Full wwPDB X-ray Structure Validation Report (i)

May 18, 2022 – 01:21 pm BST

PDB ID	:	5JKK
Title	:	Crystal structure of the negatively supercharged variant Ftn(neg) of human heavy chain ferritin
Authors	:	Kuenzle, M.; Beck, T.
Deposited on	:	2016-04-26
Resolution	:	1.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

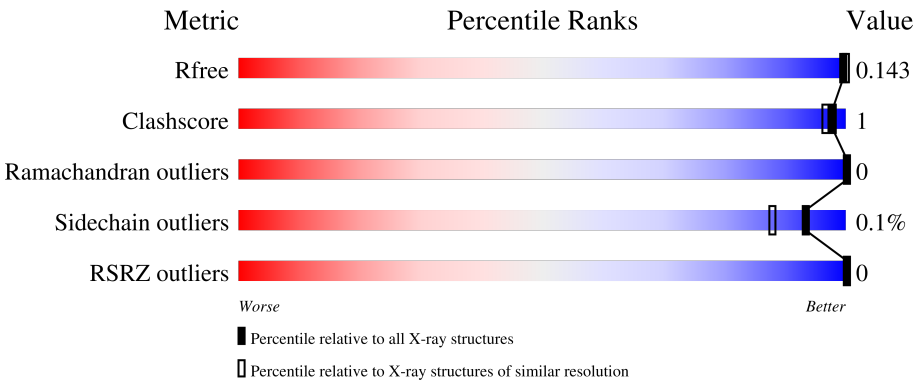
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	85% 8% • 6%
1	B	183	84% 9% • 6%
1	C	183	83% 11% 6%
1	D	183	85% 9% 6%
1	E	183	87% 7% 6%

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Mol	Chain	Length	Quality of chain
1	F	183	86% 8% • 6%
1	G	183	84% 10% • 6%
1	H	183	80% 14% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13086 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
			Total	C	N	O	S			
1	A	172	1422	890	246	281	5	0	0	0
1	B	172	1422	890	246	281	5	0	0	0
1	C	172	1422	890	246	281	5	0	0	0
1	D	172	1422	890	246	281	5	0	0	0
1	E	172	1422	890	246	281	5	0	0	0
1	F	172	1422	890	246	281	5	0	0	0
1	G	172	1422	890	246	281	5	0	0	0
1	H	172	1422	890	246	281	5	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLU	ALA	engineered mutation	UNP P02794
A	86	GLN	LYS	engineered mutation	UNP P02794
A	90	GLU	CYS	engineered mutation	UNP P02794
A	102	GLU	CYS	engineered mutation	UNP P02794
A	105	GLU	HIS	engineered mutation	UNP P02794
B	18	GLU	ALA	engineered mutation	UNP P02794
B	86	GLN	LYS	engineered mutation	UNP P02794
B	90	GLU	CYS	engineered mutation	UNP P02794
B	102	GLU	CYS	engineered mutation	UNP P02794
B	105	GLU	HIS	engineered mutation	UNP P02794
C	18	GLU	ALA	engineered mutation	UNP P02794
C	86	GLN	LYS	engineered mutation	UNP P02794
C	90	GLU	CYS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
C	102	GLU	CYS	engineered mutation	UNP P02794
C	105	GLU	HIS	engineered mutation	UNP P02794
D	18	GLU	ALA	engineered mutation	UNP P02794
D	86	GLN	LYS	engineered mutation	UNP P02794
D	90	GLU	CYS	engineered mutation	UNP P02794
D	102	GLU	CYS	engineered mutation	UNP P02794
D	105	GLU	HIS	engineered mutation	UNP P02794
E	18	GLU	ALA	engineered mutation	UNP P02794
E	86	GLN	LYS	engineered mutation	UNP P02794
E	90	GLU	CYS	engineered mutation	UNP P02794
E	102	GLU	CYS	engineered mutation	UNP P02794
E	105	GLU	HIS	engineered mutation	UNP P02794
F	18	GLU	ALA	engineered mutation	UNP P02794
F	86	GLN	LYS	engineered mutation	UNP P02794
F	90	GLU	CYS	engineered mutation	UNP P02794
F	102	GLU	CYS	engineered mutation	UNP P02794
F	105	GLU	HIS	engineered mutation	UNP P02794
G	18	GLU	ALA	engineered mutation	UNP P02794
G	86	GLN	LYS	engineered mutation	UNP P02794
G	90	GLU	CYS	engineered mutation	UNP P02794
G	102	GLU	CYS	engineered mutation	UNP P02794
G	105	GLU	HIS	engineered mutation	UNP P02794
H	18	GLU	ALA	engineered mutation	UNP P02794
H	86	GLN	LYS	engineered mutation	UNP P02794
H	90	GLU	CYS	engineered mutation	UNP P02794
H	102	GLU	CYS	engineered mutation	UNP P02794
H	105	GLU	HIS	engineered mutation	UNP P02794

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0
3	C	3	Total Mg 3 3	0	0
3	D	2	Total Mg 2 2	0	0
3	E	3	Total Mg 3 3	0	0
3	F	3	Total Mg 3 3	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	211	Total O 211 211	0	0
5	B	216	Total O 216 216	0	0
5	C	215	Total O 215 215	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	D	208	208	208	0	0
			Total	O		
5	E	201	201	201	0	0
			Total	O		
5	F	213	213	213	0	0
			Total	O		
5	G	206	206	206	0	0
			Total	O		
5	H	211	211	211	0	0

3 Residue-property plots (i)

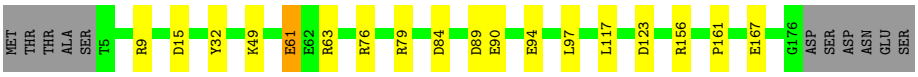
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:

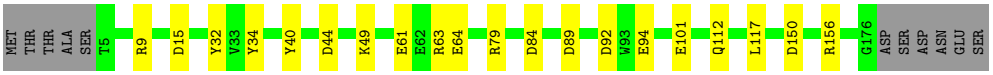
• Molecule 1: Ferritin heavy chain

Chain B:



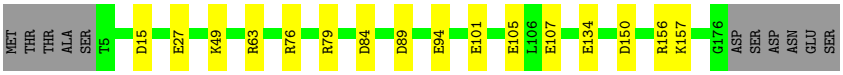
• Molecule 1: Ferritin heavy chain

Chain C:



• Molecule 1: Ferritin heavy chain

Chain D:



• Molecule 1: Ferritin heavy chain

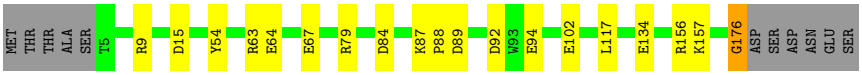
Chain E:

• Molecule 1: Ferritin heavy chain

Chain F:

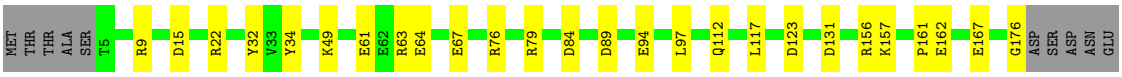
• Molecule 1: Ferritin heavy chain

Chain G:



• Molecule 1: Ferritin heavy chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α, β, γ	180.98Å 180.98Å 180.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.37 – 1.60 48.37 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.37-1.60) 99.9 (48.37-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.98 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.124 , 0.143 0.124 , 0.143	Depositor DCC
R_{free} test set	12488 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	9.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.075 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13086	wwPDB-VP
Average B, all atoms (Å^2)	11.0	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 43.81 % 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 1.6717e-04. 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.24	5/1450 (0.3%)	1.28	13/1953 (0.7%)
1	B	1.24	5/1450 (0.3%)	1.26	17/1953 (0.9%)
1	C	1.24	5/1450 (0.3%)	1.27	19/1953 (1.0%)
1	D	1.24	8/1450 (0.6%)	1.31	14/1953 (0.7%)
1	E	1.21	3/1450 (0.2%)	1.30	13/1953 (0.7%)
1	F	1.28	9/1450 (0.6%)	1.31	15/1953 (0.8%)
1	G	1.26	7/1450 (0.5%)	1.35	17/1953 (0.9%)
1	H	1.35	8/1450 (0.6%)	1.26	17/1953 (0.9%)
All	All	1.26	50/11600 (0.4%)	1.29	125/15624 (0.8%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	94	GLU	CD-OE1	14.21	1.41	1.25
1	F	94	GLU	CD-OE1	12.97	1.40	1.25
1	C	94	GLU	CD-OE1	11.51	1.38	1.25
1	H	64	GLU	CD-OE2	11.05	1.37	1.25
1	G	94	GLU	CD-OE1	10.72	1.37	1.25
1	B	94	GLU	CD-OE1	9.87	1.36	1.25
1	H	64	GLU	CG-CD	9.11	1.65	1.51
1	A	94	GLU	CG-CD	9.10	1.65	1.51
1	F	64	GLU	CG-CD	7.93	1.63	1.51
1	F	94	GLU	CG-CD	7.81	1.63	1.51
1	H	94	GLU	CG-CD	7.64	1.63	1.51
1	B	61	GLU	CD-OE2	7.56	1.33	1.25
1	B	167	GLU	CD-OE1	7.29	1.33	1.25
1	A	94	GLU	CD-OE1	6.83	1.33	1.25
1	H	162	GLU	CD-OE1	6.70	1.33	1.25
1	E	156	ARG	CZ-NH1	6.53	1.41	1.33
1	B	94	GLU	CG-CD	6.50	1.61	1.51
1	D	94	GLU	CD-OE1	6.40	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	61	GLU	CD-OE2	6.35	1.32	1.25
1	C	101	GLU	CD-OE1	-6.21	1.18	1.25
1	E	63	ARG	CZ-NH2	6.17	1.41	1.33
1	G	94	GLU	CG-CD	6.06	1.61	1.51
1	D	94	GLU	CG-CD	5.80	1.60	1.51
1	F	34	TYR	CE2-CZ	-5.78	1.31	1.38
1	H	167	GLU	CD-OE1	5.75	1.31	1.25
1	E	140	GLU	CD-OE2	5.69	1.31	1.25
1	C	40	TYR	CE2-CZ	-5.66	1.31	1.38
1	G	64	GLU	CG-CD	5.61	1.60	1.51
1	D	27	GLU	CD-OE2	5.57	1.31	1.25
1	G	102	GLU	CD-OE2	-5.56	1.19	1.25
1	H	61	GLU	CD-OE1	5.49	1.31	1.25
1	G	54	TYR	CG-CD2	-5.42	1.32	1.39
1	D	156	ARG	CZ-NH1	5.38	1.40	1.33
1	A	40	TYR	CE2-CZ	-5.32	1.31	1.38
1	D	134	GLU	CD-OE2	-5.32	1.19	1.25
1	D	107	GLU	CD-OE2	5.31	1.31	1.25
1	D	105	GLU	CG-CD	5.29	1.59	1.51
1	F	94	GLU	CB-CG	-5.29	1.42	1.52
1	A	34	TYR	CE2-CZ	-5.24	1.31	1.38
1	G	156	ARG	CZ-NH1	5.21	1.39	1.33
1	C	64	GLU	CG-CD	5.20	1.59	1.51
1	G	134	GLU	CD-OE2	-5.18	1.20	1.25
1	F	156	ARG	CZ-NH1	5.17	1.39	1.33
1	F	54	TYR	CE1-CZ	-5.15	1.31	1.38
1	H	67	GLU	CD-OE1	-5.11	1.20	1.25
1	F	101	GLU	CD-OE1	-5.09	1.20	1.25
1	A	156	ARG	CZ-NH1	5.08	1.39	1.33
1	F	67	GLU	CD-OE1	-5.07	1.20	1.25
1	D	101	GLU	CD-OE1	-5.07	1.20	1.25
1	B	90	GLU	CD-OE2	-5.04	1.20	1.25

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	63	ARG	NE-CZ-NH1	-18.35	111.12	120.30
1	E	63	ARG	NE-CZ-NH1	-16.17	112.22	120.30
1	G	84	ASP	CB-CG-OD1	15.93	132.64	118.30
1	F	63	ARG	NE-CZ-NH1	-14.76	112.92	120.30
1	C	63	ARG	NE-CZ-NH1	-14.04	113.28	120.30
1	A	63	ARG	NE-CZ-NH1	-13.84	113.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	79	ARG	NE-CZ-NH2	-13.26	113.67	120.30
1	G	156	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	H	63	ARG	NE-CZ-NH1	-12.36	114.12	120.30
1	D	63	ARG	NE-CZ-NH2	12.30	126.45	120.30
1	E	63	ARG	NE-CZ-NH2	12.15	126.38	120.30
1	D	84	ASP	CB-CG-OD1	11.77	128.90	118.30
1	E	15	ASP	CB-CG-OD2	-11.51	107.94	118.30
1	G	15	ASP	CB-CG-OD2	-11.25	108.18	118.30
1	A	79	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	E	89	ASP	CB-CG-OD2	-10.62	108.74	118.30
1	A	15	ASP	CB-CG-OD2	-10.48	108.87	118.30
1	B	63	ARG	NE-CZ-NH1	-10.34	115.13	120.30
1	F	79	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	G	63	ARG	NE-CZ-NH1	-10.26	115.17	120.30
1	C	15	ASP	CB-CG-OD2	-10.17	109.15	118.30
1	B	89	ASP	CB-CG-OD2	-9.96	109.33	118.30
1	A	84	ASP	CB-CG-OD1	9.90	127.21	118.30
1	F	84	ASP	CB-CG-OD1	9.81	127.13	118.30
1	C	63	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	D	156	ARG	NE-CZ-NH2	-9.51	115.54	120.30
1	H	15	ASP	CB-CG-OD2	-9.35	109.88	118.30
1	C	156	ARG	NE-CZ-NH2	-9.21	115.70	120.30
1	H	63	ARG	NE-CZ-NH2	9.21	124.90	120.30
1	E	156	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	E	84	ASP	CB-CG-OD1	8.94	126.35	118.30
1	G	89	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	G	156	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	H	79	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	D	76	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	H	79	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	G	79	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	A	63	ARG	NE-CZ-NH2	8.24	124.42	120.30
1	B	156	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	A	89	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	C	89	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	H	9	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	63	ARG	NE-CZ-NH2	8.01	124.31	120.30
1	H	117	LEU	CB-CG-CD1	8.00	124.59	111.00
1	F	156	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	B	117	LEU	CB-CG-CD1	7.78	124.22	111.00
1	F	89	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	H	89	ASP	CB-CG-OD2	-7.67	111.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	79	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	79	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	A	156	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	F	63	ARG	NE-CZ-NH2	7.55	124.08	120.30
1	F	15	ASP	CB-CG-OD2	-7.46	111.58	118.30
1	C	34	TYR	CD1-CE1-CZ	-7.40	113.14	119.80
1	F	92	ASP	CB-CG-OD1	7.40	124.96	118.30
1	C	150	ASP	CB-CG-OD1	7.39	124.95	118.30
1	B	84	ASP	CB-CG-OD1	7.34	124.91	118.30
1	D	150	ASP	CB-CG-OD2	-7.32	111.72	118.30
1	F	34	TYR	CB-CG-CD1	-7.29	116.63	121.00
1	D	15	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	B	79	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	G	67	GLU	OE1-CD-OE2	7.14	131.87	123.30
1	C	84	ASP	CB-CG-OD1	7.05	124.64	118.30
1	G	9	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	H	123	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	G	9	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	E	79	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	H	84	ASP	CB-CG-OD1	6.83	124.44	118.30
1	D	89	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	D	76	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	G	79	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	B	15	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	E	34	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	G	157	LYS	CD-CE-NZ	6.61	126.91	111.70
1	G	92	ASP	CB-CG-OD1	6.58	124.22	118.30
1	E	156	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	F	156	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	E	92	ASP	CB-CG-OD1	6.49	124.14	118.30
1	G	117	LEU	CB-CG-CD1	6.35	121.80	111.00
1	C	156	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	C	94	GLU	CG-CD-OE2	-6.21	105.89	118.30
1	B	9	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	E	9	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	9	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	B	79	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	E	79	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	9	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	156	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	F	94	GLU	CG-CD-OE2	-5.94	106.41	118.30
1	G	176	GLY	CA-C-O	-5.94	109.91	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	94	GLU	CA-CB-CG	5.94	126.46	113.40
1	D	84	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	34	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	C	44	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	150	ASP	CB-CG-OD1	5.86	123.58	118.30
1	H	94	GLU	CG-CD-OE2	-5.85	106.61	118.30
1	B	49	LYS	CD-CE-NZ	5.84	125.13	111.70
1	C	150	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	171	ASP	CB-CG-OD1	5.71	123.44	118.30
1	G	63	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	F	9	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	H	156	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	F	34	TYR	CD1-CE1-CZ	-5.51	114.84	119.80
1	C	32	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	E	15	ASP	OD1-CG-OD2	5.47	133.70	123.30
1	B	123	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	84	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	32	TYR	CB-CG-CD1	5.31	124.19	121.00
1	B	76	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	H	22	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	F	123	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	H	157	LYS	CD-CE-NZ	5.24	123.75	111.70
1	G	84	ASP	OD1-CG-OD2	-5.21	113.41	123.30
1	C	79	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	H	34	TYR	CD1-CE1-CZ	-5.18	115.14	119.80
1	D	49	LYS	CD-CE-NZ	5.14	123.53	111.70
1	A	32	TYR	CB-CG-CD1	5.12	124.07	121.00
1	C	92	ASP	CB-CG-OD1	5.11	122.90	118.30
1	H	131	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	49	LYS	CD-CE-NZ	5.07	123.35	111.70
1	B	156	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	94	GLU	CG-CD-OE2	-5.04	108.22	118.30
1	C	34	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	C	117	LEU	CB-CG-CD1	5.02	119.54	111.00
1	H	76	ARG	NE-CZ-NH2	-5.00	117.80	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	1422	0	1354	4	1
1	B	1422	0	1354	2	0
1	C	1422	0	1354	1	0
1	D	1422	0	1354	1	0
1	E	1422	0	1354	2	0
1	F	1422	0	1354	0	1
1	G	1422	0	1354	2	0
1	H	1422	0	1354	4	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	211	0	0	2	5
5	B	216	0	0	1	0
5	C	215	0	0	1	0
5	D	208	0	0	0	0
5	E	201	0	0	2	2
5	F	213	0	0	0	4
5	G	206	0	0	1	4
5	H	211	0	0	3	1
All	All	13086	0	10832	16	11

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 1.

All (16) 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:A:86:GLN:OE1	5:A:301:HOH:O	1.83	0.95
1:H:112:GLN:OE1	5:H:301:HOH:O	1.96	0.83
1:C:112:GLN:OE1	5:C:301:HOH:O	2.05	0.74
1:G:176:GLY:O	5:G:301:HOH:O	2.09	0.70
1:B:61:GLU:OE2	5:B:301:HOH:O	2.16	0.60
1:B:97:LEU:HD23	1:B:161:PRO:HD3	1.88	0.55
1:H:97:LEU:HD23	1:H:161:PRO:HD3	1.90	0.53
1:E:49:LYS:HE3	5:E:400:HOH:O	2.13	0.48
1:A:97:LEU:HD23	1:A:161:PRO:HD3	1.96	0.46
1:E:72:LEU:HD13	1:E:72:LEU:C	2.37	0.44
1:H:176:GLY:C	5:H:401:HOH:O	2.57	0.43
1:H:49:LYS:NZ	5:H:306:HOH:O	2.52	0.42
1:A:110:VAL:HG11	5:A:343:HOH:O	2.20	0.42
1:D:157:LYS:HE3	5:E:352:HOH:O	2.20	0.42
1:G:87:LYS:HA	1:G:88:PRO:HD3	1.96	0.41
1:A:72:LEU:HD13	1:A:72:LEU:C	2.42	0.41

All (11) 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:A:84:ASP:OD2	5:A:301:HOH:O[4_577]	1.89	0.31
5:F:364:HOH:O	5:G:361:HOH:O[7_665]	1.92	0.28
5:A:329:HOH:O	5:A:373:HOH:O[10_656]	1.94	0.26
5:A:301:HOH:O	5:F:334:HOH:O[10_656]	1.97	0.23
5:E:342:HOH:O	5:E:383:HOH:O[10_656]	1.97	0.23
5:E:342:HOH:O	5:E:342:HOH:O[7_665]	2.04	0.16
5:F:357:HOH:O	5:G:361:HOH:O[7_665]	2.04	0.16
5:A:373:HOH:O	5:A:373:HOH:O[10_656]	2.09	0.11
1:F:84:ASP:OD2	5:A:301:HOH:O[7_665]	2.16	0.04
5:F:357:HOH:O	5:G:323:HOH:O[7_665]	2.16	0.04
5:G:323:HOH:O	5:H:317:HOH:O[10_656]	2.19	0.01

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	170/183 (93%)	168 (99%)	2 (1%)	0	100	100
1	B	170/183 (93%)	167 (98%)	3 (2%)	0	100	100
1	C	170/183 (93%)	168 (99%)	2 (1%)	0	100	100
1	D	170/183 (93%)	168 (99%)	2 (1%)	0	100	100
1	E	170/183 (93%)	168 (99%)	2 (1%)	0	100	100
1	F	170/183 (93%)	168 (99%)	2 (1%)	0	100	100
1	G	170/183 (93%)	167 (98%)	3 (2%)	0	100	100
1	H	170/183 (93%)	168 (99%)	2 (1%)	0	100	100
All	All	1360/1464 (93%)	1342 (99%)	18 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	154/164 (94%)	154 (100%)	0	100	100
1	B	154/164 (94%)	154 (100%)	0	100	100
1	C	154/164 (94%)	154 (100%)	0	100	100
1	D	154/164 (94%)	154 (100%)	0	100	100
1	E	154/164 (94%)	154 (100%)	0	100	100
1	F	154/164 (94%)	154 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	154/164 (94%)	154 (100%)	0	100	100
1	H	154/164 (94%)	153 (99%)	1 (1%)	86	77
All	All	1232/1312 (94%)	1231 (100%)	1 (0%)	93	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	32	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	A	86	GLN

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 29 ligands modelled in this entry, 29 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	172/183 (93%)	-0.58	0	100	100	6, 8, 18, 26	0
1	B	172/183 (93%)	-0.58	0	100	100	6, 8, 19, 23	0
1	C	172/183 (93%)	-0.56	0	100	100	6, 8, 19, 24	0
1	D	172/183 (93%)	-0.58	0	100	100	6, 8, 19, 23	0
1	E	172/183 (93%)	-0.58	0	100	100	6, 8, 20, 25	0
1	F	172/183 (93%)	-0.60	0	100	100	6, 8, 19, 26	0
1	G	172/183 (93%)	-0.58	0	100	100	6, 8, 19, 26	0
1	H	172/183 (93%)	-0.54	0	100	100	6, 8, 19, 24	0
All	All	1376/1464 (93%)	-0.57	0	100	100	6, 8, 19, 26	0

There are no RSRZ outliers to report.

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
3	MG	D	203	1/1	0.88	0.08	13,13,13,13	1
3	MG	C	202	1/1	0.92	0.10	12,12,12,12	1
3	MG	A	204	1/1	0.93	0.28	30,30,30,30	1
3	MG	B	202	1/1	0.93	0.09	12,12,12,12	1
3	MG	F	202	1/1	0.93	0.12	12,12,12,12	1
3	MG	G	202	1/1	0.93	0.11	12,12,12,12	1
3	MG	H	202	1/1	0.93	0.15	23,23,23,23	0
3	MG	C	203	1/1	0.94	0.28	32,32,32,32	0
3	MG	A	203	1/1	0.96	0.09	12,12,12,12	1
3	MG	E	202	1/1	0.97	0.07	11,11,11,11	1
2	FE	E	201	1/1	0.99	0.11	18,18,18,18	0
2	FE	F	201	1/1	0.99	0.11	18,18,18,18	0
2	FE	G	201	1/1	0.99	0.12	18,18,18,18	0
3	MG	D	204	1/1	0.99	0.15	10,10,10,10	1
2	FE	H	201	1/1	0.99	0.12	18,18,18,18	0
2	FE	A	202	1/1	0.99	0.36	27,27,27,27	1
3	MG	F	204	1/1	0.99	0.17	11,11,11,11	1
2	FE	B	201	1/1	0.99	0.11	19,19,19,19	0
2	FE	C	201	1/1	0.99	0.12	18,18,18,18	0
2	FE	D	201	1/1	1.00	0.12	18,18,18,18	0
3	MG	E	203	1/1	1.00	0.09	8,8,8,8	1
3	MG	E	204	1/1	1.00	0.04	6,6,6,6	1
2	FE	D	202	1/1	1.00	0.22	12,12,12,12	1
3	MG	F	203	1/1	1.00	0.06	9,9,9,9	0
3	MG	C	204	1/1	1.00	0.07	7,7,7,7	1
2	FE	A	201	1/1	1.00	0.12	18,18,18,18	0
3	MG	B	203	1/1	1.00	0.05	8,8,8,8	0
4	CL	A	205	1/1	1.00	0.06	9,9,9,9	0
4	CL	D	205	1/1	1.00	0.56	2,2,2,2	1

6.5 Other polymers (i)

There are no such residues in this entry.