



Full wwPDB NMR Structure Validation Report ⓘ

Feb 28, 2026 – 05:40 PM UTC

PDB ID : 2L27 / pdb_00002L27
Title : NMR Structure of the ECD1 of CRF-R1 in complex with a peptide agonist
Authors : Grace, C.R.R.; Perrin, M.H.; Gulyas, J.R.R.; Rivier, J.E.; Vale, W.W.; Riek, R.R.
Deposited on : 2010-08-12

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

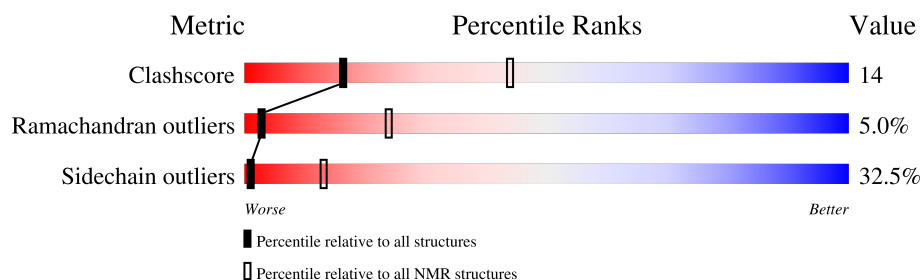
1 Overall quality at a glance

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	84	32% 52% • 12%
2	B	38	45% 42% 13%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 13 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:129-A:136, A:142-A:207, B:325-B:341 (91)	1.73	13
2	B:309-B:324 (16)	0.83	3

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1866 atoms, of which 917 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Corticotropin-releasing factor receptor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	84	Total	C	H	N	O	S	0
			1256	400	607	116	127	6	

- Molecule 2 is a protein called peptide agonist.

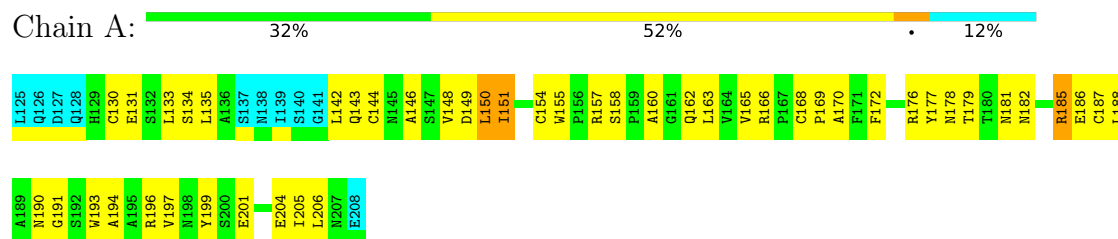
Mol	Chain	Residues	Atoms					Trace
2	B	38	Total	C	H	N	O	0
			610	190	310	49	61	

4 Residue-property plots

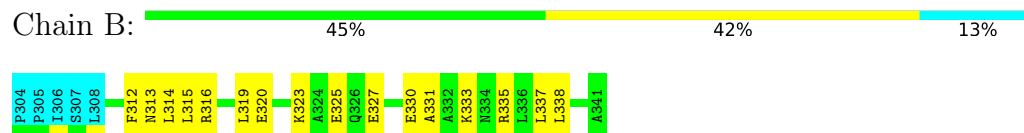
4.1 Average score per residue in the NMR ensemble

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: Corticotropin-releasing factor receptor 1



- Molecule 2: peptide agonist

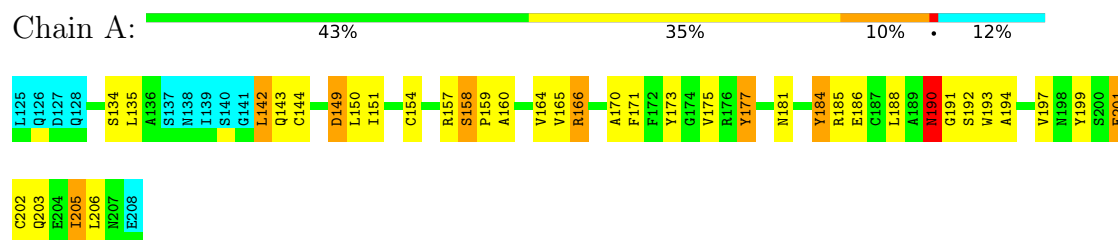


4.2 Scores per residue for each member of the ensemble

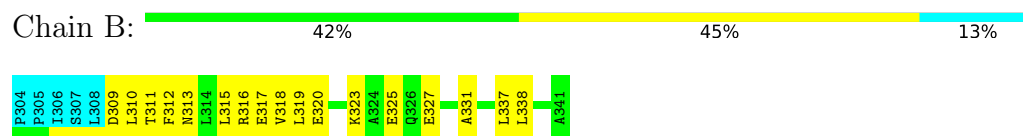
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Corticotropin-releasing factor receptor 1

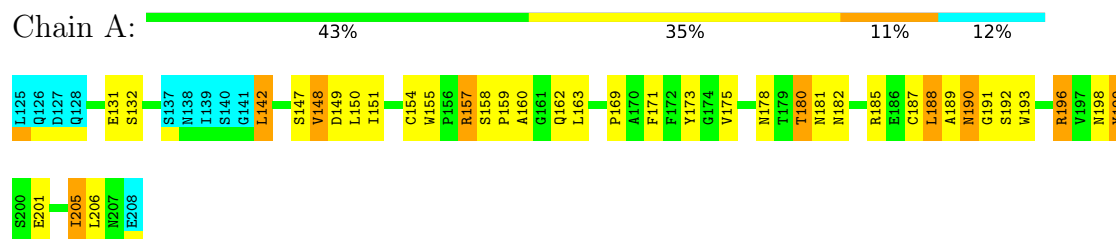


- Molecule 2: peptide agonist

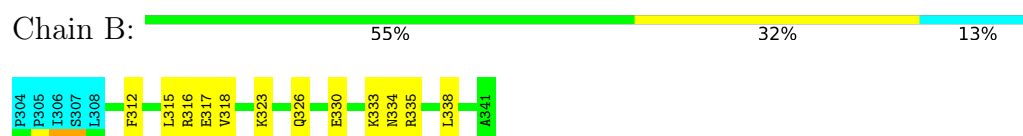


4.2.2 Score per residue for model 2

- Molecule 1: Corticotropin-releasing factor receptor 1

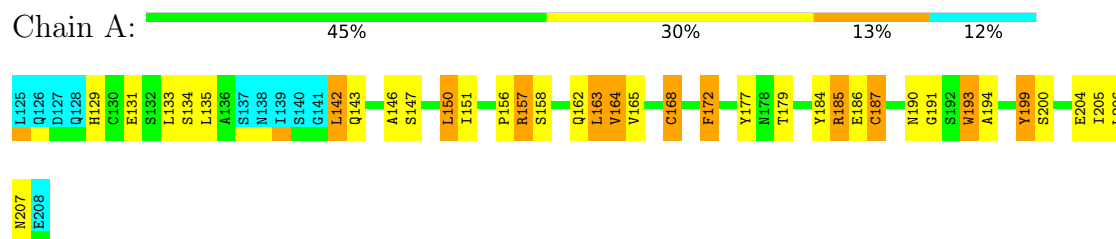


- Molecule 2: peptide agonist

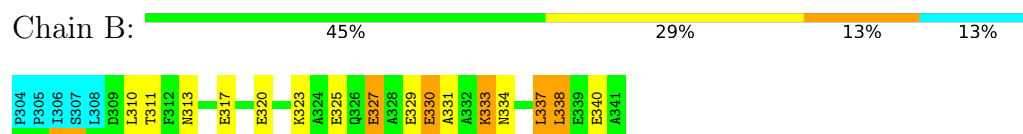


4.2.3 Score per residue for model 3

- Molecule 1: Corticotropin-releasing factor receptor 1

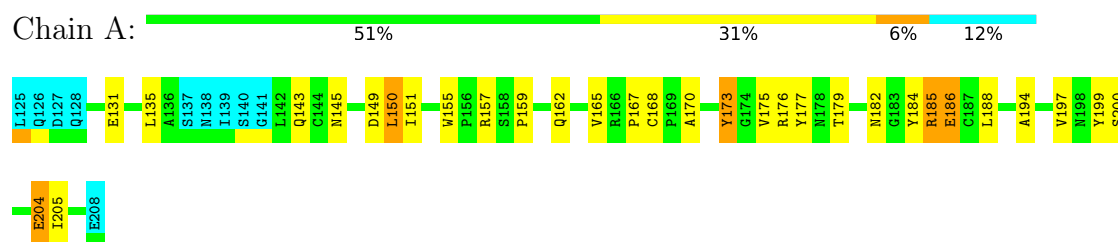


- Molecule 2: peptide agonist

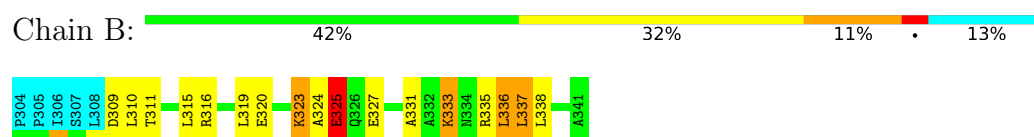


4.2.4 Score per residue for model 4

- Molecule 1: Corticotropin-releasing factor receptor 1

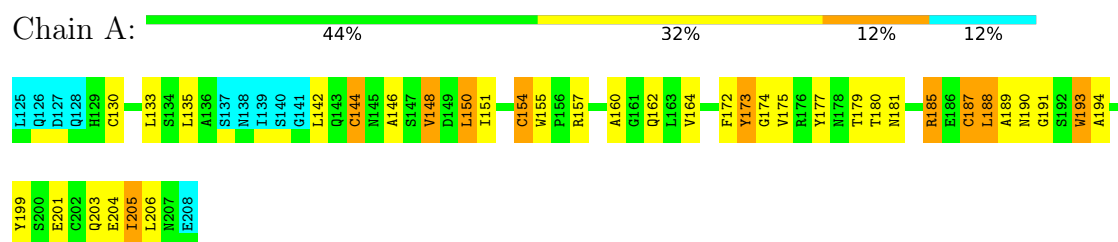


- Molecule 2: peptide agonist

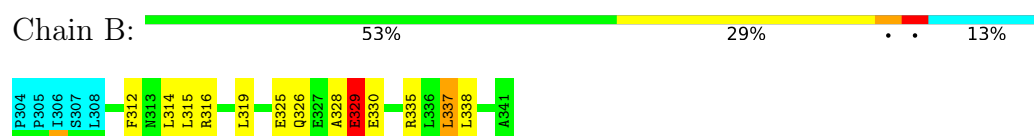


4.2.5 Score per residue for model 5

- Molecule 1: Corticotropin-releasing factor receptor 1

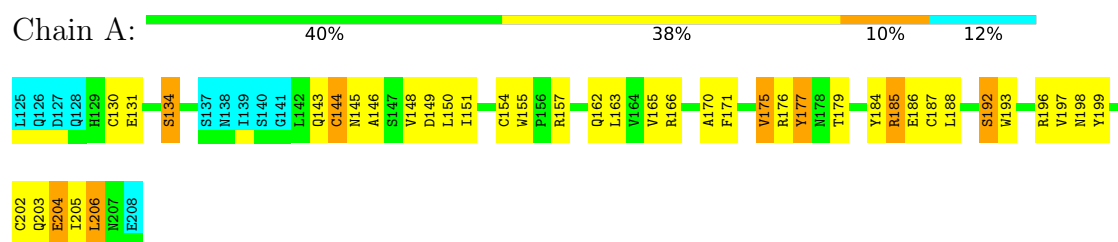


- Molecule 2: peptide agonist

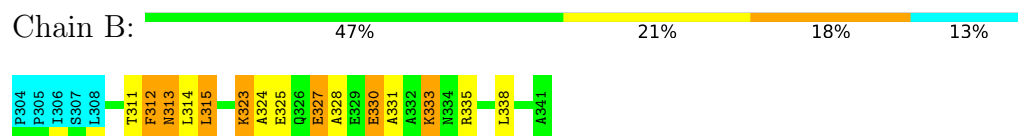


4.2.6 Score per residue for model 6

- Molecule 1: Corticotropin-releasing factor receptor 1

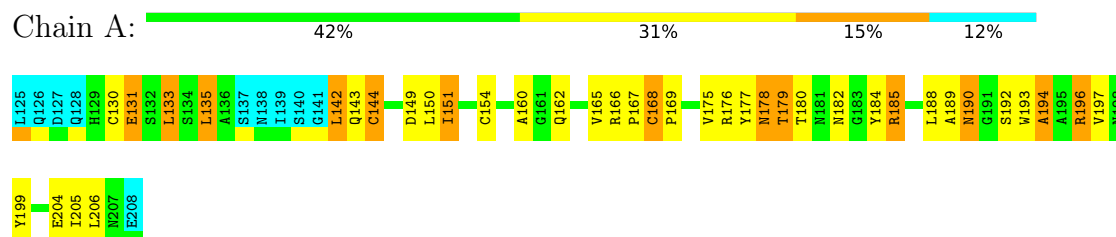


- Molecule 2: peptide agonist

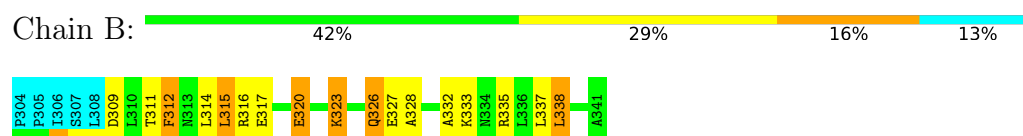


4.2.7 Score per residue for model 7

- Molecule 1: Corticotropin-releasing factor receptor 1

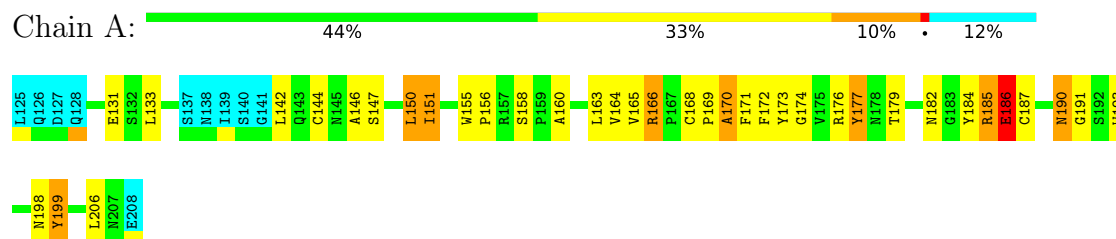


- Molecule 2: peptide agonist

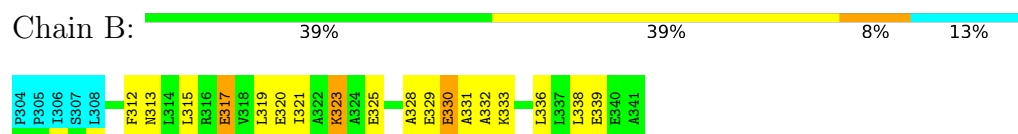


4.2.8 Score per residue for model 8

- Molecule 1: Corticotropin-releasing factor receptor 1

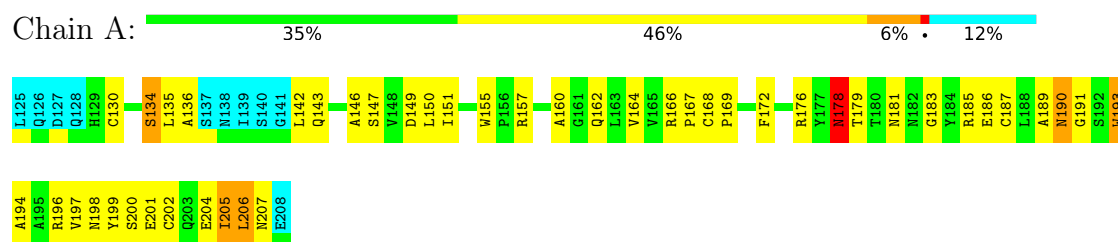


- Molecule 2: peptide agonist

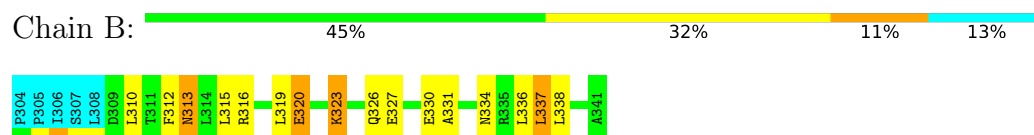


4.2.9 Score per residue for model 9

- Molecule 1: Corticotropin-releasing factor receptor 1

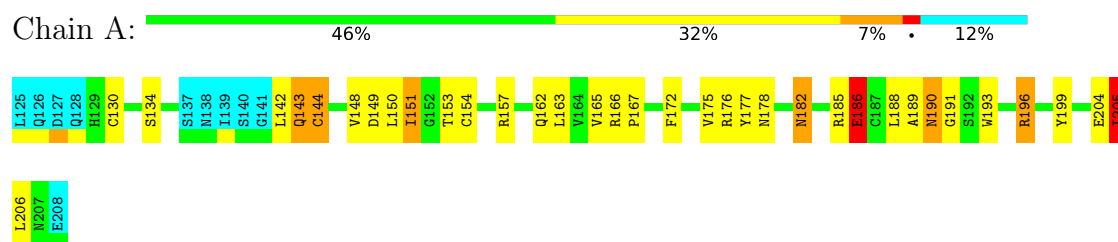


- Molecule 2: peptide agonist

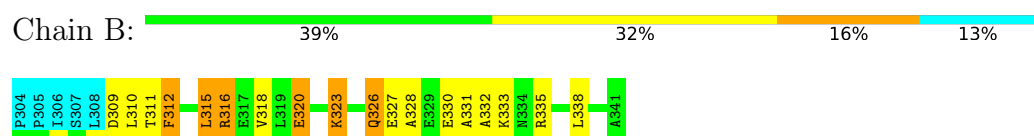


4.2.10 Score per residue for model 10

- Molecule 1: Corticotropin-releasing factor receptor 1

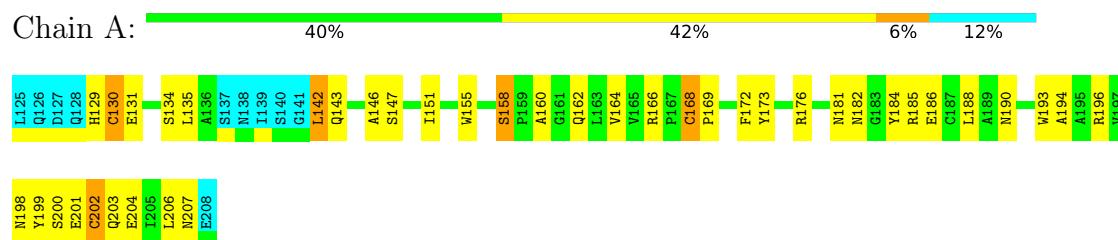


- Molecule 2: peptide agonist

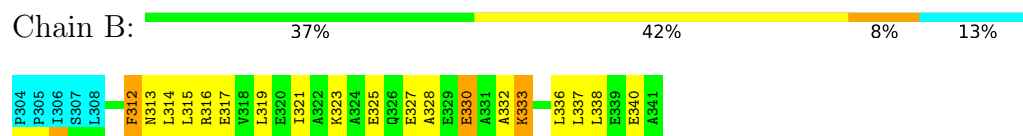


4.2.11 Score per residue for model 11

- Molecule 1: Corticotropin-releasing factor receptor 1

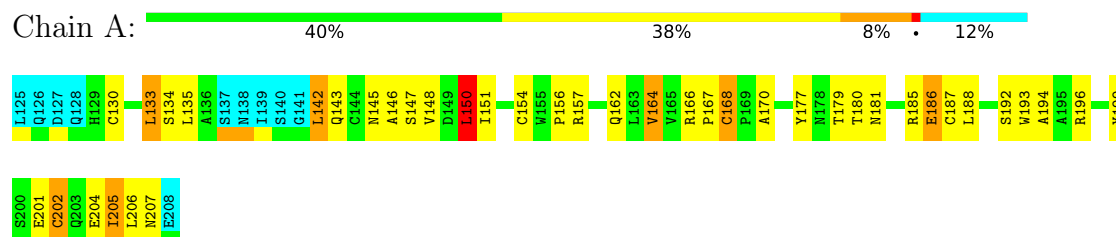


- Molecule 2: peptide agonist

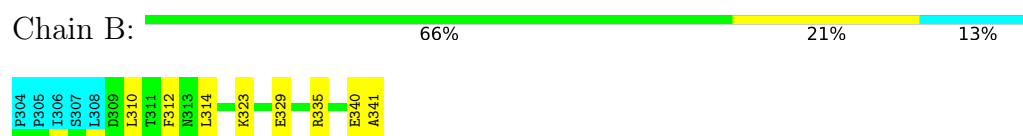


4.2.12 Score per residue for model 12

- Molecule 1: Corticotropin-releasing factor receptor 1

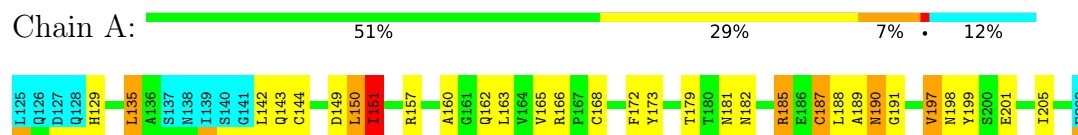


- Molecule 2: peptide agonist

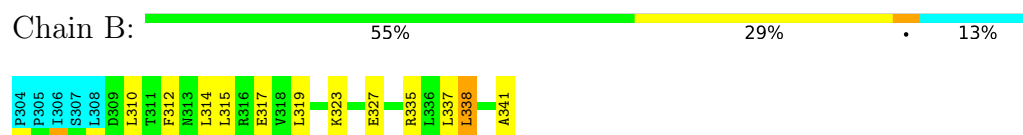


4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Corticotropin-releasing factor receptor 1



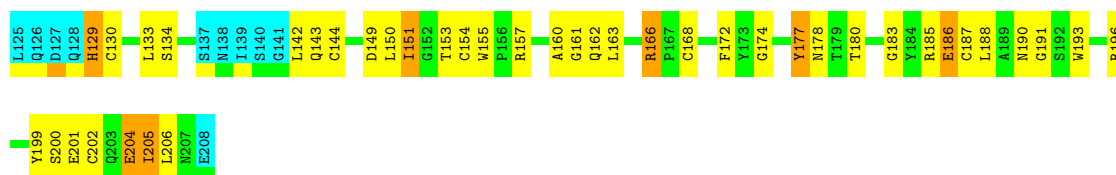
- Molecule 2: peptide agonist



4.2.14 Score per residue for model 14

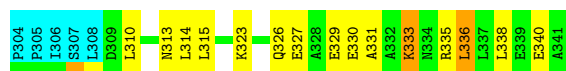
- Molecule 1: Corticotropin-releasing factor receptor 1





- Molecule 2: peptide agonist

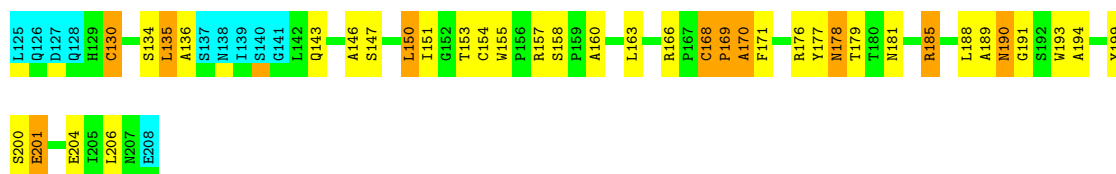
Chain B: 47% 34% 5% 13%



4.2.15 Score per residue for model 15

- Molecule 1: Corticotropin-releasing factor receptor 1

Chain A: 43% 33% 12% 12%



- Molecule 2: peptide agonist

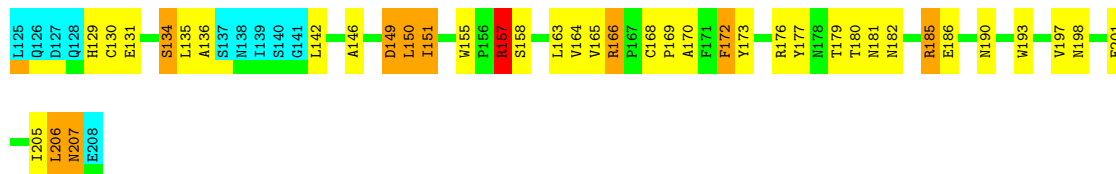
Chain B: 45% 37% 5% 13%



4.2.16 Score per residue for model 16

- Molecule 1: Corticotropin-releasing factor receptor 1

Chain A: 42% 35% 11% 12%



- Molecule 2: peptide agonist

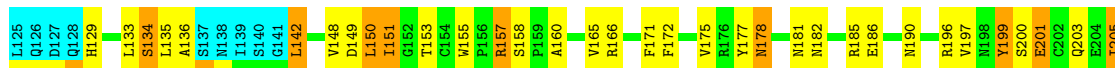
Chain B: 50% 34% 13%



4.2.17 Score per residue for model 17

- Molecule 1: Corticotropin-releasing factor receptor 1

Chain A:



- Molecule 2: peptide agonist

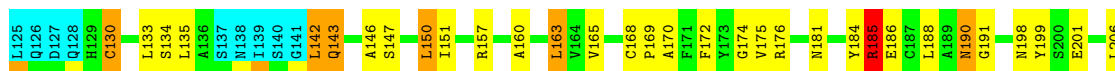
Chain B:



4.2.18 Score per residue for model 18

- Molecule 1: Corticotropin-releasing factor receptor 1

Chain A:



- Molecule 2: peptide agonist

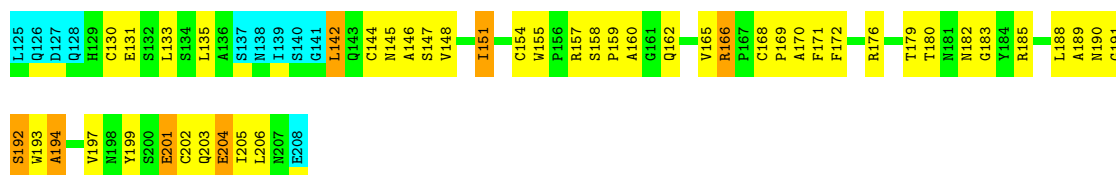
Chain B:



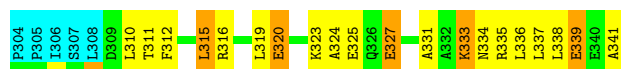
4.2.19 Score per residue for model 19

- Molecule 1: Corticotropin-releasing factor receptor 1

Chain A:

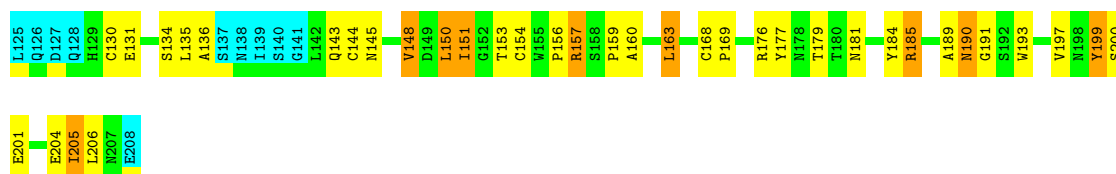


- Molecule 2: peptide agonist



4.2.20 Score per residue for model 20

- Molecule 1: Corticotropin-releasing factor receptor 1



- Molecule 2: peptide agonist



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	573	538	537	18±4
2	B	264	267	267	7±3
All	All	16740	16100	16080	465

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:328:ALA:HA	2:B:332:ALA:HB2	0.83	1.50	15	1
1:A:160:ALA:HB1	1:A:189:ALA:HA	0.82	1.51	19	8
1:A:175:VAL:HG21	1:A:204:GLU:HG2	0.78	1.53	6	1
1:A:151:ILE:HG21	2:B:338:LEU:HG	0.78	1.55	14	1
1:A:170:ALA:HB1	1:A:176:ARG:O	0.77	1.80	6	1
1:A:150:LEU:HD22	2:B:341:ALA:HB2	0.77	1.55	12	1
1:A:177:TYR:HA	1:A:205:ILE:HD11	0.74	1.57	20	1
1:A:178:ASN:HB2	1:A:205:ILE:HD11	0.74	1.56	14	1
1:A:142:LEU:HD12	1:A:160:ALA:HB3	0.72	1.59	11	1
1:A:185:ARG:O	1:A:194:ALA:HB3	0.71	1.85	11	2
1:A:175:VAL:HG21	1:A:204:GLU:CG	0.70	2.16	6	2
1:A:134:SER:HB2	1:A:146:ALA:HB3	0.67	1.65	9	1
1:A:150:LEU:HD13	1:A:151:ILE:N	0.67	2.04	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:327:GLU:O	2:B:331:ALA:HB3	0.67	1.90	15	3
1:A:178:ASN:HB2	1:A:205:ILE:HD12	0.66	1.65	10	2
1:A:142:LEU:HD22	1:A:160:ALA:HB3	0.66	1.63	2	1
1:A:130:CYS:O	1:A:146:ALA:HB1	0.66	1.91	9	1
1:A:179:THR:O	1:A:179:THR:HG23	0.66	1.90	19	7
1:A:170:ALA:HB2	1:A:179:THR:HG23	0.65	1.66	12	1
1:A:175:VAL:HG11	1:A:204:GLU:CD	0.65	2.16	7	1
1:A:185:ARG:HD3	1:A:194:ALA:HB3	0.65	1.68	3	1
1:A:151:ILE:HG22	2:B:337:LEU:HG	0.64	1.66	16	1
1:A:130:CYS:HB3	1:A:146:ALA:HB1	0.64	1.69	15	3
1:A:142:LEU:HD12	1:A:160:ALA:CB	0.64	2.22	11	1
2:B:325:GLU:HA	2:B:328:ALA:HB3	0.63	1.69	15	2
2:B:327:GLU:HA	2:B:331:ALA:HB3	0.63	1.70	9	4
1:A:165:VAL:HG22	1:A:182:ASN:HB3	0.62	1.72	13	3
1:A:130:CYS:CB	1:A:146:ALA:HB1	0.62	2.24	19	1
1:A:149:ASP:HB3	1:A:151:ILE:HD13	0.61	1.72	17	2
1:A:181:ASN:HB2	1:A:201:GLU:HB3	0.61	1.72	1	3
1:A:150:LEU:HD23	1:A:151:ILE:HG23	0.61	1.73	16	2
2:B:333:LYS:HA	2:B:336:LEU:HD23	0.60	1.74	14	1
1:A:163:LEU:HD21	1:A:184:TYR:CD1	0.59	2.32	20	1
1:A:142:LEU:HB3	1:A:160:ALA:HB3	0.59	1.72	7	2
1:A:151:ILE:HD11	1:A:199:TYR:CE1	0.59	2.33	15	1
1:A:170:ALA:HB2	1:A:179:THR:HB	0.59	1.74	4	1
1:A:178:ASN:CB	1:A:205:ILE:HD11	0.59	2.28	14	1
1:A:155:TRP:CE3	1:A:166:ARG:HD3	0.59	2.33	16	1
2:B:312:PHE:CD2	2:B:315:LEU:HD21	0.58	2.33	10	2
1:A:151:ILE:HD11	1:A:199:TYR:CE2	0.58	2.33	5	2
1:A:155:TRP:CH2	1:A:197:VAL:HG21	0.58	2.34	4	1
1:A:155:TRP:CH2	1:A:166:ARG:HB3	0.58	2.34	6	1
2:B:312:PHE:CD2	2:B:315:LEU:HD11	0.57	2.34	7	2
2:B:334:ASN:O	2:B:338:LEU:HD22	0.57	1.99	17	1
1:A:204:GLU:HG2	1:A:206:LEU:HD21	0.57	1.75	19	1
1:A:185:ARG:HG2	1:A:197:VAL:HG13	0.57	1.74	9	1
1:A:199:TYR:HB3	2:B:338:LEU:HD12	0.57	1.76	17	2
1:A:206:LEU:HD22	2:B:327:GLU:HB3	0.56	1.75	6	1
1:A:177:TYR:O	1:A:178:ASN:CB	0.56	2.52	17	1
1:A:206:LEU:HD22	1:A:207:ASN:N	0.56	2.14	16	1
1:A:155:TRP:CD2	1:A:185:ARG:HG3	0.56	2.36	16	1
1:A:205:ILE:HD13	1:A:205:ILE:N	0.56	2.16	20	4
1:A:142:LEU:HD22	1:A:160:ALA:CB	0.56	2.31	17	2
1:A:181:ASN:CB	1:A:201:GLU:HB3	0.56	2.31	1	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:ARG:CG	1:A:197:VAL:HG13	0.56	2.31	9	1
1:A:206:LEU:HD22	2:B:327:GLU:CD	0.55	2.26	11	1
1:A:150:LEU:N	1:A:150:LEU:HD22	0.55	2.16	16	1
1:A:177:TYR:HA	1:A:204:GLU:HA	0.55	1.79	3	1
1:A:150:LEU:HD23	2:B:337:LEU:HB2	0.55	1.79	3	1
1:A:142:LEU:HD21	1:A:190:ASN:N	0.55	2.17	9	1
2:B:317:GLU:HG3	2:B:318:VAL:N	0.55	2.16	1	2
1:A:135:LEU:O	1:A:136:ALA:HB3	0.54	2.02	9	1
1:A:187:CYS:HA	1:A:194:ALA:HA	0.54	1.78	3	1
1:A:167:PRO:HA	1:A:182:ASN:HA	0.54	1.80	10	3
1:A:204:GLU:OE1	2:B:331:ALA:HB1	0.54	2.02	4	1
1:A:181:ASN:HB3	1:A:201:GLU:HB3	0.54	1.78	15	6
1:A:144:CYS:HB2	1:A:193:TRP:CE2	0.54	2.38	7	3
2:B:337:LEU:C	2:B:337:LEU:HD13	0.54	2.27	17	3
1:A:150:LEU:C	1:A:151:ILE:HD13	0.54	2.27	8	1
1:A:150:LEU:HB3	1:A:151:ILE:HD13	0.54	1.79	8	1
1:A:206:LEU:HD21	2:B:326:GLN:HG3	0.54	1.79	14	1
1:A:142:LEU:HD22	1:A:160:ALA:HB2	0.54	1.79	18	2
1:A:185:ARG:HD3	1:A:194:ALA:CB	0.53	2.32	3	1
1:A:199:TYR:HB3	2:B:338:LEU:HG	0.53	1.81	6	1
1:A:146:ALA:HB1	1:A:155:TRP:O	0.53	2.03	11	1
1:A:163:LEU:HA	1:A:186:GLU:HA	0.53	1.80	8	1
1:A:199:TYR:CD2	2:B:338:LEU:HD13	0.53	2.39	2	1
2:B:328:ALA:O	2:B:329:GLU:C	0.53	2.52	5	1
2:B:334:ASN:O	2:B:338:LEU:HD23	0.53	2.04	2	2
1:A:199:TYR:HB3	2:B:338:LEU:HD23	0.53	1.81	14	1
1:A:169:PRO:O	1:A:170:ALA:HB2	0.53	2.04	15	1
1:A:149:ASP:HB3	1:A:151:ILE:CD1	0.53	2.34	17	2
1:A:178:ASN:HB3	1:A:205:ILE:HD12	0.52	1.81	9	1
1:A:181:ASN:HB2	1:A:202:CYS:HA	0.52	1.80	12	1
1:A:176:ARG:HB2	1:A:206:LEU:HB2	0.52	1.81	9	1
2:B:333:LYS:NZ	2:B:334:ASN:OD1	0.52	2.38	19	1
1:A:148:VAL:HG13	1:A:154:CYS:CA	0.52	2.35	2	1
1:A:149:ASP:C	1:A:150:LEU:HD22	0.52	2.30	13	1
1:A:133:LEU:HD21	1:A:157:ARG:HB2	0.52	1.80	12	1
1:A:149:ASP:HB3	1:A:150:LEU:HD22	0.52	1.80	1	1
1:A:176:ARG:O	1:A:177:TYR:HB2	0.52	2.04	7	2
1:A:148:VAL:HG22	1:A:154:CYS:HA	0.51	1.81	6	1
1:A:185:ARG:CZ	1:A:197:VAL:HG13	0.51	2.36	20	1
1:A:184:TYR:O	1:A:197:VAL:HG23	0.51	2.06	4	1
1:A:163:LEU:HD11	1:A:184:TYR:CE2	0.51	2.41	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:CYS:SG	1:A:179:THR:HA	0.51	2.46	9	2
1:A:130:CYS:O	1:A:133:LEU:HD23	0.51	2.05	12	1
1:A:148:VAL:HA	1:A:154:CYS:HA	0.50	1.83	10	3
2:B:324:ALA:O	2:B:325:GLU:C	0.50	2.54	4	3
1:A:197:VAL:HG22	2:B:341:ALA:O	0.50	2.06	17	1
1:A:148:VAL:HG13	1:A:154:CYS:HA	0.50	1.82	2	1
1:A:160:ALA:HA	1:A:187:CYS:SG	0.50	2.47	2	1
1:A:168:CYS:HB2	1:A:169:PRO:HD2	0.50	1.84	9	2
1:A:146:ALA:CB	1:A:156:PRO:HA	0.50	2.37	8	1
2:B:319:LEU:HD12	2:B:320:GLU:N	0.50	2.22	19	1
1:A:151:ILE:HG22	1:A:173:TYR:CE2	0.50	2.42	4	1
1:A:165:VAL:HG22	1:A:182:ASN:HB2	0.50	1.81	10	1
1:A:148:VAL:HG12	1:A:154:CYS:HB2	0.50	1.83	19	1
2:B:326:GLN:HG2	2:B:327:GLU:N	0.49	2.21	7	1
2:B:320:GLU:HA	2:B:323:LYS:CG	0.49	2.37	10	1
2:B:313:ASN:HA	2:B:316:ARG:HB3	0.49	1.83	17	1
2:B:327:GLU:HB2	2:B:331:ALA:HB3	0.49	1.82	20	1
2:B:323:LYS:NZ	2:B:324:ALA:HB2	0.49	2.22	6	1
2:B:330:GLU:O	2:B:333:LYS:NZ	0.49	2.41	6	3
1:A:151:ILE:HD11	1:A:199:TYR:CZ	0.49	2.43	7	1
1:A:150:LEU:CD2	1:A:151:ILE:HG23	0.49	2.36	15	2
2:B:337:LEU:C	2:B:337:LEU:HD12	0.49	2.32	9	1
1:A:168:CYS:O	1:A:179:THR:HG22	0.49	2.07	12	2
1:A:185:ARG:HG2	1:A:197:VAL:HG22	0.49	1.85	1	1
1:A:130:CYS:O	1:A:146:ALA:HB3	0.49	2.07	11	1
1:A:165:VAL:CG2	1:A:182:ASN:HB3	0.49	2.38	16	2
1:A:150:LEU:O	2:B:337:LEU:HD11	0.49	2.08	17	1
1:A:193:TRP:O	1:A:194:ALA:HB2	0.49	2.08	7	2
1:A:134:SER:CB	1:A:146:ALA:HB3	0.49	2.37	9	1
1:A:179:THR:O	1:A:179:THR:CG2	0.49	2.59	19	2
1:A:187:CYS:SG	1:A:193:TRP:CZ3	0.48	3.06	5	1
2:B:327:GLU:HA	2:B:331:ALA:CB	0.48	2.36	14	2
1:A:160:ALA:HB1	1:A:189:ALA:CA	0.48	2.36	5	3
1:A:181:ASN:HB3	1:A:201:GLU:HB2	0.48	1.84	17	1
1:A:199:TYR:HB3	2:B:338:LEU:HB3	0.48	1.84	14	1
1:A:188:LEU:HD23	1:A:192:SER:HB3	0.48	1.85	1	1
1:A:155:TRP:CH2	1:A:166:ARG:HB2	0.48	2.44	16	3
1:A:155:TRP:CE2	1:A:185:ARG:HD2	0.48	2.43	17	1
1:A:185:ARG:HD3	1:A:193:TRP:CE3	0.48	2.42	2	1
1:A:150:LEU:HB3	2:B:337:LEU:HD11	0.48	1.85	4	1
1:A:185:ARG:O	1:A:186:GLU:HB2	0.48	2.08	10	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:333:LYS:HA	2:B:336:LEU:HD21	0.48	1.85	4	1
1:A:185:ARG:O	1:A:186:GLU:CB	0.48	2.62	12	2
1:A:199:TYR:HB3	2:B:338:LEU:CD1	0.48	2.39	13	2
1:A:204:GLU:C	1:A:205:ILE:HD13	0.48	2.34	14	1
1:A:185:ARG:HA	1:A:197:VAL:HG12	0.48	1.86	16	1
1:A:155:TRP:HZ2	1:A:197:VAL:HG23	0.48	1.69	19	1
2:B:327:GLU:HG3	2:B:328:ALA:N	0.47	2.23	6	1
1:A:175:VAL:HG13	1:A:177:TYR:CE2	0.47	2.44	7	1
2:B:328:ALA:O	2:B:332:ALA:HB2	0.47	2.09	11	3
1:A:197:VAL:HG11	1:A:199:TYR:CE2	0.47	2.44	7	2
1:A:186:GLU:HB2	1:A:196:ARG:NH1	0.47	2.24	10	1
1:A:158:SER:HB2	1:A:193:TRP:CH2	0.47	2.45	11	1
2:B:315:LEU:HD12	2:B:316:ARG:N	0.47	2.25	5	2
1:A:192:SER:OG	1:A:193:TRP:N	0.47	2.47	19	4
1:A:169:PRO:O	1:A:171:PHE:N	0.47	2.48	19	2
1:A:161:GLY:O	1:A:187:CYS:HB3	0.47	2.09	14	1
1:A:202:CYS:HB2	2:B:338:LEU:CD2	0.47	2.40	14	1
1:A:205:ILE:HD13	1:A:205:ILE:H	0.47	1.70	2	1
2:B:320:GLU:O	2:B:323:LYS:NZ	0.47	2.42	18	3
1:A:156:PRO:O	1:A:157:ARG:C	0.47	2.58	20	1
1:A:200:SER:HA	2:B:338:LEU:HD12	0.47	1.87	20	1
1:A:151:ILE:HA	1:A:173:TYR:OH	0.47	2.09	4	1
1:A:146:ALA:HB2	1:A:157:ARG:HB3	0.47	1.86	16	1
1:A:155:TRP:CD2	1:A:185:ARG:HD3	0.46	2.44	17	1
1:A:158:SER:OG	1:A:159:PRO:HD2	0.46	2.10	2	3
1:A:173:TYR:CD1	1:A:174:GLY:N	0.46	2.84	5	1
1:A:131:GLU:HA	1:A:146:ALA:HB3	0.46	1.87	6	1
1:A:175:VAL:HG13	1:A:177:TYR:CD2	0.46	2.45	10	1
1:A:197:VAL:CG1	2:B:341:ALA:HB1	0.46	2.40	19	1
1:A:202:CYS:HB2	2:B:338:LEU:HD12	0.46	1.88	1	1
1:A:147:SER:O	1:A:154:CYS:HA	0.46	2.10	15	1
1:A:145:ASN:O	1:A:146:ALA:HB3	0.46	2.10	12	1
2:B:336:LEU:C	2:B:336:LEU:HD12	0.46	2.35	14	1
1:A:160:ALA:HB1	1:A:190:ASN:N	0.46	2.25	1	1
1:A:145:ASN:O	1:A:193:TRP:NE1	0.46	2.37	6	2
1:A:155:TRP:CZ3	1:A:166:ARG:HD3	0.46	2.44	16	1
2:B:324:ALA:HA	2:B:327:GLU:HG2	0.46	1.88	20	1
1:A:144:CYS:HB2	1:A:158:SER:OG	0.46	2.10	8	1
1:A:177:TYR:CE2	1:A:202:CYS:HB3	0.45	2.46	14	1
1:A:176:ARG:NH1	1:A:177:TYR:O	0.45	2.45	20	1
1:A:197:VAL:HG21	1:A:199:TYR:CE1	0.45	2.46	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:TYR:CG	1:A:204:GLU:HG3	0.45	2.46	12	1
1:A:163:LEU:HA	1:A:186:GLU:HG3	0.45	1.89	18	1
1:A:135:LEU:O	1:A:136:ALA:C	0.45	2.59	15	1
1:A:151:ILE:HG22	2:B:337:LEU:HD23	0.45	1.86	19	2
1:A:184:TYR:CG	1:A:184:TYR:O	0.45	2.69	7	1
1:A:197:VAL:HB	1:A:199:TYR:CD2	0.45	2.46	13	1
1:A:150:LEU:HD22	1:A:150:LEU:C	0.45	2.36	15	1
1:A:148:VAL:HG22	1:A:154:CYS:CB	0.45	2.41	6	1
1:A:151:ILE:HG21	1:A:172:PHE:CZ	0.45	2.47	13	2
1:A:155:TRP:CZ3	1:A:185:ARG:HB2	0.45	2.46	15	1
1:A:155:TRP:CZ2	1:A:197:VAL:HG21	0.45	2.46	4	1
2:B:320:GLU:O	2:B:324:ALA:N	0.45	2.48	15	1
1:A:142:LEU:HB3	1:A:160:ALA:CB	0.45	2.41	19	1
1:A:187:CYS:SG	1:A:193:TRP:CH2	0.45	3.09	5	1
1:A:199:TYR:HB2	2:B:338:LEU:O	0.45	2.12	7	1
2:B:330:GLU:O	2:B:333:LYS:HG2	0.45	2.11	15	2
1:A:172:PHE:HB3	1:A:177:TYR:CD2	0.45	2.47	17	1
1:A:143:GLN:HG2	1:A:159:PRO:HA	0.45	1.89	20	1
1:A:146:ALA:HA	1:A:155:TRP:O	0.45	2.12	19	3
1:A:196:ARG:NH1	1:A:198:ASN:OD1	0.45	2.44	9	1
1:A:177:TYR:CA	1:A:205:ILE:HD11	0.45	2.35	20	1
1:A:148:VAL:HG22	1:A:154:CYS:HB2	0.44	1.88	2	1
1:A:155:TRP:CZ3	1:A:164:VAL:HG13	0.44	2.47	11	1
2:B:313:ASN:O	2:B:314:LEU:C	0.44	2.60	6	1
1:A:156:PRO:HG2	1:A:164:VAL:HG11	0.44	1.88	12	1
1:A:170:ALA:O	1:A:179:THR:HG21	0.44	2.11	16	1
1:A:165:VAL:HB	1:A:184:TYR:HB3	0.44	1.89	18	1
2:B:336:LEU:O	2:B:339:GLU:HG3	0.44	2.12	19	1
1:A:144:CYS:HB2	1:A:193:TRP:CZ2	0.44	2.47	5	1
1:A:185:ARG:CZ	1:A:193:TRP:CB	0.44	2.96	8	1
1:A:142:LEU:HB2	1:A:160:ALA:HB2	0.44	1.90	11	1
1:A:181:ASN:CG	1:A:201:GLU:HB3	0.44	2.37	20	1
1:A:131:GLU:HG2	1:A:146:ALA:HB3	0.44	1.89	3	1
1:A:151:ILE:HG21	1:A:172:PHE:HZ	0.44	1.72	3	1
1:A:165:VAL:O	1:A:165:VAL:HG13	0.44	2.13	7	1
1:A:206:LEU:O	2:B:323:LYS:NZ	0.44	2.39	8	1
1:A:206:LEU:HD11	2:B:323:LYS:HD2	0.44	1.90	9	1
1:A:172:PHE:CE2	2:B:338:LEU:HD11	0.44	2.47	16	1
1:A:183:GLY:HA3	1:A:199:TYR:CD1	0.44	2.48	19	1
1:A:135:LEU:O	1:A:136:ALA:CB	0.44	2.65	9	1
1:A:148:VAL:O	1:A:148:VAL:HG13	0.44	2.12	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:206:LEU:HD11	2:B:326:GLN:CD	0.44	2.38	14	1
1:A:178:ASN:N	1:A:205:ILE:HD12	0.44	2.27	2	1
1:A:156:PRO:O	1:A:157:ARG:CG	0.44	2.66	3	1
2:B:331:ALA:HB1	2:B:335:ARG:HB2	0.44	1.90	6	1
1:A:165:VAL:HG22	1:A:182:ASN:CB	0.44	2.41	13	1
2:B:315:LEU:HD12	2:B:315:LEU:C	0.44	2.38	13	1
1:A:185:ARG:NH2	1:A:194:ALA:O	0.44	2.44	1	1
1:A:151:ILE:O	1:A:153:THR:N	0.44	2.49	10	1
1:A:165:VAL:HA	1:A:184:TYR:HA	0.44	1.89	4	3
1:A:148:VAL:HG13	1:A:154:CYS:N	0.43	2.27	2	1
1:A:163:LEU:HD23	1:A:184:TYR:CB	0.43	2.43	3	1
2:B:312:PHE:O	2:B:315:LEU:HG	0.43	2.13	16	4
2:B:334:ASN:HA	2:B:337:LEU:HD23	0.43	1.89	9	1
1:A:142:LEU:HB2	1:A:160:ALA:CB	0.43	2.42	11	1
2:B:333:LYS:HG3	2:B:334:ASN:N	0.43	2.28	19	1
1:A:167:PRO:O	1:A:168:CYS:CB	0.43	2.65	12	1
2:B:314:LEU:O	2:B:318:VAL:HG23	0.43	2.12	17	1
1:A:142:LEU:HD23	1:A:160:ALA:HB3	0.43	1.90	1	1
2:B:334:ASN:O	2:B:337:LEU:HG	0.43	2.13	3	1
2:B:323:LYS:O	2:B:326:GLN:HG3	0.43	2.13	10	1
1:A:155:TRP:CE2	1:A:185:ARG:HB2	0.43	2.48	11	1
1:A:185:ARG:HB3	1:A:197:VAL:CG1	0.43	2.43	13	1
1:A:144:CYS:O	1:A:193:TRP:NE1	0.43	2.47	20	1
1:A:153:THR:HG21	1:A:185:ARG:CZ	0.43	2.44	20	1
2:B:320:GLU:O	2:B:323:LYS:HG3	0.43	2.13	7	2
1:A:155:TRP:CZ3	1:A:166:ARG:HB2	0.43	2.48	11	2
2:B:327:GLU:O	2:B:332:ALA:N	0.43	2.42	20	1
2:B:327:GLU:CA	2:B:331:ALA:HB3	0.43	2.44	1	1
2:B:336:LEU:HD12	2:B:337:LEU:N	0.43	2.29	4	1
2:B:320:GLU:HA	2:B:323:LYS:HG3	0.43	1.91	10	1
1:A:155:TRP:CZ2	1:A:185:ARG:HB2	0.43	2.49	2	1
1:A:185:ARG:NH1	1:A:193:TRP:CZ3	0.43	2.87	5	1
1:A:199:TYR:CG	2:B:338:LEU:HD12	0.43	2.48	8	1
1:A:166:ARG:N	1:A:183:GLY:O	0.43	2.48	14	2
1:A:168:CYS:HB3	1:A:169:PRO:HD2	0.43	1.89	11	2
1:A:144:CYS:O	1:A:157:ARG:HA	0.43	2.13	6	2
1:A:172:PHE:O	1:A:174:GLY:N	0.43	2.49	14	2
1:A:169:PRO:O	1:A:170:ALA:HB3	0.43	2.14	8	1
1:A:167:PRO:HA	1:A:181:ASN:O	0.43	2.13	9	1
2:B:316:ARG:O	2:B:318:VAL:N	0.43	2.51	10	1
1:A:155:TRP:HB3	1:A:193:TRP:CE2	0.43	2.49	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:ASP:HB3	1:A:185:ARG:NE	0.43	2.29	14	1
1:A:154:CYS:O	1:A:166:ARG:NH1	0.43	2.43	15	1
1:A:197:VAL:HG12	1:A:199:TYR:H	0.43	1.74	20	1
1:A:185:ARG:CD	1:A:193:TRP:CE3	0.42	3.02	1	1
2:B:330:GLU:OE1	2:B:333:LYS:NZ	0.42	2.44	6	3
1:A:181:ASN:HB3	1:A:201:GLU:CB	0.42	2.44	15	1
1:A:151:ILE:HG22	2:B:337:LEU:CD1	0.42	2.44	17	1
1:A:199:TYR:O	2:B:338:LEU:HD23	0.42	2.13	6	1
2:B:312:PHE:CG	2:B:315:LEU:HD11	0.42	2.49	6	1
1:A:196:ARG:O	1:A:196:ARG:CG	0.42	2.67	7	1
1:A:150:LEU:HD23	2:B:337:LEU:HD22	0.42	1.90	17	1
2:B:331:ALA:O	2:B:335:ARG:N	0.42	2.52	6	1
1:A:177:TYR:CE1	1:A:204:GLU:HG3	0.42	2.48	15	1
1:A:185:ARG:HB3	1:A:193:TRP:CZ3	0.42	2.49	16	1
1:A:180:THR:HG23	1:A:201:GLU:HB3	0.42	1.91	19	1
1:A:150:LEU:HG	2:B:341:ALA:HB1	0.42	1.90	20	1
1:A:206:LEU:HD13	2:B:326:GLN:OE1	0.42	2.13	20	1
2:B:324:ALA:HA	2:B:327:GLU:CG	0.42	2.44	20	1
2:B:331:ALA:O	2:B:332:ALA:C	0.42	2.61	8	1
1:A:153:THR:HG21	1:A:166:ARG:HG2	0.42	1.91	15	1
1:A:185:ARG:NE	1:A:197:VAL:HG13	0.42	2.29	20	1
1:A:185:ARG:HB3	1:A:197:VAL:HG13	0.42	1.90	13	1
2:B:329:GLU:O	2:B:333:LYS:NZ	0.42	2.42	20	1
1:A:165:VAL:CG2	1:A:182:ASN:CB	0.42	2.98	8	1
2:B:317:GLU:HA	2:B:320:GLU:HG2	0.42	1.91	8	1
1:A:168:CYS:HB3	1:A:169:PRO:CD	0.42	2.44	11	1
1:A:168:CYS:O	1:A:179:THR:OG1	0.42	2.37	3	1
1:A:148:VAL:HG22	1:A:154:CYS:CA	0.42	2.45	6	1
1:A:165:VAL:HG23	1:A:184:TYR:CD1	0.42	2.50	6	1
2:B:312:PHE:O	2:B:313:ASN:C	0.42	2.61	9	2
1:A:143:GLN:HA	1:A:159:PRO:HA	0.42	1.91	4	1
1:A:206:LEU:HD13	2:B:327:GLU:CG	0.42	2.44	11	1
1:A:185:ARG:HG2	1:A:197:VAL:HB	0.42	1.90	4	2
1:A:134:SER:HA	1:A:157:ARG:HG2	0.42	1.92	6	1
1:A:134:SER:O	1:A:157:ARG:NH2	0.42	2.52	17	1
1:A:148:VAL:O	1:A:150:LEU:N	0.42	2.53	20	1
1:A:148:VAL:O	1:A:185:ARG:NH2	0.41	2.49	2	1
2:B:337:LEU:HD12	2:B:338:LEU:CD2	0.41	2.44	5	1
1:A:172:PHE:HB2	1:A:177:TYR:HB2	0.41	1.92	10	1
1:A:164:VAL:O	1:A:184:TYR:HA	0.41	2.15	11	1
2:B:309:ASP:O	2:B:313:ASN:N	0.41	2.53	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:ARG:HG3	1:A:158:SER:N	0.41	2.29	16	1
1:A:196:ARG:HD3	1:A:196:ARG:O	0.41	2.14	10	1
1:A:136:ALA:O	1:A:157:ARG:NH2	0.41	2.41	15	1
1:A:134:SER:O	1:A:136:ALA:N	0.41	2.53	16	1
1:A:178:ASN:O	1:A:179:THR:HG22	0.41	2.15	7	1
1:A:186:GLU:O	1:A:194:ALA:HB3	0.41	2.15	12	1
1:A:197:VAL:HG23	2:B:341:ALA:O	0.41	2.16	13	1
2:B:317:GLU:HG3	2:B:321:ILE:HD12	0.41	1.92	8	1
1:A:129:HIS:ND1	1:A:129:HIS:C	0.41	2.79	14	1
1:A:168:CYS:SG	1:A:169:PRO:HD2	0.41	2.56	7	1
2:B:330:GLU:O	2:B:333:LYS:HG3	0.41	2.15	14	1
1:A:150:LEU:H	1:A:150:LEU:HD13	0.41	1.75	16	1
1:A:200:SER:HB3	2:B:338:LEU:O	0.41	2.16	20	1
1:A:170:ALA:HB1	1:A:177:TYR:O	0.41	2.16	4	1
1:A:185:ARG:HB3	1:A:197:VAL:HA	0.41	1.93	7	1
1:A:183:GLY:O	1:A:185:ARG:NH1	0.41	2.49	9	1
2:B:317:GLU:HB3	2:B:321:ILE:HD12	0.41	1.92	11	1
1:A:149:ASP:HB3	1:A:185:ARG:CZ	0.41	2.46	14	1
1:A:160:ALA:CB	1:A:189:ALA:HA	0.41	2.37	15	1
2:B:320:GLU:OE2	2:B:323:LYS:NZ	0.41	2.47	16	1
1:A:134:SER:HB2	1:A:157:ARG:HG2	0.41	1.91	3	1
1:A:149:ASP:HA	1:A:185:ARG:NH2	0.41	2.30	2	1
1:A:148:VAL:HG12	1:A:151:ILE:O	0.41	2.15	5	1
1:A:133:LEU:O	1:A:135:LEU:HD23	0.41	2.16	7	1
1:A:142:LEU:O	1:A:143:GLN:CB	0.41	2.69	12	1
1:A:155:TRP:HB3	1:A:193:TRP:CH2	0.41	2.51	14	1
1:A:206:LEU:HG	2:B:323:LYS:HD3	0.41	1.91	17	1
1:A:146:ALA:HB2	1:A:157:ARG:N	0.41	2.31	18	1
1:A:165:VAL:O	1:A:166:ARG:HG2	0.41	2.16	8	1
2:B:316:ARG:O	2:B:319:LEU:HG	0.41	2.16	19	1
2:B:314:LEU:O	2:B:317:GLU:HG3	0.41	2.16	20	1
2:B:312:PHE:O	2:B:316:ARG:HB2	0.40	2.17	19	1
1:A:193:TRP:O	1:A:194:ALA:HB3	0.40	2.15	9	2
1:A:178:ASN:OD1	1:A:180:THR:HB	0.40	2.15	14	1
1:A:170:ALA:O	1:A:171:PHE:CB	0.40	2.69	1	1
1:A:187:CYS:SG	1:A:193:TRP:CE3	0.40	3.15	3	1
1:A:160:ALA:HA	1:A:187:CYS:HB3	0.40	1.92	13	1
1:A:199:TYR:HB3	2:B:338:LEU:O	0.40	2.16	2	1
1:A:185:ARG:CZ	1:A:193:TRP:CE3	0.40	3.04	5	1
1:A:172:PHE:CZ	2:B:338:LEU:HD11	0.40	2.52	14	1
1:A:175:VAL:CG1	1:A:177:TYR:CD2	0.40	3.05	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:ASN:CB	1:A:201:GLU:HB2	0.40	2.47	17	1
1:A:175:VAL:CG1	1:A:177:TYR:CD1	0.40	3.05	1	1
1:A:188:LEU:HB2	1:A:192:SER:O	0.40	2.17	2	1
1:A:151:ILE:HB	1:A:172:PHE:CZ	0.40	2.52	11	1
1:A:143:GLN:CG	1:A:159:PRO:HA	0.40	2.47	20	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	74/84 (88%)	51±3 (69±5%)	18±4 (24±5%)	5±2 (7±2%)	2	17
2	B	32/38 (84%)	28±2 (87±7%)	4±2 (12±7%)	0±0 (1±1%)	18	68
All	All	2120/2440 (87%)	1585 (75%)	429 (20%)	106 (5%)	3	24

All 39 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	191	GLY	13
1	A	190	ASN	10
1	A	173	TYR	8
1	A	186	GLU	7
1	A	164	VAL	6
1	A	147	SER	4
1	A	151	ILE	4
1	A	170	ALA	4
1	A	150	LEU	3
1	A	192	SER	3
1	A	194	ALA	3
1	A	178	ASN	3
1	A	157	ARG	2
1	A	145	ASN	2
2	B	329	GLU	2
1	A	177	TYR	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	179	THR	2
1	A	160	ALA	2
1	A	168	CYS	2
1	A	202	CYS	2
2	B	310	LEU	2
1	A	169	PRO	2
1	A	134	SER	2
1	A	166	ARG	1
1	A	180	THR	1
1	A	196	ARG	1
1	A	142	LEU	1
2	B	325	GLU	1
1	A	175	VAL	1
1	A	188	LEU	1
1	A	171	PHE	1
1	A	189	ALA	1
1	A	205	ILE	1
1	A	135	LEU	1
1	A	162	GLN	1
1	A	174	GLY	1
1	A	185	ARG	1
1	A	203	GLN	1
1	A	136	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	62/71 (87%)	43±2 (69±4%)	19±2 (31±4%)	1	15
2	B	27/32 (84%)	17±2 (64±9%)	10±2 (36±9%)	1	9
All	All	1780/2060 (86%)	1201 (67%)	579 (33%)	1	13

All 77 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	150	LEU	17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	190	ASN	16
1	A	205	ILE	16
2	B	323	LYS	16
1	A	135	LEU	14
1	A	142	LEU	14
1	A	151	ILE	13
1	A	206	LEU	13
1	A	188	LEU	13
2	B	333	LYS	13
2	B	335	ARG	13
1	A	162	GLN	12
1	A	185	ARG	12
1	A	199	TYR	11
2	B	312	PHE	11
2	B	330	GLU	11
2	B	338	LEU	11
1	A	134	SER	10
1	A	157	ARG	10
1	A	166	ARG	10
2	B	319	LEU	10
1	A	130	CYS	10
1	A	143	GLN	9
2	B	315	LEU	9
2	B	316	ARG	9
1	A	163	LEU	9
1	A	133	LEU	9
1	A	168	CYS	9
1	A	204	GLU	9
2	B	325	GLU	8
1	A	131	GLU	8
1	A	196	ARG	8
2	B	314	LEU	8
1	A	144	CYS	7
1	A	149	ASP	7
2	B	310	LEU	7
2	B	311	THR	7
2	B	320	GLU	7
1	A	198	ASN	7
1	A	186	GLU	7
1	A	187	CYS	7
1	A	200	SER	7
1	A	207	ASN	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	B	340	GLU	7
1	A	176	ARG	7
1	A	201	GLU	6
2	B	337	LEU	6
2	B	313	ASN	6
2	B	327	GLU	6
2	B	329	GLU	6
2	B	336	LEU	6
1	A	158	SER	5
1	A	177	TYR	5
1	A	203	GLN	5
1	A	180	THR	5
2	B	326	GLN	5
1	A	129	HIS	5
1	A	172	PHE	5
1	A	193	TRP	5
2	B	317	GLU	5
1	A	154	CYS	4
1	A	147	SER	4
1	A	182	ASN	4
1	A	202	CYS	4
1	A	148	VAL	3
1	A	175	VAL	3
2	B	309	ASP	3
1	A	178	ASN	3
1	A	171	PHE	3
1	A	184	TYR	2
1	A	164	VAL	2
2	B	339	GLU	2
1	A	153	THR	2
1	A	132	SER	1
1	A	179	THR	1
1	A	197	VAL	1
1	A	165	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided