



Full wwPDB NMR Structure Validation Report ⓘ

Nov 21, 2023 – 12:07 AM EST

PDB ID : 2L7U
BMRB ID : 17378
Title : Structure of CEL-PEP-RAGE V domain complex
Authors : Xue, J.; Rai, V.; Schmidt, A.; Frolov, S.; Reverdatto, S.; Singer, D.; Chabierski, S.; Xie, J.; Burz, D.; Shekhtman, A.; Hoffman, R.
Deposited on : 2010-12-23

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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
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) : 2.36

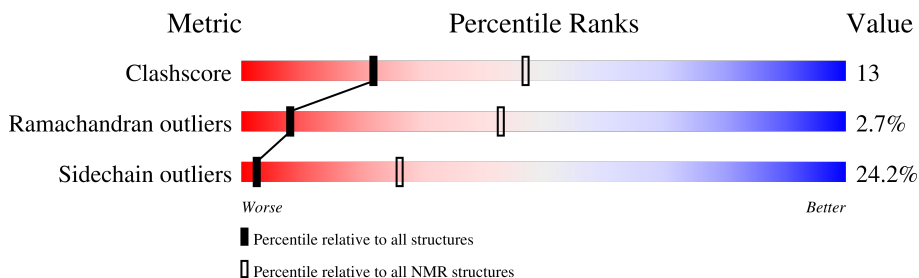
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 76%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	105	
2	B	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	B	KPI	4	-	15

2 Ensemble composition and analysis i

This entry contains 25 models. Model 15 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*.

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:3-A:24, A:28-A:45, A:56-A:101 (86)	0.42	15

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 5 clusters and 4 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1600 atoms, of which 723 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Advanced glycosylation end product-specific receptor.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	105	1494	513	681	153	144	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q15109
A	2	SER	-	expression tag	UNP Q15109

- Molecule 2 is a protein called Serum albumin peptide.

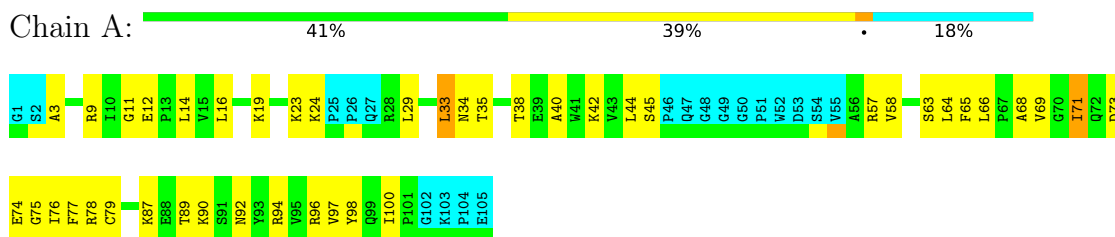
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	7	106	39	42	8	17	0

4 Residue-property plots [i](#)

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: Advanced glycosylation end product-specific receptor



- Molecule 2: Serum albumin peptide

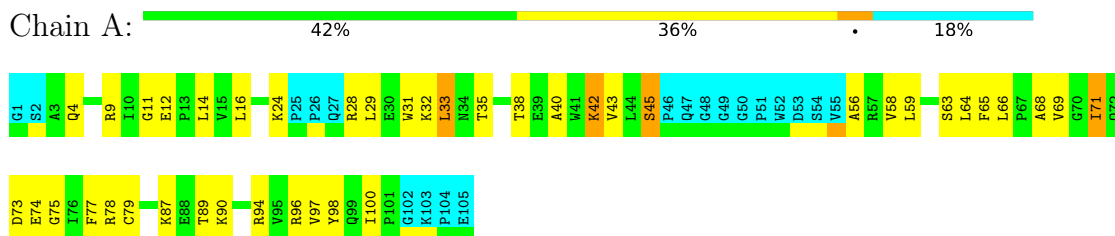


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Advanced glycosylation end product-specific receptor



- Molecule 2: Serum albumin peptide

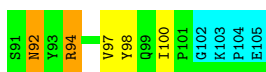
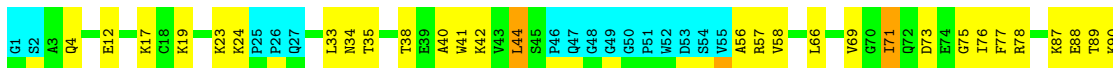
Chain B:  100%



4.2.2 Score per residue for model 2

- Molecule 1: Advanced glycosylation end product-specific receptor

Chain A:  50% 29% 18%



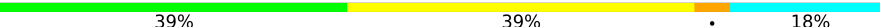
- Molecule 2: Serum albumin peptide

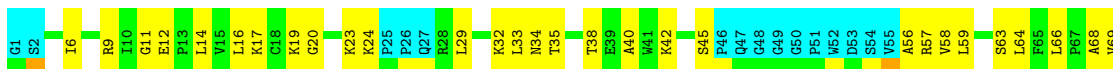
Chain B:  100%



4.2.3 Score per residue for model 3

- Molecule 1: Advanced glycosylation end product-specific receptor

Chain A:  39% 39% 18%



- Molecule 2: Serum albumin peptide

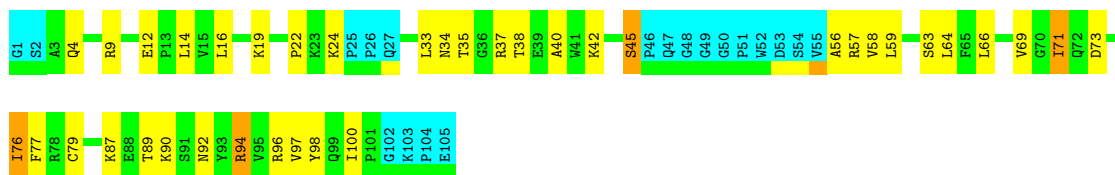
Chain B:  100%



4.2.4 Score per residue for model 4

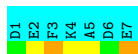
- Molecule 1: Advanced glycosylation end product-specific receptor

Chain A:  46% 32% 18%



- Molecule 2: Serum albumin peptide

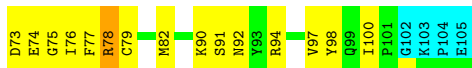
Chain B: 100%



4.2.5 Score per residue for model 5

- Molecule 1: Advanced glycosylation end product-specific receptor

Chain A: 40% 35% 7% 18%



- Molecule 2: Serum albumin peptide

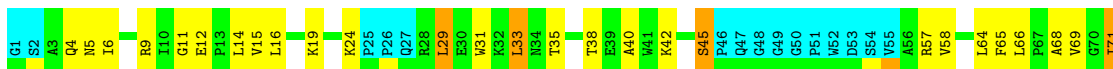
Chain B: 100%



4.2.6 Score per residue for model 6

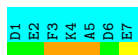
- Molecule 1: Advanced glycosylation end product-specific receptor

Chain A: 42% 34% 6% 18%



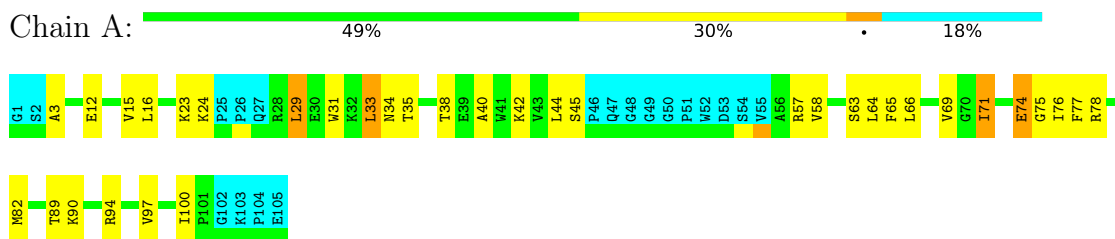
- Molecule 2: Serum albumin peptide

Chain B: 100%

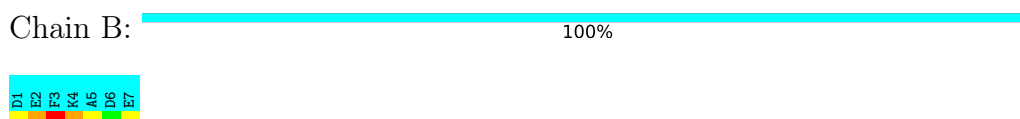


4.2.7 Score per residue for model 7

- Molecule 1: Advanced glycosylation end product-specific receptor

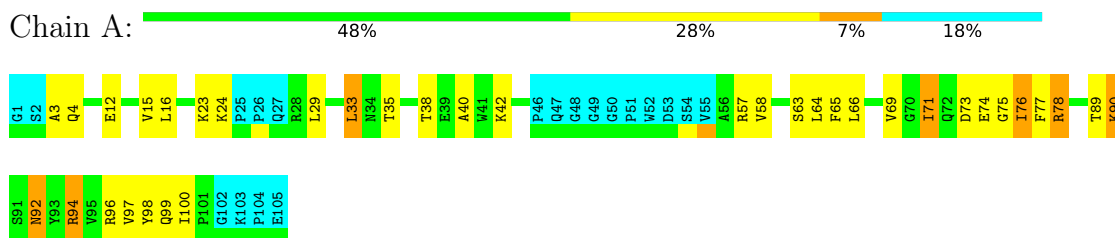


- Molecule 2: Serum albumin peptide



4.2.8 Score per residue for model 8

- Molecule 1: Advanced glycosylation end product-specific receptor

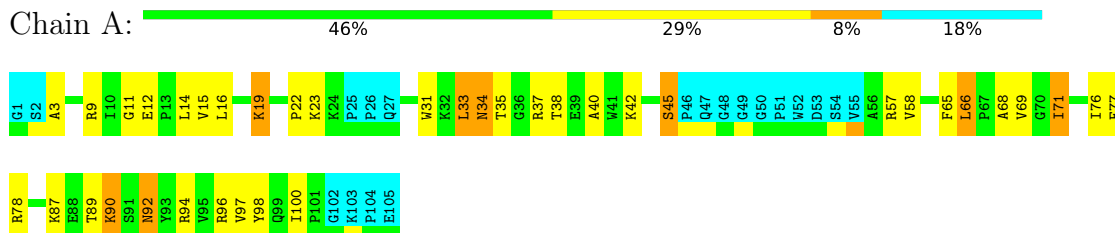


- Molecule 2: Serum albumin peptide

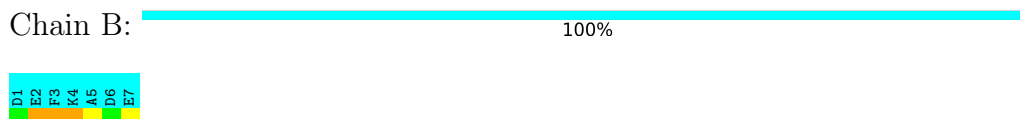


4.2.9 Score per residue for model 9

- Molecule 1: Advanced glycosylation end product-specific receptor

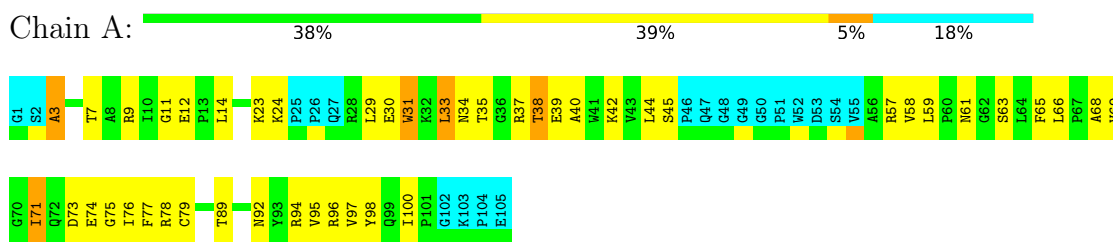


- Molecule 2: Serum albumin peptide

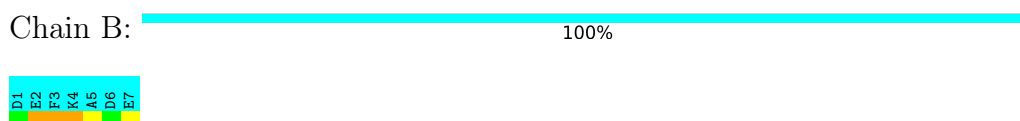


4.2.10 Score per residue for model 10

- Molecule 1: Advanced glycosylation end product-specific receptor

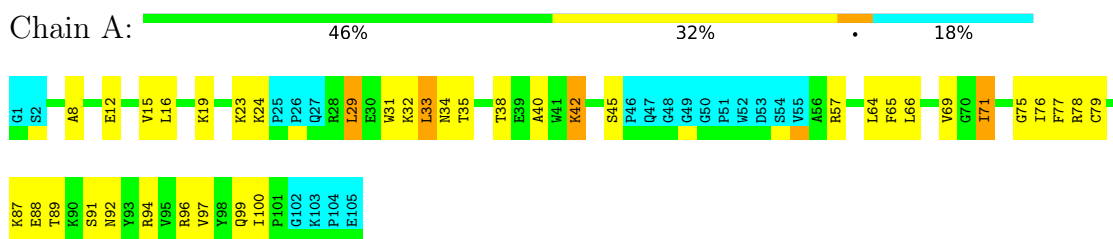


- Molecule 2: Serum albumin peptide

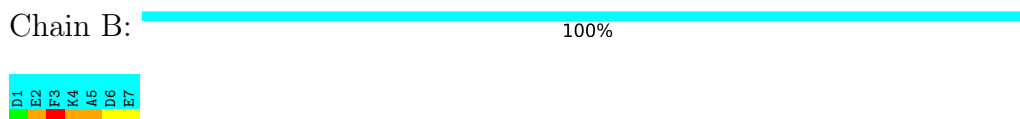


4.2.11 Score per residue for model 11

- Molecule 1: Advanced glycosylation end product-specific receptor

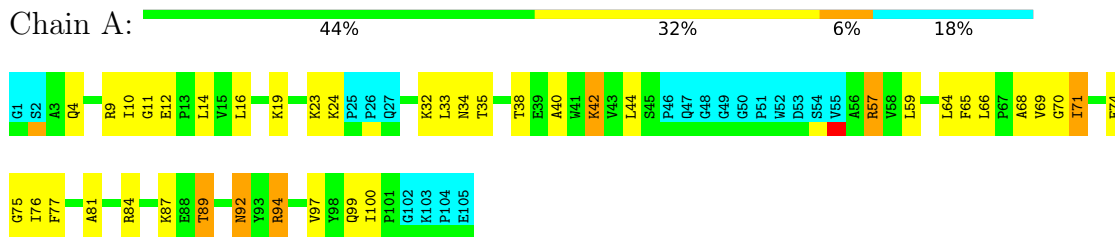


- Molecule 2: Serum albumin peptide



4.2.12 Score per residue for model 12

- Molecule 1: Advanced glycosylation end product-specific receptor

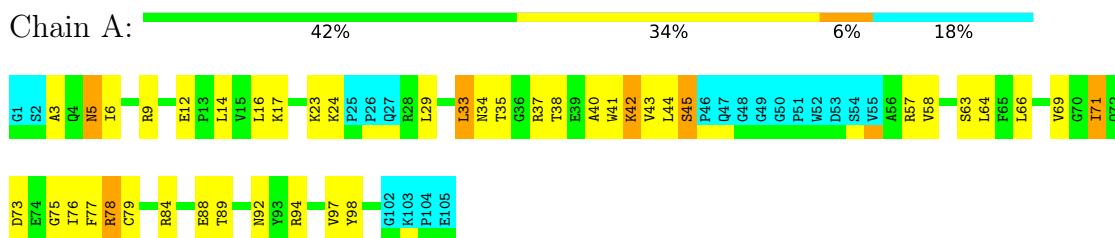


- Molecule 2: Serum albumin peptide

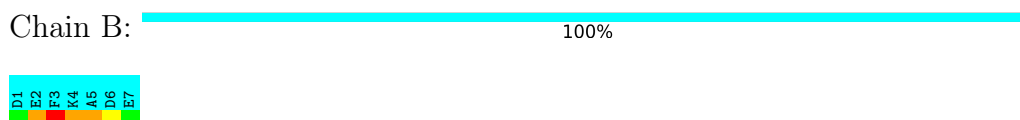


4.2.13 Score per residue for model 13

- Molecule 1: Advanced glycosylation end product-specific receptor

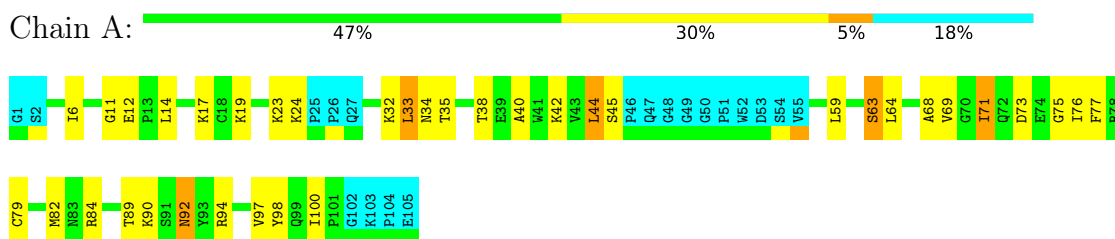


- Molecule 2: Serum albumin peptide



4.2.14 Score per residue for model 14

- Molecule 1: Advanced glycosylation end product-specific receptor



- Molecule 2: Serum albumin peptide

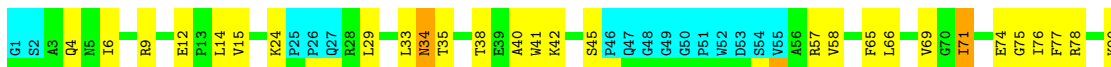




4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Advanced glycosylation end product-specific receptor

Chain A: 51% 28% 18%



- Molecule 2: Serum albumin peptide

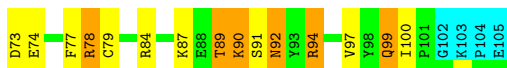
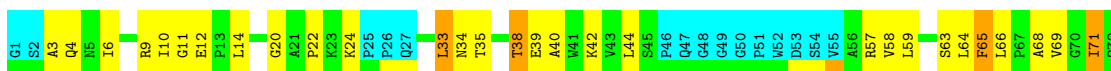
Chain B: 100%



4.2.16 Score per residue for model 16

- Molecule 1: Advanced glycosylation end product-specific receptor

Chain A: 40% 32% 10% 18%



- Molecule 2: Serum albumin peptide

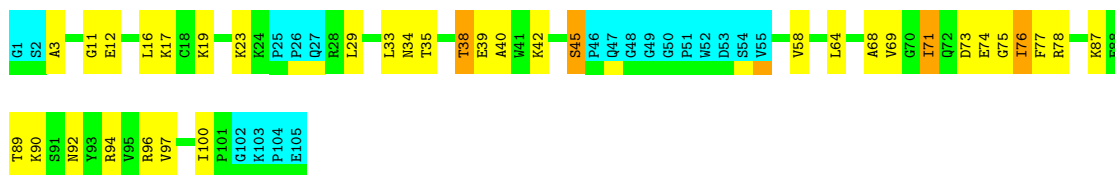
Chain B: 100%



4.2.17 Score per residue for model 17

- Molecule 1: Advanced glycosylation end product-specific receptor

Chain A: 49% 30% 18%



- Molecule 2: Serum albumin peptide

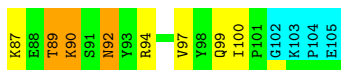
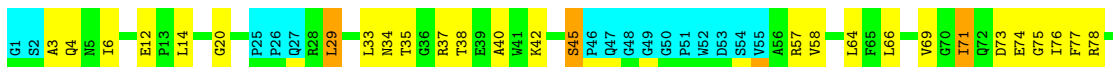
Chain B: 100%



4.2.18 Score per residue for model 18

- Molecule 1: Advanced glycosylation end product-specific receptor

Chain A: 49% 28% 6% 18%



- Molecule 2: Serum albumin peptide

Chain B: 100%



4.2.19 Score per residue for model 19

- Molecule 1: Advanced glycosylation end product-specific receptor

Chain A: 45% 32% 5% 18%



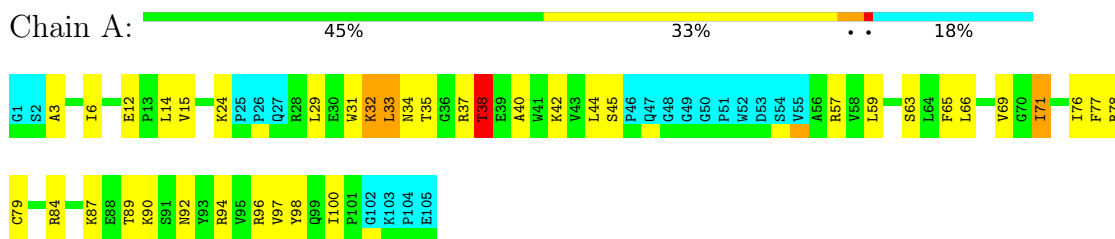
- Molecule 2: Serum albumin peptide

Chain B: 100%

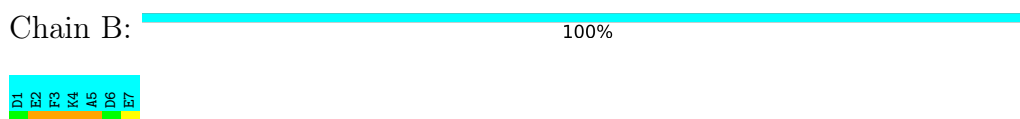


4.2.20 Score per residue for model 20

- Molecule 1: Advanced glycosylation end product-specific receptor

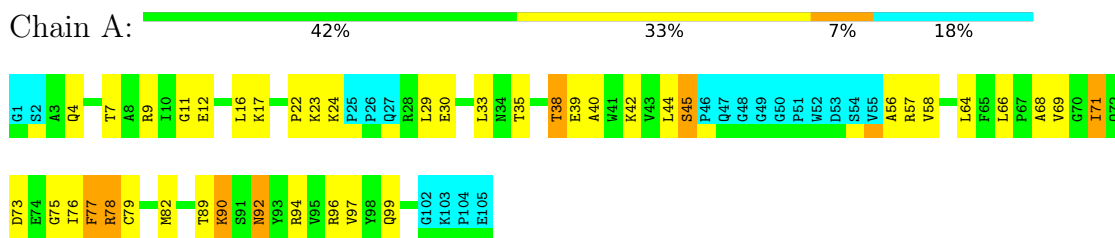


- Molecule 2: Serum albumin peptide



4.2.21 Score per residue for model 21

- Molecule 1: Advanced glycosylation end product-specific receptor

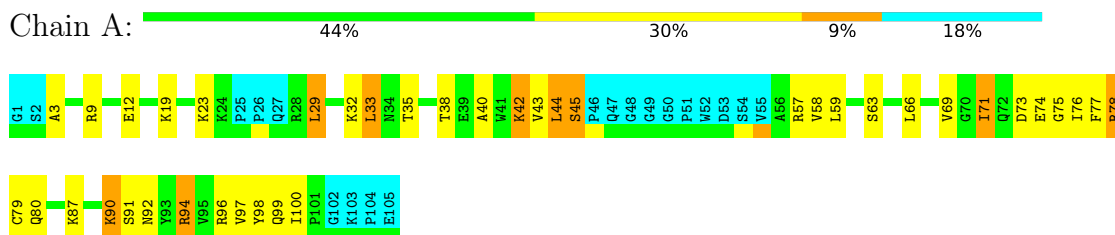


- Molecule 2: Serum albumin peptide



4.2.22 Score per residue for model 22

- Molecule 1: Advanced glycosylation end product-specific receptor



- Molecule 2: Serum albumin peptide

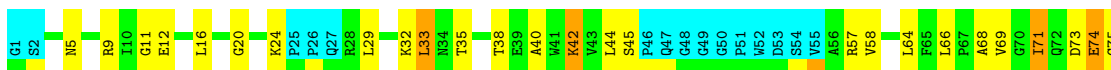
Chain B:  100%



4.2.23 Score per residue for model 23

- Molecule 1: Advanced glycosylation end product-specific receptor

Chain A:  49% 25% 9% 18%



- Molecule 2: Serum albumin peptide

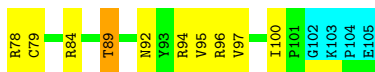
Chain B:  100%



4.2.24 Score per residue for model 24

- Molecule 1: Advanced glycosylation end product-specific receptor

Chain A:  46% 30% 5% 18%



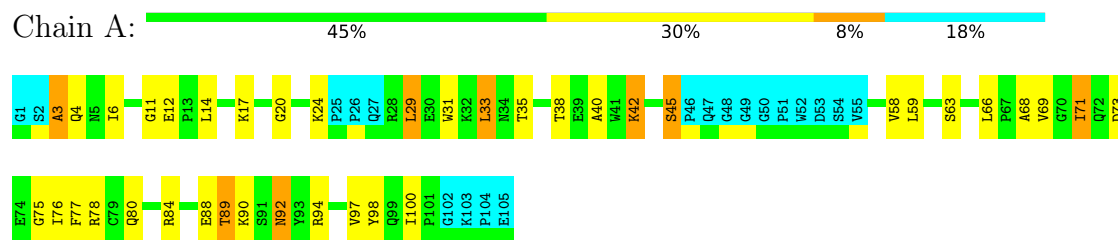
- Molecule 2: Serum albumin peptide

Chain B:  100%



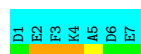
4.2.25 Score per residue for model 25

- Molecule 1: Advanced glycosylation end product-specific receptor



- Molecule 2: Serum albumin peptide

Chain B:  100%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 30 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
CYANA	structure solution	2.1
CYANA	refinement	2.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1092
Number of shifts mapped to atoms	959
Number of unparsed shifts	0
Number of shifts with mapping errors	133
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

6 Model quality i

6.1 Standard geometry i

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

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 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	681	592	713	18±4
2	B	0	0	0	0±0
All	All	17025	14800	17843	451

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:HD21	1:A:44:LEU:HD23	0.93	1.41	22	1
1:A:8:ALA:HB1	1:A:69:VAL:HG21	0.82	1.52	11	2
1:A:16:LEU:HD12	1:A:64:LEU:HD23	0.77	1.54	21	11
1:A:66:LEU:HD22	1:A:69:VAL:HG12	0.74	1.60	16	19
1:A:29:LEU:HD11	1:A:31:TRP:CE3	0.74	2.17	10	1
1:A:33:LEU:N	1:A:33:LEU:HD13	0.74	1.97	22	1
1:A:33:LEU:HD21	1:A:44:LEU:HD22	0.74	1.60	13	1
1:A:35:THR:O	1:A:40:ALA:HB3	0.73	1.84	21	25
1:A:6:ILE:HG21	1:A:14:LEU:HD11	0.72	1.61	15	6
1:A:45:SER:O	1:A:58:VAL:HG21	0.72	1.84	6	15
1:A:12:GLU:O	1:A:69:VAL:HG22	0.72	1.85	8	25

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:HD13	1:A:77:PHE:CE2	0.72	2.20	5	7
1:A:33:LEU:HD12	1:A:77:PHE:CE2	0.71	2.20	25	2
1:A:71:ILE:HA	1:A:97:VAL:HG21	0.70	1.62	8	25
1:A:44:LEU:HD11	1:A:64:LEU:HD13	0.70	1.62	14	1
1:A:33:LEU:HD21	1:A:35:THR:HG23	0.69	1.64	6	2
1:A:33:LEU:HD11	1:A:35:THR:HG23	0.69	1.63	10	3
1:A:33:LEU:HD22	1:A:77:PHE:CE2	0.67	2.24	15	7
1:A:33:LEU:HD12	1:A:77:PHE:CD2	0.67	2.25	22	2
1:A:33:LEU:HD22	1:A:34:ASN:N	0.67	2.04	10	3
1:A:75:GLY:C	1:A:76:ILE:HD12	0.67	2.10	7	13
1:A:33:LEU:HD22	1:A:77:PHE:CD2	0.66	2.25	14	2
1:A:33:LEU:HD21	1:A:44:LEU:HD12	0.66	1.67	23	3
1:A:33:LEU:HD13	1:A:77:PHE:CD2	0.65	2.26	4	5
1:A:75:GLY:O	1:A:76:ILE:HD13	0.64	1.92	22	5
1:A:32:LYS:C	1:A:33:LEU:HD13	0.64	2.13	22	1
1:A:66:LEU:HD22	1:A:69:VAL:CG1	0.64	2.23	12	6
1:A:33:LEU:HD12	1:A:42:LYS:HE3	0.63	1.69	11	3
1:A:16:LEU:HD13	1:A:77:PHE:CD2	0.62	2.29	19	2
1:A:33:LEU:HD11	1:A:77:PHE:CE2	0.62	2.30	9	1
1:A:33:LEU:C	1:A:33:LEU:HD13	0.61	2.16	10	3
1:A:11:GLY:HA2	1:A:68:ALA:HB1	0.61	1.71	1	14
1:A:32:LYS:O	1:A:33:LEU:HD23	0.61	1.96	20	3
1:A:37:ARG:O	1:A:38:THR:HG23	0.60	1.96	20	2
1:A:74:GLU:CD	1:A:97:VAL:HG22	0.59	2.18	17	3
1:A:75:GLY:C	1:A:76:ILE:HD13	0.59	2.18	22	5
1:A:33:LEU:HD23	1:A:42:LYS:HE3	0.59	1.75	22	1
1:A:16:LEU:HD13	1:A:77:PHE:CG	0.58	2.33	6	1
1:A:5:ASN:O	1:A:6:ILE:HD12	0.58	1.98	13	2
1:A:33:LEU:HD22	1:A:42:LYS:HE3	0.58	1.76	1	2
1:A:59:LEU:HD11	1:A:65:PHE:HB2	0.58	1.74	10	2
1:A:29:LEU:HD13	1:A:31:TRP:CE2	0.58	2.34	1	2
1:A:57:ARG:O	1:A:64:LEU:HD12	0.57	1.99	12	4
1:A:33:LEU:O	1:A:33:LEU:HD23	0.57	1.99	25	1
1:A:56:ALA:HB2	1:A:66:LEU:HD23	0.57	1.75	3	4
1:A:20:GLY:CA	1:A:89:THR:HG21	0.57	2.29	24	6
1:A:66:LEU:CD2	1:A:69:VAL:HG12	0.57	2.30	8	6
1:A:33:LEU:HD11	1:A:44:LEU:HG	0.57	1.77	14	1
1:A:14:LEU:O	1:A:66:LEU:HD12	0.56	2.00	12	8
1:A:29:LEU:HD11	1:A:31:TRP:CE2	0.56	2.34	11	1
1:A:33:LEU:HD12	1:A:77:PHE:HA	0.55	1.78	21	1
1:A:33:LEU:HD11	1:A:35:THR:CG2	0.55	2.30	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:HD12	1:A:77:PHE:HB2	0.55	1.79	6	1
1:A:29:LEU:HD12	1:A:29:LEU:O	0.55	2.01	1	6
1:A:6:ILE:CG2	1:A:14:LEU:HD11	0.55	2.32	14	5
1:A:44:LEU:HD13	1:A:64:LEU:HD13	0.54	1.77	7	1
1:A:29:LEU:HD22	1:A:31:TRP:CZ2	0.54	2.37	7	2
1:A:33:LEU:N	1:A:33:LEU:CD1	0.54	2.69	22	1
1:A:29:LEU:HD11	1:A:31:TRP:CZ2	0.54	2.38	11	1
1:A:33:LEU:HD12	1:A:34:ASN:N	0.54	2.18	19	3
1:A:64:LEU:HD12	1:A:65:PHE:N	0.54	2.18	16	3
1:A:74:GLU:HG3	1:A:97:VAL:HG22	0.54	1.79	7	3
1:A:59:LEU:HD12	1:A:63:SER:CB	0.53	2.34	20	6
1:A:15:VAL:HG22	1:A:65:PHE:CD1	0.53	2.39	8	3
1:A:33:LEU:HD21	1:A:35:THR:CG2	0.53	2.33	6	2
1:A:29:LEU:HD13	1:A:31:TRP:CZ3	0.52	2.40	5	1
1:A:59:LEU:HD12	1:A:63:SER:HB3	0.52	1.80	14	1
1:A:59:LEU:HD12	1:A:63:SER:HB2	0.52	1.80	25	7
1:A:33:LEU:CD2	1:A:44:LEU:HD22	0.51	2.34	13	1
1:A:32:LYS:HE2	1:A:43:VAL:HG22	0.51	1.81	1	1
1:A:29:LEU:HD12	1:A:30:GLU:N	0.51	2.20	10	1
1:A:15:VAL:HG22	1:A:65:PHE:CD2	0.51	2.41	5	5
1:A:33:LEU:CD1	1:A:35:THR:HG23	0.51	2.36	8	6
1:A:32:LYS:C	1:A:33:LEU:HD23	0.51	2.25	14	3
1:A:33:LEU:HD22	1:A:33:LEU:H	0.51	1.66	22	1
1:A:29:LEU:HD13	1:A:31:TRP:CZ2	0.50	2.41	7	2
1:A:44:LEU:CD1	1:A:64:LEU:HD13	0.50	2.36	14	2
1:A:69:VAL:O	1:A:69:VAL:HG23	0.50	2.07	15	5
1:A:33:LEU:HD23	1:A:34:ASN:N	0.50	2.22	17	1
1:A:33:LEU:HD11	1:A:44:LEU:HB2	0.50	1.83	22	1
1:A:5:ASN:C	1:A:6:ILE:HD12	0.50	2.28	24	2
1:A:33:LEU:HD22	1:A:35:THR:HG23	0.50	1.84	17	1
1:A:29:LEU:HD13	1:A:31:TRP:CD1	0.50	2.42	19	1
1:A:16:LEU:HD12	1:A:77:PHE:CD2	0.49	2.43	1	2
1:A:44:LEU:CD1	1:A:64:LEU:HD22	0.49	2.37	14	1
1:A:16:LEU:HD12	1:A:64:LEU:CD2	0.49	2.38	3	2
1:A:76:ILE:HG23	1:A:94:ARG:HD2	0.49	1.83	20	1
1:A:16:LEU:CD1	1:A:64:LEU:HD23	0.49	2.38	8	4
1:A:3:ALA:HB1	1:A:94:ARG:HH11	0.49	1.68	9	3
1:A:16:LEU:HD13	1:A:64:LEU:HD23	0.48	1.84	5	1
1:A:29:LEU:HD11	1:A:31:TRP:CZ3	0.48	2.43	10	1
1:A:10:ILE:HD11	1:A:71:ILE:HG13	0.48	1.85	19	1
1:A:33:LEU:HD12	1:A:42:LYS:CE	0.48	2.39	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:HD23	1:A:77:PHE:CG	0.47	2.43	12	2
1:A:64:LEU:HD21	1:A:77:PHE:CE2	0.47	2.45	11	1
1:A:77:PHE:CE1	1:A:95:VAL:HG21	0.47	2.45	10	2
1:A:76:ILE:HD12	1:A:76:ILE:N	0.47	2.25	18	6
1:A:29:LEU:HD13	1:A:31:TRP:NE1	0.47	2.25	19	1
1:A:74:GLU:CG	1:A:97:VAL:HG22	0.47	2.40	5	2
1:A:33:LEU:HD21	1:A:44:LEU:CD1	0.47	2.39	7	2
1:A:33:LEU:CD2	1:A:44:LEU:HD12	0.46	2.37	23	1
1:A:58:VAL:HG13	1:A:63:SER:O	0.46	2.10	8	6
1:A:41:TRP:CZ2	1:A:43:VAL:HG22	0.46	2.45	13	1
1:A:33:LEU:HD23	1:A:44:LEU:CD1	0.46	2.41	24	2
1:A:33:LEU:HD13	1:A:77:PHE:CG	0.45	2.46	18	2
1:A:33:LEU:HD22	1:A:34:ASN:H	0.45	1.69	10	3
1:A:33:LEU:HD23	1:A:77:PHE:CD2	0.45	2.47	12	1
1:A:35:THR:HG22	1:A:75:GLY:HA3	0.45	1.87	1	2
1:A:33:LEU:HD21	1:A:44:LEU:CD2	0.45	2.40	13	1
1:A:44:LEU:HD12	1:A:64:LEU:HD22	0.44	1.89	14	1
1:A:33:LEU:HD12	1:A:76:ILE:O	0.44	2.13	15	1
1:A:78:ARG:CZ	1:A:92:ASN:HB2	0.44	2.42	25	1
1:A:29:LEU:HD11	1:A:31:TRP:CD2	0.44	2.48	10	1
1:A:71:ILE:HG12	1:A:97:VAL:HG21	0.44	1.89	9	13
1:A:32:LYS:HG3	1:A:43:VAL:HG13	0.44	1.89	22	1
1:A:29:LEU:HD22	1:A:31:TRP:CH2	0.43	2.49	7	1
1:A:20:GLY:HA3	1:A:89:THR:HG21	0.43	1.90	25	3
1:A:33:LEU:HD13	1:A:77:PHE:CD1	0.43	2.48	18	1
1:A:33:LEU:HD22	1:A:42:LYS:CE	0.43	2.44	25	2
1:A:76:ILE:HD12	1:A:94:ARG:HE	0.42	1.74	6	1
1:A:81:ALA:HB3	1:A:89:THR:OG1	0.42	2.14	12	1
1:A:29:LEU:HD21	1:A:31:TRP:CH2	0.41	2.50	10	1
1:A:33:LEU:N	1:A:33:LEU:HD22	0.41	2.31	22	1
1:A:56:ALA:HB2	1:A:66:LEU:HG	0.41	1.92	2	1
1:A:38:THR:HG23	1:A:39:GLU:HG3	0.41	1.92	16	4
1:A:33:LEU:C	1:A:33:LEU:CD1	0.41	2.87	10	1
1:A:15:VAL:O	1:A:16:LEU:HD23	0.41	2.16	11	1
1:A:10:ILE:HD11	1:A:99:GLN:HB2	0.41	1.93	16	1
1:A:32:LYS:O	1:A:78:ARG:O	0.41	2.39	20	1
1:A:44:LEU:HD11	1:A:64:LEU:CD1	0.40	2.40	14	1
1:A:33:LEU:HD21	1:A:44:LEU:CG	0.40	2.46	7	1
1:A:35:THR:HG21	1:A:73:ASP:O	0.40	2.16	24	1
1:A:33:LEU:C	1:A:33:LEU:HD23	0.40	2.37	1	1
1:A:10:ILE:HG23	1:A:70:GLY:HA2	0.40	1.93	12	1

6.3 Torsion angles [i](#)

6.3.1 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 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	86/105 (82%)	79±1 (91±1%)	5±1 (6±1%)	2±1 (3±1%)	8	43
2	B	0	-	-	-	-	-
All	All	2150/2800 (77%)	1966 (91%)	126 (6%)	58 (3%)	8	43

All 6 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	38	THR	25
1	A	98	TYR	14
1	A	3	ALA	10
1	A	22	PRO	5
1	A	19	LYS	3
1	A	24	LYS	1

6.3.2 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 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	72/86 (84%)	55±3 (76±4%)	17±3 (24±4%)	2	26
2	B	0	-	-	-	-
All	All	1800/2275 (79%)	1365 (76%)	435 (24%)	2	26

All 48 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	42	LYS	25
1	A	71	ILE	25

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Mol	Chain	Res	Type	Models (Total)
1	A	89	THR	22
1	A	100	ILE	22
1	A	24	LYS	19
1	A	73	ASP	19
1	A	45	SER	18
1	A	78	ARG	18
1	A	57	ARG	18
1	A	33	LEU	16
1	A	9	ARG	15
1	A	23	LYS	15
1	A	87	LYS	14
1	A	79	CYS	13
1	A	96	ARG	13
1	A	92	ASN	13
1	A	4	GLN	12
1	A	74	GLU	12
1	A	90	LYS	11
1	A	94	ARG	11
1	A	19	LYS	10
1	A	29	LEU	10
1	A	99	GLN	8
1	A	17	LYS	7
1	A	44	LEU	7
1	A	37	ARG	7
1	A	84	ARG	7
1	A	34	ASN	6
1	A	88	GLU	5
1	A	32	LYS	4
1	A	31	TRP	4
1	A	82	MET	4
1	A	91	SER	3
1	A	76	ILE	3
1	A	28	ARG	2
1	A	41	TRP	2
1	A	7	THR	2
1	A	38	THR	2
1	A	80	GLN	2
1	A	12	GLU	1
1	A	66	LEU	1
1	A	61	ASN	1
1	A	5	ASN	1
1	A	98	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	63	SER	1
1	A	65	PHE	1
1	A	30	GLU	1
1	A	77	PHE	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](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Counts	Bond lengths	
						RMSZ	#Z>2
2	KPI	B	4	2	11,13,14	4.06±0.01	4±0 (36±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
2	KPI	B	4	2	10,15,17	5.17±0.02	6±0 (62±4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KPI	B	4	2	-	1±0,13,14,16	-

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	4	KPI	O2-CX2	10.58	1.50	1.22	2	25
2	B	4	KPI	O1-CX2	6.83	1.50	1.30	19	25
2	B	4	KPI	CX2-CX1	4.04	1.54	1.49	25	25
2	B	4	KPI	C1-CX1	2.44	1.54	1.49	13	25

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
2	B	4	KPI	O2-CX2-CX1	9.39	109.39	121.38	12	25
2	B	4	KPI	C1-CX1-CX2	9.03	109.39	118.17	12	25
2	B	4	KPI	O1-CX2-O2	6.22	109.38	123.61	5	25
2	B	4	KPI	C1-CX1-NZ	5.24	109.42	123.11	11	25
2	B	4	KPI	CE-NZ-CX1	4.53	109.36	121.70	15	25
2	B	4	KPI	O1-CX2-CX1	3.18	109.44	116.35	8	25
2	B	4	KPI	CX2-CX1-NZ	2.86	121.96	114.98	9	6

There are no chirality outliers.

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

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	4	KPI	C1-CX1-NZ-CE	8
2	B	4	KPI	CX2-CX1-NZ-CE	8
2	B	4	KPI	NZ-CX1-CX2-O1	2

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no monosaccharides 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 i

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 72% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping i

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1092
Number of shifts mapped to atoms	959
Number of unparsed shifts	0
Number of shifts with mapping errors	133
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 133 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	GLN	HB2	1.981	0.020	1
1	A	4	GLN	HG2	2.464	0.020	1
1	A	5	ASN	HB2	2.67	0.020	1
1	A	9	ARG	HB2	1.604	0.020	2
1	A	9	ARG	HG2	1.295	0.020	1
1	A	9	ARG	HD2	3.071	0.020	1
1	A	10	ILE	HG12	1.065	0.020	1
1	A	12	GLU	HB2	1.887	0.020	1
1	A	12	GLU	HG2	2.114	0.020	1
1	A	13	PRO	HB2	2.225	0.020	1
1	A	14	LEU	HB2	1.267	0.020	2
1	A	16	LEU	HB2	1.548	0.020	1
1	A	17	LYS	HB2	1.681	0.020	1
1	A	17	LYS	HG2	1.386	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	LYS	HE2	3.208	0.020	1
1	A	18	CYS	HB2	2.277	0.020	2
1	A	19	LYS	HB2	1.826	0.020	1
1	A	19	LYS	HG2	1.401	0.020	1
1	A	19	LYS	HD2	1.705	0.020	1
1	A	19	LYS	HE2	2.949	0.020	1
1	A	22	PRO	HB2	1.945	0.020	1
1	A	23	LYS	HB2	1.826	0.020	1
1	A	23	LYS	HG2	1.395	0.020	1
1	A	23	LYS	HD2	1.661	0.020	1
1	A	23	LYS	HE2	2.904	0.020	1
1	A	24	LYS	HB2	1.78	0.020	1
1	A	24	LYS	HD2	1.674	0.020	1
1	A	24	LYS	HE2	2.934	0.020	1
1	A	28	ARG	HB2	1.719	0.020	1
1	A	28	ARG	HG2	1.598	0.020	1
1	A	28	ARG	HD2	3.253	0.020	1
1	A	29	LEU	HB2	1.556	0.020	1
1	A	30	GLU	HB2	2.054	0.020	1
1	A	30	GLU	HG2	2.297	0.020	1
1	A	32	LYS	HB2	1.328	0.020	1
1	A	32	LYS	HG2	1.006	0.020	1
1	A	32	LYS	HD2	1.765	0.020	1
1	A	32	LYS	HE2	2.889	0.020	1
1	A	33	LEU	HB2	1.066	0.020	1
1	A	34	ASN	HB2	2.585	0.020	1
1	A	37	ARG	HB2	1.387	0.020	1
1	A	37	ARG	HG2	1.737	0.020	1
1	A	37	ARG	HD2	2.949	0.020	1
1	A	39	GLU	HB2	1.932	0.020	1
1	A	39	GLU	HG2	2.19	0.020	1
1	A	41	TRP	HB2	2.984	0.020	2
1	A	42	LYS	HB2	1.472	0.020	1
1	A	42	LYS	HG2	1.364	0.020	1
1	A	42	LYS	HD2	1.902	0.020	1
1	A	42	LYS	HE2	2.828	0.020	1
1	A	44	LEU	HB2	1.423	0.020	1
1	A	45	SER	HB2	3.872	0.020	1
1	A	46	PRO	HB2	2.375	0.020	2
1	A	47	GLN	HB2	2.034	0.020	1
1	A	47	GLN	HG2	2.297	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	PRO	HB2	2.063	0.020	2
1	A	52	TRP	HB2	3.409	0.020	2
1	A	53	ASP	HB2	2.645	0.020	2
1	A	54	SER	HB2	3.736	0.020	1
1	A	57	ARG	HB2	1.751	0.020	1
1	A	57	ARG	HG2	1.358	0.020	1
1	A	57	ARG	HD2	3.091	0.020	1
1	A	59	LEU	HB2	1.731	0.020	1
1	A	60	PRO	HB2	2.299	0.020	2
1	A	61	ASN	HB2	3.146	0.020	2
1	A	63	SER	HB2	3.611	0.020	1
1	A	64	LEU	HB2	1.947	0.020	1
1	A	65	PHE	HB2	2.801	0.020	2
1	A	66	LEU	HB2	1.524	0.020	1
1	A	67	PRO	HB2	1.932	0.020	2
1	A	71	ILE	HG12	1.401	0.020	2
1	A	72	GLN	HB2	2.188	0.020	1
1	A	72	GLN	HG2	2.327	0.020	1
1	A	73	ASP	HB2	2.728	0.020	2
1	A	74	GLU	HB2	2.063	0.020	2
1	A	74	GLU	HG2	2.464	0.020	1
1	A	76	ILE	HG12	0.978	0.020	1
1	A	77	PHE	HB2	2.904	0.020	1
1	A	78	ARG	HB2	1.768	0.020	1
1	A	78	ARG	HG2	1.355	0.020	1
1	A	78	ARG	HD2	2.965	0.020	1
1	A	79	CYS	HB2	2.812	0.020	1
1	A	80	GLN	HB2	1.899	0.020	1
1	A	82	MET	HB2	1.798	0.020	1
1	A	82	MET	HG2	2.957	0.020	1
1	A	83	ASN	HB2	2.858	0.020	1
1	A	85	ASN	HB2	2.857	0.020	2
1	A	87	LYS	HB2	1.555	0.020	1
1	A	87	LYS	HG2	1.325	0.020	1
1	A	87	LYS	HD2	1.629	0.020	1
1	A	87	LYS	HE2	2.889	0.020	1
1	A	88	GLU	HB2	1.686	0.020	1
1	A	88	GLU	HG2	2.008	0.020	1
1	A	90	LYS	HB2	1.801	0.020	1
1	A	90	LYS	HG2	1.325	0.020	1
1	A	90	LYS	HD2	1.872	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	90	LYS	HE2	2.889	0.020	1
1	A	91	SER	HB2	3.753	0.020	1
1	A	92	ASN	HB2	2.489	0.020	1
1	A	93	TYR	HB2	3.08	0.020	1
1	A	94	ARG	HB2	1.965	0.020	2
1	A	94	ARG	HG2	1.401	0.020	2
1	A	94	ARG	HD2	3.101	0.020	1
1	A	96	ARG	HB2	1.686	0.020	1
1	A	96	ARG	HG2	1.431	0.020	1
1	A	96	ARG	HD2	2.964	0.020	1
1	A	98	TYR	HB2	3.572	0.020	1
1	A	99	GLN	HB2	2.063	0.020	2
1	A	99	GLN	HG2	2.312	0.020	1
1	A	100	ILE	HG12	1.386	0.020	2
1	A	101	PRO	HB2	2.151	0.020	2
1	A	103	LYS	HB2	1.598	0.020	1
1	A	104	PRO	HB2	2.129	0.020	2
1	A	105	GLU	HB2	1.762	0.020	1
1	A	105	GLU	HG2	2.19	0.020	1
1	B	2	GLU	HB2	1.759	0.020	2
1	B	2	GLU	HG2	1.96	0.020	2
1	B	3	PHE	HB2	2.968	0.020	2
1	B	4	MCL	H	8.008	0.020	1
1	B	4	MCL	HA	4.114	0.020	1
1	B	4	MCL	HB2	1.618	0.020	1
1	B	4	MCL	HD2	1.531	0.020	1
1	B	4	MCL	HD3	1.531	0.020	1
1	B	4	MCL	HE2	3.977	0.020	1
1	B	4	MCL	HE3	2.856	0.020	1
1	B	4	MCL	HG2	1.217	0.020	1
1	B	4	MCL	HG3	1.217	0.020	1
1	B	4	MCL	H11	1.732	0.020	1
1	B	4	MCL	H12	1.732	0.020	1
1	B	4	MCL	H13	1.732	0.020	1
1	B	6	ASP	HB2	2.619	0.020	2
1	B	7	GLU	HB2	1.93	0.020	2
1	B	7	GLU	HG2	2.154	0.020	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	96	-0.06 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	84	0.23 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}'$	83	-5.03 ± 0.35	Should be applied
^{15}N	92	-0.72 ± 0.37	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 76%, i.e. 929 atoms were assigned a chemical shift out of a possible 1227. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	399/427 (93%)	170/174 (98%)	150/172 (87%)	79/81 (98%)
Sidechain	530/738 (72%)	379/477 (79%)	151/219 (69%)	0/42 (0%)
Aromatic	0/62 (0%)	0/30 (0%)	0/30 (0%)	0/2 (0%)
Overall	929/1227 (76%)	549/681 (81%)	301/421 (71%)	79/125 (63%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 1079 atoms were assigned a chemical shift out of a possible 1506. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	483/547 (88%)	212/224 (95%)	179/222 (81%)	92/101 (91%)
Sidechain	591/875 (68%)	425/563 (75%)	166/267 (62%)	0/45 (0%)
Aromatic	5/84 (6%)	5/41 (12%)	0/40 (0%)	0/3 (0%)
Overall	1079/1506 (72%)	642/828 (78%)	345/529 (65%)	92/149 (62%)

7.1.4 Statistically unusual chemical shifts [i](#)

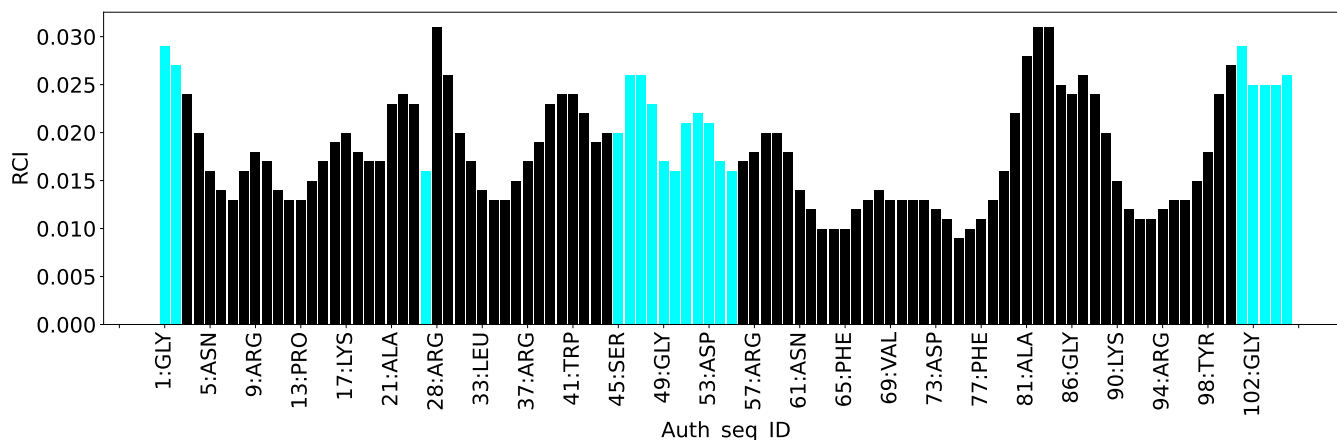
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	35	THR	HB	2.05	2.57 – 5.77	-6.6
1	A	2	SER	CB	73.64	56.28 – 71.32	6.5
1	A	75	GLY	C	184.57	164.92 – 182.89	5.9
1	A	63	SER	C	184.66	166.15 – 183.14	5.9

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

