



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:25 AM GMT

PDB ID : 3AOC  
Title : Structures of the multidrug exporter AcrB reveal a proximal multisite drug-binding pocket  
Authors : Nakashima, R.; Sakurai, K.; Yamaguchi, A.  
Deposited on : 2010-09-23  
Resolution : 3.34 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

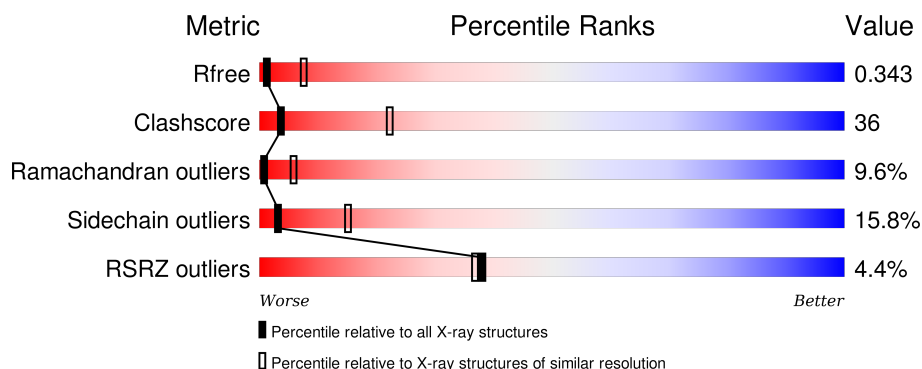
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.34 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))
$R_{free}$	91344	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	1053	<div> <div>4%</div> <div>38%</div> <div>46%</div> <div>12%</div> <div>• •</div> </div>
1	B	1053	<div> <div>5%</div> <div>35%</div> <div>47%</div> <div>14%</div> <div>• •</div> </div>
1	C	1053	<div> <div>4%</div> <div>39%</div> <div>47%</div> <div>10%</div> <div>• •</div> </div>

## 2 Entry composition

There are 3 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.

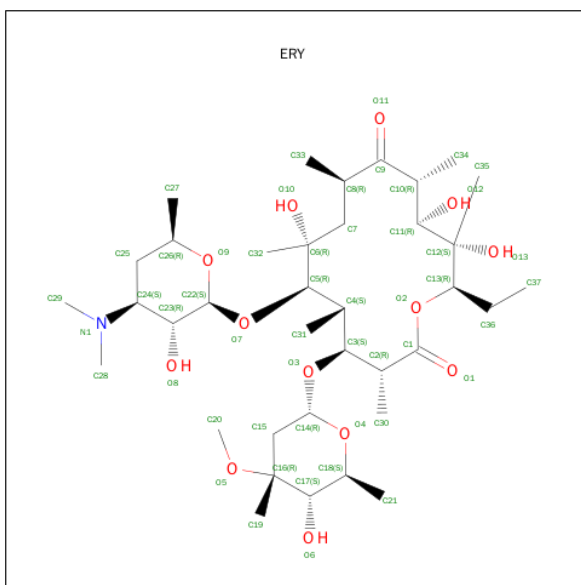
- Molecule 1 is a protein called Acriflavine resistance protein B.

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 ERYTHROMYCIN A (three-letter code: ERY) (formula:  $C_{37}H_{67}NO_{13}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			51	37	1	13		

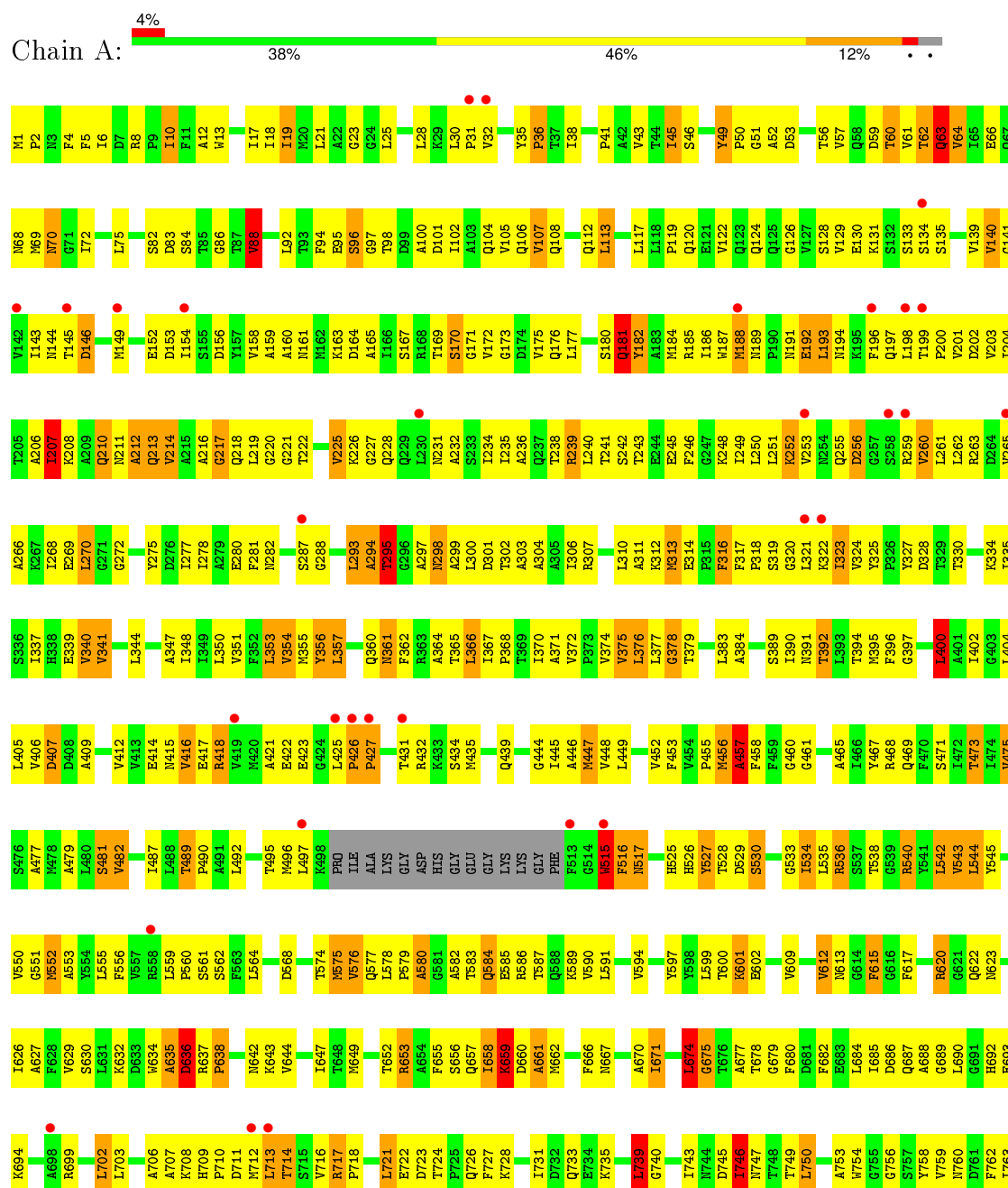
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	2	Total O 2 2	0	0
3	C	1	Total O 1 1	0	0

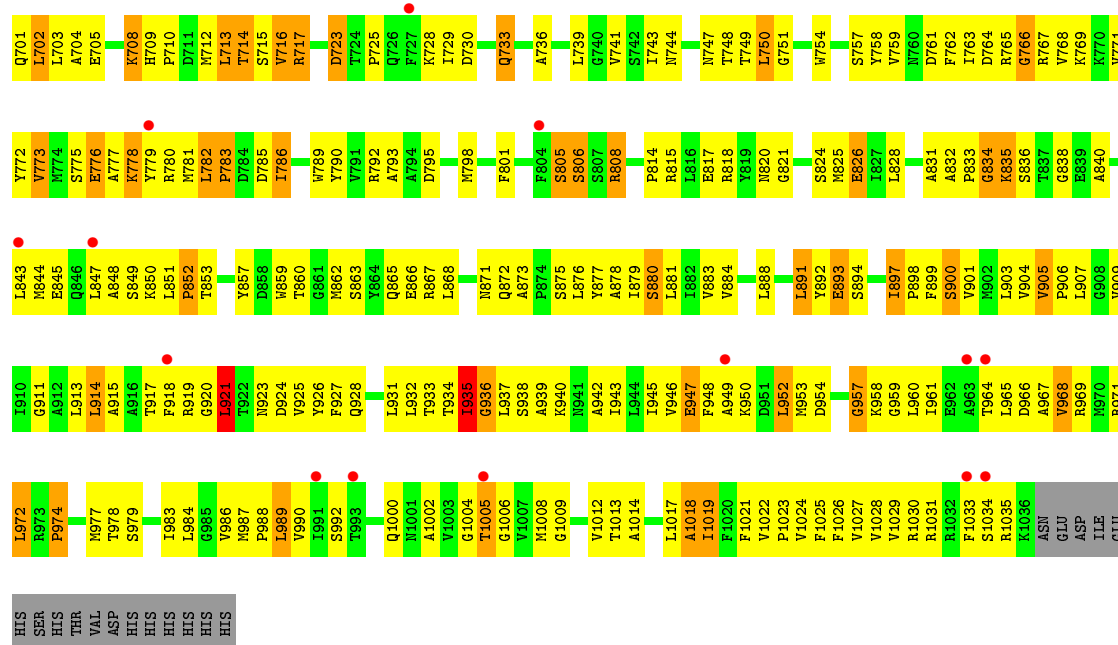
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

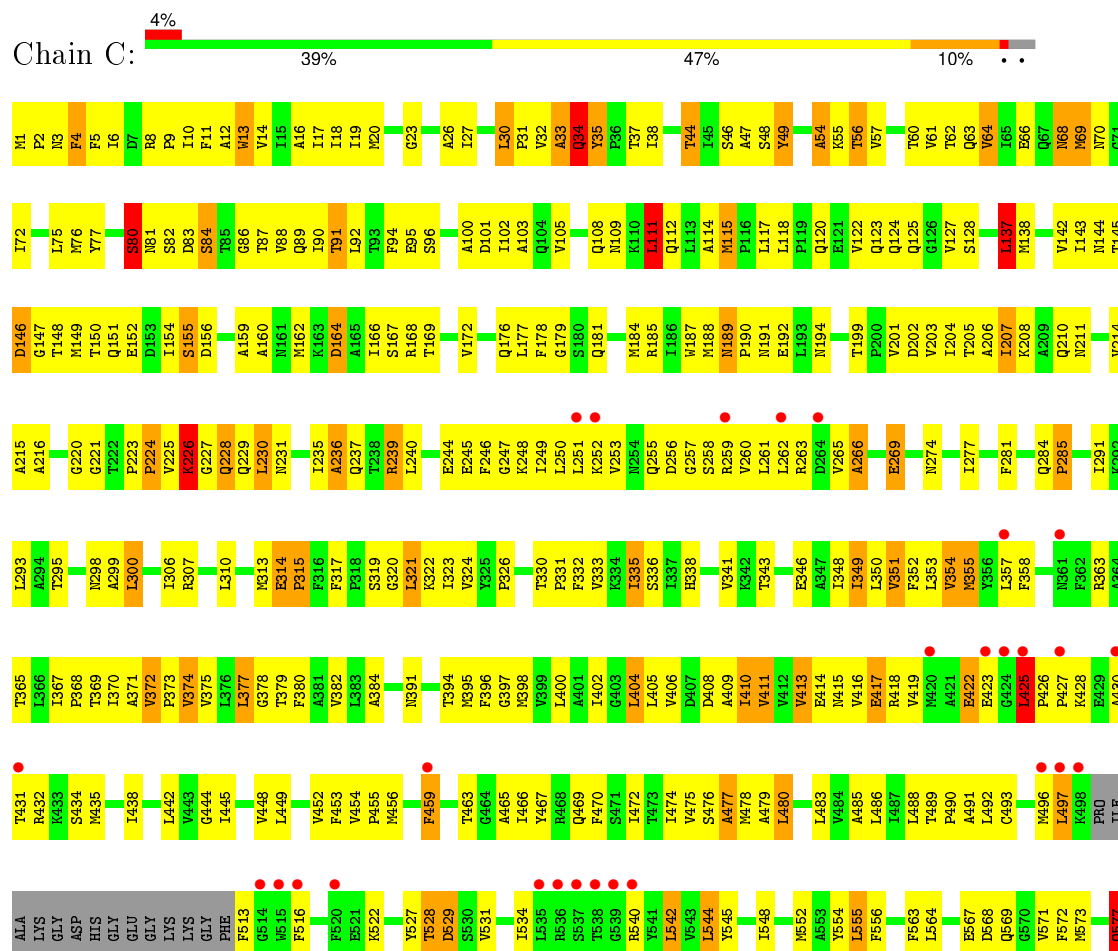
- Molecule 1: Acriflavine resistance protein B







• Molecule 1: Acriflavine resistance protein B



G1009	L876	R941	L578	R650	E722	G796	L876	R941	G1009
G1010	L877	A942	P579	R653	D723	Q797	L877	A942	G1010
M1011	A878	L943	R586	A654	T724	M798	A878	L943	M1011
A1014	L879	L944	T587	F655	P725	V799	L879	L944	A1014
T1015	S880	L945	Q588	S656	P800	F801	S880	L945	T1015
V1016	L881	V946	V589	Q657	P726	S802	L881	V946	V1016
L1017	L882	E947	V590	L658	F727	F803	L882	E947	L1017
A1018	V883	F948	L591	A661	I731	A803	V883	F948	A1018
I1019	V884	A949	N592	N662	D732	F804	V884	A949	I1019
F1020	L885	K950	E593	E734	Q733	S805	L885	K950	F1020
F1021	L886	D951	V594	E736	E734	S806	L886	D951	F1021
V1022	C887	K952	T595	V663	K735	S807	C887	K952	V1022
P1023	L888	D953	H596	F664	A736	R808	L888	D953	P1023
V1024	A889	D954	Y597	L688	Q737	W809	A889	D954	V1024
F1025	E893	G957	Y598	L671	L738	G812	E893	G957	F1025
V1028	S894	K958	E606	V672	A739	R815	S894	K958	V1028
V1029	W895	G959	T599	V673	G740	S896	W895	G959	V1029
R1030	L860	L961	K601	E673	V741	R818	L860	L961	R1030
R1031	E962	A963	E802	L674	S742	Y819	E962	A963	R1031
R1032	A963	F964	K603	G675	I743	N820	A963	F964	R1032
F1033	T964	L965	N604	T676	I746	S900	T964	L965	F1033
S1034	L965	V968	N605	G679	L750	V901	L965	V968	S1034
R1035	V969	R969	E607	F680	G751	W902	V969	R969	R1035
K1036	S608	S979	S608	D681	A752	L903	K1036	S979	K1036
ASN	V970	R970	V609	F682	W754	V904	ASN	R970	ASN
GLU	R971	R971	F610	E683	A754	V905	GLU	R971	GLU
ASP	L972	R972	A611	L684	G754	P906	ASP	R972	ASP
ILE	R973	R973	V612	L684	G754	L907	ILE	R973	ILE
GLU	R974	R974	NG13	D686	G759	G908	GLU	R974	GLU
HIS	R975	R975	G614	Q687	V760	V909	HIS	R975	HIS
SER	L976	R976	F615	A688	D761	I910	SER	R976	SER
HIS	N977	R977	G616	G689	F762	G911	HIS	N977	HIS
THR	T978	R978	F617	L690	I763	A912	THR	T978	THR
VAL	S979	R979	A618	G691	I763	L913	VAL	S979	VAL
ASP	F982	R982	G619	H692	R767	E839	ASP	F982	ASP
HIS	L983	R983	R620	E693	V768	A840	HIS	L983	HIS
HIS	L984	R984	T624	E694	K769	M841	HIS	L984	HIS
HIS	G985	R985	F628	L695	K770	E842	HIS	G985	HIS
HIS	V986	R986	V629	T696	V771	L843	HIS	V986	HIS
HIS	V987	R987	S630	R699	M774	Q846	HIS	V987	HIS
HIS	P988	R988	L631	L702	S775	L847	HIS	P988	HIS
HIS	V990	R990	D633	E705	K778	L851	HIS	V990	HIS
HIS	T993	R993	W634	K708	Y779	P852	HIS	T993	HIS
HIS	S997	R997	A635	H709	M781	W859	HIS	S997	HIS
HIS	G998	R998	D636	M712	L782	G861	HIS	G998	HIS
HIS	A999	R999	R637	L713	P783	M862	HIS	A999	HIS
HIS	V1003	R1003	E641	T714	I786	Q865	HIS	V1003	HIS
HIS	G1004	R1004	N642	S715	W789	E866	HIS	G1004	HIS
HIS	T1005	R1005	K643	V716	Y790	R867	HIS	T1005	HIS
HIS	G1006	R1006	A646	M719	V791	L868	HIS	G1006	HIS
HIS	V1007	R1007	T647	G720	R792	N871	HIS	V1007	HIS
HIS	M1008	R1008	M649	L721	D795	Q872	HIS	M1008	HIS



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	225.28Å 134.21Å 162.05Å 90.00° 98.20° 90.00°	Depositor
Resolution (Å)	45.73 – 3.34 45.73 – 3.34	Depositor EDS
% Data completeness (in resolution range)	95.4 (45.73-3.34) 95.4 (45.73-3.34)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.91 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.273 , 0.344 0.269 , 0.343	Depositor DCC
$R_{free}$ test set	3329 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	97.8	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 74.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	1 of 66210 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ERY

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	0.61	0/7920	0.77	6/10756 (0.1%)
1	B	0.59	0/7920	0.75	4/10756 (0.0%)
1	C	0.63	0/7920	0.78	6/10756 (0.1%)
All	All	0.61	0/23760	0.77	16/32268 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	457	ALA	N-CA-CB	-19.94	82.18	110.10
1	A	456	MET	N-CA-C	7.14	130.27	111.00
1	C	960	LEU	CA-CB-CG	6.55	130.38	115.30
1	B	960	LEU	CA-CB-CG	6.32	129.83	115.30
1	C	578	LEU	CA-CB-CG	6.10	129.34	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	510	0
1	B	7774	0	7931	626	0
1	C	7774	0	7931	611	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	51	0	67	10	0
3	A	2	0	0	1	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	23378	0	23860	1686	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 36.

The worst 5 of 1686 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:456:MET:HG3	1:B:467:TYR:HB3	1.24	1.16
1:A:145:THR:HG22	1:A:320:GLY:HA3	1.15	1.13
1:A:710:PRO:HA	1:A:713:LEU:HD22	1.19	1.12
1:A:638:PRO:HD2	1:A:642:ASN:HD22	1.04	1.07
1:A:714:THR:HG23	1:A:832:ALA:HA	1.33	1.06

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%)	715 (70%)	198 (19%)	105 (10%)	1	5
1	B	1018/1053 (97%)	694 (68%)	214 (21%)	110 (11%)	0	4
1	C	1018/1053 (97%)	734 (72%)	207 (20%)	77 (8%)	1	10
All	All	3054/3159 (97%)	2143 (70%)	619 (20%)	292 (10%)	1	6

5 of 292 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	A	134	SER
1	A	160	ALA
1	A	170	SER
1	A	188	MET

### 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%)	699 (84%)	134 (16%)	3	14
1	B	833/859 (97%)	700 (84%)	133 (16%)	3	15
1	C	833/859 (97%)	705 (85%)	128 (15%)	3	16
All	All	2499/2577 (97%)	2104 (84%)	395 (16%)	3	15

5 of 395 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	244	GLU
1	B	595	THR
1	C	761	ASP
1	B	259	ARG
1	B	395	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	189	ASN
1	B	415	ASN
1	C	588	GLN
1	B	191	ASN
1	B	228	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ERY	C	3402	-	53,53,53	0.98	1 (1%)	82,82,82	1.67	19 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ERY	C	3402	-	-	0/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3402	ERY	O2-C1	4.89	1.45	1.34

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	C	3402	ERY	C13-O2-C1	-3.38	112.42	118.12
2	C	3402	ERY	O12-C11-C12	-3.03	101.69	106.79
2	C	3402	ERY	C25-C24-N1	-3.02	106.77	115.70
2	C	3402	ERY	C33-C8-C7	-2.69	104.06	109.69
2	C	3402	ERY	O7-C5-C4	-2.34	107.65	111.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3402	ERY	10	0

## 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%)	0.18	39 (3%) 44 43	58, 111, 150, 192	0
1	B	1022/1053 (97%)	0.24	51 (4%) 32 32	69, 115, 154, 179	0
1	C	1022/1053 (97%)	0.19	46 (4%) 37 36	55, 109, 160, 188	0
All	All	3066/3159 (97%)	0.21	136 (4%) 38 37	55, 113, 155, 192	0

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	520	PHE	9.7
1	A	497	LEU	5.8
1	B	963	ALA	5.6
1	C	537	SER	5.3
1	A	259	ARG	4.7

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ERY	C	3402	51/51	0.85	0.33	1.19	58,68,74,79	51

## 6.5 Other polymers [i](#)

There are no such residues in this entry.