



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 05:10 PM UTC

PDB ID : 1JNB / pdb_00001jnb
Title : CONNECTOR PROTEIN FROM BACTERIOPHAGE PHI29
Authors : Simpson, A.A.; Leiman, P.G.; Tao, Y.; He, Y.; Badasso, M.O.; Jardine, P.J.;
Anderson, D.L.; Rossmann, M.G.
Deposited on : 2001-07-23
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:

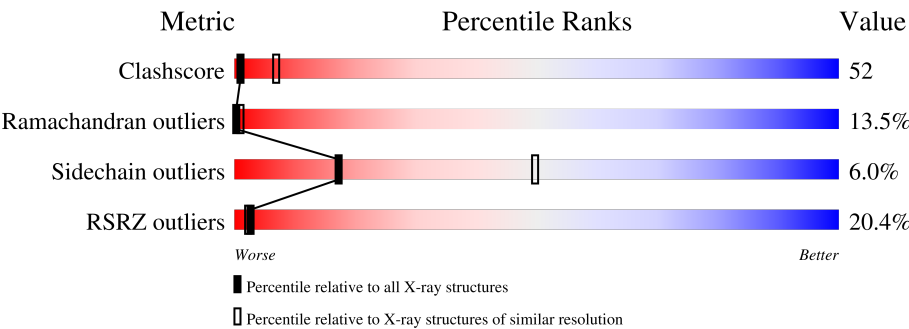
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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	14% 33%34%14%•17%
1	B	309	17% 34%33%14%•17%
1	C	309	20% 34%34%14%•17%
1	D	309	17% 32%35%14%•17%
1	E	309	22% 35%32%14%•17%
1	F	309	21% 34%33%15%•17%
1	G	309	16% 33%33%14%•17%

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Mol	Chain	Length	Quality of chain
1	H	309	18%32%35%15%•17%
1	I	309	17%35%32%15%•17%
1	J	309	12%33%34%14%•17%
1	K	309	17%33%34%14%•17%
1	L	309	14%34%32%15%•17%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25236 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.

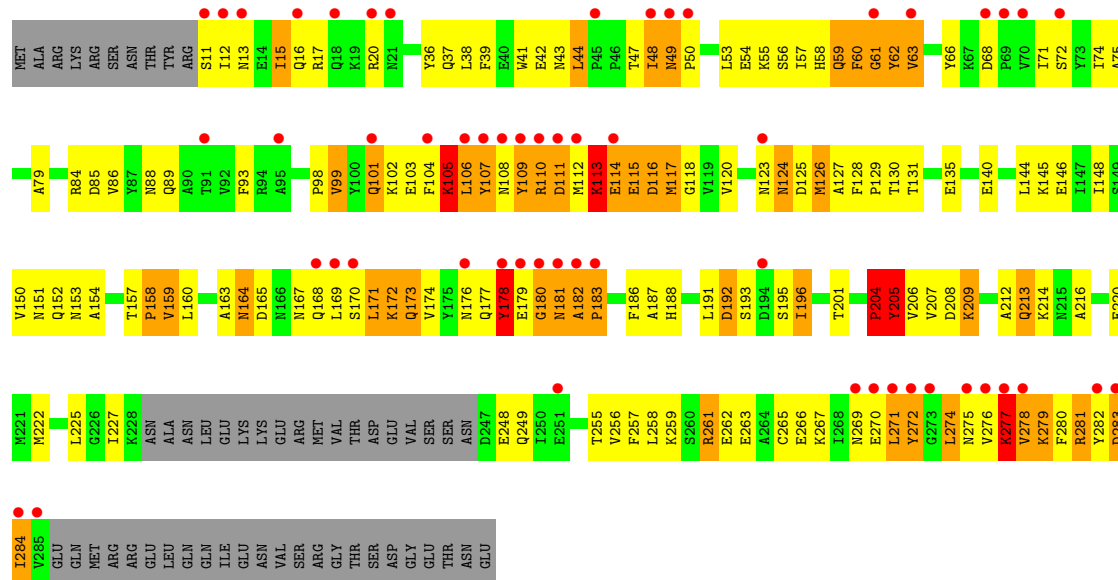
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2103	1350	347	399	7			
1	B	257	Total	C	N	O	S	0	0	0
			2103	1350	347	399	7			
1	C	257	Total	C	N	O	S	0	0	0
			2103	1350	347	399	7			
1	D	257	Total	C	N	O	S	0	0	0
			2103	1350	347	399	7			
1	E	257	Total	C	N	O	S	0	0	0
			2103	1350	347	399	7			
1	F	257	Total	C	N	O	S	0	0	0
			2103	1350	347	399	7			
1	G	257	Total	C	N	O	S	0	0	0
			2103	1350	347	399	7			
1	H	257	Total	C	N	O	S	0	0	0
			2103	1350	347	399	7			
1	I	257	Total	C	N	O	S	0	0	0
			2103	1350	347	399	7			
1	J	257	Total	C	N	O	S	0	0	0
			2103	1350	347	399	7			
1	K	257	Total	C	N	O	S	0	0	0
			2103	1350	347	399	7			
1	L	257	Total	C	N	O	S	0	0	0
			2103	1350	347	399	7			



ARG
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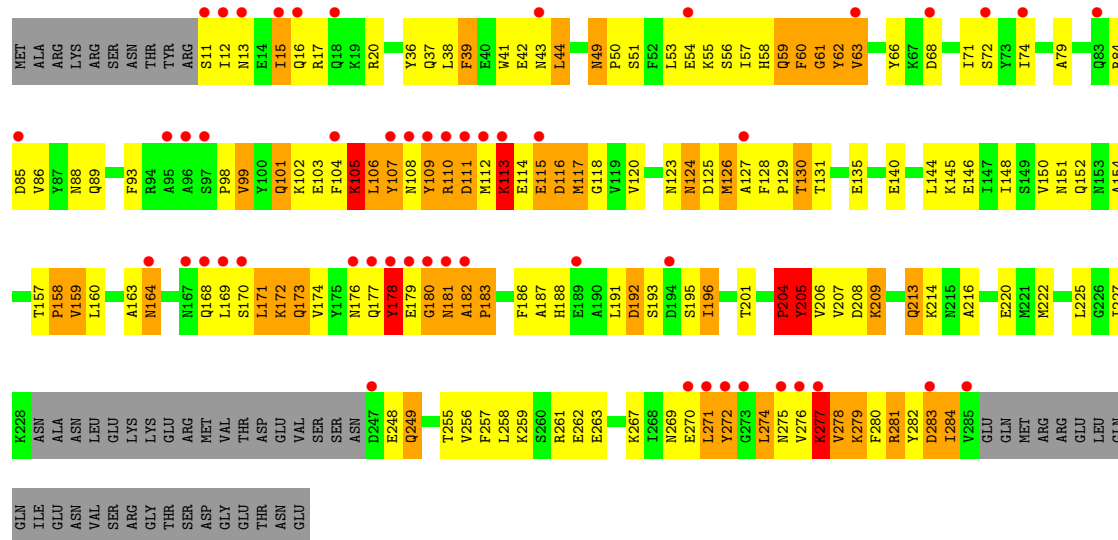
● Molecule 1: UPPER COLLAR PROTEIN

Chain H: 18% 32% 35% 15% 17%



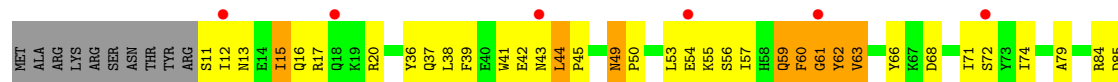
● Molecule 1: UPPER COLLAR PROTEIN

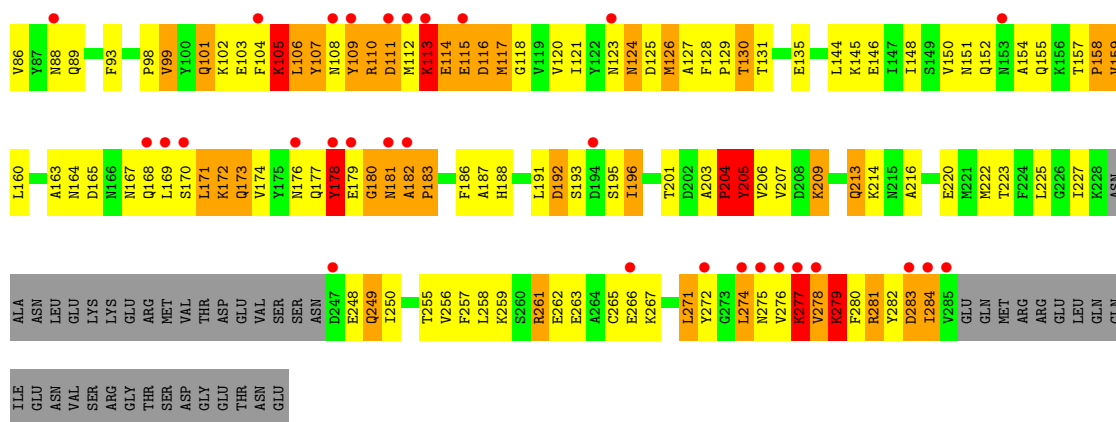
Chain I: 17% 35% 32% 15% 17%



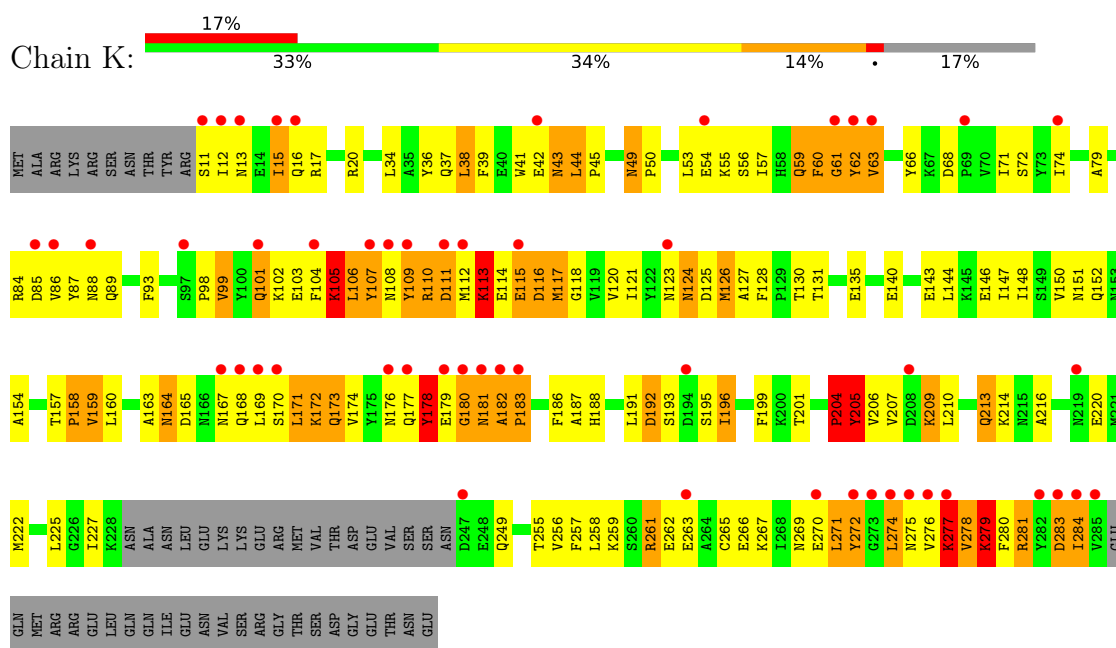
● Molecule 1: UPPER COLLAR PROTEIN

Chain J: 12% 33% 34% 14% 17%

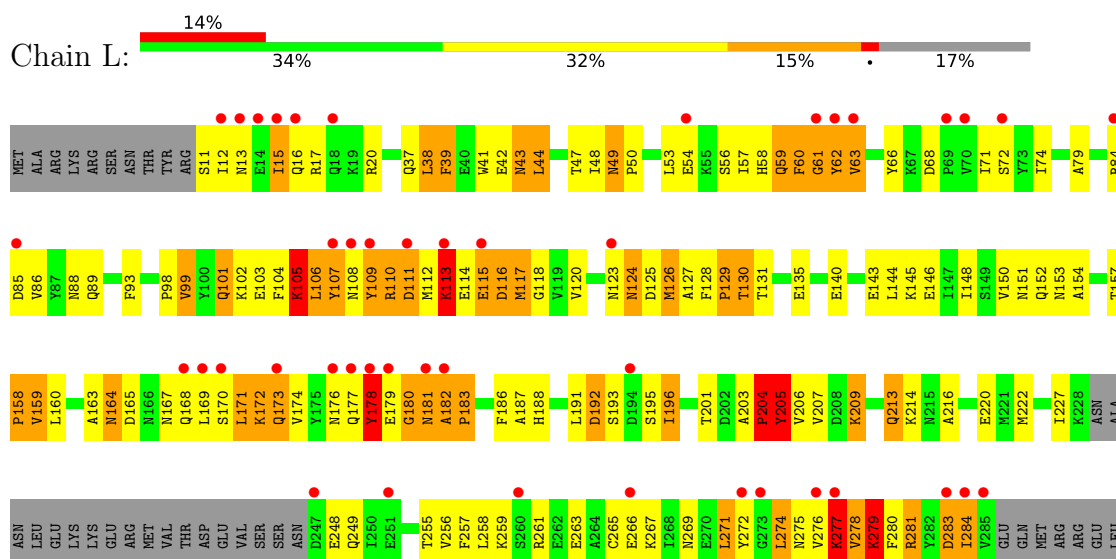




● Molecule 1: UPPER COLLAR PROTEIN



● Molecule 1: UPPER COLLAR PROTEIN



GLN
GLN
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GLY
THR
SER
ASP
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THR
ASN
GLU

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 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (9.00-3.20) 94.9 (9.00-3.20)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.81 (at 3.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.284 , 0.301 0.282 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 84.4	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	0.82	EDS
Total number of atoms	25236	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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	0.56	0/2150	1.06	16/2913 (0.5%)
1	B	0.55	0/2150	1.05	16/2913 (0.5%)
1	C	0.54	0/2150	1.05	14/2913 (0.5%)
1	D	0.52	0/2150	1.05	17/2913 (0.6%)
1	E	0.49	0/2150	1.04	16/2913 (0.5%)
1	F	0.53	0/2150	1.04	18/2913 (0.6%)
1	G	0.52	0/2150	1.05	18/2913 (0.6%)
1	H	0.51	0/2150	1.04	13/2913 (0.4%)
1	I	0.55	0/2150	1.05	13/2913 (0.4%)
1	J	0.55	0/2150	1.07	16/2913 (0.5%)
1	K	0.53	0/2150	1.05	18/2913 (0.6%)
1	L	0.55	0/2150	1.05	17/2913 (0.6%)
All	All	0.53	0/25800	1.05	192/34956 (0.5%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	12

There are no bond length outliers.

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	157	THR	N-CA-C	9.35	124.65	108.75
1	A	116	ASP	N-CA-C	-9.11	98.54	111.56
1	K	116	ASP	N-CA-C	-8.94	98.78	111.56
1	G	116	ASP	N-CA-C	-8.92	98.81	111.56
1	F	116	ASP	N-CA-C	-8.88	98.86	111.56

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	TYR	Sidechain
1	B	205	TYR	Sidechain
1	C	205	TYR	Sidechain
1	D	205	TYR	Sidechain
1	E	205	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	2103	0	2052	242	0
1	B	2103	0	2052	241	0
1	C	2103	0	2052	271	0
1	D	2103	0	2052	269	1
1	E	2103	0	2052	226	0
1	F	2103	0	2052	241	0
1	G	2103	0	2052	258	0
1	H	2103	0	2052	241	0
1	I	2103	0	2052	235	1
1	J	2103	0	2052	239	0
1	K	2103	0	2052	237	0
1	L	2103	0	2052	231	0
All	All	25236	0	24624	2577	1

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 52.

The worst 5 of 2577 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:159:VAL:HG11	1:L:201:THR:HG23	1.25	1.18
1:G:87:TYR:OH	1:H:48:ILE:HA	1.43	1.18
1:H:201:THR:HG23	1:I:159:VAL:HG11	1.29	1.12
1:D:87:TYR:OH	1:E:48:ILE:HA	1.50	1.10
1:C:110:ARG:HH22	1:D:72:SER:HB2	1.12	1.09

All (1) 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:D:272:TYR:OH	1:I:62:TYR:OH[3_445]	2.12	0.08

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%)	181 (72%)	38 (15%)	34 (13%)	0	1
1	B	253/309 (82%)	182 (72%)	37 (15%)	34 (13%)	0	1
1	C	253/309 (82%)	179 (71%)	40 (16%)	34 (13%)	0	1
1	D	253/309 (82%)	181 (72%)	38 (15%)	34 (13%)	0	1
1	E	253/309 (82%)	181 (72%)	38 (15%)	34 (13%)	0	1
1	F	253/309 (82%)	180 (71%)	38 (15%)	35 (14%)	0	1
1	G	253/309 (82%)	181 (72%)	38 (15%)	34 (13%)	0	1
1	H	253/309 (82%)	180 (71%)	38 (15%)	35 (14%)	0	1
1	I	253/309 (82%)	181 (72%)	37 (15%)	35 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	253/309 (82%)	182 (72%)	37 (15%)	34 (13%)	0	1
1	K	253/309 (82%)	181 (72%)	39 (15%)	33 (13%)	0	1
1	L	253/309 (82%)	181 (72%)	38 (15%)	34 (13%)	0	1
All	All	3036/3708 (82%)	2170 (72%)	456 (15%)	410 (14%)	0	1

5 of 410 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	TYR
1	A	105	LYS
1	A	107	TYR
1	A	113	LYS
1	A	117	MET

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	229/277 (83%)	215 (94%)	14 (6%)	17	49
1	B	229/277 (83%)	215 (94%)	14 (6%)	17	49
1	C	229/277 (83%)	216 (94%)	13 (6%)	18	51
1	D	229/277 (83%)	216 (94%)	13 (6%)	18	51
1	E	229/277 (83%)	215 (94%)	14 (6%)	17	49
1	F	229/277 (83%)	216 (94%)	13 (6%)	18	51
1	G	229/277 (83%)	215 (94%)	14 (6%)	17	49
1	H	229/277 (83%)	215 (94%)	14 (6%)	17	49
1	I	229/277 (83%)	216 (94%)	13 (6%)	18	51
1	J	229/277 (83%)	215 (94%)	14 (6%)	17	49
1	K	229/277 (83%)	215 (94%)	14 (6%)	17	49
1	L	229/277 (83%)	215 (94%)	14 (6%)	17	49
All	All	2748/3324 (83%)	2584 (94%)	164 (6%)	17	50

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	178	TYR
1	K	196	ILE
1	I	213	GLN
1	J	204	PRO
1	L	49	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 198 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	29	ASN
1	I	167	ASN
1	H	108	ASN
1	H	177	GLN
1	J	32	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 ⓘ

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%)	0.74	43 (16%) 4 3	18, 45, 98, 120	0
1	B	257/309 (83%)	0.94	54 (21%) 2 2	18, 52, 97, 121	0
1	C	257/309 (83%)	1.06	62 (24%) 2 2	21, 55, 100, 124	0
1	D	257/309 (83%)	1.01	52 (20%) 3 2	20, 58, 109, 127	0
1	E	257/309 (83%)	1.23	68 (26%) 1 1	23, 72, 113, 123	0
1	F	257/309 (83%)	1.06	64 (24%) 2 2	19, 61, 104, 120	0
1	G	257/309 (83%)	0.94	49 (19%) 3 2	21, 57, 102, 127	0
1	H	257/309 (83%)	1.06	55 (21%) 2 2	17, 64, 111, 124	0
1	I	257/309 (83%)	0.86	51 (19%) 3 2	19, 46, 90, 116	0
1	J	257/309 (83%)	0.64	36 (14%) 6 5	22, 43, 87, 115	0
1	K	257/309 (83%)	0.84	52 (20%) 3 2	17, 53, 96, 127	0
1	L	257/309 (83%)	0.72	44 (17%) 4 3	19, 48, 98, 116	0
All	All	3084/3708 (83%)	0.93	630 (20%) 3 2	17, 53, 106, 127	0

The worst 5 of 630 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	182	ALA	8.9
1	C	109	TYR	7.9
1	I	272	TYR	7.7
1	J	109	TYR	7.6
1	G	182	ALA	7.3

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.