



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:25 AM GMT

PDB ID : 3AOB
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 : 3.35 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
<http://wwpdb.org/validation/2016/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
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

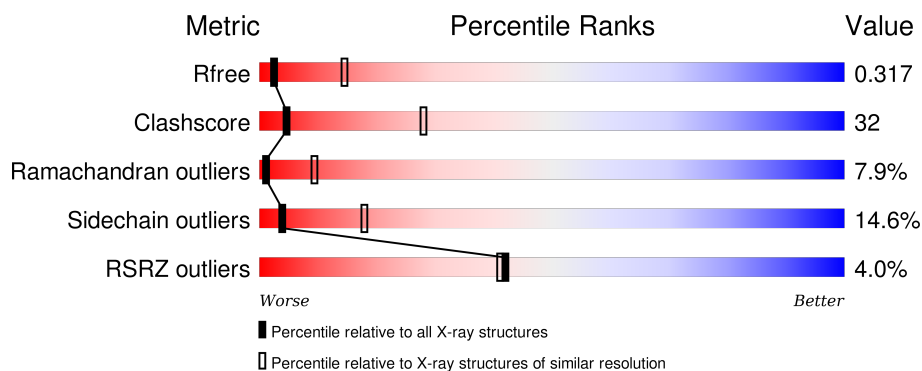
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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. 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>3%</div> <div>44%</div> <div>42%</div> <div>10%</div> <div>..</div> </div>
1	B	1053	<div> <div>5%</div> <div>39%</div> <div>47%</div> <div>11%</div> <div>.</div> </div>
1	C	1053	<div> <div>4%</div> <div>42%</div> <div>43%</div> <div>11%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	RFP	C	2002	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23385 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.

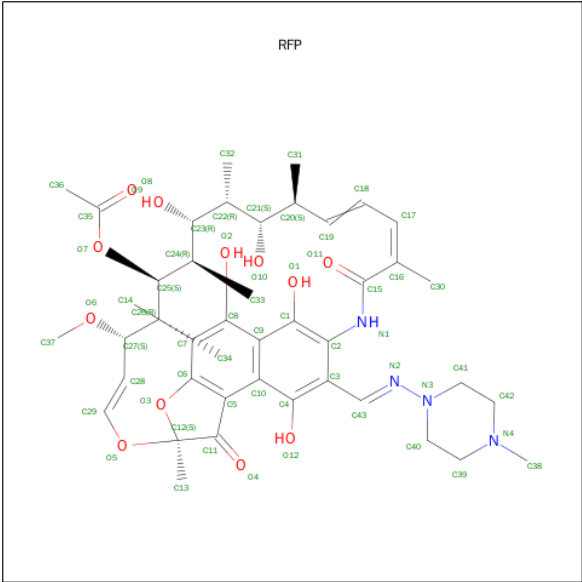
- Molecule 1 is a protein called Acriflavine resistance protein B.

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 RIFAMPICIN (three-letter code: RFP) (formula: C₄₃H₅₈N₄O₁₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			59	43	4	12		

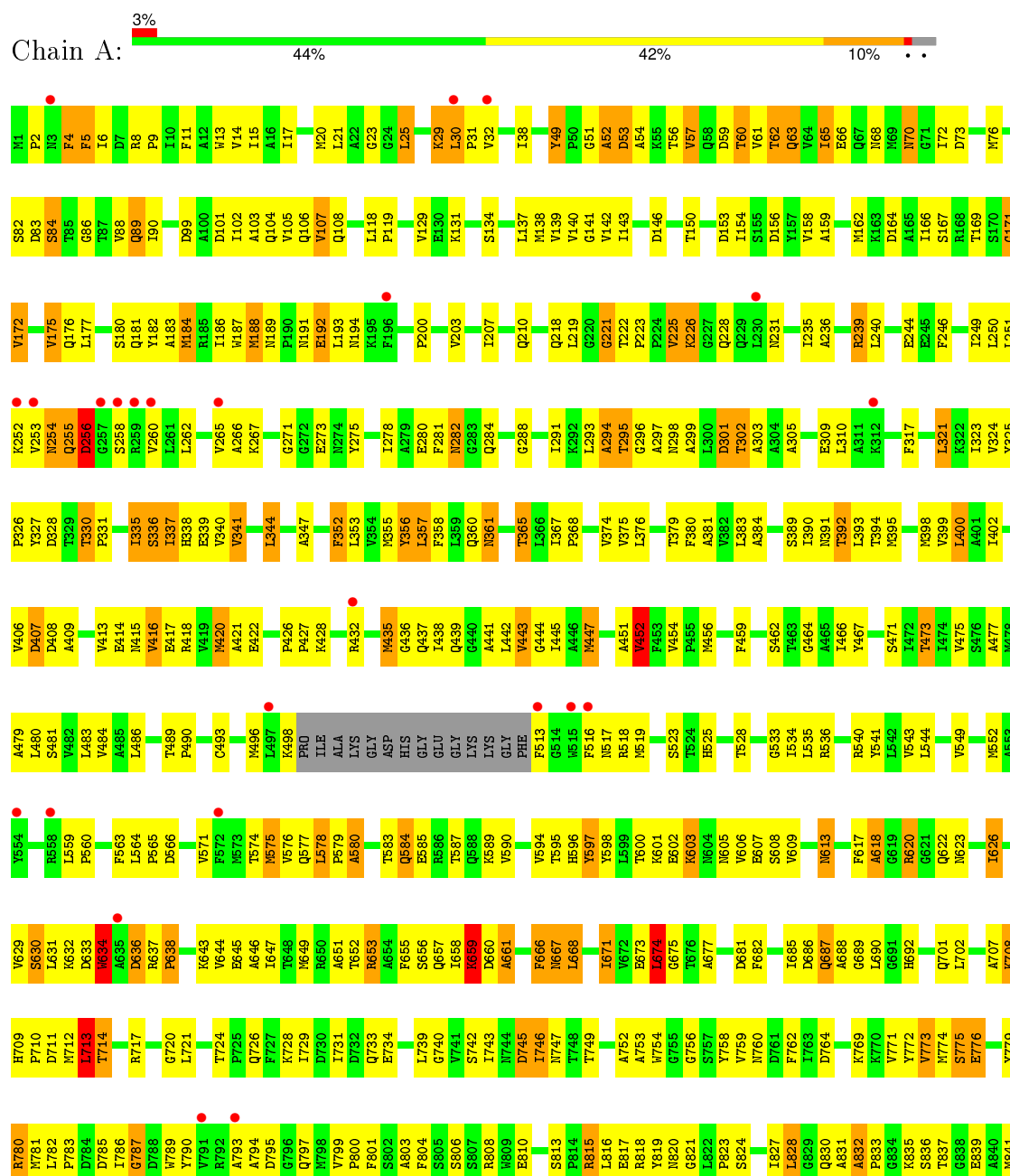
- Molecule 3 is water.

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

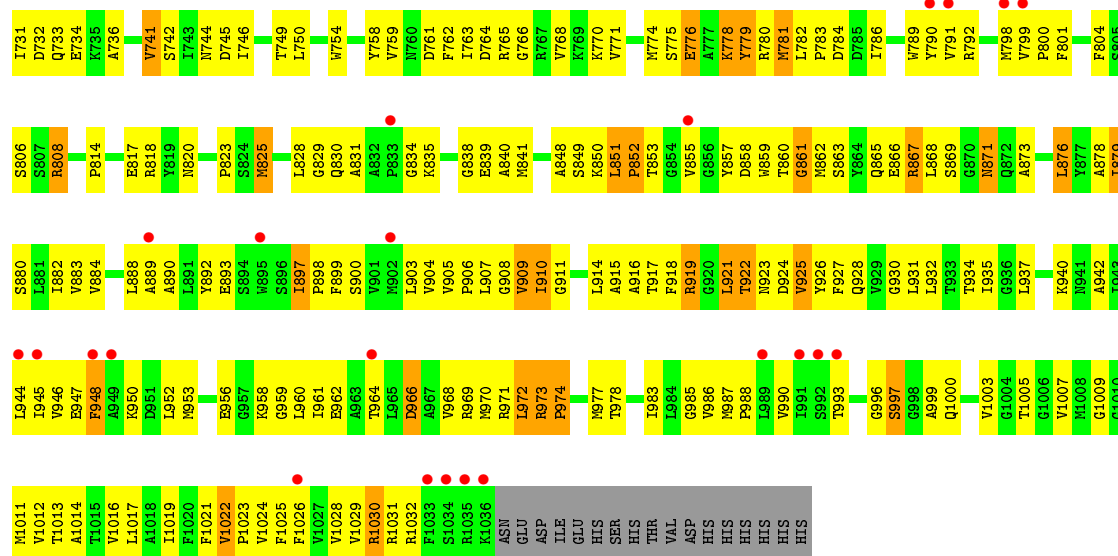
3 Residue-property plots

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.

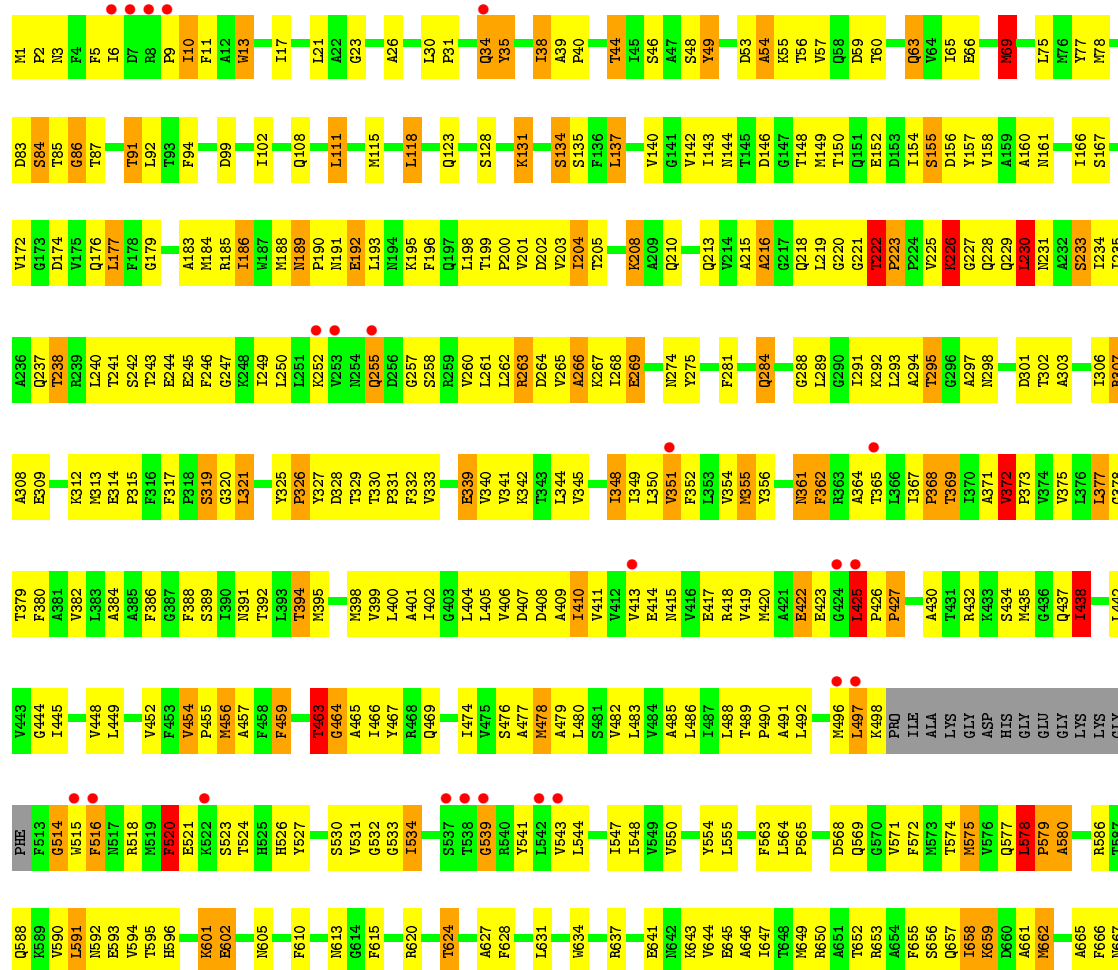
• Molecule 1: Acriflavine resistance protein B







• Molecule 1: Acriflavine resistance protein B



V1029	L668	S805	Y892	I961	V1029
R1030	V741	S806	E893	E962	R1030
R1031	S742	S807	E894	A963	R1031
R1032	I743	R808	W895	T964	R1032
R1035	I746	S813	S896	L965	R1035
K1036	N747	P814	I897	D966	K1036
ASN	T748	R815	P898	A967	ASN
GLU	T749	L816	F899	V968	GLU
ASP	L750	R817	S900	R969	ASP
ILE	G751	R818	V901	M970	ILE
GLU	A752	Y819	M902	R971	GLU
HIS	A753	N820	L903	L975	HIS
SER	W754	S824	V904	L976	SER
HIS	G755	M825	L907	M977	HIS
THR	G756	G829	G908	T978	THR
VAL	S757	N830	V909	S979	VAL
ASP	Y758	A831	I910	L980	ASP
HIS	V759	A832	G911	A915	HIS
HIS	N760	P833	L914	F918	HIS
HIS	F761	G834	A915	L921	HIS
HIS	I762	K835	F918	V925	HIS
HIS	D764	S836	L921	Y926	HIS
HIS	R765	T837	L921	F927	HIS
HIS	G766	G838	V925	G930	HIS
HIS	R767	E839	Y926	L931	HIS
HIS	T696	A840	F927	L932	HIS
HIS	Q697	M841	G934	T933	HIS
HIS	A698	F842	G935	I935	HIS
HIS	N700	L843	I935	G936	HIS
HIS	A706	F844	G936	L937	HIS
HIS	A707	E845	S938	S938	HIS
HIS	K708	Q846	N941	N941	HIS
HIS	H709	L847	A942	A942	HIS
HIS	P710	A848	I943	L943	HIS
HIS	D711	L851	L944	V945	HIS
HIS	D712	G854	V946	F947	HIS
HIS	L713	G854	F948	A949	HIS
HIS	T714	L868	A949	L952	HIS
HIS	S715	S869	L952	M953	HIS
HIS	V716	G870	D954	D954	HIS
HIS	R717	N871	K955	K955	HIS
HIS	G720	Q872	E956	E956	HIS
HIS	L721	A873	G957	G957	HIS
HIS	E722	S875	K958	K958	HIS
HIS	Q726	L876	G959	G959	HIS
HIS	F727	V884	L960	L960	HIS
HIS	I731	F885	V884	V884	HIS
HIS	D732	L886	D954	D954	HIS
HIS	Q733	C887	K955	K955	HIS
HIS	A736	P800	E956	E956	HIS
HIS	Q737	F801	G957	G957	HIS
HIS	A738	S802	K958	K958	HIS
HIS	F738	A803	G959	G959	HIS
HIS	F804	F804	L960	L960	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.90Å 134.31Å 161.77Å 90.00° 98.10° 90.00°	Depositor
Resolution (Å)	48.91 – 3.35 48.91 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.91-3.35) 97.7 (48.91-3.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.64 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.261 , 0.326 0.256 , 0.317	Depositor DCC
R_{free} test set	3350 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 71.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 66713 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23385	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 2.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.62	0/7920	0.75	2/10756 (0.0%)
1	B	0.58	0/7920	0.76	4/10756 (0.0%)
1	C	0.62	0/7920	0.76	5/10756 (0.0%)
All	All	0.61	0/23760	0.76	11/32268 (0.0%)

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	C	0	2

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	TYR	N-CA-CB	-12.26	88.53	110.60
1	B	355	MET	CB-CA-C	10.91	132.23	110.40
1	C	321	LEU	CA-CB-CG	8.34	134.48	115.30
1	B	960	LEU	CA-CB-CG	6.20	129.56	115.30
1	B	352	PHE	CB-CA-C	6.12	122.65	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	221	GLY	Peptide
1	C	222	THR	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	460	0
1	B	7774	0	7931	536	0
1	C	7774	0	7931	577	0
2	C	59	0	57	10	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	23385	0	23850	1518	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 32.

The worst 5 of 1518 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:A:447:MET:HB3	1:A:887:CYS:SG	1.82	1.20
1:C:222:THR:HG23	1:C:223:PRO:CD	1.73	1.17
1:C:815:ARG:HH11	1:C:815:ARG:HG2	1.09	1.17
1:C:146:ASP:HB3	1:C:148:THR:HG23	1.31	1.12
1:A:379:THR:HG21	1:A:477:ALA:HA	1.27	1.12

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%)	769 (76%)	174 (17%)	75 (7%)	1	11
1	B	1018/1053 (97%)	742 (73%)	193 (19%)	83 (8%)	1	9
1	C	1018/1053 (97%)	754 (74%)	182 (18%)	82 (8%)	1	9
All	All	3054/3159 (97%)	2265 (74%)	549 (18%)	240 (8%)	1	9

5 of 240 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	VAL
1	A	188	MET
1	A	239	ARG
1	A	256	ASP
1	A	293	LEU

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%)	712 (86%)	121 (14%)	4	18
1	B	833/859 (97%)	705 (85%)	128 (15%)	3	16
1	C	833/859 (97%)	718 (86%)	115 (14%)	4	20
All	All	2499/2577 (97%)	2135 (85%)	364 (15%)	4	18

5 of 364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	295	THR
1	B	642	ASN
1	C	695	LEU
1	B	343	THR
1	B	497	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	151	GLN
1	B	526	HIS
1	C	700	ASN
1	B	161	ASN
1	B	213	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	RFP	C	2002	-	63,63,63	1.75	3 (4%)	82,94,94	1.95	16 (19%)

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	RFP	C	2002	-	-	0/60/85/85	0/1/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2002	RFP	O5-C29	2.86	1.48	1.39
2	C	2002	RFP	O7-C35	5.39	1.47	1.35
2	C	2002	RFP	O4-C11	11.34	1.43	1.21

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2002	RFP	O4-C11-C5	-8.13	115.09	132.02
2	C	2002	RFP	O4-C11-C12	-3.12	112.25	119.93
2	C	2002	RFP	C30-C16-C17	-2.89	116.36	123.22
2	C	2002	RFP	C12-C11-C5	-2.78	101.03	107.53
2	C	2002	RFP	C32-C22-C21	2.01	115.38	111.24

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	2002	RFP	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, 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%)	0.09	30 (2%) 55 56	40, 90, 124, 144	0
1	B	1022/1053 (97%)	0.24	53 (5%) 31 30	57, 97, 133, 162	0
1	C	1022/1053 (97%)	0.11	41 (4%) 42 41	35, 89, 138, 167	0
All	All	3066/3159 (97%)	0.15	124 (4%) 42 41	35, 92, 134, 167	0

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1036	LYS	6.3
1	C	538	THR	5.9
1	B	1034	SER	5.1
1	A	515	TRP	5.1
1	C	870	GLY	5.1

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, 95th 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(\AA^2)	Q<0.9
2	RFP	C	2002	59/59	0.83	0.34	2.22	100,104,105,105	59

6.5 Other polymers [i](#)

There are no such residues in this entry.