



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 05:27 pm BST

PDB ID : 2DHH
Title : Crystal structure of a multidrug transporter reveal a functionally rotating mechanism
Authors : Murakami, S.; Nakashima, R.; Yamashita, E.; Matsumoto, T.
Deposited on : 2006-03-23
Resolution : 2.80 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	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

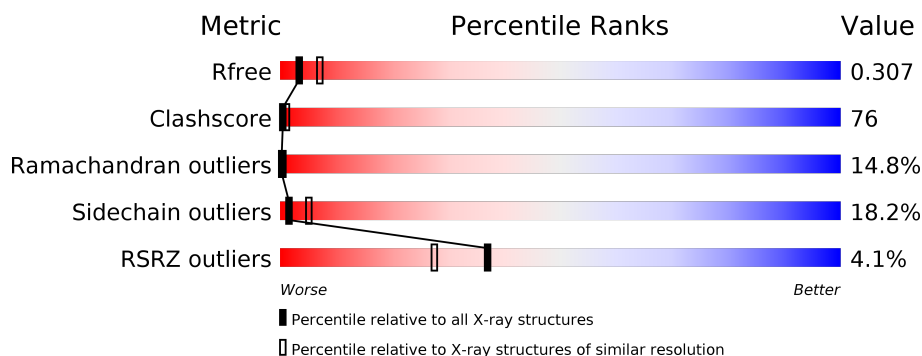
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	1053	<div> <div>4%</div> <div>23% 49% 20% 5% .</div> </div>
1	B	1053	<div> <div>4%</div> <div>19% 55% 21% . .</div> </div>
1	C	1053	<div> <div>4%</div> <div>18% 53% 22% 5% .</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23378 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 ACRB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	B	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	C	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	EXPRESSION TAG	UNP P31224
A	1051	HIS	-	EXPRESSION TAG	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224
B	1050	HIS	-	EXPRESSION TAG	UNP P31224
B	1051	HIS	-	EXPRESSION TAG	UNP P31224
B	1052	HIS	-	EXPRESSION TAG	UNP P31224
B	1053	HIS	-	EXPRESSION TAG	UNP P31224
C	1050	HIS	-	EXPRESSION TAG	UNP P31224
C	1051	HIS	-	EXPRESSION TAG	UNP P31224
C	1052	HIS	-	EXPRESSION TAG	UNP P31224
C	1053	HIS	-	EXPRESSION TAG	UNP P31224

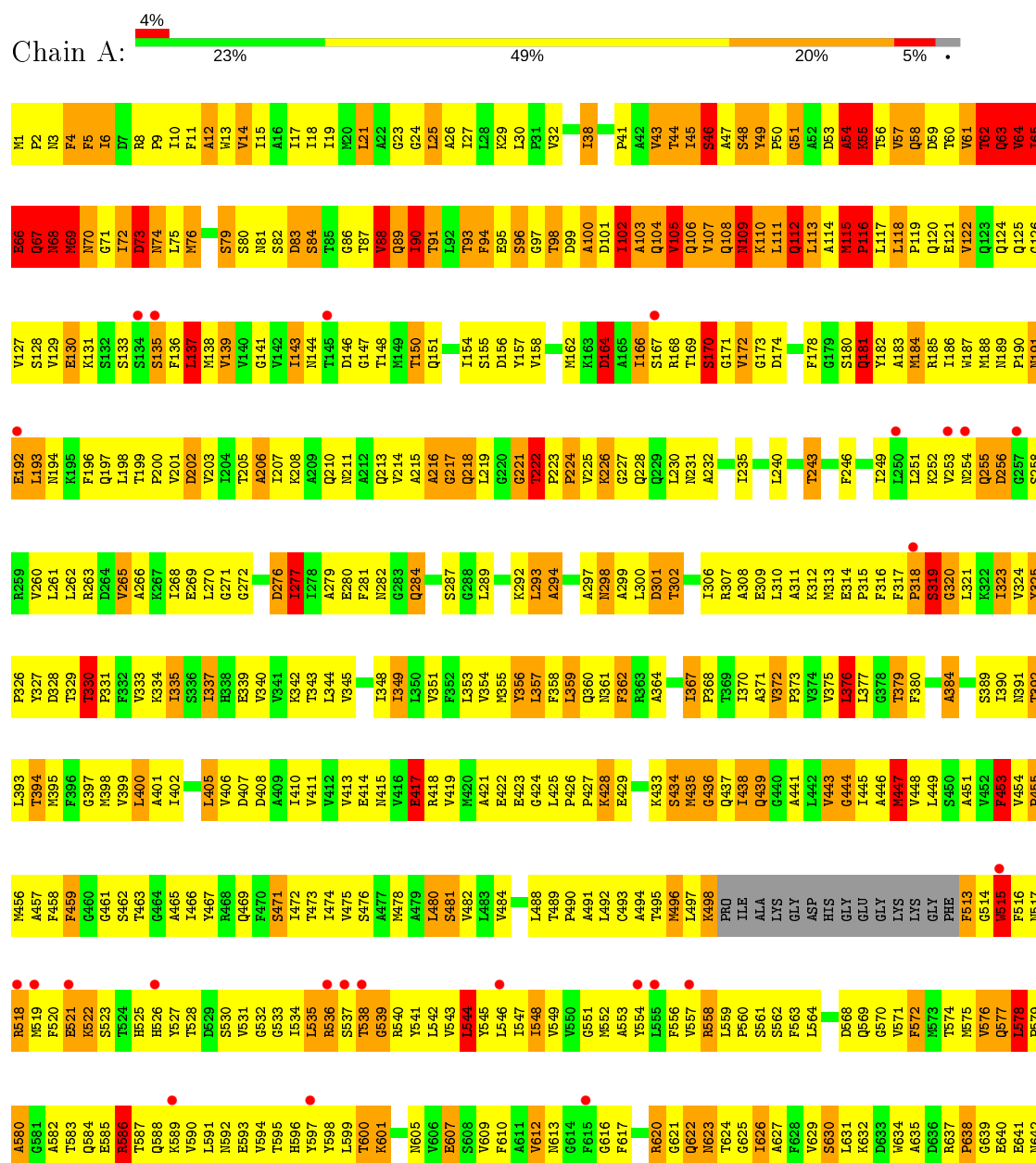
- Molecule 2 is water.

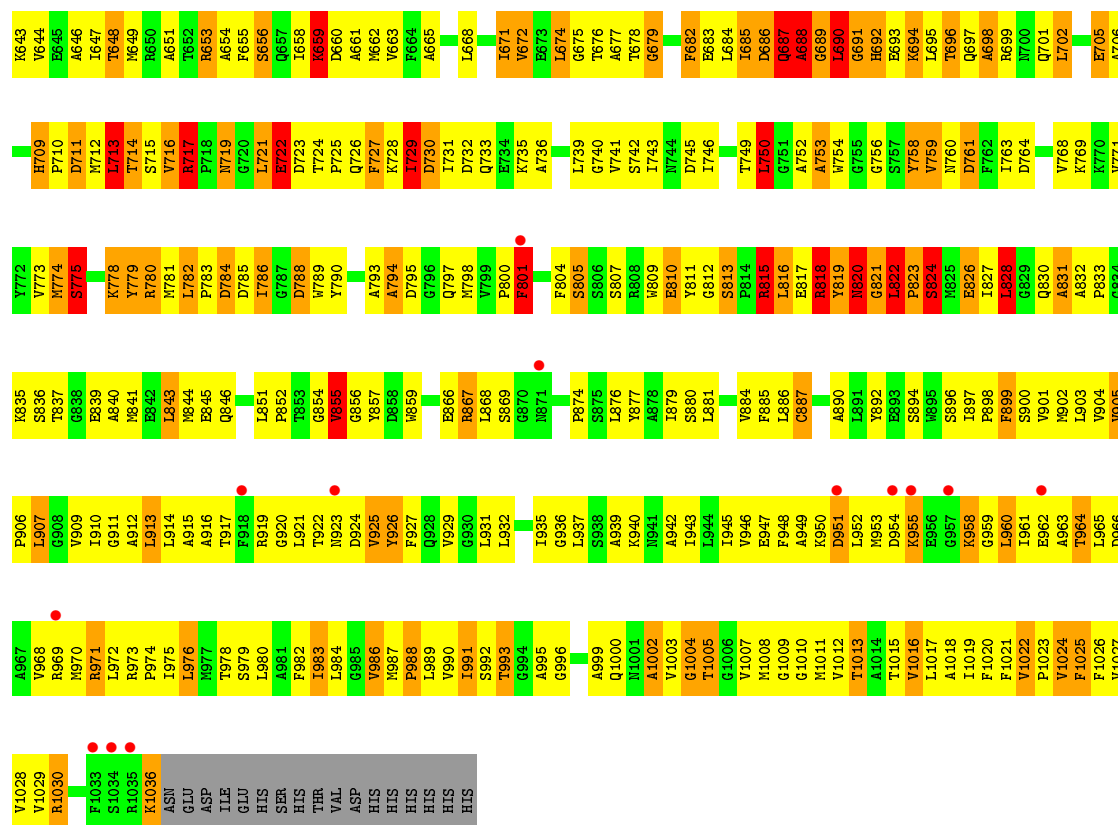
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	B	8	Total	O	0	0
			8	8		
2	C	26	Total	O	0	0
			26	26		

3 Residue-property plots

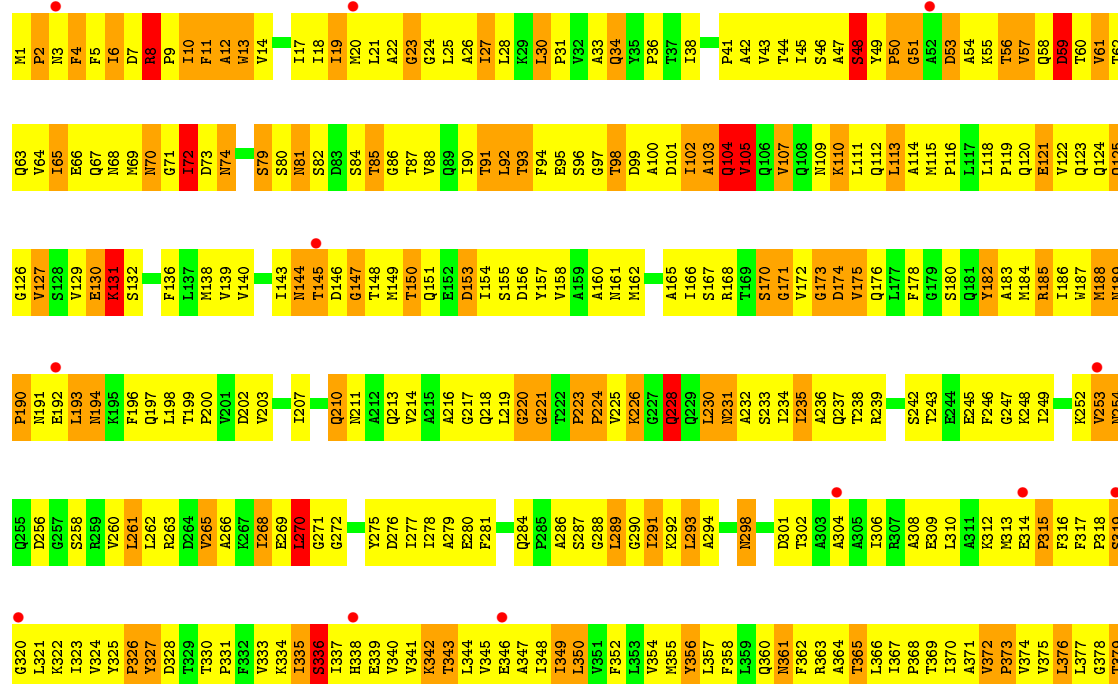
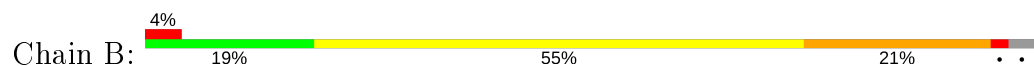
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

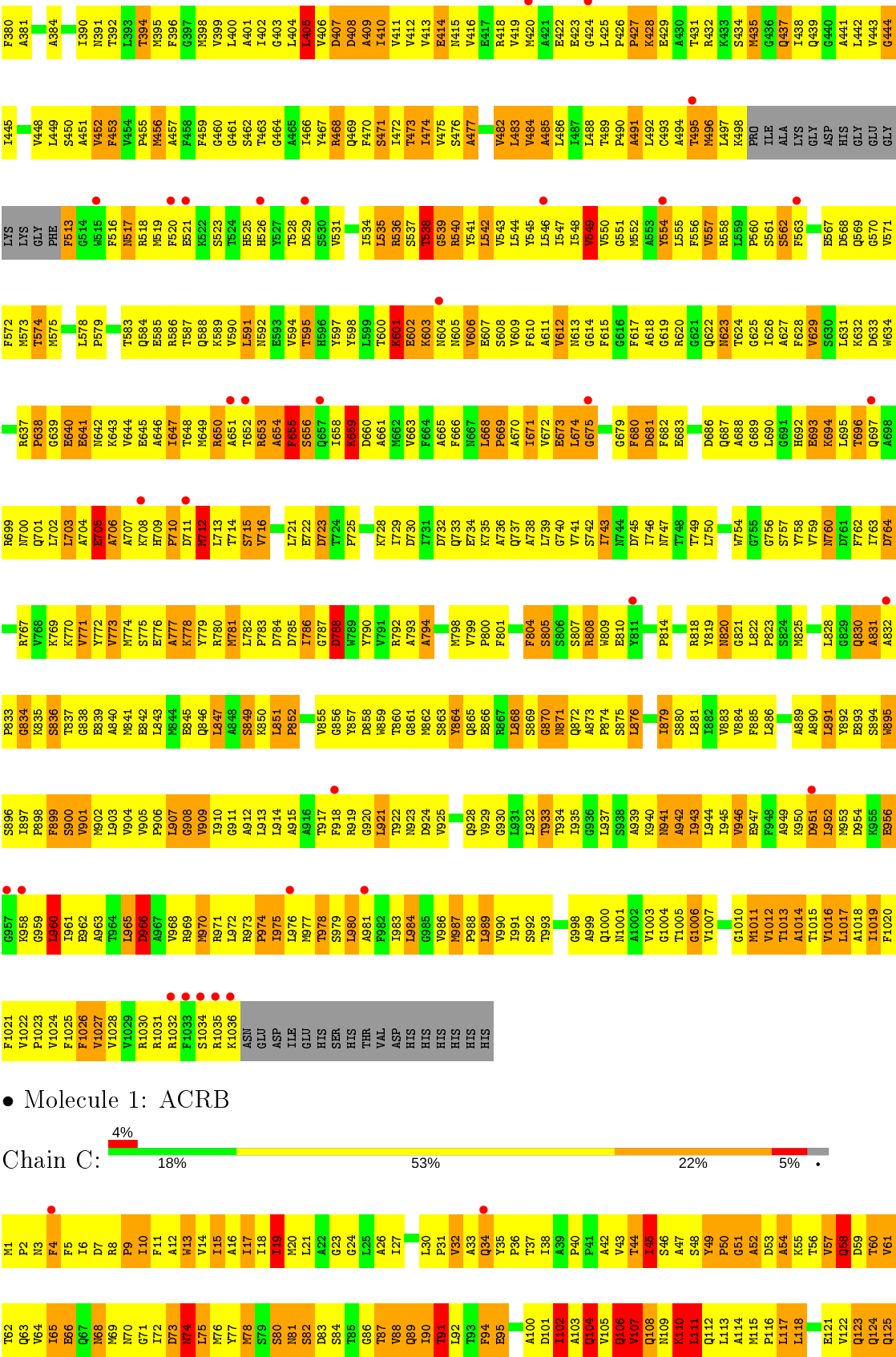
• Molecule 1: ACRB





• Molecule 1: ACRB





T933	T934	T935	G936	L937	S938	A939	K940	R941	A942	I943	L944	T945	I946	E947	F948	A949	K950	D951	L952	P953	D954	G957	K958	G959	L960	T961	E962	A963	T964	L965	D966	A967	V968	R969	K970	R971	L972	R973	P974	I975	I976	R977	T978	S979	L980	A981	F982	L983	L984	G985	V986	N987	P988	L989	T993	G994									
S813	P814	R815	L816	E817	R818	R819	M820	G821	L822	P823	S824	M825	E826	L827	L828	G829	R830	A831	A832	P833	G834	S835	S836	T837	G838	E839	A840	M841	E842	L843	M844	P845	P846	L847	A848	S849	R850	L851	P852	T853	G854	V855	G856	R857	D858	M859	L860	T861	G862	S863	Y864	V865	P866	R867	L868	S869	G870	M871	Q872						
L750	G751	A752	A753	G754	G755	T756	V757	L758	D759	D760	F761	F762	I763	D764	R765	R766	R767	V768	K769	R770	R771	V772	Y773	M774	S775	E776	A777	R778	Y779	R780	M781	L782	P783	R784	I785	I786	G787	D788	M789	Y790	Y791	R792	A793	G796	Q797	M798	V799	P800	F801	S802	A803	P804	S805	Y806	R807	R808	M809	E810	G812						
S813	P814	R815	L816	E817	R818	R819	M820	G821	L822	P823	S824	M825	E826	L827	L828	G829	R830	A831	A832	P833	G834	S835	S836	T837	G838	E839	A840	M841	E842	L843	M844	P845	P846	L847	A848	S849	R850	L851	P852	T853	G854	V855	G856	R857	D858	M859	L860	T861	G862	S863	Y864	V865	P866	R867	L868	S869	G870	M871	Q872						
A873	P874	S875	L876	Y877	A878	L879	S880	L881	L882	R883	V884	P885	L886	C887	L888	A889	K890	L891	R892	E893	S894	M895	S896	L897	P898	R899	S900	E901	N902	L903	V904	V905	P906	L907	G908	V909	I910	G911	A912	L913	L914	I915	A916	T917	F918	R919	G920	L921	T922	N923	D924	V925	P926	F927	Q928	V929	G930	L931	L932						
K248	L249	L250	L251	K252	V253	N254	G257	S258	R259	V260	L261	L262	R263	D264	V265	A266	K267	L268	E269	L270	T271	G272	E273	N274	L277	L278	A279	E280	F281	N282	G283	Q284	P285	A286	S287	G288	L289	G290	L291	K292	L293	A294	G295	G296	A297	N298	L299	L300	D301	T302	A303	A304	T305	L306	R307	A308	E309								
L310	A311	K312	K313	E314	P315	F316	F317	P318	S319	G320	L321	K322	T323	V324	Y325	P326	P327	D328	T329	T330	P331	F332	V333	V334	T335	S336	P337	R338	E339	V340	V341	F342	T343	L344	V345	E346	A347	L348	I349	L350	V351	F352	L353	V354	P355	G356	L357	F358	L359	Q360	N361	F362	A363	A364	T365	L366	L367	P368	T369						
L370	A371	V372	V373	V374	V375	L376	L377	I378	T379	F380	L383	F386	G387	F388	S389	L390	N391	T392	L393	T394	K395	F396	M397	N398	L400	L401	A402	G403	L404	L405	V406	D407	D408	A409	I410	V411	V412	V413	E414	N415	V416	E417	P355	R418	V419	M420	A421	E422	E423	G424	L425	R426	A427	L428	P429	K428	E429	A430	T431	S442	Y443	T444	E445	F446	G447
R432	K433	S434	M435	G436	Q437	L438	Q439	A441	L442	V443	G444	I445	A446	M447	V448	L449	S450	A451	V452	F453	G454	P455	M456	A457	F458	F459	G460	G461	S462	T463	A464	A465	I466	Y467	Q468	Q469	F470	S471	I474	V475	S476	A477	M478	G479	L480	S481	V482	L483	V484	A485	L486	I487	L488	T489	P490	A491	L492								
C493	A494	T495	T496	L497	K498	P499	I499	ALA	GLY	ASP	HIS	GLY	GLU	GLY	M447	L449	S450	A451	V452	F453	G454	P455	M456	A457	F458	F459	G460	G461	S462	T463	A464	A465	I466	Y467	Q468	Q469	F470	S471	I474	V475	S476	A477	M478	G479	L480	S481	V482	L483	V484	A485	L486	I487	L488	T489	P490	A491	L492								
A553	Y554	L555	F556	V557	R558	L559	P560	F561	S562	F563	L564	D568	Q569	G570	V571	F572	M573	T574	Y575	V576	M577	L578	P579	R586	S587	Q588	E589	F590	S591	V592	M593	V594	T595	H596	Y597	V598	L599	T600	K601	E602	L603	V606	E607	S608	V609	F610	L611	V612	N613	G614	L615	I616	F617	A618	V619	R620									
G621	Q622	M623	G624	G625	I626	A627	F628	V629	K632	D633	M634	D638	Q639	E640	N641	E642	G643	V644	E645	A646	I647	T648	M649	R650	R653	A654	F655	M656	S657	Q658	L659	E660	K661	M662	V663	F664	A665	G666	N667	L668	P669	A670	I671	V672	E673	E674	G675	T678	G679	F680	D681	F682	L683	E684	E685	L686	T687	R688							
Q687	A688	G689	L690	G691	H692	E693	K694	L695	T696	F697	A698	R699	T700	L701	L702	L703	A704	E705	A706	A707	K708	H709	P710	D711	M712	L713	T714	S715	M716	F717	P718	N719	E720	L721	E722	D723	T724	F725	Q726	F727	K728	I729	D730	I731	D732	Q733	E734	K735	A738	S742	I743	Y744	D745	I746	N747	L748	T749								
L750	G751	A752	A753	G754	G755	T756	V757	L758	D759	D760	F761	F762	I763	D764	R765	R766	R767	V768	K769	R770	R771	V772	Y773	M774	S775	E776	A777	R778	Y779	R780	M781	L782	P783	R784	I785	I786	G787	D788	M789	Y790	Y791	R792	A793	G796	Q797	M798	V799	P800	F801	S802	A803	P804	S805	Y806	R807	R808	M809	E810	G812						
S813	P814	R815	L816	E817	R818	R819	M820	G821	L822	P823	S824	M825	E826	L827	L828	G829	R830	A831	A832	P833	G834	S835	S836	T837	G838	E839	A840	M841	E842	L843	M844	P845	P846	L847	A848	S849	R850	L851	P852	T853	G854	V855	G856	R857	D858	M859	L860	T861	G862	S863	Y864	V865	P866	R867	L868	S869	G870	M871	Q872						
A873	P874	S875	L876	Y877	A878	L879	S880	L881	L882	R883	V884	P885	L886	C887	L888	A889	K890	L891	R892	E893	S894	M895	S896	L897	P898	R899	S900	E901	N902	L903	V904	V905	P906	L907	G908	V909	I910	G911	A912	L913	L914	I915	A916	T917	F918	R919	G920	L921	T922	N923	D924	V925	P926	F927	Q928	V929	G930	L931	L932						
T933	T934	T935	G936	L937	S938	A939	K940	R941	A942	I943	L944	T945	I946	E947	F948	A949	K950	D951	L952	P953	D954	G957	K958	G959	L960	T961	E962	A963	T964	L965	D966	A967	V968	R969	K970	R971	L972	R973	P974	I975	I976	R977	T978	S979	L980	A981	F982	L983	L984	G985	V986	N987	P988	L989	T993	G994									

S997	G998	A999	Q1000	V1003	G1004	V1007	M1008	G1009	G1010	M1011	V1012	T1013	A1014	T1015	V1016	L1017	A1018	I1019	F1020	F1021	V1022	P1023	V1024	F1025	F1026	V1027	V1028	V1029	R1030	R1031	R1032	F1033	S1034	R1035	K1036	ASN	GLU	ASP	ASP	ILE	GLU	HIS	HIS	SER	HIS	THR	VAL	ASP	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.87Å 134.42Å 163.19Å 90.00° 97.71° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (10.00-2.80) 99.0 (10.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.268 , 0.307 0.262 , 0.307	Depositor DCC
R_{free} test set	5752 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 104.1	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	0.92	EDS
Total number of atoms	23378	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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	1.50	104/7920 (1.3%)	1.28	74/10756 (0.7%)
1	B	1.02	6/7920 (0.1%)	1.05	18/10756 (0.2%)
1	C	1.54	94/7920 (1.2%)	1.33	82/10756 (0.8%)
All	All	1.37	204/23760 (0.9%)	1.23	174/32268 (0.5%)

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	A	0	4
1	B	0	2
1	C	0	6
All	All	0	12

The worst 5 of 204 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	GLN	CB-CG	23.76	2.16	1.52
1	C	129	VAL	CB-CG2	21.03	1.97	1.52
1	C	167	SER	N-CA	20.35	1.87	1.46
1	A	818	ARG	CG-CD	20.25	2.02	1.51
1	C	166	ILE	CA-CB	20.11	2.01	1.54

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	ASP	CB-CG-OD1	-17.91	102.18	118.30
1	C	767	ARG	CD-NE-CZ	-16.19	100.94	123.60
1	C	168	ARG	N-CA-C	10.95	140.57	111.00
1	A	818	ARG	NE-CZ-NH2	9.96	125.28	120.30
1	A	111	LEU	CB-CA-C	-9.93	91.33	110.20

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	THR	Mainchain
1	A	65	ILE	Mainchain
1	A	66	GLU	Peptide
1	A	818	ARG	Mainchain
1	B	102	ILE	Peptide

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	7774	0	7931	1178	0
1	B	7774	0	7931	1189	0
1	C	7774	0	7931	1304	0
2	A	22	0	0	30	0
2	B	8	0	0	6	0
2	C	26	0	0	35	0
All	All	23378	0	23793	3559	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 76.

The worst 5 of 3559 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:C:127:VAL:CB	1:C:127:VAL:CA	1.75	1.63
1:C:158:VAL:CG2	1:C:158:VAL:CB	1.77	1.60
1:A:69:MET:CG	1:A:69:MET:CB	1.74	1.60
1:C:58:GLN:CG	1:C:58:GLN:CB	1.74	1.55
1:A:68:ASN:CA	1:A:68:ASN:N	1.70	1.55

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	
1	A	1018/1053 (97%)	621 (61%)	243 (24%)	154 (15%)	0	0
1	B	1018/1053 (97%)	611 (60%)	259 (25%)	148 (14%)	0	0
1	C	1018/1053 (97%)	642 (63%)	225 (22%)	151 (15%)	0	0
All	All	3054/3159 (97%)	1874 (61%)	727 (24%)	453 (15%)	0	0

5 of 453 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	63	GLN
1	A	64	VAL
1	A	65	ILE
1	A	67	GLN

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	
1	A	833/859 (97%)	678 (81%)	155 (19%)	1	5
1	B	833/859 (97%)	688 (83%)	145 (17%)	2	6
1	C	833/859 (97%)	679 (82%)	154 (18%)	1	5
All	All	2499/2577 (97%)	2045 (82%)	454 (18%)	1	5

5 of 454 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	253	VAL
1	B	653	ARG
1	C	762	PHE
1	B	293	LEU
1	B	452	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	189	ASN
1	B	437	GLN
1	C	439	GLN
1	B	210	GLN
1	B	231	ASN

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 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	A	1022/1053 (97%)	-0.06	38 (3%)	41	31	5, 97, 116, 127	0
1	B	1022/1053 (97%)	0.05	44 (4%)	35	25	49, 102, 116, 127	0
1	C	1022/1053 (97%)	-0.06	44 (4%)	35	25	5, 94, 118, 127	0
All	All	3066/3159 (97%)	-0.02	126 (4%)	37	27	5, 99, 117, 127	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1034	SER	11.4
1	C	870	GLY	8.3
1	C	513	PHE	6.5
1	C	538	THR	6.4
1	C	536	ARG	5.7

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.