



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:10 PM GMT

PDB ID : 3W9I
Title : Structural basis for the inhibition of bacterial multidrug exporters
Authors : Sakurai, K.; Nakashima, R.; Hayashi, K.; Yamaguchi, A.
Deposited on : 2013-04-04
Resolution : 2.71 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

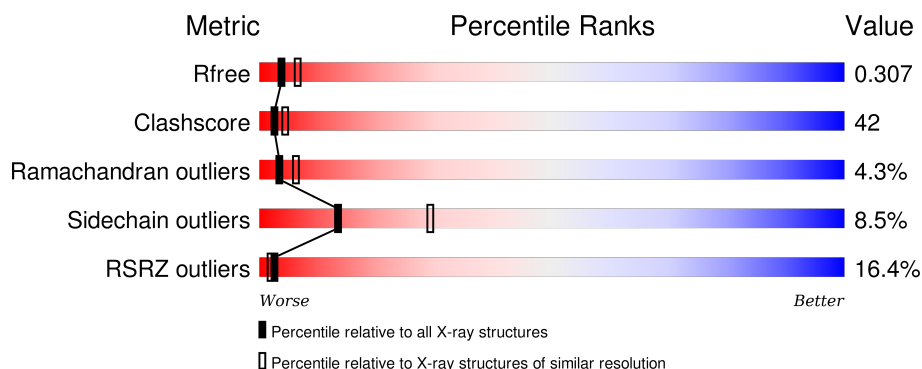
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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	1046	<div> <div>14%</div> <div>36%</div> <div>54%</div> <div>7%</div> </div>
1	B	1046	<div> <div>13%</div> <div>42%</div> <div>48%</div> <div>8%</div> </div>
1	C	1046	<div> <div>19%</div> <div>34%</div> <div>54%</div> <div>9%</div> </div>
1	D	1046	<div> <div>15%</div> <div>36%</div> <div>54%</div> <div>7%</div> </div>
1	E	1046	<div> <div>17%</div> <div>40%</div> <div>52%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	1046	

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	LMT	A	1101	-	-	-	X
2	LMT	A	1102	-	-	-	X
2	LMT	B	2001	-	-	-	X
2	LMT	B	2002	-	-	-	X
2	LMT	C	2001	-	-	-	X
2	LMT	C	2002	-	-	-	X
2	LMT	D	2001	-	-	-	X
2	LMT	D	2002	-	-	-	X
2	LMT	D	2003	-	-	-	X
2	LMT	E	2001	-	-	X	X
2	LMT	E	2002	-	-	X	X
2	LMT	E	2003	-	-	-	X
2	LMT	F	2002	-	-	-	X

2 Entry composition ⓘ

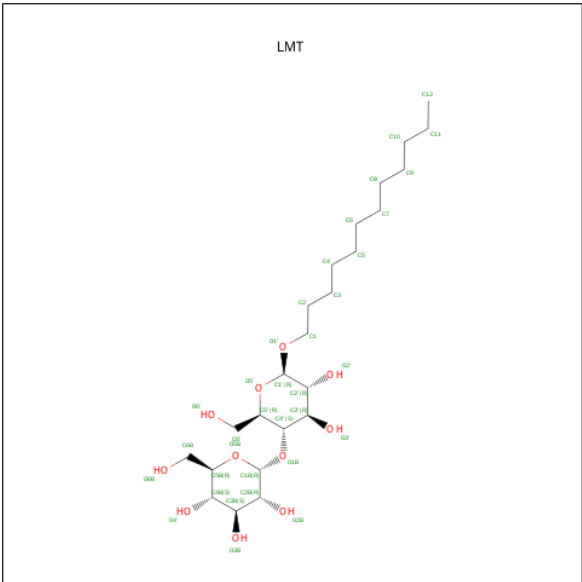
There are 3 unique types of molecules in this entry. The entry contains 47305 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Multidrug resistance protein MexB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1017	Total	C	N	O	S	0	0	0
			7718	4972	1279	1427	40			
1	B	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	C	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	D	1020	Total	C	N	O	S	0	0	0
			7744	4990	1283	1431	40			
1	E	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	F	1033	Total	C	N	O	S	0	0	0
			7840	5046	1302	1452	40			

- Molecule 2 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 35 24 11	0	0
2	A	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	F	1	Total C O 35 24 11	0	0
2	F	1	Total C O 35 24 11	0	0

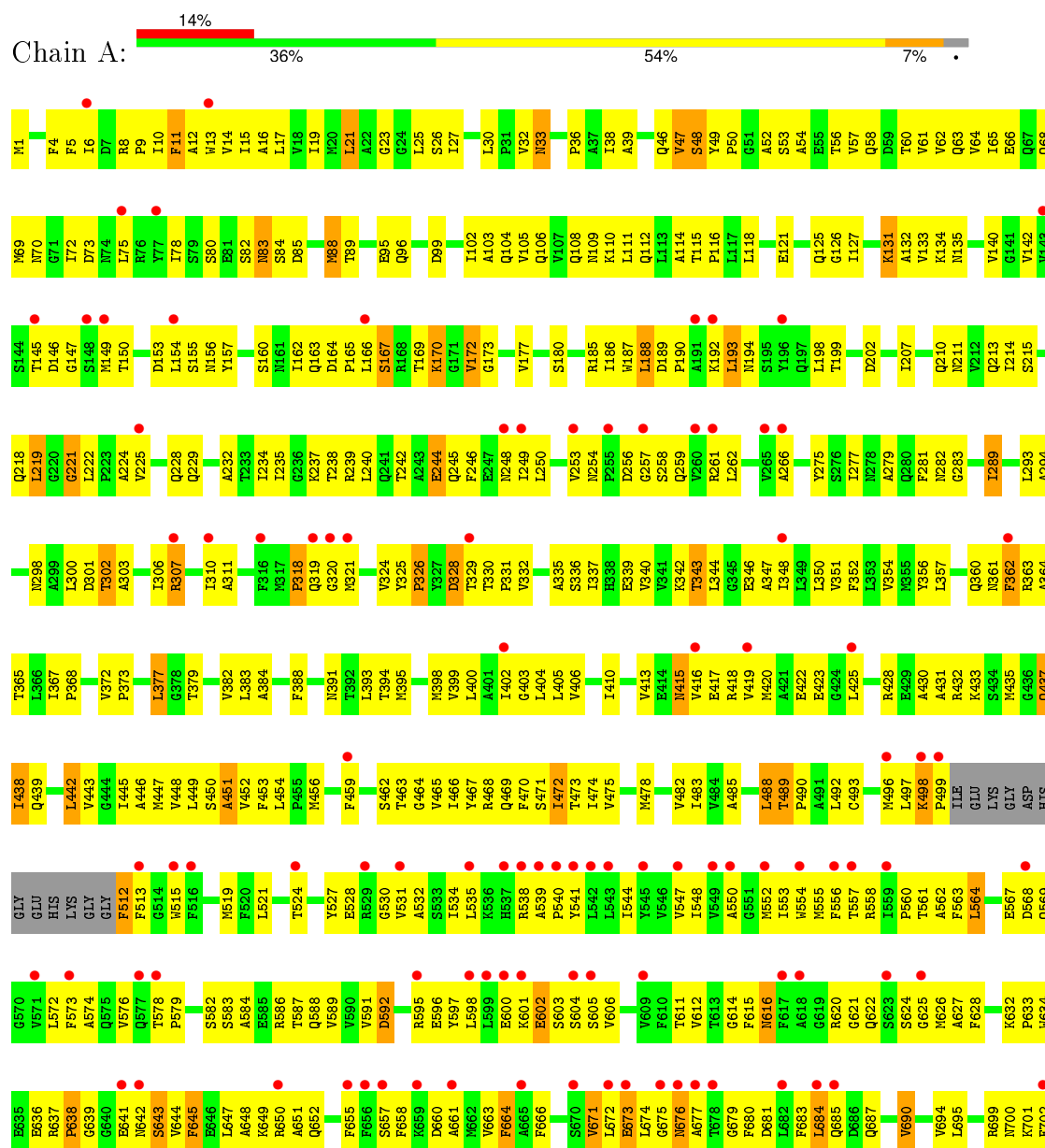
- Molecule 3 is water.

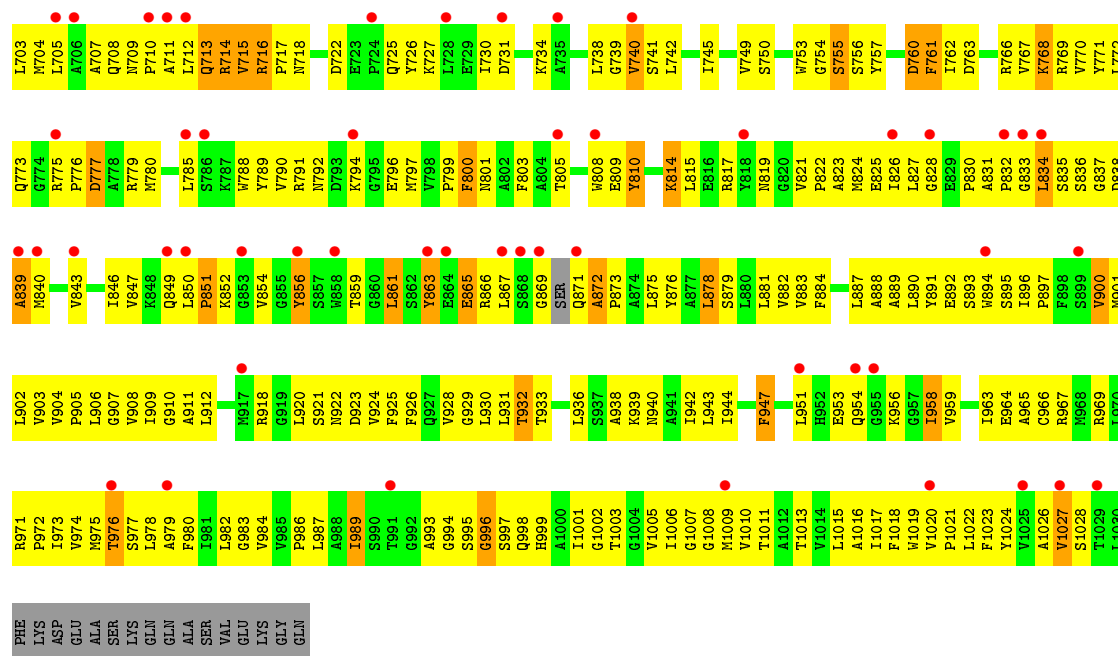
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	3	Total O 3 3	0	0
3	C	1	Total O 1 1	0	0
3	D	2	Total O 2 2	0	0

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.

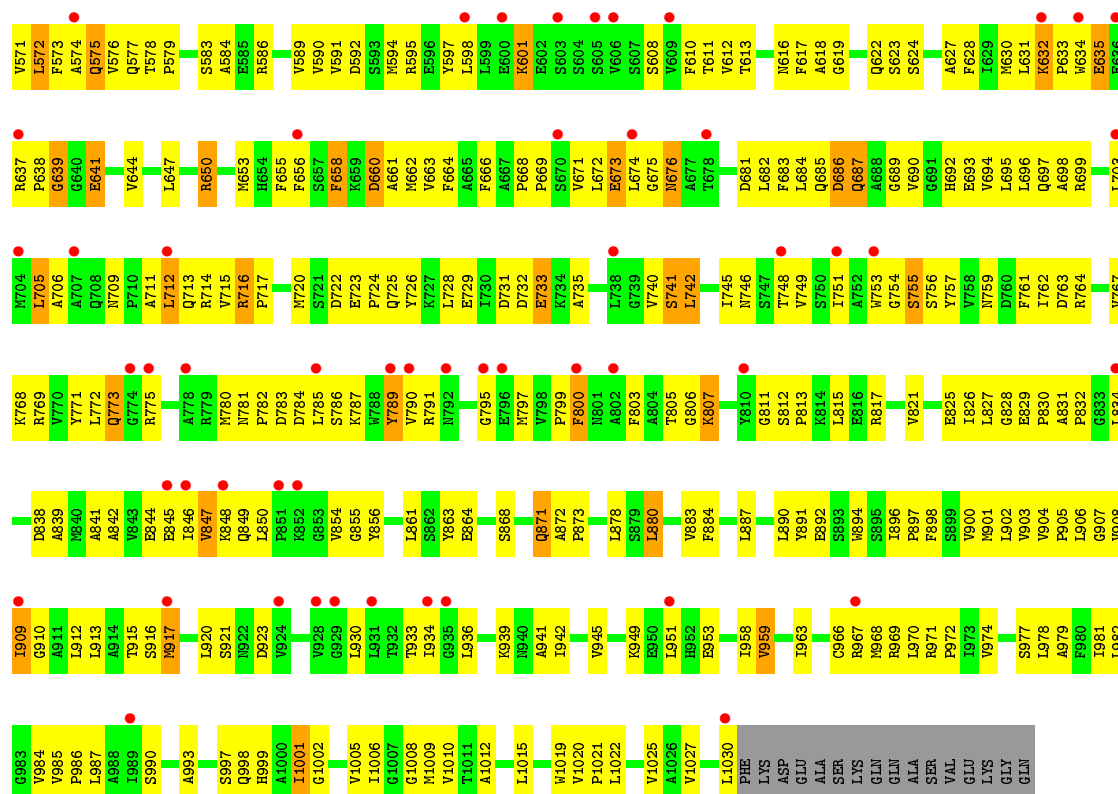
• Molecule 1: Multidrug resistance protein MexB



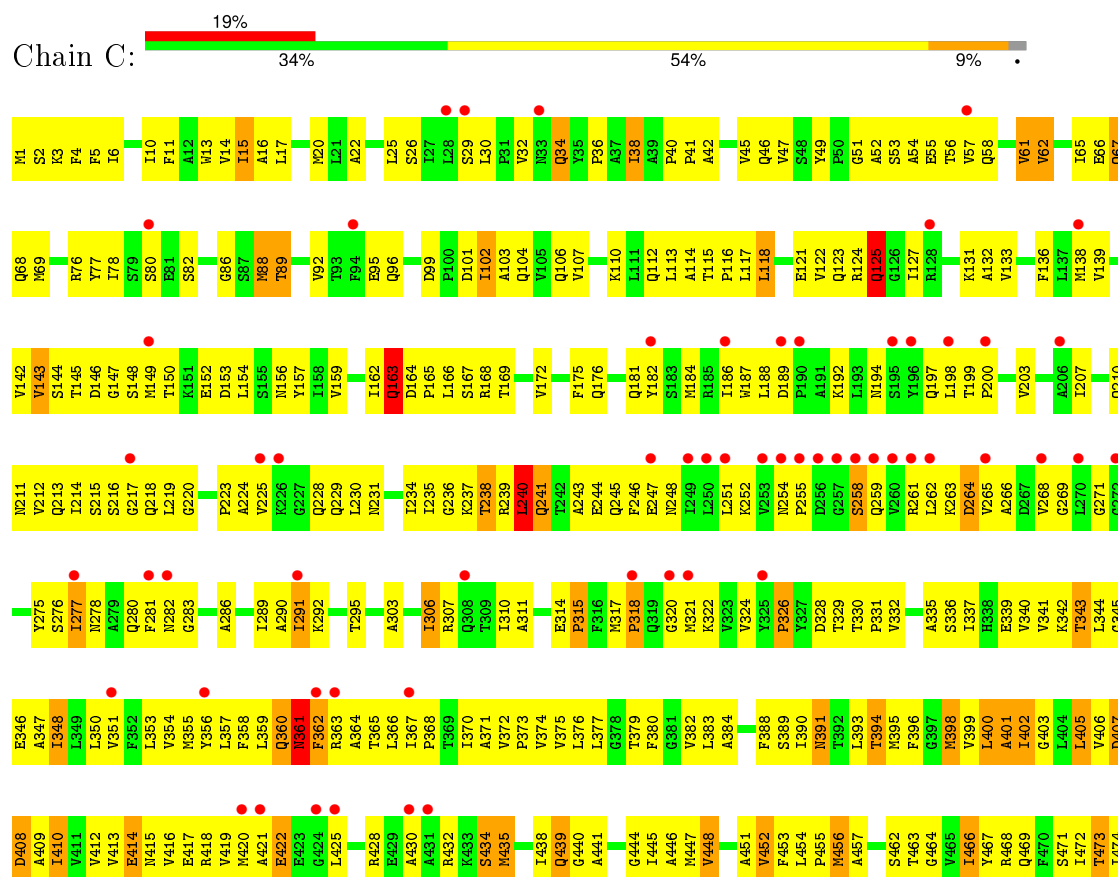


• Molecule 1: Multidrug resistance protein MexB

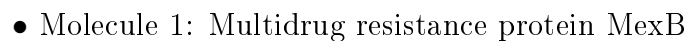


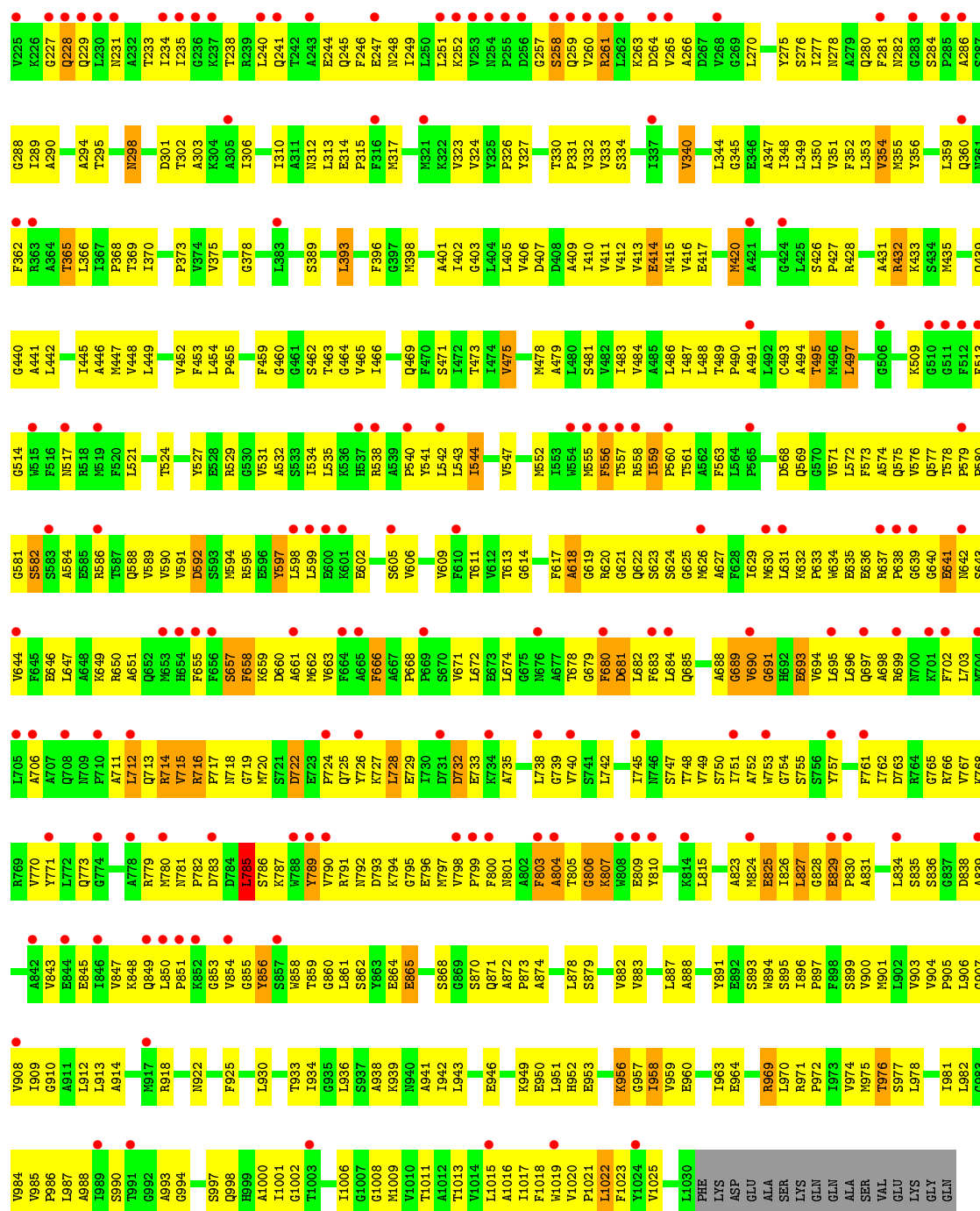


• Molecule 1: Multidrug resistance protein MexB

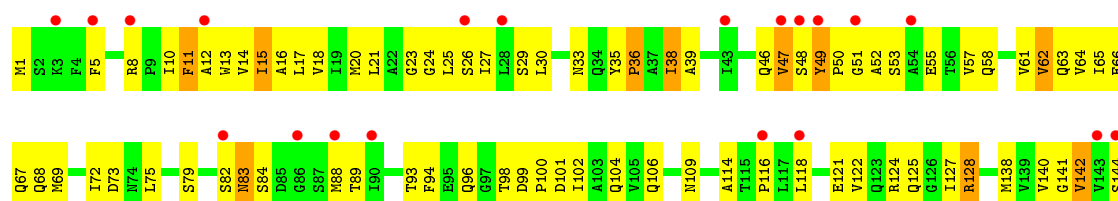








• Molecule 1: Multidrug resistance protein MexB



V1019	K939	L875	E809	Q739	G679	M616	I544	V482	V412	L344	S276	Q213	T145
V1020	K940	L876	Y810	V740	F680	F617	T545	I483	V413	G945	I277	I214	D146
P1021	A941	L880	G811	S741	D681	A618	V546	V494	E417	G946	N278	S216	G147
L1022	I942	L881	S812	L742	L682	G619	V547	A485	R418	A347	A279	S216	S148
F1023	L943	L882	P813	A743	L683	L742	I548	I486	R418	A485	Q280	G217	M149
Y1024	L944	V882	K814	D744	F684	G621	V549	I487	V419	L349	F281	Q218	T150
V1025	V945	V883	L815	I745	G685	Q622	M552	L488	W420	L350	N282	L219	E151
A1026	E946	L884	E816	N746	D686	Q623	I553	T489	W421	V351	G283	G220	E152
V1027	F947	L885	R817	I747	G687	S623	M554	P490	A422	V354	S284	P223	D153
L1030	E950	C886	Y818	T748	A688	G625	M555	A491	E423	M355	P285	P223	S155
F1031	Q954	L887	N819	V749	G689	W626	M555	L492	Q424	A224	A286	A224	L156
K1032	L888	A888	P822	S750	V690	A627	B558	Q493	L425	Y356	S287	V225	N157
D1033	L889	L889	L822	I751	G691	F628	B559	L497	R428	F358	I289	Q228	I158
GLU	L890	L890	A823	A752	H682	L629	I559	K498	R429	F359	I289	Q229	I159
ALA	E891	E891	M824	F753	H683	W630	P560	R498	A430	Q360	A290	Q229	S160
SER	E892	E892	E825	G754	F694	L631	T561	P499	A431	N361	I291	L230	
LYS	S893	S893	I826	S755	L695	G632	A562	I500	A431	K292	N231	A231	
GLN	W894	W894	L827	V758	L696	P633	F563	E501	K433	F362	A232	T293	D164
GLN	S895	S895	G828	N759	G697	W634	L564	K502	K433	R363	A294	T293	P165
ALA	L896	L896	E829		A698	B635		G503	S434	A364	A294	I234	L166
ALA	R897	R897	P830		A699	B636		D504	N435	G296	G296	I235	L167
SER	F898	F898	A831		W700	W637		H505	Q436	L366	A297	G236	R168
VAL	S899	S899		I762	F701	P638		G506	Q437	L367	N298	K237	T169
GLU	V974	V900	L634	D763	F702	G639	V571	E507	I438	P368	A299	T238	
LYS	W975	W901		K768	L703	G640	L572	H508	Q439	T369	L300	R239	V172
GLY	T976	L902		R769	W784	B641	F573	K509		L370	D301	L240	
GLN		V903	G837	Q773	L705	W642		G510	T445	V372	A302	Q241	V177
	F980	V904	D838		A706	S643	V576	G511	A446	V372	I303	T242	F178
	L981	P905	M840		A707	W644	T577	F512	N447	P373	A243	A243	
	L982	L906	A841	A778	Q708	F645	T578	F513	V448	V374	I306	E244	Y182
	G983	G907	A842	R779	W709	B646		G514	L449	V375	I306	Q245	S183
	V984	V908	W843	W780	P710	L647		W515		L376	I310	F246	M184
	V985	V909	E844	R781	A711	A648	G581	F516	W452	L377	A311		S183
	P986	G910	E845	Q782	L712	W649	S582	N517	F453	G378	N312	T249	I186
	L987	L912	W847	D783	Q713	W650	A584	R518	L454	T379	L313	L250	L187
		L913	K848	W784	R714	A651		M519	P455	F380	E314	L251	L188
	S990	A914	Q849	L785	W715	Q652	T587	F520	W456	G381	P315	K252	D189
	T991	T915	Q849	S786	R716	W653		L521	A457	V382	F316	Y253	P190
	S995	S916	L850	K787	R717	B654		S522		F388	M317	N254	A191
	G996	L920	G853	W788	W718	W655	V591	T523	Q461		P318	P255	K192
	S997	S921	K852	Y789	Q719	F656	M594	T524	S462	N391	Q319	G257	L193
	Q998	I922	V654	R791	W720		B595	H525	T463	T392	G320	G257	N194
	A1000	D923	G856	N792	D722	A661	E596	G526	Q464	L393	M321	K322	S195
	I1001	V924	T857	D793	E723	A662	T597	Y527	W465	T394	K322	Y259	Y196
		F925	W858	K794	P724	F664	E597	E528	L466	M395	V323	V260	Q197
	G1007	F926	T859	G795	Q725	A665	L599	R529	W467	F396	V324	K261	L198
	G1008	Q927	W797	Y796	Y726	E665	E800	G530	Q469		Y325	L262	T199
	M1009	V928	G860	W798	K727	F666	K801	V531		L400	K326	K263	P200
			L861	P799	L728	A667	E802	A532	F470	L401	Y327	D264	G201
		G929	S862	F799	E729	P668	S803	S533	S471	I402	G328	V265	D202
		L930	W863	F800	P669	P669	S804	I534	L472	I402	T329	A266	V203
		L931	E864	N801	D731	P670	S805	L535	W473	G403	T330	D267	S204
	A1012	T932	E865	A802	D732	W671	V606	K536	L474	L404	P331	V268	S205
	T1013	T933	R866	F803	D733	L672	S607	H537	W475	L405	V332	G269	A206
	V1014	I934	L867	R804	K734	B673	S608	R538	S476	V406	V333	L270	I207
	L1015	G935		T805	K735	L674		A539	A477	D407		G271	Q208
		L936	A872	G806	A735	L675	T611	P540	W478	D408		G272	A209
	I1017	S937	K807	W807	S736	G675	W612	F541	A479	A409		Q273	Q210
	F1018	A938	A874	W808	L738	W678	V612	L543	S481	L480		D274	M211

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	124.81Å 133.98Å 150.47Å 87.14° 69.49° 88.54°	Depositor
Resolution (Å)	48.33 – 2.71 48.33 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.0 (48.33-2.71) 95.8 (48.33-2.71)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.282 , 0.315 0.278 , 0.307	Depositor DCC
R_{free} test set	12073 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	69.8	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.6	EDS
Estimated twinning fraction	0.000 for -h,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 240857 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47305	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: LMT

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	0.48	0/7873	0.65	0/10701
1	B	0.53	0/7971	0.70	2/10833 (0.0%)
1	C	0.45	0/7971	0.62	1/10833 (0.0%)
1	D	0.45	0/7901	0.63	0/10739
1	E	0.41	0/7971	0.59	0/10833
1	F	0.44	0/8000	0.61	0/10871
All	All	0.46	0/47687	0.63	3/64810 (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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	686	ASP	CB-CG-OD2	5.92	123.63	118.30
1	C	401	ALA	CB-CA-C	-5.41	101.99	110.10
1	B	432	ARG	NE-CZ-NH2	-5.34	117.63	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	675	GLY	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	7718	0	7858	683	0
1	B	7812	0	7944	628	0
1	C	7812	0	7944	758	0
1	D	7744	0	7886	710	0
1	E	7812	0	7944	626	0
1	F	7840	0	7970	668	0
2	A	70	0	92	12	0
2	B	140	0	184	28	0
2	C	70	0	92	18	0
2	D	105	0	138	14	0
2	E	105	0	138	33	0
2	F	70	0	92	8	0
3	A	1	0	0	1	0
3	B	3	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
All	All	47305	0	48282	3970	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 42.

The worst 5 of 3970 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:E:142:VAL:HG21	1:E:158:ILE:HD11	1.33	1.10
1:D:454:LEU:CD1	2:D:2001:LMT:H101	1.82	1.09
1:E:435:MET:O	1:E:439:GLN:HB2	1.53	1.09
1:A:343:THR:HG21	1:A:998:GLN:HE22	1.16	1.08
1:B:359:LEU:HD22	1:B:417:GLU:HG2	1.34	1.07

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	1011/1046 (97%)	834 (82%)	139 (14%)	38 (4%)	4	8
1	B	1028/1046 (98%)	878 (85%)	123 (12%)	27 (3%)	7	15
1	C	1028/1046 (98%)	814 (79%)	161 (16%)	53 (5%)	2	4
1	D	1016/1046 (97%)	815 (80%)	156 (15%)	45 (4%)	3	6
1	E	1028/1046 (98%)	839 (82%)	147 (14%)	42 (4%)	3	7
1	F	1031/1046 (99%)	837 (81%)	133 (13%)	61 (6%)	2	3
All	All	6142/6276 (98%)	5017 (82%)	859 (14%)	266 (4%)	3	6

5 of 266 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	PRO
1	A	603	SER
1	A	673	GLU
1	A	714	ARG
1	A	740	VAL

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	832/854 (97%)	759 (91%)	73 (9%)	12	28
1	B	841/854 (98%)	762 (91%)	79 (9%)	11	24
1	C	841/854 (98%)	762 (91%)	79 (9%)	11	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	835/854 (98%)	766 (92%)	69 (8%)	14	31
1	E	841/854 (98%)	784 (93%)	57 (7%)	20	43
1	F	844/854 (99%)	771 (91%)	73 (9%)	13	28
All	All	5034/5124 (98%)	4604 (92%)	430 (8%)	13	29

5 of 430 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	486	LEU
1	D	163	GLN
1	F	486	LEU
1	C	595	ARG
1	C	902	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 206 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	616	ASN
1	D	231	ASN
1	F	437	GLN
1	C	708	GLN
1	D	63	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

16 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	LMT	A	1101	-	36,36,36	0.82	1 (2%)	47,47,47	1.75	16 (34%)
2	LMT	A	1102	-	36,36,36	0.67	1 (2%)	47,47,47	1.69	12 (25%)
2	LMT	B	2001	-	36,36,36	0.46	0	47,47,47	1.28	4 (8%)
2	LMT	B	2002	-	36,36,36	0.75	1 (2%)	47,47,47	1.79	11 (23%)
2	LMT	B	2003	-	36,36,36	0.80	1 (2%)	47,47,47	1.62	10 (21%)
2	LMT	B	2004	-	36,36,36	0.47	0	47,47,47	1.06	3 (6%)
2	LMT	C	2001	-	36,36,36	0.72	1 (2%)	47,47,47	1.29	5 (10%)
2	LMT	C	2002	-	36,36,36	0.69	1 (2%)	47,47,47	1.34	6 (12%)
2	LMT	D	2001	-	36,36,36	0.92	2 (5%)	47,47,47	1.47	7 (14%)
2	LMT	D	2002	-	36,36,36	0.64	0	47,47,47	1.35	5 (10%)
2	LMT	D	2003	-	36,36,36	0.77	1 (2%)	47,47,47	1.46	5 (10%)
2	LMT	E	2001	-	36,36,36	0.66	1 (2%)	47,47,47	1.15	3 (6%)
2	LMT	E	2002	-	36,36,36	0.94	1 (2%)	47,47,47	1.48	9 (19%)
2	LMT	E	2003	-	36,36,36	0.73	1 (2%)	47,47,47	1.52	7 (14%)
2	LMT	F	2001	-	36,36,36	0.80	1 (2%)	47,47,47	2.03	14 (29%)
2	LMT	F	2002	-	36,36,36	0.82	1 (2%)	47,47,47	1.40	6 (12%)

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	LMT	A	1101	-	-	0/21/61/61	0/2/2/2
2	LMT	A	1102	-	-	0/21/61/61	0/2/2/2
2	LMT	B	2001	-	-	0/21/61/61	0/2/2/2
2	LMT	B	2002	-	-	0/21/61/61	0/2/2/2
2	LMT	B	2003	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	B	2004	-	-	0/21/61/61	0/2/2/2
2	LMT	C	2001	-	-	0/21/61/61	0/2/2/2
2	LMT	C	2002	-	-	0/21/61/61	0/2/2/2
2	LMT	D	2001	-	-	0/21/61/61	0/2/2/2
2	LMT	D	2002	-	-	0/21/61/61	0/2/2/2
2	LMT	D	2003	-	-	0/21/61/61	0/2/2/2
2	LMT	E	2001	-	-	0/21/61/61	0/2/2/2
2	LMT	E	2002	-	-	0/21/61/61	0/2/2/2
2	LMT	E	2003	-	-	0/21/61/61	0/2/2/2
2	LMT	F	2001	-	-	0/21/61/61	0/2/2/2
2	LMT	F	2002	-	-	0/21/61/61	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	LMT	O1'-C1'	2.06	1.43	1.40
2	D	2001	LMT	O1B-C1B	2.20	1.47	1.41
2	E	2003	LMT	O1'-C1'	2.37	1.44	1.40
2	C	2002	LMT	O1'-C1'	2.48	1.44	1.40
2	A	1102	LMT	O1'-C1'	2.54	1.44	1.40

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2001	LMT	C3'-C4'-C5'	-4.99	99.55	110.84
2	B	2001	LMT	C1B-O1B-C4'	-4.29	106.80	118.01
2	B	2001	LMT	C1-O1'-C1'	-4.09	106.80	113.94
2	A	1101	LMT	C2'-C3'-C4'	-3.96	100.91	109.60
2	F	2001	LMT	O5'-C5'-C4'	-3.78	101.76	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 113 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	LMT	6	0
2	A	1102	LMT	6	0
2	B	2001	LMT	18	0
2	B	2002	LMT	1	0
2	B	2003	LMT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2004	LMT	4	0
2	C	2001	LMT	4	0
2	C	2002	LMT	14	0
2	D	2001	LMT	9	0
2	D	2002	LMT	3	0
2	D	2003	LMT	2	0
2	E	2001	LMT	21	0
2	E	2002	LMT	23	0
2	F	2001	LMT	6	0
2	F	2002	LMT	2	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	1017/1046 (97%)	0.94	150 (14%) 3 2	32, 75, 118, 160	0
1	B	1030/1046 (98%)	0.91	134 (13%) 5 4	29, 69, 112, 139	0
1	C	1030/1046 (98%)	1.08	195 (18%) 2 1	38, 77, 131, 172	0
1	D	1020/1046 (97%)	0.92	154 (15%) 3 2	29, 77, 121, 165	0
1	E	1030/1046 (98%)	0.99	174 (16%) 2 2	37, 83, 126, 159	0
1	F	1033/1046 (98%)	1.11	204 (19%) 1 1	39, 78, 132, 178	0
All	All	6160/6276 (98%)	0.99	1011 (16%) 2 2	29, 76, 125, 178	0

The worst 5 of 1011 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	742	LEU	15.0
1	C	738	LEU	11.9
1	E	599	LEU	10.2
1	B	253	VAL	10.0
1	E	774	GLY	9.7

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, 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(Å ²)	Q<0.9
2	LMT	E	2001	35/35	0.86	0.43	5.16	67,74,100,103	0
2	LMT	E	2002	35/35	0.71	0.38	5.10	67,106,124,132	0
2	LMT	B	2002	35/35	0.65	0.41	5.08	63,106,135,137	0
2	LMT	F	2002	35/35	0.66	0.39	4.27	76,118,147,148	0
2	LMT	B	2001	35/35	0.65	0.37	3.89	75,97,124,139	0
2	LMT	E	2003	35/35	0.66	0.35	3.71	67,94,108,124	0
2	LMT	C	2002	35/35	0.70	0.36	3.63	80,105,146,151	0
2	LMT	D	2001	35/35	0.61	0.55	3.37	47,65,79,89	35
2	LMT	D	2002	35/35	0.73	0.34	3.05	69,111,137,144	0
2	LMT	A	1101	35/35	0.80	0.36	2.88	60,86,132,142	0
2	LMT	A	1102	35/35	0.74	0.38	2.40	64,90,115,120	0
2	LMT	D	2003	35/35	0.75	0.39	2.08	70,98,134,144	0
2	LMT	C	2001	35/35	0.75	0.42	1.81	43,66,94,103	0
2	LMT	B	2004	35/35	0.85	0.33	1.73	62,69,78,84	0
2	LMT	F	2001	35/35	0.70	0.38	1.39	82,104,126,139	0
2	LMT	B	2003	35/35	0.81	0.25	0.19	71,82,104,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.