Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 11:45 AM EDT

PDB ID	:	3A1M
Title	:	A fusion protein of a beta helix region of gene product 5 and the foldon region of bacteriophage T4
Authors	:	Yokoi, N.; Suzuki, A.; Hikage, T.; Koshiyama, T.; Terauchi, M.; Yutani, K.; Kanamaru, S.; Arisaka, F.; Yamane, T.; Watanabe, Y.; Ueno, T.
Deposited on	:	2009-04-11
Resolution	:	2.00 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:

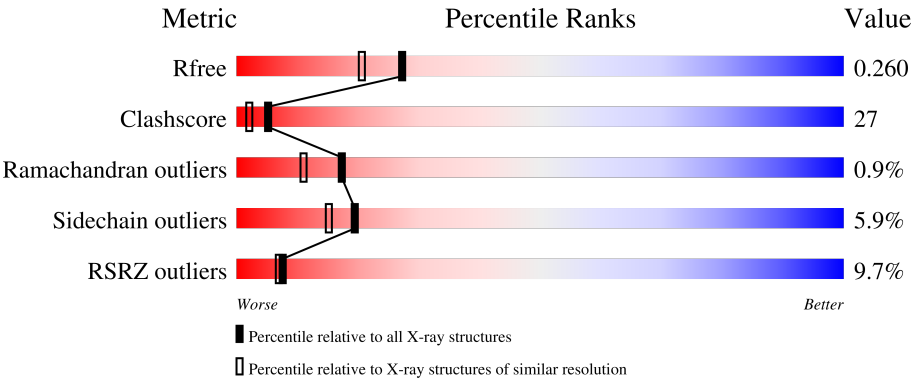
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	139	11% 56% 22% 19%
1	B	139	13% 55% 19% 6% 19%
1	C	139	14% 53% 20% 6% 20%
1	D	139	% 54% 7% 39%
1	E	139	% 50% 11% 39%

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Mol	Chain	Length	Quality of chain
1	F	139	

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	K	A	140	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4820 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 chimera of thrombin cleavage site, Tail-associated lysozyme, Fibritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	0	5	0
			856	531	140	183	2			
1	B	112	Total	C	N	O	S	0	5	0
			856	531	140	183	2			
1	C	111	Total	C	N	O	S	0	5	0
			847	526	139	180	2			
1	D	85	Total	C	N	O	S	0	2	0
			626	383	104	137	2			
1	E	85	Total	C	N	O	S	0	2	0
			626	383	104	137	2			
1	F	85	Total	C	N	O	S	0	3	0
			630	386	104	138	2			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	LEU	VAL	engineered mutation	UNP P16009
A	102	SER	-	linker	UNP P16009
A	103	VAL	-	linker	UNP P16009
A	104	GLU	-	linker	UNP P16009
A	132	VAL	-	expression tag	UNP P10104
A	133	GLU	-	expression tag	UNP P10104
A	134	HIS	-	expression tag	UNP P10104
A	135	HIS	-	expression tag	UNP P10104
A	136	HIS	-	expression tag	UNP P10104
A	137	HIS	-	expression tag	UNP P10104
A	138	HIS	-	expression tag	UNP P10104
A	139	HIS	-	expression tag	UNP P10104
B	16	LEU	VAL	engineered mutation	UNP P16009
B	102	SER	-	linker	UNP P16009
B	103	VAL	-	linker	UNP P16009
B	104	GLU	-	linker	UNP P16009

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Chain	Residue	Modelled	Actual	Comment	Reference
B	132	VAL	-	expression tag	UNP P10104
B	133	GLU	-	expression tag	UNP P10104
B	134	HIS	-	expression tag	UNP P10104
B	135	HIS	-	expression tag	UNP P10104
B	136	HIS	-	expression tag	UNP P10104
B	137	HIS	-	expression tag	UNP P10104
B	138	HIS	-	expression tag	UNP P10104
B	139	HIS	-	expression tag	UNP P10104
C	16	LEU	VAL	engineered mutation	UNP P16009
C	102	SER	-	linker	UNP P16009
C	103	VAL	-	linker	UNP P16009
C	104	GLU	-	linker	UNP P16009
C	132	VAL	-	expression tag	UNP P10104
C	133	GLU	-	expression tag	UNP P10104
C	134	HIS	-	expression tag	UNP P10104
C	135	HIS	-	expression tag	UNP P10104
C	136	HIS	-	expression tag	UNP P10104
C	137	HIS	-	expression tag	UNP P10104
C	138	HIS	-	expression tag	UNP P10104
C	139	HIS	-	expression tag	UNP P10104
D	16	LEU	VAL	engineered mutation	UNP P16009
D	102	SER	-	linker	UNP P16009
D	103	VAL	-	linker	UNP P16009
D	104	GLU	-	linker	UNP P16009
D	132	VAL	-	expression tag	UNP P10104
D	133	GLU	-	expression tag	UNP P10104
D	134	HIS	-	expression tag	UNP P10104
D	135	HIS	-	expression tag	UNP P10104
D	136	HIS	-	expression tag	UNP P10104
D	137	HIS	-	expression tag	UNP P10104
D	138	HIS	-	expression tag	UNP P10104
D	139	HIS	-	expression tag	UNP P10104
E	16	LEU	VAL	engineered mutation	UNP P16009
E	102	SER	-	linker	UNP P16009
E	103	VAL	-	linker	UNP P16009
E	104	GLU	-	linker	UNP P16009
E	132	VAL	-	expression tag	UNP P10104
E	133	GLU	-	expression tag	UNP P10104
E	134	HIS	-	expression tag	UNP P10104
E	135	HIS	-	expression tag	UNP P10104
E	136	HIS	-	expression tag	UNP P10104
E	137	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
E	138	HIS	-	expression tag	UNP P10104
E	139	HIS	-	expression tag	UNP P10104
F	16	LEU	VAL	engineered mutation	UNP P16009
F	102	SER	-	linker	UNP P16009
F	103	VAL	-	linker	UNP P16009
F	104	GLU	-	linker	UNP P16009
F	132	VAL	-	expression tag	UNP P10104
F	133	GLU	-	expression tag	UNP P10104
F	134	HIS	-	expression tag	UNP P10104
F	135	HIS	-	expression tag	UNP P10104
F	136	HIS	-	expression tag	UNP P10104
F	137	HIS	-	expression tag	UNP P10104
F	138	HIS	-	expression tag	UNP P10104
F	139	HIS	-	expression tag	UNP P10104

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0

- Molecule 3 is water.

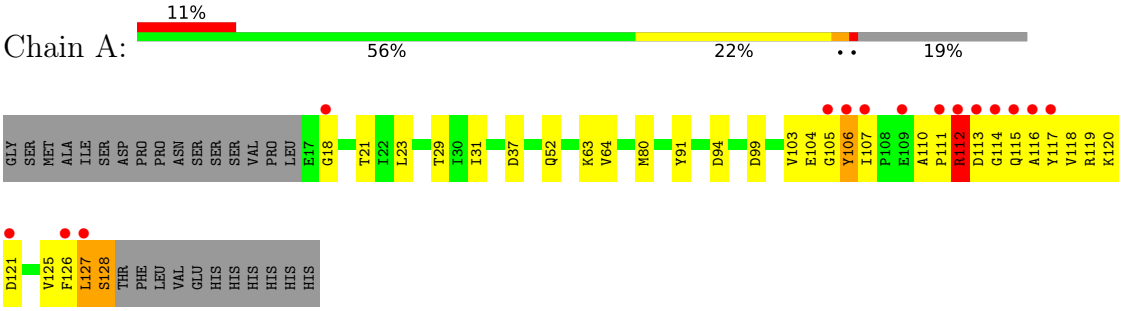
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	83	Total O 83 83	0	0
3	B	73	Total O 73 73	0	0
3	C	86	Total O 86 86	0	0
3	D	49	Total O 49 49	0	0
3	E	41	Total O 41 41	0	0
3	F	45	Total O 45 45	0	0

3 Residue-property plots (i)

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.

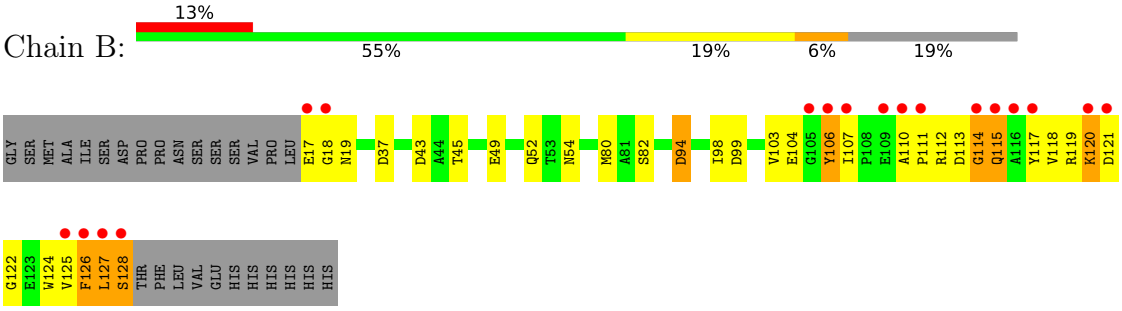
• Molecule 1: chimera of thrombin cleavage site, Tail-associated lysozyme, Fibritin

Chain A:



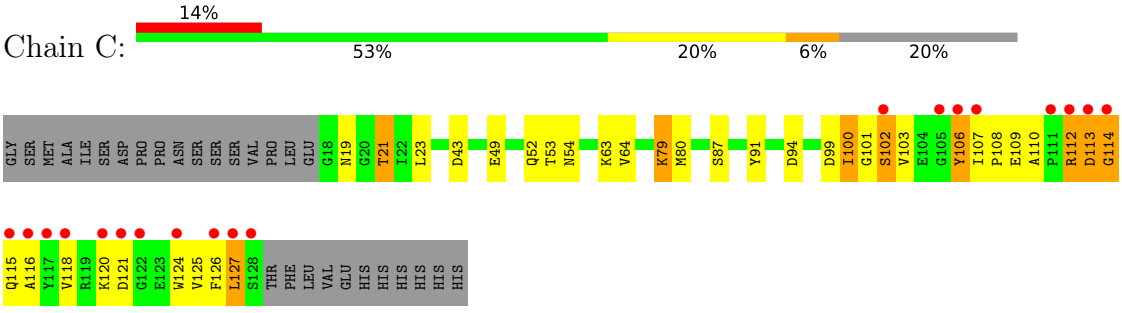
• Molecule 1: chimera of thrombin cleavage site, Tail-associated lysozyme, Fibritin

Chain B:



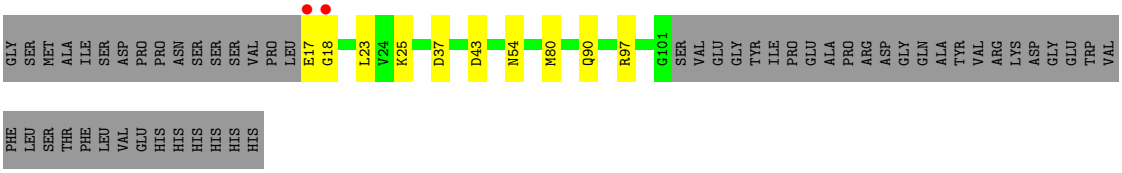
• Molecule 1: chimera of thrombin cleavage site, Tail-associated lysozyme, Fibritin

Chain C:



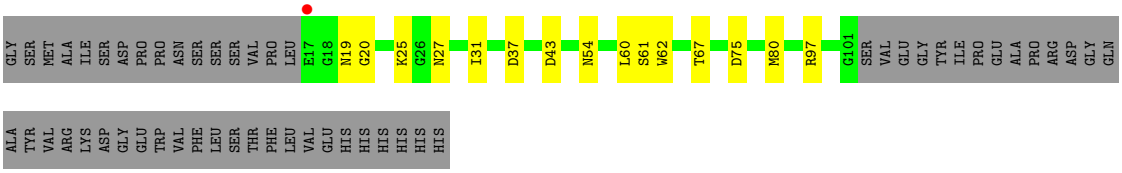
• Molecule 1: chimera of thrombin cleavage site, Tail-associated lysozyme, Fibritin

Chain D:



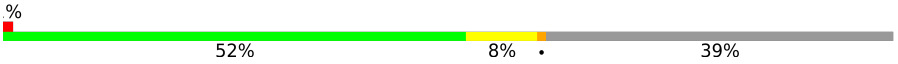
• Molecule 1: chimera of thrombin cleavage site, Tail-associated lysozyme, Fibritin

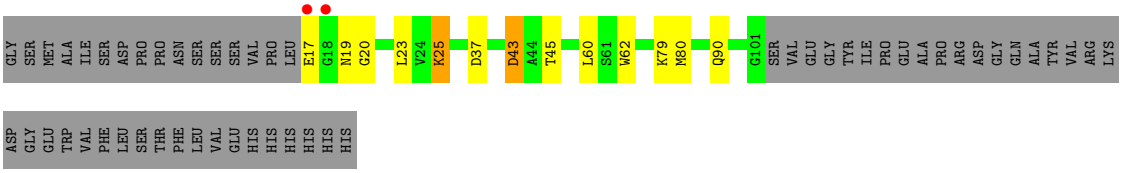
Chain E:



• Molecule 1: chimera of thrombin cleavage site, Tail-associated lysozyme, Fibritin

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	98.81Å 57.01Å 136.59Å 90.00° 103.90° 90.00°	Depositor
Resolution (Å)	29.17 – 2.00 29.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.0 (29.17-2.00) 88.9 (29.17-2.00)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	7.33 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.223 , 0.268 0.214 , 0.260	Depositor DCC
R_{free} test set	2253 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.480 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.487 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4820	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.81% 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

Bond lengths and bond angles in the following residue types are not validated in this section: K

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	1.25	2/884 (0.2%)	1.05	1/1203 (0.1%)
1	B	1.18	0/884	1.08	3/1203 (0.2%)
1	C	1.17	2/875 (0.2%)	1.06	3/1191 (0.3%)
1	D	1.00	0/638	1.04	2/867 (0.2%)
1	E	0.97	0/638	0.99	2/867 (0.2%)
1	F	0.99	0/645	1.00	2/877 (0.2%)
All	All	1.12	4/4564 (0.1%)	1.04	13/6208 (0.2%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	TYR	CE1-CZ	6.89	1.47	1.38
1	C	64	VAL	CB-CG2	6.38	1.66	1.52
1	C	91	TYR	CE1-CZ	5.89	1.46	1.38
1	A	64	VAL	CB-CG2	5.78	1.65	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	43	ASP	CB-CG-OD1	8.77	126.19	118.30
1	C	94	ASP	CB-CG-OD1	8.57	126.02	118.30
1	A	94	ASP	CB-CG-OD1	7.55	125.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	43	ASP	CB-CG-OD1	7.24	124.82	118.30
1	F	43	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	B	94	ASP	CB-CG-OD1	6.61	124.25	118.30
1	D	43	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	C	43	ASP	CB-CG-OD1	6.32	123.98	118.30
1	B	43	ASP	CB-CG-OD1	5.93	123.64	118.30
1	E	43	ASP	CB-CG-OD1	5.42	123.18	118.30
1	E	75	ASP	CB-CG-OD1	5.21	122.98	118.30
1	C	49	GLU	CA-CB-CG	-5.18	102.00	113.40
1	B	49	GLU	CA-CB-CG	-5.04	102.32	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ARG	Peptide

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	856	0	826	92	0
1	B	856	0	826	71	0
1	C	847	0	820	96	0
1	D	626	0	606	19	0
1	E	626	0	606	17	0
1	F	630	0	613	20	0
2	A	1	0	0	2	0
2	D	1	0	0	0	0
3	A	83	0	0	1	0
3	B	73	0	0	5	0
3	C	86	0	0	5	0
3	D	49	0	0	6	0
3	E	41	0	0	3	0
3	F	45	0	0	8	0
All	All	4820	0	4297	230	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 27.

All (230) 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:120:LYS:HG2	1:A:125:VAL:CG2	1.58	1.33
1:A:120:LYS:CG	1:A:125:VAL:HG21	1.66	1.24
1:B:127:LEU:CD1	1:C:118:VAL:HG11	1.66	1.23
1:A:120:LYS:CD	1:A:125:VAL:HG21	1.72	1.18
1:A:103:VAL:HG23	1:C:106:TYR:OH	1.47	1.13
1:A:106:TYR:HD2	1:A:106:TYR:O	1.31	1.09
1:A:115:GLN:HB2	1:A:126:PHE:CE1	1.87	1.09
1:A:120:LYS:HG2	1:A:125:VAL:HG23	1.35	1.08
1:A:120:LYS:CG	1:A:125:VAL:CG2	2.24	1.08
1:C:116:ALA:O	1:C:127:LEU:HB2	1.53	1.08
1:B:17:GLU:HB2	1:F:19:ASN:O	1.52	1.07
3:D:185:HOH:O	1:E:97:ARG:HD2	1.54	1.06
1:B:17:GLU:HG3	1:F:20:GLY:HA2	1.13	1.06
1:C:112:ARG:HH11	1:C:112:ARG:HG2	1.15	1.05
1:B:120:LYS:HG2	1:B:125:VAL:HG21	1.33	1.04
1:A:120:LYS:HD2	1:A:125:VAL:HG21	1.38	1.03
1:C:120:LYS:HE3	1:C:125:VAL:HG21	1.39	1.03
1:B:118:VAL:HG12	1:C:118:VAL:HG12	1.40	1.03
1:A:120:LYS:CE	1:C:116:ALA:HB2	1.89	1.02
1:B:113:ASP:OD1	1:B:113:ASP:O	1.79	1.01
1:A:120:LYS:NZ	1:C:116:ALA:HB2	1.76	1.01
1:A:106:TYR:O	1:A:106:TYR:CD2	2.14	1.00
1:A:103:VAL:CG2	1:C:106:TYR:OH	2.08	1.00
1:A:115:GLN:CB	1:A:126:PHE:CZ	2.46	0.98
1:B:18:GLY:HA2	1:F:17:GLU:N	1.78	0.98
1:A:120:LYS:HZ3	1:A:125:VAL:HG11	1.31	0.96
1:C:120:LYS:CE	1:C:125:VAL:HG21	1.96	0.94
1:A:120:LYS:HE3	1:C:116:ALA:HB2	1.47	0.94
1:C:120:LYS:HE3	1:C:125:VAL:CG2	1.98	0.94
1:A:37[B]:ASP:OD1	1:B:45[B]:THR:OG1	1.85	0.93
1:D:54:ASN:CG	3:D:373:HOH:O	2.05	0.93
1:A:127:LEU:O	1:A:127:LEU:HD23	1.68	0.93
1:A:112:ARG:HH21	1:B:122:GLY:HA3	1.32	0.92
1:B:127:LEU:HD13	1:C:118:VAL:HG11	1.52	0.91
1:C:52:GLN:HE21	1:C:54:ASN:HD21	1.19	0.90
1:A:106:TYR:HB2	1:C:106:TYR:CE2	2.07	0.89
1:B:127:LEU:HD12	1:C:118:VAL:HG11	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLN:HB3	1:A:126:PHE:CZ	2.09	0.88
1:F:37[B]:ASP:OD2	3:F:371:HOH:O	1.91	0.87
1:F:43:ASP:OD2	3:F:332:HOH:O	1.92	0.86
1:B:120:LYS:HG2	1:B:125:VAL:CG2	2.04	0.86
1:A:23:LEU:HD13	1:E:25:LYS:HD3	1.57	0.85
1:A:18:GLY:HA2	1:D:17:GLU:N	1.91	0.85
1:C:112:ARG:HH11	1:C:112:ARG:CG	1.91	0.84
1:A:115:GLN:HB2	1:A:126:PHE:HE1	1.40	0.83
3:B:326:HOH:O	1:D:18:GLY:HA3	1.78	0.83
1:B:106:TYR:CE1	1:C:103:VAL:HG11	2.14	0.82
1:E:67:THR:HG21	3:F:321:HOH:O	1.80	0.82
1:A:106:TYR:CD2	1:A:106:TYR:C	2.49	0.82
1:D:37[B]:ASP:OD2	3:D:328:HOH:O	1.97	0.82
1:B:125:VAL:HG12	1:B:126:PHE:N	1.94	0.82
1:A:103:VAL:HG21	1:C:106:TYR:CE1	2.15	0.81
1:B:106:TYR:OH	1:C:103:VAL:CG1	2.28	0.81
1:B:106:TYR:O	1:B:107:ILE:HG12	1.80	0.80
1:A:115:GLN:CB	1:A:126:PHE:CE1	2.65	0.79
1:A:115:GLN:OE1	1:A:126:PHE:CE1	2.36	0.79
1:B:106:TYR:CE2	1:C:106:TYR:HB2	2.17	0.79
1:A:115:GLN:HB2	1:A:126:PHE:CZ	2.16	0.78
1:A:115:GLN:CB	1:A:126:PHE:HZ	1.91	0.78
1:A:115:GLN:HB3	1:A:126:PHE:HZ	1.45	0.77
1:A:120:LYS:HZ1	1:C:116:ALA:HB2	1.50	0.77
1:B:52:GLN:HE21	1:B:54:ASN:HD21	1.30	0.77
1:F:37[B]:ASP:OD2	3:F:161:HOH:O	2.01	0.77
1:E:67:THR:CG2	3:F:321:HOH:O	2.32	0.76
1:C:106:TYR:HD1	1:C:106:TYR:O	1.69	0.76
1:C:106:TYR:CD1	1:C:106:TYR:C	2.59	0.75
1:A:126:PHE:O	1:A:127:LEU:CB	2.34	0.75
1:B:17:GLU:CB	1:F:19:ASN:O	2.35	0.75
1:B:118:VAL:HG12	1:C:118:VAL:CG1	2.16	0.75
1:A:120:LYS:CG	1:A:125:VAL:HG23	2.06	0.74
1:D:97:ARG:HD2	3:F:286:HOH:O	1.87	0.74
1:C:120:LYS:HB3	1:C:125:VAL:HG23	1.69	0.73
2:A:140:K:K	3:B:161:HOH:O	1.99	0.73
1:C:106:TYR:O	1:C:106:TYR:CD1	2.42	0.73
1:B:115:GLN:NE2	1:B:126:PHE:CZ	2.57	0.73
1:C:52:GLN:NE2	1:C:54:ASN:HD21	1.85	0.73
1:C:120:LYS:CD	1:C:125:VAL:HG21	2.19	0.73
1:C:112:ARG:NH1	1:C:112:ARG:H	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ALA:O	1:C:127:LEU:CB	2.36	0.73
2:A:140:K:K	3:C:158:HOH:O	1.99	0.72
1:A:120:LYS:HZ3	1:A:125:VAL:CG1	2.01	0.72
1:B:106:TYR:OH	1:C:103:VAL:HG13	1.89	0.71
1:B:106:TYR:CZ	1:C:103:VAL:HG11	2.25	0.71
1:B:99[B]:ASP:OD1	1:B:104:GLU:OE2	2.10	0.70
1:C:79:LYS:CE	3:C:293:HOH:O	2.39	0.70
1:C:112:ARG:HG2	1:C:112:ARG:NH1	1.97	0.69
1:B:37[B]:ASP:OD1	3:B:153:HOH:O	2.09	0.69
1:E:37[A]:ASP:OD1	3:E:331:HOH:O	2.09	0.69
1:A:103:VAL:HG21	1:C:106:TYR:HE1	1.58	0.69
1:A:106:TYR:CB	1:C:106:TYR:CE2	2.75	0.69
1:B:52:GLN:NE2	3:B:378:HOH:O	2.20	0.68
1:B:18:GLY:CA	1:F:17:GLU:N	2.55	0.68
1:A:113:ASP:OD2	1:A:117:TYR:OH	2.10	0.67
1:C:127:LEU:HD22	1:C:127:LEU:O	1.94	0.67
1:A:52:GLN:NE2	3:A:352:HOH:O	2.21	0.66
1:A:112:ARG:CG	1:A:112:ARG:HH11	2.08	0.66
1:A:126:PHE:O	1:A:127:LEU:HB3	1.95	0.66
1:B:114:GLY:HA2	1:C:121:ASP:OD1	1.96	0.66
1:D:54:ASN:ND2	3:D:373:HOH:O	2.21	0.66
1:A:112:ARG:HH21	1:B:122:GLY:CA	2.08	0.65
1:B:125:VAL:HG12	1:B:126:PHE:H	1.59	0.65
1:A:18:GLY:CA	1:D:17:GLU:N	2.60	0.65
1:A:115:GLN:OE1	1:A:126:PHE:HE1	1.79	0.64
1:A:120:LYS:NZ	1:C:116:ALA:CB	2.57	0.64
1:B:52:GLN:NE2	1:B:54:ASN:HD21	1.95	0.64
1:D:90:GLN:HE21	1:E:97:ARG:HD2	1.63	0.64
1:C:120:LYS:HB3	1:C:125:VAL:CG2	2.27	0.64
1:A:118:VAL:CG2	1:C:116:ALA:HB1	2.28	0.64
1:D:97:ARG:HD2	1:F:90:GLN:HE21	1.63	0.64
1:B:127:LEU:HD13	1:C:118:VAL:HG21	1.79	0.63
1:B:127:LEU:CD1	1:C:118:VAL:CG1	2.60	0.63
1:A:112:ARG:HH11	1:A:112:ARG:HG2	1.63	0.62
1:C:79:LYS:HE3	3:C:293:HOH:O	1.97	0.62
1:A:120:LYS:HB3	1:C:116:ALA:HA	1.80	0.62
1:C:52:GLN:HE21	1:C:54:ASN:ND2	1.95	0.62
1:E:27:ASN:OD1	3:E:372:HOH:O	2.16	0.62
1:E:54:ASN:CG	3:E:375:HOH:O	2.38	0.62
1:A:118:VAL:HG21	1:C:116:ALA:HB1	1.82	0.61
1:B:125:VAL:CG1	1:B:126:PHE:N	2.61	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:VAL:HG21	1:C:106:TYR:OH	1.98	0.61
1:B:106:TYR:CE2	1:C:106:TYR:CB	2.84	0.61
1:C:19:ASN:HD22	1:E:20:GLY:C	2.04	0.61
1:A:103:VAL:CG2	1:C:106:TYR:CZ	2.84	0.60
1:A:103:VAL:HG21	1:C:106:TYR:CZ	2.36	0.60
1:C:79:LYS:HE2	3:C:293:HOH:O	1.98	0.59
1:B:127:LEU:HD13	1:C:118:VAL:CG1	2.29	0.59
1:A:107:ILE:HG23	1:A:119:ARG:CZ	2.32	0.59
1:A:107:ILE:HG23	1:A:119:ARG:NH1	2.17	0.58
1:D:90:GLN:HE21	1:E:97:ARG:CD	2.14	0.58
1:A:120:LYS:HZ1	1:C:116:ALA:CB	2.15	0.58
1:B:125:VAL:CG1	1:B:126:PHE:H	2.16	0.58
1:A:23:LEU:CD1	1:E:25:LYS:HD3	2.32	0.58
1:B:113:ASP:OD1	1:B:113:ASP:C	2.41	0.57
1:B:126:PHE:O	1:B:128:SER:N	2.36	0.57
1:B:120:LYS:HG3	1:B:120:LYS:O	2.04	0.57
1:A:120:LYS:HE3	1:C:116:ALA:CB	2.30	0.57
1:A:31:ILE:HB	1:C:23:LEU:HD12	1.87	0.56
1:A:112:ARG:CG	1:A:112:ARG:NH1	2.66	0.56
1:A:29:THR:HB	1:C:21:THR:HB	1.87	0.56
1:B:117:TYR:HA	1:B:125:VAL:O	2.06	0.56
1:C:100:ILE:O	1:C:103:VAL:HG12	2.05	0.56
1:C:112:ARG:CG	1:C:112:ARG:O	2.54	0.56
1:A:107:ILE:HD13	1:A:119:ARG:NE	2.22	0.56
1:D:90:GLN:HG2	1:E:97:ARG:HD3	1.86	0.56
1:A:118:VAL:HG12	1:C:118:VAL:HG13	1.88	0.55
1:E:37[A]:ASP:OD2	1:F:45[A]:THR:OG1	2.21	0.55
1:B:115:GLN:HB3	1:B:126:PHE:CE1	2.42	0.55
1:B:114:GLY:HA2	1:C:121:ASP:CG	2.26	0.55
1:B:17:GLU:CG	1:F:20:GLY:HA2	2.09	0.54
1:D:17:GLU:CD	3:D:320:HOH:O	2.45	0.54
1:A:107:ILE:CG2	1:A:119:ARG:CZ	2.85	0.54
1:A:106:TYR:CE1	1:B:106:TYR:HB2	2.43	0.53
1:B:127:LEU:HD11	1:C:118:VAL:HG11	1.80	0.53
1:C:120:LYS:HD3	1:C:125:VAL:HG21	1.90	0.53
1:D:54:ASN:ND2	3:D:212:HOH:O	2.33	0.53
1:B:106:TYR:OH	1:C:103:VAL:CG2	2.56	0.53
1:C:52:GLN:NE2	3:C:337:HOH:O	2.32	0.53
1:B:106:TYR:O	1:B:107:ILE:CG1	2.54	0.52
1:C:110:ALA:HA	1:C:124:TRP:CD1	2.43	0.52
1:A:111:PRO:HG2	1:A:117:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:GLN:HE21	1:B:54:ASN:ND2	2.04	0.52
1:B:118:VAL:CG1	1:C:118:VAL:HG12	2.28	0.52
1:B:17:GLU:OE1	1:B:17:GLU:HA	2.10	0.52
1:B:106:TYR:CZ	1:C:103:VAL:CG1	2.90	0.52
1:B:118:VAL:CG1	1:C:118:VAL:CG1	2.88	0.51
1:B:45[B]:THR:HG22	1:C:53:THR:HB	1.92	0.50
1:C:112:ARG:O	1:C:112:ARG:HG3	2.11	0.50
1:A:114:GLY:HA2	1:B:121:ASP:OD2	2.11	0.50
1:A:121:ASP:OD1	1:C:113:ASP:O	2.30	0.50
1:A:118:VAL:HG12	1:C:118:VAL:CG1	2.42	0.49
1:A:128:SER:O	1:A:128:SER:OG	2.28	0.48
1:A:125:VAL:HG12	1:A:126:PHE:N	2.27	0.48
1:C:21:THR:HG22	1:E:19:ASN:HD21	1.77	0.48
1:B:106:TYR:OH	1:C:103:VAL:HG11	2.05	0.48
1:A:126:PHE:O	1:A:127:LEU:HB2	2.11	0.48
1:C:99[A]:ASP:OD1	1:C:102:SER:HA	2.13	0.47
1:A:115:GLN:CG	1:A:126:PHE:HZ	2.27	0.47
1:D:23:LEU:HD21	1:D:25:LYS:NZ	2.30	0.47
1:C:112:ARG:CG	1:C:112:ARG:NH1	2.60	0.47
1:F:23:LEU:HD23	1:F:23:LEU:C	2.35	0.46
1:A:126:PHE:CD2	1:A:126:PHE:C	2.88	0.46
1:A:118:VAL:HG11	1:C:127:LEU:CD1	2.46	0.46
1:A:117:TYR:CD2	1:A:126:PHE:HA	2.51	0.46
1:B:124:TRP:CZ2	1:C:107:ILE:HD13	2.51	0.46
1:B:98:ILE:O	1:B:104:GLU:HG3	2.15	0.45
1:A:115:GLN:CG	1:A:126:PHE:CZ	2.99	0.45
1:F:25:LYS:HZ2	1:F:25:LYS:HG2	1.58	0.45
1:B:82:SER:HA	1:C:87:SER:HB2	1.99	0.45
1:A:18:GLY:C	1:D:17:GLU:N	2.69	0.45
1:A:63:LYS:HE2	3:B:178:HOH:O	2.17	0.45
1:F:90:GLN:NE2	3:F:286:HOH:O	2.41	0.45
1:A:99[B]:ASP:OD1	1:A:104:GLU:OE1	2.34	0.45
1:B:114:GLY:CA	1:C:121:ASP:OD1	2.63	0.45
1:A:106:TYR:CE1	1:B:106:TYR:CB	3.00	0.44
1:D:23:LEU:HD13	1:E:31:ILE:HB	1.98	0.44
1:A:120:LYS:HG3	1:A:125:VAL:CG2	2.38	0.44
1:A:127:LEU:O	1:A:127:LEU:CD2	2.52	0.44
1:A:110:ALA:O	1:A:111:PRO:C	2.54	0.44
1:B:127:LEU:HD13	1:C:118:VAL:CG2	2.48	0.44
1:F:60:LEU:HD21	1:F:62:TRP:HE1	1.83	0.44
1:D:17:GLU:CG	1:D:17:GLU:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ARG:HH11	1:C:112:ARG:H	1.64	0.43
1:C:99[A]:ASP:OD1	1:C:102:SER:CA	2.67	0.43
1:B:106:TYR:HE1	1:C:103:VAL:HG11	1.79	0.43
1:C:113:ASP:HB3	1:C:114:GLY:H	1.32	0.43
1:A:125:VAL:CG1	1:A:126:PHE:N	2.81	0.43
1:F:19:ASN:HB3	3:F:205:HOH:O	2.18	0.43
1:A:118:VAL:HG11	1:C:127:LEU:HD12	2.00	0.42
1:C:127:LEU:O	1:C:127:LEU:CD2	2.65	0.42
1:B:110:ALA:O	1:B:111:PRO:C	2.55	0.42
1:B:126:PHE:HD1	1:B:126:PHE:HA	1.76	0.42
1:A:106:TYR:CB	1:C:106:TYR:HE2	2.31	0.42
1:B:106:TYR:CD2	1:C:106:TYR:HD2	2.37	0.42
1:D:90:GLN:NE2	1:E:97:ARG:HH11	2.17	0.42
1:E:60:LEU:HD21	1:E:62:TRP:HE1	1.84	0.42
1:B:106:TYR:C	1:B:107:ILE:CG1	2.89	0.42
1:D:23:LEU:HD21	1:D:25:LYS:HZ3	1.85	0.42
1:B:18:GLY:C	1:F:17:GLU:N	2.73	0.41
1:A:107:ILE:HD13	1:A:119:ARG:CD	2.50	0.41
1:B:19:ASN:HD22	1:F:20:GLY:C	2.23	0.41
1:A:105:GLY:O	1:C:108:PRO:HA	2.20	0.41
1:A:106:TYR:OH	1:B:103:VAL:HG12	2.21	0.41
1:F:17:GLU:O	1:F:17:GLU:HG3	2.19	0.41
1:C:126:PHE:CD2	1:C:126:PHE:N	2.89	0.40
1:F:79:LYS:HB2	1:F:79:LYS:HE3	1.66	0.40
1:A:21:THR:HG22	1:A:23:LEU:HD12	2.03	0.40
1:B:94:ASP:OD1	1:C:101:GLY:HA2	2.20	0.40
1:C:99[A]:ASP:OD1	1:C:102:SER:C	2.59	0.40
1:A:116:ALA:O	1:A:126:PHE:O	2.39	0.40
1:A:120:LYS:HG3	1:A:120:LYS:O	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	115/139 (83%)	110 (96%)	4 (4%)	1 (1%)	17 11
1	B	115/139 (83%)	109 (95%)	4 (4%)	2 (2%)	9 4
1	C	114/139 (82%)	107 (94%)	5 (4%)	2 (2%)	8 3
1	D	85/139 (61%)	85 (100%)	0	0	100 100
1	E	85/139 (61%)	84 (99%)	1 (1%)	0	100 100
1	F	86/139 (62%)	85 (99%)	1 (1%)	0	100 100
All	All	600/834 (72%)	580 (97%)	15 (2%)	5 (1%)	17 13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	LEU
1	B	127	LEU
1	C	102	SER
1	B	114	GLY
1	C	114	GLY

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	95/115 (83%)	91 (96%)	4 (4%)	30 27
1	B	95/115 (83%)	87 (92%)	8 (8%)	11 7
1	C	94/115 (82%)	83 (88%)	11 (12%)	5 3
1	D	70/115 (61%)	69 (99%)	1 (1%)	67 72
1	E	70/115 (61%)	67 (96%)	3 (4%)	29 26
1	F	71/115 (62%)	69 (97%)	2 (3%)	43 44
All	All	495/690 (72%)	466 (94%)	29 (6%)	19 15

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	MET
1	A	106	TYR
1	A	112	ARG
1	A	128	SER
1	B	80	MET
1	B	106	TYR
1	B	112	ARG
1	B	115	GLN
1	B	119	ARG
1	B	120	LYS
1	B	126	PHE
1	B	128	SER
1	C	21	THR
1	C	63	LYS
1	C	79	LYS
1	C	80	MET
1	C	100	ILE
1	C	106	TYR
1	C	109	GLU
1	C	112	ARG
1	C	113	ASP
1	C	115	GLN
1	C	127	LEU
1	D	80	MET
1	E	61[A]	SER
1	E	61[B]	SER
1	E	80	MET
1	F	25	LYS
1	F	80	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	54	ASN
1	A	115	GLN
1	B	19	ASN
1	B	52	GLN
1	B	115	GLN
1	C	19	ASN
1	C	52	GLN
1	D	19	ASN
1	D	52	GLN

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Mol	Chain	Res	Type
1	D	54	ASN
1	D	90	GLN
1	E	19	ASN
1	E	90	GLN
1	F	90	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	112/139 (80%)	0.83	15 (13%)	3	2	14, 22, 78, 83	0
1	B	112/139 (80%)	0.72	18 (16%)	1	1	14, 22, 74, 81	0
1	C	111/139 (79%)	0.81	19 (17%)	1	1	13, 22, 74, 78	0
1	D	85/139 (61%)	0.27	2 (2%)	59	57	25, 30, 42, 63	0
1	E	85/139 (61%)	0.20	1 (1%)	79	78	25, 30, 41, 62	0
1	F	85/139 (61%)	0.22	2 (2%)	59	57	24, 30, 42, 65	0
All	All	590/834 (70%)	0.54	57 (9%)	7	7	13, 28, 73, 83	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	ALA	11.0
1	C	106	TYR	6.6
1	C	116	ALA	6.4
1	A	114	GLY	6.1
1	B	116	ALA	6.0
1	C	121	ASP	5.7
1	C	114	GLY	5.5
1	A	106	TYR	5.4
1	A	126	PHE	4.8
1	A	111	PRO	4.8
1	B	127	LEU	4.7
1	C	105	GLY	4.6
1	A	115	GLN	4.4
1	C	107	ILE	4.0
1	C	113	ASP	4.0
1	B	107	ILE	4.0
1	B	126	PHE	3.9
1	B	18	GLY	3.9
1	A	121	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	18	GLY	3.6
1	C	127	LEU	3.5
1	C	111	PRO	3.4
1	D	17	GLU	3.3
1	B	106	TYR	3.3
1	A	112	ARG	3.3
1	B	115	GLN	3.3
1	B	121	ASP	3.2
1	C	117	TYR	3.1
1	B	105	GLY	3.1
1	B	17	GLU	3.1
1	C	126	PHE	3.1
1	B	128	SER	3.0
1	C	102	SER	2.9
1	A	127	LEU	2.9
1	E	17	GLU	2.9
1	C	122	GLY	2.8
1	F	17	GLU	2.7
1	A	117	TYR	2.7
1	B	110	ALA	2.7
1	B	114	GLY	2.7
1	A	105	GLY	2.6
1	C	124	TRP	2.6
1	A	107	ILE	2.6
1	C	112	ARG	2.5
1	B	109	GLU	2.3
1	C	115	GLN	2.3
1	B	117	TYR	2.3
1	D	18	GLY	2.3
1	C	128	SER	2.3
1	A	109	GLU	2.3
1	C	120	LYS	2.2
1	A	18	GLY	2.2
1	C	118	VAL	2.1
1	B	120	LYS	2.1
1	B	111	PRO	2.1
1	A	113	ASP	2.1
1	B	125	VAL	2.1

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	K	D	140	1/1	0.89	0.04	55,55,55,55	0
2	K	A	140	1/1	0.92	0.12	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.