



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 10:09 PM GMT

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 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/ValidationPDFNotes.html>

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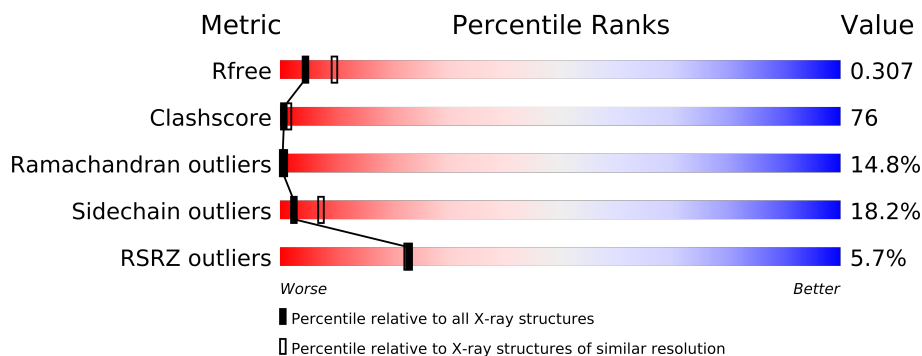
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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  $\geq 3$ , 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	A	1053	
1	B	1053	
1	C	1053	

## 2 Entry composition

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

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

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

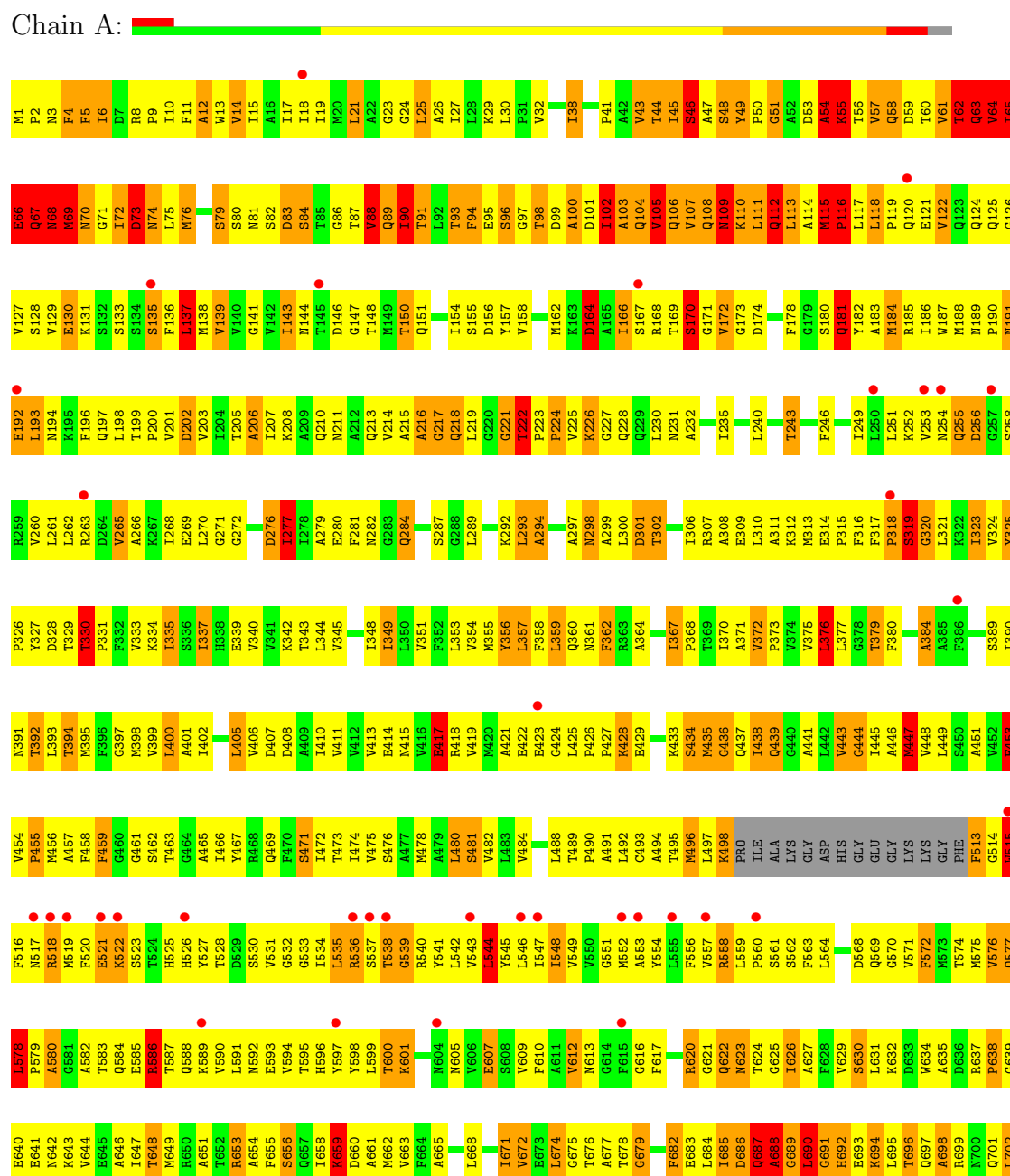
- Molecule 2 is water.

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

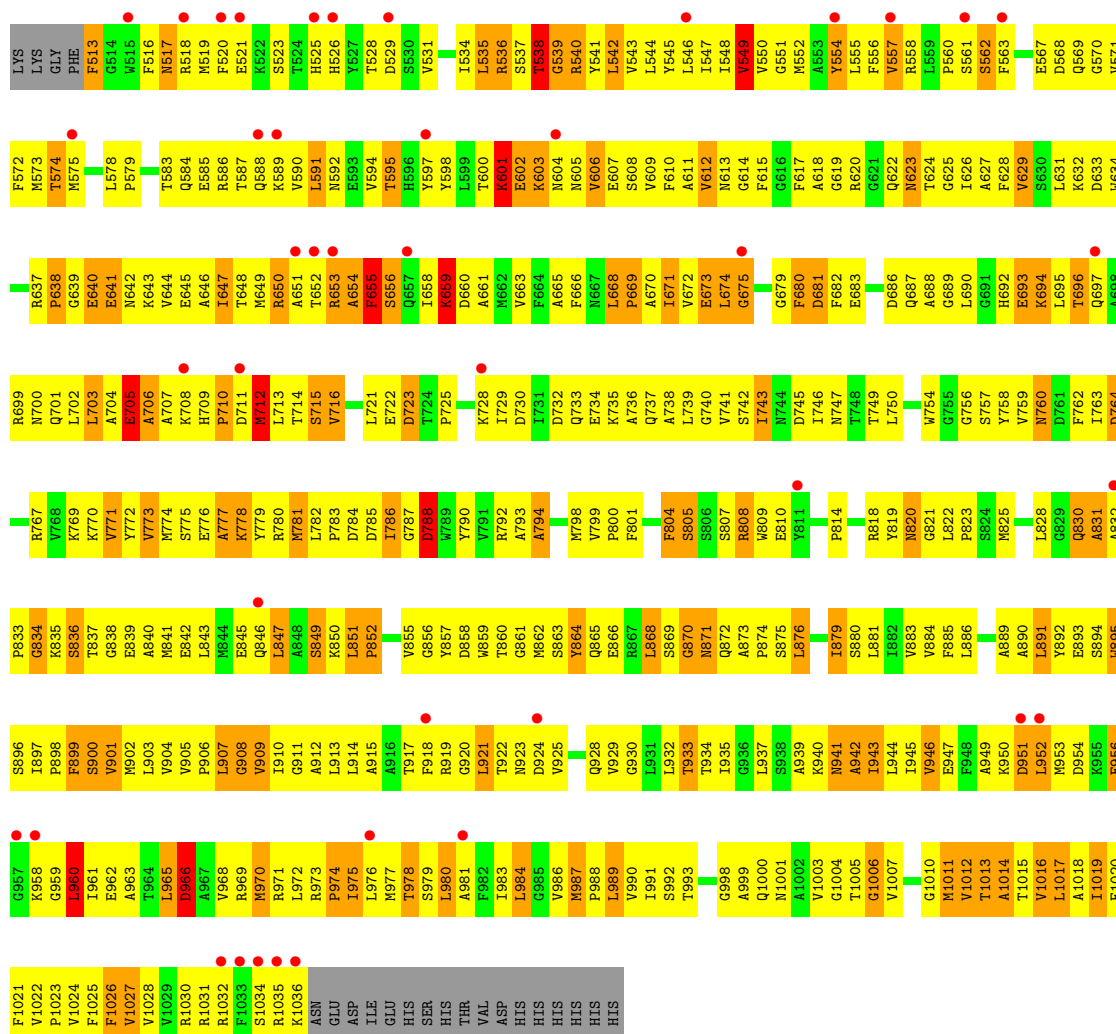
### 3 Residue-property plots

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: ACRB







T993	L932	Q872	G812	T749	D686	G621	A553	C493	R432	L370	L310
G994	T933	A873	S813	L750	Q687	Q622	T654	A494	K433	A371	A311
S997	T934	P874	R814	G751	A688	M623	T555	T495	S434	V372	K312
G998	L935	S875	R815	A752	Q689	T624	F566	M496	M435	P373	M313
A999	G936	L876	L816	A753	G691	G625	V557	L497	G436	V374	E314
Q1000	L937	T877	E817	A754	G692	T626	R568	K498	Q437	V375	P315
	S938	A878	R818	G755	H692	A627	L559	P80	K438	L376	F316
	A939	L879	R819		H693	F628	P560	I1E	Q439	L377	F317
V1003	K940	S880	M820	Y758	K694	V629	S561	ALA	Q440	G378	P318
G1004	N941	L881	G821	V759	L695		S562	LYS	A441	T379	S319
	A942	L882	L822	N760	T896		F563	GLY	L442	F380	G320
V1007	L943	R883	P823	D761	Q697	K632	L564	ASP	V443		L321
M1008	I944	V884	S824	F762	D698	D634		HIS	G444		L322
G1009	T945	F885	M825	I763	R699	A635	D588	GLY	I445		I323
	V946	L886	E826	D764	N700		Q569	GLU	A446		V324
E947	F948	C887	L827	R765	Q701	G639	Q570	GLY	M447	G387	V325
V1013	F949	L888	L828	G766	L702	E640	V571	LYS	F388	G388	P326
A1014	K950	A889	G829	R767	L703	E641	F572	LYS	L448	S389	P327
T1015	D951	A890	Q830	V768	A704	M642	M673	GLY	S450	L390	D328
V1016	L952	L891	A831	K769	E705	K643	T574	PHE	A451	N391	T329
L1017	M953	A892	A832	R770	A706	V644	P575	F513	V452	T392	T330
A1018	D954	S894	P833	Y771	K708	E646	V576	G514	F453	L393	P331
I1019	G957	S895	K835	W772	H709	T647	Q577	F516	V454	T394	F332
F1020	K958	L896	S836	M774	P710	T648	L578	N517	M456	N395	V333
F1021	G959	I897	T837	S775	D711	M649	P579	R518	A457	F396	K334
V1022	L960	P898	G838	E776	M712	R650		M519	F458	G397	I335
P1024	L961	S900	E839	A777	L713		R586	F520	F459	N399	S336
F1025	E962	V901	M840	K778	T714	R653	T587	E521	G460	V399	I337
A1026	A963	M902	A841	W779	S715	A654	Q588	K522	G461	L400	H338
V1027	T964	L903	E842	R780	V716	F655	V590	S523	G462	A401	E339
L965	D966	V904	L843	K781	R717	S656	L591	T524	S462	I402	V340
V1029	P967	P905	M844	L782	F718	Q657	N592	H525	T463	G403	V341
R1031	V968	L907	Q846	D784	N719	T658	V594	Y527	G464	L404	K342
R1032	R969	G908	L847	I786	E722	D660	T595	T529	A465	L405	T343
F1033	N970	V909	S849	G787	D723	M652	H596	D529	Y467	D407	V345
S1034	L972	G911	R850	D788	T724		Y597	S530	R468	A408	E346
K1036	R973	A912	L851	W789	T725	F663	V598	G532	Q469	A409	L347
ASN	P974	L913	T852	W790	Q726	A665	T600	G533	F470	I410	I348
GLU	L975	G914	T853	V791	F727	F666	K601	L534	S475	V411	I349
ASP	L976	A915	G854	R792	F727	L667	E602	L534	S476	V412	L350
ILE	M977	A916	V855	A793	K728	L668	K603	L534	A477	V413	V351
GLU	T978	T917	G856	G796	I729	F669		R536	A478	E414	F352
HIS	S979	F918	T857	Q797	D730		V606	T538	M479	V415	L353
SER	L980	R919	D858	Q797	D732	I671	E507	G539	R418	E417	M355
HIS	A981	G920	W859	W798	Q733	V672	S608	R540	L480	R418	Y356
THR	F982	L921	T860	V799	E734	E673	V609	Y541	S481	V419	L357
VAL	L983	T922	G861	P800	K735	L674	T610	L542	V482	M420	F358
ASP	L984	N923	M862	F801	A738	G675	A611	Y543	L483	A421	L359
HIS	G985	D924	S863	S802			V612	L544	V484	E422	Q360
HIS	V986	V925	Y864	A803	S742	T678	N613	Y545	A485	E423	N361
HIS	M987	Y926	Q865	F804	I743	G679	G614	L546	L486	G424	F362
HIS	P988	F927	E866	S805	I744	F680	P615	I547	L425	L425	A364
HIS	L989	Q928	R867	R808	D745	D681	G616	I548	L487	P426	A364
HIS	V990	V929	L868	W809	I746	F682	P617	V549	L488	P427	T365
HIS	I991	G870	S869	E810	I747	E683	A618	V550	T489	K428	L366
	S992	L931	N871	Y811	T748	T685	G619	G551	P490	E429	L367
							L684	M552	A491	A430	P368
									L492	T431	T369

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.268 , 0.307 0.265 , 0.307	Depositor DCC
$R_{free}$ test set	5752 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.4	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 74.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 115025 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities 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	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 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	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

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 76.

The worst 5 of 3559 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:127:VAL:CB	1:C:127:VAL:CA	1.75	1.63
1:C:158:VAL:CB	1:C:158:VAL:CG2	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	1
1	B	1018/1053 (97%)	611 (60%)	259 (25%)	148 (14%)	0	1
1	C	1018/1053 (97%)	642 (63%)	225 (22%)	151 (15%)	0	1
All	All	3054/3159 (97%)	1874 (61%)	727 (24%)	453 (15%)	0	1

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%)	2	7
1	B	833/859 (97%)	688 (83%)	145 (17%)	3	8
1	C	833/859 (97%)	679 (82%)	154 (18%)	2	7
All	All	2499/2577 (97%)	2045 (82%)	454 (18%)	2	7

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

Mol	Chain	Res	Type
1	B	253	VAL

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains in this entry.

## 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, 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	A	1022/1053 (97%)	0.05	54 (5%) 25 26	5, 97, 116, 127	0
1	B	1022/1053 (97%)	0.15	61 (5%) 21 21	49, 102, 116, 127	0
1	C	1022/1053 (97%)	0.05	61 (5%) 21 21	5, 94, 118, 127	0
All	All	3066/3159 (97%)	0.08	176 (5%) 23 23	5, 99, 117, 127	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1034	SER	14.1
1	C	870	GLY	9.9
1	C	538	THR	8.2
1	C	869	SER	6.5
1	C	513	PHE	6.5

### 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.