Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:27 PM GMT

PDB ID	:	4LLN
Title	:	Crystal structure of S. aureus MepR-DNA complex
Authors	:	Birukou, I.; Brennan, R.G.
Deposited on	:	2013-07-09
Resolution	:	2.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

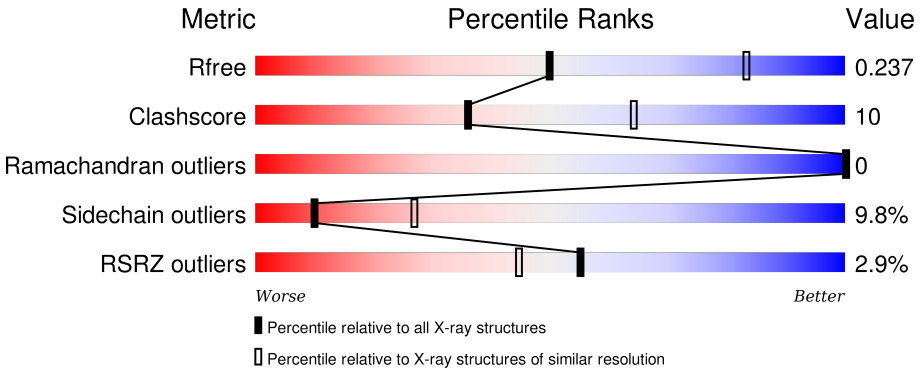
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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 <=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	140	67% 26%
1	B	140	% 74% 22%
1	C	140	3% 77% 16%
1	D	140	5% 81% 17%
1	I	140	4% 77% 18%

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Mol	Chain	Length	Quality of chain
1	J	140	6% 84% 16%
2	E	24	8% 8% 75% 17%
2	F	24	25% 71%
2	G	24	25% 54% 21%
2	H	24	42% 50% 8%
2	K	24	33% 46% 21%
2	L	24	33% 67%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9286 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 MepR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1050	659	178	208	5			
1	B	138	Total	C	N	O	S	0	0	0
			1086	682	190	209	5			
1	C	136	Total	C	N	O	S	0	0	0
			1071	673	185	208	5			
1	D	139	Total	C	N	O	S	0	1	0
			1058	664	180	209	5			
1	I	137	Total	C	N	O	S	0	0	0
			1064	663	186	210	5			
1	J	140	Total	C	N	O	S	0	0	0
			1023	639	180	199	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q5Y812
A	1	ASN	-	EXPRESSION TAG	UNP Q5Y812
B	0	SER	-	EXPRESSION TAG	UNP Q5Y812
B	1	ASN	-	EXPRESSION TAG	UNP Q5Y812
C	0	SER	-	EXPRESSION TAG	UNP Q5Y812
C	1	ASN	-	EXPRESSION TAG	UNP Q5Y812
D	0	SER	-	EXPRESSION TAG	UNP Q5Y812
D	1	ASN	-	EXPRESSION TAG	UNP Q5Y812
I	0	SER	-	EXPRESSION TAG	UNP Q5Y812
I	1	ASN	-	EXPRESSION TAG	UNP Q5Y812
J	0	SER	-	EXPRESSION TAG	UNP Q5Y812
J	1	ASN	-	EXPRESSION TAG	UNP Q5Y812

- Molecule 2 is a DNA chain called Palindromized mepR operator sequence.

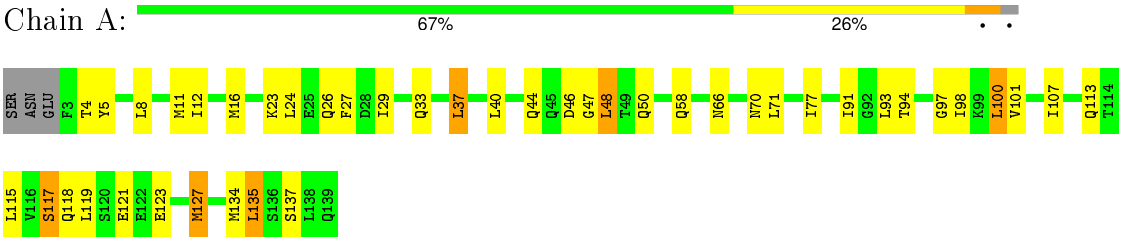
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	24	Total	C	N	O	P	0	0	0
			489	238	86	142	23			
2	H	24	Total	C	N	O	P	0	0	0
			489	238	86	142	23			
2	E	24	Total	C	N	O	P	0	0	0
			489	238	86	142	23			
2	F	24	Total	C	N	O	P	0	0	0
			489	238	86	142	23			
2	K	24	Total	C	N	O	P	0	0	0
			489	238	86	142	23			
2	L	24	Total	C	N	O	P	0	0	0
			489	238	86	142	23			

3 Residue-property plots (i)

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.

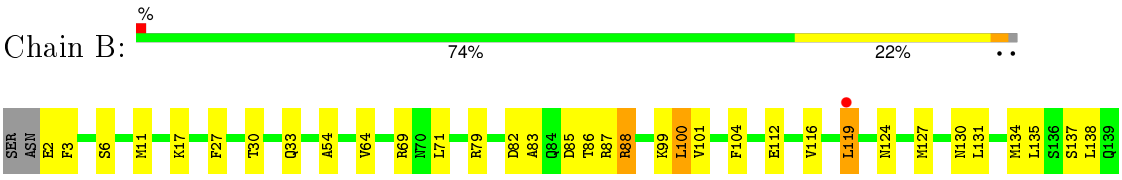
- Molecule 1: MepR

Chain A:



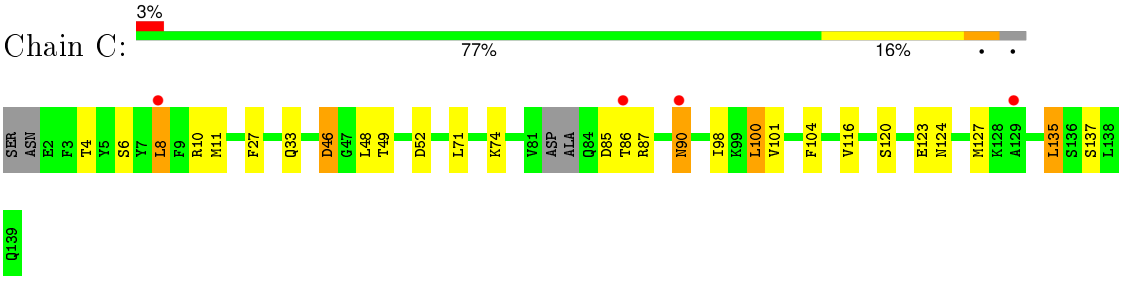
- Molecule 1: MepR

Chain B:



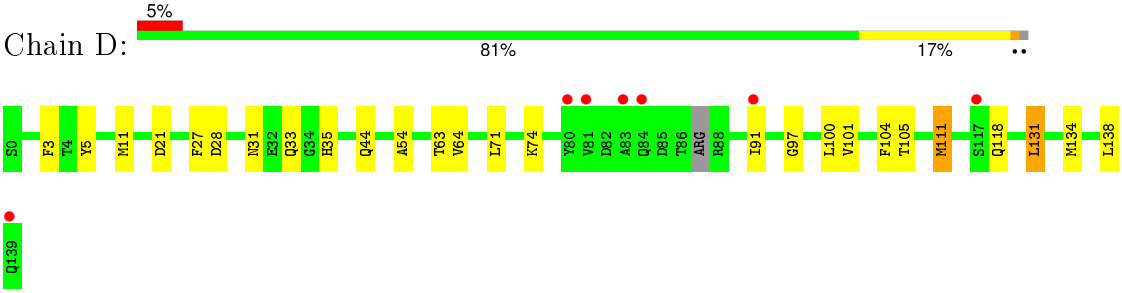
- Molecule 1: MepR

Chain C:



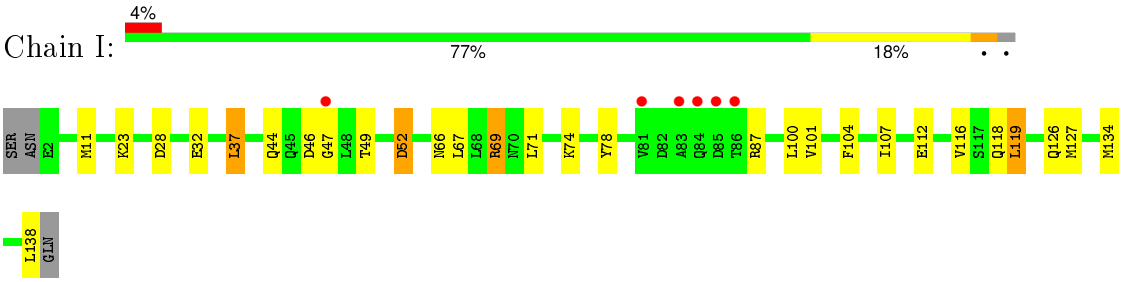
- Molecule 1: MepR

Chain D:



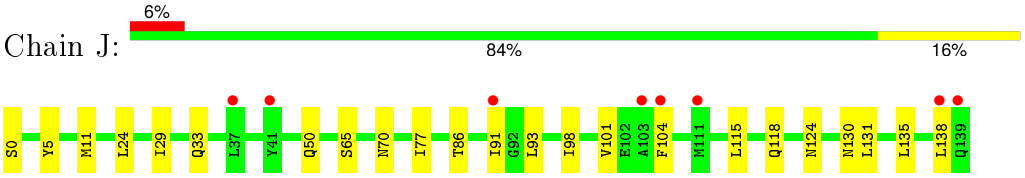
- Molecule 1: MepR

Chain I:



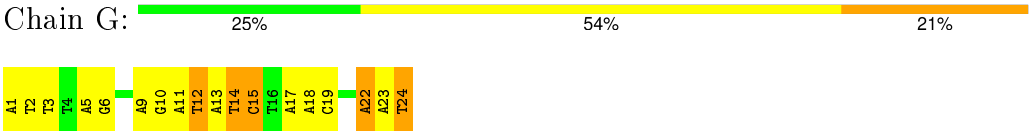
• Molecule 1: MepR

Chain J:



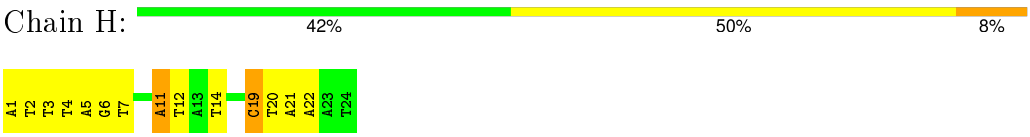
• Molecule 2: Palindromized mepR operator sequence

Chain G:



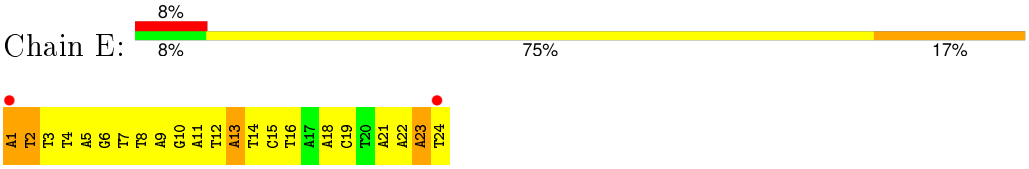
• Molecule 2: Palindromized mepR operator sequence

Chain H:



• Molecule 2: Palindromized mepR operator sequence

Chain E:



• Molecule 2: Palindromized mepR operator sequence

Chain F:

• Molecule 2: Palindromized mepR operator sequence

Chain K:

• Molecule 2: Palindromized mepR operator sequence

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.34Å 76.23Å 109.41Å 90.61° 104.75° 106.27°	Depositor
Resolution (Å)	44.84 – 2.84 44.84 – 2.84	Depositor EDS
% Data completeness (in resolution range)	89.0 (44.84-2.84) 88.0 (44.84-2.84)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.206 , 0.241 0.199 , 0.237	Depositor DCC
R_{free} test set	1996 reflections (4.18%)	DCC
Wilson B-factor (Å^2)	70.9	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 47825 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9286	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.25	0/1064	0.49	0/1442
1	B	0.24	0/1100	0.45	0/1481
1	C	0.24	0/1084	0.43	0/1459
1	D	0.22	0/1075	0.41	0/1454
1	I	0.23	0/1077	0.43	0/1455
1	J	0.22	0/1036	0.38	0/1405
2	E	0.50	0/548	1.31	8/844 (0.9%)
2	F	0.51	0/548	1.14	1/844 (0.1%)
2	G	0.50	0/548	1.22	5/844 (0.6%)
2	H	0.46	0/548	1.10	3/844 (0.4%)
2	K	0.51	0/548	1.27	6/844 (0.7%)
2	L	0.48	0/548	1.13	0/844
All	All	0.34	0/9724	0.80	23/13760 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	15	DC	O4'-C1'-N1	8.38	113.86	108.00
2	K	9	DA	O4'-C1'-N9	8.36	113.85	108.00
2	K	10	DG	O4'-C1'-N9	8.08	113.66	108.00
2	E	23	DA	O4'-C1'-N9	7.45	113.21	108.00
2	K	19	DC	O4'-C1'-N1	7.45	113.21	108.00
2	E	24	DT	O4'-C1'-N1	-6.89	103.18	108.00
2	G	14	DT	O4'-C1'-N1	6.85	112.80	108.00
2	E	13	DA	O4'-C1'-N9	6.68	112.68	108.00
2	H	19	DC	O4'-C1'-N1	6.62	112.63	108.00
2	K	23	DA	O4'-C1'-N9	6.54	112.58	108.00
2	G	22	DA	O4'-C1'-N9	6.35	112.45	108.00
2	G	12	DT	O4'-C1'-N1	6.15	112.31	108.00
2	K	22	DA	O4'-C1'-N9	6.12	112.28	108.00
2	E	24	DT	C5-C4-O4	-6.07	120.65	124.90
2	G	24	DT	O4'-C1'-N1	5.57	111.90	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	24	DT	N3-C4-O4	5.48	123.19	119.90
2	F	17	DA	O4'-C1'-N9	-5.37	104.24	108.00
2	H	11	DA	O4'-C1'-N9	5.29	111.71	108.00
2	E	2	DT	O4'-C1'-N1	5.27	111.69	108.00
2	E	24	DT	P-O5'-C5'	5.17	129.17	120.90
2	K	14	DT	O4'-C1'-N1	5.11	111.58	108.00
2	H	14	DT	O4'-C1'-N1	5.06	111.54	108.00
2	E	1	DA	C3'-C2'-C1'	-5.03	96.47	102.50

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	1050	0	984	26	0
1	B	1086	0	1059	24	0
1	C	1071	0	1039	14	0
1	D	1058	0	980	13	0
1	I	1064	0	1018	14	0
1	J	1023	0	921	12	0
2	E	489	0	276	18	0
2	F	489	0	276	11	0
2	G	489	0	276	17	0
2	H	489	0	276	8	0
2	K	489	0	276	23	0
2	L	489	0	276	10	0
All	All	9286	0	7657	162	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 10.

All (162) 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)
2:L:5:DA:H2"	2:L:6:DG:H5"	1.53	0.90
2:H:3:DT:H2"	2:H:4:DT:H5"	1.56	0.86
2:G:23:DA:H2"	2:G:24:DT:H5'	1.60	0.83
2:K:22:DA:H2"	2:K:23:DA:H5"	1.64	0.79
2:E:2:DT:H1'	2:E:3:DT:H5'	1.62	0.79
2:E:13:DA:H2"	2:E:14:DT:H5"	1.66	0.77
2:K:1:DA:H2"	2:K:2:DT:H5"	1.66	0.75
2:K:19:DC:H2"	2:K:20:DT:H5'	1.69	0.72
1:B:119:LEU:O	1:B:124:ASN:ND2	2.25	0.69
2:H:19:DC:H2"	2:H:20:DT:H5'	1.76	0.68
2:G:1:DA:H2"	2:G:2:DT:H5"	1.77	0.67
2:H:11:DA:H2"	2:H:12:DT:H5'	1.76	0.67
1:I:37:LEU:HD21	1:I:71:LEU:HD21	1.78	0.66
2:F:5:DA:H2"	2:F:6:DG:H5"	1.79	0.65
2:E:13:DA:C2'	2:E:14:DT:H5"	2.28	0.63
1:I:119:LEU:HD21	1:J:130:ASN:HB3	1.81	0.63
2:E:18:DA:H1'	2:E:19:DC:H5'	1.81	0.61
1:A:12:ILE:HG12	1:B:135:LEU:HB2	1.82	0.60
1:C:135:LEU:HD21	1:D:11:MET:HB3	1.84	0.60
1:B:27:PHE:HB3	1:B:100:LEU:HD21	1.83	0.59
1:A:119:LEU:HD21	1:B:130:ASN:HB3	1.84	0.59
1:C:87:ARG:NH1	2:E:4:DT:O2	2.35	0.59
2:K:10:DG:H2"	2:K:11:DA:O5'	2.03	0.59
1:A:8:LEU:HB3	1:B:131:LEU:HD23	1.84	0.58
2:G:10:DG:H1'	2:G:11:DA:H5'	1.85	0.58
2:G:12:DT:H2"	2:G:13:DA:H8	1.68	0.58
1:B:86:THR:OG1	2:G:23:DA:OP1	2.13	0.57
2:E:23:DA:H5"	2:E:23:DA:H8	1.69	0.57
1:B:30:THR:OG1	2:G:13:DA:OP1	2.19	0.57
2:F:19:DC:H2"	2:F:20:DT:H5'	1.85	0.57
2:L:4:DT:H4'	2:L:5:DA:OP1	2.04	0.57
1:J:70:ASN:ND2	2:K:13:DA:OP2	2.37	0.56
2:K:1:DA:C2'	2:K:2:DT:H5"	2.35	0.56
2:K:22:DA:H2"	2:K:23:DA:H8	1.70	0.56
1:D:101:VAL:HA	1:D:104:PHE:CE2	2.40	0.56
1:D:33:GLN:HB3	1:D:71:LEU:HD21	1.89	0.55
2:E:1:DA:H4'	2:E:2:DT:OP1	2.07	0.55
1:A:50:GLN:HG2	1:A:91:ILE:HD11	1.87	0.55
2:K:7:DT:H1'	2:K:8:DT:H5'	1.88	0.55
1:A:115:LEU:HD21	1:B:138:LEU:HD21	1.89	0.54
2:F:21:DA:H1'	2:F:22:DA:H5'	1.89	0.54
1:J:50:GLN:HG2	1:J:91:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LYS:HD2	1:A:107:ILE:HG23	1.90	0.53
2:E:3:DT:H1'	2:E:4:DT:H5'	1.91	0.52
1:A:94:THR:O	1:A:98:ILE:HG13	2.09	0.52
2:F:1:DA:H2"	2:F:2:DT:H6	1.75	0.52
2:L:20:DT:H1'	2:L:21:DA:H5'	1.91	0.52
2:E:21:DA:H1'	2:E:22:DA:H5'	1.90	0.52
1:I:28:ASP:OD2	1:I:74:LYS:NZ	2.43	0.52
2:K:5:DA:H2"	2:K:6:DG:H5"	1.92	0.51
2:K:19:DC:H2"	2:K:20:DT:C5'	2.38	0.51
1:I:49:THR:OG1	1:I:52:ASP:OD1	2.24	0.51
1:D:28:ASP:O	1:D:74:LYS:NZ	2.40	0.51
1:A:113:GLN:O	1:A:117:SER:OG	2.28	0.51
2:G:12:DT:H2"	2:G:13:DA:H5'	1.91	0.51
2:G:5:DA:H1'	2:G:6:DG:H5'	1.91	0.51
2:G:23:DA:H2"	2:G:24:DT:C5'	2.38	0.51
2:L:15:DC:H2"	2:L:16:DT:H5'	1.93	0.51
1:B:134:MET:O	1:B:137:SER:OG	2.18	0.50
1:A:134:MET:O	1:A:137:SER:OG	2.19	0.50
1:C:8:LEU:HD23	1:D:131:LEU:HD23	1.93	0.50
1:C:101:VAL:HA	1:C:104:PHE:CE2	2.47	0.50
1:J:33:GLN:HG3	2:K:13:DA:OP1	2.11	0.50
2:E:10:DG:H2"	2:E:11:DA:O5'	2.10	0.50
1:I:66:ASN:O	1:I:69:ARG:HG3	2.12	0.50
2:K:8:DT:H2"	2:K:9:DA:O5'	2.12	0.50
1:C:120:SER:HB3	1:C:123:GLU:HB2	1.94	0.49
2:H:6:DG:H2"	2:H:7:DT:H5'	1.94	0.49
2:E:5:DA:H2"	2:E:6:DG:O5'	2.12	0.49
1:A:33:GLN:HB3	1:A:71:LEU:HD21	1.92	0.49
1:C:46:ASP:OD1	1:C:46:ASP:N	2.44	0.49
2:G:18:DA:H1'	2:G:19:DC:H5'	1.93	0.49
1:J:24:LEU:HD22	1:J:29:ILE:HD11	1.95	0.49
1:I:101:VAL:HA	1:I:104:PHE:CE2	2.48	0.49
2:K:9:DA:H2"	2:K:10:DG:C5'	2.43	0.48
2:F:7:DT:H5'	2:F:7:DT:H6	1.78	0.48
1:B:112:GLU:O	1:B:116:VAL:HG23	2.13	0.48
1:I:46:ASP:HB3	1:I:47:GLY:C	2.33	0.48
1:C:6:SER:O	1:C:10:ARG:HB2	2.14	0.48
1:C:85:ASP:OD1	1:C:86:THR:N	2.44	0.48
2:F:17:DA:H1'	2:F:18:DA:H5'	1.94	0.48
2:F:23:DA:H2'	2:F:24:DT:C6	2.48	0.48
2:E:12:DT:H2"	2:E:13:DA:O5'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:19:DC:H2"	2:L:20:DT:O5'	2.13	0.48
2:F:15:DC:H2"	2:F:16:DT:H5'	1.96	0.47
2:E:6:DG:H2"	2:E:7:DT:H5'	1.96	0.47
1:A:37:LEU:HB3	1:A:101:VAL:HG22	1.97	0.47
1:I:23:LYS:HD2	1:I:107:ILE:HG23	1.95	0.47
1:D:63:THR:HG21	2:E:14:DT:H5'	1.95	0.47
1:B:33:GLN:HG3	2:G:13:DA:OP1	2.14	0.47
2:G:17:DA:H1'	2:G:18:DA:H5'	1.97	0.47
1:D:111:MET:SD	1:D:111:MET:N	2.88	0.47
1:D:54:ALA:HA	1:D:64:VAL:HG21	1.97	0.47
1:A:135:LEU:HD11	1:B:11:MET:HB3	1.96	0.47
1:D:31:ASN:OD1	1:D:35[B]:HIS:NE2	2.47	0.47
1:I:46:ASP:N	1:I:47:GLY:HA2	2.30	0.46
1:A:123:GLU:O	1:A:127:MET:HB2	2.16	0.46
1:B:33:GLN:HB3	1:B:71:LEU:HD21	1.98	0.46
2:K:22:DA:H2"	2:K:23:DA:C8	2.51	0.46
1:A:8:LEU:O	1:A:12:ILE:HG13	2.15	0.46
1:A:16:MET:HE1	1:B:6:SER:HA	1.97	0.45
2:K:22:DA:C2'	2:K:23:DA:H5"	2.42	0.45
2:G:22:DA:H4'	2:G:23:DA:OP1	2.16	0.45
2:H:1:DA:H1'	2:H:2:DT:H5'	1.98	0.45
1:A:58:GLN:HG3	1:B:11:MET:SD	2.56	0.45
2:F:8:DT:H1'	2:F:9:DA:H5'	1.97	0.45
1:B:100:LEU:HD22	1:B:104:PHE:HD2	1.82	0.45
1:C:116:VAL:HG12	1:D:5:TYR:HE2	1.82	0.45
1:D:27:PHE:HB3	1:D:100:LEU:HD11	1.98	0.45
1:J:77:ILE:HG12	1:J:93:LEU:HD23	1.99	0.45
2:F:17:DA:H2"	2:F:18:DA:O5'	2.17	0.45
2:E:8:DT:H1'	2:E:9:DA:H5'	1.98	0.44
1:B:101:VAL:HA	1:B:104:PHE:CE2	2.52	0.44
2:K:6:DG:H1'	2:K:7:DT:H5'	2.00	0.44
1:A:77:ILE:HG22	1:A:93:LEU:HD23	2.00	0.44
1:A:97:GLY:O	1:A:101:VAL:HG23	2.18	0.44
2:K:11:DA:H2"	2:K:12:DT:H5'	1.99	0.43
1:J:86:THR:HB	2:K:22:DA:H4'	2.00	0.43
1:A:40:LEU:O	1:A:44:GLN:HB2	2.18	0.43
2:K:9:DA:H2'	2:K:10:DG:C8	2.54	0.43
1:I:116:VAL:HG12	1:J:5:TYR:HE2	1.82	0.43
1:C:49:THR:H	1:C:52:ASP:HB2	1.82	0.43
2:K:9:DA:H2"	2:K:10:DG:O5'	2.18	0.43
1:A:24:LEU:HD22	1:A:29:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD22	1:B:134:MET:HE2	2.01	0.43
1:J:65:SER:OG	2:L:7:DT:OP2	2.31	0.43
2:G:2:DT:C6	2:G:3:DT:H72	2.54	0.43
2:L:1:DA:H1'	2:L:2:DT:H5'	2.01	0.42
1:I:49:THR:HB	2:K:6:DG:OP1	2.20	0.42
1:D:101:VAL:O	1:D:105:THR:OG1	2.31	0.42
1:A:37:LEU:HD12	1:A:37:LEU:HA	1.92	0.42
1:B:54:ALA:HA	1:B:64:VAL:HG21	2.01	0.42
2:G:9:DA:H1'	2:G:10:DG:H5'	2.01	0.42
2:E:15:DC:H2"	2:E:16:DT:H5'	2.01	0.42
1:B:82:ASP:OD1	1:B:83:ALA:N	2.53	0.42
1:A:46:ASP:N	1:A:47:GLY:HA2	2.34	0.42
1:J:101:VAL:HA	1:J:104:PHE:CE2	2.54	0.42
2:E:15:DC:H2'	2:E:16:DT:C6	2.54	0.42
1:A:48:LEU:HG	1:A:48:LEU:H	1.49	0.42
1:C:27:PHE:HB3	1:C:100:LEU:HD21	2.02	0.42
2:L:23:DA:H2"	2:L:24:DT:H5'	2.01	0.42
1:A:66:ASN:O	1:A:70:ASN:ND2	2.48	0.42
1:B:88:ARG:HB2	2:H:5:DA:H4'	2.02	0.41
2:L:17:DA:H1'	2:L:18:DA:H5'	2.01	0.41
1:I:32:GLU:H	1:I:32:GLU:CD	2.23	0.41
2:K:9:DA:C8	2:K:9:DA:H5"	2.55	0.41
1:C:100:LEU:HA	1:C:100:LEU:HD23	1.86	0.41
1:C:90:ASN:N	1:C:90:ASN:OD1	2.52	0.41
1:B:85:ASP:OD1	1:B:87:ARG:HG2	2.21	0.41
2:H:21:DA:H1'	2:H:22:DA:H5'	2.02	0.41
1:J:131:LEU:HD12	1:J:131:LEU:HA	1.89	0.41
1:A:27:PHE:HB3	1:A:100:LEU:HD21	2.03	0.41
1:C:33:GLN:HG2	1:C:71:LEU:HD21	2.02	0.41
2:G:22:DA:H1'	2:G:23:DA:C8	2.56	0.41
1:D:97:GLY:O	1:D:101:VAL:HG23	2.21	0.41
1:B:69:ARG:NH2	2:H:7:DT:H3'	2.36	0.41
2:E:5:DA:H2'	2:E:6:DG:C8	2.55	0.41
1:I:87:ARG:HD3	2:L:22:DA:N3	2.36	0.41
1:B:99:LYS:NZ	2:F:11:DA:OP1	2.41	0.40
2:K:9:DA:H2"	2:K:10:DG:H5'	2.03	0.40
1:I:134:MET:HB3	1:J:115:LEU:HD11	2.04	0.40
2:G:14:DT:H2"	2:G:15:DC:O5'	2.22	0.40

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	135/140 (96%)	131 (97%)	4 (3%)	0	100	100
1	B	136/140 (97%)	134 (98%)	2 (2%)	0	100	100
1	C	132/140 (94%)	131 (99%)	1 (1%)	0	100	100
1	D	136/140 (97%)	134 (98%)	2 (2%)	0	100	100
1	I	135/140 (96%)	133 (98%)	2 (2%)	0	100	100
1	J	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
All	All	812/840 (97%)	796 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	107/127 (84%)	95 (89%)	12 (11%)	7	21
1	B	114/127 (90%)	106 (93%)	8 (7%)	19	45
1	C	113/127 (89%)	100 (88%)	13 (12%)	7	19
1	D	106/127 (84%)	97 (92%)	9 (8%)	13	35
1	I	111/127 (87%)	97 (87%)	14 (13%)	5	15
1	J	95/127 (75%)	88 (93%)	7 (7%)	17	42
All	All	646/762 (85%)	583 (90%)	63 (10%)	10	27

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	TYR
1	A	11	MET
1	A	26	GLN
1	A	37	LEU
1	A	48	LEU
1	A	100	LEU
1	A	117	SER
1	A	118	GLN
1	A	121	GLU
1	A	127	MET
1	A	135	LEU
1	B	2	GLU
1	B	3	PHE
1	B	17	LYS
1	B	79	ARG
1	B	88	ARG
1	B	100	LEU
1	B	119	LEU
1	B	127	MET
1	C	4	THR
1	C	8	LEU
1	C	11	MET
1	C	46	ASP
1	C	48	LEU
1	C	74	LYS
1	C	90	ASN
1	C	98	ILE
1	C	100	LEU
1	C	124	ASN
1	C	127	MET
1	C	135	LEU
1	C	137	SER
1	D	3	PHE
1	D	21	ASP
1	D	44	GLN
1	D	91	ILE
1	D	111	MET
1	D	118	GLN
1	D	131	LEU
1	D	134	MET
1	D	138	LEU

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Mol	Chain	Res	Type
1	I	11	MET
1	I	37	LEU
1	I	44	GLN
1	I	52	ASP
1	I	67	LEU
1	I	69	ARG
1	I	78	TYR
1	I	100	LEU
1	I	112	GLU
1	I	118	GLN
1	I	119	LEU
1	I	126	GLN
1	I	127	MET
1	I	138	LEU
1	J	0	SER
1	J	11	MET
1	J	98	ILE
1	J	118	GLN
1	J	124	ASN
1	J	135	LEU
1	J	138	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	50	GLN
1	B	18	GLN
1	C	50	GLN
1	I	118	GLN
1	J	118	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	137/140 (97%)	0.06	0 100 100	37, 61, 92, 103	2 (1%)
1	B	138/140 (98%)	0.11	1 (0%) 89 85	38, 61, 91, 109	2 (1%)
1	C	136/140 (97%)	0.20	4 (2%) 55 45	34, 70, 112, 136	2 (1%)
1	D	139/140 (99%)	0.38	7 (5%) 32 23	46, 87, 120, 143	2 (1%)
1	I	137/140 (97%)	0.23	6 (4%) 38 28	37, 68, 111, 134	2 (1%)
1	J	140/140 (100%)	0.12	8 (5%) 27 18	54, 86, 116, 126	2 (1%)
2	E	24/24 (100%)	-0.07	2 (8%) 14 7	56, 80, 117, 128	0
2	F	24/24 (100%)	-0.25	0 100 100	49, 85, 118, 129	0
2	G	24/24 (100%)	-0.51	0 100 100	55, 70, 85, 89	0
2	H	24/24 (100%)	-0.48	0 100 100	53, 70, 85, 91	0
2	K	24/24 (100%)	-0.76	0 100 100	59, 82, 95, 99	0
2	L	24/24 (100%)	-0.47	0 100 100	57, 85, 107, 112	0
All	All	971/984 (98%)	0.09	28 (2%) 55 45	34, 73, 114, 143	12 (1%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	81	VAL	4.8
1	C	86	THR	4.6
1	J	104	PHE	4.5
1	J	91	ILE	3.6
1	D	84	GLN	3.4
1	I	86	THR	3.2
2	E	1	DA	3.1
1	D	91	ILE	3.1
1	D	117	SER	3.0
1	J	41	TYR	2.9
1	D	139	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	80	TYR	2.8
1	I	83	ALA	2.6
1	D	83	ALA	2.6
2	E	24	DT	2.6
1	J	103	ALA	2.5
1	C	129	ALA	2.4
1	J	111	MET	2.4
1	C	8	LEU	2.3
1	I	85	ASP	2.2
1	B	119	LEU	2.2
1	J	139	GLN	2.1
1	I	81	VAL	2.1
1	J	138	LEU	2.1
1	I	47	GLY	2.1
1	C	90	ASN	2.0
1	I	84	GLN	2.0
1	J	37	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.