



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:30 PM GMT

PDB ID : 4XZG
Title : Crystal structure of HIRAN domain of human HLTF
Authors : Ikegaya, Y.; Hara, K.; Hashimoto, H.
Deposited on : 2015-02-04
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

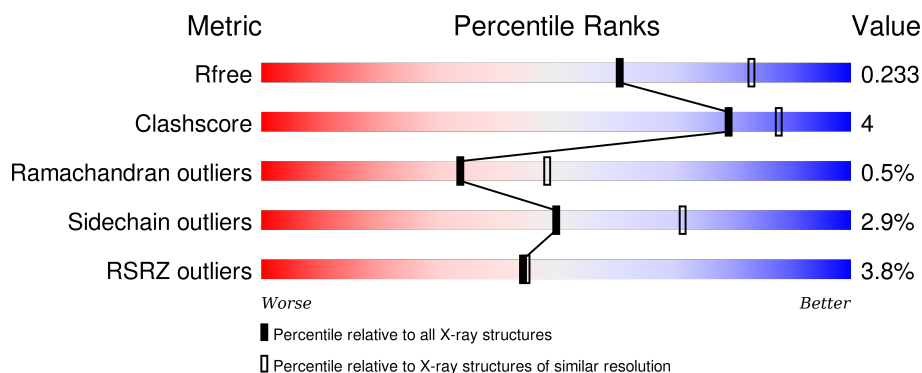
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	138	<div> <div>3%</div> <div>80% 7% 12%</div> </div>
1	B	138	<div> <div>3%</div> <div>78% 9% 12%</div> </div>
1	C	138	<div> <div>%</div> <div>80% 7% • 13%</div> </div>
1	D	138	<div> <div>3%</div> <div>80% 7% • 12%</div> </div>
1	E	138	<div> <div>4%</div> <div>78% 10% 12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	138	<div><div></div><div>3%</div><div>76%</div><div>12%</div><div>12%</div></div>
1	G	138	<div><div></div><div>4%</div><div>78%</div><div>9%</div><div>• 11%</div></div>
1	H	138	<div><div></div><div>2%</div><div>80%</div><div>9%</div><div>12%</div></div>
1	I	138	<div><div></div><div>7%</div><div>73%</div><div>14%</div><div>• 12%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8853 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 Helicase-like transcription factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			939	596	171	168	4			
1	B	121	Total	C	N	O	S	0	0	0
			939	596	171	168	4			
1	C	120	Total	C	N	O	S	0	0	0
			928	587	170	167	4			
1	D	121	Total	C	N	O	S	0	0	0
			939	596	171	168	4			
1	E	121	Total	C	N	O	S	0	0	0
			939	596	171	168	4			
1	F	122	Total	C	N	O	S	0	0	0
			951	605	172	170	4			
1	G	123	Total	C	N	O	S	0	0	0
			959	611	173	171	4			
1	H	122	Total	C	N	O	S	0	0	0
			944	599	172	169	4			
1	I	122	Total	C	N	O	S	0	0	0
			951	605	172	170	4			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	expression tag	UNP Q14527
A	38	ARG	-	expression tag	UNP Q14527
A	39	GLY	-	expression tag	UNP Q14527
A	40	SER	-	expression tag	UNP Q14527
A	41	HIS	-	expression tag	UNP Q14527
A	42	HIS	-	expression tag	UNP Q14527
A	43	HIS	-	expression tag	UNP Q14527
A	44	HIS	-	expression tag	UNP Q14527
A	45	HIS	-	expression tag	UNP Q14527
A	46	HIS	-	expression tag	UNP Q14527
A	47	GLY	-	expression tag	UNP Q14527

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Chain	Residue	Modelled	Actual	Comment	Reference
A	48	SER	-	expression tag	UNP Q14527
A	49	GLU	-	expression tag	UNP Q14527
A	50	ASN	-	expression tag	UNP Q14527
A	51	LEU	-	expression tag	UNP Q14527
A	52	TYR	-	expression tag	UNP Q14527
A	53	PHE	-	expression tag	UNP Q14527
A	54	GLN	-	expression tag	UNP Q14527
A	55	GLY	-	expression tag	UNP Q14527
A	56	GLY	-	expression tag	UNP Q14527
B	37	MET	-	expression tag	UNP Q14527
B	38	ARG	-	expression tag	UNP Q14527
B	39	GLY	-	expression tag	UNP Q14527
B	40	SER	-	expression tag	UNP Q14527
B	41	HIS	-	expression tag	UNP Q14527
B	42	HIS	-	expression tag	UNP Q14527
B	43	HIS	-	expression tag	UNP Q14527
B	44	HIS	-	expression tag	UNP Q14527
B	45	HIS	-	expression tag	UNP Q14527
B	46	HIS	-	expression tag	UNP Q14527
B	47	GLY	-	expression tag	UNP Q14527
B	48	SER	-	expression tag	UNP Q14527
B	49	GLU	-	expression tag	UNP Q14527
B	50	ASN	-	expression tag	UNP Q14527
B	51	LEU	-	expression tag	UNP Q14527
B	52	TYR	-	expression tag	UNP Q14527
B	53	PHE	-	expression tag	UNP Q14527
B	54	GLN	-	expression tag	UNP Q14527
B	55	GLY	-	expression tag	UNP Q14527
B	56	GLY	-	expression tag	UNP Q14527
C	37	MET	-	expression tag	UNP Q14527
C	38	ARG	-	expression tag	UNP Q14527
C	39	GLY	-	expression tag	UNP Q14527
C	40	SER	-	expression tag	UNP Q14527
C	41	HIS	-	expression tag	UNP Q14527
C	42	HIS	-	expression tag	UNP Q14527
C	43	HIS	-	expression tag	UNP Q14527
C	44	HIS	-	expression tag	UNP Q14527
C	45	HIS	-	expression tag	UNP Q14527
C	46	HIS	-	expression tag	UNP Q14527
C	47	GLY	-	expression tag	UNP Q14527
C	48	SER	-	expression tag	UNP Q14527
C	49	GLU	-	expression tag	UNP Q14527

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Chain	Residue	Modelled	Actual	Comment	Reference
C	50	ASN	-	expression tag	UNP Q14527
C	51	LEU	-	expression tag	UNP Q14527
C	52	TYR	-	expression tag	UNP Q14527
C	53	PHE	-	expression tag	UNP Q14527
C	54	GLN	-	expression tag	UNP Q14527
C	55	GLY	-	expression tag	UNP Q14527
C	56	GLY	-	expression tag	UNP Q14527
D	37	MET	-	expression tag	UNP Q14527
D	38	ARG	-	expression tag	UNP Q14527
D	39	GLY	-	expression tag	UNP Q14527
D	40	SER	-	expression tag	UNP Q14527
D	41	HIS	-	expression tag	UNP Q14527
D	42	HIS	-	expression tag	UNP Q14527
D	43	HIS	-	expression tag	UNP Q14527
D	44	HIS	-	expression tag	UNP Q14527
D	45	HIS	-	expression tag	UNP Q14527
D	46	HIS	-	expression tag	UNP Q14527
D	47	GLY	-	expression tag	UNP Q14527
D	48	SER	-	expression tag	UNP Q14527
D	49	GLU	-	expression tag	UNP Q14527
D	50	ASN	-	expression tag	UNP Q14527
D	51	LEU	-	expression tag	UNP Q14527
D	52	TYR	-	expression tag	UNP Q14527
D	53	PHE	-	expression tag	UNP Q14527
D	54	GLN	-	expression tag	UNP Q14527
D	55	GLY	-	expression tag	UNP Q14527
D	56	GLY	-	expression tag	UNP Q14527
E	37	MET	-	expression tag	UNP Q14527
E	38	ARG	-	expression tag	UNP Q14527
E	39	GLY	-	expression tag	UNP Q14527
E	40	SER	-	expression tag	UNP Q14527
E	41	HIS	-	expression tag	UNP Q14527
E	42	HIS	-	expression tag	UNP Q14527
E	43	HIS	-	expression tag	UNP Q14527
E	44	HIS	-	expression tag	UNP Q14527
E	45	HIS	-	expression tag	UNP Q14527
E	46	HIS	-	expression tag	UNP Q14527
E	47	GLY	-	expression tag	UNP Q14527
E	48	SER	-	expression tag	UNP Q14527
E	49	GLU	-	expression tag	UNP Q14527
E	50	ASN	-	expression tag	UNP Q14527
E	51	LEU	-	expression tag	UNP Q14527

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Chain	Residue	Modelled	Actual	Comment	Reference
E	52	TYR	-	expression tag	UNP Q14527
E	53	PHE	-	expression tag	UNP Q14527
E	54	GLN	-	expression tag	UNP Q14527
E	55	GLY	-	expression tag	UNP Q14527
E	56	GLY	-	expression tag	UNP Q14527
F	37	MET	-	expression tag	UNP Q14527
F	38	ARG	-	expression tag	UNP Q14527
F	39	GLY	-	expression tag	UNP Q14527
F	40	SER	-	expression tag	UNP Q14527
F	41	HIS	-	expression tag	UNP Q14527
F	42	HIS	-	expression tag	UNP Q14527
F	43	HIS	-	expression tag	UNP Q14527
F	44	HIS	-	expression tag	UNP Q14527
F	45	HIS	-	expression tag	UNP Q14527
F	46	HIS	-	expression tag	UNP Q14527
F	47	GLY	-	expression tag	UNP Q14527
F	48	SER	-	expression tag	UNP Q14527
F	49	GLU	-	expression tag	UNP Q14527
F	50	ASN	-	expression tag	UNP Q14527
F	51	LEU	-	expression tag	UNP Q14527
F	52	TYR	-	expression tag	UNP Q14527
F	53	PHE	-	expression tag	UNP Q14527
F	54	GLN	-	expression tag	UNP Q14527
F	55	GLY	-	expression tag	UNP Q14527
F	56	GLY	-	expression tag	UNP Q14527
G	37	MET	-	expression tag	UNP Q14527
G	38	ARG	-	expression tag	UNP Q14527
G	39	GLY	-	expression tag	UNP Q14527
G	40	SER	-	expression tag	UNP Q14527
G	41	HIS	-	expression tag	UNP Q14527
G	42	HIS	-	expression tag	UNP Q14527
G	43	HIS	-	expression tag	UNP Q14527
G	44	HIS	-	expression tag	UNP Q14527
G	45	HIS	-	expression tag	UNP Q14527
G	46	HIS	-	expression tag	UNP Q14527
G	47	GLY	-	expression tag	UNP Q14527
G	48	SER	-	expression tag	UNP Q14527
G	49	GLU	-	expression tag	UNP Q14527
G	50	ASN	-	expression tag	UNP Q14527
G	51	LEU	-	expression tag	UNP Q14527
G	52	TYR	-	expression tag	UNP Q14527
G	53	PHE	-	expression tag	UNP Q14527

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Chain	Residue	Modelled	Actual	Comment	Reference
G	54	GLN	-	expression tag	UNP Q14527
G	55	GLY	-	expression tag	UNP Q14527
G	56	GLY	-	expression tag	UNP Q14527
H	37	MET	-	expression tag	UNP Q14527
H	38	ARG	-	expression tag	UNP Q14527
H	39	GLY	-	expression tag	UNP Q14527
H	40	SER	-	expression tag	UNP Q14527
H	41	HIS	-	expression tag	UNP Q14527
H	42	HIS	-	expression tag	UNP Q14527
H	43	HIS	-	expression tag	UNP Q14527
H	44	HIS	-	expression tag	UNP Q14527
H	45	HIS	-	expression tag	UNP Q14527
H	46	HIS	-	expression tag	UNP Q14527
H	47	GLY	-	expression tag	UNP Q14527
H	48	SER	-	expression tag	UNP Q14527
H	49	GLU	-	expression tag	UNP Q14527
H	50	ASN	-	expression tag	UNP Q14527
H	51	LEU	-	expression tag	UNP Q14527
H	52	TYR	-	expression tag	UNP Q14527
H	53	PHE	-	expression tag	UNP Q14527
H	54	GLN	-	expression tag	UNP Q14527
H	55	GLY	-	expression tag	UNP Q14527
H	56	GLY	-	expression tag	UNP Q14527
I	37	MET	-	expression tag	UNP Q14527
I	38	ARG	-	expression tag	UNP Q14527
I	39	GLY	-	expression tag	UNP Q14527
I	40	SER	-	expression tag	UNP Q14527
I	41	HIS	-	expression tag	UNP Q14527
I	42	HIS	-	expression tag	UNP Q14527
I	43	HIS	-	expression tag	UNP Q14527
I	44	HIS	-	expression tag	UNP Q14527
I	45	HIS	-	expression tag	UNP Q14527
I	46	HIS	-	expression tag	UNP Q14527
I	47	GLY	-	expression tag	UNP Q14527
I	48	SER	-	expression tag	UNP Q14527
I	49	GLU	-	expression tag	UNP Q14527
I	50	ASN	-	expression tag	UNP Q14527
I	51	LEU	-	expression tag	UNP Q14527
I	52	TYR	-	expression tag	UNP Q14527
I	53	PHE	-	expression tag	UNP Q14527
I	54	GLN	-	expression tag	UNP Q14527
I	55	GLY	-	expression tag	UNP Q14527

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Chain	Residue	Modelled	Actual	Comment	Reference
I	56	GLY	-	expression tag	UNP Q14527

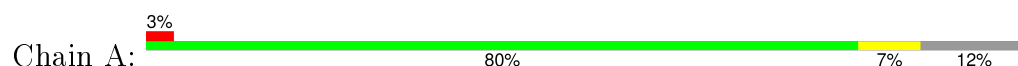
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	48	Total O 48 48	0	0
2	B	58	Total O 58 58	0	0
2	C	45	Total O 45 45	0	0
2	D	30	Total O 30 30	0	0
2	E	27	Total O 27 27	0	0
2	F	47	Total O 47 47	0	0
2	G	45	Total O 45 45	0	0
2	H	49	Total O 49 49	0	0
2	I	15	Total O 15 15	0	0

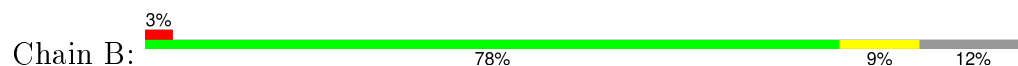
3 Residue-property plots [i](#)

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.

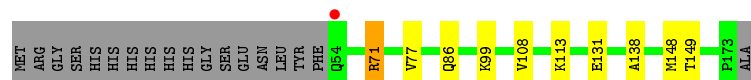
- Molecule 1: Helicase-like transcription factor



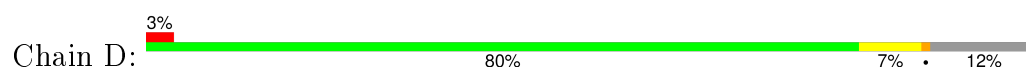
- Molecule 1: Helicase-like transcription factor



- Molecule 1: Helicase-like transcription factor



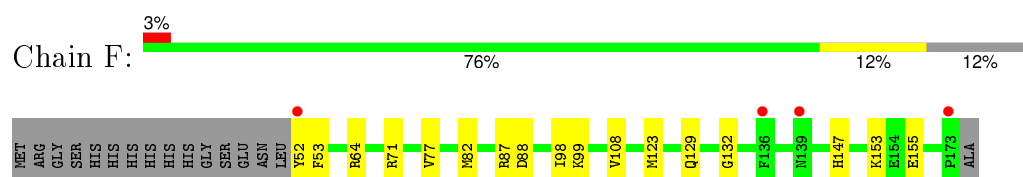
- Molecule 1: Helicase-like transcription factor



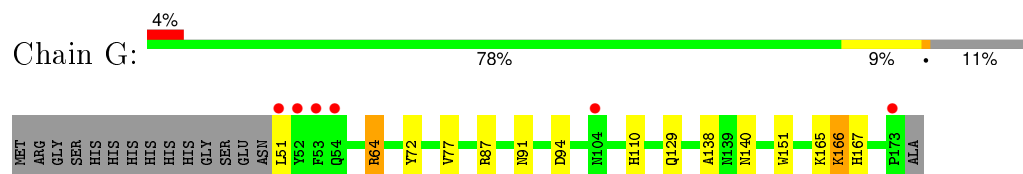
- Molecule 1: Helicase-like transcription factor



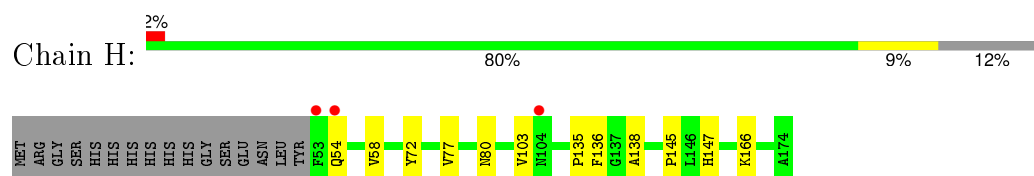
- Molecule 1: Helicase-like transcription factor



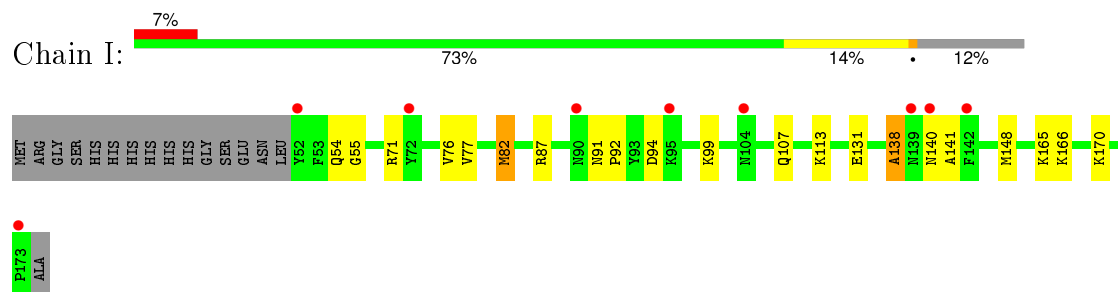
- Molecule 1: Helicase-like transcription factor



- Molecule 1: Helicase-like transcription factor



- Molecule 1: Helicase-like transcription factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.44Å 129.44Å 143.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-2.40) 99.8 (19.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.214 , 0.231 0.215 , 0.233	Depositor DCC
R_{free} test set	2430 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	6 of 48174 reflections (0.012%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8853	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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 34.50 % 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 6.7538e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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	0.75	0/959	0.87	1/1293 (0.1%)
1	B	0.75	0/959	0.81	0/1293
1	C	0.71	0/947	0.83	0/1277
1	D	0.71	0/959	0.83	1/1293 (0.1%)
1	E	0.68	0/959	0.77	0/1293
1	F	0.70	0/972	0.81	1/1311 (0.1%)
1	G	0.66	0/980	0.84	1/1322 (0.1%)
1	H	0.71	0/964	0.81	0/1300
1	I	0.65	0/972	0.75	0/1311
All	All	0.70	0/8671	0.81	4/11693 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	F	87	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	87	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	D	87	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	G	87	ARG	NE-CZ-NH1	5.56	123.08	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	939	0	935	6	0
1	B	939	0	935	7	0
1	C	928	0	926	7	0
1	D	939	0	935	5	0
1	E	939	0	935	5	0
1	F	951	0	944	7	0
1	G	959	0	955	12	0
1	H	944	0	940	6	0
1	I	951	0	944	11	0
2	A	48	0	0	0	0
2	B	58	0	0	2	0
2	C	45	0	0	1	0
2	D	30	0	0	1	0
2	E	27	0	0	0	0
2	F	47	0	0	1	0
2	G	45	0	0	3	0
2	H	49	0	0	0	0
2	I	15	0	0	0	0
All	All	8853	0	8449	60	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 4.

All (60) 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:G:64:ARG:HH11	1:G:64:ARG:HG2	1.42	0.83
1:B:77:VAL:HG13	1:B:138:ALA:HB1	1.66	0.77
1:C:71:ARG:NH1	1:H:80:ASN:HD22	1.83	0.77
1:A:91:ASN:HA	1:G:72:TYR:OH	1.86	0.74
1:E:78:ASN:O	1:E:81:GLU:HB2	1.89	0.72
1:D:68:VAL:HG12	1:D:143:THR:HG22	1.69	0.72
1:F:64:ARG:HD3	1:F:147:HIS:CE1	2.25	0.72
1:C:71:ARG:HH12	1:H:80:ASN:HD22	1.38	0.67
1:I:77:VAL:HG13	1:I:138:ALA:HB1	1.75	0.66
1:G:77:VAL:O	1:G:138:ALA:HB1	1.96	0.65
1:B:92:PRO:HG2	1:B:93:TYR:CE2	2.32	0.64
1:A:170:LYS:NZ	1:E:131:GLU:OE2	2.31	0.64
1:A:92:PRO:HD3	1:G:72:TYR:CE2	2.32	0.63
1:B:71:ARG:HG2	2:B:232:HOH:O	1.99	0.62
1:F:155:GLU:HG3	2:F:245:HOH:O	1.99	0.62
1:H:136:PHE:CE1	1:H:145:PRO:HG3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:91:ASN:HB3	1:I:94:ASP:O	2.02	0.59
1:C:86:GLN:OE1	1:C:99:LYS:HD2	2.02	0.59
1:D:149:THR:HG23	2:D:222:HOH:O	2.02	0.59
1:A:136:PHE:CE2	1:A:145:PRO:HG3	2.38	0.58
1:G:91:ASN:HB3	1:G:94:ASP:O	2.04	0.57
1:G:64:ARG:HH11	1:G:64:ARG:CG	2.17	0.55
1:D:53:PHE:N	1:D:53:PHE:CD1	2.75	0.54
1:G:129:GLN:HG2	1:G:151:TRP:HB2	1.92	0.51
1:A:68:VAL:HG12	1:A:143:THR:HG22	1.93	0.50
1:F:82:MET:HG3	1:F:132:GLY:O	2.12	0.50
1:B:122:ILE:HG13	1:B:163:GLN:HG2	1.94	0.49
1:C:77:VAL:O	1:C:138:ALA:HB1	2.15	0.47
1:B:92:PRO:HD3	1:H:72:TYR:HE2	1.79	0.47
1:G:165:LYS:HD2	2:G:242:HOH:O	2.15	0.47
1:H:77:VAL:O	1:H:138:ALA:HB1	2.15	0.47
1:C:77:VAL:CG2	1:C:108:VAL:HG21	2.46	0.46
1:I:131:GLU:O	1:I:148:MET:HA	2.15	0.46
1:F:77:VAL:CG2	1:F:108:VAL:HG21	2.45	0.46
1:B:155:GLU:HG3	2:B:207:HOH:O	2.16	0.45
1:F:98:ILE:HD13	1:F:123:MET:SD	2.57	0.45
1:E:71:ARG:HD3	1:E:142:PHE:CE2	2.52	0.45
1:I:54:GLN:CG	1:I:55:GLY:H	2.30	0.45
1:C:149:THR:HG23	2:C:236:HOH:O	2.17	0.44
1:D:91:ASN:HB3	1:D:94:ASP:O	2.17	0.44
1:I:91:ASN:HA	1:I:92:PRO:HD2	1.72	0.44
1:G:140:ASN:HB3	2:G:232:HOH:O	2.16	0.44
1:F:153:LYS:HB3	1:F:155:GLU:OE2	2.18	0.43
1:I:140:ASN:OD1	1:I:141:ALA:N	2.51	0.43
1:D:131:GLU:O	1:D:148:MET:HA	2.18	0.43
1:I:99:LYS:HG2	1:I:107:GLN:NE2	2.34	0.43
1:H:135:PRO:HG3	1:H:147:HIS:CD2	2.54	0.42
1:G:166:LYS:HG2	1:G:167:HIS:CD2	2.54	0.42
1:G:110:HIS:HB3	2:G:229:HOH:O	2.18	0.42
1:I:76:VAL:HG12	1:I:77:VAL:N	2.34	0.42
1:F:88:ASP:HB2	1:F:99:LYS:HG3	2.02	0.41
1:G:64:ARG:HG2	1:G:64:ARG:NH1	2.22	0.41
1:B:53:PHE:HB3	1:B:153:LYS:HE2	2.03	0.41
1:C:131:GLU:O	1:C:148:MET:HA	2.21	0.41
1:I:165:LYS:O	1:I:166:LYS:C	2.58	0.41
1:E:63:LEU:HD12	1:E:63:LEU:HA	1.82	0.41
1:E:99:LYS:HB2	1:E:99:LYS:HE3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:87:ARG:HA	1:I:87:ARG:HD2	1.87	0.41
1:I:82:MET:C	1:I:82:MET:SD	3.00	0.40
1:A:98:ILE:HD13	1:A:123:MET:SD	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/138 (86%)	114 (96%)	5 (4%)	0	100	100
1	B	119/138 (86%)	115 (97%)	3 (2%)	1 (1%)	24	35
1	C	118/138 (86%)	116 (98%)	2 (2%)	0	100	100
1	D	119/138 (86%)	116 (98%)	3 (2%)	0	100	100
1	E	119/138 (86%)	111 (93%)	6 (5%)	2 (2%)	11	14
1	F	120/138 (87%)	116 (97%)	3 (2%)	1 (1%)	24	35
1	G	121/138 (88%)	118 (98%)	3 (2%)	0	100	100
1	H	120/138 (87%)	118 (98%)	2 (2%)	0	100	100
1	I	120/138 (87%)	111 (92%)	8 (7%)	1 (1%)	24	35
All	All	1075/1242 (87%)	1035 (96%)	35 (3%)	5 (0%)	34	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	138	ALA
1	I	138	ALA
1	E	72	TYR
1	B	135	PRO
1	F	53	PHE

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	98/112 (88%)	98 (100%)	0	100	100
1	B	98/112 (88%)	96 (98%)	2 (2%)	63	81
1	C	97/112 (87%)	95 (98%)	2 (2%)	61	80
1	D	98/112 (88%)	95 (97%)	3 (3%)	47	69
1	E	98/112 (88%)	93 (95%)	5 (5%)	29	46
1	F	99/112 (88%)	96 (97%)	3 (3%)	48	70
1	G	100/112 (89%)	97 (97%)	3 (3%)	48	70
1	H	98/112 (88%)	94 (96%)	4 (4%)	37	57
1	I	99/112 (88%)	95 (96%)	4 (4%)	38	58
All	All	885/1008 (88%)	859 (97%)	26 (3%)	50	71

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	82	MET
1	B	158	LYS
1	C	71	ARG
1	C	113	LYS
1	D	53	PHE
1	D	113	LYS
1	D	129	GLN
1	E	82	MET
1	E	85	LEU
1	E	129	GLN
1	E	140	ASN
1	E	166	LYS
1	F	52	TYR
1	F	71	ARG
1	F	129	GLN
1	G	51	LEU
1	G	64	ARG
1	G	166	LYS

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Mol	Chain	Res	Type
1	H	54	GLN
1	H	58	VAL
1	H	103	VAL
1	H	166	LYS
1	I	71	ARG
1	I	82	MET
1	I	113	LYS
1	I	170	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	78	ASN
1	B	90	ASN
1	B	104	ASN
1	E	79	ASN
1	E	104	ASN
1	F	104	ASN
1	F	147	HIS
1	H	80	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	121/138 (87%)	-0.13	4 (3%)	50	50	24, 39, 71, 102	0
1	B	121/138 (87%)	0.02	4 (3%)	50	50	26, 39, 74, 128	0
1	C	120/138 (86%)	-0.23	1 (0%)	87	87	26, 40, 64, 85	0
1	D	121/138 (87%)	0.04	4 (3%)	50	50	27, 47, 83, 143	0
1	E	121/138 (87%)	0.08	6 (4%)	32	33	29, 51, 90, 106	0
1	F	122/138 (88%)	-0.07	4 (3%)	50	50	22, 41, 77, 98	0
1	G	123/138 (89%)	-0.01	6 (4%)	33	34	29, 46, 73, 98	0
1	H	122/138 (88%)	-0.11	3 (2%)	61	60	24, 40, 69, 94	0
1	I	122/138 (88%)	0.30	9 (7%)	17	17	27, 54, 98, 117	0
All	All	1093/1242 (88%)	-0.01	41 (3%)	44	45	22, 44, 83, 143	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	93	TYR	6.8
1	I	139	ASN	5.1
1	B	53	PHE	4.5
1	G	52	TYR	4.0
1	E	54	GLN	4.0
1	C	54	GLN	3.9
1	D	53	PHE	3.8
1	D	54	GLN	3.6
1	B	173	PRO	3.5
1	I	173	PRO	3.5
1	G	54	GLN	3.4
1	E	136	PHE	3.4
1	A	54	GLN	3.4
1	I	90	ASN	3.3
1	D	136	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	71	ARG	3.3
1	F	136	PHE	3.2
1	F	139	ASN	3.2
1	A	136	PHE	3.2
1	A	139	ASN	3.1
1	I	72	TYR	3.0
1	G	173	PRO	3.0
1	G	51	LEU	2.9
1	B	139	ASN	2.9
1	F	52	TYR	2.7
1	H	53	PHE	2.7
1	I	52	TYR	2.6
1	E	137	GLY	2.6
1	G	53	PHE	2.5
1	I	95	LYS	2.5
1	B	137	GLY	2.5
1	E	140	ASN	2.4
1	I	140	ASN	2.4
1	I	104	ASN	2.3
1	F	173	PRO	2.3
1	I	142	PHE	2.3
1	E	139	ASN	2.2
1	H	104	ASN	2.1
1	H	54	GLN	2.1
1	A	53	PHE	2.0
1	G	104	ASN	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.