Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2026 – 04:08 PM EDT

PDB ID	:	35VU / pdb_000035vu
Title	:	Crystal structure of apo DUF190
Authors	:	Stockbridge, R.B.; Peralta, C.M.
Deposited on	:	2026-05-20
Resolution	:	2.20 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:

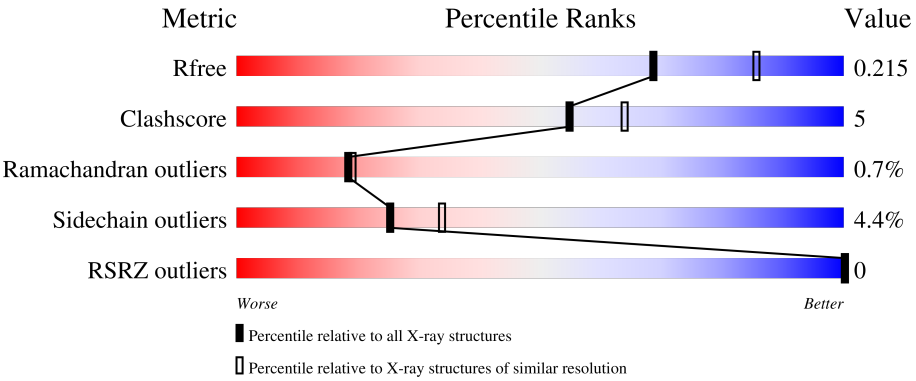
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.20 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))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 <=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	70% 11% • 16%
1	B	122	80% • • 16%
1	C	122	67% 13% • 17%
1	D	122	76% 7% • 16%
1	E	122	70% 11% • 17%

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Mol	Chain	Length	Quality of chain
1	F	122	
1	G	122	
1	H	122	
1	I	122	
1	J	122	
1	K	122	
1	L	122	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10571 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 DUF190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	104	Total	C	N	O	S	0	1	0
			848	545	145	155	3			
1	B	102	Total	C	N	O	S	0	2	0
			836	538	143	152	3			
1	E	101	Total	C	N	O	S	0	1	0
			822	531	138	150	3			
1	A	102	Total	C	N	O	S	0	0	0
			821	529	138	151	3			
1	C	101	Total	C	N	O	S	0	1	0
			832	535	143	151	3			
1	D	103	Total	C	N	O	S	0	2	0
			836	538	141	155	2			
1	F	104	Total	C	N	O	S	0	0	0
			840	540	143	154	3			
1	G	103	Total	C	N	O	S	0	1	0
			832	534	143	153	2			
1	H	102	Total	C	N	O	S	0	0	0
			826	532	140	151	3			
1	J	101	Total	C	N	O	S	0	1	0
			827	533	140	151	3			
1	K	100	Total	C	N	O	S	0	1	0
			803	514	138	149	2			
1	L	103	Total	C	N	O	S	0	1	0
			836	538	141	154	3			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	116	GLY	-	expression tag	UNP A0A1W1WVA9
I	117	GLY	-	expression tag	UNP A0A1W1WVA9
I	118	SER	-	expression tag	UNP A0A1W1WVA9
I	119	LEU	-	expression tag	UNP A0A1W1WVA9
I	120	VAL	-	expression tag	UNP A0A1W1WVA9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	121	PRO	-	expression tag	UNP A0A1W1WVA9
I	122	ARG	-	expression tag	UNP A0A1W1WVA9
B	116	GLY	-	expression tag	UNP A0A1W1WVA9
B	117	GLY	-	expression tag	UNP A0A1W1WVA9
B	118	SER	-	expression tag	UNP A0A1W1WVA9
B	119	LEU	-	expression tag	UNP A0A1W1WVA9
B	120	VAL	-	expression tag	UNP A0A1W1WVA9
B	121	PRO	-	expression tag	UNP A0A1W1WVA9
B	122	ARG	-	expression tag	UNP A0A1W1WVA9
E	116	GLY	-	expression tag	UNP A0A1W1WVA9
E	117	GLY	-	expression tag	UNP A0A1W1WVA9
E	118	SER	-	expression tag	UNP A0A1W1WVA9
E	119	LEU	-	expression tag	UNP A0A1W1WVA9
E	120	VAL	-	expression tag	UNP A0A1W1WVA9
E	121	PRO	-	expression tag	UNP A0A1W1WVA9
E	122	ARG	-	expression tag	UNP A0A1W1WVA9
A	116	GLY	-	expression tag	UNP A0A1W1WVA9
A	117	GLY	-	expression tag	UNP A0A1W1WVA9
A	118	SER	-	expression tag	UNP A0A1W1WVA9
A	119	LEU	-	expression tag	UNP A0A1W1WVA9
A	120	VAL	-	expression tag	UNP A0A1W1WVA9
A	121	PRO	-	expression tag	UNP A0A1W1WVA9
A	122	ARG	-	expression tag	UNP A0A1W1WVA9
C	116	GLY	-	expression tag	UNP A0A1W1WVA9
C	117	GLY	-	expression tag	UNP A0A1W1WVA9
C	118	SER	-	expression tag	UNP A0A1W1WVA9
C	119	LEU	-	expression tag	UNP A0A1W1WVA9
C	120	VAL	-	expression tag	UNP A0A1W1WVA9
C	121	PRO	-	expression tag	UNP A0A1W1WVA9
C	122	ARG	-	expression tag	UNP A0A1W1WVA9
D	116	GLY	-	expression tag	UNP A0A1W1WVA9
D	117	GLY	-	expression tag	UNP A0A1W1WVA9
D	118	SER	-	expression tag	UNP A0A1W1WVA9
D	119	LEU	-	expression tag	UNP A0A1W1WVA9
D	120	VAL	-	expression tag	UNP A0A1W1WVA9
D	121	PRO	-	expression tag	UNP A0A1W1WVA9
D	122	ARG	-	expression tag	UNP A0A1W1WVA9
F	116	GLY	-	expression tag	UNP A0A1W1WVA9
F	117	GLY	-	expression tag	UNP A0A1W1WVA9
F	118	SER	-	expression tag	UNP A0A1W1WVA9
F	119	LEU	-	expression tag	UNP A0A1W1WVA9
F	120	VAL	-	expression tag	UNP A0A1W1WVA9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	121	PRO	-	expression tag	UNP A0A1W1WVA9
F	122	ARG	-	expression tag	UNP A0A1W1WVA9
G	116	GLY	-	expression tag	UNP A0A1W1WVA9
G	117	GLY	-	expression tag	UNP A0A1W1WVA9
G	118	SER	-	expression tag	UNP A0A1W1WVA9
G	119	LEU	-	expression tag	UNP A0A1W1WVA9
G	120	VAL	-	expression tag	UNP A0A1W1WVA9
G	121	PRO	-	expression tag	UNP A0A1W1WVA9
G	122	ARG	-	expression tag	UNP A0A1W1WVA9
H	116	GLY	-	expression tag	UNP A0A1W1WVA9
H	117	GLY	-	expression tag	UNP A0A1W1WVA9
H	118	SER	-	expression tag	UNP A0A1W1WVA9
H	119	LEU	-	expression tag	UNP A0A1W1WVA9
H	120	VAL	-	expression tag	UNP A0A1W1WVA9
H	121	PRO	-	expression tag	UNP A0A1W1WVA9
H	122	ARG	-	expression tag	UNP A0A1W1WVA9
J	116	GLY	-	expression tag	UNP A0A1W1WVA9
J	117	GLY	-	expression tag	UNP A0A1W1WVA9
J	118	SER	-	expression tag	UNP A0A1W1WVA9
J	119	LEU	-	expression tag	UNP A0A1W1WVA9
J	120	VAL	-	expression tag	UNP A0A1W1WVA9
J	121	PRO	-	expression tag	UNP A0A1W1WVA9
J	122	ARG	-	expression tag	UNP A0A1W1WVA9
K	116	GLY	-	expression tag	UNP A0A1W1WVA9
K	117	GLY	-	expression tag	UNP A0A1W1WVA9
K	118	SER	-	expression tag	UNP A0A1W1WVA9
K	119	LEU	-	expression tag	UNP A0A1W1WVA9
K	120	VAL	-	expression tag	UNP A0A1W1WVA9
K	121	PRO	-	expression tag	UNP A0A1W1WVA9
K	122	ARG	-	expression tag	UNP A0A1W1WVA9
L	116	GLY	-	expression tag	UNP A0A1W1WVA9
L	117	GLY	-	expression tag	UNP A0A1W1WVA9
L	118	SER	-	expression tag	UNP A0A1W1WVA9
L	119	LEU	-	expression tag	UNP A0A1W1WVA9
L	120	VAL	-	expression tag	UNP A0A1W1WVA9
L	121	PRO	-	expression tag	UNP A0A1W1WVA9
L	122	ARG	-	expression tag	UNP A0A1W1WVA9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	45	Total O 45 45	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	53	Total O 53 53	0	0
2	E	57	Total O 57 57	0	0
2	A	49	Total O 49 49	0	0
2	C	46	Total O 46 46	0	0
2	D	59	Total O 59 59	0	0
2	F	51	Total O 51 51	0	0
2	G	51	Total O 51 51	0	0
2	H	53	Total O 53 53	0	0
2	J	43	Total O 43 43	0	0
2	K	52	Total O 52 52	0	0
2	L	53	Total O 53 53	0	0

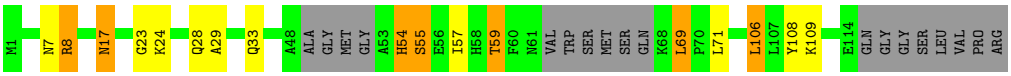
3 Residue-property plots (i)

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: DUF190

Chain I:





- Molecule 1: DUF190

Chain B:

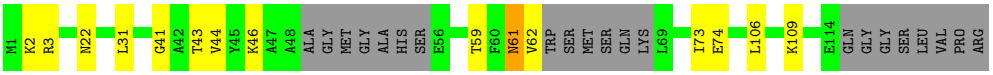




- Molecule 1: DUF190

Chain E:





- Molecule 1: DUF190

Chain A:

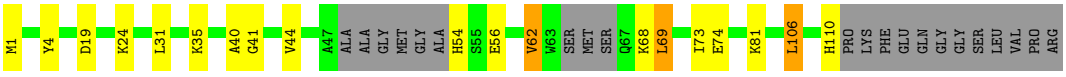




- Molecule 1: DUF190

Chain C:

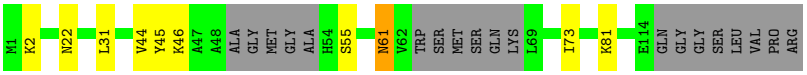




- Molecule 1: DUF190

Chain D:

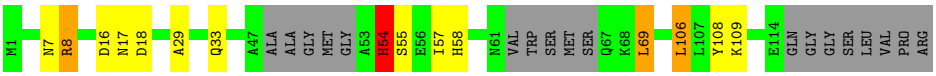




• Molecule 1: DUF190

Chain F:

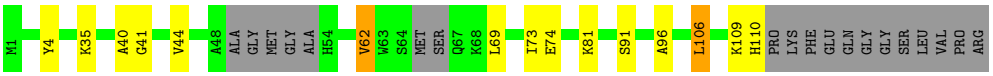




• Molecule 1: DUF190

Chain G:

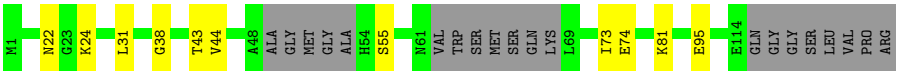




• Molecule 1: DUF190

Chain H:

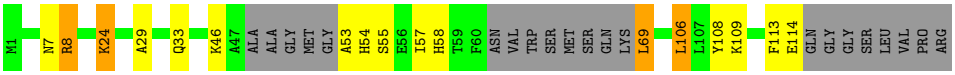




• Molecule 1: DUF190

Chain J:

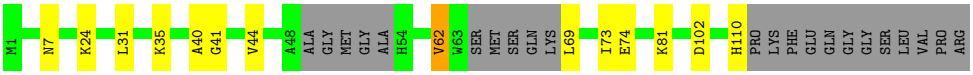




• Molecule 1: DUF190

Chain K:

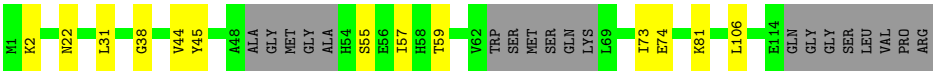




• Molecule 1: DUF190

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	58.91Å 58.91Å 348.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.96 – 2.20 48.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.96-2.20) 100.0 (48.96-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.64 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.191 , 0.215 0.192 , 0.215	Depositor DCC
R_{free} test set	3338 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 15.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.469 for -h,-k,l 0.480 for h,-h-k,-l 0.470 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10571	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.30	0/834	0.48	0/1120
1	B	0.31	0/853	0.49	0/1147
1	C	0.36	0/846	0.56	0/1137
1	D	0.31	0/852	0.45	0/1146
1	E	0.31	0/838	0.45	0/1126
1	F	0.31	0/854	0.50	0/1147
1	G	0.31	0/846	0.47	0/1140
1	H	0.32	0/840	0.45	0/1128
1	I	0.30	0/862	0.46	0/1157
1	J	0.30	0/841	0.47	0/1129
1	K	0.30	0/815	0.44	0/1098
1	L	0.31	0/849	0.45	0/1141
All	All	0.31	0/10130	0.47	0/13616

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	F	0	1
1	I	0	1
1	J	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	ARG	Sidechain
1	F	8	ARG	Sidechain
1	I	8	ARG	Sidechain
1	J	8	ARG	Sidechain

5.2 Too-close contacts (i)

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	821	0	839	13	0
1	B	836	0	853	3	1
1	C	832	0	849	13	0
1	D	836	0	851	5	0
1	E	822	0	847	10	0
1	F	840	0	854	9	0
1	G	832	0	835	10	0
1	H	826	0	844	7	0
1	I	848	0	867	15	1
1	J	827	0	845	13	0
1	K	803	0	807	9	0
1	L	836	0	853	8	0
2	A	49	0	0	1	0
2	B	53	0	0	0	0
2	C	46	0	0	1	1
2	D	59	0	0	0	0
2	E	57	0	0	1	0
2	F	51	0	0	1	0
2	G	51	0	0	2	0
2	H	53	0	0	1	1
2	I	45	0	0	1	0
2	J	43	0	0	2	0
2	K	52	0	0	2	0
2	L	53	0	0	0	0
All	All	10571	0	10144	96	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 5.

All (96) 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:69:LEU:O	2:A:201:HOH:O	1.76	1.01
1:G:91:SER:OG	2:G:201:HOH:O	1.82	0.95
1:F:69:LEU:O	2:F:201:HOH:O	2.01	0.77
1:E:44:VAL:HG22	1:E:73:ILE:HG12	1.69	0.75
1:D:44:VAL:HG22	1:D:73:ILE:HG12	1.70	0.74
1:L:44:VAL:HG22	1:L:73:ILE:HG12	1.70	0.74
1:H:44:VAL:HG22	1:H:73:ILE:HG12	1.70	0.74
1:J:69:LEU:O	2:J:201:HOH:O	2.08	0.70
1:I:69:LEU:O	2:I:201:HOH:O	2.11	0.68
1:C:35:LYS:NZ	1:C:41:GLY:H	1.91	0.68
1:E:2:LYS:HD2	1:E:106:LEU:HD11	1.76	0.68
1:G:44:VAL:HG22	1:G:73:ILE:HG12	1.75	0.68
1:K:44:VAL:HG22	1:K:73:ILE:HG12	1.76	0.67
1:K:41:GLY:HA3	1:L:59:THR:HG23	1.78	0.66
1:G:35:LYS:NZ	1:G:41:GLY:H	1.94	0.65
1:L:2:LYS:HD2	1:L:106:LEU:HD11	1.79	0.64
1:C:44:VAL:HG22	1:C:73:ILE:HG12	1.80	0.64
1:J:7:ASN:HB3	2:J:202:HOH:O	1.97	0.64
1:F:54:HIS:HB3	1:H:43:THR:HG21	1.82	0.62
1:B:44:VAL:HG22	1:B:73:ILE:HG12	1.82	0.62
1:K:7:ASN:HD21	1:K:102:ASP:HB3	1.65	0.61
1:C:35:LYS:HZ1	1:C:41:GLY:H	1.50	0.59
1:I:55:SER:O	1:I:59:THR:HG23	2.02	0.58
1:I:54:HIS:HB3	1:E:43:THR:HG21	1.86	0.57
1:F:7:ASN:O	1:F:8:ARG:HD2	2.05	0.56
1:I:23:GLY:O	1:I:24:LYS:HE2	2.05	0.56
1:A:106:LEU:HD11	1:A:108:TYR:CE2	2.41	0.56
1:I:59:THR:HG22	1:E:41:GLY:O	2.05	0.56
1:I:7[A]:ASN:O	1:I:8:ARG:HD2	2.06	0.56
1:I:109:LYS:HG2	1:B:62:VAL:HG22	1.88	0.55
1:A:7:ASN:O	1:A:8:ARG:HD2	2.07	0.55
1:G:35:LYS:HZ2	1:G:41:GLY:H	1.53	0.54
1:F:109:LYS:HG2	1:G:62:VAL:HG22	1.89	0.54
1:J:53:ALA:HA	1:L:45:TYR:CZ	2.42	0.54
1:J:7:ASN:O	1:J:8:ARG:HD2	2.07	0.54
1:G:4:TYR:HA	1:G:106:LEU:HD23	1.91	0.53
1:L:31:LEU:HD11	1:L:44:VAL:HG23	1.91	0.53
1:I:17:ASN:HA	1:I:71:LEU:HD22	1.91	0.53
1:A:58:HIS:O	1:A:60:PHE:N	2.42	0.53
1:H:38:GLY:O	1:H:81:LYS:NZ	2.41	0.52
1:J:57:ILE:HD12	1:J:57:ILE:H	1.75	0.52
1:D:31:LEU:HD11	1:D:44:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:7:ASN:ND2	2:K:201:HOH:O	2.07	0.52
1:H:31:LEU:HD11	1:H:44:VAL:HG23	1.93	0.51
1:H:24:LYS:HG3	2:H:218:HOH:O	2.11	0.50
1:A:53:ALA:HA	1:D:45:TYR:CZ	2.48	0.49
1:F:55:SER:HB2	1:H:74:GLU:HG2	1.94	0.49
1:I:59:THR:HG21	2:E:211:HOH:O	2.13	0.48
1:B:41:GLY:HA3	1:E:59:THR:HG23	1.95	0.48
1:J:106:LEU:HD11	1:J:108:TYR:CE2	2.48	0.48
1:I:55:SER:HB2	1:E:74:GLU:OE2	2.11	0.48
1:J:24:LYS:HD2	1:J:24:LYS:HA	1.71	0.48
1:J:109:LYS:HG2	1:K:62:VAL:HG22	1.96	0.48
1:E:31:LEU:HD11	1:E:44:VAL:HG23	1.95	0.48
1:A:109:LYS:HG2	1:C:62:VAL:HG22	1.96	0.47
1:C:40:ALA:N	2:C:201:HOH:O	2.08	0.47
1:J:55:SER:HB2	1:L:74:GLU:HG2	1.97	0.46
1:E:46:LYS:HE3	1:E:46:LYS:HB2	1.60	0.46
1:K:40:ALA:N	2:K:202:HOH:O	2.07	0.46
1:C:69:LEU:HD12	1:C:69:LEU:HA	1.72	0.46
1:C:4:TYR:HA	1:C:106:LEU:HD23	1.99	0.45
1:I:106:LEU:HD11	1:I:108:TYR:CE2	2.52	0.45
1:C:24:LYS:HE2	1:C:24:LYS:HB3	1.76	0.44
1:G:74:GLU:HG2	1:H:55:SER:HB2	2.00	0.44
1:K:74:GLU:OE2	1:L:55:SER:OG	2.29	0.44
1:E:3:ARG:HD3	1:E:109:LYS:HD3	2.00	0.44
1:G:40:ALA:N	2:G:202:HOH:O	2.11	0.44
1:I:7[B]:ASN:O	1:I:8:ARG:HD2	2.18	0.43
1:J:7:ASN:C	1:J:8:ARG:HD2	2.44	0.43
1:I:29:ALA:O	1:I:33:GLN:HG3	2.19	0.43
1:J:54:HIS:ND1	1:J:58:HIS:HB2	2.34	0.43
1:A:8:ARG:HD2	1:A:8:ARG:HA	1.91	0.43
1:A:24:LYS:HD3	1:A:24:LYS:HA	1.83	0.43
1:F:29:ALA:O	1:F:33:GLN:HG3	2.18	0.43
1:J:29:ALA:O	1:J:33:GLN:HG3	2.18	0.43
1:A:10:LYS:HE2	1:C:56:GLU:OE2	2.18	0.42
1:F:106:LEU:HD11	1:F:108:TYR:CE2	2.54	0.42
1:F:7:ASN:C	1:F:8:ARG:HD2	2.45	0.42
1:L:38:GLY:O	1:L:81:LYS:NZ	2.44	0.42
1:C:1:MET:HE3	1:C:1:MET:HB3	1.90	0.42
1:F:16:ASP:OD2	1:F:18:ASP:HB2	2.20	0.42
1:C:31:LEU:HD21	1:C:44:VAL:HG23	2.01	0.42
1:I:7[A]:ASN:C	1:I:8:ARG:HD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:57:ILE:HD12	1:I:57:ILE:H	1.86	0.41
1:A:29:ALA:O	1:A:33:GLN:HG3	2.21	0.41
1:J:113:PHE:O	1:J:114:GLU:HB2	2.21	0.41
1:C:74:GLU:OE2	1:D:55[B]:SER:HB2	2.21	0.41
1:G:62:VAL:HG11	1:G:96:ALA:N	2.36	0.41
1:C:35:LYS:HZ3	1:C:41:GLY:H	1.68	0.41
1:A:90:ASP:OD1	1:D:2:LYS:HD2	2.22	0.40
1:K:31:LEU:HD21	1:K:44:VAL:HG23	2.03	0.40
1:A:58:HIS:O	1:A:61:ASN:N	2.54	0.40
1:G:35:LYS:HZ1	1:G:41:GLY:H	1.67	0.40
1:A:7:ASN:C	1:A:8:ARG:HD2	2.46	0.40
1:K:31:LEU:HD11	1:K:44:VAL:HG23	2.03	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)
2:C:246:HOH:O	2:H:251:HOH:O[3_654]	2.12	0.08
1:I:28:GLN:OE1	1:B:110:HIS:NE2[1_445]	2.17	0.03

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	96/122 (79%)	93 (97%)	1 (1%)	2 (2%)	5 3
1	B	98/122 (80%)	93 (95%)	5 (5%)	0	100 100
1	C	96/122 (79%)	92 (96%)	4 (4%)	0	100 100
1	D	99/122 (81%)	98 (99%)	0	1 (1%)	12 11
1	E	96/122 (79%)	93 (97%)	3 (3%)	0	100 100
1	F	98/122 (80%)	94 (96%)	1 (1%)	3 (3%)	3 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	98/122 (80%)	94 (96%)	4 (4%)	0	100	100
1	H	96/122 (79%)	95 (99%)	1 (1%)	0	100	100
1	I	99/122 (81%)	97 (98%)	1 (1%)	1 (1%)	12	11
1	J	96/122 (79%)	94 (98%)	1 (1%)	1 (1%)	12	11
1	K	95/122 (78%)	92 (97%)	3 (3%)	0	100	100
1	L	98/122 (80%)	97 (99%)	1 (1%)	0	100	100
All	All	1165/1464 (80%)	1132 (97%)	25 (2%)	8 (1%)	18	19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	THR
1	I	54	HIS
1	A	58	HIS
1	D	61	ASN
1	F	54	HIS
1	F	58	HIS
1	J	46	LYS
1	F	57	ILE

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	88/103 (85%)	85 (97%)	3 (3%)	32	44
1	B	90/103 (87%)	89 (99%)	1 (1%)	65	79
1	C	90/103 (87%)	82 (91%)	8 (9%)	9	10
1	D	90/103 (87%)	86 (96%)	4 (4%)	25	34
1	E	89/103 (86%)	85 (96%)	4 (4%)	24	33
1	F	90/103 (87%)	86 (96%)	4 (4%)	25	34
1	G	88/103 (85%)	82 (93%)	6 (7%)	14	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	89/103 (86%)	87 (98%)	2 (2%)	45 61
1	I	91/103 (88%)	86 (94%)	5 (6%)	19 24
1	J	89/103 (86%)	86 (97%)	3 (3%)	32 44
1	K	85/103 (82%)	79 (93%)	6 (7%)	13 16
1	L	90/103 (87%)	88 (98%)	2 (2%)	45 61
All	All	1069/1236 (86%)	1021 (96%)	48 (4%)	25 33

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	17	ASN
1	I	55	SER
1	I	59	THR
1	I	69	LEU
1	I	106	LEU
1	B	62	VAL
1	E	22	ASN
1	E	61[A]	ASN
1	E	61[B]	ASN
1	E	62	VAL
1	A	17	ASN
1	A	69	LEU
1	A	106	LEU
1	C	19	ASP
1	C	54	HIS
1	C	62	VAL
1	C	68	LYS
1	C	69	LEU
1	C	81	LYS
1	C	106	LEU
1	C	110	HIS
1	D	22	ASN
1	D	46	LYS
1	D	61	ASN
1	D	81	LYS
1	F	17	ASN
1	F	54	HIS
1	F	69	LEU
1	F	106	LEU
1	G	62	VAL

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Mol	Chain	Res	Type
1	G	69	LEU
1	G	81	LYS
1	G	106	LEU
1	G	109	LYS
1	G	110	HIS
1	H	22	ASN
1	H	95	GLU
1	J	24	LYS
1	J	69	LEU
1	J	106	LEU
1	K	24	LYS
1	K	35	LYS
1	K	62	VAL
1	K	69	LEU
1	K	81	LYS
1	K	110	HIS
1	L	22	ASN
1	L	57	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	33	GLN
1	A	22	ASN
1	A	61	ASN
1	C	28	GLN
1	D	33	GLN
1	G	32	HIS
1	H	33	GLN
1	K	7	ASN
1	L	7	ASN
1	L	33	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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	102/122 (83%)	-1.48	0	100	100	10, 22, 52, 74	0
1	B	102/122 (83%)	-1.48	0	100	100	7, 19, 51, 72	2 (1%)
1	C	101/122 (82%)	-1.48	0	100	100	7, 18, 50, 58	1 (0%)
1	D	103/122 (84%)	-1.42	0	100	100	9, 19, 53, 71	2 (1%)
1	E	101/122 (82%)	-1.49	0	100	100	9, 19, 47, 65	1 (0%)
1	F	104/122 (85%)	-1.45	0	100	100	10, 23, 60, 77	0
1	G	103/122 (84%)	-1.48	0	100	100	7, 19, 54, 69	1 (0%)
1	H	102/122 (83%)	-1.49	0	100	100	9, 19, 53, 72	0
1	I	104/122 (85%)	-1.46	0	100	100	8, 23, 58, 73	1 (0%)
1	J	101/122 (82%)	-1.46	0	100	100	10, 21, 52, 64	1 (0%)
1	K	100/122 (81%)	-1.47	0	100	100	7, 19, 51, 59	1 (1%)
1	L	103/122 (84%)	-1.46	0	100	100	8, 19, 55, 73	1 (0%)
All	All	1226/1464 (83%)	-1.47	0	100	100	7, 20, 54, 77	11 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.