



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:17 PM 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.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

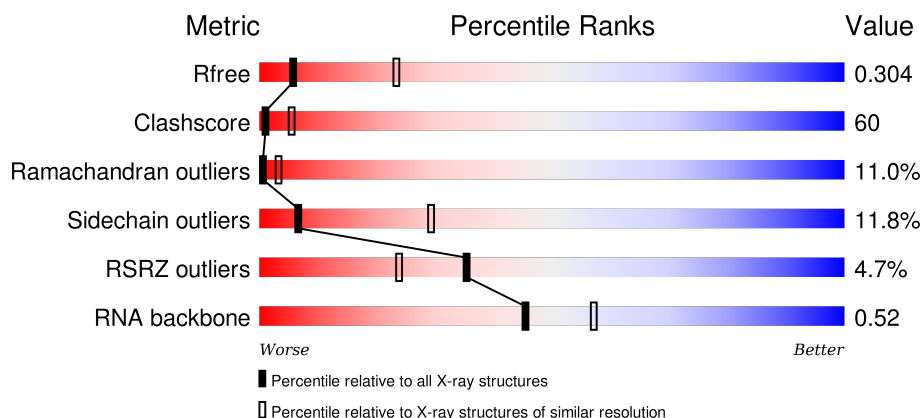
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)
RNA backbone	2183	1004 (3.72-2.72)

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

Mol	Chain	Length	Quality of chain
1	C	88	<div> <div>6%</div> <div>27% 44% 22% 7%</div> </div>
1	D	88	<div> <div>8%</div> <div>36% 39% 22% .</div> </div>
2	A	967	<div> <div>3%</div> <div>21% 60% 16% ..</div> </div>
2	B	967	<div> <div>6%</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			

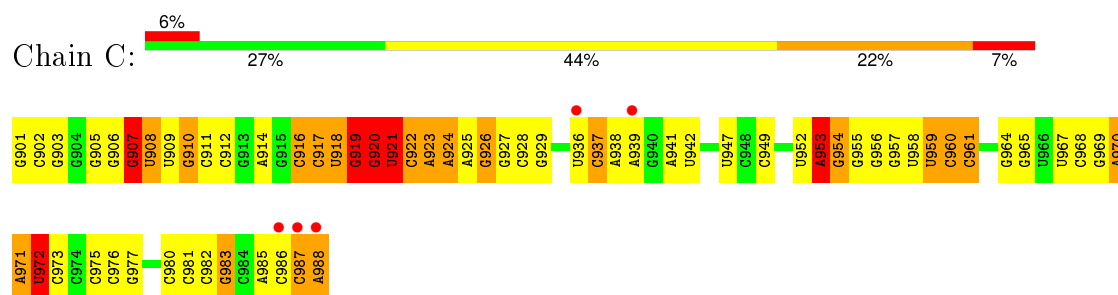
- Molecule 2 is a protein called Leucyl-tRNA synthetase.

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			

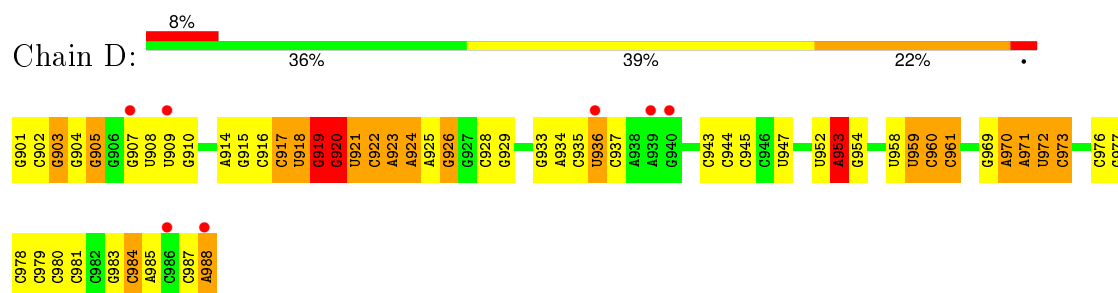
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

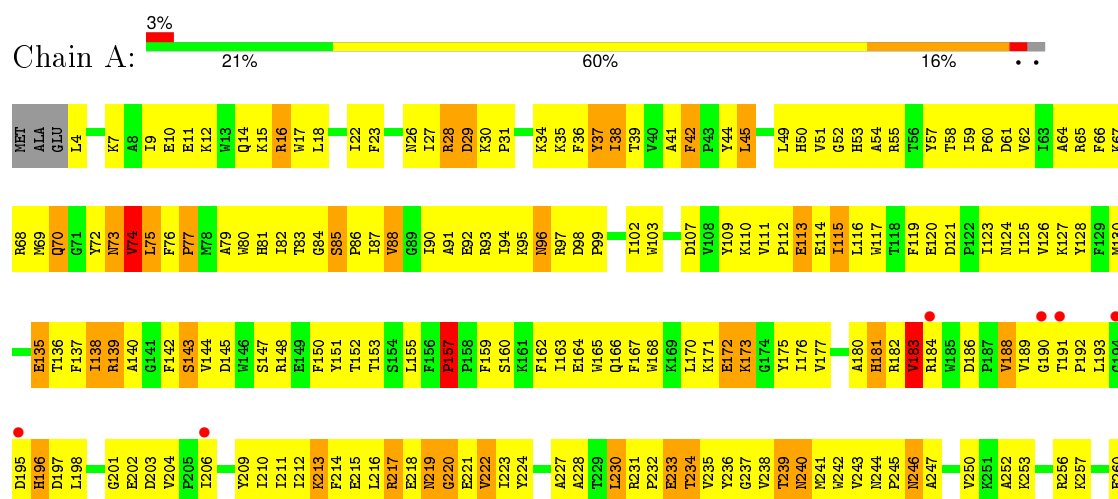
#### • Molecule 1: tRNA

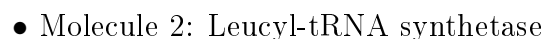


#### • Molecule 1: tRNA



#### • Molecule 2: Leucyl-tRNA synthetase





K954	K955	Q956	A957	N958	P959	L960	K961	P962	A963	F965	L966	E967	L890	M891	K892	L893	S894	E895	L896	G900	K901	E902	V903	A904	K905	I906	V907	Q908	K909	L910	I911	E912	E913	R914	T915	F916	D917	K918	R919	R920	I921	N922	E923	E924	K925	L927	R928	E929	A930	F931	F932	F933	M934	E935	I938	G939	I940	E941	I942	I943	I944	N945	P946	D949	K950	G951	E952	K953	H633	M634	P635	K636	G637	V640	M641	G644	T645	L646	E647	F648	K649	K650	M651	S652	K653	S654	K655	V658	R659	M660	F661	L662	D663	L665	A670	D671	R674	L675	Y676	L677	M678	S679	L680	A681	E682	F683	D684	F687	D688	V689	R690	E693	V694	G695	K696	L697	R698	I701	E702	R703	F704	Y705	E706	L707	I708	S709	Q710	F711	E712	L713	Y714	K717	G718	M719	V720	L721	S652	L722	R723	D724	I725	D726	R727	M728	M729	L730	R731	R732	L733	N734	I737	K738	E739	T740	T741	N742	A743	L744	E745	E746	F747	R748	T749	R750	T751	A752	V753	Q754	M755	A756	F757	Y758	S759	I760	M761	M762	D763	L764	R765	M766	L767	R769	R770	T771	R774	D775	D776	E777	A778	K779	R780	V781	L782	L783	S652	R784	T785	L786	V789	M790	V791	R792	L793	M794	A795	P796	L797	T798	K799	R800	A801	Y802	C802	E803	E804	L805	R806	E807	D808	M809	K810	G811	E812	F813	V815	S816	L817	A818	K819	N820	P821	E822	P823	V824	E825	E826	H827	L828	A866	T865	T866	E867	D868	M869	K870	M871	K872	V877	S878	E879	K880	R881	D882	F883	K884	S885	S886	M887	E888	E889	L896	D197	M198	K199	E200	G201	E202	D203	V204	L206	I210	I211	I212	K213	F214	E215	L216	K217	E218	M219	G220	E221	V222	T223	Y224	L225	P226	E227	K228	L229	A228	T229	R230	K231	P232	I235	V236	R237	T234	V235	Y236	G237	V238	N240	E241	W242	V243	N244	I247	L248	P429	E430	M431	L432	F433	K434	G435	A436	A437	E438	D501	L503	D504	K505	S506	C508	A509	R510	K511	I512	G513	L514	G515	T516	F517	L518	E519	L520	S521	L522	E523	M524	V525	I526	E527	S528	L529	S530	D531	S532	S533	T533	E534	Y535	M536	A537	Y538	Y539	T540	I541	S542	R543	I545	N546	K547	L548	R549	E551	F552	K553	L554	D555	P556	E557	K558	L559	T560	P561	E562	F563	F564	D565	Y566	F568	A569	R570	S573	K576	E577	L580	E581	K582	K583	T584	G585	I586	P587	I590	I591	H592	E593	M594	E596	E597	A604	F598	E599	Y600	M601	Y602	M606	R607	C608	S609	L613	I614	P615	M616	H617	L618	T619	F620	F621	L622	F623	N624	H625	V626	F629	R630	E631	E632	K381	L382	G383	I384	K385	S386	Q387	K388	D389	K390	E391	K392	L393	E394	Q395	A396	T397	K398	T399	I400	Y401	K402	A403	E404	Y405	H406	K407	G408	F409	K410	K411	K412	P413	Y415	E416	G417	K418	V419	Q421	V422	V423	K424	E425	A426	I427	A428	K429	E430	M431	L432	F433	K434	G435	A436	A437	E438	D501	L503	D504	K505	S506	C508	A509	R510	K511	I512	G513	L514	G515	T516	F517	L518	E519	L520	S521	L522	E523	M524	V525	I526	E527	S528	L529	S530	D531	S532	S533	T533	E534	Y535	M536	A537	Y538	Y539	T540	I541	S542	R543	I545	N546	K547	L548	R549	E551	F552	K553	L554	D555	P556	E557	K558	L559	T560	P561	E562	F563	F564	D565	Y566	F568	A569	R570	S573	K576	E577	L580	E581	K582	K583	T584	G585	I586	P587	I590	I591	H592	E593	M594	E596	E597	A604	F598	E599	Y600	M601	Y602	M606	R607	C608	S609	L613	I614	P615	M616	H617	L618	T619	F620	F621	L622	F623	N624	H625	V626	F629	R630	E631	E632	K381	L382	G383	I384	K385	S386	Q387	K388	D389	K390	E391	K392	L393	E394	Q395	A396	T397	K398	T399	I400	Y401	K402	A403	E404	Y405	H406	K407	G408	F409	K410	K411	K412	P413	Y415	E416	G417	K418	V419	Q421	V422	V423	K424	E425	A426	I427	A428	K429	E430	M431	L432	F433	K434	G435	A436	A437	E438	D501	L503	D504	K505	S506	C508	A509	R510	K511	I512	G513	L514	G515	T516	F517	L518	E519	L520	S521	L522	E523	M524	V525	I526	E527	S528	L529	S530	D531	S532	S533	T533	E534	Y535	M536	A537	Y538	Y539	T540	I541	S542	R543	I545	N546	K547	L548	R549	E551	F552	K553	L554	D555	P556	E557	K558	L559	T560	P561	E562	F563	F564	D565	Y566	F568	A569	R570	S573	K576	E577	L580	E581	K582	K583	T584	G585	I586	P587	I590	I591	H592	E593	M594	E596	E597	A604	F598	E599	Y600	M601	Y602	M606	R607	C608	S609	L613	I614	P615	M616	H617	L618	T619	F620	F621	L622	F623	N624	H625	V626	F629	R630	E631	E632	K381	L382	G383	I384	K385	S386	Q387	K388	D389	K390	E391	K392	L393	E394	Q395	A396	T397	K398	T399	I400	Y401	K402	A403	E404	Y405	H406	K407	G408	F409	K410	K411	K412	P413	Y415	E416	G417	K418	V419	Q421	V422	V423	K424	E425	A426	I427	A428	K429	E430	M431	L432	F433	K434	G435	A436	A437	E438	D501	L503	D504	K505	S506	C508	A509	R510	K511	I512	G513	L514	G515	T516	F517	L518	E519	L520	S521	L522	E523	M524	V525	I526	E527	S528	L529	S530	D531	S532	S533	T533	E534	Y535	M536	A537	Y538	Y539	T540	I541	S542	R543	I545	N546	K547	L548	R549	E551	F552	K553	L554	D555	P556	E557	K558	L559	T560	P561	E562	F563	F564	D565	Y566	F568	A569	R570	S573	K576	E577	L580	E581	K582	K583	T584	G585	I586	P587	I590	I591	H592	E593	M594	E596	E597	A604	F598	E599	Y600	M601	Y602	M606	R607	C608	S609	L613	I614	P615	M616	H617	L618	T619	F620	F621	L622	F623	N624	H625	V626	F629	R630	E631	E632	K381	L382	G383	I384	K385	S386	Q387	K388	D389	K390	E391	K392	L393	E394	Q395	A396	T397	K398	T399	I400	Y401	K402	A403	E404	Y405	H406	K407	G408	F409	K410	K411	K412	P413	Y415	E416	G417	K418	V419	Q421	V422	V423	K424	E425	A426	I427	A428	K429	E430	M431	L432	F433	K434	G435	A436	A437	E438	D501	L503	D504	K505	S506	C508	A509	R510	K511	I512	G513	L514	G515	T516	F517	L518	E519	L520	S521	L522	E523	M524	V525	I526	E527	S528	L529	S530	D531	S532	S533	T533	E534	Y535	M536	A537	Y538	Y539	T540	I541	S542	R543	I545	N546	K547	L548	R549	E551	F552	K553	L554	D555	P556	E557	K558	L559	T560	P561	E562	F563	F564	D565	Y566	F568	A569	R570	S573	K576	E577	L580	E581	K582	K583	T584	G585	I586	P587	I590	I591	H592	E593	M594	E596	E597	A604	F598	E599	Y600	M601	Y602	M606	R607	C608	S609	L613	I614	P615	M616	H617	L618	T619	F620	F621	L622	F623	N624	H625	V626	F629	R630	E631	E632	K381	L382	G383	I384	K385	S386	Q387	K388	D389	K390	E391	K392	L393	E394	Q395	A396	T397	K398	T399	I400	Y401	K402	A403	E404	Y405	H406	K407	G408	F409	K410	K411	K412	P413	Y415	E416	G417	K418	V419	Q421	V422	V423	K424	E425	A426	I427	A428	K429	E430	M431	L432	F433	K434	G435	A436	A437	E438	D501	L503	D504	K505	S506	C508	A509	R510	K511	I512	G513	L514	G515	T516	F517	L518	E519	L520	S521	L522	E523	M524	V525	I526	E527	S528	L529	S530	D531	S532	S533	T533	E534	Y535	M536	A537	Y538	Y539	T540	I541	S542	R543	I545	N546	K547	L548	R549	E551	F552	K553	L554	D555	P556	E557	K558	L559	T560	P561	E562	F563	F564	D565	Y566	F568	A569	R570	S573	K576	E577	L580	E581	K582	K583	T584	G585	I586	P587	I590	I591	H592	E593	M594	E596	E597	A604	F598	E599	Y600	M601	Y602	M606	R607	C608	S609	L613	I614	P615	M616	H617	L618	T619	F620	F621	L622	F623	N624	H625	V626	F629	R630	E631	E632	K381	L382	G383	I384	K385	S386	Q387	K388	D389	K390	E391	K392	L393	E394	Q395	A396	T397	K398	T399	I400	Y401	K402	A403	E404	Y405	H406	K407	G408	F409	K410	K411	K412	P413	Y415	E416	G417	K418	V419	Q421	V422	V423	K424	E425	A426	I427	A428	K429	E430	M431	L432	F433	K434	G435	A436	A437	E438	D501	L503	D504	K505	S506	C508	A509	R510	K511	I512	G513	L514	G515	T516	F517	L518	E519	L520	S521	L522	E523	M524	V525	I526	E527	S528	L529	S530	D531	S532	S533	T533	E534	Y535	M536	A537	Y538	Y539	T540	I541	S542	R543	I545	N546	K547	L548	R549	E551	F552	K553	L554	D555	P556	E557	K558	L559	T560	P561	E562	F563	F564	D565	Y566	F568	A569	R570	S573	K576	E577	L580	E581	K582	K583	T584	G585	I586	P587	I590	I591	H592	E593	M594	E596	E597	A604	F598	E599	Y600	M601	Y602	M606	R607	C608	S609	L613	I614	P615	M616	H617	L618	T619	F620	F621	L622	F623	N624	H625	V626	F629	R630	E631	E632	K381	L382	G383	I384	K385	S386	Q387	K388	D389	K390	E391	K392	L393	E394	Q395	A396	T397	K398	T399	I400	Y401	K402	A403	E404	Y405	H406	K407	G408	F409	K410	K411	K412	P413	Y415	E416	G417	K418	V419	Q421	V422	V423	K424	E425	A426	I427	A428	K429	E430	M431	L432	F433	K434	G435	A436	A437	E438	D501	L503	D504	K505	S506	C508	A509	R510	K511	I512	G513	L514	G515	T516	F517	L518	E519	L520	S521	L522	E523	M524	V525</
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	--------

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	75.5	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 76.5	EDS
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 49816 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	19578	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

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

## 5 Model quality

### 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

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	24
2	B	841/857 (98%)	752 (89%)	89 (11%)	8	34
All	All	1682/1714 (98%)	1483 (88%)	199 (12%)	6	29

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

Mol	Chain	Res	Type
2	A	829	ASN

*Continued on next page...*

*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 ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	87/88 (98%)	24 (27%)	7 (8%)
1	D	87/88 (98%)	22 (25%)	8 (9%)
All	All	174/176 (98%)	46 (26%)	15 (8%)

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

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	972	U
1	D	907	G
1	D	960	C
1	C	970	A
1	D	953	A

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	88/88 (100%)	0.24	5 (5%) 27 17	53, 78, 126, 149	0
1	D	88/88 (100%)	0.45	7 (7%) 15 9	53, 91, 146, 150	0
2	A	948/967 (98%)	-0.06	30 (3%) 51 38	8, 59, 131, 150	0
2	B	948/967 (98%)	0.29	55 (5%) 26 16	48, 102, 149, 150	0
All	All	2072/2110 (98%)	0.13	97 (4%) 35 24	8, 82, 143, 150	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	407	LYS	5.5
1	D	936	U	5.5
2	B	524	TRP	5.3
1	D	939	A	5.1
2	B	236	TYR	5.1

### 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.