Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 09:13 AM EDT

PDB ID	:	3D6X
Title	:	Crystal structure of Campylobacter jejuni FabZ
Authors	:	Yokoyama, T.; Yeo, H.J.
Deposited on	:	2008-05-20
Resolution	:	2.59 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:

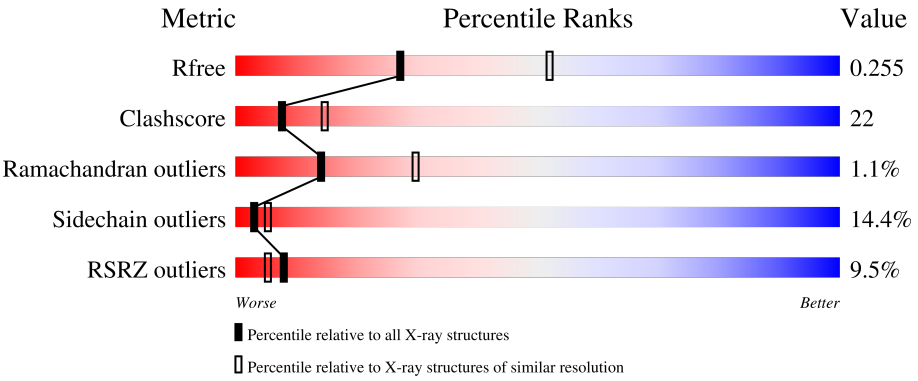
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	146	10% 66% 23% 5% 6%
1	B	146	4% 62% 25% 8%
1	C	146	5% 60% 27% 6%
1	D	146	10% 59% 29% 8%
1	E	146	14% 58% 30% 8%

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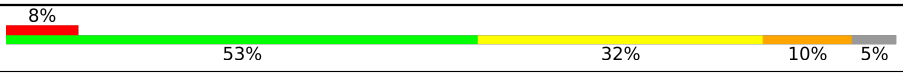
Mol	Chain	Length	Quality of chain
1	F	146	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6635 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 (3R)-hydroxymyristoyl-[acyl-carrier-protein] dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	Se	0	0	0
			1082	706	180	189	7			
1	B	141	Total	C	N	O	Se	0	0	0
			1114	725	184	197	8			
1	C	140	Total	C	N	O	Se	0	0	0
			1105	720	183	194	8			
1	D	140	Total	C	N	O	Se	0	0	0
			1105	720	183	194	8			
1	E	140	Total	C	N	O	Se	0	0	0
			1107	720	183	196	8			
1	F	139	Total	C	N	O	Se	0	1	0
			1107	721	183	194	9			

- Molecule 2 is water.

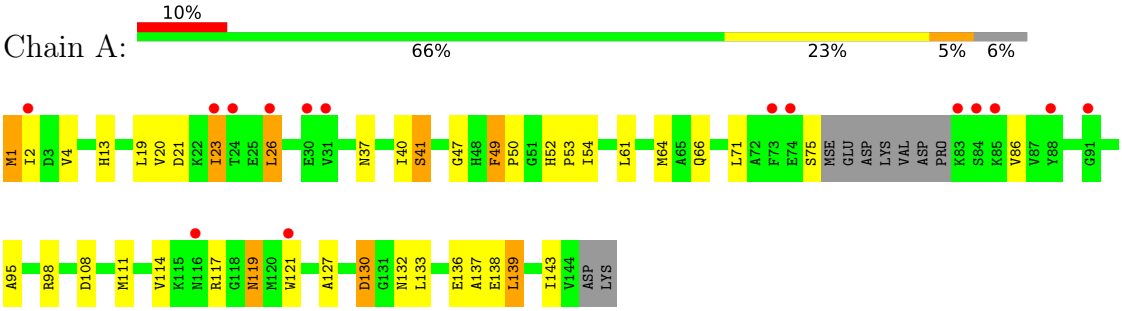
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	5	Total	O	0	0
			5	5		
2	C	3	Total	O	0	0
			3	3		
2	D	3	Total	O	0	0
			3	3		
2	F	1	Total	O	0	0
			1	1		

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.

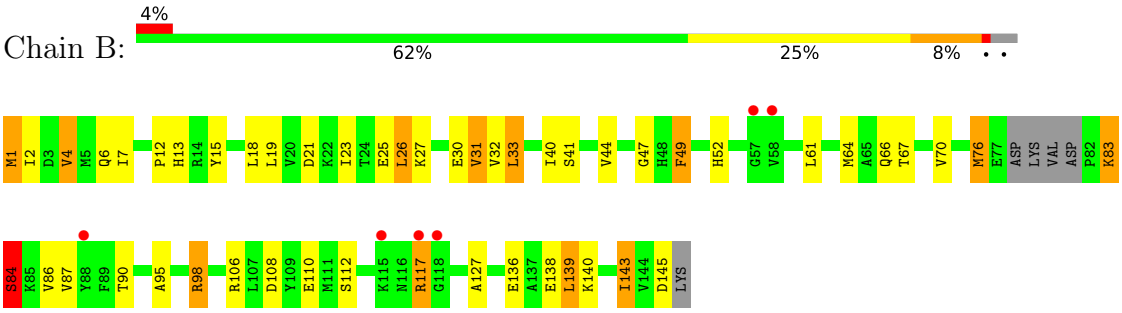
• Molecule 1: (3R)-hydroxymyristoyl-[acyl-carrier-protein] dehydratase

Chain A:



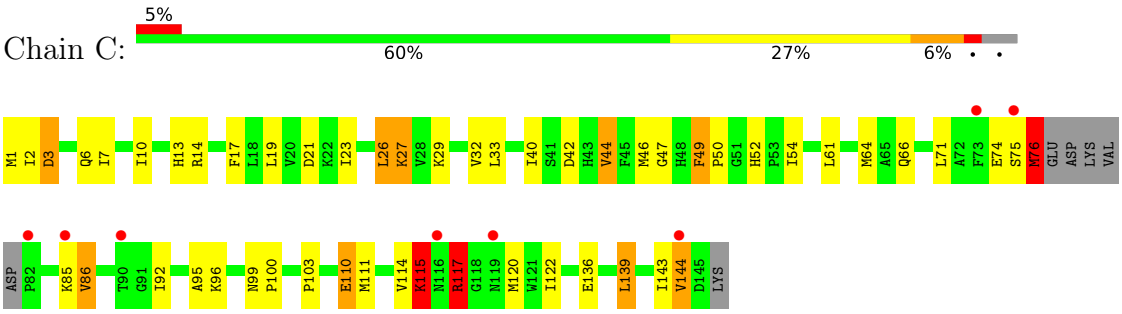
• Molecule 1: (3R)-hydroxymyristoyl-[acyl-carrier-protein] dehydratase

Chain B:



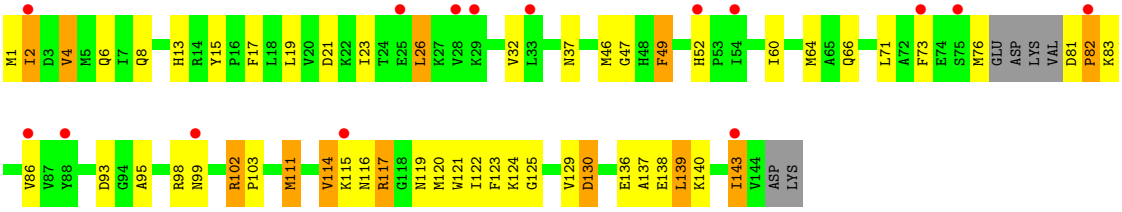
• Molecule 1: (3R)-hydroxymyristoyl-[acyl-carrier-protein] dehydratase

Chain C:

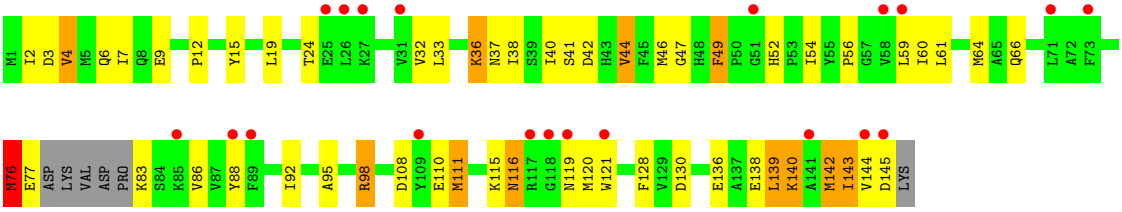


• Molecule 1: (3R)-hydroxymyristoyl-[acyl-carrier-protein] dehydratase

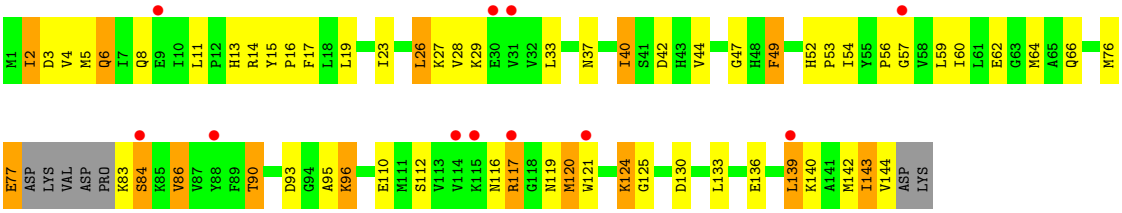
Chain D:



• Molecule 1: (3R)-hydroxymyristoyl-[acyl-carrier-protein] dehydratase



• Molecule 1: (3R)-hydroxymyristoyl-[acyl-carrier-protein] dehydratase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.59Å 93.40Å 126.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.16 – 2.59 33.83 – 2.59	Depositor EDS
% Data completeness (in resolution range)	87.8 (75.16-2.59) 87.9 (33.83-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.254 0.216 , 0.255	Depositor DCC
R_{free} test set	1490 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 60.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6635	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% 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	0.63	0/1100	0.75	0/1473
1	B	0.72	0/1132	0.85	1/1514 (0.1%)
1	C	1.22	6/1123 (0.5%)	1.21	6/1502 (0.4%)
1	D	0.60	1/1123 (0.1%)	0.73	0/1503
1	E	0.58	1/1124 (0.1%)	0.70	0/1503
1	F	0.61	0/1124	0.78	0/1502
All	All	0.76	8/6726 (0.1%)	0.85	7/8997 (0.1%)

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	B	0	1
1	C	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	ARG	NE-CZ	24.36	1.64	1.33
1	C	115	LYS	CE-NZ	19.09	1.96	1.49
1	C	117	ARG	CZ-NH1	8.65	1.44	1.33
1	C	115	LYS	CG-CD	7.97	1.79	1.52
1	C	76	MSE	C-O	7.94	1.38	1.23
1	C	117	ARG	CD-NE	7.73	1.59	1.46
1	E	116	ASN	CG-ND2	6.94	1.50	1.32
1	D	117	ARG	CZ-NH1	5.64	1.40	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	117	ARG	NE-CZ-NH2	-32.60	104.00	120.30
1	C	117	ARG	NH1-CZ-NH2	9.55	129.91	119.40
1	C	117	ARG	CD-NE-CZ	-7.45	113.17	123.60
1	C	117	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	26	LEU	CA-CB-CG	5.42	127.75	115.30
1	C	115	LYS	CD-CE-NZ	-5.36	99.36	111.70
1	C	40	ILE	CB-CA-C	-5.05	101.50	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	84	SER	Peptide
1	C	117	ARG	Sidechain

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	1082	0	1107	39	0
1	B	1114	0	1134	63	0
1	C	1105	0	1128	60	0
1	D	1105	0	1127	50	0
1	E	1107	0	1126	45	0
1	F	1107	0	1130	51	0
2	A	3	0	0	0	0
2	B	5	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	F	1	0	0	0	0
All	All	6635	0	6752	293	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 22.

All (293) 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:C:115:LYS:CD	1:C:115:LYS:CG	1.79	1.57
1:C:115:LYS:NZ	1:C:115:LYS:CE	1.96	1.27
1:C:117:ARG:HD2	1:C:120:MSE:HE3	1.26	1.18
1:D:111:MSE:HE2	1:D:123:PHE:HB3	1.27	1.10
1:C:61:LEU:HD23	1:C:64:MSE:CE	1.83	1.08
1:B:83:LYS:CG	1:B:84:SER:H	1.69	1.03
1:B:83:LYS:CD	1:B:84:SER:H	1.72	1.03
1:B:61:LEU:HD23	1:B:64:MSE:CE	1.88	1.03
1:E:98:ARG:HH11	1:E:98:ARG:CG	1.74	0.99
1:B:61:LEU:HD23	1:B:64:MSE:HE2	1.43	0.98
1:A:53:PRO:HD3	1:F:5[B]:MSE:HE3	1.42	0.98
1:B:98:ARG:HG2	1:B:98:ARG:HH11	1.29	0.95
1:C:61:LEU:HD23	1:C:64:MSE:HE1	1.50	0.94
1:B:98:ARG:HH11	1:B:98:ARG:CG	1.79	0.94
1:D:111:MSE:CE	1:D:123:PHE:HB3	1.96	0.94
1:C:117:ARG:HD2	1:C:120:MSE:CE	1.97	0.93
1:D:102:ARG:HH11	1:D:102:ARG:CG	1.82	0.93
1:B:15:TYR:CE2	1:C:46:MSE:HE2	2.05	0.92
1:C:19:LEU:H	1:C:66:GLN:HE22	1.15	0.92
1:D:102:ARG:HH11	1:D:102:ARG:HG2	1.33	0.91
1:E:76:MSE:HE3	1:E:76:MSE:HA	1.53	0.91
1:B:83:LYS:HG3	1:B:84:SER:H	1.36	0.88
1:F:19:LEU:H	1:F:66:GLN:HE22	1.22	0.88
1:F:64:MSE:HE3	1:F:125:GLY:HA3	1.56	0.87
1:E:98:ARG:HH11	1:E:98:ARG:HG2	1.36	0.87
1:D:2:ILE:HG23	1:D:23:ILE:HB	1.57	0.87
1:B:83:LYS:HG3	1:B:84:SER:N	1.90	0.86
1:F:2:ILE:HG23	1:F:23:ILE:HB	1.58	0.85
1:B:83:LYS:CG	1:B:84:SER:N	2.39	0.84
1:C:61:LEU:HA	1:C:64:MSE:HE3	1.59	0.83
1:B:117:ARG:HH11	1:B:117:ARG:HG3	1.42	0.83
1:E:42:ASP:OD1	1:E:44:VAL:HG23	1.77	0.83
1:A:19:LEU:H	1:A:66:GLN:HE22	1.26	0.83
1:D:138:GLU:C	1:D:139:LEU:HD23	1.99	0.82
1:B:61:LEU:HA	1:B:64:MSE:HE2	1.61	0.81
1:A:111:MSE:HE1	1:A:139:LEU:HD12	1.63	0.80
1:A:119:ASN:ND2	1:A:143:ILE:O	2.15	0.79
1:F:117:ARG:HB2	1:F:120:MSE:SE	2.31	0.79
1:A:52:HIS:CE1	1:A:54:ILE:HD11	2.18	0.79
1:A:119:ASN:ND2	1:A:143:ILE:HB	1.97	0.79
1:D:19:LEU:H	1:D:66:GLN:HE22	1.30	0.79
1:B:12:PRO:HD2	1:B:13:HIS:HD2	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:PRO:HG2	1:E:4:VAL:HG21	1.66	0.78
1:C:117:ARG:CD	1:C:120:MSE:HE3	2.10	0.76
1:B:117:ARG:HH11	1:B:117:ARG:CG	1.98	0.76
1:B:4:VAL:HG21	1:C:103:PRO:HB2	1.69	0.75
1:B:83:LYS:HD2	1:B:84:SER:H	1.51	0.74
1:C:115:LYS:CD	1:C:115:LYS:CB	2.65	0.74
1:B:61:LEU:CD2	1:B:64:MSE:CE	2.65	0.74
1:F:42:ASP:OD1	1:F:44:VAL:HG22	1.87	0.74
1:D:102:ARG:HG2	1:D:102:ARG:NH1	1.96	0.74
1:B:76:MSE:SE	1:B:143:ILE:HD11	2.39	0.73
1:F:52:HIS:CD2	1:F:54:ILE:HD13	2.24	0.72
1:B:1:MSE:HB3	1:B:2:ILE:HD12	1.71	0.72
1:E:33:LEU:HD22	1:E:110:GLU:HG2	1.72	0.72
1:D:111:MSE:CE	1:D:123:PHE:CB	2.68	0.72
1:C:6:GLN:O	1:C:10:ILE:HD12	1.90	0.71
1:C:61:LEU:HD23	1:C:64:MSE:HE3	1.71	0.71
1:B:19:LEU:H	1:B:66:GLN:HE22	1.35	0.71
1:B:61:LEU:HD23	1:B:64:MSE:HE1	1.73	0.71
1:B:83:LYS:CD	1:B:84:SER:N	2.52	0.71
1:C:114:VAL:HG22	1:C:122:ILE:HG22	1.73	0.70
1:C:19:LEU:H	1:C:66:GLN:NE2	1.89	0.70
1:E:98:ARG:HH11	1:E:98:ARG:HG3	1.56	0.70
1:B:15:TYR:HE2	1:C:46:MSE:HE2	1.53	0.70
1:B:12:PRO:HD2	1:B:13:HIS:CD2	2.27	0.69
1:E:98:ARG:HG2	1:E:98:ARG:NH1	2.06	0.69
1:B:98:ARG:HG2	1:B:98:ARG:NH1	2.08	0.68
1:D:98:ARG:HD3	1:D:99:ASN:HD21	1.57	0.68
1:B:83:LYS:HD2	1:B:84:SER:N	2.09	0.67
1:F:19:LEU:H	1:F:66:GLN:NE2	1.91	0.67
1:F:2:ILE:CG2	1:F:23:ILE:HB	2.25	0.67
1:B:32:VAL:CG1	1:B:67:THR:HG22	2.24	0.67
1:F:2:ILE:HG23	1:F:23:ILE:O	1.95	0.67
1:F:142:MSE:O	1:F:143:ILE:HD12	1.94	0.67
1:A:117:ARG:HG3	1:A:117:ARG:HH11	1.60	0.66
1:D:139:LEU:HD23	1:D:139:LEU:N	2.09	0.66
1:B:98:ARG:CG	1:B:98:ARG:NH1	2.49	0.66
1:F:57:GLY:HA2	1:F:60:ILE:HD12	1.79	0.65
1:C:13:HIS:O	1:C:14:ARG:HD3	1.97	0.65
1:E:76:MSE:HA	1:E:76:MSE:CE	2.24	0.65
1:E:111:MSE:HE1	1:E:139:LEU:HG	1.78	0.65
1:B:2:ILE:HG23	1:B:6:GLN:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:CD1	1:C:71:LEU:HD13	2.29	0.63
1:D:111:MSE:HE3	1:D:125:GLY:CA	2.28	0.63
1:B:61:LEU:CD2	1:B:64:MSE:HE1	2.29	0.63
1:C:26:LEU:HD13	1:C:71:LEU:HD13	1.81	0.63
1:C:114:VAL:CG2	1:C:122:ILE:HG22	2.28	0.63
1:B:25:GLU:HB2	1:B:33:LEU:HB2	1.79	0.63
1:A:111:MSE:HE1	1:A:139:LEU:CD1	2.29	0.63
1:C:13:HIS:CD2	1:C:13:HIS:H	2.15	0.63
1:B:49:PHE:HB2	1:B:52:HIS:O	1.98	0.63
1:D:19:LEU:H	1:D:66:GLN:NE2	1.95	0.62
1:F:49:PHE:HB2	1:F:52:HIS:O	2.00	0.61
1:D:81:ASP:N	1:D:82:PRO:HD3	2.15	0.61
1:E:98:ARG:CG	1:E:98:ARG:NH1	2.47	0.61
1:F:64:MSE:CE	1:F:125:GLY:HA3	2.29	0.61
1:E:49:PHE:HB2	1:E:52:HIS:O	2.01	0.61
1:A:49:PHE:HB2	1:A:52:HIS:O	2.01	0.60
1:C:49:PHE:HB2	1:C:52:HIS:O	2.02	0.60
1:F:86:VAL:HG13	1:F:144:VAL:HB	1.84	0.60
1:D:26:LEU:C	1:D:26:LEU:HD12	2.22	0.59
1:D:116:ASN:ND2	1:D:121:TRP:CZ2	2.70	0.59
1:B:32:VAL:HG13	1:B:67:THR:HG22	1.85	0.59
1:B:13:HIS:CD2	1:B:13:HIS:H	2.20	0.59
1:E:19:LEU:H	1:E:66:GLN:HE22	1.49	0.59
1:E:139:LEU:N	1:E:139:LEU:HD22	2.18	0.59
1:F:53:PRO:O	1:F:54:ILE:HD12	2.03	0.58
1:F:96:LYS:NZ	1:F:96:LYS:HB3	2.17	0.58
1:B:19:LEU:H	1:B:66:GLN:NE2	2.00	0.58
1:D:49:PHE:HB2	1:D:52:HIS:O	2.04	0.57
1:C:26:LEU:HD11	1:C:71:LEU:CD1	2.33	0.57
1:D:119:ASN:HA	1:D:143:ILE:HD11	1.84	0.57
1:B:90:THR:OG1	1:B:140:LYS:HE2	2.04	0.57
1:C:61:LEU:CD2	1:C:64:MSE:HE1	2.30	0.57
1:A:4:VAL:HG21	1:F:40:ILE:HG12	1.85	0.57
1:B:4:VAL:HG22	1:B:21:ASP:O	2.04	0.57
1:C:115:LYS:CD	1:C:115:LYS:NZ	2.67	0.57
1:B:32:VAL:HG11	1:B:67:THR:HG22	1.87	0.56
1:D:120:MSE:HE2	1:D:122:ILE:HD11	1.86	0.56
1:F:5[B]:MSE:CE	1:F:8:GLN:HE22	2.17	0.56
1:F:144:VAL:HG12	1:F:144:VAL:O	2.05	0.56
1:F:33:LEU:CD2	1:F:110:GLU:HG2	2.36	0.56
1:C:2:ILE:HB	1:C:23:ILE:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:CD1	1:C:71:LEU:CD1	2.84	0.56
1:F:2:ILE:HG13	1:F:2:ILE:O	2.03	0.56
1:B:87:VAL:HG22	1:B:143:ILE:HB	1.89	0.55
1:A:53:PRO:HD3	1:F:5[B]:MSE:CE	2.28	0.55
1:B:117:ARG:CG	1:B:117:ARG:NH1	2.64	0.55
1:C:86:VAL:HG12	1:C:144:VAL:O	2.06	0.55
1:D:111:MSE:HE1	1:D:123:PHE:CB	2.36	0.55
1:B:95:ALA:HA	1:B:136:GLU:O	2.07	0.55
1:B:23:ILE:CD1	1:B:70:VAL:HG11	2.37	0.55
1:B:76:MSE:SE	1:B:143:ILE:CD1	3.04	0.55
1:A:2:ILE:HB	1:A:23:ILE:HB	1.89	0.54
1:B:139:LEU:N	1:B:139:LEU:CD2	2.70	0.54
1:C:115:LYS:CG	1:C:115:LYS:CE	2.79	0.54
1:F:64:MSE:HE2	1:F:139:LEU:HD21	1.90	0.54
1:F:144:VAL:O	1:F:144:VAL:CG1	2.55	0.54
1:C:3:ASP:O	1:C:7:ILE:HD12	2.08	0.54
1:E:3:ASP:O	1:E:7:ILE:HG13	2.08	0.54
1:B:33:LEU:HD22	1:B:110:GLU:HG2	1.90	0.53
1:E:33:LEU:CD2	1:E:110:GLU:HG2	2.36	0.53
1:F:52:HIS:HD2	1:F:54:ILE:HD13	1.70	0.52
1:D:26:LEU:HD13	1:D:71:LEU:HD13	1.91	0.52
1:D:119:ASN:HA	1:D:143:ILE:CD1	2.40	0.52
1:C:42:ASP:OD1	1:C:44:VAL:HG22	2.09	0.52
1:D:47:GLY:C	1:D:49:PHE:H	2.11	0.52
1:A:19:LEU:H	1:A:66:GLN:NE2	2.00	0.52
1:C:13:HIS:CD2	1:C:13:HIS:N	2.77	0.52
1:A:40:ILE:HD12	1:A:41:SER:N	2.25	0.51
1:A:121:TRP:HE1	1:A:143:ILE:HD11	1.76	0.51
1:E:12:PRO:HG2	1:F:49:PHE:CE2	2.45	0.51
1:F:33:LEU:HD22	1:F:110:GLU:HG2	1.91	0.51
1:D:60:ILE:O	1:D:64:MSE:HG3	2.11	0.51
1:C:75:SER:C	1:C:76:MSE:HG3	2.32	0.51
1:B:61:LEU:HA	1:B:64:MSE:CE	2.37	0.50
1:C:29:LYS:HG3	1:C:75:SER:HB3	1.93	0.50
1:D:2:ILE:HG13	1:D:6:GLN:HB2	1.94	0.50
1:C:26:LEU:C	1:C:26:LEU:HD12	2.32	0.50
1:D:13:HIS:H	1:D:13:HIS:CD2	2.28	0.50
1:E:144:VAL:HG12	1:E:145:ASP:H	1.77	0.50
1:F:117:ARG:CB	1:F:120:MSE:SE	3.06	0.50
1:E:56:PRO:HD2	1:E:59:LEU:HD12	1.94	0.50
1:F:76:MSE:O	1:F:77:GLU:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:VAL:HG12	1:E:145:ASP:N	2.27	0.50
1:D:26:LEU:CD1	1:D:71:LEU:HD13	2.42	0.50
1:D:111:MSE:HE2	1:D:123:PHE:CB	2.17	0.50
1:D:111:MSE:HE3	1:D:124:LYS:C	2.32	0.50
1:F:13:HIS:O	1:F:14:ARG:HD3	2.12	0.50
1:D:116:ASN:ND2	1:D:121:TRP:CE2	2.80	0.50
1:A:53:PRO:CD	1:F:5[B]:MSE:HE3	2.30	0.50
1:D:4:VAL:HG13	1:D:21:ASP:O	2.12	0.50
1:B:23:ILE:HD12	1:B:70:VAL:HG11	1.93	0.49
1:E:120:MSE:HG3	1:E:142:MSE:SE	2.62	0.49
1:E:36:LYS:HD2	1:E:38:ILE:HD13	1.95	0.49
1:B:83:LYS:HE2	1:B:84:SER:OG	2.12	0.49
1:C:95:ALA:HA	1:C:136:GLU:O	2.12	0.49
1:B:108:ASP:O	1:B:127:ALA:HA	2.13	0.49
1:F:56:PRO:HD2	1:F:59:LEU:HD12	1.95	0.49
1:A:40:ILE:HD12	1:A:40:ILE:C	2.33	0.49
1:D:37:ASN:HB3	1:E:37:ASN:HB3	1.94	0.49
1:C:13:HIS:H	1:C:13:HIS:HD2	1.59	0.49
1:E:138:GLU:C	1:E:139:LEU:HD22	2.34	0.49
1:A:13:HIS:CD2	1:A:13:HIS:H	2.31	0.48
1:B:2:ILE:HG23	1:B:6:GLN:CB	2.42	0.48
1:C:26:LEU:HD11	1:C:71:LEU:HD12	1.94	0.48
1:A:121:TRP:HE1	1:A:143:ILE:CD1	2.26	0.48
1:A:26:LEU:HD13	1:A:71:LEU:CD1	2.43	0.48
1:D:111:MSE:HE1	1:D:123:PHE:HB2	1.95	0.48
1:B:18:LEU:C	1:B:19:LEU:HD23	2.34	0.48
1:B:30:GLU:HB3	1:B:31:VAL:HG12	1.95	0.48
1:B:40:ILE:C	1:B:40:ILE:HD12	2.34	0.48
1:A:121:TRP:NE1	1:A:143:ILE:HD11	2.28	0.48
1:C:3:ASP:OD1	1:C:3:ASP:C	2.52	0.48
1:C:92:ILE:HG12	1:C:139:LEU:HD13	1.95	0.48
1:E:92:ILE:HG12	1:E:139:LEU:HD13	1.96	0.48
1:D:73:PHE:HD2	1:D:76:MSE:HE2	1.79	0.47
1:F:62:GLU:O	1:F:66:GLN:HG3	2.13	0.47
1:D:111:MSE:HE3	1:D:125:GLY:N	2.30	0.47
1:C:86:VAL:O	1:C:143:ILE:HA	2.13	0.47
1:F:47:GLY:C	1:F:49:PHE:H	2.18	0.47
1:C:96:LYS:NZ	1:C:96:LYS:HB3	2.28	0.47
1:F:2:ILE:CG2	1:F:23:ILE:O	2.62	0.47
1:E:139:LEU:N	1:E:139:LEU:CD2	2.77	0.47
1:B:47:GLY:C	1:B:49:PHE:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ARG:CG	1:D:102:ARG:NH1	2.52	0.47
1:E:120:MSE:SE	1:E:140:LYS:HE3	2.65	0.47
1:B:13:HIS:HD2	1:B:13:HIS:H	1.62	0.47
1:E:120:MSE:C	1:E:121:TRP:HD1	2.18	0.47
1:A:26:LEU:HD13	1:A:71:LEU:HD13	1.97	0.46
1:E:60:ILE:O	1:E:64:MSE:HG3	2.15	0.46
1:F:2:ILE:HD12	1:F:6:GLN:HB3	1.97	0.46
1:B:1:MSE:HE3	1:B:1:MSE:HA	1.97	0.46
1:C:96:LYS:NZ	1:C:96:LYS:CB	2.77	0.46
1:D:4:VAL:O	1:D:8:GLN:HG3	2.16	0.46
1:D:114:VAL:HG23	1:D:122:ILE:O	2.15	0.46
1:F:5[B]:MSE:HE1	1:F:8:GLN:HE22	1.81	0.46
1:B:40:ILE:HD12	1:B:41:SER:N	2.30	0.46
1:B:139:LEU:N	1:B:139:LEU:HD23	2.30	0.46
1:B:13:HIS:CD2	1:B:13:HIS:N	2.82	0.46
1:E:95:ALA:HA	1:E:136:GLU:O	2.16	0.45
1:C:96:LYS:HB3	1:C:96:LYS:HZ3	1.81	0.45
1:D:95:ALA:HA	1:D:136:GLU:O	2.15	0.45
1:A:20:VAL:HG11	1:A:23:ILE:HD11	1.97	0.45
1:A:49:PHE:HA	1:A:50:PRO:HD2	1.82	0.45
1:E:32:VAL:CG1	1:E:111:MSE:HB3	2.46	0.45
1:C:33:LEU:CD2	1:C:110:GLU:HG3	2.47	0.45
1:A:23:ILE:N	1:A:23:ILE:HD13	2.31	0.45
1:F:95:ALA:HA	1:F:136:GLU:O	2.16	0.45
1:C:13:HIS:C	1:C:14:ARG:HD3	2.38	0.45
1:D:115:LYS:HB2	1:D:115:LYS:HE2	1.79	0.45
1:C:120:MSE:O	1:C:120:MSE:HG3	2.16	0.44
1:D:15:TYR:CE2	1:E:46:MSE:HE2	2.51	0.44
1:F:116:ASN:OD1	1:F:121:TRP:CE2	2.70	0.44
1:B:2:ILE:HG22	1:B:7:ILE:HG13	1.99	0.44
1:D:98:ARG:HD3	1:D:99:ASN:ND2	2.26	0.44
1:A:95:ALA:HA	1:A:136:GLU:O	2.17	0.44
1:A:37:ASN:HB3	1:F:37:ASN:HB3	1.98	0.44
1:A:47:GLY:C	1:A:49:PHE:H	2.20	0.44
1:C:32:VAL:HG13	1:C:111:MSE:HB2	2.00	0.44
1:E:3:ASP:C	1:E:3:ASP:OD2	2.55	0.44
1:F:90:THR:HG23	1:F:140:LYS:HD2	1.99	0.44
1:C:99:ASN:HB3	1:C:100:PRO:HD2	2.00	0.44
1:F:5[B]:MSE:CE	1:F:8:GLN:NE2	2.80	0.44
1:C:26:LEU:HD12	1:C:27:LYS:N	2.33	0.44
1:D:120:MSE:CE	1:D:122:ILE:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:LEU:HB3	1:F:13:HIS:HD2	1.83	0.44
1:A:21:ASP:OD1	1:F:40:ILE:CD1	2.66	0.43
1:E:119:ASN:O	1:E:143:ILE:HG23	2.17	0.43
1:C:61:LEU:HA	1:C:64:MSE:CE	2.37	0.43
1:D:120:MSE:CE	1:D:140:LYS:HE2	2.48	0.43
1:E:47:GLY:C	1:E:49:PHE:H	2.22	0.43
1:E:76:MSE:HB3	1:E:77:GLU:H	1.57	0.43
1:A:117:ARG:HG3	1:A:117:ARG:NH1	2.32	0.43
1:B:98:ARG:HH11	1:B:98:ARG:HG3	1.71	0.43
1:C:47:GLY:C	1:C:49:PHE:H	2.22	0.43
1:C:86:VAL:CG1	1:C:144:VAL:O	2.65	0.43
1:C:32:VAL:HG12	1:C:71:LEU:HD22	2.00	0.43
1:C:61:LEU:CD2	1:C:64:MSE:CE	2.76	0.43
1:A:1:MSE:C	1:A:2:ILE:HG13	2.39	0.42
1:E:61:LEU:HA	1:E:64:MSE:HE2	2.00	0.42
1:E:83:LYS:HE3	1:E:83:LYS:HB3	1.70	0.42
1:A:108:ASP:O	1:A:127:ALA:HA	2.19	0.42
1:F:119:ASN:HB2	1:F:143:ILE:HB	2.00	0.42
1:A:40:ILE:C	1:A:40:ILE:CD1	2.87	0.42
1:B:40:ILE:HG13	1:C:21:ASP:OD1	2.19	0.42
1:D:102:ARG:HH11	1:D:102:ARG:HG3	1.75	0.42
1:A:64:MSE:HE1	1:A:137:ALA:HB3	2.02	0.42
1:C:49:PHE:HA	1:C:50:PRO:HD2	1.84	0.42
1:C:52:HIS:NE2	1:C:54:ILE:HD11	2.35	0.42
1:F:26:LEU:CD1	1:F:26:LEU:C	2.89	0.42
1:F:83:LYS:HB2	1:F:84:SER:H	1.63	0.42
1:A:139:LEU:N	1:A:139:LEU:HD23	2.35	0.42
1:B:98:ARG:NH1	1:B:98:ARG:HG3	2.31	0.41
1:D:32:VAL:CG1	1:D:111:MSE:HB2	2.50	0.41
1:F:124:LYS:O	1:F:124:LYS:HG3	2.16	0.41
1:A:13:HIS:CD2	1:A:13:HIS:N	2.88	0.41
1:A:61:LEU:HA	1:A:64:MSE:HE2	2.02	0.41
1:A:138:GLU:C	1:A:139:LEU:HD23	2.40	0.41
1:E:120:MSE:C	1:E:121:TRP:CD1	2.93	0.41
1:F:15:TYR:CD1	1:F:16:PRO:HA	2.55	0.41
1:F:19:LEU:N	1:F:66:GLN:HE22	2.03	0.41
1:A:130:ASP:N	1:A:130:ASP:OD1	2.53	0.41
1:C:6:GLN:O	1:C:7:ILE:C	2.59	0.41
1:E:6:GLN:O	1:E:9:GLU:HB3	2.21	0.41
1:E:19:LEU:H	1:E:66:GLN:NE2	2.18	0.41
1:E:52:HIS:NE2	1:E:54:ILE:HD11	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:LEU:HD23	1:E:59:LEU:HA	1.87	0.40
1:E:108:ASP:HB2	1:E:128:PHE:HB2	2.02	0.40
1:D:46:MSE:HE2	1:E:15:TYR:CE2	2.56	0.40
1:D:129:VAL:HG12	1:D:130:ASP:OD2	2.22	0.40
1:D:137:ALA:HB3	1:D:139:LEU:HD21	2.03	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	133/146 (91%)	127 (96%)	5 (4%)	1 (1%)	19	39
1	B	137/146 (94%)	129 (94%)	7 (5%)	1 (1%)	22	43
1	C	136/146 (93%)	127 (93%)	8 (6%)	1 (1%)	22	43
1	D	136/146 (93%)	129 (95%)	4 (3%)	3 (2%)	6	12
1	E	136/146 (93%)	127 (93%)	7 (5%)	2 (2%)	10	21
1	F	136/146 (93%)	130 (96%)	5 (4%)	1 (1%)	22	43
All	All	814/876 (93%)	769 (94%)	36 (4%)	9 (1%)	14	30

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	PHE
1	B	49	PHE
1	C	49	PHE
1	D	49	PHE
1	D	82	PRO
1	E	49	PHE
1	D	83	LYS

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Mol	Chain	Res	Type
1	F	49	PHE
1	E	76	MSE

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	117/118 (99%)	104 (89%)	13 (11%)	6 11
1	B	121/118 (102%)	102 (84%)	19 (16%)	2 4
1	C	120/118 (102%)	106 (88%)	14 (12%)	5 10
1	D	120/118 (102%)	106 (88%)	14 (12%)	5 10
1	E	120/118 (102%)	101 (84%)	19 (16%)	2 4
1	F	120/118 (102%)	96 (80%)	24 (20%)	1 2
All	All	718/708 (101%)	615 (86%)	103 (14%)	3 5

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	23	ILE
1	A	26	LEU
1	A	41	SER
1	A	75	SER
1	A	86	VAL
1	A	98	ARG
1	A	114	VAL
1	A	119	ASN
1	A	130	ASP
1	A	132	ASN
1	A	133	LEU
1	A	139	LEU
1	B	1	MSE
1	B	4	VAL
1	B	26	LEU

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Mol	Chain	Res	Type
1	B	27	LYS
1	B	31	VAL
1	B	33	LEU
1	B	44	VAL
1	B	76	MSE
1	B	83	LYS
1	B	84	SER
1	B	86	VAL
1	B	98	ARG
1	B	106	ARG
1	B	112	SER
1	B	117	ARG
1	B	138	GLU
1	B	139	LEU
1	B	143	ILE
1	B	145	ASP
1	C	1	MSE
1	C	3	ASP
1	C	17	PHE
1	C	26	LEU
1	C	27	LYS
1	C	44	VAL
1	C	74	GLU
1	C	76	MSE
1	C	85	LYS
1	C	86	VAL
1	C	110	GLU
1	C	115	LYS
1	C	139	LEU
1	C	144	VAL
1	D	1	MSE
1	D	2	ILE
1	D	4	VAL
1	D	17	PHE
1	D	26	LEU
1	D	86	VAL
1	D	93	ASP
1	D	102	ARG
1	D	111	MSE
1	D	114	VAL
1	D	117	ARG
1	D	130	ASP

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Mol	Chain	Res	Type
1	D	139	LEU
1	D	143	ILE
1	E	2	ILE
1	E	4	VAL
1	E	24	THR
1	E	36	LYS
1	E	40	ILE
1	E	41	SER
1	E	44	VAL
1	E	76	MSE
1	E	86	VAL
1	E	88	TYR
1	E	98	ARG
1	E	111	MSE
1	E	115	LYS
1	E	116	ASN
1	E	130	ASP
1	E	139	LEU
1	E	140	LYS
1	E	142	MSE
1	E	143	ILE
1	F	2	ILE
1	F	3	ASP
1	F	4	VAL
1	F	6	GLN
1	F	17	PHE
1	F	26	LEU
1	F	27	LYS
1	F	28	VAL
1	F	29	LYS
1	F	40	ILE
1	F	77	GLU
1	F	84	SER
1	F	86	VAL
1	F	90	THR
1	F	93	ASP
1	F	96	LYS
1	F	112	SER
1	F	117	ARG
1	F	120	MSE
1	F	124	LYS
1	F	130	ASP

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Mol	Chain	Res	Type
1	F	133	LEU
1	F	139	LEU
1	F	143	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	66	GLN
1	A	119	ASN
1	A	132	ASN
1	B	13	HIS
1	B	66	GLN
1	B	116	ASN
1	B	132	ASN
1	C	8	GLN
1	C	13	HIS
1	C	66	GLN
1	D	13	HIS
1	D	52	HIS
1	D	66	GLN
1	D	99	ASN
1	E	66	GLN
1	F	8	GLN
1	F	13	HIS
1	F	52	HIS
1	F	66	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 (i)

There are no ligands in this entry.

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, 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	130/146 (89%)	0.56	15 (11%) 4 3	51, 56, 61, 68	0
1	B	133/146 (91%)	0.29	6 (4%) 33 26	52, 56, 62, 70	0
1	C	132/146 (90%)	0.44	8 (6%) 21 16	52, 56, 62, 66	0
1	D	132/146 (90%)	0.68	15 (11%) 5 3	51, 56, 62, 69	0
1	E	132/146 (90%)	0.78	20 (15%) 2 1	51, 56, 61, 69	0
1	F	131/146 (89%)	0.62	11 (8%) 11 7	49, 56, 61, 69	0
All	All	790/876 (90%)	0.56	75 (9%) 8 5	49, 56, 62, 70	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	144	VAL	5.0
1	D	88	TYR	4.7
1	A	73	PHE	4.7
1	F	88	TYR	4.7
1	A	121	TRP	4.5
1	F	114	VAL	4.5
1	C	119	ASN	4.5
1	E	118	GLY	4.4
1	C	144	VAL	4.3
1	E	31	VAL	4.2
1	D	28	VAL	4.0
1	E	88	TYR	3.9
1	F	121	TRP	3.9
1	E	27	LYS	3.8
1	B	117	ARG	3.8
1	B	118	GLY	3.8
1	E	85	LYS	3.7
1	A	83	LYS	3.6
1	A	85	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	26	LEU	3.5
1	F	31	VAL	3.5
1	D	75	SER	3.4
1	D	73	PHE	3.3
1	D	2	ILE	3.2
1	E	51	GLY	3.1
1	E	25	GLU	3.0
1	A	88	TYR	2.9
1	D	29	LYS	2.9
1	B	88	TYR	2.9
1	F	115	LYS	2.8
1	C	85	LYS	2.8
1	E	117	ARG	2.8
1	D	52	HIS	2.8
1	F	9	GLU	2.7
1	A	23	ILE	2.7
1	E	145	ASP	2.7
1	E	141	ALA	2.7
1	D	86	VAL	2.7
1	D	115	LYS	2.6
1	E	73	PHE	2.6
1	A	2	ILE	2.6
1	A	24	THR	2.5
1	C	73	PHE	2.5
1	E	121	TRP	2.5
1	E	119	ASN	2.5
1	F	139	LEU	2.4
1	D	25	GLU	2.4
1	B	115	LYS	2.4
1	D	82	PRO	2.4
1	F	30	GLU	2.4
1	C	116	ASN	2.4
1	E	58	VAL	2.4
1	A	91	GLY	2.3
1	D	99	ASN	2.3
1	B	57	GLY	2.3
1	F	117	ARG	2.3
1	F	57	GLY	2.3
1	E	71	LEU	2.3
1	A	116	ASN	2.2
1	E	109	TYR	2.2
1	A	26	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	82	PRO	2.2
1	A	84	SER	2.2
1	D	143	ILE	2.2
1	A	31	VAL	2.1
1	B	58	VAL	2.1
1	A	30	GLU	2.1
1	D	54	ILE	2.1
1	D	33	LEU	2.1
1	E	89	PHE	2.1
1	F	84	SER	2.1
1	C	90	THR	2.1
1	A	74	GLU	2.1
1	C	75	SER	2.0
1	E	59	LEU	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.