



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:09 PM BST

PDB ID : 1NYA
Title : NMR SOLUTION STRUCTURE OF CALERYTHRIN, AN EF-HAND
CALCIUM-BINDING PROTEIN
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Deposited on : 2003-02-12

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

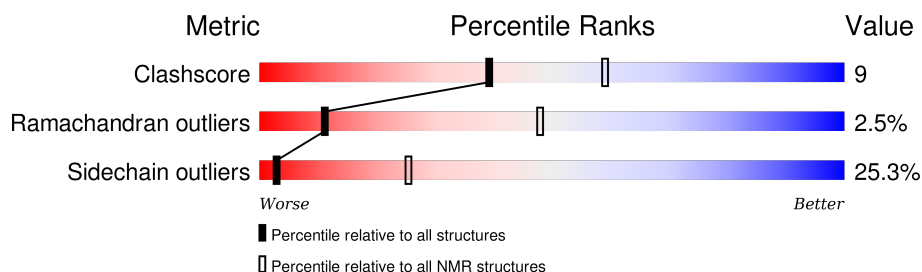
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	176	 63% 24% • 11%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:159 (156)	0.35	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 11, 12, 13, 14, 15, 16, 17, 20
2	18, 19
Single-model clusters	10

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2631 atoms, of which 1285 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calerythrin.

Mol	Chain	Residues	Atoms						Trace
1	A	176	Total	C	H	N	O	S	0
			2628	839	1285	230	271	3	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ILE	THR	ENGINEERED	UNP P06495
A	108	VAL	TRP	ENGINEERED	UNP P06495

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

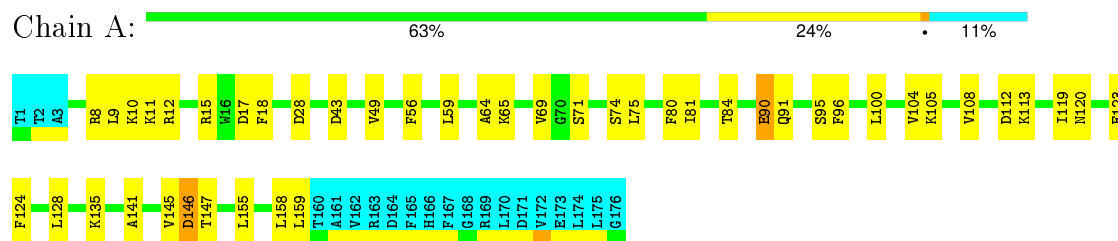
Mol	Chain	Residues	Atoms	
2	A	3	Total	Ca
			3	3

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Calerythrin

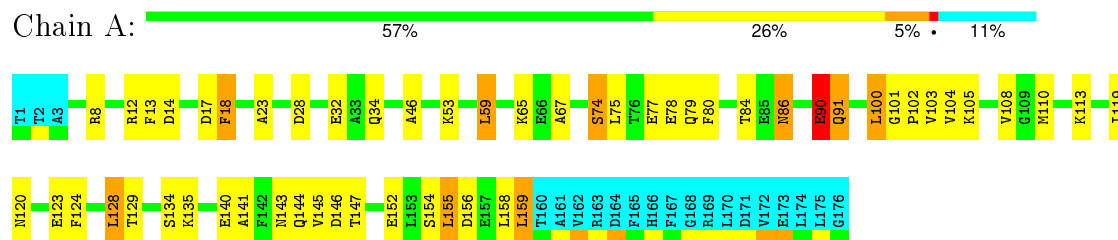


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

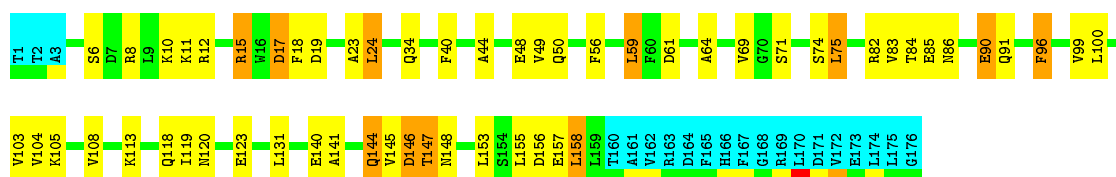
- Molecule 1: Calerythrin



4.2.2 Score per residue for model 2

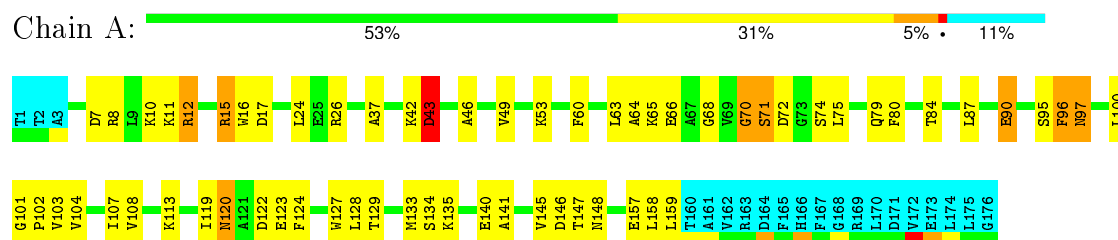
- Molecule 1: Calerythrin





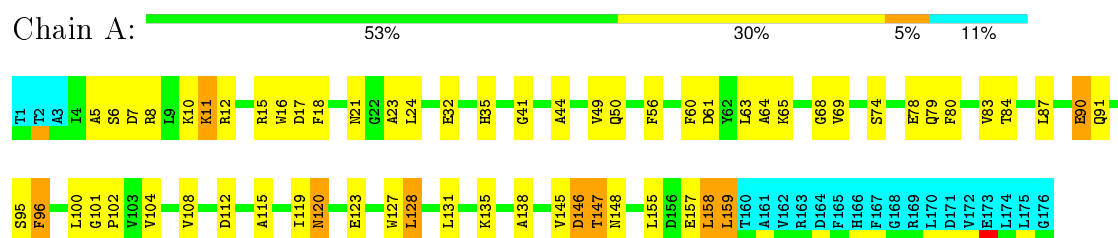
4.2.3 Score per residue for model 3

- Molecule 1: Calerythrin



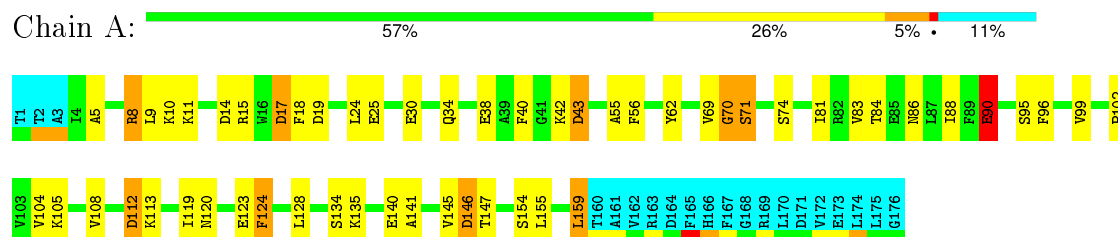
4.2.4 Score per residue for model 4

- Molecule 1: Calerythrin



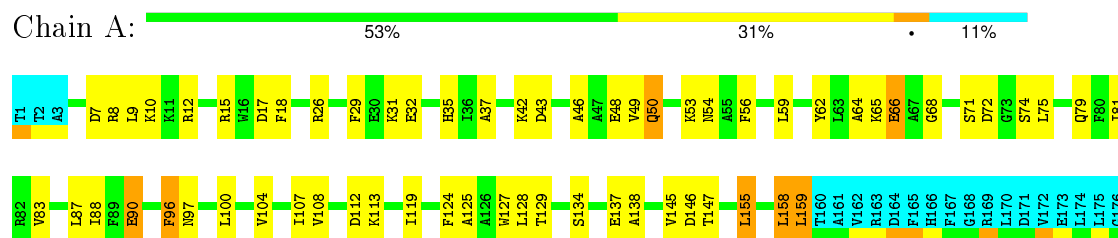
4.2.5 Score per residue for model 5

- Molecule 1: Calerythrin



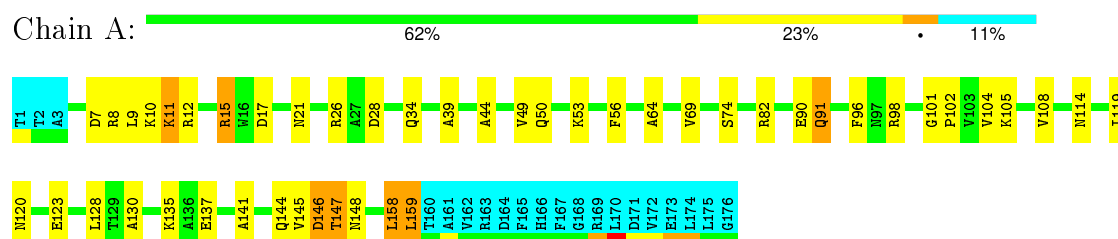
4.2.6 Score per residue for model 6

- Molecule 1: Calerythrin



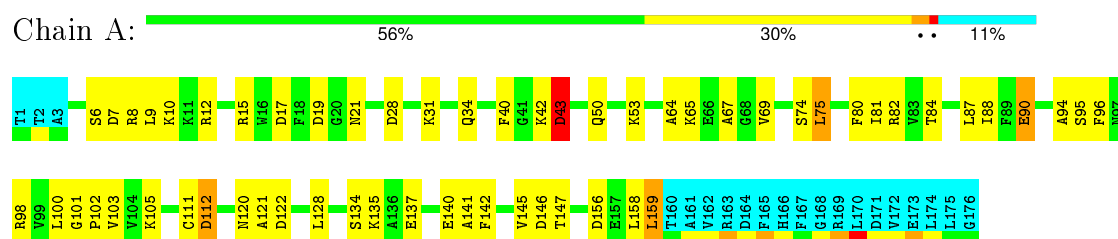
4.2.7 Score per residue for model 7

- Molecule 1: Calerythrin



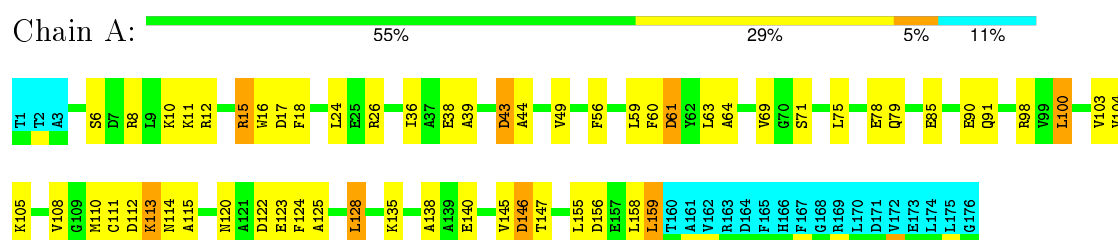
4.2.8 Score per residue for model 8

- Molecule 1: Calerythrin



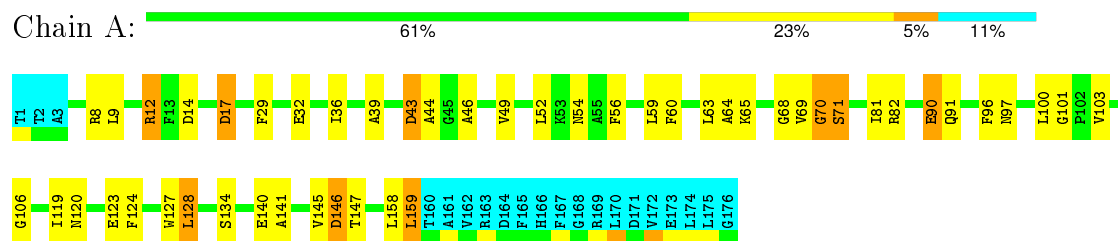
4.2.9 Score per residue for model 9

- Molecule 1: Calerythrin



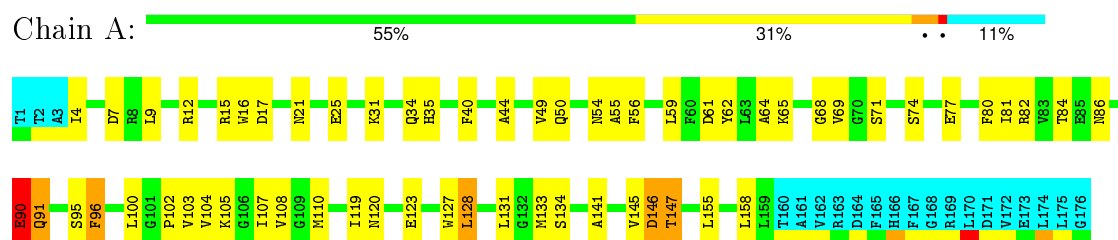
4.2.10 Score per residue for model 10

- Molecule 1: Calerythrin



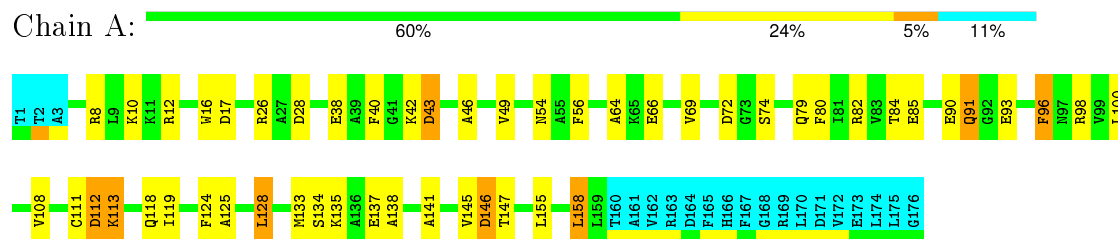
4.2.11 Score per residue for model 11

- Molecule 1: Calerythrin



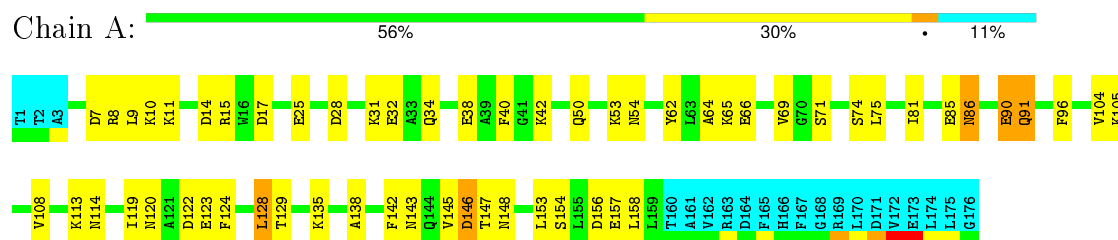
4.2.12 Score per residue for model 12

- Molecule 1: Calerythrin



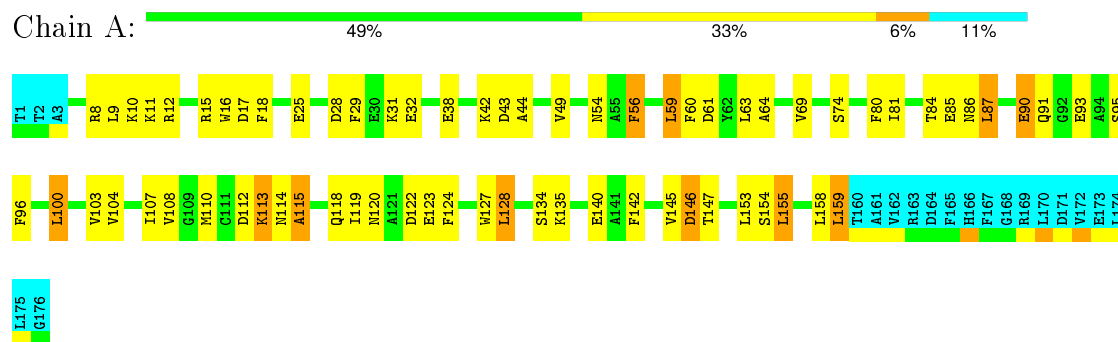
4.2.13 Score per residue for model 13

- Molecule 1: Calerythrin



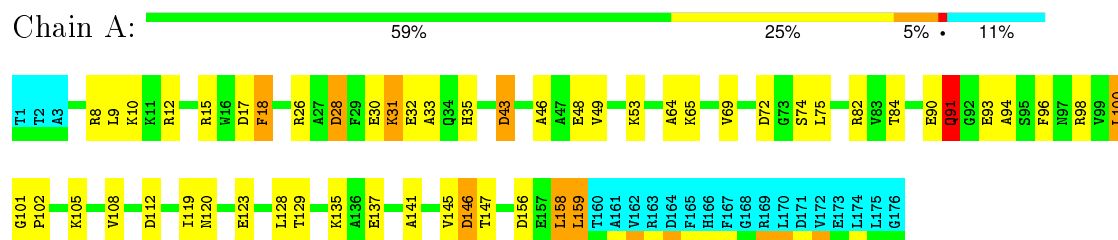
4.2.14 Score per residue for model 14

- Molecule 1: Calerythrin



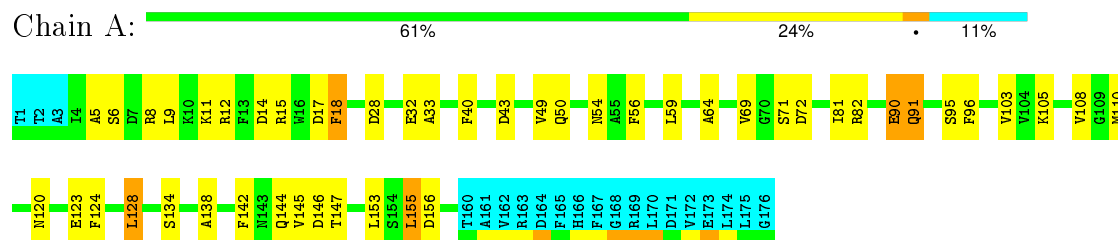
4.2.15 Score per residue for model 15

- Molecule 1: Calerythrin



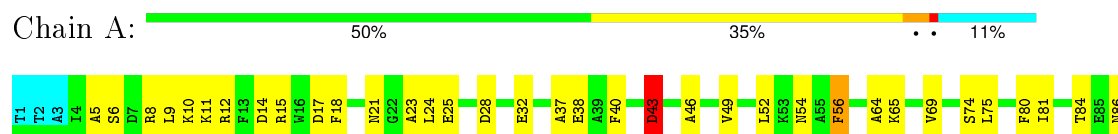
4.2.16 Score per residue for model 16

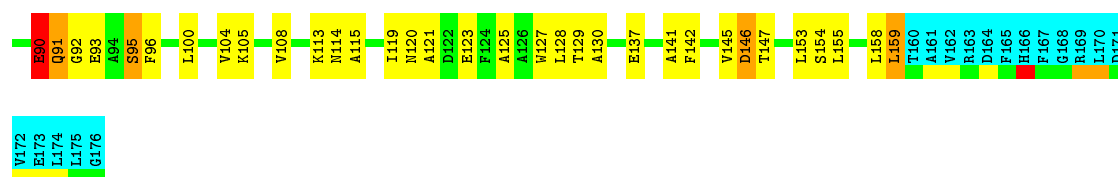
- Molecule 1: Calerythrin



4.2.17 Score per residue for model 17

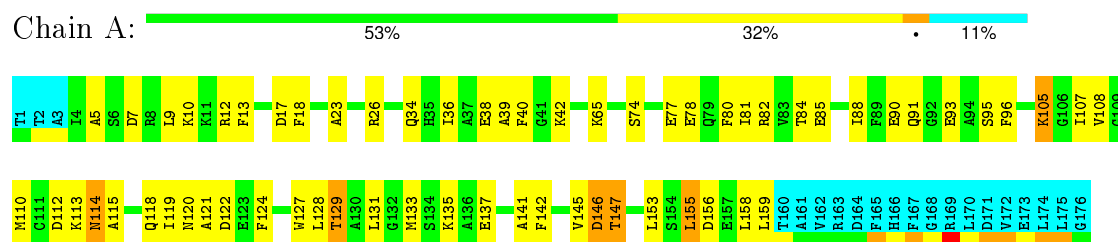
- Molecule 1: Calerythrin





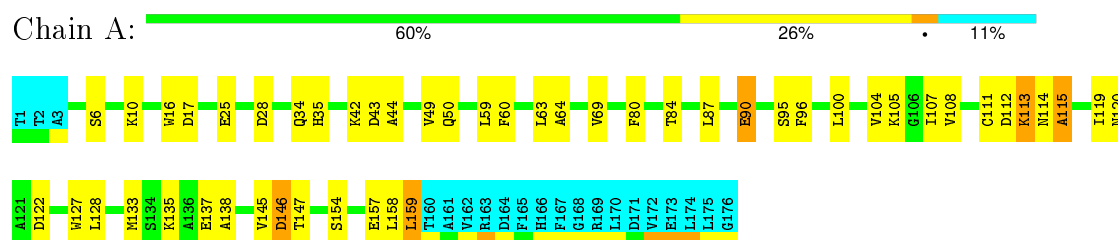
4.2.18 Score per residue for model 18

- Molecule 1: Calerythrin



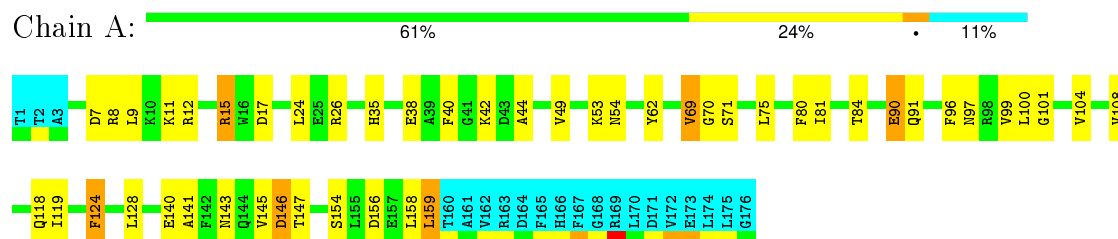
4.2.19 Score per residue for model 19

- Molecule 1: Calerythrin



4.2.20 Score per residue for model 20

- Molecule 1: Calerythrin



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 225 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	structure solution	3.1
X-PLOR	refinement	3.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1186	1129	1128	22±5
All	All	23780	22580	22560	434

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 9.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:VAL:HG13	1:A:153:LEU:HD21	0.89	1.40	14	2
1:A:104:VAL:O	1:A:108:VAL:HG23	0.81	1.75	4	11
1:A:44:ALA:O	1:A:49:VAL:HG11	0.78	1.78	7	9
1:A:29:PHE:CE2	1:A:59:LEU:HD12	0.76	2.15	6	1
1:A:107:ILE:HG21	1:A:127:TRP:CZ2	0.76	2.14	6	4
1:A:64:ALA:HB1	1:A:69:VAL:O	0.75	1.81	14	13
1:A:9:LEU:HD13	1:A:81:ILE:HG23	0.72	1.59	13	9
1:A:124:PHE:CE2	1:A:128:LEU:HD11	0.72	2.20	16	8
1:A:108:VAL:HG13	1:A:119:ILE:HD11	0.72	1.60	15	8
1:A:141:ALA:O	1:A:145:VAL:HG23	0.72	1.84	7	13
1:A:100:LEU:HD13	1:A:103:VAL:HB	0.71	1.62	9	3
1:A:104:VAL:CG1	1:A:158:LEU:HD13	0.70	2.16	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LEU:HD12	1:A:81:ILE:HG23	0.69	1.62	14	1
1:A:119:ILE:HG13	1:A:158:LEU:HD11	0.68	1.65	18	9
1:A:96:PHE:CE2	1:A:100:LEU:HD22	0.68	2.24	17	2
1:A:107:ILE:HG21	1:A:127:TRP:CE2	0.67	2.24	6	1
1:A:104:VAL:HG12	1:A:158:LEU:HD13	0.66	1.66	2	1
1:A:60:PHE:HA	1:A:63:LEU:HD12	0.66	1.67	19	2
1:A:96:PHE:CE1	1:A:100:LEU:HD22	0.65	2.27	2	6
1:A:145:VAL:CG1	1:A:153:LEU:HD21	0.65	2.22	13	3
1:A:21:ASN:ND2	1:A:23:ALA:HB3	0.65	2.07	4	2
1:A:142:PHE:CD2	1:A:153:LEU:HD11	0.65	2.27	17	1
1:A:108:VAL:HG13	1:A:119:ILE:CD1	0.64	2.22	17	5
1:A:100:LEU:HD12	1:A:104:VAL:HG23	0.63	1.69	14	1
1:A:108:VAL:HA	1:A:119:ILE:HD11	0.63	1.70	18	1
1:A:80:PHE:O	1:A:84:THR:HG23	0.62	1.93	17	3
1:A:108:VAL:HG21	1:A:155:LEU:HD22	0.61	1.72	16	1
1:A:108:VAL:HG21	1:A:155:LEU:CD2	0.61	2.25	1	3
1:A:104:VAL:HG21	1:A:159:LEU:HD22	0.60	1.72	1	1
1:A:62:TYR:CD1	1:A:99:VAL:HG21	0.60	2.32	20	1
1:A:24:LEU:HB3	1:A:75:LEU:HD12	0.60	1.72	2	1
1:A:124:PHE:CD2	1:A:128:LEU:HD11	0.60	2.32	16	2
1:A:125:ALA:O	1:A:129:THR:HG23	0.60	1.96	6	2
1:A:59:LEU:HD12	1:A:103:VAL:HG21	0.59	1.72	1	1
1:A:128:LEU:HD13	1:A:138:ALA:HA	0.59	1.73	16	2
1:A:108:VAL:HG22	1:A:119:ILE:HD11	0.59	1.75	14	3
1:A:79:GLN:O	1:A:83:VAL:HG23	0.59	1.97	6	2
1:A:108:VAL:HG21	1:A:155:LEU:HD12	0.58	1.75	4	1
1:A:119:ILE:CG1	1:A:158:LEU:HD11	0.58	2.28	18	5
1:A:96:PHE:CZ	1:A:100:LEU:HD22	0.58	2.34	10	1
1:A:59:LEU:HD13	1:A:103:VAL:HG21	0.57	1.75	16	3
1:A:128:LEU:HD22	1:A:138:ALA:HA	0.57	1.77	13	1
1:A:59:LEU:HD13	1:A:59:LEU:C	0.56	2.21	9	1
1:A:159:LEU:HD23	1:A:159:LEU:N	0.56	2.14	10	7
1:A:159:LEU:N	1:A:159:LEU:HD23	0.56	2.15	9	5
1:A:155:LEU:HD13	1:A:159:LEU:HD21	0.56	1.77	6	1
1:A:29:PHE:CZ	1:A:59:LEU:HD12	0.56	2.34	6	1
1:A:142:PHE:CD1	1:A:153:LEU:HD12	0.56	2.36	16	1
1:A:127:TRP:NE1	1:A:131:LEU:HD11	0.55	2.17	4	2
1:A:84:THR:O	1:A:88:ILE:HD12	0.55	2.01	18	1
1:A:155:LEU:HA	1:A:158:LEU:HD12	0.55	1.78	14	1
1:A:108:VAL:HG21	1:A:155:LEU:CD1	0.55	2.30	4	1
1:A:70:GLY:O	1:A:71:SER:CB	0.55	2.55	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:LEU:HD11	1:A:96:PHE:CE2	0.55	2.37	14	1
1:A:59:LEU:HD22	1:A:99:VAL:HG12	0.54	1.77	2	1
1:A:155:LEU:CD1	1:A:159:LEU:HD21	0.54	2.31	6	1
1:A:9:LEU:CD2	1:A:84:THR:HG21	0.54	2.32	15	1
1:A:59:LEU:HD23	1:A:103:VAL:HG21	0.54	1.78	2	1
1:A:5:ALA:O	1:A:9:LEU:HD12	0.54	2.03	18	2
1:A:145:VAL:HG11	1:A:153:LEU:HD11	0.54	1.80	13	2
1:A:23:ALA:HB1	1:A:74:SER:HB2	0.54	1.78	18	2
1:A:9:LEU:HD13	1:A:81:ILE:CG2	0.53	2.33	10	1
1:A:59:LEU:CD1	1:A:103:VAL:HG21	0.53	2.33	1	1
1:A:80:PHE:CE1	1:A:84:THR:CG2	0.53	2.92	4	3
1:A:104:VAL:CG1	1:A:158:LEU:HD22	0.53	2.34	7	1
1:A:114:ASN:O	1:A:115:ALA:HB3	0.52	2.04	19	5
1:A:100:LEU:O	1:A:103:VAL:HG22	0.52	2.04	8	1
1:A:46:ALA:HB3	1:A:49:VAL:HG23	0.52	1.81	12	2
1:A:9:LEU:CD1	1:A:81:ILE:HG23	0.52	2.35	5	1
1:A:87:LEU:CD1	1:A:96:PHE:CD2	0.52	2.93	14	1
1:A:96:PHE:HE1	1:A:100:LEU:HD22	0.52	1.65	2	1
1:A:39:ALA:HB1	1:A:130:ALA:O	0.51	2.05	7	1
1:A:9:LEU:HD13	1:A:81:ILE:HA	0.51	1.83	8	1
1:A:145:VAL:HB	1:A:153:LEU:HD21	0.51	1.83	18	1
1:A:62:TYR:HB2	1:A:99:VAL:HG21	0.51	1.82	5	1
1:A:37:ALA:HB2	1:A:49:VAL:HG13	0.51	1.82	17	2
1:A:127:TRP:O	1:A:130:ALA:HB3	0.50	2.06	17	1
1:A:107:ILE:HD13	1:A:127:TRP:CZ2	0.50	2.41	18	2
1:A:52:LEU:HD11	1:A:56:PHE:CE2	0.50	2.42	17	1
1:A:59:LEU:C	1:A:59:LEU:HD13	0.49	2.28	6	1
1:A:145:VAL:O	1:A:147:THR:N	0.49	2.45	6	20
1:A:36:ILE:O	1:A:39:ALA:HB3	0.49	2.08	10	1
1:A:108:VAL:HG21	1:A:155:LEU:HD21	0.49	1.84	1	1
1:A:80:PHE:CZ	1:A:84:THR:HG21	0.48	2.42	4	1
1:A:124:PHE:CE2	1:A:128:LEU:CD1	0.48	2.96	3	1
1:A:9:LEU:HD22	1:A:84:THR:HG21	0.48	1.85	15	1
1:A:49:VAL:HG13	1:A:50:GLN:N	0.48	2.24	4	5
1:A:111:CYS:O	1:A:113:LYS:N	0.48	2.46	12	1
1:A:100:LEU:HD12	1:A:103:VAL:HG21	0.48	1.85	3	1
1:A:87:LEU:CD1	1:A:96:PHE:CE2	0.48	2.97	14	1
1:A:59:LEU:HD11	1:A:100:LEU:CD2	0.48	2.39	14	1
1:A:80:PHE:CD1	1:A:84:THR:OG1	0.47	2.68	8	7
1:A:9:LEU:HD13	1:A:81:ILE:HG12	0.47	1.85	5	1
1:A:62:TYR:CE1	1:A:66:GLU:OE1	0.47	2.68	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:PHE:O	1:A:145:VAL:HG12	0.47	2.10	13	2
1:A:23:ALA:HB1	1:A:74:SER:HB3	0.47	1.87	2	1
1:A:62:TYR:CE2	1:A:66:GLU:OE2	0.47	2.68	6	1
1:A:108:VAL:HG12	1:A:112:ASP:OD2	0.47	2.10	5	2
1:A:128:LEU:HD23	1:A:133:MET:HG3	0.47	1.86	11	1
1:A:80:PHE:CE1	1:A:84:THR:OG1	0.46	2.66	11	4
1:A:59:LEU:O	1:A:59:LEU:HD13	0.46	2.10	6	2
1:A:142:PHE:CE1	1:A:153:LEU:HD12	0.46	2.45	16	1
1:A:124:PHE:O	1:A:128:LEU:HD12	0.46	2.11	13	2
1:A:101:GLY:N	1:A:102:PRO:HD2	0.45	2.27	8	6
1:A:59:LEU:HD13	1:A:59:LEU:O	0.45	2.11	9	1
1:A:43:ASP:O	1:A:49:VAL:HG21	0.45	2.11	6	2
1:A:104:VAL:HG21	1:A:159:LEU:CD2	0.45	2.41	20	1
1:A:32:GLU:OE1	1:A:56:PHE:CE2	0.45	2.69	14	1
1:A:18:PHE:CE2	1:A:32:GLU:N	0.45	2.85	16	2
1:A:108:VAL:HG12	1:A:112:ASP:CG	0.45	2.31	6	1
1:A:11:LYS:O	1:A:15:ARG:N	0.45	2.48	20	10
1:A:43:ASP:CB	1:A:46:ALA:HB2	0.45	2.42	3	2
1:A:145:VAL:CG1	1:A:153:LEU:HD11	0.45	2.42	13	2
1:A:29:PHE:CZ	1:A:63:LEU:HD11	0.45	2.47	10	1
1:A:86:ASN:O	1:A:90:GLU:N	0.44	2.50	11	6
1:A:67:ALA:CB	1:A:75:LEU:CD2	0.44	2.96	1	2
1:A:32:GLU:O	1:A:36:ILE:CG1	0.44	2.65	10	1
1:A:120:ASN:O	1:A:123:GLU:N	0.44	2.51	16	14
1:A:69:VAL:HG22	1:A:70:GLY:N	0.44	2.25	20	1
1:A:55:ALA:CB	1:A:102:PRO:O	0.44	2.65	11	2
1:A:124:PHE:CD2	1:A:153:LEU:CD1	0.44	3.01	18	1
1:A:111:CYS:O	1:A:112:ASP:C	0.44	2.56	8	2
1:A:94:ALA:O	1:A:98:ARG:CG	0.44	2.66	15	2
1:A:16:TRP:CZ2	1:A:32:GLU:OE2	0.44	2.71	4	1
1:A:112:ASP:OD1	1:A:115:ALA:N	0.43	2.51	4	1
1:A:112:ASP:O	1:A:113:LYS:HB2	0.43	2.13	12	3
1:A:21:ASN:OD1	1:A:21:ASN:N	0.43	2.49	11	2
1:A:29:PHE:CZ	1:A:63:LEU:CD1	0.43	3.02	10	1
1:A:37:ALA:CB	1:A:49:VAL:HG13	0.43	2.44	3	2
1:A:112:ASP:O	1:A:113:LYS:CB	0.43	2.66	12	3
1:A:86:ASN:N	1:A:86:ASN:OD1	0.43	2.51	13	1
1:A:96:PHE:CZ	1:A:100:LEU:CD2	0.43	3.01	10	1
1:A:40:PHE:CZ	1:A:111:CYS:SG	0.43	3.12	12	2
1:A:128:LEU:O	1:A:133:MET:CG	0.43	2.67	19	3
1:A:91:GLN:N	1:A:91:GLN:OE1	0.43	2.52	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:ALA:HB2	1:A:142:PHE:CE2	0.43	2.49	8	1
1:A:43:ASP:N	1:A:43:ASP:OD1	0.43	2.52	8	1
1:A:18:PHE:CE1	1:A:31:LYS:HB3	0.42	2.48	15	1
1:A:100:LEU:O	1:A:103:VAL:CG2	0.42	2.67	8	1
1:A:21:ASN:HD21	1:A:23:ALA:HB3	0.42	1.71	4	1
1:A:59:LEU:CD2	1:A:99:VAL:HG12	0.42	2.44	2	1
1:A:43:ASP:HB3	1:A:46:ALA:HB2	0.42	1.91	3	1
1:A:124:PHE:CG	1:A:153:LEU:CD1	0.42	3.02	18	1
1:A:13:PHE:CD1	1:A:77:GLU:HA	0.42	2.49	18	1
1:A:13:PHE:CE1	1:A:77:GLU:N	0.42	2.87	18	1
1:A:107:ILE:HG21	1:A:127:TRP:CH2	0.42	2.49	6	1
1:A:100:LEU:HD12	1:A:104:VAL:CG2	0.42	2.45	1	2
1:A:148:ASN:ND2	1:A:157:GLU:OE2	0.42	2.53	3	3
1:A:64:ALA:O	1:A:68:GLY:N	0.42	2.53	3	5
1:A:18:PHE:CE2	1:A:31:LYS:HB2	0.42	2.50	15	1
1:A:13:PHE:CD2	1:A:77:GLU:OE1	0.42	2.73	1	1
1:A:19:ASP:N	1:A:19:ASP:OD1	0.42	2.52	5	2
1:A:49:VAL:CG1	1:A:50:GLN:N	0.42	2.83	4	1
1:A:128:LEU:HD12	1:A:138:ALA:HA	0.42	1.91	6	2
1:A:33:ALA:HB3	1:A:53:LYS:HG3	0.42	1.91	15	1
1:A:60:PHE:O	1:A:63:LEU:N	0.42	2.53	9	4
1:A:40:PHE:CE2	1:A:111:CYS:SG	0.42	3.11	8	1
1:A:148:ASN:ND2	1:A:157:GLU:OE1	0.42	2.53	13	1
1:A:134:SER:CB	1:A:137:GLU:OE1	0.42	2.68	8	1
1:A:52:LEU:HD13	1:A:106:GLY:HA3	0.42	1.91	10	1
1:A:124:PHE:CD2	1:A:128:LEU:CD1	0.42	3.02	16	1
1:A:120:ASN:OD1	1:A:123:GLU:N	0.42	2.53	5	1
1:A:125:ALA:HA	1:A:138:ALA:HB1	0.41	1.90	9	2
1:A:80:PHE:O	1:A:84:THR:CG2	0.41	2.68	1	1
1:A:97:ASN:O	1:A:101:GLY:N	0.41	2.53	20	3
1:A:108:VAL:O	1:A:112:ASP:N	0.41	2.51	6	1
1:A:18:PHE:CE2	1:A:28:ASP:O	0.41	2.73	15	1
1:A:12:ARG:NH2	1:A:16:TRP:CZ2	0.41	2.88	3	1
1:A:129:THR:HG23	1:A:133:MET:O	0.41	2.14	18	1
1:A:12:ARG:O	1:A:16:TRP:CE3	0.41	2.73	9	1
1:A:36:ILE:O	1:A:39:ALA:N	0.41	2.53	9	3
1:A:119:ILE:HG21	1:A:124:PHE:CD1	0.41	2.49	5	2
1:A:62:TYR:OH	1:A:91:GLN:NE2	0.41	2.53	11	1
1:A:80:PHE:CD1	1:A:84:THR:CG2	0.41	3.03	17	2
1:A:105:LYS:HG2	1:A:155:LEU:CD2	0.41	2.46	18	1
1:A:61:ASP:OD1	1:A:61:ASP:N	0.41	2.53	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:ALA:HA	1:A:142:PHE:CE2	0.41	2.51	18	1
1:A:83:VAL:HG23	1:A:84:THR:N	0.41	2.31	5	2
1:A:92:GLY:N	1:A:95:SER:OG	0.41	2.54	17	1
1:A:26:ARG:NH2	1:A:71:SER:OG	0.41	2.54	20	1
1:A:12:ARG:CZ	1:A:16:TRP:CZ2	0.41	3.04	3	1
1:A:127:TRP:CD1	1:A:127:TRP:O	0.41	2.74	10	1
1:A:18:PHE:CZ	1:A:31:LYS:HB3	0.41	2.50	15	1
1:A:100:LEU:O	1:A:104:VAL:HG23	0.41	2.16	17	1
1:A:80:PHE:O	1:A:84:THR:CB	0.41	2.69	20	2
1:A:21:ASN:N	1:A:21:ASN:OD1	0.41	2.52	7	1
1:A:142:PHE:CD1	1:A:153:LEU:CD1	0.41	3.04	16	1
1:A:33:ALA:HB2	1:A:56:PHE:CD2	0.41	2.51	16	1
1:A:43:ASP:HB2	1:A:46:ALA:HB2	0.40	1.93	17	1
1:A:114:ASN:O	1:A:115:ALA:CB	0.40	2.68	19	1
1:A:19:ASP:OD1	1:A:19:ASP:N	0.40	2.53	2	1
1:A:46:ALA:O	1:A:50:GLN:CG	0.40	2.70	6	1
1:A:16:TRP:CH2	1:A:29:PHE:CE2	0.40	3.09	14	1
1:A:44:ALA:O	1:A:49:VAL:CG1	0.40	2.67	10	1
1:A:121:ALA:HA	1:A:142:PHE:CD2	0.40	2.51	17	1

6.3 Torsion angles ⓘ

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	156/176 (89%)	140±3 (90±2%)	12±2 (8±1%)	4±1 (2±1%)	11	48
All	All	3120/3520 (89%)	2799 (90%)	244 (8%)	77 (2%)	11	48

All 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	90	GLU	20
1	A	146	ASP	20
1	A	91	GLN	13

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Mol	Chain	Res	Type	Models (Total)
1	A	43	ASP	6
1	A	70	GLY	3
1	A	71	SER	3
1	A	17	ASP	3
1	A	42	LYS	2
1	A	112	ASP	2
1	A	46	ALA	2
1	A	115	ALA	2
1	A	41	GLY	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	117/133 (88%)	87±4 (75±4%)	30±4 (25±4%)	3	25
All	All	2340/2660 (88%)	1749 (75%)	591 (25%)	3	25

All 83 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	17	ASP	20
1	A	8	ARG	17
1	A	128	LEU	16
1	A	12	ARG	15
1	A	10	LYS	15
1	A	146	ASP	15
1	A	96	PHE	14
1	A	159	LEU	14
1	A	105	LYS	13
1	A	135	LYS	13
1	A	74	SER	13
1	A	90	GLU	13
1	A	18	PHE	11
1	A	113	LYS	11
1	A	65	LYS	11
1	A	43	ASP	11

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Mol	Chain	Res	Type	Models (Total)
1	A	56	PHE	11
1	A	95	SER	10
1	A	155	LEU	10
1	A	158	LEU	10
1	A	15	ARG	10
1	A	28	ASP	10
1	A	156	ASP	9
1	A	75	LEU	9
1	A	91	GLN	9
1	A	82	ARG	9
1	A	140	GLU	9
1	A	7	ASP	9
1	A	134	SER	9
1	A	34	GLN	9
1	A	54	ASN	9
1	A	38	GLU	8
1	A	42	LYS	8
1	A	40	PHE	8
1	A	26	ARG	7
1	A	53	LYS	7
1	A	122	ASP	7
1	A	24	LEU	7
1	A	137	GLU	7
1	A	154	SER	7
1	A	6	SER	7
1	A	110	MET	6
1	A	87	LEU	6
1	A	85	GLU	6
1	A	71	SER	6
1	A	35	HIS	6
1	A	100	LEU	6
1	A	25	GLU	6
1	A	31	LYS	6
1	A	14	ASP	6
1	A	93	GLU	5
1	A	61	ASP	5
1	A	120	ASN	5
1	A	118	GLN	5
1	A	72	ASP	5
1	A	129	THR	5
1	A	147	THR	5
1	A	32	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	50	GLN	4
1	A	78	GLU	4
1	A	59	LEU	4
1	A	79	GLN	4
1	A	143	ASN	3
1	A	69	VAL	3
1	A	11	LYS	3
1	A	48	GLU	3
1	A	114	ASN	3
1	A	66	GLU	3
1	A	98	ARG	3
1	A	86	ASN	3
1	A	16	TRP	2
1	A	144	GLN	2
1	A	124	PHE	2
1	A	97	ASN	2
1	A	30	GLU	2
1	A	112	ASP	2
1	A	111	CYS	2
1	A	131	LEU	2
1	A	152	GLU	1
1	A	148	ASN	1
1	A	9	LEU	1
1	A	4	ILE	1
1	A	77	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided