Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:17 PM GMT

PDB ID	:	3WNW
Title	:	Structure of Mouse H-chain modified ferritin
Authors	:	Zarivach, R.; Lewin, L.
Deposited on	:	2013-12-17
Resolution	:	2.24 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

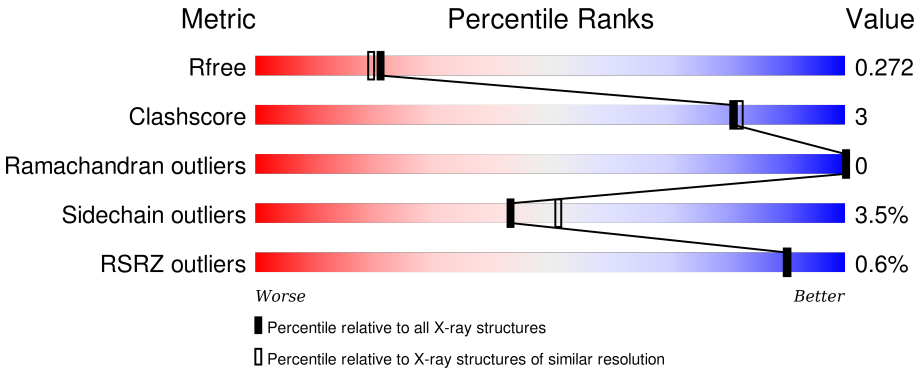
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	212	71% 10% • 18%
1	B	212	72% 8% • 18%
1	C	212	71% 9% • 18%
1	D	212	73% 8% 18%
1	E	212	70% 10% • 18%

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Mol	Chain	Length	Quality of chain
1	F	212	74% 8% 18%
1	G	212	70% 10% 18%
1	H	212	68% 13% 18%
1	I	212	70% 10% 18%
1	J	212	% 74% 8% 18%
1	K	212	74% 7% 18%
1	L	212	74% 8% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	E	201	-	-	-	X
4	GOL	A	204	-	-	-	X
4	GOL	A	205	-	-	-	X
4	GOL	C	205	-	-	-	X
4	GOL	D	203	-	-	-	X
4	GOL	E	204	-	-	-	X
4	GOL	K	203	-	-	-	X
4	GOL	K	204	-	-	-	X
4	GOL	L	202	-	-	-	X
4	GOL	L	203	-	-	-	X
5	K	B	203	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18648 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 Ferritin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	1	0
			1423	892	251	272	8			
1	B	173	Total	C	N	O	S	0	3	0
			1435	901	250	276	8			
1	C	173	Total	C	N	O	S	0	2	0
			1426	894	249	275	8			
1	D	173	Total	C	N	O	S	0	0	0
			1415	887	248	272	8			
1	E	173	Total	C	N	O	S	0	2	0
			1432	898	253	273	8			
1	F	174	Total	C	N	O	S	0	1	0
			1433	898	254	273	8			
1	G	174	Total	C	N	O	S	0	2	0
			1437	902	253	274	8			
1	H	173	Total	C	N	O	S	0	2	0
			1431	897	254	272	8			
1	I	173	Total	C	N	O	S	0	4	0
			1440	903	252	277	8			
1	J	174	Total	C	N	O	S	0	0	0
			1425	893	251	273	8			
1	K	173	Total	C	N	O	S	0	2	0
			1430	897	251	274	8			
1	L	174	Total	C	N	O	S	0	3	0
			1449	909	254	278	8			

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	GLY	-	EXPRESSION TAG	UNP P09528
A	-16	SER	-	EXPRESSION TAG	UNP P09528
A	-15	HIS	-	EXPRESSION TAG	UNP P09528
A	-14	MET	-	EXPRESSION TAG	UNP P09528
A	-13	ALA	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	SER	-	EXPRESSION TAG	UNP P09528
A	-11	MET	-	EXPRESSION TAG	UNP P09528
A	-10	THR	-	EXPRESSION TAG	UNP P09528
A	-9	GLY	-	EXPRESSION TAG	UNP P09528
A	-8	GLY	-	EXPRESSION TAG	UNP P09528
A	-7	GLN	-	EXPRESSION TAG	UNP P09528
A	-6	GLN	-	EXPRESSION TAG	UNP P09528
A	-5	MET	-	EXPRESSION TAG	UNP P09528
A	-4	GLY	-	EXPRESSION TAG	UNP P09528
A	-3	ARG	-	EXPRESSION TAG	UNP P09528
A	-2	GLY	-	EXPRESSION TAG	UNP P09528
A	-1	SER	-	EXPRESSION TAG	UNP P09528
A	182	GLY	-	EXPRESSION TAG	UNP P09528
A	183	ASP	-	EXPRESSION TAG	UNP P09528
A	184	ILE	-	EXPRESSION TAG	UNP P09528
A	185	GLU	-	EXPRESSION TAG	UNP P09528
A	186	SER	-	EXPRESSION TAG	UNP P09528
A	187	ALA	-	EXPRESSION TAG	UNP P09528
A	188	GLN	-	EXPRESSION TAG	UNP P09528
A	189	SER	-	EXPRESSION TAG	UNP P09528
A	190	ASP	-	EXPRESSION TAG	UNP P09528
A	191	GLU	-	EXPRESSION TAG	UNP P09528
A	192	GLU	-	EXPRESSION TAG	UNP P09528
A	193	VAL	-	EXPRESSION TAG	UNP P09528
A	194	GLU	-	EXPRESSION TAG	UNP P09528
B	-17	GLY	-	EXPRESSION TAG	UNP P09528
B	-16	SER	-	EXPRESSION TAG	UNP P09528
B	-15	HIS	-	EXPRESSION TAG	UNP P09528
B	-14	MET	-	EXPRESSION TAG	UNP P09528
B	-13	ALA	-	EXPRESSION TAG	UNP P09528
B	-12	SER	-	EXPRESSION TAG	UNP P09528
B	-11	MET	-	EXPRESSION TAG	UNP P09528
B	-10	THR	-	EXPRESSION TAG	UNP P09528
B	-9	GLY	-	EXPRESSION TAG	UNP P09528
B	-8	GLY	-	EXPRESSION TAG	UNP P09528
B	-7	GLN	-	EXPRESSION TAG	UNP P09528
B	-6	GLN	-	EXPRESSION TAG	UNP P09528
B	-5	MET	-	EXPRESSION TAG	UNP P09528
B	-4	GLY	-	EXPRESSION TAG	UNP P09528
B	-3	ARG	-	EXPRESSION TAG	UNP P09528
B	-2	GLY	-	EXPRESSION TAG	UNP P09528
B	-1	SER	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
B	182	GLY	-	EXPRESSION TAG	UNP P09528
B	183	ASP	-	EXPRESSION TAG	UNP P09528
B	184	ILE	-	EXPRESSION TAG	UNP P09528
B	185	GLU	-	EXPRESSION TAG	UNP P09528
B	186	SER	-	EXPRESSION TAG	UNP P09528
B	187	ALA	-	EXPRESSION TAG	UNP P09528
B	188	GLN	-	EXPRESSION TAG	UNP P09528
B	189	SER	-	EXPRESSION TAG	UNP P09528
B	190	ASP	-	EXPRESSION TAG	UNP P09528
B	191	GLU	-	EXPRESSION TAG	UNP P09528
B	192	GLU	-	EXPRESSION TAG	UNP P09528
B	193	VAL	-	EXPRESSION TAG	UNP P09528
B	194	GLU	-	EXPRESSION TAG	UNP P09528
C	-17	GLY	-	EXPRESSION TAG	UNP P09528
C	-16	SER	-	EXPRESSION TAG	UNP P09528
C	-15	HIS	-	EXPRESSION TAG	UNP P09528
C	-14	MET	-	EXPRESSION TAG	UNP P09528
C	-13	ALA	-	EXPRESSION TAG	UNP P09528
C	-12	SER	-	EXPRESSION TAG	UNP P09528
C	-11	MET	-	EXPRESSION TAG	UNP P09528
C	-10	THR	-	EXPRESSION TAG	UNP P09528
C	-9	GLY	-	EXPRESSION TAG	UNP P09528
C	-8	GLY	-	EXPRESSION TAG	UNP P09528
C	-7	GLN	-	EXPRESSION TAG	UNP P09528
C	-6	GLN	-	EXPRESSION TAG	UNP P09528
C	-5	MET	-	EXPRESSION TAG	UNP P09528
C	-4	GLY	-	EXPRESSION TAG	UNP P09528
C	-3	ARG	-	EXPRESSION TAG	UNP P09528
C	-2	GLY	-	EXPRESSION TAG	UNP P09528
C	-1	SER	-	EXPRESSION TAG	UNP P09528
C	182	GLY	-	EXPRESSION TAG	UNP P09528
C	183	ASP	-	EXPRESSION TAG	UNP P09528
C	184	ILE	-	EXPRESSION TAG	UNP P09528
C	185	GLU	-	EXPRESSION TAG	UNP P09528
C	186	SER	-	EXPRESSION TAG	UNP P09528
C	187	ALA	-	EXPRESSION TAG	UNP P09528
C	188	GLN	-	EXPRESSION TAG	UNP P09528
C	189	SER	-	EXPRESSION TAG	UNP P09528
C	190	ASP	-	EXPRESSION TAG	UNP P09528
C	191	GLU	-	EXPRESSION TAG	UNP P09528
C	192	GLU	-	EXPRESSION TAG	UNP P09528
C	193	VAL	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
C	194	GLU	-	EXPRESSION TAG	UNP P09528
D	-17	GLY	-	EXPRESSION TAG	UNP P09528
D	-16	SER	-	EXPRESSION TAG	UNP P09528
D	-15	HIS	-	EXPRESSION TAG	UNP P09528
D	-14	MET	-	EXPRESSION TAG	UNP P09528
D	-13	ALA	-	EXPRESSION TAG	UNP P09528
D	-12	SER	-	EXPRESSION TAG	UNP P09528
D	-11	MET	-	EXPRESSION TAG	UNP P09528
D	-10	THR	-	EXPRESSION TAG	UNP P09528
D	-9	GLY	-	EXPRESSION TAG	UNP P09528
D	-8	GLY	-	EXPRESSION TAG	UNP P09528
D	-7	GLN	-	EXPRESSION TAG	UNP P09528
D	-6	GLN	-	EXPRESSION TAG	UNP P09528
D	-5	MET	-	EXPRESSION TAG	UNP P09528
D	-4	GLY	-	EXPRESSION TAG	UNP P09528
D	-3	ARG	-	EXPRESSION TAG	UNP P09528
D	-2	GLY	-	EXPRESSION TAG	UNP P09528
D	-1	SER	-	EXPRESSION TAG	UNP P09528
D	182	GLY	-	EXPRESSION TAG	UNP P09528
D	183	ASP	-	EXPRESSION TAG	UNP P09528
D	184	ILE	-	EXPRESSION TAG	UNP P09528
D	185	GLU	-	EXPRESSION TAG	UNP P09528
D	186	SER	-	EXPRESSION TAG	UNP P09528
D	187	ALA	-	EXPRESSION TAG	UNP P09528
D	188	GLN	-	EXPRESSION TAG	UNP P09528
D	189	SER	-	EXPRESSION TAG	UNP P09528
D	190	ASP	-	EXPRESSION TAG	UNP P09528
D	191	GLU	-	EXPRESSION TAG	UNP P09528
D	192	GLU	-	EXPRESSION TAG	UNP P09528
D	193	VAL	-	EXPRESSION TAG	UNP P09528
D	194	GLU	-	EXPRESSION TAG	UNP P09528
E	-17	GLY	-	EXPRESSION TAG	UNP P09528
E	-16	SER	-	EXPRESSION TAG	UNP P09528
E	-15	HIS	-	EXPRESSION TAG	UNP P09528
E	-14	MET	-	EXPRESSION TAG	UNP P09528
E	-13	ALA	-	EXPRESSION TAG	UNP P09528
E	-12	SER	-	EXPRESSION TAG	UNP P09528
E	-11	MET	-	EXPRESSION TAG	UNP P09528
E	-10	THR	-	EXPRESSION TAG	UNP P09528
E	-9	GLY	-	EXPRESSION TAG	UNP P09528
E	-8	GLY	-	EXPRESSION TAG	UNP P09528
E	-7	GLN	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	GLN	-	EXPRESSION TAG	UNP P09528
E	-5	MET	-	EXPRESSION TAG	UNP P09528
E	-4	GLY	-	EXPRESSION TAG	UNP P09528
E	-3	ARG	-	EXPRESSION TAG	UNP P09528
E	-2	GLY	-	EXPRESSION TAG	UNP P09528
E	-1	SER	-	EXPRESSION TAG	UNP P09528
E	182	GLY	-	EXPRESSION TAG	UNP P09528
E	183	ASP	-	EXPRESSION TAG	UNP P09528
E	184	ILE	-	EXPRESSION TAG	UNP P09528
E	185	GLU	-	EXPRESSION TAG	UNP P09528
E	186	SER	-	EXPRESSION TAG	UNP P09528
E	187	ALA	-	EXPRESSION TAG	UNP P09528
E	188	GLN	-	EXPRESSION TAG	UNP P09528
E	189	SER	-	EXPRESSION TAG	UNP P09528
E	190	ASP	-	EXPRESSION TAG	UNP P09528
E	191	GLU	-	EXPRESSION TAG	UNP P09528
E	192	GLU	-	EXPRESSION TAG	UNP P09528
E	193	VAL	-	EXPRESSION TAG	UNP P09528
E	194	GLU	-	EXPRESSION TAG	UNP P09528
F	-17	GLY	-	EXPRESSION TAG	UNP P09528
F	-16	SER	-	EXPRESSION TAG	UNP P09528
F	-15	HIS	-	EXPRESSION TAG	UNP P09528
F	-14	MET	-	EXPRESSION TAG	UNP P09528
F	-13	ALA	-	EXPRESSION TAG	UNP P09528
F	-12	SER	-	EXPRESSION TAG	UNP P09528
F	-11	MET	-	EXPRESSION TAG	UNP P09528
F	-10	THR	-	EXPRESSION TAG	UNP P09528
F	-9	GLY	-	EXPRESSION TAG	UNP P09528
F	-8	GLY	-	EXPRESSION TAG	UNP P09528
F	-7	GLN	-	EXPRESSION TAG	UNP P09528
F	-6	GLN	-	EXPRESSION TAG	UNP P09528
F	-5	MET	-	EXPRESSION TAG	UNP P09528
F	-4	GLY	-	EXPRESSION TAG	UNP P09528
F	-3	ARG	-	EXPRESSION TAG	UNP P09528
F	-2	GLY	-	EXPRESSION TAG	UNP P09528
F	-1	SER	-	EXPRESSION TAG	UNP P09528
F	182	GLY	-	EXPRESSION TAG	UNP P09528
F	183	ASP	-	EXPRESSION TAG	UNP P09528
F	184	ILE	-	EXPRESSION TAG	UNP P09528
F	185	GLU	-	EXPRESSION TAG	UNP P09528
F	186	SER	-	EXPRESSION TAG	UNP P09528
F	187	ALA	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
F	188	GLN	-	EXPRESSION TAG	UNP P09528
F	189	SER	-	EXPRESSION TAG	UNP P09528
F	190	ASP	-	EXPRESSION TAG	UNP P09528
F	191	GLU	-	EXPRESSION TAG	UNP P09528
F	192	GLU	-	EXPRESSION TAG	UNP P09528
F	193	VAL	-	EXPRESSION TAG	UNP P09528
F	194	GLU	-	EXPRESSION TAG	UNP P09528
G	-17	GLY	-	EXPRESSION TAG	UNP P09528
G	-16	SER	-	EXPRESSION TAG	UNP P09528
G	-15	HIS	-	EXPRESSION TAG	UNP P09528
G	-14	MET	-	EXPRESSION TAG	UNP P09528
G	-13	ALA	-	EXPRESSION TAG	UNP P09528
G	-12	SER	-	EXPRESSION TAG	UNP P09528
G	-11	MET	-	EXPRESSION TAG	UNP P09528
G	-10	THR	-	EXPRESSION TAG	UNP P09528
G	-9	GLY	-	EXPRESSION TAG	UNP P09528
G	-8	GLY	-	EXPRESSION TAG	UNP P09528
G	-7	GLN	-	EXPRESSION TAG	UNP P09528
G	-6	GLN	-	EXPRESSION TAG	UNP P09528
G	-5	MET	-	EXPRESSION TAG	UNP P09528
G	-4	GLY	-	EXPRESSION TAG	UNP P09528
G	-3	ARG	-	EXPRESSION TAG	UNP P09528
G	-2	GLY	-	EXPRESSION TAG	UNP P09528
G	-1	SER	-	EXPRESSION TAG	UNP P09528
G	182	GLY	-	EXPRESSION TAG	UNP P09528
G	183	ASP	-	EXPRESSION TAG	UNP P09528
G	184	ILE	-	EXPRESSION TAG	UNP P09528
G	185	GLU	-	EXPRESSION TAG	UNP P09528
G	186	SER	-	EXPRESSION TAG	UNP P09528
G	187	ALA	-	EXPRESSION TAG	UNP P09528
G	188	GLN	-	EXPRESSION TAG	UNP P09528
G	189	SER	-	EXPRESSION TAG	UNP P09528
G	190	ASP	-	EXPRESSION TAG	UNP P09528
G	191	GLU	-	EXPRESSION TAG	UNP P09528
G	192	GLU	-	EXPRESSION TAG	UNP P09528
G	193	VAL	-	EXPRESSION TAG	UNP P09528
G	194	GLU	-	EXPRESSION TAG	UNP P09528
H	-17	GLY	-	EXPRESSION TAG	UNP P09528
H	-16	SER	-	EXPRESSION TAG	UNP P09528
H	-15	HIS	-	EXPRESSION TAG	UNP P09528
H	-14	MET	-	EXPRESSION TAG	UNP P09528
H	-13	ALA	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-12	SER	-	EXPRESSION TAG	UNP P09528
H	-11	MET	-	EXPRESSION TAG	UNP P09528
H	-10	THR	-	EXPRESSION TAG	UNP P09528
H	-9	GLY	-	EXPRESSION TAG	UNP P09528
H	-8	GLY	-	EXPRESSION TAG	UNP P09528
H	-7	GLN	-	EXPRESSION TAG	UNP P09528
H	-6	GLN	-	EXPRESSION TAG	UNP P09528
H	-5	MET	-	EXPRESSION TAG	UNP P09528
H	-4	GLY	-	EXPRESSION TAG	UNP P09528
H	-3	ARG	-	EXPRESSION TAG	UNP P09528
H	-2	GLY	-	EXPRESSION TAG	UNP P09528
H	-1	SER	-	EXPRESSION TAG	UNP P09528
H	182	GLY	-	EXPRESSION TAG	UNP P09528
H	183	ASP	-	EXPRESSION TAG	UNP P09528
H	184	ILE	-	EXPRESSION TAG	UNP P09528
H	185	GLU	-	EXPRESSION TAG	UNP P09528
H	186	SER	-	EXPRESSION TAG	UNP P09528
H	187	ALA	-	EXPRESSION TAG	UNP P09528
H	188	GLN	-	EXPRESSION TAG	UNP P09528
H	189	SER	-	EXPRESSION TAG	UNP P09528
H	190	ASP	-	EXPRESSION TAG	UNP P09528
H	191	GLU	-	EXPRESSION TAG	UNP P09528
H	192	GLU	-	EXPRESSION TAG	UNP P09528
H	193	VAL	-	EXPRESSION TAG	UNP P09528
H	194	GLU	-	EXPRESSION TAG	UNP P09528
I	-17	GLY	-	EXPRESSION TAG	UNP P09528
I	-16	SER	-	EXPRESSION TAG	UNP P09528
I	-15	HIS	-	EXPRESSION TAG	UNP P09528
I	-14	MET	-	EXPRESSION TAG	UNP P09528
I	-13	ALA	-	EXPRESSION TAG	UNP P09528
I	-12	SER	-	EXPRESSION TAG	UNP P09528
I	-11	MET	-	EXPRESSION TAG	UNP P09528
I	-10	THR	-	EXPRESSION TAG	UNP P09528
I	-9	GLY	-	EXPRESSION TAG	UNP P09528
I	-8	GLY	-	EXPRESSION TAG	UNP P09528
I	-7	GLN	-	EXPRESSION TAG	UNP P09528
I	-6	GLN	-	EXPRESSION TAG	UNP P09528
I	-5	MET	-	EXPRESSION TAG	UNP P09528
I	-4	GLY	-	EXPRESSION TAG	UNP P09528
I	-3	ARG	-	EXPRESSION TAG	UNP P09528
I	-2	GLY	-	EXPRESSION TAG	UNP P09528
I	-1	SER	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
I	182	GLY	-	EXPRESSION TAG	UNP P09528
I	183	ASP	-	EXPRESSION TAG	UNP P09528
I	184	ILE	-	EXPRESSION TAG	UNP P09528
I	185	GLU	-	EXPRESSION TAG	UNP P09528
I	186	SER	-	EXPRESSION TAG	UNP P09528
I	187	ALA	-	EXPRESSION TAG	UNP P09528
I	188	GLN	-	EXPRESSION TAG	UNP P09528
I	189	SER	-	EXPRESSION TAG	UNP P09528
I	190	ASP	-	EXPRESSION TAG	UNP P09528
I	191	GLU	-	EXPRESSION TAG	UNP P09528
I	192	GLU	-	EXPRESSION TAG	UNP P09528
I	193	VAL	-	EXPRESSION TAG	UNP P09528
I	194	GLU	-	EXPRESSION TAG	UNP P09528
J	-17	GLY	-	EXPRESSION TAG	UNP P09528
J	-16	SER	-	EXPRESSION TAG	UNP P09528
J	-15	HIS	-	EXPRESSION TAG	UNP P09528
J	-14	MET	-	EXPRESSION TAG	UNP P09528
J	-13	ALA	-	EXPRESSION TAG	UNP P09528
J	-12	SER	-	EXPRESSION TAG	UNP P09528
J	-11	MET	-	EXPRESSION TAG	UNP P09528
J	-10	THR	-	EXPRESSION TAG	UNP P09528
J	-9	GLY	-	EXPRESSION TAG	UNP P09528
J	-8	GLY	-	EXPRESSION TAG	UNP P09528
J	-7	GLN	-	EXPRESSION TAG	UNP P09528
J	-6	GLN	-	EXPRESSION TAG	UNP P09528
J	-5	MET	-	EXPRESSION TAG	UNP P09528
J	-4	GLY	-	EXPRESSION TAG	UNP P09528
J	-3	ARG	-	EXPRESSION TAG	UNP P09528
J	-2	GLY	-	EXPRESSION TAG	UNP P09528
J	-1	SER	-	EXPRESSION TAG	UNP P09528
J	182	GLY	-	EXPRESSION TAG	UNP P09528
J	183	ASP	-	EXPRESSION TAG	UNP P09528
J	184	ILE	-	EXPRESSION TAG	UNP P09528
J	185	GLU	-	EXPRESSION TAG	UNP P09528
J	186	SER	-	EXPRESSION TAG	UNP P09528
J	187	ALA	-	EXPRESSION TAG	UNP P09528
J	188	GLN	-	EXPRESSION TAG	UNP P09528
J	189	SER	-	EXPRESSION TAG	UNP P09528
J	190	ASP	-	EXPRESSION TAG	UNP P09528
J	191	GLU	-	EXPRESSION TAG	UNP P09528
J	192	GLU	-	EXPRESSION TAG	UNP P09528
J	193	VAL	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
J	194	GLU	-	EXPRESSION TAG	UNP P09528
K	-17	GLY	-	EXPRESSION TAG	UNP P09528
K	-16	SER	-	EXPRESSION TAG	UNP P09528
K	-15	HIS	-	EXPRESSION TAG	UNP P09528
K	-14	MET	-	EXPRESSION TAG	UNP P09528
K	-13	ALA	-	EXPRESSION TAG	UNP P09528
K	-12	SER	-	EXPRESSION TAG	UNP P09528
K	-11	MET	-	EXPRESSION TAG	UNP P09528
K	-10	THR	-	EXPRESSION TAG	UNP P09528
K	-9	GLY	-	EXPRESSION TAG	UNP P09528
K	-8	GLY	-	EXPRESSION TAG	UNP P09528
K	-7	GLN	-	EXPRESSION TAG	UNP P09528
K	-6	GLN	-	EXPRESSION TAG	UNP P09528
K	-5	MET	-	EXPRESSION TAG	UNP P09528
K	-4	GLY	-	EXPRESSION TAG	UNP P09528
K	-3	ARG	-	EXPRESSION TAG	UNP P09528
K	-2	GLY	-	EXPRESSION TAG	UNP P09528
K	-1	SER	-	EXPRESSION TAG	UNP P09528
K	182	GLY	-	EXPRESSION TAG	UNP P09528
K	183	ASP	-	EXPRESSION TAG	UNP P09528
K	184	ILE	-	EXPRESSION TAG	UNP P09528
K	185	GLU	-	EXPRESSION TAG	UNP P09528
K	186	SER	-	EXPRESSION TAG	UNP P09528
K	187	ALA	-	EXPRESSION TAG	UNP P09528
K	188	GLN	-	EXPRESSION TAG	UNP P09528
K	189	SER	-	EXPRESSION TAG	UNP P09528
K	190	ASP	-	EXPRESSION TAG	UNP P09528
K	191	GLU	-	EXPRESSION TAG	UNP P09528
K	192	GLU	-	EXPRESSION TAG	UNP P09528
K	193	VAL	-	EXPRESSION TAG	UNP P09528
K	194	GLU	-	EXPRESSION TAG	UNP P09528
L	-17	GLY	-	EXPRESSION TAG	UNP P09528
L	-16	SER	-	EXPRESSION TAG	UNP P09528
L	-15	HIS	-	EXPRESSION TAG	UNP P09528
L	-14	MET	-	EXPRESSION TAG	UNP P09528
L	-13	ALA	-	EXPRESSION TAG	UNP P09528
L	-12	SER	-	EXPRESSION TAG	UNP P09528
L	-11	MET	-	EXPRESSION TAG	UNP P09528
L	-10	THR	-	EXPRESSION TAG	UNP P09528
L	-9	GLY	-	EXPRESSION TAG	UNP P09528
L	-8	GLY	-	EXPRESSION TAG	UNP P09528
L	-7	GLN	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-6	GLN	-	EXPRESSION TAG	UNP P09528
L	-5	MET	-	EXPRESSION TAG	UNP P09528
L	-4	GLY	-	EXPRESSION TAG	UNP P09528
L	-3	ARG	-	EXPRESSION TAG	UNP P09528
L	-2	GLY	-	EXPRESSION TAG	UNP P09528
L	-1	SER	-	EXPRESSION TAG	UNP P09528
L	182	GLY	-	EXPRESSION TAG	UNP P09528
L	183	ASP	-	EXPRESSION TAG	UNP P09528
L	184	ILE	-	EXPRESSION TAG	UNP P09528
L	185	GLU	-	EXPRESSION TAG	UNP P09528
L	186	SER	-	EXPRESSION TAG	UNP P09528
L	187	ALA	-	EXPRESSION TAG	UNP P09528
L	188	GLN	-	EXPRESSION TAG	UNP P09528
L	189	SER	-	EXPRESSION TAG	UNP P09528
L	190	ASP	-	EXPRESSION TAG	UNP P09528
L	191	GLU	-	EXPRESSION TAG	UNP P09528
L	192	GLU	-	EXPRESSION TAG	UNP P09528
L	193	VAL	-	EXPRESSION TAG	UNP P09528
L	194	GLU	-	EXPRESSION TAG	UNP P09528

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Mg 2 2	0	0
2	J	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	K	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	I	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0

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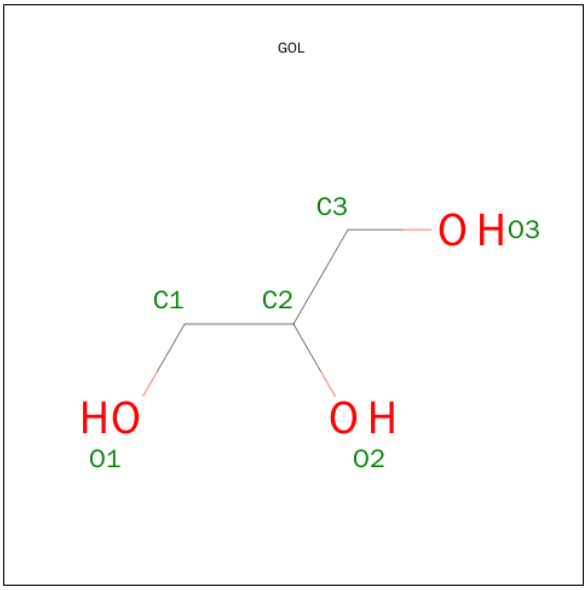
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0
3	A	1	Total Fe 1 1	0	0
3	C	1	Total Fe 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	K	1	Total C O 6 3 3	0	0
4	K	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	124	Total O 124 124	0	0
6	B	117	Total O 117 117	0	0
6	C	103	Total O 103 103	0	0
6	D	130	Total O 130 130	0	0
6	E	114	Total O 114 114	0	0
6	F	105	Total O 105 105	0	0

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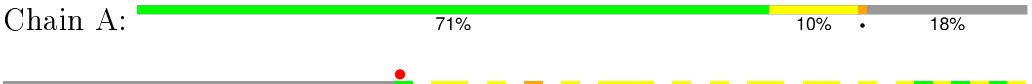
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	147	Total O 147 147	0	0
6	H	114	Total O 114 114	0	0
6	I	102	Total O 102 102	0	0
6	J	96	Total O 96 96	0	0
6	K	110	Total O 110 110	0	0
6	L	112	Total O 112 112	0	0

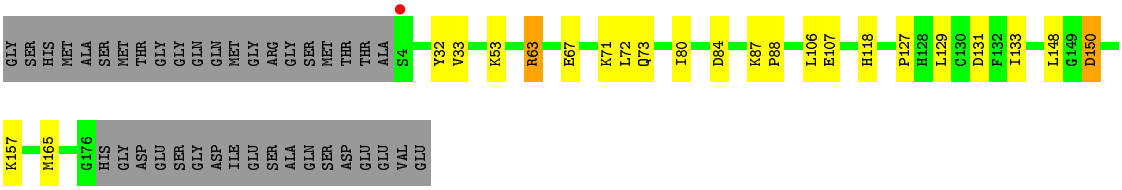
3 Residue-property plots (i)

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

- Molecule 1: Ferritin heavy chain

Chain A:





- Molecule 1: Ferritin heavy chain

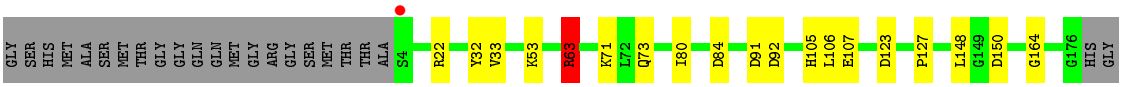
Chain B:

- Molecule 1: Ferritin heavy chain

Chain C:

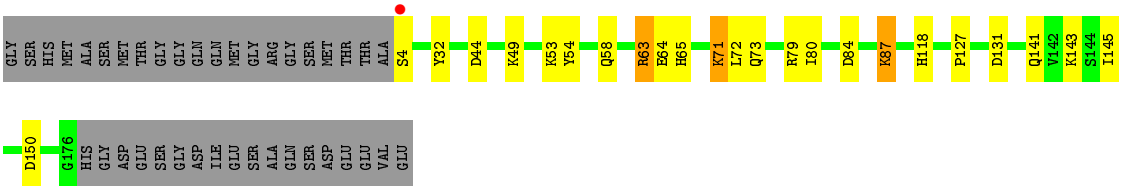
- Molecule 1: Ferritin heavy chain

Chain D:



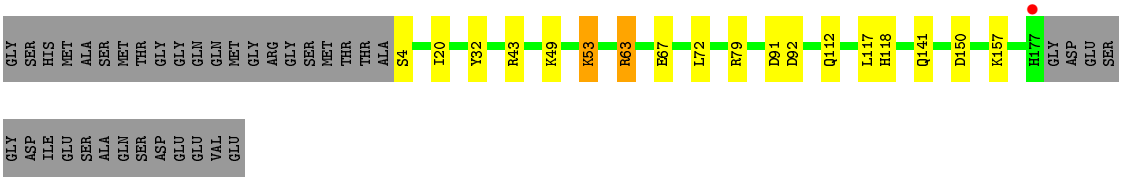
- Molecule 1: Ferritin heavy chain

Chain E:



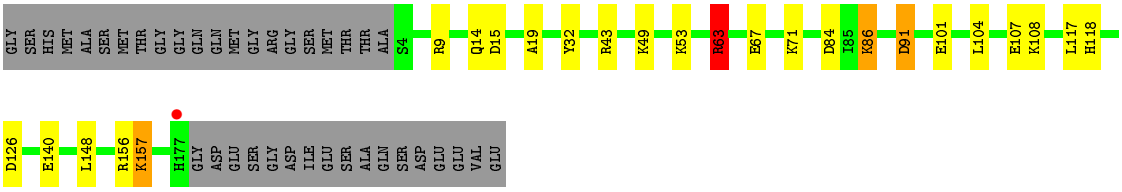
- Molecule 1: Ferritin heavy chain

Chain F:



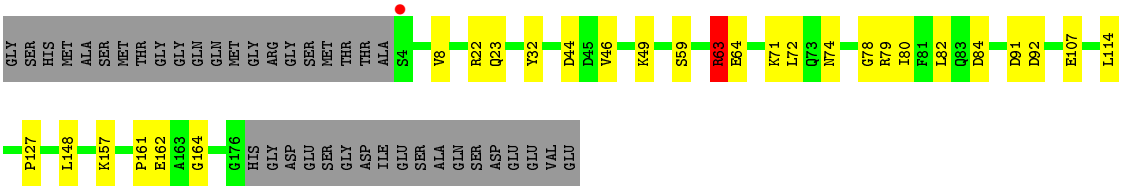
- Molecule 1: Ferritin heavy chain

Chain G:



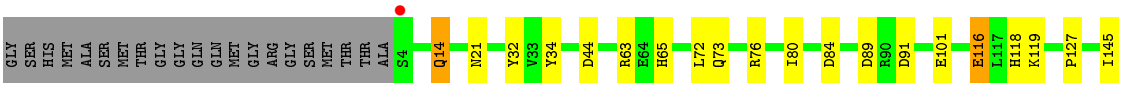
- Molecule 1: Ferritin heavy chain

Chain H:



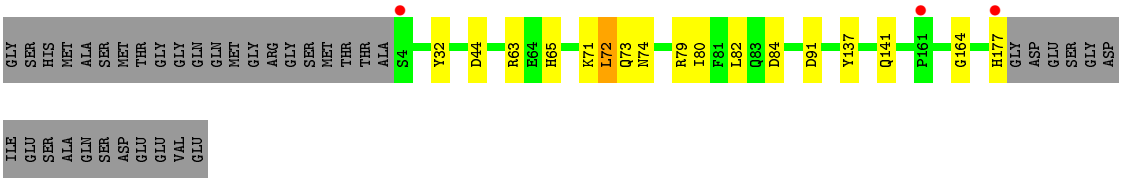
- Molecule 1: Ferritin heavy chain

Chain I:



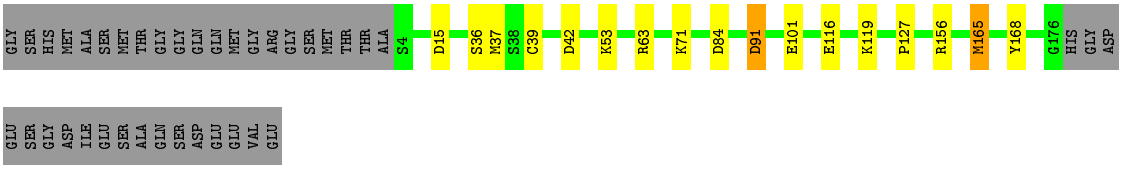
• Molecule 1: Ferritin heavy chain

Chain J:



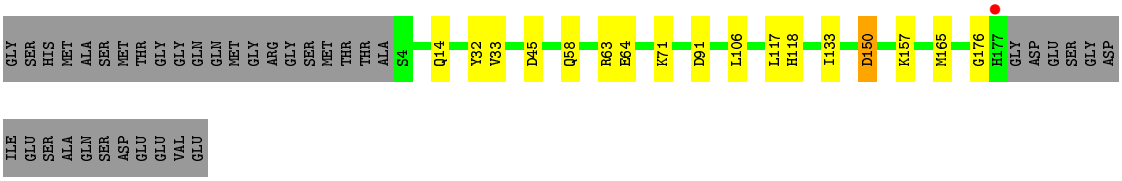
• Molecule 1: Ferritin heavy chain

Chain K:



• Molecule 1: Ferritin heavy chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	218.15Å 218.15Å 147.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 2.24 49.81 – 2.24	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.86-2.24) 94.5 (49.81-2.24)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.220 , 0.265 0.228 , 0.272	Depositor DCC
R_{free} test set	8125 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	13.8	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	58 of 160208 reflections (0.036%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18648	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.51 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.1694e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, K, FE

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	0.99	0/1455	0.98	2/1957 (0.1%)
1	B	1.03	2/1470 (0.1%)	1.04	8/1978 (0.4%)
1	C	0.98	0/1461	1.04	6/1966 (0.3%)
1	D	1.00	1/1444 (0.1%)	1.00	4/1943 (0.2%)
1	E	1.02	0/1464	1.00	5/1968 (0.3%)
1	F	0.96	0/1466	1.00	5/1972 (0.3%)
1	G	0.97	1/1473 (0.1%)	0.99	9/1981 (0.5%)
1	H	1.00	0/1466	1.00	7/1971 (0.4%)
1	I	1.05	1/1481 (0.1%)	1.02	5/1992 (0.3%)
1	J	0.97	0/1455	0.98	5/1958 (0.3%)
1	K	1.05	1/1462 (0.1%)	1.02	5/1966 (0.3%)
1	L	0.97	0/1491	0.99	5/2006 (0.2%)
All	All	1.00	6/17588 (0.0%)	1.00	66/23658 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	GLU	CG-CD	6.76	1.62	1.51
1	B	64	GLU	CD-OE1	6.12	1.32	1.25
1	I	34	TYR	CE1-CZ	-5.82	1.30	1.38
1	G	140	GLU	CD-OE2	5.33	1.31	1.25
1	D	123	ASP	CB-CG	5.26	1.62	1.51
1	K	168	TYR	CE1-CZ	-5.07	1.31	1.38

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	79	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	E	79	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	J	84	ASP	CB-CG-OD1	9.18	126.56	118.30
1	H	84	ASP	CB-CG-OD1	8.88	126.30	118.30
1	D	63	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	A	150	ASP	CB-CG-OD1	8.02	125.52	118.30
1	K	165	MET	CG-SD-CE	7.86	112.78	100.20
1	L	63	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	C	79	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	C	165	MET	CG-SD-CE	7.29	111.86	100.20
1	J	79	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	D	84	ASP	CB-CG-OD1	7.17	124.75	118.30
1	B	92	ASP	CB-CG-OD1	7.09	124.68	118.30
1	G	126	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	K	15	ASP	CB-CG-OD1	6.92	124.53	118.30
1	D	63	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	G	84	ASP	CB-CG-OD1	6.76	124.38	118.30
1	H	63[A]	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	H	63[B]	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	K	37	MET	CG-SD-CE	6.65	110.85	100.20
1	B	90	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	76	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	G	63	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	150	ASP	CB-CG-OD1	6.37	124.03	118.30
1	H	91	ASP	CB-CG-OD2	6.37	124.03	118.30
1	I	84	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	165	MET	CG-SD-CE	6.30	110.27	100.20
1	L	63	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	G	84	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	F	43	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	84	ASP	CB-CG-OD1	6.08	123.78	118.30
1	I	76	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	91	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	K	84	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	120	LEU	CA-CB-CG	5.78	128.59	115.30
1	L	45	ASP	CB-CG-OD1	5.73	123.46	118.30
1	L	150	ASP	CB-CG-OD1	5.72	123.45	118.30
1	G	43	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	F	63[A]	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	F	63[B]	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	J	91	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	9	ARG	NE-CZ-NH2	-5.64	117.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	84	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	76	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	I	89	ASP	CB-CG-OD1	5.54	123.29	118.30
1	H	63[A]	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	H	63[B]	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	90	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	L	176	GLY	N-CA-C	5.51	126.89	113.10
1	K	91	ASP	CB-CG-OD1	5.45	123.20	118.30
1	F	92	ASP	CB-CG-OD1	5.44	123.20	118.30
1	I	165	MET	CG-SD-CE	5.44	108.91	100.20
1	F	79	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	I	76	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	G	63	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	E	79	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	84	ASP	CB-CG-OD1	5.27	123.04	118.30
1	G	9	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	J	63	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	B	15	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	22	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	E	84	ASP	CB-CG-OD1	5.10	122.89	118.30
1	E	63[A]	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	E	63[B]	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	G	15	ASP	CB-CG-OD1	5.04	122.83	118.30
1	G	43	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	46	VAL	Peptide

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	1423	0	1377	13	0
1	B	1435	0	1388	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1426	0	1375	14	0
1	D	1415	0	1364	12	0
1	E	1432	0	1389	14	0
1	F	1433	0	1384	7	0
1	G	1437	0	1392	11	0
1	H	1431	0	1390	20	0
1	I	1440	0	1395	16	0
1	J	1425	0	1371	8	0
1	K	1430	0	1384	14	0
1	L	1449	0	1401	7	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	G	2	0	0	0	0
2	H	1	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	H	1	0	0	0	0
4	A	12	0	16	0	0
4	C	12	0	16	0	0
4	D	12	0	16	0	0
4	E	12	0	16	1	0
4	K	12	0	16	0	0
4	L	12	0	16	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	124	0	0	1	0
6	B	117	0	0	1	0
6	C	103	0	0	5	0
6	D	130	0	0	3	0
6	E	114	0	0	2	0
6	F	105	0	0	1	0
6	G	147	0	0	3	0
6	H	114	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	102	0	0	2	0
6	J	96	0	0	0	0
6	K	110	0	0	4	0
6	L	112	0	0	2	0
All	All	18648	0	16706	113	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 3.

All (113) 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:22[B]:ARG:NH2	6:H:406:HOH:O	2.01	0.93
1:K:91:ASP:OD2	6:K:394:HOH:O	1.94	0.84
1:H:63[B]:ARG:NH1	1:K:63:ARG:HG2	1.94	0.83
1:E:71[B]:LYS:HE3	4:E:203:GOL:O1	1.80	0.81
1:K:119[B]:LYS:HD2	6:K:327:HOH:O	1.85	0.77
1:D:63:ARG:HG2	1:I:63[A]:ARG:NH2	2.00	0.76
1:C:164:GLY:O	6:C:401:HOH:O	2.03	0.75
1:G:63:ARG:HG2	6:G:431:HOH:O	1.89	0.73
1:G:63:ARG:HD2	1:G:67:GLU:OE1	1.88	0.72
1:D:22:ARG:HD3	6:D:423:HOH:O	1.94	0.67
1:H:164:GLY:O	6:H:333:HOH:O	2.15	0.64
1:I:14:GLN:HE21	1:I:14:GLN:H	1.45	0.64
1:C:139:SER:HB2	6:C:314:HOH:O	1.99	0.63
1:E:131:ASP:OD1	6:E:412:HOH:O	2.16	0.62
1:E:72:LEU:HD13	1:E:72:LEU:C	2.22	0.60
1:L:33:VAL:HG11	1:L:106:LEU:HD22	1.84	0.59
1:H:63[B]:ARG:HH12	1:K:63:ARG:HG2	1.68	0.59
1:B:131:ASP:OD1	6:B:397:HOH:O	2.17	0.58
1:A:131:ASP:OD1	6:A:405:HOH:O	2.17	0.58
1:C:72:LEU:HD13	1:C:72:LEU:C	2.23	0.58
1:G:91:ASP:HB3	6:G:392:HOH:O	2.03	0.58
1:L:58[C]:GLN:HG3	6:L:391:HOH:O	2.03	0.57
1:E:150:ASP:OD1	1:I:44:ASP:HA	2.05	0.56
1:D:164:GLY:HA3	1:G:157:LYS:O	2.06	0.55
1:C:150:ASP:OD1	1:E:44:ASP:HA	2.06	0.55
1:A:129:LEU:O	1:A:133:ILE:HG12	2.07	0.54
1:I:157:LYS:HE2	6:K:404:HOH:O	2.07	0.54
1:I:21:ASN:HD21	1:I:80:ILE:HA	1.74	0.53
1:J:72:LEU:HD13	1:J:72:LEU:C	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:119[B]:LYS:CD	6:K:327:HOH:O	2.50	0.52
1:F:53:LYS:HE3	6:F:357:HOH:O	2.08	0.52
1:A:72:LEU:HD13	1:A:72:LEU:C	2.30	0.52
1:J:65:HIS:HB3	1:J:137:TYR:HE2	1.74	0.52
1:D:33:VAL:HG11	1:D:106:LEU:HD22	1.93	0.51
1:J:73:GLN:HG2	1:J:80:ILE:HG13	1.93	0.51
1:B:63:ARG:NH1	1:B:67:GLU:OE1	2.39	0.51
1:F:72:LEU:C	1:F:72:LEU:HD13	2.30	0.51
1:D:63:ARG:HG2	1:I:63[A]:ARG:HH22	1.73	0.50
1:B:65:HIS:HB3	1:B:137:TYR:HE2	1.77	0.50
1:D:91:ASP:OD1	6:D:401:HOH:O	2.20	0.50
1:D:63:ARG:HG2	1:I:63[A]:ARG:HH21	1.76	0.50
1:H:72:LEU:HD13	1:H:72:LEU:C	2.32	0.50
1:A:107:GLU:HG3	1:A:148:LEU:CD1	2.42	0.49
1:H:63[B]:ARG:HH11	1:K:63:ARG:HG2	1.74	0.49
1:C:42:ASP:HB3	1:J:74:ASN:ND2	2.28	0.48
1:H:59:SER:OG	1:K:63:ARG:NH1	2.37	0.48
1:C:36:SER:HB2	1:J:82:LEU:CD1	2.44	0.48
1:C:65:HIS:CD2	6:C:402:HOH:O	2.67	0.47
1:A:150:ASP:OD1	1:J:44:ASP:HA	2.15	0.47
1:A:157:LYS:O	1:J:164:GLY:HA3	2.14	0.47
1:E:73:GLN:HG2	1:E:80:ILE:HG13	1.95	0.47
1:H:92:ASP:C	1:H:92:ASP:OD1	2.54	0.46
1:K:116:GLU:HA	1:K:119[B]:LYS:HD2	1.98	0.46
1:I:65:HIS:CD2	6:I:397:HOH:O	2.69	0.46
1:D:73:GLN:HG2	1:D:80:ILE:HG13	1.98	0.46
1:H:161:PRO:HD2	1:H:162:GLU:OE1	2.15	0.45
1:A:118:HIS:CE1	1:C:127:PRO:HB3	2.52	0.45
1:E:127:PRO:HB3	1:F:118:HIS:CE1	2.51	0.45
1:L:14:GLN:NE2	6:L:318:HOH:O	2.50	0.45
1:F:20:ILE:HD13	1:F:117:LEU:HD21	1.98	0.45
1:I:101:GLU:OE1	1:I:156:ARG:NH2	2.50	0.45
1:F:63[A]:ARG:NE	1:F:67:GLU:OE1	2.47	0.45
1:H:107:GLU:HG3	1:H:148:LEU:CD1	2.47	0.45
1:H:78:GLY:O	1:H:79:ARG:NH1	2.50	0.44
1:K:101:GLU:OE1	1:K:156:ARG:NH2	2.50	0.44
1:H:164:GLY:HA3	1:L:157:LYS:O	2.17	0.44
1:B:44:ASP:HA	1:F:150:ASP:OD1	2.18	0.44
1:A:33:VAL:HG11	1:A:106:LEU:HD22	1.99	0.44
1:A:73:GLN:HG2	1:A:80:ILE:HG13	1.98	0.44
1:A:63[B]:ARG:NE	1:A:67:GLU:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PRO:HB3	1:B:118:HIS:CE1	2.53	0.44
1:G:101:GLU:OE1	1:G:156:ARG:NH2	2.49	0.43
1:H:8:VAL:HB	1:I:145:ILE:HG22	2.01	0.43
1:I:73:GLN:HG2	1:I:80:ILE:HG13	2.01	0.43
1:C:63:ARG:HG2	6:C:381:HOH:O	2.19	0.43
1:B:154:ASN:O	1:B:158:MET:HG3	2.19	0.43
1:C:157:LYS:NZ	6:C:382:HOH:O	2.41	0.42
1:E:141:GLN:O	1:E:145:ILE:HD12	2.19	0.42
1:A:63[A]:ARG:HD3	1:A:67:GLU:OE1	2.19	0.42
1:H:80:ILE:HD13	1:K:39:CYS:HB3	2.01	0.42
1:I:167:GLU:HG3	6:I:333:HOH:O	2.18	0.42
1:B:73:GLN:HG2	1:B:80:ILE:HG13	2.01	0.42
1:E:54:TYR:O	1:E:58:GLN:HG2	2.19	0.42
1:C:133:ILE:HG22	1:C:138:LEU:HG	2.02	0.42
1:K:127:PRO:HB3	1:L:118:HIS:CE1	2.53	0.42
1:G:14:GLN:NE2	6:G:407:HOH:O	2.50	0.42
1:D:92:ASP:OD1	1:D:92:ASP:C	2.57	0.42
1:E:72:LEU:HD13	1:E:72:LEU:O	2.19	0.42
1:H:74:ASN:HD22	1:K:42:ASP:HB3	1.84	0.42
1:E:72:LEU:C	1:E:72:LEU:CD1	2.88	0.42
1:A:87:LYS:HA	1:A:88:PRO:HD3	1.92	0.41
1:C:42:ASP:HB3	1:J:74:ASN:HD22	1.83	0.41
1:G:118:HIS:CE1	1:I:127:PRO:HB3	2.54	0.41
1:G:107:GLU:HG3	1:G:148:LEU:CD1	2.51	0.41
1:C:79:ARG:HD3	1:C:79:ARG:HA	1.92	0.41
1:B:164:GLY:HA3	1:F:157:LYS:O	2.19	0.41
1:D:107:GLU:HG3	1:D:148:LEU:CD1	2.51	0.41
1:I:72:LEU:HD13	1:I:72:LEU:C	2.41	0.41
1:H:44:ASP:HA	1:L:150:ASP:OD1	2.21	0.41
1:G:86:LYS:HA	1:G:86:LYS:HD2	1.90	0.41
1:H:127:PRO:HB3	1:I:118:HIS:CE1	2.55	0.41
1:H:74:ASN:ND2	1:K:42:ASP:HB3	2.36	0.41
1:G:19:ALA:HB1	1:G:117:LEU:HD13	2.01	0.41
1:D:105:HIS:HD2	6:D:374:HOH:O	2.03	0.41
1:D:127:PRO:HB3	1:E:118:HIS:CE1	2.56	0.41
1:C:78:GLY:O	1:C:79:ARG:NH1	2.54	0.40
1:B:82:LEU:O	1:E:87:LYS:HE3	2.22	0.40
1:G:104:LEU:HG	1:G:108[B]:LYS:HE2	2.02	0.40
1:H:82:LEU:CD1	1:K:36:SER:HB2	2.51	0.40
1:E:65:HIS:CD2	6:E:319:HOH:O	2.74	0.40
1:L:117:LEU:HG	1:L:133:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:GLN:NE2	1:H:114:LEU:HG	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/212 (81%)	170 (99%)	2 (1%)	0	100	100
1	B	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
1	C	173/212 (82%)	170 (98%)	3 (2%)	0	100	100
1	D	171/212 (81%)	168 (98%)	3 (2%)	0	100	100
1	E	173/212 (82%)	171 (99%)	2 (1%)	0	100	100
1	F	173/212 (82%)	169 (98%)	4 (2%)	0	100	100
1	G	174/212 (82%)	173 (99%)	1 (1%)	0	100	100
1	H	173/212 (82%)	170 (98%)	3 (2%)	0	100	100
1	I	175/212 (82%)	173 (99%)	2 (1%)	0	100	100
1	J	172/212 (81%)	169 (98%)	3 (2%)	0	100	100
1	K	173/212 (82%)	171 (99%)	2 (1%)	0	100	100
1	L	176/212 (83%)	171 (97%)	5 (3%)	0	100	100
All	All	2079/2544 (82%)	2045 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	154/182 (85%)	148 (96%)	6 (4%)	39	45
1	B	156/182 (86%)	152 (97%)	4 (3%)	54	64
1	C	155/182 (85%)	151 (97%)	4 (3%)	54	64
1	D	153/182 (84%)	149 (97%)	4 (3%)	54	64
1	E	155/182 (85%)	144 (93%)	11 (7%)	18	16
1	F	155/182 (85%)	148 (96%)	7 (4%)	34	37
1	G	156/182 (86%)	148 (95%)	8 (5%)	29	30
1	H	155/182 (85%)	148 (96%)	7 (4%)	34	37
1	I	157/182 (86%)	150 (96%)	7 (4%)	34	37
1	J	154/182 (85%)	149 (97%)	5 (3%)	46	56
1	K	155/182 (85%)	152 (98%)	3 (2%)	65	75
1	L	158/182 (87%)	153 (97%)	5 (3%)	46	56
All	All	1863/2184 (85%)	1792 (96%)	71 (4%)	43	47

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	53	LYS
1	A	63[A]	ARG
1	A	63[B]	ARG
1	A	71	LYS
1	A	165	MET
1	B	63	ARG
1	B	64	GLU
1	B	71	LYS
1	B	165	MET
1	C	49	LYS
1	C	53	LYS
1	C	71	LYS
1	C	165	MET
1	D	32	TYR
1	D	53	LYS
1	D	63	ARG
1	D	71	LYS

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Mol	Chain	Res	Type
1	E	4	SER
1	E	32	TYR
1	E	49	LYS
1	E	53	LYS
1	E	63[A]	ARG
1	E	63[B]	ARG
1	E	64	GLU
1	E	71[A]	LYS
1	E	71[B]	LYS
1	E	87	LYS
1	E	143	LYS
1	F	4	SER
1	F	32	TYR
1	F	49	LYS
1	F	53	LYS
1	F	91	ASP
1	F	112	GLN
1	F	141	GLN
1	G	32	TYR
1	G	49	LYS
1	G	53	LYS
1	G	63	ARG
1	G	71	LYS
1	G	86	LYS
1	G	91	ASP
1	G	157	LYS
1	H	32	TYR
1	H	49	LYS
1	H	63[A]	ARG
1	H	63[B]	ARG
1	H	64	GLU
1	H	71	LYS
1	H	157	LYS
1	I	14	GLN
1	I	32	TYR
1	I	91[A]	ASP
1	I	91[B]	ASP
1	I	116[A]	GLU
1	I	116[B]	GLU
1	I	119	LYS
1	J	32	TYR
1	J	71	LYS

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Mol	Chain	Res	Type
1	J	72	LEU
1	J	141	GLN
1	J	177	HIS
1	K	53	LYS
1	K	71	LYS
1	K	165	MET
1	L	32	TYR
1	L	64	GLU
1	L	71	LYS
1	L	91	ASP
1	L	165	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	105	HIS
1	F	177	HIS
1	H	10	GLN
1	I	14	GLN
1	I	21	ASN
1	I	23	GLN
1	L	14	GLN
1	L	57	HIS
1	L	177	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 26 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	204	-	5,5,5	0.35	0	5,5,5	1.17	0
4	GOL	A	205	-	5,5,5	0.52	0	5,5,5	0.99	0
4	GOL	C	204	-	5,5,5	0.71	0	5,5,5	1.06	0
4	GOL	C	205	-	5,5,5	0.82	0	5,5,5	2.59	2 (40%)
4	GOL	D	203	-	5,5,5	0.60	0	5,5,5	1.63	1 (20%)
4	GOL	D	204	-	5,5,5	0.40	0	5,5,5	0.82	0
4	GOL	E	203	-	5,5,5	0.63	0	5,5,5	1.20	1 (20%)
4	GOL	E	204	-	5,5,5	0.62	0	5,5,5	1.07	0
4	GOL	K	203	-	5,5,5	0.81	0	5,5,5	1.35	1 (20%)
4	GOL	K	204	-	5,5,5	0.48	0	5,5,5	1.14	0
4	GOL	L	202	-	5,5,5	0.20	0	5,5,5	0.58	0
4	GOL	L	203	-	5,5,5	0.49	0	5,5,5	1.55	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	204	-	-	0/4/4/4	0/0/0/0
4	GOL	A	205	-	-	0/4/4/4	0/0/0/0
4	GOL	C	204	-	-	0/4/4/4	0/0/0/0
4	GOL	C	205	-	-	0/4/4/4	0/0/0/0
4	GOL	D	203	-	-	0/4/4/4	0/0/0/0
4	GOL	D	204	-	-	0/4/4/4	0/0/0/0
4	GOL	E	203	-	-	0/4/4/4	0/0/0/0
4	GOL	E	204	-	-	0/4/4/4	0/0/0/0
4	GOL	K	203	-	-	0/4/4/4	0/0/0/0
4	GOL	K	204	-	-	0/4/4/4	0/0/0/0
4	GOL	L	202	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	L	203	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	205	GOL	C3-C2-C1	-3.47	97.51	111.12
4	L	203	GOL	C3-C2-C1	-2.83	100.02	111.12
4	E	203	GOL	O2-C2-C1	2.23	118.86	108.65
4	D	203	GOL	O3-C3-C2	2.40	121.81	110.18
4	K	203	GOL	O2-C2-C1	2.62	120.66	108.65
4	C	205	GOL	O2-C2-C3	4.06	127.27	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	203	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	173/212 (81%)	-0.43	1 (0%) 90 90	8, 13, 25, 42	0
1	B	173/212 (81%)	-0.43	1 (0%) 90 90	9, 13, 27, 48	0
1	C	173/212 (81%)	-0.38	1 (0%) 90 90	9, 13, 26, 48	0
1	D	173/212 (81%)	-0.47	1 (0%) 90 90	8, 13, 25, 46	0
1	E	173/212 (81%)	-0.35	1 (0%) 90 90	9, 14, 28, 51	0
1	F	174/212 (82%)	-0.42	1 (0%) 90 90	9, 13, 27, 61	0
1	G	174/212 (82%)	-0.44	1 (0%) 90 90	8, 12, 27, 70	0
1	H	173/212 (81%)	-0.45	1 (0%) 90 90	9, 13, 26, 51	0
1	I	173/212 (81%)	-0.44	1 (0%) 90 90	9, 13, 26, 46	0
1	J	174/212 (82%)	-0.41	3 (1%) 73 75	8, 13, 28, 71	0
1	K	173/212 (81%)	-0.40	0 100 100	9, 13, 27, 48	0
1	L	174/212 (82%)	-0.44	1 (0%) 90 90	9, 13, 27, 71	0
All	All	2080/2544 (81%)	-0.42	13 (0%) 90 90	8, 13, 27, 71	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	177	HIS	4.9
1	J	177	HIS	4.7
1	J	4	SER	3.9
1	A	4	SER	3.7
1	L	177	HIS	3.6
1	E	4	SER	3.5
1	C	4	SER	3.4
1	H	4	SER	3.4
1	G	177	HIS	3.3
1	B	4	SER	2.4
1	J	161	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	4	SER	2.2
1	I	4	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	K	204	6/6	0.91	0.23	6.38	20,21,26,35	0
4	GOL	C	205	6/6	0.82	0.19	6.34	21,23,26,31	0
2	MG	E	201	1/1	0.89	0.20	5.02	38,38,38,38	0
4	GOL	L	203	6/6	0.89	0.19	4.71	20,24,25,28	0
4	GOL	D	203	6/6	0.82	0.21	4.55	22,26,30,32	0
4	GOL	A	204	6/6	0.90	0.17	3.98	25,29,33,35	0
5	K	B	203	1/1	0.97	0.19	3.25	40,40,40,40	0
4	GOL	K	203	6/6	0.91	0.17	3.20	19,22,26,29	0
4	GOL	E	204	6/6	0.90	0.17	2.36	18,25,27,27	0
4	GOL	L	202	6/6	0.94	0.12	2.22	21,22,23,23	0
4	GOL	A	205	6/6	0.89	0.13	2.09	22,26,27,27	0
4	GOL	D	204	6/6	0.90	0.15	1.90	20,24,27,28	0
2	MG	K	201	1/1	0.92	0.12	1.51	42,42,42,42	0
4	GOL	E	203	6/6	0.84	0.21	0.86	21,26,30,35	0
4	GOL	C	204	6/6	0.94	0.10	-0.24	21,23,24,25	0
2	MG	C	201	1/1	0.94	0.09	-0.87	26,26,26,26	0
2	MG	C	202	1/1	0.97	0.09	-0.97	23,23,23,23	0
2	MG	E	202	1/1	0.93	0.10	-1.45	28,28,28,28	0
2	MG	I	201	1/1	0.93	0.07	-1.51	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	K	202	1/1	0.96	0.06	-1.66	19,19,19,19	0
2	MG	F	201	1/1	0.98	0.07	-2.34	24,24,24,24	0
2	MG	I	202	1/1	0.96	0.07	-2.51	19,19,19,19	0
2	MG	G	201	1/1	0.98	0.05	-3.22	25,25,25,25	0
2	MG	J	201	1/1	0.89	0.06	-3.60	28,28,28,28	0
2	MG	L	201	1/1	0.98	0.05	-4.29	25,25,25,25	0
3	FE	A	203	1/1	0.99	0.07	-4.67	31,31,31,31	0
3	FE	C	203	1/1	1.00	0.04	-4.70	33,33,33,33	0
2	MG	H	201	1/1	0.94	0.07	-5.85	23,23,23,23	0
2	MG	J	202	1/1	0.96	0.10	-	21,21,21,21	0
5	K	C	206	1/1	0.94	0.22	-	53,53,53,53	0
2	MG	A	201	1/1	0.97	0.06	-	28,28,28,28	0
2	MG	G	202	1/1	0.97	0.05	-	18,18,18,18	0
3	FE	H	202	1/1	0.99	0.07	-	34,34,34,34	1
2	MG	A	202	1/1	0.95	0.08	-	23,23,23,23	0
2	MG	D	202	1/1	0.98	0.05	-	20,20,20,20	0
2	MG	D	201	1/1	0.93	0.07	-	24,24,24,24	0
2	MG	B	201	1/1	0.92	0.06	-	25,25,25,25	0
3	FE	B	202	1/1	0.99	0.05	-	32,32,32,32	1

6.5 Other polymers (i)

There are no such residues in this entry.