Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 12:37 AM EDT

PDB ID	:	5K58
Title	:	Structure of the K. pneumonia SlmA-DNA complex bound to the C-terminal of the cell division protein FtsZ
Authors	:	Schumacher, M.
Deposited on	:	2016-05-23
Resolution	:	2.77 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

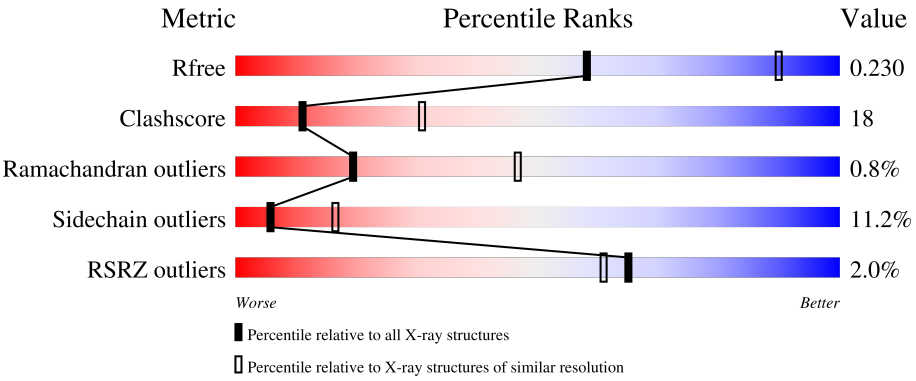
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 of 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 <=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	190	2% 55% 41% ·
1	B	190	2% 54% 39% 6% ·
1	E	190	3% 62% 36% ·
1	F	190	% 59% 36% · ·
2	R	12	17% 83%

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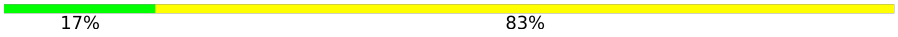
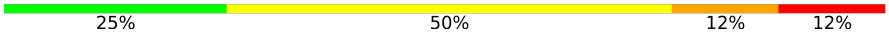
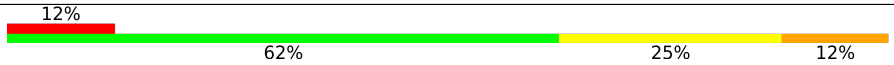
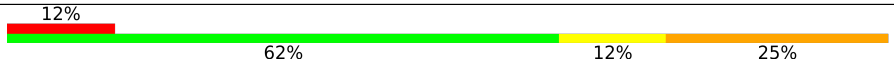
Mol	Chain	Length	Quality of chain
2	T	12	
3	K	8	
3	L	8	
3	M	8	
3	N	8	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6973 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 Nucleoid occlusion factor SlmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	190	Total	C	N	O	S	0	0	0
			1543	969	281	286	7			
1	F	189	Total	C	N	O	S	0	0	0
			1532	963	277	285	7			
1	A	190	Total	C	N	O	S	0	0	0
			1543	969	281	286	7			
1	B	189	Total	C	N	O	S	0	0	0
			1532	963	277	285	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	140	MET	LEU	engineered mutation	UNP A7ZTJ2
F	140	MET	LEU	engineered mutation	UNP A7ZTJ2
A	140	MET	LEU	engineered mutation	UNP A7ZTJ2
B	140	MET	LEU	engineered mutation	UNP A7ZTJ2

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	12	Total	C	N	O	P	0	0	0
			243	117	45	70	11			
2	T	12	Total	C	N	O	P	0	0	0
			243	117	45	70	11			

- Molecule 3 is a protein called Octapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	L	8	Total	C	N	O	0	0	0
			67	45	11	11			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	K	8	Total C N O 67 45 11 11	0	0	0
3	N	8	Total C N O 67 45 11 11	0	0	0
3	M	8	Total C N O 67 45 11 11	0	0	0

- Molecule 4 is water.

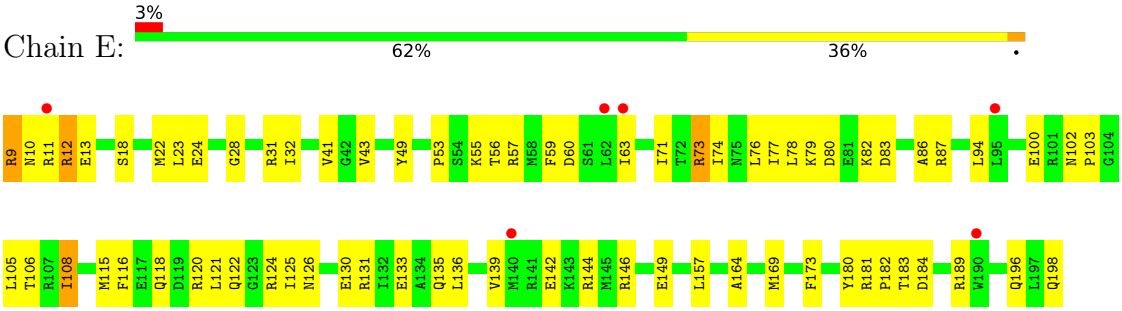
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	11	Total O 11 11	0	0
4	F	20	Total O 20 20	0	0
4	A	16	Total O 16 16	0	0
4	B	13	Total O 13 13	0	0
4	R	3	Total O 3 3	0	0
4	T	3	Total O 3 3	0	0
4	M	3	Total O 3 3	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

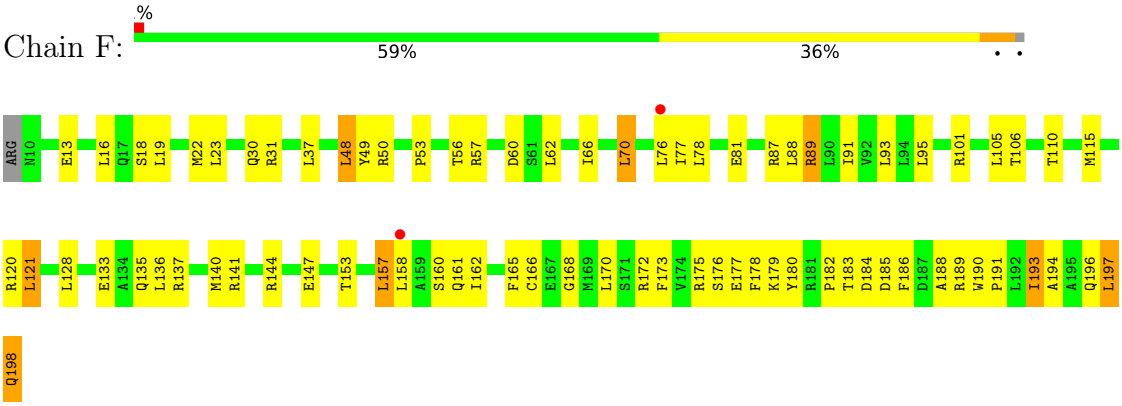
• Molecule 1: Nucleoid occlusion factor SlmA

Chain E:



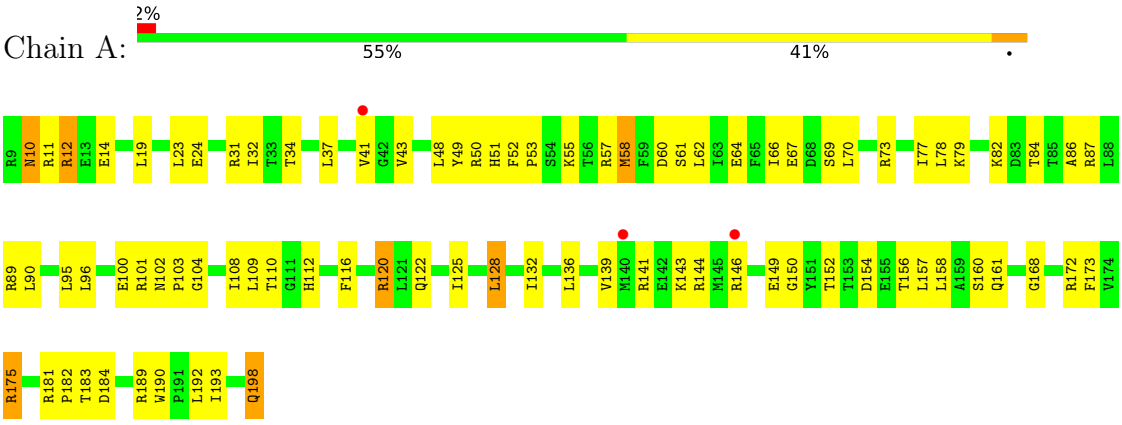
• Molecule 1: Nucleoid occlusion factor SlmA

Chain F:



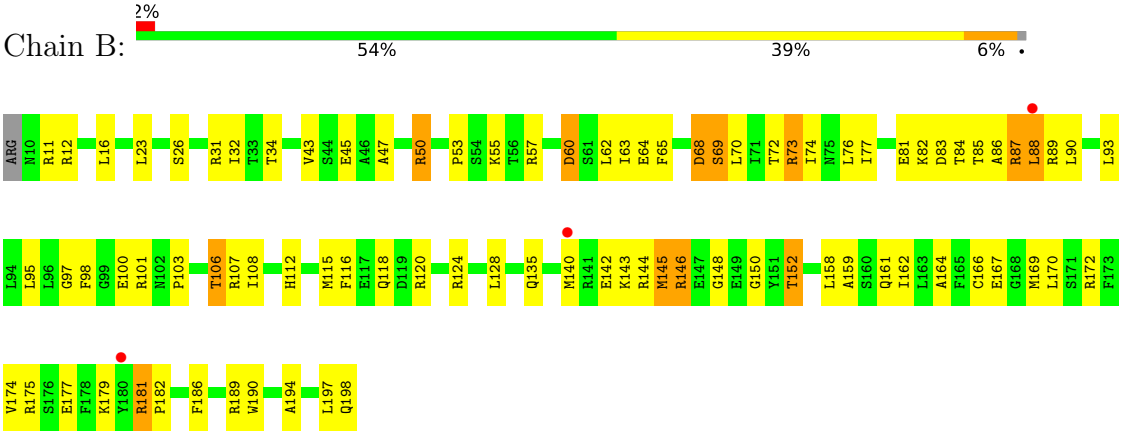
• Molecule 1: Nucleoid occlusion factor SlmA

Chain A:



• Molecule 1: Nucleoid occlusion factor SlmA

Chain B:



• Molecule 2: DNA (5'-D(*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*C)-3')

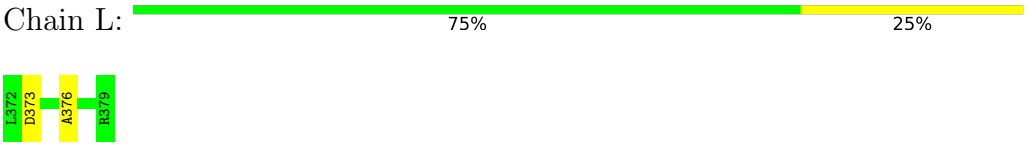
Chain R:

• Molecule 2: DNA (5'-D(*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*C)-3')

Chain T:

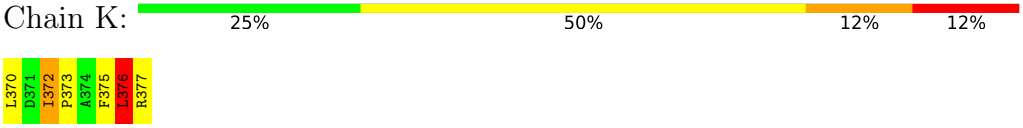
• Molecule 3: Octapeptide

Chain L:



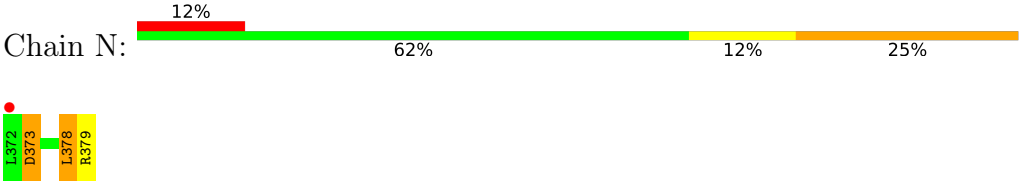
• Molecule 3: Octapeptide

Chain K:



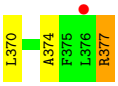
• Molecule 3: Octapeptide

Chain N:



• Molecule 3: Octapeptide

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	84.80Å 84.80Å 161.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.44 – 2.77 43.44 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.44-2.77) 98.1 (43.44-2.77)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.247 , 0.268 0.217 , 0.230	Depositor DCC
R_{free} test set	2004 reflections (6.19%)	wwPDB-VP
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 31.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.315 for -h,-k,l 0.326 for h,-h-k,-l 0.296 for -k,-h,-l	Xtriage
Reported twinning fraction	0.360 for -h,-k,l	Depositor
Outliers	0 of 32384 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6973	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.28	0/1563	0.49	0/2097
1	B	0.30	0/1552	0.52	0/2083
1	E	0.28	0/1563	0.52	0/2097
1	F	0.31	0/1552	0.56	1/2083 (0.0%)
2	R	0.63	0/272	0.99	0/418
2	T	0.59	0/272	0.98	0/418
3	K	0.33	0/68	0.59	0/90
3	L	0.26	0/68	0.40	0/90
3	M	0.41	0/68	0.70	0/90
3	N	0.31	0/68	0.59	0/90
All	All	0.33	0/7046	0.58	1/9556 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	50	ARG	NE-CZ-NH1	5.16	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1543	0	1577	59	0
1	B	1532	0	1564	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1543	0	1577	48	0
1	F	1532	0	1564	61	0
2	R	243	0	137	13	0
2	T	243	0	137	14	0
3	K	67	0	70	6	0
3	L	67	0	70	2	0
3	M	67	0	70	3	0
3	N	67	0	70	2	0
4	A	16	0	0	4	0
4	B	13	0	0	5	0
4	E	11	0	0	5	0
4	F	20	0	0	8	0
4	M	3	0	0	2	0
4	R	3	0	0	5	0
4	T	3	0	0	2	0
All	All	6973	0	6836	247	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 18.

All (247) 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:F:162:ILE:HD12	1:F:193:ILE:HD11	1.47	0.94
1:B:93:LEU:HD11	1:B:186:PHE:CZ	2.11	0.85
1:A:10:ASN:OD1	4:A:201:HOH:O	1.93	0.85
1:F:22:MET:SD	4:F:220:HOH:O	2.33	0.85
1:F:140:MET:SD	1:F:158:LEU:HB3	2.20	0.81
1:B:169:MET:SD	4:B:213:HOH:O	2.39	0.81
1:B:172:ARG:HG2	1:B:175:ARG:HH21	1.46	0.81
1:F:137:ARG:HB3	1:F:141:ARG:HH12	1.47	0.80
1:F:144:ARG:NH1	4:F:202:HOH:O	2.06	0.80
1:B:140:MET:CE	1:B:159:ALA:HA	2.11	0.80
1:F:176:SER:OG	4:F:201:HOH:O	2.00	0.79
1:E:28:GLY:O	4:E:201:HOH:O	2.01	0.78
1:A:78:LEU:HA	1:A:87:ARG:HD2	1.66	0.78
1:A:96:LEU:HB3	1:A:183:THR:HG22	1.68	0.76
1:A:181:ARG:HB2	1:A:184:ASP:HB2	1.66	0.75
1:F:141:ARG:NH2	4:F:205:HOH:O	2.17	0.75
1:B:107:ARG:NH2	1:B:177:GLU:OE1	2.20	0.75
1:B:63:ILE:HG21	1:B:124:ARG:HG2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:ILE:HD11	1:E:125:ILE:HD11	1.71	0.70
1:F:147:GLU:OE1	4:F:203:HOH:O	2.09	0.70
1:F:56:THR:HG23	1:F:121:LEU:HD11	1.72	0.69
1:B:166:CYS:O	4:B:201:HOH:O	2.10	0.69
1:F:165:PHE:O	4:F:204:HOH:O	2.10	0.69
1:A:12:ARG:HG3	1:A:51:HIS:HB3	1.74	0.68
1:A:144:ARG:HH11	1:A:150:GLY:N	1.93	0.66
1:A:110:THR:OG1	4:A:202:HOH:O	2.13	0.66
1:E:115:MET:HE1	4:F:211:HOH:O	1.96	0.65
1:F:140:MET:CE	1:F:158:LEU:HG	2.27	0.65
2:T:12:DA:OP1	4:T:101:HOH:O	2.15	0.65
1:E:12:ARG:NH2	4:E:202:HOH:O	2.14	0.64
1:B:53:PRO:HD2	1:B:57:ARG:HG3	1.79	0.64
1:B:115:MET:N	4:B:203:HOH:O	2.30	0.64
2:R:9:DC:N4	4:R:102:HOH:O	2.30	0.64
1:F:37:LEU:HG	1:F:48:LEU:HD21	1.80	0.64
1:F:178:PHE:N	4:F:201:HOH:O	2.32	0.63
1:F:60:ASP:OD2	1:F:120:ARG:NH2	2.26	0.63
1:B:82:LYS:O	1:B:146:ARG:NH1	2.32	0.62
1:A:32:ILE:O	1:A:55:LYS:HE2	2.00	0.62
1:F:140:MET:HE1	1:F:158:LEU:HG	1.82	0.62
1:A:67:GLU:HA	1:A:128:LEU:HD12	1.82	0.62
1:F:53:PRO:HD2	1:F:57:ARG:HG3	1.82	0.61
1:A:84:THR:HG23	1:A:139:VAL:HG12	1.83	0.60
1:B:118:GLN:HB3	1:B:120:ARG:HG2	1.83	0.60
1:F:31:ARG:HH21	2:R:12:DA:H5"	1.66	0.59
1:A:84:THR:HB	1:A:143:LYS:HD3	1.84	0.59
1:B:144:ARG:HG2	1:B:150:GLY:HA2	1.84	0.59
1:B:100:GLU:HB2	1:B:182:PRO:HD2	1.84	0.59
4:R:101:HOH:O	2:T:11:DC:N3	2.31	0.58
1:E:74:ILE:HG21	1:E:135:GLN:HG3	1.85	0.58
1:E:133:GLU:OE1	1:F:172:ARG:NH2	2.37	0.58
1:B:140:MET:HE1	1:B:159:ALA:HA	1.86	0.58
1:E:131:ARG:O	1:E:135:GLN:HG2	2.04	0.58
2:R:3:DT:H2"	2:R:4:DG:C8	2.39	0.57
1:E:102:ASN:HB3	1:E:105:LEU:HD13	1.85	0.57
1:A:31:ARG:HH22	1:B:31:ARG:HH11	1.50	0.57
1:A:101:ARG:HG3	3:L:376:ALA:HB2	1.84	0.57
1:E:24:GLU:HG3	1:E:103:PRO:HB2	1.86	0.57
1:B:186:PHE:CZ	1:B:190:TRP:HB2	2.39	0.57
1:A:175:ARG:NH2	1:B:167:GLU:OE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:GLU:HB2	1:B:124:ARG:HH21	1.70	0.57
1:E:53:PRO:HG2	1:E:57:ARG:HG3	1.87	0.57
1:F:91:ILE:HG21	1:F:136:LEU:HD11	1.86	0.57
1:F:137:ARG:HB3	1:F:141:ARG:NH1	2.17	0.57
1:A:172:ARG:HD3	1:A:175:ARG:NH2	2.20	0.57
1:B:158:LEU:O	1:B:162:ILE:HG12	2.05	0.56
1:A:10:ASN:OD1	1:A:10:ASN:N	2.24	0.56
1:B:142:GLU:HB3	1:B:146:ARG:HD2	1.86	0.56
1:A:86:ALA:O	1:A:90:LEU:HG	2.05	0.56
1:F:193:ILE:HG12	1:F:196:GLN:NE2	2.21	0.56
1:A:58:MET:O	1:A:61:SER:OG	2.22	0.56
1:F:140:MET:SD	1:F:158:LEU:HD23	2.46	0.55
1:F:77:ILE:O	1:F:81:GLU:N	2.35	0.55
1:A:66:ILE:HG22	1:A:128:LEU:HD11	1.86	0.55
1:B:158:LEU:HD21	1:B:197:LEU:HD23	1.87	0.55
1:E:31:ARG:HG3	1:E:116:PHE:HB3	1.89	0.55
1:F:101:ARG:HG3	3:M:374:ALA:HB2	1.89	0.55
1:B:81:GLU:O	1:B:87:ARG:NH1	2.37	0.54
1:B:140:MET:HE3	1:B:159:ALA:HA	1.89	0.54
2:T:4:DG:H1'	2:T:5:DA:H5'	1.89	0.54
1:F:133:GLU:O	1:F:137:ARG:HG3	2.07	0.54
1:E:73:ARG:O	1:E:77:ILE:HG13	2.07	0.53
1:F:140:MET:CE	1:F:158:LEU:CG	2.86	0.53
1:F:191:PRO:HA	1:F:194:ALA:HB3	1.90	0.53
1:B:45:GLU:OE2	2:T:13:DC:N4	2.30	0.53
1:B:88:LEU:HD21	1:B:197:LEU:HD11	1.90	0.53
1:E:73:ARG:HG2	1:E:94:LEU:HD11	1.91	0.53
1:B:144:ARG:O	1:B:148:GLY:N	2.39	0.53
1:E:73:ARG:NH2	3:N:373:ASP:OD2	2.42	0.53
1:A:100:GLU:HA	1:A:173:PHE:CE2	2.44	0.53
1:B:26:SER:HA	1:B:177:GLU:OE2	2.10	0.52
1:A:37:LEU:O	1:A:41:VAL:HG23	2.09	0.52
1:B:170:LEU:O	1:B:174:VAL:HG23	2.10	0.52
1:E:118:GLN:HB3	1:E:120:ARG:HG2	1.90	0.52
1:E:41:VAL:HB	1:E:43:VAL:HG22	1.92	0.51
1:B:194:ALA:HA	1:B:197:LEU:HG	1.93	0.51
1:A:19:LEU:O	1:A:23:LEU:HB2	2.11	0.51
1:A:102:ASN:HD21	3:L:376:ALA:HA	1.75	0.51
1:E:18:SER:O	1:E:22:MET:HG3	2.11	0.51
1:A:82:LYS:HB2	1:A:146:ARG:CZ	2.41	0.50
1:A:24:GLU:HB2	1:A:103:PRO:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:ASP:O	1:F:189:ARG:HG3	2.11	0.50
1:E:126:ASN:O	1:E:130:GLU:HG2	2.11	0.50
2:R:11:DC:H2"	2:R:12:DA:N7	2.26	0.50
2:T:11:DC:H2"	2:T:12:DA:C8	2.47	0.50
1:A:157:LEU:HD12	1:B:189:ARG:NH2	2.26	0.50
1:F:89:ARG:HB2	1:F:190:TRP:CZ2	2.47	0.50
1:F:140:MET:CE	1:F:158:LEU:HB3	2.41	0.50
1:E:196:GLN:OE1	1:F:196:GLN:NE2	2.44	0.49
1:A:50:ARG:HH11	2:T:2:DG:H8	1.59	0.49
1:B:69:SER:O	1:B:73:ARG:HD2	2.12	0.49
4:R:101:HOH:O	2:T:11:DC:N4	2.43	0.49
1:A:89:ARG:HB2	1:A:190:TRP:CE2	2.48	0.49
1:B:145:MET:SD	1:B:145:MET:N	2.83	0.49
3:K:375:PHE:O	3:K:377:ARG:N	2.45	0.48
1:B:16:LEU:HD13	1:B:62:LEU:HD13	1.93	0.48
1:B:11:ARG:NE	4:B:206:HOH:O	2.47	0.48
1:B:83:ASP:O	1:B:87:ARG:HB2	2.12	0.48
1:E:74:ILE:HD13	1:E:135:GLN:HG3	1.95	0.48
1:F:106:THR:O	1:F:110:THR:HG23	2.13	0.48
1:B:77:ILE:HD13	1:B:90:LEU:HB2	1.96	0.48
1:B:63:ILE:HG12	1:B:108:ILE:HG21	1.96	0.48
1:E:9:ARG:NH2	1:E:10:ASN:OD1	2.42	0.48
1:F:136:LEU:O	1:F:140:MET:HG3	2.14	0.48
1:F:158:LEU:O	1:F:161:GLN:HB3	2.14	0.48
1:A:73:ARG:O	1:A:77:ILE:HG13	2.13	0.48
1:B:84:THR:HG21	1:B:143:LYS:HB2	1.95	0.48
1:F:196:GLN:C	1:F:198:GLN:H	2.18	0.47
1:E:135:GLN:O	1:E:139:VAL:HG23	2.14	0.47
1:F:188:ALA:O	1:F:191:PRO:HD2	2.15	0.47
1:A:32:ILE:HG22	1:A:37:LEU:HB2	1.95	0.47
1:B:83:ASP:HB3	1:B:86:ALA:HB3	1.96	0.47
1:B:103:PRO:O	1:B:106:THR:HG22	2.13	0.47
1:E:83:ASP:HB3	1:E:86:ALA:HB3	1.94	0.47
1:E:149:GLU:HB3	4:E:205:HOH:O	2.12	0.47
1:E:164:ALA:O	1:F:168:GLY:HA3	2.14	0.47
1:F:88:LEU:HD23	1:F:197:LEU:HD13	1.95	0.47
1:F:140:MET:HE1	1:F:158:LEU:CB	2.44	0.47
1:E:196:GLN:HA	1:E:198:GLN:NE2	2.28	0.47
1:B:23:LEU:HD13	1:B:32:ILE:HD11	1.96	0.47
1:B:86:ALA:O	1:B:90:LEU:HG	2.15	0.47
1:A:31:ARG:HB3	1:A:116:PHE:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HD11	1:A:132:ILE:HG21	1.97	0.47
1:B:47:ALA:HA	1:B:50:ARG:HG2	1.95	0.47
1:A:50:ARG:NH1	2:T:2:DG:H8	2.12	0.47
1:A:79:LYS:HA	1:A:82:LYS:NZ	2.30	0.47
1:A:62:LEU:HD23	1:A:108:ILE:HD11	1.97	0.47
1:E:100:GLU:OE1	1:E:183:THR:OG1	2.30	0.47
1:B:152:THR:N	1:B:198:GLN:O	2.44	0.47
3:N:378:LEU:HD23	3:N:379:ARG:H	1.81	0.46
1:E:57:ARG:NH1	1:E:60:ASP:OD2	2.48	0.46
1:E:142:GLU:O	1:E:146:ARG:HD3	2.15	0.46
2:R:4:DG:C6	2:R:5:DA:C6	3.04	0.46
1:F:140:MET:HE1	1:F:158:LEU:HB3	1.98	0.46
1:A:70:LEU:HD21	1:A:128:LEU:HD11	1.97	0.46
1:B:64:GLU:HB2	1:B:124:ARG:NH2	2.30	0.46
1:B:70:LEU:O	1:B:74:ILE:HG22	2.16	0.46
1:B:31:ARG:HG3	1:B:116:PHE:CD2	2.51	0.45
2:T:6:DG:H2"	2:T:7:DT:O5'	2.17	0.45
2:R:2:DG:H2"	2:R:3:DT:O5'	2.17	0.45
4:R:101:HOH:O	2:T:11:DC:C4	2.70	0.45
1:A:143:LYS:HZ3	1:A:149:GLU:CD	2.20	0.45
2:T:3:DT:H2"	2:T:4:DG:N7	2.32	0.45
1:F:18:SER:O	1:F:22:MET:HG3	2.16	0.45
2:R:2:DG:H2'	2:R:3:DT:C7	2.47	0.45
1:E:59:PHE:O	1:E:63:ILE:HG13	2.17	0.45
1:E:74:ILE:HG21	1:E:135:GLN:CG	2.46	0.44
1:A:152:THR:H	1:A:198:GLN:C	2.20	0.44
1:F:49:TYR:CE1	2:R:13:DC:H2'	2.52	0.44
1:B:55:LYS:NZ	4:T:101:HOH:O	2.50	0.44
1:B:57:ARG:HA	1:B:60:ASP:HB2	1.97	0.44
1:E:116:PHE:CZ	1:F:115:MET:HB3	2.53	0.44
1:F:172:ARG:HG2	1:F:175:ARG:HH21	1.82	0.44
1:F:193:ILE:HD13	1:F:193:ILE:O	2.17	0.44
1:A:53:PRO:HG2	1:A:57:ARG:HG3	1.99	0.44
1:A:122:GLN:O	1:A:125:ILE:HG12	2.17	0.44
1:E:173:PHE:HE1	1:E:181:ARG:HD3	1.82	0.44
1:F:140:MET:HE1	1:F:158:LEU:CG	2.44	0.44
2:R:11:DC:H2"	2:R:12:DA:C8	2.53	0.44
2:R:11:DC:H42	2:T:4:DG:H1	1.64	0.44
1:E:82:LYS:HA	1:E:87:ARG:NH1	2.33	0.44
1:F:140:MET:HE2	1:F:158:LEU:HG	1.99	0.44
1:A:144:ARG:HH11	1:A:150:GLY:H	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:MET:HE1	1:B:158:LEU:C	2.38	0.44
1:A:11:ARG:HH22	1:A:41:VAL:CG1	2.30	0.44
1:A:193:ILE:HD11	1:B:161:GLN:HE22	1.81	0.44
3:K:372:ILE:H	3:K:372:ILE:HG12	1.68	0.44
1:F:179:LYS:HE3	1:F:179:LYS:HB3	1.65	0.44
1:B:62:LEU:HD11	3:K:375:PHE:CZ	2.52	0.43
1:A:23:LEU:HD21	1:A:108:ILE:HG13	1.99	0.43
1:E:49:TYR:OH	2:T:8:DA:H2"	2.18	0.43
1:E:100:GLU:CD	1:E:181:ARG:HB3	2.39	0.43
1:A:189:ARG:O	1:A:192:LEU:N	2.48	0.43
1:E:124:ARG:NH2	4:E:207:HOH:O	2.51	0.43
1:B:106:THR:HG23	1:B:174:VAL:HG22	2.00	0.43
1:E:181:ARG:HA	1:E:182:PRO:HD2	1.90	0.43
1:F:78:LEU:HD22	1:F:87:ARG:CZ	2.48	0.43
1:A:34:THR:HG21	1:A:49:TYR:OH	2.19	0.43
1:E:73:ARG:HD2	1:E:73:ARG:N	2.33	0.43
1:E:100:GLU:OE1	1:E:181:ARG:HB3	2.19	0.43
1:B:88:LEU:HG	1:B:190:TRP:HH2	1.84	0.43
1:A:160:SER:HB2	4:B:207:HOH:O	2.18	0.43
2:R:5:DA:H2"	2:R:6:DG:C8	2.54	0.43
1:E:136:LEU:HA	1:E:136:LEU:HD23	1.80	0.43
1:B:68:ASP:O	1:B:72:THR:HG22	2.18	0.43
1:E:32:ILE:O	1:E:55:LYS:NZ	2.43	0.43
1:E:169:MET:SD	4:E:211:HOH:O	2.62	0.42
1:E:189:ARG:NH1	1:F:160:SER:OG	2.46	0.42
1:F:93:LEU:HB2	1:F:186:PHE:CE2	2.54	0.42
1:F:173:PHE:CD1	1:F:182:PRO:HD3	2.54	0.42
1:B:98:PHE:HE1	3:K:373:PRO:HG2	1.84	0.42
1:B:103:PRO:HD2	3:K:376:LEU:HD21	2.01	0.42
1:B:97:GLY:O	1:B:101:ARG:HD3	2.19	0.42
1:F:196:GLN:O	1:F:198:GLN:N	2.50	0.42
1:A:24:GLU:HB3	1:A:104:GLY:CA	2.49	0.42
1:A:84:THR:CB	1:A:143:LYS:HD3	2.47	0.42
1:F:137:ARG:O	1:F:141:ARG:NH1	2.47	0.42
3:M:377:ARG:NH2	4:M:403:HOH:O	2.51	0.42
1:A:10:ASN:O	1:A:14:GLU:HG3	2.19	0.42
1:F:19:LEU:O	1:F:23:LEU:HD12	2.20	0.42
1:F:91:ILE:HG21	1:F:136:LEU:CD1	2.49	0.42
1:E:78:LEU:C	1:E:80:ASP:H	2.23	0.42
1:A:82:LYS:HA	1:A:87:ARG:NH1	2.34	0.42
1:B:65:PHE:O	1:B:69:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:4:DG:O6	4:R:101:HOH:O	2.21	0.42
2:T:6:DG:H2"	2:T:7:DT:H2'	2.01	0.42
1:B:62:LEU:HD12	1:B:62:LEU:HA	1.61	0.41
1:F:95:LEU:HD12	1:F:166:CYS:SG	2.60	0.41
1:A:120:ARG:HB3	1:A:120:ARG:NH1	2.36	0.41
1:F:16:LEU:HD22	1:F:62:LEU:HD13	2.01	0.41
1:A:51:HIS:ND1	4:A:203:HOH:O	2.16	0.41
3:M:377:ARG:NH1	4:M:401:HOH:O	2.40	0.41
1:A:112:HIS:CE1	1:B:112:HIS:NE2	2.89	0.41
1:B:76:LEU:HD23	3:K:370:LEU:HD23	2.01	0.41
1:F:62:LEU:HG	1:F:105:LEU:HD21	2.03	0.41
1:B:63:ILE:CG2	1:B:124:ARG:HG2	2.46	0.41
1:E:120:ARG:HG3	1:E:121:LEU:HG	2.02	0.41
1:E:106:THR:HG21	1:E:173:PHE:HD2	1.84	0.41
1:E:189:ARG:NH1	1:F:157:LEU:HG	2.36	0.41
1:A:69:SER:O	1:A:73:ARG:HB2	2.21	0.41
1:A:181:ARG:HA	1:A:182:PRO:HD3	1.79	0.40
2:R:6:DG:H2"	2:R:7:DT:O5'	2.21	0.40
1:A:168:GLY:HA3	1:B:164:ALA:O	2.21	0.40
1:B:140:MET:HE1	1:B:159:ALA:CA	2.52	0.40
1:B:181:ARG:HA	1:B:182:PRO:HD3	1.95	0.40
1:F:66:ILE:O	1:F:70:LEU:HB2	2.22	0.40
1:A:51:HIS:N	4:A:203:HOH:O	2.50	0.40
1:A:128:LEU:O	1:A:132:ILE:HG13	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	188/190 (99%)	173 (92%)	15 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	187/190 (98%)	167 (89%)	18 (10%)	2 (1%)	14 38
1	E	188/190 (99%)	170 (90%)	17 (9%)	1 (0%)	29 58
1	F	187/190 (98%)	171 (91%)	15 (8%)	1 (0%)	29 58
3	K	6/8 (75%)	5 (83%)	0	1 (17%)	0 0
3	L	6/8 (75%)	6 (100%)	0	0	100 100
3	M	6/8 (75%)	5 (83%)	1 (17%)	0	100 100
3	N	6/8 (75%)	2 (33%)	3 (50%)	1 (17%)	0 0
All	All	774/792 (98%)	699 (90%)	69 (9%)	6 (1%)	19 47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	376	LEU
3	N	373	ASP
1	F	197	LEU
1	E	79	LYS
1	B	95	LEU
1	B	68	ASP

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	166/166 (100%)	147 (89%)	19 (11%)	5 16
1	B	165/166 (99%)	146 (88%)	19 (12%)	5 15
1	E	166/166 (100%)	151 (91%)	15 (9%)	9 26
1	F	165/166 (99%)	147 (89%)	18 (11%)	6 17
3	K	7/7 (100%)	5 (71%)	2 (29%)	0 1
3	L	7/7 (100%)	6 (86%)	1 (14%)	3 9
3	M	7/7 (100%)	5 (71%)	2 (29%)	0 1
3	N	7/7 (100%)	6 (86%)	1 (14%)	3 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	690/692 (100%)	613 (89%)	77 (11%)	6 16

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	9	ARG
1	E	11	ARG
1	E	12	ARG
1	E	13	GLU
1	E	23	LEU
1	E	56	THR
1	E	71	ILE
1	E	73	ARG
1	E	76	LEU
1	E	108	ILE
1	E	122	GLN
1	E	144	ARG
1	E	157	LEU
1	E	180	TYR
1	E	184	ASP
1	F	13	GLU
1	F	30	GLN
1	F	48	LEU
1	F	70	LEU
1	F	76	LEU
1	F	89	ARG
1	F	121	LEU
1	F	128	LEU
1	F	135	GLN
1	F	153	THR
1	F	157	LEU
1	F	170	LEU
1	F	177	GLU
1	F	180	TYR
1	F	183	THR
1	F	184	ASP
1	F	193	ILE
1	F	198	GLN
1	A	10	ASN
1	A	12	ARG
1	A	43	VAL
1	A	48	LEU

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Mol	Chain	Res	Type
1	A	52	PHE
1	A	58	MET
1	A	60	ASP
1	A	64	GLU
1	A	109	LEU
1	A	120	ARG
1	A	128	LEU
1	A	136	LEU
1	A	141	ARG
1	A	154	ASP
1	A	156	THR
1	A	158	LEU
1	A	161	GLN
1	A	175	ARG
1	A	198	GLN
1	B	12	ARG
1	B	34	THR
1	B	43	VAL
1	B	50	ARG
1	B	60	ASP
1	B	69	SER
1	B	73	ARG
1	B	85	THR
1	B	87	ARG
1	B	88	LEU
1	B	89	ARG
1	B	106	THR
1	B	128	LEU
1	B	135	GLN
1	B	145	MET
1	B	146	ARG
1	B	152	THR
1	B	179	LYS
1	B	181	ARG
3	L	373	ASP
3	K	372	ILE
3	K	376	LEU
3	N	378	LEU
3	M	370	LEU
3	M	377	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	75	ASN
1	B	161	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 monosaccharides 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	190/190 (100%)	0.40	3 (1%) 72 69	37, 57, 74, 92	0
1	B	189/190 (99%)	0.43	3 (1%) 72 69	36, 55, 73, 80	0
1	E	190/190 (100%)	0.42	6 (3%) 47 42	32, 56, 71, 81	0
1	F	189/190 (99%)	0.35	2 (1%) 80 78	35, 52, 69, 84	0
2	R	12/12 (100%)	0.01	0 100 100	57, 64, 71, 77	0
2	T	12/12 (100%)	-0.08	0 100 100	52, 62, 71, 72	0
3	K	8/8 (100%)	0.94	0 100 100	68, 72, 76, 79	0
3	L	8/8 (100%)	0.61	0 100 100	71, 74, 78, 90	0
3	M	8/8 (100%)	1.18	1 (12%) 3 2	64, 69, 73, 74	0
3	N	8/8 (100%)	0.37	1 (12%) 3 2	60, 68, 79, 81	0
All	All	814/816 (99%)	0.40	16 (1%) 65 61	32, 56, 74, 92	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	376	LEU	3.1
1	E	63	ILE	2.8
1	F	158	LEU	2.7
1	B	180	TYR	2.6
1	A	146	ARG	2.5
1	E	190	TRP	2.4
3	N	372	LEU	2.3
1	A	41	VAL	2.2
1	E	11	ARG	2.2
1	B	88	LEU	2.2
1	E	95	LEU	2.1
1	A	140	MET	2.1
1	F	76	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	140	MET	2.1
1	E	62	LEU	2.0
1	B	140	MET	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.