Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2L27
Title	:	NMR Structure of the ECD1 of CRF-R1 in complex with a peptide agonist
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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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

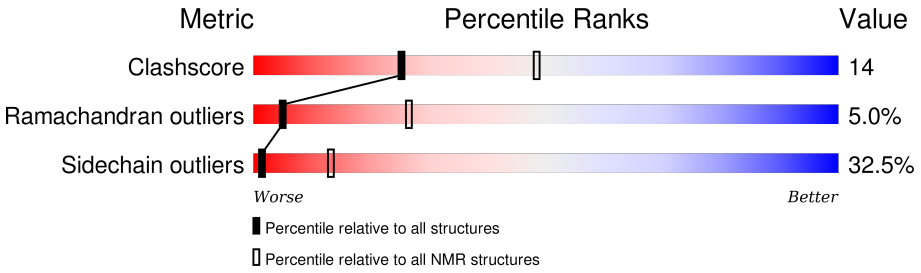
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	84	30% 56% • 12%
2	B	38	50% 37% 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)	1.00	13
2	B:309-B:324 (16)	0.48	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 Seven transmembrane helix receptor.

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 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: Seven transmembrane helix receptor

Chain A:

• Molecule 2: peptide agonist

Chain B:

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

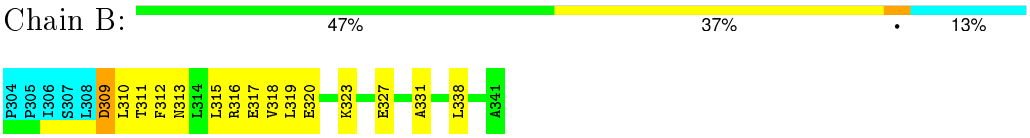
4.2.1 Score per residue for model 1

• Molecule 1: Seven transmembrane helix receptor

Chain A:

• Molecule 2: peptide agonist

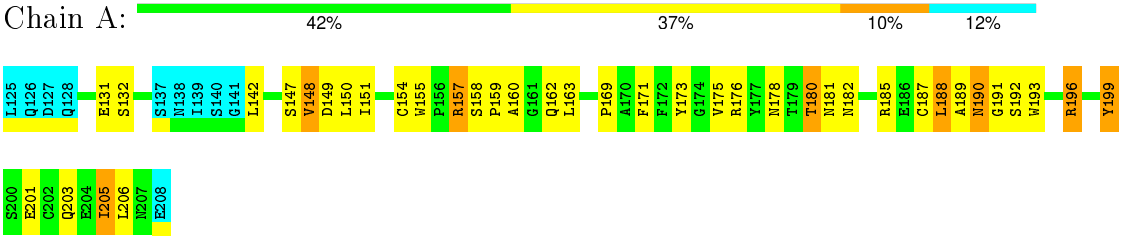
Chain B:



4.2.2 Score per residue for model 2

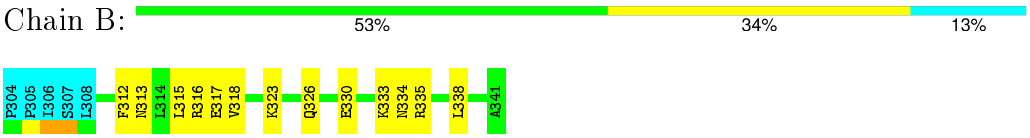
- Molecule 1: Seven transmembrane helix receptor

Chain A:



- Molecule 2: peptide agonist

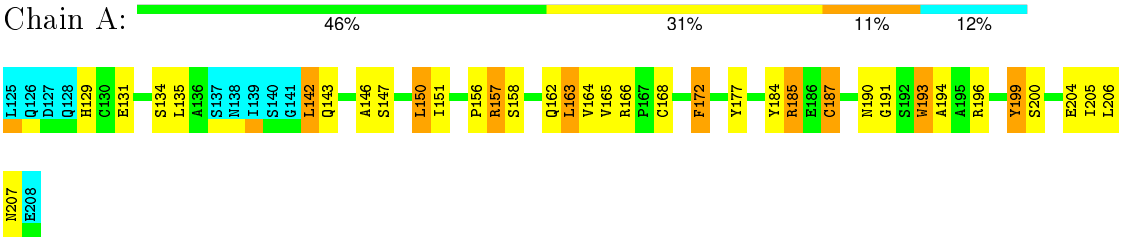
Chain B:



4.2.3 Score per residue for model 3

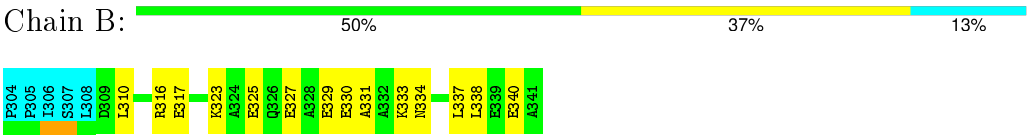
- Molecule 1: Seven transmembrane helix receptor

Chain A:



- Molecule 2: peptide agonist

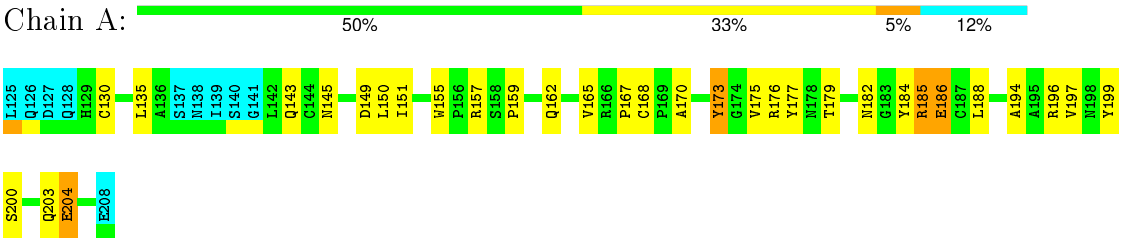
Chain B:



4.2.4 Score per residue for model 4

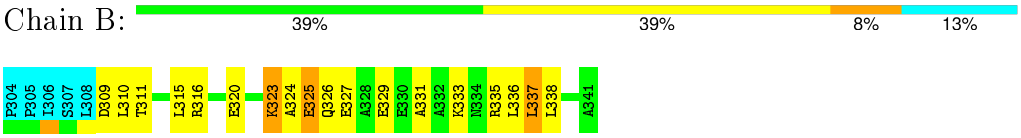
- Molecule 1: Seven transmembrane helix receptor

Chain A:



- Molecule 2: peptide agonist

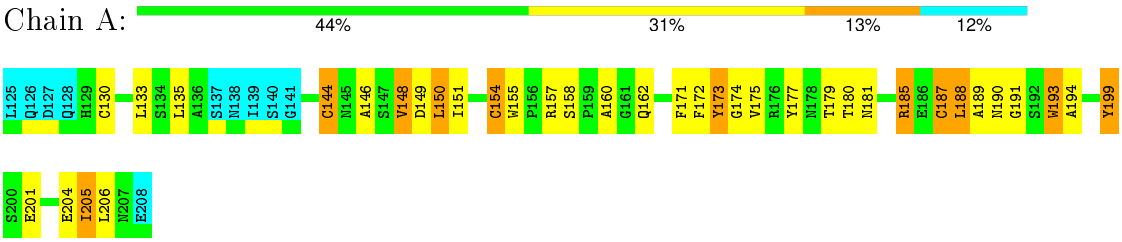
Chain B:



4.2.5 Score per residue for model 5

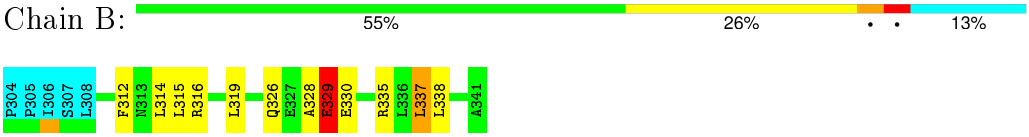
- Molecule 1: Seven transmembrane helix receptor

Chain A:



- Molecule 2: peptide agonist

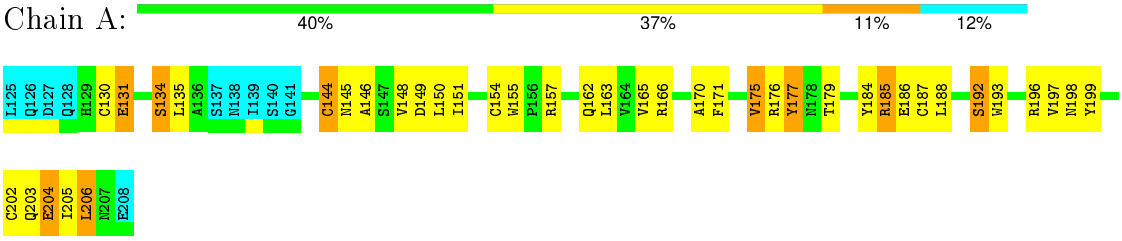
Chain B:



4.2.6 Score per residue for model 6

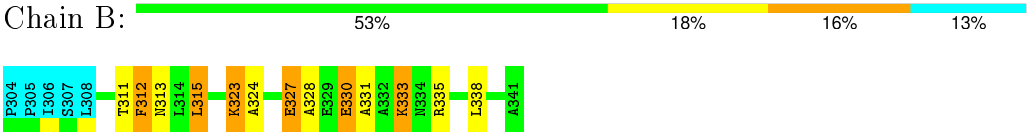
- Molecule 1: Seven transmembrane helix receptor

Chain A:



- Molecule 2: peptide agonist

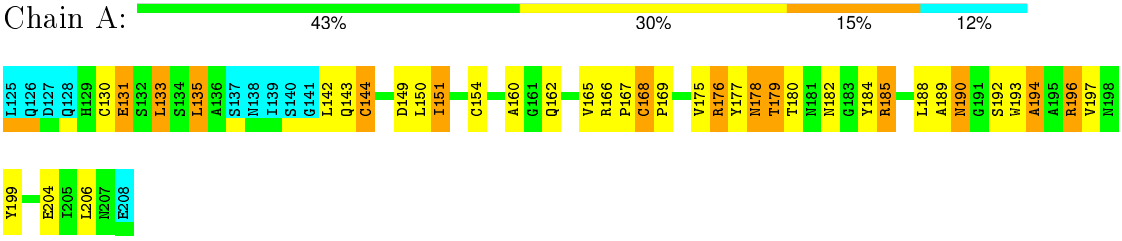
Chain B:



4.2.7 Score per residue for model 7

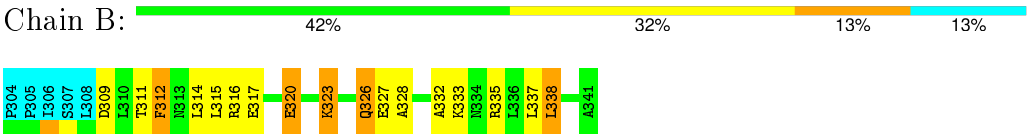
- Molecule 1: Seven transmembrane helix receptor

Chain A:



- Molecule 2: peptide agonist

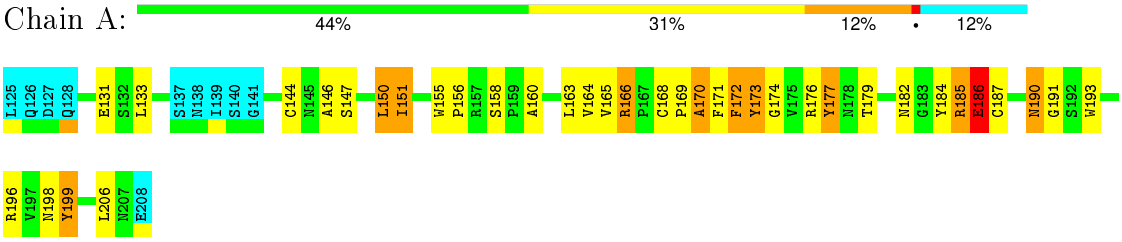
Chain B:



4.2.8 Score per residue for model 8

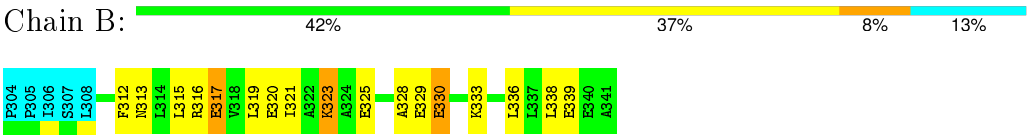
- Molecule 1: Seven transmembrane helix receptor

Chain A:



- Molecule 2: peptide agonist

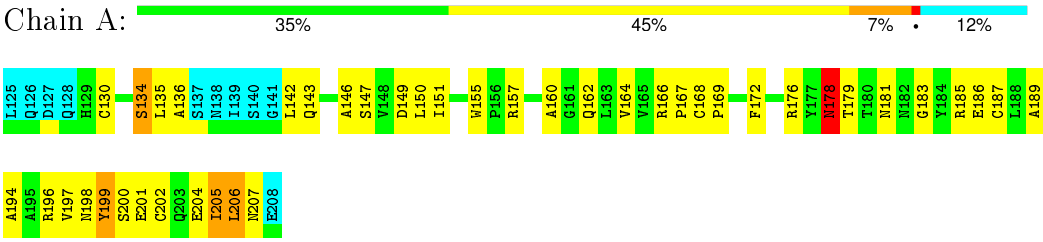
Chain B:



4.2.9 Score per residue for model 9

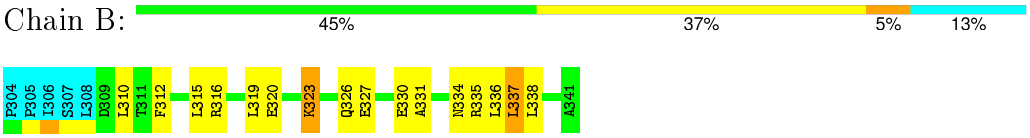
- Molecule 1: Seven transmembrane helix receptor

Chain A:



• Molecule 2: peptide agonist

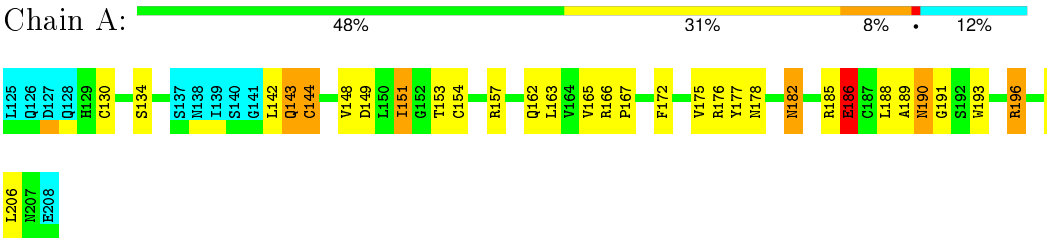
Chain B:



4.2.10 Score per residue for model 10

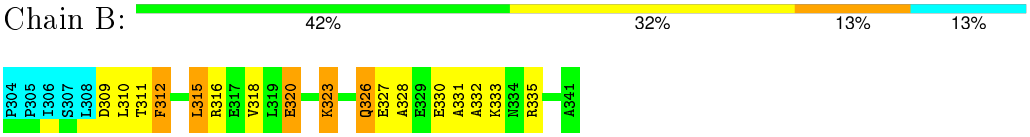
• Molecule 1: Seven transmembrane helix receptor

Chain A:



• Molecule 2: peptide agonist

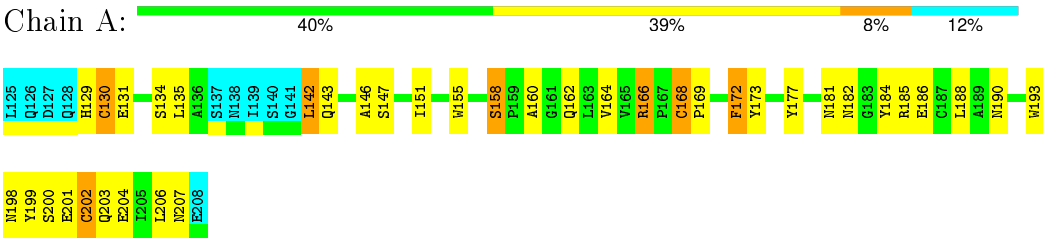
Chain B:



4.2.11 Score per residue for model 11

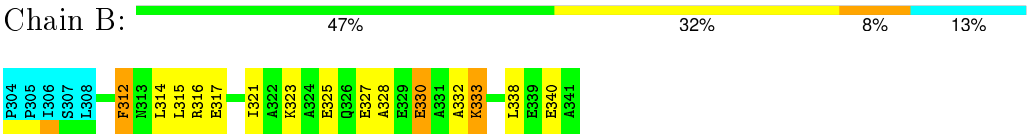
• Molecule 1: Seven transmembrane helix receptor

Chain A:



• Molecule 2: peptide agonist

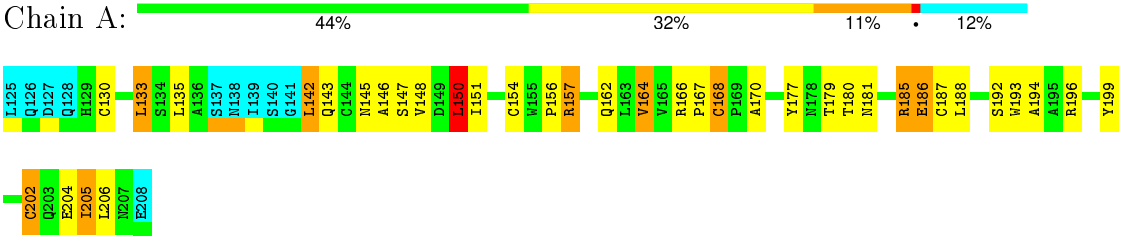
Chain B:



4.2.12 Score per residue for model 12

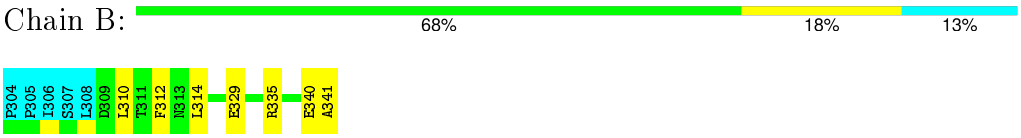
- Molecule 1: Seven transmembrane helix receptor

Chain A:



- Molecule 2: peptide agonist

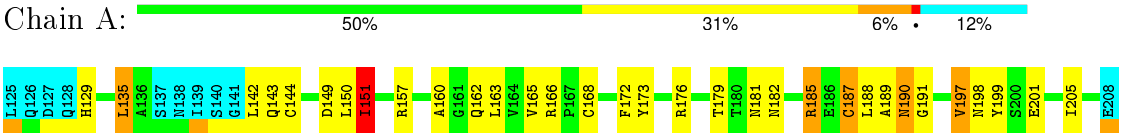
Chain B:



4.2.13 Score per residue for model 13 (medoid)

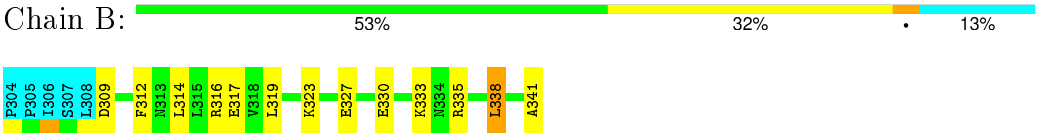
- Molecule 1: Seven transmembrane helix receptor

Chain A:



- Molecule 2: peptide agonist

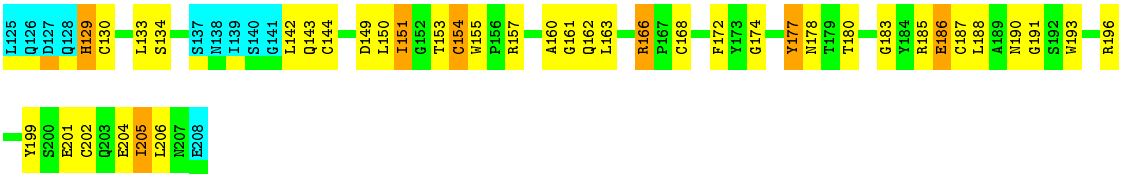
Chain B:



4.2.14 Score per residue for model 14

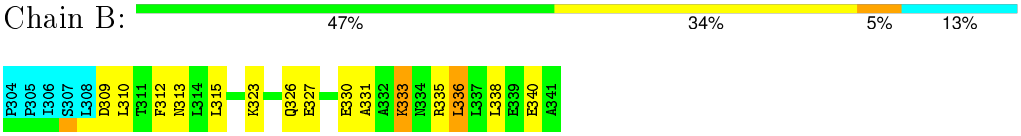
- Molecule 1: Seven transmembrane helix receptor

Chain A:



- Molecule 2: peptide agonist

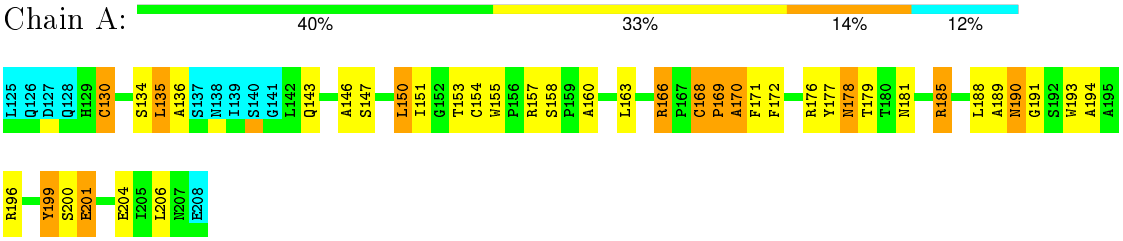
Chain B:



4.2.15 Score per residue for model 15

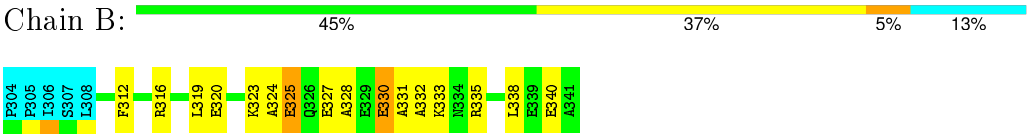
- Molecule 1: Seven transmembrane helix receptor

Chain A:



- Molecule 2: peptide agonist

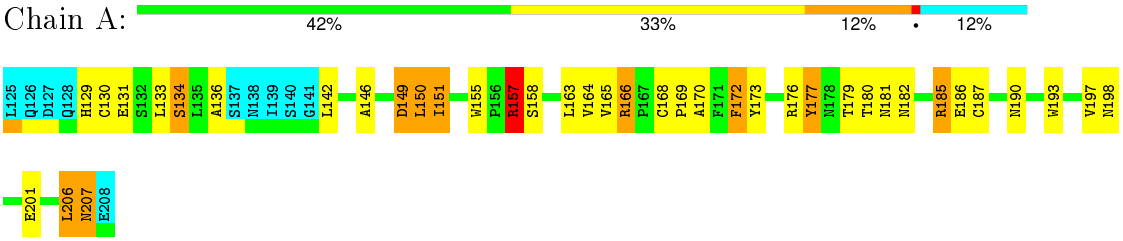
Chain B:



4.2.16 Score per residue for model 16

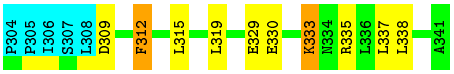
- Molecule 1: Seven transmembrane helix receptor

Chain A:



- Molecule 2: peptide agonist

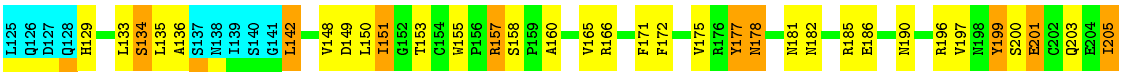
Chain B:



4.2.17 Score per residue for model 17

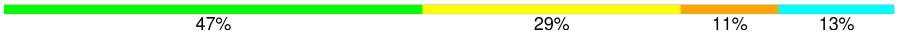
- Molecule 1: Seven transmembrane helix receptor

Chain A:



- Molecule 2: peptide agonist

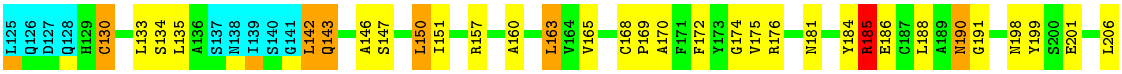
Chain B:



4.2.18 Score per residue for model 18

- Molecule 1: Seven transmembrane helix receptor

Chain A:



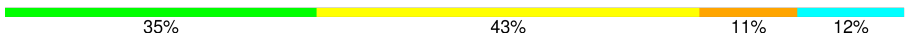
- Molecule 2: peptide agonist

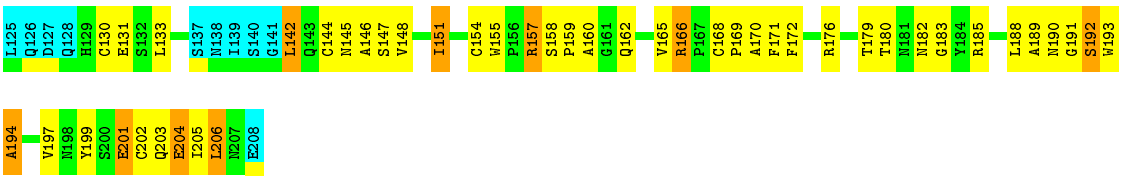
Chain B:

4.2.19 Score per residue for model 19

- Molecule 1: Seven transmembrane helix receptor

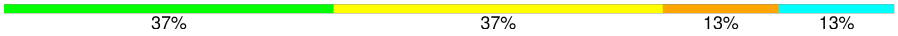
Chain A:





- Molecule 2: peptide agonist

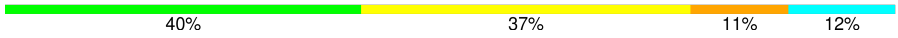
Chain B:



4.2.20 Score per residue for model 20

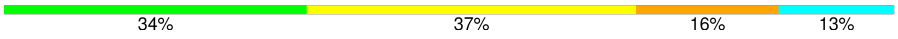
- Molecule 1: Seven transmembrane helix receptor

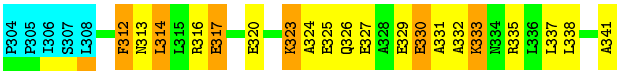
Chain A:



- Molecule 2: peptide agonist

Chain B:





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. 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	573	538	537	18±4
2	B	264	267	267	6±3
All	All	16740	16100	16080	449

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:150:LEU:HD13	1:A:151:ILE:N	0.67	2.04	15	1
1:A:134:SER:HB2	1:A:146:ALA:HB3	0.67	1.65	9	1

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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:HG23	1:A:179:THR:O	0.66	1.90	19	4
1:A:170:ALA:HB2	1:A:179:THR:HG23	0.65	1.66	12	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:179:THR:O	1:A:179:THR:HG23	0.61	1.96	20	3
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
1:A:175:VAL:HG11	1:A:204:GLU:CD	0.60	2.16	7	1
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:178:ASN:CB	1:A:205:ILE:HD11	0.59	2.28	14	1
1:A:170:ALA:HB2	1:A:179:THR:HB	0.59	1.74	4	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
1:A:204:GLU:HG2	1:A:206:LEU:HD21	0.57	1.75	19	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:199:TYR:HB3	2:B:338:LEU:HD12	0.57	1.76	17	2
1:A:185:ARG:HG2	1:A:197:VAL:HG13	0.57	1.74	9	1
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	3
1:A:142:LEU:HD22	1:A:160:ALA:CB	0.56	2.31	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:ASN:CB	1:A:201:GLU:HB3	0.56	2.31	1	8
1:A:185:ARG:CG	1:A:197:VAL:HG13	0.56	2.31	9	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:167:PRO:HA	1:A:182:ASN:HA	0.54	1.80	10	3
1:A:187:CYS:HA	1:A:194:ALA:HA	0.54	1.78	3	1
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
1:A:206:LEU:HD21	2:B:326:GLN:HG3	0.54	1.79	14	1
1:A:150:LEU:HB3	1:A:151:ILE:HD13	0.54	1.79	8	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
1:A:199:TYR:HB3	2:B:338:LEU:HD23	0.53	1.81	14	1
2:B:334:ASN:O	2:B:338:LEU:HD23	0.53	2.04	2	2
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
1:A:148:VAL:HG13	1:A:154:CYS:CA	0.52	2.35	2	1
1:A:133:LEU:HD21	1:A:157:ARG:HB2	0.52	1.80	12	1
1:A:176:ARG:O	1:A:177:TYR:HB2	0.52	2.04	7	2
1:A:149:ASP:HB3	1:A:150:LEU:HD22	0.52	1.80	1	1
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:206:LEU:HD22	2:B:327:GLU:CD	0.51	2.26	11	1
1:A:163:LEU:HD11	1:A:184:TYR:CE2	0.51	2.41	6	1
1:A:130:CYS:O	1:A:133:LEU:HD23	0.51	2.05	12	1
1:A:184:TYR:O	1:A:197:VAL:HG23	0.51	2.06	4	1
1:A:168:CYS:SG	1:A:179:THR:HA	0.51	2.46	9	2
1:A:148:VAL:HA	1:A:154:CYS:HA	0.50	1.83	10	3
1:A:197:VAL:HG22	2:B:341:ALA:O	0.50	2.06	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:326:GLN:HG2	2:B:327:GLU:N	0.49	2.21	7	1
2:B:327:GLU:HB2	2:B:331:ALA:HB3	0.49	1.82	20	1
2:B:337:LEU:C	2:B:337:LEU:HD13	0.49	2.27	17	1
2:B:323:LYS:NZ	2:B:324:ALA:HB2	0.49	2.22	6	1
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
1:A:150:LEU:C	1:A:151:ILE:HD13	0.49	2.27	8	1
1:A:168:CYS:O	1:A:179:THR:HG22	0.49	2.07	12	2
1:A:130:CYS:O	1:A:146:ALA:HB3	0.49	2.07	11	1
1:A:150:LEU:O	2:B:337:LEU:HD11	0.49	2.08	17	1
1:A:165:VAL:CG2	1:A:182:ASN:HB3	0.49	2.38	16	2
1:A:185:ARG:HG2	1:A:197:VAL:HG22	0.49	1.85	1	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	1
2:B:327:GLU:HA	2:B:331:ALA:CB	0.48	2.36	14	2
1:A:187:CYS:SG	1:A:193:TRP:CZ3	0.48	3.06	5	1
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: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:188:LEU:HD23	1:A:192:SER:HB3	0.48	1.85	1	1
1:A:185:ARG:HD3	1:A:193:TRP:CE3	0.48	2.42	2	1
2:B:328:ALA:O	2:B:329:GLU:C	0.48	2.52	5	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
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:155:TRP:HZ2	1:A:197:VAL:HG23	0.48	1.69	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:ARG:HA	1:A:197:VAL:HG12	0.48	1.86	16	1
2:B:327:GLU:HG3	2:B:328:ALA:N	0.47	2.23	6	1
2:B:328:ALA:O	2:B:332:ALA:HB2	0.47	2.09	11	3
1:A:175:VAL:HG13	1:A:177:TYR:CE2	0.47	2.44	7	1
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
1:A:149:ASP:C	1:A:150:LEU:HD22	0.47	2.30	13	1
2:B:315:LEU:HD12	2:B:316:ARG:N	0.47	2.25	5	2
2:B:330:GLU:O	2:B:333:LYS:NZ	0.47	2.41	6	4
1:A:192:SER:OG	1:A:193:TRP:N	0.47	2.47	19	4
1:A:202:CYS:HB2	2:B:338:LEU:CD2	0.47	2.40	14	1
1:A:161:GLY:O	1:A:187:CYS:HB3	0.47	2.09	14	1
1:A:169:PRO:O	1:A:171:PHE:N	0.47	2.48	19	2
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	2
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:131:GLU:HA	1:A:146:ALA:HB3	0.46	1.87	6	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: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
1:A:145:ASN:O	1:A:193:TRP:NE1	0.46	2.37	6	2
1:A:160:ALA:HB1	1:A:190:ASN:N	0.46	2.25	1	1
1:A:155:TRP:CZ3	1:A:166:ARG:HD3	0.46	2.44	16	1
2:B:324:ALA:O	2:B:325:GLU:C	0.46	2.54	4	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
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:197:VAL:HB	1:A:199:TYR:CD2	0.45	2.46	13	1
1:A:151:ILE:HG22	2:B:337:LEU:HD23	0.45	1.86	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:184:TYR:O	1:A:184:TYR:CG	0.45	2.69	7	1
1:A:151:ILE:HG21	1:A:172:PHE:CZ	0.45	2.47	13	2
1:A:148:VAL:HG22	1:A:154:CYS:CB	0.45	2.41	6	1
1:A:155:TRP:CZ3	1:A:185:ARG:HB2	0.45	2.46	15	1
1:A:142:LEU:HB3	1:A:160:ALA:CB	0.45	2.41	19	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:187:CYS:SG	1:A:193:TRP:CH2	0.45	3.09	5	1
1:A:172:PHE:HB3	1:A:177:TYR:CD2	0.45	2.47	17	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: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:179:THR:CG2	1:A:179:THR:O	0.45	2.65	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:337:LEU:HD12	2:B:337:LEU:C	0.44	2.32	9	1
1:A:156:PRO:HG2	1:A:164:VAL:HG11	0.44	1.88	12	1
1:A:205:ILE:N	1:A:205:ILE:HD13	0.44	2.28	5	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:170:ALA:O	1:A:179:THR:HG21	0.44	2.11	16	1
1:A:144:CYS:HB2	1:A:193:TRP:CZ2	0.44	2.47	5	1
1:A:142:LEU:HB2	1:A:160:ALA:HB2	0.44	1.90	11	1
1:A:185:ARG:CZ	1:A:193:TRP:CB	0.44	2.96	8	1
1:A:206:LEU:O	2:B:323:LYS:NZ	0.44	2.39	8	1
1:A:183:GLY:HA3	1:A:199:TYR:CD1	0.44	2.48	19	1
1:A:151:ILE:HG21	1:A:172:PHE:HZ	0.44	1.72	3	1
1:A:131:GLU:HG2	1:A:146:ALA:HB3	0.44	1.89	3	1
1:A:165:VAL:HG13	1:A:165:VAL:O	0.44	2.13	7	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:148:VAL:HG13	1:A:148:VAL:O	0.44	2.12	10	1
1:A:135:LEU:O	1:A:136:ALA:CB	0.44	2.65	9	1
1:A:165:VAL:HG22	1:A:182:ASN:CB	0.44	2.41	13	1
2:B:331:ALA:HB1	2:B:335:ARG:HB2	0.44	1.90	6	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
1:A:151:ILE:O	1:A:153:THR:N	0.44	2.49	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:ARG:NH2	1:A:194:ALA:O	0.44	2.44	1	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:142:LEU:HB2	1:A:160:ALA:CB	0.43	2.42	11	1
2:B:312:PHE:O	2:B:315:LEU:HG	0.43	2.13	16	4
2:B:333:LYS:HG3	2:B:334:ASN:N	0.43	2.28	19	1
1:A:163:LEU:HD23	1:A:184:TYR:CB	0.43	2.43	3	1
2:B:334:ASN:HA	2:B:337:LEU:HD23	0.43	1.89	9	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:185:ARG:HB3	1:A:197:VAL:CG1	0.43	2.43	13	1
1:A:155:TRP:CE2	1:A:185:ARG:HB2	0.43	2.48	11	1
2:B:323:LYS:O	2:B:326:GLN:HG3	0.43	2.13	10	1
2:B:334:ASN:O	2:B:337:LEU:HG	0.43	2.13	3	1
1:A:142:LEU:HD23	1:A:160:ALA:HB3	0.43	1.90	1	1
1:A:153:THR:HG21	1:A:185:ARG:CZ	0.43	2.44	20	1
1:A:144:CYS:O	1:A:193:TRP:NE1	0.43	2.47	20	1
1:A:155:TRP:CZ3	1:A:166:ARG:HB2	0.43	2.48	11	2
2:B:320:GLU:O	2:B:323:LYS:HG3	0.43	2.13	7	2
2:B:327:GLU:O	2:B:332:ALA:N	0.43	2.42	20	1
2:B:320:GLU:HA	2:B:323:LYS:HG3	0.43	1.91	10	1
2:B:336:LEU:HD12	2:B:337:LEU:N	0.43	2.29	4	1
2:B:327:GLU:CA	2:B:331:ALA:HB3	0.43	2.44	1	1
1:A:166:ARG:N	1:A:183:GLY:O	0.43	2.48	14	2
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: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
2:B:316:ARG:O	2:B:318:VAL:N	0.43	2.51	10	1
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
1:A:204:GLU:C	1:A:205:ILE:HD13	0.43	2.34	14	1
1:A:149:ASP:HB3	1:A:185:ARG:NE	0.43	2.29	14	1
1:A:196:ARG:CG	1:A:196:ARG:O	0.43	2.67	7	1
1:A:154:CYS:O	1:A:166:ARG:NH1	0.43	2.43	15	1
1:A:155:TRP:HB3	1:A:193:TRP:CE2	0.43	2.49	9	1
1:A:197:VAL:HG12	1:A:199:TYR:H	0.43	1.74	20	1
1:A:151:ILE:HG22	2:B:337:LEU:CD1	0.42	2.44	17	1
1:A:185:ARG:CD	1:A:193:TRP:CE3	0.42	3.02	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:ASN:HB3	1:A:201:GLU:CB	0.42	2.44	15	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: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:180:THR:HG23	1:A:201:GLU:HB3	0.42	1.91	19	1
1:A:177:TYR:CE1	1:A:204:GLU:HG3	0.42	2.48	15	1
2:B:324:ALA:HA	2:B:327:GLU:CG	0.42	2.44	20	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
1:A:185:ARG:HB3	1:A:193:TRP:CZ3	0.42	2.49	16	1
2:B:330:GLU:OE1	2:B:333:LYS:NZ	0.42	2.44	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:168:CYS:HB3	1:A:169:PRO:CD	0.42	2.44	11	1
2:B:317:GLU:HA	2:B:320:GLU:HG2	0.42	1.91	8	1
1:A:165:VAL:CG2	1:A:182:ASN:CB	0.42	2.98	8	1
1:A:156:PRO:O	1:A:157:ARG:C	0.42	2.58	20	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
1:A:206:LEU:HD13	2:B:327:GLU:CG	0.42	2.44	11	1
2:B:333:LYS:NZ	2:B:334:ASN:OD1	0.42	2.38	19	1
1:A:143:GLN:HA	1:A:159:PRO:HA	0.42	1.91	4	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
1:A:164:VAL:O	1:A:184:TYR:HA	0.41	2.15	11	1
1:A:172:PHE:HB2	1:A:177:TYR:HB2	0.41	1.92	10	1
2:B:337:LEU:HD12	2:B:338:LEU:CD2	0.41	2.44	5	1
2:B:309:ASP:O	2:B:313:ASN:N	0.41	2.53	1	1
1:A:157:ARG:HG3	1:A:158:SER:N	0.41	2.29	16	1
1:A:196:ARG:O	1:A:196:ARG:HD3	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:197:VAL:HG23	2:B:341:ALA:O	0.41	2.16	13	1
2:B:336:LEU:C	2:B:336:LEU:HD12	0.41	2.35	14	1
1:A:186:GLU:O	1:A:194:ALA:HB3	0.41	2.15	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:178:ASN:O	1:A:179:THR:HG22	0.41	2.15	7	1
2:B:317:GLU:HG3	2:B:321:ILE:HD12	0.41	1.92	8	1
2:B:330:GLU:O	2:B:333:LYS:HG3	0.41	2.15	14	1
1:A:168:CYS:SG	1:A:169:PRO:HD2	0.41	2.56	7	1
1:A:200:SER:HB3	2:B:338:LEU:O	0.41	2.16	20	1
1:A:150:LEU:H	1:A:150:LEU:HD13	0.41	1.75	16	1
1:A:149:ASP:HB3	1:A:185:ARG:CZ	0.41	2.46	14	1
2:B:317:GLU:HB3	2:B:321:ILE:HD12	0.41	1.92	11	1
1:A:185:ARG:HB3	1:A:197:VAL:HA	0.41	1.93	7	1
1:A:170:ALA:HB1	1:A:177:TYR:O	0.41	2.16	4	1
1:A:160:ALA:CB	1:A:189:ALA:HA	0.41	2.37	15	1
1:A:183:GLY:O	1:A:185:ARG:NH1	0.41	2.49	9	1
1:A:134:SER:HB2	1:A:157:ARG:HG2	0.41	1.91	3	1
1:A:155:TRP:HB3	1:A:193:TRP:CH2	0.41	2.51	14	1
1:A:149:ASP:HA	1:A:185:ARG:NH2	0.41	2.30	2	1
1:A:142:LEU:O	1:A:143:GLN:CB	0.41	2.69	12	1
1:A:148:VAL:HG12	1:A:151:ILE:O	0.41	2.15	5	1
1:A:146:ALA:HB2	1:A:157:ARG:N	0.41	2.31	18	1
1:A:206:LEU:HG	2:B:323:LYS:HD3	0.41	1.91	17	1
1:A:133:LEU:O	1:A:135:LEU:HD23	0.41	2.16	7	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:135:LEU:O	1:A:136:ALA:C	0.40	2.59	15	1
1:A:178:ASN:OD1	1:A:180:THR:HB	0.40	2.15	14	1
1:A:193:TRP:O	1:A:194:ALA:HB3	0.40	2.15	9	2
1:A:150:LEU:C	1:A:150:LEU:HD22	0.40	2.36	15	1
1:A:160:ALA:HA	1:A:187:CYS:HB3	0.40	1.92	13	1
1:A:187:CYS:SG	1:A:193:TRP:CE3	0.40	3.15	3	1
1:A:170:ALA:O	1:A:171:PHE:CB	0.40	2.69	1	1
1:A:172:PHE:CZ	2:B:338:LEU:HD11	0.40	2.52	14	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:175:VAL:CG1	1:A:177:TYR:CD2	0.40	3.05	17	1
1:A:181:ASN:CB	1:A:201:GLU:HB2	0.40	2.47	17	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:175:VAL:CG1	1:A:177:TYR:CD1	0.40	3.05	1	1
1:A:143:GLN:CG	1:A:159:PRO:HA	0.40	2.47	20	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	74/84 (88%)	51±3 (69±5%)	18±4 (24±5%)	5±2 (7±2%)	3 18
2	B	32/38 (84%)	28±2 (87±7%)	4±2 (12±7%)	0±0 (1±1%)	29 74
All	All	2120/2440 (87%)	1585 (75%)	429 (20%)	106 (5%)	5 26

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	170	ALA	4
1	A	151	ILE	4
1	A	147	SER	4
1	A	194	ALA	3
1	A	150	LEU	3
1	A	192	SER	3
1	A	178	ASN	3
2	B	310	LEU	2
2	B	329	GLU	2
1	A	134	SER	2
1	A	202	CYS	2
1	A	168	CYS	2
1	A	177	TYR	2
1	A	169	PRO	2
1	A	157	ARG	2
1	A	145	ASN	2
1	A	160	ALA	2
1	A	179	THR	2
1	A	203	GLN	1
2	B	325	GLU	1
1	A	162	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	135	LEU	1
1	A	189	ALA	1
1	A	205	ILE	1
1	A	136	ALA	1
1	A	166	ARG	1
1	A	171	PHE	1
1	A	180	THR	1
1	A	142	LEU	1
1	A	175	VAL	1
1	A	188	LEU	1
1	A	185	ARG	1
1	A	196	ARG	1
1	A	174	GLY	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	62/71 (87%)	42±2 (68±4%)	20±2 (32±4%)	1 14
2	B	27/32 (84%)	18±2 (66±7%)	9±2 (34±7%)	1 12
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)
2	B	323	LYS	16
1	A	190	ASN	16
2	B	312	PHE	14
1	A	206	LEU	14
2	B	335	ARG	14
1	A	199	TYR	14
1	A	185	ARG	14
2	B	316	ARG	13
1	A	166	ARG	13
1	A	135	LEU	13
1	A	150	LEU	13

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Mol	Chain	Res	Type	Models (Total)
1	A	151	ILE	13
1	A	188	LEU	13
1	A	196	ARG	13
1	A	162	GLN	12
1	A	205	ILE	12
1	A	157	ARG	12
1	A	142	LEU	11
2	B	330	GLU	11
2	B	333	LYS	11
1	A	130	CYS	11
1	A	176	ARG	10
1	A	134	SER	9
1	A	133	LEU	9
1	A	168	CYS	9
1	A	131	GLU	8
1	A	172	PHE	8
1	A	204	GLU	8
1	A	177	TYR	8
1	A	187	CYS	8
2	B	315	LEU	8
2	B	319	LEU	8
1	A	163	LEU	8
1	A	149	ASP	8
1	A	143	GLN	8
2	B	329	GLU	7
1	A	144	CYS	7
2	B	314	LEU	7
1	A	207	ASN	7
2	B	338	LEU	7
2	B	310	LEU	6
2	B	313	ASN	6
2	B	311	THR	6
2	B	309	ASP	6
1	A	203	GLN	6
2	B	326	GLN	6
1	A	158	SER	6
2	B	340	GLU	6
1	A	186	GLU	6
1	A	198	ASN	6
1	A	200	SER	6
2	B	317	GLU	5
1	A	193	TRP	5

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Mol	Chain	Res	Type	Models (Total)
1	A	180	THR	5
2	B	320	GLU	5
1	A	129	HIS	5
1	A	201	GLU	5
1	A	154	CYS	5
2	B	325	GLU	5
1	A	182	ASN	4
1	A	171	PHE	4
2	B	337	LEU	4
1	A	202	CYS	4
1	A	147	SER	4
2	B	336	LEU	4
2	B	327	GLU	4
1	A	148	VAL	3
1	A	175	VAL	3
1	A	178	ASN	3
2	B	339	GLU	2
1	A	153	THR	2
1	A	184	TYR	2
1	A	165	VAL	1
1	A	132	SER	1
1	A	173	TYR	1
1	A	197	VAL	1
1	A	179	THR	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided