WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 02:26 PM JST

PDB ID	:	7CPC
Title	:	His-Mediated Reversible Self-assembly of Ferritin Nanocage with Ni binding
Authors	:	Gu, C.; Zhang, T.; Zhao, G.
Deposited on	:	2020-08-06
Resolution	:	2.80 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Rfree		0.269
Clashscore		7
Ramachandran outliers		0.3%
Sidechain outliers		2.5%
RSRZ outliers		0.1%

Worse   Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
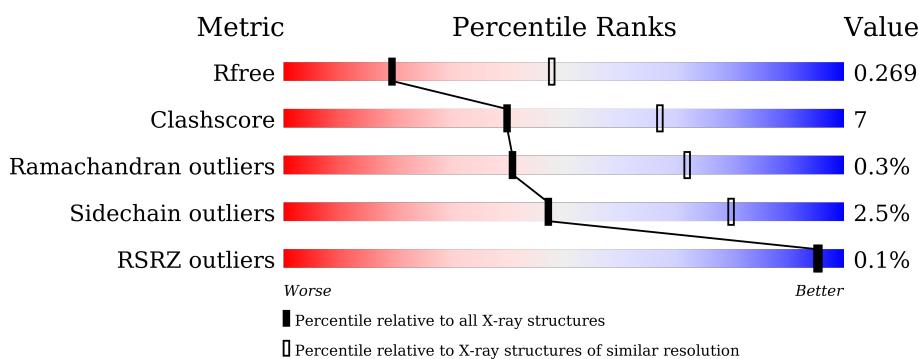
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	169	83% 14% ··
1	B	169	79% 20% ··
1	C	169	86% 12% ·
1	D	169	74% 23% ··
1	E	169	% 78% 19% ··
1	F	169	81% 18% ·

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8254 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	167	Total	C	N	O	S	0	0	0
			1372	859	238	268	7			
1	A	167	Total	C	N	O	S	0	0	0
			1372	859	238	268	7			
1	C	167	Total	C	N	O	S	0	0	0
			1372	859	238	268	7			
1	D	167	Total	C	N	O	S	0	0	0
			1372	859	238	268	7			
1	E	167	Total	C	N	O	S	0	0	0
			1372	859	238	268	7			
1	F	167	Total	C	N	O	S	0	0	0
			1372	859	238	268	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	89	ARG	GLN	engineered mutation	UNP T2B7E1
B	157	HIS	-	expression tag	UNP T2B7E1
B	158	HIS	-	expression tag	UNP T2B7E1
B	159	HIS	-	expression tag	UNP T2B7E1
B	160	HIS	-	expression tag	UNP T2B7E1
B	161	HIS	-	expression tag	UNP T2B7E1
B	162	HIS	-	expression tag	UNP T2B7E1
B	163	GLU	-	expression tag	UNP T2B7E1
B	164	TYR	-	expression tag	UNP T2B7E1
B	165	MET	-	expression tag	UNP T2B7E1
B	166	PHE	-	expression tag	UNP T2B7E1
B	167	ASP	-	expression tag	UNP T2B7E1
B	168	LYS	-	expression tag	UNP T2B7E1
B	169	GLU	-	expression tag	UNP T2B7E1
B	170	LEU	-	expression tag	UNP T2B7E1
B	171	ASN	-	expression tag	UNP T2B7E1
A	89	ARG	GLN	engineered mutation	UNP T2B7E1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	157	HIS	-	expression tag	UNP T2B7E1
A	158	HIS	-	expression tag	UNP T2B7E1
A	159	HIS	-	expression tag	UNP T2B7E1
A	160	HIS	-	expression tag	UNP T2B7E1
A	161	HIS	-	expression tag	UNP T2B7E1
A	162	HIS	-	expression tag	UNP T2B7E1
A	163	GLU	-	expression tag	UNP T2B7E1
A	164	TYR	-	expression tag	UNP T2B7E1
A	165	MET	-	expression tag	UNP T2B7E1
A	166	PHE	-	expression tag	UNP T2B7E1
A	167	ASP	-	expression tag	UNP T2B7E1
A	168	LYS	-	expression tag	UNP T2B7E1
A	169	GLU	-	expression tag	UNP T2B7E1
A	170	LEU	-	expression tag	UNP T2B7E1
A	171	ASN	-	expression tag	UNP T2B7E1
C	89	ARG	GLN	engineered mutation	UNP T2B7E1
C	157	HIS	-	expression tag	UNP T2B7E1
C	158	HIS	-	expression tag	UNP T2B7E1
C	159	HIS	-	expression tag	UNP T2B7E1
C	160	HIS	-	expression tag	UNP T2B7E1
C	161	HIS	-	expression tag	UNP T2B7E1
C	162	HIS	-	expression tag	UNP T2B7E1
C	163	GLU	-	expression tag	UNP T2B7E1
C	164	TYR	-	expression tag	UNP T2B7E1
C	165	MET	-	expression tag	UNP T2B7E1
C	166	PHE	-	expression tag	UNP T2B7E1
C	167	ASP	-	expression tag	UNP T2B7E1
C	168	LYS	-	expression tag	UNP T2B7E1
C	169	GLU	-	expression tag	UNP T2B7E1
C	170	LEU	-	expression tag	UNP T2B7E1
C	171	ASN	-	expression tag	UNP T2B7E1
D	89	ARG	GLN	engineered mutation	UNP T2B7E1
D	157	HIS	-	expression tag	UNP T2B7E1
D	158	HIS	-	expression tag	UNP T2B7E1
D	159	HIS	-	expression tag	UNP T2B7E1
D	160	HIS	-	expression tag	UNP T2B7E1
D	161	HIS	-	expression tag	UNP T2B7E1
D	162	HIS	-	expression tag	UNP T2B7E1
D	163	GLU	-	expression tag	UNP T2B7E1
D	164	TYR	-	expression tag	UNP T2B7E1
D	165	MET	-	expression tag	UNP T2B7E1
D	166	PHE	-	expression tag	UNP T2B7E1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	167	ASP	-	expression tag	UNP T2B7E1
D	168	LYS	-	expression tag	UNP T2B7E1
D	169	GLU	-	expression tag	UNP T2B7E1
D	170	LEU	-	expression tag	UNP T2B7E1
D	171	ASN	-	expression tag	UNP T2B7E1
E	89	ARG	GLN	engineered mutation	UNP T2B7E1
E	157	HIS	-	expression tag	UNP T2B7E1
E	158	HIS	-	expression tag	UNP T2B7E1
E	159	HIS	-	expression tag	UNP T2B7E1
E	160	HIS	-	expression tag	UNP T2B7E1
E	161	HIS	-	expression tag	UNP T2B7E1
E	162	HIS	-	expression tag	UNP T2B7E1
E	163	GLU	-	expression tag	UNP T2B7E1
E	164	TYR	-	expression tag	UNP T2B7E1
E	165	MET	-	expression tag	UNP T2B7E1
E	166	PHE	-	expression tag	UNP T2B7E1
E	167	ASP	-	expression tag	UNP T2B7E1
E	168	LYS	-	expression tag	UNP T2B7E1
E	169	GLU	-	expression tag	UNP T2B7E1
E	170	LEU	-	expression tag	UNP T2B7E1
E	171	ASN	-	expression tag	UNP T2B7E1
F	89	ARG	GLN	engineered mutation	UNP T2B7E1
F	157	HIS	-	expression tag	UNP T2B7E1
F	158	HIS	-	expression tag	UNP T2B7E1
F	159	HIS	-	expression tag	UNP T2B7E1
F	160	HIS	-	expression tag	UNP T2B7E1
F	161	HIS	-	expression tag	UNP T2B7E1
F	162	HIS	-	expression tag	UNP T2B7E1
F	163	GLU	-	expression tag	UNP T2B7E1
F	164	TYR	-	expression tag	UNP T2B7E1
F	165	MET	-	expression tag	UNP T2B7E1
F	166	PHE	-	expression tag	UNP T2B7E1
F	167	ASP	-	expression tag	UNP T2B7E1
F	168	LYS	-	expression tag	UNP T2B7E1
F	169	GLU	-	expression tag	UNP T2B7E1
F	170	LEU	-	expression tag	UNP T2B7E1
F	171	ASN	-	expression tag	UNP T2B7E1

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Fe 1	0	0
3	A	1	Total 1	Fe 1	0	0
3	C	1	Total 1	Fe 1	0	0
3	D	1	Total 1	Fe 1	0	0
3	E	1	Total 1	Fe 1	0	0
3	F	1	Total 1	Fe 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	O 1	0	0
4	A	2	Total 2	O 2	0	0
4	C	1	Total 1	O 1	0	0
4	D	1	Total 1	O 1	0	0
4	E	3	Total 3	O 3	0	0
4	F	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

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: Ferritin
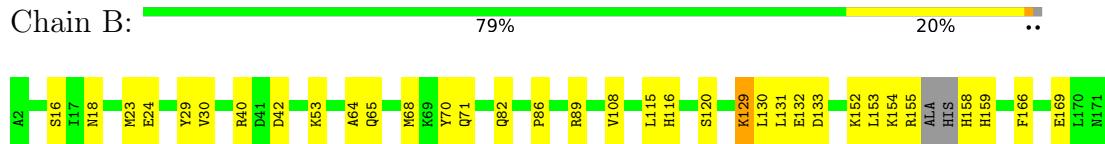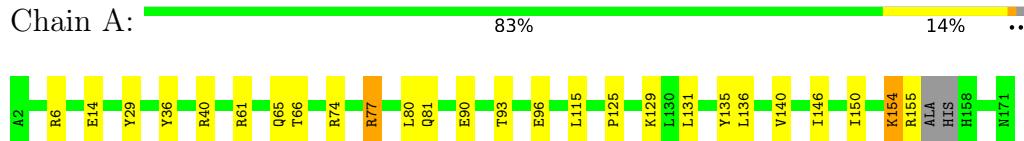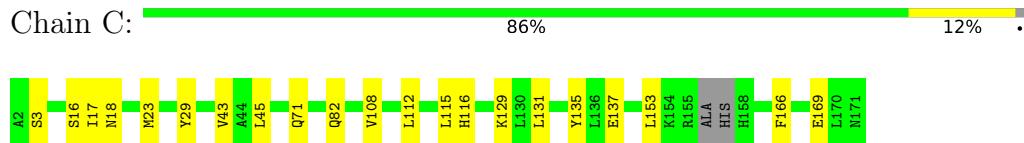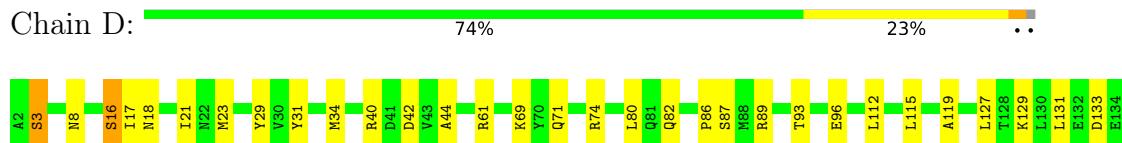
Chain B:

- Molecule 1: Ferritin

Chain A:

- Molecule 1: Ferritin

Chain C:

- Molecule 1: Ferritin

Chain D:

- Molecule 1: Ferritin

Chain E:

K154 R155 ALA HIS H158 H159 H160 N171

• Molecule 1: Ferritin

Chain F:

81%　　　　　　　　　　　18%

A2 S16 Q20 E24 L25 Y29 V30 S33 Y36 R40 D41 D42 E60 M68 K69 Y70 G76 R77 I78 I83 R89 E90 W91 L95 L115 L130 L131 I150 L153 K154 R155 ALA HIS H158 H162 F166 D167 K168 N171
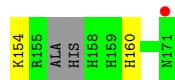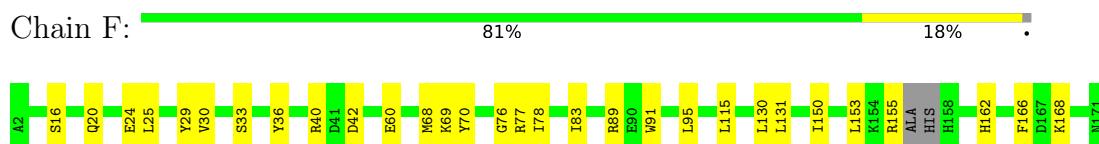
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	125.84Å 125.84Å 176.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.27 – 2.80 40.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.27-2.80) 95.0 (40.81-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.195 , 0.270 0.196 , 0.269	Depositor DCC
R_{free} test set	2010 reflections (6.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 0.8	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.043 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.024 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.026 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.034 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.068 for -h,k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8254	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.44	0/1399	0.56	0/1878
1	B	0.44	0/1399	0.54	0/1878
1	C	0.44	0/1399	0.53	0/1878
1	D	0.44	0/1399	0.57	0/1878
1	E	0.46	0/1399	0.56	0/1878
1	F	0.45	0/1399	0.54	0/1878
All	All	0.44	0/8394	0.55	0/11268

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	LYS	Peptide
1	B	158	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1372	0	1311	20	0
1	B	1372	0	1311	19	1
1	C	1372	0	1311	13	1
1	D	1372	0	1311	40	0
1	E	1372	0	1311	24	0
1	F	1372	0	1311	24	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	E	2	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	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
All	All	8254	0	7866	117	1

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 7.

All (117) 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:D:86:PRO:HB2	1:D:89:ARG:HH12	1.08	1.10
1:D:86:PRO:HB2	1:D:89:ARG:NH1	1.75	1.02
1:D:86:PRO:CB	1:D:89:ARG:HH12	1.72	1.01
1:D:161:HIS:CE1	1:D:165:MET:CE	2.52	0.93
1:D:161:HIS:CE1	1:D:165:MET:HE1	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:SER:HB3	1:F:115:LEU:HD13	1.65	0.78
1:D:86:PRO:CG	1:D:89:ARG:HH12	1.99	0.74
1:B:16:SER:HB3	1:B:115:LEU:HD13	1.70	0.74
1:D:161:HIS:CE1	1:D:165:MET:HE3	2.22	0.72
1:D:115:LEU:HG	1:D:131:LEU:HD11	1.70	0.72
1:F:155:ARG:HG2	1:F:162:HIS:CD2	2.24	0.71
1:B:115:LEU:HG	1:B:131:LEU:HD11	1.72	0.70
1:C:112:LEU:HD13	1:C:135:TYR:HB3	1.73	0.69
1:F:76:GLY:O	1:F:77:ARG:NH1	2.24	0.69
1:A:129:LYS:HE2	1:C:137:GLU:HG3	1.76	0.66
1:D:18:ASN:OD1	1:D:71:GLN:NE2	2.29	0.65
1:A:36:TYR:HE2	1:F:69:LYS:HG3	1.62	0.65
1:C:17:ILE:HD13	1:C:115:LEU:HD21	1.79	0.64
1:D:144:LYS:NZ	1:D:148:ASP:OD1	2.30	0.64
1:F:115:LEU:HG	1:F:131:LEU:HD11	1.80	0.63
1:D:16:SER:HB3	1:D:115:LEU:HD13	1.81	0.62
1:E:115:LEU:HG	1:E:131:LEU:HD11	1.81	0.61
1:B:116:HIS:CE1	1:E:125:PRO:HB3	2.36	0.60
1:C:18:ASN:OD1	1:C:71:GLN:NE2	2.34	0.59
1:F:40:ARG:NH2	1:F:42:ASP:OD2	2.35	0.59
1:C:16:SER:HB3	1:C:115:LEU:HD13	1.84	0.59
1:A:40:ARG:HH12	1:A:90:GLU:HG2	1.68	0.59
1:B:70:TYR:CD1	1:B:130:LEU:HD13	2.37	0.58
1:E:28:SER:HB3	1:E:60:GLU:HB2	1.85	0.58
1:F:89:ARG:CZ	1:F:89:ARG:HB2	2.33	0.58
1:B:23:MET:HE1	1:B:108:VAL:HA	1.86	0.57
1:F:70:TYR:CD1	1:F:130:LEU:HD22	2.39	0.57
1:B:155:ARG:HH12	1:D:159:HIS:HB2	1.69	0.57
1:E:16:SER:HB3	1:E:115:LEU:HD13	1.85	0.57
1:D:80:LEU:HD13	1:E:29:TYR:CE1	2.40	0.56
1:A:80:LEU:HD12	1:F:33:SER:HB2	1.86	0.56
1:A:93:THR:OG1	1:A:96:GLU:HG3	2.04	0.56
1:B:70:TYR:HD1	1:B:130:LEU:HD13	1.70	0.55
1:E:98:LEU:HD11	1:E:149:MET:HE2	1.86	0.55
1:E:18:ASN:OD1	1:E:71:GLN:NE2	2.39	0.55
1:E:6:ARG:NH1	1:E:14:GLU:OE1	2.25	0.55
1:D:31:TYR:CD1	1:D:34:MET:CE	2.90	0.55
1:A:6:ARG:NH1	1:A:14:GLU:OE1	2.27	0.54
1:E:129:LYS:NZ	1:E:133:ASP:OD2	2.41	0.54
1:C:115:LEU:HG	1:C:131:LEU:HD11	1.91	0.53
1:D:129:LYS:HE2	1:D:133:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:LEU:HB3	1:E:29:TYR:OH	2.09	0.53
1:B:129:LYS:HE3	1:B:133:ASP:OD2	2.10	0.51
1:D:86:PRO:CG	1:D:89:ARG:NH1	2.72	0.51
1:D:112:LEU:HD13	1:D:135:TYR:HB3	1.93	0.51
1:B:40:ARG:NH2	1:B:42:ASP:OD2	2.43	0.51
1:B:169:GLU:HG3	1:D:168:LYS:HZ1	1.76	0.51
1:D:31:TYR:CD1	1:D:34:MET:HE3	2.45	0.51
1:F:153:LEU:HD13	1:F:166:PHE:CD1	2.46	0.51
1:F:33:SER:OG	1:F:89:ARG:HG3	2.11	0.51
1:D:69:LYS:HG3	1:E:36:TYR:HE2	1.75	0.50
1:E:95:LEU:O	1:E:99:GLN:HG3	2.12	0.49
1:B:155:ARG:NH1	1:D:159:HIS:HB2	2.28	0.49
1:A:154:LYS:O	1:A:155:ARG:HB2	2.12	0.49
1:B:65:GLN:HA	1:B:68:MET:HE3	1.94	0.49
1:C:23:MET:HE1	1:C:108:VAL:HA	1.95	0.49
1:C:169:GLU:HG3	1:F:168:LYS:NZ	2.28	0.49
1:A:65:GLN:HB3	1:F:36:TYR:OH	2.12	0.49
1:A:129:LYS:HE2	1:C:137:GLU:CG	2.43	0.48
1:F:60:GLU:HA	1:F:60:GLU:OE1	2.13	0.48
1:D:161:HIS:ND1	1:D:165:MET:HE3	2.29	0.48
1:F:95:LEU:HD11	1:F:150:ILE:HG23	1.95	0.47
1:D:161:HIS:HE1	1:D:165:MET:HE1	1.71	0.47
1:B:24:GLU:HB2	1:B:64:ALA:HB2	1.95	0.47
1:D:3:SER:OG	1:E:41:ASP:OD2	2.33	0.47
1:D:149:MET:HB3	1:D:166:PHE:HZ	1.80	0.47
1:E:70:TYR:CD1	1:E:130:LEU:HD22	2.50	0.47
1:A:125:PRO:HB3	1:C:116:HIS:CE1	2.50	0.46
1:B:153:LEU:HD13	1:B:166:PHE:CD1	2.50	0.46
1:A:81:GLN:OE1	1:D:82:GLN:HB2	2.16	0.46
1:C:153:LEU:HD13	1:C:166:PHE:CD1	2.50	0.46
1:B:18:ASN:OD1	1:B:71:GLN:NE2	2.48	0.46
1:B:152:LYS:HE2	1:D:44:ALA:O	2.16	0.45
1:D:31:TYR:HA	1:D:34:MET:HE2	1.98	0.45
1:F:89:ARG:HB2	1:F:89:ARG:NH2	2.32	0.45
1:A:77:ARG:HD2	1:F:40:ARG:NE	2.32	0.45
1:A:40:ARG:NH1	1:A:90:GLU:HG2	2.32	0.44
1:F:68:MET:HE3	1:F:78:ILE:HG21	1.98	0.44
1:D:61:ARG:NH2	1:E:61:ARG:HE	2.15	0.44
1:D:93:THR:OG1	1:D:96:GLU:HG3	2.18	0.44
1:E:103:ASP:O	1:E:107:GLN:HG3	2.18	0.44
1:D:86:PRO:HG2	1:D:89:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HG	1:A:131:LEU:HD11	2.00	0.44
1:A:74:ARG:HA	1:A:74:ARG:HD2	1.72	0.44
1:A:136:LEU:O	1:A:140:VAL:HG23	2.18	0.43
1:A:66:THR:HB	1:A:135:TYR:OH	2.17	0.43
1:E:130:LEU:HD12	1:E:134:GLU:HG3	2.00	0.43
1:F:25:LEU:HD13	1:F:83:ILE:HD11	2.00	0.43
1:F:77:ARG:HA	1:F:77:ARG:HD3	1.73	0.43
1:A:77:ARG:HA	1:A:77:ARG:HD3	1.61	0.43
1:D:119:ALA:HB2	1:D:127:LEU:HD23	2.00	0.43
1:B:132:GLU:HB3	1:E:129:LYS:HD2	2.01	0.43
1:F:20:GLN:O	1:F:24:GLU:HG2	2.19	0.43
1:D:82:GLN:CD	1:E:82:GLN:HG3	2.39	0.42
1:E:144:LYS:NZ	1:E:148:ASP:OD1	2.47	0.42
1:D:23:MET:HE3	1:D:23:MET:HB3	1.87	0.42
1:E:20:GLN:NE2	1:E:23:MET:HE2	2.34	0.42
1:F:30:VAL:HG13	1:F:91:TRP:CH2	2.54	0.42
1:C:169:GLU:OE1	1:F:168:LYS:HD2	2.20	0.42
1:C:43:VAL:HG12	1:C:45:LEU:HD12	2.01	0.42
1:D:40:ARG:NE	1:E:77:ARG:NH1	2.68	0.42
1:D:86:PRO:CB	1:D:89:ARG:NH1	2.51	0.42
1:D:17:ILE:O	1:D:21:ILE:HG13	2.20	0.42
1:E:101:ALA:O	1:E:105:GLU:HG2	2.20	0.42
1:F:16:SER:CB	1:F:115:LEU:HD13	2.44	0.41
1:D:8:ASN:O	1:D:74:ARG:NH2	2.54	0.41
1:A:61:ARG:O	1:A:65:GLN:HG3	2.20	0.41
1:D:42:ASP:OD1	1:D:42:ASP:N	2.44	0.41
1:A:146:ILE:O	1:A:150:ILE:HG13	2.20	0.41
1:E:16:SER:CB	1:E:115:LEU:HD13	2.50	0.41
1:B:64:ALA:O	1:B:68:MET:HG3	2.20	0.41
1:B:30:VAL:HG22	1:B:86:PRO:HB3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLN:OE1	1:C:82:GLN:NE2[7_455]	2.09	0.11

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	163/169 (96%)	159 (98%)	4 (2%)	0	100	100
1	B	163/169 (96%)	158 (97%)	4 (2%)	1 (1%)	25	56
1	C	163/169 (96%)	157 (96%)	6 (4%)	0	100	100
1	D	163/169 (96%)	156 (96%)	6 (4%)	1 (1%)	25	56
1	E	163/169 (96%)	157 (96%)	5 (3%)	1 (1%)	25	56
1	F	163/169 (96%)	159 (98%)	4 (2%)	0	100	100
All	All	978/1014 (96%)	946 (97%)	29 (3%)	3 (0%)	41	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	LYS
1	D	87	SER
1	E	154	LYS

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	147/148 (99%)	145 (99%)	2 (1%)	67	90
1	B	147/148 (99%)	141 (96%)	6 (4%)	30	64
1	C	147/148 (99%)	144 (98%)	3 (2%)	55	84
1	D	147/148 (99%)	141 (96%)	6 (4%)	30	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	147/148 (99%)	143 (97%)	4 (3%)	44	78
1	F	147/148 (99%)	146 (99%)	1 (1%)	84	95
All	All	882/888 (99%)	860 (98%)	22 (2%)	47	80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	29	TYR
1	B	53	LYS
1	B	89	ARG
1	B	120	SER
1	B	129	LYS
1	B	159	HIS
1	A	29	TYR
1	A	77	ARG
1	C	3	SER
1	C	29	TYR
1	C	129	LYS
1	D	3	SER
1	D	16	SER
1	D	29	TYR
1	D	155	ARG
1	D	159	HIS
1	D	171	ASN
1	E	29	TYR
1	E	41	ASP
1	E	61	ARG
1	E	160	HIS
1	F	29	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	162	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 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	167/169 (98%)	-0.38	0	100	100	17, 25, 42, 63	0
1	B	167/169 (98%)	-0.46	0	100	100	16, 24, 38, 53	0
1	C	167/169 (98%)	-0.36	0	100	100	17, 25, 43, 63	0
1	D	167/169 (98%)	-0.38	0	100	100	16, 25, 41, 58	0
1	E	167/169 (98%)	-0.33	1 (0%)	89	86	15, 26, 41, 54	0
1	F	167/169 (98%)	-0.38	0	100	100	18, 24, 43, 59	0
All	All	1002/1014 (98%)	-0.38	1 (0%)	95	95	15, 25, 43, 63	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	171	ASN	2.6

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	NI	C	201	1/1	0.96	0.12	52,52,52,52	0
3	FE	A	203	1/1	0.98	0.08	47,47,47,47	0
2	NI	B	201	1/1	0.99	0.18	33,33,33,33	0
2	NI	E	201	1/1	0.99	0.13	37,37,37,37	1
2	NI	E	202	1/1	0.99	0.13	57,57,57,57	1
3	FE	B	202	1/1	0.99	0.08	47,47,47,47	0
2	NI	A	202	1/1	0.99	0.09	59,59,59,59	1
3	FE	C	202	1/1	0.99	0.09	46,46,46,46	0
3	FE	D	201	1/1	0.99	0.10	41,41,41,41	0
3	FE	E	203	1/1	0.99	0.09	49,49,49,49	0
3	FE	F	201	1/1	0.99	0.09	46,46,46,46	0
2	NI	A	201	1/1	1.00	0.18	31,31,31,31	1

6.5 Other polymers ⓘ

There are no such residues in this entry.