



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 06:44 pm BST

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

<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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
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

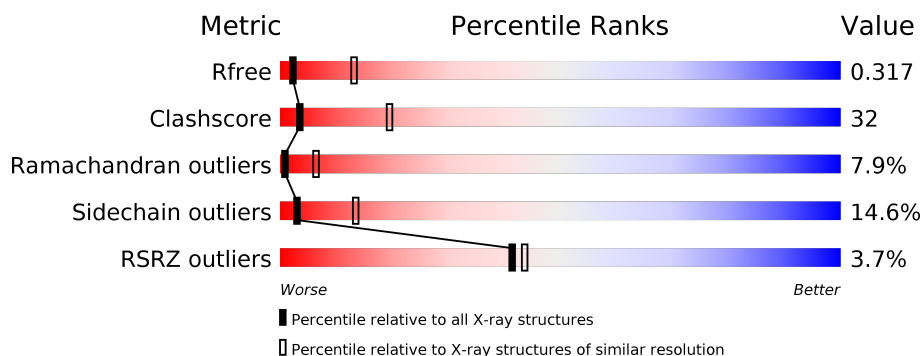
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (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 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>3%</div> <div> <div></div> <div>44%</div> <div>42%</div> <div>10%</div> <div>••</div> </div> </div>
1	B	1053	<div> <div>4%</div> <div> <div></div> <div>39%</div> <div>47%</div> <div>11%</div> <div>•</div> </div> </div>
1	C	1053	<div> <div>4%</div> <div> <div></div> <div>42%</div> <div>43%</div> <div>11%</div> <div>••</div> </div> </div>

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: $C_{43}H_{58}N_4O_{12}$).



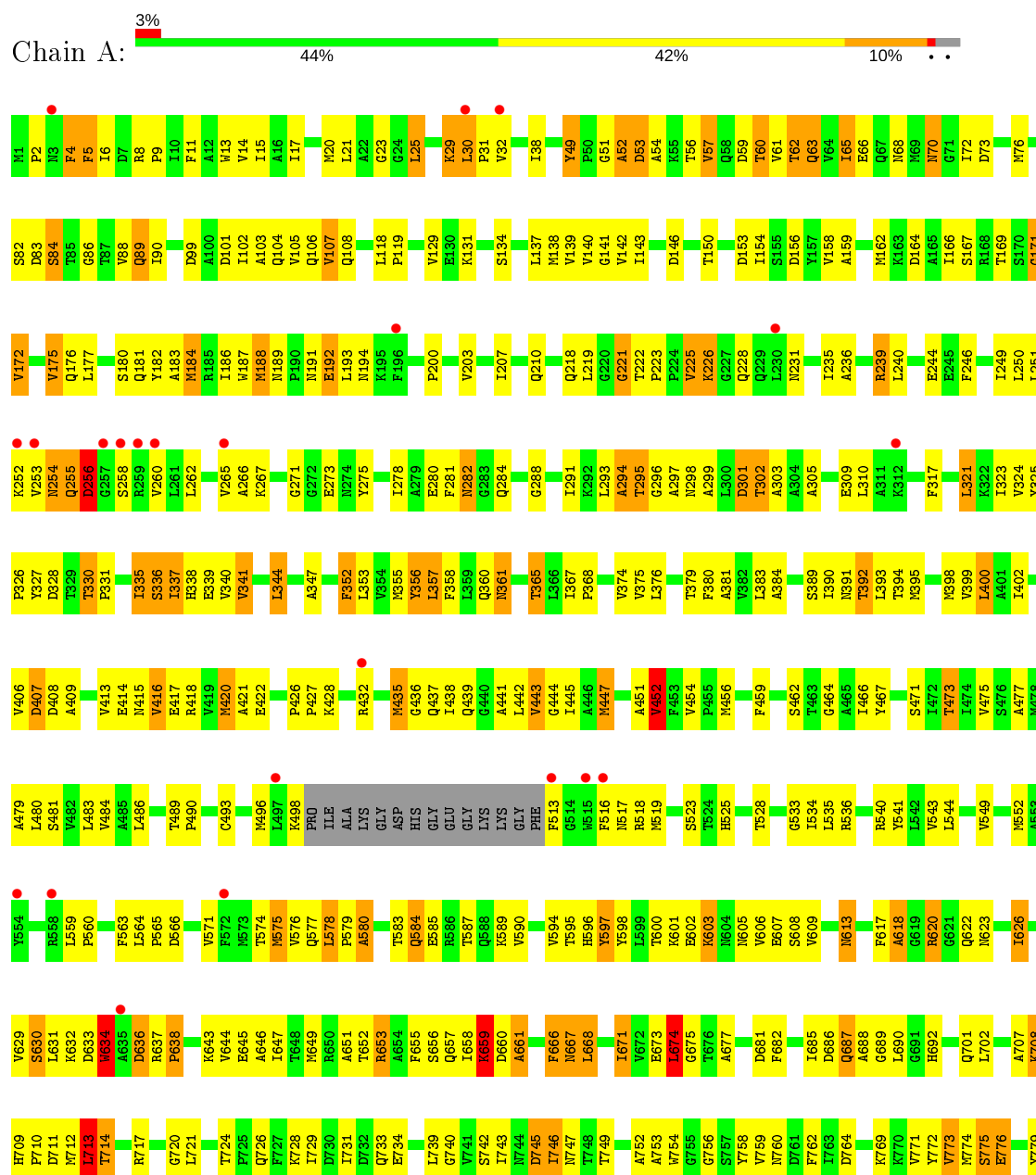
- Molecule 3 is water.

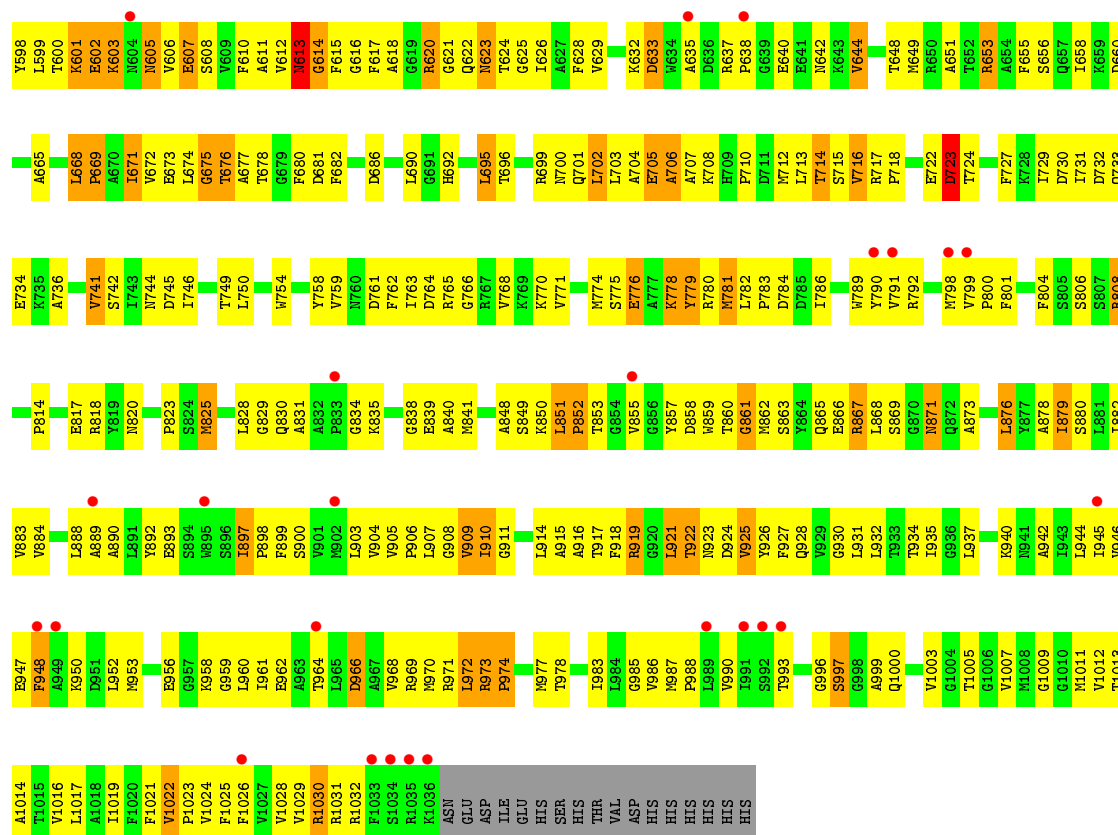


3 Residue-property plots

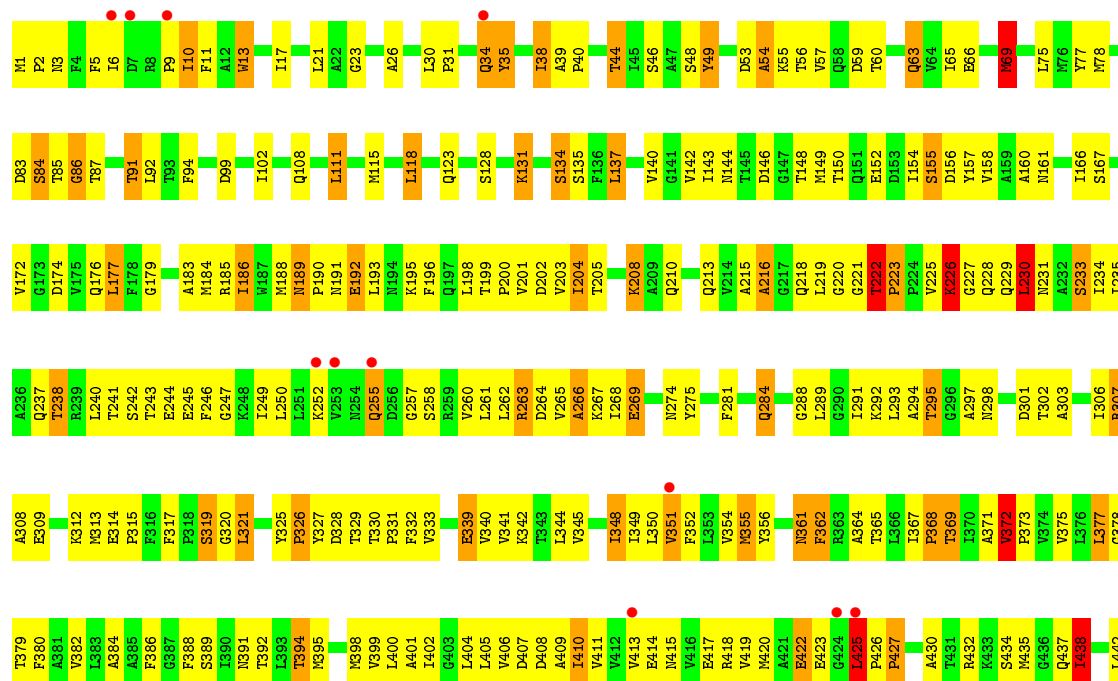
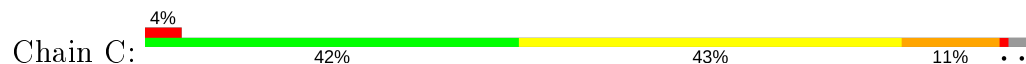
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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





• Molecule 1: Acriflavine resistance protein B



V1029	V443	PHE	Q588	L668	V741	S805	Y892	I961	V1029
R1030	G444	FS13	R589	I671	S742	S806	E893	E962	R1030
R1031	I445	G514	V590	V672	I743	S807	E894	A963	R1031
R1032	V448	W515	L591	E673	I746	R808	W895	T964	R1032
R1035	L449	FS16	N592	L674	N747	S813	S896	D966	R1035
ASN	V452	FS18	E593	G675	T748	R814	P898	A967	ASN
GLU	F453	FS19	N594	G676	T749	R815	F899	V968	GLU
ASP	P455	FS20	T595	G677	L750	L816	S900	R969	ASP
ILE	V454	E521	E601	G678	A752	R817	V901	M970	ILE
GLU	P455	FS22	R601	G679	A753	R818	H902	R971	GLU
HIS	M456	FS23	E602	F680	A754	Y819	V904	I975	HIS
HIS	A457	FS24	R605	E683	G755	N820	V904	L976	HIS
HIS	F458	FS25	L605	L684	G756	S824	L907	M977	HIS
HIS	F459	FS26	F610	L685	G757	M825	G908	T977	HIS
HIS	T463	FS27	F610	L686	S757	G829	V909	T978	HIS
HIS	G464	S530	N613	Q687	Y758	Q829	V910	S979	HIS
HIS	A465	V531	G614	Q687	V759	Q830	V911	L980	HIS
HIS	I466	G532	F615	A688	N760	A831	G911	A981	HIS
HIS	Y467	G533	R620	G889	D761	A832	L914	F982	HIS
HIS	Q469	FS34	T624	L690	D763	P833	A915	L984	HIS
HIS	I474	S537	G624	G691	D764	G834	F918	G985	HIS
HIS	V475	TS38	A627	E693	R765	K835	L921	V986	HIS
HIS	S476	G539	F628	E694	G766	S836	L921	M987	HIS
HIS	A477	FS40	F628	L695	R767	T837	V925	P988	HIS
HIS	M478	Y541	L631	T696	V768	G838	V926	S992	HIS
HIS	A479	L542	N634	Q697	R770	E839	F927	T993	HIS
HIS	L480	L544	R637	A698	V771	M841	G930	G994	HIS
HIS	S481	L547	A706	N700	Y772	E842	L931	A995	HIS
HIS	V482	FS48	A707	A706	V773	L843	L932	G996	HIS
HIS	L483	V549	K708	K708	M774	E845	L933	S997	HIS
HIS	A485	V550	H709	H709	S775	Q846	T933	G998	HIS
HIS	L486	Y554	K643	K643	K778	L847	T934	Q1000	HIS
HIS	L487	L595	V644	V644	Y779	A848	T935	G1004	HIS
HIS	T489	FS63	A646	A646	R780	L851	G936	T1005	HIS
HIS	P490	L564	T647	T647	M781	G854	L937	G1006	HIS
HIS	A491	P665	L647	L647	L782	L851	S938	V1007	HIS
HIS	L492	D668	T648	T648	P783	G854	N941	M1008	HIS
HIS	M496	Q569	V649	V649	D784	L868	A942	M1011	HIS
HIS	L497	Q570	R650	R650	D785	S869	I943	V1012	HIS
HIS	PRO	FS71	A691	A691	I786	G870	L944	T1013	HIS
HIS	ILE	V571	F655	F655	G787	Q871	I945	A1014	HIS
HIS	ALA	FS72	A654	A654	D788	Q872	V946	T1015	HIS
HIS	LYS	N573	S656	S656	Y790	A873	E947	V1016	HIS
HIS	GLY	TS74	Q657	Q657	V791	P874	F948	L1017	HIS
HIS	GLY	FS75	L658	L658	R792	S875	A949	A1018	HIS
HIS	ASP	V576	K659	K659	G796	V884	L952	I1019	HIS
HIS	HIS	Q577	D660	D660	V799	F885	M953	V1022	HIS
HIS	GLY	L578	A661	A661	P800	L886	D954	P1023	HIS
HIS	GLY	P579	N662	N662	F801	C887	E956	V1024	HIS
HIS	LYS	A580	A665	A665	S802	L888	G957	F1025	HIS
HIS	GLY	TS87	F666	F666	A803	A889	R988	V1026	HIS
HIS	GLY	TS87	N667	N667	A738	A890	G959	V1027	HIS
HIS	GLY	TS87				L960		V1028	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	Depositor
R, R_{free}	0.261 , 0.326 0.256 , 0.317	Depositor DCC
R_{free} test set	3350 reflections (5.02%)	wwPDB-VP
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
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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	7
1	B	1018/1053 (97%)	742 (73%)	193 (19%)	83 (8%)	1	6
1	C	1018/1053 (97%)	754 (74%)	182 (18%)	82 (8%)	1	6
All	All	3054/3159 (97%)	2265 (74%)	549 (18%)	240 (8%)	1	6

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%)	3	14
1	B	833/859 (97%)	705 (85%)	128 (15%)	2	12
1	C	833/859 (97%)	718 (86%)	115 (14%)	3	15
All	All	2499/2577 (97%)	2135 (85%)	364 (15%)	3	13

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	1.98	3 (4%)	94,94,94	1.83	14 (14%)

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	-	-	16/60/85/85	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2002	RFP	O4-C11	13.30	1.43	1.21
2	C	2002	RFP	O7-C35	5.55	1.47	1.35
2	C	2002	RFP	O5-C29	3.39	1.48	1.39

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2002	RFP	O4-C11-C5	-8.76	115.09	131.81
2	C	2002	RFP	C41-C42-N4	5.45	116.96	110.80
2	C	2002	RFP	O7-C35-C36	4.49	119.35	111.09
2	C	2002	RFP	O4-C11-C12	-4.08	112.25	120.56
2	C	2002	RFP	O3-C6-C7	3.96	127.95	121.14

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

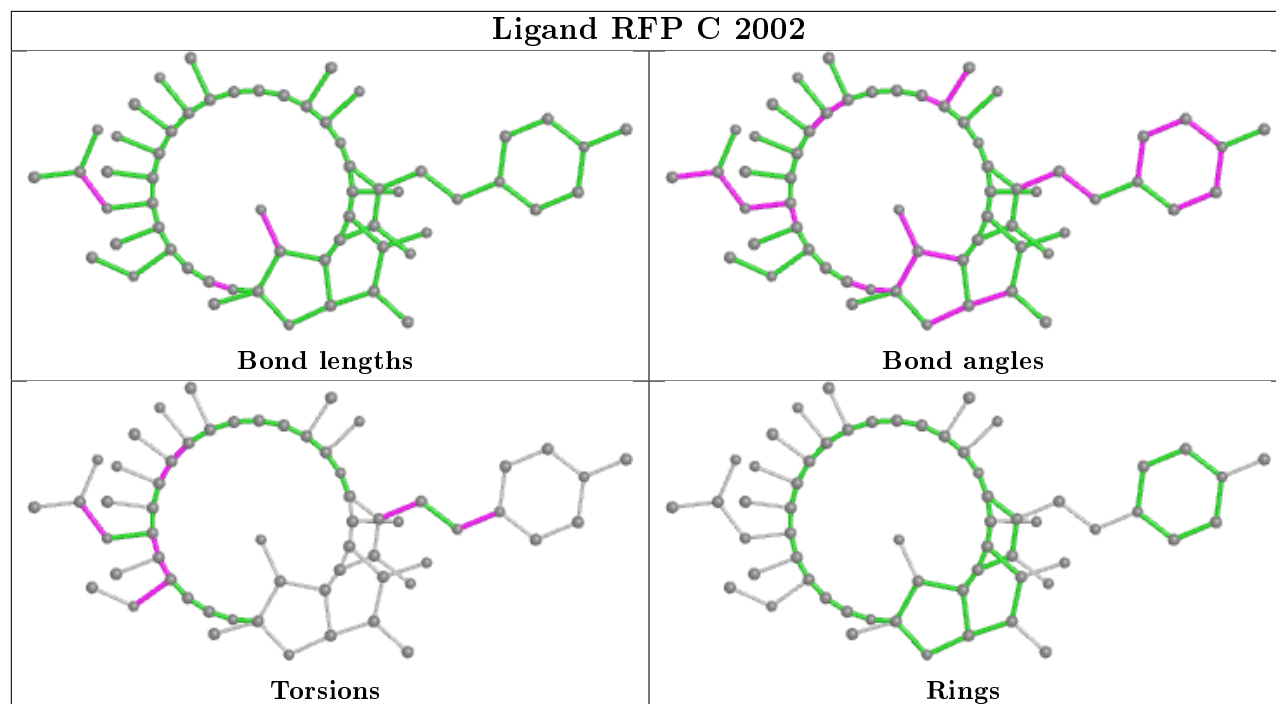
Mol	Chain	Res	Type	Atoms
2	C	2002	RFP	C2-C3-C43-N2
2	C	2002	RFP	C4-C3-C43-N2
2	C	2002	RFP	C26-C27-O6-C37
2	C	2002	RFP	C28-C27-O6-C37
2	C	2002	RFP	C36-C35-O7-C25

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	30 (2%) 51 54	40, 90, 124, 144	0
1	B	1022/1053 (97%)	0.21	45 (4%) 34 37	57, 97, 133, 162	0
1	C	1022/1053 (97%)	0.09	38 (3%) 41 43	35, 89, 138, 167	0
All	All	3066/3159 (97%)	0.12	113 (3%) 41 43	35, 92, 134, 167	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1036	LYS	6.1
1	C	538	THR	5.7
1	C	870	GLY	5.0
1	B	1034	SER	4.9
1	A	515	TRP	4.9

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](#)

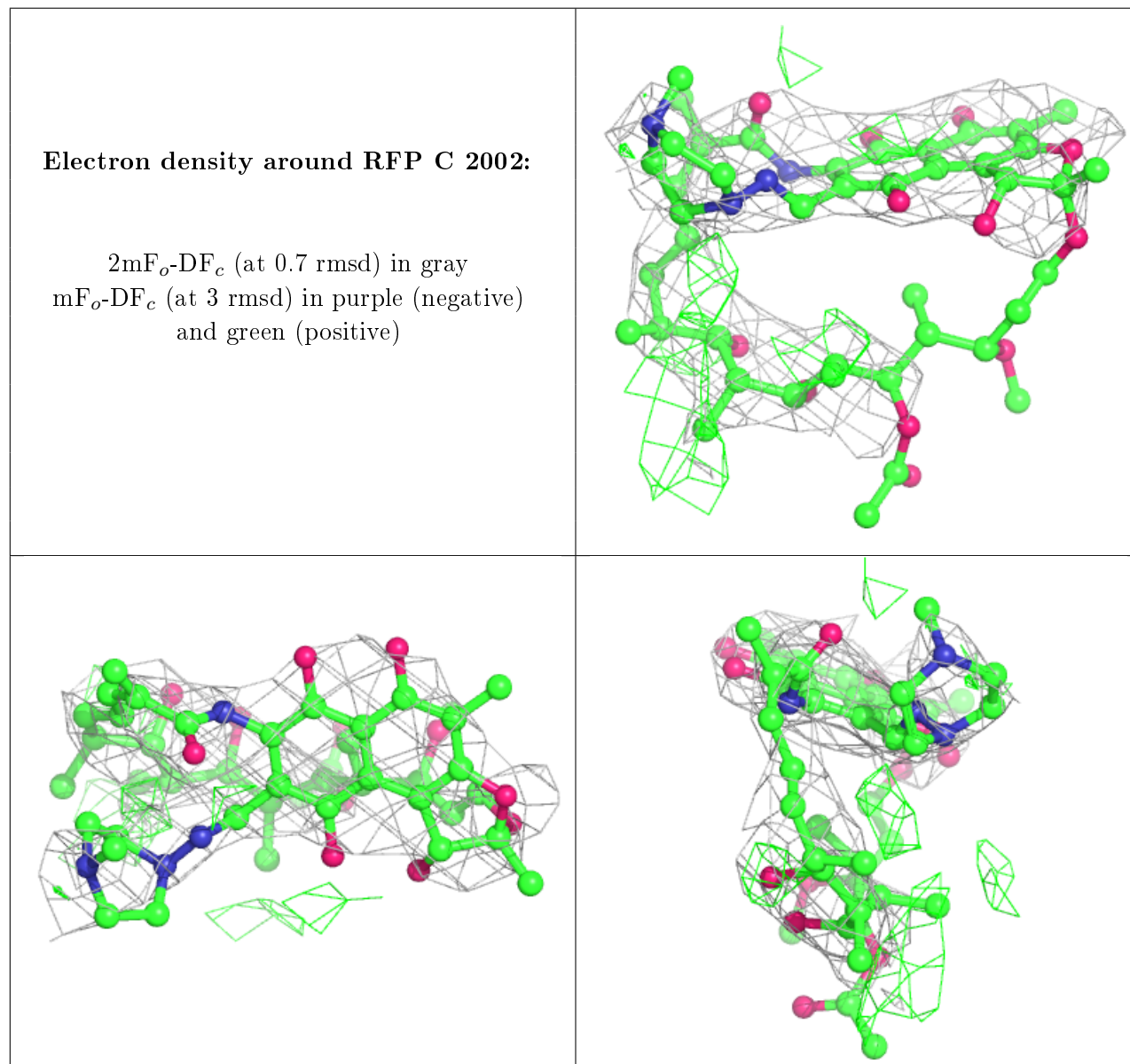
There are no carbohydrates in this entry.

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. 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	B-factors(\AA^2)	Q<0.9
2	RFP	C	2002	59/59	0.83	0.34	100,104,105,105	59

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.