



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 1, 2023 – 02:43 PM JST

PDB ID : 5I8I
Title : Crystal Structure of the K. lactis Urea Amidolyase
Authors : Zhao, J.; Xiang, S.
Deposited on : 2016-02-19
Resolution : 6.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

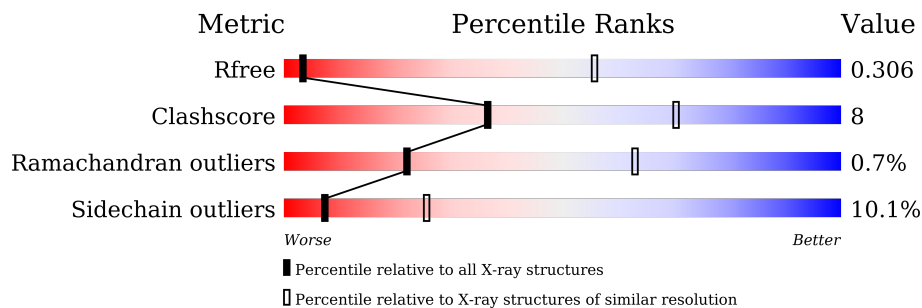
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 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	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)

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

Mol	Chain	Length	Quality of chain
1	A	1829	
1	B	1829	
1	C	1829	
1	D	1829	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 51722 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 Urea Amidolyase.

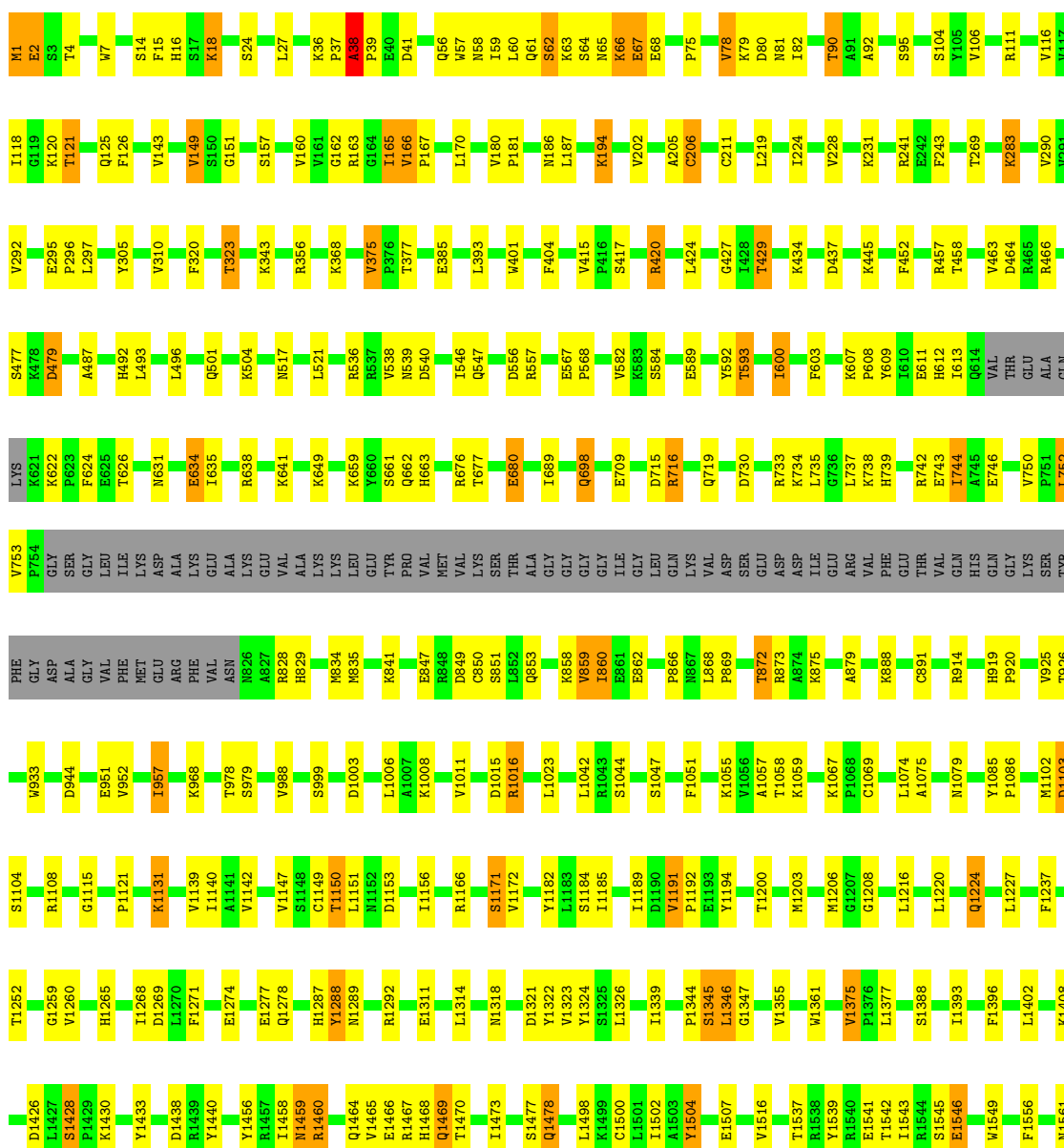
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1660	12939	8253	2183	2456	47	0	0	0
1	B	1658	12922	8243	2181	2452	46	0	0	0
1	C	1660	12939	8253	2183	2456	47	0	0	0
1	D	1658	12922	8243	2181	2452	46	0	0	0

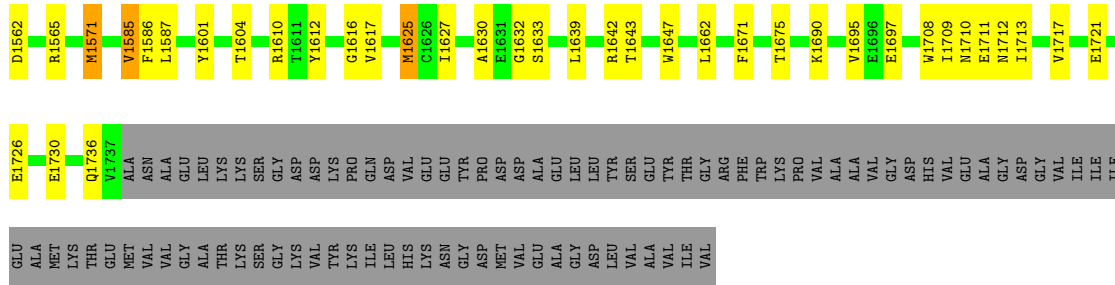
3 Residue-property plots

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. 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. 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.

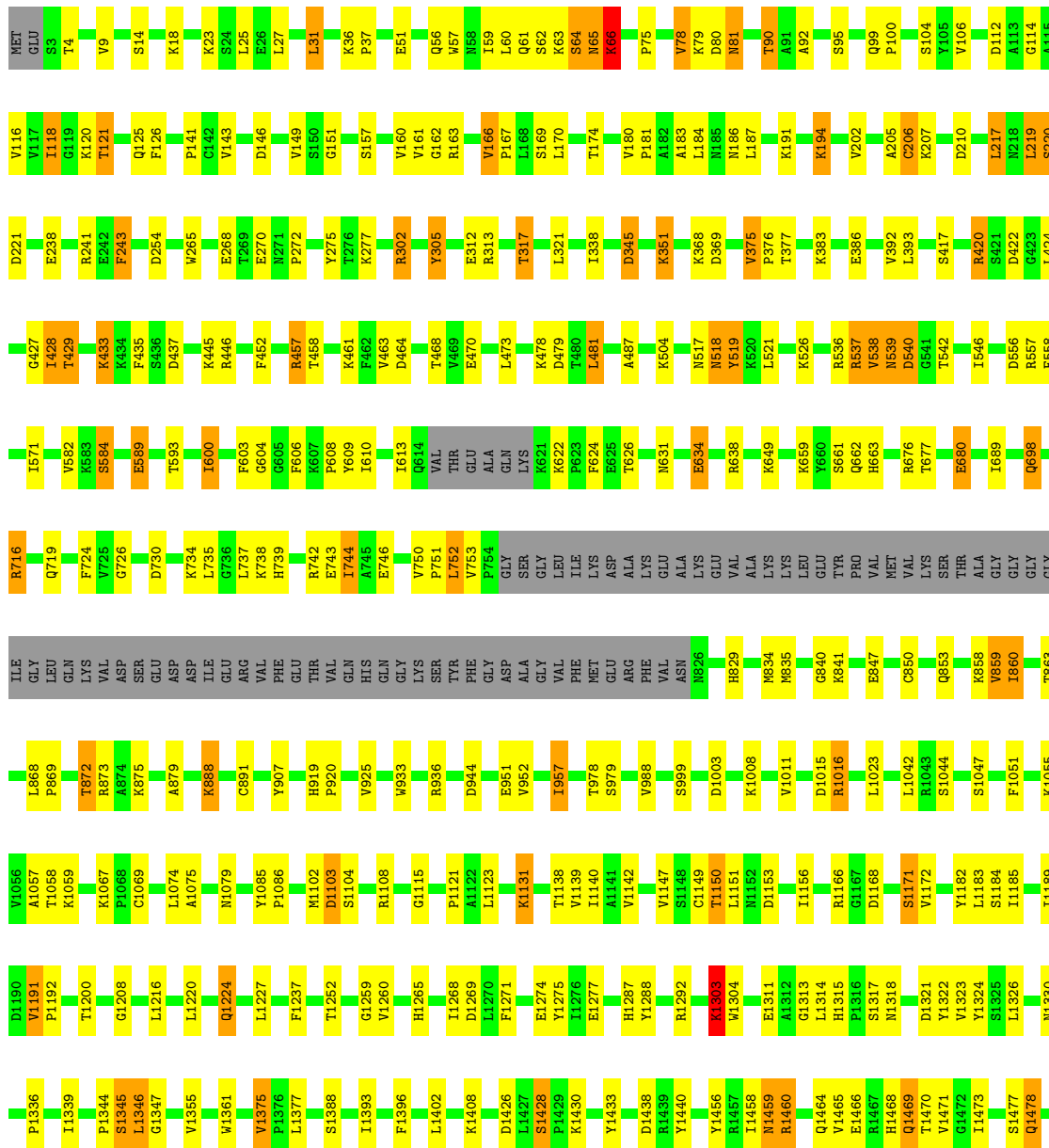
- Molecule 1: Urea Amidolyase

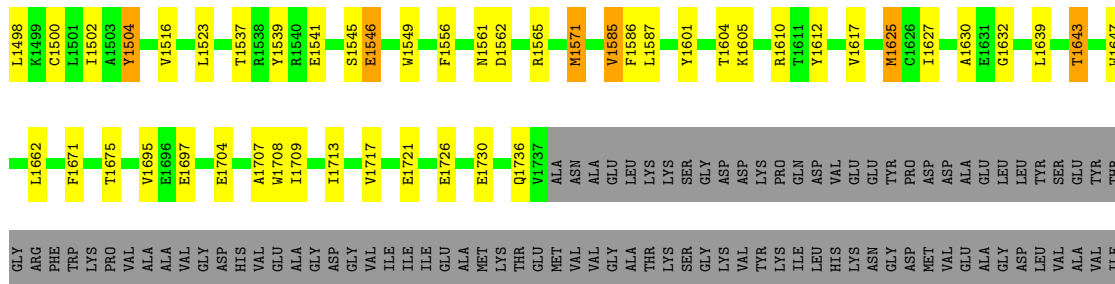
Chain A:





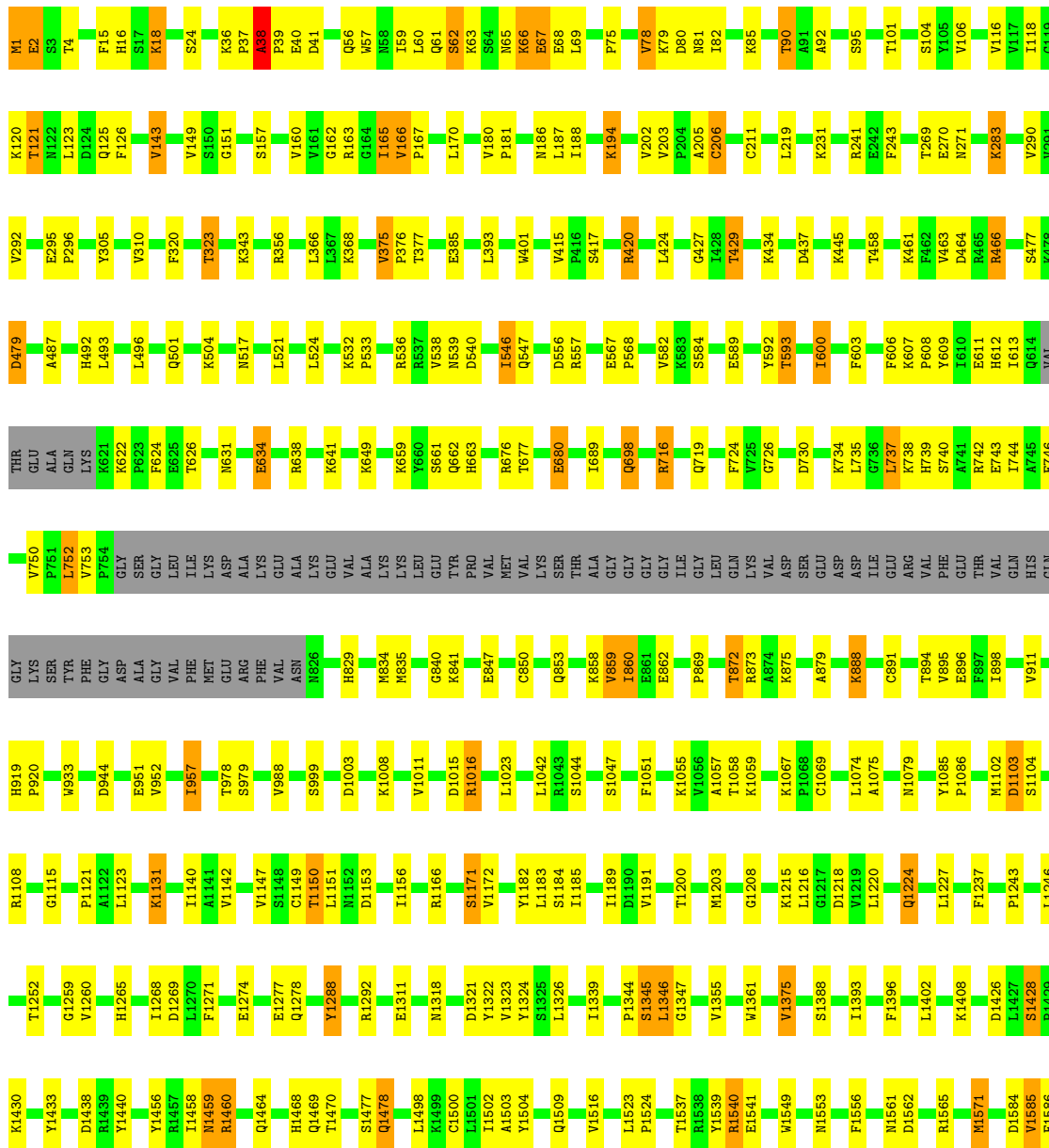
• Molecule 1: Urea Amidolyase





VAL

• Molecule 1: Urea Amidolyase



L1587	L1601	Y1606	R1610	Y1611	Y1612	G1616	V1617	M1625	C1626	I1627	A1630	F1631	G1632	S1633	L1639	R1642	T1643	V1647	L1662	F1671	T1675	V1695	E1696	E1697	W1708	I1709	N1710	E1711	N1712	I1713	V1717	E1721	E1726	E1730	Q1736	V1737	ALA	ASN	ALA	GLU						
LEU	LYS	SER	GLY	LYS	PRO	GLN	VAL	GLU	TYR	ASP	ASP	VAL	ALA	GLU	LEU	LEU	TYR	THR	GLY	ARG	PHE	TRP	LYS	VAL	ALA	VAL	GLY	ASP	HIS	VAL	GLU	ALA	VAL	ILE	ILE	GLU	ALA	MET	LYS	THR	GLU	MET	VAL	VAL	GLY	
ALA	THR	LYS	SER	GLY	LYS	ILE	LYS	ASN	GLY	ASP	MET	VAL	GLU	ALA	GLY	ASP	VAL	VAL	ILE	VAL	THR	LYS	VAL	ALA	VAL	VAL	THR	LYS	VAL	GLU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA

● Molecule 1: Urea Amidolyase



MET	GLU	S3	T4	W7	S8	V9	S14	S17	K18	K23	S24	L25	E26	L27	L28	E29	N30	L31	L32	K33	P37	E51	H55	Q56	W57	N58	I59	L60	Q61	S62	K63	K66	P75	V78	K79	D80	N81	T90	A91	A92	S95	Q99	P100	T101	S104						
Y106	V106	G114	A115	V116	V117	I118	G119	K120	T121	Q125	V143	V149	S150	G151	S157	V160	V161	G162	R163	V166	P167	L168	S169	L170	T174	N185	N186	L187	K191	K194	V202	A205	C206	K207	A92	S95	D210	C211	L217	N218	I219	S220									
D221	E238	R241	E242	F243	D254	W265	E268	T269	N271	P272	Y275	Z276	K277	R302	D479	Y305	E312	R313	T317	L321	I338	D345	K351	K368	D369	V375	P376	T377	P382	V392	L393	S417	R420	S421	D422	G427	I428	T429													
K433	K434	F435	S436	D437	K445	R446	T458	K461	F462	V463	T468	V469	E470	L473	K478	D479	T480	L481	A487	K504	S516	M517	N518	Y519	K520	L521	Y522	K526	L531	K532	P533	R536	R537	V538	N539	D540	G541	T542	I546	D556	R557	P588	I571								
V582	R583	S584	E589	T593	I600	F603	G604	G605	P606	P608	V609	I610	G614	VAL	THR	GLU	ALA	GLN	LYS	K621	K622	P623	F624	E625	T626	N631	E634	R638	K649	K659	Q662	R676	T677	E680	I689	Q698	I701	P702	R716												
Q719	D730	K734	L735	G736	L737	K738	H739	R742	E743	I744	A745	E746	V750	P751	L752	V753	P754	GLY	SER	GLU	ALA	GLY	LEU	ILE	LYS	ASP	ALA	ARG	PHE	VAL	ASN	H826	H829	M834	N835	G840	K841	S1044	E847	C850	S851	L852	Q853	K858	V859	T860	E861	E862	P869	T872	R873
A874	K875	A879	K888	C891	H919	P920	W933	D944	A951	V952	I957	K968	T978	S979	V988	S1148	C1149	T1150	L1151	N1152	D1153	I1156	R1166	S1171	V1172	Y1182	L1183	S1184	I1186	I1189	D1190	V1191	T1200	A1057	M1203	K1059	G1208	K1067	F1068	C1069	L1074										
A1075	M1079	Y1085	P1086	D1103	S1104	R1108	G1115	P1121	A1122	L1123	K1131	T1138	V1139	I1140	A1141	V1142	V1147	S1148	C1149	T1150	L1151	N1152	D1153	I1156	R1166	S1171	V1172	Y1182	L1183	S1184	I1186	I1189	D1190	V1191	T1200	A1057	M1203	K1059	G1208	K1067	F1068	C1069	L1074								
Q1224	L1227	F1237	P1243	L1246	T1252	G1259	V1260	H1265	I1268	D1269	L1270	F1271	K1430	Y1433	D1438	R1439	Y1440	Y1456	R1457	N1458	M1459	R1460	Q1464	H1468	Q1469	T1470	S1477	Q1478	L1498	K1499	C1500	D1501	I1502	A1503	Y1504	Q1509	S1345	V1516	G1347	L1523	T1537	R1538									
V1375	P1376	L1377	S1388	K1391	S1392	I1393	F1396	L1402	K1408	D1426	F1586	L1427	S1428	P1429	K1430	Y1433	D1438	R1439	Y1440	Y1456	R1457	N1458	M1459	R1460	Q1464	H1468	Q1469	T1470	S1477	Q1478	L1498	K1499	C1500	D1501	I1502	A1503	Y1504	Q1509	S1345	V1516	G1347	L1523	T1537	R1538							
Y1539	R1540	E1541	T1542	V1549	F1556	N1561	D1562	R1565	M1571	V1585	F1586	L1587	Y1601	K1605	R1610	T1611	Y1612	V1617	M1625	C1626	I1627	G1632	S1633	L1639	T1643	V1647	D1654	L1662	F1671	T1675	F1691	V1695	F1696	E1697	W1708	I1709															

M1710	GLU	GLU
E1711	ALA	ALA
M1712	GLY	GLY
I1713	ASP	ASP
V1717	GLY	VAL
	VAL	ILE
E1721	ILE	ILE
	ILE	ILE
E1726	GLU	GLU
	ALA	ALA
E1730	MET	MET
	LYS	LYS
Q1736	THR	THR
V1737	GLU	MET
	ALA	VAL
	ASN	VAL
	ALA	VAL
	GLU	GLY
	LEU	ALA
	LYS	THR
	LYS	LYS
	LYS	SER
	GLY	SER
	ASP	LYS
	ASP	VAL
	LYS	TYR
	LYS	LYS
	PRO	LYS
	GLN	ILE
	ASP	LEU
	VAL	HIS
	GLU	LYS
	GLU	ASN
	TYR	GLY
	PRO	ASP
	ASP	MET
	ASP	VAL
	ASP	VAL
	ALA	GLU
	GLU	ALA
	LEU	GLY
	LEU	ASP
	LEU	LEU
	TYR	VAL
	SER	ALA
	GLU	VAL
	TYR	ALA
	THR	VAL
	GLY	ILE
	ARG	VAL
	PHE	THR
	TRP	LYS
	LYS	PRO
	PRO	VAL
	VAL	ALA
	ALA	ALA
	VAL	VAL
	GLY	GLY
	ASP	ASP
	HIS	HIS
	VAL	VAL

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.74Å 181.94Å 549.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 6.50 29.98 – 6.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.98-6.50) 96.0 (29.98-6.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 6.58Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.278 , 0.302 0.281 , 0.306	Depositor DCC
R_{free} test set	1017 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	216.1	Xtrriage
Anisotropy	0.897	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 238.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	51722	wwPDB-VP
Average B, all atoms (Å ²)	308.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.40	1/13231 (0.0%)	0.70	4/17964 (0.0%)
1	B	0.51	2/13214 (0.0%)	0.86	23/17942 (0.1%)
1	C	0.39	1/13231 (0.0%)	0.69	5/17964 (0.0%)
1	D	0.49	3/13214 (0.0%)	0.83	21/17942 (0.1%)
All	All	0.45	7/52890 (0.0%)	0.77	53/71812 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	3
1	D	0	6
All	All	0	13

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1546	GLU	CG-CD	-7.32	1.41	1.51
1	C	1288	TYR	CD2-CE2	6.77	1.49	1.39
1	B	1546	GLU	CG-CD	-5.72	1.43	1.51
1	D	17	SER	CA-CB	5.61	1.61	1.52
1	D	1288	TYR	CD2-CE2	5.39	1.47	1.39

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	556	ASP	N-CA-CB	-8.99	94.41	110.60
1	B	556	ASP	N-CA-CB	-8.84	94.69	110.60
1	A	1504	TYR	CB-CG-CD1	-8.11	116.14	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1504	TYR	CB-CG-CD1	-7.93	116.24	121.00
1	D	422	ASP	N-CA-CB	-7.68	96.78	110.60

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1469	GLN	Mainchain
1	A	539	ASN	Peptide
1	B	1469	GLN	Mainchain
1	B	539	ASN	Peptide
1	C	539	ASN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12939	0	12896	226	0
1	B	12922	0	12878	218	1
1	C	12939	0	12896	203	1
1	D	12922	0	12878	215	0
All	All	51722	0	51548	813	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 8.

The worst 5 of 813 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:B:59:ILE:O	1:B:62:SER:OG	1.78	1.01
1:B:79:LYS:HA	1:B:121:THR:HG22	1.45	0.97
1:C:1509:GLN:NE2	1:D:101:THR:O	1.97	0.97
1:D:79:LYS:HA	1:D:121:THR:HG22	1.45	0.95
1:A:493:LEU:HB2	1:A:496:LEU:HD12	1.47	0.94

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1288:TYR:OH	1:C:1541:GLU:OE2[2_455]	1.97	0.23

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	1654/1829 (90%)	1540 (93%)	101 (6%)	13 (1%)	19 60
1	B	1652/1829 (90%)	1544 (94%)	97 (6%)	11 (1%)	22 63
1	C	1654/1829 (90%)	1539 (93%)	102 (6%)	13 (1%)	19 60
1	D	1652/1829 (90%)	1544 (94%)	97 (6%)	11 (1%)	22 63
All	All	6612/7316 (90%)	6167 (93%)	397 (6%)	48 (1%)	22 63

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ALA
1	A	1166	ARG
1	A	1711	GLU
1	B	1166	ARG
1	C	38	ALA

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	1413/1547 (91%)	1275 (90%)	138 (10%)	8	27
1	B	1411/1547 (91%)	1264 (90%)	147 (10%)	7	25
1	C	1413/1547 (91%)	1274 (90%)	139 (10%)	8	27
1	D	1411/1547 (91%)	1263 (90%)	148 (10%)	7	24
All	All	5648/6188 (91%)	5076 (90%)	572 (10%)	7	25

5 of 572 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	428	ILE
1	D	538	VAL
1	D	420	ARG
1	D	1015	ASP
1	B	600	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	65	ASN
1	D	1459	ASN
1	C	829	HIS
1	D	1509	GLN
1	D	829	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.