



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:48 PM GMT

PDB ID : 3A68
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 validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

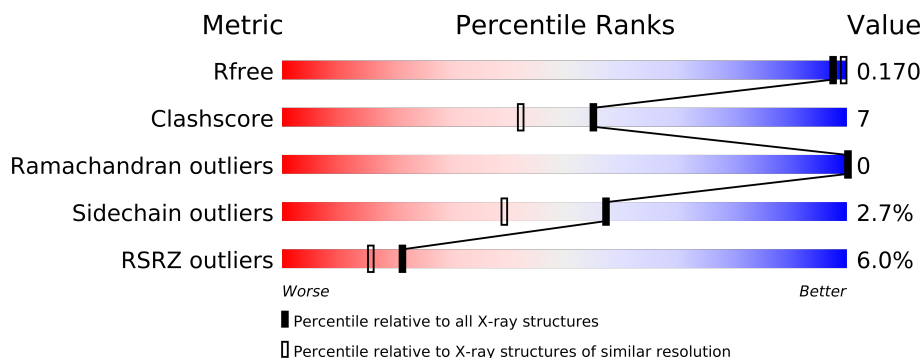
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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.












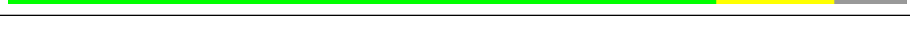
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	212	
1	B	212	
1	C	212	
1	D	212	
1	E	212	
1	F	212	
1	G	212	
1	H	212	
1	I	212	
1	J	212	
1	K	212	
1	L	212	
1	M	212	
1	N	212	

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Mol	Chain	Length	Quality of chain
1	O	212	
1	P	212	
1	Q	212	
1	R	212	
1	S	212	
1	T	212	
1	U	212	
1	V	212	
1	W	212	
1	X	212	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	A	216	-	X
2	CA	A	351[A]	-	X
2	CA	B	213	-	X
2	CA	C	216	-	X
2	CA	C	403	-	X
2	CA	D	213	-	X
2	CA	D	215	-	X
2	CA	D	404	-	X
2	CA	E	216	-	X
2	CA	F	216	-	X
2	CA	F	406	-	X
2	CA	G	213	-	X
2	CA	G	216	-	X
2	CA	H	213	-	X
2	CA	H	216	-	X
2	CA	H	408	-	X
2	CA	I	216	-	X
2	CA	J	216	-	X
2	CA	K	216	-	X
2	CA	K	371	-	X
2	CA	K	411	-	X
2	CA	L	215	-	X
2	CA	L	216	-	X
2	CA	M	216	-	X
2	CA	M	413	-	X
2	CA	N	213	-	X
2	CA	N	216	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	CA	N	414	-	X
2	CA	O	216	-	X
2	CA	O	415	-	X
2	CA	P	216	-	X
2	CA	Q	213	-	X
2	CA	Q	215	-	X
2	CA	Q	216	-	X
2	CA	Q	417	-	X
2	CA	R	216	-	X
2	CA	R	418	-	X
2	CA	S	213	-	X
2	CA	S	216	-	X
2	CA	T	213	-	X
2	CA	T	216	-	X
2	CA	T	420	-	X
2	CA	U	215	-	X
2	CA	V	224	-	X
2	CA	W	234	-	X
2	CA	W	423	-	X
2	CA	X	244	-	X
2	CA	X	352[B]	-	X
2	CA	X	424	-	X
3	ACY	G	217	-	X
3	ACY	I	217	-	X
3	ACY	S	217	-	X
3	ACY	V	213	-	X
3	ACY	X	213	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 44039 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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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 (three-letter code: CA) (formula: Ca).

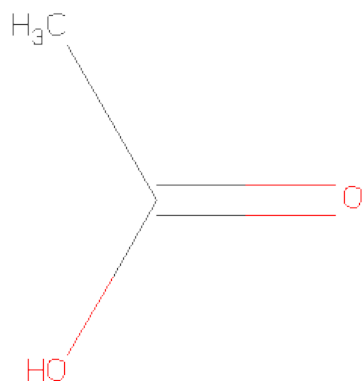
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	5	Total	Ca	0	0
			5	5		
2	K	7	Total	Ca	0	0
			7	7		
2	B	5	Total	Ca	0	0
			5	5		
2	W	5	Total	Ca	0	0
			5	5		
2	N	6	Total	Ca	0	1
			6	6		
2	X	6	Total	Ca	0	1
			6	6		
2	S	5	Total	Ca	0	0
			5	5		
2	J	6	Total	Ca	0	1
			6	6		
2	E	7	Total	Ca	0	0
			7	7		
2	V	5	Total	Ca	0	0
			5	5		
2	A	7	Total	Ca	0	1
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	R	5	Total 5	Ca 5	0	0
2	M	5	Total 5	Ca 5	0	0
2	D	5	Total 5	Ca 5	0	0
2	I	6	Total 6	Ca 6	0	0
2	U	4	Total 4	Ca 4	0	0
2	L	7	Total 7	Ca 7	0	0
2	G	5	Total 5	Ca 5	0	0
2	Q	6	Total 6	Ca 6	0	0
2	H	5	Total 5	Ca 5	0	0
2	C	7	Total 7	Ca 7	0	0
2	T	5	Total 5	Ca 5	0	0
2	O	7	Total 7	Ca 7	0	0
2	F	5	Total 5	Ca 5	0	0

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

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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		

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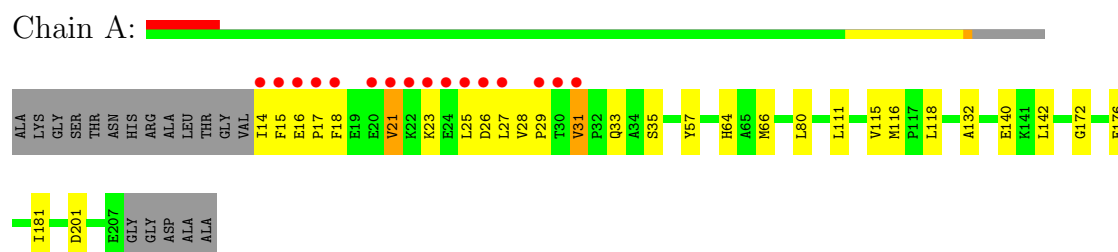
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	179	Total 181	O 181	0	2
4	Q	187	Total 192	O 192	0	5
4	R	194	Total 197	O 197	0	3
4	S	183	Total 184	O 184	0	1
4	T	182	Total 183	O 183	0	1
4	U	186	Total 190	O 190	0	4
4	V	186	Total 188	O 188	0	2
4	W	175	Total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

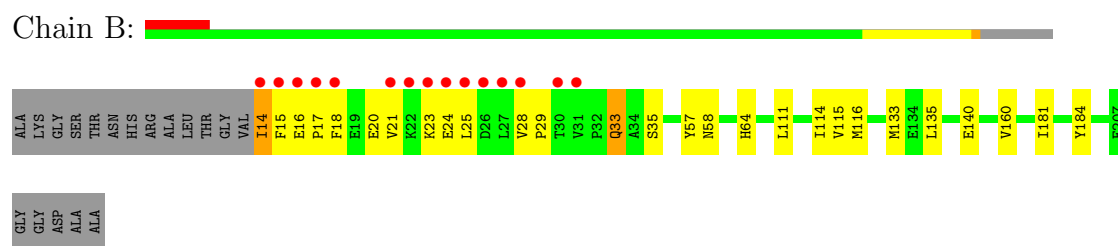
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

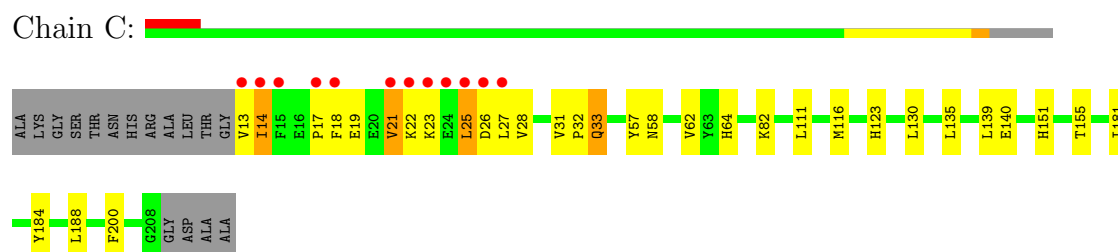
- Molecule 1: Ferritin-4, chloroplastic



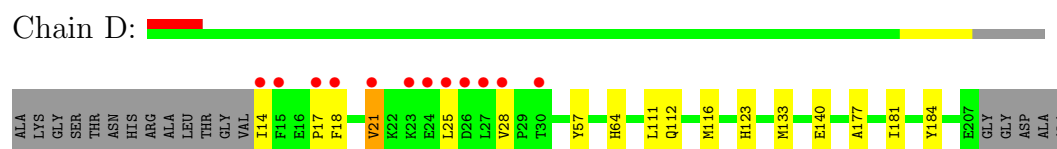
- Molecule 1: Ferritin-4, chloroplastic



- Molecule 1: Ferritin-4, chloroplastic

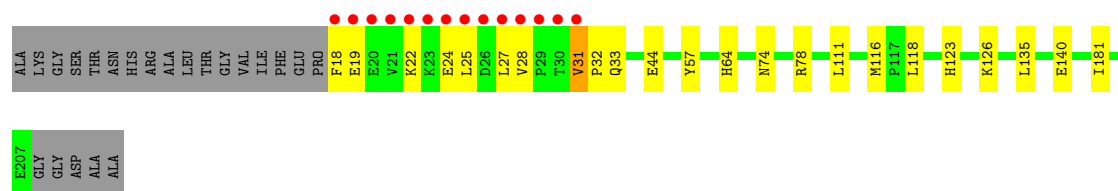


- Molecule 1: Ferritin-4, chloroplastic



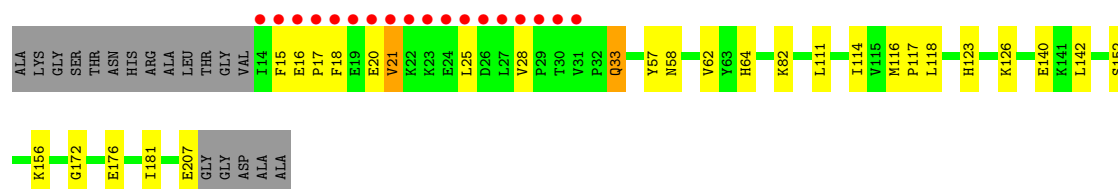
- Molecule 1: Ferritin-4, chloroplastic





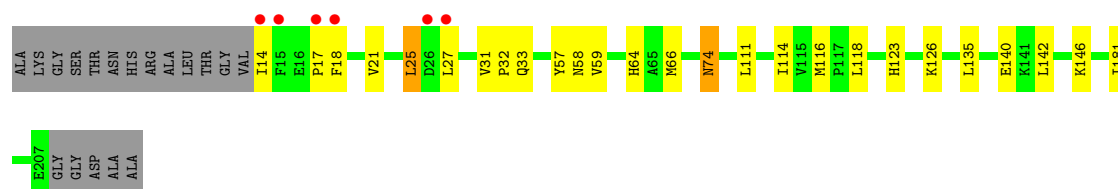
- Molecule 1: Ferritin-4, chloroplastic

Chain F:



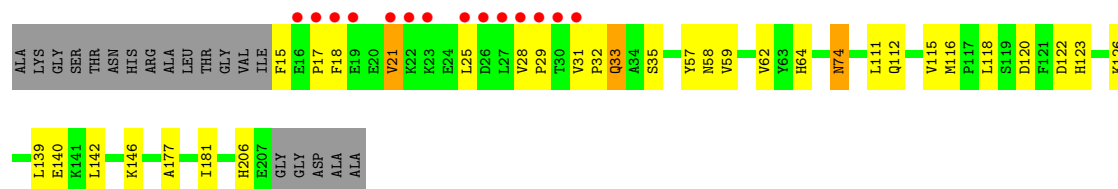
- Molecule 1: Ferritin-4, chloroplastic

Chain G:



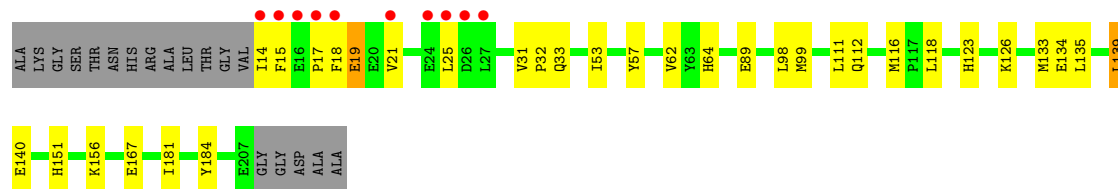
- Molecule 1: Ferritin-4, chloroplastic

Chain H:



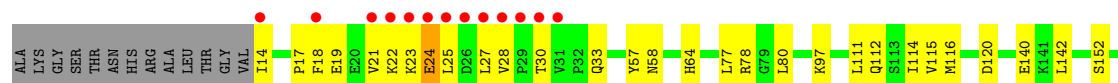
- Molecule 1: Ferritin-4, chloroplastic

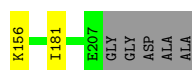
Chain I:



- Molecule 1: Ferritin-4, chloroplastic

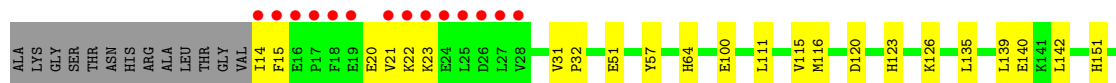
Chain J:





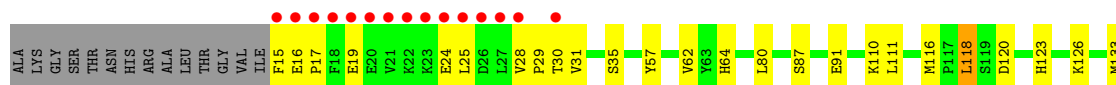
- Molecule 1: Ferritin-4, chloroplastic

Chain K:



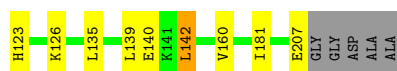
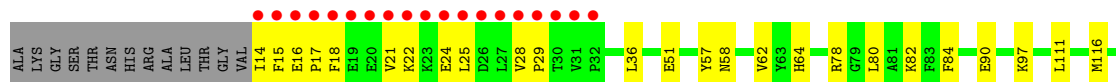
- Molecule 1: Ferritin-4, chloroplastic

Chain L:



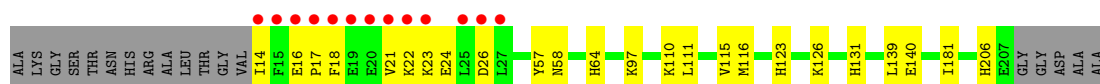
- Molecule 1: Ferritin-4, chloroplastic

Chain M:



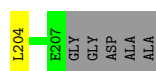
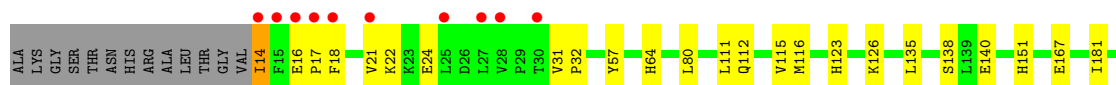
- Molecule 1: Ferritin-4, chloroplastic

Chain N:



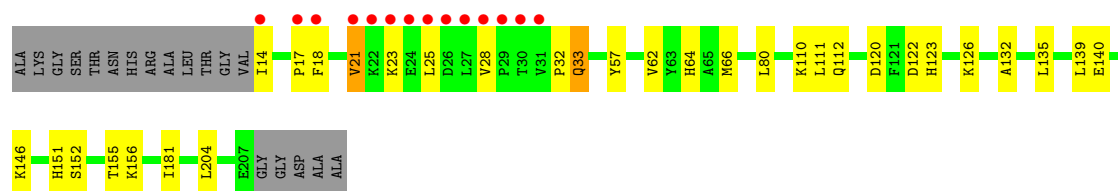
- Molecule 1: Ferritin-4, chloroplastic

Chain O:



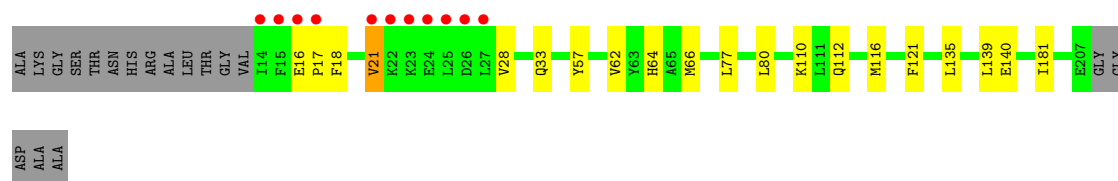
- Molecule 1: Ferritin-4, chloroplastic

Chain P:



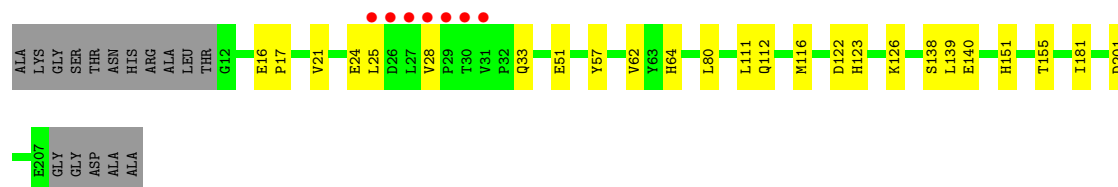
- Molecule 1: Ferritin-4, chloroplastic

Chain Q:



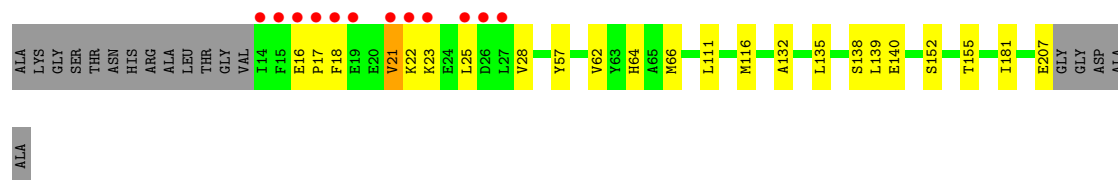
- Molecule 1: Ferritin-4, chloroplastic

Chain R:



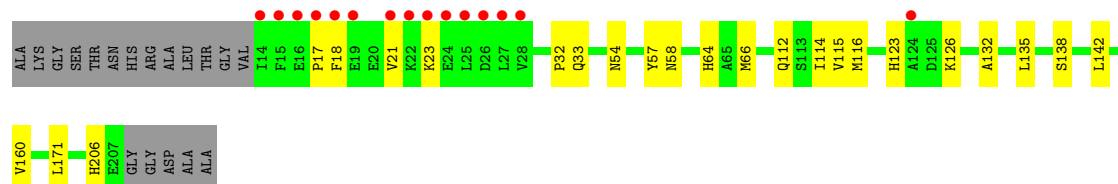
- Molecule 1: Ferritin-4, chloroplastic

Chain S:



- Molecule 1: Ferritin-4, chloroplastic

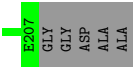
Chain T:



- Molecule 1: Ferritin-4, chloroplastic

Chain U:





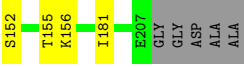
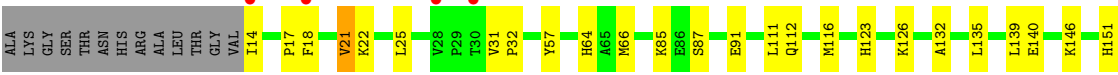
• Molecule 1: Ferritin-4, chloroplastic

Chain V:



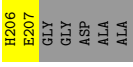
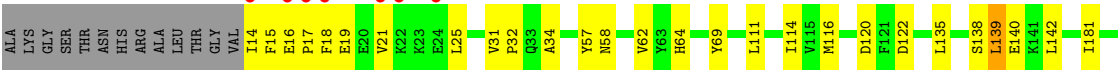
• Molecule 1: Ferritin-4, chloroplastic

Chain W:



• Molecule 1: Ferritin-4, chloroplastic

Chain X:



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)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.142 , 0.173 0.139 , 0.170	Depositor DCC
R_{free} test set	27426 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.2	EDS
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 546458 reflections	Xtriage
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

Xtriage'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.

5 Model quality

5.1 Standard geometry

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	0.28	0/1685	0.42	0/2270
1	B	0.28	0/1673	0.42	0/2254
1	C	0.28	0/1720	0.41	0/2317
1	D	0.28	0/1684	0.42	0/2268
1	E	0.28	0/1645	0.42	0/2212
1	F	0.28	0/1693	0.42	0/2280
1	G	0.27	0/1668	0.42	0/2248
1	H	0.27	0/1685	0.41	0/2270
1	I	0.27	0/1722	0.42	0/2320
1	J	0.28	0/1695	0.43	0/2284
1	K	0.27	0/1646	0.42	0/2217
1	L	0.27	0/1644	0.41	0/2215
1	M	0.28	0/1701	0.42	0/2292
1	N	0.27	0/1674	0.42	0/2255
1	O	0.29	0/1701	0.43	0/2291
1	P	0.27	0/1682	0.41	0/2265
1	Q	0.28	0/1696	0.43	0/2283
1	R	0.28	0/1686	0.42	0/2272
1	S	0.27	0/1669	0.42	0/2248
1	T	0.26	0/1700	0.41	0/2290
1	U	0.28	0/1703	0.42	0/2292
1	V	0.26	0/1704	0.41	0/2294
1	W	0.26	0/1699	0.40	0/2288
1	X	0.28	0/1730	0.41	0/2329
All	All	0.27	0/40505	0.42	0/54554

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1631	0	1611	30	0
1	B	1631	0	1601	35	0
1	C	1675	0	1635	42	0
1	D	1639	0	1607	23	0
1	E	1591	0	1575	20	0
1	F	1636	0	1610	42	0
1	G	1623	0	1595	30	0
1	H	1631	0	1604	35	0
1	I	1662	0	1643	33	0
1	J	1644	0	1617	26	0
1	K	1607	0	1571	22	0
1	L	1605	0	1576	27	0
1	M	1644	0	1626	37	0
1	N	1620	0	1597	25	0
1	O	1647	0	1614	29	0
1	P	1632	0	1599	29	0
1	Q	1639	0	1631	21	0
1	R	1635	0	1607	26	0
1	S	1618	0	1606	25	0
1	T	1653	0	1616	28	0
1	U	1643	0	1632	23	0
1	V	1645	0	1626	27	0
1	W	1648	0	1618	21	0
1	X	1664	0	1642	27	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	6	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	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0
4	S	184	0	0	3	0
4	T	183	0	0	7	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	525	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 525 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	174 (97%)	5 (3%)	56	38
1	B	178/179 (99%)	174 (98%)	4 (2%)	64	48
1	C	183/179 (102%)	176 (96%)	7 (4%)	44	24
1	D	179/179 (100%)	176 (98%)	3 (2%)	73	61
1	E	175/179 (98%)	170 (97%)	5 (3%)	55	37
1	F	180/179 (101%)	176 (98%)	4 (2%)	64	48
1	G	177/179 (99%)	172 (97%)	5 (3%)	56	38
1	H	179/179 (100%)	173 (97%)	6 (3%)	49	29
1	I	184/179 (103%)	179 (97%)	5 (3%)	57	39
1	J	180/179 (101%)	172 (96%)	8 (4%)	39	18
1	K	174/179 (97%)	168 (97%)	6 (3%)	49	29
1	L	174/179 (97%)	169 (97%)	5 (3%)	55	37
1	M	181/179 (101%)	174 (96%)	7 (4%)	43	23
1	N	178/179 (99%)	175 (98%)	3 (2%)	73	61
1	O	181/179 (101%)	178 (98%)	3 (2%)	73	61
1	P	179/179 (100%)	172 (96%)	7 (4%)	43	23
1	Q	181/179 (101%)	177 (98%)	4 (2%)	64	48
1	R	179/179 (100%)	176 (98%)	3 (2%)	73	61
1	S	178/179 (99%)	175 (98%)	3 (2%)	73	61
1	T	181/179 (101%)	176 (97%)	5 (3%)	56	38
1	U	182/179 (102%)	179 (98%)	3 (2%)	75	63
1	V	182/179 (102%)	177 (97%)	5 (3%)	57	39
1	W	181/179 (101%)	177 (98%)	4 (2%)	64	48
1	X	185/179 (103%)	180 (97%)	5 (3%)	57	39
All	All	4310/4296 (100%)	4195 (97%)	115 (3%)	57	39

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	20	GLU
1	M	51	GLU
1	W	21	VAL
1	K	51[A]	GLU
1	L	30	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	206	HIS
1	L	123	HIS
1	U	206	HIS
1	I	58	ASN
1	J	54	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	217	-	3,3,3	0.65	0	3,3,3	0.70	0
3	ACY	E	217	-	3,3,3	0.66	0	3,3,3	0.66	0
3	ACY	F	217	-	3,3,3	0.68	0	3,3,3	0.55	0
3	ACY	G	217	-	3,3,3	0.64	0	3,3,3	0.68	0
3	ACY	H	217	-	3,3,3	0.67	0	3,3,3	0.65	0
3	ACY	I	217	-	3,3,3	0.66	0	3,3,3	0.66	0
3	ACY	J	217	-	3,3,3	0.64	0	3,3,3	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACY	L	217	-	3,3,3	0.64	0	3,3,3	0.63	0
3	ACY	M	217	-	3,3,3	0.66	0	3,3,3	0.63	0
3	ACY	O	217	-	3,3,3	0.66	0	3,3,3	0.60	0
3	ACY	P	217	-	3,3,3	0.66	0	3,3,3	0.69	0
3	ACY	Q	217	-	3,3,3	0.67	0	3,3,3	0.60	0
3	ACY	R	217	-	3,3,3	0.64	0	3,3,3	0.72	0
3	ACY	S	217	-	3,3,3	0.64	0	3,3,3	0.71	0
3	ACY	T	217	-	3,3,3	0.67	0	3,3,3	0.61	0
3	ACY	V	213	-	3,3,3	0.64	0	3,3,3	0.70	0
3	ACY	W	213	-	3,3,3	0.68	0	3,3,3	0.60	0
3	ACY	X	213	-	3,3,3	0.70	0	3,3,3	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACY	A	217	-	-	0/0/0/0	0/0/0/0
3	ACY	E	217	-	-	0/0/0/0	0/0/0/0
3	ACY	F	217	-	-	0/0/0/0	0/0/0/0
3	ACY	G	217	-	-	0/0/0/0	0/0/0/0
3	ACY	H	217	-	-	0/0/0/0	0/0/0/0
3	ACY	I	217	-	-	0/0/0/0	0/0/0/0
3	ACY	J	217	-	-	0/0/0/0	0/0/0/0
3	ACY	L	217	-	-	0/0/0/0	0/0/0/0
3	ACY	M	217	-	-	0/0/0/0	0/0/0/0
3	ACY	O	217	-	-	0/0/0/0	0/0/0/0
3	ACY	P	217	-	-	0/0/0/0	0/0/0/0
3	ACY	Q	217	-	-	0/0/0/0	0/0/0/0
3	ACY	R	217	-	-	0/0/0/0	0/0/0/0
3	ACY	S	217	-	-	0/0/0/0	0/0/0/0
3	ACY	T	217	-	-	0/0/0/0	0/0/0/0
3	ACY	V	213	-	-	0/0/0/0	0/0/0/0
3	ACY	W	213	-	-	0/0/0/0	0/0/0/0
3	ACY	X	213	-	-	0/0/0/0	0/0/0/0

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.

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, 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%)	-0.29	16 (8%) 12 8	6, 11, 83, 104	0
1	B	194/212 (91%)	-0.33	15 (7%) 13 10	7, 12, 76, 106	0
1	C	196/212 (92%)	-0.44	12 (6%) 21 15	7, 13, 50, 98	0
1	D	194/212 (91%)	-0.39	12 (6%) 20 14	7, 12, 71, 103	0
1	E	190/212 (89%)	-0.30	14 (7%) 14 10	6, 12, 83, 124	0
1	F	194/212 (91%)	-0.36	18 (9%) 9 6	6, 12, 71, 100	0
1	G	194/212 (91%)	-0.53	6 (3%) 47 39	6, 12, 51, 86	0
1	H	193/212 (91%)	-0.39	14 (7%) 15 10	6, 12, 64, 101	0
1	I	194/212 (91%)	-0.41	10 (5%) 26 20	6, 13, 66, 88	0
1	J	194/212 (91%)	-0.35	13 (6%) 17 12	6, 12, 65, 97	0
1	K	194/212 (91%)	-0.35	14 (7%) 15 11	6, 13, 74, 101	0
1	L	193/212 (91%)	-0.30	15 (7%) 13 9	6, 13, 86, 109	0
1	M	194/212 (91%)	-0.26	19 (9%) 8 6	7, 12, 85, 114	0
1	N	194/212 (91%)	-0.44	13 (6%) 17 12	6, 13, 61, 103	0
1	O	194/212 (91%)	-0.44	10 (5%) 26 20	5, 11, 65, 106	0
1	P	194/212 (91%)	-0.38	14 (7%) 15 11	6, 13, 52, 93	0
1	Q	194/212 (91%)	-0.47	11 (5%) 23 17	4, 11, 67, 104	0
1	R	196/212 (92%)	-0.50	7 (3%) 41 33	6, 12, 63, 94	0
1	S	194/212 (91%)	-0.41	12 (6%) 20 14	6, 11, 69, 91	0
1	T	194/212 (91%)	-0.37	15 (7%) 13 10	6, 13, 73, 100	0
1	U	194/212 (91%)	-0.53	9 (4%) 31 24	5, 12, 63, 96	0
1	V	194/212 (91%)	-0.54	6 (3%) 47 39	7, 13, 54, 100	0
1	W	194/212 (91%)	-0.55	4 (2%) 60 54	7, 12, 52, 84	0
1	X	194/212 (91%)	-0.51	7 (3%) 41 33	7, 12, 49, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
All	All	4654/5088 (91%)	-0.41	286 (6%)	21 15	4, 12, 68, 124	0

The worst 5 of 286 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	ILE	13.2
1	A	14	ILE	12.1
1	E	27	LEU	11.3
1	D	14	ILE	10.1
1	E	21	VAL	9.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CA	T	420	1/1	0.20	241.00	56,56,56,56	0
2	CA	O	415	1/1	0.22	43.86	66,66,66,66	0
2	CA	T	216	1/1	0.33	36.87	80,80,80,80	0
2	CA	W	423	1/1	0.21	25.00	68,68,68,68	0
2	CA	X	424	1/1	0.14	17.25	55,55,55,55	0
2	CA	V	224	1/1	0.25	15.95	77,77,77,77	0
2	CA	M	216	1/1	0.19	15.64	56,56,56,56	0
2	CA	Q	417	1/1	0.13	14.11	63,63,63,63	0
2	CA	J	216	1/1	0.15	13.15	48,48,48,48	0
2	CA	K	411	1/1	0.14	12.20	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	N	213	1/1	0.13	10.25	28,28,28,28	0
2	CA	W	234	1/1	0.18	9.64	60,60,60,60	0
2	CA	X	244	1/1	0.16	9.60	39,39,39,39	0
2	CA	K	371	1/1	0.23	9.54	58,58,58,58	0
2	CA	R	418	1/1	0.13	9.15	68,68,68,68	0
2	CA	A	216	1/1	0.16	8.89	48,48,48,48	0
2	CA	P	216	1/1	0.18	8.75	42,42,42,42	0
2	CA	O	216	1/1	0.19	8.71	43,43,43,43	0
2	CA	N	216	1/1	0.20	8.57	44,44,44,44	0
2	CA	S	216	1/1	0.23	8.47	66,66,66,66	0
2	CA	B	213	1/1	0.10	8.22	27,27,27,27	0
2	CA	X	352[B]	1/1	0.20	8.12	30,30,30,30	1
2	CA	H	408	1/1	0.16	8.00	69,69,69,69	0
2	CA	H	216	1/1	0.17	7.24	47,47,47,47	0
2	CA	D	215	1/1	0.14	7.16	48,48,48,48	0
2	CA	D	404	1/1	0.15	7.09	63,63,63,63	0
2	CA	R	216	1/1	0.17	6.92	49,49,49,49	0
2	CA	C	403	1/1	0.11	6.50	60,60,60,60	0
2	CA	L	216	1/1	0.18	6.49	55,55,55,55	0
2	CA	G	216	1/1	0.16	6.28	53,53,53,53	0
2	CA	M	413	1/1	0.12	5.67	45,45,45,45	0
2	CA	F	216	1/1	0.17	5.39	38,38,38,38	0
2	CA	Q	216	1/1	0.12	5.26	42,42,42,42	0
2	CA	K	216	1/1	0.15	4.98	51,51,51,51	0
2	CA	E	216	1/1	0.15	4.79	39,39,39,39	0
2	CA	U	215	1/1	0.12	4.73	37,37,37,37	0
2	CA	F	406	1/1	0.13	4.60	59,59,59,59	0
2	CA	N	414	1/1	0.13	4.05	52,52,52,52	0
2	CA	G	213	1/1	0.07	3.95	26,26,26,26	0
3	ACY	X	213	4/4	0.19	3.93	14,21,41,90	0
2	CA	L	215	1/1	0.13	3.44	28,28,28,28	0
3	ACY	G	217	4/4	0.23	3.11	16,20,33,83	0
2	CA	T	213	1/1	0.07	3.09	29,29,29,29	0
3	ACY	S	217	4/4	0.17	2.93	18,19,47,56	0
2	CA	Q	215	1/1	0.12	2.73	35,35,35,35	0
2	CA	S	213	1/1	0.11	2.71	28,28,28,28	0
2	CA	I	216	1/1	0.15	2.69	54,54,54,54	0
2	CA	Q	213	1/1	0.08	2.69	26,26,26,26	0
3	ACY	I	217	4/4	0.20	2.68	24,25,48,84	0
3	ACY	V	213	4/4	0.20	2.57	19,21,39,86	0
2	CA	H	213	1/1	0.07	2.45	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	C	216	1/1	0.13	2.37	44,44,44,44	0
2	CA	D	213	1/1	0.10	2.27	26,26,26,26	0
2	CA	A	351[A]	1/1	0.10	2.09	10,10,10,10	1
3	ACY	W	213	4/4	0.19	1.95	20,26,38,43	0
2	CA	V	221	1/1	0.06	1.84	22,22,22,22	0
2	CA	N	215	1/1	0.10	1.80	28,28,28,28	0
3	ACY	O	217	4/4	0.17	1.65	18,21,63,65	0
2	CA	K	215	1/1	0.11	1.60	34,34,34,34	0
2	CA	B	216	1/1	0.10	1.52	39,39,39,39	0
3	ACY	Q	217	4/4	0.14	1.50	14,20,57,59	0
2	CA	I	332	1/1	0.12	1.35	24,24,24,24	0
3	ACY	L	217	4/4	0.17	1.27	19,28,34,50	0
2	CA	I	213	1/1	0.07	1.26	24,24,24,24	0
2	CA	C	323	1/1	0.11	1.25	33,33,33,33	0
2	CA	I	215	1/1	0.12	1.23	23,23,23,23	0
3	ACY	A	217	4/4	0.17	1.19	18,22,40,51	0
2	CA	X	241	1/1	0.06	1.16	22,22,22,22	0
2	CA	B	402	1/1	0.10	1.10	51,51,51,51	0
2	CA	O	342	1/1	0.10	1.05	21,21,21,21	0
2	CA	D	214	1/1	0.08	0.89	33,33,33,33	0
2	CA	U	214	1/1	0.08	0.80	33,33,33,33	0
3	ACY	P	217	4/4	0.15	0.79	23,24,35,52	0
3	ACY	H	217	4/4	0.20	0.79	18,26,36,65	0
3	ACY	T	217	4/4	0.15	0.78	23,24,51,72	0
2	CA	C	213	1/1	0.07	0.78	28,28,28,28	0
3	ACY	M	217	4/4	0.18	0.73	19,26,46,55	0
3	ACY	F	217	4/4	0.15	0.64	19,20,48,73	0
3	ACY	R	217	4/4	0.14	0.56	23,23,35,38	0
3	ACY	E	217	4/4	0.18	0.51	24,24,35,51	0
2	CA	A	353	1/1	0.08	0.28	26,26,26,26	0
2	CA	L	214	1/1	0.07	0.28	28,28,28,28	0
2	CA	F	213	1/1	0.06	0.25	20,20,20,20	0
3	ACY	J	217	4/4	0.12	0.17	24,27,41,51	0
2	CA	C	215	1/1	0.09	0.02	20,20,20,20	0
2	CA	J	362[B]	1/1	0.07	-0.21	28,28,28,28	1
2	CA	C	321	1/1	0.07	-0.41	31,31,31,31	0
2	CA	S	215	1/1	0.07	-0.44	24,24,24,24	0
2	CA	F	214	1/1	0.06	-0.54	23,23,23,23	0
2	CA	T	215	1/1	0.07	-0.54	23,23,23,23	0
2	CA	K	214	1/1	0.07	-0.62	30,30,30,30	0
2	CA	E	215	1/1	0.06	-0.69	28,28,28,28	0
2	CA	E	312	1/1	0.06	-0.82	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	J	214	1/1	0.05	-1.05	18,18,18,18	0
2	CA	R	214	1/1	0.06	-1.19	19,19,19,19	0
2	CA	W	231	1/1	0.04	-1.20	21,21,21,21	0
2	CA	I	214	1/1	0.06	-1.29	25,25,25,25	0
2	CA	U	213	1/1	0.04	-1.31	21,21,21,21	0
2	CA	Q	214	1/1	0.05	-1.36	22,22,22,22	0
2	CA	N	361[A]	1/1	0.06	-1.40	12,12,12,12	1
2	CA	C	214	1/1	0.06	-1.53	20,20,20,20	0
2	CA	O	341	1/1	0.05	-1.54	24,24,24,24	0
2	CA	P	215	1/1	0.04	-1.54	17,17,17,17	0
2	CA	P	213	1/1	0.04	-1.57	22,22,22,22	0
2	CA	D	331	1/1	0.04	-1.60	23,23,23,23	0
2	CA	M	213	1/1	0.04	-1.63	23,23,23,23	0
2	CA	G	215	1/1	0.05	-1.76	19,19,19,19	0
2	CA	K	373	1/1	0.05	-1.99	28,28,28,28	0
2	CA	W	232	1/1	0.04	-2.07	18,18,18,18	0
2	CA	O	215	1/1	0.04	-2.35	17,17,17,17	0
2	CA	A	214	1/1	0.04	-2.57	19,19,19,19	0
2	CA	A	215	1/1	0.04	-2.60	16,16,16,16	0
2	CA	E	214	1/1	0.04	-2.67	19,19,19,19	0
2	CA	E	213	1/1	0.04	-2.85	19,19,19,19	0
2	CA	E	311	1/1	0.03	-2.86	19,19,19,19	0
2	CA	F	215	1/1	0.04	-2.96	19,19,19,19	0
2	CA	A	213	1/1	0.03	-3.10	19,19,19,19	0
2	CA	H	214	1/1	0.04	-3.10	16,16,16,16	0
2	CA	N	214	1/1	0.04	-3.17	21,21,21,21	0
2	CA	R	215	1/1	0.04	-3.20	17,17,17,17	0
2	CA	K	213	1/1	0.04	-3.25	26,26,26,26	0
2	CA	J	215	1/1	0.04	-3.28	18,18,18,18	0
2	CA	L	382	1/1	0.05	-3.56	21,21,21,21	0
2	CA	X	242	1/1	0.03	-3.62	19,19,19,19	0
2	CA	V	223	1/1	0.04	-3.63	21,21,21,21	0
2	CA	L	381	1/1	0.04	-3.78	14,14,14,14	0
2	CA	G	214	1/1	0.03	-3.80	19,19,19,19	0
2	CA	T	214	1/1	0.04	-4.11	23,23,23,23	0
2	CA	M	215	1/1	0.03	-4.37	18,18,18,18	0
2	CA	Q	363	1/1	0.03	-4.40	29,29,29,29	0
2	CA	P	214	1/1	0.03	-4.90	22,22,22,22	0
2	CA	M	214	1/1	0.04	-4.94	19,19,19,19	0
2	CA	O	214	1/1	0.03	-5.31	17,17,17,17	0
2	CA	H	215	1/1	0.03	-5.34	17,17,17,17	0
2	CA	W	233	1/1	0.02	-5.40	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	X	243	1/1	0.03	-5.53	19,19,19,19	0
2	CA	J	213	1/1	0.05	-5.81	23,23,23,23	0
2	CA	O	213	1/1	0.04	-6.99	20,20,20,20	0
2	CA	V	222	1/1	0.03	-7.41	20,20,20,20	0
2	CA	S	214	1/1	0.03	-7.48	17,17,17,17	0
2	CA	B	214	1/1	0.03	-8.01	16,16,16,16	0
2	CA	R	213	1/1	0.03	-12.50	19,19,19,19	0
2	CA	L	213	1/1	0.03	-12.98	22,22,22,22	0
2	CA	B	215	1/1	0.02	-16.10	16,16,16,16	0
2	CA	I	409	1/1	0.17	-	66,66,66,66	0
2	CA	E	405	1/1	0.21	-	80,80,80,80	0
2	CA	G	407	1/1	0.23	-	62,62,62,62	0
2	CA	V	422	1/1	0.15	-	64,64,64,64	0
2	CA	P	416	1/1	0.18	-	72,72,72,72	0
2	CA	L	412	1/1	0.09	-	47,47,47,47	0
2	CA	J	410	1/1	0.18	-	77,77,77,77	0
2	CA	A	401	1/1	0.10	-	52,52,52,52	0
2	CA	U	421	1/1	0.22	-	68,68,68,68	0
2	CA	S	419	1/1	0.17	-	77,77,77,77	0

6.5 Other polymers ⓘ

There are no such residues in this entry.