wwPDB X-ray Structure Validation Summary Report (i)

Oct 22, 2023 – 04:41 PM EDT

PDB ID	:	3A9Q
Title	:	Crystal Structure Analysis of E173A variant of the soybean ferritin SFER4
Authors	:	Masuda, T.; Goto, F.; Yoshihara, T.; Mikami, B.
Deposited on	:	2009-11-05
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

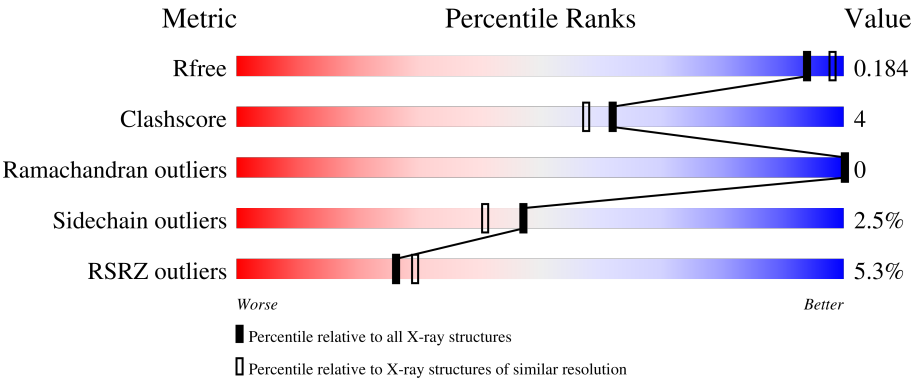
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	212	7% 82% 8% • 8%
1	B	212	8% 82% 9% • 8%
1	C	212	2% 78% 13% 8%
1	D	212	4% 80% 11% 8%
1	E	212	% 75% 7% • 16%

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Mol	Chain	Length	Quality of chain
1	F	212	9% 83% 8% 8%
1	G	212	82% 8% • 9%
1	H	212	8% 80% 10% 9%
1	I	212	2% 78% 13% 9%
1	J	212	5% 81% 10% • 8%
1	K	212	7% 83% 7% 9%
1	L	212	8% 82% 8% 9%
1	M	212	8% 75% 14% • 9%
1	N	212	4% 82% 9% 9%
1	O	212	6% 83% 8% 9%
1	P	212	4% 79% 11% • 9%
1	Q	212	8% 80% 10% • 9%
1	R	212	2% 83% 8% • 8%
1	S	212	5% 84% 7% 9%
1	T	212	6% 82% 10% 8%
1	U	212	3% 81% 9% • 9%
1	V	212	% 83% 8% 9%
1	W	212	4% 83% 8% 8%
1	X	212	2% 84% 7% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 42812 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
1	A	194	Total	C	N	O	S	0	9	0
			1621	1033	270	312	6			
1	B	194	Total	C	N	O	S	0	11	0
			1633	1039	271	316	7			
1	C	194	Total	C	N	O	S	0	16	0
			1669	1059	277	328	5			
1	D	194	Total	C	N	O	S	0	15	0
			1661	1056	273	326	6			
1	E	178	Total	C	N	O	S	0	11	0
			1492	945	252	289	6			
1	F	194	Total	C	N	O	S	0	12	0
			1636	1043	271	316	6			
1	G	193	Total	C	N	O	S	0	10	0
			1617	1027	269	315	6			
1	H	193	Total	C	N	O	S	0	12	0
			1631	1037	272	317	5			
1	I	193	Total	C	N	O	S	0	20	0
			1677	1069	274	328	6			
1	J	194	Total	C	N	O	S	0	11	0
			1637	1041	275	316	5			
1	K	193	Total	C	N	O	S	0	6	0
			1599	1013	270	311	5			
1	L	193	Total	C	N	O	S	0	9	0
			1618	1029	270	314	5			
1	M	193	Total	C	N	O	S	0	15	0
			1651	1050	275	320	6			
1	N	193	Total	C	N	O	S	0	13	0
			1631	1036	270	319	6			
1	O	193	Total	C	N	O	S	0	16	0
			1657	1051	274	327	5			
1	P	193	Total	C	N	O	S	0	12	0
			1631	1035	270	321	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	193	Total	C	N	O	S	0	13	0
			1630	1040	271	312	7			
1	R	196	Total	C	N	O	S	0	11	0
			1643	1043	275	319	6			
1	S	193	Total	C	N	O	S	0	12	0
			1622	1033	269	315	5			
1	T	194	Total	C	N	O	S	0	13	0
			1650	1049	274	321	6			
1	U	193	Total	C	N	O	S	0	15	0
			1641	1045	271	318	7			
1	V	193	Total	C	N	O	S	0	13	0
			1633	1037	270	320	6			
1	W	194	Total	C	N	O	S	0	13	0
			1649	1048	275	320	6			
1	X	194	Total	C	N	O	S	0	15	0
			1652	1050	272	322	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	ALA	GLU	engineered mutation	UNP Q948P5
B	173	ALA	GLU	engineered mutation	UNP Q948P5
C	173	ALA	GLU	engineered mutation	UNP Q948P5
D	173	ALA	GLU	engineered mutation	UNP Q948P5
E	173	ALA	GLU	engineered mutation	UNP Q948P5
F	173	ALA	GLU	engineered mutation	UNP Q948P5
G	173	ALA	GLU	engineered mutation	UNP Q948P5
H	173	ALA	GLU	engineered mutation	UNP Q948P5
I	173	ALA	GLU	engineered mutation	UNP Q948P5
J	173	ALA	GLU	engineered mutation	UNP Q948P5
K	173	ALA	GLU	engineered mutation	UNP Q948P5
L	173	ALA	GLU	engineered mutation	UNP Q948P5
M	173	ALA	GLU	engineered mutation	UNP Q948P5
N	173	ALA	GLU	engineered mutation	UNP Q948P5
O	173	ALA	GLU	engineered mutation	UNP Q948P5
P	173	ALA	GLU	engineered mutation	UNP Q948P5
Q	173	ALA	GLU	engineered mutation	UNP Q948P5
R	173	ALA	GLU	engineered mutation	UNP Q948P5
S	173	ALA	GLU	engineered mutation	UNP Q948P5
T	173	ALA	GLU	engineered mutation	UNP Q948P5
U	173	ALA	GLU	engineered mutation	UNP Q948P5
V	173	ALA	GLU	engineered mutation	UNP Q948P5
W	173	ALA	GLU	engineered mutation	UNP Q948P5

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Chain	Residue	Modelled	Actual	Comment	Reference
X	173	ALA	GLU	engineered mutation	UNP Q948P5

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Ca 5 5	0	1
2	B	6	Total Ca 6 6	0	2
2	C	5	Total Ca 6 6	0	1
2	D	4	Total Ca 4 4	0	2
2	E	5	Total Ca 5 5	0	2
2	F	6	Total Ca 6 6	0	2
2	G	6	Total Ca 6 6	0	2
2	H	5	Total Ca 5 5	0	2
2	I	5	Total Ca 6 6	0	1
2	J	5	Total Ca 6 6	0	1
2	K	6	Total Ca 6 6	0	2
2	L	6	Total Ca 7 7	0	1
2	M	5	Total Ca 5 5	0	2
2	N	6	Total Ca 6 6	0	2
2	O	5	Total Ca 5 5	0	0
2	P	5	Total Ca 6 6	0	1
2	Q	4	Total Ca 4 4	0	2
2	R	6	Total Ca 6 6	0	2
2	S	5	Total Ca 5 5	0	2

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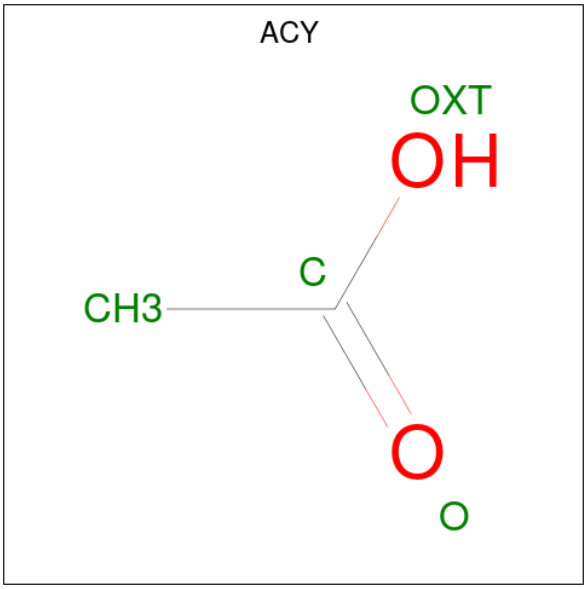
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	T	5	Total Ca 5 5	0	2
2	U	4	Total Ca 4 4	0	2
2	V	5	Total Ca 5 5	0	2
2	W	4	Total Ca 4 4	0	0
2	X	7	Total Ca 7 7	0	2

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	158	Total O 158 158	0	0
4	B	149	Total O 149 149	0	0
4	C	143	Total O 143 143	0	0
4	D	130	Total O 130 130	0	0
4	E	150	Total O 150 150	0	0
4	F	146	Total O 146 146	0	0
4	G	155	Total O 155 155	0	0

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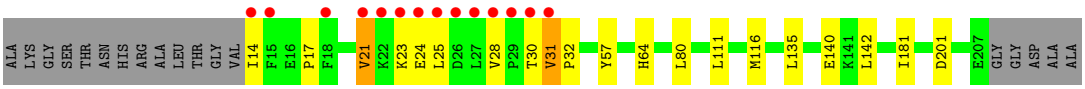
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	143	Total O 145 145	0	2
4	I	133	Total O 133 133	0	0
4	J	142	Total O 142 142	0	0
4	K	129	Total O 129 129	0	0
4	L	136	Total O 136 136	0	0
4	M	134	Total O 134 134	0	0
4	N	144	Total O 145 145	0	1
4	O	162	Total O 162 162	0	0
4	P	136	Total O 136 136	0	0
4	Q	147	Total O 148 148	0	1
4	R	150	Total O 150 150	0	0
4	S	137	Total O 137 137	0	0
4	T	135	Total O 135 135	0	0
4	U	135	Total O 135 135	0	0
4	V	146	Total O 146 146	0	0
4	W	137	Total O 137 137	0	0
4	X	148	Total O 148 148	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.

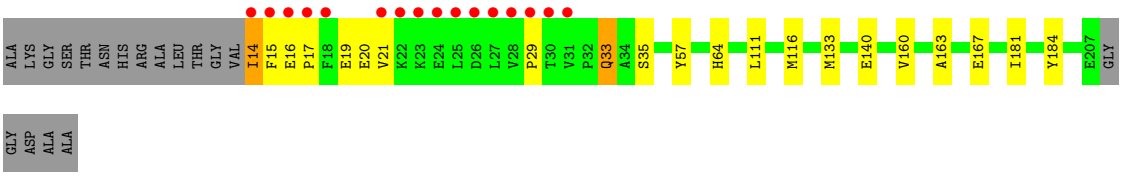
• Molecule 1: Ferritin-4, chloroplastic

Chain A:



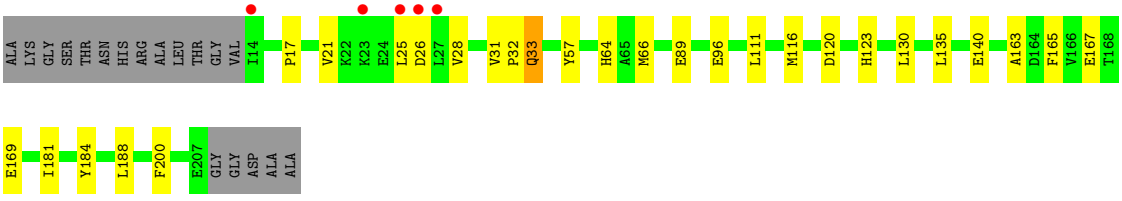
• Molecule 1: Ferritin-4, chloroplastic

Chain B:



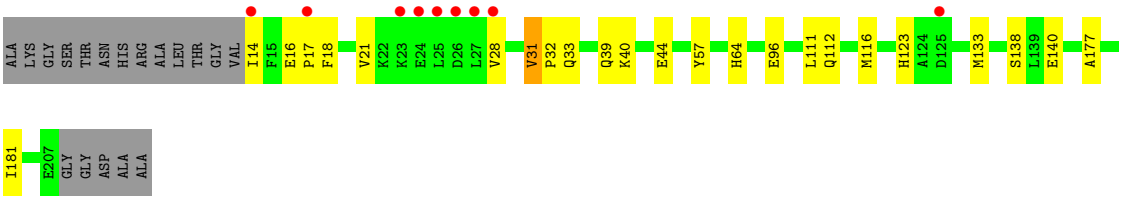
• Molecule 1: Ferritin-4, chloroplastic

Chain C:



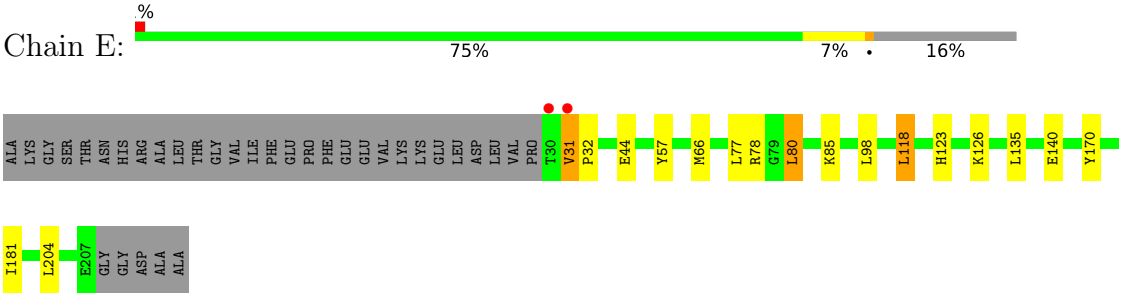
• Molecule 1: Ferritin-4, chloroplastic

Chain D:



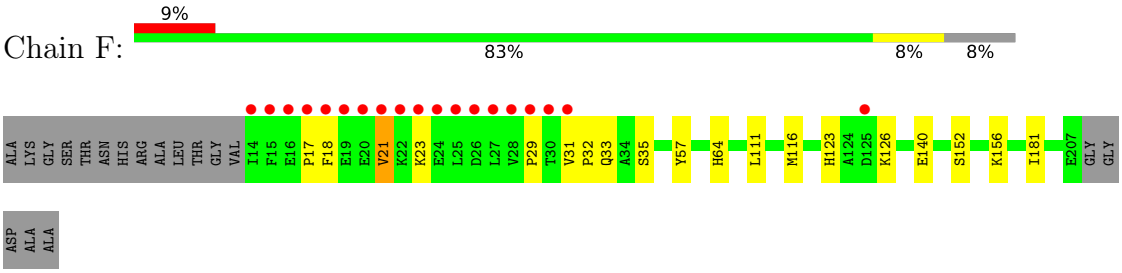
• Molecule 1: Ferritin-4, chloroplastic

Chain E:



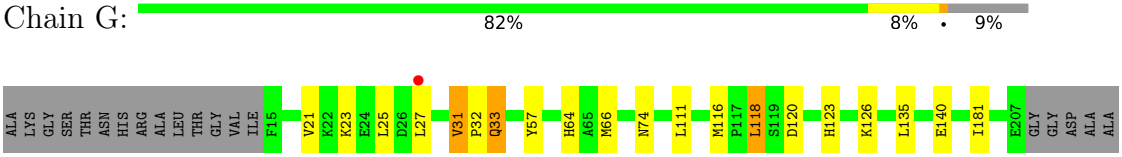
• Molecule 1: Ferritin-4, chloroplastic

Chain F:



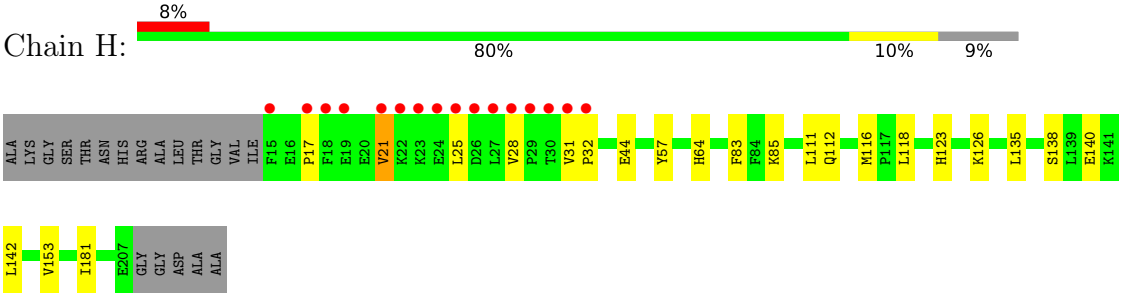
• Molecule 1: Ferritin-4, chloroplastic

Chain G:



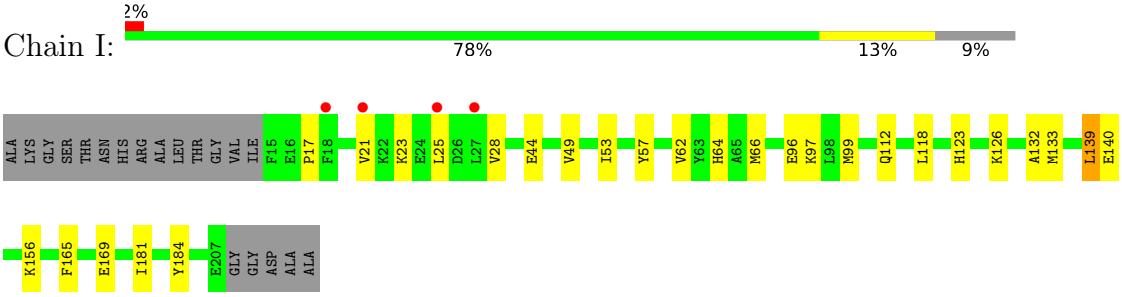
• Molecule 1: Ferritin-4, chloroplastic

Chain H:



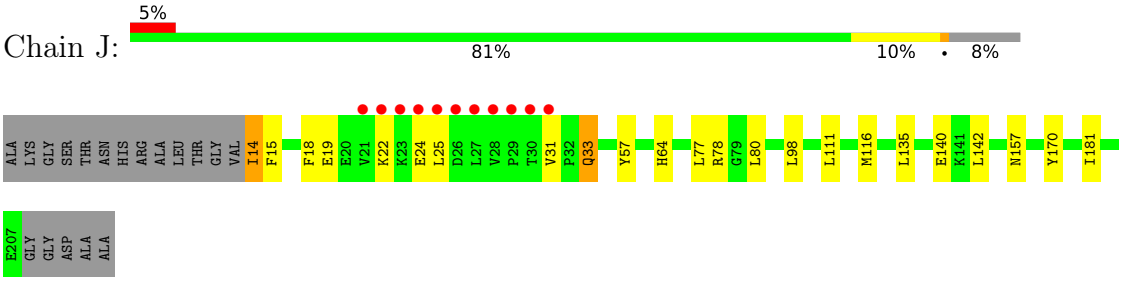
• Molecule 1: Ferritin-4, chloroplastic

Chain I:



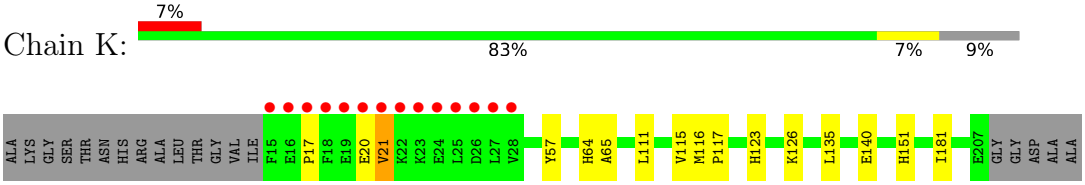
• Molecule 1: Ferritin-4, chloroplastic

Chain J:



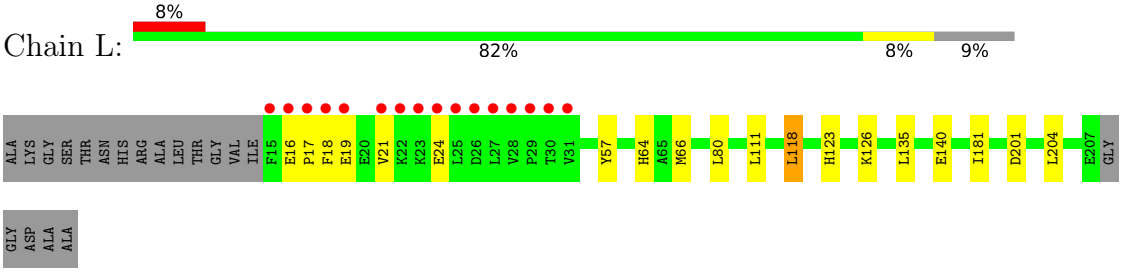
• Molecule 1: Ferritin-4, chloroplastic

Chain K:



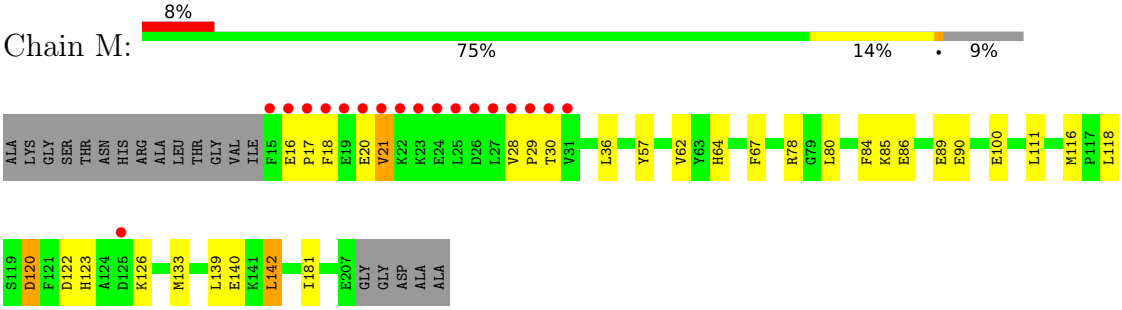
• Molecule 1: Ferritin-4, chloroplastic

Chain L:



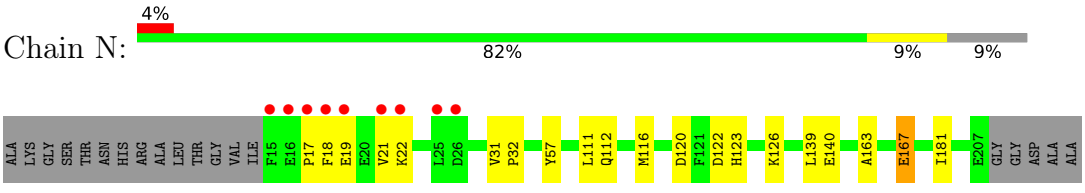
• Molecule 1: Ferritin-4, chloroplastic

Chain M:



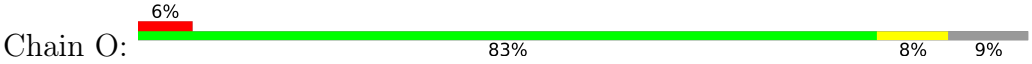
• Molecule 1: Ferritin-4, chloroplastic

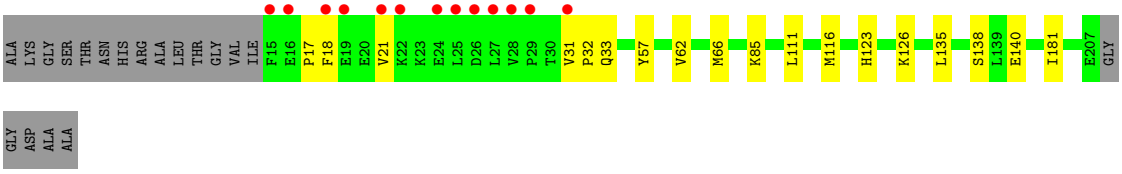
Chain N:



• Molecule 1: Ferritin-4, chloroplastic

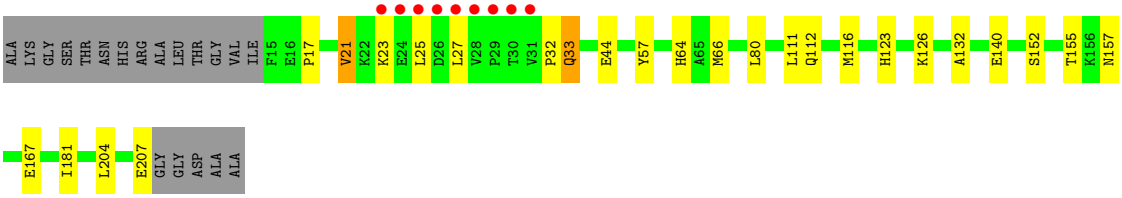
Chain O:





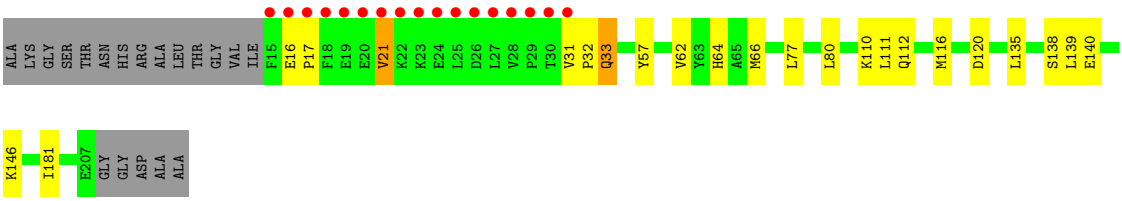
• Molecule 1: Ferritin-4, chloroplastic

Chain P:



• Molecule 1: Ferritin-4, chloroplastic

Chain Q:

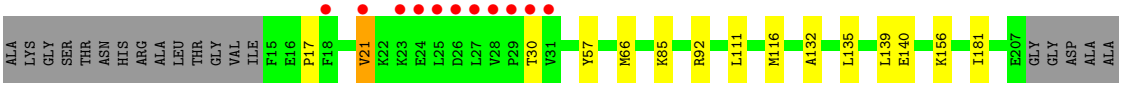


• Molecule 1: Ferritin-4, chloroplastic

Chain R:

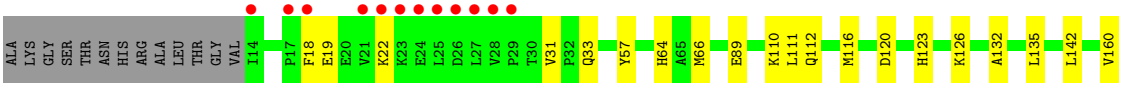
• Molecule 1: Ferritin-4, chloroplastic

Chain S:



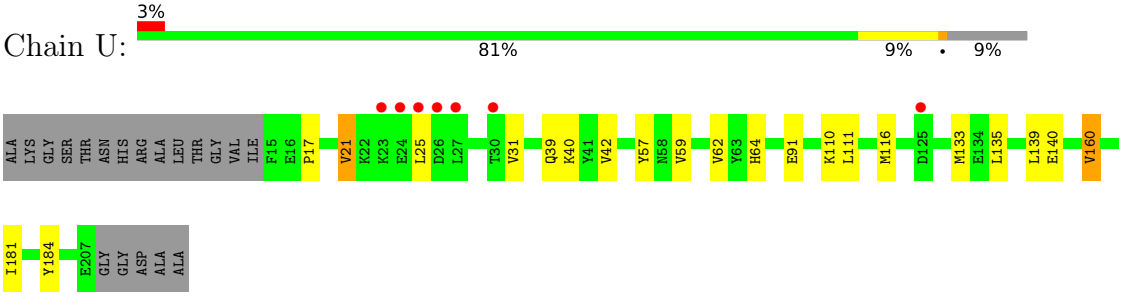
• Molecule 1: Ferritin-4, chloroplastic

Chain T:



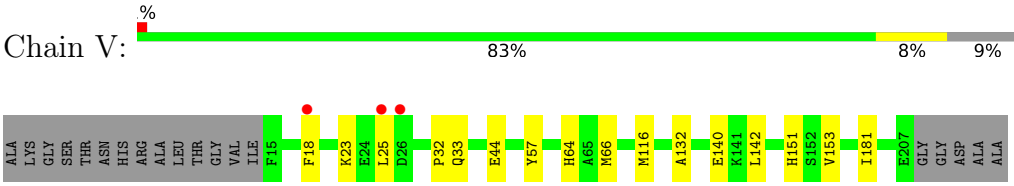
• Molecule 1: Ferritin-4, chloroplastic

Chain U:



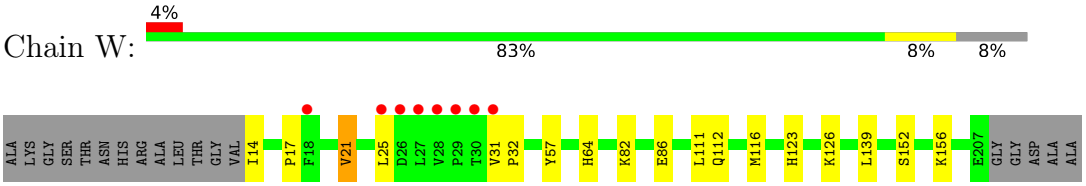
• Molecule 1: Ferritin-4, chloroplastic

Chain V:



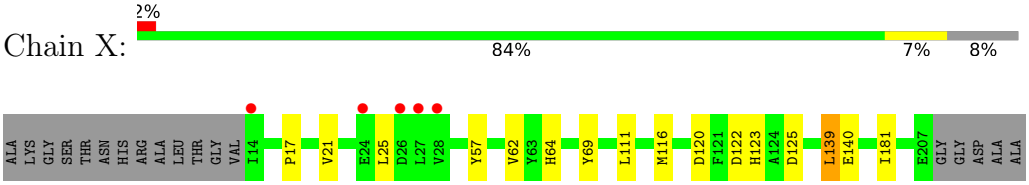
• Molecule 1: Ferritin-4, chloroplastic

Chain W:



• Molecule 1: Ferritin-4, chloroplastic

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	223.50Å 221.82Å 122.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 1.90 49.90 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.67-1.90) 99.0 (49.90-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.15 (at 1.90Å)	Xtriage
Refinement program	CNS, PHENIX (phenix.refine)	Depositor
R, R_{free}	0.150 , 0.185 0.150 , 0.184	Depositor DCC
R_{free} test set	23785 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	15.2	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	42812	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 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.34	0/1672	0.47	0/2253
1	B	0.34	0/1684	0.47	0/2270
1	C	0.33	0/1729	0.46	0/2329
1	D	0.33	0/1721	0.44	0/2318
1	E	0.33	0/1547	0.46	0/2080
1	F	0.33	0/1696	0.45	0/2285
1	G	0.33	0/1671	0.46	0/2252
1	H	0.33	0/1688	0.45	0/2274
1	I	0.31	0/1752	0.45	0/2361
1	J	0.32	0/1691	0.46	0/2279
1	K	0.31	0/1641	0.45	0/2211
1	L	0.32	0/1666	0.45	0/2245
1	M	0.33	0/1717	0.46	0/2313
1	N	0.33	0/1697	0.47	0/2286
1	O	0.34	0/1726	0.47	0/2325
1	P	0.32	0/1687	0.44	0/2272
1	Q	0.33	0/1693	0.46	0/2279
1	R	0.33	0/1700	0.46	0/2291
1	S	0.34	0/1682	0.46	0/2266
1	T	0.32	0/1706	0.44	0/2298
1	U	0.34	0/1707	0.45	0/2298
1	V	0.34	0/1692	0.45	0/2278
1	W	0.31	0/1703	0.45	0/2294
1	X	0.32	0/1718	0.46	0/2313
All	All	0.33	0/40586	0.46	0/54670

There are no bond length outliers.

There are no bond angle outliers.

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	1621	0	1604	20	0
1	B	1633	0	1610	18	0
1	C	1669	0	1639	23	0
1	D	1661	0	1633	24	0
1	E	1492	0	1476	13	0
1	F	1636	0	1623	13	0
1	G	1617	0	1587	20	0
1	H	1631	0	1608	17	0
1	I	1677	0	1662	24	0
1	J	1637	0	1614	22	0
1	K	1599	0	1561	14	0
1	L	1618	0	1591	16	0
1	M	1651	0	1634	26	0
1	N	1631	0	1607	16	0
1	O	1657	0	1629	14	0
1	P	1631	0	1596	18	0
1	Q	1630	0	1628	22	0
1	R	1643	0	1617	17	0
1	S	1622	0	1608	11	0
1	T	1650	0	1623	15	0
1	U	1641	0	1628	22	0
1	V	1633	0	1606	13	0
1	W	1649	0	1627	16	0
1	X	1652	0	1631	16	0
2	A	5	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	4	0	0	0	0
2	E	5	0	0	0	0
2	F	6	0	0	0	0
2	G	6	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	6	0	0	0	0
2	L	7	0	0	0	0
2	M	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	6	0	0	0	0
2	O	5	0	0	0	0
2	P	6	0	0	0	0
2	Q	4	0	0	0	0
2	R	6	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	4	0	0	0	0
2	X	7	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	0	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	0	0
4	A	158	0	0	0	0
4	B	149	0	0	1	0
4	C	143	0	0	0	0
4	D	130	0	0	1	0
4	E	150	0	0	1	0
4	F	146	0	0	0	0
4	G	155	0	0	0	0
4	H	145	0	0	1	0
4	I	133	0	0	2	0
4	J	142	0	0	2	0
4	K	129	0	0	3	0
4	L	136	0	0	0	0
4	M	134	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	145	0	0	1	0
4	O	162	0	0	0	0
4	P	136	0	0	2	0
4	Q	148	0	0	2	0
4	R	150	0	0	0	0
4	S	137	0	0	1	0
4	T	135	0	0	2	0
4	U	135	0	0	2	0
4	V	146	0	0	1	0
4	W	137	0	0	2	0
4	X	148	0	0	0	0
All	All	42812	0	38696	341	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 4.

The worst 5 of 341 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:T:123:HIS:HD2	1:T:126:LYS:H	1.22	0.86
1:I:21:VAL:HG11	1:W:139[A]:LEU:HD23	1.59	0.83
1:U:133[B]:MET:HE3	1:U:181:ILE:HG23	1.62	0.81
1:T:123:HIS:CD2	1:T:126:LYS:H	1.99	0.79
1:K:123:HIS:HD2	1:K:126:LYS:H	1.31	0.78

There are no symmetry-related clashes.

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	201/212 (95%)	201 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	203/212 (96%)	203 (100%)	0	0	100	100
1	C	208/212 (98%)	208 (100%)	0	0	100	100
1	D	207/212 (98%)	206 (100%)	1 (0%)	0	100	100
1	E	186/212 (88%)	186 (100%)	0	0	100	100
1	F	204/212 (96%)	204 (100%)	0	0	100	100
1	G	201/212 (95%)	201 (100%)	0	0	100	100
1	H	203/212 (96%)	203 (100%)	0	0	100	100
1	I	211/212 (100%)	211 (100%)	0	0	100	100
1	J	203/212 (96%)	202 (100%)	1 (0%)	0	100	100
1	K	197/212 (93%)	197 (100%)	0	0	100	100
1	L	200/212 (94%)	200 (100%)	0	0	100	100
1	M	206/212 (97%)	206 (100%)	0	0	100	100
1	N	204/212 (96%)	204 (100%)	0	0	100	100
1	O	208/212 (98%)	208 (100%)	0	0	100	100
1	P	202/212 (95%)	202 (100%)	0	0	100	100
1	Q	204/212 (96%)	204 (100%)	0	0	100	100
1	R	205/212 (97%)	204 (100%)	1 (0%)	0	100	100
1	S	203/212 (96%)	203 (100%)	0	0	100	100
1	T	204/212 (96%)	204 (100%)	0	0	100	100
1	U	206/212 (97%)	205 (100%)	1 (0%)	0	100	100
1	V	203/212 (96%)	203 (100%)	0	0	100	100
1	W	205/212 (97%)	205 (100%)	0	0	100	100
1	X	207/212 (98%)	207 (100%)	0	0	100	100
All	All	4881/5088 (96%)	4877 (100%)	4 (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	177/178 (99%)	172 (97%)	5 (3%)	43	36
1	B	179/178 (101%)	175 (98%)	4 (2%)	52	47
1	C	184/178 (103%)	178 (97%)	6 (3%)	38	29
1	D	183/178 (103%)	180 (98%)	3 (2%)	62	60
1	E	163/178 (92%)	157 (96%)	6 (4%)	34	25
1	F	180/178 (101%)	176 (98%)	4 (2%)	52	47
1	G	177/178 (99%)	170 (96%)	7 (4%)	31	22
1	H	179/178 (101%)	175 (98%)	4 (2%)	52	47
1	I	187/178 (105%)	181 (97%)	6 (3%)	39	30
1	J	179/178 (101%)	174 (97%)	5 (3%)	43	36
1	K	173/178 (97%)	169 (98%)	4 (2%)	50	45
1	L	176/178 (99%)	173 (98%)	3 (2%)	60	57
1	M	182/178 (102%)	174 (96%)	8 (4%)	28	19
1	N	180/178 (101%)	178 (99%)	2 (1%)	73	73
1	O	184/178 (103%)	183 (100%)	1 (0%)	88	89
1	P	179/178 (101%)	175 (98%)	4 (2%)	52	47
1	Q	180/178 (101%)	174 (97%)	6 (3%)	38	29
1	R	180/178 (101%)	175 (97%)	5 (3%)	43	36
1	S	179/178 (101%)	176 (98%)	3 (2%)	60	57
1	T	181/178 (102%)	175 (97%)	6 (3%)	38	29
1	U	182/178 (102%)	176 (97%)	6 (3%)	38	29
1	V	180/178 (101%)	177 (98%)	3 (2%)	60	57
1	W	181/178 (102%)	177 (98%)	4 (2%)	52	47
1	X	183/178 (103%)	179 (98%)	4 (2%)	52	47
All	All	4308/4272 (101%)	4199 (98%)	109 (2%)	47	41

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	21	VAL
1	P	64	HIS
1	V	57	TYR
1	M	57	TYR
1	N	57	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	206	HIS
1	T	206	HIS
1	P	112	GLN
1	R	123	HIS
1	W	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 148 ligands modelled in this entry, 130 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	S	218	-	3,3,3	0.78	0	3,3,3	0.79	0
3	ACY	T	218	-	3,3,3	0.79	0	3,3,3	0.71	0
3	ACY	W	231	-	3,3,3	0.82	0	3,3,3	0.71	0
3	ACY	I	218	-	3,3,3	0.77	0	3,3,3	0.83	0
3	ACY	E	218	-	3,3,3	0.83	0	3,3,3	0.66	0
3	ACY	L	219	-	3,3,3	0.79	0	3,3,3	0.77	0
3	ACY	J	218	-	3,3,3	0.77	0	3,3,3	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ACY	Q	217	-	3,3,3	0.84	0	3,3,3	0.62	0
3	ACY	P	218	-	3,3,3	0.78	0	3,3,3	0.76	0
3	ACY	R	219	-	3,3,3	0.75	0	3,3,3	0.93	0
3	ACY	F	219	-	3,3,3	0.79	0	3,3,3	0.75	0
3	ACY	A	217	-	3,3,3	0.78	0	3,3,3	0.83	0
3	ACY	G	219	-	3,3,3	0.79	0	3,3,3	0.73	0
3	ACY	M	218	-	3,3,3	0.81	0	3,3,3	0.73	0
3	ACY	V	221	-	3,3,3	0.79	0	3,3,3	0.76	0
3	ACY	O	218	-	3,3,3	0.79	0	3,3,3	0.70	0
3	ACY	H	218	-	3,3,3	0.76	0	3,3,3	0.85	0
3	ACY	X	241	-	3,3,3	0.80	0	3,3,3	0.71	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	194/212 (91%)	-0.22	14 (7%)	15	17	8, 13, 65, 106	0
1	B	194/212 (91%)	-0.18	16 (8%)	11	13	8, 13, 69, 96	0
1	C	194/212 (91%)	-0.49	5 (2%)	56	58	8, 13, 42, 81	0
1	D	194/212 (91%)	-0.33	9 (4%)	32	35	9, 14, 56, 89	0
1	E	178/212 (83%)	-0.62	2 (1%)	80	82	8, 13, 32, 73	0
1	F	194/212 (91%)	-0.23	19 (9%)	7	8	7, 13, 62, 94	0
1	G	193/212 (91%)	-0.55	1 (0%)	91	92	9, 13, 43, 75	0
1	H	193/212 (91%)	-0.23	16 (8%)	11	13	7, 14, 66, 93	0
1	I	193/212 (91%)	-0.53	4 (2%)	63	66	8, 15, 46, 70	0
1	J	194/212 (91%)	-0.26	11 (5%)	23	26	7, 14, 55, 100	0
1	K	193/212 (91%)	-0.25	14 (7%)	15	16	9, 16, 63, 91	0
1	L	193/212 (91%)	-0.17	16 (8%)	11	13	8, 15, 74, 100	0
1	M	193/212 (91%)	-0.27	18 (9%)	8	10	9, 13, 69, 92	0
1	N	193/212 (91%)	-0.42	9 (4%)	31	34	8, 14, 50, 82	0
1	O	193/212 (91%)	-0.34	13 (6%)	17	20	7, 12, 60, 86	0
1	P	193/212 (91%)	-0.33	9 (4%)	31	34	9, 15, 52, 93	0
1	Q	193/212 (91%)	-0.33	17 (8%)	10	11	7, 13, 65, 95	0
1	R	196/212 (92%)	-0.51	5 (2%)	56	58	7, 13, 45, 90	0
1	S	193/212 (91%)	-0.35	11 (5%)	23	26	7, 12, 53, 89	0
1	T	194/212 (91%)	-0.38	12 (6%)	20	23	9, 15, 55, 91	0
1	U	193/212 (91%)	-0.48	7 (3%)	42	45	8, 13, 50, 89	0
1	V	193/212 (91%)	-0.55	3 (1%)	72	74	8, 14, 41, 78	0
1	W	194/212 (91%)	-0.48	8 (4%)	37	40	10, 15, 55, 89	0
1	X	194/212 (91%)	-0.50	5 (2%)	56	58	8, 14, 46, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	4629/5088 (90%)	-0.37	244 (5%)	26	29	7, 14, 57, 106	0

The worst 5 of 244 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	28	VAL	11.1
1	L	27	LEU	10.8
1	M	27	LEU	10.4
1	A	14	ILE	9.8
1	A	27	LEU	9.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	R	218	1/1	0.28	0.32	93,93,93,93	0
2	CA	O	216	1/1	0.33	0.31	95,95,95,95	0
2	CA	P	216	1/1	0.49	0.25	77,77,77,77	0
2	CA	F	218[B]	1/1	0.56	0.34	57,57,57,57	1
2	CA	S	216[B]	1/1	0.61	0.25	46,46,46,46	1
2	CA	R	217[B]	1/1	0.62	0.31	51,51,51,51	1
2	CA	M	217[B]	1/1	0.74	0.20	41,41,41,41	1
2	CA	P	217[A]	1/1	0.74	0.17	49,49,49,49	1
2	CA	P	217[B]	1/1	0.74	0.17	29,29,29,29	1
2	CA	O	215	1/1	0.75	0.15	65,65,65,65	0
2	CA	U	215[B]	1/1	0.77	0.19	50,50,50,50	1
2	CA	E	217[B]	1/1	0.79	0.19	40,40,40,40	1
2	CA	Q	216[B]	1/1	0.79	0.28	52,52,52,52	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACY	I	218	4/4	0.79	0.20	20,28,54,110	0
2	CA	V	215	1/1	0.80	0.12	71,71,71,71	0
2	CA	H	217	1/1	0.81	0.14	66,66,66,66	0
2	CA	K	218	1/1	0.83	0.12	52,52,52,52	0
2	CA	K	216[A]	1/1	0.83	0.13	36,36,36,36	1
2	CA	T	215[A]	1/1	0.84	0.18	37,37,37,37	1
2	CA	D	216[B]	1/1	0.84	0.20	45,45,45,45	1
2	CA	N	213	1/1	0.85	0.11	46,46,46,46	0
2	CA	N	218[B]	1/1	0.85	0.13	42,42,42,42	1
2	CA	J	216	1/1	0.85	0.17	69,69,69,69	0
2	CA	D	214	1/1	0.86	0.12	61,61,61,61	0
2	CA	B	218[B]	1/1	0.86	0.26	53,53,53,53	1
2	CA	H	216[B]	1/1	0.88	0.17	45,45,45,45	1
2	CA	X	213	1/1	0.88	0.17	52,52,52,52	0
2	CA	U	216	1/1	0.88	0.10	50,50,50,50	0
3	ACY	T	218	4/4	0.88	0.16	20,22,59,75	0
2	CA	V	216[A]	1/1	0.89	0.12	31,31,31,31	1
2	CA	O	217	1/1	0.89	0.12	46,46,46,46	0
2	CA	G	218[B]	1/1	0.90	0.15	38,38,38,38	1
2	CA	X	217[A]	1/1	0.90	0.14	35,35,35,35	1
2	CA	J	215[A]	1/1	0.90	0.13	27,27,27,27	1
2	CA	J	215[B]	1/1	0.90	0.13	49,49,49,49	1
2	CA	A	216[B]	1/1	0.91	0.12	54,54,54,54	1
2	CA	F	216	1/1	0.91	0.10	52,52,52,52	0
2	CA	A	216[A]	1/1	0.91	0.12	28,28,28,28	1
3	ACY	V	221	4/4	0.91	0.19	18,20,47,104	0
3	ACY	W	231	4/4	0.91	0.17	18,23,36,48	0
2	CA	C	217	1/1	0.92	0.12	58,58,58,58	0
2	CA	T	217	1/1	0.92	0.14	59,59,59,59	0
2	CA	C	216[A]	1/1	0.92	0.12	25,25,25,25	1
2	CA	D	215[A]	1/1	0.92	0.10	36,36,36,36	1
2	CA	C	216[B]	1/1	0.92	0.12	40,40,40,40	1
2	CA	S	217	1/1	0.92	0.10	56,56,56,56	0
2	CA	C	214	1/1	0.93	0.09	36,36,36,36	0
2	CA	X	214	1/1	0.93	0.08	52,52,52,52	0
3	ACY	M	218	4/4	0.93	0.17	19,26,34,39	0
2	CA	T	216[B]	1/1	0.94	0.07	25,25,25,25	1
2	CA	B	216	1/1	0.94	0.11	54,54,54,54	0
2	CA	H	215[A]	1/1	0.94	0.10	27,27,27,27	1
3	ACY	A	217	4/4	0.94	0.14	21,26,35,48	0
2	CA	B	214	1/1	0.94	0.11	52,52,52,52	0
2	CA	L	217[A]	1/1	0.94	0.08	23,23,23,23	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACY	P	218	4/4	0.94	0.16	18,21,45,60	0
3	ACY	Q	217	4/4	0.94	0.14	16,23,31,46	0
3	ACY	R	219	4/4	0.94	0.15	17,27,32,57	0
3	ACY	S	218	4/4	0.94	0.14	16,18,60,62	0
2	CA	L	217[B]	1/1	0.94	0.08	34,34,34,34	1
2	CA	V	217[B]	1/1	0.94	0.10	33,33,33,33	1
2	CA	W	215	1/1	0.94	0.09	53,53,53,53	0
3	ACY	F	219	4/4	0.95	0.13	20,22,39,82	0
3	ACY	G	219	4/4	0.95	0.18	21,22,50,98	0
2	CA	S	215[A]	1/1	0.95	0.08	27,27,27,27	1
2	CA	I	213	1/1	0.95	0.10	48,48,48,48	0
2	CA	I	216[A]	1/1	0.95	0.08	25,25,25,25	1
2	CA	Q	215[A]	1/1	0.95	0.08	23,23,23,23	1
2	CA	M	216[A]	1/1	0.95	0.07	27,27,27,27	1
2	CA	R	216[A]	1/1	0.95	0.07	25,25,25,25	1
2	CA	I	216[B]	1/1	0.95	0.08	35,35,35,35	1
2	CA	E	216[A]	1/1	0.95	0.07	23,23,23,23	1
3	ACY	E	218	4/4	0.95	0.13	19,20,30,51	0
3	ACY	X	241	4/4	0.95	0.20	23,24,35,99	0
2	CA	L	216	1/1	0.96	0.06	31,31,31,31	0
2	CA	F	217[A]	1/1	0.96	0.08	25,25,25,25	1
2	CA	B	217[A]	1/1	0.96	0.06	20,20,20,20	1
3	ACY	J	218	4/4	0.96	0.09	19,24,31,68	0
2	CA	M	215	1/1	0.96	0.07	44,44,44,44	0
3	ACY	O	218	4/4	0.96	0.12	16,20,38,63	0
2	CA	G	217[A]	1/1	0.96	0.10	29,29,29,29	1
2	CA	F	214	1/1	0.96	0.08	36,36,36,36	0
2	CA	K	217[B]	1/1	0.96	0.08	32,32,32,32	1
2	CA	N	217[A]	1/1	0.96	0.07	26,26,26,26	1
2	CA	X	218[B]	1/1	0.96	0.06	27,27,27,27	1
2	CA	X	219	1/1	0.96	0.07	58,58,58,58	0
2	CA	U	214[A]	1/1	0.96	0.07	24,24,24,24	1
2	CA	A	215	1/1	0.96	0.06	49,49,49,49	0
2	CA	K	215	1/1	0.97	0.04	33,33,33,33	0
3	ACY	L	219	4/4	0.97	0.12	18,24,31,37	0
2	CA	W	216	1/1	0.97	0.12	46,46,46,46	0
2	CA	I	217	1/1	0.97	0.05	48,48,48,48	0
3	ACY	H	218	4/4	0.97	0.13	19,19,33,72	0
2	CA	G	216	1/1	0.97	0.09	42,42,42,42	0
2	CA	G	214	1/1	0.98	0.05	18,18,18,18	0
2	CA	L	218	1/1	0.98	0.07	48,48,48,48	0
2	CA	J	217	1/1	0.98	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	K	213	1/1	0.98	0.04	26,26,26,26	0
2	CA	M	214	1/1	0.99	0.06	17,17,17,17	0
2	CA	E	215	1/1	0.99	0.04	19,19,19,19	0
2	CA	J	213	1/1	0.99	0.04	23,23,23,23	0
2	CA	U	213	1/1	0.99	0.04	18,18,18,18	0
2	CA	J	214	1/1	0.99	0.05	19,19,19,19	0
2	CA	G	215	1/1	0.99	0.10	33,33,33,33	0
2	CA	N	214	1/1	0.99	0.05	29,29,29,29	0
2	CA	V	213	1/1	0.99	0.03	25,25,25,25	0
2	CA	V	214	1/1	0.99	0.04	18,18,18,18	0
2	CA	N	215	1/1	0.99	0.04	19,19,19,19	0
2	CA	N	216	1/1	0.99	0.06	38,38,38,38	0
2	CA	B	215	1/1	0.99	0.04	24,24,24,24	0
2	CA	W	214	1/1	0.99	0.06	20,20,20,20	0
2	CA	C	215	1/1	0.99	0.03	27,27,27,27	0
2	CA	O	214	1/1	0.99	0.04	14,14,14,14	0
2	CA	F	213	1/1	0.99	0.04	22,22,22,22	0
2	CA	H	214	1/1	0.99	0.04	16,16,16,16	0
2	CA	X	216	1/1	0.99	0.04	18,18,18,18	0
2	CA	K	214	1/1	0.99	0.06	21,21,21,21	0
2	CA	P	213	1/1	0.99	0.07	31,31,31,31	0
2	CA	P	214	1/1	0.99	0.04	23,23,23,23	0
2	CA	P	215	1/1	0.99	0.04	22,22,22,22	0
2	CA	B	213	1/1	0.99	0.04	14,14,14,14	0
2	CA	F	215	1/1	0.99	0.04	21,21,21,21	0
2	CA	C	213	1/1	0.99	0.06	17,17,17,17	0
2	CA	Q	214	1/1	0.99	0.05	18,18,18,18	0
2	CA	E	213	1/1	0.99	0.05	28,28,28,28	0
2	CA	L	213	1/1	0.99	0.05	21,21,21,21	0
2	CA	R	213	1/1	0.99	0.06	36,36,36,36	0
2	CA	R	215	1/1	0.99	0.06	18,18,18,18	0
2	CA	L	214	1/1	0.99	0.05	21,21,21,21	0
2	CA	L	215	1/1	0.99	0.07	26,26,26,26	0
2	CA	I	214	1/1	0.99	0.03	25,25,25,25	0
2	CA	S	213	1/1	0.99	0.04	26,26,26,26	0
2	CA	S	214	1/1	0.99	0.05	16,16,16,16	0
2	CA	I	215	1/1	0.99	0.03	19,19,19,19	0
2	CA	E	214	1/1	0.99	0.06	17,17,17,17	0
2	CA	G	213	1/1	0.99	0.04	27,27,27,27	0
2	CA	T	213	1/1	0.99	0.03	25,25,25,25	0
2	CA	T	214	1/1	1.00	0.04	20,20,20,20	0
2	CA	Q	213	1/1	1.00	0.03	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	M	213	1/1	1.00	0.04	23,23,23,23	0
2	CA	O	213	1/1	1.00	0.03	19,19,19,19	0
2	CA	W	213	1/1	1.00	0.04	25,25,25,25	0
2	CA	A	214	1/1	1.00	0.05	17,17,17,17	0
2	CA	A	213	1/1	1.00	0.04	20,20,20,20	0
2	CA	R	214	1/1	1.00	0.03	22,22,22,22	0
2	CA	H	213	1/1	1.00	0.04	22,22,22,22	0
2	CA	D	213	1/1	1.00	0.04	17,17,17,17	0
2	CA	X	215	1/1	1.00	0.03	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.