Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2022 – 06:18 pm GMT

PDB ID	:	6S5L
Title	:	Anabaena Apo-C-Terminal Domain Homolog Of The Orange Carotenoid Protein In Native Conditions
Authors	:	Harris, D.; Muzzopappa, F.; Kirilovsky, D.; Adir, N.
Deposited on	:	2019-07-01
Resolution	:	2.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

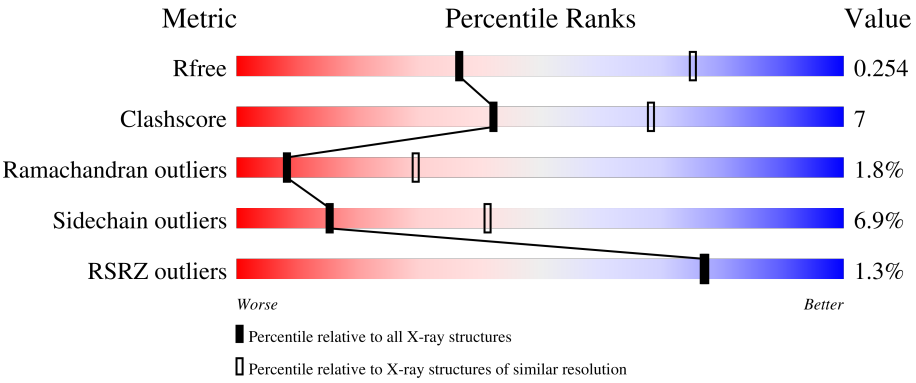
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	140	76% 11% • 11%
1	B	140	2% 77% 11% • 11%
1	C	140	% 74% 16% • 10%
1	D	140	2% 81% 11% • 8%
1	E	140	71% 16% • 11%

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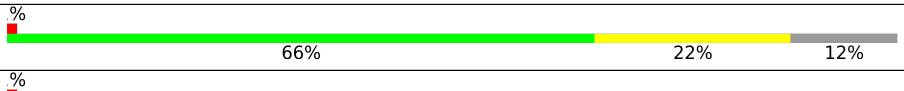
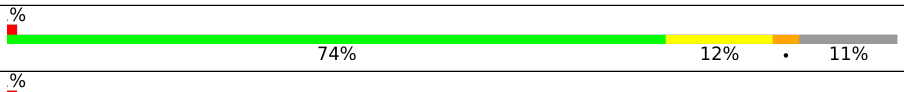
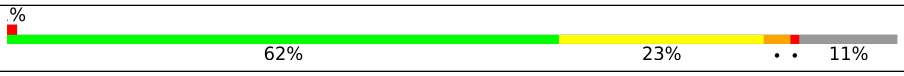
Mol	Chain	Length	Quality of chain
1	F	140	
1	G	140	
1	H	140	
1	I	140	
1	J	140	
1	K	140	
1	L	140	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11429 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 All4940 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			947	608	153	184	2			
1	B	124	Total	C	N	O	S	0	0	0
			936	601	152	181	2			
1	C	126	Total	C	N	O	S	0	0	0
			954	611	155	186	2			
1	D	129	Total	C	N	O	S	0	0	0
			975	626	158	189	2			
1	E	124	Total	C	N	O	S	0	0	0
			937	600	153	182	2			
1	F	129	Total	C	N	O	S	0	0	0
			975	626	158	189	2			
1	G	125	Total	C	N	O	S	0	0	0
			942	604	153	183	2			
1	H	124	Total	C	N	O	S	0	0	0
			939	602	152	183	2			
1	I	124	Total	C	N	O	S	0	0	0
			937	602	152	181	2			
1	J	123	Total	C	N	O	S	0	0	0
			928	595	151	180	2			
1	K	125	Total	C	N	O	S	0	0	0
			946	605	154	185	2			
1	L	124	Total	C	N	O	S	0	0	0
			939	602	152	183	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	5	Total	O	0	0
			5	5		

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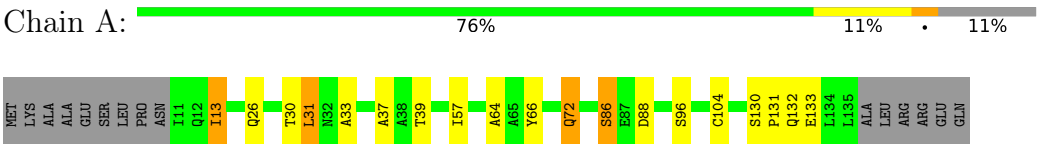
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	9	Total O 9 9	0	0
2	D	6	Total O 6 6	0	0
2	E	6	Total O 6 6	0	0
2	F	8	Total O 8 8	0	0
2	G	7	Total O 7 7	0	0
2	H	6	Total O 6 6	0	0
2	I	3	Total O 3 3	0	0
2	J	7	Total O 7 7	0	0
2	K	2	Total O 2 2	0	0
2	L	7	Total O 7 7	0	0

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.

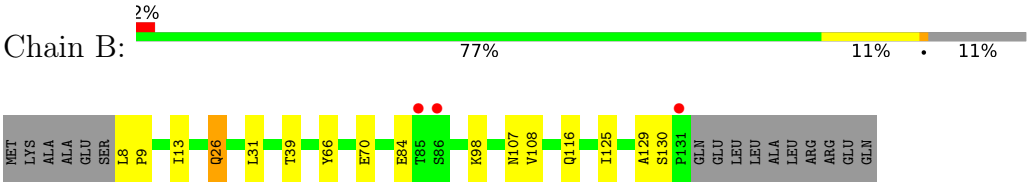
• Molecule 1: All4940 protein

Chain A:



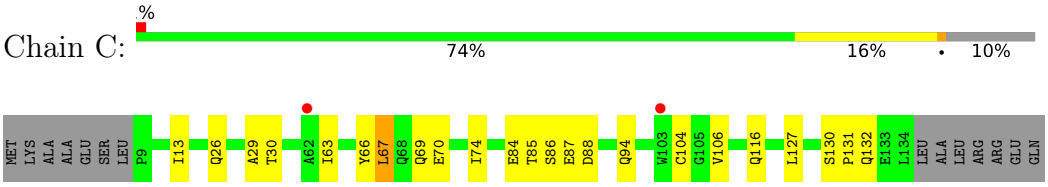
• Molecule 1: All4940 protein

Chain B:



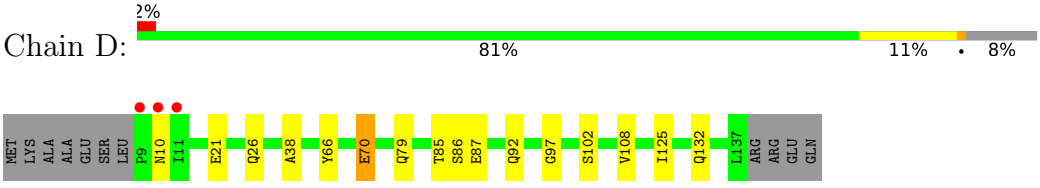
• Molecule 1: All4940 protein

Chain C:



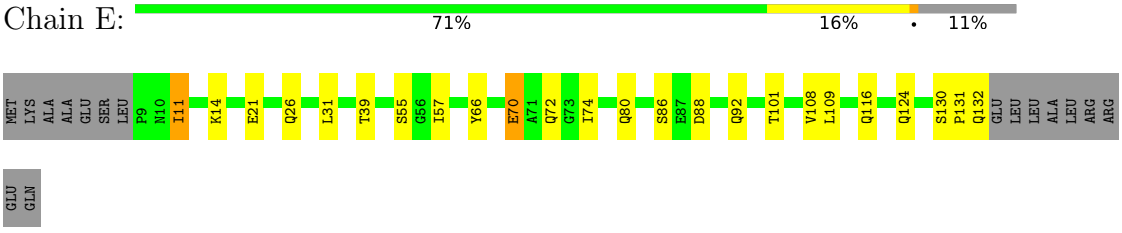
• Molecule 1: All4940 protein

Chain D:



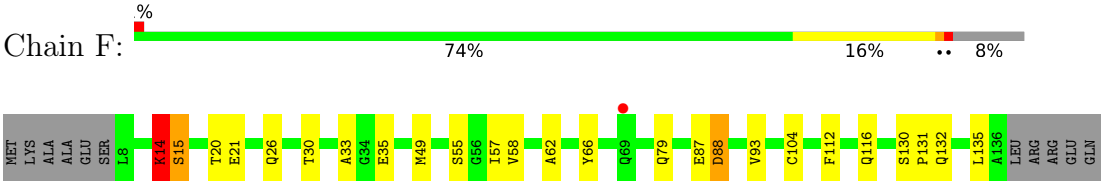
• Molecule 1: All4940 protein

Chain E:



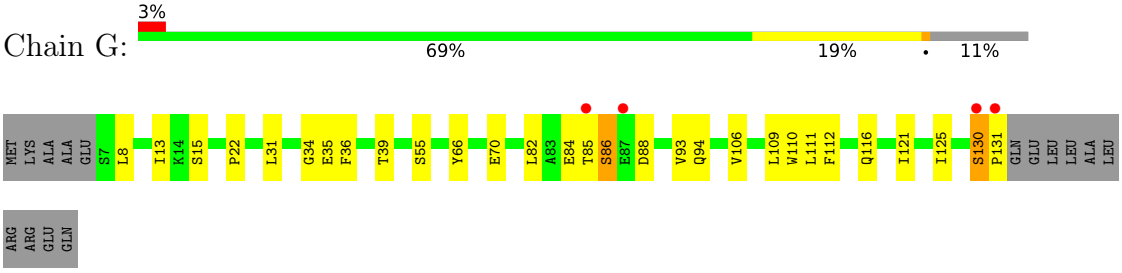
• Molecule 1: All4940 protein

Chain F:



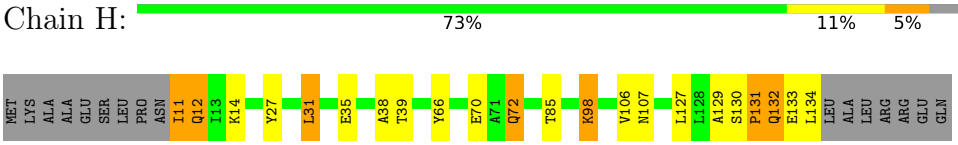
• Molecule 1: All4940 protein

Chain G:



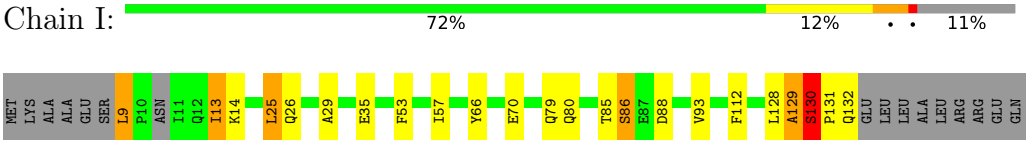
• Molecule 1: All4940 protein

Chain H:



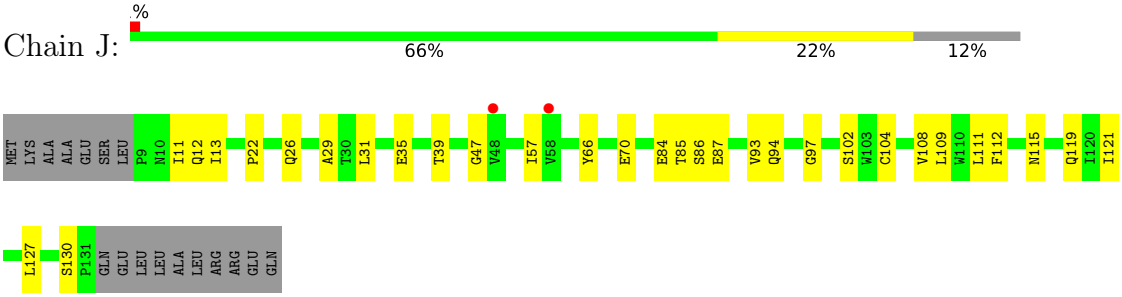
• Molecule 1: All4940 protein

Chain I:



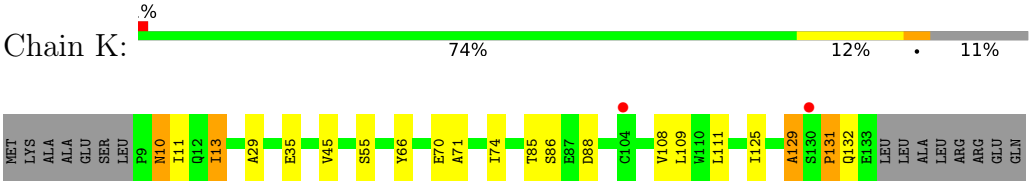
• Molecule 1: All4940 protein

Chain J:



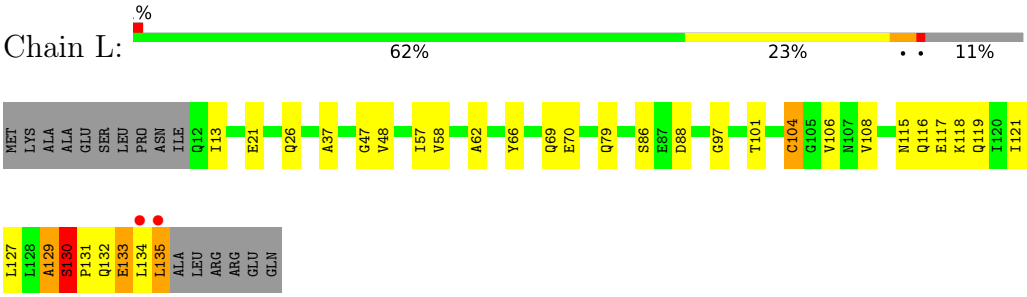
• Molecule 1: All4940 protein

Chain K:



• Molecule 1: All4940 protein

Chain L:


%
62%
23%
11%
MET LYS ALA ALA GLU SER LEU PRO ASN ILE Q12 I13 E21 Q26 A37 G47 V48 I57 V58 A62 Y66 Q69 E70 Q79 S86 E87 D88 G97 T101 C104 G105 V106 N107 V108 N115 Q116 E117 K118 Q119 I120 I121 H122 T123 Q124 I125 K126
L127 L128 A129 S130 P131 Q132 E133 L134 L135 ALA LEU ARG ARG GLU GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.65Å 112.28Å 318.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.99 – 2.90 46.18 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.99-2.90) 99.8 (46.18-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.209 , 0.254 0.216 , 0.254	Depositor DCC
R_{free} test set	2692 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	65.8	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11429	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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	0.68	0/966	0.81	0/1317
1	B	0.67	0/956	0.80	0/1305
1	C	0.67	0/974	0.77	0/1328
1	D	0.71	0/995	0.82	0/1357
1	E	0.71	0/957	0.80	0/1305
1	F	0.69	0/995	0.84	0/1358
1	G	0.66	0/962	0.80	0/1313
1	H	0.66	0/958	0.85	0/1306
1	I	0.67	0/957	0.82	0/1306
1	J	0.63	0/948	0.77	0/1293
1	K	0.64	0/966	0.79	0/1317
1	L	0.67	0/958	0.81	1/1306 (0.1%)
All	All	0.67	0/11592	0.81	1/15811 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	129	ALA	C-N-CA	5.17	134.62	121.70

There are no chirality outliers.

There are no planarity outliers.

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	947	0	941	16	1
1	B	936	0	928	11	0
1	C	954	0	943	14	0
1	D	975	0	971	7	0
1	E	937	0	927	15	0
1	F	975	0	969	17	0
1	G	942	0	933	20	0
1	H	939	0	929	12	0
1	I	937	0	931	16	0
1	J	928	0	919	17	1
1	K	946	0	933	13	0
1	L	939	0	929	26	0
2	A	8	0	0	0	0
2	B	5	0	0	0	0
2	C	9	0	0	1	0
2	D	6	0	0	0	0
2	E	6	0	0	1	0
2	F	8	0	0	2	0
2	G	7	0	0	1	0
2	H	6	0	0	0	0
2	I	3	0	0	0	0
2	J	7	0	0	0	0
2	K	2	0	0	0	0
2	L	7	0	0	3	0
All	All	11429	0	11253	157	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 7.

All (157) 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:30:THR:O	1:F:33:ALA:O	1.56	1.21
1:K:11:ILE:HG21	1:K:35:GLU:OE1	1.71	0.89
1:A:30:THR:O	1:A:33:ALA:O	1.95	0.84
1:F:88:ASP:N	1:F:88:ASP:OD1	2.09	0.80
1:I:13:ILE:HG12	1:I:29:ALA:HB2	1.64	0.77
1:L:127:LEU:N	1:L:127:LEU:HD22	2.02	0.74
1:L:135:LEU:HD23	1:L:135:LEU:O	1.92	0.69
1:I:13:ILE:CD1	1:I:25:LEU:HD13	2.24	0.67
1:G:130:SER:HB3	1:G:131:PRO:HD2	1.76	0.66
1:H:130:SER:HB2	1:H:131:PRO:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLN:CG	1:E:26:GLN:HE22	2.10	0.65
1:B:26:GLN:HE21	1:J:22:PRO:HA	1.62	0.65
1:L:134:LEU:N	1:L:134:LEU:HD23	2.11	0.64
1:H:35:GLU:O	1:H:38:ALA:N	2.31	0.64
1:E:31:LEU:HD12	1:E:74:ILE:HD11	1.81	0.63
1:L:21:GLU:OE1	1:L:118:LYS:NZ	2.32	0.63
1:H:31:LEU:CD2	1:H:39:THR:HG21	2.32	0.59
1:K:86:SER:OG	1:K:88:ASP:OD1	2.21	0.58
1:G:15:SER:HG	1:I:9:LEU:N	2.01	0.58
1:J:11:ILE:HG22	1:J:29:ALA:HB1	1.85	0.58
1:C:106:VAL:HG21	1:C:127:LEU:HD23	1.85	0.58
1:G:31:LEU:CD2	1:G:39:THR:HG21	2.34	0.57
1:C:63:ILE:O	1:C:67:LEU:HD22	2.04	0.57
1:A:96:SER:OG	1:J:94:GLN:NE2	2.31	0.57
1:L:130:SER:HB3	1:L:131:PRO:HD3	1.85	0.57
1:B:31:LEU:CD2	1:B:39:THR:HG21	2.35	0.57
1:J:11:ILE:CG2	1:J:29:ALA:HB1	2.36	0.56
1:K:109:LEU:HD21	1:K:111:LEU:HD21	1.87	0.56
1:C:26:GLN:HE22	1:D:26:GLN:HG3	1.71	0.56
1:D:79:GLN:HG2	1:D:97:GLY:HA2	1.87	0.55
1:F:14:LYS:O	1:F:15:SER:CB	2.53	0.55
1:L:131:PRO:HD2	2:L:205:HOH:O	2.06	0.55
1:B:98:LYS:HE2	1:B:107:ASN:HD21	1.73	0.54
1:F:20:THR:OG1	1:L:117:GLU:HG2	2.08	0.54
1:J:31:LEU:CD2	1:J:39:THR:HG21	2.37	0.54
1:A:26:GLN:HG3	1:E:26:GLN:HE22	1.72	0.54
1:H:132:GLN:O	1:H:132:GLN:NE2	2.40	0.54
1:B:13:ILE:HG21	1:J:26:GLN:HE22	1.72	0.53
1:F:26:GLN:HE22	1:L:26:GLN:CG	2.21	0.53
1:L:127:LEU:N	1:L:127:LEU:CD2	2.72	0.52
1:A:57:ILE:CD1	1:A:66:TYR:CD1	2.93	0.52
1:I:93:VAL:HB	1:I:112:PHE:HB2	1.92	0.52
1:I:13:ILE:CG1	1:I:29:ALA:HB2	2.36	0.52
1:L:119:GLN:HG2	2:L:203:HOH:O	2.10	0.52
1:A:64:ALA:CB	1:E:11:ILE:HD11	2.41	0.51
1:C:88:ASP:O	1:C:116:GLN:NE2	2.43	0.51
1:E:66:TYR:CE1	1:E:70:GLU:HG3	2.45	0.51
1:G:34:GLY:O	1:G:36:PHE:N	2.43	0.51
1:D:66:TYR:CE1	1:D:70:GLU:HG3	2.45	0.51
1:K:11:ILE:CG2	1:K:35:GLU:OE1	2.51	0.51
1:C:26:GLN:HE22	1:D:26:GLN:CG	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:LEU:HD21	1:G:111:LEU:HD21	1.92	0.50
1:F:14:LYS:O	1:F:15:SER:HB3	2.11	0.50
1:F:21:GLU:HB2	2:F:204:HOH:O	2.11	0.50
1:I:57:ILE:HD11	1:I:66:TYR:CD2	2.47	0.50
1:C:116:GLN:HG3	2:C:209:HOH:O	2.11	0.50
1:F:57:ILE:HD11	1:F:66:TYR:CD1	2.47	0.50
1:H:130:SER:O	1:H:131:PRO:C	2.50	0.50
1:L:132:GLN:O	1:L:132:GLN:HG3	2.11	0.50
1:C:130:SER:O	1:C:132:GLN:N	2.45	0.49
1:G:116:GLN:HG3	2:G:206:HOH:O	2.11	0.49
1:J:109:LEU:HD21	1:J:111:LEU:HD21	1.94	0.49
1:A:37:ALA:HA	1:E:11:ILE:CD1	2.43	0.49
1:A:130:SER:O	1:A:132:GLN:N	2.46	0.49
1:J:11:ILE:HD11	1:J:35:GLU:OE2	2.13	0.48
1:F:130:SER:O	1:F:132:GLN:N	2.46	0.48
1:I:129:ALA:HB1	1:I:131:PRO:HD2	1.94	0.48
1:E:80:GLN:HG3	1:G:94:GLN:HE21	1.79	0.48
1:G:66:TYR:CE1	1:G:70:GLU:HG3	2.48	0.48
1:A:13:ILE:HG22	1:A:13:ILE:O	2.15	0.47
1:A:13:ILE:O	1:A:13:ILE:CG2	2.62	0.47
1:J:97:GLY:O	1:J:108:VAL:N	2.45	0.47
1:C:69:GLN:HG3	1:C:70:GLU:HG2	1.97	0.47
1:G:130:SER:HB3	1:G:131:PRO:CD	2.42	0.47
1:L:106:VAL:HG23	1:L:108:VAL:HG22	1.96	0.47
1:G:130:SER:CB	1:G:131:PRO:HD2	2.44	0.46
1:H:72:GLN:HE21	1:L:69:GLN:HB2	1.79	0.46
1:H:106:VAL:HG21	1:H:127:LEU:HD23	1.98	0.46
1:L:115:ASN:HB3	1:L:121:ILE:HD11	1.96	0.46
1:J:13:ILE:HB	1:J:29:ALA:HB2	1.97	0.46
1:L:58:VAL:O	1:L:62:ALA:HB3	2.15	0.46
1:E:31:LEU:CD2	1:E:39:THR:HG21	2.45	0.46
1:A:86:SER:HB2	1:A:88:ASP:OD1	2.16	0.46
1:B:98:LYS:HG2	1:B:107:ASN:ND2	2.31	0.46
1:G:13:ILE:HG21	1:I:26:GLN:HE22	1.80	0.46
1:A:31:LEU:HD12	1:A:39:THR:HG21	1.98	0.45
1:B:98:LYS:HE2	1:B:107:ASN:ND2	2.30	0.45
1:G:34:GLY:O	1:G:36:PHE:CD1	2.69	0.45
1:I:13:ILE:HD13	1:I:25:LEU:HD13	1.97	0.45
1:E:21:GLU:HB2	2:E:206:HOH:O	2.16	0.45
1:G:22:PRO:HB3	1:I:26:GLN:HG3	1.97	0.45
1:K:108:VAL:HG13	1:K:125:ILE:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLN:HG2	1:E:26:GLN:HE22	1.81	0.45
1:C:13:ILE:CD1	1:C:29:ALA:HB1	2.47	0.45
1:I:128:LEU:O	1:I:129:ALA:HB2	2.17	0.45
1:H:11:ILE:N	1:K:13:ILE:O	2.50	0.45
1:K:66:TYR:CE1	1:K:70:GLU:HG3	2.52	0.45
1:E:88:ASP:O	1:E:116:GLN:NE2	2.47	0.44
1:B:8:LEU:HB3	1:B:9:PRO:CD	2.47	0.44
1:B:13:ILE:HD13	1:J:26:GLN:NE2	2.32	0.44
1:D:108:VAL:HG13	1:D:125:ILE:HG23	1.99	0.44
1:C:66:TYR:CE1	1:C:70:GLU:HG3	2.53	0.44
1:J:127:LEU:HD22	1:J:127:LEU:N	2.32	0.44
1:F:57:ILE:HD13	1:F:66:TYR:CG	2.53	0.44
1:L:47:GLY:HA2	1:L:121:ILE:O	2.18	0.44
1:F:26:GLN:HE22	1:L:26:GLN:HG3	1.82	0.44
1:A:72:GLN:N	1:A:72:GLN:OE1	2.50	0.44
1:K:129:ALA:HB1	1:K:132:GLN:HE21	1.83	0.44
1:H:14:LYS:HA	1:K:10:ASN:HB2	2.00	0.44
1:K:71:ALA:HA	1:K:74:ILE:HD12	2.00	0.44
1:J:93:VAL:HB	1:J:112:PHE:HB2	2.00	0.43
1:J:57:ILE:HD13	1:J:66:TYR:CG	2.53	0.43
1:L:88:ASP:O	1:L:116:GLN:NE2	2.51	0.43
1:F:35:GLU:OE1	1:L:37:ALA:HB3	2.18	0.43
1:G:110:TRP:CD1	1:G:125:ILE:HG12	2.54	0.43
1:C:84:GLU:OE2	1:C:94:GLN:OE1	2.37	0.43
1:F:93:VAL:HB	1:F:112:PHE:HB2	2.00	0.43
1:G:130:SER:CB	1:G:131:PRO:CD	2.96	0.43
1:K:129:ALA:HB1	1:K:132:GLN:NE2	2.34	0.43
1:G:86:SER:HB2	1:G:88:ASP:OD1	2.19	0.43
1:F:57:ILE:CD1	1:F:66:TYR:CD1	3.01	0.43
1:I:57:ILE:HD13	1:I:66:TYR:CG	2.54	0.43
1:A:57:ILE:HD13	1:A:66:TYR:HB2	2.01	0.42
1:L:86:SER:HB2	1:L:88:ASP:OD1	2.19	0.42
1:E:108:VAL:HG12	1:E:109:LEU:N	2.34	0.42
1:F:49:MET:CE	2:F:208:HOH:O	2.66	0.42
1:F:57:ILE:CD1	1:F:66:TYR:CG	3.02	0.42
1:I:66:TYR:CE2	1:I:70:GLU:HG3	2.54	0.42
1:A:57:ILE:HD11	1:A:66:TYR:CD1	2.53	0.42
1:E:80:GLN:NE2	1:G:94:GLN:HG3	2.35	0.42
1:I:130:SER:N	1:I:131:PRO:CD	2.82	0.42
1:B:108:VAL:HG13	1:B:125:ILE:HG23	2.01	0.42
1:J:115:ASN:HD21	1:J:119:GLN:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:13:ILE:HB	1:K:29:ALA:HB2	2.01	0.42
1:L:57:ILE:HD11	1:L:66:TYR:CD2	2.55	0.42
1:H:27:TYR:O	1:H:31:LEU:HB2	2.19	0.42
1:I:57:ILE:HD13	1:I:66:TYR:CB	2.50	0.41
1:H:98:LYS:HG2	1:H:107:ASN:ND2	2.35	0.41
1:J:66:TYR:CZ	1:J:70:GLU:HG2	2.55	0.41
1:C:30:THR:HG22	1:D:38:ALA:HB2	2.02	0.41
1:F:58:VAL:O	1:F:62:ALA:HB3	2.21	0.41
1:L:108:VAL:CG1	1:L:125:ILE:HG23	2.49	0.41
1:C:30:THR:CG2	1:D:38:ALA:HB2	2.50	0.41
1:I:86:SER:HB2	1:I:88:ASP:OD1	2.20	0.41
1:K:109:LEU:CD2	1:K:111:LEU:HD21	2.49	0.41
1:L:124:GLN:HB2	2:L:202:HOH:O	2.20	0.41
1:E:80:GLN:HB2	1:G:82:LEU:HD23	2.01	0.41
1:J:47:GLY:HA2	1:J:121:ILE:O	2.20	0.41
1:L:48:VAL:O	1:L:122:HIS:HA	2.21	0.41
1:L:121:ILE:HG22	1:L:122:HIS:HD2	1.86	0.41
1:G:93:VAL:HB	1:G:112:PHE:HB2	2.03	0.40
1:B:66:TYR:CE1	1:B:70:GLU:HG3	2.56	0.40
1:E:57:ILE:HD13	1:E:66:TYR:CG	2.56	0.40
1:C:104:CYS:HB3	1:G:106:VAL:HG13	2.04	0.40
1:H:66:TYR:CE1	1:H:70:GLU:HG3	2.57	0.40
1:B:8:LEU:CB	1:B:9:PRO:CD	2.99	0.40
1:L:79:GLN:HG2	1:L:97:GLY:HA2	2.03	0.40

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:A:104:CYS:SG	1:J:104:CYS:SG[4_545]	1.73	0.47

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	123/140 (88%)	115 (94%)	6 (5%)	2 (2%)	9 32
1	B	122/140 (87%)	113 (93%)	7 (6%)	2 (2%)	9 32
1	C	124/140 (89%)	117 (94%)	6 (5%)	1 (1%)	19 51
1	D	127/140 (91%)	125 (98%)	2 (2%)	0	100 100
1	E	122/140 (87%)	114 (93%)	6 (5%)	2 (2%)	9 32
1	F	127/140 (91%)	115 (91%)	8 (6%)	4 (3%)	4 16
1	G	123/140 (88%)	114 (93%)	7 (6%)	2 (2%)	9 32
1	H	122/140 (87%)	112 (92%)	7 (6%)	3 (2%)	5 21
1	I	122/140 (87%)	115 (94%)	3 (2%)	4 (3%)	4 15
1	J	121/140 (86%)	112 (93%)	9 (7%)	0	100 100
1	K	123/140 (88%)	115 (94%)	6 (5%)	2 (2%)	9 32
1	L	122/140 (87%)	109 (89%)	8 (7%)	5 (4%)	3 11
All	All	1478/1680 (88%)	1376 (93%)	75 (5%)	27 (2%)	8 29

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	130	SER
1	E	130	SER
1	F	14	LYS
1	F	135	LEU
1	G	35	GLU
1	H	12	GLN
1	H	131	PRO
1	K	131	PRO
1	L	130	SER
1	A	131	PRO
1	B	129	ALA
1	C	131	PRO
1	F	15	SER
1	F	131	PRO
1	H	129	ALA
1	I	129	ALA
1	K	129	ALA
1	I	35	GLU
1	L	13	ILE
1	L	129	ALA

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Mol	Chain	Res	Type
1	I	53	PHE
1	L	104	CYS
1	A	13	ILE
1	L	133	GLU
1	E	131	PRO
1	G	130	SER
1	I	130	SER

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	99/111 (89%)	95 (96%)	4 (4%)	31	65
1	B	98/111 (88%)	95 (97%)	3 (3%)	40	74
1	C	100/111 (90%)	95 (95%)	5 (5%)	24	57
1	D	102/111 (92%)	93 (91%)	9 (9%)	10	30
1	E	98/111 (88%)	88 (90%)	10 (10%)	7	22
1	F	102/111 (92%)	95 (93%)	7 (7%)	15	41
1	G	99/111 (89%)	93 (94%)	6 (6%)	18	48
1	H	98/111 (88%)	89 (91%)	9 (9%)	9	27
1	I	98/111 (88%)	88 (90%)	10 (10%)	7	22
1	J	97/111 (87%)	90 (93%)	7 (7%)	14	39
1	K	99/111 (89%)	93 (94%)	6 (6%)	18	48
1	L	98/111 (88%)	92 (94%)	6 (6%)	18	48
All	All	1188/1332 (89%)	1106 (93%)	82 (7%)	15	41

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	72	GLN
1	A	86	SER

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Mol	Chain	Res	Type
1	A	133	GLU
1	B	26	GLN
1	B	84	GLU
1	B	116	GLN
1	C	67	LEU
1	C	74	ILE
1	C	85	THR
1	C	86	SER
1	C	87	GLU
1	D	10	ASN
1	D	21	GLU
1	D	70	GLU
1	D	85	THR
1	D	86	SER
1	D	87	GLU
1	D	92	GLN
1	D	102	SER
1	D	132	GLN
1	E	11	ILE
1	E	14	LYS
1	E	55	SER
1	E	70	GLU
1	E	72	GLN
1	E	86	SER
1	E	92	GLN
1	E	101	THR
1	E	124	GLN
1	E	132	GLN
1	F	14	LYS
1	F	55	SER
1	F	79	GLN
1	F	87	GLU
1	F	88	ASP
1	F	104	CYS
1	F	116	GLN
1	G	8	LEU
1	G	55	SER
1	G	84	GLU
1	G	85	THR
1	G	86	SER
1	G	121	ILE
1	H	11	ILE

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Mol	Chain	Res	Type
1	H	12	GLN
1	H	31	LEU
1	H	72	GLN
1	H	85	THR
1	H	98	LYS
1	H	132	GLN
1	H	133	GLU
1	H	134	LEU
1	I	9	LEU
1	I	13	ILE
1	I	14	LYS
1	I	25	LEU
1	I	79	GLN
1	I	80	GLN
1	I	85	THR
1	I	86	SER
1	I	130	SER
1	I	132	GLN
1	J	12	GLN
1	J	84	GLU
1	J	85	THR
1	J	86	SER
1	J	87	GLU
1	J	102	SER
1	J	130	SER
1	K	10	ASN
1	K	13	ILE
1	K	45	VAL
1	K	55	SER
1	K	85	THR
1	K	131	PRO
1	L	70	GLU
1	L	101	THR
1	L	104	CYS
1	L	130	SER
1	L	133	GLU
1	L	135	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN

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Mol	Chain	Res	Type
1	B	26	GLN
1	B	107	ASN
1	C	94	GLN
1	D	79	GLN
1	D	92	GLN
1	D	94	GLN
1	E	26	GLN
1	E	80	GLN
1	E	92	GLN
1	E	94	GLN
1	E	124	GLN
1	E	132	GLN
1	F	26	GLN
1	F	94	GLN
1	F	122	HIS
1	F	132	GLN
1	G	26	GLN
1	G	72	GLN
1	G	94	GLN
1	G	122	HIS
1	H	72	GLN
1	H	94	GLN
1	H	107	ASN
1	I	26	GLN
1	I	122	HIS
1	J	26	GLN
1	J	72	GLN
1	J	94	GLN
1	J	107	ASN
1	J	119	GLN
1	J	122	HIS
1	J	124	GLN
1	K	122	HIS
1	K	132	GLN
1	L	122	HIS
1	L	124	GLN

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 monosaccharides 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	125/140 (89%)	-0.23	0 100 100	36, 59, 108, 155	0
1	B	124/140 (88%)	-0.08	3 (2%) 59 56	45, 68, 106, 141	0
1	C	126/140 (90%)	-0.12	2 (1%) 72 71	40, 65, 114, 137	0
1	D	129/140 (92%)	-0.12	3 (2%) 60 58	43, 61, 117, 142	0
1	E	124/140 (88%)	-0.08	0 100 100	39, 66, 111, 142	0
1	F	129/140 (92%)	0.01	1 (0%) 86 86	41, 70, 118, 128	0
1	G	125/140 (89%)	-0.06	4 (3%) 47 43	41, 66, 104, 152	0
1	H	124/140 (88%)	-0.15	0 100 100	42, 72, 115, 149	0
1	I	124/140 (88%)	-0.15	0 100 100	43, 70, 115, 132	0
1	J	123/140 (87%)	-0.04	2 (1%) 72 71	42, 73, 111, 128	0
1	K	125/140 (89%)	-0.04	2 (1%) 72 71	45, 71, 111, 144	0
1	L	124/140 (88%)	-0.12	2 (1%) 72 71	30, 67, 109, 130	0
All	All	1502/1680 (89%)	-0.10	19 (1%) 77 77	30, 68, 115, 155	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	9	PRO	4.3
1	G	130	SER	3.7
1	D	10	ASN	3.6
1	B	131	PRO	3.2
1	B	85	THR	3.1
1	F	69	GLN	2.9
1	K	104	CYS	2.7
1	G	87	GLU	2.6
1	J	58	VAL	2.6
1	C	62	ALA	2.5
1	C	103	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	135	LEU	2.5
1	L	134	LEU	2.5
1	D	11	ILE	2.4
1	G	131	PRO	2.3
1	B	86	SER	2.2
1	K	130	SER	2.2
1	J	48	VAL	2.1
1	G	85	THR	2.1

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.