



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:35 PM UTC

PDB ID : 3A68 / pdb_00003a68
Title : Crystal structure of plant ferritin reveals a novel metal binding site that functions as a transit site for metal transfer in ferritin
Authors : Masuda, T.; Goto, F.; Yoshihara, T.; Mikami, B.
Deposited on : 2009-08-26
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

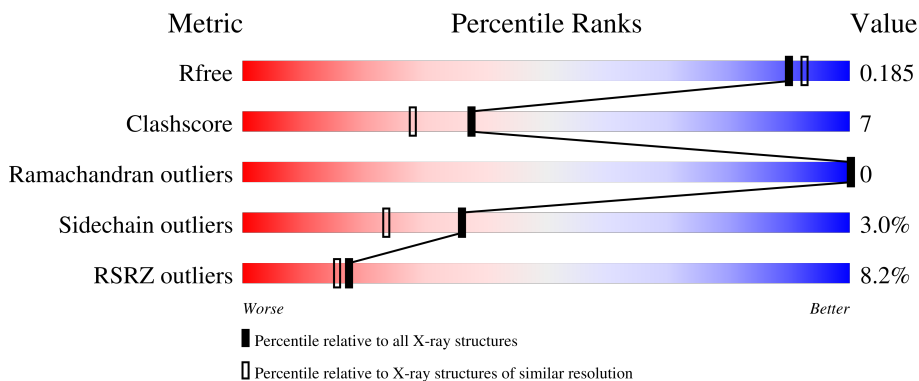
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	212	 9% 76% 13% • 8%
1	B	212	 9% 79% 11% • 8%
1	C	212	 7% 76% 15% • 8%
1	D	212	 8% 82% 8% • 8%
1	E	212	 7% 77% 10% • 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	212	 9% 77% 12% 8%
1	G	212	 6% 79% 12% 8%
1	H	212	 8% 74% 16% 9%
1	I	212	 8% 75% 15% 8%
1	J	212	 8% 77% 13% 8%
1	K	212	 8% 80% 11% 8%
1	L	212	 8% 75% 15% 9%
1	M	212	 8% 75% 15% 8%
1	N	212	 6% 80% 11% 8%
1	O	212	 8% 78% 12% 8%
1	P	212	 8% 76% 14% 8%
1	Q	212	 8% 82% 9% 8%
1	R	212	 7% 81% 12% 8%
1	S	212	 7% 80% 11% 8%
1	T	212	 8% 80% 11% 8%
1	U	212	 7% 79% 12% 8%
1	V	212	 6% 77% 14% 8%
1	W	212	 6% 78% 13% 8%
1	X	212	 6% 78% 13% 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 44039 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-4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	194	Total 1631	C 1039	N 270	O 316	S 6	0	10	0
1	B	194	Total 1631	C 1036	N 273	O 315	S 7	0	9	0
1	C	196	Total 1675	C 1060	N 282	O 328	S 5	0	13	0
1	D	194	Total 1639	C 1041	N 273	O 319	S 6	0	10	0
1	E	190	Total 1591	C 1010	N 266	O 309	S 6	0	10	0
1	F	194	Total 1636	C 1039	N 272	O 319	S 6	0	11	0
1	G	194	Total 1623	C 1032	N 271	O 314	S 6	0	8	0
1	H	193	Total 1631	C 1036	N 273	O 317	S 5	0	11	0
1	I	194	Total 1662	C 1059	N 274	O 323	S 6	0	15	0
1	J	194	Total 1644	C 1044	N 277	O 318	S 5	0	11	0
1	K	194	Total 1607	C 1019	N 271	O 312	S 5	0	5	0
1	L	193	Total 1605	C 1020	N 270	O 310	S 5	0	6	0
1	M	194	Total 1644	C 1045	N 276	O 317	S 6	0	12	0
1	N	194	Total 1620	C 1029	N 271	O 314	S 6	0	9	0
1	O	194	Total 1647	C 1045	N 274	O 323	S 5	0	12	0
1	P	194	Total 1632	C 1036	N 271	O 320	S 5	0	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	194	Total	C	N	O	S	0	12	0
			1639	1045	272	315	7			
1	R	196	Total	C	N	O	S	0	9	0
			1635	1037	275	317	6			
1	S	194	Total	C	N	O	S	0	9	0
			1618	1031	270	312	5			
1	T	194	Total	C	N	O	S	0	12	0
			1653	1048	277	322	6			
1	U	194	Total	C	N	O	S	0	13	0
			1643	1047	272	317	7			
1	V	194	Total	C	N	O	S	0	13	0
			1645	1046	273	320	6			
1	W	194	Total	C	N	O	S	0	12	0
			1648	1045	275	322	6			
1	X	194	Total	C	N	O	S	0	16	0
			1664	1058	273	325	8			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

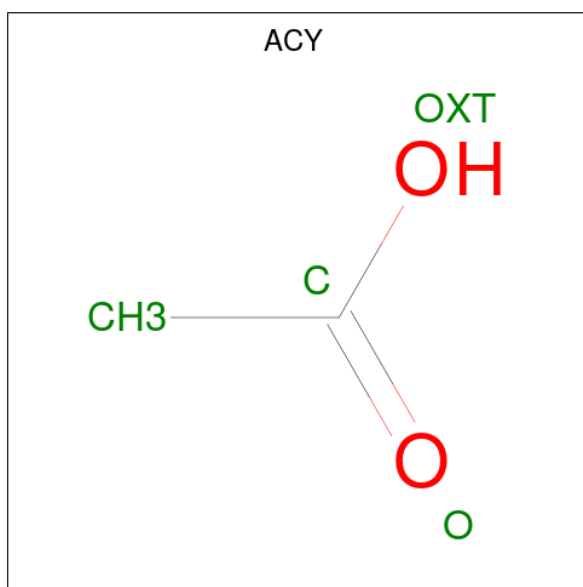
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Ca	0	1
			7	7		
2	B	5	Total	Ca	0	0
			5	5		
2	C	7	Total	Ca	0	0
			7	7		
2	D	5	Total	Ca	0	0
			5	5		
2	E	7	Total	Ca	0	0
			7	7		
2	F	5	Total	Ca	0	0
			5	5		
2	G	5	Total	Ca	0	0
			5	5		
2	H	5	Total	Ca	0	0
			5	5		
2	I	6	Total	Ca	0	0
			6	6		
2	J	6	Total	Ca	0	1
			6	6		
2	K	7	Total	Ca	0	0
			7	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	7	Total 7	Ca 7	0	0
2	M	5	Total 5	Ca 5	0	0
2	N	6	Total 6	Ca 6	0	1
2	O	7	Total 7	Ca 7	0	0
2	P	5	Total 5	Ca 5	0	0
2	Q	6	Total 6	Ca 6	0	0
2	R	5	Total 5	Ca 5	0	0
2	S	5	Total 5	Ca 5	0	0
2	T	5	Total 5	Ca 5	0	0
2	U	4	Total 4	Ca 4	0	0
2	V	5	Total 5	Ca 5	0	0
2	W	5	Total 5	Ca 5	0	0
2	X	6	Total 6	Ca 6	0	1

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	M	1	Total C O 4 2 2	0	0
3	O	1	Total C O 4 2 2	0	0
3	P	1	Total C O 4 2 2	0	0
3	Q	1	Total C O 4 2 2	0	0
3	R	1	Total C O 4 2 2	0	0
3	S	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	T	1	Total	C	O	0	0
			4	2	2		
3	V	1	Total	C	O	0	0
			4	2	2		
3	W	1	Total	C	O	0	0
			4	2	2		
3	X	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	201	Total	O	0	5
			206	206		
4	B	193	Total	O	0	2
			195	195		
4	C	206	Total	O	0	4
			210	210		
4	D	167	Total	O	0	2
			169	169		
4	E	190	Total	O	0	2
			192	192		
4	F	188	Total	O	0	2
			190	190		
4	G	197	Total	O	0	2
			199	199		
4	H	194	Total	O	0	3
			197	197		
4	I	187	Total	O	0	0
			187	187		
4	J	195	Total	O	0	2
			197	197		
4	K	181	Total	O	0	2
			183	183		
4	L	168	Total	O	0	2
			170	170		
4	M	182	Total	O	0	0
			182	182		
4	N	201	Total	O	0	0
			201	201		
4	O	191	Total	O	0	2
			193	193		

Continued on next page...


Continued from previous page...

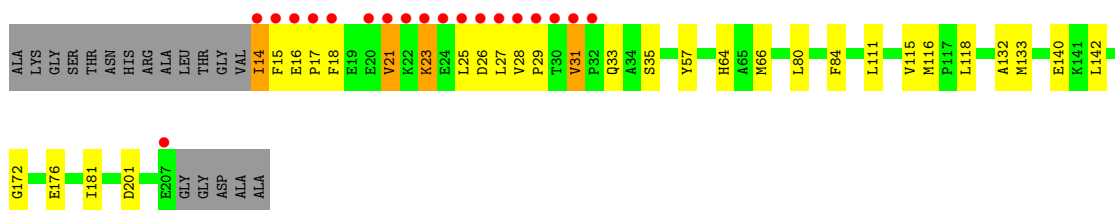
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	179	Total 181	O 181	0	2
4	Q	187	Total 192	O 192	0	5
4	R	194	Total 197	O 197	0	3
4	S	183	Total 184	O 184	0	1
4	T	182	Total 183	O 183	0	1
4	U	186	Total 190	O 190	0	4
4	V	186	Total 188	O 188	0	2
4	W	175	Total 178	O 178	0	3
4	X	201	Total 204	O 204	0	3

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.

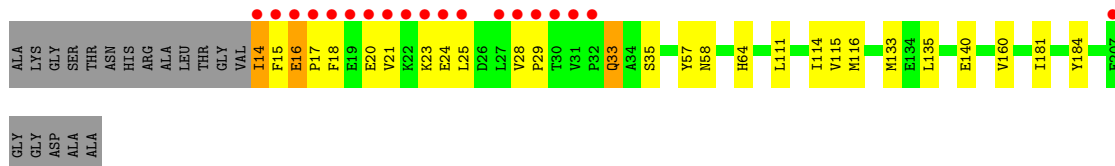
- Molecule 1: Ferritin-4, chloroplastic

Chain A: 




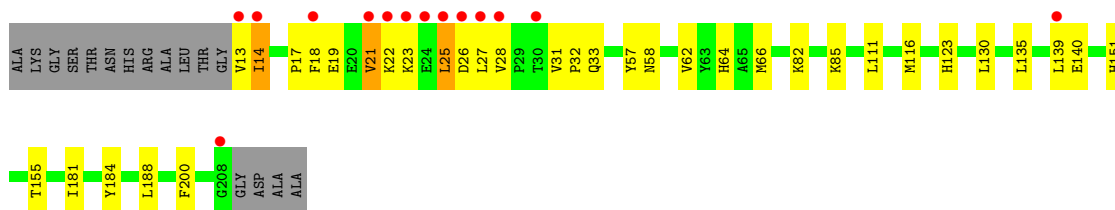
- Molecule 1: Ferritin-4, chloroplastic

Chain B: 




- Molecule 1: Ferritin-4, chloroplastic

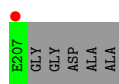
Chain C: 



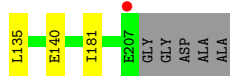
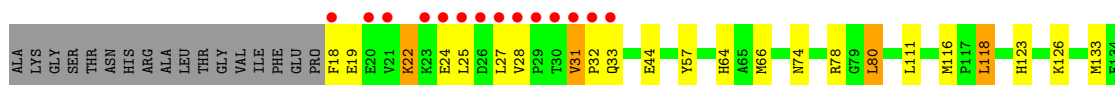
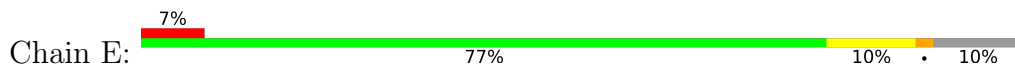
- Molecule 1: Ferritin-4, chloroplastic

Chain D: 

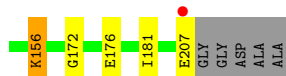
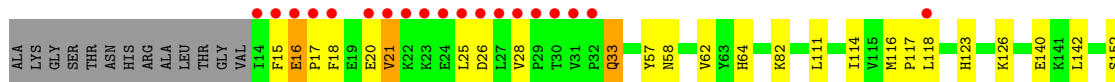
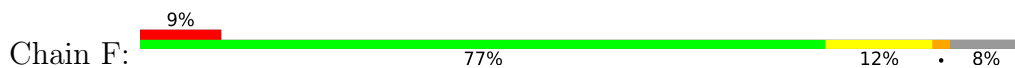




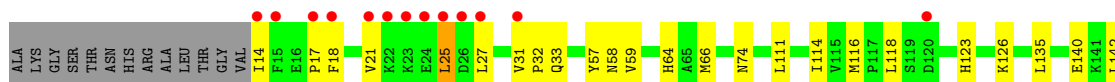
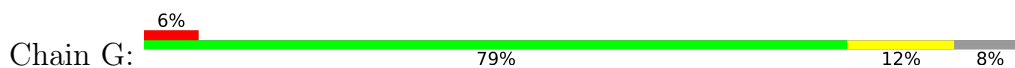
- Molecule 1: Ferritin-4, chloroplastic



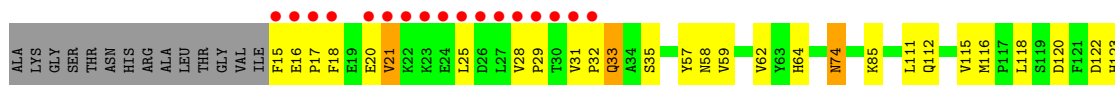
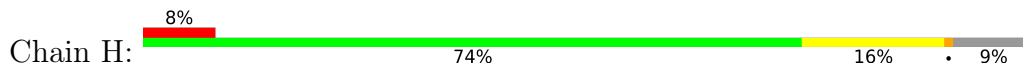
- Molecule 1: Ferritin-4, chloroplastic



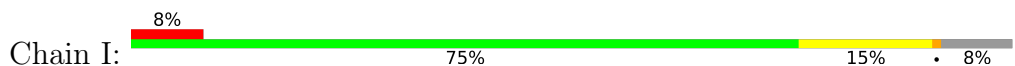
- Molecule 1: Ferritin-4, chloroplastic

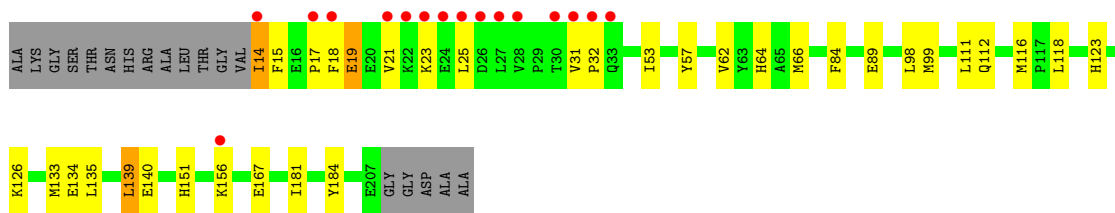


- Molecule 1: Ferritin-4, chloroplastic

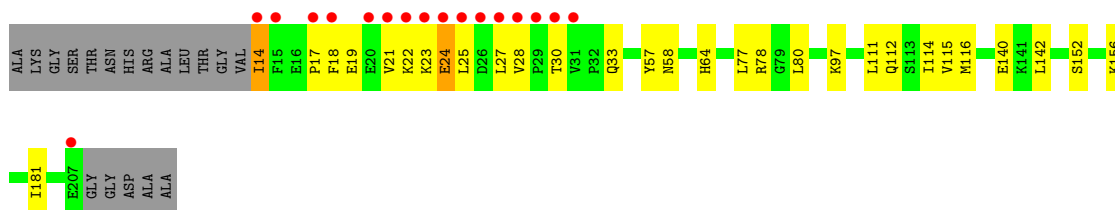
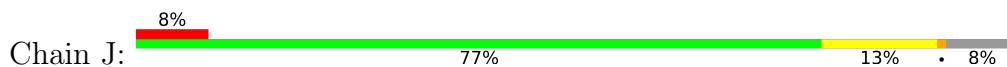


- Molecule 1: Ferritin-4, chloroplastic

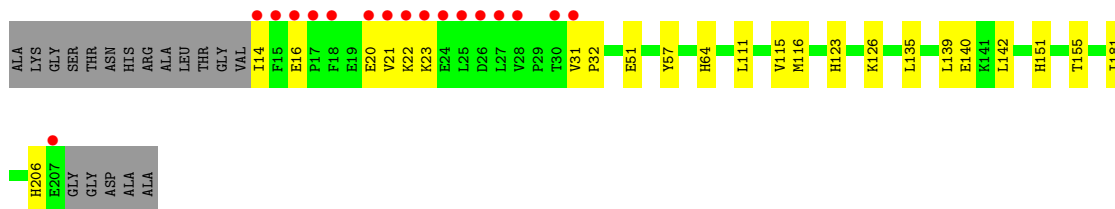
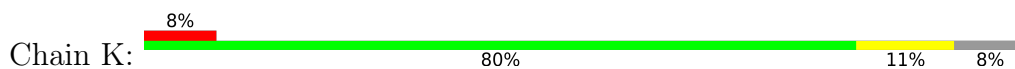




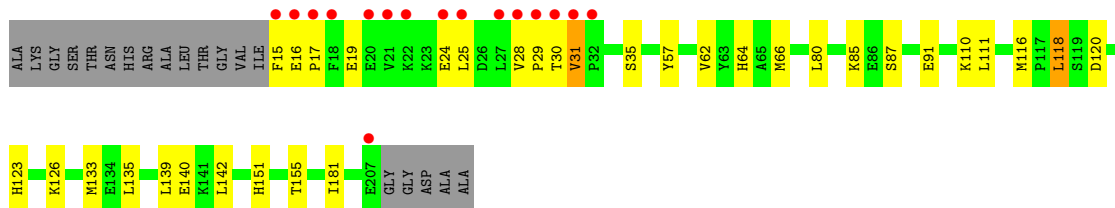
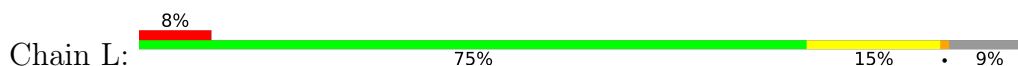
- Molecule 1: Ferritin-4, chloroplastic



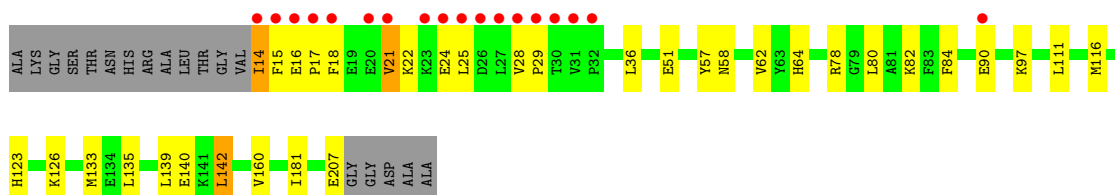
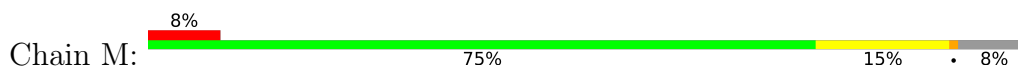
- Molecule 1: Ferritin-4, chloroplastic



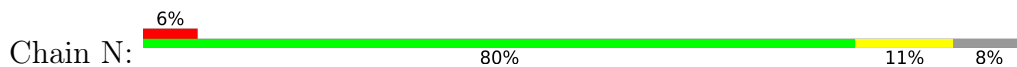
- Molecule 1: Ferritin-4, chloroplastic



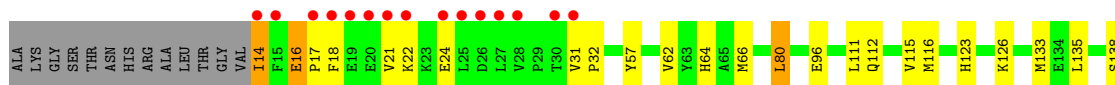
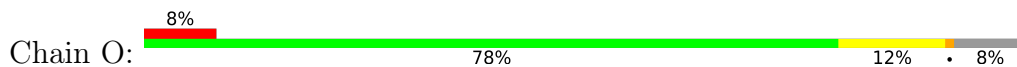
- Molecule 1: Ferritin-4, chloroplastic



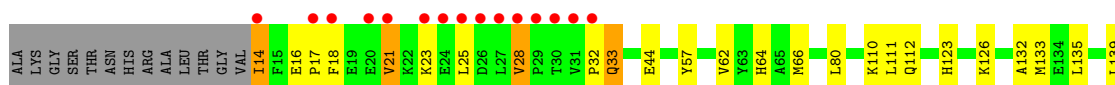
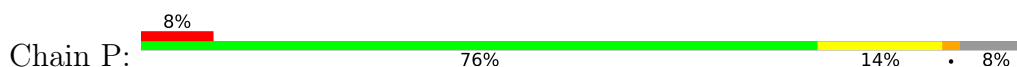
• Molecule 1: Ferritin-4, chloroplastic



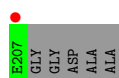
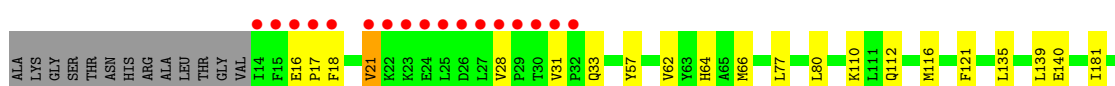
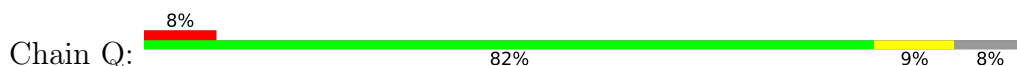
• Molecule 1: Ferritin-4, chloroplastic



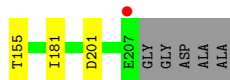
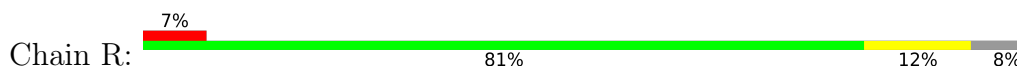
• Molecule 1: Ferritin-4, chloroplastic



• Molecule 1: Ferritin-4, chloroplastic

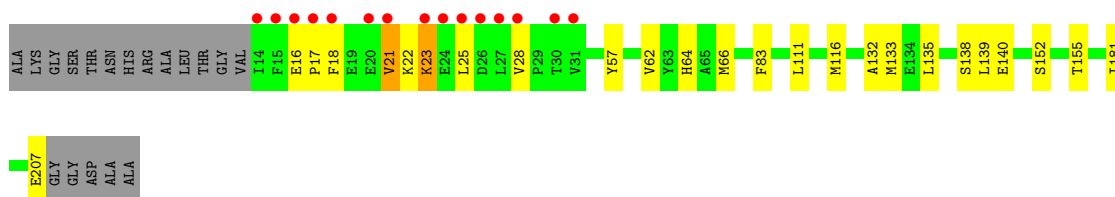


• Molecule 1: Ferritin-4, chloroplastic



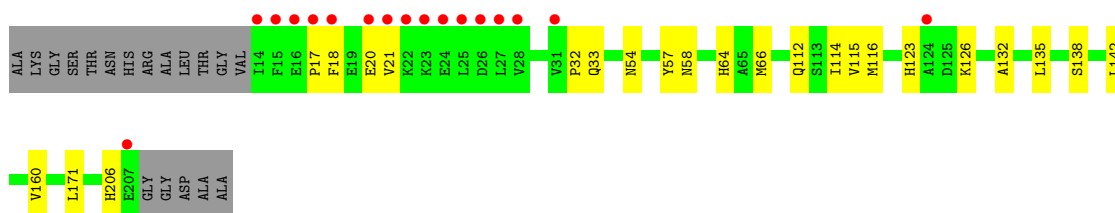
- Molecule 1: Ferritin-4, chloroplastic

Chain S: 7% 80% 11% 8%



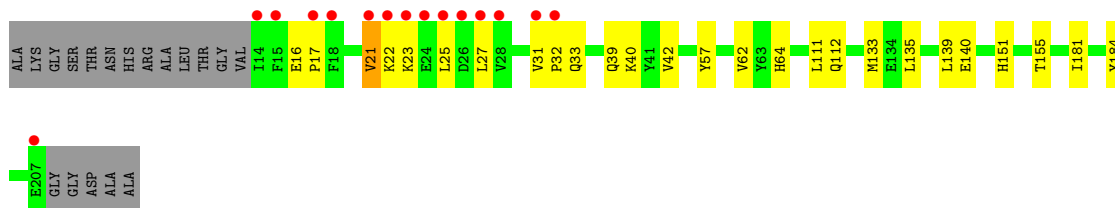
- Molecule 1: Ferritin-4, chloroplastic

Chain T: 8% 80% 11% 8%



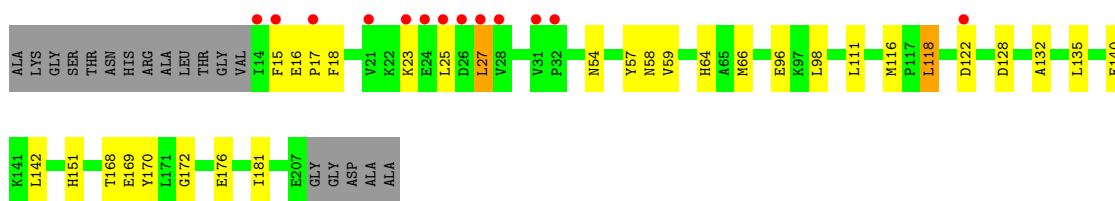
- Molecule 1: Ferritin-4, chloroplastic

Chain U: 7% 79% 12% 8%



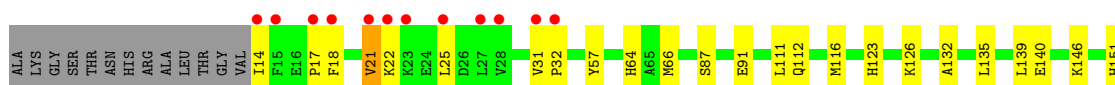
- Molecule 1: Ferritin-4, chloroplastic

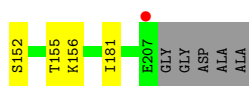
Chain V: 6% 77% 14% 8%



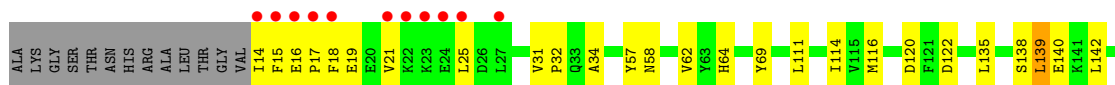
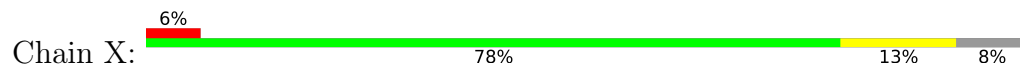
- Molecule 1: Ferritin-4, chloroplastic

Chain W: 6% 78% 13% 8%





- Molecule 1: Ferritin-4, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	222.61Å 220.89Å 122.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 1.80 49.47 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.47-1.80) 98.8 (49.47-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.69 (at 1.79Å)	Xtrriage
Refinement program	CNS, PHENIX (phenix.refine)	Depositor
R, R_{free}	0.142 , 0.173 0.159 , 0.185	Depositor DCC
R_{free} test set	27445 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtrriage
Anisotropy	0.590	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.011 for k,h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	44039	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.33	0/1685	0.63	0/2270
1	B	0.34	0/1673	0.64	2/2254 (0.1%)
1	C	0.33	0/1720	0.60	0/2317
1	D	0.32	0/1684	0.63	0/2268
1	E	0.32	0/1645	0.60	0/2212
1	F	0.33	0/1693	0.63	2/2280 (0.1%)
1	G	0.33	0/1668	0.61	0/2248
1	H	0.33	0/1685	0.63	2/2270 (0.1%)
1	I	0.31	0/1722	0.59	0/2320
1	J	0.32	0/1695	0.63	0/2284
1	K	0.32	0/1646	0.64	2/2217 (0.1%)
1	L	0.33	0/1644	0.65	2/2215 (0.1%)
1	M	0.33	0/1701	0.61	0/2292
1	N	0.33	0/1674	0.63	0/2255
1	O	0.32	0/1701	0.61	2/2291 (0.1%)
1	P	0.31	0/1682	0.63	2/2265 (0.1%)
1	Q	0.33	0/1696	0.61	0/2283
1	R	0.33	0/1686	0.63	0/2272
1	S	0.33	0/1669	0.61	0/2248
1	T	0.31	0/1700	0.61	0/2290
1	U	0.32	0/1703	0.62	2/2292 (0.1%)
1	V	0.32	0/1704	0.60	0/2294
1	W	0.32	0/1699	0.60	0/2288
1	X	0.32	0/1730	0.61	0/2329
All	All	0.32	0/40505	0.62	16/54554 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
-----	-------	-----	------	-------	---	-------------	----------

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	16	GLU	CA-C-N	6.57	126.07	119.24
1	F	16	GLU	C-N-CA	6.57	126.07	119.24
1	B	16	GLU	CA-C-N	6.49	125.99	119.24
1	B	16	GLU	C-N-CA	6.49	125.99	119.24
1	O	16	GLU	CA-C-N	6.04	125.66	119.56

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	1631	0	1611	32	0
1	B	1631	0	1601	35	0
1	C	1675	0	1635	44	0
1	D	1639	0	1607	25	0
1	E	1591	0	1575	22	0
1	F	1636	0	1610	43	0
1	G	1623	0	1595	30	0
1	H	1631	0	1604	36	0
1	I	1662	0	1643	36	0
1	J	1644	0	1617	26	0
1	K	1607	0	1571	20	0
1	L	1605	0	1576	30	0
1	M	1644	0	1626	38	0
1	N	1620	0	1597	25	0
1	O	1647	0	1614	33	0
1	P	1632	0	1599	29	0
1	Q	1639	0	1631	21	0
1	R	1635	0	1607	27	0
1	S	1618	0	1606	25	0
1	T	1653	0	1616	27	0
1	U	1643	0	1632	22	0
1	V	1645	0	1626	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1648	0	1618	22	0
1	X	1664	0	1642	28	0
2	A	7	0	0	0	0
2	B	5	0	0	0	0
2	C	7	0	0	0	0
2	D	5	0	0	0	0
2	E	7	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	6	0	0	0	0
2	J	6	0	0	0	0
2	K	7	0	0	0	0
2	L	7	0	0	0	0
2	M	5	0	0	0	0
2	N	6	0	0	0	0
2	O	7	0	0	0	0
2	P	5	0	0	0	0
2	Q	6	0	0	0	0
2	R	5	0	0	0	0
2	S	5	0	0	0	0
2	T	5	0	0	0	0
2	U	4	0	0	0	0
2	V	5	0	0	0	0
2	W	5	0	0	0	0
2	X	6	0	0	0	0
3	A	4	0	3	0	0
3	E	4	0	3	0	0
3	F	4	0	3	0	0
3	G	4	0	3	0	0
3	H	4	0	3	0	0
3	I	4	0	3	0	0
3	J	4	0	3	0	0
3	L	4	0	3	0	0
3	M	4	0	3	0	0
3	O	4	0	3	0	0
3	P	4	0	3	0	0
3	Q	4	0	3	0	0
3	R	4	0	3	0	0
3	S	4	0	3	1	0
3	T	4	0	3	0	0
3	V	4	0	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	W	4	0	3	0	0
3	X	4	0	3	1	0
4	A	206	0	0	1	0
4	B	195	0	0	3	0
4	C	210	0	0	8	0
4	D	169	0	0	2	0
4	E	192	0	0	4	0
4	F	190	0	0	2	0
4	G	199	0	0	7	0
4	H	197	0	0	8	0
4	I	187	0	0	1	0
4	J	197	0	0	3	0
4	K	183	0	0	3	0
4	L	170	0	0	3	0
4	M	182	0	0	5	0
4	N	201	0	0	7	0
4	O	193	0	0	0	0
4	P	181	0	0	1	0
4	Q	192	0	0	2	0
4	R	197	0	0	2	0
4	S	184	0	0	3	0
4	T	183	0	0	6	0
4	U	190	0	0	6	0
4	V	188	0	0	4	0
4	W	178	0	0	2	0
4	X	204	0	0	2	0
All	All	44039	0	38713	547	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 547 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:N:58[B]:ASN:HD21	1:Q:17:PRO:HG3	1.13	1.09
1:N:58[B]:ASN:ND2	1:Q:17:PRO:HG3	1.72	1.02
1:A:17:PRO:HG3	1:H:58[B]:ASN:HD21	1.33	0.94
1:C:31:VAL:HB	1:C:33:GLN:HE21	1.35	0.91
1:L:16:GLU:HG2	1:L:19:GLU:HG2	1.53	0.90

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	202/212 (95%)	201 (100%)	1 (0%)	0	100	100
1	B	201/212 (95%)	200 (100%)	1 (0%)	0	100	100
1	C	207/212 (98%)	207 (100%)	0	0	100	100
1	D	202/212 (95%)	202 (100%)	0	0	100	100
1	E	197/212 (93%)	197 (100%)	0	0	100	100
1	F	203/212 (96%)	203 (100%)	0	0	100	100
1	G	200/212 (94%)	200 (100%)	0	0	100	100
1	H	202/212 (95%)	202 (100%)	0	0	100	100
1	I	207/212 (98%)	205 (99%)	2 (1%)	0	100	100
1	J	203/212 (96%)	201 (99%)	2 (1%)	0	100	100
1	K	197/212 (93%)	197 (100%)	0	0	100	100
1	L	197/212 (93%)	197 (100%)	0	0	100	100
1	M	204/212 (96%)	202 (99%)	2 (1%)	0	100	100
1	N	201/212 (95%)	200 (100%)	1 (0%)	0	100	100
1	O	204/212 (96%)	204 (100%)	0	0	100	100
1	P	201/212 (95%)	200 (100%)	1 (0%)	0	100	100
1	Q	204/212 (96%)	203 (100%)	1 (0%)	0	100	100
1	R	203/212 (96%)	203 (100%)	0	0	100	100
1	S	201/212 (95%)	201 (100%)	0	0	100	100
1	T	203/212 (96%)	202 (100%)	1 (0%)	0	100	100
1	U	205/212 (97%)	204 (100%)	1 (0%)	0	100	100
1	V	204/212 (96%)	204 (100%)	0	0	100	100
1	W	204/212 (96%)	204 (100%)	0	0	100	100
1	X	208/212 (98%)	208 (100%)	0	0	100	100
All	All	4860/5088 (96%)	4847 (100%)	13 (0%)	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	179/179 (100%)	172 (96%)	7 (4%)	28	16
1	B	178/179 (99%)	174 (98%)	4 (2%)	45	34
1	C	183/179 (102%)	177 (97%)	6 (3%)	33	21
1	D	179/179 (100%)	175 (98%)	4 (2%)	45	34
1	E	175/179 (98%)	166 (95%)	9 (5%)	21	9
1	F	180/179 (101%)	174 (97%)	6 (3%)	33	21
1	G	177/179 (99%)	173 (98%)	4 (2%)	44	33
1	H	179/179 (100%)	173 (97%)	6 (3%)	32	20
1	I	184/179 (103%)	179 (97%)	5 (3%)	39	27
1	J	180/179 (101%)	173 (96%)	7 (4%)	28	16
1	K	174/179 (97%)	169 (97%)	5 (3%)	37	25
1	L	174/179 (97%)	169 (97%)	5 (3%)	37	25
1	M	181/179 (101%)	172 (95%)	9 (5%)	22	10
1	N	178/179 (99%)	175 (98%)	3 (2%)	53	45
1	O	181/179 (101%)	176 (97%)	5 (3%)	38	26
1	P	179/179 (100%)	172 (96%)	7 (4%)	28	16
1	Q	181/179 (101%)	176 (97%)	5 (3%)	38	26
1	R	179/179 (100%)	176 (98%)	3 (2%)	53	45
1	S	178/179 (99%)	174 (98%)	4 (2%)	45	34
1	T	181/179 (101%)	176 (97%)	5 (3%)	38	26
1	U	182/179 (102%)	178 (98%)	4 (2%)	45	34
1	V	182/179 (102%)	177 (97%)	5 (3%)	39	27
1	W	181/179 (101%)	177 (98%)	4 (2%)	45	34
1	X	185/179 (103%)	180 (97%)	5 (3%)	39	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4310/4296 (100%)	4183 (97%)	127 (3%)	36 25

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	64	HIS
1	U	22	LYS
1	M	51	GLU
1	U	21	VAL
1	W	21	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	94	HIS
1	S	58	ASN
1	O	144	ASN
1	Q	144	ASN
1	T	123	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 154 ligands modelled in this entry, 136 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACY	X	213	-	3,3,3	0.87	0	3,3,3	0.68	0
3	ACY	L	217	-	3,3,3	0.81	0	3,3,3	0.76	0
3	ACY	V	213	-	3,3,3	0.81	0	3,3,3	0.83	0
3	ACY	W	213	-	3,3,3	0.85	0	3,3,3	0.73	0
3	ACY	R	217	-	3,3,3	0.81	0	3,3,3	0.86	0
3	ACY	T	217	-	3,3,3	0.84	0	3,3,3	0.74	0
3	ACY	J	217	-	3,3,3	0.81	0	3,3,3	0.81	0
3	ACY	G	217	-	3,3,3	0.81	0	3,3,3	0.81	0
3	ACY	I	217	-	3,3,3	0.83	0	3,3,3	0.79	0
3	ACY	M	217	-	3,3,3	0.83	0	3,3,3	0.75	0
3	ACY	F	217	-	3,3,3	0.85	0	3,3,3	0.67	0
3	ACY	S	217	-	3,3,3	0.80	0	3,3,3	0.85	0
3	ACY	O	217	-	3,3,3	0.84	0	3,3,3	0.72	0
3	ACY	P	217	-	3,3,3	0.83	0	3,3,3	0.83	0
3	ACY	A	217	-	3,3,3	0.82	0	3,3,3	0.83	0
3	ACY	E	217	-	3,3,3	0.83	0	3,3,3	0.79	0
3	ACY	Q	217	-	3,3,3	0.84	0	3,3,3	0.73	0
3	ACY	H	217	-	3,3,3	0.84	0	3,3,3	0.79	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	213	ACY	1	0
3	S	217	ACY	1	0

5.7 Other polymers [i](#)

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 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	194/212 (91%)	-0.24	19 (9%) 13 11	6, 11, 83, 104	10 (5%)
1	B	194/212 (91%)	-0.27	19 (9%) 13 11	5, 12, 76, 106	9 (4%)
1	C	196/212 (92%)	-0.24	14 (7%) 22 20	5, 12, 50, 98	13 (6%)
1	D	194/212 (91%)	-0.30	18 (9%) 14 12	5, 12, 71, 103	10 (5%)
1	E	190/212 (89%)	-0.28	15 (7%) 18 16	6, 11, 83, 124	10 (5%)
1	F	194/212 (91%)	-0.19	20 (10%) 12 10	4, 12, 71, 100	11 (5%)
1	G	194/212 (91%)	-0.39	13 (6%) 24 22	6, 12, 51, 86	8 (4%)
1	H	193/212 (91%)	-0.29	17 (8%) 15 13	6, 12, 64, 101	11 (5%)
1	I	194/212 (91%)	-0.21	16 (8%) 17 15	5, 12, 66, 88	15 (7%)
1	J	194/212 (91%)	-0.16	17 (8%) 15 13	6, 12, 65, 97	11 (5%)
1	K	194/212 (91%)	-0.21	17 (8%) 15 13	6, 13, 74, 101	5 (2%)
1	L	193/212 (91%)	-0.20	16 (8%) 17 15	5, 13, 86, 109	6 (3%)
1	M	194/212 (91%)	-0.17	18 (9%) 14 12	7, 12, 85, 114	12 (6%)
1	N	194/212 (91%)	-0.33	12 (6%) 26 25	6, 12, 61, 103	9 (4%)
1	O	194/212 (91%)	-0.32	16 (8%) 17 15	5, 11, 62, 106	12 (6%)
1	P	194/212 (91%)	-0.22	16 (8%) 17 15	6, 13, 52, 93	10 (5%)
1	Q	194/212 (91%)	-0.33	18 (9%) 14 12	4, 11, 67, 104	12 (6%)
1	R	196/212 (92%)	-0.30	15 (7%) 19 17	6, 11, 63, 94	9 (4%)
1	S	194/212 (91%)	-0.38	15 (7%) 19 17	5, 11, 69, 91	9 (4%)
1	T	194/212 (91%)	-0.24	17 (8%) 15 13	6, 13, 73, 100	12 (6%)
1	U	194/212 (91%)	-0.37	15 (7%) 19 17	4, 11, 63, 96	13 (6%)
1	V	194/212 (91%)	-0.37	13 (6%) 24 22	6, 12, 51, 100	13 (6%)
1	W	194/212 (91%)	-0.36	13 (6%) 24 22	6, 12, 52, 84	12 (6%)
1	X	194/212 (91%)	-0.35	12 (6%) 26 25	6, 11, 49, 96	16 (8%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4654/5088 (91%)	-0.28	381 (8%) 17 15	4, 12, 68, 124	258 (5%)

The worst 5 of 381 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	14	ILE	8.2
1	E	21	VAL	8.0
1	B	14	ILE	8.0
1	A	14	ILE	7.9
1	O	18	PHE	7.7

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 oligosaccharides 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	CA	T	216	1/1	0.56	0.23	80,80,80,80	0
2	CA	E	405	1/1	0.63	0.22	80,80,80,80	0
2	CA	V	224	1/1	0.64	0.22	77,77,77,77	0
2	CA	S	216	1/1	0.66	0.20	66,66,66,66	0
2	CA	K	371	1/1	0.68	0.25	58,58,58,58	0
2	CA	G	407	1/1	0.72	0.21	62,62,62,62	0
2	CA	P	416	1/1	0.73	0.18	72,72,72,72	0
2	CA	I	409	1/1	0.76	0.19	66,66,66,66	0
2	CA	J	410	1/1	0.77	0.16	77,77,77,77	0
2	CA	M	216	1/1	0.78	0.18	56,56,56,56	0
2	CA	O	415	1/1	0.79	0.24	66,66,66,66	0
2	CA	S	419	1/1	0.79	0.18	77,77,77,77	0
2	CA	L	216	1/1	0.80	0.20	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	U	421	1/1	0.80	0.21	68,68,68,68	0
2	CA	H	408	1/1	0.80	0.17	69,69,69,69	0
2	CA	W	234	1/1	0.80	0.16	60,60,60,60	0
2	CA	W	423	1/1	0.82	0.18	68,68,68,68	0
2	CA	D	404	1/1	0.83	0.19	63,63,63,63	0
2	CA	V	422	1/1	0.83	0.17	64,64,64,64	0
2	CA	R	418	1/1	0.83	0.19	68,68,68,68	0
2	CA	F	406	1/1	0.83	0.17	59,59,59,59	0
2	CA	X	352[B]	1/1	0.83	0.16	30,30,30,30	1
2	CA	X	424	1/1	0.83	0.18	55,55,55,55	0
2	CA	T	420	1/1	0.84	0.20	56,56,56,56	0
2	CA	G	216	1/1	0.84	0.17	53,53,53,53	0
2	CA	N	414	1/1	0.85	0.21	52,52,52,52	0
2	CA	C	403	1/1	0.85	0.17	60,60,60,60	0
2	CA	H	216	1/1	0.85	0.20	47,47,47,47	0
2	CA	D	215	1/1	0.86	0.13	48,48,48,48	0
2	CA	I	216	1/1	0.86	0.16	54,54,54,54	0
2	CA	Q	417	1/1	0.86	0.18	63,63,63,63	0
2	CA	R	216	1/1	0.86	0.18	49,49,49,49	0
2	CA	A	216	1/1	0.87	0.16	48,48,48,48	0
3	ACY	E	217	4/4	0.87	0.17	24,24,35,51	0
2	CA	J	216	1/1	0.89	0.15	48,48,48,48	0
2	CA	N	216	1/1	0.89	0.16	44,44,44,44	0
3	ACY	S	217	4/4	0.89	0.19	18,19,47,56	0
2	CA	K	216	1/1	0.90	0.16	51,51,51,51	0
3	ACY	I	217	4/4	0.90	0.15	24,25,48,84	0
3	ACY	L	217	4/4	0.90	0.15	19,28,34,50	0
2	CA	B	402	1/1	0.90	0.15	51,51,51,51	0
3	ACY	W	213	4/4	0.90	0.18	20,26,38,43	0
2	CA	K	411	1/1	0.91	0.20	47,47,47,47	0
2	CA	Q	216	1/1	0.91	0.15	42,42,42,42	0
2	CA	C	216	1/1	0.91	0.13	44,44,44,44	0
3	ACY	M	217	4/4	0.91	0.18	19,26,46,55	0
2	CA	A	401	1/1	0.91	0.13	52,52,52,52	0
3	ACY	T	217	4/4	0.91	0.17	23,24,51,72	0
3	ACY	V	213	4/4	0.91	0.20	19,21,39,86	0
3	ACY	A	217	4/4	0.91	0.18	18,22,40,51	0
3	ACY	X	213	4/4	0.91	0.17	14,21,41,90	0
3	ACY	R	217	4/4	0.92	0.13	23,23,35,38	0
2	CA	P	216	1/1	0.92	0.17	42,42,42,42	0
3	ACY	F	217	4/4	0.92	0.16	19,20,48,73	0
3	ACY	H	217	4/4	0.92	0.18	18,26,36,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ACY	O	217	4/4	0.92	0.18	18,21,63,65	0
3	ACY	P	217	4/4	0.92	0.14	23,24,35,52	0
2	CA	X	244	1/1	0.93	0.18	39,39,39,39	0
2	CA	E	216	1/1	0.93	0.15	39,39,39,39	0
3	ACY	G	217	4/4	0.93	0.19	16,20,33,83	0
2	CA	M	413	1/1	0.94	0.11	45,45,45,45	0
3	ACY	J	217	4/4	0.94	0.12	24,27,41,51	0
2	CA	L	412	1/1	0.94	0.13	47,47,47,47	0
2	CA	C	321	1/1	0.94	0.07	31,31,31,31	0
2	CA	O	216	1/1	0.95	0.18	43,43,43,43	0
2	CA	B	216	1/1	0.95	0.13	39,39,39,39	0
2	CA	J	362[B]	1/1	0.95	0.08	28,28,28,28	1
3	ACY	Q	217	4/4	0.95	0.15	14,20,57,59	0
2	CA	C	323	1/1	0.95	0.14	33,33,33,33	0
2	CA	D	214	1/1	0.96	0.12	33,33,33,33	0
2	CA	Q	215	1/1	0.96	0.15	35,35,35,35	0
2	CA	E	215	1/1	0.96	0.07	28,28,28,28	0
2	CA	Q	213	1/1	0.97	0.10	26,26,26,26	0
2	CA	F	216	1/1	0.97	0.18	38,38,38,38	0
2	CA	K	373	1/1	0.97	0.06	28,28,28,28	0
2	CA	E	312	1/1	0.97	0.10	26,26,26,26	0
2	CA	L	215	1/1	0.97	0.13	28,28,28,28	0
2	CA	O	341	1/1	0.97	0.04	24,24,24,24	0
2	CA	O	342	1/1	0.97	0.10	21,21,21,21	0
2	CA	K	213	1/1	0.97	0.05	26,26,26,26	0
2	CA	T	214	1/1	0.97	0.06	23,23,23,23	0
2	CA	K	215	1/1	0.97	0.13	34,34,34,34	0
2	CA	A	353	1/1	0.97	0.10	26,26,26,26	0
2	CA	U	214	1/1	0.97	0.12	33,33,33,33	0
2	CA	U	215	1/1	0.97	0.13	37,37,37,37	0
2	CA	T	213	1/1	0.98	0.07	29,29,29,29	0
2	CA	C	214	1/1	0.98	0.07	20,20,20,20	0
2	CA	I	214	1/1	0.98	0.07	25,25,25,25	0
2	CA	P	213	1/1	0.98	0.04	22,22,22,22	0
2	CA	L	382	1/1	0.98	0.08	21,21,21,21	0
2	CA	K	214	1/1	0.98	0.08	30,30,30,30	0
2	CA	D	331	1/1	0.98	0.05	23,23,23,23	0
2	CA	Q	214	1/1	0.98	0.05	22,22,22,22	0
2	CA	I	332	1/1	0.98	0.12	24,24,24,24	0
2	CA	A	351[A]	1/1	0.98	0.04	10,10,10,10	1
2	CA	N	361[A]	1/1	0.98	0.05	12,12,12,12	1
2	CA	H	214	1/1	0.98	0.05	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	O	213	1/1	0.98	0.05	20,20,20,20	0
2	CA	S	213	1/1	0.98	0.13	28,28,28,28	0
2	CA	C	213	1/1	0.98	0.07	28,28,28,28	0
2	CA	L	214	1/1	0.98	0.09	28,28,28,28	0
2	CA	E	311	1/1	0.99	0.04	19,19,19,19	0
2	CA	S	214	1/1	0.99	0.05	17,17,17,17	0
2	CA	S	215	1/1	0.99	0.10	24,24,24,24	0
2	CA	D	213	1/1	0.99	0.11	26,26,26,26	0
2	CA	M	213	1/1	0.99	0.05	23,23,23,23	0
2	CA	M	214	1/1	0.99	0.05	19,19,19,19	0
2	CA	M	215	1/1	0.99	0.06	18,18,18,18	0
2	CA	T	215	1/1	0.99	0.09	23,23,23,23	0
2	CA	B	213	1/1	0.99	0.13	27,27,27,27	0
2	CA	F	213	1/1	0.99	0.07	20,20,20,20	0
2	CA	U	213	1/1	0.99	0.06	21,21,21,21	0
2	CA	N	213	1/1	0.99	0.12	28,28,28,28	0
2	CA	N	214	1/1	0.99	0.05	21,21,21,21	0
2	CA	N	215	1/1	0.99	0.13	28,28,28,28	0
2	CA	V	221	1/1	0.99	0.07	22,22,22,22	0
2	CA	V	222	1/1	0.99	0.04	20,20,20,20	0
2	CA	V	223	1/1	0.99	0.07	21,21,21,21	0
2	CA	J	213	1/1	0.99	0.05	23,23,23,23	0
2	CA	J	214	1/1	0.99	0.06	18,18,18,18	0
2	CA	W	231	1/1	0.99	0.05	21,21,21,21	0
2	CA	W	232	1/1	0.99	0.06	18,18,18,18	0
2	CA	J	215	1/1	0.99	0.07	18,18,18,18	0
2	CA	F	214	1/1	0.99	0.07	23,23,23,23	0
2	CA	X	241	1/1	0.99	0.07	22,22,22,22	0
2	CA	X	242	1/1	0.99	0.05	19,19,19,19	0
2	CA	O	214	1/1	0.99	0.04	17,17,17,17	0
2	CA	F	215	1/1	0.99	0.06	19,19,19,19	0
2	CA	C	215	1/1	0.99	0.12	20,20,20,20	0
2	CA	B	214	1/1	0.99	0.04	16,16,16,16	0
2	CA	G	213	1/1	0.99	0.06	26,26,26,26	0
2	CA	G	214	1/1	0.99	0.03	19,19,19,19	0
2	CA	P	214	1/1	0.99	0.04	22,22,22,22	0
2	CA	P	215	1/1	0.99	0.07	17,17,17,17	0
2	CA	A	214	1/1	0.99	0.06	19,19,19,19	0
2	CA	E	213	1/1	0.99	0.06	19,19,19,19	0
2	CA	H	213	1/1	0.99	0.08	22,22,22,22	0
2	CA	E	214	1/1	0.99	0.03	19,19,19,19	0
2	CA	L	213	1/1	0.99	0.06	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	215	1/1	0.99	0.06	16,16,16,16	0
2	CA	Q	363	1/1	0.99	0.05	29,29,29,29	0
2	CA	A	213	1/1	0.99	0.06	19,19,19,19	0
2	CA	R	213	1/1	0.99	0.04	19,19,19,19	0
2	CA	R	214	1/1	0.99	0.07	19,19,19,19	0
2	CA	R	215	1/1	0.99	0.06	17,17,17,17	0
2	CA	I	213	1/1	0.99	0.07	24,24,24,24	0
2	CA	L	381	1/1	0.99	0.03	14,14,14,14	0
2	CA	G	215	1/1	1.00	0.07	19,19,19,19	0
2	CA	W	233	1/1	1.00	0.04	15,15,15,15	0
2	CA	H	215	1/1	1.00	0.06	17,17,17,17	0
2	CA	B	215	1/1	1.00	0.04	16,16,16,16	0
2	CA	I	215	1/1	1.00	0.14	23,23,23,23	0
2	CA	O	215	1/1	1.00	0.07	17,17,17,17	0
2	CA	X	243	1/1	1.00	0.06	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.