Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 01:15 pm GMT

PDB ID	:	8PP4
Title	:	Binary crystal structure of positively supercharged ferritin variant Ftn(pos) and reduced charge negatively supercharged ferritin variant Ftn(neg)-m3 (Mg formate condition)
Authors	:	Lang, L.; Beck, T.
Deposited on	:	2023-07-06
Resolution	:	2.00 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:

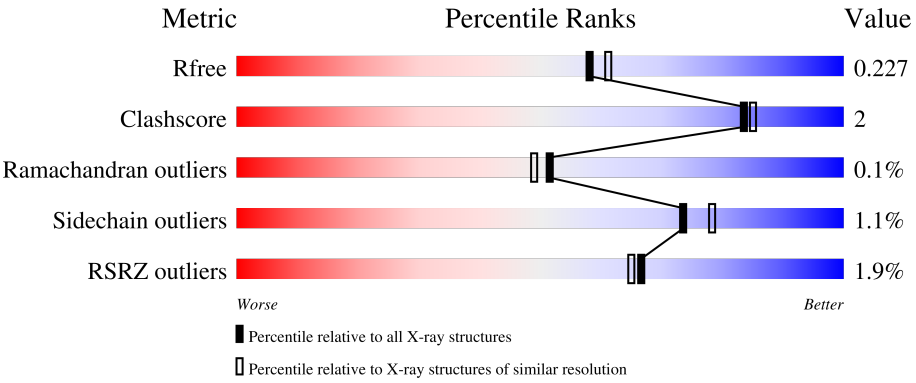
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	183	2% 86% 7% · 6%
1	B	183	2% 91% · 6%
1	C	183	2% 90% · 6%
1	D	183	% 90% · 6%
1	E	183	2% 88% 6% 6%

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Mol	Chain	Length	Quality of chain
1	F	183	2% 89% 5% 6%
2	G	182	2% 88% 7% 5%
2	H	182	3% 90% 5%
2	I	182	2% 88% 7% 5%
2	J	182	3% 89% 5% 5%
2	K	182	2% 89% 6% 5%
2	L	182	2% 87% 7% 5%

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
3	FE	C	202	-	-	-	X
4	MG	H	203	-	-	-	X
4	MG	J	202	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 35183 atoms, of which 16971 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	172	Total	C	H	N	O	S	42	3	0
			2919	919	1459	265	271	5			
1	B	172	Total	C	H	N	O	S	42	0	0
			2861	903	1429	258	266	5			
1	C	172	Total	C	H	N	O	S	42	3	0
			2905	917	1452	260	271	5			
1	D	172	Total	C	H	N	O	S	42	3	0
			2914	918	1459	263	269	5			
1	E	172	Total	C	H	N	O	S	42	3	0
			2918	919	1460	264	270	5			
1	F	172	Total	C	H	N	O	S	42	0	0
			2861	903	1429	258	266	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	LYS	ALA	engineered mutation	UNP P02794
A	25	ARG	ASN	engineered mutation	UNP P02794
A	86	GLN	LYS	engineered mutation	UNP P02794
A	90	LYS	CYS	engineered mutation	UNP P02794
A	98	ARG	ASN	engineered mutation	UNP P02794
A	102	LYS	CYS	engineered mutation	UNP P02794
A	105	LYS	HIS	engineered mutation	UNP P02794
A	109	LYS	ASN	engineered mutation	UNP P02794
A	123	LYS	ASP	engineered mutation	UNP P02794
A	162	ARG	GLU	engineered mutation	UNP P02794
B	18	LYS	ALA	engineered mutation	UNP P02794
B	25	ARG	ASN	engineered mutation	UNP P02794
B	86	GLN	LYS	engineered mutation	UNP P02794
B	90	LYS	CYS	engineered mutation	UNP P02794
B	98	ARG	ASN	engineered mutation	UNP P02794
B	102	LYS	CYS	engineered mutation	UNP P02794
B	105	LYS	HIS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
B	109	LYS	ASN	engineered mutation	UNP P02794
B	123	LYS	ASP	engineered mutation	UNP P02794
B	162	ARG	GLU	engineered mutation	UNP P02794
C	18	LYS	ALA	engineered mutation	UNP P02794
C	25	ARG	ASN	engineered mutation	UNP P02794
C	86	GLN	LYS	engineered mutation	UNP P02794
C	90	LYS	CYS	engineered mutation	UNP P02794
C	98	ARG	ASN	engineered mutation	UNP P02794
C	102	LYS	CYS	engineered mutation	UNP P02794
C	105	LYS	HIS	engineered mutation	UNP P02794
C	109	LYS	ASN	engineered mutation	UNP P02794
C	123	LYS	ASP	engineered mutation	UNP P02794
C	162	ARG	GLU	engineered mutation	UNP P02794
D	18	LYS	ALA	engineered mutation	UNP P02794
D	25	ARG	ASN	engineered mutation	UNP P02794
D	86	GLN	LYS	engineered mutation	UNP P02794
D	90	LYS	CYS	engineered mutation	UNP P02794
D	98	ARG	ASN	engineered mutation	UNP P02794
D	102	LYS	CYS	engineered mutation	UNP P02794
D	105	LYS	HIS	engineered mutation	UNP P02794
D	109	LYS	ASN	engineered mutation	UNP P02794
D	123	LYS	ASP	engineered mutation	UNP P02794
D	162	ARG	GLU	engineered mutation	UNP P02794
E	18	LYS	ALA	engineered mutation	UNP P02794
E	25	ARG	ASN	engineered mutation	UNP P02794
E	86	GLN	LYS	engineered mutation	UNP P02794
E	90	LYS	CYS	engineered mutation	UNP P02794
E	98	ARG	ASN	engineered mutation	UNP P02794
E	102	LYS	CYS	engineered mutation	UNP P02794
E	105	LYS	HIS	engineered mutation	UNP P02794
E	109	LYS	ASN	engineered mutation	UNP P02794
E	123	LYS	ASP	engineered mutation	UNP P02794
E	162	ARG	GLU	engineered mutation	UNP P02794
F	18	LYS	ALA	engineered mutation	UNP P02794
F	25	ARG	ASN	engineered mutation	UNP P02794
F	86	GLN	LYS	engineered mutation	UNP P02794
F	90	LYS	CYS	engineered mutation	UNP P02794
F	98	ARG	ASN	engineered mutation	UNP P02794
F	102	LYS	CYS	engineered mutation	UNP P02794
F	105	LYS	HIS	engineered mutation	UNP P02794
F	109	LYS	ASN	engineered mutation	UNP P02794
F	123	LYS	ASP	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
F	162	ARG	GLU	engineered mutation	UNP P02794

- Molecule 2 is a protein called Ferritin heavy chain, N-terminally processed.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	173	Total	C	H	N	O	S	48	5	0
			2859	913	1401	254	281	10			
2	H	172	Total	C	H	N	O	S	48	2	0
			2799	892	1373	249	276	9			
2	I	172	Total	C	H	N	O	S	47	2	0
			2810	895	1381	250	276	8			
2	J	172	Total	C	H	N	O	S	47	2	0
			2803	894	1374	249	278	8			
2	K	173	Total	C	H	N	O	S	46	2	0
			2825	900	1386	252	280	7			
2	L	172	Total	C	H	N	O	S	47	1	0
			2788	889	1368	248	275	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	18	GLU	ALA	engineered mutation	UNP P02794
G	86	GLN	LYS	engineered mutation	UNP P02794
H	18	GLU	ALA	engineered mutation	UNP P02794
H	86	GLN	LYS	engineered mutation	UNP P02794
I	18	GLU	ALA	engineered mutation	UNP P02794
I	86	GLN	LYS	engineered mutation	UNP P02794
J	18	GLU	ALA	engineered mutation	UNP P02794
J	86	GLN	LYS	engineered mutation	UNP P02794
K	18	GLU	ALA	engineered mutation	UNP P02794
K	86	GLN	LYS	engineered mutation	UNP P02794
L	18	GLU	ALA	engineered mutation	UNP P02794
L	86	GLN	LYS	engineered mutation	UNP P02794

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total Fe 2 2	0	0
3	D	1	Total Fe 1 1	0	0
3	E	1	Total Fe 1 1	0	0
3	F	1	Total Fe 1 1	0	0
3	G	1	Total Fe 1 1	0	0
3	H	1	Total Fe 1 1	0	0
3	I	1	Total Fe 1 1	0	0
3	J	1	Total Fe 1 1	0	0
3	K	1	Total Fe 1 1	0	0
3	L	2	Total Fe 2 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	D	2	Total Mg 2 2	0	0
4	H	2	Total Mg 2 2	0	0
4	I	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total Cl 1 1	0	0

- Molecule 6 is water.

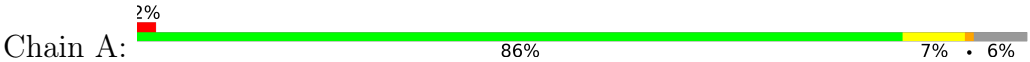
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	103	Total O 103 103	0	0
6	B	116	Total O 116 116	0	0
6	C	105	Total O 106 106	0	1
6	D	106	Total O 106 106	0	0
6	E	94	Total O 94 94	0	0
6	F	92	Total O 92 92	0	0
6	G	58	Total O 58 58	0	0
6	H	47	Total O 47 47	0	0
6	I	52	Total O 52 52	0	0
6	J	50	Total O 50 50	0	0
6	K	42	Total O 42 42	0	0
6	L	31	Total O 31 31	0	0

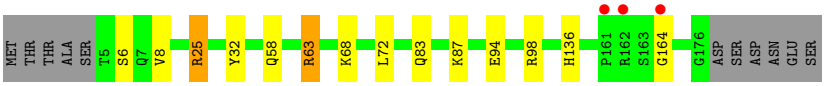
3 Residue-property plots (i)

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 heavy chain

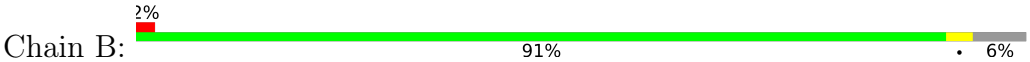
Chain A:

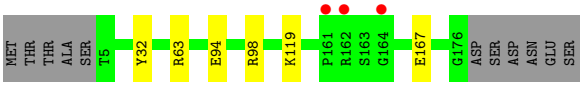




• Molecule 1: Ferritin heavy chain

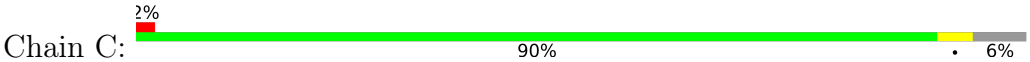
Chain B:





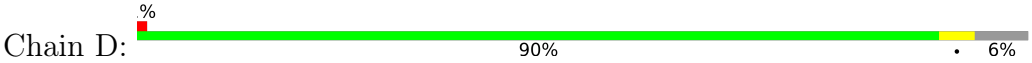
• Molecule 1: Ferritin heavy chain

Chain C:



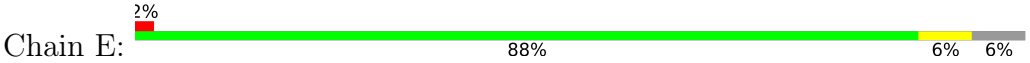
• Molecule 1: Ferritin heavy chain

Chain D:



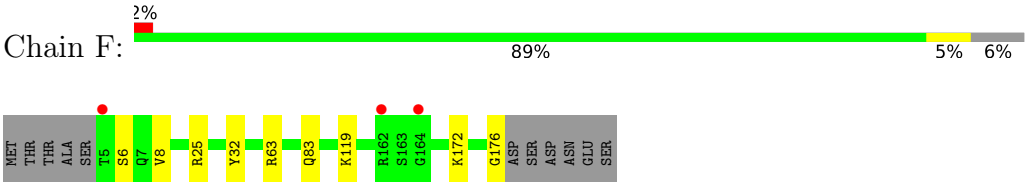
• Molecule 1: Ferritin heavy chain

Chain E:



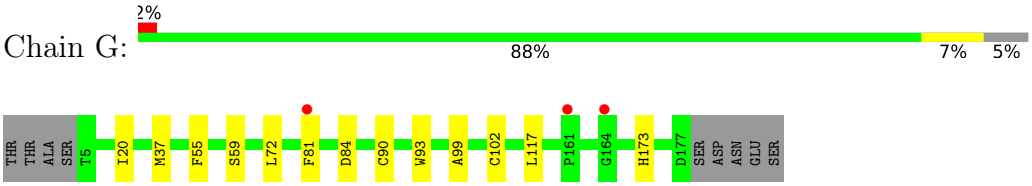
• Molecule 1: Ferritin heavy chain

Chain F:



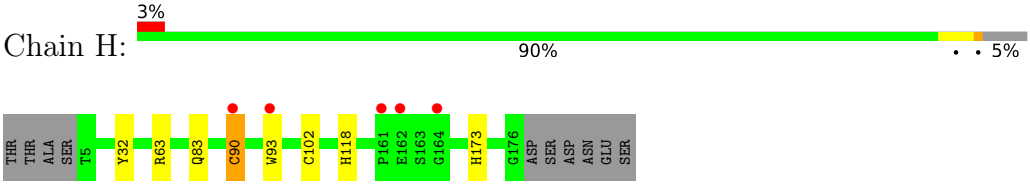
• Molecule 2: Ferritin heavy chain, N-terminally processed

Chain G:



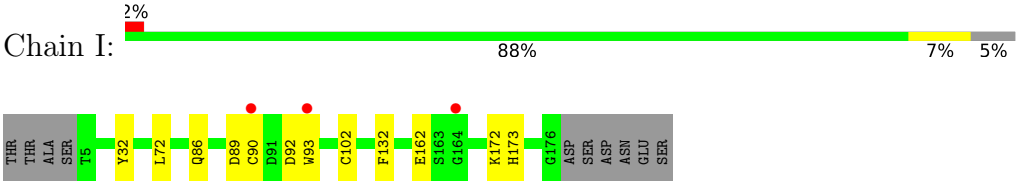
• Molecule 2: Ferritin heavy chain, N-terminally processed

Chain H:



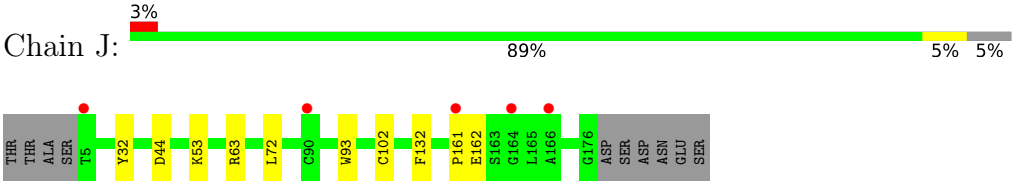
• Molecule 2: Ferritin heavy chain, N-terminally processed

Chain I:



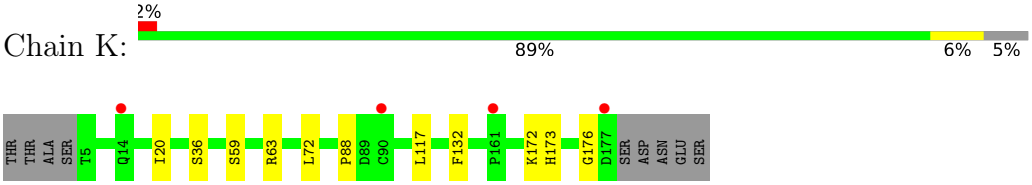
• Molecule 2: Ferritin heavy chain, N-terminally processed

Chain J:



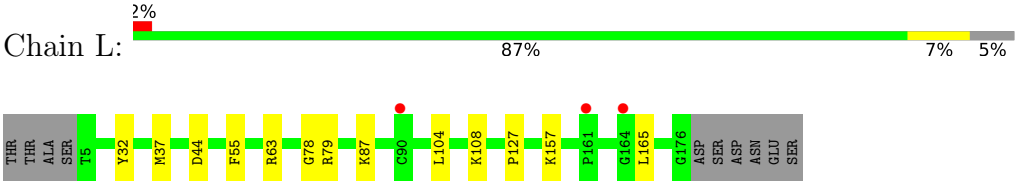
• Molecule 2: Ferritin heavy chain, N-terminally processed

Chain K:



• Molecule 2: Ferritin heavy chain, N-terminally processed

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	127.04Å 127.04Å 176.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 2.00 49.31 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.36-2.00) 99.7 (49.31-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.181 , 0.221 0.189 , 0.227	Depositor DCC
R_{free} test set	9421 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	35183	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.76	1/1488 (0.1%)	0.88	4/1993 (0.2%)
1	B	0.78	0/1460	0.80	0/1957
1	C	0.75	0/1487	0.85	2/1992 (0.1%)
1	D	0.77	1/1489 (0.1%)	0.80	0/1994
1	E	0.74	0/1489	0.84	1/1994 (0.1%)
1	F	0.75	0/1460	0.86	1/1957 (0.1%)
2	G	0.73	0/1491	0.82	0/2008
2	H	0.76	0/1458	0.80	1/1964 (0.1%)
2	I	0.74	0/1461	0.81	0/1967
2	J	0.75	0/1461	0.82	0/1968
2	K	0.73	0/1471	0.80	0/1981
2	L	0.74	0/1452	0.81	0/1956
All	All	0.75	2/17667 (0.0%)	0.83	9/23731 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	147	GLU	CD-OE2	-7.28	1.17	1.25
1	A	164	GLY	C-O	5.13	1.31	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	A	25	ARG	NE-CZ-NH1	-7.50	116.55	120.30
2	H	63	ARG	CG-CD-NE	7.29	127.10	111.80
1	C	98	ARG	CG-CD-NE	-6.98	97.15	111.80
1	A	63[A]	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	63[B]	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	F	176	GLY	CA-C-O	-5.69	110.35	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	176	GLY	CA-C-O	-5.60	110.53	120.60
1	C	98	ARG	NE-CZ-NH2	-5.57	117.51	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1460	1459	1446	10	0
1	B	1432	1429	1419	4	0
1	C	1453	1452	1443	8	0
1	D	1455	1459	1450	4	0
1	E	1458	1460	1449	5	3
1	F	1432	1429	1419	4	3
2	G	1458	1401	1385	19	0
2	H	1426	1373	1362	7	0
2	I	1429	1381	1370	7	1
2	J	1429	1374	1363	6	0
2	K	1439	1386	1375	10	0
2	L	1420	1368	1358	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	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
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	2	0	0	1	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
4	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	C	1	0	0	1	0
5	G	1	0	0	1	0
5	L	1	0	0	1	0
6	A	103	0	0	1	3
6	B	116	0	0	1	1
6	C	106	0	0	3	2
6	D	106	0	0	1	1
6	E	94	0	0	1	0
6	F	92	0	0	1	0
6	G	58	0	0	4	0
6	H	47	0	0	0	0
6	I	52	0	0	2	0
6	J	50	0	0	0	0
6	K	42	0	0	1	0
6	L	31	0	0	0	0
All	All	18212	16971	16839	83	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 2.

All (83) 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)
5:C:203:CL:CL	6:C:317:HOH:O	2.13	1.03
1:A:63[B]:ARG:NH2	1:C:63:ARG:HD3	1.88	0.89
3:L:202:FE:FE	5:L:203:CL:CL	1.66	0.84
2:I:89:ASP:O	6:I:301:HOH:O	1.96	0.82
1:A:63[B]:ARG:HH21	1:C:63:ARG:HD3	1.48	0.77
2:H:93:TRP:HZ3	2:H:102[B]:CYS:HG	1.37	0.72
2:G:90[B]:CYS:SG	2:G:93:TRP:CE3	2.84	0.71
2:K:63:ARG:NH1	2:L:63:ARG:HD3	2.09	0.68
6:G:311:HOH:O	2:H:173:HIS:CE1	2.48	0.66
1:B:94:GLU:OE1	1:B:98:ARG:NH1	2.29	0.65
1:A:25:ARG:HD3	1:A:83:GLN:HB2	1.79	0.64
2:J:93:TRP:HZ3	2:J:102[A]:CYS:HG	1.45	0.62
1:C:25:ARG:NH2	2:G:84:ASP:OD2	2.31	0.62
2:G:90[B]:CYS:SG	2:G:93:TRP:CD2	2.92	0.62
2:G:93:TRP:HZ3	2:G:102[B]:CYS:HG	1.46	0.61
2:I:93:TRP:HZ3	2:I:102[B]:CYS:SG	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:93:TRP:HZ3	2:H:102[B]:CYS:SG	2.24	0.60
2:K:63:ARG:NH1	2:L:63:ARG:CD	2.64	0.60
1:A:94:GLU:OE1	1:A:98:ARG:NH1	2.36	0.58
2:I:172[B]:LYS:HG3	2:K:173:HIS:HB3	1.85	0.58
2:G:20:ILE:HD13	2:G:117:LEU:HD21	1.87	0.57
2:G:173:HIS:CE1	6:G:311:HOH:O	2.57	0.57
2:I:93:TRP:CZ3	2:I:102[B]:CYS:SG	2.97	0.57
2:G:90[B]:CYS:SG	2:G:93:TRP:CZ3	3.00	0.55
5:G:202:CL:CL	6:G:311:HOH:O	2.55	0.55
1:A:72:LEU:C	1:A:72:LEU:HD13	2.28	0.54
1:E:72:LEU:HD22	1:E:132:PHE:CE2	2.43	0.54
1:F:25:ARG:HD3	1:F:83:GLN:HB2	1.89	0.54
2:G:93:TRP:HZ3	2:G:102[B]:CYS:SG	2.30	0.53
2:K:172[A]:LYS:HE2	6:K:313:HOH:O	2.07	0.53
2:G:37[A]:MET:HE3	2:G:99:ALA:HB1	1.91	0.53
2:J:72:LEU:HD22	2:J:132:PHE:CE1	2.44	0.53
2:G:72:LEU:C	2:G:72:LEU:HD13	2.30	0.52
2:K:59:SER:OG	2:L:63:ARG:NH2	2.42	0.52
1:A:87:LYS:HE2	2:G:81[B]:PHE:CZ	2.44	0.52
2:G:93:TRP:CZ3	2:G:102[B]:CYS:SG	3.00	0.51
1:A:68:LYS:HE2	1:A:136:HIS:CG	2.46	0.51
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.45	0.51
1:B:63:ARG:NH2	1:D:59:SER:OG	2.44	0.50
1:A:6:SER:OG	1:A:8:VAL:HG22	2.11	0.49
1:A:58:GLN:OE1	6:A:301:HOH:O	2.20	0.49
2:H:118:HIS:CE1	2:L:127:PRO:HB3	2.48	0.48
1:B:167:GLU:OE1	6:B:301:HOH:O	2.19	0.48
1:E:172[A]:LYS:HE2	6:E:321:HOH:O	2.13	0.48
2:L:37:MET:HE3	2:L:55:PHE:CD1	2.48	0.48
2:H:90[B]:CYS:SG	2:H:93:TRP:CD2	3.06	0.48
2:J:93:TRP:HZ3	2:J:102[A]:CYS:SG	2.36	0.47
2:H:90[B]:CYS:SG	2:H:93:TRP:CE3	3.07	0.47
2:J:161:PRO:HD2	2:J:162:GLU:OE1	2.15	0.47
2:G:37[B]:MET:HE2	2:G:102[B]:CYS:HB3	1.97	0.46
1:C:153:THR:O	1:C:157:LYS:HG2	2.15	0.46
2:G:37[A]:MET:HE1	2:G:55:PHE:CE1	2.50	0.46
1:D:72:LEU:C	1:D:72:LEU:HD13	2.36	0.46
2:G:37[A]:MET:CE	2:G:99:ALA:HB1	2.46	0.45
1:D:87:LYS:NZ	6:D:305:HOH:O	2.49	0.45
2:K:63:ARG:HH12	2:L:63:ARG:HD3	1.82	0.45
1:E:160:ALA:HB1	1:E:161:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:20:ILE:HD13	2:K:117:LEU:HD21	2.00	0.44
2:K:72:LEU:HD22	2:K:132:PHE:CE1	2.53	0.44
1:C:5:THR:N	6:C:308:HOH:O	2.51	0.44
1:F:119:LYS:HE3	1:F:119:LYS:HB2	1.85	0.44
2:H:93:TRP:CZ3	2:H:102[B]:CYS:SG	3.05	0.44
2:J:72:LEU:HD22	2:J:132:PHE:CD1	2.53	0.43
1:B:63:ARG:HD3	1:D:63[A]:ARG:NH1	2.33	0.43
1:C:134:GLU:OE1	6:C:301:HOH:O	2.21	0.43
1:A:63[B]:ARG:HH21	1:C:63:ARG:CD	2.24	0.43
2:L:165:LEU:HA	2:L:165:LEU:HD12	1.85	0.43
6:G:311:HOH:O	2:I:173:HIS:CE1	2.72	0.43
1:F:172:LYS:HE2	6:F:315:HOH:O	2.19	0.42
2:G:59:SER:OG	2:J:63:ARG:NH2	2.50	0.42
1:C:79:ARG:HD3	1:C:79:ARG:HA	1.90	0.42
2:I:72:LEU:HD22	2:I:132:PHE:CE1	2.55	0.42
2:K:63:ARG:NH1	2:L:63:ARG:HD2	2.34	0.42
2:L:37:MET:CE	2:L:55:PHE:CD1	3.03	0.42
1:E:20:ILE:HD13	1:E:117:LEU:HD21	2.01	0.41
2:L:78:GLY:O	2:L:79:ARG:NH1	2.53	0.41
2:K:36:SER:HB2	2:K:88:PRO:HG2	2.03	0.41
2:G:37[A]:MET:CE	2:G:55:PHE:CE1	3.04	0.41
2:G:37[A]:MET:CE	2:G:55:PHE:CZ	3.04	0.41
2:G:37[A]:MET:HE2	2:G:55:PHE:CZ	2.56	0.41
2:I:172[A]:LYS:HE2	6:I:316:HOH:O	2.20	0.41
2:L:104:LEU:O	2:L:108:LYS:HG3	2.20	0.40
1:F:6:SER:OG	1:F:8:VAL:HG22	2.21	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)
6:D:305:HOH:O	6:D:305:HOH:O[2_765]	1.89	0.31
1:E:63[A]:ARG:HH21	1:F:63:ARG:HG2[4_575]	1.29	0.31
6:A:329:HOH:O	6:B:303:HOH:O[4_575]	1.91	0.29
2:I:86:GLN:OE1	2:I:86:GLN:OE1[2_765]	1.92	0.28
1:E:59:SER:HG	1:F:63:ARG:HH22[4_575]	1.34	0.26
6:A:329:HOH:O	6:C:326:HOH:O[4_575]	1.95	0.25
6:A:329:HOH:O	6:C:302:HOH:O[4_575]	2.09	0.11
1:E:59:SER:OG	1:F:63:ARG:HH22[4_575]	1.57	0.03

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	173/183 (94%)	169 (98%)	4 (2%)	0	100	100
1	B	170/183 (93%)	166 (98%)	4 (2%)	0	100	100
1	C	173/183 (94%)	171 (99%)	2 (1%)	0	100	100
1	D	173/183 (94%)	168 (97%)	4 (2%)	1 (1%)	25	19
1	E	173/183 (94%)	168 (97%)	5 (3%)	0	100	100
1	F	170/183 (93%)	169 (99%)	1 (1%)	0	100	100
2	G	176/182 (97%)	171 (97%)	5 (3%)	0	100	100
2	H	172/182 (94%)	169 (98%)	3 (2%)	0	100	100
2	I	172/182 (94%)	168 (98%)	4 (2%)	0	100	100
2	J	172/182 (94%)	170 (99%)	2 (1%)	0	100	100
2	K	173/182 (95%)	169 (98%)	3 (2%)	1 (1%)	25	19
2	L	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
All	All	2068/2190 (94%)	2025 (98%)	41 (2%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	162	ARG
2	K	176	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	157/164 (96%)	156 (99%)	1 (1%)	86 90
1	B	154/164 (94%)	152 (99%)	2 (1%)	69 74
1	C	157/164 (96%)	157 (100%)	0	100 100
1	D	157/164 (96%)	156 (99%)	1 (1%)	86 90
1	E	157/164 (96%)	156 (99%)	1 (1%)	86 90
1	F	154/164 (94%)	153 (99%)	1 (1%)	86 90
2	G	159/163 (98%)	159 (100%)	0	100 100
2	H	156/163 (96%)	152 (97%)	4 (3%)	46 48
2	I	156/163 (96%)	152 (97%)	4 (3%)	46 48
2	J	156/163 (96%)	153 (98%)	3 (2%)	57 61
2	K	157/163 (96%)	157 (100%)	0	100 100
2	L	155/163 (95%)	151 (97%)	4 (3%)	46 48
All	All	1875/1962 (96%)	1854 (99%)	21 (1%)	73 78

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	B	32	TYR
1	B	119	LYS
1	D	163	SER
1	E	32	TYR
1	F	32	TYR
2	H	32	TYR
2	H	83	GLN
2	H	90[A]	CYS
2	H	90[B]	CYS
2	I	32	TYR
2	I	90	CYS
2	I	92	ASP
2	I	162	GLU
2	J	32	TYR
2	J	44	ASP
2	J	53	LYS
2	L	32	TYR
2	L	44	ASP
2	L	87	LYS
2	L	157	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	58	GLN
2	G	14	GLN
2	I	25	ASN
2	L	141	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 24 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

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	172/183 (93%)	-0.02	3 (1%)	70	68	24, 28, 45, 95	0
1	B	172/183 (93%)	0.01	3 (1%)	70	68	24, 28, 45, 94	0
1	C	172/183 (93%)	0.06	3 (1%)	70	68	25, 28, 46, 94	0
1	D	172/183 (93%)	-0.04	2 (1%)	79	78	24, 29, 46, 86	0
1	E	172/183 (93%)	0.08	3 (1%)	70	68	23, 31, 49, 90	0
1	F	172/183 (93%)	-0.01	3 (1%)	70	68	27, 32, 51, 96	0
2	G	173/182 (95%)	0.14	3 (1%)	70	68	30, 36, 55, 72	0
2	H	172/182 (94%)	0.15	5 (2%)	51	50	31, 37, 55, 69	0
2	I	172/182 (94%)	0.07	3 (1%)	70	68	30, 36, 54, 77	0
2	J	172/182 (94%)	0.14	5 (2%)	51	50	31, 37, 57, 85	0
2	K	173/182 (95%)	0.20	4 (2%)	60	59	29, 39, 56, 81	0
2	L	172/182 (94%)	0.17	3 (1%)	70	68	31, 40, 62, 91	0
All	All	2066/2190 (94%)	0.08	40 (1%)	66	65	23, 35, 53, 96	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	GLY	5.3
1	B	162	ARG	5.2
1	B	161	PRO	5.0
1	B	164	GLY	4.8
1	C	164	GLY	4.7
1	A	162	ARG	4.6
1	E	162	ARG	4.4
1	C	162	ARG	3.9
1	F	164	GLY	3.8
1	D	161	PRO	3.7
1	F	162	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	161	PRO	3.4
2	G	81[A]	PHE	3.1
1	E	164	GLY	3.1
2	J	164	GLY	3.1
2	L	164	GLY	3.0
2	K	90	CYS	3.0
2	I	164	GLY	2.8
2	G	164	GLY	2.8
2	I	90	CYS	2.8
1	A	161	PRO	2.7
2	J	161	PRO	2.7
2	H	93	TRP	2.7
2	H	164	GLY	2.6
2	H	162	GLU	2.6
1	F	5	THR	2.5
2	J	90	CYS	2.5
1	E	161	PRO	2.5
2	K	177	ASP	2.4
1	C	161	PRO	2.4
2	H	90[A]	CYS	2.4
2	L	161	PRO	2.3
2	K	161	PRO	2.3
2	K	14	GLN	2.2
1	D	162	ARG	2.2
2	L	90	CYS	2.1
2	I	93	TRP	2.1
2	G	161	PRO	2.1
2	J	166	ALA	2.1
2	J	5	THR	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, 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	B-factors(Å^2)	Q<0.9
3	FE	C	202	1/1	0.61	0.72	432,432,432,432	0
4	MG	H	203	1/1	0.71	0.47	64,64,64,64	0
4	MG	J	202	1/1	0.77	0.44	64,64,64,64	0
5	CL	L	203	1/1	0.83	0.09	44,44,44,44	1
4	MG	D	203	1/1	0.92	0.15	73,73,73,73	0
3	FE	L	202	1/1	0.95	0.10	123,123,123,123	1
4	MG	H	202	1/1	0.96	0.07	40,40,40,40	0
4	MG	I	202	1/1	0.97	0.09	36,36,36,36	0
3	FE	B	201	1/1	0.98	0.09	34,34,34,34	0
4	MG	B	202	1/1	0.98	0.12	32,32,32,32	0
3	FE	H	201	1/1	0.98	0.06	46,46,46,46	0
3	FE	L	201	1/1	0.98	0.09	52,52,52,52	0
3	FE	E	201	1/1	0.99	0.10	36,36,36,36	0
3	FE	F	201	1/1	0.99	0.09	37,37,37,37	0
4	MG	D	202	1/1	0.99	0.08	32,32,32,32	0
3	FE	G	201	1/1	0.99	0.06	44,44,44,44	0
3	FE	A	201	1/1	0.99	0.08	34,34,34,34	0
3	FE	I	201	1/1	0.99	0.06	45,45,45,45	0
3	FE	J	201	1/1	0.99	0.09	49,49,49,49	0
3	FE	K	201	1/1	0.99	0.07	49,49,49,49	0
5	CL	G	202	1/1	0.99	0.08	33,33,33,33	0
3	FE	D	201	1/1	0.99	0.08	35,35,35,35	0
3	FE	C	201	1/1	1.00	0.10	34,34,34,34	0
5	CL	C	203	1/1	1.00	0.09	29,29,29,29	1

6.5 Other polymers (i)

There are no such residues in this entry.