Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:12 am BST

PDB ID	:	5XPB
Title	:	Crystal Structure of Selenomethionine labelled Drep4 CIDE domain
Authors	:	Park, H.H.; Jeong, J.H.
Deposited on	:	2017-06-01
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

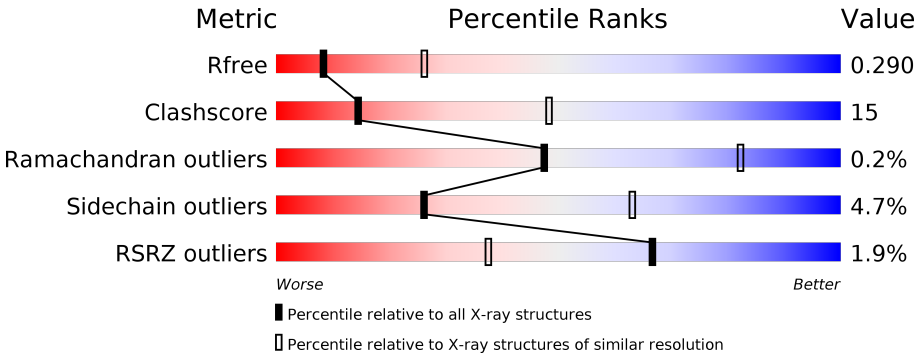
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	100	56% 29% 15%
1	B	100	2% 55% 31% 12%
1	C	100	2% 59% 25% 13%
1	D	100	57% 26% 14%
1	E	100	3% 61% 24% 15%
1	F	100	56% 29% 14%

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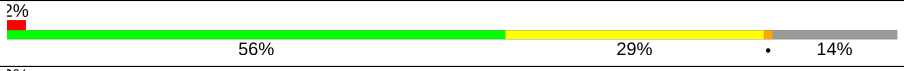
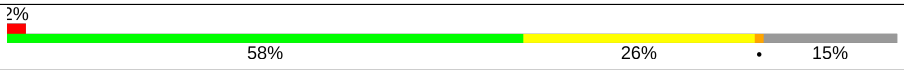
Mol	Chain	Length	Quality of chain
1	G	100	
1	H	100	
1	I	100	
1	J	100	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6748 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 DNAation factor-related protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	Se	0	0	0
			667	428	106	131	2			
1	B	88	Total	C	N	O	Se	0	0	0
			687	441	109	134	3			
1	C	87	Total	C	N	O	Se	0	0	0
			683	439	108	133	3			
1	D	86	Total	C	N	O	Se	0	0	0
			675	433	107	132	3			
1	E	85	Total	C	N	O	Se	0	0	0
			667	428	106	131	2			
1	F	86	Total	C	N	O	Se	0	0	0
			675	433	107	132	3			
1	G	86	Total	C	N	O	Se	0	0	0
			675	433	107	132	3			
1	H	86	Total	C	N	O	Se	0	0	0
			675	433	107	132	3			
1	I	85	Total	C	N	O	Se	0	0	0
			667	428	106	131	2			
1	J	86	Total	C	N	O	Se	0	0	0
			675	433	107	132	3			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	LEU	-	expression tag	UNP Q9V3H0
A	132	GLU	-	expression tag	UNP Q9V3H0
A	133	HIS	-	expression tag	UNP Q9V3H0
A	134	HIS	-	expression tag	UNP Q9V3H0
A	135	HIS	-	expression tag	UNP Q9V3H0
A	136	HIS	-	expression tag	UNP Q9V3H0
A	137	HIS	-	expression tag	UNP Q9V3H0
A	138	HIS	-	expression tag	UNP Q9V3H0
B	131	LEU	-	expression tag	UNP Q9V3H0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	132	GLU	-	expression tag	UNP Q9V3H0
B	133	HIS	-	expression tag	UNP Q9V3H0
B	134	HIS	-	expression tag	UNP Q9V3H0
B	135	HIS	-	expression tag	UNP Q9V3H0
B	136	HIS	-	expression tag	UNP Q9V3H0
B	137	HIS	-	expression tag	UNP Q9V3H0
B	138	HIS	-	expression tag	UNP Q9V3H0
C	131	LEU	-	expression tag	UNP Q9V3H0
C	132	GLU	-	expression tag	UNP Q9V3H0
C	133	HIS	-	expression tag	UNP Q9V3H0
C	134	HIS	-	expression tag	UNP Q9V3H0
C	135	HIS	-	expression tag	UNP Q9V3H0
C	136	HIS	-	expression tag	UNP Q9V3H0
C	137	HIS	-	expression tag	UNP Q9V3H0
C	138	HIS	-	expression tag	UNP Q9V3H0
D	131	LEU	-	expression tag	UNP Q9V3H0
D	132	GLU	-	expression tag	UNP Q9V3H0
D	133	HIS	-	expression tag	UNP Q9V3H0
D	134	HIS	-	expression tag	UNP Q9V3H0
D	135	HIS	-	expression tag	UNP Q9V3H0
D	136	HIS	-	expression tag	UNP Q9V3H0
D	137	HIS	-	expression tag	UNP Q9V3H0
D	138	HIS	-	expression tag	UNP Q9V3H0
E	131	LEU	-	expression tag	UNP Q9V3H0
E	132	GLU	-	expression tag	UNP Q9V3H0
E	133	HIS	-	expression tag	UNP Q9V3H0
E	134	HIS	-	expression tag	UNP Q9V3H0
E	135	HIS	-	expression tag	UNP Q9V3H0
E	136	HIS	-	expression tag	UNP Q9V3H0
E	137	HIS	-	expression tag	UNP Q9V3H0
E	138	HIS	-	expression tag	UNP Q9V3H0
F	131	LEU	-	expression tag	UNP Q9V3H0
F	132	GLU	-	expression tag	UNP Q9V3H0
F	133	HIS	-	expression tag	UNP Q9V3H0
F	134	HIS	-	expression tag	UNP Q9V3H0
F	135	HIS	-	expression tag	UNP Q9V3H0
F	136	HIS	-	expression tag	UNP Q9V3H0
F	137	HIS	-	expression tag	UNP Q9V3H0
F	138	HIS	-	expression tag	UNP Q9V3H0
G	131	LEU	-	expression tag	UNP Q9V3H0
G	132	GLU	-	expression tag	UNP Q9V3H0
G	133	HIS	-	expression tag	UNP Q9V3H0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	134	HIS	-	expression tag	UNP Q9V3H0
G	135	HIS	-	expression tag	UNP Q9V3H0
G	136	HIS	-	expression tag	UNP Q9V3H0
G	137	HIS	-	expression tag	UNP Q9V3H0
G	138	HIS	-	expression tag	UNP Q9V3H0
H	131	LEU	-	expression tag	UNP Q9V3H0
H	132	GLU	-	expression tag	UNP Q9V3H0
H	133	HIS	-	expression tag	UNP Q9V3H0
H	134	HIS	-	expression tag	UNP Q9V3H0
H	135	HIS	-	expression tag	UNP Q9V3H0
H	136	HIS	-	expression tag	UNP Q9V3H0
H	137	HIS	-	expression tag	UNP Q9V3H0
H	138	HIS	-	expression tag	UNP Q9V3H0
I	131	LEU	-	expression tag	UNP Q9V3H0
I	132	GLU	-	expression tag	UNP Q9V3H0
I	133	HIS	-	expression tag	UNP Q9V3H0
I	134	HIS	-	expression tag	UNP Q9V3H0
I	135	HIS	-	expression tag	UNP Q9V3H0
I	136	HIS	-	expression tag	UNP Q9V3H0
I	137	HIS	-	expression tag	UNP Q9V3H0
I	138	HIS	-	expression tag	UNP Q9V3H0
J	131	LEU	-	expression tag	UNP Q9V3H0
J	132	GLU	-	expression tag	UNP Q9V3H0
J	133	HIS	-	expression tag	UNP Q9V3H0
J	134	HIS	-	expression tag	UNP Q9V3H0
J	135	HIS	-	expression tag	UNP Q9V3H0
J	136	HIS	-	expression tag	UNP Q9V3H0
J	137	HIS	-	expression tag	UNP Q9V3H0
J	138	HIS	-	expression tag	UNP Q9V3H0

- Molecule 2 is water.

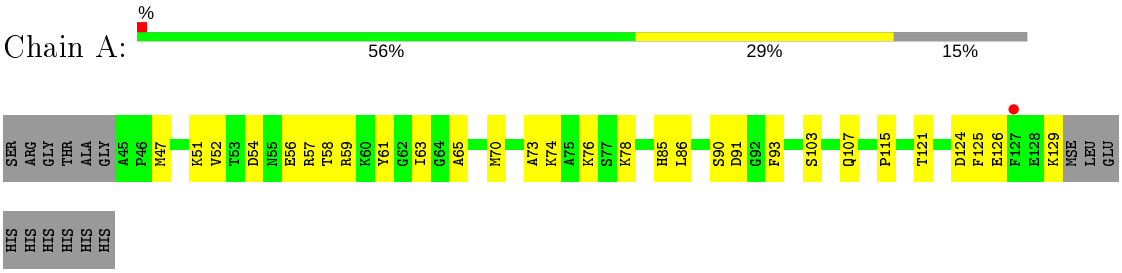
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O 1 1	0	0
2	H	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

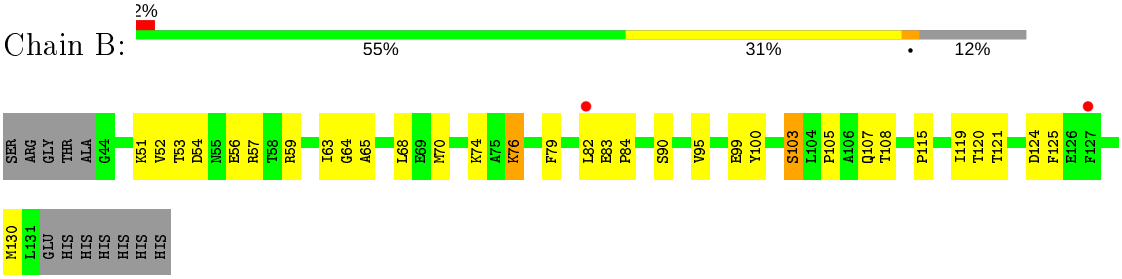
- Molecule 1: DNAation factor-related protein 4

Chain A:



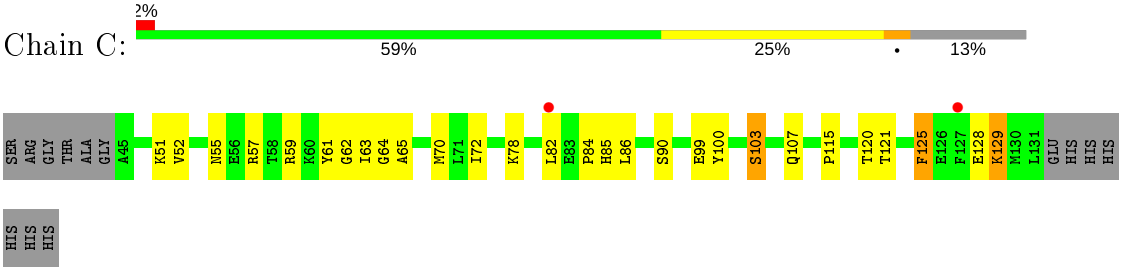
- Molecule 1: DNAation factor-related protein 4

Chain B:



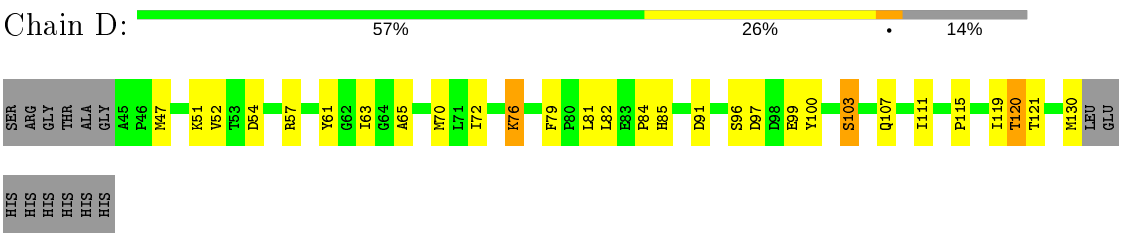
- Molecule 1: DNAation factor-related protein 4

Chain C:



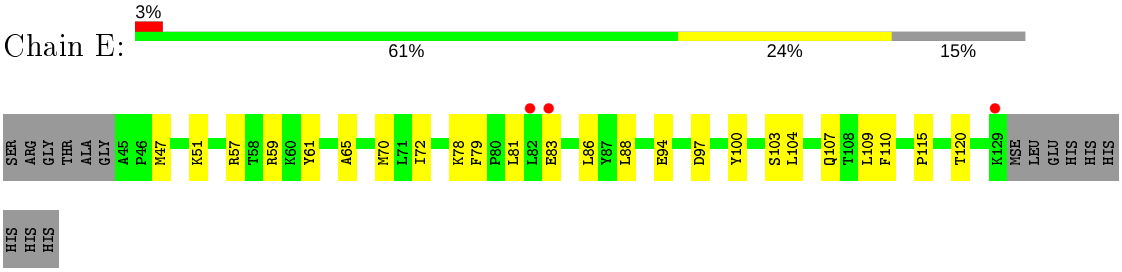
- Molecule 1: DNAation factor-related protein 4

Chain D:



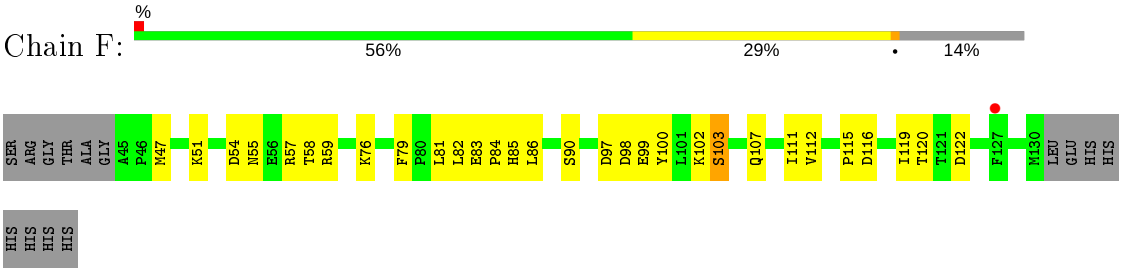
• Molecule 1: DNAation factor-related protein 4

Chain E:



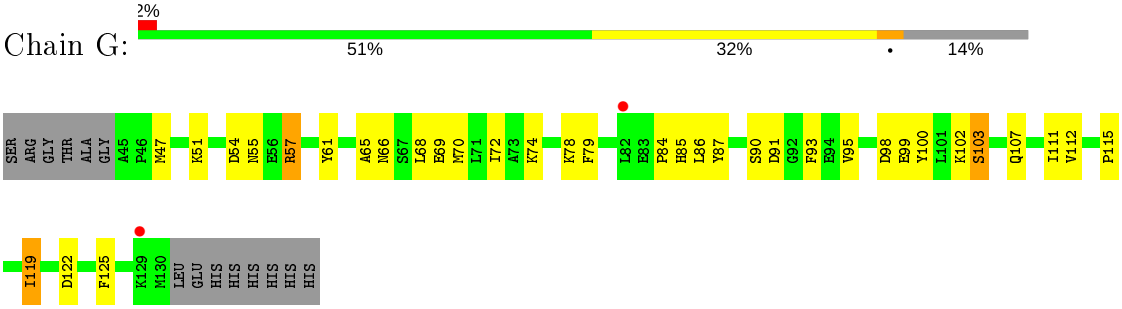
• Molecule 1: DNAation factor-related protein 4

Chain F:



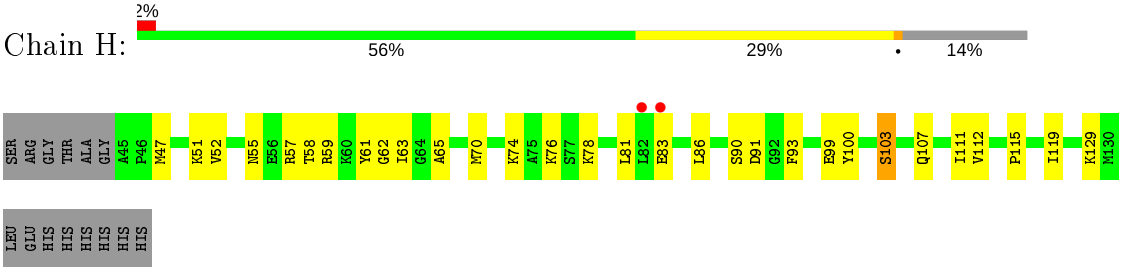
• Molecule 1: DNAation factor-related protein 4

Chain G:



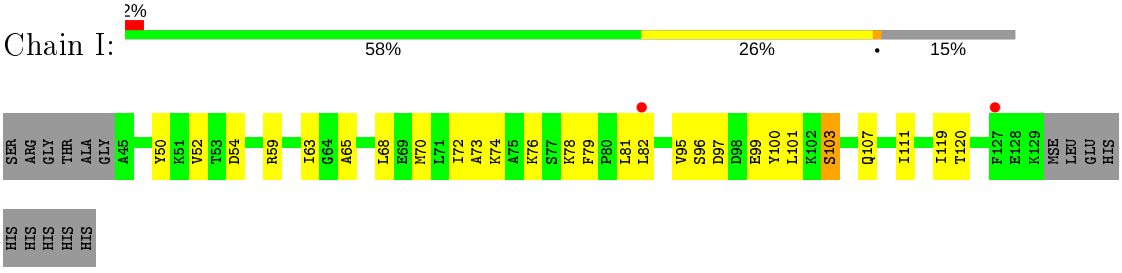
• Molecule 1: DNAation factor-related protein 4

Chain H:



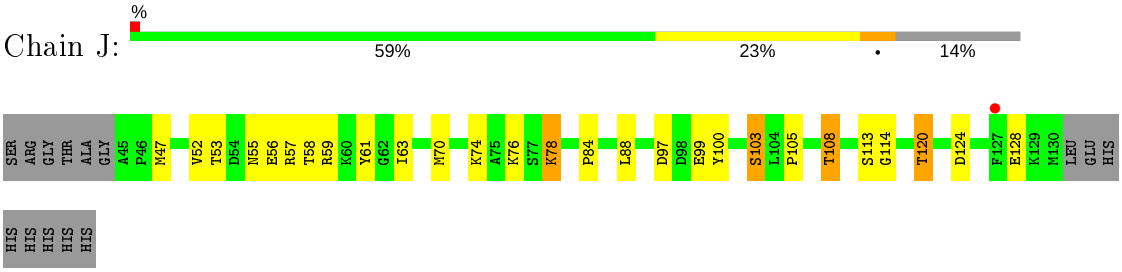
• Molecule 1: DNAation factor-related protein 4

Chain I:



• Molecule 1: DNAation factor-related protein 4

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.51Å 103.72Å 103.82Å 102.46° 105.81° 105.77°	Depositor
Resolution (Å)	29.83 – 3.00 29.83 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.6 (29.83-3.00) 91.6 (29.83-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 3.00Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.216 , 0.263 0.240 , 0.290	Depositor DCC
R_{free} test set	1992 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 19.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.449 for h,-h-k,-h-l 0.033 for -h,h+l,h+k 0.030 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6748	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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	0.58	0/679	0.74	0/914
1	B	0.59	0/698	0.73	0/937
1	C	0.67	0/694	0.80	1/932 (0.1%)
1	D	0.61	0/686	0.71	0/921
1	E	0.57	0/679	0.71	0/914
1	F	0.63	0/686	0.76	0/921
1	G	0.61	0/686	0.78	2/921 (0.2%)
1	H	0.58	0/686	0.68	0/921
1	I	0.60	0/679	0.72	0/914
1	J	0.57	0/686	0.72	1/921 (0.1%)
All	All	0.60	0/6859	0.74	4/9216 (0.0%)

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	F	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	125	PHE	CB-CG-CD1	-7.05	115.86	120.80
1	G	119	ILE	CA-CB-CG1	-6.00	99.60	111.00
1	G	57	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	J	88	LEU	CB-CG-CD1	-5.13	102.28	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	116	ASP	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	667	0	659	24	0
1	B	687	0	681	25	0
1	C	683	0	679	25	0
1	D	675	0	668	22	0
1	E	667	0	659	16	0
1	F	675	0	668	19	0
1	G	675	0	668	33	0
1	H	675	0	668	29	0
1	I	667	0	659	19	0
1	J	675	0	668	18	0
2	B	1	0	0	0	0
2	H	1	0	0	0	0
All	All	6748	0	6677	207	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 15.

All (207) 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:G:65:ALA:HA	1:G:70:MSE:HE3	1.60	0.83
1:E:59:ARG:NH1	1:E:78:LYS:O	2.12	0.82
1:H:59:ARG:NH2	1:H:78:LYS:O	2.11	0.82
1:C:51:LYS:NZ	1:D:91:ASP:OD2	2.13	0.81
1:D:76:LYS:NZ	1:D:82:LEU:O	2.17	0.77
1:H:57:ARG:NH2	1:H:111:ILE:HD11	2.01	0.75
1:C:107:GLN:NE2	1:D:103:SER:OG	2.20	0.74
1:G:47:MSE:HE3	1:H:99:GLU:HG2	1.68	0.74
1:E:79:PHE:HB3	1:E:81:LEU:HD12	1.70	0.74
1:H:129:LYS:HA	1:H:129:LYS:HE3	1.70	0.74
1:D:51:LYS:HE2	1:D:107:GLN:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LYS:HE3	1:B:107:GLN:HB3	1.73	0.71
1:F:57:ARG:NH1	1:F:122:ASP:OD2	2.25	0.69
1:B:76:LYS:HE2	1:B:84:PRO:HG3	1.75	0.69
1:B:64:GLY:HA3	1:C:99:GLU:HB2	1.75	0.68
1:I:59:ARG:NH2	1:I:78:LYS:O	2.26	0.68
1:B:54:ASP:HB3	1:B:79:PHE:HE2	1.58	0.67
1:D:54:ASP:HB3	1:D:79:PHE:HE2	1.60	0.67
1:C:65:ALA:HA	1:C:70:MSE:SE	2.45	0.67
1:D:76:LYS:HB2	1:D:84:PRO:HG3	1.75	0.67
1:B:121:THR:HG23	1:B:124:ASP:H	1.62	0.64
1:G:91:ASP:HB3	1:G:93:PHE:HD1	1.62	0.64
1:A:54:ASP:OD2	1:A:57:ARG:N	2.30	0.64
1:J:61:TYR:CE1	1:J:78:LYS:HD2	2.32	0.64
1:A:54:ASP:OD1	1:A:58:THR:HG22	1.97	0.64
1:D:57:ARG:NH2	1:D:120:THR:O	2.31	0.63
1:F:51:LYS:HE2	1:F:107:GLN:HB3	1.81	0.63
1:A:61:TYR:CE1	1:A:78:LYS:HD2	2.34	0.63
1:A:107:GLN:NE2	1:B:103:SER:OG	2.32	0.62
1:G:72:ILE:HD11	1:G:84:PRO:O	1.98	0.62
1:E:51:LYS:HE2	1:E:107:GLN:HB3	1.79	0.62
1:I:54:ASP:HB3	1:I:79:PHE:HE1	1.64	0.62
1:C:125:PHE:CZ	1:C:129:LYS:HE2	2.35	0.62
1:G:91:ASP:HB3	1:G:93:PHE:CD1	2.34	0.61
1:A:125:PHE:HD2	1:A:126:GLU:HG2	1.66	0.61
1:J:124:ASP:O	1:J:128:GLU:HG3	2.01	0.61
1:C:55:ASN:OD1	1:C:120:THR:OG1	2.18	0.61
1:H:58:THR:HG22	1:H:59:ARG:HG2	1.83	0.61
1:B:76:LYS:HE3	1:B:84:PRO:HD3	1.83	0.61
1:G:55:ASN:OD1	1:G:119:ILE:HG23	2.01	0.60
1:B:54:ASP:HB3	1:B:79:PHE:CE2	2.36	0.60
1:G:86:LEU:HB2	1:G:95:VAL:HG12	1.84	0.60
1:C:55:ASN:HD21	1:C:120:THR:H	1.50	0.60
1:H:47:MSE:CE	1:I:99:GLU:HG2	2.31	0.60
1:H:111:ILE:HD12	1:H:119:ILE:CG2	2.32	0.60
1:G:107:GLN:NE2	1:H:103:SER:OG	2.35	0.59
1:C:61:TYR:CE2	1:C:78:LYS:HD2	2.37	0.59
1:H:129:LYS:HA	1:H:129:LYS:CE	2.33	0.58
1:D:85:HIS:CD2	1:D:115:PRO:HA	2.38	0.58
1:A:85:HIS:CE1	1:A:115:PRO:HB3	2.38	0.58
1:F:76:LYS:HB2	1:F:84:PRO:HG3	1.85	0.57
1:H:76:LYS:NZ	1:H:81:LEU:O	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:57:ARG:NH2	1:J:120:THR:O	2.34	0.57
1:G:57:ARG:HG3	1:G:125:PHE:CE1	2.39	0.57
1:A:59:ARG:NE	1:A:59:ARG:HA	2.20	0.57
1:E:88:LEU:HD21	1:E:104:LEU:HD13	1.85	0.57
1:A:91:ASP:HB3	1:A:93:PHE:CD1	2.39	0.57
1:J:52:VAL:HG21	1:J:63:ILE:HD12	1.87	0.56
1:I:100:TYR:O	1:I:103:SER:HB3	2.06	0.56
1:F:55:ASN:OD1	1:F:119:ILE:HG23	2.05	0.56
1:G:87:TYR:CG	1:G:119:ILE:HD12	2.41	0.56
1:A:51:LYS:HE2	1:A:107:GLN:HB3	1.88	0.55
1:F:97:ASP:OD2	1:F:99:GLU:HB2	2.07	0.55
1:D:107:GLN:NE2	1:E:103:SER:OG	2.40	0.55
1:I:107:GLN:NE2	1:J:103:SER:OG	2.40	0.55
1:C:128:GLU:HG2	1:C:129:LYS:HZ2	1.72	0.55
1:F:100:TYR:O	1:F:103:SER:HB3	2.07	0.55
1:A:52:VAL:HG21	1:A:63:ILE:HD12	1.87	0.55
1:B:100:TYR:O	1:B:103:SER:HB3	2.06	0.54
1:J:97:ASP:OD2	1:J:99:GLU:N	2.39	0.54
1:D:65:ALA:HA	1:D:70:MSE:SE	2.57	0.54
1:B:51:LYS:HE2	1:C:100:TYR:OH	2.07	0.54
1:I:65:ALA:HA	1:I:70:MSE:SE	2.57	0.54
1:D:54:ASP:HB3	1:D:79:PHE:CE2	2.43	0.54
1:H:47:MSE:HE1	1:H:70:MSE:SE	2.57	0.54
1:C:62:GLY:O	1:D:96:SER:OG	2.23	0.54
1:J:105:PRO:HG2	1:J:108:THR:HG23	1.89	0.54
1:H:111:ILE:HD12	1:H:119:ILE:HG23	1.90	0.53
1:G:100:TYR:O	1:G:103:SER:HB3	2.07	0.53
1:B:65:ALA:HA	1:B:70:MSE:SE	2.58	0.53
1:F:85:HIS:CE1	1:F:115:PRO:HG3	2.43	0.53
1:J:59:ARG:NH2	1:J:78:LYS:O	2.41	0.53
1:G:85:HIS:ND1	1:G:115:PRO:HA	2.23	0.53
1:A:91:ASP:HB3	1:A:93:PHE:HD1	1.72	0.52
1:B:68:LEU:HD22	1:B:95:VAL:HG12	1.91	0.52
1:G:95:VAL:HG23	1:G:100:TYR:HD2	1.75	0.52
1:H:100:TYR:O	1:H:103:SER:HB3	2.09	0.52
1:A:54:ASP:OD1	1:A:56:GLU:HB2	2.10	0.52
1:C:85:HIS:CE1	1:C:115:PRO:HG3	2.45	0.52
1:E:65:ALA:HA	1:E:70:MSE:SE	2.60	0.52
1:H:52:VAL:HG21	1:H:63:ILE:HD12	1.92	0.51
1:A:65:ALA:HA	1:A:70:MSE:SE	2.61	0.51
1:I:72:ILE:HD12	1:I:73:ALA:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HG23	1:A:59:ARG:N	2.26	0.51
1:C:107:GLN:HE22	1:D:103:SER:HG	1.57	0.51
1:C:59:ARG:NH1	1:C:78:LYS:O	2.43	0.51
1:G:66:ASN:H	1:G:70:MSE:HE3	1.76	0.51
1:H:47:MSE:HE3	1:I:99:GLU:HG2	1.93	0.51
1:C:121:THR:O	1:C:125:PHE:N	2.42	0.51
1:E:61:TYR:CE1	1:E:78:LYS:HD3	2.46	0.51
1:I:54:ASP:HB3	1:I:79:PHE:CE1	2.46	0.50
1:J:56:GLU:O	1:J:58:THR:HG23	2.12	0.50
1:G:68:LEU:HD11	1:G:86:LEU:HD12	1.93	0.50
1:G:69:GLU:O	1:G:72:ILE:HG22	2.11	0.50
1:D:100:TYR:O	1:D:103:SER:HB3	2.12	0.49
1:B:70:MSE:HE2	1:B:74:LYS:NZ	2.27	0.49
1:H:47:MSE:HE2	1:I:99:GLU:HG2	1.94	0.49
1:G:111:ILE:HG21	1:G:119:ILE:HD13	1.95	0.49
1:I:111:ILE:HG21	1:I:119:ILE:HD12	1.94	0.48
1:D:52:VAL:HG21	1:D:63:ILE:HD12	1.95	0.48
1:G:57:ARG:HH12	1:G:122:ASP:HB3	1.77	0.48
1:E:88:LEU:HD21	1:E:104:LEU:CD1	2.44	0.48
1:A:47:MSE:HG2	1:B:99:GLU:HB3	1.94	0.48
1:G:66:ASN:H	1:G:70:MSE:CE	2.26	0.48
1:F:47:MSE:HE2	1:G:99:GLU:HG2	1.95	0.48
1:C:100:TYR:O	1:C:103:SER:HB3	2.14	0.48
1:B:105:PRO:HG2	1:B:108:THR:HG23	1.95	0.47
1:A:54:ASP:CG	1:A:56:GLU:H	2.18	0.47
1:J:70:MSE:HE2	1:J:74:LYS:CE	2.43	0.47
1:A:73:ALA:O	1:A:76:LYS:HB3	2.13	0.47
1:J:76:LYS:HB2	1:J:84:PRO:HG3	1.97	0.47
1:J:100:TYR:O	1:J:103:SER:HB3	2.14	0.47
1:E:100:TYR:O	1:E:103:SER:HB3	2.14	0.47
1:D:61:TYR:HD2	1:E:94:GLU:HB3	1.80	0.47
1:F:82:LEU:HD23	1:F:83:GLU:H	1.80	0.47
1:I:52:VAL:HG21	1:I:63:ILE:HD12	1.96	0.47
1:B:53:THR:HG21	1:B:57:ARG:HD3	1.98	0.46
1:C:125:PHE:CE1	1:C:129:LYS:HE2	2.49	0.46
1:C:128:GLU:HG2	1:C:129:LYS:NZ	2.30	0.46
1:F:54:ASP:HB3	1:F:79:PHE:CE1	2.50	0.46
1:A:59:ARG:HA	1:A:59:ARG:HE	1.80	0.46
1:A:70:MSE:O	1:A:74:LYS:HG3	2.16	0.46
1:F:54:ASP:OD2	1:F:58:THR:OG1	2.34	0.46
1:F:98:ASP:OD1	1:F:102:LYS:NZ	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:61:TYR:CD1	1:J:78:LYS:HD2	2.51	0.46
1:J:70:MSE:HE2	1:J:74:LYS:HE3	1.98	0.46
1:B:52:VAL:HG21	1:B:63:ILE:HD12	1.97	0.45
1:A:121:THR:HG23	1:A:124:ASP:H	1.81	0.45
1:A:86:LEU:HA	1:A:86:LEU:HD23	1.65	0.45
1:I:68:LEU:HD22	1:I:95:VAL:HG12	1.98	0.45
1:B:125:PHE:C	1:B:125:PHE:CD2	2.89	0.45
1:B:70:MSE:HE2	1:B:74:LYS:CE	2.47	0.45
1:H:61:TYR:CE1	1:H:78:LYS:HD2	2.51	0.45
1:F:85:HIS:ND1	1:F:115:PRO:HG3	2.32	0.45
1:H:65:ALA:HA	1:H:70:MSE:SE	2.67	0.45
1:G:87:TYR:N	1:G:87:TYR:CD2	2.85	0.45
1:G:51:LYS:HE2	1:G:107:GLN:HB3	2.00	0.44
1:D:72:ILE:HG23	1:D:84:PRO:HG2	1.99	0.44
1:H:57:ARG:CZ	1:H:111:ILE:HD11	2.47	0.44
1:C:52:VAL:HG21	1:C:63:ILE:HD12	1.99	0.44
1:I:76:LYS:HE2	1:I:82:LEU:O	2.18	0.44
1:J:47:MSE:HE2	1:J:47:MSE:HB2	1.81	0.44
1:E:51:LYS:O	1:E:109:LEU:HD12	2.16	0.44
1:H:91:ASP:HB3	1:H:93:PHE:CD1	2.52	0.44
1:I:70:MSE:O	1:I:74:LYS:HG3	2.18	0.44
1:F:47:MSE:CE	1:G:99:GLU:HG2	2.48	0.43
1:C:86:LEU:HA	1:C:86:LEU:HD23	1.70	0.43
1:C:82:LEU:HA	1:C:82:LEU:HD23	1.84	0.43
1:G:111:ILE:CG2	1:G:119:ILE:HD13	2.48	0.43
1:H:107:GLN:NE2	1:I:103:SER:OG	2.47	0.43
1:H:86:LEU:HD23	1:H:86:LEU:HA	1.78	0.43
1:B:83:GLU:O	1:B:115:PRO:HD3	2.19	0.42
1:J:53:THR:HG21	1:J:57:ARG:HG2	2.01	0.42
1:F:54:ASP:HB3	1:F:79:PHE:HE1	1.84	0.42
1:G:98:ASP:OD2	1:G:102:LYS:NZ	2.52	0.42
1:H:91:ASP:HB3	1:H:93:PHE:HD1	1.83	0.42
1:H:55:ASN:HA	1:H:111:ILE:HD13	2.00	0.42
1:H:70:MSE:O	1:H:74:LYS:HG3	2.19	0.42
1:E:88:LEU:HD23	1:E:110:PHE:CE1	2.54	0.42
1:F:81:LEU:H	1:F:81:LEU:HD12	1.84	0.42
1:D:76:LYS:HG3	1:D:76:LYS:O	2.17	0.42
1:F:111:ILE:HG13	1:F:119:ILE:HG21	2.01	0.42
1:G:70:MSE:SE	1:G:74:LYS:HE3	2.70	0.42
1:G:78:LYS:HB3	1:G:78:LYS:HE2	1.82	0.42
1:A:59:ARG:HB3	1:A:61:TYR:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:MSE:CG	1:A:74:LYS:HE3	2.49	0.42
1:C:125:PHE:O	1:C:129:LYS:HD2	2.19	0.42
1:G:47:MSE:CE	1:H:99:GLU:HG2	2.46	0.42
1:D:111:ILE:HG21	1:D:119:ILE:HD12	2.02	0.41
1:G:98:ASP:OD1	1:G:102:LYS:NZ	2.53	0.41
1:B:70:MSE:HE2	1:B:74:LYS:HE3	2.02	0.41
1:C:64:GLY:HA3	1:D:99:GLU:HB3	2.02	0.41
1:I:120:THR:H	1:I:120:THR:HG1	1.58	0.41
1:B:76:LYS:CE	1:B:84:PRO:HD3	2.49	0.41
1:E:47:MSE:HE2	1:E:47:MSE:HB2	1.91	0.41
1:I:50:TYR:CE1	1:I:101:LEU:HD11	2.55	0.41
1:J:113:SER:OG	1:J:114:GLY:N	2.53	0.41
1:D:47:MSE:HB2	1:D:47:MSE:HE2	1.82	0.41
1:J:55:ASN:OD1	1:J:120:THR:OG1	2.37	0.41
1:C:57:ARG:HG2	1:C:125:PHE:CE1	2.55	0.41
1:H:51:LYS:HE2	1:H:107:GLN:HB3	2.03	0.41
1:C:72:ILE:HD11	1:C:86:LEU:HG	2.03	0.41
1:E:72:ILE:HD11	1:E:86:LEU:HG	2.02	0.41
1:G:84:PRO:HB2	1:G:112:VAL:CG2	2.51	0.41
1:F:86:LEU:HD23	1:F:112:VAL:HG22	2.03	0.41
1:B:70:MSE:O	1:B:74:LYS:HG3	2.21	0.40
1:D:81:LEU:HA	1:D:81:LEU:HD13	1.69	0.40
1:F:107:GLN:NE2	1:G:103:SER:HG	2.19	0.40
1:G:54:ASP:HB3	1:G:79:PHE:CE1	2.57	0.40
1:H:83:GLU:O	1:H:115:PRO:HD3	2.22	0.40
1:A:58:THR:CG2	1:A:59:ARG:N	2.84	0.40
1:H:62:GLY:O	1:I:96:SER:OG	2.31	0.40
1:G:61:TYR:CD1	1:G:78:LYS:NZ	2.78	0.40
1:B:82:LEU:HD23	1:B:82:LEU:O	2.22	0.40
1:E:57:ARG:NH2	1:E:120:THR:O	2.52	0.40
1:B:119:ILE:HD12	1:B:120:THR:C	2.41	0.40
1:E:83:GLU:HG2	1:E:115:PRO:HG3	2.04	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	83/100 (83%)	78 (94%)	5 (6%)	0	100 100
1	B	86/100 (86%)	82 (95%)	4 (5%)	0	100 100
1	C	85/100 (85%)	78 (92%)	6 (7%)	1 (1%)	13 48
1	D	84/100 (84%)	79 (94%)	5 (6%)	0	100 100
1	E	83/100 (83%)	76 (92%)	7 (8%)	0	100 100
1	F	84/100 (84%)	80 (95%)	4 (5%)	0	100 100
1	G	84/100 (84%)	77 (92%)	7 (8%)	0	100 100
1	H	84/100 (84%)	81 (96%)	3 (4%)	0	100 100
1	I	83/100 (83%)	78 (94%)	4 (5%)	1 (1%)	13 48
1	J	84/100 (84%)	81 (96%)	3 (4%)	0	100 100
All	All	840/1000 (84%)	790 (94%)	48 (6%)	2 (0%)	47 82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	81	LEU
1	C	84	PRO

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	72/81 (89%)	69 (96%)	3 (4%)	30 66
1	B	74/81 (91%)	68 (92%)	6 (8%)	11 40
1	C	74/81 (91%)	71 (96%)	3 (4%)	30 67
1	D	73/81 (90%)	67 (92%)	6 (8%)	11 39
1	E	72/81 (89%)	71 (99%)	1 (1%)	67 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	73/81 (90%)	69 (94%)	4 (6%)	21 57
1	G	73/81 (90%)	71 (97%)	2 (3%)	44 77
1	H	73/81 (90%)	70 (96%)	3 (4%)	30 67
1	I	72/81 (89%)	70 (97%)	2 (3%)	43 77
1	J	73/81 (90%)	69 (94%)	4 (6%)	21 57
All	All	729/810 (90%)	695 (95%)	34 (5%)	26 63

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	SER
1	A	103	SER
1	A	129	LYS
1	B	56	GLU
1	B	59	ARG
1	B	76	LYS
1	B	90	SER
1	B	103	SER
1	B	130	MSE
1	C	90	SER
1	C	103	SER
1	C	129	LYS
1	D	76	LYS
1	D	97	ASP
1	D	103	SER
1	D	120	THR
1	D	121	THR
1	D	130	MSE
1	E	97	ASP
1	F	59	ARG
1	F	90	SER
1	F	103	SER
1	F	120	THR
1	G	90	SER
1	G	103	SER
1	H	90	SER
1	H	103	SER
1	H	112	VAL
1	I	97	ASP
1	I	103	SER

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Mol	Chain	Res	Type
1	J	78	LYS
1	J	103	SER
1	J	108	THR
1	J	120	THR

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

Mol	Chain	Res	Type
1	C	55	ASN
1	C	107	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	83/100 (83%)	0.18	1 (1%) 79 54	38, 60, 97, 114	0
1	B	85/100 (85%)	0.21	2 (2%) 59 30	34, 60, 100, 117	0
1	C	84/100 (84%)	0.13	2 (2%) 59 30	33, 50, 94, 109	0
1	D	83/100 (83%)	0.16	0 100 100	32, 52, 90, 103	0
1	E	83/100 (83%)	0.27	3 (3%) 42 17	31, 48, 88, 110	0
1	F	83/100 (83%)	0.17	1 (1%) 79 54	36, 57, 109, 129	0
1	G	83/100 (83%)	0.15	2 (2%) 59 30	38, 61, 104, 131	0
1	H	83/100 (83%)	0.14	2 (2%) 59 30	36, 52, 83, 110	0
1	I	83/100 (83%)	0.21	2 (2%) 59 30	32, 52, 91, 104	0
1	J	83/100 (83%)	0.15	1 (1%) 79 54	37, 50, 91, 97	0
All	All	833/1000 (83%)	0.18	16 (1%) 66 37	31, 54, 97, 131	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	82	LEU	4.1
1	B	82	LEU	3.4
1	G	129	LYS	3.3
1	G	82	LEU	3.2
1	I	82	LEU	3.0
1	H	82	LEU	2.9
1	E	129	LYS	2.8
1	F	127	PHE	2.7
1	I	127	PHE	2.6
1	C	127	PHE	2.6
1	C	82	LEU	2.4
1	J	127	PHE	2.3
1	A	127	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	83	GLU	2.1
1	E	83	GLU	2.0
1	B	127	PHE	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 carbohydrates 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.