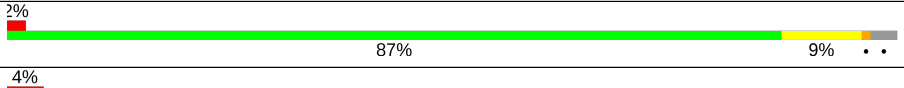
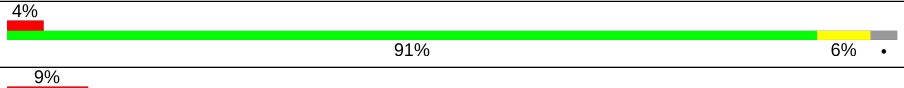
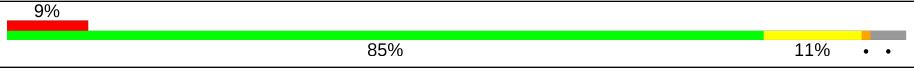
Mol	Chain	Length	Quality of chain
1	G	330	
1	H	330	
1	I	330	
1	J	330	
1	K	330	
1	L	330	

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
F	152	CSO	VAL	ENGINEERED MUTATION	UNP F7J696
F	169	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
F	199	ILE	VAL	ENGINEERED MUTATION	UNP F7J696
F	209	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
F	215	CYS	GLY	ENGINEERED MUTATION	UNP F7J696
F	217	ASN	GLY	ENGINEERED MUTATION	UNP F7J696
F	223	PRO	SER	ENGINEERED MUTATION	UNP F7J696
F	269	PRO	LEU	ENGINEERED MUTATION	UNP F7J696
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
G	152	CSO	VAL	ENGINEERED MUTATION	UNP F7J696
G	169	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
G	199	ILE	VAL	ENGINEERED MUTATION	UNP F7J696
G	209	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
G	215	CYS	GLY	ENGINEERED MUTATION	UNP F7J696
G	217	ASN	GLY	ENGINEERED MUTATION	UNP F7J696
G	223	PRO	SER	ENGINEERED MUTATION	UNP F7J696
G	269	PRO	LEU	ENGINEERED MUTATION	UNP F7J696
G	273	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
G	282	SER	THR	ENGINEERED MUTATION	UNP F7J696
G	284	GLY	ALA	ENGINEERED MUTATION	UNP F7J696
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
H	136	PHE	GLY	ENGINEERED MUTATION	UNP F7J696
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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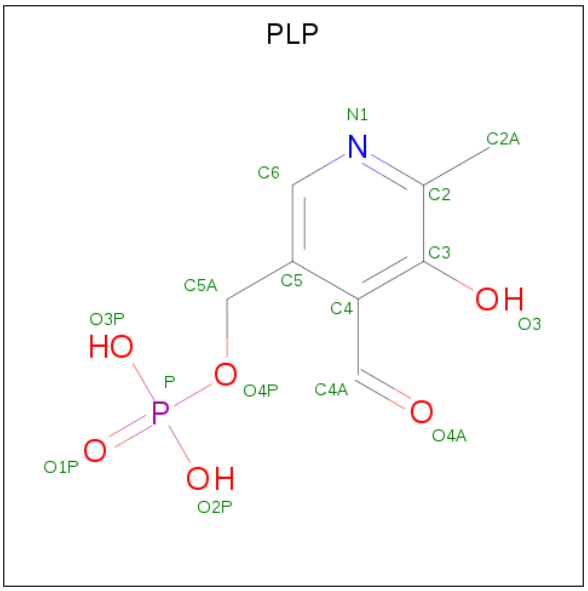
Chain	Residue	Modelled	Actual	Comment	Reference
K	217	ASN	GLY	ENGINEERED MUTATION	UNP F7J696
K	223	PRO	SER	ENGINEERED MUTATION	UNP F7J696
K	269	PRO	LEU	ENGINEERED MUTATION	UNP F7J696
K	273	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
K	282	SER	THR	ENGINEERED MUTATION	UNP F7J696
K	284	GLY	ALA	ENGINEERED MUTATION	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: $C_8H_{10}NO_6P$).



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.

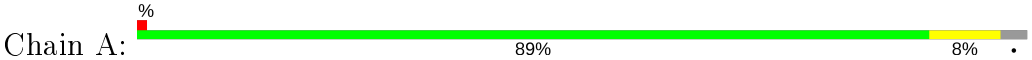
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	174	Total O 174 174	0	0
3	B	182	Total O 182 182	0	0
3	C	161	Total O 161 161	0	0
3	D	179	Total O 179 179	0	0
3	E	124	Total O 124 124	0	0
3	F	144	Total O 144 144	0	0
3	G	199	Total O 199 199	0	0
3	H	183	Total O 183 183	0	0
3	I	119	Total O 119 119	0	0
3	J	137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

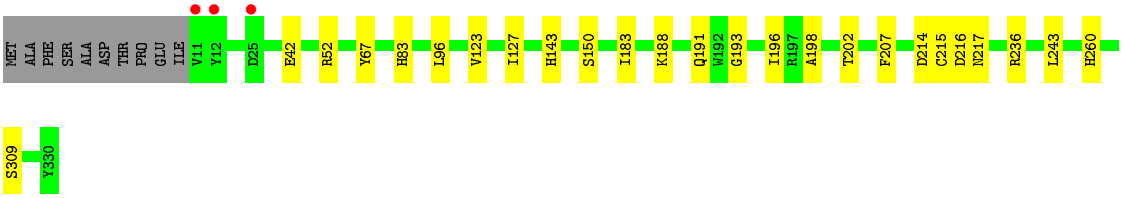
3 Residue-property plots (i)

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: (R)-amine transaminase

Chain A:



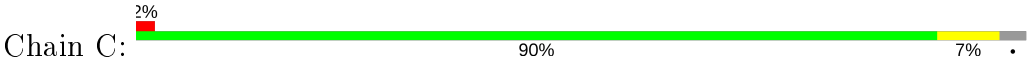


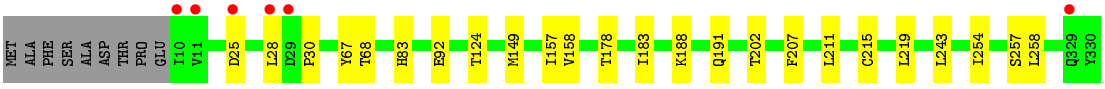
- Molecule 1: (R)-amine transaminase

Chain B:

- Molecule 1: (R)-amine transaminase

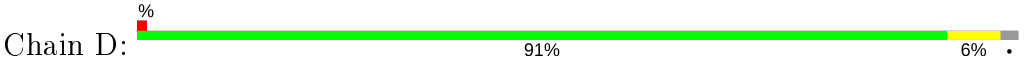
Chain C:

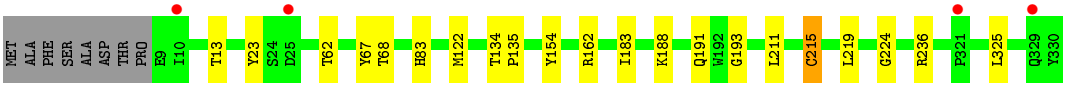




- Molecule 1: (R)-amine transaminase

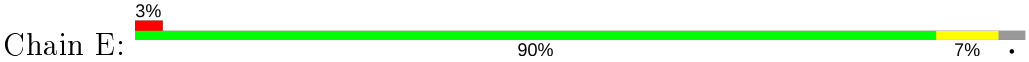
Chain D:

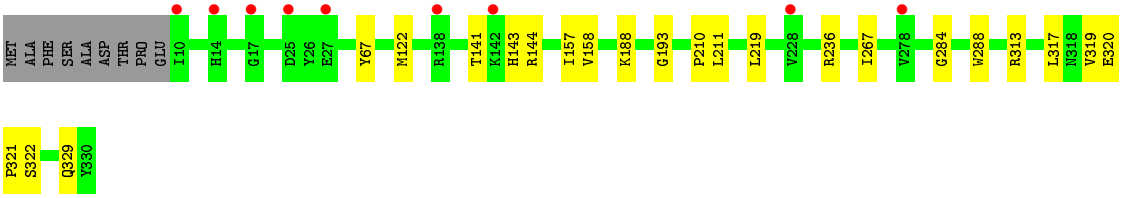




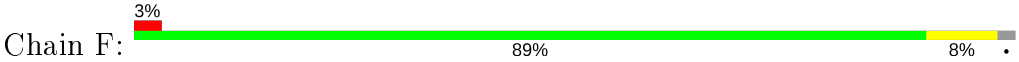
- Molecule 1: (R)-amine transaminase

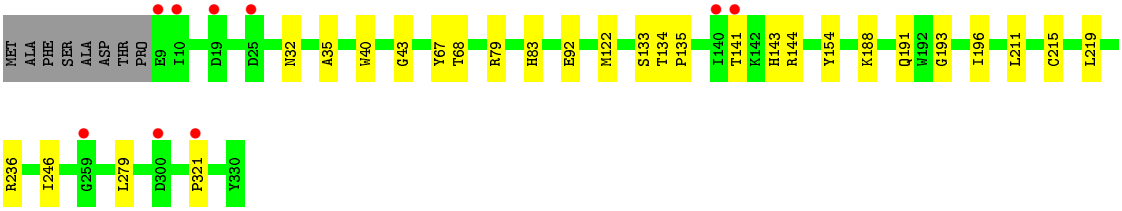
Chain E:



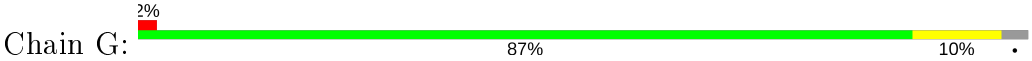


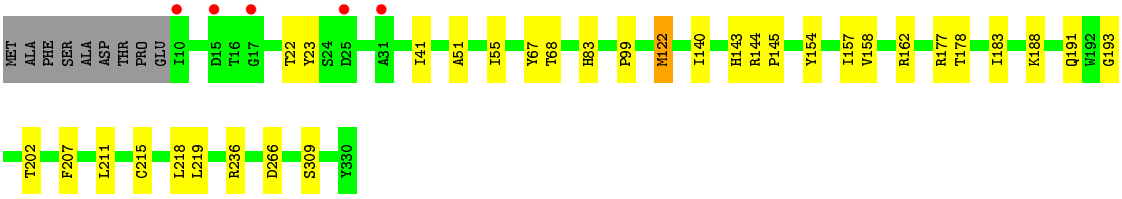
• Molecule 1: (R)-amine transaminase



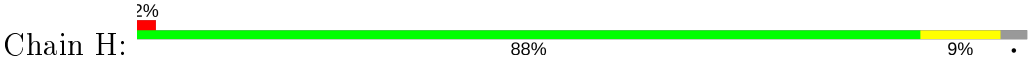


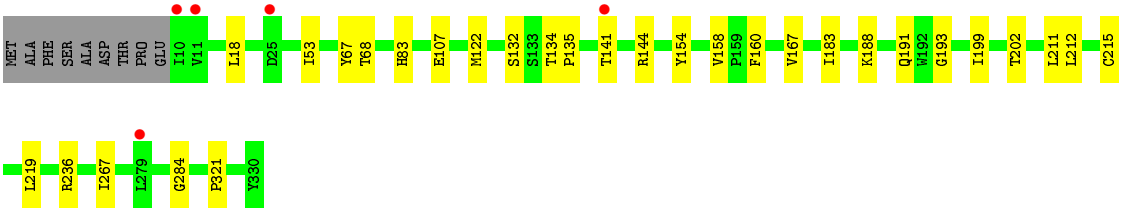
• Molecule 1: (R)-amine transaminase



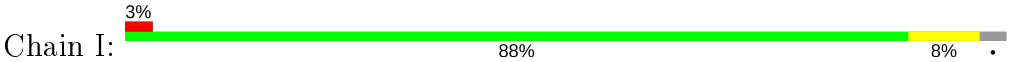


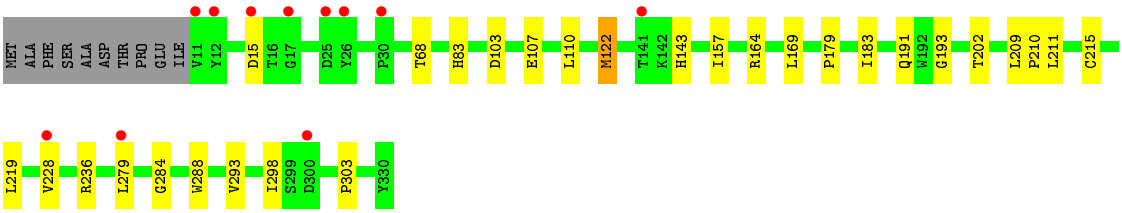
• Molecule 1: (R)-amine transaminase





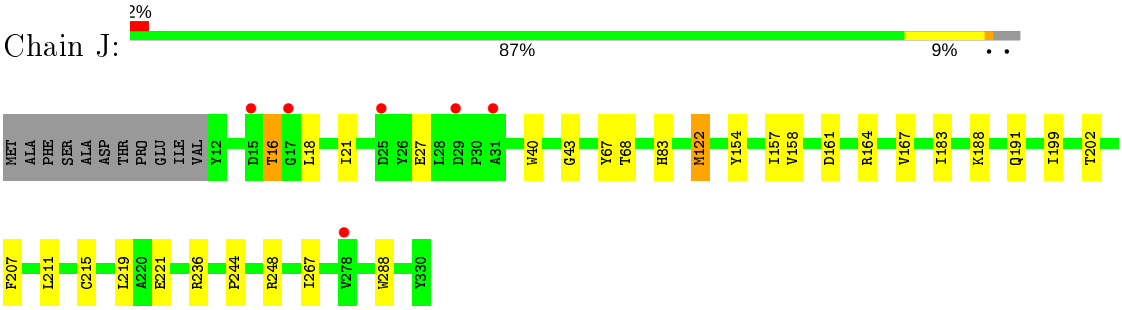
• Molecule 1: (R)-amine transaminase





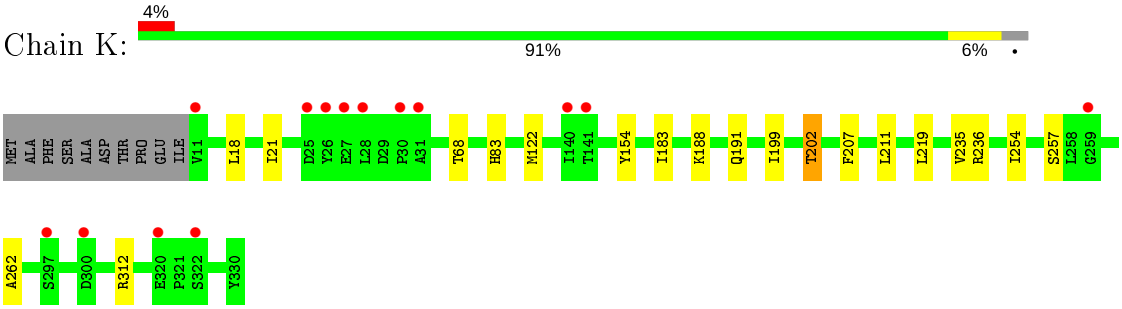
• Molecule 1: (R)-amine transaminase

Chain J:



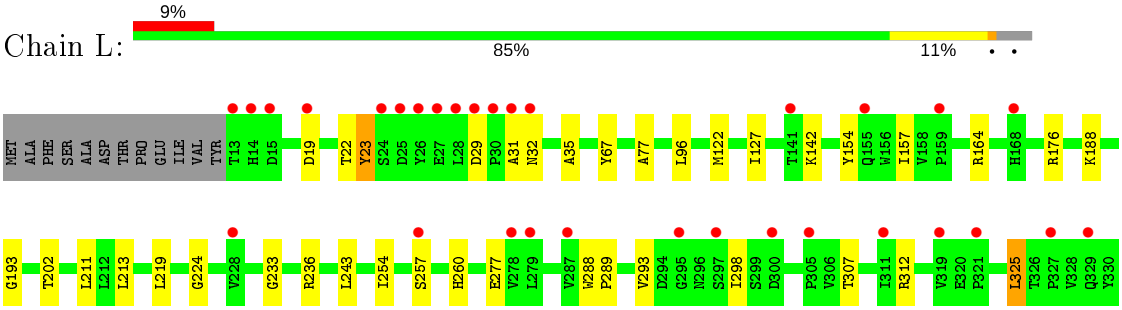
• Molecule 1: (R)-amine transaminase

Chain K:



• Molecule 1: (R)-amine transaminase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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 (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32226	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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(^{o})	Ideal(^{o})
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

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.

All (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
1:L:22:THR:O	1:L:23:TYR:HB2	1.85	0.77
1:D:236:ARG:HD2	3:D:570:HOH:O	1.85	0.74
1:D:193:GLY:H	1:F:191:GLN:HE22	1.35	0.74
1:A:143:HIS:CD2	3:A:612:HOH:O	2.40	0.74
1:C:191:GLN:HE22	1:E:193:GLY:H	1.35	0.73
1:A:191:GLN:HE22	1:B:193:GLY:H	1.35	0.73
1:J:16:THR:HG22	1:J:18:LEU:H	1.55	0.72
1:E:320:GLU:O	1:E:322:SER:N	2.24	0.70
1:K:122:MET:HG2	1:K:154:TYR:HA	1.73	0.70
1:A:143:HIS:NE2	3:A:612:HOH:O	2.26	0.68
1:C:157:ILE:HG23	1:C:158:VAL:HG13	1.77	0.67
1:I:236:ARG:HD2	3:I:520:HOH:O	1.95	0.67
1:J:68:THR:OG1	1:J:83:HIS:HD2	1.78	0.66
1:A:215[A]:CYS:SG	3:H:537:HOH:O	2.53	0.66
1:G:68:THR:OG1	1:G:83:HIS:HD2	1.79	0.65
1:A:193:GLY:H	1:B:191:GLN:HE22	1.44	0.65
1:G:191:GLN:HE22	1:H:193:GLY:H	1.44	0.65
1:L:67:TYR:CE2	1:L:188:LYS:HE3	2.31	0.64
1:F:122:MET:HG2	1:F:154:TYR:HA	1.80	0.63
1:A:196:ILE:HD12	3:A:556:HOH:O	1.97	0.63
1:A:207:PHE:O	1:B:138:ARG:NH2	2.31	0.63
1:D:122:MET:HG2	1:D:154:TYR:HA	1.81	0.63
1:G:67:TYR:CZ	1:G:188:LYS:HE3	2.34	0.63
1:F:211:LEU:HD21	1:F:219:LEU:HG	1.82	0.62
1:G:193:GLY:H	1:H:191:GLN:HE22	1.46	0.62
3:B:622:HOH:O	1:G:215[A]:CYS:SG	2.56	0.61
1:C:67:TYR:CE2	1:C:188:LYS:HE3	2.36	0.60
1:J:191:GLN:HE22	1:L:193:GLY:H	1.50	0.60
1:D:67:TYR:CE2	1:D:188:LYS:HE3	2.36	0.60
1:J:67:TYR:CE2	1:J:188:LYS:HE3	2.38	0.59
1:D:191:GLN:HE22	1:F:193:GLY:H	1.51	0.58
1:J:122:MET:HE3	1:J:154:TYR:CD2	2.37	0.58
1:C:68:THR:OG1	1:C:83:HIS:HD2	1.85	0.58
1:G:67:TYR:CE2	1:G:188:LYS:HE3	2.38	0.58
1:I:83:HIS:HE1	3:I:506:HOH:O	1.85	0.58
1:A:236:ARG:HD2	3:A:607:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:TYR:CZ	1:F:188:LYS:HE3	2.39	0.58
1:B:83:HIS:HE1	3:B:501:HOH:O	1.86	0.58
1:D:83:HIS:HE1	3:D:502:HOH:O	1.88	0.57
1:I:179:PRO:HG3	1:I:215[B]:CYS:SG	2.45	0.57
1:A:42:GLU:OE2	1:B:52:ARG:NH2	2.33	0.56
1:F:67:TYR:CE2	1:F:188:LYS:HE3	2.40	0.56
1:L:188:LYS:HD2	1:L:243:LEU:HD21	1.87	0.56
1:F:32:ASN:HB3	1:F:35:ALA:HB2	1.88	0.56
3:A:595:HOH:O	1:H:215[B]:CYS:SG	2.28	0.56
1:J:158:VAL:HG11	1:J:167:VAL:HG21	1.86	0.56
1:I:193:GLY:H	1:K:191:GLN:HE22	1.53	0.56
1:B:68:THR:OG1	1:B:83:HIS:HD2	1.89	0.55
1:K:236:ARG:NH1	3:K:553:HOH:O	2.38	0.55
1:I:183:ILE:HD13	1:I:191:GLN:OE1	2.06	0.55
3:C:615:HOH:O	1:I:215[A]:CYS:SG	2.58	0.55
1:E:157:ILE:HG21	1:E:288:TRP:CH2	2.42	0.55
1:F:236:ARG:HD3	3:F:579:HOH:O	2.05	0.55
1:H:183:ILE:HD13	1:H:191:GLN:NE2	2.21	0.55
1:G:202:THR:HG22	1:G:207:PHE:O	2.07	0.55
1:I:202:THR:HG21	1:I:210:PRO:HD3	1.89	0.55
1:B:67:TYR:CE2	1:B:188:LYS:HE3	2.42	0.55
1:H:67:TYR:CE2	1:H:188:LYS:HE3	2.41	0.54
1:H:107:GLU:HG2	3:H:602:HOH:O	2.07	0.54
1:H:188:LYS:NZ	2:H:401:PLP:C4A	2.70	0.54
1:H:68:THR:OG1	1:H:83:HIS:HD2	1.90	0.53
1:E:236:ARG:NH1	3:E:571:HOH:O	2.42	0.53
1:F:133:SER:HG	1:F:143:HIS:CE1	2.23	0.53
1:H:122:MET:CE	1:H:284:GLY:HA2	2.36	0.53
1:H:67:TYR:CZ	1:H:188:LYS:HE3	2.44	0.53
1:G:157:ILE:HG23	1:G:158:VAL:HG13	1.90	0.52
1:J:40:TRP:CZ2	1:J:43:GLY:HA2	2.44	0.52
1:K:199:ILE:O	1:K:202:THR:HB	2.10	0.52
1:J:183:ILE:HD13	1:J:191:GLN:NE2	2.24	0.52
1:A:83:HIS:HE1	3:A:570:HOH:O	1.92	0.52
1:G:188:LYS:NZ	2:G:401:PLP:C4A	2.73	0.52
1:I:122:MET:HE2	1:I:284:GLY:HA2	1.91	0.52
1:D:183:ILE:HD13	1:D:191:GLN:NE2	2.25	0.52
1:G:55:ILE:CD1	1:H:53:ILE:HG23	2.40	0.52
1:G:55:ILE:HD13	1:H:53:ILE:HG23	1.92	0.52
1:I:228:VAL:HB	1:I:279:LEU:HG	1.92	0.51
1:J:236:ARG:HD3	3:J:533:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:83:HIS:HE1	3:J:522:HOH:O	1.93	0.51
1:D:188:LYS:NZ	2:D:401:PLP:C4A	2.74	0.51
1:L:22:THR:N	3:L:584:HOH:O	2.23	0.51
1:E:188:LYS:NZ	2:E:401:PLP:C4A	2.74	0.51
1:D:188:LYS:NZ	2:D:401:PLP:O4A	2.44	0.51
1:E:122:MET:CE	1:E:284:GLY:HA2	2.35	0.50
1:I:293:VAL:HG23	1:I:298:ILE:HD11	1.93	0.50
1:C:178:THR:HG21	1:C:183:ILE:HB	1.94	0.50
1:C:67:TYR:CE1	1:C:188:LYS:HG2	2.47	0.50
1:G:236:ARG:HD2	3:G:541:HOH:O	2.11	0.50
1:E:319:VAL:HG23	3:E:532:HOH:O	2.10	0.50
1:L:277:GLU:OE1	1:L:307:THR:N	2.42	0.50
1:D:215[B]:CYS:HG	1:J:215:CYS:HG	1.59	0.49
1:J:236:ARG:CD	3:J:533:HOH:O	2.61	0.49
1:A:183:ILE:HD13	1:A:191:GLN:NE2	2.28	0.49
1:H:188:LYS:HZ1	2:H:401:PLP:C4A	2.26	0.49
1:H:18:LEU:HD23	1:H:160:PHE:HB3	1.95	0.48
1:L:157:ILE:HG21	1:L:288:TRP:CH2	2.48	0.48
1:C:183:ILE:HD13	1:C:191:GLN:NE2	2.28	0.48
1:B:240:ARG:CZ	1:G:218:LEU:HD12	2.43	0.48
1:G:218:LEU:HD13	1:G:266:ASP:HB3	1.96	0.48
1:E:157:ILE:HG23	1:E:158:VAL:HG13	1.94	0.48
1:E:67:TYR:CE2	1:E:188:LYS:HE3	2.48	0.48
1:K:183:ILE:HD13	1:K:191:GLN:NE2	2.29	0.48
1:F:40:TRP:CZ2	1:F:43:GLY:HA2	2.48	0.48
1:C:211:LEU:HD21	1:C:219:LEU:HG	1.96	0.47
1:D:67:TYR:CZ	1:D:188:LYS:HE3	2.50	0.47
1:H:122:MET:HE3	1:H:154:TYR:CG	2.49	0.47
1:C:254:ILE:O	1:C:257:SER:HB2	2.14	0.47
1:L:233:GLY:O	1:L:260:HIS:ND1	2.47	0.47
1:H:211:LEU:HD21	1:H:219:LEU:HG	1.96	0.47
1:L:22:THR:O	1:L:23:TYR:CB	2.60	0.47
1:K:18:LEU:HD12	1:K:21:ILE:HD12	1.97	0.47
1:G:162[B]:ARG:CZ	3:G:617:HOH:O	2.63	0.47
1:I:211:LEU:HD21	1:I:219:LEU:HG	1.96	0.47
1:F:141:THR:O	1:F:144:ARG:NH1	2.46	0.46
1:F:83:HIS:HE1	3:F:507:HOH:O	1.98	0.46
1:B:215[A]:CYS:SG	3:G:605:HOH:O	2.61	0.46
1:E:329:GLN:HG2	1:E:329:GLN:O	2.15	0.46
1:H:141:THR:O	1:H:144:ARG:NH1	2.48	0.46
1:J:199:ILE:O	1:J:202:THR:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LEU:HD21	1:B:219:LEU:HG	1.96	0.46
1:F:68:THR:OG1	1:F:83:HIS:HD2	1.96	0.46
1:L:96:LEU:HD21	1:L:127:ILE:HG22	1.97	0.46
1:J:211:LEU:HD21	1:J:219:LEU:HG	1.96	0.46
1:J:219:LEU:HD22	1:J:267:ILE:CG2	2.46	0.46
1:D:211:LEU:HD21	1:D:219:LEU:HG	1.98	0.46
1:K:211:LEU:HD21	1:K:219:LEU:HG	1.96	0.46
1:E:313:ARG:O	1:E:317:LEU:HG	2.15	0.46
1:K:68:THR:OG1	1:K:83:HIS:HD2	1.99	0.46
1:L:122:MET:HG2	1:L:154:TYR:HA	1.97	0.46
1:E:211:LEU:HD21	1:E:219:LEU:HG	1.97	0.46
1:G:22:THR:HG22	1:G:23:TYR:O	2.16	0.46
1:C:188:LYS:HD2	1:C:243:LEU:CD2	2.46	0.45
1:H:321:PRO:HB2	1:I:110:LEU:HD13	1.97	0.45
1:L:289:PRO:HB3	1:L:307:THR:HG21	1.98	0.45
1:I:68:THR:OG1	1:I:83:HIS:HD2	2.00	0.45
1:C:215[B]:CYS:HG	1:I:215[B]:CYS:HB2	1.81	0.45
1:E:67:TYR:CZ	1:E:188:LYS:HE3	2.52	0.45
1:F:188:LYS:NZ	2:F:401:PLP:C4A	2.79	0.45
1:G:211:LEU:HD21	1:G:219:LEU:HG	1.99	0.45
1:K:188:LYS:HZ1	2:K:401:PLP:C4A	2.29	0.45
1:H:199:ILE:O	1:H:202:THR:OG1	2.30	0.45
1:B:188:LYS:NZ	2:B:401:PLP:O4A	2.50	0.45
1:G:122:MET:CE	1:G:154:TYR:CD2	3.00	0.45
1:G:99:PRO:HD3	1:G:145:PRO:HB2	1.98	0.45
1:B:90:ASN:ND2	1:B:188:LYS:H	2.14	0.45
1:H:122:MET:HG3	1:H:154:TYR:HA	1.98	0.44
1:J:67:TYR:CE1	1:J:188:LYS:HG2	2.52	0.44
1:G:140:ILE:HD12	1:G:140:ILE:H	1.82	0.44
1:A:52:ARG:NH2	1:B:42:GLU:OE2	2.51	0.44
1:L:29:ASP:OD1	1:L:31:ALA:HB3	2.17	0.44
1:C:124:THR:O	1:C:149:MET:HA	2.18	0.44
1:L:224:GLY:HA2	2:L:401:PLP:C3	2.47	0.44
1:A:188:LYS:HD2	1:A:243:LEU:HD21	2.00	0.44
1:K:202:THR:HG23	1:K:207:PHE:O	2.18	0.44
1:G:202:THR:CG2	1:G:207:PHE:O	2.66	0.43
1:I:103:ASP:O	1:I:107:GLU:HG3	2.18	0.43
1:J:244:PRO:HA	1:J:248:ARG:NH2	2.33	0.43
1:K:254:ILE:O	1:K:257:SER:HB2	2.18	0.43
1:B:157:ILE:HG21	1:B:288:TRP:CH2	2.54	0.43
1:B:53:ILE:HG22	1:B:148:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:TYR:CE1	1:B:188:LYS:HG2	2.54	0.43
1:C:188:LYS:HD2	1:C:243:LEU:HD22	2.01	0.43
1:G:162[B]:ARG:NE	3:G:617:HOH:O	2.52	0.43
1:F:79:ARG:HD3	1:F:246:ILE:CG2	2.49	0.43
1:G:83:HIS:HE1	3:G:522:HOH:O	2.01	0.43
1:I:164:ARG:O	1:I:303:PRO:HG2	2.19	0.43
1:C:202:THR:HG22	1:C:207:PHE:O	2.19	0.42
1:D:68:THR:OG1	1:D:83:HIS:HD2	2.01	0.42
1:E:188:LYS:HZ1	2:E:401:PLP:C4A	2.31	0.42
1:I:143:HIS:CE1	3:I:562:HOH:O	2.71	0.42
1:G:188:LYS:NZ	2:G:401:PLP:O4A	2.52	0.42
1:F:134:THR:HB	1:F:135:PRO:CD	2.50	0.42
1:A:123:VAL:HA	1:A:150:SER:O	2.20	0.42
1:I:157:ILE:HG21	1:I:288:TRP:CH2	2.54	0.42
1:L:293:VAL:HG23	1:L:298:ILE:HD11	2.02	0.42
1:A:260:HIS:HE1	1:C:258:LEU:O	2.03	0.42
1:G:178:THR:HG21	1:G:183:ILE:HB	2.01	0.42
1:J:188:LYS:NZ	2:J:401:PLP:O4A	2.53	0.42
1:K:235:VAL:O	1:K:262:ALA:HA	2.20	0.42
1:G:41:ILE:HD12	1:G:51:ALA:HA	2.00	0.41
1:J:221:GLU:OE1	2:J:401:PLP:N1	2.53	0.41
1:L:236:ARG:HD2	3:L:544:HOH:O	2.18	0.41
1:D:134:THR:HB	1:D:135:PRO:CD	2.50	0.41
1:A:191:GLN:HE22	1:B:193:GLY:N	2.12	0.41
1:J:122:MET:HE3	1:J:154:TYR:CE2	2.55	0.41
1:A:198:ALA:O	1:A:202:THR:HG23	2.20	0.41
1:C:28:LEU:O	1:C:30:PRO:HD3	2.19	0.41
1:L:254:ILE:O	1:L:257:SER:HB2	2.21	0.41
1:E:141:THR:O	1:E:144:ARG:NH1	2.53	0.41
1:F:67:TYR:CE1	1:F:188:LYS:HG2	2.55	0.41
1:A:96:LEU:HD13	1:A:127:ILE:HG22	2.02	0.41
1:G:183:ILE:HD13	1:G:191:GLN:NE2	2.36	0.41
1:L:211:LEU:HD21	1:L:219:LEU:HG	2.03	0.41
1:D:13:THR:HA	1:D:23:TYR:CD2	2.55	0.41
1:J:16:THR:HG21	1:J:21:ILE:O	2.21	0.41
1:K:183:ILE:HD13	1:K:191:GLN:HE21	1.86	0.41
1:L:77:ALA:O	1:L:325:LEU:HA	2.20	0.41
1:D:62:THR:HB	1:F:196:ILE:HD11	2.03	0.41
1:F:279:LEU:C	1:F:279:LEU:HD12	2.41	0.41
1:H:212:LEU:HD12	1:H:212:LEU:N	2.35	0.41
1:L:32:ASN:HB3	1:L:35:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASP:O	1:A:217:ASN:HB2	2.21	0.41
1:D:67:TYR:CE1	1:D:188:LYS:HG2	2.56	0.41
1:E:143:HIS:CD2	3:E:568:HOH:O	2.73	0.41
1:L:19:ASP:OD2	1:L:312:ARG:NH1	2.54	0.41
1:A:67:TYR:CE2	1:A:188:LYS:HE3	2.56	0.40
1:I:169:LEU:HD12	1:I:209:LEU:O	2.20	0.40
1:C:83:HIS:HE1	3:C:507:HOH:O	2.04	0.40
1:H:132:SER:HB2	1:H:144:ARG:HB2	2.02	0.40
1:H:219:LEU:HD22	1:H:267:ILE:CG2	2.52	0.40
1:J:157:ILE:HG21	1:J:288:TRP:CH2	2.56	0.40
1:L:176:ARG:HG2	1:L:213:LEU:O	2.21	0.40
1:H:158:VAL:HG11	1:H:167:VAL:HG21	2.02	0.40
2:H:401:PLP:O4A	3:H:603:HOH:O	2.21	0.40
1:B:243:LEU:HA	1:B:244:PRO:HD3	1.98	0.40
1:J:202:THR:HG23	1:J:207:PHE:O	2.19	0.40
1:A:52:ARG:O	1:B:52:ARG:NH1	2.55	0.40
1:D:224:GLY:HA2	2:D:401:PLP:C3	2.52	0.40
1:H:134:THR:HB	1:H:135:PRO:CD	2.51	0.40
1:H:236:ARG:HD3	3:H:608:HOH:O	2.21	0.40
1:J:18:LEU:HD21	1:J:164:ARG:HB2	2.02	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	318/330 (96%)	308 (97%)	8 (2%)	2 (1%)	25 26
1	F	320/330 (97%)	308 (96%)	11 (3%)	1 (0%)	41 46
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%)	41 46
All	All	3825/3960 (97%)	3694 (97%)	127 (3%)	4 (0%)	51 60

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 (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	274/280 (98%)	273 (100%)	1 (0%)	91 96
1	B	276/280 (99%)	276 (100%)	0	100 100
1	C	274/280 (98%)	272 (99%)	2 (1%)	84 91
1	D	275/280 (98%)	271 (98%)	4 (2%)	65 78
1	E	272/280 (97%)	272 (100%)	0	100 100
1	F	275/280 (98%)	274 (100%)	1 (0%)	91 96
1	G	275/280 (98%)	271 (98%)	4 (2%)	65 78
1	H	274/280 (98%)	274 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	273/280 (98%)	271 (99%)	2 (1%)	84 91
1	J	272/280 (97%)	268 (98%)	4 (2%)	65 78
1	K	273/280 (98%)	271 (99%)	2 (1%)	84 91
1	L	270/280 (96%)	266 (98%)	4 (2%)	65 78
All	All	3283/3360 (98%)	3259 (99%)	24 (1%)	84 91

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	SER
1	C	25	ASP
1	C	92	GLU
1	D	162	ARG
1	D	215[A]	CYS
1	D	215[B]	CYS
1	D	325	LEU
1	F	92	GLU
1	G	122	MET
1	G	143	HIS
1	G	144	ARG
1	G	309	SER
1	I	15	ASP
1	I	122	MET
1	J	16	THR
1	J	27	GLU
1	J	122	MET
1	J	161	ASP
1	K	202	THR
1	K	312	ARG
1	L	142	LYS
1	L	164	ARG
1	L	202	THR
1	L	325	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	83	HIS
1	A	90	ASN

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Mol	Chain	Res	Type
1	A	143	HIS
1	A	191	GLN
1	A	260	HIS
1	B	83	HIS
1	B	90	ASN
1	B	191	GLN
1	B	260	HIS
1	C	74	ASN
1	C	83	HIS
1	C	90	ASN
1	C	191	GLN
1	D	83	HIS
1	D	173	GLN
1	D	191	GLN
1	D	260	HIS
1	D	308	GLN
1	E	83	HIS
1	E	173	GLN
1	F	74	ASN
1	F	83	HIS
1	F	90	ASN
1	F	173	GLN
1	F	191	GLN
1	F	318	ASN
1	G	74	ASN
1	G	83	HIS
1	G	186	GLN
1	G	191	GLN
1	H	14	HIS
1	H	83	HIS
1	H	155	GLN
1	H	191	GLN
1	I	83	HIS
1	I	173	GLN
1	J	83	HIS
1	J	173	GLN
1	J	191	GLN
1	K	74	ASN
1	K	83	HIS
1	K	173	GLN
1	K	191	GLN
1	K	203	HIS

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Mol	Chain	Res	Type
1	K	329	GLN
1	L	173	GLN

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	0.67	0	0,6,8	0.00	-
1	CSO	K	152	1	3,6,7	1.23	0	0,6,8	0.00	-
1	CSO	H	152	1	3,6,7	0.79	0	0,6,8	0.00	-
1	CSO	J	152	1	3,6,7	0.77	0	0,6,8	0.00	-
1	CSO	I	152	1	3,6,7	0.80	0	0,6,8	0.00	-
1	CSO	G	152	1	3,6,7	0.56	0	0,6,8	0.00	-
1	CSO	D	152	1	3,6,7	0.84	0	0,6,8	0.00	-
1	CSO	F	152	1	3,6,7	0.68	0	0,6,8	0.00	-
1	CSO	C	152	1	3,6,7	0.71	0	0,6,8	0.00	-
1	CSO	E	152	1	3,6,7	0.55	0	0,6,8	0.00	-
1	CSO	B	152	1	3,6,7	0.68	0	0,6,8	0.00	-
1	CSO	L	152	1	3,6,7	0.59	0	0,6,8	0.00	-

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	-
1	CSO	K	152	1	-	1/1/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	H	152	1	-	0/1/5/7	-
1	CSO	J	152	1	-	0/1/5/7	-
1	CSO	I	152	1	-	0/1/5/7	-
1	CSO	G	152	1	-	0/1/5/7	-
1	CSO	D	152	1	-	0/1/5/7	-
1	CSO	F	152	1	-	0/1/5/7	-
1	CSO	C	152	1	-	0/1/5/7	-
1	CSO	E	152	1	-	0/1/5/7	-
1	CSO	B	152	1	-	0/1/5/7	-
1	CSO	L	152	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	K	152	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	E	401	-	16,16,16	2.93	3 (18%)	20,23,23	1.57	6 (30%)
2	PLP	F	401	-	16,16,16	2.84	3 (18%)	20,23,23	1.58	5 (25%)
2	PLP	G	401	-	16,16,16	2.90	3 (18%)	20,23,23	1.67	5 (25%)
2	PLP	A	401	-	16,16,16	2.85	3 (18%)	20,23,23	1.59	4 (20%)
2	PLP	B	401	-	16,16,16	2.98	3 (18%)	20,23,23	1.70	6 (30%)
2	PLP	C	401	-	16,16,16	2.92	3 (18%)	20,23,23	1.50	4 (20%)
2	PLP	H	401	-	16,16,16	2.61	3 (18%)	20,23,23	1.82	4 (20%)
2	PLP	I	401	-	16,16,16	2.93	3 (18%)	20,23,23	1.37	5 (25%)
2	PLP	J	401	-	16,16,16	2.93	3 (18%)	20,23,23	1.63	5 (25%)
2	PLP	K	401	-	16,16,16	3.30	3 (18%)	20,23,23	1.52	3 (15%)
2	PLP	D	401	-	16,16,16	2.64	3 (18%)	20,23,23	1.59	4 (20%)
2	PLP	L	401	-	16,16,16	3.01	3 (18%)	20,23,23	1.47	4 (20%)

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	401	-	-	0/8/8/8	0/1/1/1
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	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	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	D	401	-	-	0/8/8/8	0/1/1/1
2	PLP	L	401	-	-	0/8/8/8	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	401	PLP	C3-C2	8.74	1.49	1.40
2	E	401	PLP	C3-C2	8.46	1.49	1.40
2	B	401	PLP	C3-C2	8.28	1.49	1.40
2	A	401	PLP	C3-C2	8.14	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	401	PLP	C3-C2	8.12	1.49	1.40
2	J	401	PLP	C3-C2	8.12	1.49	1.40
2	I	401	PLP	C3-C2	7.96	1.48	1.40
2	G	401	PLP	C3-C2	7.59	1.48	1.40
2	F	401	PLP	C3-C2	7.48	1.48	1.40
2	C	401	PLP	C3-C2	7.22	1.48	1.40
2	K	401	PLP	C4-C5	7.14	1.51	1.42
2	C	401	PLP	C4-C5	6.37	1.50	1.42
2	L	401	PLP	C4-C5	6.32	1.49	1.42
2	D	401	PLP	C3-C2	6.22	1.47	1.40
2	K	401	PLP	C4-C3	6.20	1.50	1.40
2	H	401	PLP	C3-C2	6.19	1.47	1.40
2	I	401	PLP	C4-C5	6.16	1.49	1.42
2	F	401	PLP	C4-C5	6.12	1.49	1.42
2	C	401	PLP	C4-C3	6.09	1.50	1.40
2	G	401	PLP	C4-C5	5.82	1.49	1.42
2	D	401	PLP	C4-C5	5.80	1.49	1.42
2	G	401	PLP	C4-C3	5.75	1.49	1.40
2	B	401	PLP	C4-C3	5.74	1.49	1.40
2	J	401	PLP	C4-C5	5.73	1.49	1.42
2	L	401	PLP	C4-C3	5.65	1.49	1.40
2	D	401	PLP	C4-C3	5.61	1.49	1.40
2	H	401	PLP	C4-C5	5.61	1.49	1.42
2	H	401	PLP	C4-C3	5.60	1.49	1.40
2	A	401	PLP	C4-C3	5.57	1.49	1.40
2	B	401	PLP	C4-C5	5.54	1.48	1.42
2	E	401	PLP	C4-C3	5.48	1.49	1.40
2	E	401	PLP	C4-C5	5.33	1.48	1.42
2	F	401	PLP	C4-C3	5.19	1.48	1.40
2	J	401	PLP	C4-C3	5.18	1.48	1.40
2	I	401	PLP	C4-C3	5.04	1.48	1.40
2	A	401	PLP	C4-C5	4.96	1.48	1.42

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	401	PLP	O4A-C4A-C4	-4.20	115.75	124.91
2	K	401	PLP	C3-C4-C5	-4.13	115.09	118.26
2	D	401	PLP	C4-C3-C2	-4.09	117.66	120.19
2	G	401	PLP	C4-C3-C2	-3.99	117.72	120.19
2	L	401	PLP	C4-C3-C2	-3.93	117.75	120.19
2	J	401	PLP	C4-C3-C2	-3.83	117.82	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	401	PLP	C4-C3-C2	-3.71	117.89	120.19
2	B	401	PLP	C4-C3-C2	-3.54	118.00	120.19
2	A	401	PLP	C4-C3-C2	-3.54	118.00	120.19
2	C	401	PLP	C4-C3-C2	-3.47	118.04	120.19
2	E	401	PLP	C4-C3-C2	-3.38	118.10	120.19
2	H	401	PLP	C6-N1-C2	3.19	125.08	119.17
2	D	401	PLP	O4A-C4A-C4	-3.10	118.15	124.91
2	F	401	PLP	C4-C3-C2	-2.92	118.38	120.19
2	D	401	PLP	C6-N1-C2	2.88	124.50	119.17
2	C	401	PLP	C3-C4-C5	-2.86	116.06	118.26
2	J	401	PLP	C2A-C2-C3	-2.79	117.44	120.89
2	A	401	PLP	O4A-C4A-C4	-2.71	119.00	124.91
2	G	401	PLP	O4A-C4A-C4	-2.69	119.05	124.91
2	C	401	PLP	C3-C4-C4A	2.69	123.71	119.90
2	A	401	PLP	C3-C4-C5	-2.63	116.24	118.26
2	F	401	PLP	C3-C4-C5	-2.61	116.26	118.26
2	B	401	PLP	C2A-C2-C3	-2.61	117.67	120.89
2	H	401	PLP	C2A-C2-N1	2.58	122.71	117.67
2	K	401	PLP	C6-N1-C2	2.52	123.83	119.17
2	F	401	PLP	O4A-C4A-C4	-2.49	119.49	124.91
2	B	401	PLP	O4A-C4A-C4	-2.46	119.54	124.91
2	G	401	PLP	O2P-P-O4P	-2.44	100.23	106.73
2	F	401	PLP	C6-N1-C2	2.44	123.68	119.17
2	E	401	PLP	C6-N1-C2	2.43	123.67	119.17
2	G	401	PLP	C6-N1-C2	2.41	123.63	119.17
2	B	401	PLP	C2A-C2-N1	2.40	122.37	117.67
2	I	401	PLP	C3-C4-C5	-2.40	116.42	118.26
2	L	401	PLP	O4A-C4A-C4	-2.37	119.74	124.91
2	I	401	PLP	O3P-P-O2P	2.35	116.62	107.64
2	L	401	PLP	C6-N1-C2	2.32	123.47	119.17
2	J	401	PLP	C3-C4-C5	-2.31	116.49	118.26
2	E	401	PLP	C3-C4-C5	-2.28	116.51	118.26
2	I	401	PLP	C4-C3-C2	-2.24	118.80	120.19
2	B	401	PLP	C6-N1-C2	2.23	123.30	119.17
2	B	401	PLP	C3-C4-C5	-2.23	116.55	118.26
2	C	401	PLP	C6-N1-C2	2.19	123.23	119.17
2	E	401	PLP	O3P-P-O4P	-2.19	100.91	106.73
2	A	401	PLP	C6-N1-C2	2.11	123.07	119.17
2	F	401	PLP	C2A-C2-N1	2.10	121.78	117.67
2	D	401	PLP	C2A-C2-N1	2.09	121.75	117.67
2	E	401	PLP	C3-C4-C4A	2.09	122.85	119.90
2	J	401	PLP	C3-C4-C4A	2.08	122.84	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	PLP	O4A-C4A-C4	-2.06	120.41	124.91
2	L	401	PLP	C3-C4-C5	-2.03	116.70	118.26
2	G	401	PLP	C2A-C2-N1	2.02	121.62	117.67
2	K	401	PLP	C3-C4-C4A	2.01	122.75	119.90
2	J	401	PLP	O4A-C4A-C4	-2.01	120.54	124.91
2	I	401	PLP	C2A-C2-C3	-2.00	118.42	120.89
2	I	401	PLP	C2A-C2-N1	2.00	121.58	117.67

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	E	401	PLP	2	0
2	F	401	PLP	1	0
2	G	401	PLP	2	0
2	B	401	PLP	1	0
2	H	401	PLP	3	0
2	J	401	PLP	2	0
2	K	401	PLP	1	0
2	D	401	PLP	3	0
2	L	401	PLP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	319/330 (96%)	-0.19	3 (0%)	84	83	22, 29, 45, 63	0
1	B	322/330 (97%)	-0.23	5 (1%)	72	70	21, 28, 42, 74	0
1	C	320/330 (96%)	-0.20	6 (1%)	66	65	22, 31, 45, 61	0
1	D	321/330 (97%)	-0.23	4 (1%)	79	77	19, 27, 41, 60	0
1	E	320/330 (96%)	0.06	9 (2%)	53	51	24, 37, 55, 69	0
1	F	321/330 (97%)	-0.07	9 (2%)	53	51	20, 32, 49, 68	0
1	G	320/330 (96%)	-0.14	5 (1%)	72	70	19, 29, 47, 60	0
1	H	320/330 (96%)	-0.21	5 (1%)	72	70	19, 29, 44, 61	0
1	I	319/330 (96%)	-0.01	11 (3%)	45	43	25, 36, 52, 69	0
1	J	318/330 (96%)	-0.06	6 (1%)	66	65	22, 33, 54, 67	0
1	K	319/330 (96%)	0.13	14 (4%)	34	32	25, 38, 53, 69	0
1	L	317/330 (96%)	0.58	31 (9%)	7	6	31, 55, 73, 84	0
All	All	3836/3960 (96%)	-0.05	108 (2%)	53	51	19, 33, 58, 84	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	28	LEU	5.2
1	A	11	VAL	5.1
1	L	15	ASP	4.7
1	F	141	THR	4.6
1	G	10	ILE	4.6
1	D	10	ILE	4.5
1	K	11	VAL	4.4
1	B	9	GLU	4.4
1	L	300	ASP	4.2
1	E	25	ASP	4.2
1	B	8	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	278	VAL	4.0
1	E	10	ILE	3.9
1	I	11	VAL	3.9
1	B	10	ILE	3.9
1	L	25	ASP	3.8
1	G	31	ALA	3.7
1	L	31	ALA	3.7
1	I	25	ASP	3.7
1	H	10	ILE	3.7
1	L	13	THR	3.6
1	F	10	ILE	3.6
1	K	31	ALA	3.6
1	L	321	PRO	3.6
1	C	11	VAL	3.5
1	F	9	GLU	3.5
1	K	25	ASP	3.5
1	K	30	PRO	3.4
1	I	141	THR	3.4
1	B	11	VAL	3.3
1	L	228	VAL	3.3
1	K	27	GLU	3.3
1	F	140	ILE	3.2
1	J	25	ASP	3.2
1	I	30	PRO	3.2
1	L	279	LEU	3.2
1	L	27	GLU	3.1
1	I	15	ASP	3.0
1	C	10	ILE	3.0
1	L	141	THR	2.9
1	K	140	ILE	2.8
1	K	141	THR	2.7
1	B	72	VAL	2.7
1	K	28	LEU	2.7
1	I	228	VAL	2.7
1	J	15	ASP	2.7
1	L	297	SER	2.6
1	A	25	ASP	2.6
1	I	279	LEU	2.6
1	D	329	GLN	2.5
1	K	320	GLU	2.5
1	A	12	TYR	2.5
1	L	319	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	300	ASP	2.5
1	G	15	ASP	2.4
1	F	259	GLY	2.4
1	L	29	ASP	2.4
1	F	300	ASP	2.4
1	L	26	TYR	2.4
1	E	17	GLY	2.4
1	G	17	GLY	2.4
1	L	19	ASP	2.4
1	E	278	VAL	2.4
1	L	329	GLN	2.4
1	H	25	ASP	2.3
1	L	14	HIS	2.3
1	L	168	HIS	2.3
1	C	329	GLN	2.3
1	L	30	PRO	2.3
1	J	278	VAL	2.3
1	E	138	ARG	2.3
1	L	287	VAL	2.3
1	L	305	PRO	2.3
1	K	259	GLY	2.2
1	L	24	SER	2.2
1	G	25	ASP	2.2
1	H	141	THR	2.2
1	L	311	ILE	2.2
1	K	322	SER	2.2
1	F	321	PRO	2.2
1	H	279	LEU	2.2
1	L	295	GLY	2.2
1	E	228	VAL	2.1
1	H	11	VAL	2.1
1	J	31	ALA	2.1
1	E	27	GLU	2.1
1	C	25	ASP	2.1
1	J	29	ASP	2.1
1	D	321	PRO	2.1
1	E	14	HIS	2.1
1	I	12	TYR	2.1
1	F	25	ASP	2.1
1	L	32	ASN	2.1
1	I	17	GLY	2.1
1	J	17	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	26	TYR	2.1
1	K	26	TYR	2.1
1	E	142	LYS	2.1
1	C	29	ASP	2.1
1	D	25	ASP	2.1
1	L	159	PRO	2.1
1	L	155	GLN	2.0
1	F	19	ASP	2.0
1	K	297	SER	2.0
1	K	300	ASP	2.0
1	L	327	PRO	2.0
1	C	28	LEU	2.0
1	L	257	SER	2.0

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. The B-factors column lists the minimum, median, 95^{th} 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
1	CSO	K	152	7/8	0.79	0.15	39,41,47,47	0
1	CSO	L	152	7/8	0.86	0.14	51,51,53,53	0
1	CSO	C	152	7/8	0.88	0.12	30,32,35,36	0
1	CSO	F	152	7/8	0.92	0.11	27,29,34,35	0
1	CSO	I	152	7/8	0.92	0.09	39,40,41,43	0
1	CSO	E	152	7/8	0.92	0.12	30,31,35,36	0
1	CSO	D	152	7/8	0.92	0.11	24,25,28,29	0
1	CSO	A	152	7/8	0.93	0.10	28,29,31,33	0
1	CSO	J	152	7/8	0.93	0.10	35,37,44,44	0
1	CSO	B	152	7/8	0.95	0.09	28,28,31,34	0
1	CSO	G	152	7/8	0.95	0.09	25,27,30,30	0
1	CSO	H	152	7/8	0.96	0.08	24,25,28,30	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	K	401	16/16	0.94	0.14	29,36,42,47	0
2	PLP	L	401	16/16	0.94	0.12	34,43,51,54	0
2	PLP	J	401	16/16	0.95	0.12	22,27,36,39	0
2	PLP	B	401	16/16	0.95	0.14	22,27,30,31	0
2	PLP	I	401	16/16	0.95	0.12	22,34,41,43	0
2	PLP	A	401	16/16	0.96	0.12	24,28,36,38	0
2	PLP	G	401	16/16	0.96	0.12	22,25,31,35	0
2	PLP	C	401	16/16	0.96	0.13	25,30,36,38	0
2	PLP	D	401	16/16	0.96	0.11	20,23,32,32	0
2	PLP	H	401	16/16	0.96	0.13	24,25,31,35	0
2	PLP	E	401	16/16	0.97	0.10	28,38,43,43	0
2	PLP	F	401	16/16	0.97	0.10	24,29,33,33	0

6.5 Other polymers

There are no such residues in this entry.