



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:15 AM GMT

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
<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

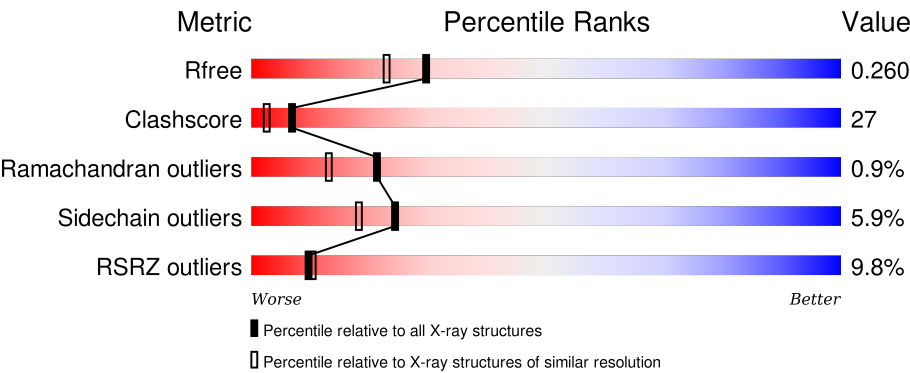
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 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	139	<div><div>11%</div><div>56%</div><div>22%</div><div>••</div><div>19%</div></div>
1	B	139	<div><div>14%</div><div>55%</div><div>19%</div><div>6%</div><div>19%</div></div>
1	C	139	<div><div>14%</div><div>53%</div><div>20%</div><div>6%</div><div>20%</div></div>
1	D	139	<div><div>%</div><div>54%</div><div>7%</div><div>39%</div></div>
1	E	139	<div><div>%</div><div>50%</div><div>11%</div><div>39%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	139	<p>%</p> <p>52% 8% 39%</p>

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

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, Fibrin.

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	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	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	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	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	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	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

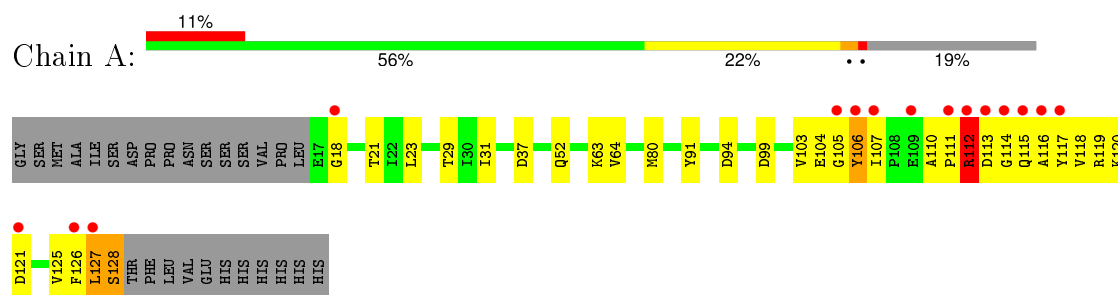
- Molecule 3 is water.

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

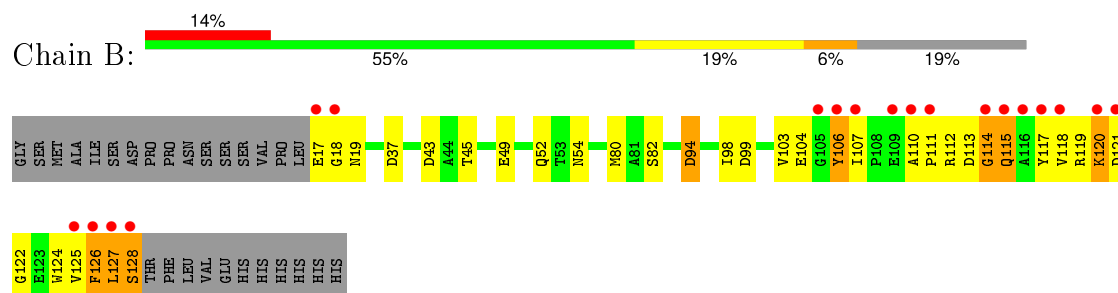
3 Residue-property plots

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.

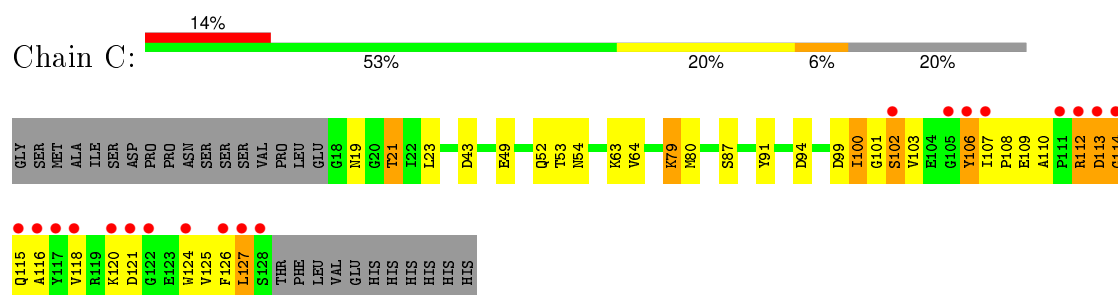
- Molecule 1: chimera of thrombin cleavage site, Tail-associated lysozyme, Fibrin



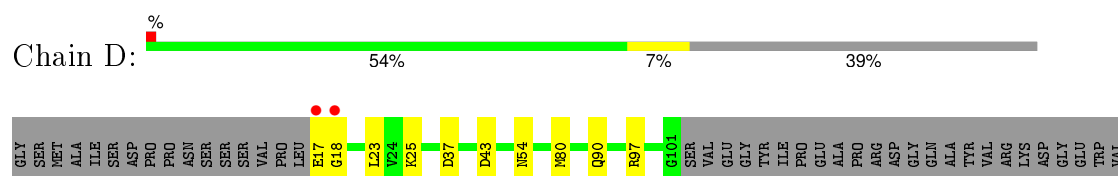
- Molecule 1: chimera of thrombin cleavage site, Tail-associated lysozyme, Fibrin



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



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



PHE
LEU
SER
THR
PHE
LEU
VAL
GLU
HIS
HIS
HIS
HIS
HIS
HIS

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



GLY
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ARG
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LYS
SER
ASP
PRO
TRP
ASN
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PHE
SER
SER
SER
VAL
PRO
LEU
LEU
VAL
E17
G18
N19
G20
K25
G26
N27
I31
D37
D43
N54
L60
S61
W62
T67
D75
M80
R87
G101
SER
VAL
GLU
GLY
TYR
ILE
PRO
GLU
ALA
PRO
ARG
ASP
GLY
GLN

ALA
TYR
VAL
ARG
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- Molecule 1: chimera of thrombin cleavage site, Tail-associated lysozyme, Fibrin



GLY
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LEU
VAL
E17
G18
N19
G20
L23
V24
K25
D37
D43
A44
T45
L60
S61
W62
K79
M80
Q90
G101
SER
VAL
GLU
GLY
TYR
ILE
PRO
GLU
ALA
PRO
ARG
ASP
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4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	7.33 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.223 , 0.268 0.214 , 0.260	Depositor DCC
R_{free} test set	2253 reflections (5.33%)	DCC
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 , 40.9	EDS
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
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	5 of 44534 reflections (0.011%)	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.*

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: 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(°)	Ideal(°)
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(°)	Ideal(°)
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 ⓘ

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:115:GLN:HB2	1:A:126:PHE:CE1	1.87	1.09
1:A:106:TYR:O	1:A:106:TYR:HD2	1.31	1.09
1:A:120:LYS:CG	1:A:125:VAL:CG2	2.24	1.08
1:A:120:LYS:HG2	1:A:125:VAL:HG23	1.35	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:HG2	1:C:112:ARG:HH11	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:HD23	1:A:127:LEU:O	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:CG	1:C:112:ARG:HH11	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:C	1:A:106:TYR:CD2	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:118:VAL:HG12	1:C:118:VAL:CG1	2.16	0.75
1:B:17:GLU:CB	1:F:19:ASN:O	2.35	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
1:C:106:TYR:CD1	1:C:106:TYR:O	2.42	0.73
2:A:140:K:K	3:B:161:HOH:O	1.99	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:116:ALA:O	1:C:127:LEU:CB	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ARG:H	1:C:112:ARG:NH1	1.87	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:O	1:C:127:LEU:HD22	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:120:LYS:NZ	1:C:116:ALA:CB	2.57	0.64
1:A:115:GLN:OE1	1:A:126:PHE:HE1	1.79	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:126:PHE:O	1:B:128:SER:N	2.36	0.57
1:B:113:ASP:OD1	1:B:113:ASP:C	2.41	0.57
1:B:120:LYS:O	1:B:120:LYS:HG3	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:C:100:ILE:O	1:C:103:VAL:HG12	2.05	0.56
1:B:117:TYR:HA	1:B:125:VAL:O	2.06	0.56
1:C:112:ARG:O	1:C:112:ARG:CG	2.54	0.56
1:D:90:GLN:HG2	1:E:97:ARG:HD3	1.86	0.56
1:A:107:ILE:HD13	1:A:119:ARG:NE	2.22	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:B:127:LEU:HD11	1:C:118:VAL:HG11	1.80	0.53
1:A:106:TYR:CE1	1:B:106:TYR:HB2	2.43	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:118:VAL:CG1	1:C:118:VAL:HG12	2.28	0.52
1:B:52:GLN:HE21	1:B:54:ASN:ND2	2.04	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:OG	1:A:128:SER:O	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:C	1:F:23:LEU:HD23	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:F:90:GLN:NE2	3:F:286:HOH:O	2.41	0.45
1:A:63:LYS:HE2	3:B:178:HOH:O	2.17	0.45
1:B:114:GLY:CA	1:C:121:ASP:OD1	2.63	0.45
1:A:99[B]:ASP:OD1	1:A:104:GLU:OE1	2.34	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:CD2	1:A:127:LEU:O	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:O	1:D:17:GLU:CG	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ARG:H	1:C:112:ARG:HH11	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:126:PHE:HD1	1:B:126:PHE:HA	1.76	0.42
1:B:110:ALA:O	1:B:111:PRO:C	2.55	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: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:A:105:GLY:O	1:C:108:PRO:HA	2.20	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:C:99[A]:ASP:OD1	1:C:102:SER:C	2.59	0.40
1:B:94:ASP:OD1	1:C:101:GLY:HA2	2.20	0.40
1:A:120:LYS:O	1:A:120:LYS:HG3	2.22	0.40
1:A:116:ALA:O	1:A:126:PHE:O	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	21	13
1	B	115/139 (83%)	109 (95%)	4 (4%)	2 (2%)	11	4
1	C	114/139 (82%)	107 (94%)	5 (4%)	2 (2%)	11	4
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%)	21	15

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 ⓘ

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%)	36	31
1	B	95/115 (83%)	87 (92%)	8 (8%)	14	8
1	C	94/115 (82%)	83 (88%)	11 (12%)	7	3
1	D	70/115 (61%)	69 (99%)	1 (1%)	74	77
1	E	70/115 (61%)	67 (96%)	3 (4%)	35	30
1	F	71/115 (62%)	69 (97%)	2 (3%)	51	50
All	All	495/690 (72%)	466 (94%)	29 (6%)	24	18

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

Some 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 [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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [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 ⓘ

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, 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	112/139 (80%)	0.91	15 (13%) 4 5	14, 22, 78, 83	0
1	B	112/139 (80%)	0.80	19 (16%) 2 3	14, 22, 74, 81	0
1	C	111/139 (79%)	0.89	19 (17%) 2 2	13, 22, 74, 78	0
1	D	85/139 (61%)	0.33	2 (2%) 62 63	25, 30, 42, 63	0
1	E	85/139 (61%)	0.26	1 (1%) 81 81	25, 30, 41, 62	0
1	F	85/139 (61%)	0.29	2 (2%) 62 63	24, 30, 42, 65	0
All	All	590/834 (70%)	0.62	58 (9%) 10 10	13, 28, 73, 83	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	ALA	11.5
1	C	106	TYR	6.8
1	C	116	ALA	6.8
1	B	116	ALA	6.4
1	A	114	GLY	6.4
1	C	121	ASP	5.9
1	C	114	GLY	5.8
1	A	106	TYR	5.6
1	A	126	PHE	5.1
1	A	111	PRO	5.0
1	B	127	LEU	5.0
1	C	105	GLY	4.8
1	A	115	GLN	4.6
1	C	107	ILE	4.3
1	B	107	ILE	4.3
1	C	113	ASP	4.2
1	B	126	PHE	4.1
1	B	18	GLY	4.1
1	F	18	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	121	ASP	3.8
1	C	127	LEU	3.7
1	C	111	PRO	3.6
1	B	106	TYR	3.4
1	D	17	GLU	3.4
1	A	112	ARG	3.4
1	B	115	GLN	3.4
1	B	121	ASP	3.4
1	B	105	GLY	3.3
1	C	117	TYR	3.3
1	C	126	PHE	3.2
1	B	17	GLU	3.2
1	B	128	SER	3.1
1	A	127	LEU	3.1
1	C	102	SER	3.1
1	E	17	GLU	3.0
1	C	122	GLY	3.0
1	B	110	ALA	2.9
1	F	17	GLU	2.9
1	A	117	TYR	2.8
1	A	107	ILE	2.8
1	B	114	GLY	2.8
1	C	124	TRP	2.8
1	A	105	GLY	2.8
1	C	112	ARG	2.6
1	B	109	GLU	2.4
1	D	18	GLY	2.4
1	C	115	GLN	2.4
1	B	117	TYR	2.4
1	C	128	SER	2.4
1	A	109	GLU	2.4
1	C	118	VAL	2.3
1	C	120	LYS	2.3
1	A	18	GLY	2.3
1	B	125	VAL	2.3
1	B	111	PRO	2.2
1	A	113	ASP	2.2
1	B	120	LYS	2.2
1	B	118	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 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	K	A	140	1/1	0.92	0.12	-0.30	39,39,39,39	0
2	K	D	140	1/1	0.88	0.04	-6.98	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.