



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:55 PM UTC

PDB ID : 2QFD / pdb_00002qfd
Title : Crystal structure of the regulatory domain of human RIG-I with bound Hg
Authors : Cui, S.; Lammens, A.; Lammens, K.; Hopfner, K.P.
Deposited on : 2007-06-27
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

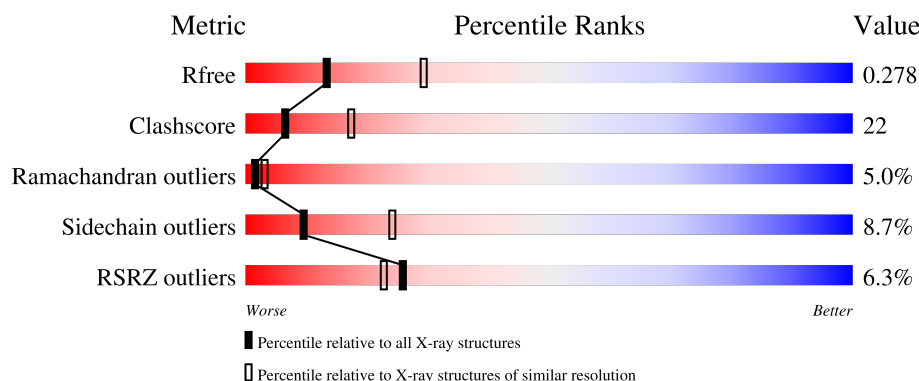
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	145	% 58% 21% 5% 17%
1	B	145	2% 56% 23% 5% 17%
1	C	145	3% 43% 34% 6% 17%
1	D	145	% 50% 27% 6% 17%
1	E	145	6% 41% 32% 10% 17%

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Mol	Chain	Length	Quality of chain
1	F	145	3% 40% 34% 9% 17%
1	G	145	7% 53% 25% 5% 17%
1	H	145	6% 47% 28% 7% 17%
1	I	145	6% 40% 35% 7% 17%
1	J	145	17% 46% 30% 6% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10092 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 Probable ATP-dependent RNA helicase DDX58.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	36	0	0
			998	648	169	173	8			
1	B	121	Total	C	N	O	S	73	0	0
			998	648	169	173	8			
1	C	121	Total	C	N	O	S	85	0	0
			998	648	169	173	8			
1	D	121	Total	C	N	O	S	130	0	0
			998	648	169	173	8			
1	E	121	Total	C	N	O	S	109	0	0
			998	648	169	173	8			
1	F	121	Total	C	N	O	S	86	0	0
			998	648	169	173	8			
1	G	121	Total	C	N	O	S	123	0	0
			998	648	169	173	8			
1	H	121	Total	C	N	O	S	98	0	0
			998	648	169	173	8			
1	I	121	Total	C	N	O	S	86	0	0
			998	648	169	173	8			
1	J	121	Total	C	N	O	S	176	0	0
			998	648	169	173	8			

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	781	MET	-	expression tag	UNP O95786
A	782	GLY	-	expression tag	UNP O95786
A	783	SER	-	expression tag	UNP O95786
A	784	SER	-	expression tag	UNP O95786
A	785	HIS	-	expression tag	UNP O95786
A	786	HIS	-	expression tag	UNP O95786
A	787	HIS	-	expression tag	UNP O95786
A	788	HIS	-	expression tag	UNP O95786
A	789	HIS	-	expression tag	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
A	790	HIS	-	expression tag	UNP O95786
A	791	SER	-	expression tag	UNP O95786
A	792	SER	-	expression tag	UNP O95786
A	793	GLY	-	expression tag	UNP O95786
A	794	LEU	-	expression tag	UNP O95786
A	795	VAL	-	expression tag	UNP O95786
A	796	PRO	-	expression tag	UNP O95786
A	797	ARG	-	expression tag	UNP O95786
A	798	GLY	-	expression tag	UNP O95786
A	799	SER	-	expression tag	UNP O95786
A	800	HIS	-	expression tag	UNP O95786
A	801	MET	-	expression tag	UNP O95786
B	781	MET	-	expression tag	UNP O95786
B	782	GLY	-	expression tag	UNP O95786
B	783	SER	-	expression tag	UNP O95786
B	784	SER	-	expression tag	UNP O95786
B	785	HIS	-	expression tag	UNP O95786
B	786	HIS	-	expression tag	UNP O95786
B	787	HIS	-	expression tag	UNP O95786
B	788	HIS	-	expression tag	UNP O95786
B	789	HIS	-	expression tag	UNP O95786
B	790	HIS	-	expression tag	UNP O95786
B	791	SER	-	expression tag	UNP O95786
B	792	SER	-	expression tag	UNP O95786
B	793	GLY	-	expression tag	UNP O95786
B	794	LEU	-	expression tag	UNP O95786
B	795	VAL	-	expression tag	UNP O95786
B	796	PRO	-	expression tag	UNP O95786
B	797	ARG	-	expression tag	UNP O95786
B	798	GLY	-	expression tag	UNP O95786
B	799	SER	-	expression tag	UNP O95786
B	800	HIS	-	expression tag	UNP O95786
B	801	MET	-	expression tag	UNP O95786
C	781	MET	-	expression tag	UNP O95786
C	782	GLY	-	expression tag	UNP O95786
C	783	SER	-	expression tag	UNP O95786
C	784	SER	-	expression tag	UNP O95786
C	785	HIS	-	expression tag	UNP O95786
C	786	HIS	-	expression tag	UNP O95786
C	787	HIS	-	expression tag	UNP O95786
C	788	HIS	-	expression tag	UNP O95786
C	789	HIS	-	expression tag	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
C	790	HIS	-	expression tag	UNP O95786
C	791	SER	-	expression tag	UNP O95786
C	792	SER	-	expression tag	UNP O95786
C	793	GLY	-	expression tag	UNP O95786
C	794	LEU	-	expression tag	UNP O95786
C	795	VAL	-	expression tag	UNP O95786
C	796	PRO	-	expression tag	UNP O95786
C	797	ARG	-	expression tag	UNP O95786
C	798	GLY	-	expression tag	UNP O95786
C	799	SER	-	expression tag	UNP O95786
C	800	HIS	-	expression tag	UNP O95786
C	801	MET	-	expression tag	UNP O95786
D	781	MET	-	expression tag	UNP O95786
D	782	GLY	-	expression tag	UNP O95786
D	783	SER	-	expression tag	UNP O95786
D	784	SER	-	expression tag	UNP O95786
D	785	HIS	-	expression tag	UNP O95786
D	786	HIS	-	expression tag	UNP O95786
D	787	HIS	-	expression tag	UNP O95786
D	788	HIS	-	expression tag	UNP O95786
D	789	HIS	-	expression tag	UNP O95786
D	790	HIS	-	expression tag	UNP O95786
D	791	SER	-	expression tag	UNP O95786
D	792	SER	-	expression tag	UNP O95786
D	793	GLY	-	expression tag	UNP O95786
D	794	LEU	-	expression tag	UNP O95786
D	795	VAL	-	expression tag	UNP O95786
D	796	PRO	-	expression tag	UNP O95786
D	797	ARG	-	expression tag	UNP O95786
D	798	GLY	-	expression tag	UNP O95786
D	799	SER	-	expression tag	UNP O95786
D	800	HIS	-	expression tag	UNP O95786
D	801	MET	-	expression tag	UNP O95786
E	781	MET	-	expression tag	UNP O95786
E	782	GLY	-	expression tag	UNP O95786
E	783	SER	-	expression tag	UNP O95786
E	784	SER	-	expression tag	UNP O95786
E	785	HIS	-	expression tag	UNP O95786
E	786	HIS	-	expression tag	UNP O95786
E	787	HIS	-	expression tag	UNP O95786
E	788	HIS	-	expression tag	UNP O95786
E	789	HIS	-	expression tag	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
E	790	HIS	-	expression tag	UNP O95786
E	791	SER	-	expression tag	UNP O95786
E	792	SER	-	expression tag	UNP O95786
E	793	GLY	-	expression tag	UNP O95786
E	794	LEU	-	expression tag	UNP O95786
E	795	VAL	-	expression tag	UNP O95786
E	796	PRO	-	expression tag	UNP O95786
E	797	ARG	-	expression tag	UNP O95786
E	798	GLY	-	expression tag	UNP O95786
E	799	SER	-	expression tag	UNP O95786
E	800	HIS	-	expression tag	UNP O95786
E	801	MET	-	expression tag	UNP O95786
F	781	MET	-	expression tag	UNP O95786
F	782	GLY	-	expression tag	UNP O95786
F	783	SER	-	expression tag	UNP O95786
F	784	SER	-	expression tag	UNP O95786
F	785	HIS	-	expression tag	UNP O95786
F	786	HIS	-	expression tag	UNP O95786
F	787	HIS	-	expression tag	UNP O95786
F	788	HIS	-	expression tag	UNP O95786
F	789	HIS	-	expression tag	UNP O95786
F	790	HIS	-	expression tag	UNP O95786
F	791	SER	-	expression tag	UNP O95786
F	792	SER	-	expression tag	UNP O95786
F	793	GLY	-	expression tag	UNP O95786
F	794	LEU	-	expression tag	UNP O95786
F	795	VAL	-	expression tag	UNP O95786
F	796	PRO	-	expression tag	UNP O95786
F	797	ARG	-	expression tag	UNP O95786
F	798	GLY	-	expression tag	UNP O95786
F	799	SER	-	expression tag	UNP O95786
F	800	HIS	-	expression tag	UNP O95786
F	801	MET	-	expression tag	UNP O95786
G	781	MET	-	expression tag	UNP O95786
G	782	GLY	-	expression tag	UNP O95786
G	783	SER	-	expression tag	UNP O95786
G	784	SER	-	expression tag	UNP O95786
G	785	HIS	-	expression tag	UNP O95786
G	786	HIS	-	expression tag	UNP O95786
G	787	HIS	-	expression tag	UNP O95786
G	788	HIS	-	expression tag	UNP O95786
G	789	HIS	-	expression tag	UNP O95786

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G	790	HIS	-	expression tag	UNP O95786
G	791	SER	-	expression tag	UNP O95786
G	792	SER	-	expression tag	UNP O95786
G	793	GLY	-	expression tag	UNP O95786
G	794	LEU	-	expression tag	UNP O95786
G	795	VAL	-	expression tag	UNP O95786
G	796	PRO	-	expression tag	UNP O95786
G	797	ARG	-	expression tag	UNP O95786
G	798	GLY	-	expression tag	UNP O95786
G	799	SER	-	expression tag	UNP O95786
G	800	HIS	-	expression tag	UNP O95786
G	801	MET	-	expression tag	UNP O95786
H	781	MET	-	expression tag	UNP O95786
H	782	GLY	-	expression tag	UNP O95786
H	783	SER	-	expression tag	UNP O95786
H	784	SER	-	expression tag	UNP O95786
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H	786	HIS	-	expression tag	UNP O95786
H	787	HIS	-	expression tag	UNP O95786
H	788	HIS	-	expression tag	UNP O95786
H	789	HIS	-	expression tag	UNP O95786
H	790	HIS	-	expression tag	UNP O95786
H	791	SER	-	expression tag	UNP O95786
H	792	SER	-	expression tag	UNP O95786
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I	794	LEU	-	expression tag	UNP O95786
I	795	VAL	-	expression tag	UNP O95786
I	796	PRO	-	expression tag	UNP O95786
I	797	ARG	-	expression tag	UNP O95786
I	798	GLY	-	expression tag	UNP O95786
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I	800	HIS	-	expression tag	UNP O95786
I	801	MET	-	expression tag	UNP O95786
J	781	MET	-	expression tag	UNP O95786
J	782	GLY	-	expression tag	UNP O95786
J	783	SER	-	expression tag	UNP O95786
J	784	SER	-	expression tag	UNP O95786
J	785	HIS	-	expression tag	UNP O95786
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J	787	HIS	-	expression tag	UNP O95786
J	788	HIS	-	expression tag	UNP O95786
J	789	HIS	-	expression tag	UNP O95786
J	790	HIS	-	expression tag	UNP O95786
J	791	SER	-	expression tag	UNP O95786
J	792	SER	-	expression tag	UNP O95786
J	793	GLY	-	expression tag	UNP O95786
J	794	LEU	-	expression tag	UNP O95786
J	795	VAL	-	expression tag	UNP O95786
J	796	PRO	-	expression tag	UNP O95786
J	797	ARG	-	expression tag	UNP O95786
J	798	GLY	-	expression tag	UNP O95786
J	799	SER	-	expression tag	UNP O95786
J	800	HIS	-	expression tag	UNP O95786
J	801	MET	-	expression tag	UNP O95786

- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Hg 1 1	0	0
2	B	1	Total Hg 1 1	0	0
2	C	1	Total Hg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Hg 1 1	0	0
2	E	1	Total Hg 1 1	0	0
2	F	1	Total Hg 1 1	0	0
2	G	1	Total Hg 1 1	0	0
2	H	1	Total Hg 1 1	0	0
2	I	1	Total Hg 1 1	0	0
2	J	1	Total Hg 1 1	0	0

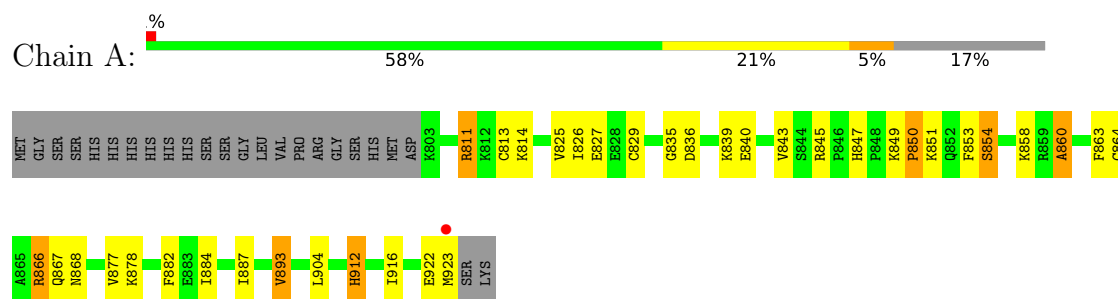
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O 27 27	0	0
3	B	25	Total O 25 25	0	0
3	C	12	Total O 12 12	0	0
3	D	15	Total O 15 15	0	0
3	E	8	Total O 8 8	0	0
3	F	4	Total O 4 4	0	0
3	G	8	Total O 8 8	0	0
3	H	3	Total O 3 3	0	0

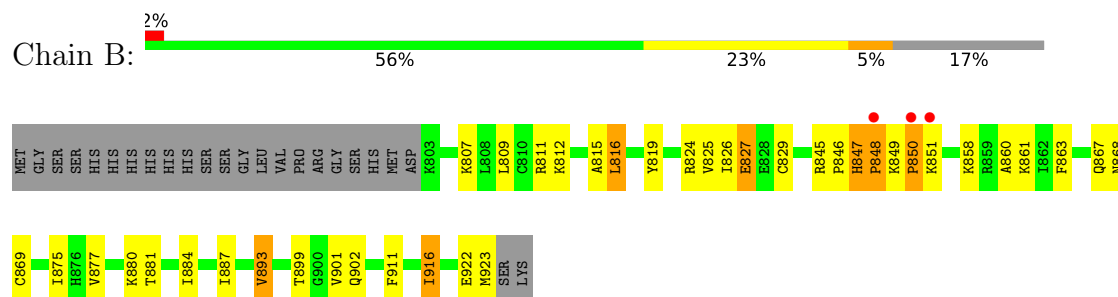
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

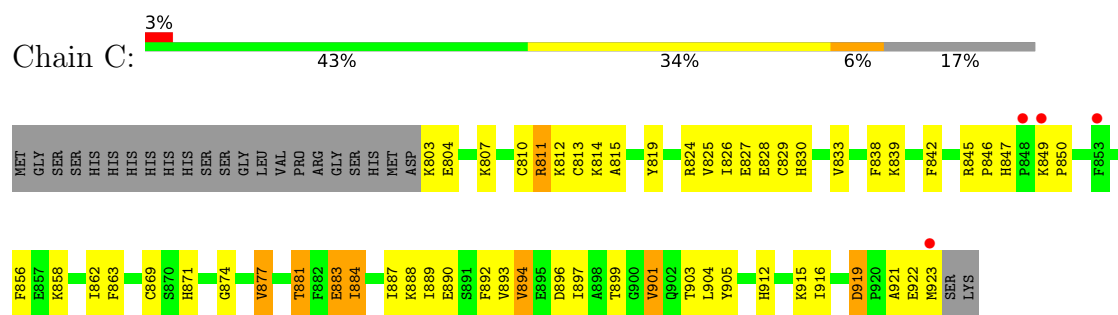
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



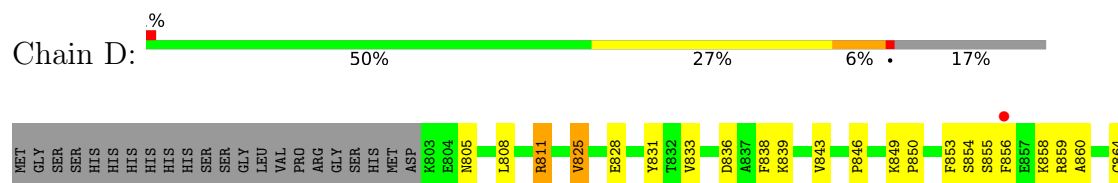
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



- Molecule 1: Probable ATP-dependent RNA helicase DDX58

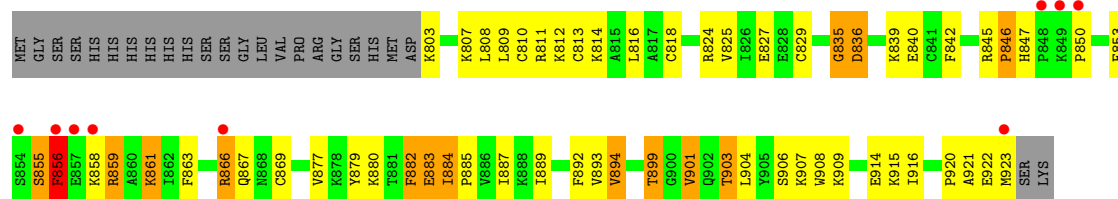


- Molecule 1: Probable ATP-dependent RNA helicase DDX58

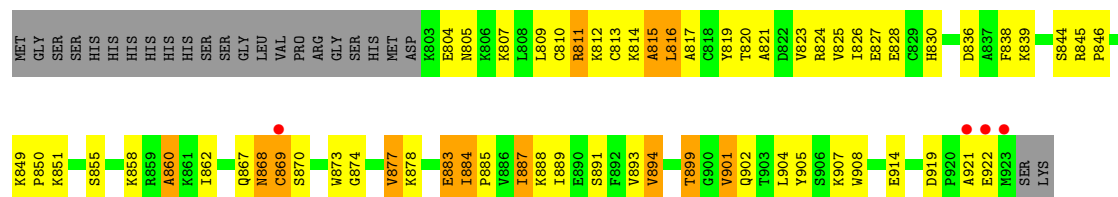




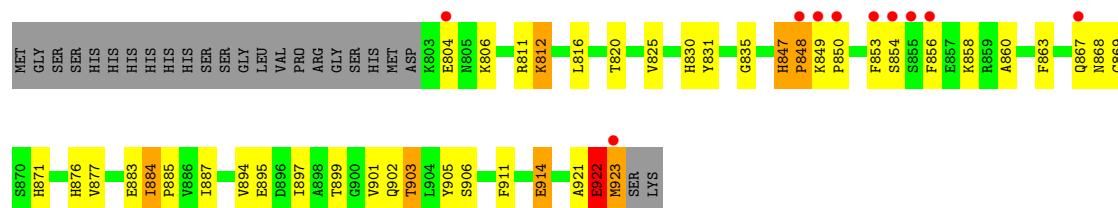
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



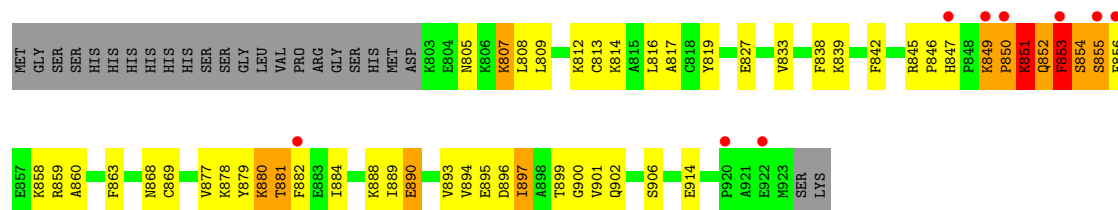
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



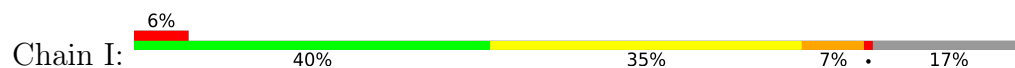
- Molecule 1: Probable ATP-dependent RNA helicase DDX58

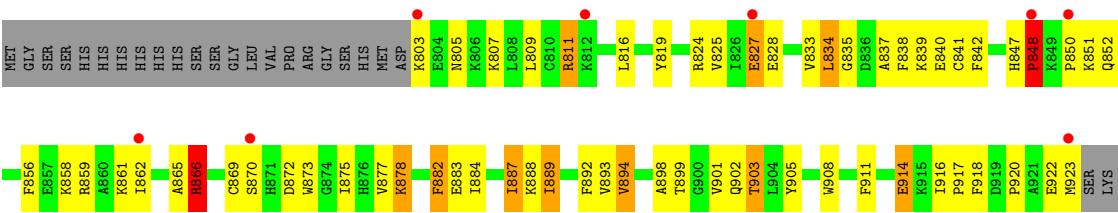


- Molecule 1: Probable ATP-dependent RNA helicase DDX58

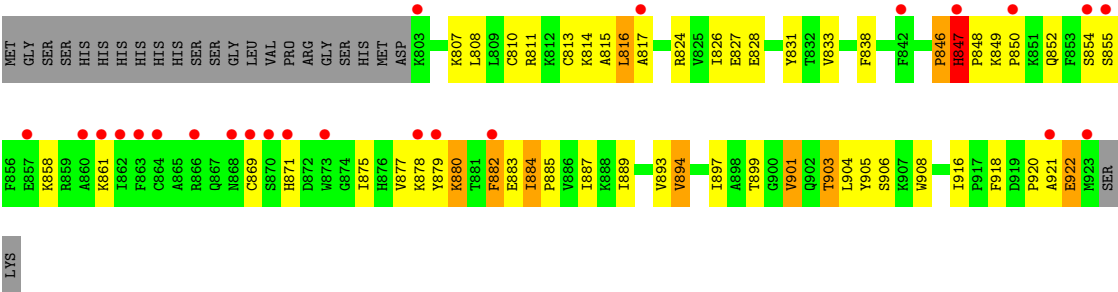
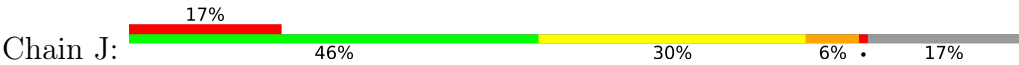


- Molecule 1: Probable ATP-dependent RNA helicase DDX58





● Molecule 1: Probable ATP-dependent RNA helicase DDX58



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.15Å 76.54Å 137.90Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-2.70) 97.8 (20.00-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.276 0.241 , 0.278	Depositor DCC
R_{free} test set	5544 reflections (10.17%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10092	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG

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	0.54	0/1026	1.11	11/1380 (0.8%)
1	B	0.53	0/1026	1.04	5/1380 (0.4%)
1	C	0.46	0/1026	1.02	5/1380 (0.4%)
1	D	0.46	0/1026	0.97	4/1380 (0.3%)
1	E	0.47	0/1026	1.02	5/1380 (0.4%)
1	F	0.44	0/1026	0.99	5/1380 (0.4%)
1	G	0.39	0/1026	0.99	6/1380 (0.4%)
1	H	0.45	0/1026	1.09	5/1380 (0.4%)
1	I	0.39	0/1026	0.96	5/1380 (0.4%)
1	J	0.42	0/1026	0.97	6/1380 (0.4%)
All	All	0.46	0/10260	1.02	57/13800 (0.4%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	852	GLN	N-CA-C	15.16	129.40	111.82
1	H	853	PHE	N-CA-C	8.52	122.05	110.55
1	G	922	GLU	N-CA-C	-7.84	94.10	110.80
1	J	847	HIS	C-N-CD	-7.77	103.50	120.60
1	E	835	GLY	N-CA-C	7.72	122.41	110.91
1	I	884	ILE	N-CA-C	7.35	117.31	109.01
1	J	852	GLN	N-CA-C	7.20	121.31	112.23
1	E	882	PHE	N-CA-C	7.18	120.12	110.35
1	A	912	HIS	N-CA-C	7.18	121.05	108.56
1	A	835	GLY	N-CA-C	7.09	120.23	112.29
1	E	887	ILE	N-CA-C	7.03	118.77	109.21
1	A	840	GLU	N-CA-C	-6.93	104.85	113.38
1	I	889	ILE	N-CA-C	6.93	117.69	110.62
1	F	887	ILE	N-CA-C	6.81	119.25	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	877	VAL	N-CA-C	6.76	117.07	108.82
1	E	899	THR	N-CA-C	6.47	119.33	111.82
1	A	825	VAL	N-CA-C	6.38	117.05	107.80
1	G	887	ILE	N-CA-C	6.38	118.85	108.97
1	G	906	SER	N-CA-C	-6.34	106.51	114.56
1	D	916	ILE	N-CA-C	6.26	114.01	108.63
1	A	887	ILE	N-CA-C	6.24	118.77	109.17
1	F	877	VAL	N-CA-C	6.23	117.89	108.80
1	F	825	VAL	N-CA-C	6.07	116.85	107.99
1	A	893	VAL	N-CA-C	-6.04	99.65	108.11
1	D	906	SER	N-CA-C	-6.04	106.89	114.56
1	B	887	ILE	N-CA-C	6.03	118.31	108.97
1	G	812	LYS	N-CA-C	6.00	117.69	111.03
1	I	887	ILE	N-CA-C	5.97	116.90	108.36
1	B	827	GLU	N-CA-C	-5.84	98.21	108.08
1	I	898	ALA	N-CA-C	-5.76	104.69	110.97
1	H	851	LYS	N-CA-C	-5.72	98.62	110.80
1	C	912	HIS	N-CA-C	5.72	118.51	108.56
1	I	882	PHE	N-CA-C	5.66	118.95	109.95
1	A	916	ILE	N-CA-C	5.66	113.47	107.76
1	C	884	ILE	N-CA-C	5.64	115.39	109.01
1	C	896	ASP	N-CA-C	-5.61	101.33	110.20
1	J	847	HIS	CA-C-N	5.60	140.45	127.00
1	J	847	HIS	C-N-CA	5.60	140.45	127.00
1	B	827	GLU	CA-C-N	-5.51	113.39	121.99
1	B	827	GLU	C-N-CA	-5.51	113.39	121.99
1	H	845	ARG	CA-C-N	5.48	126.69	119.84
1	H	845	ARG	C-N-CA	5.48	126.69	119.84
1	F	899	THR	N-CA-C	5.44	120.03	112.90
1	J	887	ILE	N-CA-C	5.37	116.97	109.55
1	A	860	ALA	N-CA-C	5.37	116.31	108.14
1	B	916	ILE	CB-CA-C	-5.32	106.00	110.94
1	A	877	VAL	N-CA-C	5.27	116.50	108.80
1	A	884	ILE	N-CA-C	5.25	114.75	108.45
1	D	897	ILE	N-CA-C	5.23	115.44	110.42
1	G	847	HIS	N-CA-C	5.23	114.32	108.25
1	D	887	ILE	N-CA-C	5.23	117.08	108.97
1	C	887	ILE	N-CA-C	5.22	117.37	108.86
1	G	835	GLY	N-CA-C	5.16	118.48	111.72
1	A	854	SER	N-CA-C	5.15	116.97	111.36
1	F	860	ALA	N-CA-C	5.12	115.92	108.14
1	J	906	SER	N-CA-C	-5.09	107.05	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	856	PHE	N-CA-C	5.01	116.03	108.07

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	998	0	993	24	0
1	B	998	0	993	25	0
1	C	998	0	993	47	0
1	D	998	0	994	36	0
1	E	998	0	996	44	0
1	F	998	0	993	51	0
1	G	998	0	994	29	0
1	H	998	0	995	47	0
1	I	998	0	993	51	0
1	J	998	0	993	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	27	0	0	1	0
3	B	25	0	0	1	0
3	C	12	0	0	1	0
3	D	15	0	0	1	0
3	E	8	0	0	0	0
3	F	4	0	0	1	0
3	G	8	0	0	2	0
3	H	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10092	0	9937	384	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 22.

All (384) 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:H:897:ILE:HD12	1:H:897:ILE:H	1.20	1.05
1:D:858:LYS:HA	1:D:877:VAL:HG12	1.39	1.03
1:D:897:ILE:HD13	1:D:897:ILE:H	1.23	1.00
1:D:897:ILE:H	1:D:897:ILE:CD1	1.81	0.92
1:D:894:VAL:HG13	1:D:903:THR:HG23	1.51	0.91
1:D:897:ILE:HD13	1:D:897:ILE:N	1.85	0.91
1:I:866:ARG:HB3	1:I:866:ARG:HH11	1.34	0.90
1:J:858:LYS:HA	1:J:877:VAL:HG12	1.53	0.89
1:G:858:LYS:HA	1:G:877:VAL:HG12	1.54	0.88
1:H:859:ARG:HD2	1:H:878:LYS:HB2	1.57	0.87
1:I:894:VAL:HG13	1:I:903:THR:HG23	1.54	0.87
1:A:866:ARG:HG2	1:A:866:ARG:HH11	1.40	0.86
1:D:880:LYS:O	1:D:881:THR:HG22	1.75	0.86
1:H:888:LYS:HB2	1:H:890:GLU:OE2	1.78	0.84
1:B:848:PRO:HG3	1:B:861:LYS:HG3	1.58	0.83
1:G:894:VAL:HG11	1:G:905:TYR:HE2	1.41	0.83
1:H:897:ILE:HD12	1:H:897:ILE:N	1.95	0.81
1:G:894:VAL:HG13	1:G:903:THR:HG23	1.62	0.81
1:H:890:GLU:H	1:H:890:GLU:CD	1.90	0.80
1:E:858:LYS:HA	1:E:877:VAL:HG12	1.67	0.77
1:J:878:LYS:HA	1:J:883:GLU:HA	1.66	0.77
1:H:858:LYS:HA	1:H:877:VAL:HG12	1.69	0.74
1:E:839:LYS:HA	1:E:842:PHE:CE1	2.23	0.74
1:F:891:SER:HA	3:F:112:HOH:O	1.87	0.74
1:A:864:CYS:SG	1:A:866:ARG:HB2	2.28	0.73
1:J:810:CYS:HB3	1:J:813:CYS:O	1.88	0.73
1:C:811:ARG:HA	1:C:893:VAL:HG23	1.71	0.73
1:I:899:THR:OG1	1:I:901:VAL:HG12	1.89	0.73
1:B:847:HIS:N	1:B:848:PRO:HD2	2.04	0.72
1:J:899:THR:OG1	1:J:901:VAL:HG12	1.90	0.72
1:H:807:LYS:HE2	1:H:816:LEU:HD23	1.72	0.72
1:E:836:ASP:HA	1:E:839:LYS:HD2	1.70	0.71
1:D:903:THR:HG22	3:D:102:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:899:THR:HG23	1:G:901:VAL:HG12	1.72	0.71
1:G:847:HIS:HB3	1:G:848:PRO:HD2	1.71	0.71
1:I:847:HIS:O	1:I:848:PRO:C	2.34	0.71
1:I:866:ARG:HB3	1:I:866:ARG:NH1	2.06	0.70
1:H:893:VAL:CG1	1:H:902:GLN:HB3	2.21	0.69
1:B:827:GLU:O	3:B:28:HOH:O	2.10	0.69
1:I:878:LYS:HB2	1:I:878:LYS:NZ	2.06	0.69
1:I:848:PRO:O	1:I:850:PRO:HD3	1.94	0.68
1:G:847:HIS:CB	1:G:848:PRO:HD2	2.22	0.68
1:J:894:VAL:HG13	1:J:903:THR:HG23	1.75	0.68
1:F:807:LYS:HD2	1:F:809:LEU:HD21	1.76	0.68
1:G:894:VAL:HG11	1:G:905:TYR:CE2	2.28	0.67
1:B:850:PRO:HG3	1:B:858:LYS:HB3	1.75	0.67
1:D:894:VAL:HG11	1:D:905:TYR:CE2	2.30	0.67
1:C:919:ASP:OD1	1:C:921:ALA:HB3	1.95	0.67
1:J:884:ILE:HD13	1:J:884:ILE:H	1.59	0.67
1:D:894:VAL:CG1	1:D:903:THR:HG23	2.24	0.67
1:C:829:CYS:HB3	1:E:829:CYS:HB3	1.76	0.66
1:A:912:HIS:HD2	3:A:6:HOH:O	1.79	0.65
1:E:884:ILE:HD13	1:E:884:ILE:H	1.60	0.65
1:C:858:LYS:HA	1:C:877:VAL:HG12	1.78	0.65
1:C:899:THR:OG1	1:C:901:VAL:HG12	1.96	0.65
1:J:816:LEU:CD2	1:J:817:ALA:H	2.09	0.65
1:E:920:PRO:C	1:E:922:GLU:H	2.05	0.65
1:A:845:ARG:O	1:A:860:ALA:HB1	1.97	0.65
1:C:812:LYS:HB3	1:C:869:CYS:SG	2.37	0.65
1:E:809:LEU:HD23	1:E:816:LEU:HA	1.79	0.65
1:G:867:GLN:O	1:G:868:ASN:HB2	1.95	0.64
1:D:894:VAL:HG11	1:D:905:TYR:HE2	1.60	0.64
1:I:878:LYS:HB2	1:I:878:LYS:HZ3	1.62	0.64
1:D:884:ILE:HD13	1:D:884:ILE:H	1.62	0.64
1:C:803:LYS:HG3	1:C:804:GLU:H	1.63	0.63
1:H:897:ILE:H	1:H:897:ILE:CD1	1.88	0.63
1:A:866:ARG:HG2	1:A:866:ARG:NH1	2.15	0.62
1:H:895:GLU:HG3	1:H:902:GLN:HG2	1.82	0.62
1:J:813:CYS:O	1:J:815:ALA:N	2.29	0.62
1:C:883:GLU:OE1	1:C:883:GLU:N	2.21	0.62
1:H:853:PHE:O	1:H:854:SER:HB2	1.98	0.62
1:F:919:ASP:C	1:F:921:ALA:H	2.08	0.61
1:G:903:THR:HG22	3:G:118:HOH:O	1.99	0.61
1:G:921:ALA:O	1:G:922:GLU:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:846:PRO:HA	1:D:860:ALA:HB2	1.81	0.61
1:C:812:LYS:HD3	1:C:869:CYS:SG	2.41	0.61
1:F:811:ARG:HA	1:F:893:VAL:HG23	1.83	0.61
1:F:812:LYS:CD	1:F:869:CYS:HB2	2.31	0.61
1:A:836:ASP:HA	1:A:839:LYS:HD2	1.83	0.61
1:B:847:HIS:H	1:B:848:PRO:HD2	1.64	0.60
1:E:811:ARG:HA	1:E:893:VAL:HG23	1.82	0.60
1:A:836:ASP:HA	1:A:839:LYS:CD	2.31	0.60
1:C:919:ASP:OD2	1:C:922:GLU:HG3	2.01	0.60
1:F:812:LYS:CE	1:F:869:CYS:HB2	2.32	0.60
1:F:827:GLU:HG2	1:F:855:SER:OG	2.01	0.60
1:H:847:HIS:O	1:H:849:LYS:N	2.36	0.59
1:I:842:PHE:CD2	1:I:862:ILE:HG23	2.37	0.59
1:J:813:CYS:C	1:J:815:ALA:H	2.11	0.59
1:B:807:LYS:HG2	1:B:819:TYR:CE2	2.38	0.59
1:E:812:LYS:HG3	1:E:869:CYS:SG	2.42	0.59
1:I:922:GLU:HG3	1:I:923:MET:H	1.67	0.58
1:F:810:CYS:HB2	1:F:873:TRP:HZ2	1.69	0.58
1:A:811:ARG:HA	1:A:893:VAL:HG23	1.85	0.58
1:I:838:PHE:O	1:I:841:CYS:HB2	2.03	0.58
1:C:922:GLU:O	1:C:923:MET:HG3	2.04	0.58
1:C:811:ARG:HD3	1:C:892:PHE:O	2.04	0.58
1:F:887:ILE:HG13	1:F:908:TRP:HZ2	1.69	0.57
1:E:811:ARG:HD3	1:E:892:PHE:O	2.05	0.57
1:I:878:LYS:NZ	1:I:883:GLU:HG2	2.20	0.57
1:J:813:CYS:O	1:J:813:CYS:SG	2.62	0.57
1:D:864:CYS:SG	1:D:866:ARG:HB2	2.44	0.57
1:E:861:LYS:HB3	1:E:863:PHE:CE1	2.38	0.57
1:C:829:CYS:SG	1:C:830:HIS:CE1	2.98	0.57
1:B:922:GLU:O	1:B:923:MET:HB2	2.05	0.57
1:C:813:CYS:O	1:C:814:LYS:HB2	2.05	0.57
1:H:827:GLU:OE2	1:H:855:SER:HB3	2.05	0.57
1:E:813:CYS:O	1:E:814:LYS:HB2	2.04	0.57
1:I:862:ILE:HG22	1:I:873:TRP:HB2	1.87	0.56
1:C:889:ILE:HD13	1:C:905:TYR:HB2	1.85	0.56
1:I:811:ARG:HA	1:I:893:VAL:HG23	1.88	0.56
1:C:863:PHE:HA	1:C:871:HIS:O	2.05	0.56
1:F:812:LYS:HE2	1:F:869:CYS:HB2	1.88	0.56
1:J:816:LEU:HD22	1:J:817:ALA:H	1.71	0.56
1:D:890:GLU:O	1:D:890:GLU:HG2	2.05	0.56
1:F:826:ILE:HB	1:F:830:HIS:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:855:SER:O	1:E:879:TYR:HD1	1.88	0.56
1:H:890:GLU:CD	1:H:890:GLU:N	2.62	0.56
1:E:894:VAL:HG22	1:E:903:THR:HG23	1.88	0.56
1:J:824:ARG:HD3	1:J:916:ILE:HB	1.86	0.56
1:C:824:ARG:HD3	1:C:916:ILE:HB	1.88	0.55
1:D:833:VAL:HB	1:D:838:PHE:CD2	2.41	0.55
1:G:895:GLU:OE1	1:G:902:GLN:NE2	2.32	0.55
1:H:879:TYR:O	1:H:881:THR:N	2.39	0.55
1:J:884:ILE:HB	1:J:885:PRO:HD2	1.87	0.55
3:C:91:HOH:O	1:E:909:LYS:HB3	2.05	0.55
1:I:856:PHE:CG	1:I:877:VAL:HG21	2.42	0.55
1:F:899:THR:CG2	1:F:901:VAL:HG12	2.37	0.55
1:I:848:PRO:O	1:I:850:PRO:CD	2.55	0.55
1:C:881:THR:HG23	1:C:881:THR:O	2.07	0.54
1:E:808:LEU:HD12	1:E:818:CYS:SG	2.47	0.54
1:E:810:CYS:HB3	1:E:813:CYS:SG	2.46	0.54
1:I:847:HIS:O	1:I:848:PRO:O	2.25	0.54
1:J:883:GLU:O	1:J:883:GLU:HG3	2.07	0.54
1:C:899:THR:OG1	1:C:901:VAL:CG1	2.56	0.54
1:G:884:ILE:HD13	1:G:884:ILE:H	1.73	0.54
1:G:899:THR:CG2	1:G:901:VAL:HG12	2.37	0.54
1:A:826:ILE:HG22	1:A:827:GLU:HG2	1.88	0.53
1:F:816:LEU:C	1:F:816:LEU:CD2	2.81	0.53
1:A:878:LYS:HA	1:A:882:PHE:O	2.08	0.53
1:C:827:GLU:O	1:C:828:GLU:HB2	2.09	0.53
1:A:866:ARG:HH11	1:A:866:ARG:CG	2.18	0.53
1:D:811:ARG:HA	1:D:893:VAL:HG23	1.89	0.53
1:D:856:PHE:CD2	1:D:877:VAL:HG21	2.44	0.53
1:H:896:ASP:CG	1:H:899:THR:HB	2.33	0.53
1:J:833:VAL:HB	1:J:838:PHE:CD2	2.44	0.53
1:F:813:CYS:SG	1:F:815:ALA:HB2	2.48	0.53
1:F:894:VAL:HG11	1:F:905:TYR:HE2	1.74	0.52
1:J:893:VAL:HG22	1:J:904:LEU:CD2	2.38	0.52
1:C:828:GLU:OE2	1:E:915:LYS:NZ	2.41	0.52
1:D:880:LYS:NZ	1:D:880:LYS:HB3	2.24	0.52
1:F:823:VAL:O	1:F:824:ARG:NH1	2.37	0.52
1:F:849:LYS:N	1:F:850:PRO:HD3	2.24	0.52
1:F:812:LYS:HD3	1:F:869:CYS:HB2	1.91	0.52
1:F:846:PRO:HA	1:F:860:ALA:HB2	1.90	0.52
1:G:883:GLU:HG3	1:G:883:GLU:O	2.09	0.52
1:F:844:SER:H	1:H:881:THR:HG21	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:884:ILE:HD13	1:J:884:ILE:N	2.24	0.52
1:B:893:VAL:CG1	1:B:902:GLN:HB3	2.40	0.52
1:D:889:ILE:HB	1:D:908:TRP:CE2	2.45	0.52
1:C:811:ARG:HA	1:C:893:VAL:CG2	2.40	0.52
1:B:893:VAL:HG13	1:B:902:GLN:HB3	1.92	0.52
1:I:807:LYS:HG2	1:I:816:LEU:HD13	1.91	0.52
1:C:919:ASP:OD1	1:C:919:ASP:C	2.52	0.51
1:H:807:LYS:NZ	1:H:809:LEU:HD21	2.25	0.51
1:F:893:VAL:HG22	1:F:904:LEU:CD2	2.40	0.51
1:I:827:GLU:O	1:I:828:GLU:HB2	2.11	0.51
1:E:811:ARG:CZ	1:E:904:LEU:HD22	2.41	0.51
1:E:907:LYS:HD3	1:G:867:GLN:OE1	2.11	0.51
1:J:879:TYR:OH	1:J:880:LYS:HE3	2.10	0.51
1:B:899:THR:OG1	1:B:901:VAL:HG23	2.10	0.51
1:C:810:CYS:O	1:C:814:LYS:HA	2.10	0.51
1:C:829:CYS:HG	1:C:830:HIS:CE1	2.29	0.51
1:E:859:ARG:NH1	1:E:883:GLU:OE1	2.43	0.51
1:F:862:ILE:HG22	1:F:873:TRP:HB2	1.92	0.51
1:H:813:CYS:O	1:H:814:LYS:HB2	2.11	0.51
1:B:824:ARG:HD3	1:B:916:ILE:HB	1.91	0.51
1:F:812:LYS:HG3	1:F:813:CYS:N	2.26	0.50
1:F:810:CYS:HB2	1:F:873:TRP:CZ2	2.46	0.50
1:F:899:THR:HB	1:F:901:VAL:HG12	1.92	0.50
1:I:858:LYS:HA	1:I:877:VAL:HG12	1.94	0.50
1:B:858:LYS:HE2	1:B:875:ILE:HG21	1.94	0.50
1:F:894:VAL:HG11	1:F:905:TYR:CE2	2.47	0.50
1:J:807:LYS:O	1:J:894:VAL:HA	2.12	0.50
1:A:847:HIS:HD2	1:A:858:LYS:NZ	2.10	0.50
1:H:896:ASP:HB3	1:H:900:GLY:H	1.77	0.50
1:G:894:VAL:HG12	1:G:903:THR:O	2.11	0.50
1:A:811:ARG:HD2	1:A:904:LEU:HD22	1.94	0.50
1:C:825:VAL:HG21	1:C:915:LYS:HB3	1.94	0.50
1:G:894:VAL:CG1	1:G:903:THR:HG23	2.37	0.50
1:H:854:SER:O	1:H:856:PHE:N	2.45	0.49
1:F:867:GLN:O	1:F:868:ASN:HB2	2.11	0.49
1:I:811:ARG:HD3	1:I:892:PHE:O	2.12	0.49
1:H:890:GLU:OE1	1:H:906:SER:O	2.31	0.49
1:E:840:GLU:O	1:E:840:GLU:HG3	2.11	0.49
1:H:807:LYS:HZ3	1:H:807:LYS:HB3	1.77	0.49
1:C:811:ARG:HD2	1:C:893:VAL:HG22	1.95	0.49
1:I:920:PRO:C	1:I:922:GLU:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:893:VAL:HG11	1:H:902:GLN:HB3	1.94	0.48
1:J:816:LEU:HD23	1:J:817:ALA:H	1.78	0.48
1:E:812:LYS:HG3	1:E:813:CYS:N	2.29	0.48
1:F:919:ASP:O	1:F:921:ALA:N	2.40	0.48
1:I:920:PRO:C	1:I:922:GLU:N	2.70	0.48
1:A:922:GLU:O	1:A:923:MET:HB2	2.14	0.48
1:E:884:ILE:HD13	1:E:884:ILE:N	2.27	0.48
1:H:880:LYS:O	1:H:881:THR:HB	2.13	0.48
1:B:845:ARG:HD2	1:B:863:PHE:CE1	2.48	0.48
1:C:922:GLU:O	1:C:923:MET:CB	2.60	0.48
1:F:893:VAL:CG1	1:F:902:GLN:HB3	2.43	0.48
1:I:837:ALA:O	1:I:840:GLU:N	2.46	0.48
1:H:816:LEU:HD13	1:H:816:LEU:C	2.39	0.48
1:B:826:ILE:HD11	1:B:884:ILE:CD1	2.44	0.48
1:J:826:ILE:HD12	1:J:918:PHE:HB2	1.96	0.48
1:C:826:ILE:HD11	1:C:884:ILE:CD1	2.44	0.47
1:D:858:LYS:HA	1:D:877:VAL:CG1	2.28	0.47
1:F:893:VAL:HG22	1:F:904:LEU:HD21	1.97	0.47
1:E:866:ARG:HG2	1:E:866:ARG:HH11	1.79	0.47
1:F:807:LYS:CD	1:F:809:LEU:HD21	2.42	0.47
1:F:889:ILE:HB	1:F:908:TRP:CE2	2.49	0.47
1:G:847:HIS:HB3	1:G:848:PRO:CD	2.42	0.47
1:E:813:CYS:O	1:E:814:LYS:CB	2.62	0.47
1:H:816:LEU:HD13	1:H:817:ALA:N	2.30	0.47
1:I:859:ARG:NH2	1:I:878:LYS:HD2	2.29	0.47
1:E:906:SER:O	1:E:907:LYS:HG2	2.15	0.47
1:I:865:ALA:O	1:I:866:ARG:C	2.57	0.47
1:I:887:ILE:HG13	1:I:887:ILE:O	2.14	0.47
1:D:879:TYR:CZ	1:D:880:LYS:HE2	2.50	0.47
1:D:880:LYS:O	1:D:881:THR:CG2	2.57	0.47
1:E:812:LYS:CG	1:E:869:CYS:SG	3.02	0.47
1:E:899:THR:OG1	1:E:901:VAL:HG13	2.15	0.47
1:H:856:PHE:CD2	1:H:877:VAL:HG21	2.50	0.47
1:C:893:VAL:HG13	1:C:904:LEU:CD2	2.45	0.47
1:E:867:GLN:C	1:E:869:CYS:H	2.22	0.47
1:G:806:LYS:O	1:G:820:THR:HG23	2.15	0.47
1:G:884:ILE:HB	1:G:885:PRO:HD2	1.97	0.47
1:H:807:LYS:CG	1:H:819:TYR:CE1	2.97	0.47
1:I:889:ILE:HB	1:I:908:TRP:CE2	2.50	0.47
1:C:922:GLU:O	1:C:923:MET:CG	2.64	0.46
1:I:807:LYS:CG	1:I:816:LEU:HD13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:851:LYS:H	1:I:858:LYS:HD3	1.81	0.46
1:H:853:PHE:O	1:H:854:SER:CB	2.62	0.46
1:J:920:PRO:O	1:J:922:GLU:O	2.33	0.46
1:G:922:GLU:O	1:G:923:MET:O	2.33	0.46
1:F:858:LYS:HA	1:F:877:VAL:HG12	1.96	0.46
1:H:839:LYS:HA	1:H:842:PHE:CE1	2.51	0.46
1:A:867:GLN:HG2	1:A:868:ASN:ND2	2.31	0.46
1:D:872:ASP:OD2	1:D:888:LYS:NZ	2.49	0.46
1:E:810:CYS:CB	1:E:813:CYS:HG	2.21	0.46
1:F:878:LYS:HA	1:F:883:GLU:OE1	2.16	0.46
1:H:805:ASN:O	1:H:897:ILE:HD11	2.15	0.46
1:H:896:ASP:HB3	1:H:899:THR:HB	1.98	0.46
1:I:889:ILE:CD1	1:I:911:PHE:HD2	2.29	0.46
1:F:845:ARG:O	1:F:860:ALA:HB1	2.17	0.45
1:F:869:CYS:O	1:F:870:SER:C	2.60	0.45
1:D:805:ASN:O	1:D:897:ILE:HD12	2.15	0.45
1:E:889:ILE:HB	1:E:908:TRP:CE2	2.52	0.45
1:G:899:THR:HG23	1:G:901:VAL:H	1.81	0.45
1:H:854:SER:O	1:H:855:SER:C	2.58	0.45
1:I:869:CYS:O	1:I:870:SER:C	2.58	0.45
1:C:839:LYS:HA	1:C:842:PHE:CE1	2.52	0.45
1:E:835:GLY:O	1:E:839:LYS:HG3	2.16	0.45
1:I:894:VAL:HG11	1:I:905:TYR:HE2	1.81	0.45
1:J:882:PHE:CD1	1:J:882:PHE:N	2.76	0.45
1:A:829:CYS:SG	1:B:829:CYS:SG	3.15	0.45
1:A:845:ARG:HH11	1:A:845:ARG:HG2	1.82	0.45
1:G:830:HIS:CD2	1:G:856:PHE:HZ	2.34	0.45
1:H:833:VAL:HB	1:H:838:PHE:CD2	2.52	0.45
1:B:809:LEU:HA	1:B:815:ALA:O	2.16	0.45
1:E:807:LYS:O	1:E:894:VAL:HA	2.17	0.45
1:J:882:PHE:HZ	1:J:920:PRO:HB3	1.82	0.45
1:A:853:PHE:CE2	1:A:858:LYS:HB2	2.51	0.45
1:D:879:TYR:O	1:D:880:LYS:C	2.59	0.45
1:H:807:LYS:HZ3	1:H:807:LYS:CB	2.30	0.45
1:H:896:ASP:CB	1:H:899:THR:HB	2.46	0.45
1:B:847:HIS:N	1:B:848:PRO:CD	2.79	0.44
1:C:807:LYS:O	1:C:894:VAL:HA	2.17	0.44
1:B:809:LEU:HD23	1:B:816:LEU:HA	1.99	0.44
1:C:845:ARG:O	1:C:847:HIS:N	2.49	0.44
1:E:884:ILE:N	1:E:884:ILE:CD1	2.79	0.44
1:E:920:PRO:O	1:E:922:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:911:PHE:CD1	1:G:911:PHE:C	2.96	0.44
1:H:899:THR:CG2	1:H:901:VAL:HG12	2.47	0.44
1:A:867:GLN:O	1:A:868:ASN:HB2	2.17	0.44
1:A:853:PHE:HE2	1:A:858:LYS:HD2	1.82	0.44
1:C:826:ILE:HD11	1:C:884:ILE:HD12	1.98	0.44
1:D:869:CYS:O	1:D:869:CYS:SG	2.75	0.44
1:E:856:PHE:C	1:E:856:PHE:CD2	2.96	0.44
1:E:845:ARG:O	1:E:846:PRO:C	2.61	0.44
1:D:887:ILE:HB	1:D:892:PHE:HE2	1.83	0.44
1:F:805:ASN:HD21	1:F:821:ALA:H	1.66	0.44
1:F:810:CYS:O	1:F:814:LYS:HA	2.18	0.44
1:D:916:ILE:HA	1:D:917:PRO:HD3	1.92	0.43
1:G:812:LYS:HD3	1:G:869:CYS:SG	2.58	0.43
1:B:880:LYS:C	1:B:881:THR:HG23	2.43	0.43
1:B:812:LYS:HE2	1:B:869:CYS:SG	2.58	0.43
1:C:903:THR:C	1:C:904:LEU:HD23	2.43	0.43
1:F:805:ASN:ND2	1:F:821:ALA:H	2.16	0.43
1:I:916:ILE:HA	1:I:917:PRO:HD3	1.91	0.43
1:C:803:LYS:HG3	1:C:804:GLU:N	2.32	0.43
1:I:894:VAL:HG11	1:I:905:TYR:CE2	2.52	0.43
1:J:831:TYR:N	1:J:831:TYR:CD1	2.86	0.43
1:B:867:GLN:O	1:B:868:ASN:HB2	2.18	0.43
1:C:833:VAL:HG11	1:C:838:PHE:CG	2.54	0.43
1:F:884:ILE:HB	1:F:885:PRO:HD2	1.99	0.43
1:J:894:VAL:HG11	1:J:905:TYR:HE2	1.82	0.43
1:C:862:ILE:HG12	1:C:874:GLY:C	2.44	0.43
1:C:888:LYS:HB3	1:C:890:GLU:HG2	2.01	0.43
1:D:911:PHE:C	1:D:911:PHE:CD1	2.93	0.43
1:F:836:ASP:O	1:F:839:LYS:HB2	2.18	0.43
1:J:894:VAL:HG11	1:J:905:TYR:CE2	2.54	0.43
1:D:836:ASP:O	1:D:839:LYS:HB2	2.19	0.43
1:E:884:ILE:HB	1:E:885:PRO:HD2	2.01	0.43
1:H:812:LYS:HD3	1:H:869:CYS:SG	2.59	0.43
1:H:847:HIS:CD2	1:H:860:ALA:HA	2.54	0.43
1:J:889:ILE:HB	1:J:908:TRP:CE2	2.53	0.43
1:H:807:LYS:HZ3	1:H:809:LEU:HD21	1.84	0.43
1:H:808:LEU:HD23	1:H:808:LEU:HA	1.87	0.43
1:J:808:LEU:CD2	1:J:894:VAL:HB	2.48	0.43
1:A:849:LYS:O	1:A:850:PRO:O	2.37	0.43
1:A:922:GLU:O	1:A:923:MET:CB	2.66	0.43
1:I:861:LYS:HA	1:I:875:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:810:CYS:O	1:J:811:ARG:C	2.62	0.42
1:J:877:VAL:O	1:J:884:ILE:N	2.52	0.42
1:G:860:ALA:O	1:G:876:HIS:N	2.50	0.42
1:I:805:ASN:HD21	1:I:819:TYR:HD2	1.67	0.42
1:A:863:PHE:CD1	1:A:863:PHE:N	2.87	0.42
1:A:813:CYS:O	1:A:814:LYS:HB2	2.19	0.42
1:C:830:HIS:CD2	1:C:856:PHE:CE1	3.07	0.42
1:F:819:TYR:O	1:F:820:THR:C	2.63	0.42
1:G:811:ARG:NH2	3:G:115:HOH:O	2.35	0.42
1:H:888:LYS:C	1:H:890:GLU:OE2	2.63	0.42
1:I:848:PRO:O	1:I:850:PRO:N	2.53	0.42
1:I:878:LYS:NZ	1:I:883:GLU:CG	2.82	0.42
1:F:809:LEU:HD22	1:F:815:ALA:O	2.20	0.42
1:C:813:CYS:SG	1:C:815:ALA:CB	3.08	0.42
1:E:879:TYR:O	1:E:880:LYS:HB2	2.20	0.42
1:F:813:CYS:SG	1:F:815:ALA:CB	3.08	0.42
1:I:824:ARG:HB3	1:I:918:PHE:HA	2.01	0.42
1:I:856:PHE:CD2	1:I:877:VAL:HG21	2.55	0.42
1:E:920:PRO:C	1:E:922:GLU:N	2.71	0.42
1:J:869:CYS:SG	1:J:871:HIS:HB2	2.60	0.42
1:C:889:ILE:HD13	1:C:905:TYR:CB	2.50	0.41
1:E:810:CYS:O	1:E:811:ARG:C	2.63	0.41
1:D:884:ILE:HD13	1:D:884:ILE:N	2.33	0.41
1:F:817:ALA:HB1	1:F:838:PHE:HE1	1.85	0.41
1:H:807:LYS:HG3	1:H:819:TYR:CE1	2.55	0.41
1:I:837:ALA:O	1:I:838:PHE:C	2.63	0.41
1:B:858:LYS:HA	1:B:877:VAL:HG12	2.02	0.41
1:I:824:ARG:HG2	1:I:824:ARG:HH11	1.84	0.41
1:J:861:LYS:HA	1:J:875:ILE:HA	2.02	0.41
1:E:884:ILE:H	1:E:884:ILE:CD1	2.29	0.41
1:F:805:ASN:HD21	1:F:819:TYR:HB3	1.84	0.41
1:J:920:PRO:O	1:J:921:ALA:C	2.64	0.41
1:E:824:ARG:HD3	1:E:916:ILE:HB	2.03	0.41
1:F:874:GLY:HA2	1:F:888:LYS:HD2	2.02	0.41
1:H:807:LYS:NZ	1:H:807:LYS:CB	2.82	0.41
1:B:911:PHE:C	1:B:911:PHE:CD1	2.97	0.41
1:C:919:ASP:OD1	1:C:921:ALA:N	2.53	0.41
1:F:816:LEU:C	1:F:816:LEU:HD23	2.46	0.41
1:F:919:ASP:C	1:F:921:ALA:N	2.73	0.41
1:I:833:VAL:HG11	1:I:838:PHE:CD1	2.56	0.41
1:I:872:ASP:OD2	1:I:888:LYS:CE	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:867:GLN:O	1:D:868:ASN:HB2	2.21	0.41
1:H:856:PHE:HB3	1:H:879:TYR:HA	2.02	0.41
1:I:889:ILE:CD1	1:I:911:PHE:CD2	3.04	0.41
1:D:843:VAL:HG13	1:D:865:ALA:HB2	2.01	0.41
1:D:880:LYS:NZ	1:D:880:LYS:CB	2.84	0.41
1:H:863:PHE:CD1	1:H:863:PHE:N	2.88	0.41
1:I:856:PHE:CD2	1:I:877:VAL:HG11	2.56	0.41
1:I:893:VAL:CG1	1:I:902:GLN:HB3	2.51	0.41
1:J:827:GLU:O	1:J:828:GLU:HB2	2.21	0.41
1:C:919:ASP:OD1	1:C:921:ALA:CB	2.67	0.41
1:F:811:ARG:HD2	1:F:904:LEU:HD22	2.03	0.41
1:B:826:ILE:CD1	1:B:884:ILE:HD11	2.51	0.40
1:G:863:PHE:HA	1:G:871:HIS:O	2.21	0.40
1:I:839:LYS:C	1:I:841:CYS:H	2.28	0.40
1:I:847:HIS:O	1:I:847:HIS:CG	2.74	0.40
1:B:846:PRO:HA	1:B:860:ALA:HB2	2.02	0.40
1:C:863:PHE:CD1	1:C:863:PHE:N	2.89	0.40
1:C:807:LYS:HG2	1:C:819:TYR:CE2	2.55	0.40
1:D:825:VAL:HG22	1:D:831:TYR:CE2	2.57	0.40
1:G:831:TYR:CD1	1:G:831:TYR:N	2.88	0.40
1:D:880:LYS:O	1:D:880:LYS:HG3	2.20	0.40
1:I:807:LYS:O	1:I:894:VAL:HA	2.22	0.40
1:F:814:LYS:O	1:F:815:ALA:O	2.40	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	119/145 (82%)	110 (92%)	8 (7%)	1 (1%)	16	37
1	B	119/145 (82%)	110 (92%)	4 (3%)	5 (4%)	2	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	119/145 (82%)	100 (84%)	16 (13%)	3 (2%)	4	11
1	D	119/145 (82%)	99 (83%)	12 (10%)	8 (7%)	1	1
1	E	119/145 (82%)	95 (80%)	17 (14%)	7 (6%)	1	2
1	F	119/145 (82%)	104 (87%)	11 (9%)	4 (3%)	3	7
1	G	119/145 (82%)	102 (86%)	10 (8%)	7 (6%)	1	2
1	H	119/145 (82%)	100 (84%)	10 (8%)	9 (8%)	1	1
1	I	119/145 (82%)	93 (78%)	21 (18%)	5 (4%)	2	4
1	J	119/145 (82%)	91 (76%)	18 (15%)	10 (8%)	0	1
All	All	1190/1450 (82%)	1004 (84%)	127 (11%)	59 (5%)	1	3

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	850	PRO
1	B	847	HIS
1	B	850	PRO
1	C	850	PRO
1	D	849	LYS
1	E	847	HIS
1	E	850	PRO
1	F	815	ALA
1	F	868	ASN
1	F	922	GLU
1	G	849	LYS
1	G	853	PHE
1	G	854	SER
1	G	922	GLU
1	H	849	LYS
1	H	850	PRO
1	H	851	LYS
1	H	855	SER
1	H	880	LYS
1	I	848	PRO
1	J	847	HIS
1	J	848	PRO
1	J	849	LYS
1	J	854	SER
1	J	855	SER
1	B	849	LYS

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Mol	Chain	Res	Type
1	B	851	LYS
1	E	921	ALA
1	G	848	PRO
1	H	854	SER
1	H	889	ILE
1	H	914	GLU
1	I	834	LEU
1	I	835	GLY
1	J	814	LYS
1	J	897	ILE
1	D	853	PHE
1	D	859	ARG
1	E	859	ARG
1	G	914	GLU
1	I	914	GLU
1	J	846	PRO
1	B	848	PRO
1	D	850	PRO
1	D	854	SER
1	E	855	SER
1	E	866	ARG
1	H	846	PRO
1	I	866	ARG
1	C	846	PRO
1	C	849	LYS
1	D	828	GLU
1	E	846	PRO
1	J	880	LYS
1	D	855	SER
1	D	880	LYS
1	F	828	GLU
1	G	850	PRO
1	J	922	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	110/131 (84%)	105 (96%)	5 (4%)	24	52
1	B	110/131 (84%)	106 (96%)	4 (4%)	31	60
1	C	110/131 (84%)	103 (94%)	7 (6%)	16	38
1	D	110/131 (84%)	100 (91%)	10 (9%)	9	22
1	E	110/131 (84%)	95 (86%)	15 (14%)	3	9
1	F	110/131 (84%)	99 (90%)	11 (10%)	7	19
1	G	110/131 (84%)	101 (92%)	9 (8%)	10	27
1	H	110/131 (84%)	98 (89%)	12 (11%)	6	16
1	I	110/131 (84%)	96 (87%)	14 (13%)	4	11
1	J	110/131 (84%)	101 (92%)	9 (8%)	10	27
All	All	1100/1310 (84%)	1004 (91%)	96 (9%)	9	24

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	811	ARG
1	A	843	VAL
1	A	851	LYS
1	A	854	SER
1	A	866	ARG
1	B	811	ARG
1	B	816	LEU
1	B	825	VAL
1	B	893	VAL
1	C	811	ARG
1	C	881	THR
1	C	883	GLU
1	C	894	VAL
1	C	897	ILE
1	C	901	VAL
1	C	919	ASP
1	D	808	LEU
1	D	811	ARG
1	D	825	VAL
1	D	866	ARG
1	D	880	LYS
1	D	884	ILE
1	D	894	VAL
1	D	897	ILE

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Mol	Chain	Res	Type
1	D	903	THR
1	D	909	LYS
1	E	803	LYS
1	E	825	VAL
1	E	827	GLU
1	E	836	ASP
1	E	853	PHE
1	E	856	PHE
1	E	861	LYS
1	E	882	PHE
1	E	883	GLU
1	E	884	ILE
1	E	894	VAL
1	E	901	VAL
1	E	903	THR
1	E	914	GLU
1	E	923	MET
1	F	804	GLU
1	F	811	ARG
1	F	816	LEU
1	F	851	LYS
1	F	869	CYS
1	F	883	GLU
1	F	884	ILE
1	F	894	VAL
1	F	901	VAL
1	F	907	LYS
1	F	914	GLU
1	G	804	GLU
1	G	816	LEU
1	G	825	VAL
1	G	884	ILE
1	G	897	ILE
1	G	903	THR
1	G	914	GLU
1	G	922	GLU
1	G	923	MET
1	H	807	LYS
1	H	850	PRO
1	H	851	LYS
1	H	852	GLN
1	H	853	PHE

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Mol	Chain	Res	Type
1	H	868	ASN
1	H	881	THR
1	H	882	PHE
1	H	884	ILE
1	H	890	GLU
1	H	894	VAL
1	H	897	ILE
1	I	803	LYS
1	I	809	LEU
1	I	811	ARG
1	I	825	VAL
1	I	827	GLU
1	I	834	LEU
1	I	848	PRO
1	I	852	GLN
1	I	866	ARG
1	I	878	LYS
1	I	882	PHE
1	I	894	VAL
1	I	903	THR
1	I	914	GLU
1	J	816	LEU
1	J	846	PRO
1	J	847	HIS
1	J	850	PRO
1	J	882	PHE
1	J	884	ILE
1	J	894	VAL
1	J	901	VAL
1	J	903	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	830	HIS
1	A	852	GLN
1	A	868	ASN
1	A	912	HIS
1	B	830	HIS
1	C	830	HIS
1	C	871	HIS
1	D	830	HIS

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Mol	Chain	Res	Type
1	D	902	GLN
1	E	830	HIS
1	E	876	HIS
1	F	805	ASN
1	F	830	HIS
1	F	852	GLN
1	G	830	HIS
1	H	830	HIS
1	H	867	GLN
1	I	830	HIS
1	I	871	HIS
1	I	876	HIS
1	J	830	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	121/145 (83%)	-0.44	1 (0%) 82 81	13, 33, 60, 76	14 (11%)
1	B	119/145 (82%)	-0.20	3 (2%) 58 55	9, 31, 54, 77	20 (16%)
1	C	119/145 (82%)	0.03	4 (3%) 48 44	10, 41, 67, 85	24 (20%)
1	D	112/145 (77%)	0.00	2 (1%) 67 65	9, 41, 67, 98	18 (16%)
1	E	118/145 (81%)	0.45	9 (7%) 20 17	14, 48, 79, 94	24 (20%)
1	F	120/145 (82%)	0.18	4 (3%) 49 45	12, 44, 62, 94	27 (22%)
1	G	118/145 (81%)	0.14	10 (8%) 16 14	14, 45, 69, 95	29 (24%)
1	H	118/145 (81%)	0.26	9 (7%) 20 17	25, 50, 87, 100	25 (21%)
1	I	120/145 (82%)	0.56	8 (6%) 24 21	12, 61, 91, 96	30 (25%)
1	J	116/145 (80%)	1.10	24 (20%) 2 2	16, 65, 96, 100	36 (31%)
All	All	1181/1450 (81%)	0.21	74 (6%) 26 23	9, 45, 84, 100	247 (20%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	851	LYS	15.3
1	J	868	ASN	8.5
1	J	847	HIS	7.6
1	G	853	PHE	7.1
1	D	923	MET	5.9
1	J	870	SER	5.6
1	F	923	MET	5.6
1	E	850	PRO	5.5
1	B	848	PRO	5.3
1	G	848	PRO	5.1
1	J	842	PHE	4.3
1	J	923	MET	4.3
1	I	870	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	854	SER	4.1
1	E	854	SER	4.1
1	B	850	PRO	4.0
1	I	803	LYS	3.8
1	J	855	SER	3.8
1	D	856	PHE	3.8
1	G	850	PRO	3.7
1	G	855	SER	3.6
1	E	857	GLU	3.6
1	J	866	ARG	3.6
1	G	849	LYS	3.5
1	G	923	MET	3.5
1	C	853	PHE	3.4
1	J	862	ILE	3.3
1	E	849	LYS	3.2
1	C	849	LYS	3.1
1	J	803	LYS	3.1
1	I	827	GLU	3.0
1	J	861	LYS	2.9
1	J	850	PRO	2.9
1	J	873	TRP	2.8
1	J	863	PHE	2.8
1	J	882	PHE	2.8
1	E	923	MET	2.7
1	E	848	PRO	2.7
1	J	921	ALA	2.7
1	F	922	GLU	2.6
1	J	869	CYS	2.6
1	H	922	GLU	2.6
1	F	921	ALA	2.6
1	J	857	GLU	2.6
1	H	920	PRO	2.6
1	A	923	MET	2.6
1	H	856	PHE	2.5
1	C	923	MET	2.5
1	J	864	CYS	2.5
1	I	923	MET	2.4
1	H	882	PHE	2.4
1	H	849	LYS	2.4
1	H	850	PRO	2.3
1	G	867	GLN	2.3
1	J	860	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	848	PRO	2.3
1	I	862	ILE	2.3
1	H	847	HIS	2.3
1	H	855	SER	2.3
1	J	817	ALA	2.2
1	J	879	TYR	2.2
1	E	858	LYS	2.2
1	E	856	PHE	2.2
1	J	854	SER	2.2
1	I	850	PRO	2.1
1	I	812	LYS	2.1
1	I	848	PRO	2.1
1	H	853	PHE	2.1
1	E	866	ARG	2.1
1	G	804	GLU	2.1
1	J	878	LYS	2.1
1	F	869	CYS	2.1
1	J	871	HIS	2.1
1	G	856	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HG	J	1010	1/1	0.98	0.21	48,48,48,48	1
2	HG	B	1002	1/1	0.99	0.10	44,44,44,44	1
2	HG	C	1003	1/1	0.99	0.15	37,37,37,37	1
2	HG	D	1004	1/1	0.99	0.11	49,49,49,49	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HG	E	1005	1/1	0.99	0.10	59,59,59,59	1
2	HG	F	1006	1/1	0.99	0.10	54,54,54,54	1
2	HG	H	1008	1/1	0.99	0.12	51,51,51,51	1
2	HG	I	1009	1/1	0.99	0.14	51,51,51,51	1
2	HG	A	1001	1/1	0.99	0.12	45,45,45,45	1
2	HG	G	1007	1/1	1.00	0.07	51,51,51,51	1

6.5 Other polymers [i](#)

There are no such residues in this entry.