



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:51 AM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

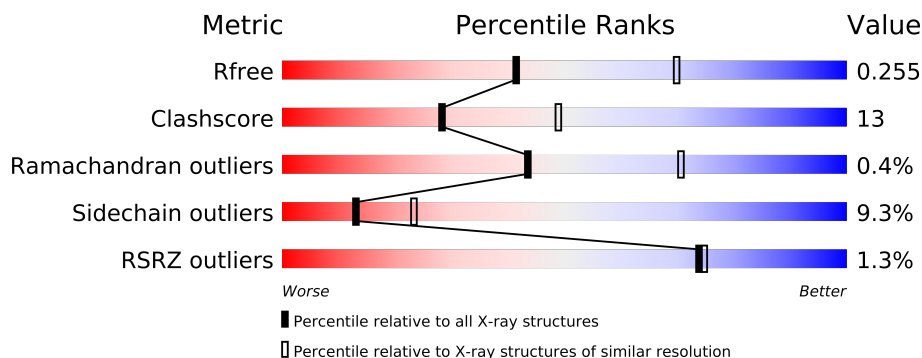
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2393 (2.68-2.60)
Clashscore	79885	2915 (2.68-2.60)
Ramachandran outliers	78287	2865 (2.68-2.60)
Sidechain outliers	78261	2865 (2.68-2.60)
RSRZ outliers	66119	2393 (2.68-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	120	
1	B	120	
1	D	120	
1	E	120	
1	G	120	
1	H	120	
2	C	141	
2	F	141	
2	I	141	
3	J	84	
3	K	84	
3	L	84	
3	M	84	
3	N	84	

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Mol	Chain	Length	Quality of chain
3	O	84	 A horizontal bar chart representing the quality of chain O. The bar is divided into four segments: a long green segment (approx. 70%), a short yellow segment (approx. 10%), a short orange segment (approx. 10%), and a short grey segment (approx. 10%).

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10508 atoms, of which 0 are hydrogen and 0 are deuterium.

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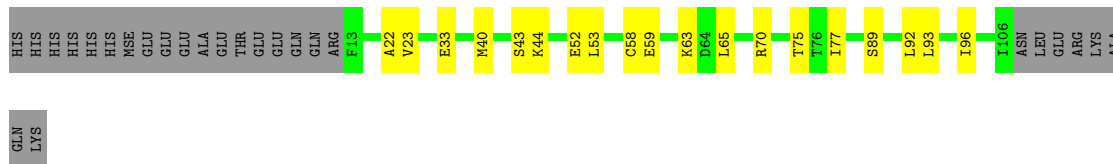
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total 3	O 3	0	0
4	E	3	Total 3	O 3	0	0
4	F	3	Total 3	O 3	0	0
4	G	8	Total 8	O 8	0	0
4	H	12	Total 12	O 12	0	0
4	I	18	Total 18	O 18	0	0
4	J	3	Total 3	O 3	0	0
4	K	13	Total 13	O 13	0	0
4	L	8	Total 8	O 8	0	0
4	M	3	Total 3	O 3	0	0
4	N	4	Total 4	O 4	0	0
4	O	8	Total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

Chain G:



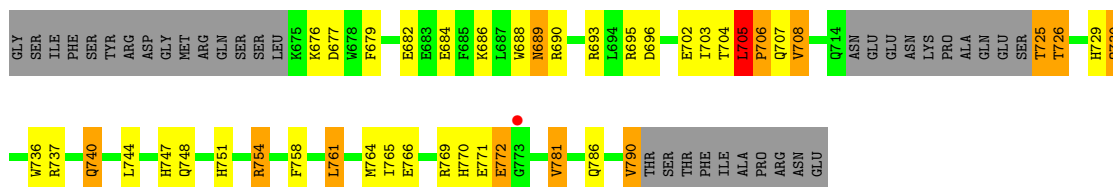
- Molecule 1: Centromere protein S

Chain H:



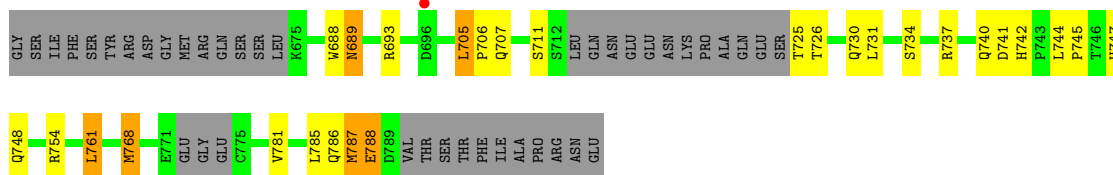
- Molecule 2: Fanconi anemia group M protein

Chain C:



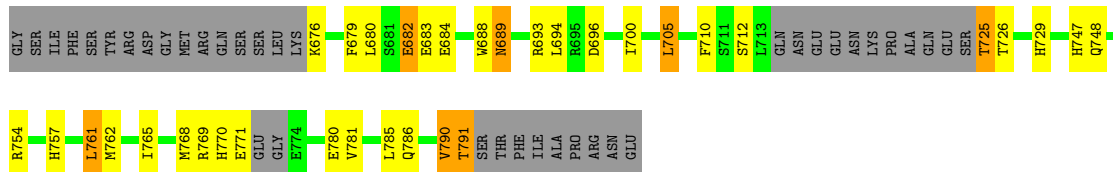
- Molecule 2: Fanconi anemia group M protein

Chain F:



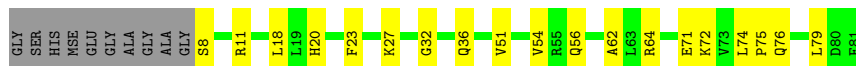
- Molecule 2: Fanconi anemia group M protein

Chain I:



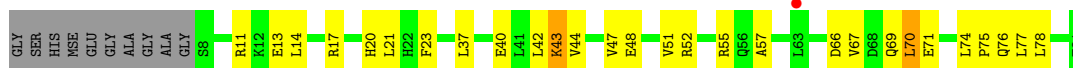
- Molecule 3: Centromere protein X

Chain J:



- Molecule 3: Centromere protein X

Chain K:



- Molecule 3: Centromere protein X

Chain L:



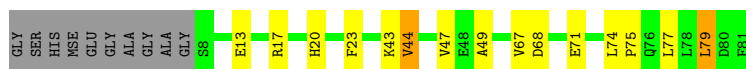
- Molecule 3: Centromere protein X

Chain M:



- Molecule 3: Centromere protein X

Chain N:



- Molecule 3: Centromere protein X

Chain O:



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	2690 reflections (5.09%)	DCC
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 , 23.0	EDS
Estimated twinning fraction	0.000 for l,k,-h 0.020 for h,-k,-l 0.012 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 52875 reflections	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.*

¹Intensities estimated from amplitudes.

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (254) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:99:LYS:HG2	3:M:40:GLU:HG2	1.54	0.86
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
3:M:66:ASP:H	3:M:69:GLN:HE21	1.43	0.67
2:I:689:ASN:HD21	2:I:693:ARG:HH11	1.41	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	Distance(Å)	Clash(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
2:F:787:MET:HA	2:F:788:GLU:CB	2.34	0.58
1:B:84:LEU:O	1:B:87:ARG:HG2	2.03	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
2:I:689:ASN:ND2	2:I:693:ARG:HD3	2.19	0.57
1:G:86:ALA:HB1	1:G:92:LEU:HD13	1.86	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:H:70:ARG:HD3	1:H:70:ARG:O	2.05	0.56
1:A:89:SER:HB3	1:A:92:LEU:HB2	1.86	0.56
2:C:771:GLU:CA	2:C:772:GLU:CB	2.77	0.56
1:E:65:LEU:HD13	1:E:85:LEU:HD11	1.88	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
3:O:74:LEU:HB3	3:O:75:PRO:HD3	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:O:11:ARG:HB3	3:O:13:GLU:OE1	2.10	0.52
2:C:729:HIS:HE1	3:J:71:GLU:OE2	1.92	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:M:19:LEU:HB3	3:M:23:PHE:CZ	2.47	0.49
3:J:20:HIS:HA	3:J:23:PHE:CD2	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:H:40:MSE:HE2	3:O:57:ALA:HB3	1.94	0.49
1:G:92:LEU:HG	2:I:710:PHE:CE2	2.47	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
2:I:762:MET:HE1	3:N:71:GLU:HG2	1.95	0.49
3:N:20:HIS:HA	3:N:23:PHE:CD2	2.47	0.49
3:J:74:LEU:HB3	3:J:75:PRO:HD3	1.94	0.48
3:L:69:GLN:NE2	3:L:69:GLN:H	2.09	0.48
3:L:15:VAL:O	3:L:19:LEU:HG	2.13	0.48
3:K:40:GLU:O	3:K:44:VAL:HG23	2.13	0.48
3:N:13:GLU:H	3:N:13:GLU:CD	2.17	0.48
1:G:86:ALA:CB	1:G:92:LEU:HD13	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:M:66:ASP:N	3:M:69:GLN:HE21	2.08	0.48
1:E:40:MSE:HE2	3:M:63:LEU:O	2.13	0.48
2:C:708:VAL:HG21	3:K:76:GLN:NE2	2.29	0.48
1:E:23:VAL:O	1:E:27:VAL:HG23	2.14	0.48
1:A:12:ARG:CG	1:A:13:PHE:H	2.22	0.48
1:D:45:GLN:HE21	1:D:45:GLN:H	1.62	0.47
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:B:74:ARG:NH2	1:B:81:ASP:OD1	2.47	0.47
2:C:736:TRP:CE3	3:J:72:LYS:HE3	2.49	0.47
2:C:769:ARG:NH2	3:K:71:GLU:OE2	2.46	0.47
1:D:65:LEU:HB3	1:D:77:ILE:HG21	1.96	0.47
1:E:42:PHE:HA	3:M:65:VAL:HG13	1.97	0.47
1:G:53:LEU:HB2	2:I:761:LEU:HD11	1.96	0.47
3:M:66:ASP:HB2	3:M:69:GLN:HE22	1.78	0.47
3:L:51:VAL:O	3:L:54:VAL:HB	2.15	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
2:F:725:THR:HG22	2:F:726:THR:N	2.28	0.46
1:B:19:LEU:HD12	3:K:21:LEU:HD22	1.98	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
2:I:700:ILE:HD12	2:I:729:HIS:HB2	1.98	0.46
1:G:27:VAL:HG21	1:G:51:SER:HA	1.97	0.46
1:E:15:TYR:O	1:E:18:ARG:HB3	2.16	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
3:K:57:ALA:HA	3:K:69:GLN:HG2	1.98	0.45
1:E:35:ALA:HB2	1:E:42:PHE:CE1	2.51	0.45
3:L:15:VAL:HG21	3:L:39:VAL:HG22	1.97	0.45
2:I:688:TRP:CH2	2:I:693:ARG:HD2	2.51	0.45
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
1:A:24:HIS:CG	2:C:688:TRP:HE1	2.34	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:744:LEU:HB3	2:F:745:PRO:HD2	1.98	0.45
1:G:24:HIS:HA	1:G:51:SER:OG	2.16	0.45
2:C:702:GLU:HG2	2:C:703:ILE:N	2.31	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:HA	1:A:93:LEU:HD23	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:711:SER:HB2	3:M:55:ARG:NH2	2.31	0.45
2:F:705:LEU:H	2:F:705:LEU:HD22	1.82	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
3:K:70:LEU:O	3:K:74:LEU:HG	2.17	0.44
2:I:769:ARG:HG2	2:I:770:HIS:CD2	2.53	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
3:L:69:GLN:NE2	3:L:69:GLN:N	2.54	0.43
2:F:734:SER:O	2:F:737:ARG:HG2	2.18	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:H:22:ALA:HA	2:I:680:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:53:LEU:HA	2:F:761: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:M:15:VAL:HG21	3:M:39:VAL:HG22	2.02	0.42
3:L:18:LEU:HA	3:L:18:LEU:HD12	1.87	0.42
2:I:689:ASN:HA	2:I:689:ASN:HD22	1.60	0.42
3:M:49:ALA:CA	3:M:77:LEU:HD11	2.47	0.41
1:B:18:ARG:HD2	2:C:786:GLN:NE2	2.35	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:H:40:MSE:CE	3:O:57:ALA:HB1	2.50	0.41
1:A:79:THR:CG2	1:A:83:LYS:HD2	2.51	0.41
1:B:74:ARG:HH21	1:B:78:ASN:CG	2.23	0.41
3:K:13:GLU:CD	3:K:13:GLU:H	2.24	0.41
2:I:790:VAL:O	2:I:791:THR:C	2.59	0.41
1:A:52:GLU:HG3	2:C:703:ILE:O	2.21	0.41
2:C:684:GLU:OE2	3:J:11:ARG:NH2	2.53	0.41
2:C:766:GLU:OE1	2:C:769:ARG:NH1	2.54	0.41
1:E:65:LEU:HD23	1:E:77:ILE:HD13	2.03	0.40
2:C:747:HIS:ND1	3:J:51:VAL:HG11	2.36	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
2:F:787:MET:CA	2:F:788:GLU:CB	2.99	0.40
1:B:53:LEU:HD11	3:K:78:LEU:HD21	2.04	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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/120 (80%)	96 (100%)	0	0	100	100
1	B	101/120 (84%)	97 (96%)	3 (3%)	1 (1%)	22	43
1	D	96/120 (80%)	96 (100%)	0	0	100	100
1	E	95/120 (79%)	91 (96%)	3 (3%)	1 (1%)	21	40
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%)	7	11
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%)	43	70

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 ⓘ

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%)	6	10
1	B	74/104 (71%)	72 (97%)	2 (3%)	57	84
1	D	71/104 (68%)	65 (92%)	6 (8%)	15	28
1	E	63/104 (61%)	59 (94%)	4 (6%)	25	47
1	G	77/104 (74%)	71 (92%)	6 (8%)	18	34
1	H	74/104 (71%)	71 (96%)	3 (4%)	41	71
2	C	90/133 (68%)	74 (82%)	16 (18%)	2	4
2	F	77/133 (58%)	67 (87%)	10 (13%)	6	10
2	I	92/133 (69%)	81 (88%)	11 (12%)	7	13
3	J	62/67 (92%)	60 (97%)	2 (3%)	51	79
3	K	59/67 (88%)	53 (90%)	6 (10%)	11	19
3	L	56/67 (84%)	49 (88%)	7 (12%)	7	12
3	M	50/67 (75%)	44 (88%)	6 (12%)	7	13
3	N	59/67 (88%)	56 (95%)	3 (5%)	33	59
3	O	63/67 (94%)	58 (92%)	5 (8%)	18	33
All	All	1042/1425 (73%)	945 (91%)	97 (9%)	13	23

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
3	O	36	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	98/120 (81%)	-0.29	3 (3%) 47 43	23, 40, 81, 95	0
1	B	103/120 (85%)	-0.22	0 100 100	27, 42, 75, 89	0
1	D	97/120 (80%)	0.04	2 (2%) 60 58	29, 51, 71, 81	0
1	E	97/120 (80%)	0.15	3 (3%) 47 43	41, 63, 80, 92	0
1	G	105/120 (87%)	-0.24	2 (1%) 64 62	28, 41, 76, 89	0
1	H	94/120 (78%)	-0.34	0 100 100	25, 38, 66, 81	0
2	C	106/141 (75%)	-0.08	1 (0%) 81 82	26, 39, 68, 72	0
2	F	100/141 (70%)	-0.00	1 (1%) 79 81	32, 54, 80, 86	0
2	I	103/141 (73%)	-0.29	0 100 100	25, 36, 58, 70	0
3	J	74/84 (88%)	-0.39	0 100 100	25, 34, 52, 59	0
3	K	74/84 (88%)	-0.23	1 (1%) 72 72	30, 38, 54, 58	0
3	L	74/84 (88%)	-0.19	2 (2%) 52 49	30, 43, 59, 72	0
3	M	74/84 (88%)	0.08	3 (4%) 35 32	35, 61, 75, 79	0
3	N	74/84 (88%)	-0.35	0 100 100	29, 38, 55, 64	0
3	O	74/84 (88%)	-0.33	0 100 100	23, 33, 50, 54	0
All	All	1347/1647 (81%)	-0.17	18 (1%) 74 75	23, 42, 74, 95	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	ILE	4.1
1	E	25	TYR	3.7
1	A	107	ASN	3.6
1	D	103	ILE	3.6
3	K	63	LEU	3.5
1	D	104	ALA	3.2
3	M	28	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	75	THR	2.8
3	M	23	PHE	2.6
3	M	25	ASP	2.6
3	L	63	LEU	2.6
3	L	64	ARG	2.4
1	E	36	LEU	2.3
2	F	696	ASP	2.3
1	G	75	THR	2.2
1	A	106	ILE	2.2
1	G	103	ILE	2.2
2	C	773	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.