



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2023 – 06:25 AM EDT

PDB ID : 1Z6O
Title : Crystal Structure of Trichoplusia ni secreted ferritin
Authors : Hamburger, A.E.; West Jr., A.P.; Hamburger, Z.A.; Hamburger, P.; Bjorkman, P.J.
Deposited on : 2005-03-22
Resolution : 1.91 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

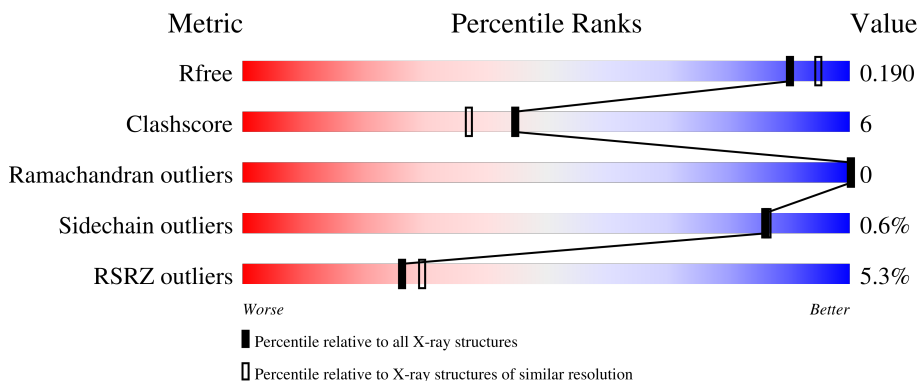
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 $\leq 5\%$. 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% 88% 12%
1	B	212	 6% 91% 9%
1	C	212	 6% 90% 10%
1	D	212	 6% 91% 9%
1	E	212	 6% 91% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	212	8% 89% 10%
1	G	212	7% 91% 9%
1	H	212	6% 89% 10%
1	I	212	10% 89% 11%
1	J	212	7% 91% 8%
1	K	212	9% 89% 10%
1	L	212	7% 90% 9%
2	M	191	3% 90% 10%
2	N	191	4% 89% 11%
2	O	191	4% 88% 12%
2	P	191	4% 91% 9%
2	Q	191	4% 90% 10%
2	R	191	3% 90% 10%
2	S	191	3% 89% 11%
2	T	191	2% 91% 9%
2	U	191	4% 90% 10%
2	V	191	2% 91% 9%
2	W	191	3% 91% 9%
2	X	191	3% 90% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 43180 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 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	Total 1699	C 1066	N 294	O 334	S 5	0	0	0
1	B	212	Total 1699	C 1066	N 294	O 334	S 5	0	0	0
1	C	212	Total 1699	C 1066	N 294	O 334	S 5	0	0	0
1	D	212	Total 1699	C 1066	N 294	O 334	S 5	0	0	0
1	E	212	Total 1699	C 1066	N 294	O 334	S 5	0	0	0
1	F	212	Total 1699	C 1066	N 294	O 334	S 5	0	0	0
1	G	212	Total 1699	C 1066	N 294	O 334	S 5	0	0	0
1	H	212	Total 1699	C 1066	N 294	O 334	S 5	0	0	0
1	I	212	Total 1699	C 1066	N 294	O 334	S 5	0	0	0
1	J	212	Total 1699	C 1066	N 294	O 334	S 5	0	0	0
1	K	212	Total 1699	C 1066	N 294	O 334	S 5	0	0	0
1	L	212	Total 1699	C 1066	N 294	O 334	S 5	0	0	0

- Molecule 2 is a protein called Ferritin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	191	Total 1526	C 955	N 267	O 293	S 11	0	0	0
2	N	191	Total 1526	C 955	N 267	O 293	S 11	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	P	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	Q	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	R	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	S	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	T	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	U	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	V	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	W	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	X	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	F	1	Total	Fe	0	0
			1	1		
3	M	1	Total	Fe	0	0
			1	1		
3	N	1	Total	Fe	0	0
			1	1		
3	O	1	Total	Fe	0	0
			1	1		
3	P	1	Total	Fe	0	0
			1	1		
3	Q	1	Total	Fe	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	R	1	Total Fe 1 1	0	0
3	S	1	Total Fe 1 1	0	0
3	T	1	Total Fe 1 1	0	0
3	U	1	Total Fe 1 1	0	0
3	V	1	Total Fe 1 1	0	0
3	W	1	Total Fe 1 1	0	0
3	X	1	Total Fe 1 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0
4	B	2	Total Ca 2 2	0	0
4	C	2	Total Ca 2 2	0	0
4	F	2	Total Ca 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	155	Total O 155 155	0	0
5	B	157	Total O 157 157	0	0
5	C	159	Total O 159 159	0	0
5	D	158	Total O 158 158	0	0
5	E	161	Total O 161 161	0	0
5	F	158	Total O 158 158	0	0

Continued on next page...

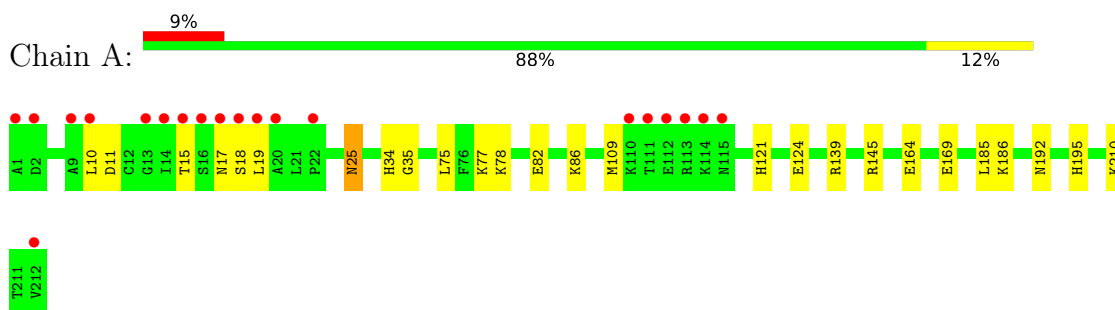
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	157	Total 157	O 157	0	0
5	H	161	Total 161	O 161	0	0
5	I	159	Total 159	O 159	0	0
5	J	158	Total 158	O 158	0	0
5	K	156	Total 156	O 156	0	0
5	L	159	Total 159	O 159	0	0
5	M	215	Total 215	O 215	0	0
5	N	214	Total 214	O 214	0	0
5	O	211	Total 211	O 211	0	0
5	P	215	Total 215	O 215	0	0
5	Q	214	Total 214	O 214	0	0
5	R	211	Total 211	O 211	0	0
5	S	214	Total 214	O 214	0	0
5	T	213	Total 213	O 213	0	0
5	U	211	Total 211	O 211	0	0
5	V	214	Total 214	O 214	0	0
5	W	214	Total 214	O 214	0	0
5	X	212	Total 212	O 212	0	0

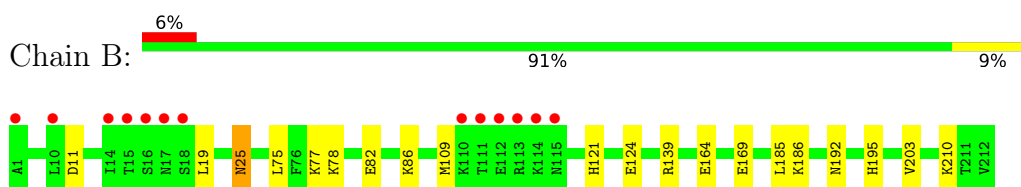
3 Residue-property plots [i](#)

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.

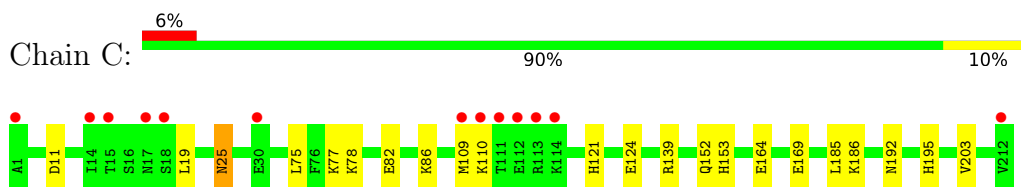
- Molecule 1: Ferritin light chain



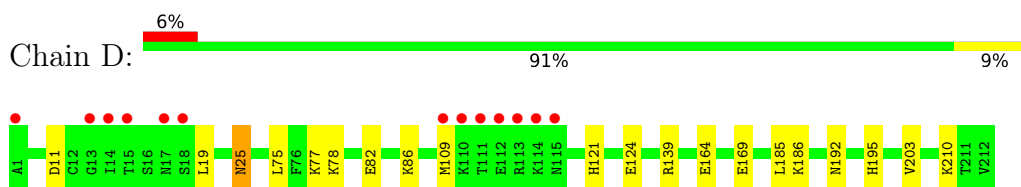
- Molecule 1: Ferritin light chain



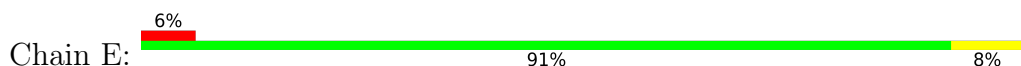
- Molecule 1: Ferritin light chain

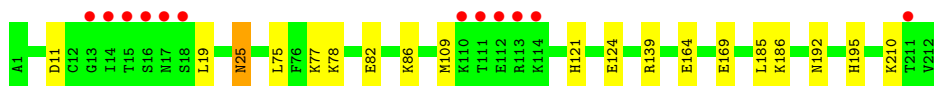


- Molecule 1: Ferritin light chain

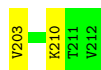
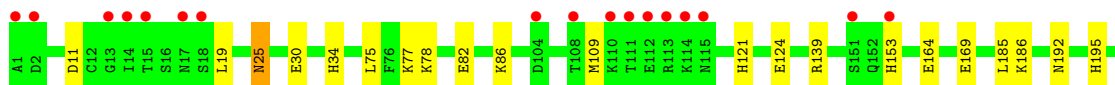
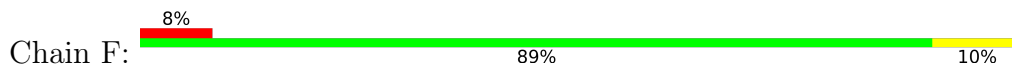


- Molecule 1: Ferritin light chain

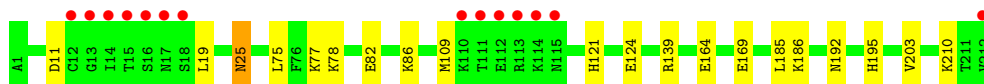
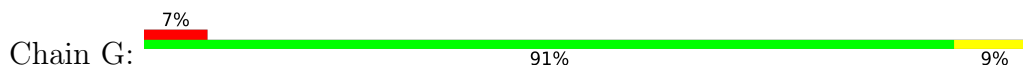




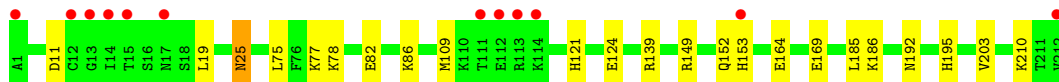
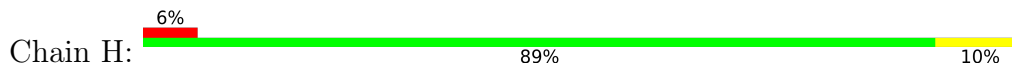
- Molecule 1: Ferritin light chain



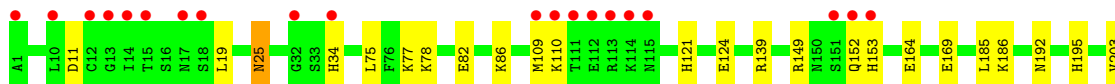
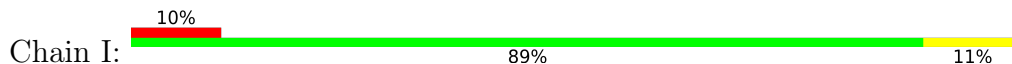
- Molecule 1: Ferritin light chain



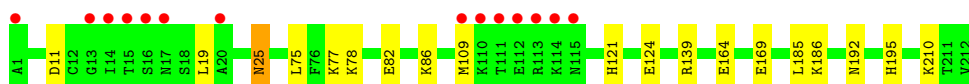
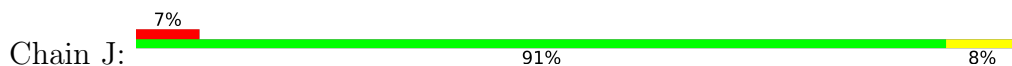
- Molecule 1: Ferritin light chain



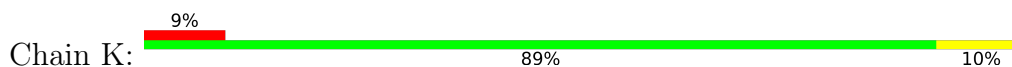
- Molecule 1: Ferritin light chain



- Molecule 1: Ferritin light chain

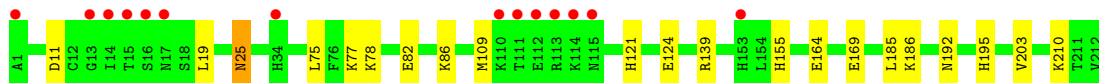
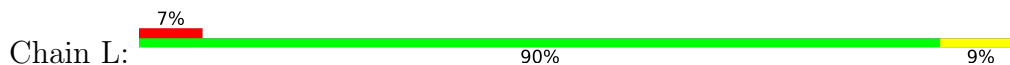


- Molecule 1: Ferritin light chain

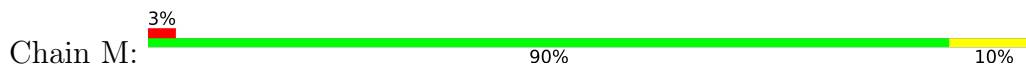




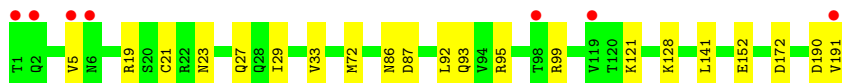
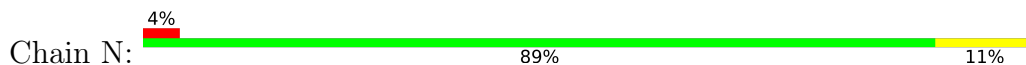
- Molecule 1: Ferritin light chain



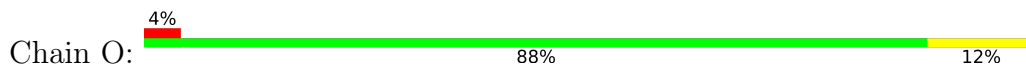
- Molecule 2: Ferritin heavy chain



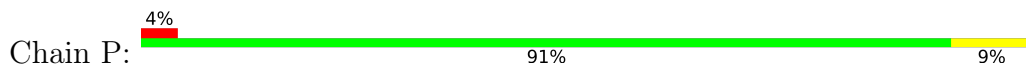
- Molecule 2: Ferritin heavy chain



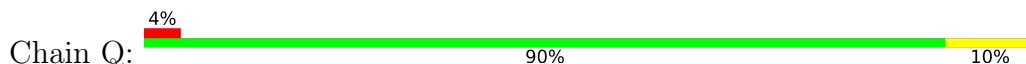
- Molecule 2: Ferritin heavy chain



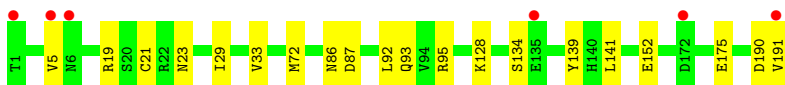
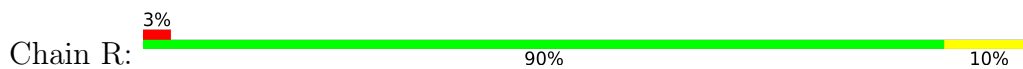
- Molecule 2: Ferritin heavy chain



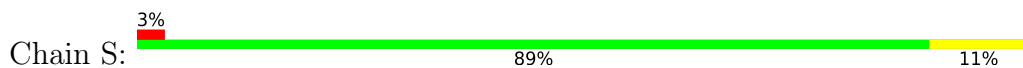
- Molecule 2: Ferritin heavy chain



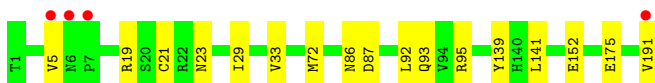
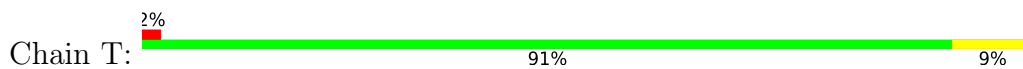
- Molecule 2: Ferritin heavy chain



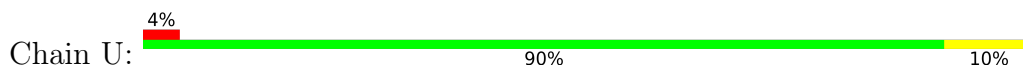
• Molecule 2: Ferritin heavy chain



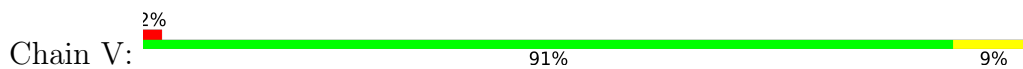
• Molecule 2: Ferritin heavy chain



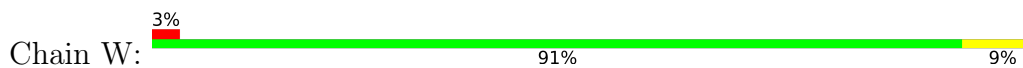
• Molecule 2: Ferritin heavy chain



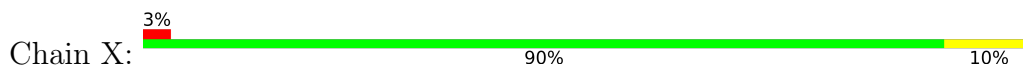
• Molecule 2: Ferritin heavy chain



• Molecule 2: Ferritin heavy chain



• Molecule 2: Ferritin heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	206.88Å 145.70Å 209.16Å 90.00° 94.93° 90.00°	Depositor
Resolution (Å)	19.98 – 1.91 29.85 – 1.91	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.98-1.91) 75.2 (29.85-1.91)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.80 (at 1.91Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.194 0.189 , 0.190	Depositor DCC
R_{free} test set	23175 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	6.5	Xtrriage
Anisotropy	0.604	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.13$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	43180	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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

5.1 Standard geometry

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

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	0.45	0/1734	0.60	0/2343
1	B	0.45	0/1734	0.61	0/2343
1	C	0.45	0/1734	0.61	0/2343
1	D	0.45	0/1734	0.60	0/2343
1	E	0.45	0/1734	0.61	0/2343
1	F	0.45	0/1734	0.60	0/2343
1	G	0.45	0/1734	0.60	0/2343
1	H	0.45	0/1734	0.60	0/2343
1	I	0.45	0/1734	0.60	0/2343
1	J	0.45	0/1734	0.60	0/2343
1	K	0.45	0/1734	0.60	0/2343
1	L	0.45	0/1734	0.60	0/2343
2	M	0.48	0/1553	0.60	0/2088
2	N	0.48	0/1553	0.60	0/2088
2	O	0.48	0/1553	0.60	0/2088
2	P	0.48	0/1553	0.60	0/2088
2	Q	0.48	0/1553	0.60	0/2088
2	R	0.48	0/1553	0.60	0/2088
2	S	0.48	0/1553	0.60	0/2088
2	T	0.48	0/1553	0.60	0/2088
2	U	0.48	0/1553	0.60	0/2088
2	V	0.48	0/1553	0.60	0/2088
2	W	0.48	0/1553	0.60	0/2088
2	X	0.48	0/1553	0.60	0/2088
All	All	0.46	0/39444	0.60	0/53172

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

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	1699	0	1613	28	10
1	B	1699	0	1613	29	0
1	C	1699	0	1613	27	16
1	D	1699	0	1613	23	0
1	E	1699	0	1613	25	0
1	F	1699	0	1613	25	14
1	G	1699	0	1613	25	0
1	H	1699	0	1613	27	18
1	I	1699	0	1613	28	16
1	J	1699	0	1613	27	0
1	K	1699	0	1613	23	10
1	L	1699	0	1613	28	0
2	M	1526	0	1500	23	1
2	N	1526	0	1500	23	18
2	O	1526	0	1500	23	5
2	P	1526	0	1500	21	0
2	Q	1526	0	1500	24	4
2	R	1526	0	1500	22	3
2	S	1526	0	1500	23	6
2	T	1526	0	1500	22	0
2	U	1526	0	1500	23	1
2	V	1526	0	1500	22	5
2	W	1526	0	1500	20	0
2	X	1526	0	1500	22	3
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	F	2	0	0	0	0
5	A	155	0	0	8	2
5	B	157	0	0	7	0
5	C	159	0	0	7	2
5	D	158	0	0	7	0
5	E	161	0	0	7	0
5	F	158	0	0	6	1
5	G	157	0	0	7	0
5	H	161	0	0	8	0
5	I	159	0	0	8	2
5	J	158	0	0	8	0
5	K	156	0	0	7	0
5	L	159	0	0	8	0
5	M	215	0	0	2	0
5	N	214	0	0	4	17
5	O	211	0	0	2	14
5	P	215	0	0	2	0
5	Q	214	0	0	2	1
5	R	211	0	0	2	0
5	S	214	0	0	2	6
5	T	213	0	0	2	0
5	U	211	0	0	2	0
5	V	214	0	0	3	3
5	W	214	0	0	2	0
5	X	212	0	0	2	7
All	All	43180	0	37356	489	99

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 6.

The worst 5 of 489 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:K:210:LYS:HE2	2:N:190:ASP:O	1.80	0.81
1:L:109:MET:CE	1:L:139:ARG:HE	1.94	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:MET:HE1	1:B:139:ARG:HE	1.45	0.81
1:F:109:MET:HE1	1:F:139:ARG:HE	1.45	0.81
1:I:109:MET:CE	1:I:139:ARG:HE	1.94	0.81

The worst 5 of 99 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:132:ASP:OD1	2:V:103:LYS:CE[4_546]	0.54	1.66
1:C:153:HIS:CE1	5:N:483:HOH:O[4_555]	0.55	1.65
1:K:17:ASN:ND2	5:X:411:HOH:O[3_545]	0.55	1.65
1:F:34:HIS:ND1	1:F:34:HIS:NE2[2_656]	0.59	1.61
1:K:35:GLY:O	2:X:103:LYS:NZ[3_545]	0.61	1.59

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	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	B	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	C	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	D	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	E	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	F	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	G	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	H	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	I	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	J	210/212 (99%)	205 (98%)	5 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	L	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
2	M	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	N	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	O	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	P	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	Q	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	R	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	S	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	T	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	U	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	V	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	W	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	X	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
All	All	4788/4836 (99%)	4704 (98%)	84 (2%)	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	177/181 (98%)	175 (99%)	2 (1%)	73	72
1	B	177/181 (98%)	175 (99%)	2 (1%)	73	72
1	C	177/181 (98%)	175 (99%)	2 (1%)	73	72
1	D	177/181 (98%)	175 (99%)	2 (1%)	73	72
1	E	177/181 (98%)	175 (99%)	2 (1%)	73	72
1	F	177/181 (98%)	175 (99%)	2 (1%)	73	72
1	G	177/181 (98%)	175 (99%)	2 (1%)	73	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	177/181 (98%)	175 (99%)	2 (1%)	73	72
1	I	177/181 (98%)	175 (99%)	2 (1%)	73	72
1	J	177/181 (98%)	175 (99%)	2 (1%)	73	72
1	K	177/181 (98%)	175 (99%)	2 (1%)	73	72
1	L	177/181 (98%)	175 (99%)	2 (1%)	73	72
2	M	167/167 (100%)	167 (100%)	0	100	100
2	N	167/167 (100%)	167 (100%)	0	100	100
2	O	167/167 (100%)	167 (100%)	0	100	100
2	P	167/167 (100%)	167 (100%)	0	100	100
2	Q	167/167 (100%)	167 (100%)	0	100	100
2	R	167/167 (100%)	167 (100%)	0	100	100
2	S	167/167 (100%)	167 (100%)	0	100	100
2	T	167/167 (100%)	167 (100%)	0	100	100
2	U	167/167 (100%)	167 (100%)	0	100	100
2	V	167/167 (100%)	167 (100%)	0	100	100
2	W	167/167 (100%)	167 (100%)	0	100	100
2	X	167/167 (100%)	167 (100%)	0	100	100
All	All	4128/4176 (99%)	4104 (99%)	24 (1%)	86	86

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	25	ASN
1	I	185	LEU
1	I	25	ASN
1	J	25	ASN
1	D	25	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	86	ASN
2	U	23	ASN
2	Q	23	ASN
2	S	23	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	V	86	ASN

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 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	212/212 (100%)	0.38	20 (9%) 8 10	16, 23, 66, 116	0
1	B	212/212 (100%)	0.22	13 (6%) 21 24	16, 23, 66, 116	0
1	C	212/212 (100%)	0.40	13 (6%) 21 24	16, 23, 66, 116	0
1	D	212/212 (100%)	0.17	13 (6%) 21 24	16, 23, 66, 116	0
1	E	212/212 (100%)	0.13	12 (5%) 23 26	16, 23, 66, 116	0
1	F	212/212 (100%)	0.31	17 (8%) 12 14	16, 23, 66, 116	0
1	G	212/212 (100%)	0.20	14 (6%) 18 20	16, 23, 66, 116	0
1	H	212/212 (100%)	0.24	12 (5%) 23 26	16, 23, 66, 116	0
1	I	212/212 (100%)	0.37	21 (9%) 7 8	16, 23, 66, 116	0
1	J	212/212 (100%)	0.16	14 (6%) 18 20	16, 23, 66, 116	0
1	K	212/212 (100%)	0.39	20 (9%) 8 10	16, 23, 66, 116	0
1	L	212/212 (100%)	0.19	14 (6%) 18 20	16, 23, 66, 116	0
2	M	191/191 (100%)	-0.13	5 (2%) 56 59	15, 21, 51, 80	0
2	N	191/191 (100%)	0.11	7 (3%) 41 44	15, 21, 51, 80	0
2	O	191/191 (100%)	0.11	8 (4%) 36 39	15, 21, 51, 80	0
2	P	191/191 (100%)	-0.10	7 (3%) 41 44	15, 21, 51, 80	0
2	Q	191/191 (100%)	-0.01	7 (3%) 41 44	15, 21, 51, 80	0
2	R	191/191 (100%)	-0.07	6 (3%) 49 52	15, 21, 51, 80	0
2	S	191/191 (100%)	-0.06	6 (3%) 49 52	15, 21, 51, 80	0
2	T	191/191 (100%)	-0.14	4 (2%) 63 66	15, 21, 51, 80	0
2	U	191/191 (100%)	-0.04	8 (4%) 36 39	15, 21, 51, 80	0
2	V	191/191 (100%)	-0.13	4 (2%) 63 66	15, 21, 51, 80	0
2	W	191/191 (100%)	-0.07	6 (3%) 49 52	15, 21, 51, 80	0
2	X	191/191 (100%)	-0.07	5 (2%) 56 59	15, 21, 51, 80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4836/4836 (100%)	0.11	256 (5%) 26 29	15, 22, 58, 116	0

The worst 5 of 256 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ILE	13.7
1	K	14	ILE	13.7
1	K	114	LYS	13.2
1	L	14	ILE	12.6
1	F	113	ARG	12.3

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
3	FE	A	301	1/1	0.91	0.07	34,34,34,34	1
4	CA	B	6303	1/1	0.93	0.09	63,63,63,63	0
4	CA	F	8303	1/1	0.93	0.10	63,63,63,63	0
4	CA	A	5303	1/1	0.94	0.10	63,63,63,63	0
3	FE	F	301	1/1	0.95	0.07	34,34,34,34	1
4	CA	C	7303	1/1	0.96	0.10	63,63,63,63	0
3	FE	C	301	1/1	0.97	0.07	34,34,34,34	1
3	FE	N	300	1/1	0.97	0.08	18,18,18,18	0
3	FE	O	300	1/1	0.99	0.09	18,18,18,18	0
4	CA	C	7302	1/1	0.99	0.09	18,18,18,18	0
4	CA	A	5302	1/1	0.99	0.07	18,18,18,18	0
3	FE	B	301	1/1	0.99	0.04	34,34,34,34	1
3	FE	U	300	1/1	1.00	0.07	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FE	V	300	1/1	1.00	0.07	18,18,18,18	0
3	FE	W	300	1/1	1.00	0.07	18,18,18,18	0
3	FE	X	300	1/1	1.00	0.05	18,18,18,18	0
3	FE	M	300	1/1	1.00	0.06	18,18,18,18	0
3	FE	P	300	1/1	1.00	0.06	18,18,18,18	0
4	CA	B	6302	1/1	1.00	0.08	18,18,18,18	0
3	FE	Q	300	1/1	1.00	0.07	18,18,18,18	0
3	FE	R	300	1/1	1.00	0.06	18,18,18,18	0
3	FE	S	300	1/1	1.00	0.05	18,18,18,18	0
4	CA	F	8302	1/1	1.00	0.06	18,18,18,18	0
3	FE	T	300	1/1	1.00	0.07	18,18,18,18	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.