



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:04 am GMT

PDB ID : 1WZ2
Title : The crystal structure of Leucyl-tRNA synthetase and tRNA(leucine) complex
Authors : Fukunaga, R.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-02-21
Resolution : 3.21 Å(reported)

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

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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
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

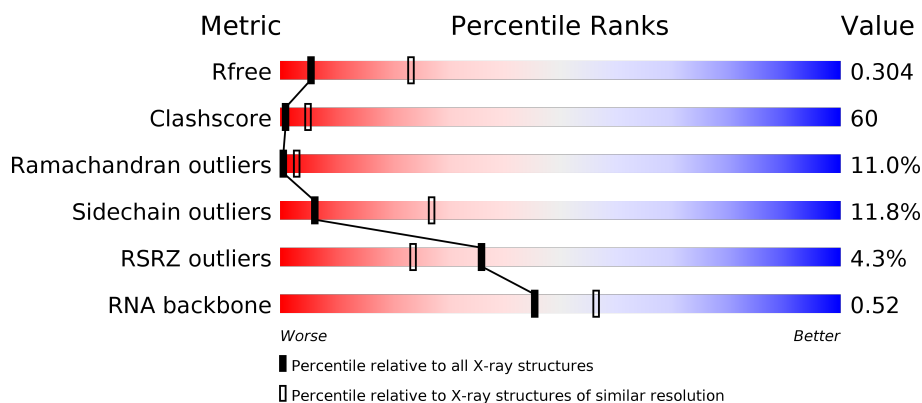
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1036 (3.24-3.20)
Clashscore	112137	1161 (3.24-3.20)
Ramachandran outliers	110173	1140 (3.24-3.20)
Sidechain outliers	110143	1139 (3.24-3.20)
RSRZ outliers	101464	1040 (3.24-3.20)
RNA backbone	2435	1055 (3.64-2.80)

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	C	88	<div> <div>5%</div> <div>27% 47% 19% 7%</div> </div>
1	D	88	<div> <div>8%</div> <div>38% 41% 18%</div> </div>
2	A	967	<div> <div>3%</div> <div>21% 60% 16%</div> </div>
2	B	967	<div> <div>5%</div> <div>22% 61% 14%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19578 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 RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	88	Total	C	N	O	P	0	0	0
			1880	836	339	617	88			
1	D	88	Total	C	N	O	P	0	0	0
			1880	836	339	617	88			

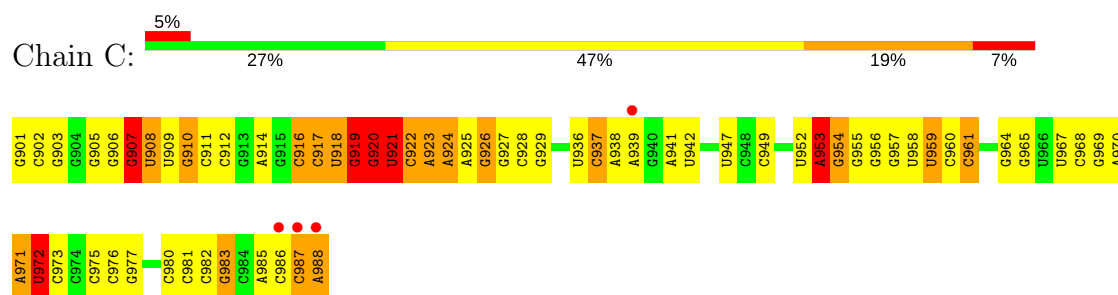
- Molecule 2 is a protein called Leucyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	948	Total	C	N	O	S	0	0	0
			7909	5132	1323	1430	24			
2	B	948	Total	C	N	O	S	0	0	0
			7909	5132	1323	1430	24			

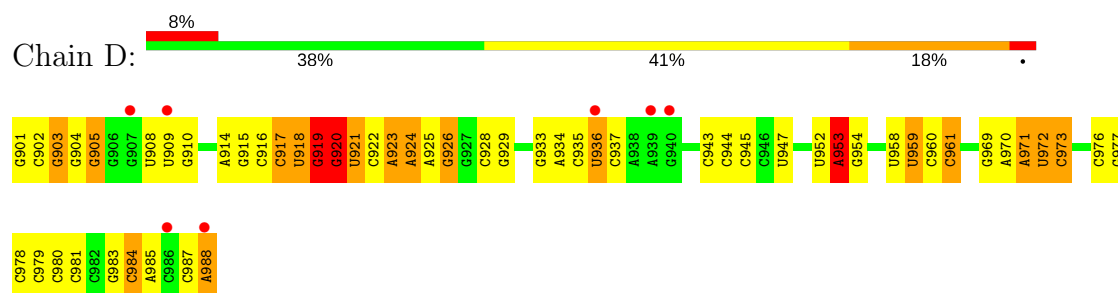
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

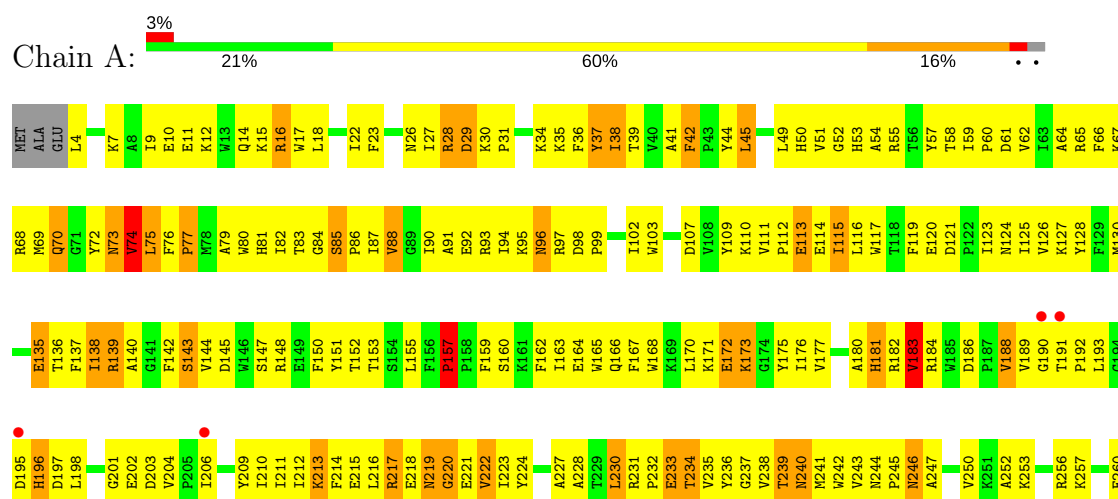
• Molecule 1: tRNA

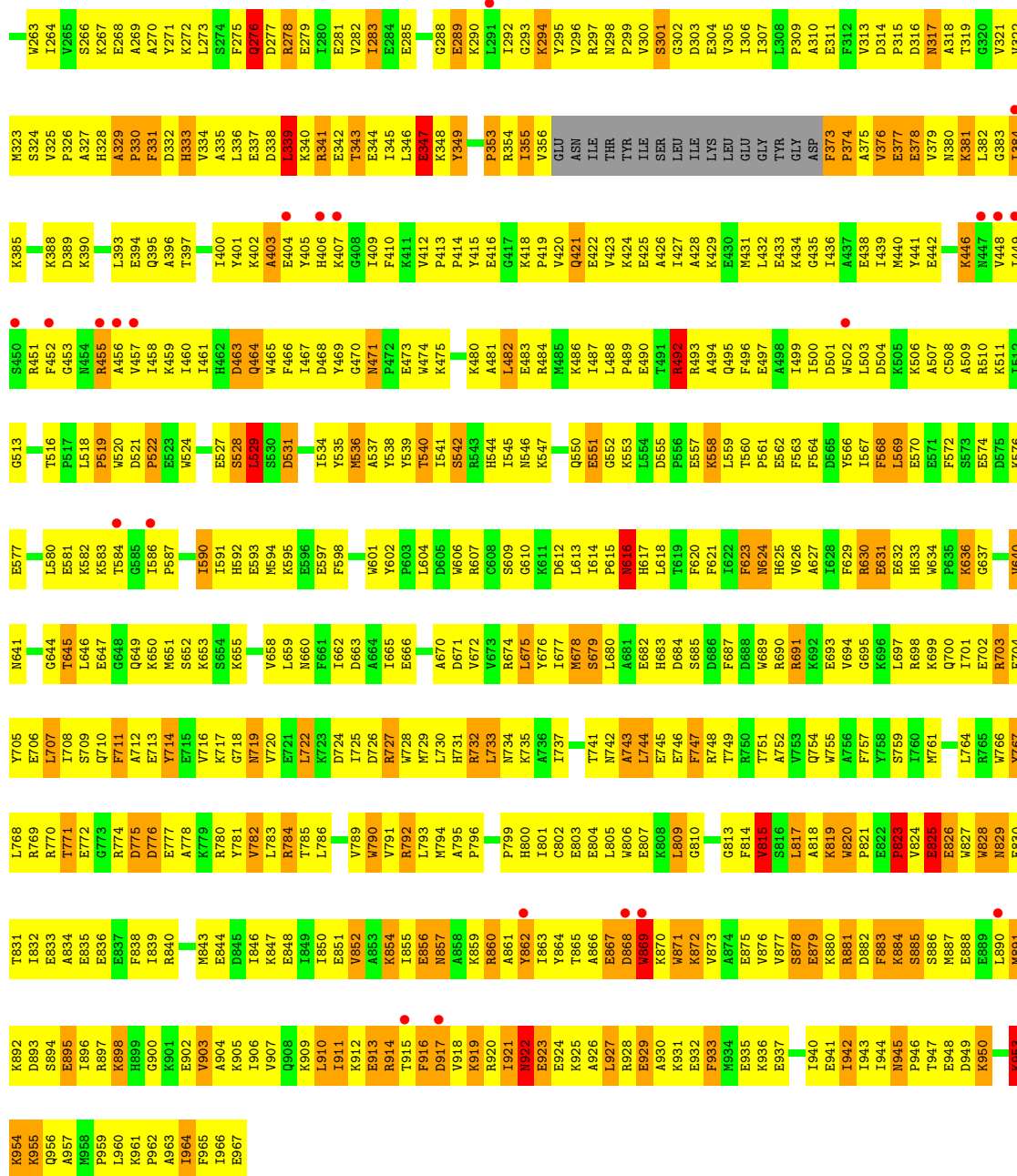


• Molecule 1: tRNA

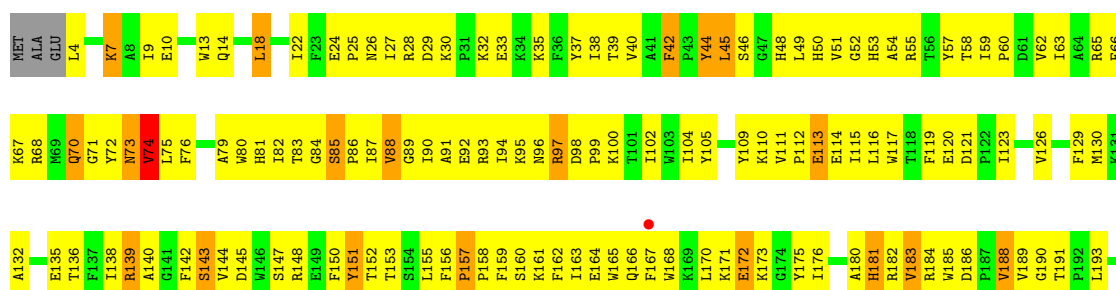


• Molecule 2: Leucyl-tRNA synthetase





• Molecule 2: Leucyl-tRNA synthetase



K954	K955	Q956	A957	M958	P959	L960	K961	P962	A963	P964	P965	I966	E967	L890	M891	K892	D893	T894	E895	L896	Q900	K901	E902	V903	A904	K905	I906	V907	K908	Q909	L910	I911	K912	E913	R914	T915	F916	D917	K918	R919	R920	I921	N922	E923	E924	K925	L926	R927	T928	E929	A930	F931	F932	F933	M934	E935	L938	G939	I940	E941	I942	I943	I944	N945	P946	D949	K950	G951	G952	K953	H827	H828	E829	T830	T831	T832	E833	A834	E835	E836	F837	F838	T839	R840	S841	H842	H843	E844	E845	T846	R847	E848	T849	E850	E851	V852	A853	K854	T855	E856	N857	A858	K859	R860	A861	T862	T863	T864	T865	A866	E867	D868	K869	K870	H871	K872	G873	F874	E875	E876	V877	E878	E879	K880	R881	D882	F883	K884	S885	S886	H887	G888	E889	R703	F704	Y705	E706	G707	V708	S709	F710	F711	A712	E713	Y714	K715	G716	K717	G718	M719	V720	E721	S722	L723	K724	D725	T726	R727	V728	M729	L730	H731	R732	L733	M734	I737	K738	E739	T740	Y741	N742	A743	E745	E746	F747	E748	T749	R750	T751	A752	V753	Q754	W755	A756	F757	Y758	S759	I760	M761	N762	D763	L764	R765	W766	Y767	L768	R769	R770	T771	R774	D775	E776	E777	A778	K779	R780	Y781	V782	L783	R784	T785	L786	V789	W790	Y791	R792	L793	M794	A795	P796	L797	T798	P799	H800	T801	C802	E803	E804	L805	W806	E807	K808	L809	G810	G811	E812	G813	V814	V815	S816	L817	A818	K819	W820	P821	E822	P823	V824	E825	E826	H827	H828	E829	T830	T831	T832	E833	A834	E835	E836	F837	F838	T839	R840	S841	H842	H843	E844	E845	T846	R847	E848	T849	E850	E851	V852	A853	K854	T855	E856	N857	A858	K859	R860	A861	T862	T863	T864	T865	A866	E867	D868	K869	K870	H871	K872	G873	F874	E875	E876	V877	E878	E879	K880	R881	D882	F883	K884	S885	S886	H887	G888	E889	D504	K505	K506	C507	S508	A509	R510	S511	L512	L513	G514	G515	T516	F517	L518	P519	W520	K521	P522	S523	W524	D525	V526	E527	S528	L529	S530	D531	S532	T533	E534	Y535	M536	A537	Y538	Y539	T540	I541	S542	R543	H544	I545	M546	K547	L548	S549	Q550	E551	G552	K553	L554	D555	P556	E557	K558	A498	T499	I500	P501	E502	F563	F564	D565	Y566	I567	F568	L569	E570	S573	K576	E577	L580	E581	K582	K583	T584	G585	I586	P587	I590	I591	H592	E593	M594	E595	E596	E597	F598	E599	Y600	W601	Y602	W606	R607	C608	S609	L613	I614	P615	M616	H617	L618	T619	V620	F621	L622	F623	N624	H625	V626	F629	R630	E631	E632	D442	F443	K446	N447	V448	T449	S450	R451	F452	O453	N454	R455	A456	V457	L458	K459	I460	T461	H462	Q464	D467	D468	Y469	G470	D471	F472	E473	N474	N475	A476	F477	A478	B479	K480	A481	L482	E483	R484	M485	K486	T487	L488	P489	E490	T491	R492	K493	A494	Q495	F496	E497	A498	T499	I500	D501	W502	L503	K381	L382	G383	I384	S385	K386	Q387	D388	K389	K390	E391	K392	L393	H394	Q395	L396	E397	D398	L399	K399	T399	I400	A401	K402	A403	T343	E344	I345	L346	E347	K407	G408	I409	F410	K290	D350	L351	D352	P353	R354	I355	V356	G417	K418	P419	V420	Q421	E422	V423	K424	E425	A426	I427	K428	E430	M431	L432	E433	F373	P374	A375	R255	I436	A437	E438	I439	L308	T309	A310	E311	F312	V313	D314	P315	D316	N317	A318	K259	E260	E261	T262	W263	L264	V265	K266	K267	E268	A269	A270	Y271	K272	L273	S274	I210	I211	I212	K213	F214	E215	R216	K217	E218	V219	N220	E221	V222	T223	Y224	K287	G288	E289	F290	K291	L291	L292	G293	K294	Y295	V296	R297	N298	P299	V300	G301	G302	D303	SER	N240	M241	W242	V243	N244	L245	L308	P309	T310	E311	A252	K253	D254	V255	R256	K257	D258	K259	E260	V321	V322	M323	S324	K325	P326	A327	H328	A329	P330	A331	D332	H333	V334	A335	L336	E337	D338	L339	K340	R341	E342	T343	I344	E284	L345	L346	E347	K347	G408	I409	F410	K290	D350	L351	D352	P353	R354	I355	V356	G417	K418	P419	V420	Q421	E422	V423	K424	E425	A426	I427	K428	E430	M431	L432	E433	F373	P374	A375	R255	I436	A437	E438	I439	L308	T309	A310	E311	F312	V313	D314	P315	D316	N317	A318	K259	E260	E261	T262	W263	L264	V265	K266	K267	E268	A269	A270	Y271	K272	L273	S274	I210	I211	I212	K213	F214	E215	R216	K217	E218	V219	N220	E221	V222	T223	Y224	K287	G288	E289	F290	K291	L291	L292	G293	K294	Y295	V296	R297	N298	P299	V300	G301	G302	D303	SER	N240	M241	W242	V243	N244	L245	L308	P309	T310	E311	A252	K253	D254	V255	R256	K257	D258	K259	E260	V321	V322	M323	S324	K325	P326	A327	H328	A329	P330	A331	D332	H333	V334	A335	L336	E337	D338	L339	K340	R341	E342	T343	I344	E284	L345	L346	E347	K347	G408	I409	F410	K290	D350	L351	D352	P353	R354	I355	V356	G417	K418	P419	V420	Q421	E422	V423	K424	E425	A426	I427	K428	E430	M431	L432	E433	F373	P374	A375	R255	I436	A437	E438	I439	L308	T309	A310	E311	F312	V313	D314	P315	D316	N317	A318	K259	E260	E261	T262	W263	L264	V265	K266	K267	E268	A269	A270	Y271	K272	L273	S274	I210	I211	I212	K213	F214	E215	R216	K217	E218	V219	N220	E221	V222	T223	Y224	K287	G288	E289	F290	K291	L291	L292	G293	K294	Y295	V296	R297	N298	P299	V300	G301	G302	D303	SER	N240	M241	W242	V243	N244	L245	L308	P309	T310	E311	A252	K253	D254	V255	R256	K257	D258	K259	E260	V321	V322	M323	S324	K325	P326	A327	H328	A329	P330	A331	D332	H333	V334	A335	L336	E337	D338	L339	K340	R341	E342	T343	I344	E284	L345	L346	E347	K347	G408	I409	F410	K290	D350	L351	D352	P353	R354	I355	V356	G417	K418	P419	V420	Q421	E422	V423	K424	E425	A426	I427	K428	E430	M431	L432	E433	F373	P374	A375	R255	I436	A437	E438	I439	L308	T309	A310	E311	F312	V313	D314	P315	D316	N317	A318	K259	E260	E261	T262	W263	L264	V265	K266	K267	E268	A269	A270	Y271	K272	L273	S274	I210	I211	I212	K213	F214	E215	R216	K217	E218	V219	N220	E221	V222	T223	Y224	K287	G288	E289	F290	K291	L291	L292	G293	K294	Y295	V296	R297	N298	P299	V300	G301	G302	D303	SER	N240	M241	W242	V243	N244	L245	L308	P309	T310	E311	A252	K253	D254	V255	R256	K257	D258	K259	E260	V321	V322	M323	S324	K325	P326	A327	H328	A329	P330	A331	D332	H333	V334	A335	L336	E337	D338	L339	K340	R341	E342	T343	I344	E284	L345	L346	E347	K347	G408	I409	F410	K290	D350	L351	D352	P353	R354	I355	V356	G417	K418	P419	V420	Q421	E422	V423	K424	E425	A426	I427	K428	E430	M431	L432	E433	F373	P374	A375	R255	I436	A437	E438	I439	L308	T309	A310	E311	F312	V313	D314	P315	D316	N317	A318	K259	E260	E261	T262	W263	L264	V265	K266	K267	E268	A269	A270	Y271	K272	L273	S274	I210	I211	I212	K213	F214	E215	R216	K217	E218	V219	N220	E221	V222	T223	Y224	K287	G288	E289	F290	K291	L291	L292	G293	K294	Y295	V296	R297	N298	P299	V300	G301	G302	D303	SER	N240	M241	W242	V243	N244	L245	L308	P309	T310	E311	A252	K253	D254	V255	R256	K257	D258	K259	E260	V321	V322	M323	S324	K325	P326	A327	H328	A329	P330	A331	D332	H333	V334	A335	L336	E337	D338	L339	K340	R341	E342	T343	I344	E284	L345	L346	E347	K347	G408	I409	F410	K290	D350	L351	D352	P353	R354	I355	V356	G417	K418	P419	V420	Q421	E422	V423	K424	E425	A426	I427	K428	E430	M431	L432	E433	F373	P374	A375	R255	I436	A437	E438	I439	L308	T309	A310	E311	F312	V313	D314	P315	D316	N317	A318	K259	E260	E261	T262	W263	L264	V265	K266	K267	E268	A269	A270	Y271	K272	L273	S274	I210	I211	I212	K213	F214	E215	R216	K217	E218	V219	N220	E221	V222	T223	Y224	K287	G288	E289	F290	K291	L291	L292	G293	K294	Y295	V296	R297	N298	P299	V300	G301	G302	D303	SER	N240	M241	W242	V243	N244	L245	L308	P309	T310	E311	A252	K253	D254	V255	R256	K257	D258	K259	E260	V321	V322	M323	S324	K325	P326	A327	H328	A329	P330	A331	D332	H333	V334	A335	L336	E337	D338	L339	K340	R341	E342	T343	I344	E284	L345	L346	E347	K347	G408	I409	F410	K290	D350	L351	D352	P353	R354	I355	V356	G417	K418	P419	V420	Q421	E422	V423	K424	E425	A426	I427	K428	E430	M431	L432	E433	F373	P374	A375	R255	I436	A437	E438	I439	L308	T309	A310	E311	F312	V313	D314	P315	D316	N317	A318	K259	E260	E261	T262	W263	L264	V265	K266	K267	E268	A269	A270	Y271	K272	L273	S274	I210	I211	I212	K213	F214	E215	R216	K217	E218	V219	N220	E221	V222	T223	Y224	K287	G288	E289	F290	K291	L291	L292	G293	K294	Y295	V296	R297	N298	P299	V300	G301	G302	D303	SER	N240	M241	W242	V243	N244	L245	L308	P309	T310	E311	A252	K253	D254	V255	R256	K257	D258	K259	E260	V321	V322	M323	S324	K325	P326	A327	H328	A329	P330	A331	D332	H333	V334	A335	L336	E337	D338	L339	K340	R341	E342	T343	I344	E284	L345	L346	E347	K347
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.55Å 231.13Å 118.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 3.21 48.69 – 3.21	Depositor EDS
% Data completeness (in resolution range)	90.7 (14.99-3.21) 90.8 (48.69-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.305 0.243 , 0.304	Depositor DCC
R_{free} test set	4957 reflections (10.07%)	DCC
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19578	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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

5.1 Standard geometry

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	C	0.55	1/2099 (0.0%)	0.82	7/3270 (0.2%)
1	D	0.52	1/2099 (0.0%)	0.81	3/3270 (0.1%)
2	A	0.59	0/8115	0.76	6/10953 (0.1%)
2	B	0.42	0/8115	0.67	2/10953 (0.0%)
All	All	0.52	2/20428 (0.0%)	0.74	18/28446 (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	C	0	6
1	D	0	5
2	A	0	2
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	901	G	OP3-P	-7.18	1.52	1.61
1	D	901	G	OP3-P	-7.06	1.52	1.61

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	675	LEU	CA-CB-CG	10.29	138.97	115.30
2	A	815	VAL	CB-CA-C	-8.02	96.17	111.40
1	C	919	G	N9-C1'-C2'	7.77	124.10	114.00
1	D	953	A	N9-C1'-C2'	7.42	123.64	114.00
1	C	907	G	N9-C1'-C2'	7.18	123.33	114.00

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	907	G	Sidechain
1	C	919	G	Sidechain
1	C	920	G	Sidechain
1	C	921	U	Sidechain
1	C	926	G	Sidechain

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	C	1880	0	956	88	0
1	D	1880	0	956	65	0
2	A	7909	0	7908	1115	0
2	B	7909	0	7908	1018	0
All	All	19578	0	17728	2256	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 60.

The worst 5 of 2256 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)
2:A:866:ALA:N	2:A:955:LYS:HZ3	1.39	1.18
2:A:30:LYS:HB2	2:A:73:ASN:HD22	1.11	1.13
2:A:170:LEU:HB3	2:A:176:ILE:HD11	1.23	1.09
2:A:616:ASN:HD22	2:A:617:HIS:N	1.51	1.08
2:A:68:ARG:HH22	2:A:143:SER:HB3	1.15	1.07

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	
2	A	944/967 (98%)	630 (67%)	211 (22%)	103 (11%)	0	3
2	B	944/967 (98%)	632 (67%)	208 (22%)	104 (11%)	0	3
All	All	1888/1934 (98%)	1262 (67%)	419 (22%)	207 (11%)	0	3

5 of 207 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	74	VAL
2	A	110	LYS
2	A	143	SER
2	A	183	VAL
2	A	188	VAL

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	
2	A	841/857 (98%)	731 (87%)	110 (13%)	5	22
2	B	841/857 (98%)	752 (89%)	89 (11%)	8	32
All	All	1682/1714 (98%)	1483 (88%)	199 (12%)	6	27

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	829	ASN

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Continued from previous page...

Mol	Chain	Res	Type
2	B	18	LEU
2	B	825	GLU
2	A	860	ARG
2	A	917	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	683	HIS
2	B	53	HIS
2	B	734	ASN
2	A	731	HIS
2	A	800	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	87/88 (98%)	24 (27%)	0
1	D	87/88 (98%)	22 (25%)	0
All	All	174/176 (98%)	46 (26%)	0

5 of 46 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	907	G
1	C	908	U
1	C	910	G
1	C	916	C
1	C	917	C

There are no RNA pucker outliers to report.

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](#)

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 [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	C	88/88 (100%)	0.20	4 (4%) 34 22	53, 78, 126, 149	0
1	D	88/88 (100%)	0.41	7 (7%) 13 8	53, 91, 146, 150	0
2	A	948/967 (98%)	-0.09	26 (2%) 55 41	8, 59, 131, 150	0
2	B	948/967 (98%)	0.26	53 (5%) 25 15	48, 102, 149, 150	0
All	All	2072/2110 (98%)	0.10	90 (4%) 36 24	8, 82, 143, 150	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	407	LYS	5.4
1	D	936	U	5.3
2	B	524	TRP	5.1
1	D	939	A	4.9
2	B	236	TYR	4.9

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.