



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:48 am GMT

PDB ID : 5FR9
Title : Structure of transaminase ATA-117 arRmut11 from *Arthrobacter* sp. KNK168 inhibited with 1-(4-Bromophenyl)-2-fluoroethylamine
Authors : Cuetos, A.; Kroutil, W.; Lavandera, I.; Grogan, G.
Deposited on : 2015-12-16
Resolution : 2.81 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

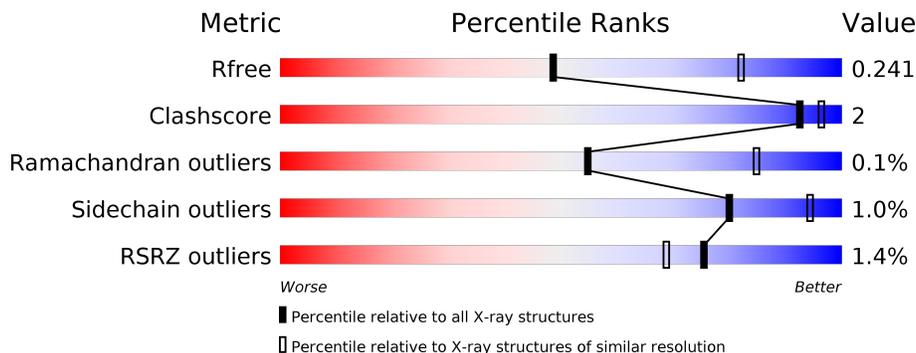
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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.



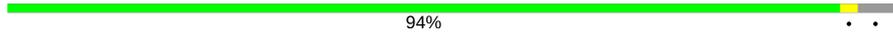
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2917 (2.84-2.80)
Clashscore	112137	3382 (2.84-2.80)
Ramachandran outliers	110173	3324 (2.84-2.80)
Sidechain outliers	110143	3326 (2.84-2.80)
RSRZ outliers	101464	2948 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	91% 5% .
1	B	333	91% . . .
1	C	333	93% . . .
1	D	333	92% . . .
1	E	333	2% 92% . .
1	F	333	% 92% . . .

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Mol	Chain	Length	Quality of chain
1	G	333	 94% . .
1	H	333	 92% . . .
1	I	333	 95% . .
1	J	333	 92% . . .
1	K	333	 91% . . .
1	L	333	 91% . . 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29531 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
			Total	C	N	O	S			
1	A	319	Total 2445	C 1559	N 413	O 467	S 6	0	0	0
1	B	320	Total 2473	C 1577	N 417	O 473	S 6	0	0	0
1	C	321	Total 2429	C 1553	N 408	O 462	S 6	0	0	0
1	D	322	Total 2496	C 1591	N 423	O 476	S 6	0	0	0
1	E	321	Total 2374	C 1519	N 403	O 446	S 6	0	0	0
1	F	322	Total 2461	C 1575	N 413	O 467	S 6	0	0	0
1	G	321	Total 2465	C 1574	N 415	O 470	S 6	0	0	0
1	H	321	Total 2469	C 1578	N 415	O 470	S 6	0	0	0
1	I	320	Total 2289	C 1465	N 392	O 427	S 5	0	0	0
1	J	319	Total 2406	C 1538	N 407	O 455	S 6	0	0	0
1	K	319	Total 2347	C 1492	N 407	O 442	S 6	0	0	0
1	L	318	Total 2280	C 1452	N 389	O 433	S 6	0	0	0

There are 372 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	331	ALA	-	EXPRESSION TAG	UNP F7J696
A	332	LEU	-	EXPRESSION TAG	UNP F7J696
A	333	GLU	-	EXPRESSION TAG	UNP F7J696
A	8	PRO	SER	ENGINEERED MUTATION	UNP F7J696
A	60	PHE	TYR	ENGINEERED MUTATION	UNP F7J696

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Chain	Residue	Modelled	Actual	Comment	Reference
A	61	TYR	LEU	ENGINEERED MUTATION	UNP F7J696
A	62	THR	HIS	ENGINEERED MUTATION	UNP F7J696
A	65	ALA	VAL	ENGINEERED MUTATION	UNP F7J696
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	CYS	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	331	ALA	-	EXPRESSION TAG	UNP F7J696
B	332	LEU	-	EXPRESSION TAG	UNP F7J696
B	333	GLU	-	EXPRESSION TAG	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	150	SER	TYR	ENGINEERED MUTATION	UNP F7J696
B	152	CYS	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
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	331	ALA	-	EXPRESSION TAG	UNP F7J696
C	332	LEU	-	EXPRESSION TAG	UNP F7J696
C	333	GLU	-	EXPRESSION TAG	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	CYS	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	331	ALA	-	EXPRESSION TAG	UNP F7J696
D	332	LEU	-	EXPRESSION TAG	UNP F7J696
D	333	GLU	-	EXPRESSION TAG	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
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	CYS	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	331	ALA	-	EXPRESSION TAG	UNP F7J696
E	332	LEU	-	EXPRESSION TAG	UNP F7J696
E	333	GLU	-	EXPRESSION TAG	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	CYS	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
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	331	ALA	-	EXPRESSION TAG	UNP F7J696
F	332	LEU	-	EXPRESSION TAG	UNP F7J696
F	333	GLU	-	EXPRESSION TAG	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	CYS	VAL	ENGINEERED MUTATION	UNP F7J696

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Chain	Residue	Modelled	Actual	Comment	Reference
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	331	ALA	-	EXPRESSION TAG	UNP F7J696
G	332	LEU	-	EXPRESSION TAG	UNP F7J696
G	333	GLU	-	EXPRESSION TAG	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
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	CYS	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

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Chain	Residue	Modelled	Actual	Comment	Reference
G	306	VAL	ILE	ENGINEERED MUTATION	UNP F7J696
G	321	PRO	SER	ENGINEERED MUTATION	UNP F7J696
H	331	ALA	-	EXPRESSION TAG	UNP F7J696
H	332	LEU	-	EXPRESSION TAG	UNP F7J696
H	333	GLU	-	EXPRESSION TAG	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	CYS	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
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	331	ALA	-	EXPRESSION TAG	UNP F7J696
I	332	LEU	-	EXPRESSION TAG	UNP F7J696
I	333	GLU	-	EXPRESSION TAG	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	CYS	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	331	ALA	-	EXPRESSION TAG	UNP F7J696
J	332	LEU	-	EXPRESSION TAG	UNP F7J696
J	333	GLU	-	EXPRESSION TAG	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
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	CYS	VAL	ENGINEERED MUTATION	UNP F7J696
J	169	LEU	ALA	ENGINEERED MUTATION	UNP F7J696
J	199	ILE	VAL	ENGINEERED MUTATION	UNP F7J696

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Chain	Residue	Modelled	Actual	Comment	Reference
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	331	ALA	-	EXPRESSION TAG	UNP F7J696
K	332	LEU	-	EXPRESSION TAG	UNP F7J696
K	333	GLU	-	EXPRESSION TAG	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	CYS	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
L	331	ALA	-	EXPRESSION TAG	UNP F7J696
L	332	LEU	-	EXPRESSION TAG	UNP F7J696
L	333	GLU	-	EXPRESSION TAG	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	CYS	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 [4-[3-(4-BROMOPHENYL)-3-OXIDANYLIDENE-PROPYL]-6-METHYL-5-OXIDANYL-PYRIDIN-3-YL]METHYL PHOSPHATE (three-letter code: 9HC) (formula: C₁₆H₁₅BrNO₆P).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	35	Total O 35 35	0	0
3	B	41	Total O 41 41	0	0
3	C	20	Total O 20 20	0	0
3	D	60	Total O 60 60	0	0
3	E	6	Total O 6 6	0	0
3	F	22	Total O 22 22	0	0
3	G	40	Total O 40 40	0	0
3	H	28	Total O 28 28	0	0
3	I	5	Total O 5 5	0	0
3	J	28	Total O 28 28	0	0
3	K	4	Total O 4 4	0	0
3	L	8	Total O 8 8	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 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

Chain F: 



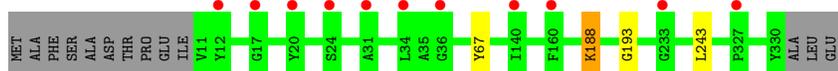
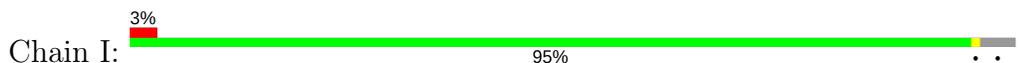
● Molecule 1: (R)-AMINE TRANSAMINASE



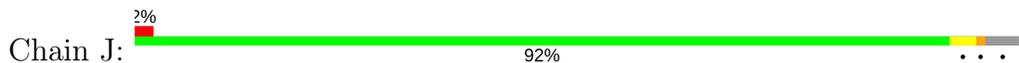
● Molecule 1: (R)-AMINE TRANSAMINASE



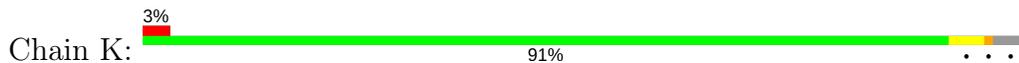
● Molecule 1: (R)-AMINE TRANSAMINASE



● Molecule 1: (R)-AMINE TRANSAMINASE



● Molecule 1: (R)-AMINE TRANSAMINASE



● Molecule 1: (R)-AMINE TRANSAMINASE



LEU
GLU

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.15Å 135.51Å 197.32Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	194.08 – 2.81 48.52 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.3 (194.08-2.81) 99.3 (48.52-2.81)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.210 , 0.239 0.214 , 0.241	Depositor DCC
R_{free} test set	5274 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	62.2	Xtrriage
Anisotropy	0.501	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29531	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.21 % 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 $6.0435e-04$. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 9HC

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	0.62	0/2508	0.73	3/3435 (0.1%)
1	B	0.64	1/2537 (0.0%)	0.73	3/3473 (0.1%)
1	C	0.64	1/2493 (0.0%)	0.77	6/3419 (0.2%)
1	D	0.67	0/2560	0.83	9/3503 (0.3%)
1	E	0.67	4/2437 (0.2%)	0.75	6/3346 (0.2%)
1	F	0.64	0/2525	0.79	10/3460 (0.3%)
1	G	0.67	1/2529 (0.0%)	0.73	2/3464 (0.1%)
1	H	0.62	0/2533	0.76	6/3469 (0.2%)
1	I	0.61	0/2347	0.69	0/3231
1	J	0.67	1/2469 (0.0%)	0.80	3/3385 (0.1%)
1	K	0.64	0/2409	0.82	11/3308 (0.3%)
1	L	0.66	0/2338	0.78	5/3216 (0.2%)
All	All	0.64	8/29685 (0.0%)	0.77	64/40709 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	85	GLU	CD-OE1	-9.46	1.15	1.25
1	E	85	GLU	CD-OE2	-7.59	1.17	1.25
1	E	85	GLU	CD-OE1	7.45	1.33	1.25
1	G	215	CYS	CB-SG	-7.16	1.70	1.82
1	C	323	SER	CA-CB	6.65	1.62	1.52
1	E	215	CYS	CB-SG	-6.42	1.71	1.82
1	E	321	PRO	C-O	5.29	1.33	1.23
1	B	17	GLY	N-CA	-5.12	1.38	1.46

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	161	ASP	CB-CG-OD2	16.71	133.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	161	ASP	CB-CG-OD1	-13.11	106.50	118.30
1	D	162	ARG	NE-CZ-NH2	-10.72	114.94	120.30
1	D	162	ARG	NE-CZ-NH1	10.43	125.52	120.30
1	L	325	LEU	CB-CG-CD1	-10.25	93.57	111.00
1	C	122	MET	CA-CB-CG	10.21	130.65	113.30
1	K	325	LEU	CB-CG-CD1	-10.08	93.86	111.00
1	K	312	ARG	NE-CZ-NH1	9.57	125.09	120.30
1	K	122	MET	CG-SD-CE	9.10	114.76	100.20
1	H	18	LEU	CB-CG-CD1	8.89	126.12	111.00
1	K	162	ARG	CG-CD-NE	8.76	130.20	111.80
1	D	52	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	E	85	GLU	CG-CD-OE1	8.57	135.45	118.30
1	D	52	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	G	208	GLU	OE1-CD-OE2	-8.36	113.27	123.30
1	C	122	MET	CG-SD-CE	8.16	113.25	100.20
1	F	19	ASP	CB-CG-OD1	8.08	125.57	118.30
1	C	162	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	F	162	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	K	19	ASP	CB-CG-OD2	-7.42	111.63	118.30
1	E	85	GLU	CG-CD-OE2	-6.93	104.44	118.30
1	H	162	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	F	52	ARG	CD-NE-CZ	6.66	132.93	123.60
1	E	321	PRO	N-CA-C	6.58	129.22	112.10
1	H	133	SER	CA-CB-OG	6.45	128.62	111.20
1	A	96	LEU	CA-CB-CG	6.43	130.09	115.30
1	D	96	LEU	CA-CB-CG	6.43	130.09	115.30
1	E	162	ARG	CG-CD-NE	6.41	125.26	111.80
1	K	312	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	96	LEU	CA-CB-CG	6.34	129.88	115.30
1	K	133	SER	CA-CB-OG	6.32	128.27	111.20
1	F	133	SER	CA-CB-OG	6.31	128.24	111.20
1	E	162	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	H	133	SER	N-CA-CB	-6.09	101.36	110.50
1	H	162	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	K	325	LEU	CA-CB-CG	5.92	128.91	115.30
1	B	96	LEU	CB-CG-CD1	5.87	120.98	111.00
1	D	96	LEU	CB-CG-CD1	5.85	120.95	111.00
1	A	96	LEU	CB-CG-CD1	5.83	120.91	111.00
1	C	162	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	236	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	F	52	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	F	133	SER	N-CA-CB	-5.75	101.88	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	23	TYR	N-CA-CB	5.72	120.90	110.60
1	F	162	ARG	CA-CB-CG	-5.72	100.82	113.40
1	C	323	SER	N-CA-CB	5.68	119.02	110.50
1	B	236	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	K	133	SER	N-CA-CB	-5.60	102.10	110.50
1	E	325	LEU	CA-CB-CG	5.54	128.04	115.30
1	F	52	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	D	325	LEU	CA-CB-CG	5.45	127.84	115.30
1	K	19	ASP	CB-CG-OD1	5.36	123.12	118.30
1	J	236	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	L	299	SER	CB-CA-C	-5.32	99.99	110.10
1	A	236	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	F	236	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	L	236	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	K	236	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	G	236	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	236	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	F	188	LYS	CD-CE-NZ	5.11	123.45	111.70
1	H	42	GLU	CG-CD-OE2	-5.03	108.25	118.30
1	L	301	GLY	N-CA-C	5.03	125.66	113.10
1	D	308	GLN	CG-CD-OE1	-5.01	111.57	121.60

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	2445	0	2348	13	0
1	B	2473	0	2383	15	0
1	C	2429	0	2301	13	1
1	D	2496	0	2413	14	0
1	E	2374	0	2191	6	0
1	F	2461	0	2364	10	0
1	G	2465	0	2368	6	0
1	H	2469	0	2379	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2289	0	2091	3	0
1	J	2406	0	2284	7	0
1	K	2347	0	2163	15	1
1	L	2280	0	2053	11	0
2	A	25	0	0	1	0
2	B	25	0	0	0	0
2	C	25	0	0	1	0
2	D	25	0	0	1	0
2	E	25	0	0	0	0
2	F	25	0	0	0	0
2	G	25	0	0	0	0
2	H	25	0	0	0	0
2	I	25	0	0	0	0
2	J	25	0	0	0	0
2	K	25	0	0	0	0
2	L	25	0	0	0	0
3	A	35	0	0	0	0
3	B	41	0	0	0	0
3	C	20	0	0	0	0
3	D	60	0	0	0	0
3	E	6	0	0	0	0
3	F	22	0	0	0	0
3	G	40	0	0	0	0
3	H	28	0	0	0	0
3	I	5	0	0	0	0
3	J	28	0	0	0	0
3	K	4	0	0	0	0
3	L	8	0	0	0	0
All	All	29531	0	27338	103	1

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 2.

All (103) 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:K:122:MET:HE2	1:K:155:GLN:H	1.05	1.17
1:F:122:MET:HE2	1:F:155:GLN:H	1.03	1.12
1:D:122:MET:HE2	1:D:155:GLN:H	0.93	1.09
1:L:122:MET:HE2	1:L:155:GLN:N	1.67	1.08
1:K:122:MET:HE2	1:K:155:GLN:N	1.70	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:MET:HE2	1:D:155:GLN:N	1.71	1.06
1:L:122:MET:HE2	1:L:155:GLN:H	0.88	1.04
1:K:122:MET:CE	1:K:155:GLN:H	1.76	0.97
1:F:122:MET:HE2	1:F:155:GLN:N	1.80	0.96
1:B:258:LEU:HD23	1:D:305:PRO:HB2	1.53	0.90
1:D:122:MET:CE	1:D:155:GLN:H	1.83	0.89
1:F:122:MET:CE	1:F:155:GLN:H	1.90	0.84
1:L:122:MET:CE	1:L:155:GLN:H	1.83	0.83
1:K:122:MET:HE3	1:K:155:GLN:O	1.84	0.78
1:J:16:THR:HG22	1:J:18:LEU:H	1.50	0.76
1:K:122:MET:CE	1:K:155:GLN:O	2.34	0.76
1:L:299:SER:O	1:L:300:ASP:CB	2.38	0.72
1:C:122:MET:HE2	1:C:155:GLN:H	1.54	0.70
1:B:16:THR:O	1:B:18:LEU:N	2.21	0.70
1:B:133:SER:OG	1:B:143:HIS:HD2	1.78	0.67
1:A:133:SER:OG	1:A:143:HIS:HD2	1.77	0.67
1:B:16:THR:HG22	1:B:160:PHE:CZ	2.30	0.67
1:E:133:SER:OG	1:E:143:HIS:HD2	1.80	0.65
1:G:52:ARG:O	1:H:52:ARG:NH1	2.28	0.65
1:D:122:MET:HG2	1:D:154:TYR:HA	1.79	0.64
1:L:122:MET:HG2	1:L:154:TYR:HA	1.80	0.64
1:G:42:GLU:OE2	1:H:52:ARG:NH2	2.31	0.63
1:F:122:MET:HG2	1:F:154:TYR:HA	1.83	0.61
1:J:191:GLN:HE22	1:L:193:GLY:H	1.48	0.60
1:C:191:GLN:HE22	1:E:193:GLY:H	1.48	0.59
1:K:122:MET:CE	1:K:155:GLN:N	2.48	0.59
1:A:52:ARG:O	1:B:52:ARG:NH1	2.35	0.59
1:G:52:ARG:NH2	1:H:42:GLU:OE2	2.36	0.59
1:J:16:THR:HG22	1:J:18:LEU:N	2.18	0.59
1:D:193:GLY:H	1:F:191:GLN:HE22	1.51	0.58
1:D:122:MET:CE	1:D:155:GLN:O	2.51	0.58
1:I:193:GLY:H	1:K:191:GLN:HE22	1.52	0.58
1:C:157:ILE:HD11	2:C:1331:9HC:CAH	2.34	0.57
1:G:193:GLY:H	1:H:191:GLN:HE22	1.52	0.57
1:A:133:SER:OG	1:A:143:HIS:CD2	2.58	0.56
1:C:122:MET:CE	1:C:155:GLN:H	2.18	0.56
1:B:133:SER:OG	1:B:143:HIS:CD2	2.58	0.56
1:L:122:MET:CE	1:L:155:GLN:O	2.54	0.56
1:A:193:GLY:H	1:B:191:GLN:HE22	1.54	0.55
1:A:191:GLN:HE22	1:B:193:GLY:H	1.54	0.54
1:B:258:LEU:CD2	1:D:305:PRO:HB2	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:MET:CE	1:F:155:GLN:O	2.55	0.54
1:E:133:SER:OG	1:E:143:HIS:CD2	2.60	0.53
1:A:305:PRO:HB2	1:C:258:LEU:HD23	1.91	0.52
1:C:122:MET:HE2	1:C:155:GLN:HB2	1.91	0.52
1:K:188:LYS:HD2	1:K:243:LEU:CD2	2.40	0.52
1:B:162:ARG:HG3	1:B:162:ARG:NH1	2.25	0.51
1:G:191:GLN:HE22	1:H:193:GLY:H	1.57	0.51
1:D:191:GLN:HE22	1:F:193:GLY:H	1.58	0.51
1:J:188:LYS:HD2	1:J:243:LEU:CD2	2.40	0.51
1:C:188:LYS:HD2	1:C:243:LEU:CD2	2.42	0.50
1:K:325:LEU:HD12	1:K:325:LEU:N	2.26	0.50
1:L:188:LYS:HD2	1:L:243:LEU:CD2	2.41	0.50
1:B:16:THR:O	1:B:16:THR:OG1	2.30	0.49
1:A:162:ARG:NH2	1:A:208:GLU:OE2	2.46	0.48
1:G:188:LYS:HD2	1:G:243:LEU:CD2	2.44	0.48
1:L:229:VAL:HG12	1:L:236:ARG:HB2	1.96	0.48
1:C:122:MET:HE2	1:C:155:GLN:N	2.27	0.48
1:A:188:LYS:HD2	1:A:243:LEU:CD2	2.43	0.48
1:J:16:THR:HG21	1:J:21:ILE:HB	1.94	0.48
1:H:188:LYS:HD2	1:H:243:LEU:CD2	2.43	0.48
1:F:188:LYS:HD2	1:F:243:LEU:CD2	2.44	0.48
1:C:330:TYR:N	1:C:330:TYR:CD1	2.82	0.48
1:D:188:LYS:HD2	1:D:243:LEU:CD2	2.44	0.47
1:F:133:SER:HG	1:F:143:HIS:CE1	2.27	0.47
1:B:188:LYS:HD2	1:B:243:LEU:CD2	2.44	0.47
1:A:258:LEU:HD23	1:C:305:PRO:HB2	1.97	0.47
1:A:96:LEU:HD13	1:A:127:ILE:HG22	1.97	0.47
1:E:188:LYS:HD2	1:E:243:LEU:CD2	2.45	0.46
1:I:188:LYS:HD2	1:I:243:LEU:CD2	2.46	0.45
1:K:122:MET:HG2	1:K:154:TYR:HA	1.98	0.45
1:D:96:LEU:HD13	1:D:127:ILE:HG22	1.99	0.45
1:I:67:TYR:CE1	1:I:188:LYS:HG2	2.53	0.43
1:B:96:LEU:HD13	1:B:127:ILE:HG22	1.99	0.43
1:C:188:LYS:HD2	1:C:243:LEU:HD22	2.01	0.43
1:C:122:MET:HE2	1:C:155:GLN:CB	2.48	0.43
1:C:122:MET:HE1	1:C:155:GLN:O	2.19	0.43
1:K:122:MET:CG	1:K:154:TYR:HA	2.49	0.43
1:A:155:GLN:HB3	2:A:1331:9HC:BR	2.74	0.42
1:D:162:ARG:NH1	1:D:208:GLU:OE2	2.52	0.42
1:E:122:MET:HE2	1:E:284:GLY:HA2	2.00	0.42
1:F:162:ARG:NH1	1:F:166:GLY:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:188:LYS:HD2	1:J:243:LEU:HD22	2.02	0.42
1:H:133:SER:HG	1:H:143:HIS:CE1	2.28	0.42
1:A:42:GLU:OE2	1:B:52:ARG:NH2	2.53	0.41
1:K:188:LYS:HD2	1:K:243:LEU:HD21	2.02	0.41
1:K:68:THR:OG1	1:K:83:HIS:HD2	2.03	0.41
1:B:68:THR:OG1	1:B:83:HIS:HD2	2.04	0.41
1:J:68:THR:OG1	1:J:83:HIS:HD2	2.04	0.41
1:H:68:THR:OG1	1:H:83:HIS:HD2	2.04	0.41
1:L:188:LYS:HD2	1:L:243:LEU:HD22	2.02	0.41
1:D:67:TYR:CE1	1:D:188:LYS:HG2	2.56	0.41
1:E:68:THR:OG1	1:E:83:HIS:HD2	2.04	0.41
1:K:188:LYS:HD2	1:K:243:LEU:HD22	2.02	0.41
1:A:188:LYS:HD2	1:A:243:LEU:HD22	2.02	0.40
1:D:155:GLN:HB3	2:D:1331:9HC:BR	2.76	0.40
1:K:199:ILE:O	1:K:202:THR:HB	2.21	0.40
1:L:199:ILE:O	1:L:202:THR:HB	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:SER:OG	1:K:19:ASP:OD1[1_455]	2.16	0.04

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	317/333 (95%)	307 (97%)	10 (3%)	0	100	100
1	B	318/333 (96%)	307 (96%)	10 (3%)	1 (0%)	44	76
1	C	319/333 (96%)	308 (97%)	11 (3%)	0	100	100
1	D	320/333 (96%)	310 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	319/333 (96%)	308 (97%)	10 (3%)	1 (0%)	44	76
1	F	320/333 (96%)	310 (97%)	10 (3%)	0	100	100
1	G	319/333 (96%)	308 (97%)	11 (3%)	0	100	100
1	H	319/333 (96%)	308 (97%)	11 (3%)	0	100	100
1	I	318/333 (96%)	307 (96%)	11 (4%)	0	100	100
1	J	317/333 (95%)	307 (97%)	10 (3%)	0	100	100
1	K	317/333 (95%)	307 (97%)	10 (3%)	0	100	100
1	L	316/333 (95%)	304 (96%)	11 (4%)	1 (0%)	44	76
All	All	3819/3996 (96%)	3691 (97%)	125 (3%)	3 (0%)	55	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	300	ASP
1	B	17	GLY
1	E	321	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	260/283 (92%)	257 (99%)	3 (1%)	75	93
1	B	265/283 (94%)	262 (99%)	3 (1%)	78	94
1	C	252/283 (89%)	249 (99%)	3 (1%)	75	93
1	D	268/283 (95%)	265 (99%)	3 (1%)	78	94
1	E	232/283 (82%)	231 (100%)	1 (0%)	93	98
1	F	260/283 (92%)	258 (99%)	2 (1%)	85	95
1	G	262/283 (93%)	261 (100%)	1 (0%)	93	98
1	H	263/283 (93%)	259 (98%)	4 (2%)	70	91
1	I	216/283 (76%)	215 (100%)	1 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	249/283 (88%)	244 (98%)	5 (2%)	60	87
1	K	231/283 (82%)	229 (99%)	2 (1%)	82	95
1	L	215/283 (76%)	212 (99%)	3 (1%)	71	91
All	All	2973/3396 (88%)	2942 (99%)	31 (1%)	80	94

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	188	LYS
1	A	309	SER
1	B	52	ARG
1	B	96	LEU
1	B	162	ARG
1	C	122	MET
1	C	188	LYS
1	C	323	SER
1	D	96	LEU
1	D	155	GLN
1	D	188	LYS
1	E	155	GLN
1	F	155	GLN
1	F	188	LYS
1	G	188	LYS
1	H	18	LEU
1	H	52	ARG
1	H	159	PRO
1	H	188	LYS
1	I	188	LYS
1	J	16	THR
1	J	85	GLU
1	J	188	LYS
1	J	309	SER
1	J	329	GLN
1	K	122	MET
1	K	152	CYS
1	L	229	VAL
1	L	309	SER
1	L	325	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such

sidechains are listed below:

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	9HC	A	1331	1	26,26,26	0.38	0	34,37,37	0.66	0
2	9HC	B	1331	1	26,26,26	0.38	0	34,37,37	0.70	1 (2%)
2	9HC	C	1331	1	26,26,26	0.42	0	34,37,37	0.72	0
2	9HC	D	1331	1	26,26,26	0.48	0	34,37,37	0.81	0
2	9HC	E	1331	1	26,26,26	0.42	0	34,37,37	0.87	1 (2%)
2	9HC	F	1331	1	26,26,26	0.45	0	34,37,37	0.81	1 (2%)
2	9HC	G	1331	1	26,26,26	0.45	0	34,37,37	0.94	2 (5%)
2	9HC	H	1331	1	26,26,26	0.52	0	34,37,37	0.72	0
2	9HC	I	1331	1	26,26,26	0.42	0	34,37,37	0.77	0
2	9HC	J	1331	1	26,26,26	0.43	0	34,37,37	0.78	1 (2%)
2	9HC	K	1331	1	26,26,26	0.44	0	34,37,37	0.85	1 (2%)
2	9HC	L	1331	1	26,26,26	0.43	0	34,37,37	0.90	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9HC	A	1331	1	-	0/15/15/15	0/2/2/2
2	9HC	B	1331	1	-	0/15/15/15	0/2/2/2
2	9HC	C	1331	1	-	0/15/15/15	0/2/2/2
2	9HC	D	1331	1	-	0/15/15/15	0/2/2/2
2	9HC	E	1331	1	-	0/15/15/15	0/2/2/2
2	9HC	F	1331	1	-	0/15/15/15	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9HC	G	1331	1	-	0/15/15/15	0/2/2/2
2	9HC	H	1331	1	-	0/15/15/15	0/2/2/2
2	9HC	I	1331	1	-	0/15/15/15	0/2/2/2
2	9HC	J	1331	1	-	0/15/15/15	0/2/2/2
2	9HC	K	1331	1	-	0/15/15/15	0/2/2/2
2	9HC	L	1331	1	-	0/15/15/15	0/2/2/2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1331	9HC	CAM-CAN-CAX	-3.41	107.28	112.60
2	L	1331	9HC	CAM-CAN-CAX	-2.87	108.13	112.60
2	B	1331	9HC	CAM-CAN-CAX	-2.58	108.59	112.60
2	G	1331	9HC	CAM-CAN-CAX	-2.40	108.85	112.60
2	J	1331	9HC	CAM-CAN-CAX	-2.31	109.00	112.60
2	F	1331	9HC	OAF-PAY-OAQ	-2.10	101.14	106.73
2	K	1331	9HC	CAM-CAN-CAX	-2.08	109.36	112.60
2	L	1331	9HC	OAQ-CAO-CAV	2.14	113.63	109.32
2	G	1331	9HC	OAQ-CAO-CAV	2.59	114.53	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1331	9HC	1	0
2	C	1331	9HC	1	0
2	D	1331	9HC	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/333 (95%)	-0.22	1 (0%) 93 92	42, 61, 88, 109	0
1	B	320/333 (96%)	-0.29	0 100 100	40, 59, 80, 96	0
1	C	321/333 (96%)	-0.29	1 (0%) 93 92	45, 66, 97, 125	0
1	D	322/333 (96%)	-0.44	0 100 100	39, 53, 76, 114	0
1	E	321/333 (96%)	0.01	8 (2%) 58 47	49, 81, 104, 116	0
1	F	322/333 (96%)	-0.26	2 (0%) 89 86	42, 62, 83, 110	0
1	G	321/333 (96%)	-0.40	0 100 100	39, 57, 83, 114	0
1	H	321/333 (96%)	-0.33	2 (0%) 89 86	40, 60, 85, 100	0
1	I	320/333 (96%)	0.11	11 (3%) 46 34	54, 81, 120, 140	0
1	J	319/333 (95%)	-0.24	7 (2%) 62 52	41, 63, 93, 115	0
1	K	319/333 (95%)	0.12	11 (3%) 46 34	51, 77, 99, 119	0
1	L	318/333 (95%)	0.15	11 (3%) 44 33	49, 81, 113, 136	0
All	All	3843/3996 (96%)	-0.18	54 (1%) 75 69	39, 66, 99, 140	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	35	ALA	5.2
1	L	121	ALA	4.9
1	I	12	TYR	4.3
1	E	328	VAL	3.8
1	I	24	SER	3.7
1	I	20	TYR	3.4
1	L	319	VAL	3.3
1	I	34	LEU	3.3
1	E	326	THR	3.2
1	K	36	GLY	3.1
1	J	26	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	25	ASP	2.8
1	L	318	ASN	2.7
1	A	28	LEU	2.7
1	E	114	ALA	2.7
1	J	29	ASP	2.7
1	I	36	GLY	2.6
1	L	14	HIS	2.5
1	I	160	PHE	2.5
1	L	77	ALA	2.5
1	J	16	THR	2.5
1	I	17	GLY	2.4
1	I	31	ALA	2.4
1	L	151	ALA	2.4
1	K	23	TYR	2.4
1	I	140	ILE	2.4
1	I	327	PRO	2.3
1	L	118	LEU	2.3
1	E	77	ALA	2.3
1	I	233	GLY	2.3
1	K	318	ASN	2.2
1	E	14	HIS	2.2
1	L	36	GLY	2.2
1	H	26	TYR	2.2
1	E	259	GLY	2.2
1	K	26	TYR	2.2
1	J	233	GLY	2.1
1	K	121	ALA	2.1
1	C	43	GLY	2.1
1	K	319	VAL	2.1
1	F	119	ARG	2.1
1	K	15	ASP	2.1
1	J	160	PHE	2.1
1	K	113	VAL	2.1
1	L	300	ASP	2.1
1	E	319	VAL	2.1
1	K	117	GLU	2.1
1	L	122	MET	2.1
1	H	215	CYS	2.0
1	E	318	ASN	2.0
1	J	23	TYR	2.0
1	F	321	PRO	2.0
1	K	215	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	24	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q < 0.9
2	9HC	J	1331	25/25	0.95	0.17	-0.01	42,51,76,88	0
2	9HC	I	1331	25/25	0.93	0.16	-0.57	53,66,77,93	0
2	9HC	A	1331	25/25	0.94	0.16	-0.68	43,61,70,86	0
2	9HC	H	1331	25/25	0.96	0.14	-0.70	44,53,68,77	0
2	9HC	K	1331	25/25	0.91	0.14	-0.86	62,75,84,101	0
2	9HC	L	1331	25/25	0.94	0.14	-0.87	59,73,97,113	0
2	9HC	E	1331	25/25	0.92	0.13	-0.97	60,76,89,101	0
2	9HC	B	1331	25/25	0.96	0.14	-0.98	45,54,69,78	0
2	9HC	F	1331	25/25	0.96	0.14	-1.00	45,53,67,75	0
2	9HC	D	1331	25/25	0.97	0.14	-1.01	36,43,58,61	0
2	9HC	C	1331	25/25	0.95	0.14	-1.16	47,59,71,80	0
2	9HC	G	1331	25/25	0.97	0.12	-1.79	36,50,63,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.