



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 06:19 PM UTC

PDB ID : 1FOU / pdb_00001fou
Title : CONNECTOR PROTEIN FROM BACTERIOPHAGE PHI29
Authors : Simpson, A.A.; Tao, Y.; Leiman, P.G.; Badasso, M.O.; He, Y.; Jardine, P.J.; Olson, N.H.; Morais, M.C.; Grimes, S.N.; Anderson, D.L.; Baker, T.S.; Rossmann, M.G.
Deposited on : 2000-08-28
Resolution : 3.20 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	:	4-5-2 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

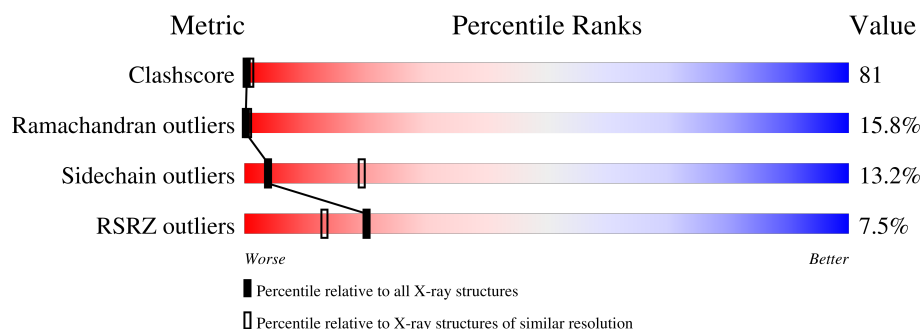
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	309	7% 17% 44% 18% • 17%
1	B	309	7% 15% 45% 19% 5% 17%
1	C	309	6% 14% 49% 18% • 17%
1	D	309	7% 11% 50% 19% • 17%
1	E	309	8% 12% 48% 21% • 17%
1	F	309	6% 17% 44% 18% 5% 17%
1	G	309	4% 15% 48% 18% • 17%

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Mol	Chain	Length	Quality of chain
1	H	309	6%14%48%17%•17%
1	I	309	5%16%47%17%•17%
1	J	309	5%13%46%20%•17%
1	K	309	6%16%47%16%•17%
1	L	309	7%20%42%19%•17%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25272 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 UPPER COLLAR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2106	1350	348	401	7			
1	B	257	Total	C	N	O	S	0	0	0
			2106	1350	348	401	7			
1	C	257	Total	C	N	O	S	0	0	0
			2106	1350	348	401	7			
1	D	257	Total	C	N	O	S	0	0	0
			2106	1350	348	401	7			
1	E	257	Total	C	N	O	S	0	0	0
			2106	1350	348	401	7			
1	F	257	Total	C	N	O	S	0	0	0
			2106	1350	348	401	7			
1	G	257	Total	C	N	O	S	0	0	0
			2106	1350	348	401	7			
1	H	257	Total	C	N	O	S	0	0	0
			2106	1350	348	401	7			
1	I	257	Total	C	N	O	S	0	0	0
			2106	1350	348	401	7			
1	J	257	Total	C	N	O	S	0	0	0
			2106	1350	348	401	7			
1	K	257	Total	C	N	O	S	0	0	0
			2106	1350	348	401	7			
1	L	257	Total	C	N	O	S	0	0	0
			2106	1350	348	401	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	LYS	LEU	conflict	UNP P04332
A	226	LEU	GLY	conflict	UNP P04332
A	227	GLN	ILE	conflict	UNP P04332
A	228	THR	LYS	conflict	UNP P04332
A	251	ASP	GLU	conflict	UNP P04332

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Chain	Residue	Modelled	Actual	Comment	Reference
B	225	LYS	LEU	conflict	UNP P04332
B	226	LEU	GLY	conflict	UNP P04332
B	227	GLN	ILE	conflict	UNP P04332
B	228	THR	LYS	conflict	UNP P04332
B	251	ASP	GLU	conflict	UNP P04332
C	225	LYS	LEU	conflict	UNP P04332
C	226	LEU	GLY	conflict	UNP P04332
C	227	GLN	ILE	conflict	UNP P04332
C	228	THR	LYS	conflict	UNP P04332
C	251	ASP	GLU	conflict	UNP P04332
D	225	LYS	LEU	conflict	UNP P04332
D	226	LEU	GLY	conflict	UNP P04332
D	227	GLN	ILE	conflict	UNP P04332
D	228	THR	LYS	conflict	UNP P04332
D	251	ASP	GLU	conflict	UNP P04332
E	225	LYS	LEU	conflict	UNP P04332
E	226	LEU	GLY	conflict	UNP P04332
E	227	GLN	ILE	conflict	UNP P04332
E	228	THR	LYS	conflict	UNP P04332
E	251	ASP	GLU	conflict	UNP P04332
F	225	LYS	LEU	conflict	UNP P04332
F	226	LEU	GLY	conflict	UNP P04332
F	227	GLN	ILE	conflict	UNP P04332
F	228	THR	LYS	conflict	UNP P04332
F	251	ASP	GLU	conflict	UNP P04332
G	225	LYS	LEU	conflict	UNP P04332
G	226	LEU	GLY	conflict	UNP P04332
G	227	GLN	ILE	conflict	UNP P04332
G	228	THR	LYS	conflict	UNP P04332
G	251	ASP	GLU	conflict	UNP P04332
H	225	LYS	LEU	conflict	UNP P04332
H	226	LEU	GLY	conflict	UNP P04332
H	227	GLN	ILE	conflict	UNP P04332
H	228	THR	LYS	conflict	UNP P04332
H	251	ASP	GLU	conflict	UNP P04332
I	225	LYS	LEU	conflict	UNP P04332
I	226	LEU	GLY	conflict	UNP P04332
I	227	GLN	ILE	conflict	UNP P04332
I	228	THR	LYS	conflict	UNP P04332
I	251	ASP	GLU	conflict	UNP P04332
J	225	LYS	LEU	conflict	UNP P04332
J	226	LEU	GLY	conflict	UNP P04332

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Chain	Residue	Modelled	Actual	Comment	Reference
J	227	GLN	ILE	conflict	UNP P04332
J	228	THR	LYS	conflict	UNP P04332
J	251	ASP	GLU	conflict	UNP P04332
K	225	LYS	LEU	conflict	UNP P04332
K	226	LEU	GLY	conflict	UNP P04332
K	227	GLN	ILE	conflict	UNP P04332
K	228	THR	LYS	conflict	UNP P04332
K	251	ASP	GLU	conflict	UNP P04332
L	225	LYS	LEU	conflict	UNP P04332
L	226	LEU	GLY	conflict	UNP P04332
L	227	GLN	ILE	conflict	UNP P04332
L	228	THR	LYS	conflict	UNP P04332
L	251	ASP	GLU	conflict	UNP P04332

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.

Chain A:

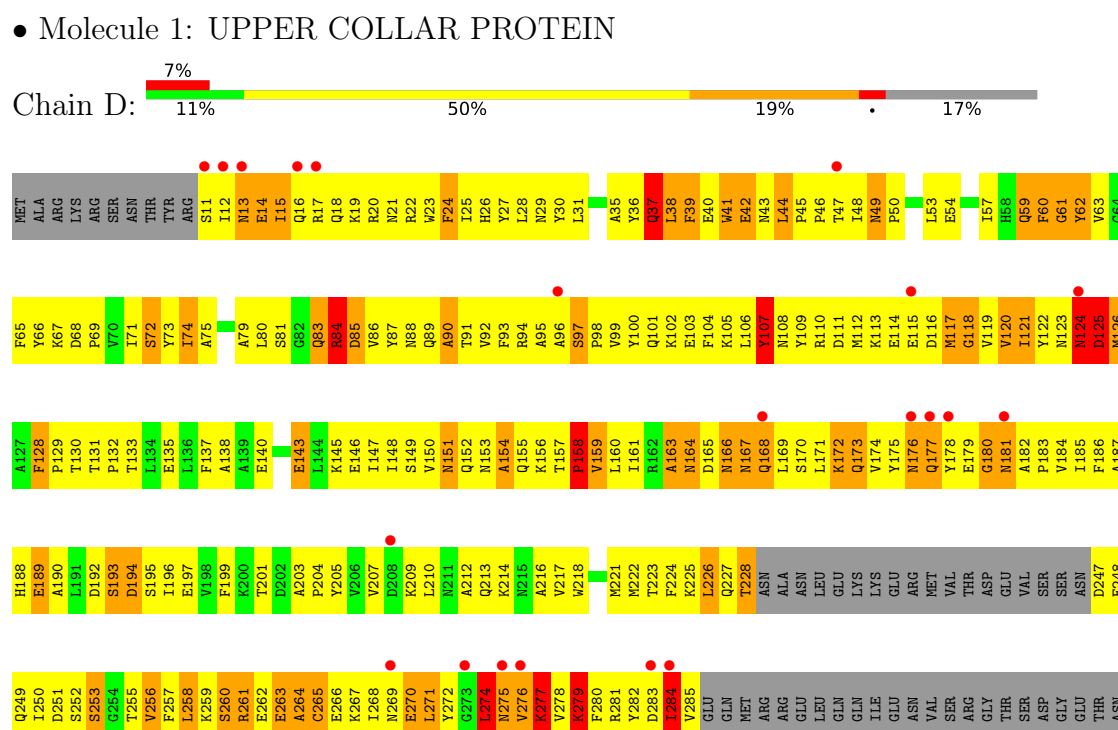
7% 17% 44% 18% 17%

Vertical bar charts (Chain A):

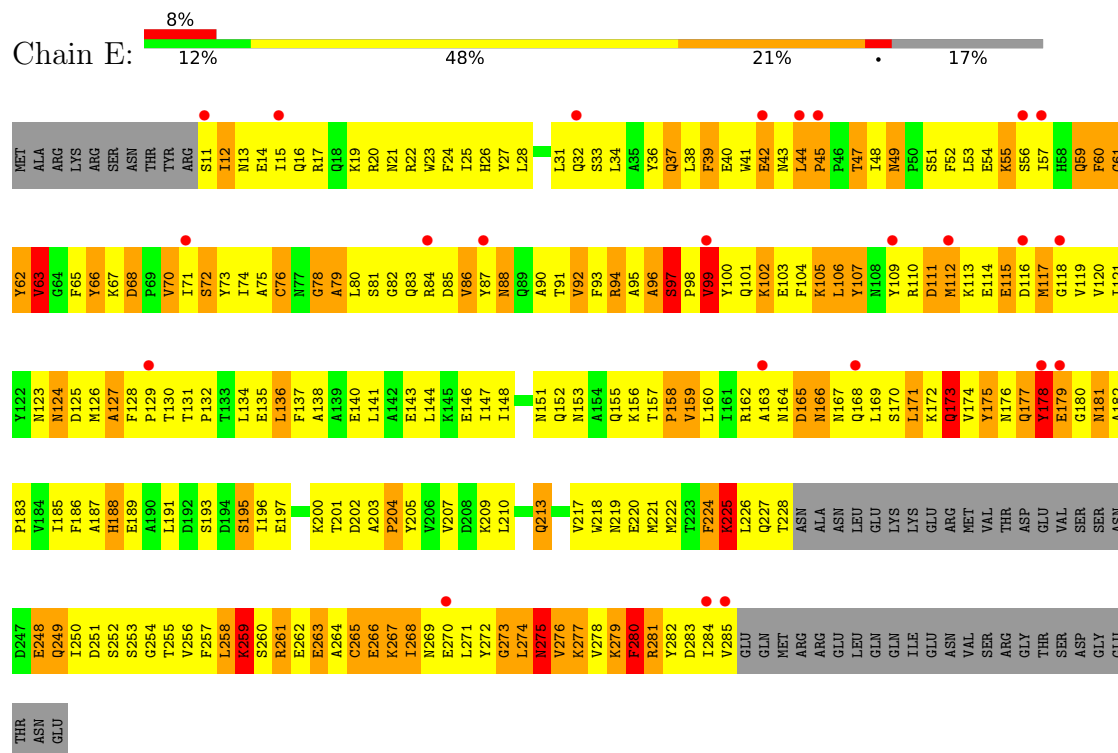
- Row 1: MET, Y66, P129, D192, L258
- Row 2: ALA, K67, T130, S193, K259
- Row 3: ARG, D68, T131, S194, K260
- Row 4: LYS, P69, T132, S195, R261
- Row 5: ARG, V70, T133, S196, R262
- Row 6: SER, T71, T134, E197, E263
- Row 7: ASN, S72, F137, V198, K264
- Row 8: THR, Y73, A138, F199, C265
- Row 9: ARG, T74, A139, K200, E266
- Row 10: S11, C76, A142, T201, M269
- Row 11: I12, M77, E143, D202, L271
- Row 12: N13, G78, A144, Y205, Y272
- Row 13: E14, A79, K145, Y206, Y273
- Row 14: I15, L80, E146, V207, G274
- Row 15: Q16, S81, I147, D208, L274
- Row 16: R17, G82, I148, K209, M275
- Row 17: Q18, Q83, S149, K210, Y276
- Row 18: K19, R84, A149, Q213, K277
- Row 19: N21, D85, V150, Q214, Y278
- Row 20: R22, G88, Q152, M219, K279
- Row 21: Y27, Q89, M153, N218, F280
- Row 22: L28, A90, Q154, A163, R281
- Row 23: M29, T91, Q155, A164, Y282
- Row 24: Y30, V92, K156, M165, L284
- Row 25: L31, F93, T157, A166, V285
- Row 26: Q32, R94, V159, L160, GLU
- Row 27: A35, A96, L161, R162, MET
- Row 28: Y36, S97, R163, A163, ARG
- Row 29: Q37, P98, M164, A164, ARG
- Row 30: L38, V99, A165, A165, GLU
- Row 31: F39, Y100, M166, A166, LEU
- Row 32: F104, F104, M167, L167, GLU
- Row 33: K105, Q168, Q168, LYS
- Row 34: L106, L169, LYS
- Row 35: Y107, S170, GLU
- Row 36: M108, L171, ARG
- Row 37: Y109, K172, MET
- Row 38: R110, Q173, VAL
- Row 39: D111, V174, THR
- Row 40: K113, Y175, ASP
- Row 41: M112, M112, GLU
- Row 42: M113, K113, SER
- Row 43: E114, Q177, VAL
- Row 44: E115, Y178, SER
- Row 45: D116, E179, SER
- Row 46: M117, G180, ASN
- Row 47: G118, D247, D247
- Row 48: E119, E248, E248
- Row 49: K124, Q249, Q249
- Row 50: V120, I250, I250
- Row 51: I121, D251, D251
- Row 52: Y122, S252, S252
- Row 53: M123, G254, G254
- Row 54: N124, H188, H188
- Row 55: D125, E189, E189
- Row 56: M126, T255, T255
- Row 57: V63, V56, V56
- Row 58: G64, F56, F56
- Row 59: Q59, F60, F60
- Row 60: G61, Y62, Y62
- Row 61: E54, K55, K55
- Row 62: L53, S56, S56
- Row 63: F52, S51, S51
- Row 64: F52, F52, F52
- Row 65: P50, P50, P50
- Row 66: P46, P46, P46
- Row 67: T47, T47, T47
- Row 68: P45, P45, P45
- Row 69: L44, L44, L44
- Row 70: M44, M44, M44
- Row 71: E42, E42, E42
- Row 72: W41, W41, W41
- Row 73: F40, F40, F40
- Row 74: L38, L38, L38
- Row 75: Q37, Q37, Q37
- Row 76: Y36, Y36, Y36
- Row 77: A35, A35, A35

Chain B:

Amino Acid	Percentage
ALA	15%
ARG	45%
LYS	19%
SER	5%
ASN	17%

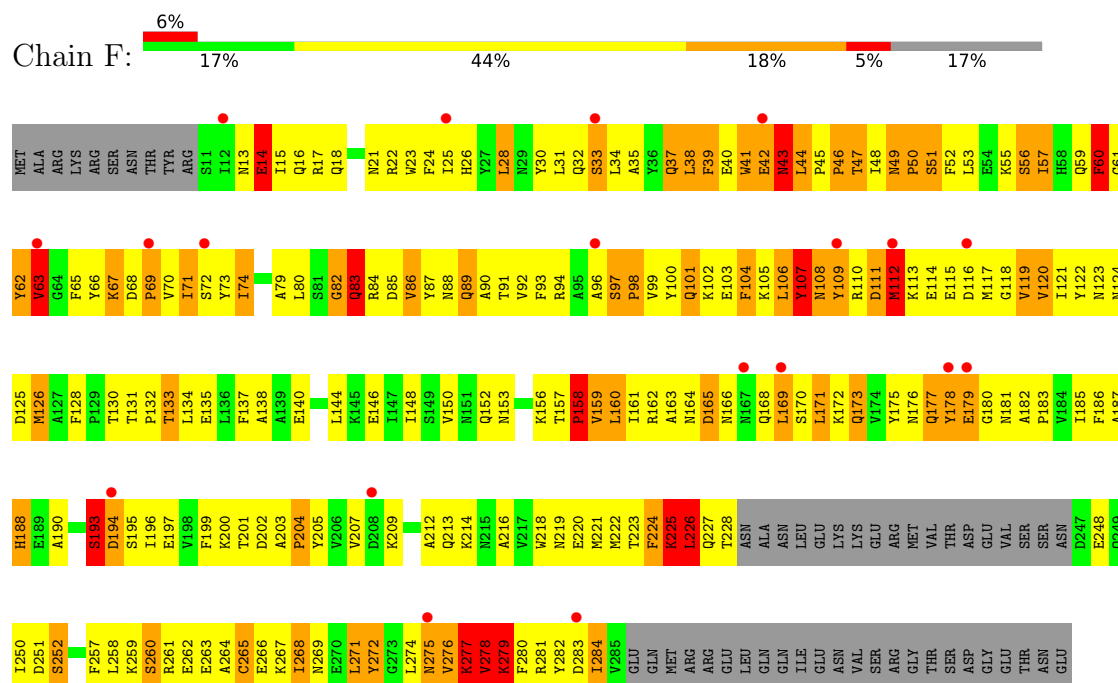


- Molecule 1: UPPER COLLAR PROTEIN



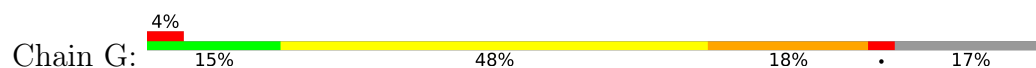
THR
ASN
GLU

- Molecule 1: UPPER COLLAR PROTEIN

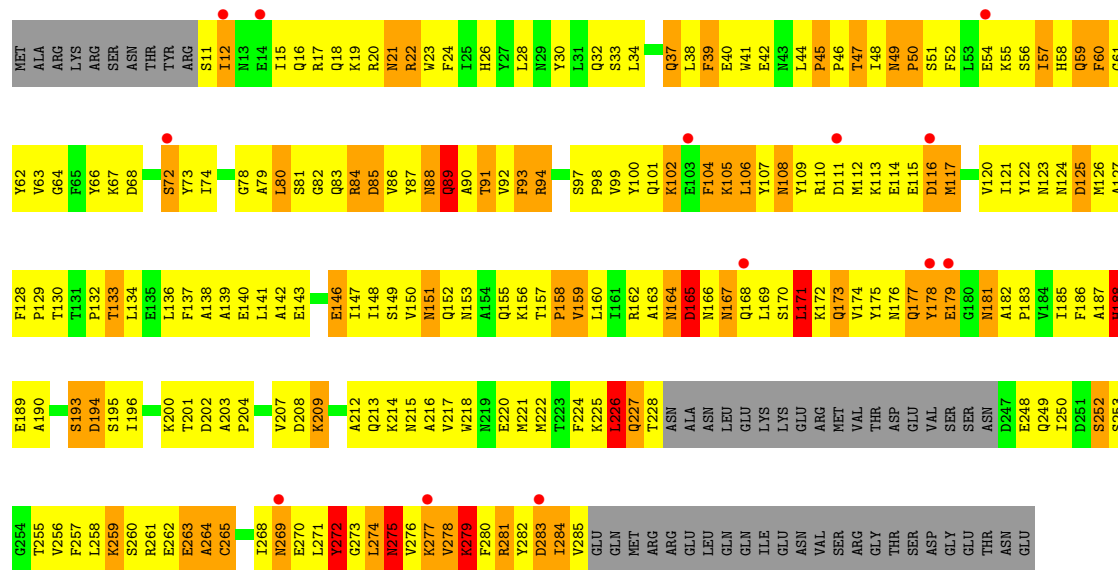


I250	
D251	
S252	

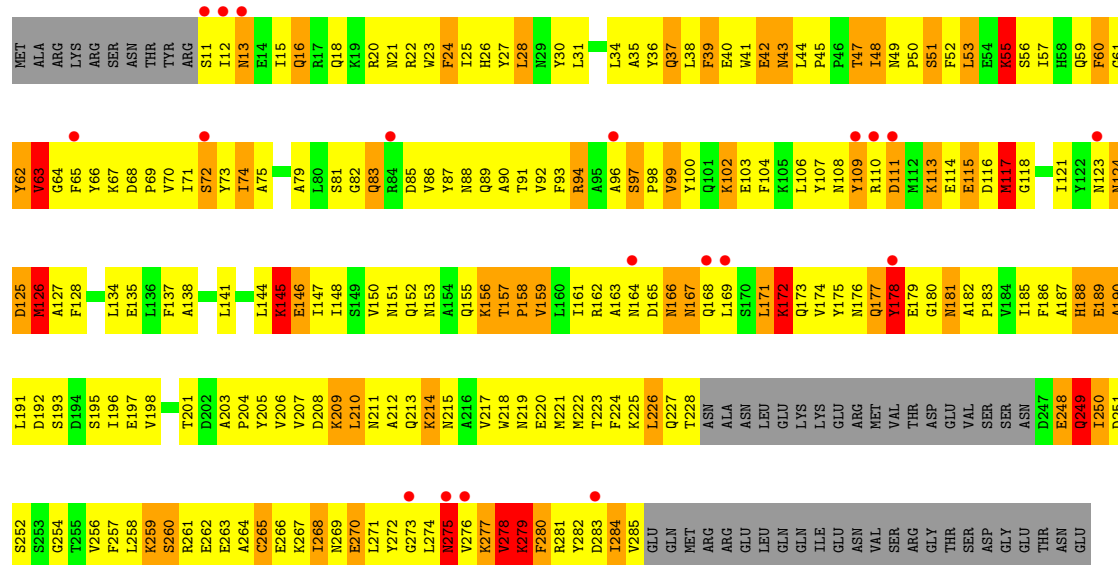
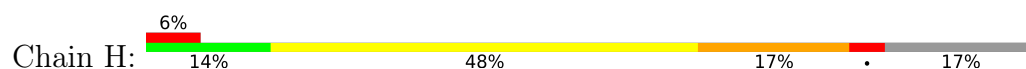
• Molecule 1: UPPER COLLAR PROTEIN



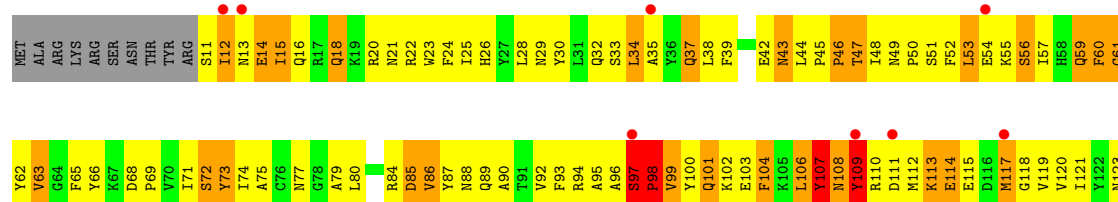
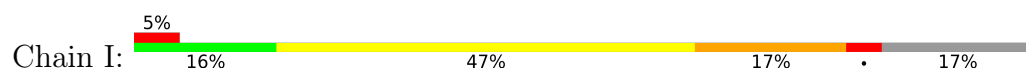
Chain G:

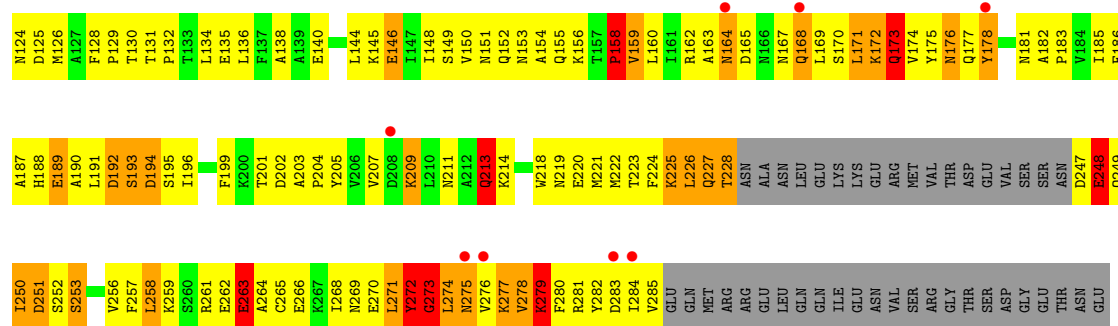


• Molecule 1: UPPER COLLAR PROTEIN

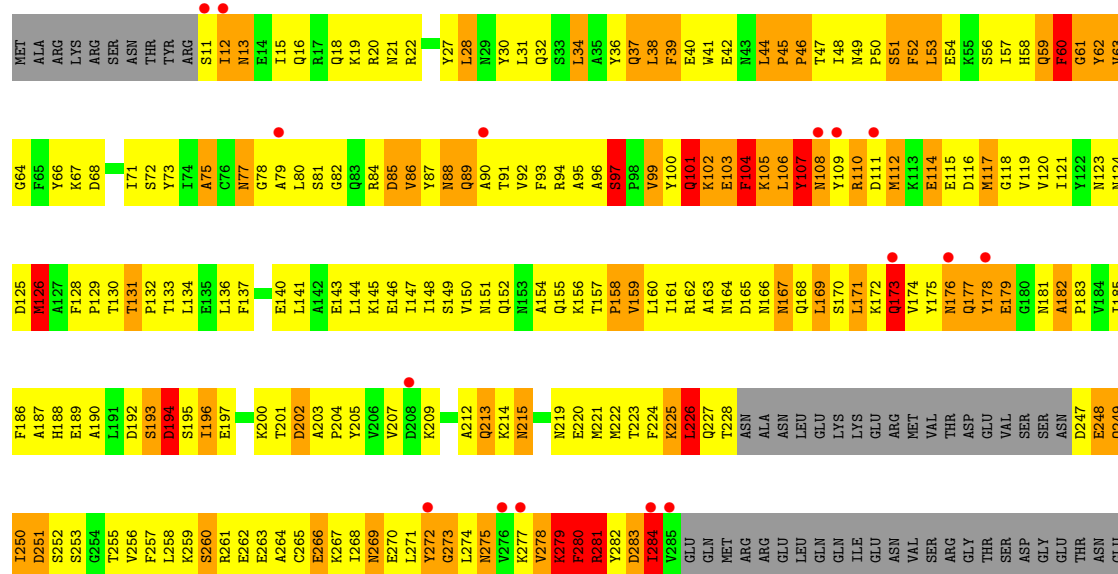


• Molecule 1: UPPER COLLAR PROTEIN

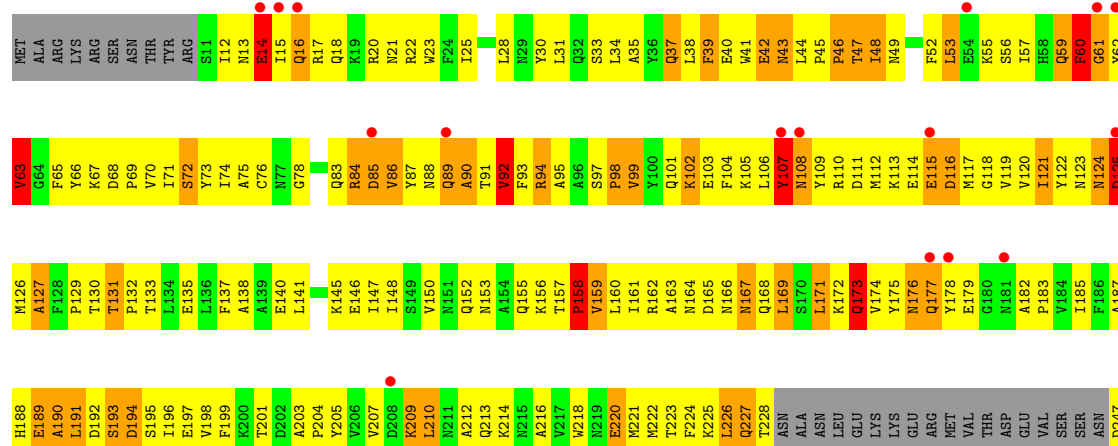
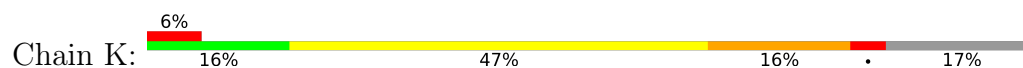


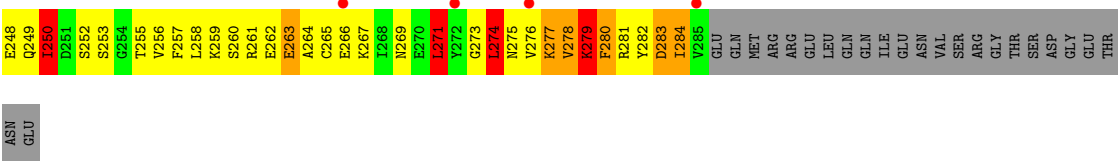


• Molecule 1: UPPER COLLAR PROTEIN

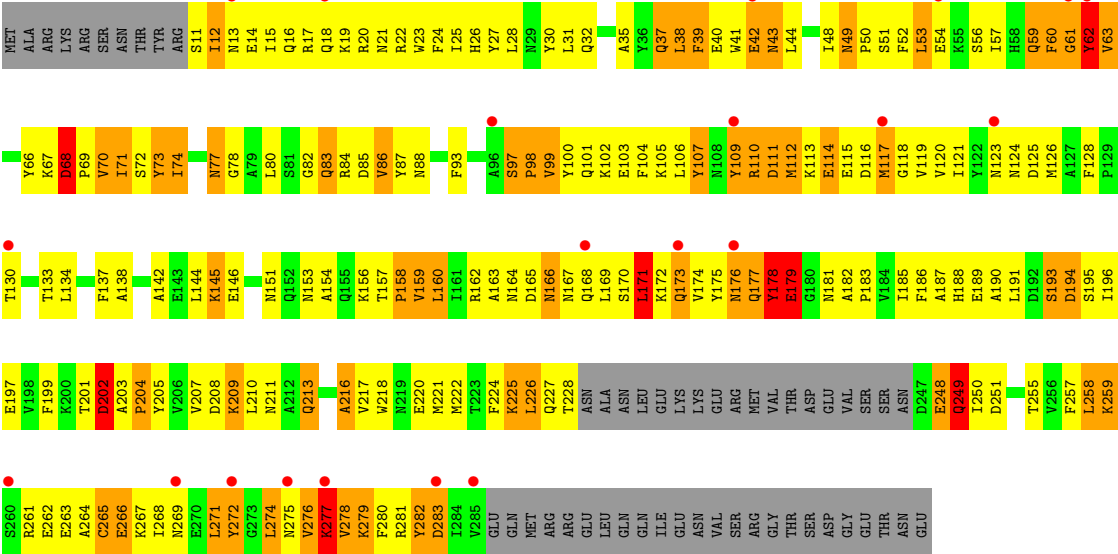
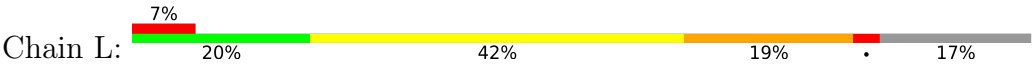


• Molecule 1: UPPER COLLAR PROTEIN





● Molecule 1: UPPER COLLAR PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.16Å 169.24Å 185.44Å 90.00° 114.10° 90.00°	Depositor
Resolution (Å)	9.00 – 3.20 9.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (9.00-3.20) 93.3 (9.00-3.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.94 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.290 , 0.360 0.277 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 78.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	25272	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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	0.59	0/2153	1.13	23/2918 (0.8%)
1	B	0.57	0/2153	1.15	23/2918 (0.8%)
1	C	0.56	0/2153	1.12	16/2918 (0.5%)
1	D	0.55	0/2153	1.15	23/2918 (0.8%)
1	E	0.52	0/2153	1.09	17/2918 (0.6%)
1	F	0.57	0/2153	1.06	18/2918 (0.6%)
1	G	0.53	0/2153	1.05	16/2918 (0.5%)
1	H	0.54	0/2153	1.10	24/2918 (0.8%)
1	I	0.60	0/2153	1.19	26/2918 (0.9%)
1	J	0.59	0/2153	1.23	26/2918 (0.9%)
1	K	0.56	0/2153	1.08	16/2918 (0.5%)
1	L	0.60	0/2153	1.08	16/2918 (0.5%)
All	All	0.57	0/25836	1.12	244/35016 (0.7%)

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	D	0	1
1	L	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 244 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	177	GLN	N-CA-C	-14.21	94.06	111.40
1	A	104	PHE	N-CA-C	13.83	122.03	108.75
1	J	177	GLN	N-CA-C	-13.68	94.71	111.40
1	L	271	LEU	N-CA-C	-11.96	97.16	112.23
1	E	177	GLN	N-CA-C	-11.88	93.38	111.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	107	TYR	Sidechain
1	L	62	TYR	Sidechain

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	2106	0	2051	322	0
1	B	2106	0	2051	358	0
1	C	2106	0	2051	390	0
1	D	2106	0	2051	422	0
1	E	2106	0	2051	387	0
1	F	2106	0	2051	351	0
1	G	2106	0	2051	383	0
1	H	2106	0	2051	364	0
1	I	2106	0	2051	363	0
1	J	2106	0	2051	389	0
1	K	2106	0	2051	370	0
1	L	2106	0	2051	332	0
All	All	25272	0	24612	4049	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 81.

The worst 5 of 4049 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:F:119:VAL:HG11	1:F:268:ILE:HB	1.31	1.11
1:I:275:ASN:HB2	1:I:277:LYS:HE3	1.18	1.11
1:C:43:ASN:HB2	1:C:277:LYS:HD2	1.33	1.10
1:D:163:ALA:HB3	1:E:187:ALA:HB2	1.26	1.10
1:K:278:VAL:HG23	1:K:279:LYS:H	1.14	1.10

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	253/309 (82%)	170 (67%)	48 (19%)	35 (14%)	0	1
1	B	253/309 (82%)	160 (63%)	49 (19%)	44 (17%)	0	0
1	C	253/309 (82%)	172 (68%)	45 (18%)	36 (14%)	0	1
1	D	253/309 (82%)	150 (59%)	60 (24%)	43 (17%)	0	0
1	E	253/309 (82%)	151 (60%)	50 (20%)	52 (21%)	0	0
1	F	253/309 (82%)	166 (66%)	47 (19%)	40 (16%)	0	0
1	G	253/309 (82%)	160 (63%)	53 (21%)	40 (16%)	0	0
1	H	253/309 (82%)	176 (70%)	41 (16%)	36 (14%)	0	1
1	I	253/309 (82%)	187 (74%)	34 (13%)	32 (13%)	0	1
1	J	253/309 (82%)	175 (69%)	39 (15%)	39 (15%)	0	0
1	K	253/309 (82%)	169 (67%)	46 (18%)	38 (15%)	0	1
1	L	253/309 (82%)	163 (64%)	46 (18%)	44 (17%)	0	0
All	All	3036/3708 (82%)	1999 (66%)	558 (18%)	479 (16%)	0	0

5 of 479 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	42	GLU
1	A	92	VAL
1	A	97	SER
1	A	105	LYS

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	230/278 (83%)	198 (86%)	32 (14%)	3	17
1	B	230/278 (83%)	199 (86%)	31 (14%)	4	19
1	C	230/278 (83%)	199 (86%)	31 (14%)	4	19
1	D	230/278 (83%)	204 (89%)	26 (11%)	5	24
1	E	230/278 (83%)	200 (87%)	30 (13%)	4	20
1	F	230/278 (83%)	193 (84%)	37 (16%)	2	13
1	G	230/278 (83%)	200 (87%)	30 (13%)	4	20
1	H	230/278 (83%)	201 (87%)	29 (13%)	4	21
1	I	230/278 (83%)	200 (87%)	30 (13%)	4	20
1	J	230/278 (83%)	198 (86%)	32 (14%)	3	17
1	K	230/278 (83%)	199 (86%)	31 (14%)	4	19
1	L	230/278 (83%)	206 (90%)	24 (10%)	7	28
All	All	2760/3336 (83%)	2397 (87%)	363 (13%)	4	19

5 of 363 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	115	GLU
1	J	104	PHE
1	H	172	LYS
1	I	160	LEU
1	J	250	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 164 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	49	ASN
1	K	83	GLN
1	I	89	GLN
1	J	49	ASN
1	K	269	ASN

5.3.3 RNA ⓘ

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	257/309 (83%)	0.47	21 (8%) 17 11	1, 7, 33, 38	0
1	B	257/309 (83%)	0.49	23 (8%) 15 10	1, 13, 32, 46	0
1	C	257/309 (83%)	0.42	17 (6%) 24 15	1, 13, 32, 39	0
1	D	257/309 (83%)	0.48	21 (8%) 17 11	1, 16, 35, 43	0
1	E	257/309 (83%)	0.54	24 (9%) 14 9	1, 21, 35, 42	0
1	F	257/309 (83%)	0.48	19 (7%) 20 13	1, 16, 35, 40	0
1	G	257/309 (83%)	0.44	13 (5%) 33 21	1, 14, 36, 51	0
1	H	257/309 (83%)	0.54	19 (7%) 20 13	1, 16, 34, 41	0
1	I	257/309 (83%)	0.41	16 (6%) 26 17	1, 9, 32, 43	0
1	J	257/309 (83%)	0.35	16 (6%) 26 17	1, 9, 30, 43	0
1	K	257/309 (83%)	0.52	20 (7%) 19 12	1, 13, 33, 47	0
1	L	257/309 (83%)	0.47	21 (8%) 17 11	1, 11, 32, 41	0
All	All	3084/3708 (83%)	0.47	230 (7%) 20 13	1, 13, 34, 51	0

The worst 5 of 230 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	ASP	8.6
1	I	13	ASN	6.8
1	L	283	ASP	5.2
1	K	61	GLY	4.9
1	D	12	ILE	4.8

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.