



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 02:55 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 validation summary 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/ValidationPDFNotes.html>

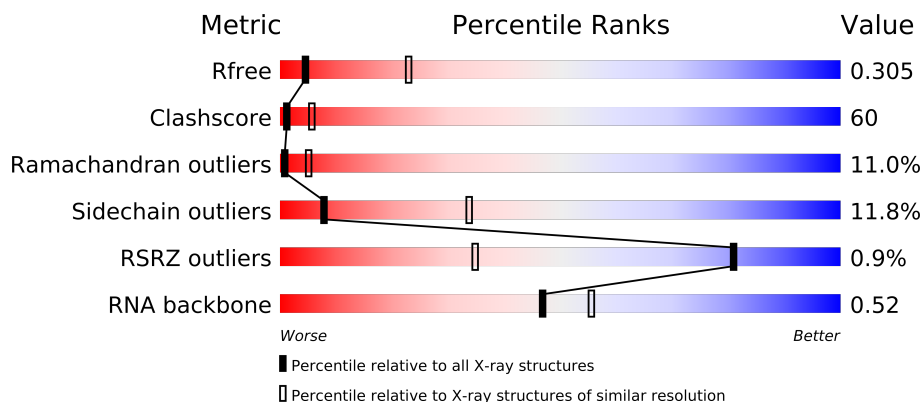
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

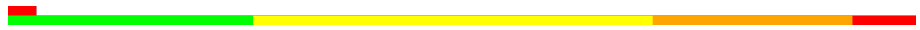


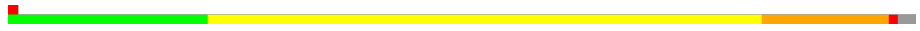
The reported resolution of this entry is 3.21 Å.

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}	66092	1205 (3.30-3.14)
Clashscore	79885	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RSRZ outliers	66119	1206 (3.30-3.14)
RNA backbone	1838	1004 (3.74-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	88	
1	D	88	
2	A	967	
2	B	967	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19578 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

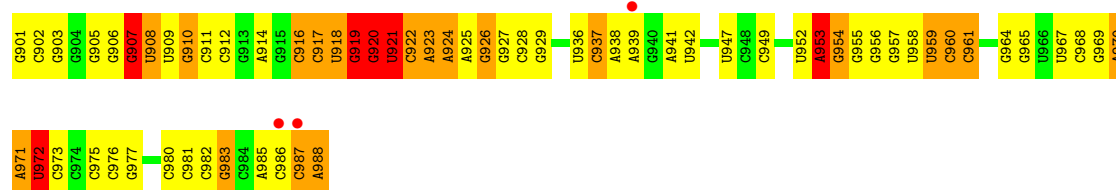
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	948	Total	C	N	O	S	0	0	0
			7909	5132	1323	1430	24			
2	B	948	Total	C	N	O	S	0	0	0
			7909	5132	1323	1430	24			

3 Residue-property plots

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.

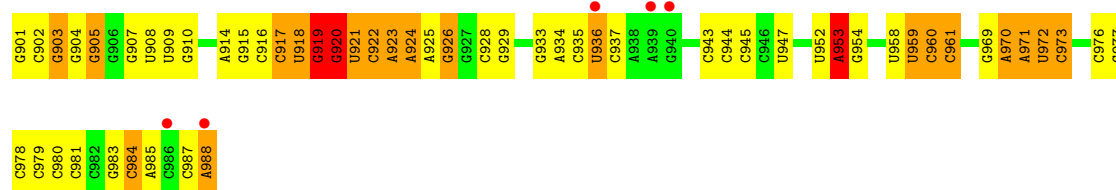
• Molecule 1: tRNA

Chain C: 



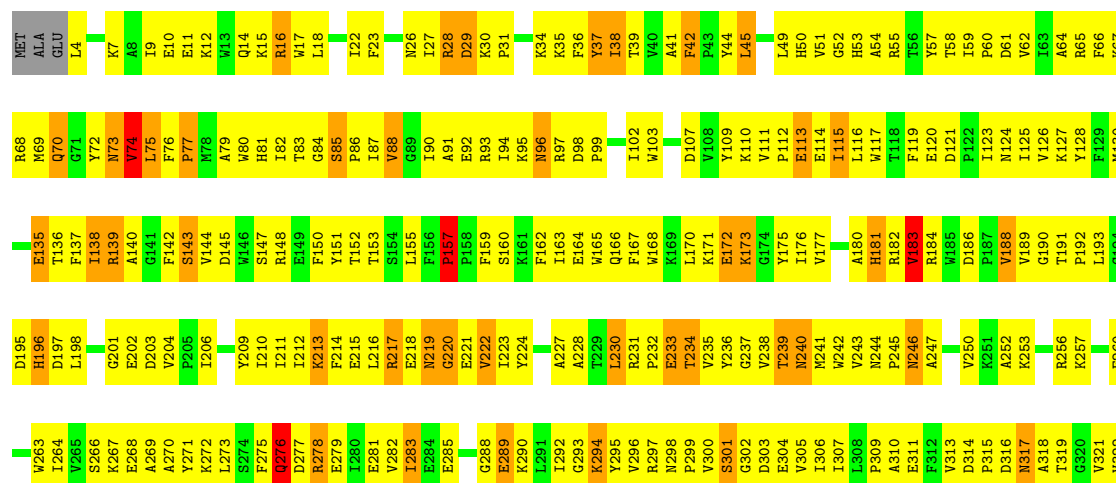
• Molecule 1: tRNA

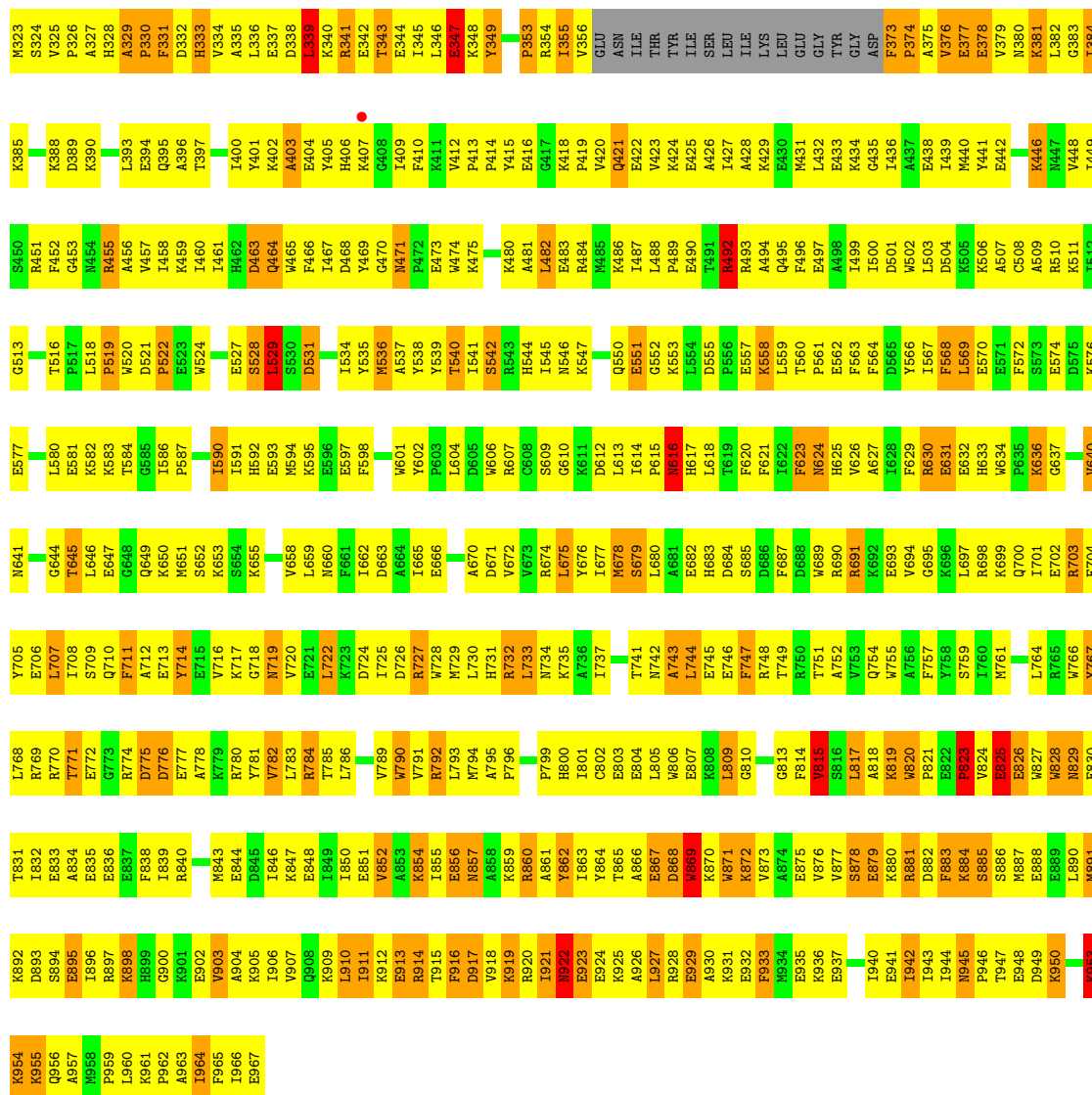
Chain D: 



• Molecule 2: Leucyl-tRNA synthetase

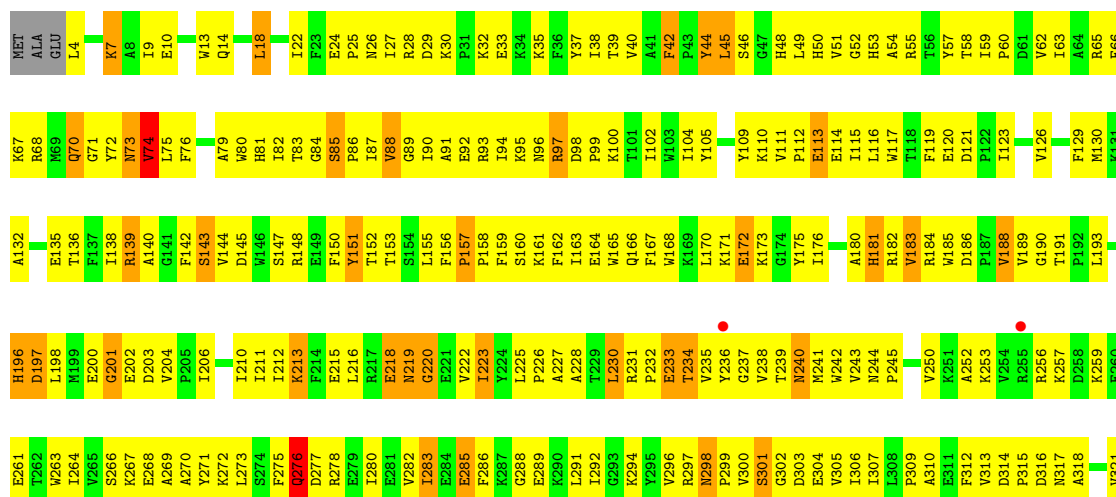
Chain A: 





• Molecule 2: Leucyl-tRNA synthetase

Chain B:



A957	D893	E830	L768	E706	K636	Y566	K506	F443	L382	V322
M958	S894	T831	R769	L707	G637	I567	A507	F446	G383	K323
P959	E895	T832	R770	I708	V640	F568	C508	K447	S324	K324
L960	I896	E833	T771	S709	N641	E570	A509	M448	V325	P326
P962	G900	E835	R774	F711	G644	S573	R510	V448	S386	A327
A963	K901	E836	D775	A712	T645	E573	K511	I449	K388	H328
T964	E902	E837	D776	E713	L646	K576	G513	S450	D389	A329
F965	V903	F838	D777	Y714	E577	E577	G514	R451	P330	F331
P966	A904	T839	A778	K717	G648	E577	G515	G453	K392	D332
E967	K905	R840	K779	K717	E648	L580	T516	N454	L393	D332
	I906	S841	R780	K718	Q649	E581	P517	R455	E394	V334
	V907	V842	N781	N719	K650	E581	L518	A456	Q395	A335
	Q908	R843	V782	V720	K651	T584	P519	K459	A396	L336
	K909	E844	L783	E721	S652	G585	W520	I460	A397	E337
	L910	D845	L784	E722	K653	E592	D521	I461	K398	D338
	E911	T846	T785	K723	S654	P587	P522	H462	T399	L339
	K912	K847	L786	I725	K655	E587	E523	D463	I400	K340
	E913	E848		D726	V658	I590	W524	Q464	Y401	R341
	R914	T849		R727	L659	I591	W525		K402	E342
	T915	I850	W789	R727	N660	E592	E527	I467	A403	T343
	F916	E851	V791	W728	F661	E593	E528	D468	E404	E344
	D917	V852	R792	M729	L662	M594	L529	Y469	Y405	T345
	V918	A853	L793	L730	D663	K595	S530	G470	H406	L346
	K919	K854	M794	H731	E664	E596	D531	K471	K407	E347
	R920	T855	A795	R732	L665	E597	S532	F472	G408	K348
	N921	E856	P796	L733	A670	F598	T533	E473	I409	K349
	E923	N857	F797	N734	D671	E599	Y534	W474	F410	D350
	E924	A858	T798	T737	E671	Y600	Y535	K475	K411	L351
	K925	R860	H800	K738	D671	W601	M536	E476	V412	D352
	A926	A861	I801	E739	R674	Y602	A537	K477	P413	P353
	L927	E862	C802	T740	L675	W606	F538	A478	P414	R354
	R928	T863	R803	T741	Y676	C608	Y539	R479	Y415	T355
	E929	E864	E804	N742	L677	R607	T540	K480	E416	V356
	A930	T865	L805	A743	M678	C608	S542	A481	G417	GLU
	K931	A866	W806	L744	S679	S609	I541	L482	K418	ASN
	E932	E867	E807	E745	L680	L613	R543	E483	P419	ILE
	F933	D868	K808	E746	A681	L614	H544	R484	V420	THR
	M934	W869	L809	F747	E682	P615	T546	M485	Q421	TYR
	E935	K870	G810	R748	H683	N616	K547	K486	E422	ILE
		W871	G811	T749	D684	H617	L548	I487	V423	SER
	L938	K872	E812	R750	E687	L618	R549	L488	K424	LEU
	G939	G813	G813	T751	T687	T619	K549	ILE	E425	ILE
	I940	S878	F814	A752	D688	F620	Q550	A426	A426	LYS
	E941	E879	V815	V753	W689	F621	E551	I427	I427	LEU
	I942	K880	S816	Q754	R690	F621	G552	A428	A428	GLU
	I943	K881	L817	W755	E693	I622	K553	K429	K429	GLY
	I944	D882	A818	A756	E694	F623	L554	E430	E430	TYR
	N945	F883	K819	F757	G695	N624	D555	M431	M431	GLY
	P946	K884	W820	Y758	K696	H625	P556	L432	L432	ASP
		P821	P821	Y758	L697	V626	E557	E497	E497	
	D949	S885	E822	S759	R698	F629	K558	A498	K434	P374
	K950	R886	P823	I760	M761	R630	L559	I499	G435	A375
	G951	N887	V824	M762	N763	E631	T560	I500	I436	V376
	G952	E888	E825	D763	L701	E632	P561	D501	A437	E377
	K953	E889	E826	L764	E702	H633	E562	W502	E438	E378
	K954	L890	W827	R765	R703	H633	F563	L503	I439	V379
	K955	M891	W828	W766	F704	W634	F564	D504	K380	N380
	Q956	K892	N829	Y767	Y705	P635	D565	K505	E442	K381

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 0.245 , 0.305	Depositor DCC
R_{free} test set	5012 reflections (11.19%)	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 , 36.2	EDS
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 49816 reflections	Xtriage
F_o, F_c correlation	0.89	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 60.

The worst 5 of 2256 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

5.3.1 Protein backbone ⓘ

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%)	1	5
2	B	944/967 (98%)	632 (67%)	208 (22%)	104 (11%)	1	5
All	All	1888/1934 (98%)	1262 (67%)	419 (22%)	207 (11%)	1	5

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 ⓘ

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%)	6	28
2	B	841/857 (98%)	752 (89%)	89 (11%)	10	38
All	All	1682/1714 (98%)	1483 (88%)	199 (12%)	8	34

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

Mol	Chain	Res	Type
2	A	829	ASN
2	B	18	LEU
2	B	825	GLU
2	A	860	ARG

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Mol	Chain	Res	Type
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.16	3 (3%)	43 9	53, 78, 126, 149	0
1	D	88/88 (100%)	0.26	5 (5%)	23 5	53, 91, 146, 150	0
2	A	948/967 (98%)	-0.10	1 (0%)	93 75	8, 59, 131, 150	0
2	B	948/967 (98%)	0.08	9 (0%)	81 35	48, 102, 149, 150	0
All	All	2072/2110 (98%)	0.01	18 (0%)	81 35	8, 82, 143, 150	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	939	A	5.3
1	D	936	U	4.2
2	B	920	ARG	3.9
1	D	986	C	3.5
2	B	236	TYR	3.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.