



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2025 – 02:31 PM JST

PDB ID : 8YKR
Title : Enhancing the Gastric Stability of Ferritin Nanocage via Computational-Assisted Disulfide Bond Engineering
Authors : Gu, C.K.; Wang, S.J.; Zhao, G.H.
Deposited on : 2024-03-05
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

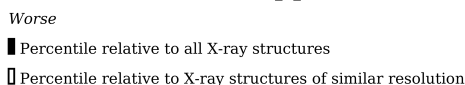
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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X-RAY DIFFRACTION

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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	A	170		..
1	B	170		..
1	C	170		..
1	D	170		..
1	E	170		..
1	F	170		..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8097 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	169	Total	C	N	O	S	0	1	0
			1348	837	227	269	15			
1	A	169	Total	C	N	O	S	0	1	0
			1348	837	227	269	15			
1	C	168	Total	C	N	O	S	0	1	0
			1343	834	226	268	15			
1	D	169	Total	C	N	O	S	0	1	0
			1348	837	227	269	15			
1	E	169	Total	C	N	O	S	0	1	0
			1348	837	227	269	15			
1	F	162	Total	C	N	O	S	0	1	0
			1293	806	214	258	15			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	44	CYS	ALA	engineered mutation	UNP T2B7E1
B	72	CYS	LYS	engineered mutation	UNP T2B7E1
B	88	ARG	GLN	conflict	UNP T2B7E1
B	125	CYS	HIS	engineered mutation	UNP T2B7E1
B	135	CYS	LEU	engineered mutation	UNP T2B7E1
B	139	CYS	VAL	engineered mutation	UNP T2B7E1
B	147	CYS	ASP	engineered mutation	UNP T2B7E1
B	155	CYS	ALA	engineered mutation	UNP T2B7E1
B	163	CYS	TYR	engineered mutation	UNP T2B7E1
A	44	CYS	ALA	engineered mutation	UNP T2B7E1
A	72	CYS	LYS	engineered mutation	UNP T2B7E1
A	88	ARG	GLN	conflict	UNP T2B7E1
A	125	CYS	HIS	engineered mutation	UNP T2B7E1
A	135	CYS	LEU	engineered mutation	UNP T2B7E1
A	139	CYS	VAL	engineered mutation	UNP T2B7E1
A	147	CYS	ASP	engineered mutation	UNP T2B7E1
A	155	CYS	ALA	engineered mutation	UNP T2B7E1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	163	CYS	TYR	engineered mutation	UNP T2B7E1
C	44	CYS	ALA	engineered mutation	UNP T2B7E1
C	72	CYS	LYS	engineered mutation	UNP T2B7E1
C	88	ARG	GLN	conflict	UNP T2B7E1
C	125	CYS	HIS	engineered mutation	UNP T2B7E1
C	135	CYS	LEU	engineered mutation	UNP T2B7E1
C	139	CYS	VAL	engineered mutation	UNP T2B7E1
C	147	CYS	ASP	engineered mutation	UNP T2B7E1
C	155	CYS	ALA	engineered mutation	UNP T2B7E1
C	163	CYS	TYR	engineered mutation	UNP T2B7E1
D	44	CYS	ALA	engineered mutation	UNP T2B7E1
D	72	CYS	LYS	engineered mutation	UNP T2B7E1
D	88	ARG	GLN	conflict	UNP T2B7E1
D	125	CYS	HIS	engineered mutation	UNP T2B7E1
D	135	CYS	LEU	engineered mutation	UNP T2B7E1
D	139	CYS	VAL	engineered mutation	UNP T2B7E1
D	147	CYS	ASP	engineered mutation	UNP T2B7E1
D	155	CYS	ALA	engineered mutation	UNP T2B7E1
D	163	CYS	TYR	engineered mutation	UNP T2B7E1
E	44	CYS	ALA	engineered mutation	UNP T2B7E1
E	72	CYS	LYS	engineered mutation	UNP T2B7E1
E	88	ARG	GLN	conflict	UNP T2B7E1
E	125	CYS	HIS	engineered mutation	UNP T2B7E1
E	135	CYS	LEU	engineered mutation	UNP T2B7E1
E	139	CYS	VAL	engineered mutation	UNP T2B7E1
E	147	CYS	ASP	engineered mutation	UNP T2B7E1
E	155	CYS	ALA	engineered mutation	UNP T2B7E1
E	163	CYS	TYR	engineered mutation	UNP T2B7E1
F	44	CYS	ALA	engineered mutation	UNP T2B7E1
F	72	CYS	LYS	engineered mutation	UNP T2B7E1
F	88	ARG	GLN	conflict	UNP T2B7E1
F	125	CYS	HIS	engineered mutation	UNP T2B7E1
F	135	CYS	LEU	engineered mutation	UNP T2B7E1
F	139	CYS	VAL	engineered mutation	UNP T2B7E1
F	147	CYS	ASP	engineered mutation	UNP T2B7E1
F	155	CYS	ALA	engineered mutation	UNP T2B7E1
F	163	CYS	TYR	engineered mutation	UNP T2B7E1

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

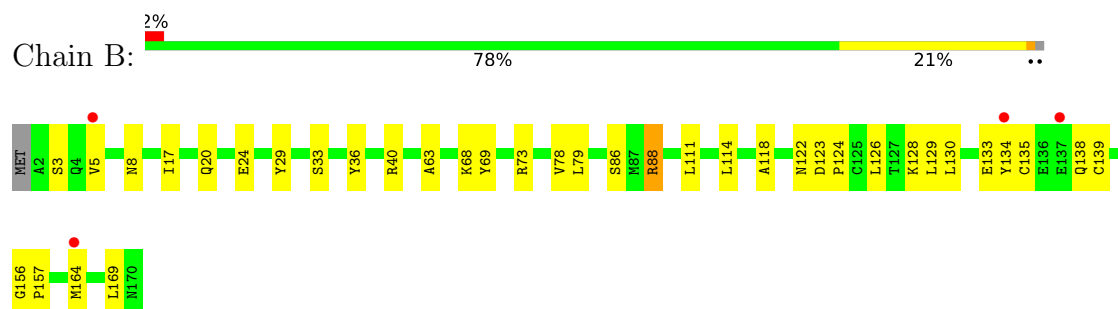
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	10	Total O 10 10	0	0
3	A	12	Total O 12 12	0	0
3	C	10	Total O 10 10	0	0
3	D	8	Total O 8 8	0	0
3	E	11	Total O 11 11	0	0
3	F	8	Total O 8 8	0	0

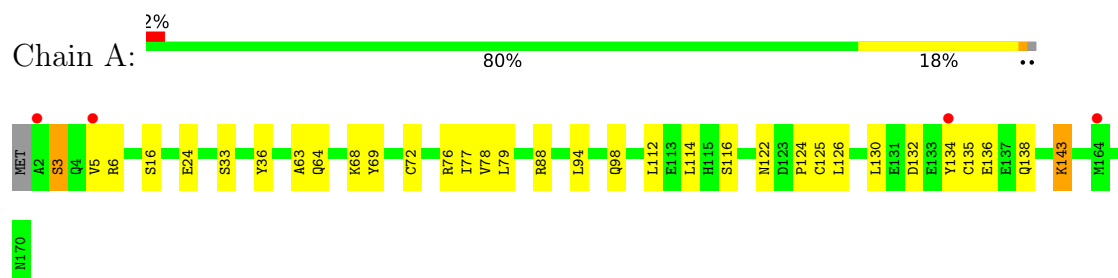
3 Residue-property plots [i](#)

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.

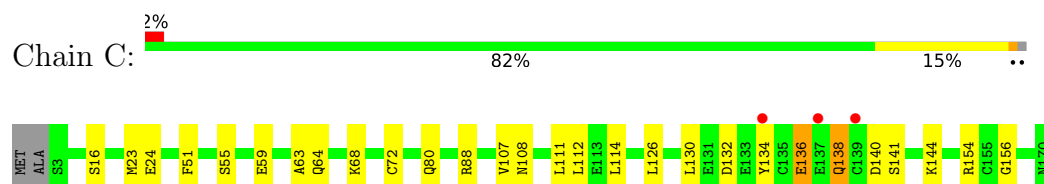
- Molecule 1: Ferritin



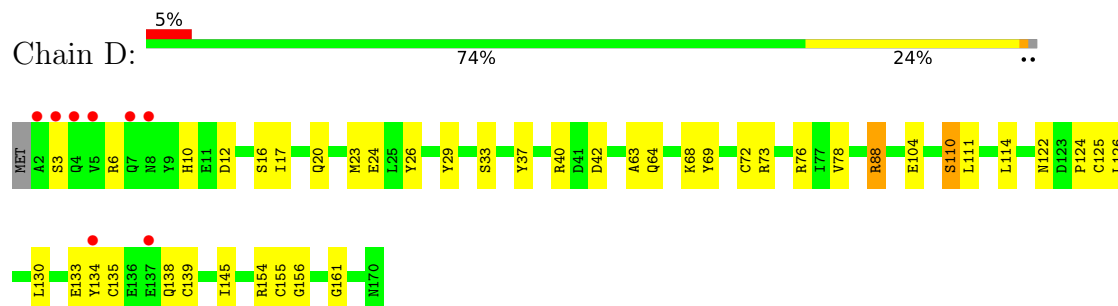
- Molecule 1: Ferritin



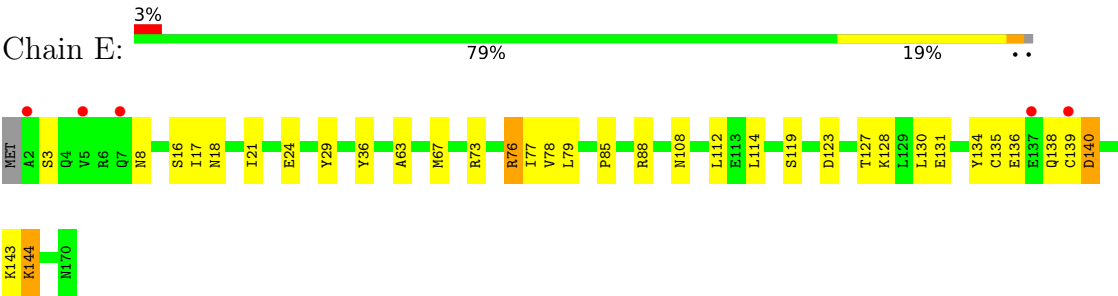
- Molecule 1: Ferritin



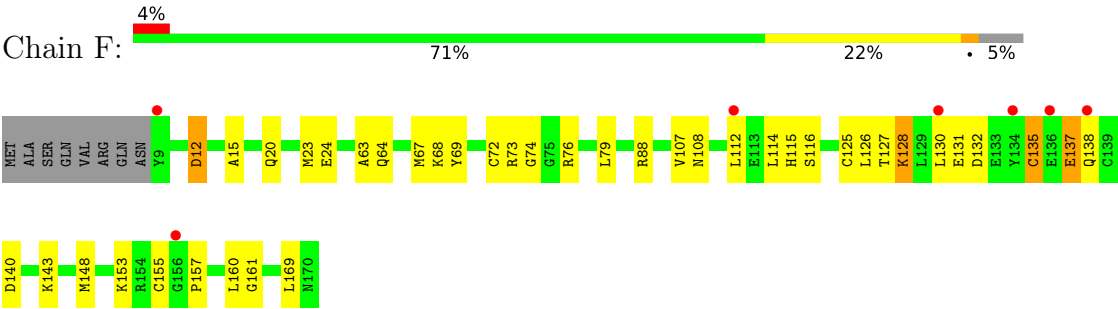
- Molecule 1: Ferritin



● Molecule 1: Ferritin



● Molecule 1: Ferritin



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	125.08Å 125.08Å 175.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.50 29.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.48-2.50) 99.9 (29.48-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.14 _ 3260: ???)	Depositor
R, R_{free}	0.185 , 0.230 0.186 , 0.231	Depositor DCC
R_{free} test set	44589 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.000 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.007 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.008 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.027 for -h,k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8097	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.52	0/1373	0.60	1/1843 (0.1%)
1	B	0.48	0/1373	0.61	1/1843 (0.1%)
1	C	0.52	0/1368	0.68	2/1836 (0.1%)
1	D	0.49	0/1373	0.59	2/1843 (0.1%)
1	E	0.56	0/1373	0.64	1/1843 (0.1%)
1	F	0.49	0/1318	0.62	2/1769 (0.1%)
All	All	0.51	0/8178	0.62	9/10977 (0.1%)

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	F	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	88	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	88	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	C	141[A]	SER	CA-C-O	6.18	133.09	120.10
1	C	141[B]	SER	CA-C-O	6.18	133.09	120.10
1	A	143	LYS	CB-CG-CD	-5.62	96.99	111.60
1	F	88	ARG	CB-CG-CD	-5.55	97.17	111.60
1	E	140	ASP	N-CA-C	-5.43	96.35	111.00
1	D	135	CYS	CA-CB-SG	-5.40	104.28	114.00
1	B	88	ARG	NE-CZ-NH1	5.39	123.00	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	12	ASP	Peptide
1	F	137	GLU	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	1348	0	1296	30	5
1	B	1348	0	1296	36	2
1	C	1343	0	1289	20	1
1	D	1348	0	1296	33	2
1	E	1348	0	1296	36	2
1	F	1293	0	1240	27	4
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	12	0	0	3	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	8	0	0	0	0
3	E	11	0	0	1	0
3	F	8	0	0	0	0
All	All	8097	0	7713	158	8

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 10.

All (158) 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:E:114:LEU:HG	1:E:130:LEU:HD11	1.32	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:LEU:HG	1:E:130:LEU:CD1	2.00	0.92
1:B:128:LYS:NZ	1:F:135:CYS:SG	2.52	0.83
1:E:108:ASN:HD21	1:E:138:GLN:HB3	1.56	0.71
1:C:114:LEU:HG	1:C:130:LEU:HD11	1.73	0.70
1:F:135:CYS:HA	1:F:138:GLN:HB2	1.72	0.70
1:B:79:LEU:HD12	1:A:33:SER:HB2	1.76	0.68
1:C:108:ASN:ND2	1:C:138:GLN:HG3	2.10	0.67
1:C:132:ASP:HA	1:C:136:GLU:CG	2.24	0.67
1:D:33:SER:OG	1:D:88:ARG:NH2	2.29	0.66
1:E:143:LYS:NZ	1:E:144:LYS:NZ	2.45	0.65
1:B:133:GLU:HG2	1:B:134:TYR:CE2	2.32	0.65
1:C:16:SER:HB3	1:C:114:LEU:HD13	1.78	0.65
1:E:108:ASN:HD21	1:E:138:GLN:CB	2.11	0.64
1:B:8:ASN:O	1:B:73:ARG:NH2	2.30	0.64
1:E:16:SER:HB3	1:E:114:LEU:HD13	1.80	0.64
1:C:108:ASN:HD22	1:C:111:LEU:HD12	1.63	0.63
1:D:78:VAL:HA	1:E:88:ARG:HD2	1.81	0.63
1:E:112:LEU:HD23	1:E:134:TYR:CE1	2.33	0.63
1:E:85:PRO:HD2	1:E:88:ARG:HH11	1.64	0.63
1:A:76:ARG:CZ	3:A:301:HOH:O	2.47	0.62
1:F:135:CYS:HA	1:F:138:GLN:HE21	1.64	0.62
1:E:112:LEU:HD21	1:E:134:TYR:CZ	2.35	0.62
1:D:23:MET:HA	1:D:23:MET:HE3	1.82	0.62
1:D:68:LYS:HG2	1:E:36:TYR:HE2	1.66	0.61
1:B:130:LEU:O	1:B:134:TYR:HB2	2.01	0.60
1:E:143:LYS:NZ	1:E:144:LYS:HZ3	1.97	0.60
1:D:23:MET:HE1	1:D:26:TYR:CD2	2.36	0.60
1:B:79:LEU:HB2	1:A:88:ARG:NH1	2.17	0.60
1:C:134:TYR:O	1:C:138:GLN:HB2	2.02	0.60
1:B:88:ARG:HH21	1:A:78:VAL:HA	1.67	0.59
1:D:69:TYR:OH	1:D:73:ARG:NH1	2.36	0.59
1:A:76:ARG:NE	3:A:301:HOH:O	2.36	0.58
1:C:51:PHE:HE1	1:C:144:LYS:HE2	1.68	0.58
1:D:23:MET:HA	1:D:23:MET:CE	2.34	0.57
1:D:20:GLN:OE1	1:D:110:SER:OG	2.22	0.57
1:F:72:CYS:O	1:F:74:GLY:N	2.38	0.56
1:E:112:LEU:CD2	1:E:134:TYR:CE1	2.88	0.56
1:E:143:LYS:HZ2	1:E:144:LYS:NZ	2.04	0.56
1:B:114:LEU:HG	1:B:130:LEU:HD11	1.87	0.56
1:F:23:MET:HG3	1:F:107:VAL:HG22	1.88	0.55
1:B:69:TYR:OH	1:B:73:ARG:NH1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:PRO:HD2	1:E:88:ARG:NH1	2.21	0.54
1:A:16:SER:HB2	1:A:114:LEU:HD13	1.88	0.54
1:A:3:SER:OG	1:A:76:ARG:NH2	2.41	0.54
1:F:131:GLU:HA	1:F:135:CYS:HB3	1.90	0.54
1:F:153:LYS:HA	1:F:157:PRO:HG3	1.89	0.54
1:C:64:GLN:O	1:C:68:LYS:HG3	2.08	0.53
1:E:8:ASN:O	1:E:73:ARG:NH2	2.41	0.53
1:F:64:GLN:O	1:F:68:LYS:HG3	2.07	0.53
1:C:132:ASP:HA	1:C:136:GLU:HG2	1.91	0.53
1:F:108:ASN:O	1:F:112:LEU:HG	2.08	0.52
1:A:114:LEU:HG	1:A:130:LEU:HD11	1.91	0.52
1:D:88:ARG:NE	1:E:79:LEU:H	2.08	0.52
1:A:94:LEU:O	1:A:98:GLN:HG3	2.10	0.51
1:D:23:MET:CE	1:D:26:TYR:CD2	2.93	0.51
1:F:137:GLU:HG3	1:F:140:ASP:HB2	1.93	0.51
1:D:37:TYR:O	1:D:40:ARG:HG3	2.10	0.51
1:B:78:VAL:HG13	1:A:88:ARG:HD3	1.93	0.51
1:C:136:GLU:OE2	1:C:136:GLU:HA	2.10	0.51
1:D:64:GLN:O	1:D:68:LYS:HG3	2.10	0.51
1:E:18:ASN:HA	1:E:21:ILE:HD12	1.92	0.51
1:A:138:GLN:O	1:A:143:LYS:HG2	2.11	0.50
1:E:112:LEU:HD21	1:E:134:TYR:CE2	2.46	0.50
1:D:104:GLU:HG3	1:D:145:ILE:HD12	1.92	0.50
1:F:24:GLU:HB2	1:F:63:ALA:HB2	1.94	0.49
1:B:68:LYS:HG3	1:A:36:TYR:HE2	1.76	0.49
1:D:154:ARG:C	1:D:156:GLY:H	2.15	0.49
1:A:24:GLU:HB2	1:A:63:ALA:HB2	1.93	0.49
1:B:88:ARG:CZ	1:A:79:LEU:H	2.25	0.49
1:F:69:TYR:CE2	1:F:126:LEU:HD13	2.48	0.48
1:A:64:GLN:O	1:A:68:LYS:HG3	2.12	0.48
1:B:118:ALA:HB2	1:B:126:LEU:HD23	1.94	0.48
1:D:133:GLU:HB2	1:D:134:TYR:CD2	2.48	0.48
1:F:20:GLN:O	1:F:24:GLU:HG2	2.14	0.48
1:A:114:LEU:HG	1:A:130:LEU:CD1	2.44	0.47
1:B:17:ILE:HD11	1:B:126:LEU:HD11	1.96	0.47
1:C:138:GLN:OE1	1:C:138:GLN:HA	2.14	0.47
1:B:88:ARG:HH21	1:A:78:VAL:CA	2.27	0.47
1:B:128:LYS:HD3	1:F:131:GLU:HB2	1.96	0.47
1:D:3:SER:HB3	1:D:6:ARG:HB2	1.97	0.47
1:B:88:ARG:NE	1:A:79:LEU:H	2.12	0.47
1:B:40:ARG:NE	3:A:301:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:GLU:HB2	1:C:63:ALA:HB2	1.96	0.46
1:F:12:ASP:HA	1:F:15:ALA:H	1.81	0.46
1:D:88:ARG:CZ	1:D:88:ARG:HB3	2.45	0.46
1:B:24:GLU:HB2	1:B:63:ALA:HB2	1.96	0.46
1:F:114:LEU:HG	1:F:130:LEU:HD11	1.97	0.46
1:B:33:SER:OG	1:B:88:ARG:NH1	2.49	0.46
1:B:33:SER:HB2	1:A:79:LEU:HD12	1.98	0.46
1:B:36:TYR:HE2	1:A:68:LYS:HG2	1.81	0.46
1:C:23:MET:HG3	1:C:107:VAL:HG22	1.98	0.46
1:E:127:THR:O	1:E:131:GLU:HB2	2.17	0.45
1:E:144:LYS:NZ	3:E:301:HOH:O	2.18	0.45
1:D:76:ARG:HD3	1:D:76:ARG:HA	1.70	0.45
1:F:155:CYS:O	1:F:161:GLY:HA3	2.16	0.45
1:C:126:LEU:O	1:C:130:LEU:HG	2.16	0.45
1:D:23:MET:HE2	1:D:26:TYR:HB3	1.99	0.45
1:D:122:ASN:O	1:D:124:PRO:HD3	2.17	0.45
1:E:17:ILE:HD13	1:E:114:LEU:HD21	1.99	0.45
1:D:10:HIS:ND1	1:D:12:ASP:OD1	2.50	0.45
1:B:134:TYR:O	1:B:138:GLN:HB2	2.17	0.45
1:E:123:ASP:O	1:E:127:THR:HG23	2.17	0.45
1:A:132:ASP:O	1:A:136:GLU:HB2	2.18	0.44
1:F:148:MET:CE	1:F:169:LEU:HD11	2.47	0.44
1:B:128:LYS:HB3	1:B:128:LYS:HE2	1.64	0.44
1:E:16:SER:CB	1:E:114:LEU:HD13	2.48	0.44
1:F:160:LEU:HD12	1:F:160:LEU:HA	1.77	0.44
1:F:128:LYS:O	1:F:132:ASP:HB2	2.18	0.44
1:A:112:LEU:HD11	1:A:134:TYR:OH	2.18	0.43
1:E:143:LYS:NZ	1:E:144:LYS:HZ1	2.16	0.43
1:F:63:ALA:O	1:F:67:MET:HG3	2.19	0.43
1:B:5:VAL:HG11	1:F:143:LYS:HA	2.00	0.43
1:B:122:ASN:O	1:B:124:PRO:HD3	2.19	0.43
1:B:169:LEU:HD12	1:B:169:LEU:HA	1.80	0.43
1:E:112:LEU:CD2	1:E:134:TYR:CZ	3.01	0.43
1:E:143:LYS:HZ3	1:E:144:LYS:NZ	2.14	0.43
1:C:154:ARG:C	1:C:156:GLY:H	2.22	0.43
1:A:3:SER:HB3	1:A:5:VAL:H	1.83	0.43
1:D:42:ASP:OD2	1:E:76:ARG:NH2	2.52	0.43
1:D:20:GLN:NE2	1:D:111:LEU:HG	2.34	0.43
1:E:24:GLU:HB2	1:E:63:ALA:HB2	2.00	0.43
1:E:143:LYS:HZ2	1:E:144:LYS:HZ1	1.67	0.43
1:A:122:ASN:O	1:A:124:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LEU:HD23	1:B:130:LEU:HA	1.89	0.42
1:D:33:SER:HB2	1:E:79:LEU:HD12	2.00	0.42
1:B:78:VAL:HA	1:A:88:ARG:HD3	2.02	0.42
1:B:133:GLU:HG2	1:B:134:TYR:CZ	2.55	0.42
1:F:112:LEU:HD21	1:F:138:GLN:OE1	2.19	0.42
1:C:134:TYR:C	1:C:138:GLN:HB2	2.40	0.42
1:E:63:ALA:O	1:E:67:MET:HG3	2.20	0.42
1:F:76:ARG:HD3	1:F:76:ARG:HA	1.88	0.42
1:A:69:TYR:CE2	1:A:126:LEU:HD13	2.55	0.41
1:C:55:SER:O	1:C:59:GLU:HG2	2.20	0.41
1:D:155:CYS:O	1:D:161:GLY:HA3	2.19	0.41
1:A:76:ARG:HA	1:A:76:ARG:HD3	1.84	0.41
1:E:130:LEU:HD23	1:E:130:LEU:HA	1.69	0.41
1:F:108:ASN:CG	1:F:138:GLN:HG3	2.40	0.41
1:B:156:GLY:HA2	1:B:157:PRO:HD3	1.90	0.41
1:D:126:LEU:O	1:D:130:LEU:HG	2.20	0.41
1:A:3:SER:HB2	1:A:6:ARG:HB2	2.03	0.41
1:C:114:LEU:HG	1:C:130:LEU:CD1	2.48	0.41
1:D:24:GLU:HB2	1:D:63:ALA:HB2	2.03	0.41
1:B:20:GLN:NE2	1:B:111:LEU:HG	2.36	0.41
1:B:88:ARG:NH2	1:A:79:LEU:H	2.19	0.41
1:B:88:ARG:NH2	1:A:77:ILE:HG22	2.36	0.41
1:D:16:SER:HB3	1:D:114:LEU:HD13	2.03	0.41
1:F:126:LEU:O	1:F:130:LEU:HG	2.21	0.41
1:D:88:ARG:HE	1:E:79:LEU:H	1.69	0.41
1:B:86:SER:HB3	1:E:78:VAL:HG11	2.03	0.40
1:D:17:ILE:HD11	1:D:126:LEU:HD11	2.03	0.40
1:D:23:MET:CE	1:D:26:TYR:HB3	2.51	0.40
1:B:69:TYR:CD1	1:B:129:LEU:HD22	2.56	0.40
1:C:108:ASN:HB3	1:C:134:TYR:CE2	2.56	0.40
1:D:23:MET:CE	1:D:26:TYR:HD2	2.35	0.40
1:C:112:LEU:HA	1:C:112:LEU:HD23	1.84	0.40
1:D:88:ARG:NH1	1:E:77:ILE:HG22	2.37	0.40
1:F:115:HIS:CE1	1:F:127:THR:HB	2.57	0.40

All (8) 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:D:72:CYS:SG	1:E:139:CYS:SG[4_655]	1.21	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:CYS:SG	1:F:125:CYS:CB[3_555]	1.28	0.92
1:B:135:CYS:SG	1:A:125:CYS:CB[4_555]	1.36	0.84
1:D:125:CYS:SG	1:E:135:CYS:SG[4_655]	1.43	0.77
1:B:135:CYS:CB	1:A:125:CYS:SG[4_555]	1.70	0.50
1:A:143:LYS:NZ	1:F:72:CYS:O[3_555]	1.85	0.35
1:A:135:CYS:CB	1:F:125:CYS:SG[3_555]	1.90	0.30
1:C:88:ARG:NH2	1:F:79:LEU:O[8_544]	1.90	0.30

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	168/170 (99%)	162 (96%)	6 (4%)	0	100	100
1	B	168/170 (99%)	164 (98%)	3 (2%)	1 (1%)	22	39
1	C	167/170 (98%)	160 (96%)	6 (4%)	1 (1%)	22	39
1	D	168/170 (99%)	160 (95%)	8 (5%)	0	100	100
1	E	168/170 (99%)	163 (97%)	5 (3%)	0	100	100
1	F	161/170 (95%)	154 (96%)	6 (4%)	1 (1%)	22	39
All	All	1000/1020 (98%)	963 (96%)	34 (3%)	3 (0%)	37	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	73	ARG
1	C	136	GLU
1	B	123	ASP

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	148/148 (100%)	145 (98%)	3 (2%)	50	75
1	B	148/148 (100%)	144 (97%)	4 (3%)	40	67
1	C	148/148 (100%)	144 (97%)	4 (3%)	40	67
1	D	148/148 (100%)	144 (97%)	4 (3%)	40	67
1	E	148/148 (100%)	140 (95%)	8 (5%)	18	37
1	F	142/148 (96%)	139 (98%)	3 (2%)	48	74
All	All	882/888 (99%)	856 (97%)	26 (3%)	36	64

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

Mol	Chain	Res	Type
1	B	3	SER
1	B	29	TYR
1	B	139	CYS
1	B	164	MET
1	A	3	SER
1	A	72	CYS
1	A	116	SER
1	C	72	CYS
1	C	80	GLN
1	C	138	GLN
1	C	140	ASP
1	D	29	TYR
1	D	110	SER
1	D	138	GLN
1	D	139	CYS
1	E	3	SER
1	E	29	TYR
1	E	76	ARG
1	E	119	SER
1	E	128	LYS
1	E	136	GLU
1	E	140	ASP

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Mol	Chain	Res	Type
1	E	144	LYS
1	F	116	SER
1	F	128	LYS
1	F	135	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	108	ASN
1	E	108	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	169/170 (99%)	-0.20	4 (2%) 59 56	32, 48, 82, 96	1 (0%)
1	B	169/170 (99%)	-0.13	4 (2%) 59 56	33, 47, 81, 104	1 (0%)
1	C	168/170 (98%)	-0.14	3 (1%) 67 64	34, 50, 81, 108	1 (0%)
1	D	169/170 (99%)	-0.11	8 (4%) 37 34	31, 48, 86, 99	1 (0%)
1	E	169/170 (99%)	-0.15	5 (2%) 52 49	32, 48, 85, 102	1 (0%)
1	F	162/170 (95%)	-0.07	7 (4%) 40 37	34, 50, 88, 103	1 (0%)
All	All	1006/1020 (98%)	-0.13	31 (3%) 51 48	31, 49, 85, 108	6 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	5	VAL	3.9
1	C	139	CYS	3.5
1	A	5	VAL	3.5
1	C	134	TYR	3.3
1	D	2	ALA	3.2
1	D	134	TYR	3.2
1	F	112	LEU	3.1
1	E	5	VAL	3.1
1	C	137	GLU	3.1
1	D	3	SER	3.0
1	B	134	TYR	2.9
1	D	137	GLU	2.9
1	F	138	GLN	2.9
1	B	164	MET	2.8
1	E	137	GLU	2.8
1	E	7	GLN	2.8
1	F	134	TYR	2.7
1	F	136	GLU	2.6
1	B	5	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	139	CYS	2.6
1	E	2	ALA	2.6
1	B	137	GLU	2.5
1	F	156	GLY	2.5
1	A	164	MET	2.5
1	A	2	ALA	2.4
1	D	8	ASN	2.3
1	F	9	TYR	2.3
1	D	4	GLN	2.3
1	D	7	GLN	2.1
1	A	134	TYR	2.1
1	F	130	LEU	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	FE	C	201	1/1	0.68	0.18	113,113,113,113	0
2	FE	D	202	1/1	0.80	0.16	114,114,114,114	0
2	FE	D	201	1/1	0.85	0.13	107,107,107,107	0
2	FE	A	201	1/1	0.88	0.09	105,105,105,105	0
2	FE	F	202	1/1	0.89	0.09	113,113,113,113	0
2	FE	F	201	1/1	0.91	0.10	113,113,113,113	0
2	FE	B	201	1/1	0.92	0.12	102,102,102,102	0
2	FE	E	202	1/1	0.93	0.12	106,106,106,106	0
2	FE	B	202	1/1	0.94	0.09	110,110,110,110	0
2	FE	E	201	1/1	0.96	0.06	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.