Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 06:40 pm BST

PDB ID	:	4DRB
Title	:	The crystal structure of FANCM bound MHF complex
Authors	:	Tao, Y.; Niu, L.; Teng, M.
Deposited on	:	2012-02-17
Resolution	:	2.63 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

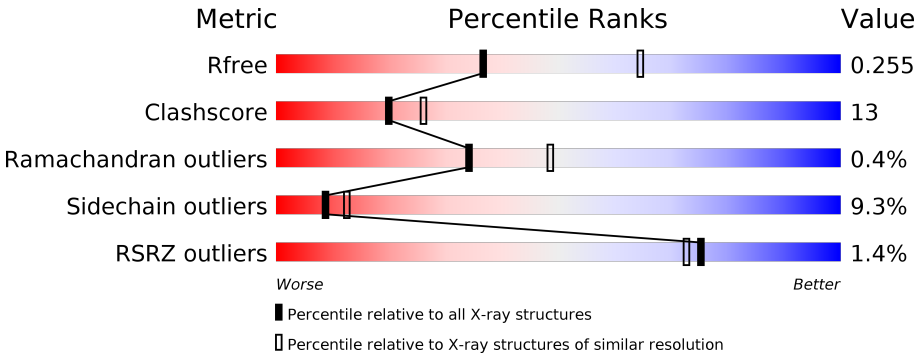
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	120	3% 53% 23% 5% 18%
1	B	120	61% 24% • 14%
1	D	120	3% 58% 22% • 19%
1	E	120	3% 59% 21% • 19%
1	G	120	% 73% 11% • 13%
1	H	120	63% 16% 22%

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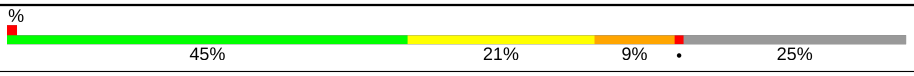
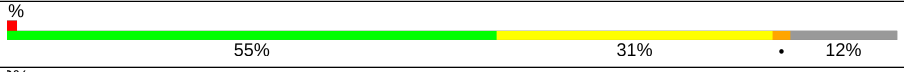
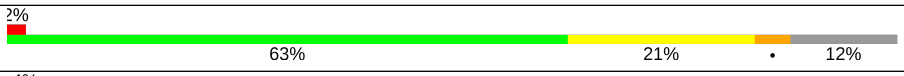
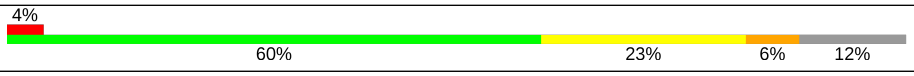
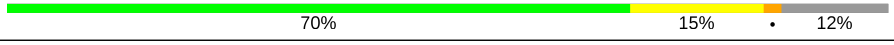
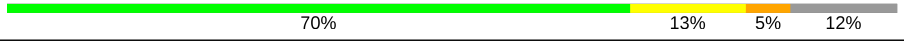
Mol	Chain	Length	Quality of chain
2	C	141	
2	F	141	
2	I	141	
3	J	84	
3	K	84	
3	L	84	
3	M	84	
3	N	84	
3	O	84	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10508 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 Centromere protein S.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	Se	0	0	0
			758	477	131	145	3	2			
1	B	103	Total	C	N	O	S	Se	0	0	0
			769	480	134	150	3	2			
1	D	97	Total	C	N	O	S	Se	0	1	0
			736	460	125	146	3	2			
1	E	97	Total	C	N	O	S	Se	0	0	0
			699	436	124	134	3	2			
1	G	105	Total	C	N	O	S	Se	0	0	0
			793	492	141	155	3	2			
1	H	94	Total	C	N	O	S	Se	0	0	0
			731	459	125	142	3	2			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
A	-4	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
A	-3	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
A	-2	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
A	-1	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
A	0	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
B	-5	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
B	-4	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
B	-3	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
B	-2	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
B	-1	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
B	0	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
D	-5	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
D	-4	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
D	-3	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
D	-2	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
D	-1	HIS	-	EXPRESSION TAG	UNP Q8N2Z9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
E	-5	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
E	-4	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
E	-3	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
E	-2	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
E	-1	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
E	0	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
G	-5	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
G	-4	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
G	-3	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
G	-2	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
G	-1	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
G	0	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
H	-5	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
H	-4	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
H	-3	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
H	-2	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
H	-1	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
H	0	HIS	-	EXPRESSION TAG	UNP Q8N2Z9

- Molecule 2 is a protein called Fanconi anemia group M protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	106	Total	C	N	O	S	0	0	0
			860	542	151	161	6			
2	F	100	Total	C	N	O	S	0	1	0
			796	505	141	144	6			
2	I	103	Total	C	N	O	S	0	1	0
			857	542	151	158	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	660	GLY	-	EXPRESSION TAG	UNP Q8IYD8
F	660	GLY	-	EXPRESSION TAG	UNP Q8IYD8
I	660	GLY	-	EXPRESSION TAG	UNP Q8IYD8

- Molecule 3 is a protein called Centromere protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	74	Total	C	N	O	Se	0	0	0
			581	371	102	107	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	74	Total	C	N	O	Se	0	0	0
			570	365	100	104	1			
3	L	74	Total	C	N	O	Se	0	0	0
			558	358	96	103	1			
3	M	74	Total	C	N	O	Se	0	0	0
			529	340	88	100	1			
3	N	74	Total	C	N	O	Se	0	0	0
			567	363	97	106	1			
3	O	74	Total	C	N	O	Se	0	0	0
			584	374	102	107	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-2	GLY	-	EXPRESSION TAG	UNP A8MT69
J	-1	SER	-	EXPRESSION TAG	UNP A8MT69
J	0	HIS	-	EXPRESSION TAG	UNP A8MT69
K	-2	GLY	-	EXPRESSION TAG	UNP A8MT69
K	-1	SER	-	EXPRESSION TAG	UNP A8MT69
K	0	HIS	-	EXPRESSION TAG	UNP A8MT69
L	-2	GLY	-	EXPRESSION TAG	UNP A8MT69
L	-1	SER	-	EXPRESSION TAG	UNP A8MT69
L	0	HIS	-	EXPRESSION TAG	UNP A8MT69
M	-2	GLY	-	EXPRESSION TAG	UNP A8MT69
M	-1	SER	-	EXPRESSION TAG	UNP A8MT69
M	0	HIS	-	EXPRESSION TAG	UNP A8MT69
N	-2	GLY	-	EXPRESSION TAG	UNP A8MT69
N	-1	SER	-	EXPRESSION TAG	UNP A8MT69
N	0	HIS	-	EXPRESSION TAG	UNP A8MT69
O	-2	GLY	-	EXPRESSION TAG	UNP A8MT69
O	-1	SER	-	EXPRESSION TAG	UNP A8MT69
O	0	HIS	-	EXPRESSION TAG	UNP A8MT69

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	10	Total	O	0	0
			10	10		
4	C	17	Total	O	0	0
			17	17		

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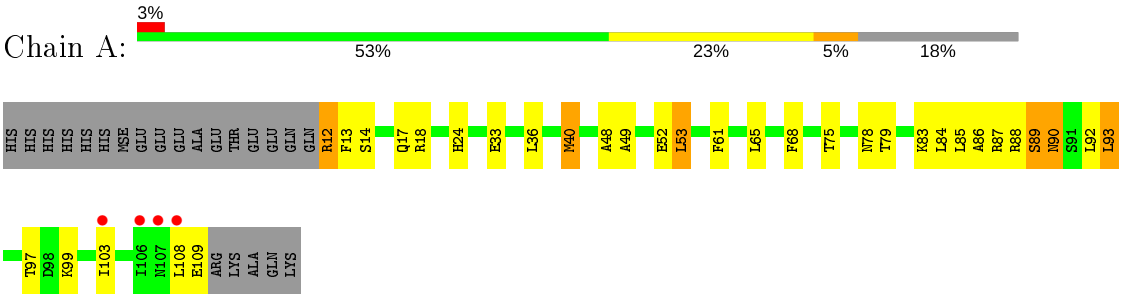
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	3	Total O 3 3	0	0
4	E	3	Total O 3 3	0	0
4	F	3	Total O 3 3	0	0
4	G	8	Total O 8 8	0	0
4	H	12	Total O 12 12	0	0
4	I	18	Total O 18 18	0	0
4	J	3	Total O 3 3	0	0
4	K	13	Total O 13 13	0	0
4	L	8	Total O 8 8	0	0
4	M	3	Total O 3 3	0	0
4	N	4	Total O 4 4	0	0
4	O	8	Total O 8 8	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.

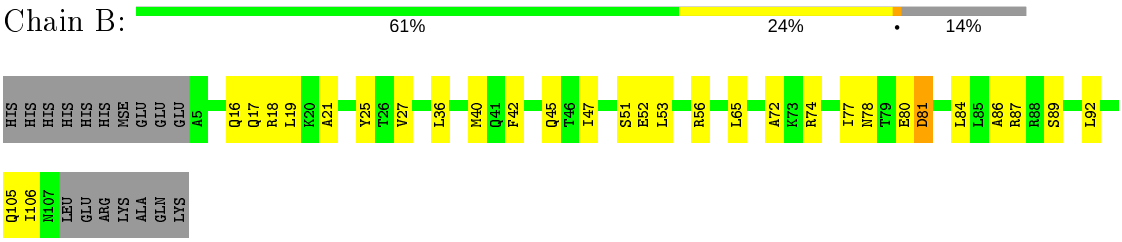
- Molecule 1: Centromere protein S

Chain A:



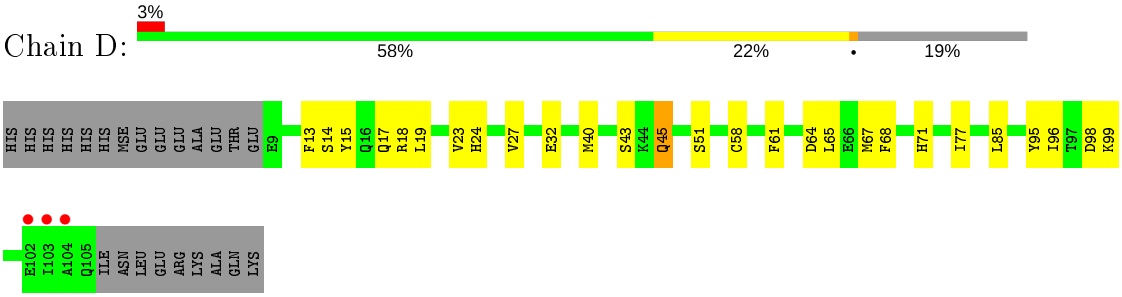
- Molecule 1: Centromere protein S

Chain B:



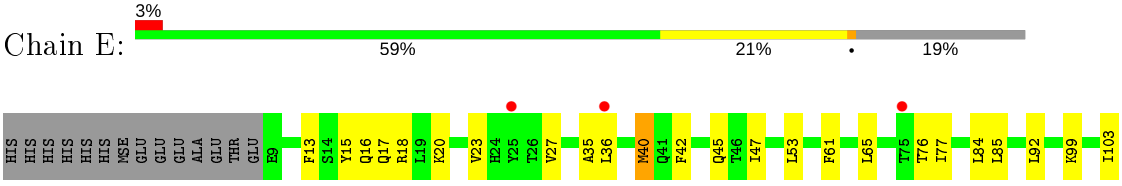
- Molecule 1: Centromere protein S

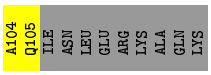
Chain D:



- Molecule 1: Centromere protein S

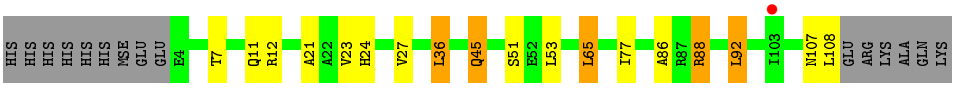
Chain E:





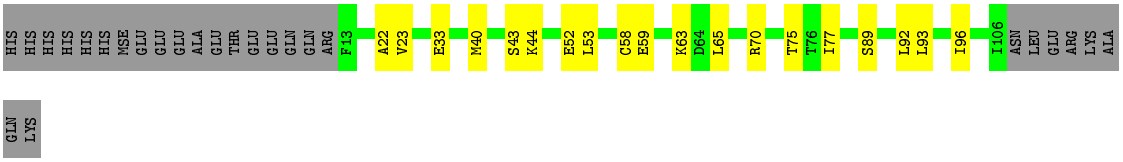
• Molecule 1: Centromere protein S

Chain G:



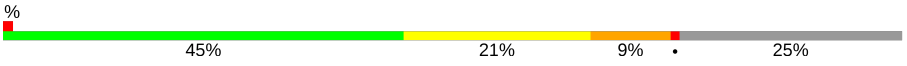
• Molecule 1: Centromere protein S

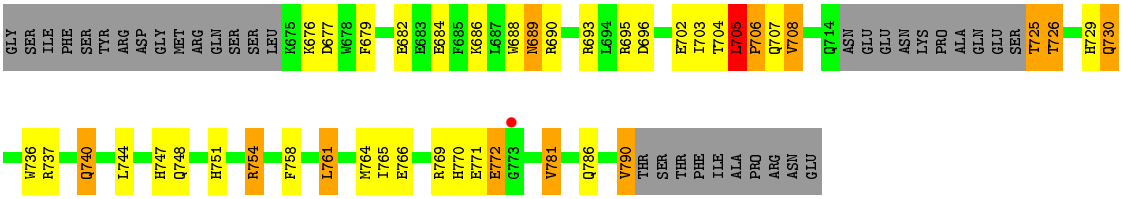
Chain H:



• Molecule 2: Fanconi anemia group M protein

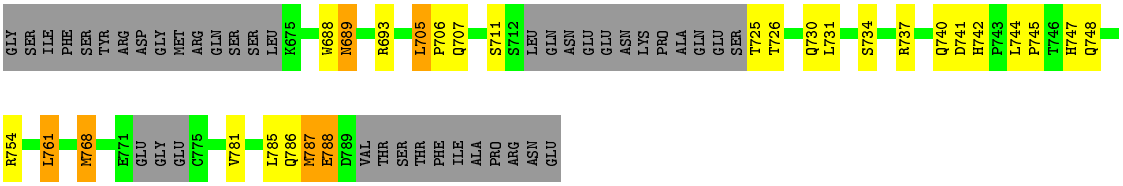
Chain C:





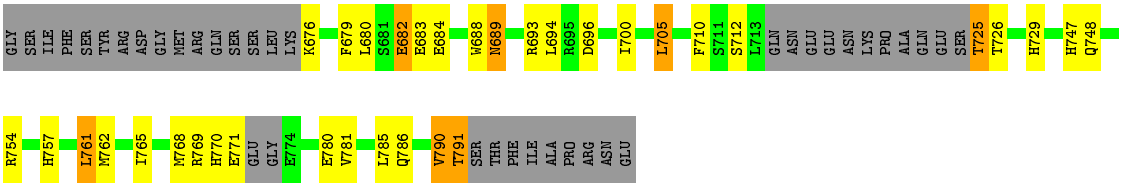
• Molecule 2: Fanconi anemia group M protein

Chain F:



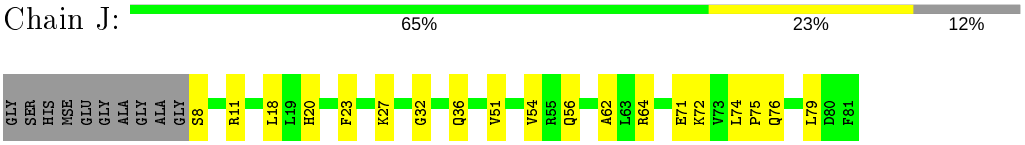
• Molecule 2: Fanconi anemia group M protein

Chain I:



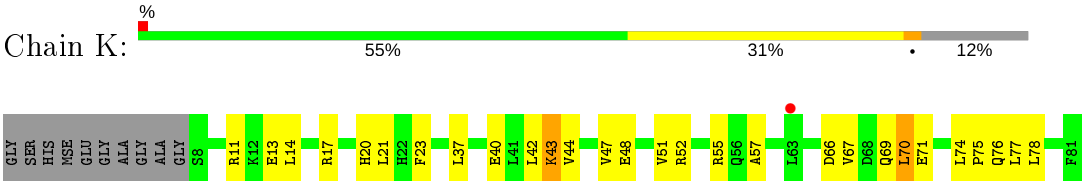
• Molecule 3: Centromere protein X

Chain J:



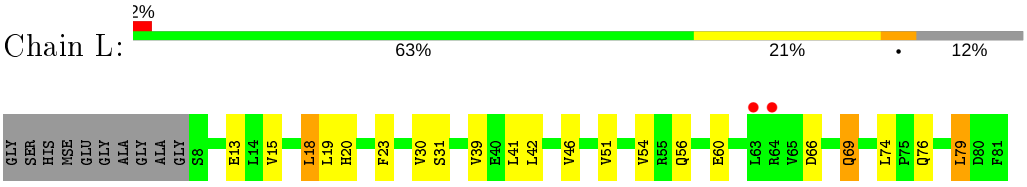
• Molecule 3: Centromere protein X

Chain K:



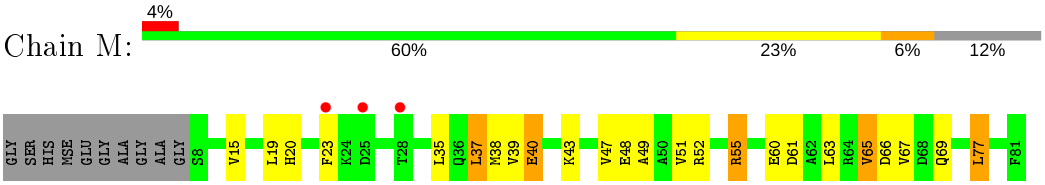
• Molecule 3: Centromere protein X

Chain L:



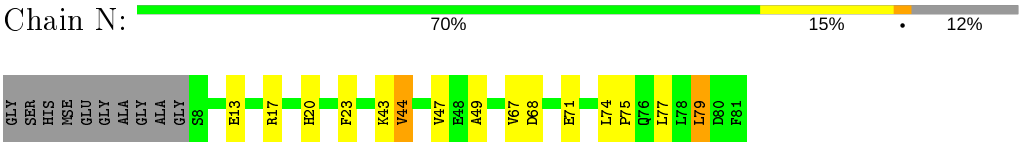
• Molecule 3: Centromere protein X

Chain M:



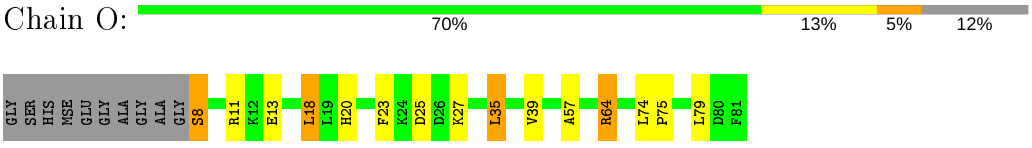
• Molecule 3: Centromere protein X

Chain N:



• Molecule 3: Centromere protein X

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.32Å 70.03Å 115.75Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	49.67 – 2.63 49.67 – 2.63	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.67-2.63) 99.6 (49.67-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.87 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.221 , 0.256 0.218 , 0.255	Depositor DCC
R_{free} test set	2691 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.020 for h,-k,-l 0.012 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10508	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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	0.22	0/765	0.36	0/1027
1	B	0.26	0/775	0.38	0/1045
1	D	0.22	0/743	0.37	0/1001
1	E	0.25	0/704	0.40	0/953
1	G	0.21	0/799	0.36	0/1074
1	H	0.22	0/738	0.34	0/991
2	C	0.25	0/882	0.45	1/1195 (0.1%)
2	F	0.21	0/818	0.38	0/1111
2	I	0.21	0/882	0.36	0/1194
3	J	0.21	0/586	0.33	0/788
3	K	0.22	0/575	0.35	0/777
3	L	0.20	0/563	0.32	0/762
3	M	0.20	0/534	0.32	0/728
3	N	0.21	0/572	0.35	0/772
3	O	0.21	0/589	0.32	0/792
All	All	0.22	0/10525	0.37	1/14210 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	705	LEU	CA-CB-CG	5.50	127.96	115.30

There are no chirality outliers.

There are no planarity outliers.

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	758	0	724	28	0
1	B	769	0	715	25	0
1	D	736	0	673	16	0
1	E	699	0	630	21	0
1	G	793	0	740	15	0
1	H	731	0	698	16	0
2	C	860	0	771	44	0
2	F	796	0	679	22	0
2	I	857	0	781	28	0
3	J	581	0	593	15	0
3	K	570	0	571	21	0
3	L	558	0	547	16	0
3	M	529	0	491	23	0
3	N	567	0	565	10	0
3	O	584	0	602	14	0
4	A	7	0	0	1	0
4	B	10	0	0	0	0
4	C	17	0	0	1	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	G	8	0	0	1	0
4	H	12	0	0	0	0
4	I	18	0	0	0	0
4	J	3	0	0	0	0
4	K	13	0	0	0	0
4	L	8	0	0	0	0
4	M	3	0	0	0	0
4	N	4	0	0	0	0
4	O	8	0	0	0	0
All	All	10508	0	9780	254	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 13.

All (254) 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)
2:C:676:LYS:HG2	2:C:677:ASP:H	1.23	1.03
2:C:771:GLU:HA	2:C:772:GLU:CB	1.94	0.95
1:A:14:SER:H	1:A:17:GLN:HE21	1.19	0.90
1:E:99:LYS:HG2	3:M:40:GLU:HG2	1.54	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:PHE:HB3	3:M:38:MSE:HE1	1.58	0.85
3:L:69:GLN:N	3:L:69:GLN:HE21	1.74	0.85
2:C:744:LEU:H	3:J:76:GLN:HE22	1.23	0.83
2:C:676:LYS:CG	2:C:677:ASP:H	1.93	0.81
2:C:676:LYS:HG2	2:C:677:ASP:N	1.95	0.81
1:E:104:ALA:O	1:E:105:GLN:CB	2.30	0.80
1:B:40:MSE:HE1	3:K:57:ALA:HB3	1.68	0.76
2:F:689:ASN:HD21	2:F:693:ARG:HH11	1.34	0.74
1:E:65:LEU:HD22	3:M:38:MSE:HE2	1.70	0.73
2:C:689:ASN:HD21	2:C:693:ARG:HH11	1.34	0.73
2:C:708:VAL:HG11	3:K:76:GLN:HG2	1.71	0.73
1:H:52:GLU:HG3	2:I:705:LEU:HD11	1.72	0.71
3:M:66:ASP:H	3:M:69:GLN:NE2	1.88	0.71
1:D:45:GLN:NE2	1:D:45:GLN:H	1.89	0.70
1:A:12:ARG:HG3	1:A:13:PHE:H	1.58	0.68
2:F:725:THR:HG22	2:F:726:THR:H	1.56	0.68
1:B:16:GLN:HE21	1:B:17:GLN:HE21	1.40	0.68
1:A:90:ASN:H	1:A:90:ASN:ND2	1.93	0.67
2:I:689:ASN:HD21	2:I:693:ARG:HH11	1.41	0.67
3:M:66:ASP:H	3:M:69:GLN:HE21	1.43	0.67
3:M:49:ALA:HA	3:M:77:LEU:HD11	1.76	0.66
1:D:14:SER:H	1:D:17:GLN:HE21	1.44	0.66
3:K:66:ASP:H	3:K:69:GLN:NE2	1.92	0.66
1:B:78:ASN:OD1	1:B:80:GLU:HG2	1.96	0.66
2:C:754:ARG:HD2	3:J:79:LEU:O	1.95	0.65
1:A:14:SER:H	1:A:17:GLN:NE2	1.93	0.65
1:E:65:LEU:HB3	1:E:77:ILE:HD13	1.79	0.65
3:N:49:ALA:HA	3:N:77:LEU:HD11	1.79	0.65
3:L:69:GLN:H	3:L:69:GLN:HE21	1.44	0.65
1:A:99:LYS:O	1:A:103:ILE:HG12	1.97	0.64
1:D:65:LEU:HB3	1:D:77:ILE:HD13	1.79	0.64
1:E:13:PHE:O	1:E:17:GLN:HG2	1.98	0.63
1:H:59:GLU:HG2	1:H:63:LYS:HD2	1.81	0.63
1:G:107:ASN:HA	1:G:108:LEU:C	2.19	0.62
3:M:60:GLU:O	3:M:61:ASP:HB2	1.98	0.62
2:F:786:GLN:O	2:F:788:GLU:HB3	2.00	0.62
2:F:711:SER:HB2	3:M:55:ARG:CZ	2.29	0.61
3:O:20:HIS:HA	3:O:23:PHE:CD1	2.35	0.61
1:B:53:LEU:HA	2:C:761:LEU:HD11	1.83	0.61
2:I:765:ILE:HG23	3:N:67:VAL:HB	1.83	0.61
2:C:740:GLN:HG3	2:C:758:PHE:HE2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ALA:HB1	1:B:92:LEU:HG	1.83	0.60
2:C:695:ARG:HG3	2:I:786:GLN:NE2	2.16	0.60
1:A:87:ARG:HH22	1:B:87:ARG:HH22	1.48	0.60
3:K:13:GLU:O	3:K:17:ARG:HG3	2.00	0.60
3:M:20:HIS:HA	3:M:23:PHE:CD2	2.37	0.60
1:B:72:ALA:HB3	1:B:74:ARG:HH11	1.67	0.60
1:G:45:GLN:H	1:G:45:GLN:NE2	1.99	0.59
3:N:74:LEU:HB3	3:N:75:PRO:HD3	1.84	0.59
2:C:725:THR:HG22	2:C:726:THR:H	1.66	0.59
3:N:13:GLU:O	3:N:17:ARG:HG3	2.02	0.59
1:H:65:LEU:HB3	1:H:77:ILE:HD13	1.82	0.59
1:B:72:ALA:HB3	1:B:74:ARG:NH1	2.18	0.59
1:E:45:GLN:HB3	2:F:768:MET:HE3	1.84	0.58
1:B:52:GLU:HG3	1:B:56:ARG:HD2	1.85	0.58
1:H:40:MSE:HE2	3:O:57:ALA:CB	2.32	0.58
1:B:84:LEU:O	1:B:87:ARG:HG2	2.03	0.58
2:F:787:MET:HA	2:F:788:GLU:CB	2.34	0.58
2:I:689:ASN:HD22	2:I:693:ARG:HD3	1.69	0.58
2:C:708:VAL:HG21	3:K:76:GLN:CD	2.24	0.58
1:G:86:ALA:HB1	1:G:92:LEU:HD13	1.86	0.57
2:I:689:ASN:ND2	2:I:693:ARG:HD3	2.19	0.57
3:J:32:GLY:O	3:J:36:GLN:HG3	2.05	0.57
2:F:747:HIS:ND1	3:L:51:VAL:HG11	2.20	0.57
1:A:108:LEU:O	1:A:109:GLU:CB	2.53	0.57
1:A:89:SER:HB3	1:A:92:LEU:HB2	1.86	0.56
1:H:70:ARG:HD3	1:H:70:ARG:O	2.05	0.56
1:E:65:LEU:HD13	1:E:85:LEU:HD11	1.88	0.56
2:C:771:GLU:CA	2:C:772:GLU:CB	2.77	0.56
3:N:43:LYS:O	3:N:47:VAL:HG13	2.05	0.56
3:K:66:ASP:H	3:K:69:GLN:HE22	1.54	0.55
1:E:65:LEU:HG	1:E:77:ILE:HG21	1.89	0.54
1:G:88:ARG:HB2	4:G:205:HOH:O	2.06	0.54
1:D:24:HIS:CG	2:F:688:TRP:HE1	2.25	0.54
2:I:790:VAL:HG12	2:I:791:THR:N	2.23	0.54
1:B:16:GLN:HE21	1:B:17:GLN:NE2	2.05	0.54
2:C:740:GLN:HG3	2:C:758:PHE:CE2	2.43	0.54
1:H:53:LEU:HD23	2:I:705:LEU:HD23	1.89	0.54
2:I:676:LYS:HA	2:I:679:PHE:CZ	2.42	0.54
1:E:65:LEU:CD2	3:M:38:MSE:HE2	2.38	0.54
1:A:90:ASN:H	1:A:90:ASN:HD22	1.55	0.53
1:A:40:MSE:HG3	3:J:54:VAL:HG13	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:74:LEU:HB3	3:O:75:PRO:HD3	1.89	0.53
1:H:44:LYS:HE2	2:I:694:LEU:HD23	1.91	0.53
1:D:98[B]:ASP:OD1	1:D:99:LYS:N	2.41	0.53
1:H:33:GLU:OE2	3:O:8:SER:HB2	2.09	0.53
1:D:95:TYR:O	1:D:98[B]:ASP:OD1	2.27	0.52
3:M:43:LYS:O	3:M:47:VAL:HG23	2.08	0.52
2:F:740:GLN:NE2	3:L:76:GLN:HE21	2.08	0.52
3:M:47:VAL:O	3:M:51:VAL:HG23	2.10	0.52
3:K:74:LEU:HB2	3:K:75:PRO:HD3	1.91	0.52
1:A:86:ALA:HB1	1:A:92:LEU:HB3	1.89	0.52
1:E:42:PHE:HB2	1:E:47:ILE:HD11	1.90	0.52
3:M:35:LEU:O	3:M:39:VAL:HG23	2.10	0.52
2:C:729:HIS:HE1	3:J:71:GLU:OE2	1.92	0.52
3:O:11:ARG:HB3	3:O:13:GLU:OE1	2.10	0.52
1:E:16:GLN:O	1:E:20:LYS:HB2	2.09	0.52
2:I:790:VAL:CG1	2:I:791:THR:N	2.72	0.52
1:A:88:ARG:HB2	4:A:204:HOH:O	2.10	0.51
1:B:25:TYR:CE2	2:C:790:VAL:HG11	2.46	0.51
3:K:51:VAL:O	3:K:55:ARG:HG2	2.11	0.51
3:M:48:GLU:O	3:M:52:ARG:HG3	2.11	0.51
1:D:27:VAL:HG21	1:D:51:SER:HA	1.93	0.50
1:B:45:GLN:NE2	1:B:45:GLN:H	2.09	0.50
2:F:787:MET:HA	2:F:788:GLU:HB3	1.94	0.50
2:I:682:GLU:HG2	2:I:683:GLU:N	2.27	0.50
1:H:40:MSE:HE2	3:O:57:ALA:HB1	1.92	0.49
3:J:20:HIS:HA	3:J:23:PHE:CD2	2.47	0.49
3:M:19:LEU:HB3	3:M:23:PHE:CZ	2.47	0.49
1:B:65:LEU:HB3	1:B:77:ILE:HD13	1.93	0.49
1:G:65:LEU:HB3	1:G:77:ILE:HG12	1.94	0.49
1:D:14:SER:O	1:D:18:ARG:HG3	2.12	0.49
3:N:44:VAL:HA	3:N:47:VAL:HG22	1.93	0.49
1:G:92:LEU:HG	2:I:710:PHE:CE2	2.47	0.49
1:H:40:MSE:HE2	3:O:57:ALA:HB3	1.94	0.49
2:C:676:LYS:HA	4:C:907:HOH:O	2.13	0.49
2:C:705:LEU:N	2:C:705:LEU:HD23	2.28	0.49
3:N:20:HIS:HA	3:N:23:PHE:CD2	2.47	0.49
2:I:762:MET:HE1	3:N:71:GLU:HG2	1.95	0.49
3:J:74:LEU:HB3	3:J:75:PRO:HD3	1.94	0.48
3:K:40:GLU:O	3:K:44:VAL:HG23	2.13	0.48
3:L:15:VAL:O	3:L:19:LEU:HG	2.13	0.48
3:L:69:GLN:NE2	3:L:69:GLN:H	2.09	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:ALA:CB	1:G:92:LEU:HD13	2.43	0.48
3:N:13:GLU:CD	3:N:13:GLU:H	2.17	0.48
1:A:12:ARG:HG3	1:A:13:PHE:N	2.28	0.48
2:F:741:ASP:OD1	2:F:742[B]:HIS:CD2	2.66	0.48
1:E:40:MSE:HE2	3:M:63:LEU:O	2.13	0.48
3:M:66:ASP:N	3:M:69:GLN:HE21	2.08	0.48
1:E:23:VAL:O	1:E:27:VAL:HG23	2.14	0.48
2:C:708:VAL:HG21	3:K:76:GLN:NE2	2.29	0.48
1:A:12:ARG:CG	1:A:13:PHE:H	2.22	0.48
1:A:40:MSE:HE1	3:J:62:ALA:O	2.14	0.47
1:A:79:THR:HG22	1:A:83:LYS:HD2	1.95	0.47
1:D:45:GLN:HE21	1:D:45:GLN:H	1.62	0.47
1:B:74:ARG:NH2	1:B:81:ASP:OD1	2.47	0.47
2:C:769:ARG:NH2	3:K:71:GLU:OE2	2.46	0.47
2:C:736:TRP:CE3	3:J:72:LYS:HE3	2.49	0.47
1:D:65:LEU:HB3	1:D:77:ILE:HG21	1.96	0.47
1:G:53:LEU:HB2	2:I:761:LEU:HD11	1.96	0.47
1:E:42:PHE:HA	3:M:65:VAL:HG13	1.97	0.47
3:L:51:VAL:O	3:L:54:VAL:HB	2.15	0.47
3:M:66:ASP:HB2	3:M:69:GLN:HE22	1.78	0.47
1:E:47:ILE:H	1:E:47:ILE:HD12	1.80	0.47
3:L:20:HIS:HA	3:L:23:PHE:CD2	2.50	0.47
2:I:684:GLU:OE2	3:O:11:ARG:NH2	2.48	0.47
2:I:757:HIS:O	2:I:761:LEU:HB2	2.15	0.47
1:G:21:ALA:HA	2:I:781:VAL:HG13	1.97	0.47
2:C:686:LYS:O	2:C:690:ARG:HG2	2.15	0.46
2:C:690:ARG:HH21	2:I:785:LEU:HD23	1.80	0.46
1:B:19:LEU:HD12	3:K:21:LEU:HD22	1.98	0.46
2:F:725:THR:HG22	2:F:726:THR:N	2.28	0.46
1:A:93:LEU:O	1:A:97:THR:HG23	2.15	0.46
2:C:705:LEU:H	2:C:705:LEU:HD23	1.80	0.46
1:E:15:TYR:O	1:E:18:ARG:HB3	2.16	0.46
1:G:27:VAL:HG21	1:G:51:SER:HA	1.97	0.46
2:I:700:ILE:HD12	2:I:729:HIS:HB2	1.98	0.46
1:A:61:PHE:O	1:A:65:LEU:HG	2.15	0.46
1:D:67:MSE:O	1:D:71:HIS:HB2	2.15	0.46
2:C:747:HIS:CD2	2:C:748:GLN:HG3	2.50	0.46
1:E:35:ALA:HB2	1:E:42:PHE:CE1	2.51	0.45
3:K:57:ALA:HA	3:K:69:GLN:HG2	1.98	0.45
3:L:15:VAL:HG21	3:L:39:VAL:HG22	1.97	0.45
1:A:24:HIS:CG	2:C:688:TRP:HE1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD13	2:C:705:LEU:HD13	1.98	0.45
1:A:68:PHE:CG	1:A:84:LEU:HD23	2.50	0.45
2:F:744:LEU:HB3	2:F:745:PRO:HD2	1.98	0.45
2:I:688:TRP:CH2	2:I:693:ARG:HD2	2.51	0.45
2:C:702:GLU:HG2	2:C:703:ILE:N	2.31	0.45
1:G:24:HIS:HA	1:G:51:SER:OG	2.16	0.45
3:O:25:ASP:OD1	3:O:27:LYS:HB2	2.17	0.45
2:F:706:PRO:HD3	2:F:731:LEU:O	2.16	0.45
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.76	0.45
3:N:75:PRO:O	3:N:79:LEU:HD22	2.15	0.45
1:B:42:PHE:HB2	1:B:47:ILE:HD11	1.98	0.45
2:F:705:LEU:H	2:F:705:LEU:HD22	1.82	0.45
2:F:711:SER:HB2	3:M:55:ARG:NH2	2.31	0.45
1:A:33:GLU:OE2	3:J:8:SER:HB3	2.17	0.45
1:B:89:SER:HB3	1:B:92:LEU:HB3	1.99	0.45
1:D:96:ILE:HA	1:D:96:ILE:HD13	1.84	0.45
2:C:705:LEU:N	2:C:705:LEU:CD2	2.80	0.44
2:C:770:HIS:CD2	3:L:13:GLU:HG3	2.52	0.44
2:C:765:ILE:HG23	3:K:67:VAL:HB	1.99	0.44
2:C:751:HIS:CE1	3:J:76:GLN:HE21	2.35	0.44
3:K:43:LYS:O	3:K:47:VAL:HG23	2.16	0.44
1:G:7:THR:O	1:G:11:GLN:HB2	2.17	0.44
3:O:35:LEU:O	3:O:39:VAL:HG23	2.18	0.44
1:G:23:VAL:O	1:G:27:VAL:HG23	2.18	0.44
2:F:688:TRP:CZ3	2:F:693:ARG:HD2	2.52	0.44
2:I:769:ARG:HG2	2:I:770:HIS:CD2	2.53	0.44
3:K:70:LEU:O	3:K:74:LEU:HG	2.17	0.44
3:L:42:LEU:O	3:L:46:VAL:HG23	2.18	0.44
1:B:106:ILE:H	1:B:106:ILE:HG13	1.51	0.44
2:I:768:MET:HB2	2:I:771:GLU:OE1	2.18	0.44
3:O:18:LEU:HD12	3:O:18:LEU:HA	1.89	0.44
3:K:42:LEU:HA	3:K:42:LEU:HD23	1.84	0.43
2:C:689:ASN:ND2	2:C:693:ARG:HH11	2.11	0.43
1:D:64:ASP:HB3	1:D:68:PHE:CE2	2.53	0.43
3:K:48:GLU:O	3:K:52:ARG:HG3	2.17	0.43
1:D:15:TYR:CZ	1:D:19:LEU:HD11	2.53	0.43
3:M:37:LEU:HD23	3:M:37:LEU:HA	1.88	0.43
2:I:725:THR:HG22	2:I:726:THR:N	2.32	0.43
3:J:27:LYS:HE2	3:J:27:LYS:HB2	1.80	0.43
3:J:64:ARG:HE	3:J:64:ARG:HB3	1.62	0.43
2:F:734:SER:O	2:F:737:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:69:GLN:NE2	3:L:69:GLN:N	2.54	0.43
1:D:19:LEU:O	1:D:23:VAL:HG23	2.18	0.43
1:E:84:LEU:HD23	1:E:84:LEU:HA	1.87	0.43
1:E:53:LEU:HA	2:F:761:LEU:HD21	2.01	0.43
1:H:22:ALA:HA	2:I:680:LEU:HD21	2.01	0.43
1:B:21:ALA:HA	2:C:781:VAL:HG13	2.01	0.43
3:L:56:GLN:O	3:L:60:GLU:HG3	2.19	0.43
1:B:27:VAL:HG21	1:B:51:SER:HA	2.01	0.43
3:K:20:HIS:HA	3:K:23:PHE:CD2	2.54	0.42
3:L:18:LEU:HA	3:L:18:LEU:HD12	1.87	0.42
3:M:15:VAL:HG21	3:M:39:VAL:HG22	2.02	0.42
2:I:689:ASN:HA	2:I:689:ASN:HD22	1.60	0.42
1:B:18:ARG:HD2	2:C:786:GLN:NE2	2.35	0.41
3:M:49:ALA:CA	3:M:77:LEU:HD11	2.47	0.41
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.84	0.41
1:A:49:ALA:O	1:A:53:LEU:HD22	2.19	0.41
2:C:704:THR:OG1	2:C:730:GLN:HG2	2.20	0.41
1:D:61:PHE:CD1	1:D:85:LEU:HD21	2.55	0.41
2:F:706:PRO:HA	2:F:730:GLN:NE2	2.36	0.41
1:H:43:SER:HB3	3:O:64:ARG:HD2	2.02	0.41
3:L:79:LEU:HD12	3:L:79:LEU:HA	1.90	0.41
1:B:89:SER:HB3	1:B:92:LEU:CB	2.51	0.41
1:H:23:VAL:CG2	3:O:18:LEU:HD21	2.51	0.41
1:H:96:ILE:HD13	1:H:96:ILE:HA	1.95	0.41
1:A:48:ALA:HB3	2:C:703:ILE:HD12	2.03	0.41
1:A:79:THR:CG2	1:A:83:LYS:HD2	2.51	0.41
1:H:40:MSE:CE	3:O:57:ALA:HB1	2.50	0.41
1:B:74:ARG:HH21	1:B:78:ASN:CG	2.23	0.41
2:C:684:GLU:OE2	3:J:11:ARG:NH2	2.53	0.41
1:A:52:GLU:HG3	2:C:703:ILE:O	2.21	0.41
2:I:790:VAL:O	2:I:791:THR:C	2.59	0.41
3:K:13:GLU:CD	3:K:13:GLU:H	2.24	0.41
2:C:766:GLU:OE1	2:C:769:ARG:NH1	2.54	0.41
2:C:747:HIS:ND1	3:J:51:VAL:HG11	2.36	0.40
1:E:65:LEU:HD23	1:E:77:ILE:HD13	2.03	0.40
1:G:36:LEU:HD22	1:G:36:LEU:HA	1.86	0.40
2:C:689:ASN:HD22	2:C:693:ARG:HD3	1.87	0.40
3:L:41:LEU:HD12	3:L:41:LEU:O	2.20	0.40
2:C:677:ASP:HB3	2:C:679:PHE:CE1	2.57	0.40
2:F:707:GLN:HB2	2:F:707:GLN:HE21	1.70	0.40
2:I:747:HIS:CD2	2:I:748:GLN:HG3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:787:MET:CA	2:F:788:GLU:CB	2.99	0.40
1:G:65:LEU:HA	1:G:65:LEU:HD12	1.78	0.40
1:H:89:SER:HB3	1:H:92:LEU:HB3	2.03	0.40
1:B:53:LEU:HD11	3:K:78:LEU:HD21	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	96/120 (80%)	96 (100%)	0	0	100 100
1	B	101/120 (84%)	97 (96%)	3 (3%)	1 (1%)	15 22
1	D	96/120 (80%)	96 (100%)	0	0	100 100
1	E	95/120 (79%)	91 (96%)	3 (3%)	1 (1%)	14 20
1	G	103/120 (86%)	103 (100%)	0	0	100 100
1	H	92/120 (77%)	92 (100%)	0	0	100 100
2	C	102/141 (72%)	94 (92%)	5 (5%)	3 (3%)	4 6
2	F	95/141 (67%)	91 (96%)	4 (4%)	0	100 100
2	I	98/141 (70%)	92 (94%)	6 (6%)	0	100 100
3	J	72/84 (86%)	71 (99%)	1 (1%)	0	100 100
3	K	72/84 (86%)	72 (100%)	0	0	100 100
3	L	72/84 (86%)	72 (100%)	0	0	100 100
3	M	72/84 (86%)	69 (96%)	3 (4%)	0	100 100
3	N	72/84 (86%)	71 (99%)	1 (1%)	0	100 100
3	O	72/84 (86%)	72 (100%)	0	0	100 100
All	All	1310/1647 (80%)	1279 (98%)	26 (2%)	5 (0%)	34 48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	105	GLN
2	C	772	GLU
2	C	706	PRO
2	C	707	GLN
1	E	103	ILE

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	75/104 (72%)	65 (87%)	10 (13%)	4 4
1	B	74/104 (71%)	72 (97%)	2 (3%)	44 63
1	D	71/104 (68%)	65 (92%)	6 (8%)	10 15
1	E	63/104 (61%)	59 (94%)	4 (6%)	18 27
1	G	77/104 (74%)	71 (92%)	6 (8%)	12 19
1	H	74/104 (71%)	71 (96%)	3 (4%)	30 47
2	C	90/133 (68%)	74 (82%)	16 (18%)	2 1
2	F	77/133 (58%)	67 (87%)	10 (13%)	4 5
2	I	92/133 (69%)	81 (88%)	11 (12%)	5 6
3	J	62/67 (92%)	60 (97%)	2 (3%)	39 56
3	K	59/67 (88%)	53 (90%)	6 (10%)	7 9
3	L	56/67 (84%)	49 (88%)	7 (12%)	4 5
3	M	50/67 (75%)	44 (88%)	6 (12%)	5 6
3	N	59/67 (88%)	56 (95%)	3 (5%)	24 37
3	O	63/67 (94%)	58 (92%)	5 (8%)	12 18
All	All	1042/1425 (73%)	945 (91%)	97 (9%)	9 12

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	18	ARG
1	A	36	LEU
1	A	40	MSE
1	A	53	LEU
1	A	75	THR
1	A	78	ASN
1	A	89	SER
1	A	90	ASN
1	A	93	LEU
1	B	36	LEU
1	B	81	ASP
2	C	682	GLU
2	C	689	ASN
2	C	696	ASP
2	C	705	LEU
2	C	706	PRO
2	C	708	VAL
2	C	725	THR
2	C	726	THR
2	C	730	GLN
2	C	737	ARG
2	C	740	GLN
2	C	754	ARG
2	C	761	LEU
2	C	764	MET
2	C	781	VAL
2	C	790	VAL
1	D	13	PHE
1	D	32	GLU
1	D	40	MSE
1	D	43	SER
1	D	45	GLN
1	D	58	CYS
1	E	36	LEU
1	E	40	MSE
1	E	76	THR
1	E	92	LEU
2	F	689	ASN
2	F	705	LEU
2	F	748	GLN
2	F	754	ARG
2	F	761	LEU

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Mol	Chain	Res	Type
2	F	768	MET
2	F	781	VAL
2	F	785	LEU
2	F	787	MET
2	F	788	GLU
1	G	12	ARG
1	G	36	LEU
1	G	45	GLN
1	G	65	LEU
1	G	88	ARG
1	G	92	LEU
1	H	58	CYS
1	H	75	THR
1	H	93	LEU
2	I	682	GLU
2	I	689	ASN
2	I	696	ASP
2	I	705	LEU
2	I	712	SER
2	I	725	THR
2	I	754	ARG
2	I	761	LEU
2	I	780	GLU
2	I	790	VAL
2	I	791	THR
3	J	18	LEU
3	J	56	GLN
3	K	11	ARG
3	K	14	LEU
3	K	37	LEU
3	K	43	LYS
3	K	70	LEU
3	K	77	LEU
3	L	18	LEU
3	L	30	VAL
3	L	31	SER
3	L	66	ASP
3	L	69	GLN
3	L	74	LEU
3	L	79	LEU
3	M	37	LEU
3	M	40	GLU

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Mol	Chain	Res	Type
3	M	55	ARG
3	M	65	VAL
3	M	67	VAL
3	M	77	LEU
3	N	44	VAL
3	N	68	ASP
3	N	79	LEU
3	O	8	SER
3	O	18	LEU
3	O	35	LEU
3	O	64	ARG
3	O	79	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	57	GLN
1	A	90	ASN
1	B	17	GLN
1	B	45	GLN
2	C	689	ASN
2	C	729	HIS
2	C	763	GLN
2	C	770	HIS
1	D	17	GLN
1	D	45	GLN
1	D	57	GLN
1	D	90	ASN
2	F	689	ASN
2	F	707	GLN
2	F	730	GLN
2	F	740	GLN
2	F	757	HIS
1	G	45	GLN
1	H	57	GLN
2	I	689	ASN
2	I	729	HIS
2	I	740	GLN
2	I	763	GLN
2	I	786	GLN
3	J	76	GLN

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Mol	Chain	Res	Type
3	K	22	HIS
3	K	56	GLN
3	K	69	GLN
3	L	22	HIS
3	L	56	GLN
3	L	69	GLN
3	M	22	HIS
3	M	56	GLN
3	M	69	GLN
3	O	22	HIS
3	O	36	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	96/120 (80%)	-0.30	4 (4%) 36 33	23, 40, 81, 95	0
1	B	101/120 (84%)	-0.30	0 100 100	27, 42, 75, 89	0
1	D	95/120 (79%)	-0.10	3 (3%) 47 44	29, 50, 71, 81	0
1	E	95/120 (79%)	0.06	3 (3%) 47 44	41, 63, 80, 92	0
1	G	103/120 (85%)	-0.31	1 (0%) 82 81	28, 41, 76, 89	0
1	H	92/120 (76%)	-0.42	0 100 100	25, 38, 66, 81	0
2	C	106/141 (75%)	-0.18	1 (0%) 84 83	26, 39, 68, 72	0
2	F	100/141 (70%)	-0.03	0 100 100	32, 54, 80, 86	0
2	I	103/141 (73%)	-0.37	0 100 100	25, 36, 58, 70	0
3	J	73/84 (86%)	-0.50	0 100 100	25, 34, 52, 59	0
3	K	73/84 (86%)	-0.34	1 (1%) 75 73	30, 38, 54, 58	0
3	L	73/84 (86%)	-0.26	2 (2%) 54 50	30, 43, 59, 72	0
3	M	73/84 (86%)	-0.02	3 (4%) 37 33	35, 61, 75, 79	0
3	N	73/84 (86%)	-0.43	0 100 100	29, 38, 55, 64	0
3	O	73/84 (86%)	-0.41	0 100 100	23, 33, 50, 54	0
All	All	1329/1647 (80%)	-0.25	18 (1%) 75 73	23, 42, 74, 95	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	ILE	4.4
1	A	107	ASN	4.4
1	E	25	TYR	3.7
1	D	103	ILE	3.6
3	K	63	LEU	3.4
3	L	64	ARG	3.4
3	M	28	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	106	ILE	3.0
1	E	75	THR	2.6
1	D	104	ALA	2.6
3	M	25	ASP	2.5
3	L	63	LEU	2.5
3	M	23	PHE	2.4
1	E	36	LEU	2.3
2	C	773	GLY	2.3
1	A	108	LEU	2.2
1	G	103	ILE	2.1
1	D	102	GLU	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.