



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 09:24 AM UTC

PDB ID : 6HLU / pdb_00006hlu
Title : Crystal structure of the LRR-Roc-COR domain of the *Chlorobium tepidum* Roco protein
Authors : Deyaert, E.; Versees, W.; Singh, R.
Deposited on : 2018-09-11
Resolution : 3.29 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

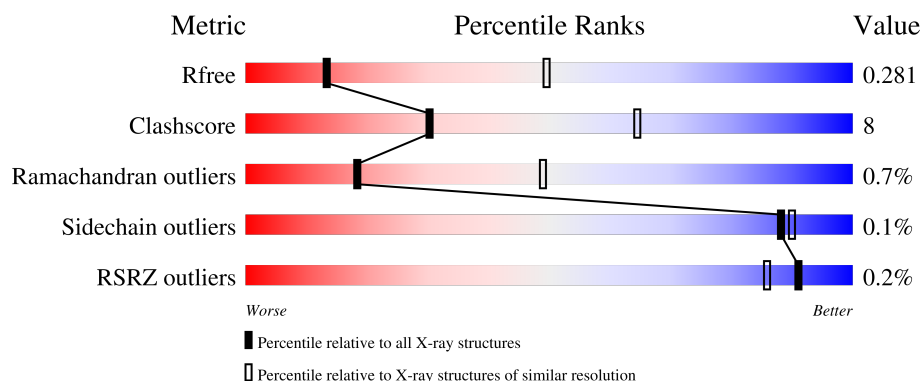
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. 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	A	974	 76% 17% 7%
1	B	974	 72% 19% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13681 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 Rab family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	908	Total	C	N	O	S	0	0	0
			6890	4379	1117	1372	22			
1	B	896	Total	C	N	O	S	0	0	0
			6791	4306	1103	1361	21			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q8KC98
A	-26	SER	-	expression tag	UNP Q8KC98
A	-25	TYR	-	expression tag	UNP Q8KC98
A	-24	TYR	-	expression tag	UNP Q8KC98
A	-23	HIS	-	expression tag	UNP Q8KC98
A	-22	HIS	-	expression tag	UNP Q8KC98
A	-21	HIS	-	expression tag	UNP Q8KC98
A	-20	HIS	-	expression tag	UNP Q8KC98
A	-19	HIS	-	expression tag	UNP Q8KC98
A	-18	HIS	-	expression tag	UNP Q8KC98
A	-17	ASP	-	expression tag	UNP Q8KC98
A	-16	TYR	-	expression tag	UNP Q8KC98
A	-15	ASP	-	expression tag	UNP Q8KC98
A	-14	ILE	-	expression tag	UNP Q8KC98
A	-13	PRO	-	expression tag	UNP Q8KC98
A	-12	THR	-	expression tag	UNP Q8KC98
A	-11	THR	-	expression tag	UNP Q8KC98
A	-10	GLU	-	expression tag	UNP Q8KC98
A	-9	ASN	-	expression tag	UNP Q8KC98
A	-8	LEU	-	expression tag	UNP Q8KC98
A	-7	TYR	-	expression tag	UNP Q8KC98
A	-6	PHE	-	expression tag	UNP Q8KC98
A	-5	GLN	-	expression tag	UNP Q8KC98
A	-4	GLY	-	expression tag	UNP Q8KC98
A	-3	ALA	-	expression tag	UNP Q8KC98

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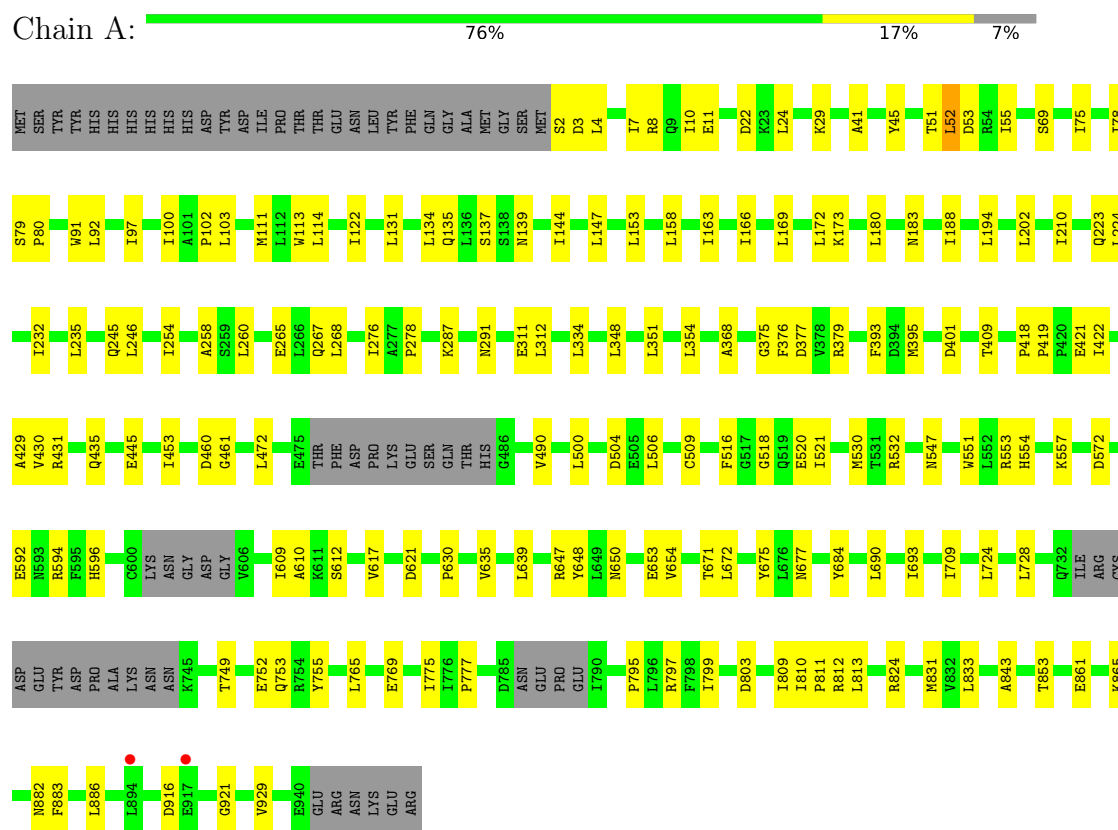
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP Q8KC98
A	-1	GLY	-	expression tag	UNP Q8KC98
A	0	SER	-	expression tag	UNP Q8KC98
B	-27	MET	-	initiating methionine	UNP Q8KC98
B	-26	SER	-	expression tag	UNP Q8KC98
B	-25	TYR	-	expression tag	UNP Q8KC98
B	-24	TYR	-	expression tag	UNP Q8KC98
B	-23	HIS	-	expression tag	UNP Q8KC98
B	-22	HIS	-	expression tag	UNP Q8KC98
B	-21	HIS	-	expression tag	UNP Q8KC98
B	-20	HIS	-	expression tag	UNP Q8KC98
B	-19	HIS	-	expression tag	UNP Q8KC98
B	-18	HIS	-	expression tag	UNP Q8KC98
B	-17	ASP	-	expression tag	UNP Q8KC98
B	-16	TYR	-	expression tag	UNP Q8KC98
B	-15	ASP	-	expression tag	UNP Q8KC98
B	-14	ILE	-	expression tag	UNP Q8KC98
B	-13	PRO	-	expression tag	UNP Q8KC98
B	-12	THR	-	expression tag	UNP Q8KC98
B	-11	THR	-	expression tag	UNP Q8KC98
B	-10	GLU	-	expression tag	UNP Q8KC98
B	-9	ASN	-	expression tag	UNP Q8KC98
B	-8	LEU	-	expression tag	UNP Q8KC98
B	-7	TYR	-	expression tag	UNP Q8KC98
B	-6	PHE	-	expression tag	UNP Q8KC98
B	-5	GLN	-	expression tag	UNP Q8KC98
B	-4	GLY	-	expression tag	UNP Q8KC98
B	-3	ALA	-	expression tag	UNP Q8KC98
B	-2	MET	-	expression tag	UNP Q8KC98
B	-1	GLY	-	expression tag	UNP Q8KC98
B	0	SER	-	expression tag	UNP Q8KC98

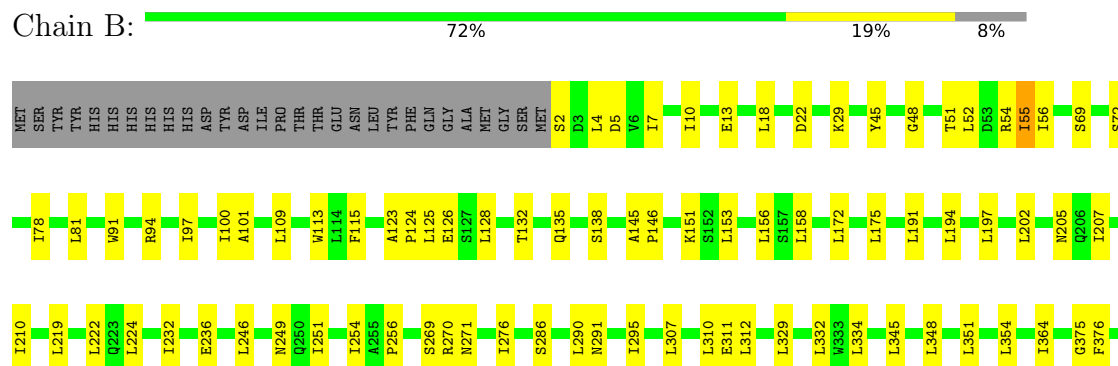
3 Residue-property plots [i](#)

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 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: Rab family protein



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E940	R385	I708	I815	I458	R386	I709	I816	I459	L386	I710	I817	I460	L387	I711	I818	I461	L388	I712	I819	I462	L389	I713	I820	I463	L390	I714	I821	I464	L391	I715	I822	I465	L392	I716	I823	I466	L393	I717	I824	I467	L394	I718	I825	I468	L395	I719	I826	I469	L396	I720	I827	I470	L397	I721	I828	I471	L398	I722	I829	I472	L399	I723	I830	I473	L400	I724	I831	I474	L401	I725	I832	I475	L402	I726	I833	I476	L403	I727	I834	I477	L404	I728	I835	I478	L405	I729	I836	I479	L406	I730	I837	I480	L407	I731	I838	I481	L408	I732	I839	I482	L409	I733	I840	I483	L410	I734	I841	I484	L411	I735	I842	I485	L412	I736	I843	I486	L413	I737	I844	I487	L414	I738	I845	I488	L415	I739	I846	I489	L416	I740	I847	I490	L417	I741	I848	I491	L418	I742	I849	I492	L419	I743	I850	I493	L420	I744	I851	I494	L421	I745	I852	I495	L422	I746	I853	I496	L423	I747	I854	I497	L424	I748	I855	I498	L425	I749	I856	I499	L426	I750	I857	I500	L427	I751	I858	I501	L428	I752	I859	I502	L429	I753	I860	I503	L430	I754	I861	I504	L431	I755	I862	I505	L432	I756	I863	I506	L433	I757	I864	I507	L434	I758	I865	I508	L435	I759	I866	I509	L436	I760	I867	I510	L437	I761	I868	I511	L438	I762	I869	I512	L439	I763	I870	I513	L440	I764	I871	I514	L441	I765	I872	I515	L442	I766	I873	I516	L443	I767	I874	I517	L444	I768	I875	I518	L445	I769	I876	I519	L446	I770	I877	I520	L447	I771	I878	I521	L448	I772	I879	I522	L449	I773	I880	I523	L450	I774	I881	I524	L451	I775	I882	I525	L452	I776	I883	I526	L453	I777	I884	I527	L454	I778	I885	I528	L455	I779	I886	I529	L456	I780	I887	I530	L457	I781	I888	I531	L458	I782	I889	I532	L459	I783	I890	I533	L460	I784	I891	I534	L461	I785	I892	I535	L462	I786	I893	I536	L463	I787	I894	I537	L464	I788	I895	I538	L465	I789	I896	I539	L466	I790	I897	I540	L467	I791	I898	I541	L468	I792	I899	I542	L469	I793	I900	I543	L470	I794	I901	I544	L471	I795	I902	I545	L472	I796	I903	I546	L473	I797	I904	I547	L474	I798	I905	I548	L475	I799	I906	I549	L476	I800	I907	I550	L477	I801	I908	I551	L478	I802	I909	I552	L479	I803	I910	I553	L480	I804	I911	I554	L481	I805	I912	I555	L482	I806	I913	I556	L483	I807	I914	I557	L484	I808	I915	I558	L485	I809	I916	I559	L486	I810	I917	I560	L487	I811	I918	I561	L488	I812	I919	I562	L489	I813	I920	I563	L490	I814	I921	I564	L491	I815	I922	I565	L492	I816	I923	I566	L493	I817	I924	I567	L494	I818	I925	I568	L495	I819	I926	I569	L496	I820	I927	I570	L497	I821	I928	I571	L498	I822	I929	I572	L499	I823	I930	I573	L500	I824	I931	I574	L501	I825	I932	I575	L502	I826	I933	I576	L503	I827	I934	I577	L504	I828	I935	I578	L505	I829	I936	I579	L506	I830	I937	I580	L507	I831	I938	I581	L508	I832	I939	I582	L509	I833	I940	I583	L510	I834	I941	I584	L511	I835	I942	I585	L512	I836	I943	I586	L513	I837	I944	I587	L514	I838	I945	I588	L515	I839	I946	I589	L516	I840	I947	I590	L517	I841	I948	I591	L518	I842	I949	I592	L519	I843	I950	I593	L520	I844	I951	I594	L521	I845	I952	I595	L522	I846	I953	I596	L523	I847	I954	I597	L524	I848	I955	I598	L525	I849	I956	I599	L526	I850	I957	I600	L527	I851	I958	I601	L528	I852	I959	I602	L529	I853	I960	I603	L530	I854	I961	I604	L531	I855	I962	I605	L532	I856	I963	I606	L533	I857	I964	I607	L534	I858	I965	I608	L535	I859	I966	I609	L536	I860	I967	I610	L537	I861	I968	I611	L538	I862	I969	I612	L539	I863	I970	I613	L540	I864	I971	I614	L541	I865	I972	I615	L542	I866	I973	I616	L543	I867	I974	I617	L544	I868	I975	I618	L545	I869	I976	I619	L546	I870	I977	I620	L547	I871	I978	I621	L548	I872	I979	I622	L549	I873	I980	I623	L550	I874	I981	I624	L551	I875	I982	I625	L552	I876	I983	I626	L553	I877	I984	I627	L554	I878	I985	I628	L555	I879	I986	I629	L556	I880	I987	I630	L557	I881	I988	I631	L558	I882	I989	I632	L559	I883	I990	I633	L560	I884	I991	I634	L561	I885	I992	I635	L562	I886	I993	I636	L563	I887	I994	I637	L564	I888	I995	I638	L565	I889	I996	I639	L566	I890	I997	I640	L567	I891	I998	I641	L568	I892	I999	I642	L569	I893	I1000	I643	L570	I894	I1001	I644	L571	I895	I1002	I645	L572	I896	I1003	I646	L573	I897	I1004	I647	L574	I898	I1005	I648	L575	I899	I1006	I649	L576	I900	I1007	I650	L577	I901	I1008	I651	L578	I902	I1009	I652	L579	I903	I1010	I653	L580	I904	I1011	I654	L581	I905	I1012	I655	L582	I906	I1013	I656	L583	I907	I1014	I657	L584	I908	I1015	I658	L585	I909	I1016	I659	L586	I910	I1017	I660	L587	I911	I1018	I661	L588	I912	I1019	I662	L589	I913	I1020	I663	L590	I914	I1021	I664	L591	I915	I1022	I665	L592	I916	I1023	I666	L593	I917	I1024	I667	L594	I918	I1025	I668	L595	I919	I1026	I669	L596	I920	I1027	I670	L597	I921	I1028	I671	L598	I922	I1029	I672	L599	I923	I1030	I673	L600	I924	I1031	I674	L601	I925	I1032	I675	L602	I926	I1033	I676	L603	I927	I1034	I677	L604	I928	I1035	I678	L605	I929	I1036	I679	L606	I930	I1037	I680	L607	I931	I1038	I681	L608	I932	I1039	I682	L609	I933	I1040	I683	L610	I934	I1041	I684	L611	I935	I1042	I685	L612	I936	I1043	I686	L613	I937	I1044	I687	L614	I938	I1045	I688	L615	I939	I1046	I689	L616	I940	I1047	I690	L617	I941	I1048	I691	L618	I942	I1049	I692	L619	I943	I1050	I693	L620	I944	I1051	I694	L621	I945	I1052	I695	L622	I946	I1053	I696	L623	I947	I1054	I697	L624	I948	I1055	I698	L625	I949	I1056	I699	L626	I950	I1057	I700	L627	I951	I1058	I701	L628	I952	I1059	I702	L629	I953	I1060	I703	L630	I954	I106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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.59Å 129.76Å 179.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.85 – 3.29 44.85 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.85-3.29) 99.1 (44.85-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.230 , 0.281 0.230 , 0.281	Depositor DCC
R_{free} test set	1686 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	85.1	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13681	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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	A	0.09	0/7010	0.28	0/9556
1	B	0.10	0/6906	0.30	0/9419
All	All	0.09	0/13916	0.29	0/18975

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	6890	0	6658	112	0
1	B	6791	0	6584	118	0
All	All	13681	0	13242	227	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 8.

The worst 5 of 227 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:557:LYS:NZ	1:B:885:ASN:O	2.10	0.83
1:A:769:GLU:OE2	1:A:824:ARG:NH1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ARG:NH1	1:A:621:ASP:O	2.14	0.80
1:B:109:LEU:HD11	1:B:128:LEU:HD23	1.63	0.80
1:A:29:LYS:NZ	1:A:45:TYR:O	2.15	0.79

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	
1	A	898/974 (92%)	806 (90%)	90 (10%)	2 (0%)	43	71
1	B	886/974 (91%)	785 (89%)	90 (10%)	11 (1%)	10	37
All	All	1784/1948 (92%)	1591 (89%)	180 (10%)	13 (1%)	18	49

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	ALA
1	B	145	ALA
1	B	270	ARG
1	B	937	ILE
1	B	55	ILE

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	745/886 (84%)	744 (100%)	1 (0%)	88	90
1	B	750/886 (85%)	750 (100%)	0	100	100
All	All	1495/1772 (84%)	1494 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	490	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	135	GLN
1	B	451	GLN
1	B	762	GLN
1	B	245	GLN
1	A	581	GLN

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 oligosaccharides 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 ⓘ

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	A	908/974 (93%)	-0.23	2 (0%) 91 86	41, 79, 116, 140	0
1	B	896/974 (91%)	-0.12	1 (0%) 92 90	57, 90, 126, 157	0
All	All	1804/1948 (92%)	-0.18	3 (0%) 91 86	41, 85, 122, 157	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	907	LEU	3.4
1	A	917	GLU	2.4
1	A	894	LEU	2.3

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 oligosaccharides 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.