



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 09:04 pm GMT

PDB ID : 2AYY
Title : Solution structure of the E.coli RcsC C-terminus (residues 700-816) containing linker region
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

<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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

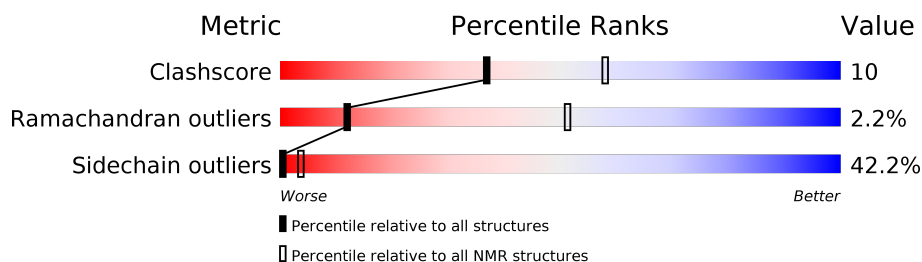
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	121	

2 Ensemble composition and analysis ⓘ

This entry contains 25 models. Model 19 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:707-A:801 (95)	0.52	19

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 3 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1852 atoms, of which 925 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1852	583	925	161	178	5	

There are 4 discrepancies between the modelled and reference sequences:

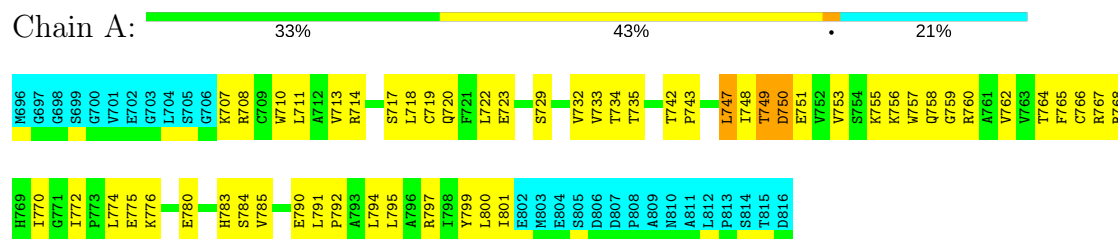
Chain	Residue	Modelled	Actual	Comment	Reference
A	696	MET	-	CLONING ARTIFACT	UNP P14376
A	697	GLY	-	CLONING ARTIFACT	UNP P14376
A	698	GLY	-	CLONING ARTIFACT	UNP P14376
A	699	SER	-	CLONING ARTIFACT	UNP P14376

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: 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

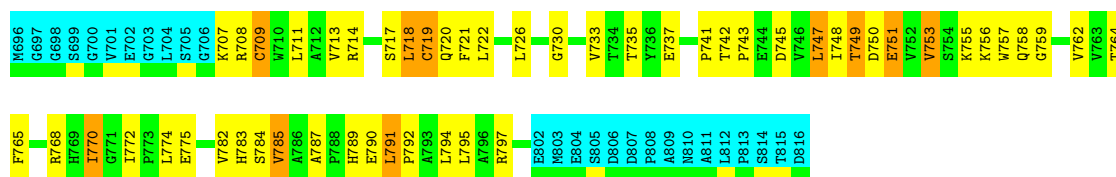
- Molecule 1: Sensor kinase protein rcsC



4.2.2 Score per residue for model 2

- Molecule 1: Sensor kinase protein rcsC

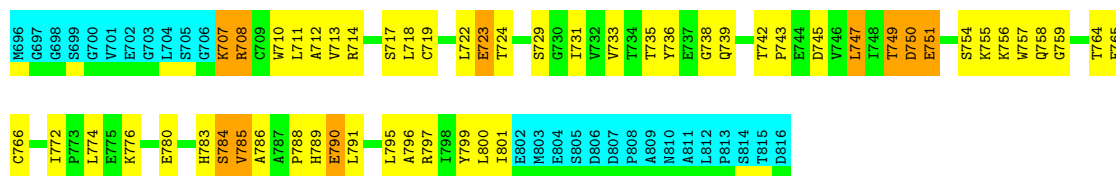




4.2.3 Score per residue for model 3

- Molecule 1: Sensor kinase protein rcsC

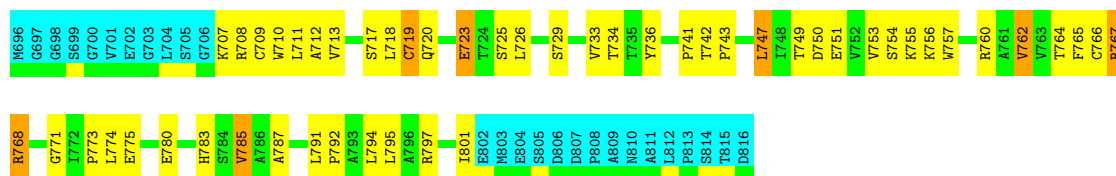
Chain A: 34% 36% 8% 21%



4.2.4 Score per residue for model 4

- Molecule 1: Sensor kinase protein rcsC

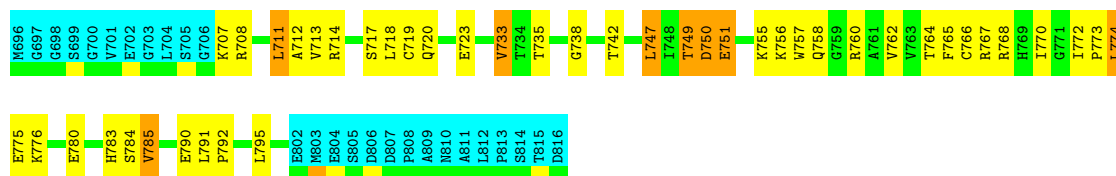
Chain A: 36% 36% 6% 21%



4.2.5 Score per residue for model 5

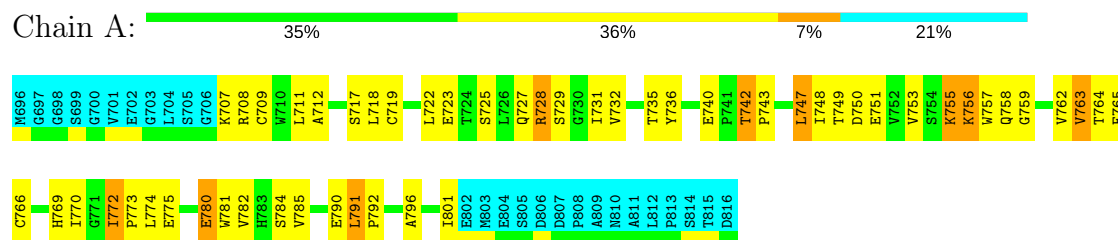
- Molecule 1: Sensor kinase protein rcsC

Chain A: 42% 30% 7% 21%



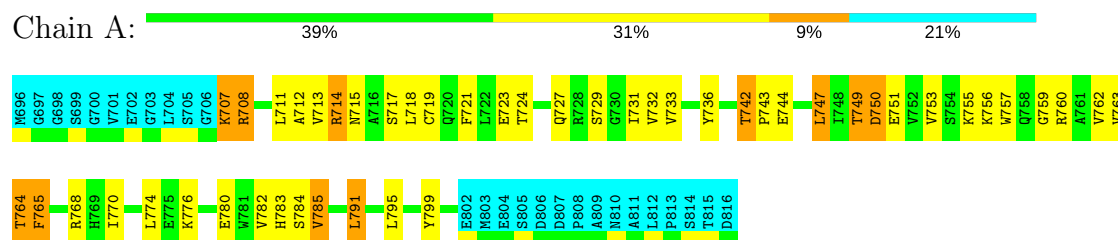
4.2.6 Score per residue for model 6

- Molecule 1: Sensor kinase protein rcsC



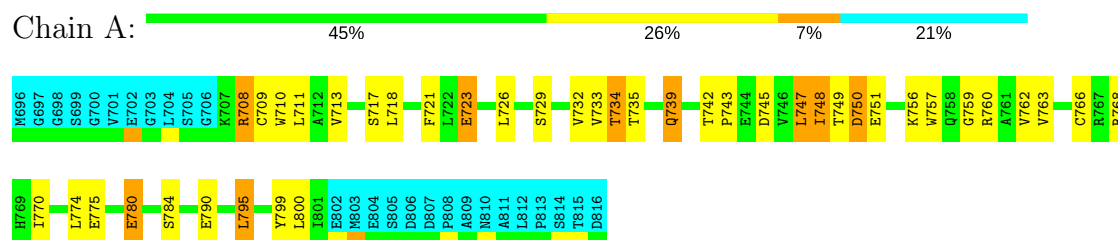
4.2.7 Score per residue for model 7

- Molecule 1: Sensor kinase protein rcsC



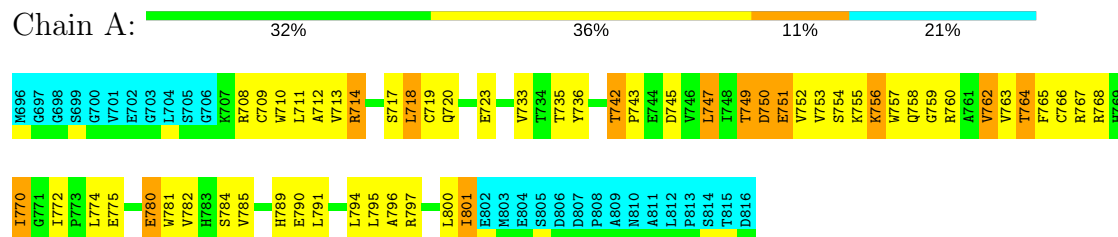
4.2.8 Score per residue for model 8

- Molecule 1: Sensor kinase protein rcsC



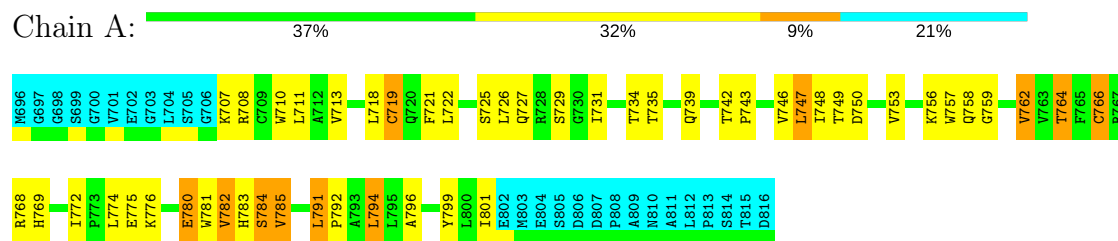
4.2.9 Score per residue for model 9

- Molecule 1: Sensor kinase protein rcsC



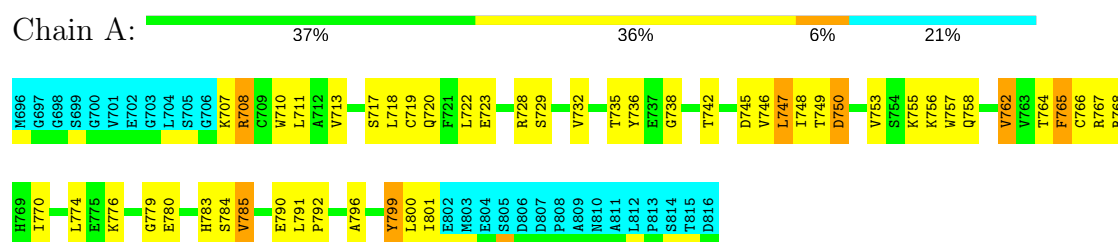
4.2.10 Score per residue for model 10

- Molecule 1: Sensor kinase protein rcsC



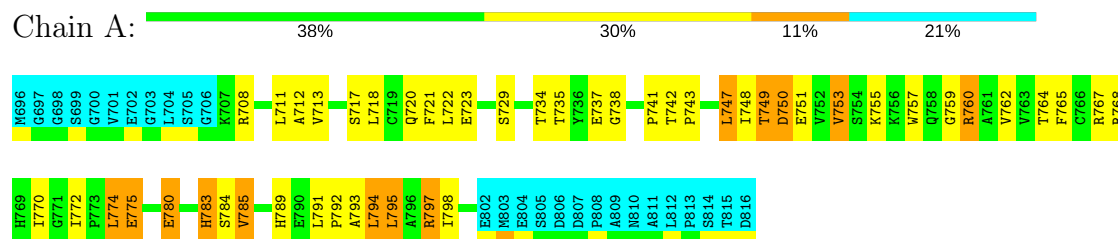
4.2.11 Score per residue for model 11

- Molecule 1: Sensor kinase protein rcsC



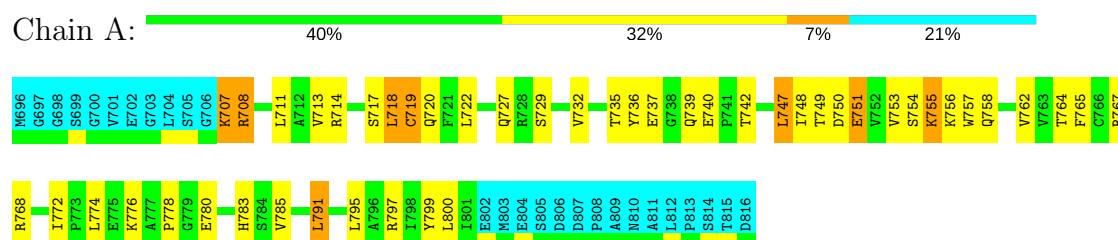
4.2.12 Score per residue for model 12

- Molecule 1: Sensor kinase protein rcsC



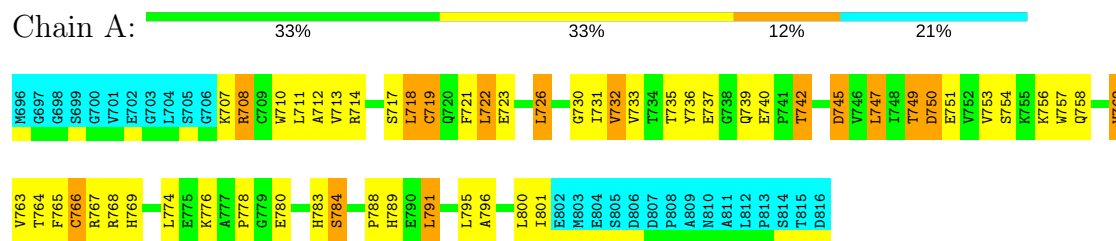
4.2.13 Score per residue for model 13

- Molecule 1: Sensor kinase protein rcsC



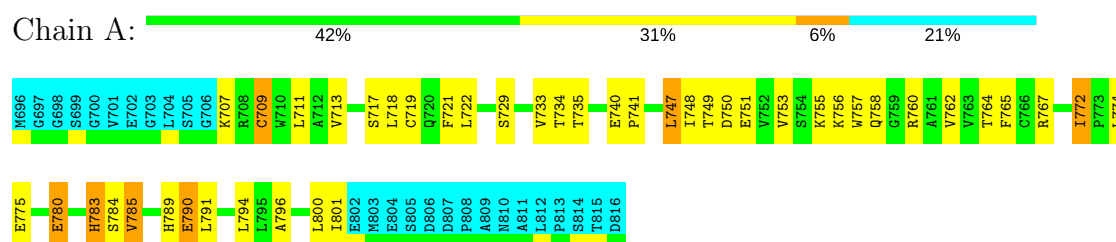
4.2.14 Score per residue for model 14

- Molecule 1: Sensor kinase protein rcsC



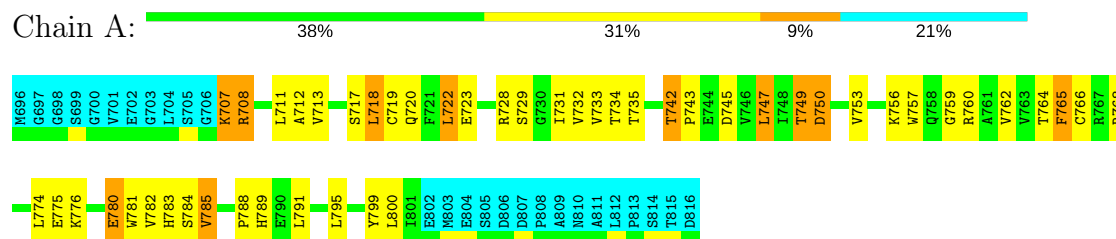
4.2.15 Score per residue for model 15

- Molecule 1: Sensor kinase protein rcsC



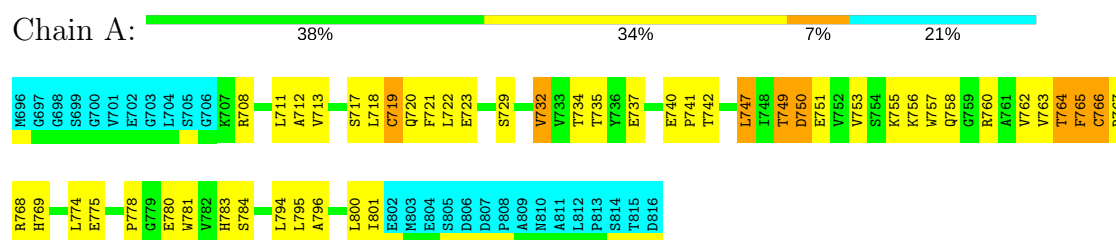
4.2.16 Score per residue for model 16

- Molecule 1: Sensor kinase protein rcsC



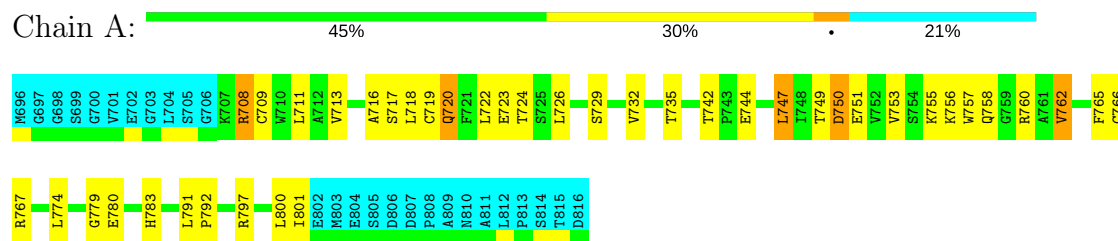
4.2.17 Score per residue for model 17

- Molecule 1: Sensor kinase protein rcsC



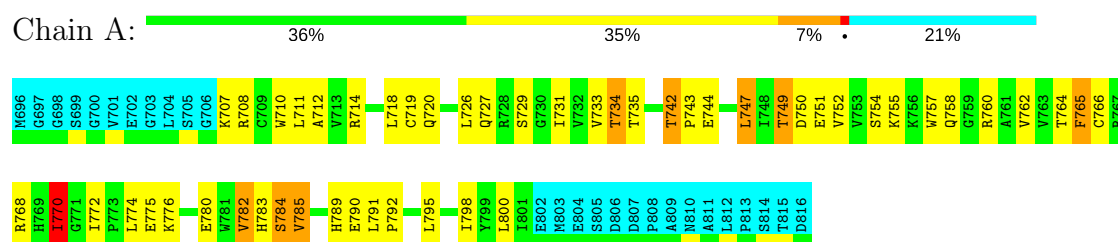
4.2.18 Score per residue for model 18

- Molecule 1: Sensor kinase protein rcsC



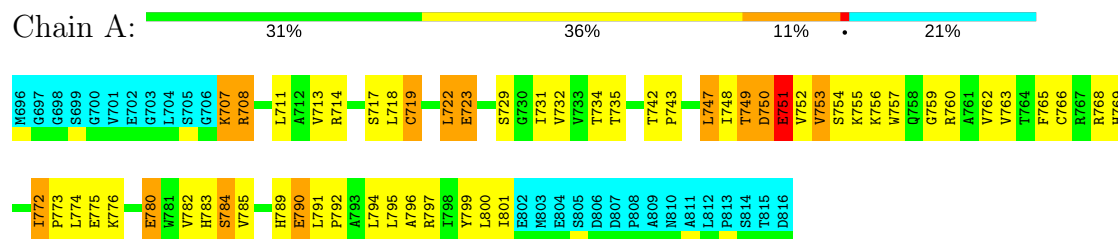
4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: Sensor kinase protein rcsC



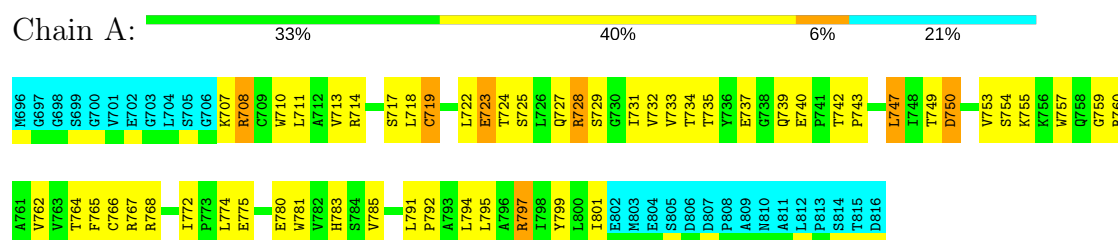
4.2.20 Score per residue for model 20

- Molecule 1: Sensor kinase protein rcsC



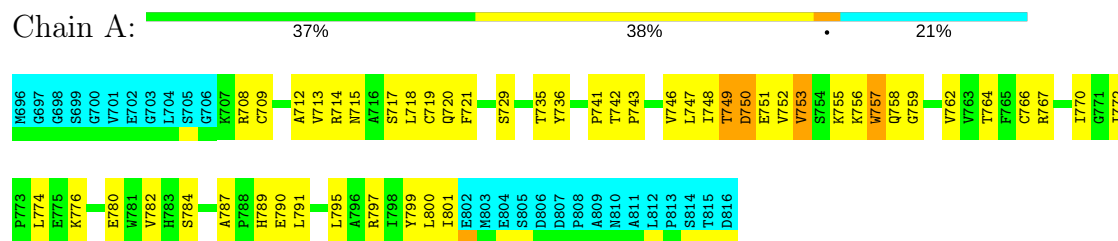
4.2.21 Score per residue for model 21

- Molecule 1: Sensor kinase protein rcsC



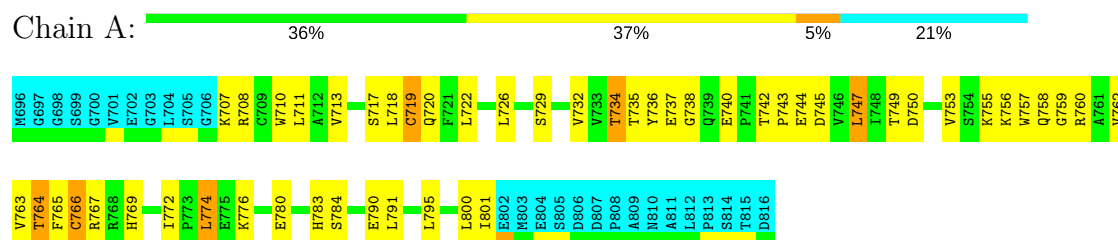
4.2.22 Score per residue for model 22

- Molecule 1: Sensor kinase protein rcsC



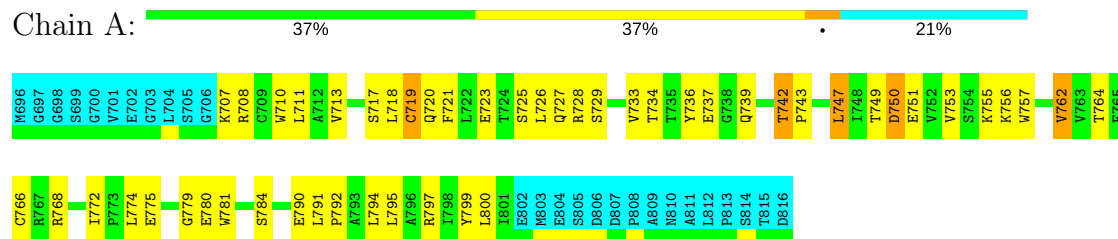
4.2.23 Score per residue for model 23

- Molecule 1: Sensor kinase protein rcsC



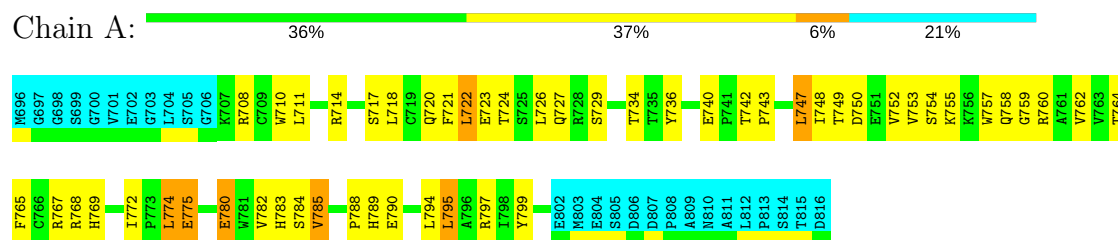
4.2.24 Score per residue for model 24

- 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. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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	753	772	769	14±4
All	All	18825	19300	19225	362

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:752:VAL:HB	1:A:770:ILE:HD13	0.73	1.60	19	1
1:A:764:THR:HG21	1:A:772:ILE:HG21	0.72	1.58	6	2
1:A:712:ALA:HB3	1:A:749:THR:HG23	0.72	1.61	3	7
1:A:718:LEU:HG	1:A:788:PRO:HB3	0.72	1.62	16	1
1:A:713:VAL:HA	1:A:750:ASP:HB3	0.71	1.62	12	9
1:A:765:PHE:HB3	1:A:785:VAL:HB	0.70	1.63	13	4
1:A:775:GLU:HA	1:A:780:GLU:HB2	0.70	1.63	9	3
1:A:765:PHE:HB3	1:A:785:VAL:HG13	0.70	1.62	2	5
1:A:749:THR:HB	1:A:753:VAL:HG21	0.70	1.63	22	4
1:A:743:PRO:HA	1:A:759:GLY:HA2	0.70	1.62	10	14
1:A:775:GLU:HG3	1:A:781:TRP:HA	0.69	1.65	24	6
1:A:710:TRP:HB3	1:A:736:TYR:HB2	0.69	1.65	25	7
1:A:712:ALA:HB3	1:A:749:THR:HG22	0.67	1.64	9	4
1:A:713:VAL:HB	1:A:719:CYS:HB2	0.66	1.65	23	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:742:THR:HG22	1:A:743:PRO:HD2	0.64	1.68	19	6
1:A:707:LYS:HG3	1:A:731:ILE:HG12	0.64	1.68	3	3
1:A:715:ASN:HB3	1:A:718:LEU:HB2	0.63	1.71	7	2
1:A:796:ALA:HA	1:A:801:ILE:HD12	0.63	1.69	15	7
1:A:747:LEU:HB2	1:A:757:TRP:CD2	0.62	2.29	18	17
1:A:756:LYS:HD2	1:A:757:TRP:H	0.61	1.56	9	2
1:A:713:VAL:HG21	1:A:722:LEU:HD21	0.60	1.72	21	2
1:A:722:LEU:HD11	1:A:748:ILE:HD13	0.60	1.73	11	1
1:A:791:LEU:HB3	1:A:792:PRO:HD3	0.60	1.74	19	10
1:A:708:ARG:HG2	1:A:732:VAL:HG13	0.60	1.72	20	12
1:A:752:VAL:HA	1:A:772:ILE:HD11	0.59	1.74	25	1
1:A:775:GLU:HA	1:A:780:GLU:O	0.59	1.97	10	4
1:A:712:ALA:HB2	1:A:736:TYR:HB3	0.59	1.72	22	3
1:A:713:VAL:HB	1:A:719:CYS:HB3	0.58	1.75	7	2
1:A:748:ILE:HG21	1:A:791:LEU:HD21	0.57	1.75	1	2
1:A:757:TRP:HB3	1:A:762:VAL:HG22	0.57	1.76	9	7
1:A:765:PHE:HB3	1:A:785:VAL:HG22	0.57	1.76	4	2
1:A:713:VAL:HG13	1:A:750:ASP:HB3	0.57	1.75	16	8
1:A:766:CYS:O	1:A:784:SER:HA	0.56	2.00	10	6
1:A:747:LEU:HG	1:A:757:TRP:CE3	0.55	2.37	11	13
1:A:718:LEU:O	1:A:722:LEU:HG	0.55	2.02	2	1
1:A:753:VAL:H	1:A:772:ILE:HD11	0.54	1.62	20	1
1:A:772:ILE:HG22	1:A:774:LEU:H	0.54	1.63	5	1
1:A:764:THR:HG21	1:A:772:ILE:HD12	0.54	1.79	22	1
1:A:773:PRO:O	1:A:774:LEU:HG	0.53	2.04	5	1
1:A:743:PRO:HA	1:A:759:GLY:CA	0.53	2.32	23	2
1:A:764:THR:O	1:A:782:VAL:HA	0.53	2.03	10	2
1:A:760:ARG:NH1	1:A:760:ARG:HA	0.53	2.19	1	1
1:A:723:GLU:HG3	1:A:724:THR:N	0.52	2.19	21	5
1:A:795:LEU:HA	1:A:798:ILE:HD12	0.52	1.81	19	2
1:A:765:PHE:CZ	1:A:791:LEU:HG	0.52	2.40	7	3
1:A:719:CYS:HA	1:A:722:LEU:HD23	0.52	1.80	14	2
1:A:764:THR:HG21	1:A:772:ILE:HG12	0.51	1.82	9	1
1:A:794:LEU:O	1:A:797:ARG:HG2	0.51	2.06	24	1
1:A:718:LEU:HD13	1:A:722:LEU:HD11	0.51	1.81	2	1
1:A:710:TRP:HZ3	1:A:739:GLN:HG3	0.51	1.66	8	1
1:A:742:THR:HB	1:A:745:ASP:OD1	0.51	2.06	14	1
1:A:765:PHE:HA	1:A:783:HIS:O	0.51	2.06	21	13
1:A:791:LEU:HB2	1:A:792:PRO:HD3	0.51	1.83	12	3
1:A:714:ARG:HB2	1:A:751:GLU:HB2	0.51	1.81	9	1
1:A:749:THR:HG22	1:A:753:VAL:HG21	0.50	1.82	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:753:VAL:HG12	1:A:755:LYS:HD2	0.50	1.83	6	1
1:A:718:LEU:HD13	1:A:791:LEU:HD21	0.50	1.83	13	1
1:A:774:LEU:HG	1:A:782:VAL:HG11	0.50	1.82	19	1
1:A:707:LYS:HB2	1:A:731:ILE:HG12	0.50	1.83	14	3
1:A:720:GLN:HA	1:A:723:GLU:HG2	0.50	1.84	4	2
1:A:747:LEU:HG	1:A:757:TRP:CZ3	0.50	2.41	2	3
1:A:747:LEU:HB2	1:A:757:TRP:CG	0.49	2.43	15	6
1:A:718:LEU:HD22	1:A:791:LEU:HD12	0.49	1.85	7	1
1:A:722:LEU:HD13	1:A:791:LEU:HG	0.49	1.84	16	1
1:A:796:ALA:HB1	1:A:801:ILE:HB	0.49	1.84	20	3
1:A:744:GLU:HA	1:A:760:ARG:CZ	0.49	2.37	7	1
1:A:774:LEU:H	1:A:774:LEU:HD23	0.49	1.68	16	1
1:A:775:GLU:HB2	1:A:782:VAL:H	0.49	1.68	9	2
1:A:708:ARG:HB3	1:A:745:ASP:OD2	0.49	2.08	14	2
1:A:741:PRO:HA	1:A:757:TRP:CH2	0.49	2.43	17	3
1:A:726:LEU:HD11	1:A:733:VAL:HB	0.48	1.83	14	1
1:A:765:PHE:CE1	1:A:783:HIS:HB3	0.48	2.43	17	3
1:A:749:THR:HG21	1:A:753:VAL:HG21	0.48	1.84	17	2
1:A:794:LEU:HA	1:A:797:ARG:HE	0.48	1.68	12	1
1:A:723:GLU:HB2	1:A:733:VAL:HG11	0.47	1.87	24	3
1:A:709:CYS:SG	1:A:733:VAL:HG12	0.47	2.50	15	1
1:A:714:ARG:HG2	1:A:750:ASP:OD1	0.47	2.09	7	1
1:A:710:TRP:HZ3	1:A:739:GLN:HE21	0.47	1.50	1	1
1:A:712:ALA:HB3	1:A:749:THR:CG2	0.47	2.37	9	1
1:A:775:GLU:HG3	1:A:780:GLU:O	0.47	2.09	17	4
1:A:741:PRO:HA	1:A:757:TRP:CZ3	0.47	2.45	22	2
1:A:713:VAL:HG13	1:A:750:ASP:CB	0.47	2.40	24	3
1:A:727:GLN:HG2	1:A:731:ILE:O	0.47	2.10	10	3
1:A:722:LEU:HG	1:A:723:GLU:N	0.47	2.24	25	4
1:A:765:PHE:CE1	1:A:791:LEU:HD13	0.47	2.45	16	1
1:A:710:TRP:HA	1:A:734:THR:O	0.46	2.10	21	4
1:A:718:LEU:HD13	1:A:791:LEU:HD11	0.46	1.87	14	1
1:A:763:VAL:HA	1:A:781:TRP:HB2	0.46	1.88	6	2
1:A:774:LEU:HD23	1:A:774:LEU:H	0.46	1.70	12	1
1:A:711:LEU:O	1:A:711:LEU:HG	0.46	2.10	5	1
1:A:747:LEU:HB3	1:A:762:VAL:HG13	0.46	1.88	11	1
1:A:722:LEU:HD13	1:A:791:LEU:HB2	0.46	1.86	14	1
1:A:736:TYR:HE2	1:A:755:LYS:HE2	0.46	1.71	13	1
1:A:775:GLU:HA	1:A:780:GLU:HG3	0.46	1.88	21	1
1:A:774:LEU:HA	1:A:782:VAL:HB	0.46	1.87	2	1
1:A:791:LEU:CB	1:A:792:PRO:HD3	0.46	2.41	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:718:LEU:HD22	1:A:791:LEU:HD23	0.46	1.88	16	1
1:A:744:GLU:HA	1:A:760:ARG:HH11	0.45	1.70	19	1
1:A:774:LEU:HD12	1:A:782:VAL:HG21	0.45	1.88	2	3
1:A:790:GLU:HG3	1:A:791:LEU:N	0.45	2.26	20	1
1:A:713:VAL:HG12	1:A:715:ASN:H	0.45	1.72	7	1
1:A:775:GLU:HB2	1:A:782:VAL:N	0.44	2.27	9	1
1:A:737:GLU:HB2	1:A:739:GLN:HE22	0.44	1.72	21	1
1:A:789:HIS:HB3	1:A:790:GLU:OE1	0.44	2.11	25	1
1:A:722:LEU:HD22	1:A:791:LEU:HD13	0.44	1.90	1	1
1:A:723:GLU:HB2	1:A:733:VAL:HG21	0.44	1.89	1	1
1:A:760:ARG:HA	1:A:760:ARG:NH1	0.44	2.28	12	1
1:A:767:ARG:O	1:A:768:ARG:HD2	0.44	2.12	4	1
1:A:713:VAL:HG22	1:A:750:ASP:HB2	0.44	1.88	21	1
1:A:790:GLU:HA	1:A:790:GLU:OE1	0.44	2.12	15	1
1:A:753:VAL:HB	1:A:772:ILE:HD12	0.43	1.89	15	1
1:A:757:TRP:HB2	1:A:762:VAL:HG13	0.43	1.90	14	1
1:A:725:SER:HA	1:A:728:ARG:NH1	0.43	2.28	21	1
1:A:707:LYS:HE3	1:A:799:TYR:CZ	0.43	2.48	13	1
1:A:709:CYS:SG	1:A:733:VAL:HG22	0.43	2.54	2	1
1:A:718:LEU:HD21	1:A:791:LEU:HD13	0.43	1.91	9	1
1:A:749:THR:HB	1:A:764:THR:HG23	0.43	1.91	1	1
1:A:765:PHE:CE1	1:A:791:LEU:HG	0.43	2.48	15	1
1:A:751:GLU:HB3	1:A:752:VAL:H	0.43	1.52	9	2
1:A:716:ALA:O	1:A:720:GLN:HB2	0.43	2.14	18	1
1:A:799:TYR:HB3	1:A:801:ILE:HG13	0.42	1.91	11	1
1:A:718:LEU:HD21	1:A:788:PRO:HA	0.42	1.91	14	1
1:A:710:TRP:HE3	1:A:736:TYR:HA	0.42	1.73	24	1
1:A:722:LEU:HD22	1:A:791:LEU:HD21	0.42	1.91	21	1
1:A:774:LEU:O	1:A:776:LYS:HG2	0.42	2.15	1	1
1:A:749:THR:HB	1:A:753:VAL:CG2	0.42	2.40	22	1
1:A:707:LYS:HB3	1:A:731:ILE:HG12	0.42	1.92	21	1
1:A:741:PRO:HB3	1:A:757:TRP:CH2	0.42	2.50	2	1
1:A:781:TRP:CZ3	1:A:794:LEU:HD21	0.42	2.50	10	1
1:A:764:THR:HB	1:A:766:CYS:SG	0.42	2.55	17	1
1:A:781:TRP:CH2	1:A:797:ARG:HD3	0.41	2.50	21	1
1:A:750:ASP:HA	1:A:765:PHE:O	0.41	2.16	5	1
1:A:775:GLU:CG	1:A:776:LYS:H	0.41	2.29	16	1
1:A:788:PRO:HA	1:A:790:GLU:OE1	0.41	2.16	3	1
1:A:774:LEU:O	1:A:780:GLU:HG3	0.41	2.15	25	1
1:A:743:PRO:HA	1:A:759:GLY:C	0.41	2.36	16	1
1:A:753:VAL:HG23	1:A:772:ILE:HD11	0.41	1.93	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:709:CYS:HB2	1:A:748:ILE:HD11	0.41	1.92	8	1
1:A:749:THR:HG21	1:A:753:VAL:HG13	0.41	1.91	16	1
1:A:747:LEU:HD12	1:A:757:TRP:HB2	0.40	1.93	8	1
1:A:710:TRP:CE3	1:A:734:THR:HB	0.40	2.51	19	1
1:A:725:SER:O	1:A:728:ARG:HB2	0.40	2.16	6	1
1:A:774:LEU:H	1:A:774:LEU:HG	0.40	1.55	23	1
1:A:743:PRO:O	1:A:760:ARG:HD2	0.40	2.16	4	1
1:A:748:ILE:HG21	1:A:795:LEU:HD11	0.40	1.93	8	1
1:A:795:LEU:HD22	1:A:795:LEU:HA	0.40	1.79	25	1
1:A:722:LEU:HD22	1:A:791:LEU:HD22	0.40	1.92	10	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	95/121 (79%)	80±2 (84±2%)	13±3 (14±3%)	2±1 (2±2%)	12	51
All	All	2375/3025 (79%)	2000 (84%)	323 (14%)	52 (2%)	12	51

All 16 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	785	VAL	8
1	A	751	GLU	7
1	A	770	ILE	6
1	A	738	GLY	5
1	A	779	GLY	4
1	A	775	GLU	4
1	A	787	ALA	3
1	A	778	PRO	3
1	A	773	PRO	3
1	A	730	GLY	2
1	A	801	ILE	2
1	A	752	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	786	ALA	1
1	A	753	VAL	1
1	A	739	GLN	1
1	A	771	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	82/101 (81%)	47±3 (58±4%)	35±3 (42±4%)	0 4
All	All	2050/2525 (81%)	1185 (58%)	865 (42%)	0 4

All 70 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	747	LEU	25
1	A	749	THR	24
1	A	742	THR	24
1	A	718	LEU	24
1	A	750	ASP	23
1	A	717	SER	23
1	A	711	LEU	23
1	A	780	GLU	22
1	A	708	ARG	22
1	A	756	LYS	21
1	A	735	THR	21
1	A	729	SER	21
1	A	755	LYS	21
1	A	762	VAL	21
1	A	774	LEU	20
1	A	784	SER	19
1	A	764	THR	19
1	A	795	LEU	19
1	A	719	CYS	18
1	A	768	ARG	18
1	A	751	GLU	16

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Mol	Chain	Res	Type	Models (Total)
1	A	758	GLN	16
1	A	766	CYS	16
1	A	800	LEU	15
1	A	720	GLN	14
1	A	707	LYS	14
1	A	767	ARG	14
1	A	753	VAL	14
1	A	790	GLU	13
1	A	760	ARG	13
1	A	714	ARG	13
1	A	799	TYR	12
1	A	785	VAL	12
1	A	776	LYS	12
1	A	797	ARG	12
1	A	723	GLU	12
1	A	722	LEU	11
1	A	794	LEU	11
1	A	721	PHE	11
1	A	734	THR	11
1	A	726	LEU	11
1	A	754	SER	10
1	A	772	ILE	10
1	A	789	HIS	10
1	A	791	LEU	9
1	A	748	ILE	9
1	A	733	VAL	9
1	A	783	HIS	8
1	A	770	ILE	8
1	A	769	HIS	8
1	A	740	GLU	8
1	A	737	GLU	7
1	A	709	CYS	7
1	A	763	VAL	7
1	A	745	ASP	7
1	A	765	PHE	6
1	A	782	VAL	6
1	A	739	GLN	6
1	A	728	ARG	6
1	A	727	GLN	5
1	A	725	SER	3
1	A	732	VAL	3
1	A	746	VAL	3

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Mol	Chain	Res	Type	Models (Total)
1	A	744	GLU	2
1	A	801	ILE	2
1	A	757	TRP	1
1	A	724	THR	1
1	A	775	GLU	1
1	A	715	ASN	1
1	A	788	PRO	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 carbohydrates 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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided