Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 02:36 PM JST

PDB ID	:	8ZYS / pdb_00008zys
Title	:	Crystal structure of HSF5 DNA-binding domain in complex with 3-site HSE DNA (25 bp)
Authors	:	Shi, X.; Zhang, Q.; Liu, W.
Deposited on	:	2024-06-18
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:

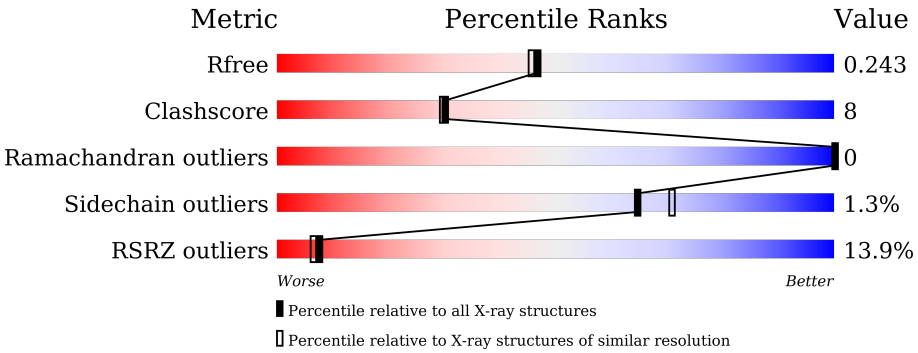
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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	129	9% 57% 16% · 26%
1	B	129	8% 64% 9% · 26%
1	C	129	24% 55% 18% 27%
1	D	129	10% 66% 8% 26%
1	E	129	8% 61% 12% 26%
1	F	129	12% 51% 16% · 30%

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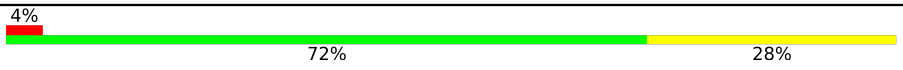
Mol	Chain	Length	Quality of chain
2	G	25	
2	I	25	
3	H	25	
3	J	25	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7166 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 Heat shock factor protein 5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	95	Total 803	C 524	N 150	O 129	0	0	0
1	B	95	Total 806	C 527	N 150	O 129	0	0	0
1	C	94	Total 791	C 513	N 149	O 129	0	0	0
1	D	95	Total 810	C 527	N 152	O 131	0	0	0
1	E	95	Total 807	C 525	N 150	O 132	0	0	0
1	F	90	Total 765	C 499	N 145	O 121	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP Q4G112
A	5	HIS	-	expression tag	UNP Q4G112
A	6	HIS	-	expression tag	UNP Q4G112
A	7	HIS	-	expression tag	UNP Q4G112
A	8	HIS	-	expression tag	UNP Q4G112
A	9	HIS	-	expression tag	UNP Q4G112
A	10	HIS	-	expression tag	UNP Q4G112
B	4	MET	-	initiating methionine	UNP Q4G112
B	5	HIS	-	expression tag	UNP Q4G112
B	6	HIS	-	expression tag	UNP Q4G112
B	7	HIS	-	expression tag	UNP Q4G112
B	8	HIS	-	expression tag	UNP Q4G112
B	9	HIS	-	expression tag	UNP Q4G112
B	10	HIS	-	expression tag	UNP Q4G112
C	4	MET	-	initiating methionine	UNP Q4G112
C	5	HIS	-	expression tag	UNP Q4G112
C	6	HIS	-	expression tag	UNP Q4G112

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Chain	Residue	Modelled	Actual	Comment	Reference
C	7	HIS	-	expression tag	UNP Q4G112
C	8	HIS	-	expression tag	UNP Q4G112
C	9	HIS	-	expression tag	UNP Q4G112
C	10	HIS	-	expression tag	UNP Q4G112
D	4	MET	-	initiating methionine	UNP Q4G112
D	5	HIS	-	expression tag	UNP Q4G112
D	6	HIS	-	expression tag	UNP Q4G112
D	7	HIS	-	expression tag	UNP Q4G112
D	8	HIS	-	expression tag	UNP Q4G112
D	9	HIS	-	expression tag	UNP Q4G112
D	10	HIS	-	expression tag	UNP Q4G112
E	4	MET	-	initiating methionine	UNP Q4G112
E	5	HIS	-	expression tag	UNP Q4G112
E	6	HIS	-	expression tag	UNP Q4G112
E	7	HIS	-	expression tag	UNP Q4G112
E	8	HIS	-	expression tag	UNP Q4G112
E	9	HIS	-	expression tag	UNP Q4G112
E	10	HIS	-	expression tag	UNP Q4G112
F	4	MET	-	initiating methionine	UNP Q4G112
F	5	HIS	-	expression tag	UNP Q4G112
F	6	HIS	-	expression tag	UNP Q4G112
F	7	HIS	-	expression tag	UNP Q4G112
F	8	HIS	-	expression tag	UNP Q4G112
F	9	HIS	-	expression tag	UNP Q4G112
F	10	HIS	-	expression tag	UNP Q4G112

- Molecule 2 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	25	Total	C	N	O	P	0	0	0
			508	243	96	145	24			
2	I	25	Total	C	N	O	P	0	0	0
			508	243	96	145	24			

- Molecule 3 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	24	Total	C	N	O	P	0	0	0
			494	235	89	146	24			
3	J	25	Total	C	N	O	P	0	0	0
			511	245	91	151	24			

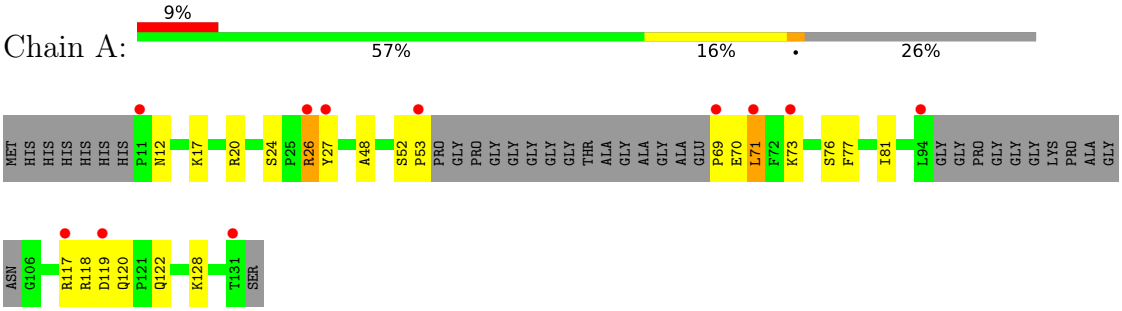
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	56	Total O 56 56	0	0
4	B	50	Total O 50 50	0	0
4	C	3	Total O 3 3	0	0
4	D	37	Total O 37 37	0	0
4	E	54	Total O 54 54	0	0
4	F	15	Total O 15 15	0	0
4	G	42	Total O 42 42	0	0
4	H	35	Total O 35 35	0	0
4	I	36	Total O 36 36	0	0
4	J	35	Total O 35 35	0	0

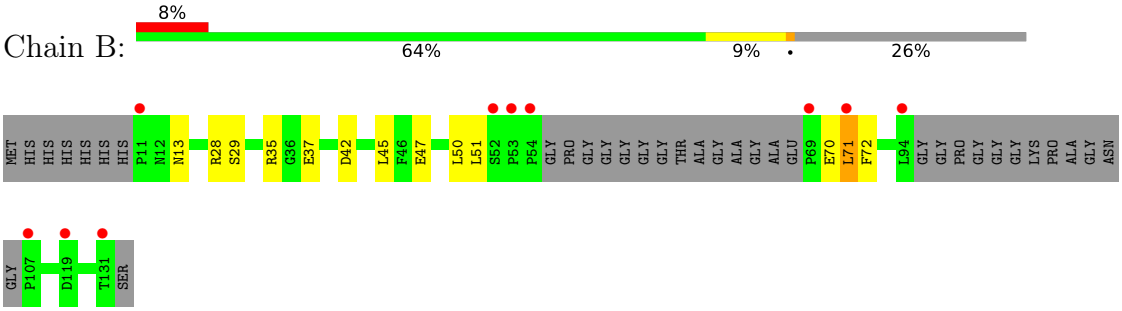
3 Residue-property plots (i)

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.

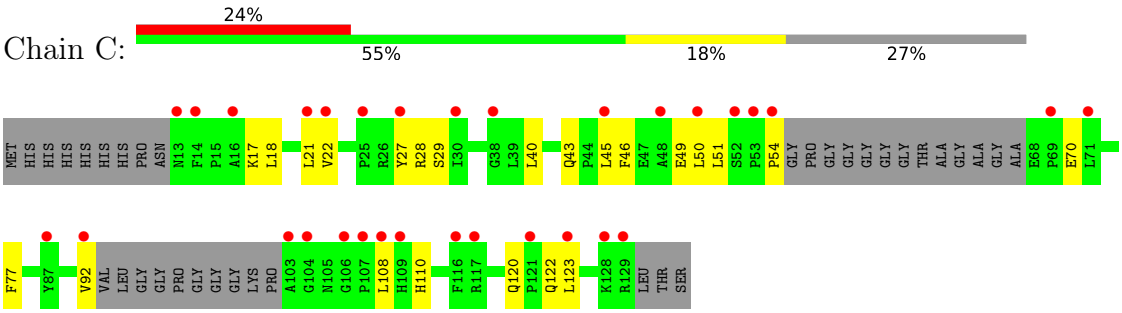
• Molecule 1: Heat shock factor protein 5



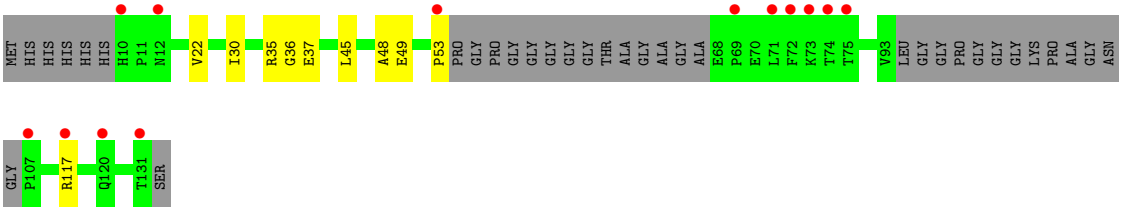
• Molecule 1: Heat shock factor protein 5



• Molecule 1: Heat shock factor protein 5

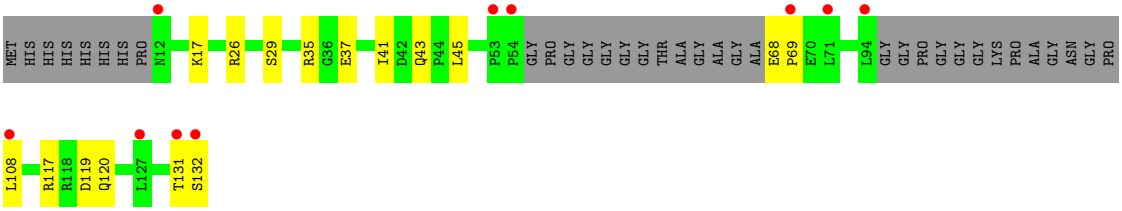


• Molecule 1: Heat shock factor protein 5



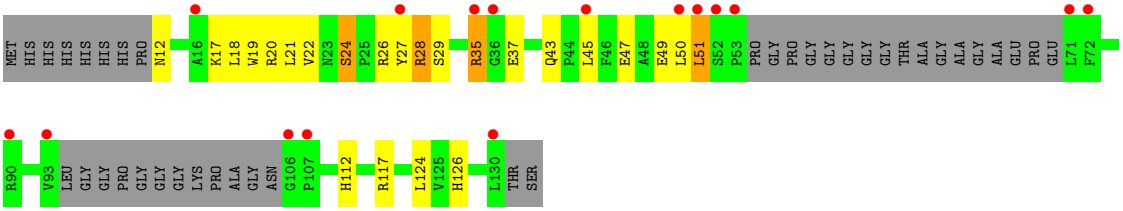
• Molecule 1: Heat shock factor protein 5

Chain E:



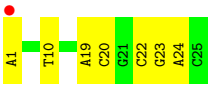
• Molecule 1: Heat shock factor protein 5

Chain F:



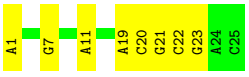
• Molecule 2: DNA (25-MER)

Chain G:



• Molecule 2: DNA (25-MER)

Chain I:



• Molecule 3: DNA (25-MER)

Chain H:

• Molecule 3: DNA (25-MER)

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.96Å 50.00Å 126.88Å 78.95° 88.54° 73.07°	Depositor
Resolution (Å)	41.51 – 2.00 41.51 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (41.51-2.00) 96.6 (41.51-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122, BUSTER 2.10.4	Depositor
R, R_{free}	0.213 , 0.241 0.213 , 0.243	Depositor DCC
R_{free} test set	6386 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-k+l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7166	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3897e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.37	0/828	0.83	6/1118 (0.5%)
1	B	0.34	0/832	0.56	0/1124
1	C	0.17	0/816	0.46	0/1102
1	D	0.32	0/836	0.62	0/1130
1	E	0.30	0/831	0.52	0/1123
1	F	0.38	0/788	0.87	5/1063 (0.5%)
2	G	0.34	0/570	0.58	0/877
2	I	0.33	0/570	0.55	0/877
3	H	0.36	0/553	0.56	0/852
3	J	0.32	0/572	0.54	0/882
All	All	0.33	0/7196	0.63	11/10148 (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	A	0	1
1	C	0	1
1	F	0	1
All	All	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	35	ARG	CB-CG-CD	-12.52	82.50	111.30
1	A	26	ARG	CD-NE-CZ	-9.40	111.24	124.40
1	A	26	ARG	CG-CD-NE	9.13	132.09	112.00
1	A	71	LEU	CB-CG-CD1	-7.65	87.74	110.70
1	F	35	ARG	CG-CD-NE	7.28	128.02	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	LEU	N-CA-CB	-6.91	100.34	110.84
1	F	35	ARG	CA-CB-CG	6.85	127.80	114.10
1	A	71	LEU	CB-CG-CD2	5.64	127.61	110.70
1	A	71	LEU	CB-CA-C	5.27	118.57	110.62
1	F	51	LEU	CA-C-N	5.03	128.25	121.20
1	F	51	LEU	C-N-CA	5.03	128.25	121.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	GLU	Peptide
1	C	28	ARG	Sidechain
1	F	28	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	803	0	810	15	0
1	B	806	0	815	12	0
1	C	791	0	784	15	0
1	D	810	0	808	8	0
1	E	807	0	809	13	0
1	F	765	0	770	20	0
2	G	508	0	282	6	0
2	I	508	0	282	7	0
3	H	494	0	272	2	0
3	J	511	0	285	8	0
4	A	56	0	0	4	2
4	B	50	0	0	3	2
4	C	3	0	0	0	0
4	D	37	0	0	4	1
4	E	54	0	0	3	1
4	F	15	0	0	6	0
4	G	42	0	0	1	0
4	H	35	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	36	0	0	1	0
4	J	35	0	0	3	0
All	All	7166	0	5917	105	3

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 8.

All (105) 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)
3:J:7:DG:N3	4:J:101:HOH:O	1.88	1.05
1:E:17:LYS:NZ	4:E:201:HOH:O	1.97	0.95
1:E:43:GLN:H	1:E:108:LEU:HD23	1.38	0.88
3:J:25:DG:N7	4:J:102:HOH:O	2.08	0.85
1:E:119:ASP:OD1	1:E:120:GLN:NE2	2.08	0.84
1:F:112:HIS:ND1	4:F:204:HOH:O	2.09	0.84
1:A:12:ASN:O	4:A:201:HOH:O	1.99	0.78
1:B:51:LEU:O	4:B:201:HOH:O	2.01	0.77
1:C:120:GLN:HB3	1:C:123:LEU:HD23	1.67	0.77
1:F:37:GLU:O	4:F:201:HOH:O	2.01	0.77
1:D:117:ARG:NH2	4:D:202:HOH:O	2.19	0.75
1:E:68:GLU:HG2	1:E:69:PRO:HD3	1.70	0.74
1:E:35:ARG:NH1	4:E:203:HOH:O	2.20	0.73
1:C:49:GLU:HG3	1:C:50:LEU:HD23	1.69	0.73
1:F:27:TYR:O	4:F:202:HOH:O	2.05	0.73
3:H:7:DG:N3	4:H:101:HOH:O	2.20	0.73
1:F:22:VAL:O	4:F:203:HOH:O	2.07	0.72
1:F:35:ARG:HB3	1:F:37:GLU:OE1	1.89	0.71
1:B:70:GLU:OE2	4:B:202:HOH:O	2.07	0.71
3:H:4:DC:H2"	3:H:5:DG:C8	2.27	0.69
1:C:21:LEU:HD21	1:C:50:LEU:HD11	1.74	0.69
1:D:36:GLY:O	4:D:201:HOH:O	2.09	0.69
2:I:7:DG:OP2	4:I:201:HOH:O	2.12	0.68
1:D:37:GLU:HG2	4:D:201:HOH:O	1.94	0.67
3:J:4:DC:H2"	3:J:5:DG:C8	2.32	0.65
3:J:25:DG:O6	4:J:103:HOH:O	2.11	0.64
1:F:37:GLU:HG3	1:F:117:ARG:HB3	1.79	0.63
1:E:131:THR:OG1	1:E:132:SER:N	2.35	0.60
1:D:117:ARG:HB2	4:D:201:HOH:O	2.01	0.59
1:A:120:GLN:OE1	1:A:122:GLN:NE2	2.37	0.58
1:D:45:LEU:O	1:D:49:GLU:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:SER:OG	1:F:26:ARG:HG3	2.03	0.58
1:F:17:LYS:O	1:F:21:LEU:HG	2.03	0.57
1:A:118:ARG:NH1	4:A:203:HOH:O	2.25	0.57
1:F:29:SER:HB3	1:F:45:LEU:HB3	1.87	0.57
1:F:43:GLN:O	1:F:47:GLU:HG3	2.06	0.56
1:A:117:ARG:CG	1:A:117:ARG:HH11	2.20	0.54
1:E:35:ARG:HH11	1:E:35:ARG:HG3	1.72	0.54
1:F:18:LEU:O	1:F:22:VAL:HG12	2.08	0.53
1:A:73:LYS:NZ	4:A:206:HOH:O	2.41	0.53
1:A:20:ARG:HB3	1:A:69:PRO:HG3	1.91	0.52
1:A:119:ASP:OD2	1:A:120:GLN:HG2	2.08	0.52
1:D:35:ARG:HB3	1:D:37:GLU:HG3	1.92	0.52
2:G:19:DA:H2"	2:G:20:DC:O5'	2.09	0.52
1:F:19:TRP:CE3	1:F:124:LEU:HD11	2.45	0.52
1:C:18:LEU:O	1:C:22:VAL:HG12	2.09	0.51
1:F:27:TYR:CD2	1:F:50:LEU:HD21	2.46	0.51
2:I:19:DA:H2"	2:I:20:DC:O5'	2.09	0.51
1:C:29:SER:HB3	1:C:45:LEU:HB3	1.92	0.51
1:B:71:LEU:HD22	1:B:72:PHE:N	2.26	0.50
1:F:126:HIS:HB3	4:F:205:HOH:O	2.11	0.50
2:I:22:DC:H2"	2:I:23:DG:C8	2.46	0.50
2:G:22:DC:H2"	2:G:23:DG:C8	2.46	0.50
1:C:49:GLU:HA	1:C:54:PRO:HA	1.94	0.50
1:E:26:ARG:HH12	1:E:68:GLU:HB2	1.76	0.50
1:B:50:LEU:O	1:B:51:LEU:HD23	2.12	0.50
2:G:10:DT:OP2	4:G:101:HOH:O	2.19	0.50
2:G:19:DA:H2'	2:G:20:DC:C6	2.46	0.49
1:A:117:ARG:HH11	1:A:117:ARG:HG3	1.76	0.49
2:I:19:DA:H2'	2:I:20:DC:C6	2.47	0.49
1:B:71:LEU:HD23	1:B:71:LEU:HA	1.59	0.48
1:C:27:TYR:HE2	1:C:70:GLU:HG3	1.78	0.48
1:C:92:VAL:HG23	1:C:110:HIS:CD2	2.49	0.48
3:J:1:DT:H2"	3:J:2:DG:N7	2.29	0.48
1:E:29:SER:HB3	1:E:45:LEU:HG	1.96	0.48
1:E:35:ARG:NH1	1:E:35:ARG:HG3	2.29	0.47
1:B:47:GLU:HA	1:B:51:LEU:HB2	1.95	0.47
1:B:13:ASN:ND2	1:B:13:ASN:H	2.13	0.47
2:G:1:DA:H5'	2:G:1:DA:H8	1.79	0.47
1:C:43:GLN:HG3	1:C:77:PHE:CE1	2.50	0.47
1:C:40:LEU:HD22	1:C:108:LEU:HD21	1.97	0.46
2:I:1:DA:H8	2:I:1:DA:H5'	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:LEU:O	1:F:51:LEU:HD23	2.15	0.46
1:E:41:ILE:O	1:E:108:LEU:HB3	2.16	0.46
1:F:45:LEU:O	1:F:49:GLU:HG2	2.15	0.46
1:B:35:ARG:HB3	1:B:37:GLU:HG3	1.97	0.46
1:A:48:ALA:O	1:A:53:PRO:HD3	2.16	0.46
1:B:13:ASN:H	1:B:13:ASN:HD22	1.63	0.46
1:F:26:ARG:C	1:F:26:ARG:HD3	2.42	0.45
1:A:20:ARG:HH21	1:A:69:PRO:HA	1.82	0.44
1:A:26:ARG:HH11	1:A:26:ARG:HD3	1.36	0.44
1:D:48:ALA:O	1:D:53:PRO:HD3	2.18	0.44
1:F:12:ASN:ND2	4:F:207:HOH:O	2.49	0.44
1:D:22:VAL:HG12	1:D:30:ILE:HG12	1.99	0.43
1:A:128:LYS:HE2	4:A:222:HOH:O	2.18	0.43
3:J:2:DG:H1'	3:J:3:DT:H5'	1.99	0.43
1:B:29:SER:HB3	1:B:45:LEU:HG	2.00	0.43
1:C:45:LEU:O	1:C:49:GLU:HG2	2.18	0.43
1:F:20:ARG:O	1:F:24:SER:HB3	2.18	0.43
1:C:122:GLN:HG2	1:C:123:LEU:HD22	1.99	0.43
1:F:26:ARG:HD3	1:F:27:TYR:N	2.33	0.43
1:C:17:LYS:HB3	1:C:17:LYS:HE3	1.80	0.42
2:I:11:DA:C2	3:J:17:DA:C2	3.07	0.42
1:C:50:LEU:O	1:C:51:LEU:HD23	2.20	0.42
2:G:23:DG:H2"	2:G:24:DA:C8	2.54	0.42
1:B:71:LEU:HD22	1:B:72:PHE:H	1.84	0.42
1:A:17:LYS:HE3	1:A:69:PRO:O	2.19	0.41
2:I:20:DC:H2"	2:I:21:DG:C8	2.55	0.41
1:E:37:GLU:OE2	1:E:117:ARG:NH1	2.52	0.41
1:B:42:ASP:HB2	4:B:206:HOH:O	2.20	0.41
1:A:77:PHE:CE2	1:A:81:ILE:HD11	2.55	0.41
3:J:1:DT:H2"	3:J:2:DG:C5	2.56	0.41
1:A:24:SER:HB3	1:A:27:TYR:HD2	1.86	0.40
1:E:35:ARG:NH1	4:E:207:HOH:O	2.52	0.40
1:C:46:PHE:O	1:C:50:LEU:HB2	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:222:HOH:O	4:B:206:HOH:O[1_455]	1.93	0.27
4:D:236:HOH:O	4:E:233:HOH:O[1_655]	2.06	0.14
4:A:221:HOH:O	4:B:243:HOH:O[1_455]	2.07	0.13

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	89/129 (69%)	87 (98%)	2 (2%)	0	100	100
1	B	89/129 (69%)	88 (99%)	1 (1%)	0	100	100
1	C	88/129 (68%)	86 (98%)	2 (2%)	0	100	100
1	D	89/129 (69%)	86 (97%)	3 (3%)	0	100	100
1	E	89/129 (69%)	88 (99%)	1 (1%)	0	100	100
1	F	84/129 (65%)	84 (100%)	0	0	100	100
All	All	528/774 (68%)	519 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	88/104 (85%)	85 (97%)	3 (3%)	32	32
1	B	89/104 (86%)	87 (98%)	2 (2%)	47	51
1	C	85/104 (82%)	85 (100%)	0	100	100
1	D	89/104 (86%)	89 (100%)	0	100	100
1	E	89/104 (86%)	89 (100%)	0	100	100
1	F	83/104 (80%)	81 (98%)	2 (2%)	44	47
All	All	523/624 (84%)	516 (99%)	7 (1%)	65	71

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	71	LEU
1	A	76	SER
1	B	28	ARG
1	B	71	LEU
1	F	24	SER
1	F	28	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	ASN
1	B	115	HIS
1	B	120	GLN
1	C	115	HIS
1	F	112	HIS

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 oligosaccharides 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	95/129 (73%)	0.87	11 (11%) 11 9	27, 45, 92, 119	0
1	B	95/129 (73%)	0.60	10 (10%) 13 12	26, 40, 90, 114	0
1	C	94/129 (72%)	1.71	31 (32%) 1 1	49, 102, 133, 143	0
1	D	95/129 (73%)	0.95	13 (13%) 8 6	30, 48, 104, 132	0
1	E	95/129 (73%)	0.66	10 (10%) 13 12	28, 41, 88, 113	0
1	F	90/129 (69%)	1.23	16 (17%) 4 4	44, 75, 100, 112	0
2	G	25/25 (100%)	-0.01	1 (4%) 43 41	31, 48, 88, 90	0
2	I	25/25 (100%)	0.06	0 100 100	32, 51, 116, 148	0
3	H	24/25 (96%)	-0.07	0 100 100	33, 48, 94, 105	0
3	J	25/25 (100%)	0.00	0 100 100	35, 53, 135, 157	0
All	All	663/874 (75%)	0.85	92 (13%) 7 6	26, 53, 114, 157	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	PRO	5.7
1	A	131	THR	5.1
1	F	71	LEU	5.1
1	A	69	PRO	5.0
1	F	130	LEU	5.0
1	D	53	PRO	4.7
1	C	53	PRO	4.6
1	E	71	LEU	4.5
1	C	54	PRO	4.4
1	F	93	VAL	4.2
1	D	131	THR	4.1
1	E	94	LEU	4.1
1	C	103	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	71	LEU	4.0
1	B	71	LEU	3.9
1	D	117	ARG	3.7
1	F	106	GLY	3.7
1	E	54	PRO	3.6
1	C	106	GLY	3.6
1	D	73	LYS	3.6
1	F	53	PRO	3.6
1	A	11	PRO	3.5
1	A	26	ARG	3.5
1	E	53	PRO	3.5
1	E	108	LEU	3.5
1	F	36	GLY	3.4
1	E	132	SER	3.3
1	C	108	LEU	3.3
1	C	52	SER	3.3
1	A	53	PRO	3.2
1	C	16	ALA	3.2
1	F	72	PHE	3.2
1	C	128	LYS	3.1
1	B	53	PRO	3.1
1	A	27	TYR	3.0
1	E	131	THR	3.0
1	B	69	PRO	3.0
1	B	107	PRO	2.9
1	B	52	SER	2.9
1	C	92	VAL	2.9
1	D	10	HIS	2.9
1	C	22	VAL	2.8
1	F	52	SER	2.8
1	F	27	TYR	2.7
1	C	71	LEU	2.7
1	D	72	PHE	2.7
1	C	48	ALA	2.7
1	E	69	PRO	2.7
1	C	129	ARG	2.7
1	F	35	ARG	2.7
1	D	71	LEU	2.6
1	C	69	PRO	2.6
1	D	12	ASN	2.6
1	B	131	THR	2.5
1	C	107	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	45	LEU	2.5
1	F	90	ARG	2.5
1	D	107	PRO	2.5
1	A	119	ASP	2.5
1	F	51	LEU	2.5
1	C	27	TYR	2.4
1	C	87	TYR	2.4
1	C	21	LEU	2.4
1	F	50	LEU	2.4
1	D	74	THR	2.4
1	C	116	PHE	2.4
1	F	45	LEU	2.3
1	C	14	PHE	2.3
1	B	94	LEU	2.3
1	C	50	LEU	2.3
1	C	25	PRO	2.3
1	C	30	ILE	2.3
1	D	75	THR	2.3
1	B	54	PRO	2.2
1	E	12	ASN	2.2
1	B	119	ASP	2.2
1	D	69	PRO	2.2
1	C	104	GLY	2.2
1	D	120	GLN	2.2
1	A	73	LYS	2.2
1	C	117	ARG	2.2
2	G	1	DA	2.1
1	A	117	ARG	2.1
1	F	16	ALA	2.1
1	C	121	PRO	2.1
1	C	13	ASN	2.1
1	C	109	HIS	2.1
1	C	38	GLY	2.1
1	F	107	PRO	2.1
1	A	94	LEU	2.1
1	C	123	LEU	2.0
1	E	127	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.