



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:01 AM UTC

PDB ID : 2FQL / pdb_00002fql
Title : Crystal structure of trimeric frataxin from the yeast *Saccharomyces cerevisiae*
Authors : Al-Karadaghi, S.; Karlberg, T.
Deposited on : 2006-01-18
Resolution : 3.01 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

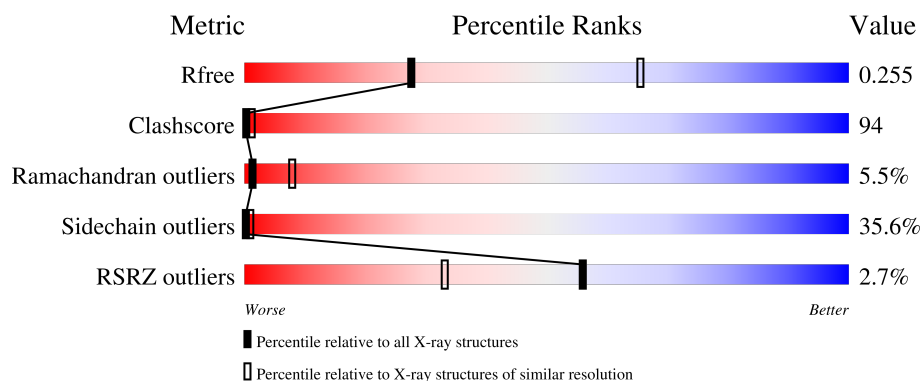
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	123	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 883 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 homolog, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	3	0	0
			883	561	143	177	2			

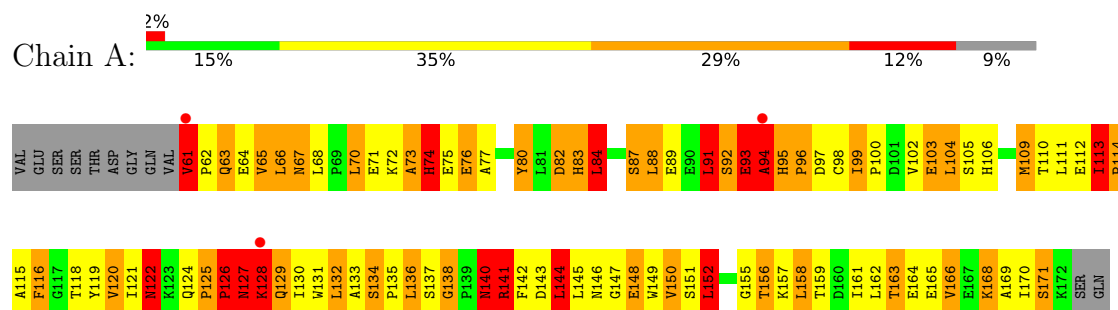
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	ALA	TYR	engineered mutation	UNP Q07540

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: Frataxin homolog, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	121.22Å 121.22Å 121.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.74 – 3.01 19.74 – 3.01	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.74-3.01) 99.5 (19.74-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.286 , 0.305 0.238 , 0.255	Depositor DCC
R_{free} test set	303 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	82.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	883	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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 ⓘ

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	2.41	37/903 (4.1%)	2.29	47/1233 (3.8%)

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
1	A	0	4

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	LYS	N-CA	20.04	1.72	1.46
1	A	129	GLN	N-CA	16.71	1.67	1.46
1	A	146	ASN	CA-C	-12.39	1.40	1.53
1	A	129	GLN	CA-C	10.25	1.66	1.52
1	A	128	LYS	CD-CE	9.46	1.80	1.52
1	A	128	LYS	CA-C	9.40	1.65	1.52
1	A	74	HIS	N-CA	9.17	1.58	1.46
1	A	127	ASN	CB-CG	8.34	1.73	1.52
1	A	128	LYS	CB-CG	7.78	1.75	1.52
1	A	120	VAL	CA-CB	-7.37	1.43	1.55
1	A	148	GLU	CG-CD	7.25	1.70	1.52
1	A	128	LYS	CE-NZ	6.88	1.70	1.49
1	A	128	LYS	CG-CD	6.85	1.73	1.52
1	A	126	PRO	C-O	-6.53	1.15	1.24
1	A	148	GLU	CB-CG	6.51	1.72	1.52
1	A	113	ILE	CA-CB	-6.47	1.45	1.54
1	A	127	ASN	CG-ND2	6.43	1.46	1.33
1	A	122	ASN	CA-C	-6.38	1.45	1.52
1	A	61	VAL	CA-C	6.30	1.66	1.52
1	A	145	LEU	CA-C	-6.19	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	LYS	C-N	6.15	1.42	1.33
1	A	93	GLU	N-CA	6.02	1.53	1.46
1	A	113	ILE	C-O	5.94	1.31	1.24
1	A	73	ALA	N-CA	-5.93	1.38	1.46
1	A	130	ILE	CA-C	5.83	1.59	1.52
1	A	94	ALA	CA-CB	5.82	1.63	1.53
1	A	75	GLU	CD-OE2	5.76	1.36	1.25
1	A	65	VAL	CA-C	-5.68	1.47	1.52
1	A	73	ALA	C-O	-5.68	1.17	1.24
1	A	129	GLN	CD-NE2	5.51	1.44	1.33
1	A	115	ALA	CA-C	5.46	1.60	1.52
1	A	94	ALA	N-CA	5.41	1.53	1.46
1	A	130	ILE	N-CA	5.37	1.53	1.46
1	A	61	VAL	CA-CB	5.25	1.68	1.54
1	A	80	TYR	CA-C	-5.24	1.46	1.52
1	A	128	LYS	C-O	5.19	1.30	1.24
1	A	127	ASN	C-N	5.00	1.40	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	GLN	N-CA-C	20.77	139.08	113.12
1	A	145	LEU	CA-C-N	-12.05	105.32	122.06
1	A	145	LEU	C-N-CA	-12.05	105.32	122.06
1	A	125	PRO	CA-C-N	11.43	134.13	119.84
1	A	125	PRO	C-N-CA	11.43	134.13	119.84
1	A	91	LEU	N-CA-C	-9.36	99.59	114.09
1	A	74	HIS	CB-CA-C	-8.88	92.75	110.42
1	A	135	PRO	N-CA-C	-8.27	103.86	114.03
1	A	122	ASN	CB-CA-C	-7.11	95.33	109.33
1	A	128	LYS	CA-C-O	-7.00	110.50	120.51
1	A	140	ASN	N-CA-C	6.80	119.66	108.99
1	A	61	VAL	CB-CA-C	6.70	124.12	111.40
1	A	138	GLY	CA-C-N	6.67	128.18	119.84
1	A	138	GLY	C-N-CA	6.67	128.18	119.84
1	A	127	ASN	CA-C-N	6.63	134.20	121.54
1	A	127	ASN	C-N-CA	6.63	134.20	121.54
1	A	166	VAL	N-CA-C	6.58	116.72	110.53
1	A	73	ALA	N-CA-C	6.57	120.16	111.75
1	A	73	ALA	CA-C-O	-6.24	113.22	120.20
1	A	82	ASP	N-CA-C	-6.18	103.14	112.04
1	A	125	PRO	N-CA-C	-6.05	103.32	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ASN	N-CA-CB	6.05	117.12	110.35
1	A	75	GLU	CA-C-N	-6.03	111.14	120.31
1	A	75	GLU	C-N-CA	-6.03	111.14	120.31
1	A	65	VAL	N-CA-C	-6.02	107.06	112.12
1	A	128	LYS	CD-CE-NZ	5.97	131.01	111.90
1	A	152	LEU	CA-CB-CG	-5.81	95.97	116.30
1	A	141	ARG	N-CA-C	5.77	118.88	109.24
1	A	92	SER	CA-C-N	5.74	132.50	121.54
1	A	92	SER	C-N-CA	5.74	132.50	121.54
1	A	113	ILE	CA-C-N	5.72	125.25	119.19
1	A	113	ILE	C-N-CA	5.72	125.25	119.19
1	A	130	ILE	CB-CA-C	-5.65	103.15	110.84
1	A	144	LEU	N-CA-C	5.65	118.43	109.96
1	A	65	VAL	CB-CA-C	-5.63	105.39	110.91
1	A	66	LEU	N-CA-C	-5.36	106.33	112.92
1	A	148	GLU	CB-CA-C	5.33	119.12	109.37
1	A	84	LEU	N-CA-C	-5.31	103.44	111.56
1	A	114	PRO	N-CA-C	-5.19	106.77	113.57
1	A	73	ALA	CA-C-N	-5.19	111.63	121.54
1	A	73	ALA	C-N-CA	-5.19	111.63	121.54
1	A	148	GLU	CB-CG-CD	5.19	121.42	112.60
1	A	134	SER	N-CA-C	5.16	116.15	109.65
1	A	147	GLY	CA-C-N	-5.14	114.59	122.87
1	A	147	GLY	C-N-CA	-5.14	114.59	122.87
1	A	96	PRO	N-CA-C	-5.12	104.89	112.26
1	A	120	VAL	CB-CA-C	-5.08	103.00	110.82

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	ASN	Peptide
1	A	126	PRO	Peptide
1	A	127	ASN	Peptide
1	A	61	VAL	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	883	0	865	164	3
All	All	883	0	865	164	3

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 94.

All (164) 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:A:128:LYS:CB	1:A:128:LYS:CG	1.75	1.57
1:A:129:GLN:N	1:A:129:GLN:CA	1.67	1.56
1:A:128:LYS:CD	1:A:128:LYS:CE	1.80	1.55
1:A:128:LYS:CE	1:A:128:LYS:NZ	1.70	1.52
1:A:128:LYS:N	1:A:128:LYS:CA	1.72	1.50
1:A:112:GLU:OE2	1:A:118:THR:HG21	1.43	1.19
1:A:92:SER:HA	1:A:99:ILE:CD1	1.74	1.18
1:A:73:ALA:O	1:A:74:HIS:HB2	1.33	1.12
1:A:92:SER:CA	1:A:99:ILE:HD11	1.82	1.09
1:A:84:LEU:HD13	1:A:109:MET:HE1	1.35	1.07
1:A:113:ILE:O	1:A:113:ILE:HG22	1.54	1.05
1:A:95:HIS:CE1	1:A:97:ASP:HA	1.91	1.05
1:A:95:HIS:O	1:A:95:HIS:CG	2.11	1.03
1:A:132:LEU:HD22	1:A:133:ALA:N	1.75	1.01
1:A:95:HIS:O	1:A:95:HIS:CD2	2.15	0.99
1:A:129:GLN:N	1:A:129:GLN:HA	1.74	0.98
1:A:95:HIS:HB2	1:A:99:ILE:CG1	1.92	0.98
1:A:95:HIS:HB2	1:A:99:ILE:HG13	1.46	0.96
1:A:73:ALA:O	1:A:74:HIS:CB	2.11	0.96
1:A:76:GLU:N	1:A:76:GLU:OE2	2.03	0.91
1:A:95:HIS:CE1	1:A:97:ASP:CA	2.53	0.91
1:A:126:PRO:C	1:A:128:LYS:H	1.78	0.90
1:A:128:LYS:HD3	1:A:152:LEU:CB	2.01	0.90
1:A:96:PRO:HD2	1:A:98:CYS:SG	2.12	0.90
1:A:63:GLN:HA	1:A:66:LEU:CD2	2.04	0.88
1:A:126:PRO:C	1:A:128:LYS:N	2.34	0.85
1:A:84:LEU:CD1	1:A:109:MET:HE1	2.07	0.82
1:A:93:GLU:C	1:A:95:HIS:H	1.89	0.80
1:A:92:SER:HA	1:A:99:ILE:HD11	0.86	0.79
1:A:137:SER:HB3	1:A:165:GLU:OE2	1.83	0.78
1:A:127:ASN:O	1:A:128:LYS:HG3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HD23	1:A:66:LEU:H	1.47	0.78
1:A:132:LEU:HD22	1:A:132:LEU:C	2.10	0.76
1:A:128:LYS:CB	1:A:152:LEU:HD13	2.15	0.76
1:A:112:GLU:HA	1:A:118:THR:HG22	1.67	0.75
1:A:140:ASN:HD22	1:A:141:ARG:H	1.31	0.75
1:A:116:PHE:CD2	1:A:116:PHE:N	2.54	0.75
1:A:128:LYS:HD2	1:A:141:ARG:HG2	1.68	0.74
1:A:95:HIS:HB2	1:A:99:ILE:HG12	1.68	0.74
1:A:168:LYS:CD	1:A:168:LYS:N	2.51	0.73
1:A:132:LEU:CD2	1:A:133:ALA:N	2.51	0.72
1:A:99:ILE:HG13	1:A:99:ILE:O	1.89	0.71
1:A:120:VAL:HG12	1:A:121:ILE:N	2.06	0.71
1:A:84:LEU:C	1:A:84:LEU:HD22	2.15	0.71
1:A:111:LEU:HB2	1:A:119:TYR:HB2	1.73	0.70
1:A:113:ILE:O	1:A:113:ILE:CG2	2.33	0.70
1:A:67:ASN:H	1:A:67:ASN:HD22	1.38	0.70
1:A:93:GLU:O	1:A:95:HIS:N	2.23	0.70
1:A:128:LYS:HD3	1:A:152:LEU:HB3	1.73	0.70
1:A:151:SER:HB3	1:A:156:THR:H	1.57	0.69
1:A:129:GLN:HG3	1:A:129:GLN:O	1.91	0.69
1:A:95:HIS:CE1	1:A:97:ASP:C	2.71	0.69
1:A:88:LEU:HB3	1:A:102:VAL:HG11	1.74	0.69
1:A:128:LYS:CG	1:A:152:LEU:HD13	2.22	0.69
1:A:158:LEU:HG	1:A:162:LEU:HD11	1.74	0.68
1:A:128:LYS:HD2	1:A:141:ARG:CG	2.24	0.68
1:A:67:ASN:HD22	1:A:67:ASN:N	1.90	0.67
1:A:132:LEU:C	1:A:132:LEU:CD2	2.67	0.66
1:A:127:ASN:O	1:A:128:LYS:CG	2.44	0.66
1:A:168:LYS:N	1:A:168:LYS:HD2	2.09	0.65
1:A:63:GLN:HA	1:A:66:LEU:HD21	1.77	0.65
1:A:151:SER:HB3	1:A:156:THR:N	2.12	0.65
1:A:93:GLU:C	1:A:95:HIS:N	2.54	0.65
1:A:140:ASN:HD22	1:A:141:ARG:N	1.96	0.64
1:A:99:ILE:CG1	1:A:99:ILE:O	2.45	0.64
1:A:93:GLU:OE1	1:A:93:GLU:N	2.31	0.64
1:A:148:GLU:HG3	1:A:157:LYS:HZ1	1.62	0.63
1:A:102:VAL:HG12	1:A:111:LEU:HD21	1.79	0.63
1:A:89:GLU:HB3	1:A:102:VAL:CG2	2.28	0.63
1:A:158:LEU:O	1:A:162:LEU:HD12	1.99	0.62
1:A:89:GLU:HA	1:A:92:SER:HB2	1.83	0.61
1:A:170:ILE:HD12	1:A:170:ILE:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:HB3	1:A:152:LEU:HD13	1.82	0.60
1:A:66:LEU:CD2	1:A:66:LEU:H	2.14	0.60
1:A:83:HIS:N	1:A:83:HIS:CD2	2.69	0.59
1:A:67:ASN:H	1:A:67:ASN:ND2	2.00	0.59
1:A:127:ASN:C	1:A:128:LYS:HG3	2.29	0.58
1:A:128:LYS:C	1:A:129:GLN:CA	2.72	0.58
1:A:84:LEU:HD22	1:A:84:LEU:O	2.02	0.58
1:A:116:PHE:CE1	1:A:136:LEU:HD22	2.39	0.57
1:A:80:TYR:CE2	1:A:158:LEU:HD21	2.40	0.56
1:A:82:ASP:C	1:A:84:LEU:H	2.13	0.56
1:A:120:VAL:CG1	1:A:121:ILE:N	2.68	0.56
1:A:122:ASN:HB2	1:A:131:TRP:HB3	1.86	0.56
1:A:159:THR:O	1:A:163:THR:HB	2.06	0.56
1:A:112:GLU:OE2	1:A:118:THR:CG2	2.36	0.56
1:A:66:LEU:HD23	1:A:66:LEU:N	2.21	0.56
1:A:128:LYS:HD2	1:A:141:ARG:HD3	1.88	0.56
1:A:63:GLN:HA	1:A:66:LEU:HD22	1.85	0.55
1:A:61:VAL:HG12	1:A:62:PRO:HD3	1.88	0.55
1:A:120:VAL:C	1:A:121:ILE:HG13	2.32	0.55
1:A:128:LYS:C	1:A:129:GLN:HA	2.31	0.55
1:A:170:ILE:O	1:A:171:SER:C	2.51	0.54
1:A:96:PRO:CD	1:A:98:CYS:SG	2.93	0.54
1:A:168:LYS:N	1:A:168:LYS:HD3	2.23	0.54
1:A:128:LYS:CB	1:A:128:LYS:N	2.66	0.53
1:A:128:LYS:HD3	1:A:152:LEU:CG	2.39	0.53
1:A:95:HIS:HE1	1:A:97:ASP:HA	1.63	0.53
1:A:83:HIS:CD2	1:A:83:HIS:H	2.28	0.52
1:A:150:VAL:HG13	1:A:151:SER:N	2.23	0.52
1:A:124:GLN:HG3	1:A:125:PRO:HD2	1.92	0.51
1:A:82:ASP:C	1:A:84:LEU:N	2.68	0.51
1:A:116:PHE:CE2	1:A:169:ALA:HB2	2.46	0.51
1:A:164:GLU:O	1:A:165:GLU:C	2.53	0.50
1:A:91:LEU:C	1:A:93:GLU:H	2.19	0.50
1:A:128:LYS:CD	1:A:141:ARG:HD3	2.41	0.50
1:A:161:ILE:O	1:A:165:GLU:HG3	2.10	0.50
1:A:102:VAL:HG12	1:A:111:LEU:CD2	2.42	0.49
1:A:64:GLU:O	1:A:64:GLU:HG2	2.12	0.49
1:A:134:SER:O	1:A:138:GLY:N	2.45	0.49
1:A:88:LEU:O	1:A:91:LEU:HB2	2.13	0.49
1:A:128:LYS:CB	1:A:152:LEU:CD1	2.90	0.49
1:A:168:LYS:HD3	1:A:168:LYS:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:HIS:O	1:A:87:SER:HB3	2.13	0.48
1:A:116:PHE:HE2	1:A:169:ALA:HB2	1.78	0.48
1:A:93:GLU:HB2	1:A:94:ALA:H	1.33	0.48
1:A:109:MET:HG2	1:A:110:THR:N	2.27	0.48
1:A:122:ASN:HD22	1:A:124:GLN:HE22	1.60	0.48
1:A:128:LYS:CD	1:A:152:LEU:HD13	2.44	0.48
1:A:128:LYS:HB3	1:A:152:LEU:CD1	2.43	0.48
1:A:116:PHE:CD1	1:A:136:LEU:HD22	2.49	0.48
1:A:80:TYR:CZ	1:A:158:LEU:HD21	2.48	0.47
1:A:88:LEU:HA	1:A:88:LEU:HD12	1.38	0.47
1:A:144:LEU:HD13	1:A:149:TRP:CE2	2.49	0.47
1:A:126:PRO:HA	1:A:128:LYS:CA	2.44	0.47
1:A:93:GLU:N	1:A:93:GLU:CD	2.71	0.47
1:A:148:GLU:HG3	1:A:157:LYS:NZ	2.29	0.47
1:A:89:GLU:HB3	1:A:102:VAL:HG21	1.97	0.46
1:A:150:VAL:HG13	1:A:155:GLY:HA2	1.97	0.46
1:A:89:GLU:C	1:A:91:LEU:H	2.23	0.45
1:A:76:GLU:N	1:A:76:GLU:CD	2.73	0.45
1:A:76:GLU:O	1:A:77:ALA:C	2.59	0.45
1:A:104:LEU:C	1:A:104:LEU:CD2	2.89	0.45
1:A:141:ARG:HH11	1:A:141:ARG:HD2	1.64	0.45
1:A:112:GLU:HA	1:A:118:THR:CG2	2.41	0.45
1:A:93:GLU:O	1:A:95:HIS:O	2.35	0.45
1:A:129:GLN:O	1:A:129:GLN:CG	2.63	0.45
1:A:142:PHE:HD1	1:A:150:VAL:C	2.26	0.44
1:A:128:LYS:HD2	1:A:141:ARG:CD	2.45	0.44
1:A:129:GLN:N	1:A:129:GLN:CB	2.68	0.43
1:A:142:PHE:HA	1:A:150:VAL:O	2.18	0.43
1:A:111:LEU:HA	1:A:111:LEU:HD23	1.43	0.43
1:A:125:PRO:HA	1:A:126:PRO:HD3	1.68	0.43
1:A:151:SER:N	1:A:156:THR:O	2.52	0.43
1:A:126:PRO:HA	1:A:128:LYS:C	2.44	0.43
1:A:89:GLU:HB3	1:A:102:VAL:HG22	2.02	0.42
1:A:116:PHE:H	1:A:116:PHE:HD2	1.66	0.42
1:A:122:ASN:HD22	1:A:124:GLN:NE2	2.17	0.42
1:A:70:LEU:HD12	1:A:70:LEU:HA	1.91	0.42
1:A:95:HIS:ND1	1:A:97:ASP:C	2.78	0.42
1:A:140:ASN:HB3	1:A:142:PHE:CE2	2.54	0.42
1:A:92:SER:C	1:A:93:GLU:OE1	2.63	0.42
1:A:119:TYR:OH	1:A:165:GLU:HB3	2.20	0.41
1:A:170:ILE:HD12	1:A:170:ILE:N	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:O	1:A:73:ALA:C	2.62	0.41
1:A:82:ASP:O	1:A:84:LEU:N	2.53	0.41
1:A:68:LEU:HB2	1:A:70:LEU:HD13	2.02	0.41
1:A:162:LEU:HD12	1:A:162:LEU:H	1.85	0.41
1:A:100:PRO:HD2	1:A:114:PRO:HD3	2.02	0.41
1:A:103:GLU:HB3	1:A:110:THR:OG1	2.21	0.41
1:A:113:ILE:HG22	1:A:116:PHE:HD2	1.85	0.41
1:A:128:LYS:CD	1:A:152:LEU:CB	2.87	0.41
1:A:113:ILE:HA	1:A:114:PRO:HD3	1.87	0.40
1:A:66:LEU:CD2	1:A:66:LEU:N	2.82	0.40

All (3) 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)
1:A:127:ASN:CA	1:A:129:GLN:NE2[7_454]	1.85	0.35
1:A:127:ASN:CB	1:A:129:GLN:NE2[7_454]	1.89	0.31
1:A:127:ASN:ND2	1:A:129:GLN:CG[7_454]	2.12	0.08

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	110/123 (89%)	79 (72%)	25 (23%)	6 (6%)	1 8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ALA
1	A	126	PRO
1	A	105	SER
1	A	127	ASN

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Mol	Chain	Res	Type
1	A	128	LYS
1	A	74	HIS

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	101/111 (91%)	65 (64%)	36 (36%)	0 1

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	65	VAL
1	A	67	ASN
1	A	70	LEU
1	A	71	GLU
1	A	76	GLU
1	A	83	HIS
1	A	84	LEU
1	A	87	SER
1	A	88	LEU
1	A	91	LEU
1	A	93	GLU
1	A	95	HIS
1	A	99	ILE
1	A	103	GLU
1	A	104	LEU
1	A	106	HIS
1	A	109	MET
1	A	113	ILE
1	A	116	PHE
1	A	127	ASN
1	A	128	LYS
1	A	132	LEU
1	A	136	LEU

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Mol	Chain	Res	Type
1	A	140	ASN
1	A	141	ARG
1	A	143	ASP
1	A	144	LEU
1	A	150	VAL
1	A	152	LEU
1	A	156	THR
1	A	158	LEU
1	A	163	THR
1	A	166	VAL
1	A	168	LYS
1	A	171	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	67	ASN
1	A	83	HIS
1	A	95	HIS
1	A	124	GLN
1	A	127	ASN
1	A	140	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [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	112/123 (91%)	-0.22	3 (2%) 56 33	43, 71, 100, 100	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	LYS	5.8
1	A	94	ALA	2.5
1	A	61	VAL	2.3

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 oligosaccharides 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.