



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:57 AM UTC

PDB ID : 2AYZ / pdb_00002ayz
Title : Solution structure of the E.coli RcsC C-terminus (residues 817-949) containing phosphoreceiver domain
Authors : Rogov, V.V.; Rogova, N.Y.; Bernhard, F.; Koglin, A.; Lohr, F.; Dotsch, V.
Deposited on : 2005-09-09

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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

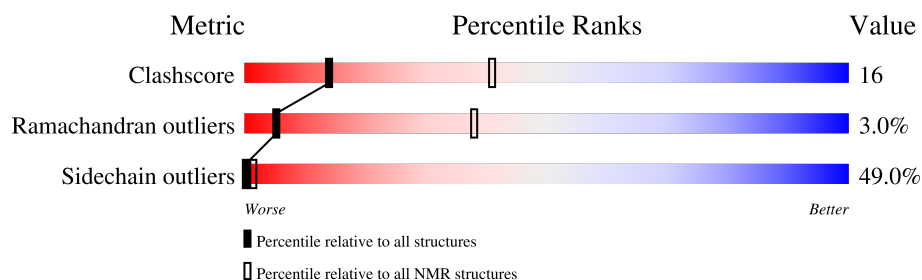
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	133	26% 53% 8% 13%

2 Ensemble composition and analysis

This entry contains 25 models. Model 24 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy and fewest violation*.

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:825-A:876, A:884-A:947 (116)	0.83	24

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 4 clusters and 10 single-model clusters were found.

Cluster number	Models
1	2, 9, 10, 18, 19, 25
2	6, 15, 20, 23, 24
3	13, 17
4	12, 16
Single-model clusters	1; 3; 4; 5; 7; 8; 11; 14; 21; 22

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2081 atoms, of which 1055 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sensor kinase protein rcsC.

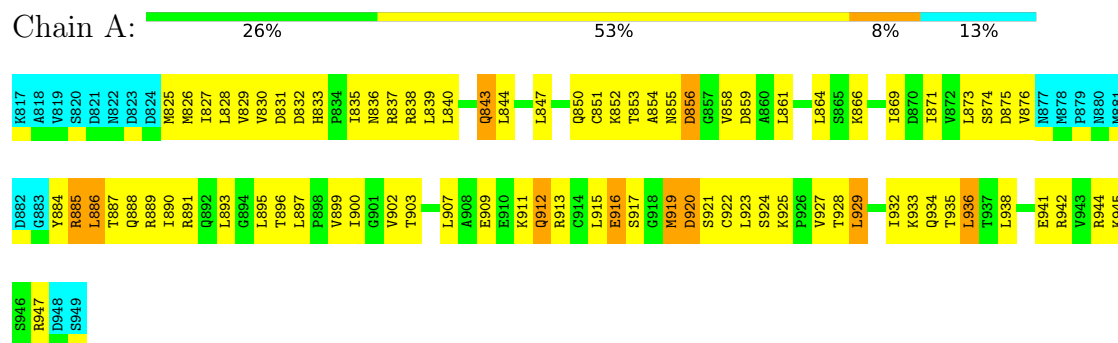
Mol	Chain	Residues	Atoms						Trace
1	A	133	Total	C	H	N	O	S	0
			2081	630	1055	185	203	8	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Sensor kinase protein rcsC

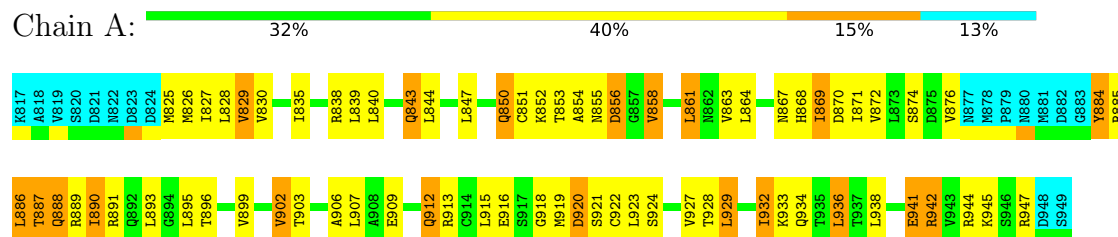


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

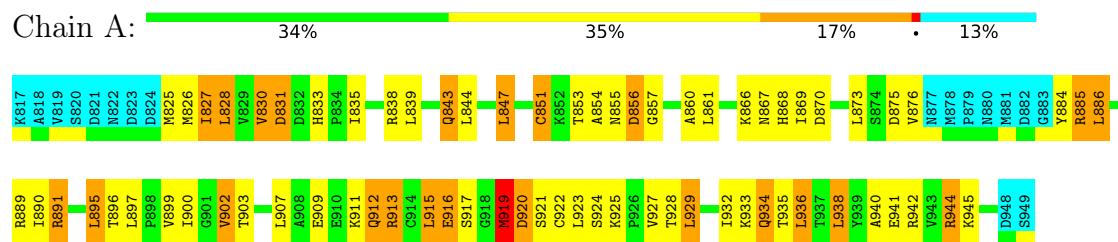
4.2.1 Score per residue for model 1

- Molecule 1: Sensor kinase protein rcsC



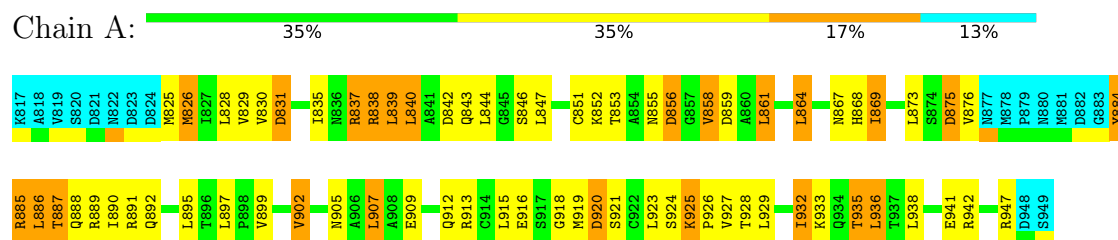
4.2.2 Score per residue for model 2

- Molecule 1: Sensor kinase protein rcsC



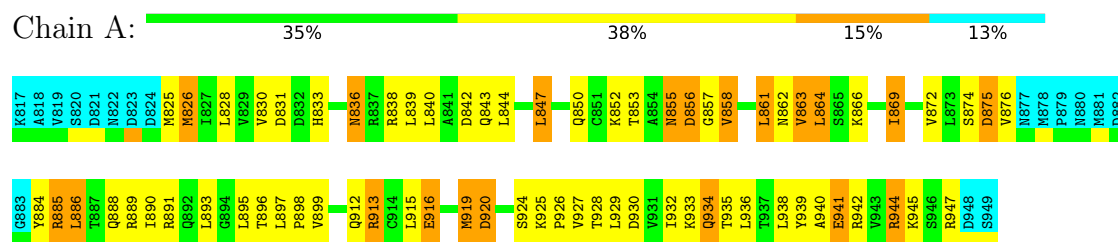
4.2.3 Score per residue for model 3

- Molecule 1: Sensor kinase protein rcsC



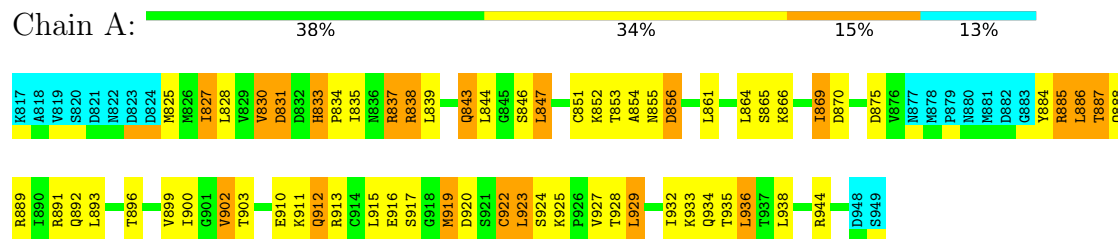
4.2.4 Score per residue for model 4

- Molecule 1: Sensor kinase protein rcsC



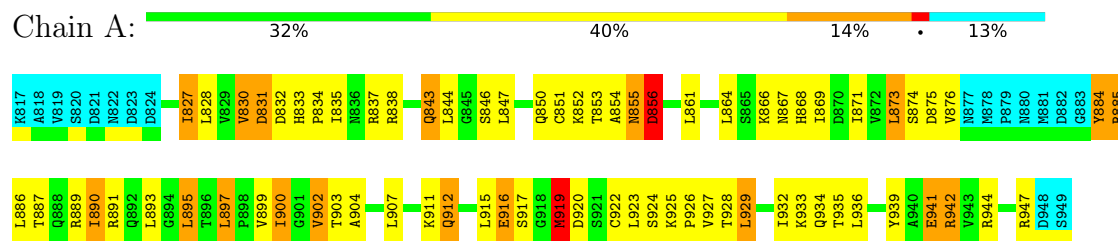
4.2.5 Score per residue for model 5

- Molecule 1: Sensor kinase protein rcsC



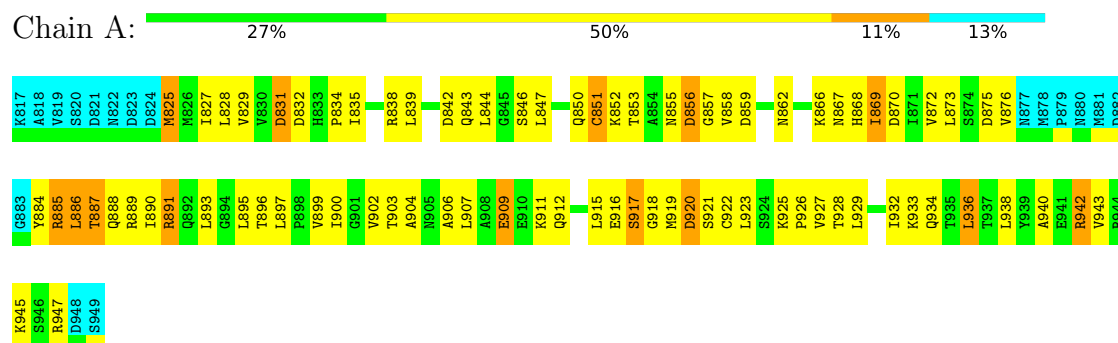
4.2.6 Score per residue for model 6

- Molecule 1: Sensor kinase protein rcsC



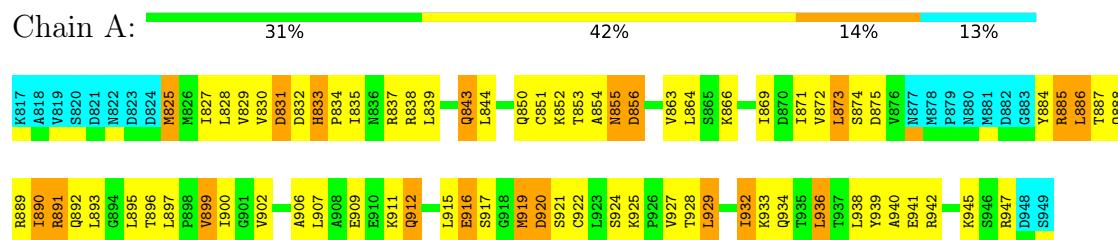
4.2.7 Score per residue for model 7

- Molecule 1: Sensor kinase protein rcsC



4.2.8 Score per residue for model 8

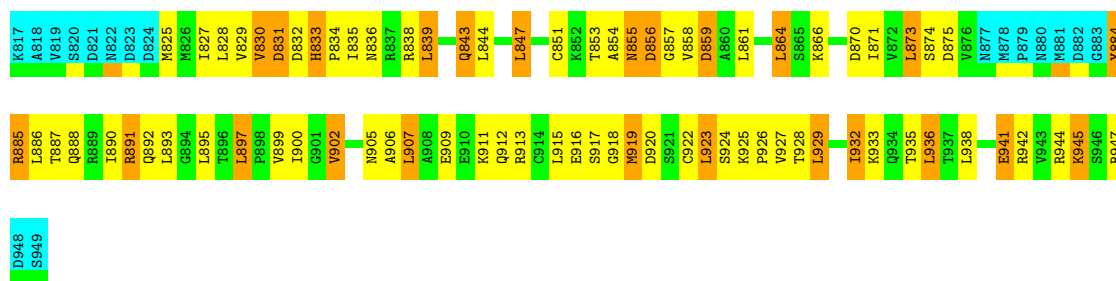
- Molecule 1: Sensor kinase protein rcsC



4.2.9 Score per residue for model 9

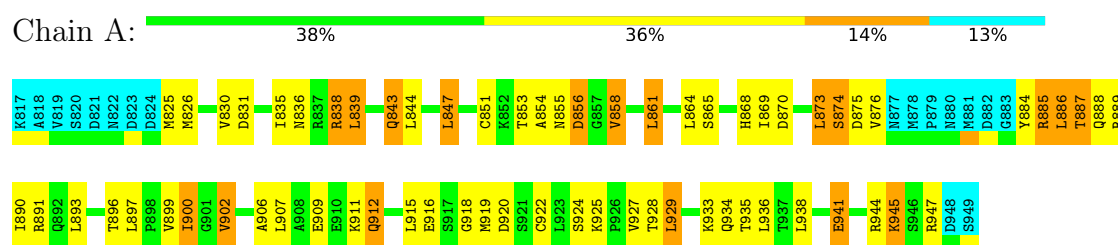
- Molecule 1: Sensor kinase protein rcsC





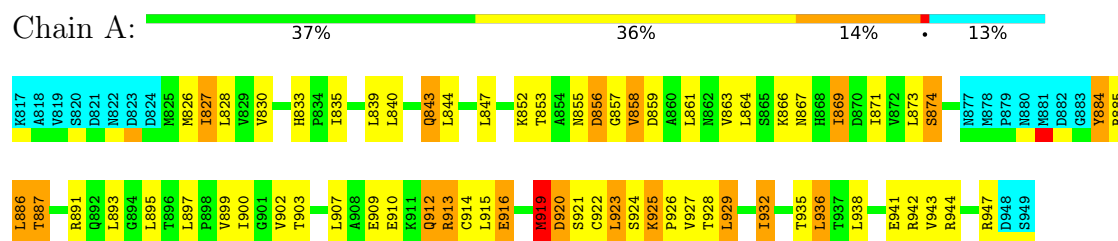
4.2.10 Score per residue for model 10

- Molecule 1: Sensor kinase protein rcsC



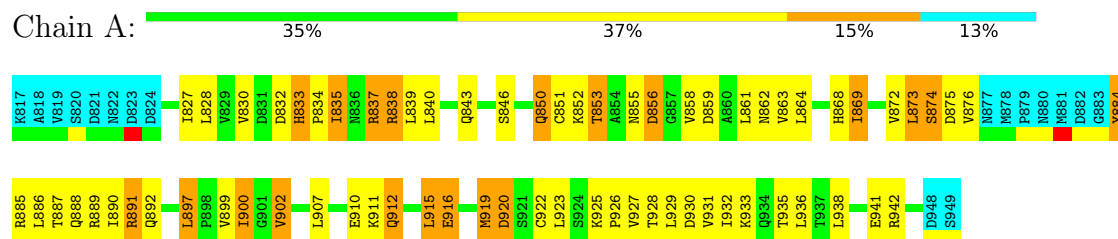
4.2.11 Score per residue for model 11

- Molecule 1: Sensor kinase protein rcsC



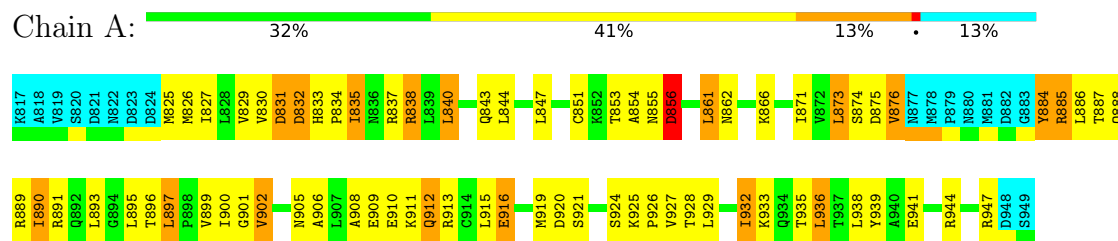
4.2.12 Score per residue for model 12

- Molecule 1: Sensor kinase protein rcsC



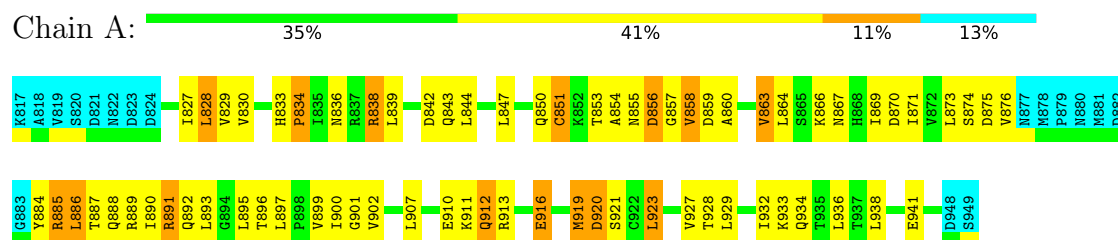
4.2.13 Score per residue for model 13

- Molecule 1: Sensor kinase protein rcsC



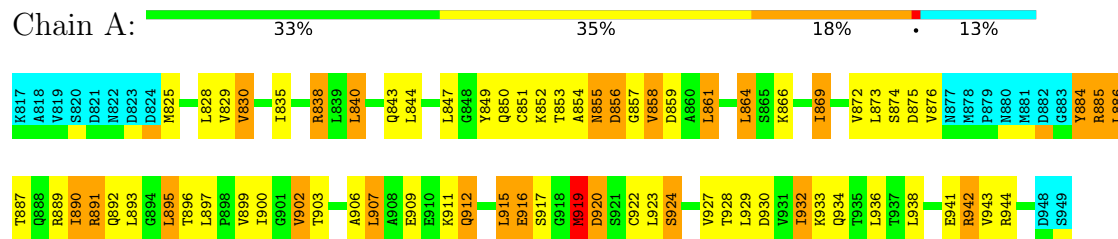
4.2.14 Score per residue for model 14

- Molecule 1: Sensor kinase protein rcsC



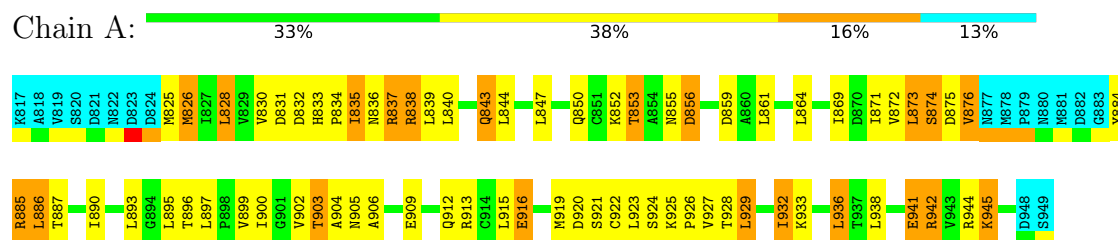
4.2.15 Score per residue for model 15

- Molecule 1: Sensor kinase protein rcsC



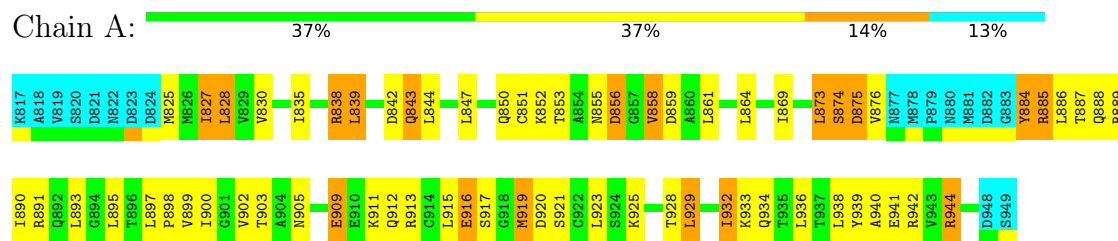
4.2.16 Score per residue for model 16

- Molecule 1: Sensor kinase protein rcsC



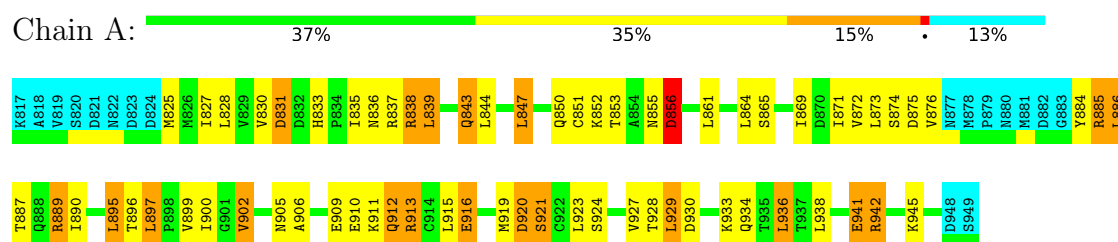
4.2.17 Score per residue for model 17

- Molecule 1: Sensor kinase protein rcsC



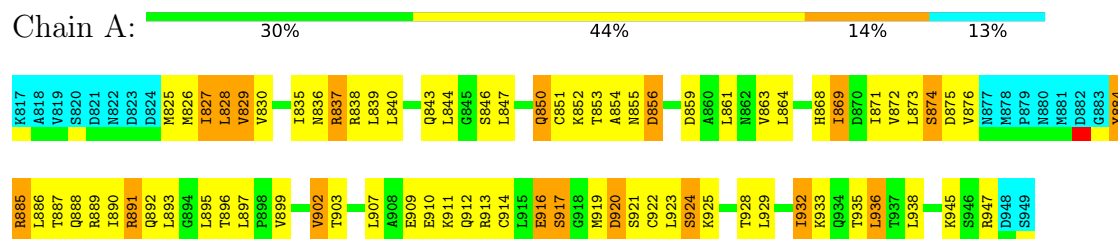
4.2.18 Score per residue for model 18

- Molecule 1: Sensor kinase protein rcsC



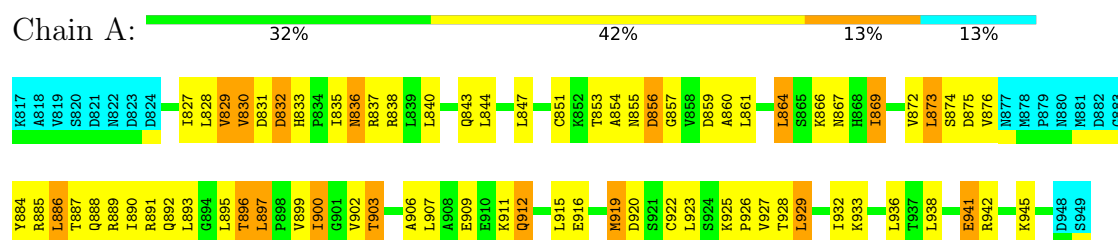
4.2.19 Score per residue for model 19

- Molecule 1: Sensor kinase protein rcsC



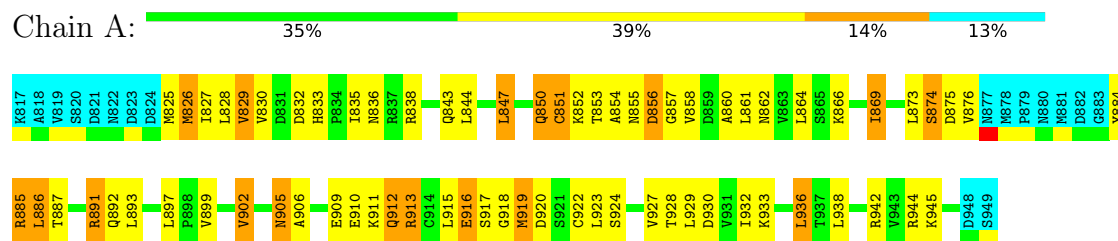
4.2.20 Score per residue for model 20

- Molecule 1: Sensor kinase protein rcsC



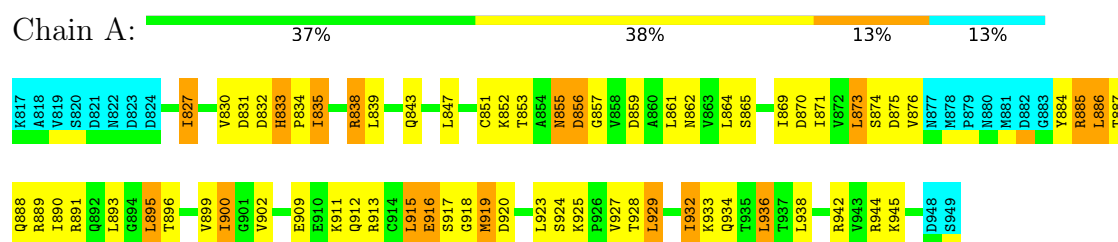
4.2.21 Score per residue for model 21

- Molecule 1: Sensor kinase protein rcsC



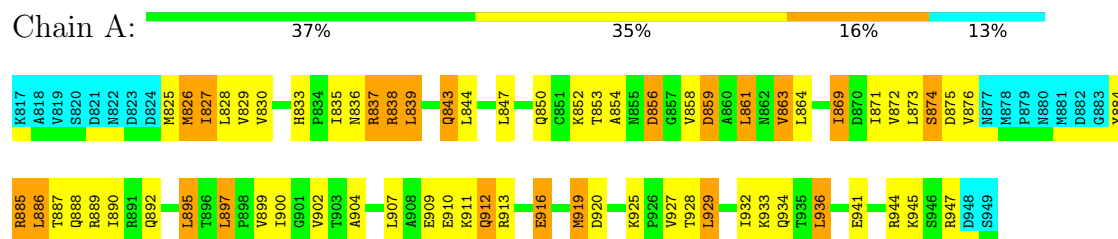
4.2.22 Score per residue for model 22

- Molecule 1: Sensor kinase protein rcsC



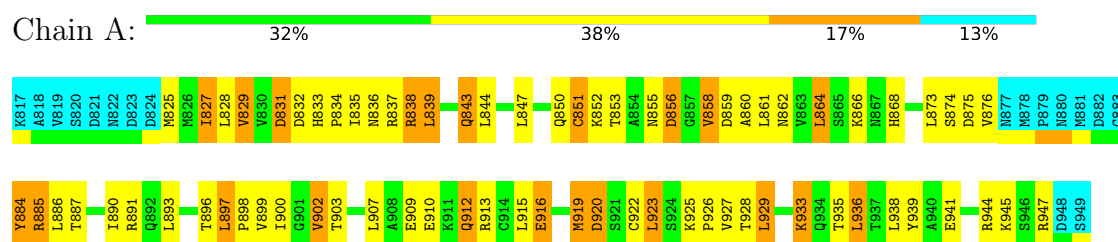
4.2.23 Score per residue for model 23

- Molecule 1: Sensor kinase protein rcsC



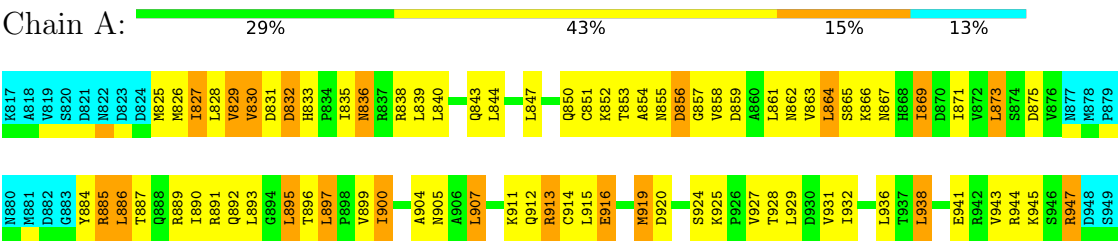
4.2.24 Score per residue for model 24 (medoid)

- Molecule 1: Sensor kinase protein rcsC



4.2.25 Score per residue for model 25

● Molecule 1: Sensor kinase protein rcsC



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Energy minimization*.

Of the 50 calculated structures, 25 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
DYANA	structure solution	1.5
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 (average) 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	0.42±0.02	0±0/909 (0.0± 0.0%)	0.73±0.02	0±1/1230 (0.0± 0.1%)
All	All	0.42	0/22725 (0.0%)	0.73	12/30750 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	833	HIS	CA-C-N	6.18	127.56	119.84	22	6
1	A	833	HIS	C-N-CA	6.18	127.56	119.84	22	6

There are no chirality outliers.

There are no planarity outliers.

6.2 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 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	901	950	948	29±4
All	All	22525	23750	23700	727

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:884:TYR:HB3	1:A:912:GLN:HB3	1.03	1.26	4	13
1:A:887:THR:HB	1:A:916:GLU:HG3	1.01	1.32	6	4
1:A:902:VAL:HG23	1:A:923:LEU:HB2	0.96	1.32	14	2
1:A:837:ARG:HA	1:A:837:ARG:HE	0.91	1.20	3	1
1:A:884:TYR:HB2	1:A:912:GLN:HB3	0.91	1.41	6	4
1:A:887:THR:HB	1:A:916:GLU:HB2	0.88	1.44	11	9
1:A:829:VAL:HB	1:A:840:LEU:HD13	0.85	1.47	13	1
1:A:864:LEU:HG	1:A:897:LEU:HD21	0.84	1.49	25	1
1:A:857:GLY:HA3	1:A:886:LEU:HG	0.81	1.53	14	3
1:A:827:ILE:HB	1:A:844:LEU:HD21	0.80	1.53	14	13
1:A:900:ILE:HG23	1:A:921:SER:HB2	0.80	1.54	18	1
1:A:856:ASP:HB3	1:A:859:ASP:HB2	0.77	1.55	23	14
1:A:899:VAL:HB	1:A:919:MET:HA	0.77	1.57	20	24
1:A:837:ARG:HG2	1:A:853:THR:HG22	0.77	1.56	12	1
1:A:828:LEU:HB2	1:A:869:ILE:HG21	0.75	1.57	15	9
1:A:906:ALA:HB3	1:A:909:GLU:HG3	0.75	1.56	9	7
1:A:837:ARG:HA	1:A:837:ARG:NE	0.75	1.96	3	1
1:A:830:VAL:HG12	1:A:854:ALA:HB3	0.74	1.59	23	1
1:A:861:LEU:HD11	1:A:890:ILE:HA	0.74	1.57	6	2
1:A:884:TYR:HB2	1:A:912:GLN:HG3	0.73	1.58	1	1
1:A:847:LEU:HD13	1:A:936:LEU:HG	0.73	1.60	18	6
1:A:857:GLY:HA3	1:A:886:LEU:HB2	0.73	1.58	20	3
1:A:884:TYR:HB3	1:A:912:GLN:HG2	0.72	1.59	13	5
1:A:887:THR:HG22	1:A:916:GLU:HB2	0.72	1.59	7	3
1:A:843:GLN:HG3	1:A:929:LEU:HD23	0.72	1.61	22	12
1:A:906:ALA:HB3	1:A:909:GLU:HB3	0.72	1.62	10	2
1:A:857:GLY:HA3	1:A:886:LEU:HD22	0.72	1.62	9	1
1:A:830:VAL:HB	1:A:874:SER:HA	0.71	1.63	12	9
1:A:888:GLN:N	1:A:916:GLU:HB3	0.71	2.01	17	6
1:A:884:TYR:CB	1:A:912:GLN:HB3	0.71	2.16	8	15
1:A:887:THR:HB	1:A:916:GLU:CB	0.71	2.16	17	5
1:A:826:MET:HA	1:A:850:GLN:HB3	0.70	1.63	4	3
1:A:873:LEU:HD23	1:A:900:ILE:HD12	0.69	1.63	12	5
1:A:826:MET:HG2	1:A:869:ILE:HG13	0.69	1.62	23	2
1:A:872:VAL:HG23	1:A:897:LEU:HD11	0.69	1.62	16	5
1:A:885:ARG:O	1:A:885:ARG:HD2	0.68	1.88	5	19
1:A:888:GLN:HB2	1:A:916:GLU:HB2	0.67	1.65	13	3
1:A:837:ARG:HD3	1:A:853:THR:HB	0.67	1.65	8	1
1:A:830:VAL:HG13	1:A:854:ALA:HB3	0.66	1.67	9	7
1:A:884:TYR:O	1:A:916:GLU:HG2	0.65	1.91	16	11
1:A:830:VAL:HG22	1:A:874:SER:HA	0.65	1.68	23	1
1:A:831:ASP:HB2	1:A:875:ASP:HB3	0.65	1.66	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:913:ARG:HA	1:A:916:GLU:OE2	0.65	1.91	22	6
1:A:884:TYR:HB3	1:A:912:GLN:CB	0.65	2.15	4	5
1:A:830:VAL:HG22	1:A:854:ALA:HB3	0.65	1.69	10	7
1:A:829:VAL:HB	1:A:840:LEU:CD1	0.65	2.22	13	1
1:A:884:TYR:C	1:A:916:GLU:HG3	0.64	2.17	9	5
1:A:895:LEU:HD22	1:A:918:GLY:HA2	0.64	1.70	22	1
1:A:887:THR:HB	1:A:916:GLU:CG	0.64	2.18	6	6
1:A:912:GLN:O	1:A:916:GLU:HG3	0.64	1.93	17	9
1:A:830:VAL:CG2	1:A:874:SER:HA	0.63	2.23	23	1
1:A:919:MET:O	1:A:920:ASP:HB2	0.63	1.92	8	12
1:A:904:ALA:HB2	1:A:925:LYS:HB2	0.63	1.70	23	4
1:A:890:ILE:HG21	1:A:899:VAL:HG21	0.63	1.70	1	1
1:A:830:VAL:O	1:A:875:ASP:HB2	0.62	1.95	17	2
1:A:903:THR:HB	1:A:909:GLU:HG2	0.62	1.68	1	2
1:A:890:ILE:HG23	1:A:895:LEU:HB2	0.62	1.71	23	1
1:A:826:MET:HB2	1:A:869:ILE:HA	0.61	1.73	21	1
1:A:886:LEU:HD13	1:A:887:THR:N	0.61	2.10	5	4
1:A:932:ILE:HG23	1:A:936:LEU:HD23	0.61	1.71	8	3
1:A:828:LEU:HG	1:A:830:VAL:HG22	0.61	1.72	15	2
1:A:875:ASP:HA	1:A:902:VAL:HB	0.60	1.71	13	8
1:A:864:LEU:HD11	1:A:872:VAL:HG21	0.60	1.72	15	3
1:A:855:ASN:O	1:A:856:ASP:HB2	0.60	1.96	2	20
1:A:832:ASP:HA	1:A:855:ASN:HB2	0.60	1.73	20	1
1:A:884:TYR:HB3	1:A:912:GLN:HG3	0.60	1.72	24	1
1:A:861:LEU:HD11	1:A:890:ILE:HG12	0.60	1.72	12	1
1:A:884:TYR:HB3	1:A:912:GLN:CG	0.59	2.28	9	4
1:A:864:LEU:HD11	1:A:897:LEU:HD21	0.59	1.75	24	1
1:A:887:THR:HA	1:A:890:ILE:HD12	0.59	1.75	23	8
1:A:875:ASP:HA	1:A:902:VAL:O	0.58	1.98	14	6
1:A:864:LEU:HG	1:A:897:LEU:CD2	0.58	2.27	25	1
1:A:861:LEU:HD11	1:A:893:LEU:HD23	0.58	1.76	9	1
1:A:855:ASN:O	1:A:856:ASP:HB3	0.58	1.98	18	1
1:A:913:ARG:HD3	1:A:922:CYS:SG	0.58	2.38	5	4
1:A:875:ASP:HA	1:A:902:VAL:HG12	0.57	1.75	9	1
1:A:884:TYR:HB2	1:A:912:GLN:CG	0.57	2.30	1	1
1:A:896:THR:H	1:A:897:LEU:HD22	0.57	1.60	20	1
1:A:887:THR:CB	1:A:916:GLU:HG3	0.57	2.21	6	1
1:A:913:ARG:HA	1:A:916:GLU:OE1	0.56	2.01	24	2
1:A:888:GLN:HB2	1:A:916:GLU:HB3	0.56	1.78	10	6
1:A:913:ARG:NH2	1:A:919:MET:H	0.56	1.97	25	2
1:A:831:ASP:OD2	1:A:836:ASN:HB2	0.56	2.00	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:856:ASP:OD2	1:A:858:VAL:HG22	0.56	2.01	3	2
1:A:843:GLN:HB3	1:A:932:ILE:HG21	0.56	1.77	15	3
1:A:884:TYR:HD1	1:A:885:ARG:N	0.56	1.98	24	1
1:A:902:VAL:HG13	1:A:923:LEU:HB2	0.55	1.77	1	2
1:A:829:VAL:HG23	1:A:840:LEU:HD23	0.55	1.77	25	4
1:A:887:THR:HG23	1:A:918:GLY:N	0.55	2.17	1	3
1:A:884:TYR:CE2	1:A:915:LEU:HB3	0.55	2.37	22	1
1:A:885:ARG:HA	1:A:916:GLU:HG3	0.55	1.78	5	1
1:A:913:ARG:HG3	1:A:919:MET:HB2	0.55	1.79	3	1
1:A:844:LEU:HD12	1:A:847:LEU:HD23	0.55	1.79	21	1
1:A:833:HIS:O	1:A:837:ARG:HB2	0.55	2.02	23	1
1:A:844:LEU:HA	1:A:847:LEU:HD12	0.54	1.79	24	2
1:A:887:THR:O	1:A:918:GLY:HA3	0.54	2.01	1	4
1:A:885:ARG:HD3	1:A:888:GLN:HB3	0.54	1.78	19	1
1:A:884:TYR:O	1:A:916:GLU:HG3	0.54	2.03	9	4
1:A:831:ASP:OD2	1:A:836:ASN:HB3	0.54	2.03	4	2
1:A:913:ARG:NH2	1:A:917:SER:HA	0.54	2.18	21	1
1:A:831:ASP:HB3	1:A:837:ARG:HG3	0.54	1.78	13	1
1:A:942:ARG:HA	1:A:945:LYS:HE2	0.54	1.78	9	1
1:A:857:GLY:HA3	1:A:886:LEU:HB3	0.54	1.80	2	1
1:A:884:TYR:CD1	1:A:885:ARG:N	0.54	2.76	24	1
1:A:832:ASP:CB	1:A:876:VAL:HA	0.54	2.33	16	1
1:A:829:VAL:HB	1:A:840:LEU:HD21	0.53	1.81	15	1
1:A:887:THR:HG23	1:A:918:GLY:H	0.53	1.62	1	3
1:A:932:ILE:O	1:A:936:LEU:HB2	0.53	2.03	23	9
1:A:925:LYS:HB3	1:A:926:PRO:HD3	0.53	1.77	12	4
1:A:898:PRO:HB2	1:A:939:TYR:HE2	0.53	1.62	24	1
1:A:858:VAL:HA	1:A:861:LEU:HD13	0.53	1.79	11	2
1:A:875:ASP:HA	1:A:902:VAL:HG22	0.53	1.81	12	1
1:A:885:ARG:O	1:A:888:GLN:HB3	0.52	2.04	22	6
1:A:884:TYR:CB	1:A:912:GLN:HG2	0.52	2.34	19	3
1:A:827:ILE:HG23	1:A:871:ILE:HB	0.52	1.80	1	7
1:A:895:LEU:HD11	1:A:897:LEU:HD22	0.52	1.81	18	1
1:A:884:TYR:HD1	1:A:916:GLU:HB3	0.52	1.63	6	1
1:A:831:ASP:HA	1:A:875:ASP:HB3	0.52	1.82	2	3
1:A:887:THR:HG21	1:A:919:MET:HG2	0.52	1.81	16	1
1:A:887:THR:HG22	1:A:916:GLU:CB	0.51	2.34	1	1
1:A:832:ASP:HA	1:A:855:ASN:OD1	0.51	2.05	25	2
1:A:886:LEU:HD13	1:A:887:THR:H	0.51	1.65	10	2
1:A:901:GLY:HA3	1:A:919:MET:SD	0.51	2.45	13	2
1:A:884:TYR:O	1:A:887:THR:HB	0.51	2.05	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:828:LEU:HD21	1:A:863:VAL:HG11	0.51	1.82	14	1
1:A:887:THR:HA	1:A:890:ILE:HG13	0.51	1.82	17	1
1:A:870:ASP:HA	1:A:947:ARG:HH21	0.51	1.65	1	1
1:A:900:ILE:HG22	1:A:923:LEU:HD11	0.51	1.83	11	1
1:A:891:ARG:HB3	1:A:918:GLY:HA3	0.51	1.81	21	1
1:A:898:PRO:HB2	1:A:939:TYR:CE2	0.50	2.42	24	3
1:A:857:GLY:HA3	1:A:886:LEU:CB	0.50	2.36	21	3
1:A:884:TYR:CG	1:A:885:ARG:N	0.50	2.79	20	10
1:A:857:GLY:HA3	1:A:886:LEU:HD13	0.50	1.82	4	2
1:A:884:TYR:CD1	1:A:912:GLN:HG2	0.50	2.40	18	3
1:A:860:ALA:O	1:A:864:LEU:HG	0.50	2.07	14	1
1:A:828:LEU:HD22	1:A:869:ILE:HD13	0.50	1.83	7	1
1:A:837:ARG:HA	1:A:840:LEU:HD21	0.50	1.83	13	1
1:A:923:LEU:HD11	1:A:935:THR:HG21	0.50	1.84	3	1
1:A:833:HIS:HB2	1:A:834:PRO:CD	0.50	2.37	12	1
1:A:885:ARG:HD2	1:A:885:ARG:C	0.50	2.31	5	3
1:A:831:ASP:HA	1:A:875:ASP:O	0.50	2.06	18	7
1:A:884:TYR:CD2	1:A:915:LEU:HB3	0.50	2.42	15	2
1:A:844:LEU:HD23	1:A:851:CYS:HA	0.50	1.84	14	3
1:A:884:TYR:CD1	1:A:916:GLU:HB3	0.50	2.42	6	1
1:A:891:ARG:HE	1:A:917:SER:HB2	0.50	1.67	7	2
1:A:943:VAL:O	1:A:947:ARG:HB2	0.49	2.07	25	1
1:A:863:VAL:HA	1:A:866:LYS:HE2	0.49	1.84	8	1
1:A:843:GLN:HG2	1:A:929:LEU:HD23	0.49	1.83	11	1
1:A:885:ARG:C	1:A:885:ARG:HD2	0.49	2.31	11	2
1:A:903:THR:O	1:A:924:SER:HA	0.49	2.07	2	2
1:A:860:ALA:O	1:A:864:LEU:HB2	0.49	2.07	24	2
1:A:925:LYS:N	1:A:926:PRO:HD2	0.49	2.23	7	7
1:A:828:LEU:HD12	1:A:872:VAL:HG22	0.49	1.83	16	1
1:A:830:VAL:HG11	1:A:860:ALA:HB2	0.49	1.84	2	1
1:A:829:VAL:HB	1:A:837:ARG:HD3	0.49	1.85	3	1
1:A:828:LEU:O	1:A:873:LEU:HG	0.49	2.07	17	1
1:A:838:ARG:HD3	1:A:839:LEU:N	0.49	2.23	3	7
1:A:895:LEU:HD13	1:A:897:LEU:HG	0.49	1.84	6	1
1:A:835:ILE:O	1:A:838:ARG:HG3	0.49	2.08	13	4
1:A:912:GLN:HA	1:A:915:LEU:HB2	0.48	1.85	2	1
1:A:829:VAL:HG12	1:A:873:LEU:HD11	0.48	1.84	13	1
1:A:830:VAL:HG21	1:A:860:ALA:HB2	0.48	1.85	21	1
1:A:864:LEU:HD21	1:A:897:LEU:HD21	0.48	1.85	9	1
1:A:887:THR:CG2	1:A:919:MET:HG2	0.48	2.38	16	1
1:A:890:ILE:HG23	1:A:895:LEU:HG	0.48	1.84	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:887:THR:HB	1:A:916:GLU:CD	0.48	2.34	19	2
1:A:942:ARG:HG3	1:A:943:VAL:N	0.48	2.23	15	2
1:A:941:GLU:O	1:A:945:LYS:HG2	0.48	2.09	16	4
1:A:828:LEU:HD13	1:A:863:VAL:HG11	0.48	1.84	4	2
1:A:888:GLN:O	1:A:891:ARG:HG3	0.47	2.09	12	2
1:A:861:LEU:HD21	1:A:890:ILE:HG13	0.47	1.85	3	1
1:A:833:HIS:HB3	1:A:834:PRO:CD	0.47	2.39	14	1
1:A:940:ALA:O	1:A:944:ARG:HB2	0.47	2.09	4	3
1:A:829:VAL:HG13	1:A:844:LEU:HD22	0.47	1.84	21	2
1:A:838:ARG:C	1:A:838:ARG:HD3	0.47	2.33	1	2
1:A:867:ASN:HD22	1:A:869:ILE:HD12	0.47	1.68	25	1
1:A:858:VAL:O	1:A:861:LEU:HG	0.47	2.09	4	4
1:A:825:MET:SD	1:A:940:ALA:HB1	0.47	2.48	8	1
1:A:941:GLU:HG3	1:A:942:ARG:N	0.47	2.24	20	7
1:A:861:LEU:HD13	1:A:890:ILE:HA	0.47	1.87	9	1
1:A:829:VAL:CB	1:A:840:LEU:HD13	0.47	2.31	13	1
1:A:847:LEU:HD21	1:A:936:LEU:HG	0.47	1.86	21	1
1:A:904:ALA:HB2	1:A:925:LYS:HD3	0.47	1.87	25	1
1:A:902:VAL:CG2	1:A:923:LEU:HB2	0.47	2.25	9	1
1:A:838:ARG:O	1:A:842:ASP:HB2	0.47	2.10	14	1
1:A:857:GLY:O	1:A:886:LEU:HD13	0.46	2.10	7	1
1:A:837:ARG:CZ	1:A:840:LEU:HD22	0.46	2.40	3	1
1:A:939:TYR:HA	1:A:942:ARG:HD2	0.46	1.87	6	1
1:A:887:THR:HA	1:A:890:ILE:HB	0.46	1.87	8	1
1:A:837:ARG:HD2	1:A:854:ALA:O	0.46	2.10	6	3
1:A:930:ASP:O	1:A:934:GLN:HG3	0.46	2.11	4	1
1:A:943:VAL:O	1:A:947:ARG:HG3	0.46	2.11	11	1
1:A:828:LEU:HD23	1:A:872:VAL:HG13	0.46	1.88	1	2
1:A:843:GLN:HB3	1:A:932:ILE:HD13	0.46	1.87	17	1
1:A:828:LEU:HD11	1:A:863:VAL:CG1	0.46	2.41	19	1
1:A:888:GLN:NE2	1:A:916:GLU:HA	0.46	2.25	7	1
1:A:858:VAL:HG22	1:A:886:LEU:HB3	0.45	1.88	14	1
1:A:873:LEU:HD23	1:A:900:ILE:HB	0.45	1.88	2	1
1:A:888:GLN:O	1:A:892:GLN:HG3	0.45	2.10	3	1
1:A:885:ARG:HD3	1:A:888:GLN:OE1	0.45	2.11	10	1
1:A:856:ASP:OD2	1:A:858:VAL:HG23	0.45	2.10	24	1
1:A:831:ASP:HB3	1:A:837:ARG:CD	0.45	2.41	3	1
1:A:888:GLN:H	1:A:916:GLU:HB3	0.45	1.71	17	1
1:A:884:TYR:CA	1:A:916:GLU:HG2	0.45	2.41	11	1
1:A:861:LEU:HB3	1:A:890:ILE:HG13	0.45	1.89	1	2
1:A:884:TYR:HD1	1:A:885:ARG:H	0.45	1.54	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:886:LEU:C	1:A:886:LEU:HD22	0.45	2.37	5	1
1:A:875:ASP:CG	1:A:925:LYS:HZ2	0.44	2.20	25	1
1:A:856:ASP:HB3	1:A:859:ASP:CB	0.44	2.41	24	2
1:A:826:MET:HA	1:A:850:GLN:CB	0.44	2.43	21	1
1:A:831:ASP:HB3	1:A:837:ARG:HD2	0.44	1.88	3	1
1:A:847:LEU:HG	1:A:936:LEU:HD23	0.44	1.89	10	1
1:A:826:MET:HB2	1:A:869:ILE:HG13	0.44	1.88	3	1
1:A:912:GLN:O	1:A:916:GLU:HG2	0.44	2.12	7	1
1:A:886:LEU:HG	1:A:887:THR:N	0.44	2.28	15	1
1:A:836:ASN:CG	1:A:925:LYS:HE3	0.44	2.37	10	1
1:A:902:VAL:HG22	1:A:923:LEU:HB2	0.44	1.89	17	1
1:A:895:LEU:O	1:A:895:LEU:HG	0.44	2.11	22	1
1:A:906:ALA:O	1:A:909:GLU:HG3	0.44	2.12	20	1
1:A:875:ASP:OD1	1:A:902:VAL:HB	0.43	2.13	5	1
1:A:913:ARG:HA	1:A:916:GLU:CD	0.43	2.38	23	2
1:A:902:VAL:HG23	1:A:925:LYS:HA	0.43	1.90	12	1
1:A:861:LEU:CD2	1:A:889:ARG:HG3	0.43	2.43	19	1
1:A:891:ARG:HA	1:A:895:LEU:HD23	0.43	1.90	2	2
1:A:873:LEU:HA	1:A:900:ILE:O	0.43	2.12	8	3
1:A:844:LEU:HD23	1:A:851:CYS:HB3	0.43	1.90	7	2
1:A:884:TYR:CG	1:A:912:GLN:HB3	0.43	2.48	5	2
1:A:856:ASP:HB3	1:A:859:ASP:H	0.43	1.73	20	1
1:A:861:LEU:HD22	1:A:890:ILE:HG13	0.43	1.90	23	1
1:A:890:ILE:CG2	1:A:895:LEU:HB3	0.43	2.44	7	1
1:A:902:VAL:CG2	1:A:925:LYS:HA	0.43	2.43	12	1
1:A:884:TYR:CD1	1:A:912:GLN:HG3	0.43	2.48	14	1
1:A:837:ARG:NH1	1:A:875:ASP:HB2	0.43	2.29	3	1
1:A:891:ARG:HA	1:A:895:LEU:HD22	0.43	1.91	9	2
1:A:830:VAL:HA	1:A:854:ALA:O	0.42	2.14	6	1
1:A:887:THR:HG22	1:A:918:GLY:H	0.42	1.73	9	1
1:A:933:LYS:HB3	1:A:933:LYS:HE2	0.42	1.47	24	1
1:A:861:LEU:CD2	1:A:890:ILE:HG12	0.42	2.44	17	1
1:A:843:GLN:HG2	1:A:929:LEU:HA	0.42	1.89	16	2
1:A:886:LEU:HD13	1:A:886:LEU:H	0.42	1.75	14	1
1:A:832:ASP:HB2	1:A:876:VAL:HA	0.42	1.91	16	1
1:A:884:TYR:C	1:A:916:GLU:HG2	0.42	2.39	16	1
1:A:828:LEU:CB	1:A:869:ILE:HG21	0.42	2.45	20	1
1:A:887:THR:HG22	1:A:918:GLY:CA	0.42	2.45	3	1
1:A:826:MET:HA	1:A:850:GLN:HB2	0.42	1.91	19	1
1:A:909:GLU:HA	1:A:912:GLN:OE1	0.42	2.14	19	1
1:A:833:HIS:HB3	1:A:834:PRO:HD2	0.42	1.91	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:826:MET:HG3	1:A:869:ILE:HA	0.41	1.91	3	1
1:A:902:VAL:HG22	1:A:923:LEU:HD12	0.41	1.91	5	3
1:A:857:GLY:CA	1:A:886:LEU:HD22	0.41	2.45	7	1
1:A:903:THR:HG21	1:A:909:GLU:HB2	0.41	1.91	17	1
1:A:919:MET:O	1:A:920:ASP:CB	0.41	2.68	18	1
1:A:884:TYR:CD1	1:A:884:TYR:N	0.41	2.88	24	1
1:A:838:ARG:HD2	1:A:839:LEU:HG	0.41	1.92	5	1
1:A:888:GLN:HB2	1:A:916:GLU:OE1	0.41	2.16	7	1
1:A:856:ASP:CB	1:A:859:ASP:HB2	0.41	2.44	16	1
1:A:886:LEU:H	1:A:886:LEU:HG	0.41	1.40	18	1
1:A:895:LEU:HD21	1:A:897:LEU:HD23	0.41	1.93	18	1
1:A:870:ASP:HA	1:A:947:ARG:NH2	0.41	2.29	1	1
1:A:890:ILE:HG22	1:A:895:LEU:HB3	0.41	1.93	25	1
1:A:825:MET:HE2	1:A:940:ALA:HA	0.41	1.93	7	1
1:A:932:ILE:HG12	1:A:936:LEU:HD23	0.41	1.93	7	1
1:A:832:ASP:HB3	1:A:876:VAL:HA	0.41	1.92	16	1
1:A:864:LEU:HG	1:A:895:LEU:HD21	0.41	1.93	3	1
1:A:919:MET:HB3	1:A:920:ASP:H	0.41	1.44	3	1
1:A:855:ASN:O	1:A:856:ASP:CB	0.41	2.69	6	1
1:A:871:ILE:HD11	1:A:940:ALA:HA	0.41	1.91	8	1
1:A:827:ILE:HG13	1:A:844:LEU:HD11	0.41	1.93	11	1
1:A:861:LEU:HD11	1:A:890:ILE:CG1	0.41	2.44	12	1
1:A:834:PRO:HA	1:A:837:ARG:HB2	0.41	1.93	13	1
1:A:858:VAL:O	1:A:861:LEU:HB2	0.41	2.16	17	1
1:A:861:LEU:HD21	1:A:890:ILE:HA	0.41	1.93	17	1
1:A:844:LEU:HD23	1:A:851:CYS:SG	0.41	2.56	21	1
1:A:856:ASP:OD1	1:A:858:VAL:HG22	0.41	2.16	12	1
1:A:891:ARG:HG2	1:A:916:GLU:O	0.41	2.16	12	1
1:A:934:GLN:O	1:A:938:LEU:HB2	0.40	2.16	2	1
1:A:831:ASP:OD2	1:A:837:ARG:HB2	0.40	2.16	6	1
1:A:895:LEU:HD12	1:A:897:LEU:HG	0.40	1.92	13	1
1:A:889:ARG:HA	1:A:889:ARG:HD3	0.40	1.73	18	1
1:A:938:LEU:O	1:A:941:GLU:HG2	0.40	2.16	25	1
1:A:906:ALA:O	1:A:907:LEU:HB2	0.40	2.16	9	1
1:A:890:ILE:HG23	1:A:895:LEU:HD22	0.40	1.93	13	1
1:A:924:SER:O	1:A:927:VAL:HG23	0.40	2.17	15	1
1:A:837:ARG:HD2	1:A:853:THR:HG22	0.40	1.92	16	1
1:A:886:LEU:H	1:A:886:LEU:HD13	0.40	1.76	21	1
1:A:830:VAL:HG12	1:A:856:ASP:H	0.40	1.75	5	1
1:A:847:LEU:HD11	1:A:932:ILE:HG23	0.40	1.92	5	1
1:A:830:VAL:HG23	1:A:873:LEU:O	0.40	2.17	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:864:LEU:HA	1:A:867:ASN:O	0.40	2.16	14	1
1:A:861:LEU:HD22	1:A:889:ARG:HG3	0.40	1.93	19	1
1:A:828:LEU:HB2	1:A:869:ILE:HG12	0.40	1.93	1	1
1:A:826:MET:HE3	1:A:826:MET:HB2	0.40	1.80	16	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	116/133 (87%)	105±2 (91±2%)	7±2 (6±2%)	3±1 (3±1%)	5	38
All	All	2900/3325 (87%)	2628 (91%)	186 (6%)	86 (3%)	5	38

All 10 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	856	ASP	25
1	A	920	ASP	25
1	A	884	TYR	9
1	A	834	PRO	9
1	A	919	MET	7
1	A	907	LEU	4
1	A	869	ILE	3
1	A	905	ASN	2
1	A	908	ALA	1
1	A	906	ALA	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	103/118 (87%)	53±3 (51±3%)	50±3 (49±3%)	0	1
All	All	2575/2950 (87%)	1314 (51%)	1261 (49%)	0	1

All 95 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	928	THR	25
1	A	929	LEU	25
1	A	853	THR	24
1	A	886	LEU	24
1	A	936	LEU	24
1	A	835	ILE	23
1	A	933	LYS	23
1	A	938	LEU	23
1	A	843	GLN	22
1	A	891	ARG	22
1	A	915	LEU	22
1	A	927	VAL	22
1	A	838	ARG	22
1	A	885	ARG	22
1	A	847	LEU	21
1	A	851	CYS	21
1	A	873	LEU	21
1	A	864	LEU	20
1	A	876	VAL	20
1	A	897	LEU	20
1	A	825	MET	19
1	A	839	LEU	19
1	A	852	LYS	19
1	A	889	ARG	19
1	A	893	LEU	19
1	A	941	GLU	19
1	A	911	LYS	19
1	A	902	VAL	18
1	A	932	ILE	18
1	A	916	GLU	18
1	A	874	SER	18
1	A	869	ILE	17
1	A	896	THR	17
1	A	912	GLN	17
1	A	924	SER	17
1	A	944	ARG	17

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Mol	Chain	Res	Type	Models (Total)
1	A	907	LEU	16
1	A	850	GLN	15
1	A	861	LEU	15
1	A	895	LEU	15
1	A	945	LYS	15
1	A	827	ILE	15
1	A	923	LEU	15
1	A	900	ILE	15
1	A	858	VAL	14
1	A	934	GLN	14
1	A	942	ARG	14
1	A	866	LYS	14
1	A	919	MET	14
1	A	922	CYS	13
1	A	833	HIS	13
1	A	921	SER	12
1	A	935	THR	12
1	A	947	ARG	12
1	A	829	VAL	11
1	A	831	ASP	11
1	A	836	ASN	11
1	A	892	GLN	11
1	A	890	ILE	10
1	A	828	LEU	10
1	A	913	ARG	10
1	A	917	SER	10
1	A	910	GLU	10
1	A	832	ASP	10
1	A	868	HIS	9
1	A	826	MET	9
1	A	830	VAL	9
1	A	909	GLU	9
1	A	837	ARG	9
1	A	844	LEU	8
1	A	862	ASN	8
1	A	903	THR	8
1	A	863	VAL	7
1	A	867	ASN	7
1	A	870	ASP	7
1	A	840	LEU	7
1	A	855	ASN	7
1	A	887	THR	6

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Mol	Chain	Res	Type	Models (Total)
1	A	846	SER	6
1	A	925	LYS	6
1	A	905	ASN	6
1	A	865	SER	5
1	A	871	ILE	5
1	A	842	ASP	4
1	A	930	ASP	4
1	A	875	ASP	3
1	A	856	ASP	3
1	A	914	CYS	3
1	A	888	GLN	2
1	A	884	TYR	2
1	A	899	VAL	2
1	A	939	TYR	2
1	A	859	ASP	2
1	A	931	VAL	2
1	A	872	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided