



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:24 AM GMT

PDB ID : 3AOD
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 : 3.30 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

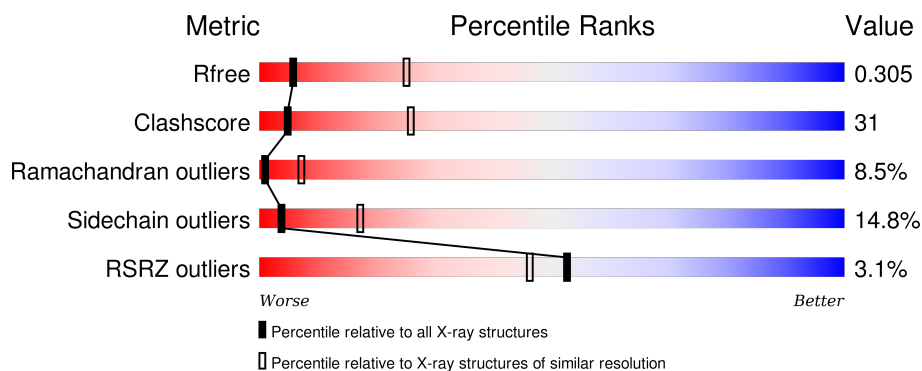
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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>43%</div> <div>42%</div> <div>11%</div> <div>..</div> </div>
1	B	1053	<div> <div>3%</div> <div>40%</div> <div>45%</div> <div>11%</div> <div>..</div> </div>
1	C	1053	<div> <div>3%</div> <div>44%</div> <div>43%</div> <div>10%</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23419 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.

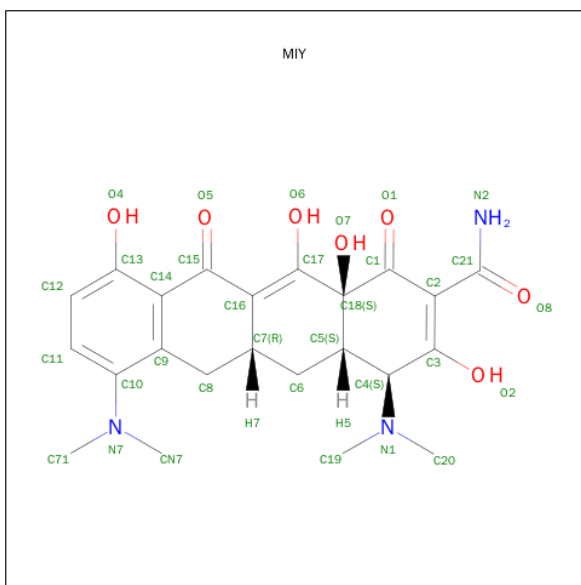
- Molecule 1 is a protein called Acriflavine resistance protein B.

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:

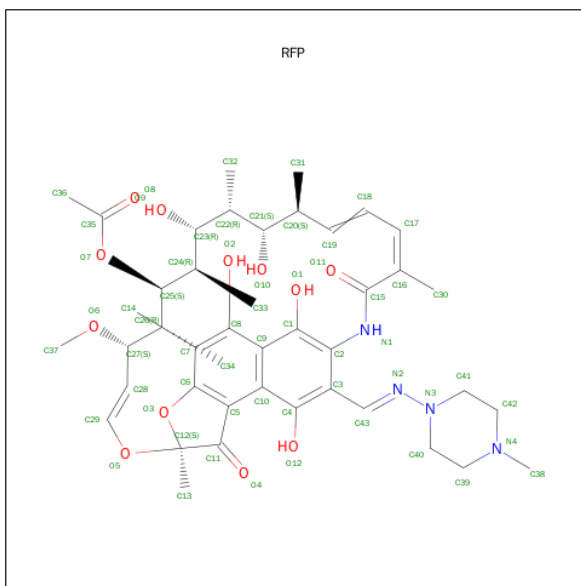
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	EXPRESSION TAG	UNP P31224
A	1051	HIS	-	EXPRESSION TAG	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224
B	1050	HIS	-	EXPRESSION TAG	UNP P31224
B	1051	HIS	-	EXPRESSION TAG	UNP P31224
B	1052	HIS	-	EXPRESSION 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 (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula: C₂₃H₂₇N₃O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	23	3	7		

- Molecule 3 is RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



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

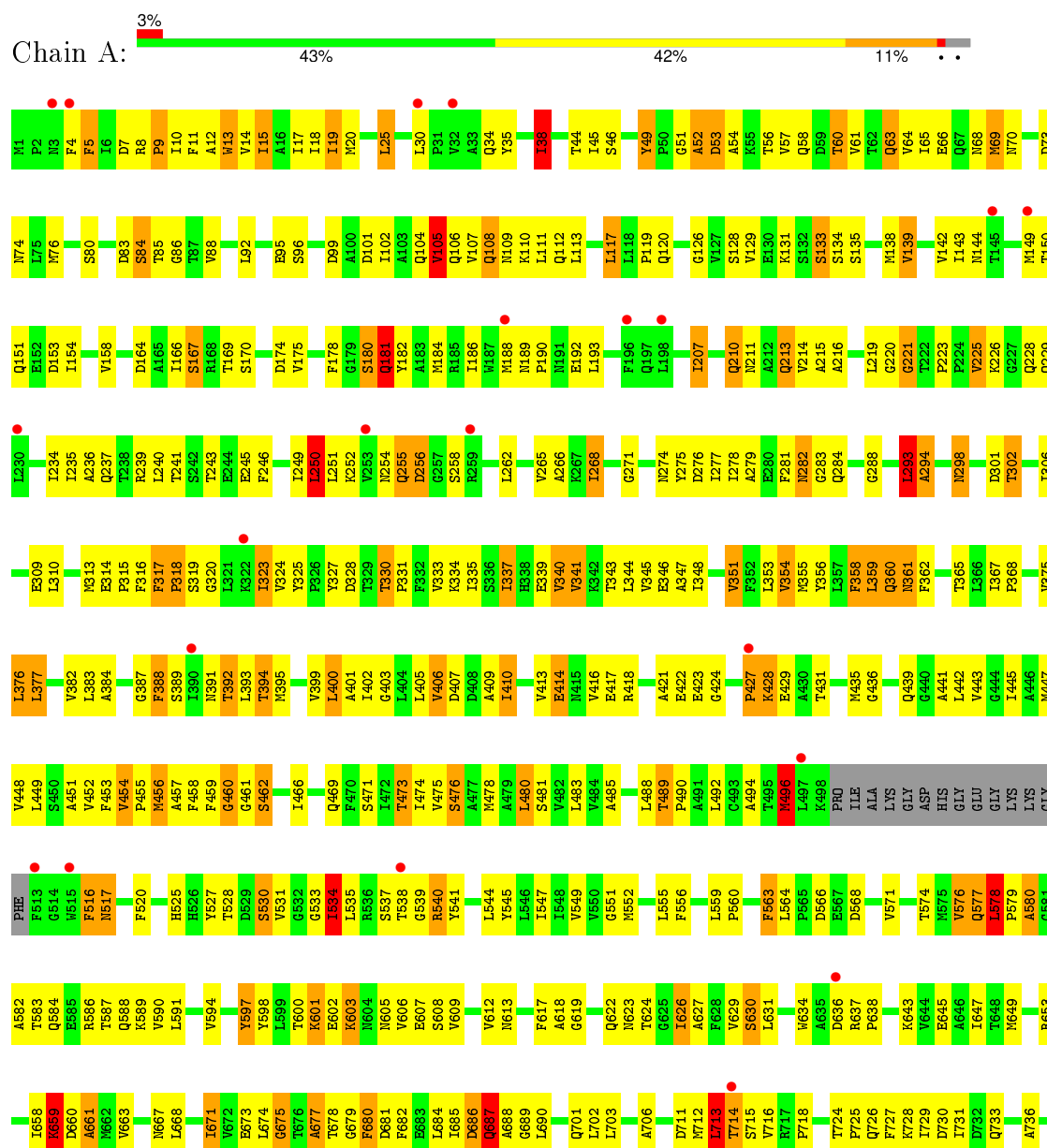
- Molecule 4 is water.

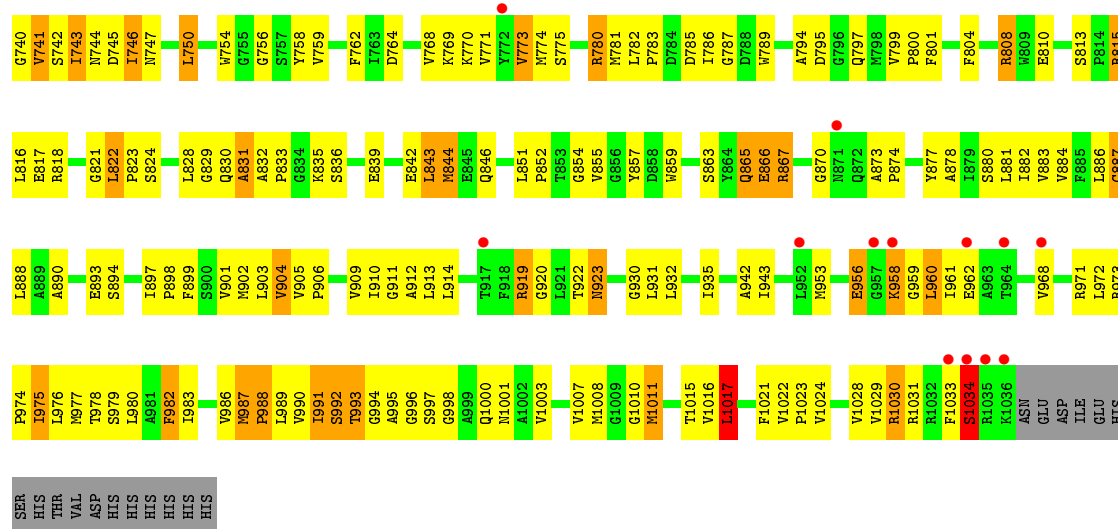
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	2	Total 2	O 2	0	0
4	C	1	Total 1	O 1	0	0

3 Residue-property plots

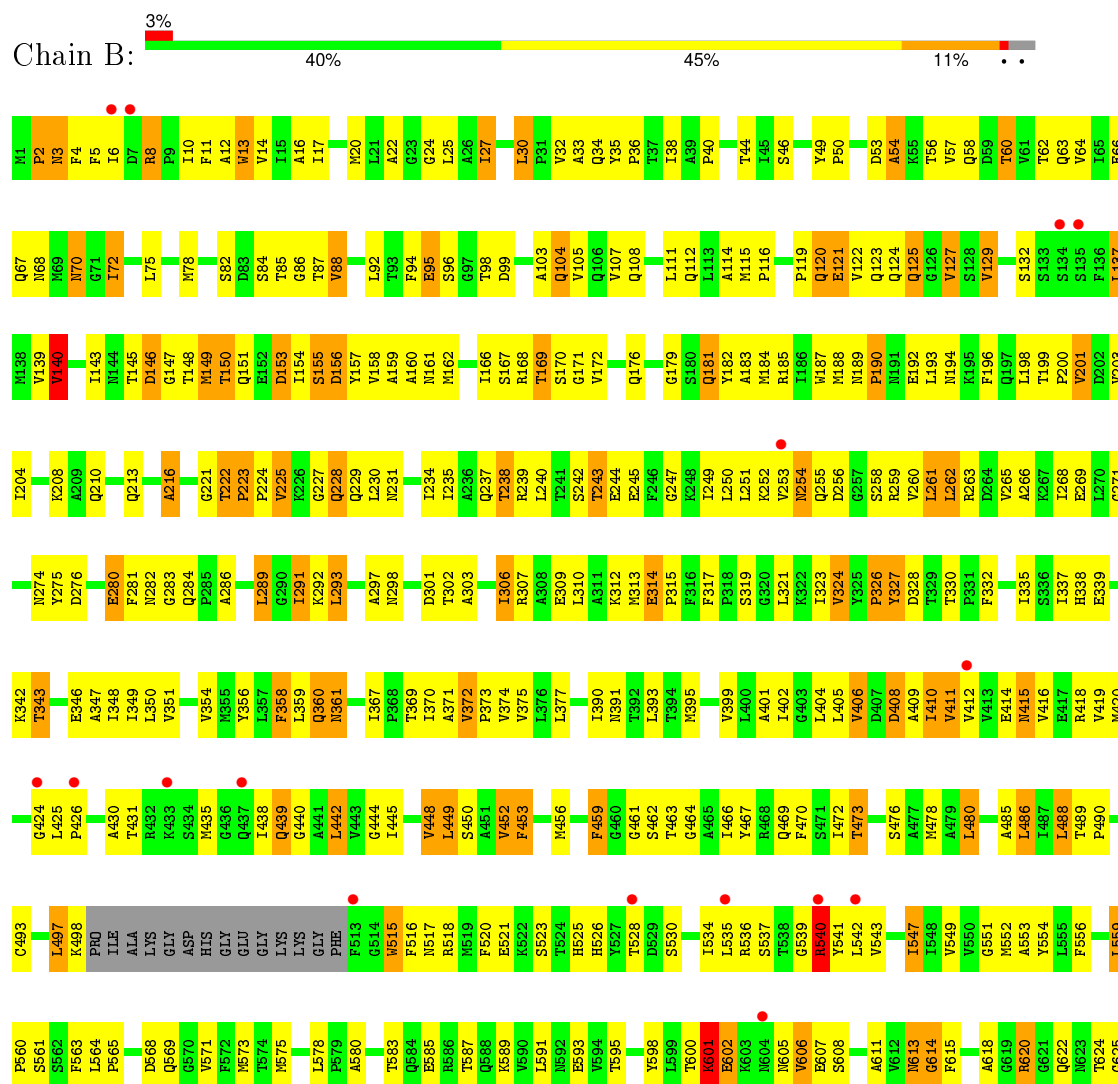
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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





Q1000	G1004	T1005	G1006	V1007	M1008	M1011	Y1012	T1013	A1014	T1015	V1016	L1017	A1018	I1019	F1020	F1021	V1022	P1023	Y1024	F1025	F1026	V1027	V1028	V1029	R1030	R1031	R1032	F1033	S1034	R1035	K1036	ASN	GLU	ASP	TLE	GLU	HIS	SER	HIS	THR	VAL	ASP	HIS	HIS	HIS	HIS								
L931	L932	T933	T934	I935	K940	N941	A942	T943	L944	T945	V946	E947	F948	A949	K950	D951	L952	K953	D954	K955	E956	G957	K958	G959	L960	T961	E962	A963	T964	L965	D966	A967	V968	R969	N970	R971	L972	R973	P974	T975	L976	N977	F982	T983	L984	G985	V986	L989	V990	T993	G994	S997	G998	A999
G854	V855	G856	V857	N859	S863	L868	S869	G870	N871	Q872	A873	P874	S875	L879	V883	V884	T885	L888	A889	A890	E893	S896	F899	S900	V901	V904	V905	P906	L907	G908	V909	T910	G911	L914	A915	R919	G920	L921	T922	V925	V926	F927	Q928	V929	G930									
V771	M774	S775	K778	T779	R780	M781	L782	P783	D784	D785	I786	W789	P792	D795	G796	Q797	M798	V799	P800	F801	S802	A803	F804	S805	S806	S807	R808	P814	R815	G821	L822	M825	Q830	A831	A832	P833	G834	K835	S836	E839	L843	M844	L847	A848	S849	K850	L851							
N623	T624	F628	V629	S630	L631	K632	D633	W634	A635	D636	R637	N642	K643	V644	I647	T648	M649	F655	S656	Q657	I658	K659	M662	V663	F664	A665	I671	V672	L674	G675	T676	A677	T678	G679	F680	D681	L684	I685	D686	Q687	L690	G691	H692	E693	K694	L695	T696	Q697	A698	R699				
L702	A707	P710	D711	M712	L713	T714	S715	V716	R717	G720	L721	E722	D723	T724	F727	K728	I729	D730	I731	D732	Q733	E734	K735	A736	Q737	A738	L739	G740	V741	S742	D745	I746	L750	G751	A752	A753	W754	G755	G756	S757	Y758	V759	M760	D761	F762	I763	D764	R767	V768	K769	K770			

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.60Å 134.50Å 162.83Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	47.50 – 3.30 47.50 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.50-3.30) 97.3 (47.50-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.67 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.258 , 0.318 0.251 , 0.305	Depositor DCC
R_{free} test set	3532 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	95.3	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.3	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 70728 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23419	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MIY, 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	0.65	0/7920	0.77	4/10756 (0.0%)
1	B	0.60	0/7920	0.76	2/10756 (0.0%)
1	C	0.65	0/7920	0.79	5/10756 (0.0%)
All	All	0.64	0/23760	0.77	11/32268 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	321	LEU	CA-CB-CG	7.38	132.26	115.30
1	B	868	LEU	CA-CB-CG	6.60	130.48	115.30
1	C	721	LEU	CA-CB-CG	6.58	130.42	115.30
1	A	400	LEU	CA-CB-CG	6.09	129.30	115.30
1	C	344	LEU	CA-CB-CG	5.79	128.62	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	537	0
1	C	7774	0	7931	503	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	33	0	24	0	0
3	C	59	0	56	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
All	All	23419	0	23873	1489	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 31.

The worst 5 of 1489 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:713:LEU:CB	1:A:832:ALA:HA	1.80	1.11
1:C:44:THR:HG23	1:C:91:THR:HB	1.33	1.10
1:C:909:VAL:HG12	1:C:931:LEU:HD21	1.11	1.09
1:B:95:GLU:O	1:B:98:THR:HG22	1.50	1.09
1:C:115:MET:HE3	1:C:127:VAL:HG11	1.33	1.08

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%)	752 (74%)	173 (17%)	93 (9%)	1	6
1	B	1018/1053 (97%)	730 (72%)	201 (20%)	87 (8%)	1	7
1	C	1018/1053 (97%)	760 (75%)	178 (18%)	80 (8%)	1	8
All	All	3054/3159 (97%)	2242 (73%)	552 (18%)	260 (8%)	1	7

5 of 260 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	A	181	GLN
1	A	182	TYR
1	A	282	ASN
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%)	707 (85%)	126 (15%)	3	16
1	B	833/859 (97%)	708 (85%)	125 (15%)	3	17
1	C	833/859 (97%)	715 (86%)	118 (14%)	4	19
All	All	2499/2577 (97%)	2130 (85%)	369 (15%)	4	17

5 of 369 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	254	ASN
1	B	601	LYS
1	C	724	THR
1	B	292	LYS
1	B	435	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	GLN
1	B	338	HIS
1	C	726	GLN
1	B	161	ASN
1	B	213	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

2 ligands are 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	MIY	A	2001	-	35,36,36	1.83	4 (11%)	40,58,58	1.91	11 (27%)
3	RFP	C	2002	-	63,63,63	1.73	3 (4%)	82,94,94	1.96	15 (18%)

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	MIY	A	2001	-	-	0/12/70/70	0/4/4/4
3	RFP	C	2002	-	-	0/60/85/85	0/1/5/5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	MIY	C18-C1	-2.08	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	MIY	C4-N1	2.04	1.51	1.47
2	A	2001	MIY	C16-C15	2.05	1.52	1.47
3	C	2002	RFP	O5-C29	2.85	1.48	1.39
3	C	2002	RFP	O7-C35	5.38	1.47	1.35

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2002	RFP	O4-C11-C5	-7.99	115.37	132.02
2	A	2001	MIY	O5-C15-C14	-5.87	110.99	122.01
2	A	2001	MIY	O5-C15-C16	-5.43	112.64	120.73
2	A	2001	MIY	O6-C17-C16	-4.09	119.93	123.84
3	C	2002	RFP	C30-C16-C17	-3.41	115.14	123.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2002	RFP	4	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%)	0.05	34 (3%)	50 43	52, 102, 136, 167	0
1	B	1022/1053 (97%)	0.13	27 (2%)	59 53	65, 106, 140, 169	0
1	C	1022/1053 (97%)	0.01	34 (3%)	50 43	49, 100, 148, 183	0
All	All	3066/3159 (97%)	0.06	95 (3%)	52 46	49, 103, 142, 183	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	872	GLN	5.9
1	C	514	GLY	5.5
1	C	515	TRP	5.3
1	A	32	VAL	5.0
1	C	425	LEU	5.0

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	MIY	A	2001	33/33	0.87	0.25	0.35	134,138,142,142	0
3	RFP	C	2002	59/59	0.91	0.26	0.17	131,136,139,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.