



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 11:45 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

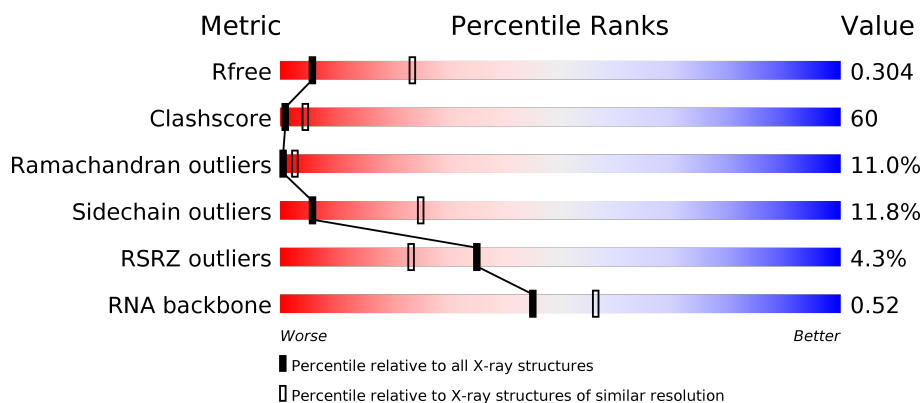
1 Overall quality at a glance

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}	111664	1145 (3.24-3.20)
Clashscore	122126	1266 (3.24-3.20)
Ramachandran outliers	120053	1245 (3.24-3.20)
Sidechain outliers	120020	1244 (3.24-3.20)
RSRZ outliers	108989	1103 (3.24-3.20)
RNA backbone	2636	1117 (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% 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>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			

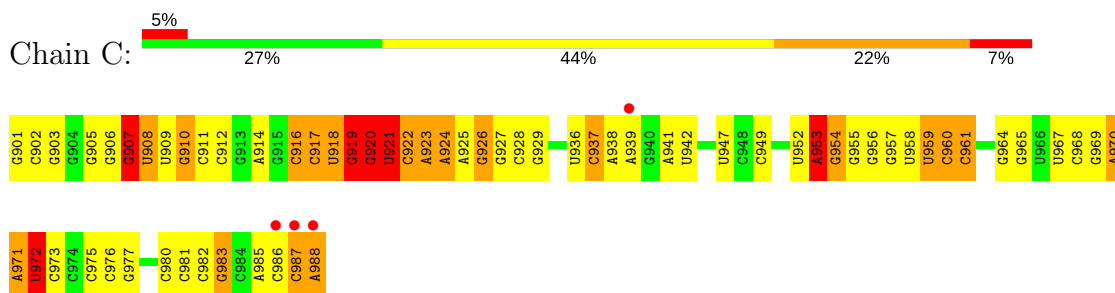
- Molecule 2 is a protein called Leucyl-tRNA synthetase.

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			

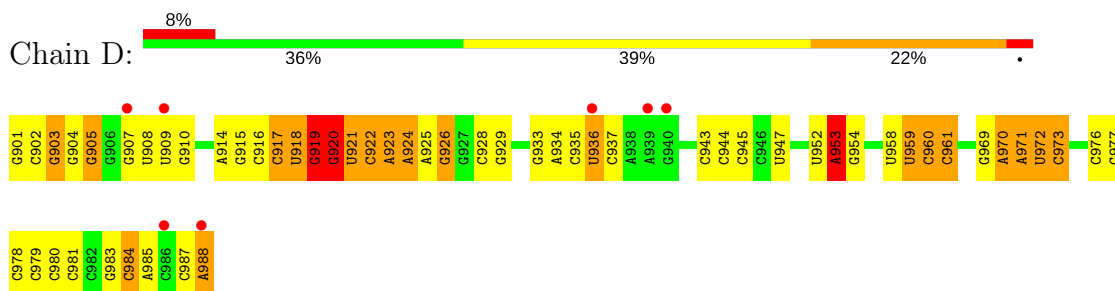
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

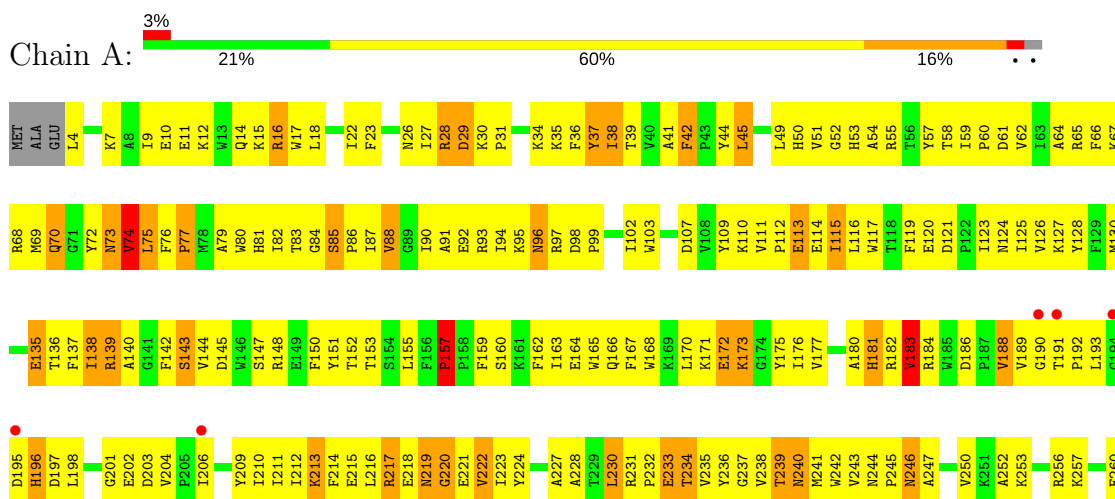
• Molecule 1: tRNA

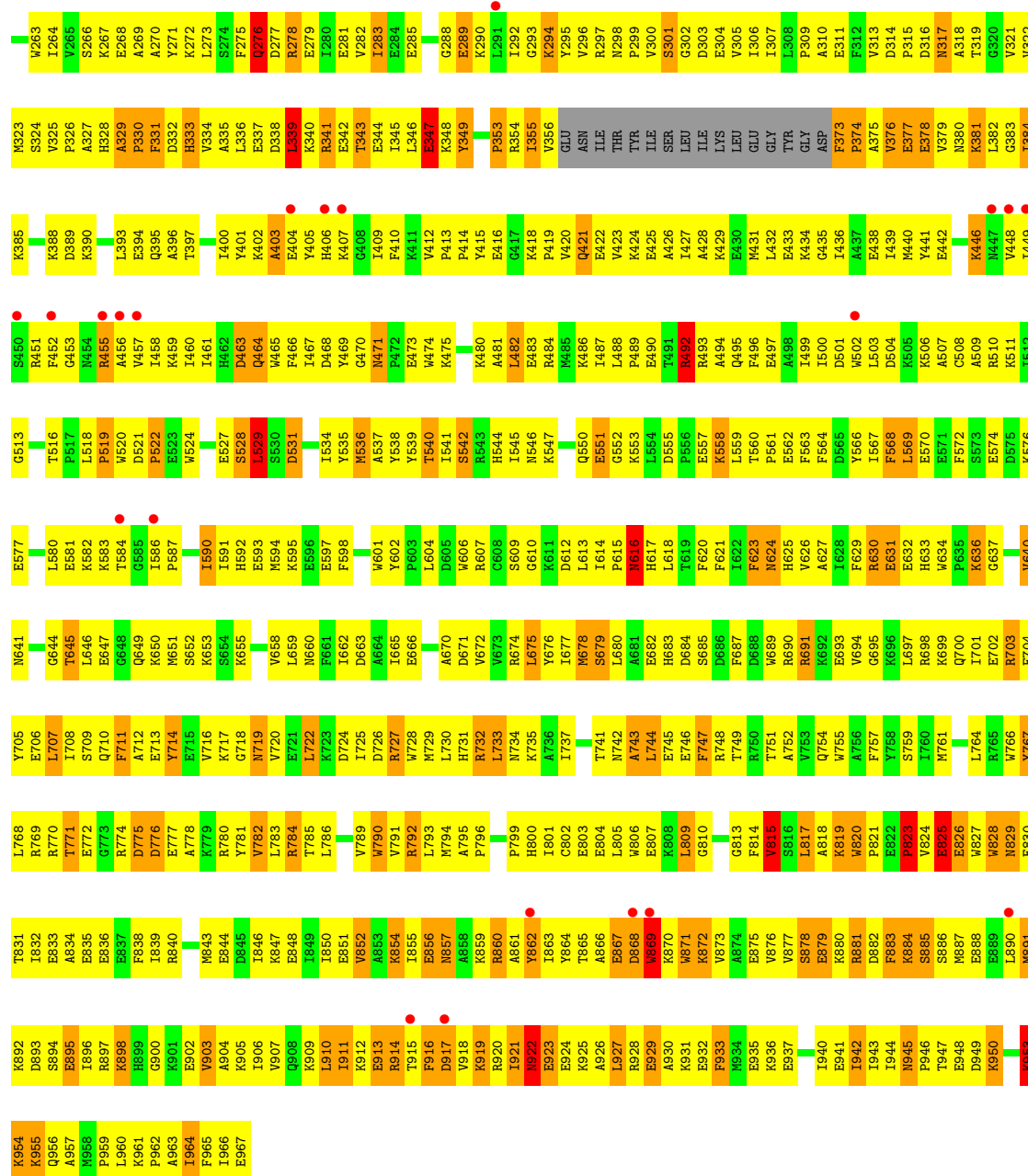


• Molecule 1: tRNA



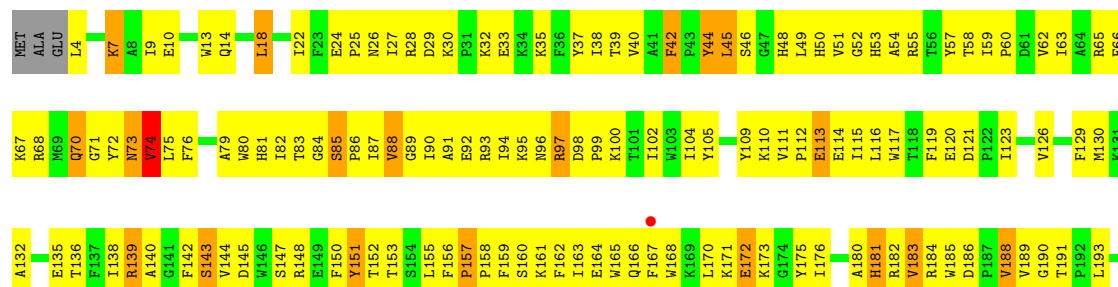
• Molecule 2: Leucyl-tRNA synthetase





• Molecule 2: Leucyl-tRNA synthetase

Chain B: 5% 22% 61% 14%



K954	K955	Q956	A957	M958	P959	L960	K961	G900	K901	E902	V903	A904	K905	I906	V907	H841	S842	H843	E844	L845	I846	K847	E848	I849	T850	F851	V852	A853	K854	I855	E856	N857	A858	K859	R860	A861	Y862	T863	Y864	T865	A866	E867	D868	K869	K870	W871	K872	G839	E940	E941	I942	I943	I944	N945	P946	D949	K950	G951	E952	K953							
L890	M891	K892	D893	T831	E832	E833	A834	E835	E836	E837	F838	I839	K840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889					
E703	F704	Y705	E706	L707	I708	S709	F710	F711	A712	E713	Y714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764						
R765	W766	Y767	L768	R769	R770	T771	R772	D773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826						
W827	W828	E829	E830	T831	I832	E833	A834	E835	E836	E837	F838	I839	K840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889					
E923	E924	K925	L927	R928	E929	A930	F931	F932	F933	M934	E935	L938	G939	E940	E941	I942	I943	I944	N945	P946	D949	K950	G951	E952	K953	E923	E924	K925	L927	R928	E929	A930	F931	F932	F933	M934	E935	L938	G939	E940	E941	I942	I943	I944	N945	P946	D949	K950	G951	E952	K953																
E261	T262	W263	L264	Y265	S266	K267	E268	A269	A270	Y271	K272	L273	E274	E275	E276	E277	E278	E279	E280	E281	E282	E283	E284	E285	E286	E287	E288	E289	E290	E291	E292	E293	E294	E295	E296	E297	E298	E299	E300	E301	E302	E303	E304	E305	E306	E307	E308	E309	E310	E311	E312	E313	E314	E315	E316	E317	E318	E319	E320								
H321	V322	M323	S324	K325	P326	A327	H328	A329	P330	F331	D332	H333	V334	A335	L336	E337	D338	E339	K340	R341	E342	T343	E344	I345	L346	E347	E348	E349	D350	P351	R352	R353	R354	I355	V356	G357	ASN	ILE	THR	TYR	ILE	E422	V423	LEU	ILE	LYS	LEU	GLY	TYR	GLY	ASP	F373	P374	A375	R376	E377	E378	V379	N380								
K381	L382	G383	I384	S385	K386	Q387	D388	K389	K390	E391	E392	L393	V394	Q395	A396	E397	K398	T399	I400	A401	K402	E403	E404	Y405	H406	K407	G408	I409	F410	E411	V412	P413	E414	Y415	E416	G417	K418	P419	V420	Q421	E422	V423	K424	E425	A426	I427	K428	E429	E430	M431	L432	E433	F373	P374	A375	R376	E377	E378	V379	N380							
E442	F443	K446	N447	V448	T449	S450	R451	F452	Q453	N454	L455	A456	V457	L458	K459	L460	T461	H462	Q463	Q464	D465	E466	S467	S468	E469	E470	E471	E472	E473	E474	E475	E476	E477	E478	E479	E480	E481	E482	E483	E484	E485	E486	E487	E488	E489	E490	E491	E492	E493	E494	E495	E496	E497	E498	E499	E500	E501	E502	E503								
D504	K505	Y506	E507	C508	A509	R510	E511	E512	E513	L514	G515	T516	F517	L518	P519	W520	K521	P522	E523	W524	E525	E526	E527	S528	L529	S530	D531	S532	T533	E534	Y535	M536	A537	Y538	Y539	E540	E541	S542	R543	E544	E545	E546	E547	E548	E549	E550	E551	E552	E553	E554	E555	E556	E557	E558	E559	E560	E561	E562	E563								
F564	D565	Y566	E567	F568	L569	E570	S571	K572	E573	E574	E575	L580	E581	K582	K583	T584	E585	E586	E587	E588	E589	E590	E591	E592	E593	E594	E595	E596	E597	E598	E599	E600	E601	E602	E603	E604	E605	E606	E607	E608	S609	L613	E614	E615	E616	E617	E618	E619	E620	E621	E622	E623	E624	E625	E626	E627	E628	E629	E630	E631	E632						
H633	W634	P635	K636	G637	V640	M641	G642	E643	E644	E645	E646	E647	E648	E649	E650	E651	E652	E653	E654	E655	E656	E657	E658	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702
R703	F704	Y705	E706	L707	I708	S709	F710	F711	A712	E713	Y714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764						
R765	W766	Y767	L768	R769	R770	T771	R772	D773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826						
W827	W828	E829	E830	T831	I832	E833	A834	E835	E836	E837	F838	I839	K840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889					
E923	E924	K925	L927	R928	E929	A930	F931	F932	F933	M934	E935	L938	G939	E940	E941	I942	I943	I944	N945	P946	D949	K950	G951	E952	K953	E923	E924	K925	L927	R928	E929	A930	F931	F932	F933	M934	E935	L938	G939	E940	E941	I942	I943	I944	N945	P946	D949	K950	G951	E952	K953																

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	5012 reflections (10.06%)	wwPDB-VP
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

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

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%)	4	20
2	B	841/857 (98%)	752 (89%)	89 (11%)	7	30
All	All	1682/1714 (98%)	1483 (88%)	199 (12%)	6	25

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

Mol	Chain	Res	Type
2	A	829	ASN

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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, 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%) 33 22	53, 78, 126, 149	0
1	D	88/88 (100%)	0.41	7 (7%) 12 7	53, 91, 146, 150	0
2	A	948/967 (98%)	-0.09	26 (2%) 54 41	8, 59, 131, 150	0
2	B	948/967 (98%)	0.26	53 (5%) 24 14	48, 102, 149, 150	0
All	All	2072/2110 (98%)	0.10	90 (4%) 35 23	8, 82, 143, 150	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	407	LYS	5.3
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.