



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:54 PM 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 X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

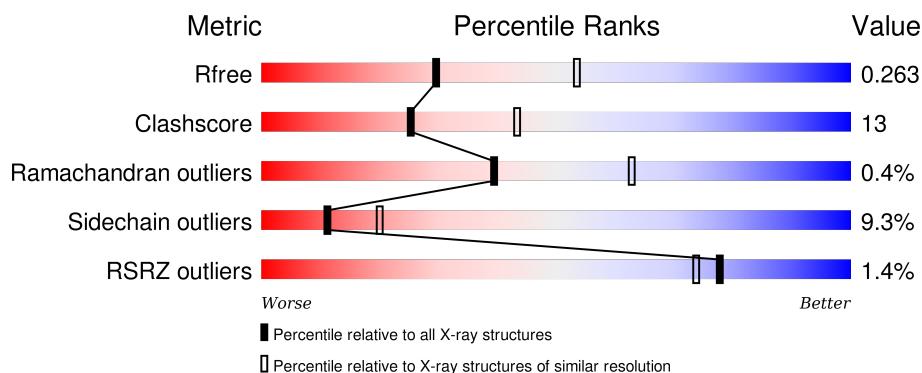
# 1 Overall quality at a glance

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.




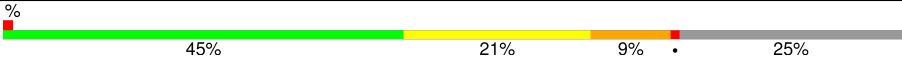








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	<div> <div>3%</div> <div>53% 23% 5% 18%</div> </div>
1	B	120	<div> <div>61% 24% • 14%</div> </div>
1	D	120	<div> <div>3%</div> <div>58% 22% • 19%</div> </div>
1	E	120	<div> <div>3%</div> <div>59% 21% • 19%</div> </div>
1	G	120	<div> <div>•</div> <div>73% 11% • 13%</div> </div>

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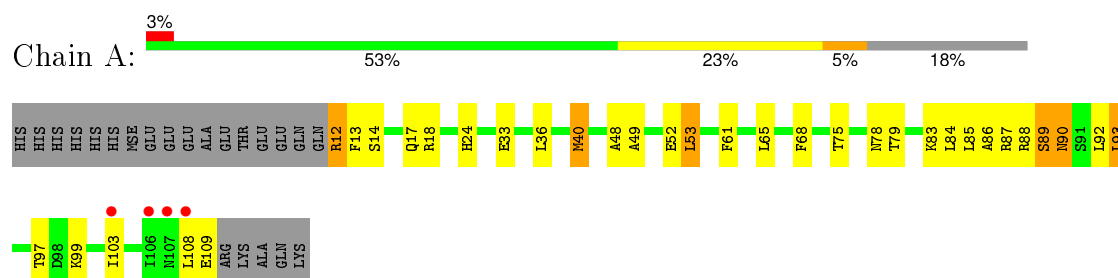
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total 3	O 3	0	0
4	E	3	Total 3	O 3	0	0
4	F	3	Total 3	O 3	0	0
4	G	8	Total 8	O 8	0	0
4	H	12	Total 12	O 12	0	0
4	I	18	Total 18	O 18	0	0
4	J	3	Total 3	O 3	0	0
4	K	13	Total 13	O 13	0	0
4	L	8	Total 8	O 8	0	0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

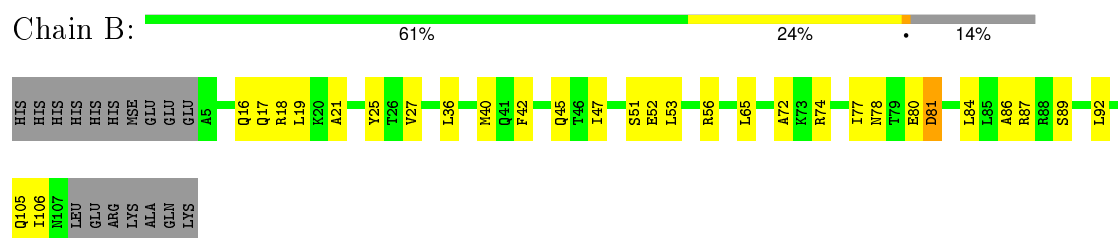
### 3 Residue-property plots [i](#)

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

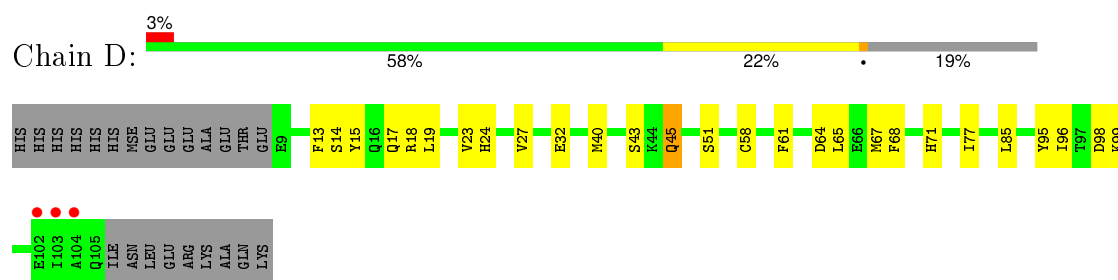
- Molecule 1: Centromere protein S



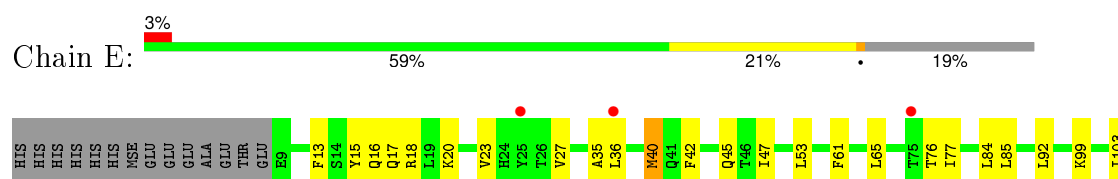
- Molecule 1: Centromere protein S



- Molecule 1: Centromere protein S



- Molecule 1: Centromere protein S





A104  
Q105  
ILE  
ASN  
LEU  
GLU  
ARG  
LYS  
ALA  
GLN  
LYS

• Molecule 1: Centromere protein S

Chain G:  73% 11% 13%

HIS HIS HIS HIS HIS HIS MSE GLU E4 T7 Q11 R12 A21 A22 V23 H24 V27 L36 Q45 S51 E52 L53 L65 I77 A86 R87 R88 L92 I103 H107 L108 GLU ARG LYS LYS ALA GLN LYS


• Molecule 1: Centromere protein S

Chain H:  63% 16% 22%

HIS HIS HIS HIS HIS HIS MSE GLU GLU GLU GLU GLU THR GLU GLN GLN ARG F13 A22 V23 E33 M40 S43 K44 N689 E52 L53 C58 E59 K63 D64 L65 R70 T75 T76 I77 S89 L92 L93 I96 I106 ASN LEU GLU ARG LYS ALA

GLN  
LYS

• Molecule 2: Fanconi anemia group M protein

Chain C:  45% 21% 9% 25%

GLY SER ILE PHE SER TYR ARG ASP GLY MET ARG GLN SER SER LEU K675 K676 D677 W678 F679 E682 E683 E684 F685 K686 W688 W689 R690 R693 L694 R695 E702 I703 T704 L705 P706 Q707 V708 Q714 ASN GLU GLU GLU ASN LYS PRO ALA GLN GLU SER T725 T726 H729 H730

W736 R737 Q740 L744 H747 Q748 H751 R754 F758 L761 M764 I765 E766 R769 H770 E771 E772 G773 V781 Q786 V790 T791 T792 P793 P794 I795 I796 A797 A798 A799 A800 A801 A802 A803 A804 A805 A806 A807 A808 A809 A810 A811 A812 A813 A814 A815 A816 A817 A818 A819 A820 A821 A822 A823 A824 A825 A826 A827 A828 A829 A830 A831 A832 A833 A834 A835 A836 A837 A838 A839 A840 A841 A842 A843 A844 A845 A846 A847 A848 A849 A850 A851 A852 A853 A854 A855 A856 A857 A858 A859 A860 A861 A862 A863 A864 A865 A866 A867 A868 A869 A870 A871 A872 A873 A874 A875 A876 A877 A878 A879 A880 A881 A882 A883 A884 A885 A886 A887 A888 A889 A890 A891 A892 A893 A894 A895 A896 A897 A898 A899 A900 A901 A902 A903 A904 A905 A906 A907 A908 A909 A910 A911 A912 A913 A914 A915 A916 A917 A918 A919 A920 A921 A922 A923 A924 A925 A926 A927 A928 A929 A930 A931 A932 A933 A934 A935 A936 A937 A938 A939 A940 A941 A942 A943 A944 A945 A946 A947 A948 A949 A950 A951 A952 A953 A954 A955 A956 A957 A958 A959 A960 A961 A962 A963 A964 A965 A966 A967 A968 A969 A970 A971 A972 A973 A974 A975 A976 A977 A978 A979 A980 A981 A982 A983 A984 A985 A986 A987 A988 A989 A990 A991 A992 A993 A994 A995 A996 A997 A998 A999 A1000

• Molecule 2: Fanconi anemia group M protein

Chain F:  51% 16% 29%

GLY SER ILE PHE SER TYR ARG ASP GLY MET ARG GLN SER SER LEU K675 W688 M689 R693 D696 L705 P706 Q707 S711 S712 LEU GLN ASN GLU GLU GLU LYS LYS PRO PRO ALA GLU SER T725 T726 Q730 L731 S734 R737 Q740 D741 H742 P743 L744 P745 H747

Q748 R754 L761 H768 E771 GLY GLU GLU G775 V781 L785 Q786 M787 E788 D789 VAL THR SER THR PHE ILE ALA PRO ARG ASN GLU

• Molecule 2: Fanconi anemia group M protein

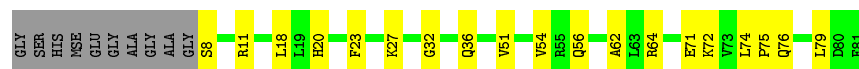
Chain I:  48% 20% 5% 27%

GLY SER ILE PHE SER TYR ARG ASP GLY MET ARG GLN SER SER LEU LEU K676 F679 L680 M689 E682 E683 E684 W688 M689 R693 L694 R695 D696 I700 L705 F710 S711 S712 L713 ASN GLU GLU GLU ASN LYS PRO PRO ALA GLN GLU SER T725 T726 H729 H747 Q748

R754 H757 L761 M762 I765 M768 R769 H770 E771 GLU GLY E774 E780 V781 L785 Q786 V790 T791 SER THR PHE ILE ALA PRO ARG ASN GLU

- Molecule 3: Centromere protein X

Chain J: 



- Molecule 3: Centromere protein X

Chain K: 



- Molecule 3: Centromere protein X

Chain L: 



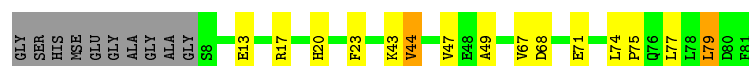
- Molecule 3: Centromere protein X

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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.87 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, $R_{free}$	0.221 , 0.256 0.224 , 0.263	Depositor DCC
$R_{free}$ test set	2693 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 40.9	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 <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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 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	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
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	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
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

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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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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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
1:A:24:HIS:CG	2:C:688:TRP:HE1	2.34	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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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: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%)	19	37
1	D	96/120 (80%)	96 (100%)	0	0	100	100
1	E	95/120 (79%)	91 (96%)	3 (3%)	1 (1%)	17	34
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%)	6	9
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%)	39	63

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%)	5	8
1	B	74/104 (71%)	72 (97%)	2 (3%)	52	78
1	D	71/104 (68%)	65 (92%)	6 (8%)	13	24
1	E	63/104 (61%)	59 (94%)	4 (6%)	22	42
1	G	77/104 (74%)	71 (92%)	6 (8%)	16	29
1	H	74/104 (71%)	71 (96%)	3 (4%)	37	64
2	C	90/133 (68%)	74 (82%)	16 (18%)	2	3
2	F	77/133 (58%)	67 (87%)	10 (13%)	5	8
2	I	92/133 (69%)	81 (88%)	11 (12%)	6	10
3	J	62/67 (92%)	60 (97%)	2 (3%)	46	73
3	K	59/67 (88%)	53 (90%)	6 (10%)	9	16
3	L	56/67 (84%)	49 (88%)	7 (12%)	6	10
3	M	50/67 (75%)	44 (88%)	6 (12%)	6	10
3	N	59/67 (88%)	56 (95%)	3 (5%)	29	53
3	O	63/67 (94%)	58 (92%)	5 (8%)	15	28
All	All	1042/1425 (73%)	945 (91%)	97 (9%)	11	20

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 [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 carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	96/120 (80%)	-0.27	4 (4%) 40 33	23, 40, 81, 95	0
1	B	101/120 (84%)	-0.26	0 100 100	27, 42, 75, 89	0
1	D	95/120 (79%)	-0.07	3 (3%) 51 45	29, 50, 71, 81	0
1	E	95/120 (79%)	0.10	3 (3%) 51 45	41, 63, 80, 92	0
1	G	103/120 (85%)	-0.28	1 (0%) 84 81	28, 41, 76, 89	0
1	H	92/120 (76%)	-0.39	0 100 100	25, 38, 66, 81	0
2	C	106/141 (75%)	-0.15	1 (0%) 85 83	26, 39, 68, 72	0
2	F	100/141 (70%)	0.00	1 (1%) 84 81	32, 54, 80, 86	0
2	I	103/141 (73%)	-0.34	0 100 100	25, 36, 58, 70	0
3	J	73/84 (86%)	-0.47	0 100 100	25, 34, 52, 59	0
3	K	73/84 (86%)	-0.31	1 (1%) 78 74	30, 38, 54, 58	0
3	L	73/84 (86%)	-0.23	2 (2%) 58 52	30, 43, 59, 72	0
3	M	73/84 (86%)	0.02	3 (4%) 41 34	35, 61, 75, 79	0
3	N	73/84 (86%)	-0.40	0 100 100	29, 38, 55, 64	0
3	O	73/84 (86%)	-0.38	0 100 100	23, 33, 50, 54	0
All	All	1329/1647 (80%)	-0.22	19 (1%) 78 74	23, 42, 74, 95	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	ILE	4.5
1	A	107	ASN	4.5
1	E	25	TYR	3.8
1	D	103	ILE	3.6
3	K	63	LEU	3.5
3	L	64	ARG	3.4
3	M	28	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	106	ILE	3.0
1	E	75	THR	2.7
1	D	104	ALA	2.7
3	M	25	ASP	2.6
3	L	63	LEU	2.5
3	M	23	PHE	2.4
2	C	773	GLY	2.3
1	E	36	LEU	2.3
1	A	108	LEU	2.2
1	G	103	ILE	2.1
1	D	102	GLU	2.1
2	F	696	ASP	2.1

## 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.