



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2024 – 09:07 am GMT

PDB ID : 9HO6
Title : Crystal Structure of the Human Frataxin protein in complex with a tailored Camelid Nanobody 16C10
Deposited on : 2024-12-11
Resolution : 2.00 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

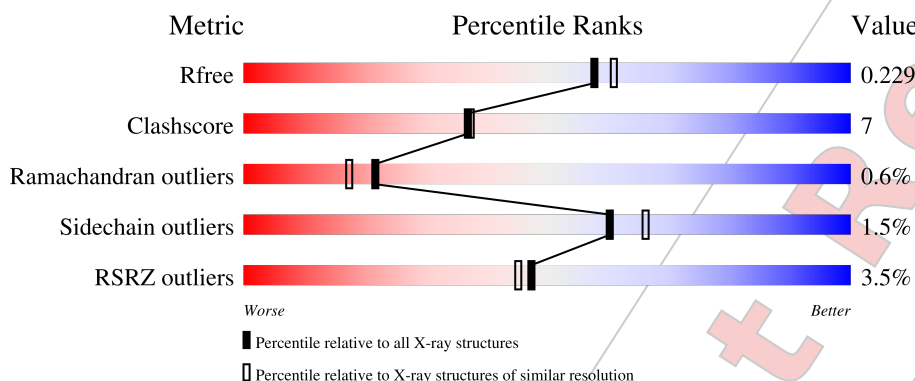
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	122	<div> <div>0%</div> <div>93%</div> <div>6%</div> </div>
1	B	122	<div> <div>2%</div> <div>90%</div> <div>7%</div> </div>
2	C	139	<div> <div>4%</div> <div>73%</div> <div>14%</div> <div>12%</div> </div>
2	D	139	<div> <div>6%</div> <div>73%</div> <div>12%</div> <div>12%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4011 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 Frataxin mature form.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	0	0	0
			953	609	149	195			
1	B	121	Total	C	N	O	0	0	0
			953	609	149	195			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q16595
B	0	MET	-	initiating methionine	UNP Q16595

- Molecule 2 is a protein called Camelid Nanobody 16C10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	123	Total	C	N	O S	0	1	0
			935	578	170	183 4			
2	C	123	Total	C	N	O S	0	1	0
			935	578	170	183 4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	D	54	Total	O	0	0
			54	54		
3	B	54	Total	O	0	0
			54	54		
3	C	65	Total	O	0	0
			65	65		

- Molecule 1: Frataxin mature form



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.90Å 81.10Å 107.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.75 – 2.00 64.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	74.0 (64.75-2.00) 74.3 (64.75-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.21rc1_4958	Depositor
R, R_{free}	0.180 , 0.227 0.180 , 0.229	Depositor DCC
R_{free} test set	1765 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtrriage
Anisotropy	0.200	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4011	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	0.42	0/975	0.57	0/1324
1	B	0.38	0/975	0.58	0/1324
2	C	0.38	0/953	0.68	1/1296 (0.1%)
2	D	0.38	0/953	0.70	2/1296 (0.2%)
All	All	0.39	0/3856	0.64	3/5240 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	D	0	2
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	98	VAL	C-N-CD	-7.34	104.46	120.60
2	C	98	VAL	C-N-CD	-7.06	105.07	120.60
2	D	18	LEU	CA-CB-CG	5.24	127.35	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	98	VAL	Peptide
2	D	98	VAL	Mainchain,Peptide

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	953	0	921	6	0
1	B	953	0	921	10	0
2	C	935	0	910	17	0
2	D	935	0	910	21	0
3	A	62	0	0	2	0
3	B	54	0	0	3	1
3	C	65	0	0	5	2
3	D	54	0	0	3	1
All	All	4011	0	3662	52	2

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

All (52) 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)
2:C:123:ALA:O	3:C:201:HOH:O	1.65	1.12
2:D:30:SER:HA	2:D:71[B]:ARG:HH12	1.31	0.92
2:D:99:PRO:HG3	1:B:107:THR:HG23	1.61	0.82
2:C:71[A]:ARG:NH1	3:C:203:HOH:O	2.21	0.72
1:B:7:GLU:OE1	3:B:201:HOH:O	2.07	0.71
2:C:88:GLU:O	3:C:202:HOH:O	2.10	0.69
2:D:108:ASP:OD2	3:D:202:HOH:O	2.11	0.68
2:C:30:SER:HB3	2:C:71[B]:ARG:HH22	1.60	0.67
1:B:19:GLU:OE2	3:B:202:HOH:O	2.13	0.66
2:D:71[A]:ARG:HD2	2:D:73:ASN:ND2	2.10	0.66
1:A:59:GLN:OE1	1:A:62:ASN:ND2	2.31	0.64
1:A:59:GLN:HG3	1:A:66:TRP:CD2	2.33	0.62
1:B:59:GLN:HG3	1:B:66:TRP:CE2	2.35	0.61
2:C:13:GLN:HG2	2:C:122:ALA:HB3	1.82	0.60
1:B:106:LYS:NZ	3:B:204:HOH:O	2.34	0.60
2:C:62:SER:HB2	3:C:252:HOH:O	2.02	0.59
2:D:12:VAL:HG21	2:D:85:LEU:HD13	1.86	0.56
2:C:18:LEU:HB2	2:C:82:MET:HE3	1.88	0.55
2:D:34:MET:HE1	2:D:71[A]:ARG:HE	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:LYS:NZ	3:D:206:HOH:O	2.40	0.55
2:D:3:GLN:HB2	2:D:25:THR:HG23	1.90	0.54
1:A:107:THR:HG22	3:A:210:HOH:O	2.08	0.53
2:C:30:SER:HA	2:C:71[B]:ARG:HH12	1.73	0.53
2:D:25:THR:HG22	3:D:225:HOH:O	2.09	0.52
2:D:18:LEU:HB2	2:D:82:MET:HE3	1.91	0.51
2:D:30:SER:HA	2:D:71[B]:ARG:NH1	2.11	0.51
1:B:119:LYS:HG3	1:B:120:ASP:N	2.25	0.51
2:D:34:MET:CE	2:D:71[A]:ARG:HE	2.23	0.51
2:D:29:PHE:CZ	2:D:34:MET:HG2	2.46	0.50
1:A:59:GLN:HG3	1:A:66:TRP:CE2	2.49	0.48
2:D:72:ASP:OD2	2:D:75:LYS:HE2	2.14	0.48
2:D:71[B]:ARG:NH2	2:D:76:ASN:OD1	2.46	0.47
1:A:56:ILE:HG12	1:A:67:LEU:HD12	1.96	0.47
1:B:57:ASN:ND2	1:B:58:LYS:O	2.47	0.46
2:D:71[A]:ARG:NH1	2:D:73:ASN:HD21	2.14	0.46
2:D:71[A]:ARG:HB3	2:D:71[A]:ARG:HH11	1.80	0.46
2:C:18:LEU:HB2	2:C:82:MET:CE	2.47	0.45
1:A:113:SER:OG	3:A:201:HOH:O	2.21	0.44
2:D:112:GLN:NE2	2:D:113:GLY:O	2.51	0.43
2:C:30:SER:CA	2:C:71[B]:ARG:HH12	2.31	0.43
2:C:29:PHE:CZ	2:C:34:MET:HG2	2.54	0.43
1:B:41:GLY:HA3	1:B:58:LYS:HD3	2.00	0.42
2:C:12:VAL:HG21	2:C:85:LEU:HD13	2.02	0.42
2:D:34:MET:SD	2:D:71[B]:ARG:NH1	2.94	0.41
2:C:30:SER:HA	2:C:71[B]:ARG:NH1	2.34	0.41
2:D:12:VAL:HG21	2:D:85:LEU:CD1	2.50	0.41
2:C:67:PHE:HA	2:C:81:GLN:O	2.19	0.41
2:D:28:ILE:HD13	2:D:28:ILE:HA	1.87	0.41
1:B:119:LYS:HB2	2:C:104:VAL:HG22	2.02	0.41
2:C:30:SER:CB	2:C:71[B]:ARG:HH12	2.33	0.41
2:C:68:THR:OG1	3:C:204:HOH:O	2.22	0.41
1:B:59:GLN:HG3	1:B:66:TRP:CD2	2.56	0.40

All (2) 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)
3:B:253:HOH:O	3:C:265:HOH:O[1_455]	1.91	0.29
3:D:238:HOH:O	3:C:250:HOH:O[4_445]	2.08	0.12

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	119/122 (98%)	116 (98%)	3 (2%)	0	100	100
1	B	119/122 (98%)	115 (97%)	3 (2%)	1 (1%)	16	12
2	C	122/139 (88%)	118 (97%)	3 (2%)	1 (1%)	16	12
2	D	122/139 (88%)	117 (96%)	4 (3%)	1 (1%)	16	12
All	All	482/522 (92%)	466 (97%)	13 (3%)	3 (1%)	22	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	99	PRO
2	C	99	PRO
1	B	120	ASP

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	104/105 (99%)	104 (100%)	0	100	100
1	B	104/105 (99%)	103 (99%)	1 (1%)	73	78
2	C	100/114 (88%)	98 (98%)	2 (2%)	50	55
2	D	100/114 (88%)	97 (97%)	3 (3%)	36	37
All	All	408/438 (93%)	402 (98%)	6 (2%)	60	66

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	25	THR
2	D	95	CYS
2	D	112	GLN
1	B	107	THR
2	C	3	GLN
2	C	95	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
2	D	73	ASN
2	C	73	ASN
2	C	115	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	121/122 (99%)	-0.26	1 (0%) 82 82	22, 31, 44, 70	0
1	B	121/122 (99%)	-0.28	2 (1%) 69 67	24, 30, 44, 81	0
2	C	123/139 (88%)	-0.06	6 (4%) 36 34	17, 31, 55, 65	1 (0%)
2	D	123/139 (88%)	-0.01	8 (6%) 26 24	16, 32, 52, 66	1 (0%)
All	All	488/522 (93%)	-0.15	17 (3%) 47 45	16, 31, 50, 81	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	ALA	7.8
1	A	121	ALA	5.9
2	D	32	ASN	3.6
2	D	123	ALA	3.3
2	C	29	PHE	3.3
2	D	31	ILE	3.1
2	C	28	ILE	3.1
2	D	29	PHE	3.0
2	C	123	ALA	3.0
2	D	28	ILE	3.0
2	C	31	ILE	2.8
2	D	27	SER	2.7
2	C	2	VAL	2.6
2	D	71[A]	ARG	2.6
1	B	88	HIS	2.2
2	D	112	GLN	2.2
2	C	32	ASN	2.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.

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