Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 01:53 PM EDT

PDB ID	:	2QFD
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 (i) 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 (1)) were used in the production of this report:

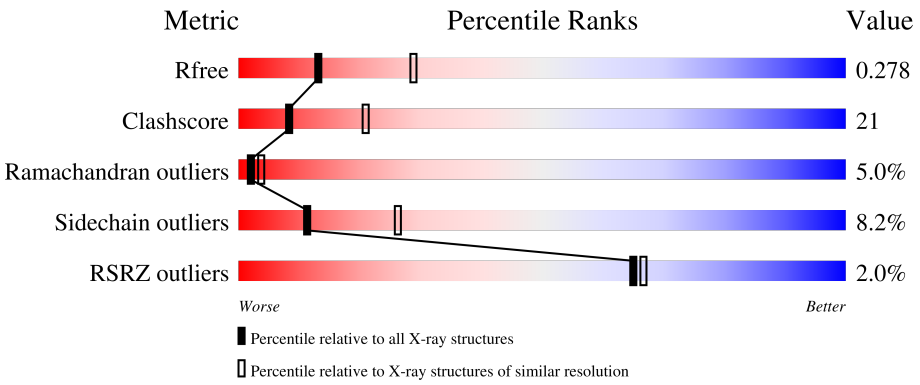
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	63% 17% • 17%
1	B	145	2% 59% 21% • 17%
1	C	145	48% 30% 5% 17%
1	D	145	% 50% 28% • • 17%
1	E	145	% 43% 33% 7% 17%

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Mol	Chain	Length	Quality of chain
1	F	145	41% 35% 7% 17%
1	G	145	3% 56% 23% • • 17%
1	H	145	% 48% 29% 7% 17%
1	I	145	% 43% 35% • • 17%
1	J	145	9% 49% 28% 6% • 17%

2 Entry composition (i)

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

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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Chain	Residue	Modelled	Actual	Comment	Reference
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
H	785	HIS	-	EXPRESSION TAG	UNP O95786
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
H	793	GLY	-	EXPRESSION TAG	UNP O95786
H	794	LEU	-	EXPRESSION TAG	UNP O95786
H	795	VAL	-	EXPRESSION TAG	UNP O95786
H	796	PRO	-	EXPRESSION TAG	UNP O95786
H	797	ARG	-	EXPRESSION TAG	UNP O95786
H	798	GLY	-	EXPRESSION TAG	UNP O95786
H	799	SER	-	EXPRESSION TAG	UNP O95786
H	800	HIS	-	EXPRESSION TAG	UNP O95786
H	801	MET	-	EXPRESSION TAG	UNP O95786
I	781	MET	-	EXPRESSION TAG	UNP O95786
I	782	GLY	-	EXPRESSION TAG	UNP O95786
I	783	SER	-	EXPRESSION TAG	UNP O95786
I	784	SER	-	EXPRESSION TAG	UNP O95786
I	785	HIS	-	EXPRESSION TAG	UNP O95786
I	786	HIS	-	EXPRESSION TAG	UNP O95786
I	787	HIS	-	EXPRESSION TAG	UNP O95786
I	788	HIS	-	EXPRESSION TAG	UNP O95786
I	789	HIS	-	EXPRESSION TAG	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
I	790	HIS	-	EXPRESSION TAG	UNP O95786
I	791	SER	-	EXPRESSION TAG	UNP O95786
I	792	SER	-	EXPRESSION TAG	UNP O95786
I	793	GLY	-	EXPRESSION TAG	UNP O95786
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
I	799	SER	-	EXPRESSION TAG	UNP O95786
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
J	786	HIS	-	EXPRESSION TAG	UNP O95786
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 (three-letter code: 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.

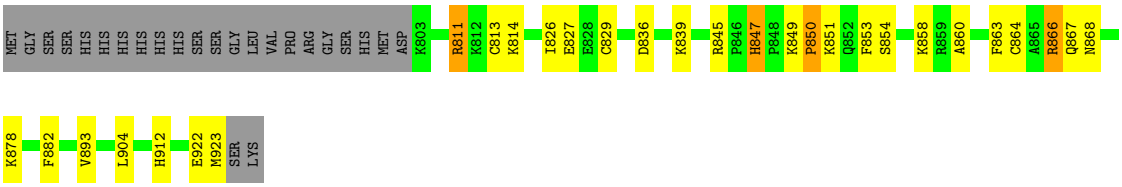
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O 27 27	0	0
3	B	25	Total O 25 25	0	0
3	C	12	Total O 12 12	0	0
3	D	15	Total O 15 15	0	0
3	E	8	Total O 8 8	0	0
3	F	4	Total O 4 4	0	0
3	G	8	Total O 8 8	0	0
3	H	3	Total O 3 3	0	0

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

Chain A:



• Molecule 1: Probable ATP-dependent RNA helicase DDX58

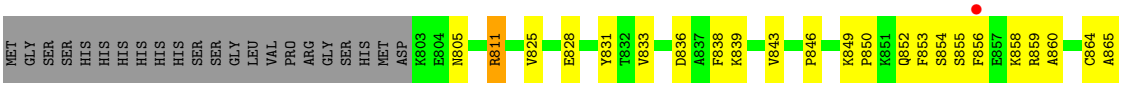
Chain B:

• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain C:

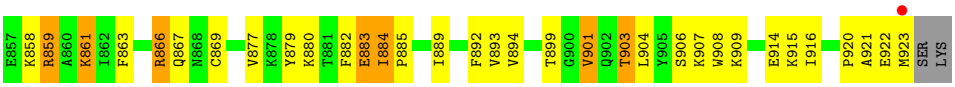
• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain D:



• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain E:

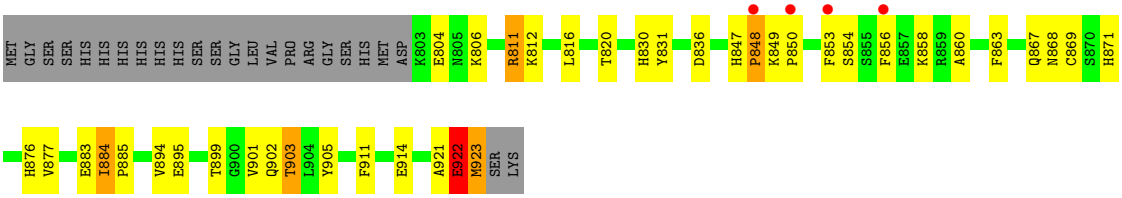


• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain F:

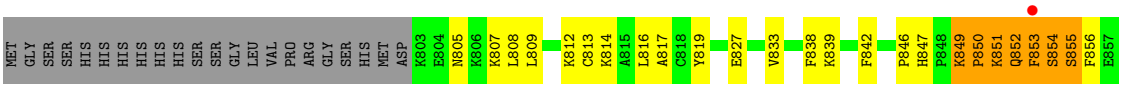
• Molecule 1: Probable ATP-dependent RNA helicase DDX58

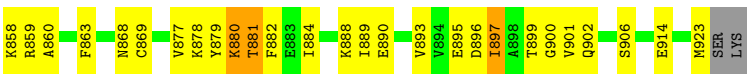
Chain G:



• Molecule 1: Probable ATP-dependent RNA helicase DDX58

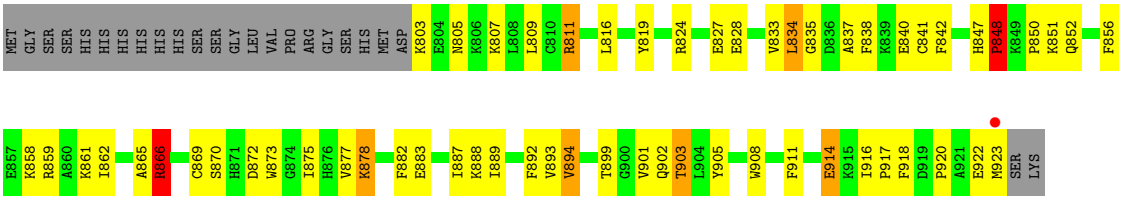
Chain H:





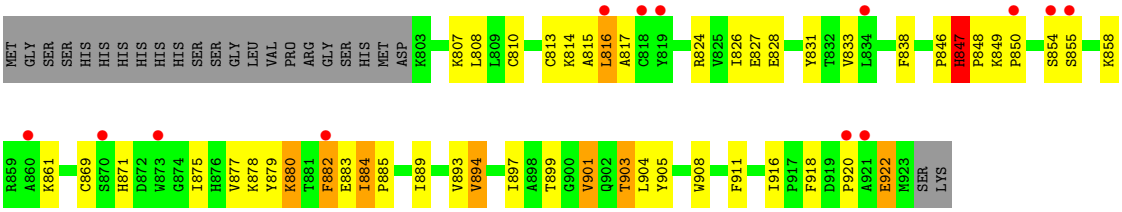
• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain I:



• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain J:



4 Data and refinement statistics (i)

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 48.51 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-2.70) 98.0 (48.51-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [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)	0.31 , 59.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.45	0/1026	0.70	0/1380
1	B	0.46	0/1026	0.71	0/1380
1	C	0.42	0/1026	0.70	0/1380
1	D	0.43	0/1026	0.64	0/1380
1	E	0.41	0/1026	0.68	0/1380
1	F	0.39	0/1026	0.64	0/1380
1	G	0.38	0/1026	0.67	1/1380 (0.1%)
1	H	0.40	0/1026	0.69	1/1380 (0.1%)
1	I	0.37	0/1026	0.60	0/1380
1	J	0.37	0/1026	0.66	1/1380 (0.1%)
All	All	0.41	0/10260	0.67	3/13800 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	847	HIS	C-N-CD	-7.77	103.50	120.60
1	H	852	GLN	N-CA-C	6.82	129.40	111.00
1	G	922	GLU	N-CA-C	-6.26	94.10	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	998	0	993	24	0
1	B	998	0	993	23	0
1	C	998	0	993	45	0
1	D	998	0	994	36	0
1	E	998	0	996	41	0
1	F	998	0	993	49	0
1	G	998	0	994	28	0
1	H	998	0	995	46	0
1	I	998	0	993	49	0
1	J	998	0	993	34	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
All	All	10092	0	9937	370	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 21.

All (370) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:890:GLU:H	1:H:890:GLU:CD	1.90	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:847:HIS:O	1:I:848:PRO:C	2.34	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: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	0.65
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:H:853:PHE:O	1:H:854:SER:HB2	1.98	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: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
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:E:920:PRO:C	1:E:922:GLU:H	2.05	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:919:ASP:C	1:F:921:ALA:H	2.08	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
1:E:855:SER:O	1:E:879:TYR:HD1	1.88	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:J:813:CYS:C	1:J:815:ALA:H	2.11	0.54

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:840:GLU:O	1:E:840:GLU:HG3	2.11	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: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:F:816:LEU:C	1:F:816:LEU:CD2	2.81	0.49
1:H:896:ASP:CG	1:H:899:THR:HB	2.33	0.49
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: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: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:828:GLU:OE2	1:E:915:LYS:NZ	2.41	0.47
1:H:890:GLU:CD	1:H:890:GLU:N	2.62	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:887:ILE:HG13	1:I:887:ILE:O	2.14	0.47
1:C:919:ASP:OD1	1:C:919:ASP:C	2.52	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: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
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:920:PRO:C	1:I:922:GLU:H	2.19	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: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:I:920:PRO:C	1:I:922:GLU:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:812:LYS:HE2	1:B:869:CYS:SG	2.58	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:H:816:LEU:HD13	1:H:816:LEU:C	2.39	0.43
1:J:894:VAL:HG11	1:J:905:TYR:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:LYS:HB3	1:C:890:GLU:HG2	2.01	0.43
1:E:867:GLN:C	1:E:869:CYS:H	2.22	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:E:920:PRO:C	1:E:922:GLU:N	2.71	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
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:I:865:ALA:O	1:I:866:ARG:C	2.57	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:G:811:ARG:NH2	3:G:115:HOH:O	2.35	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:H:854:SER:O	1:H:855:SER:C	2.58	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:J:813:CYS:C	1:J:815:ALA:N	2.72	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:D:884:ILE:HD13	1:D:884:ILE:N	2.33	0.41
1:D:911:PHE:C	1:D:911:PHE:CD1	2.93	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:B:858:LYS:HA	1:B:877:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:919:ASP:OD1	1:C:921:ALA:N	2.53	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
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:F:869:CYS:O	1:F:870:SER:C	2.60	0.41
1:F:919:ASP:C	1:F:921:ALA:N	2.73	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:869:CYS:O	1:I:870:SER:C	2.58	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: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:879:TYR:O	1:D:880:LYS:C	2.59	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%)	19	43
1	B	119/145 (82%)	110 (92%)	4 (3%)	5 (4%)	3	5
1	C	119/145 (82%)	100 (84%)	16 (13%)	3 (2%)	5	14
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	8
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%)	3	5
1	J	119/145 (82%)	91 (76%)	18 (15%)	10 (8%)	1	1
All	All	1190/1450 (82%)	1004 (84%)	127 (11%)	59 (5%)	2	4

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	F	828	GLU
1	G	850	PRO
1	J	922	GLU

5.3.2 Protein sidechains (i)

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%)	27	55
1	B	110/131 (84%)	107 (97%)	3 (3%)	44	74
1	C	110/131 (84%)	103 (94%)	7 (6%)	17	39
1	D	110/131 (84%)	101 (92%)	9 (8%)	11	26
1	E	110/131 (84%)	96 (87%)	14 (13%)	4	10
1	F	110/131 (84%)	98 (89%)	12 (11%)	6	14
1	G	110/131 (84%)	101 (92%)	9 (8%)	11	26
1	H	110/131 (84%)	100 (91%)	10 (9%)	9	21
1	I	110/131 (84%)	98 (89%)	12 (11%)	6	14
1	J	110/131 (84%)	101 (92%)	9 (8%)	11	26
All	All	1100/1310 (84%)	1010 (92%)	90 (8%)	11	26

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	811	ARG
1	A	847	HIS
1	A	851	LYS
1	A	854	SER
1	A	866	ARG
1	B	811	ARG
1	B	816	LEU
1	B	893	VAL
1	C	811	ARG
1	C	863	PHE

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Mol	Chain	Res	Type
1	C	881	THR
1	C	883	GLU
1	C	894	VAL
1	C	901	VAL
1	C	919	ASP
1	D	811	ARG
1	D	852	GLN
1	D	866	ARG
1	D	880	LYS
1	D	884	ILE
1	D	894	VAL
1	D	897	ILE
1	D	903	THR
1	D	923	MET
1	E	803	LYS
1	E	811	ARG
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	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	F	922	GLU
1	G	804	GLU
1	G	811	ARG

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Mol	Chain	Res	Type
1	G	816	LEU
1	G	836	ASP
1	G	884	ILE
1	G	903	THR
1	G	911	PHE
1	G	922	GLU
1	G	923	MET
1	H	850	PRO
1	H	851	LYS
1	H	852	GLN
1	H	853	PHE
1	H	868	ASN
1	H	881	THR
1	H	882	PHE
1	H	884	ILE
1	H	897	ILE
1	H	923	MET
1	I	803	LYS
1	I	809	LEU
1	I	811	ARG
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	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
1	J	911	PHE

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

Mol	Chain	Res	Type
1	A	852	GLN
1	A	868	ASN
1	A	912	HIS
1	B	876	HIS
1	D	830	HIS
1	E	830	HIS
1	E	867	GLN
1	E	876	HIS
1	F	805	ASN
1	F	852	GLN
1	G	830	HIS
1	H	867	GLN
1	I	830	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.37	0 100 100	17, 33, 62, 76	14 (11%)
1	B	119/145 (82%)	-0.24	3 (2%) 57 59	18, 33, 69, 85	20 (16%)
1	C	119/145 (82%)	-0.31	0 100 100	25, 43, 74, 85	24 (20%)
1	D	112/145 (77%)	-0.30	1 (0%) 84 85	26, 42, 78, 98	18 (16%)
1	E	118/145 (81%)	-0.17	1 (0%) 86 87	26, 51, 98, 100	24 (20%)
1	F	120/145 (82%)	-0.28	0 100 100	28, 47, 75, 99	27 (22%)
1	G	118/145 (81%)	-0.24	4 (3%) 45 45	32, 50, 94, 100	29 (24%)
1	H	118/145 (81%)	-0.15	1 (0%) 86 87	35, 55, 96, 100	25 (21%)
1	I	120/145 (82%)	0.08	1 (0%) 86 87	38, 65, 93, 98	30 (25%)
1	J	116/145 (80%)	0.32	13 (11%) 5 4	41, 78, 100, 100	36 (31%)
All	All	1181/1450 (81%)	-0.17	24 (2%) 65 67	17, 49, 94, 100	247 (20%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	851	LYS	5.4
1	D	856	PHE	4.3
1	J	870	SER	4.1
1	G	848	PRO	3.8
1	B	848	PRO	3.8
1	J	921	ALA	3.7
1	G	850	PRO	3.6
1	H	853	PHE	3.6
1	J	854	SER	3.2
1	I	923	MET	3.0
1	J	855	SER	2.9
1	G	853	PHE	2.8
1	E	923	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	850	PRO	2.7
1	J	819	TYR	2.6
1	J	882	PHE	2.5
1	B	850	PRO	2.4
1	G	856	PHE	2.4
1	J	816	LEU	2.3
1	J	834	LEU	2.2
1	J	860	ALA	2.2
1	J	818	CYS	2.0
1	J	920	PRO	2.0
1	J	873	TRP	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 monosaccharides 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(Å^2)	Q<0.9
2	HG	I	1009	1/1	0.97	0.15	51,51,51,51	1
2	HG	J	1010	1/1	0.97	0.16	48,48,48,48	1
2	HG	F	1006	1/1	0.98	0.10	54,54,54,54	1
2	HG	B	1002	1/1	0.99	0.10	44,44,44,44	1
2	HG	H	1008	1/1	0.99	0.13	51,51,51,51	1
2	HG	C	1003	1/1	0.99	0.17	37,37,37,37	1
2	HG	E	1005	1/1	0.99	0.14	59,59,59,59	1
2	HG	A	1001	1/1	1.00	0.13	45,45,45,45	1
2	HG	D	1004	1/1	1.00	0.12	49,49,49,49	1
2	HG	G	1007	1/1	1.00	0.08	51,51,51,51	1

6.5 Other polymers (i)

There are no such residues in this entry.