



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:34 PM UTC

PDB ID : 2DHH / pdb\_00002dhh  
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](mailto: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  
Xtrriage (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

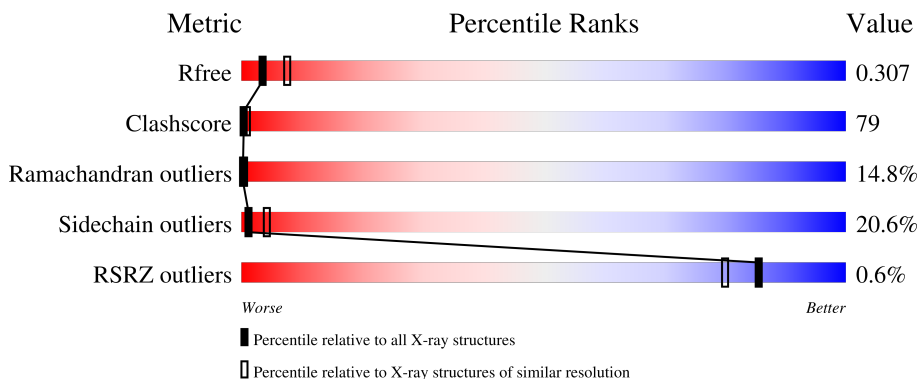
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	1053	
1	C	1053	

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	1022	7774	5003	1283	1444	44	0	0	0
1	B	1022	7774	5003	1283	1444	44	0	0	0
1	C	1022	7774	5003	1283	1444	44	0	0	0

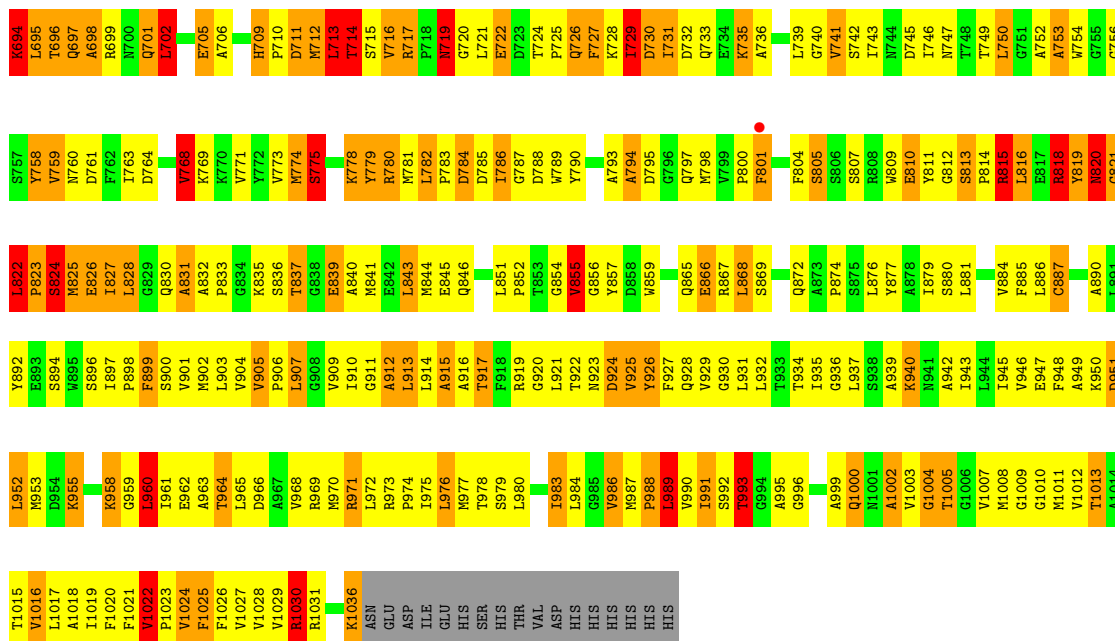
There are 12 discrepancies between the modelled and reference sequences:

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

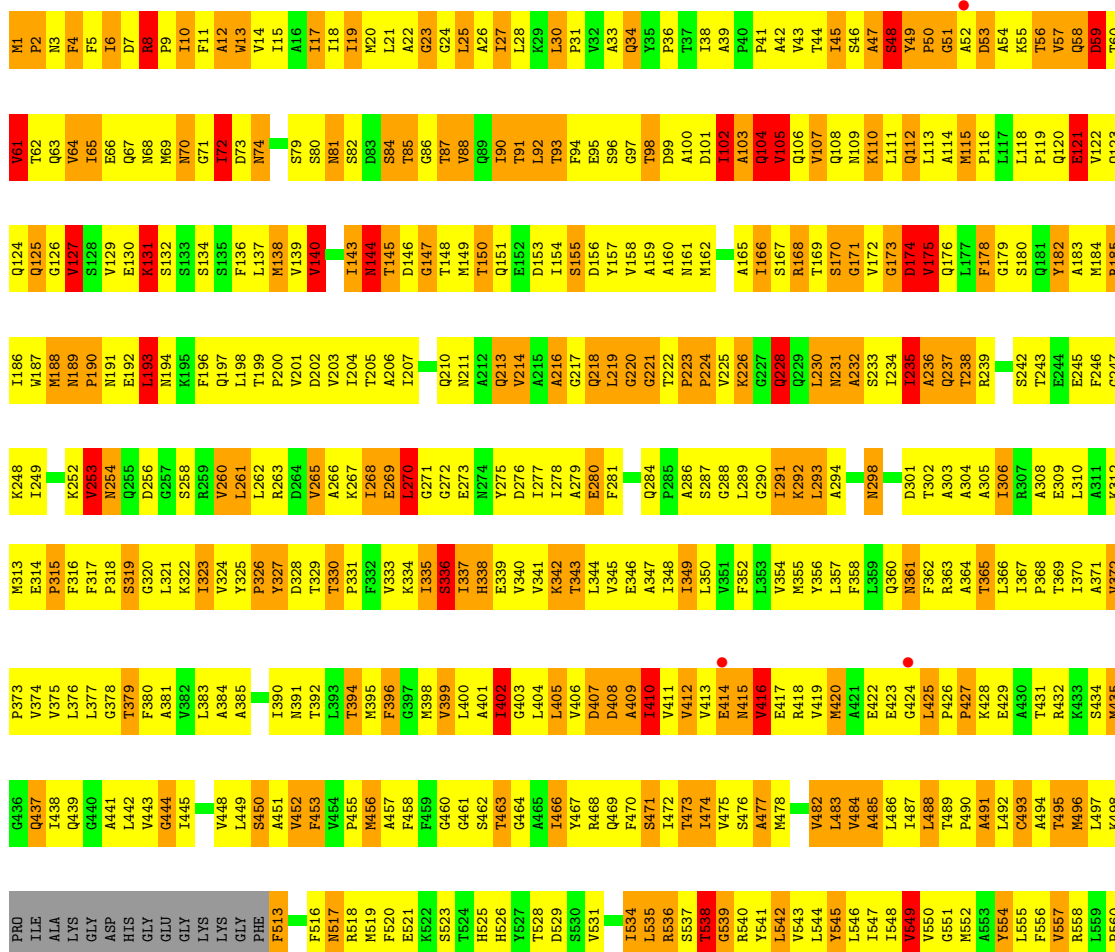
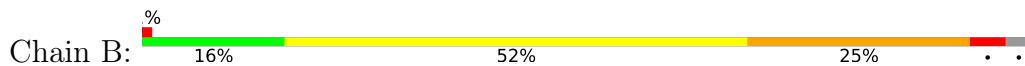
- Molecule 2 is water.

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





• Molecule 1: ACRB





VAL	L984	N923	S863	A803	S742	G679	F615	T548	L488	P427	I367
ASP	G985	D924	Y864	F804	I743	F680	G616	V649	T489	K428	P368
HIS	Y986	V925	Q865	S806	N744	D681	F617	V550	P490	K429	P369
HIS	M987	Y926	E866	S805	N745	F682	A618	G551	A491	E429	I370
HIS	P988	F927	R867	S807	I746	E683	G619	M552	L492	T431	A371
HIS	L989	Q928	L868	R808	N747	E684	R620	A553	C493	R432	V372
HIS	V990	V929	S869	M809	I748	L885	G621	Y554	A494	R433	P373
HIS	Y991	G930	G870	E810	T749	D886	Q622	L555	T495	K434	P374
	S992	N931	N871	Y811	L750	Q887	M623	F556	M496	S434	V375
	T993	L932	Q872	G751	G751	A688	N623	V557	L497	M435	V376
	G994	S933	A873	A752	A689	G689	G625	R558	G436	L376	L377
	A995	T934	R874	A753	L690	L690	I626	L559	K498	G378	G378
	G996	I935	S875	M754	G691	G691	A627	P560	PRO	L438	G379
	S997	G936	L876	L816	H692	H692	F628	S561	ALA	C440	F380
	G998	L937	Y877	E817	E693	E693	V629	S562	A441	A441	A391
	A999	S938	R818	R818	K694	K694	V629	S562	LYS	L442	A392
	Q1000	A939	I879	Y819	L695	L695	L631	L564	GLY	V392	L383
	V1003	K940	N820	N820	V759	T696	K632	L564	ASP	V443	A384
	G1004	N941	G821	G821	N760	Q697	D633	E567	HIS	G444	A385
	V1007	A942	L882	L822	D761	A698	M634	D568	GLU	A446	F386
	M1008	I944	V883	Q829	F762	R699	G639	Q569	GLY	M447	G387
	G1009	L945	R884	S824	I763	N700	E640	G570	LYS	V448	F388
	G1010	V946	L886	M825	D764	Q701	E640	V571	LYS	V449	S389
	M1011	E947	C887	E826	R765	L702	E641	F572	GLY	S450	I390
	Y1012	F948	L888	I827	G766	L703	M642	M573	PHE	A451	M391
	T1013	A949	A889	L828	R767	A704	K643	T574	F513	V452	T392
	A1014	K950	R890	G829	V768	E705	V644	M575	G514	F453	L393
	T1015	D951	L891	Q830	A706	A706	E645	V576	M515	V454	T394
	V1016	L952	R892	A831	K770	A646	E645	A577	F516	M395	M395
	L1017	M953	E893	A832	V771	K708	I647	L578	M517	M456	F396
	A1018	D954	S894	P833	Y772	H709	T648	P579	R518	A457	G397
	F1020	G957	M895	G834	W773	P710	M649	A580	M519	F458	M398
	F1021	K958	R896	S835	M774	D711	R650	R586	F520	F459	V399
	F1022	G959	I897	T837	E776	M712	R653	R587	E521	G460	L400
	P1023	F960	P898	G838	A777	L713	A654	T587	K522	G461	A401
	V1024	I961	F899	E839	K778	T714	F655	Q588	S523	T463	I402
	F1025	E962	S900	A840	Y779	R716	S656	K589	T524	T463	G403
	F1026	A963	V901	M841	R780	R717	Q657	V590	H525	G484	L404
	F1027	T964	E902	E842	L781	P718	T658	L891	H526	A485	L405
	V1028	L965	M904	L843	L782	N719	D660	N592	Y627	I466	V406
	V1029	D966	V905	M844	P783	G720	D660	E593	Y467	Y467	D407
	R1030	A967	Q906	E845	D784	L721	A661	V594	R468	R468	D408
	R1031	V968	L907	Q846	D785	E722	M662	T595	Q469	Q469	A409
	R1032	R969	G908	L847	I786	D723	V663	L597	V531	F470	I410
	F1033	M970	V909	A848	G787	T724	F664	Y698	G532	S471	V411
	S1034	R971	I910	S849	D788	P725	A665	L599	O533	V412	V413
	R1035	L972	G911	K850	W789	Q726	F666	T600	L535	V475	E414
	K1036	R973	A912	L851	Y790	F727	M667	K601	L536	S476	M415
ASN	P974	R974	L913	P852	R791	K728	L668	E602	S537	A477	V416
GLU	L975	L975	L914	T853	A792	I729	F669	K603	T538	M478	E417
ASP	L976	L976	A915	G854	A793	D730	A670	V606	G539	A479	R418
ILE	M977	M977	A916	G855	G796	D732	L671	R540	R540	L480	V419
GLU	S978	T917	T917	G856	G797	D732	V672	E607	Y541	S481	M420
GLU	S979	F918	F918	Y857	Q797	E733	E673	E610	L542	V482	A421
HIS	L980	R919	R919	D858	M798	F734	L674	F610	M543	I483	E422
SER	A981	L980	G920	M859	V799	K735	G875	A611	L544	V484	E423
HIS	F982	L921	L921	T860	P800	A738	T676	M612	Y545	A485	G424
THR		I983	T922	M862	S902		A677	N613	L546	L486	L425
							T678	G614	Y547	I487	P426

## 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) 96.7 (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)	Xtrriage
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 (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.4	Xtrriage
Anisotropy	0.444	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 78.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtrriage'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.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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	1.97	199/7920 (2.5%)	1.66	169/10756 (1.6%)
1	B	1.29	28/7920 (0.4%)	1.42	101/10756 (0.9%)
1	C	1.98	175/7920 (2.2%)	1.71	209/10756 (1.9%)
All	All	1.78	402/23760 (1.7%)	1.60	479/32268 (1.5%)

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 402 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	ILE	CA-CB	34.30	2.01	1.54
1	C	167	SER	N-CA	31.68	1.87	1.46
1	C	166	ILE	CA-C	-25.56	1.20	1.52
1	C	45	ILE	CA-CB	24.92	1.88	1.54
1	A	68	ASN	CA-CB	24.51	1.94	1.53

The worst 5 of 479 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	VAL	N-CA-C	17.57	128.00	111.48
1	C	767	ARG	CD-NE-CZ	-16.76	100.94	124.40
1	C	126	GLY	N-CA-C	-15.08	88.68	111.00
1	A	696	THR	N-CA-C	-14.55	92.20	112.13
1	A	821	GLY	N-CA-C	-14.09	98.31	115.08

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 [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	A	7774	0	7931	1227	0
1	B	7774	0	7931	1258	0
1	C	7774	0	7931	1370	0
2	A	22	0	0	31	0
2	B	8	0	0	6	0
2	C	26	0	0	35	0
All	All	23378	0	23793	3741	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 79.

The worst 5 of 3741 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:CA	1:C:127:VAL:CB	1.75	1.63
1:C:158:VAL:CB	1:C:158:VAL:CG2	1.77	1.60
1:A:69:MET:CB	1:A:69:MET:CG	1.74	1.60
1:A:65:ILE:CA	1:A:65:ILE:C	1.79	1.56
1:C:58:GLN:CB	1:C:58:GLN:CG	1.74	1.55

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	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 [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	833/859 (97%)	655 (79%)	178 (21%)	1	4
1	B	833/859 (97%)	664 (80%)	169 (20%)	1	4
1	C	833/859 (97%)	666 (80%)	167 (20%)	1	4
All	All	2499/2577 (97%)	1985 (79%)	514 (21%)	1	4

5 of 514 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	685	ILE
1	C	762	PHE
1	C	676	THR
1	B	73	ASP
1	B	59	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	437	GLN
1	B	865	GLN
1	B	517	ASN
1	B	642	ASN
1	C	104	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 [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, 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%)	-0.41	4 (0%) 88 84	5, 97, 116, 127	0
1	B	1022/1053 (97%)	-0.34	6 (0%) 85 80	49, 102, 116, 127	0
1	C	1022/1053 (97%)	-0.38	7 (0%) 84 77	5, 94, 118, 127	0
All	All	3066/3159 (97%)	-0.38	17 (0%) 85 80	5, 99, 117, 127	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	ALA	5.4
1	B	1034	SER	5.1
1	C	538	THR	4.3
1	C	194	ASN	3.6
1	B	414	GLU	3.3

### 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.