



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:07 AM GMT

PDB ID : 3KX8  
Title : Structural basis of the activity and substrate specificity of the fluoroacetyl-CoA thioesterase FIK  
Authors : Chirgadze, D.Y.; Dias, M.V.B.; Huang, F; Tosin, M.; Spiteller, D; Valentine, E.F.; Leadlay, P.F.; Spencer, J.B.; Blundell, T.L.  
Deposited on : 2009-12-02  
Resolution : 2.35 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

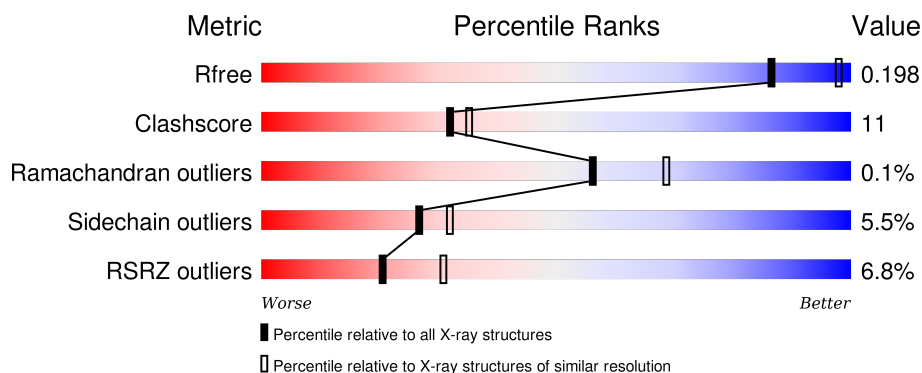
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	139	<div> <div>11%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>• •</div> </div> </div>
1	B	139	<div> <div>9%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• • •</div> </div> </div>
1	C	139	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	D	139	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• •</div> </div> </div>
1	E	139	<div> <div>9%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	139	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>76%</div><div>17%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	G	139	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>76%</div><div>19%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	H	139	<div><div><div></div><div></div><div></div></div><div><div>7%</div><div>72%</div><div>22%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8498 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 fluoroacetyl-CoA thioesterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	Se	0	1	0
			1022	651	179	186	2	4			
1	B	135	Total	C	N	O	S	Se	0	2	0
			1061	671	191	193	2	4			
1	C	132	Total	C	N	O	S	Se	0	1	0
			1026	652	183	186	2	3			
1	D	133	Total	C	N	O	S	Se	0	1	0
			1026	653	185	182	2	4			
1	E	133	Total	C	N	O	S	Se	0	1	0
			1018	649	178	185	2	4			
1	F	133	Total	C	N	O	S	Se	0	1	0
			1030	655	184	185	2	4			
1	G	133	Total	C	N	O	S	Se	0	1	0
			1018	648	178	186	2	4			
1	H	134	Total	C	N	O	S	Se	0	1	0
			1022	651	179	186	2	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		
2	B	41	Total	O	0	0
			41	41		
2	C	33	Total	O	0	0
			33	33		
2	D	26	Total	O	0	0
			26	26		
2	E	30	Total	O	0	0
			30	30		
2	F	39	Total	O	0	0
			39	39		

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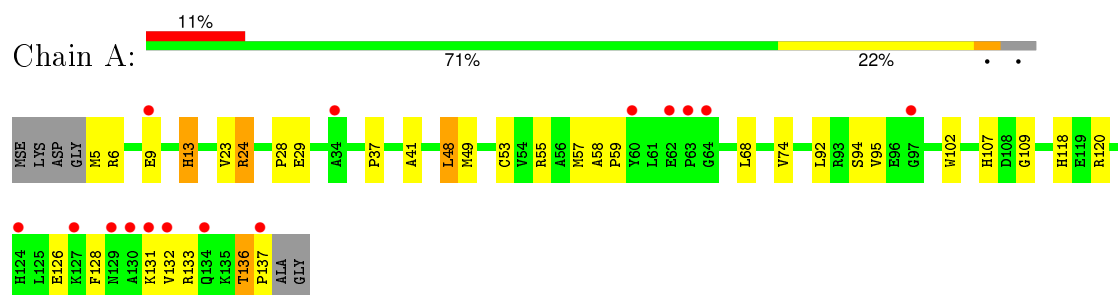
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	43	Total 43	O 43	0	0
2	H	26	Total 26	O 26	0	0

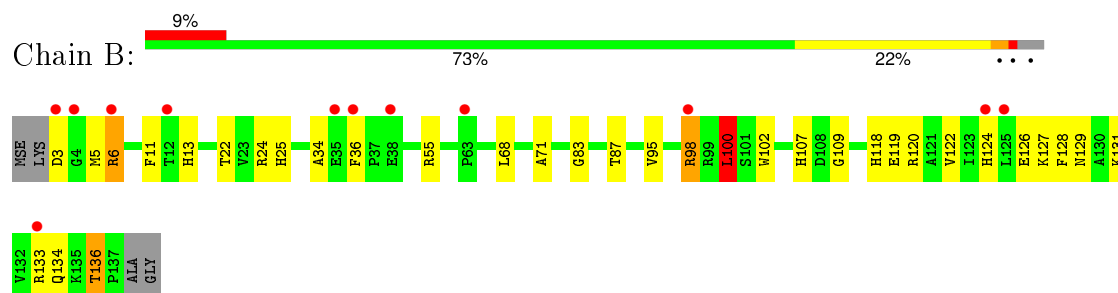
### 3 Residue-property plots [i](#)

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.

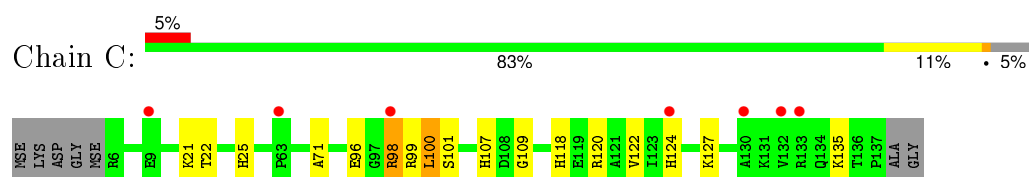
#### • Molecule 1: fluoroacetyl-CoA thioesterase



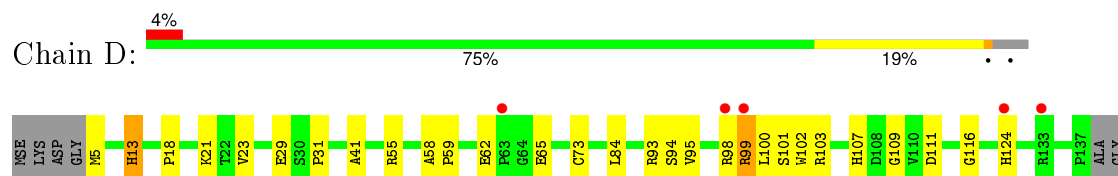
#### • Molecule 1: fluoroacetyl-CoA thioesterase



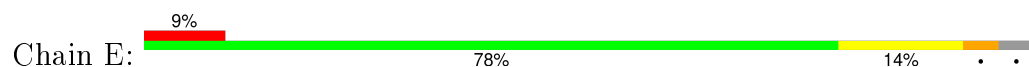
#### • Molecule 1: fluoroacetyl-CoA thioesterase

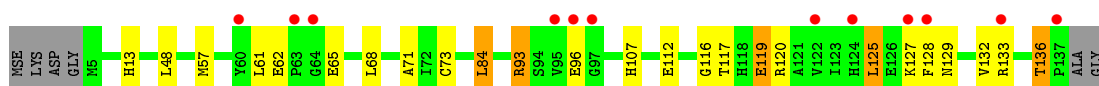


#### • Molecule 1: fluoroacetyl-CoA thioesterase

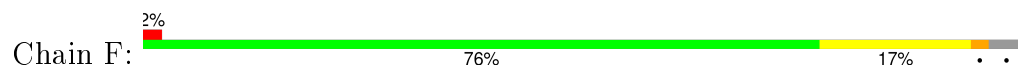


#### • Molecule 1: fluoroacetyl-CoA thioesterase

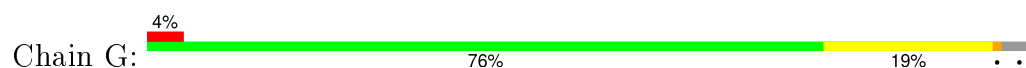




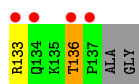
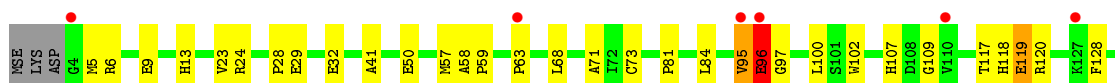
- Molecule 1: fluoroacetyl-CoA thioesterase



- Molecule 1: fluoroacetyl-CoA thioesterase



- Molecule 1: fluoroacetyl-CoA thioesterase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.91Å 71.08Å 104.35Å 90.00° 102.62° 90.00°	Depositor
Resolution (Å)	49.75 – 2.35 47.67 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.75-2.35) 95.2 (47.67-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.39 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.190 , 0.243 0.205 , 0.198	Depositor DCC
$R_{free}$ test set	2000 reflections (4.61%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 45339 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.39 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1529e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 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	0.49	0/1049	0.58	0/1426
1	B	0.49	0/1087	0.65	1/1472 (0.1%)
1	C	0.49	0/1053	0.65	1/1430 (0.1%)
1	D	0.48	0/1053	0.60	1/1430 (0.1%)
1	E	0.49	0/1045	0.63	0/1421
1	F	0.51	0/1057	0.62	0/1435
1	G	0.52	0/1045	0.58	0/1422
1	H	0.50	0/1048	0.59	0/1423
All	All	0.49	0/8437	0.61	3/11459 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	H	0	2
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	LEU	CA-CB-CG	5.39	127.69	115.30
1	D	13	HIS	N-CA-CB	-5.28	101.09	110.60
1	B	100	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	96	GLU	Peptide
1	H	63	PRO	Peptide
1	H	95	VAL	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1022	0	982	29	0
1	B	1061	0	1027	35	2
1	C	1026	0	993	10	0
1	D	1026	0	996	23	0
1	E	1018	0	976	20	0
1	F	1030	0	998	20	0
1	G	1018	0	971	29	0
1	H	1022	0	979	22	0
2	A	37	0	0	1	3
2	B	41	0	0	3	1
2	C	33	0	0	1	0
2	D	26	0	0	1	0
2	E	30	0	0	0	0
2	F	39	0	0	2	0
2	G	43	0	0	3	0
2	H	26	0	0	1	0
All	All	8498	0	7922	171	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:NH1	1:B:6:ARG:HG3	1.61	1.04
1:B:107[B]:HIS:HE1	1:D:99:ARG:NH1	1.60	0.98
1:B:6:ARG:CG	1:B:6:ARG:HH11	1.75	0.98
1:B:6:ARG:HG3	1:B:6:ARG:HH11	0.82	0.96
1:E:93:ARG:HG3	1:E:93:ARG:HH21	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107[B]:HIS:CE1	1:D:99:ARG:CZ	2.51	0.93
1:B:107[B]:HIS:HE1	1:D:99:ARG:CZ	1.81	0.92
1:B:118:HIS:HE1	1:B:120:ARG:HH11	1.17	0.92
1:B:13:HIS:CD2	1:B:55:ARG:HH11	1.88	0.90
1:A:13:HIS:HD2	1:A:55:ARG:HH11	1.19	0.88
1:F:107[B]:HIS:CD2	1:F:109:GLY:H	1.95	0.85
1:B:107[B]:HIS:CE1	1:D:99:ARG:NH1	2.45	0.84
1:B:133:ARG:HA	1:B:136:THR:HG23	1.61	0.82
1:H:24:ARG:HD3	2:H:419:HOH:O	1.79	0.82
1:B:13:HIS:CD2	1:B:55:ARG:NH1	2.52	0.78
1:G:107[A]:HIS:HD2	1:G:109:GLY:H	1.31	0.78
1:A:107[B]:HIS:HD2	1:A:109:GLY:H	1.32	0.78
1:F:107[A]:HIS:HD2	1:F:109:GLY:H	1.31	0.77
1:C:107[B]:HIS:CD2	1:C:109:GLY:H	2.04	0.76
1:C:118:HIS:HE1	1:C:120:ARG:HH11	1.34	0.75
1:G:57:MSE:HE2	1:G:102:TRP:HZ2	1.51	0.75
1:B:11:PHE:CE1	2:B:411:HOH:O	2.40	0.75
1:D:107[B]:HIS:HD2	1:D:109:GLY:H	1.36	0.74
1:G:118:HIS:HE1	1:G:120:ARG:HH11	1.36	0.73
1:G:6:ARG:O	1:G:9:GLU:HB2	1.89	0.72
1:E:93:ARG:NH2	1:E:93:ARG:HG3	2.05	0.72
1:B:13:HIS:HD2	1:B:55:ARG:NH1	1.88	0.72
1:A:118:HIS:HE1	1:A:120:ARG:HH11	1.37	0.71
1:G:107[B]:HIS:CD2	1:G:109:GLY:H	2.09	0.71
1:B:118:HIS:CE1	1:B:120:ARG:HH11	2.06	0.71
1:A:13:HIS:CD2	1:A:55:ARG:HH11	2.07	0.70
1:B:119:GLU:OE2	2:B:233:HOH:O	2.10	0.70
1:H:107[B]:HIS:HD2	1:H:109:GLY:H	1.40	0.70
1:H:96:GLU:O	1:H:96:GLU:CG	2.41	0.69
1:C:107[B]:HIS:HD2	1:C:109:GLY:H	1.42	0.67
1:H:96:GLU:O	1:H:96:GLU:HG3	1.94	0.66
1:C:101:SER:HB3	2:C:187:HOH:O	1.95	0.66
1:B:107[A]:HIS:HD2	1:B:109:GLY:H	1.44	0.66
1:A:107[B]:HIS:CD2	1:A:109:GLY:H	2.13	0.65
1:E:125:LEU:HD23	1:E:129:ASN:HD21	1.62	0.64
1:G:57:MSE:HE2	1:G:102:TRP:CZ2	2.33	0.64
1:H:96:GLU:N	1:H:97:GLY:HA2	2.14	0.63
1:D:107[B]:HIS:CD2	1:D:109:GLY:H	2.16	0.62
1:B:124:HIS:ND1	1:B:127:LYS:HG3	2.15	0.61
1:H:133:ARG:HA	1:H:136:THR:CG2	2.30	0.61
1:G:13:HIS:CE1	1:G:55:ARG:HH11	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107[B]:HIS:CD2	1:B:109:GLY:H	2.20	0.60
1:A:37:PRO:HB3	1:B:129:ASN:OD1	2.02	0.59
1:A:6:ARG:O	1:A:9:GLU:HB2	2.03	0.59
1:C:118:HIS:CE1	1:C:120:ARG:HH11	2.18	0.59
1:E:68:LEU:HD11	1:E:128:PHE:CZ	2.38	0.59
1:A:24:ARG:HG3	2:A:377:HOH:O	2.03	0.58
1:C:124:HIS:CD2	1:C:127:LYS:HB2	2.39	0.58
1:G:124:HIS:CE1	1:G:126:GLU:HB2	2.38	0.58
1:B:11:PHE:HE1	2:B:411:HOH:O	1.78	0.58
1:F:99:ARG:NH1	1:G:99:ARG:NH1	2.51	0.58
1:H:96:GLU:H	1:H:97:GLY:HA2	1.67	0.58
1:E:68:LEU:HD11	1:E:128:PHE:CE1	2.40	0.57
1:B:6:ARG:CG	1:B:6:ARG:NH1	2.46	0.57
1:E:71:ALA:HB3	1:E:119:GLU:HG3	1.85	0.57
1:B:5:MSE:HE1	1:B:102:TRP:HH2	1.69	0.57
1:H:133:ARG:HA	1:H:136:THR:HG22	1.87	0.56
1:B:107[A]:HIS:CD2	1:B:109:GLY:H	2.24	0.56
1:F:99:ARG:NH1	1:G:99:ARG:HH11	2.03	0.56
1:E:107[B]:HIS:HD2	1:E:112:GLU:CD	2.09	0.56
1:H:107[B]:HIS:CD2	1:H:109:GLY:H	2.21	0.56
1:D:5:MSE:HE1	1:D:102:TRP:HH2	1.71	0.56
1:F:22:THR:OG1	1:F:25:HIS:HD2	1.89	0.56
1:F:107[A]:HIS:HD2	1:F:109:GLY:N	2.01	0.55
1:H:71:ALA:HB3	1:H:119:GLU:HG3	1.89	0.55
1:H:57:MSE:SE	1:H:120:ARG:HD3	2.57	0.55
1:A:133:ARG:O	1:A:136:THR:HG22	2.07	0.54
1:A:107[A]:HIS:HD2	1:A:109:GLY:H	1.54	0.54
1:G:124:HIS:HE1	1:G:126:GLU:HB2	1.72	0.53
1:E:133:ARG:HA	1:E:136:THR:HG23	1.90	0.53
1:F:99:ARG:HH22	1:G:96:GLU:CD	2.12	0.53
1:G:118:HIS:CE1	1:G:120:ARG:HH11	2.23	0.52
1:B:24[B]:ARG:HG2	1:B:34:ALA:HA	1.91	0.52
1:F:98:ARG:HG3	1:F:122:VAL:HB	1.91	0.52
1:G:68:LEU:HD11	1:G:128:PHE:CZ	2.45	0.52
1:G:57:MSE:CE	1:G:120:ARG:HD3	2.40	0.51
1:D:95:VAL:HG23	1:D:100:LEU:HG	1.91	0.51
1:E:57:MSE:CE	1:E:120:ARG:HD3	2.40	0.51
1:A:137:PRO:HG3	1:B:83:GLY:HA3	1.93	0.50
1:F:103:ARG:NH1	2:F:149:HOH:O	2.36	0.50
1:E:125:LEU:HD23	1:E:129:ASN:ND2	2.27	0.50
1:H:81:PRO:HD2	1:H:84:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:MSE:HE1	1:F:67:SER:CB	2.43	0.49
1:B:87:THR:HB	1:B:107[A]:HIS:CE1	2.48	0.49
1:F:5:MSE:HG2	1:F:60:TYR:CD2	2.47	0.49
1:A:133:ARG:C	1:A:136:THR:HG22	2.33	0.49
1:F:68:LEU:HD21	1:F:128:PHE:CZ	2.48	0.48
1:G:107[A]:HIS:CD2	1:G:109:GLY:H	2.20	0.48
1:F:107[B]:HIS:CD2	1:F:109:GLY:N	2.74	0.48
1:G:12:THR:HG21	2:G:192:HOH:O	2.13	0.48
1:D:58:ALA:N	1:D:59:PRO:CD	2.77	0.48
1:F:58:ALA:N	1:F:59:PRO:CD	2.77	0.48
1:H:23:VAL:HA	1:H:41:ALA:HB2	1.94	0.48
1:H:68:LEU:HD11	1:H:128:PHE:CE1	2.48	0.47
1:E:117:THR:OG1	1:G:91:GLU:OE1	2.26	0.47
1:H:5:MSE:HE1	1:H:102:TRP:CH2	2.50	0.47
1:E:62:GLU:O	1:E:65:GLU:HB2	2.15	0.47
1:A:13:HIS:CE1	1:A:48:LEU:HD22	2.50	0.47
1:B:68:LEU:HD11	1:B:128:PHE:CE1	2.50	0.47
1:D:94:SER:HB3	1:D:101:SER:HB3	1.97	0.47
1:D:5:MSE:HE1	1:D:102:TRP:CH2	2.48	0.46
1:F:29:GLU:O	1:F:31:PRO:HD3	2.15	0.46
1:E:127:LYS:O	1:E:127:LYS:HG2	2.15	0.46
1:A:53:CYS:O	1:A:57:MSE:HG2	2.15	0.46
1:H:6:ARG:O	1:H:9:GLU:HB2	2.15	0.46
1:A:118:HIS:CE1	1:A:120:ARG:HH11	2.26	0.46
1:D:23:VAL:HA	1:D:41:ALA:HB2	1.97	0.46
1:G:24:ARG:HG2	2:G:162:HOH:O	2.15	0.46
1:A:133:ARG:O	1:A:136:THR:CG2	2.63	0.46
1:D:95:VAL:O	1:D:95:VAL:HG13	2.16	0.46
1:E:57:MSE:HE1	1:E:120:ARG:HD3	1.97	0.46
1:G:5:MSE:HE3	1:G:9:GLU:OE1	2.16	0.45
1:F:99:ARG:NH2	1:G:96:GLU:OE1	2.48	0.45
1:G:107[A]:HIS:HD2	1:G:109:GLY:N	2.06	0.45
1:F:24:ARG:HD3	2:F:357:HOH:O	2.16	0.45
1:A:13:HIS:CD2	1:A:55:ARG:NH1	2.81	0.45
1:A:5:MSE:HE1	1:A:102:TRP:HH2	1.81	0.45
1:A:5:MSE:CE	1:A:102:TRP:HH2	2.30	0.45
1:H:58:ALA:N	1:H:59:PRO:CD	2.80	0.45
1:A:68:LEU:HD11	1:A:128:PHE:CE1	2.52	0.44
1:E:132:VAL:O	1:E:136:THR:HG22	2.17	0.44
1:D:13:HIS:CE1	1:D:55:ARG:HH11	2.35	0.44
1:A:57:MSE:SE	1:A:120:ARG:HD3	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:GLU:OE1	1:H:117:THR:OG1	2.31	0.44
1:E:125:LEU:O	1:E:129:ASN:ND2	2.50	0.44
1:G:99:ARG:HG3	2:G:230:HOH:O	2.18	0.44
1:A:23:VAL:HA	1:A:41:ALA:HB2	1.98	0.44
1:D:29:GLU:O	1:D:31:PRO:HD3	2.18	0.43
1:B:118:HIS:HE1	1:B:120:ARG:NH1	2.00	0.43
1:G:5:MSE:HE2	1:G:92:LEU:HD22	2.00	0.43
1:G:57:MSE:HE1	1:G:120:ARG:HD3	2.01	0.43
1:C:22:THR:OG1	1:C:25:HIS:HD2	2.01	0.43
1:H:28:PRO:HD2	1:H:29:GLU:OE2	2.19	0.43
1:H:50:GLU:HG2	1:H:118:HIS:CE1	2.54	0.43
1:D:62:GLU:O	1:D:65:GLU:HB2	2.19	0.43
1:E:73:CYS:O	1:E:116:GLY:HA3	2.19	0.43
1:E:84:LEU:HD13	1:F:137:PRO:HG3	2.00	0.43
1:C:71:ALA:O	1:C:118:HIS:HD2	2.02	0.42
1:B:98:ARG:HG2	1:B:122:VAL:HB	2.00	0.42
1:G:55:ARG:HG2	1:H:32:GLU:HG2	2.01	0.42
1:B:24[A]:ARG:NH1	1:B:36:PHE:O	2.39	0.42
1:B:107[B]:HIS:CE1	1:D:99:ARG:NE	2.87	0.42
1:D:98:ARG:NH2	1:D:124:HIS:CE1	2.88	0.42
1:A:49:MSE:SE	1:A:74:VAL:HG11	2.70	0.42
1:D:18:PRO:HG2	1:D:21:LYS:HG2	2.01	0.42
1:D:93:ARG:NH1	2:D:409:HOH:O	2.53	0.42
1:B:71:ALA:O	1:B:118:HIS:HD2	2.03	0.41
1:A:107[B]:HIS:HD2	1:A:109:GLY:N	2.09	0.41
1:B:95:VAL:HG13	1:B:100:LEU:HD22	2.02	0.41
1:B:22:THR:OG1	1:B:25:HIS:HD2	2.02	0.41
1:F:73:CYS:O	1:F:116:GLY:HA3	2.20	0.41
1:E:132:VAL:O	1:E:136:THR:CG2	2.67	0.41
1:A:5:MSE:HE1	1:A:102:TRP:CH2	2.55	0.41
1:D:73:CYS:O	1:D:116:GLY:HA3	2.21	0.41
1:G:73:CYS:O	1:G:116:GLY:HA3	2.19	0.41
1:A:28:PRO:HD2	1:A:29:GLU:OE2	2.21	0.41
1:G:73:CYS:HA	1:H:73:CYS:HA	2.03	0.41
1:A:58:ALA:N	1:A:59:PRO:CD	2.84	0.41
1:G:133:ARG:C	1:G:135:LYS:H	2.24	0.41
1:E:107[B]:HIS:HD2	1:E:112:GLU:OE2	2.03	0.41
1:B:131:LYS:O	1:B:134:GLN:HB2	2.20	0.41
1:C:135:LYS:NZ	1:D:111:ASP:OD2	2.42	0.40
1:A:13:HIS:HE1	1:A:48:LEU:HD22	1.87	0.40
1:C:98:ARG:HG3	1:C:122:VAL:HB	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD21	1:A:95:VAL:CG2	2.52	0.40
1:D:93:ARG:NH2	1:D:103:ARG:HD3	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:422:HOH:O	2:B:412:HOH:O[2_647]	0.44	1.76
1:B:13:HIS:NE2	2:A:407:HOH:O[2_657]	1.25	0.95
1:B:13:HIS:CE1	2:A:407:HOH:O[2_657]	1.95	0.25

## 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	132/139 (95%)	130 (98%)	2 (2%)	0	100	100
1	B	135/139 (97%)	135 (100%)	0	0	100	100
1	C	131/139 (94%)	130 (99%)	1 (1%)	0	100	100
1	D	132/139 (95%)	130 (98%)	2 (2%)	0	100	100
1	E	132/139 (95%)	130 (98%)	2 (2%)	0	100	100
1	F	132/139 (95%)	132 (100%)	0	0	100	100
1	G	132/139 (95%)	128 (97%)	4 (3%)	0	100	100
1	H	133/139 (96%)	128 (96%)	4 (3%)	1 (1%)	24	26
All	All	1059/1112 (95%)	1043 (98%)	15 (1%)	1 (0%)	56	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	96	GLU

### 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	107/108 (99%)	99 (92%)	8 (8%)	17	18
1	B	112/108 (104%)	106 (95%)	6 (5%)	27	33
1	C	108/108 (100%)	104 (96%)	4 (4%)	41	53
1	D	107/108 (99%)	105 (98%)	2 (2%)	65	79
1	E	106/108 (98%)	97 (92%)	9 (8%)	13	14
1	F	108/108 (100%)	101 (94%)	7 (6%)	21	24
1	G	106/108 (98%)	101 (95%)	5 (5%)	32	41
1	H	106/108 (98%)	100 (94%)	6 (6%)	25	30
All	All	860/864 (100%)	813 (94%)	47 (6%)	27	32

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	24	ARG
1	A	48	LEU
1	A	94	SER
1	A	126	GLU
1	A	131	LYS
1	A	132	VAL
1	A	136	THR
1	B	3	ASP
1	B	6	ARG
1	B	98	ARG
1	B	100	LEU
1	B	126	GLU
1	B	136	THR
1	C	21	LYS
1	C	98	ARG
1	C	99	ARG
1	C	100	LEU
1	D	84	LEU

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Mol	Chain	Res	Type
1	D	99	ARG
1	E	13	HIS
1	E	48	LEU
1	E	61	LEU
1	E	84	LEU
1	E	93	ARG
1	E	96	GLU
1	E	119	GLU
1	E	125	LEU
1	E	136	THR
1	F	12	THR
1	F	33	PHE
1	F	68	LEU
1	F	98	ARG
1	F	99	ARG
1	F	127	LYS
1	F	133	ARG
1	G	96	GLU
1	G	105	SER
1	G	112	GLU
1	G	126	GLU
1	G	134	GLN
1	H	13	HIS
1	H	95	VAL
1	H	96	GLU
1	H	100	LEU
1	H	119	GLU
1	H	136	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	118	HIS
1	B	13	HIS
1	B	25	HIS
1	B	118	HIS
1	C	25	HIS
1	C	118	HIS
1	C	124	HIS
1	D	124	HIS
1	E	25	HIS

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Mol	Chain	Res	Type
1	E	129	ASN
1	F	25	HIS
1	F	124	HIS
1	G	13	HIS
1	G	118	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no 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	129/139 (92%)	0.60	15 (11%)	6 11	13, 25, 46, 52	0
1	B	131/139 (94%)	0.57	12 (9%)	11 18	14, 24, 42, 53	0
1	C	129/139 (92%)	0.48	7 (5%)	29 44	13, 25, 45, 50	0
1	D	129/139 (92%)	0.39	5 (3%)	43 57	13, 25, 42, 46	0
1	E	129/139 (92%)	0.44	12 (9%)	11 18	12, 23, 51, 56	0
1	F	129/139 (92%)	0.41	3 (2%)	64 76	11, 22, 35, 43	0
1	G	129/139 (92%)	0.41	6 (4%)	35 50	11, 23, 40, 51	0
1	H	130/139 (93%)	0.52	10 (7%)	16 25	14, 26, 47, 51	0
All	All	1035/1112 (93%)	0.48	70 (6%)	20 31	11, 25, 45, 56	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	LYS	6.6
1	B	3	ASP	5.9
1	H	95	VAL	4.9
1	F	133	ARG	4.7
1	A	63	PRO	4.6
1	B	36	PHE	4.3
1	B	6	ARG	4.2
1	E	124	HIS	4.2
1	A	130	ALA	4.2
1	A	134	GLN	3.9
1	E	63	PRO	3.6
1	H	96	GLU	3.5
1	E	64	GLY	3.5
1	A	124	HIS	3.5
1	A	64	GLY	3.4
1	E	137	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	97	GLY	3.3
1	B	98	ARG	3.3
1	G	134	GLN	3.3
1	D	99	ARG	3.2
1	H	134	GLN	3.2
1	H	133	ARG	3.1
1	G	126	GLU	3.1
1	B	35	GLU	3.0
1	A	62	GLU	3.0
1	B	4	GLY	2.9
1	H	110	VAL	2.9
1	C	98	ARG	2.9
1	G	136	THR	2.9
1	E	60	TYR	2.9
1	C	63	PRO	2.8
1	A	60	TYR	2.8
1	H	127	LYS	2.8
1	H	136	THR	2.8
1	E	122	VAL	2.7
1	E	96	GLU	2.7
1	H	137	PRO	2.7
1	F	124	HIS	2.6
1	C	124	HIS	2.5
1	B	125	LEU	2.5
1	C	9	GLU	2.5
1	E	127	LYS	2.4
1	B	38	GLU	2.4
1	D	98	ARG	2.4
1	A	131	LYS	2.4
1	E	133	ARG	2.4
1	G	137	PRO	2.3
1	F	125	LEU	2.3
1	H	63	PRO	2.3
1	A	132	VAL	2.3
1	H	4	GLY	2.2
1	G	38	GLU	2.2
1	A	129	ASN	2.2
1	E	128	PHE	2.2
1	A	137	PRO	2.2
1	E	95	VAL	2.2
1	A	9	GLU	2.2
1	A	34	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	24	ARG	2.1
1	C	132	VAL	2.1
1	D	133	ARG	2.1
1	E	97	GLY	2.1
1	D	124	HIS	2.1
1	B	63	PRO	2.1
1	C	133	ARG	2.1
1	B	124	HIS	2.1
1	B	12	THR	2.1
1	B	133	ARG	2.1
1	C	130	ALA	2.0
1	D	63	PRO	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.