Full wwPDB NMR Structure Validation Report (i)

Jun 15, 2024 – 09:16 PM EDT

PDB ID	:	2KSY
Title	:	Solution nmr structure of sensory rhodopsin II
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Deposited on	:	2010-01-14

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 (i) 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 (i)) were used in the production of this report:

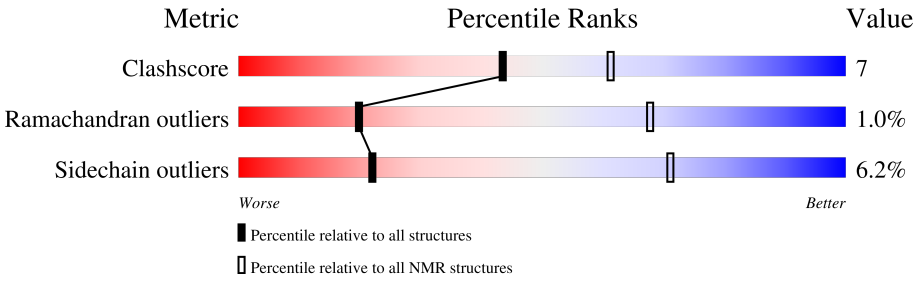
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	247	72% 13% 15%

2 Ensemble composition and analysis

This entry contains 30 models. Model 26 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:25, A:32-A:218 (210)	0.52	26

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 6 clusters and 7 single-model clusters were found.

Cluster number	Models
1	3, 8, 10, 12, 26, 27, 29
2	14, 15, 16, 18, 25, 30
3	9, 19, 20, 22
4	4, 17
5	7, 24
6	5, 21
Single-model clusters	1; 2; 6; 11; 13; 23; 28

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3834 atoms, of which 1943 are hydrogens and 0 are deuteriums.

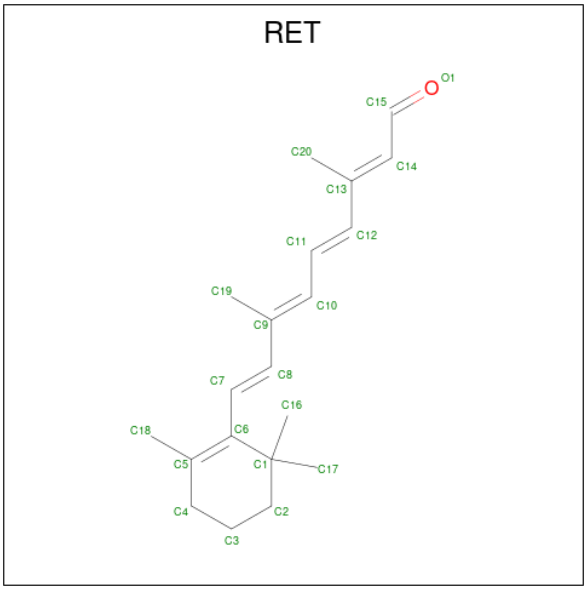
- Molecule 1 is a protein called Sensory rhodopsin II.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	247	3786	1237	1915	305	322	7	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	LEU	-	EXPRESSION TAG	UNP Q3IMZ8
A	241	GLU	-	EXPRESSION TAG	UNP Q3IMZ8
A	242	HIS	-	EXPRESSION TAG	UNP Q3IMZ8
A	243	HIS	-	EXPRESSION TAG	UNP Q3IMZ8
A	244	HIS	-	EXPRESSION TAG	UNP Q3IMZ8
A	245	HIS	-	EXPRESSION TAG	UNP Q3IMZ8
A	246	HIS	-	EXPRESSION TAG	UNP Q3IMZ8
A	247	HIS	-	EXPRESSION TAG	UNP Q3IMZ8

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



Mol	Chain	Residues	Atoms		
			Total	C	H
2	A	1	48	20	28

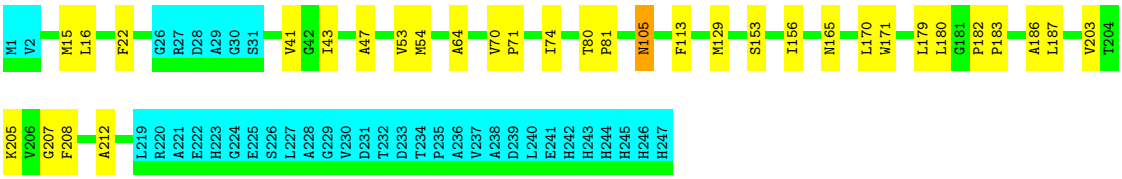
4 Residue-property plots

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: Sensory rhodopsin II

Chain A: 



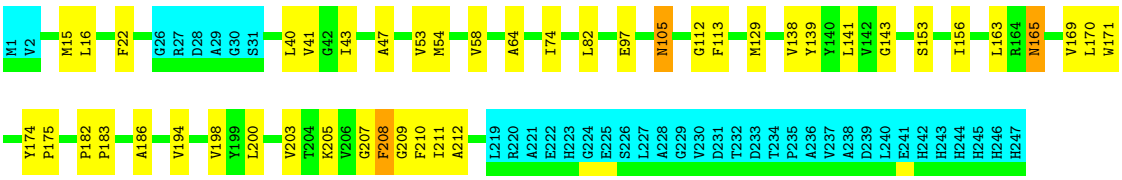
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Sensory rhodopsin II

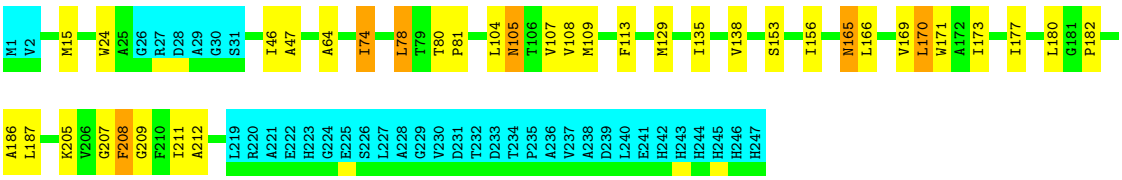
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: Sensory rhodopsin II

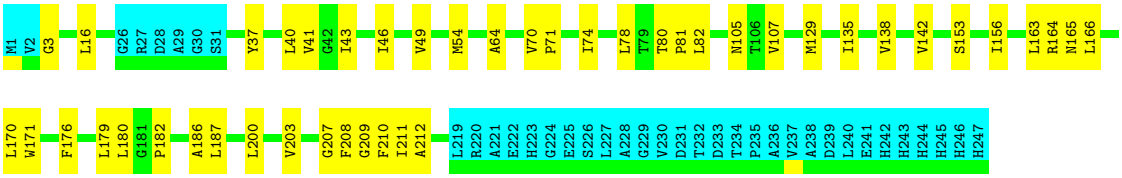
Chain A: 



4.2.3 Score per residue for model 3

• Molecule 1: Sensory rhodopsin II

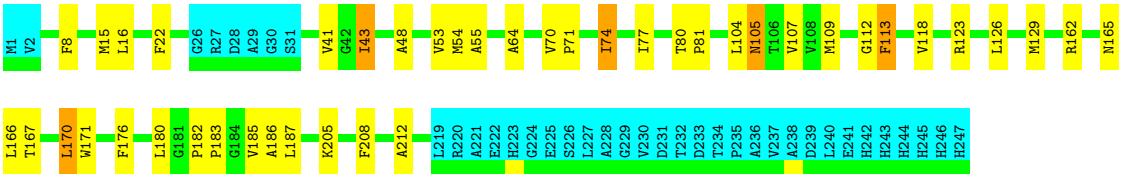
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Sensory rhodopsin II

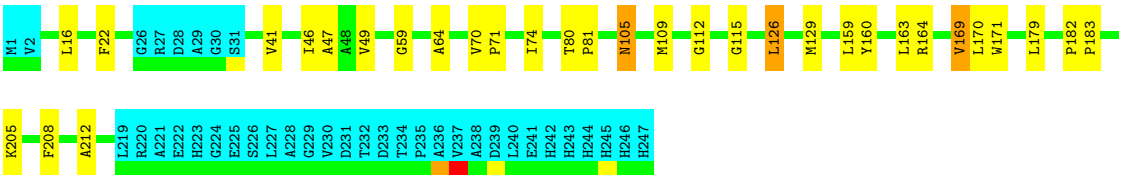
Chain A:



4.2.5 Score per residue for model 5

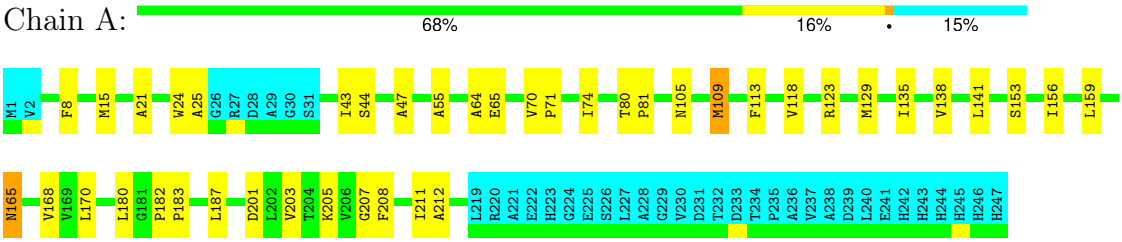
• Molecule 1: Sensory rhodopsin II

Chain A:



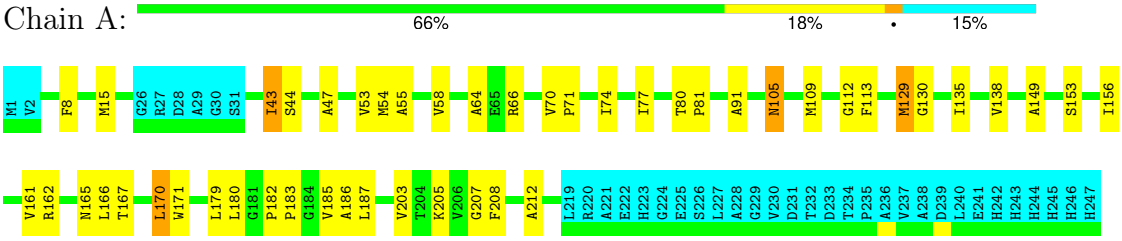
4.2.6 Score per residue for model 6

• Molecule 1: Sensory rhodopsin II



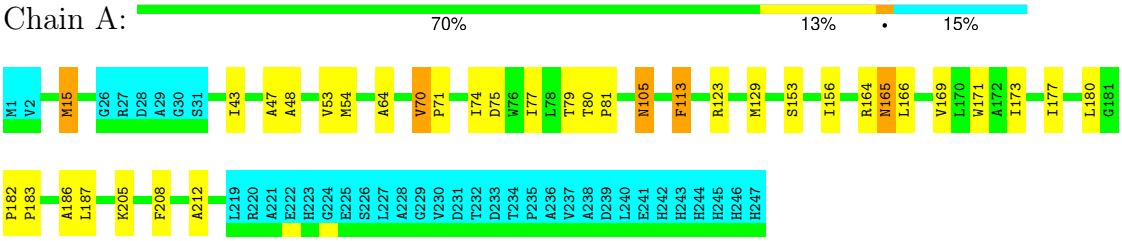
4.2.7 Score per residue for model 7

• Molecule 1: Sensory rhodopsin II



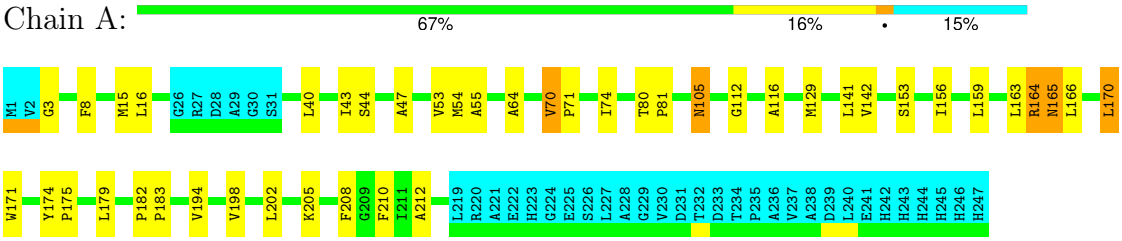
4.2.8 Score per residue for model 8

• Molecule 1: Sensory rhodopsin II



4.2.9 Score per residue for model 9

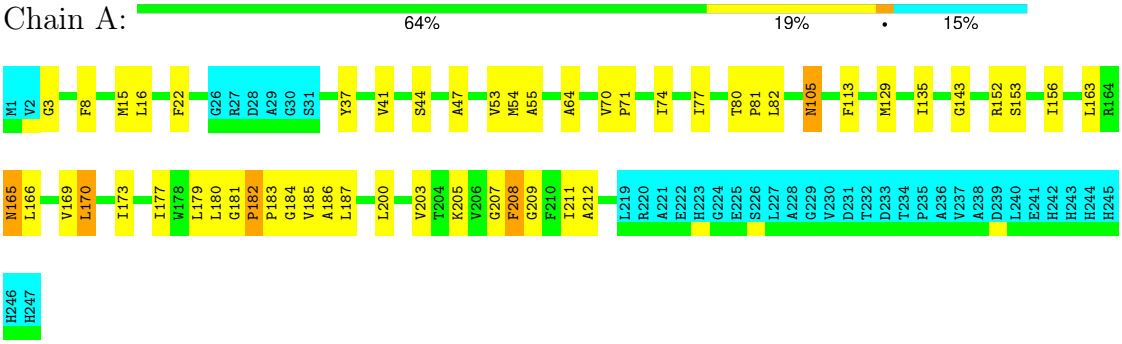
• Molecule 1: Sensory rhodopsin II



4.2.10 Score per residue for model 10

• Molecule 1: Sensory rhodopsin II

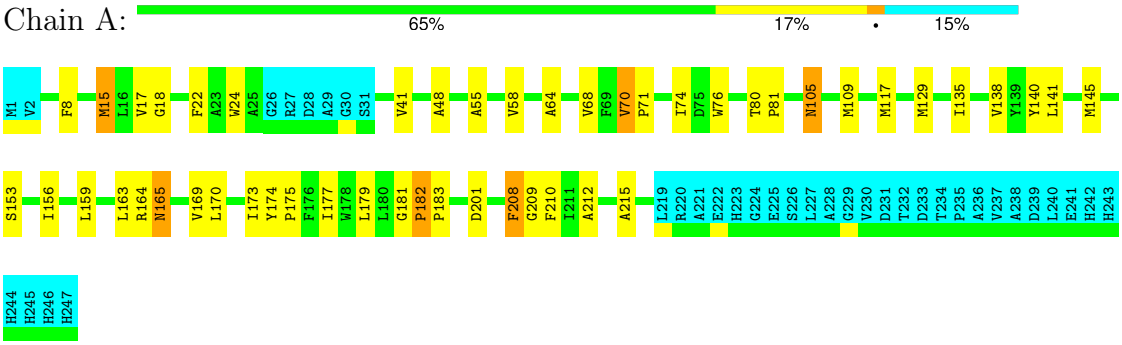
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Sensory rhodopsin II

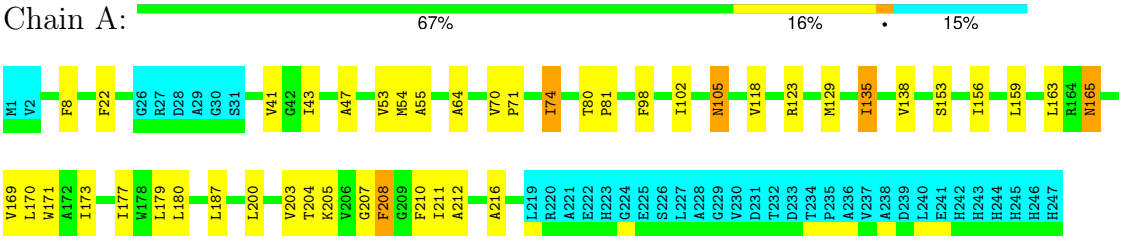
Chain A:



4.2.12 Score per residue for model 12

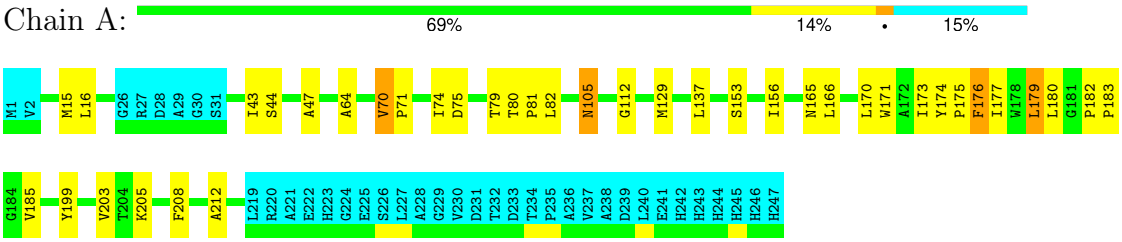
• Molecule 1: Sensory rhodopsin II

Chain A:



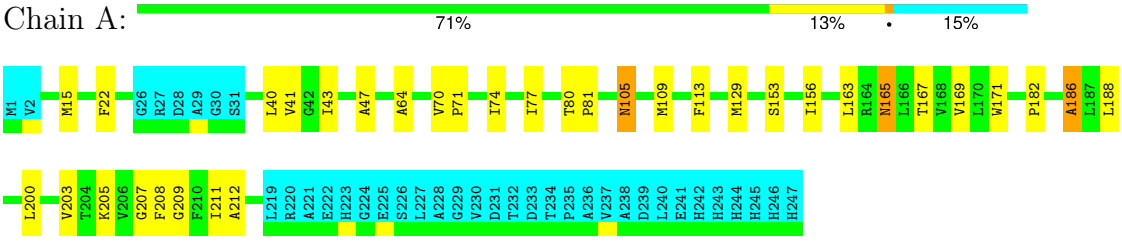
4.2.13 Score per residue for model 13

• Molecule 1: Sensory rhodopsin II



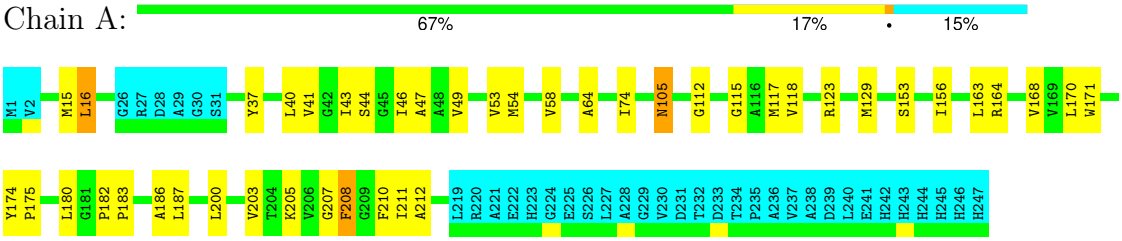
4.2.14 Score per residue for model 14

• Molecule 1: Sensory rhodopsin II



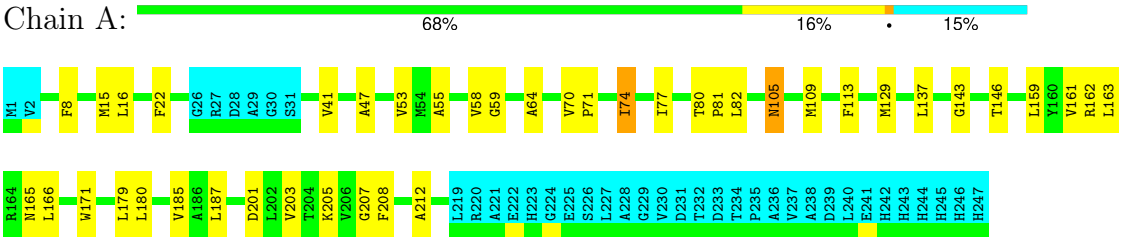
4.2.15 Score per residue for model 15

• Molecule 1: Sensory rhodopsin II



4.2.16 Score per residue for model 16

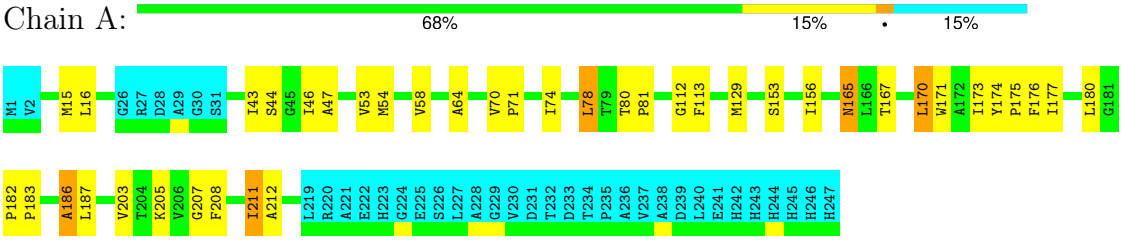
• Molecule 1: Sensory rhodopsin II



4.2.17 Score per residue for model 17

• Molecule 1: Sensory rhodopsin II

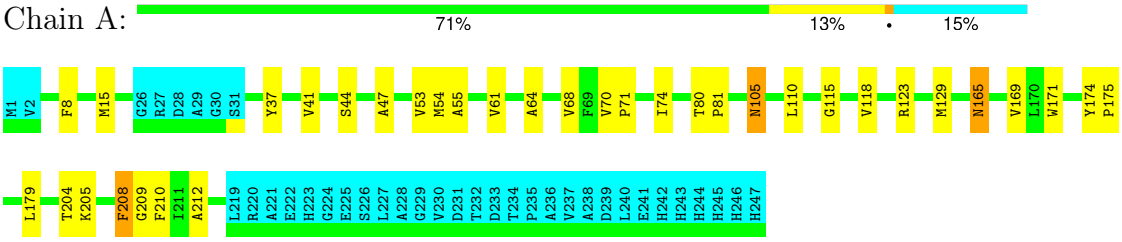
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Sensory rhodopsin II

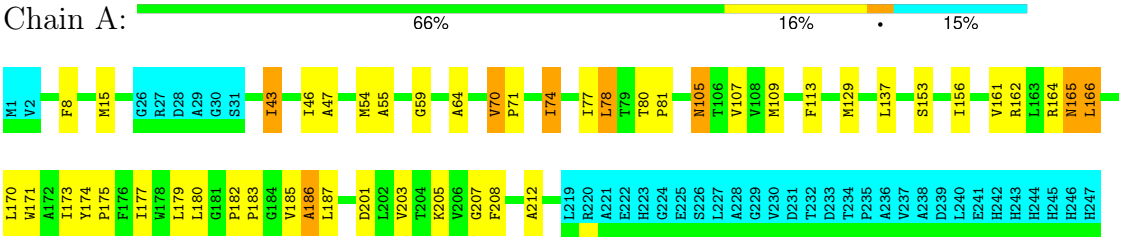
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Sensory rhodopsin II

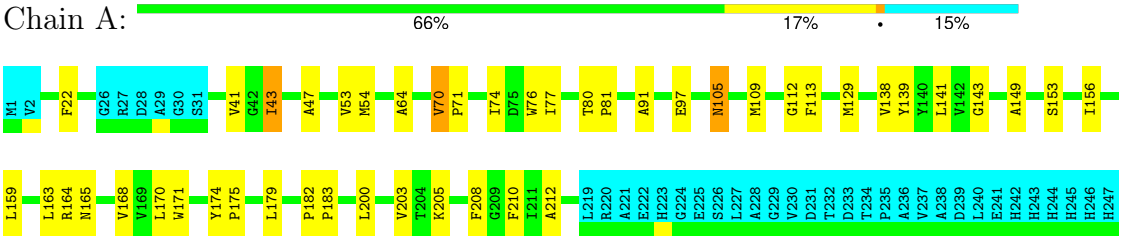
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Sensory rhodopsin II

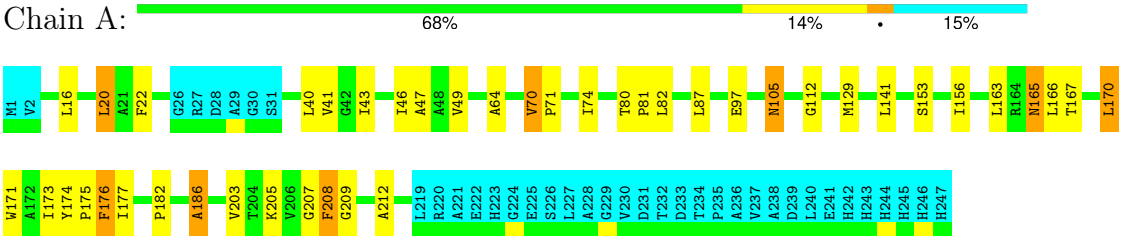
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: Sensory rhodopsin II

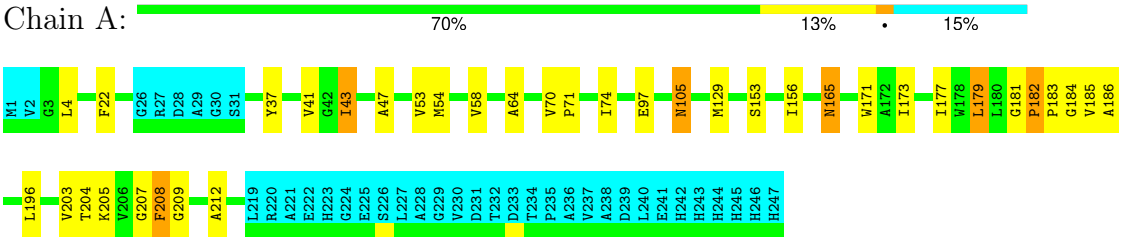
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: Sensory rhodopsin II

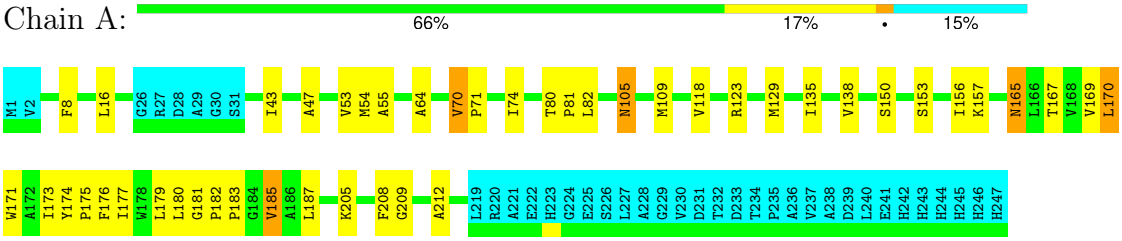
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: Sensory rhodopsin II

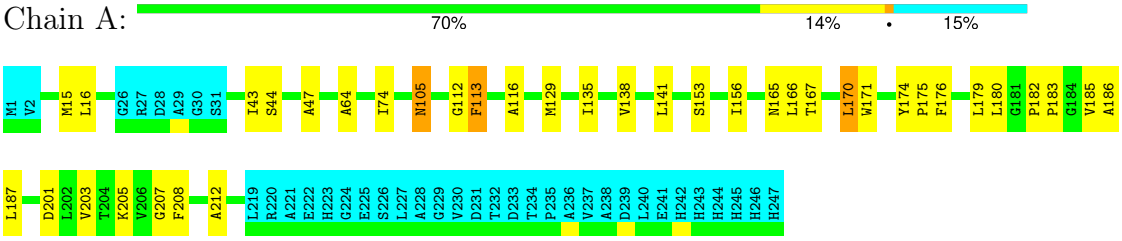
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: Sensory rhodopsin II

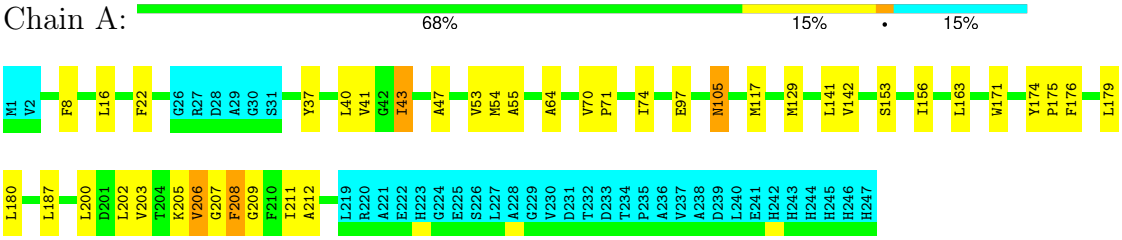
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: Sensory rhodopsin II

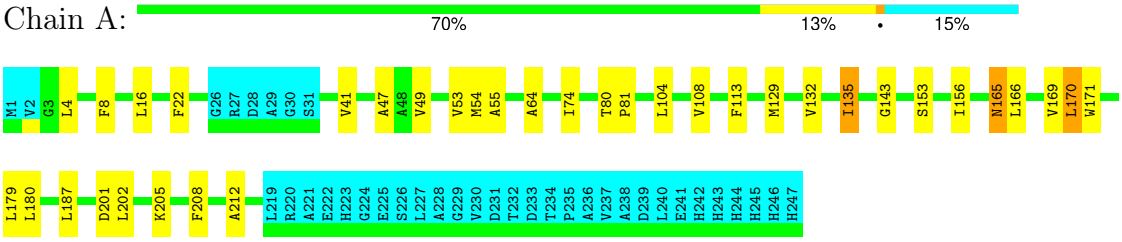
Chain A:



4.2.26 Score per residue for model 26 (medoid)

• Molecule 1: Sensory rhodopsin II

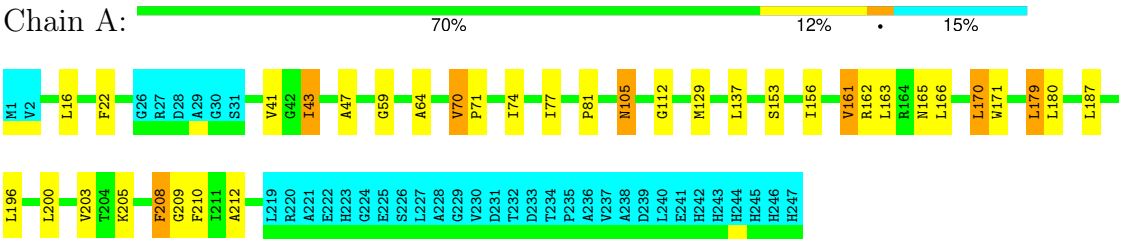
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: Sensory rhodopsin II

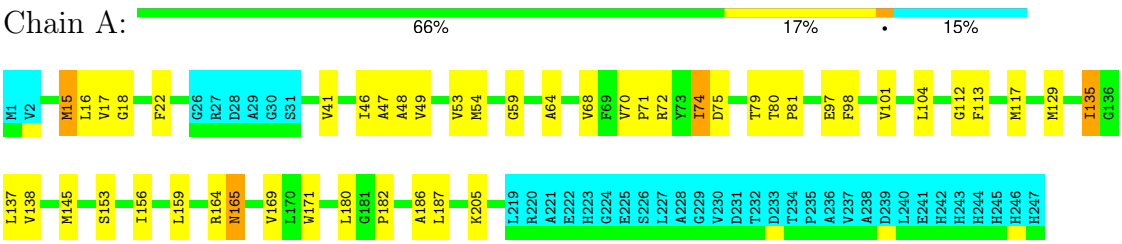
Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: Sensory rhodopsin II

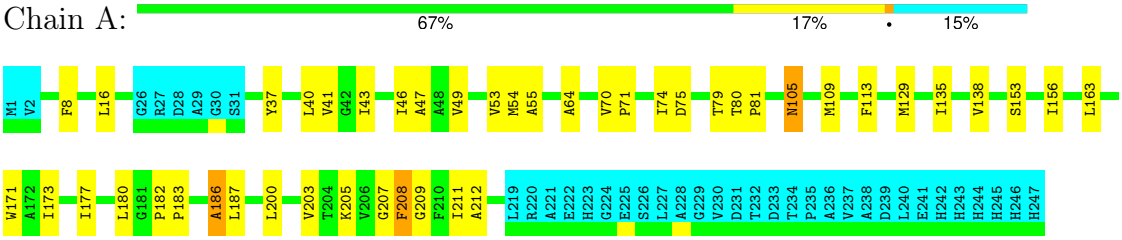
Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: Sensory rhodopsin II

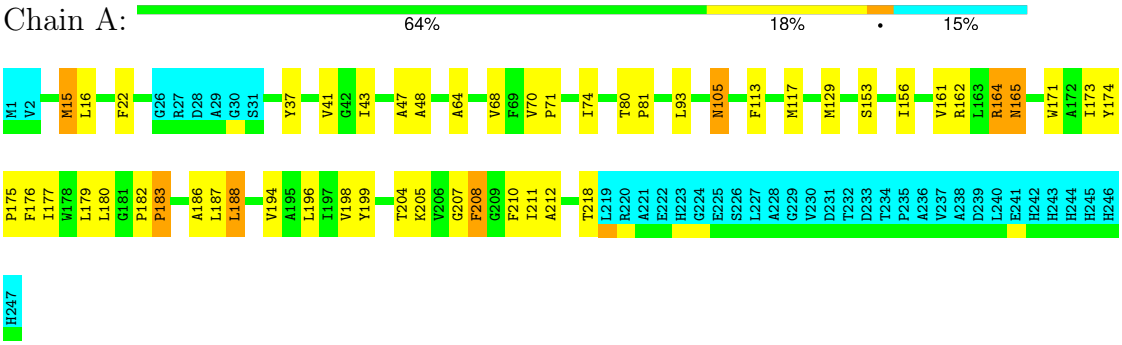
Chain A:



4.2.30 Score per residue for model 30

• Molecule 1: Sensory rhodopsin II

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing, molecular dynamics.*

Of the 100 calculated structures, 30 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
ARIA	structure solution	
CNS	structure solution	
CNS	refinement	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

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	1592	1660	1661	23±4
2	A	20	28	27	2±1
All	All	48360	50640	50636	693

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:171:TRP:HE1	2:A:301:RET:H203	0.72	1.44	18	27
1:A:173:ILE:HG22	1:A:177:ILE:CG1	0.62	2.25	13	2
1:A:138:VAL:HA	1:A:141:LEU:HD12	0.60	1.74	20	4
1:A:159:LEU:HG	1:A:163:LEU:HD11	0.60	1.74	9	1
1:A:16:LEU:O	1:A:20:LEU:HD23	0.59	1.97	21	1
1:A:70:VAL:N	1:A:71:PRO:HD2	0.58	2.13	27	12
1:A:109:MET:SD	1:A:109:MET:N	0.58	2.77	6	1
1:A:47:ALA:HB2	1:A:205:LYS:HE2	0.57	1.77	18	27
1:A:163:LEU:HD13	1:A:208:PHE:CZ	0.57	2.35	9	1
1:A:70:VAL:HG12	1:A:71:PRO:HD3	0.57	1.75	19	12
1:A:43:ILE:HG22	1:A:205:LYS:HE3	0.57	1.77	27	7

Continued on next page...

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:180:LEU:HD22	1:A:187:LEU:HD11	0.56	1.77	12	20
1:A:22:PHE:HB2	1:A:41:VAL:HG22	0.56	1.78	21	16
1:A:115:GLY:O	1:A:118:VAL:HG22	0.56	2.01	15	2
1:A:182:PRO:N	1:A:183:PRO:HD2	0.55	2.17	30	5
1:A:8:PHE:HB2	1:A:55:ALA:HB2	0.54	1.79	12	14
1:A:59:GLY:HA3	1:A:71:PRO:HD3	0.54	1.78	16	5
1:A:43:ILE:HG23	1:A:82:LEU:HD23	0.54	1.79	23	3
1:A:174:TYR:N	1:A:175:PRO:HD2	0.54	2.18	11	6
1:A:173:ILE:HG22	1:A:177:ILE:HG13	0.54	1.80	13	2
1:A:70:VAL:N	1:A:71:PRO:CD	0.54	2.71	16	19
1:A:159:LEU:HD13	1:A:215:ALA:HB3	0.54	1.80	11	1
1:A:46:ILE:O	1:A:49:VAL:HG22	0.53	2.04	28	6
1:A:46:ILE:HD12	1:A:78:LEU:HD12	0.52	1.79	19	4
1:A:185:VAL:O	1:A:185:VAL:HG23	0.52	2.04	7	3
1:A:208:PHE:O	1:A:212:ALA:N	0.52	2.42	24	25
1:A:40:LEU:HD12	1:A:43:ILE:HD11	0.52	1.81	29	4
1:A:80:THR:HB	1:A:81:PRO:HD3	0.52	1.81	26	18
1:A:80:THR:HG21	1:A:109:MET:HE1	0.52	1.82	5	8
1:A:105:ASN:HD22	1:A:105:ASN:N	0.52	2.02	7	21
1:A:170:LEU:HD22	1:A:203:VAL:HG13	0.52	1.81	21	1
1:A:15:MET:HB3	1:A:48:ALA:HB2	0.52	1.81	28	5
1:A:80:THR:N	1:A:81:PRO:HD2	0.52	2.20	28	6
1:A:59:GLY:O	1:A:70:VAL:HG13	0.51	2.05	16	1
1:A:112:GLY:HA3	2:A:301:RET:H21	0.51	1.82	5	13
1:A:53:VAL:O	1:A:58:VAL:HG22	0.51	2.06	15	3
1:A:101:VAL:HG21	1:A:145:MET:HE3	0.51	1.82	28	1
1:A:182:PRO:HA	1:A:186:ALA:HB2	0.50	1.83	3	11
1:A:173:ILE:O	1:A:177:ILE:HG12	0.50	2.06	21	5
1:A:188:LEU:HD13	1:A:188:LEU:N	0.50	2.19	30	1
1:A:141:LEU:HD13	1:A:168:VAL:HG22	0.50	1.82	20	2
1:A:194:VAL:O	1:A:198:VAL:HG22	0.50	2.07	1	3
1:A:173:ILE:HG22	1:A:177:ILE:HD11	0.50	1.82	11	8
1:A:137:LEU:HD13	1:A:138:VAL:N	0.50	2.22	28	1
1:A:153:SER:HB2	1:A:156:ILE:HG12	0.50	1.84	3	10
1:A:15:MET:SD	1:A:44:SER:HA	0.49	2.48	9	9
1:A:164:ARG:O	1:A:168:VAL:HG23	0.49	2.07	20	2
1:A:37:TYR:O	1:A:41:VAL:HG23	0.49	2.07	30	8
1:A:105:ASN:N	1:A:105:ASN:HD22	0.49	2.05	8	4
1:A:209:GLY:O	1:A:212:ALA:HB3	0.49	2.08	3	12
1:A:153:SER:HB3	1:A:156:ILE:HG12	0.49	1.84	1	16
1:A:200:LEU:O	1:A:203:VAL:HG12	0.49	2.07	10	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:LEU:HD12	1:A:142:VAL:HG23	0.49	1.84	25	1
1:A:165:ASN:O	1:A:169:VAL:HG23	0.49	2.08	2	11
1:A:161:VAL:HG12	1:A:162:ARG:N	0.49	2.22	19	3
1:A:162:ARG:O	1:A:166:LEU:HD12	0.49	2.08	7	2
1:A:143:GLY:O	1:A:146:THR:HG22	0.48	2.08	16	1
1:A:53:VAL:HG23	1:A:54:MET:N	0.48	2.23	9	17
1:A:202:LEU:O	1:A:206:VAL:HG22	0.48	2.08	25	1
1:A:163:LEU:HG	1:A:208:PHE:HB2	0.48	1.84	10	10
1:A:105:ASN:HD21	1:A:137:LEU:HD13	0.48	1.69	27	3
1:A:208:PHE:N	1:A:208:PHE:CD1	0.48	2.81	16	5
1:A:159:LEU:O	1:A:163:LEU:HG	0.48	2.08	9	2
1:A:74:ILE:O	1:A:78:LEU:HD23	0.48	2.09	2	2
1:A:115:GLY:HA2	1:A:126:LEU:HD11	0.48	1.86	5	1
1:A:141:LEU:CD1	1:A:168:VAL:HG22	0.48	2.38	20	1
1:A:167:THR:HA	1:A:170:LEU:HD11	0.48	1.85	23	6
1:A:91:ALA:HA	1:A:149:ALA:HB2	0.48	1.85	20	1
1:A:21:ALA:O	1:A:25:ALA:HB2	0.47	2.08	6	1
1:A:177:ILE:O	1:A:182:PRO:HD2	0.47	2.09	10	3
1:A:137:LEU:HD13	1:A:137:LEU:C	0.47	2.29	28	1
1:A:207:GLY:O	1:A:211:ILE:HD12	0.47	2.10	6	1
1:A:169:VAL:CG1	1:A:170:LEU:N	0.46	2.77	5	1
1:A:20:LEU:CD2	1:A:20:LEU:N	0.46	2.79	21	1
1:A:135:ILE:O	1:A:138:VAL:HG22	0.46	2.11	11	9
1:A:170:LEU:HD12	1:A:171:TRP:N	0.46	2.25	21	4
1:A:164:ARG:HG3	1:A:165:ASN:N	0.46	2.25	28	3
1:A:182:PRO:O	1:A:184:GLY:N	0.46	2.48	10	2
1:A:54:MET:HG2	1:A:71:PRO:HG2	0.46	1.86	19	2
1:A:179:LEU:HG	1:A:185:VAL:HG22	0.46	1.86	7	3
1:A:68:VAL:HG21	1:A:117:MET:SD	0.46	2.51	28	2
1:A:71:PRO:HA	1:A:74:ILE:HG22	0.46	1.88	16	2
1:A:180:LEU:HA	1:A:185:VAL:HG23	0.46	1.88	24	1
1:A:171:TRP:NE1	2:A:301:RET:H203	0.45	2.25	25	8
1:A:207:GLY:O	1:A:211:ILE:HG13	0.45	2.12	10	10
1:A:104:LEU:O	1:A:107:VAL:HG12	0.45	2.11	2	1
1:A:77:ILE:O	1:A:81:PRO:HG2	0.45	2.11	14	6
1:A:15:MET:HE3	1:A:47:ALA:CB	0.45	2.42	19	2
1:A:203:VAL:O	1:A:207:GLY:HA3	0.45	2.10	16	10
1:A:179:LEU:O	1:A:185:VAL:HG22	0.45	2.10	10	4
1:A:171:TRP:CZ2	2:A:301:RET:H202	0.45	2.47	3	1
1:A:165:ASN:N	1:A:165:ASN:HD22	0.45	2.09	1	4
1:A:40:LEU:HD12	1:A:43:ILE:HD12	0.45	1.89	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:208:PHE:O	1:A:212:ALA:HB2	0.45	2.12	2	3
1:A:208:PHE:CD1	1:A:208:PHE:C	0.44	2.90	21	1
1:A:166:LEU:O	1:A:170:LEU:HG	0.44	2.12	13	10
1:A:24:TRP:HA	1:A:24:TRP:CE3	0.44	2.48	2	2
1:A:164:ARG:NE	1:A:165:ASN:ND2	0.44	2.66	19	2
1:A:207:GLY:O	1:A:211:ILE:HG12	0.43	2.13	17	1
1:A:75:ASP:O	1:A:79:THR:HG23	0.43	2.14	8	4
1:A:204:THR:O	1:A:208:PHE:CD1	0.43	2.72	18	4
1:A:53:VAL:O	1:A:58:VAL:HG12	0.43	2.13	17	3
1:A:76:TRP:HB3	1:A:109:MET:SD	0.43	2.53	11	2
1:A:179:LEU:HD13	1:A:179:LEU:O	0.43	2.14	13	1
1:A:118:VAL:HG21	1:A:123:ARG:HB3	0.43	1.91	4	3
1:A:159:LEU:HD23	1:A:159:LEU:O	0.43	2.14	6	1
1:A:176:PHE:O	1:A:180:LEU:HG	0.43	2.14	25	7
1:A:70:VAL:N	1:A:71:PRO:HD3	0.43	2.27	16	2
1:A:105:ASN:ND2	1:A:137:LEU:HD22	0.43	2.29	16	2
1:A:17:VAL:HG13	1:A:18:GLY:N	0.42	2.29	28	2
1:A:182:PRO:N	1:A:183:PRO:CD	0.42	2.82	4	10
1:A:179:LEU:HD23	1:A:180:LEU:HD23	0.42	1.89	27	1
1:A:173:ILE:HA	1:A:176:PHE:CE2	0.42	2.49	13	2
1:A:164:ARG:HE	1:A:165:ASN:ND2	0.42	2.13	30	1
1:A:118:VAL:HG11	1:A:123:ARG:N	0.42	2.30	6	1
1:A:180:LEU:HD22	1:A:187:LEU:CD1	0.42	2.44	23	1
1:A:80:THR:HB	1:A:109:MET:HE2	0.42	1.92	6	1
1:A:165:ASN:HD22	1:A:165:ASN:N	0.42	2.12	22	2
1:A:59:GLY:HA2	1:A:70:VAL:HG22	0.42	1.92	16	1
1:A:185:VAL:CG2	1:A:187:LEU:HD21	0.42	2.44	10	1
1:A:110:LEU:HD23	1:A:110:LEU:C	0.42	2.35	18	1
1:A:161:VAL:CG1	1:A:162:ARG:N	0.42	2.82	19	1
1:A:77:ILE:O	1:A:81:PRO:HG3	0.42	2.14	27	1
1:A:161:VAL:HG23	1:A:162:ARG:N	0.41	2.30	7	2
1:A:70:VAL:HG22	1:A:71:PRO:HD3	0.41	1.90	16	1
1:A:160:TYR:O	1:A:164:ARG:HB3	0.41	2.16	5	1
1:A:139:TYR:O	1:A:143:GLY:N	0.41	2.54	20	2
1:A:91:ALA:HB2	1:A:149:ALA:HB2	0.41	1.91	7	1
1:A:164:ARG:HG3	1:A:165:ASN:HD22	0.41	1.76	28	2
1:A:132:VAL:O	1:A:135:ILE:HG13	0.41	2.15	26	1
1:A:129:MET:C	1:A:129:MET:SD	0.41	2.99	25	2
1:A:170:LEU:HD12	1:A:171:TRP:H	0.41	1.75	7	1
1:A:17:VAL:CG1	1:A:18:GLY:N	0.41	2.84	11	1
1:A:159:LEU:HD12	1:A:163:LEU:HD13	0.41	1.91	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:O	1:A:43:ILE:HG12	0.41	2.16	3	1
1:A:159:LEU:O	1:A:163:LEU:HB2	0.41	2.15	5	1
1:A:199:TYR:O	1:A:203:VAL:HG23	0.41	2.15	13	1
1:A:159:LEU:O	1:A:163:LEU:HD13	0.41	2.16	20	1
1:A:93:LEU:HD12	1:A:93:LEU:N	0.41	2.30	30	1
1:A:141:LEU:HD12	1:A:142:VAL:N	0.41	2.30	9	1
1:A:174:TYR:N	1:A:175:PRO:CD	0.41	2.84	25	8
1:A:167:THR:O	1:A:171:TRP:HB2	0.41	2.15	14	1
1:A:188:LEU:HD12	1:A:188:LEU:N	0.41	2.30	14	1
1:A:61:VAL:HG13	1:A:68:VAL:HG23	0.41	1.91	18	1
1:A:187:LEU:N	1:A:187:LEU:HD23	0.41	2.30	23	1
1:A:118:VAL:HG21	1:A:123:ARG:N	0.41	2.31	15	2
1:A:173:ILE:HG22	1:A:177:ILE:HG12	0.41	1.92	21	1
1:A:68:VAL:HG11	1:A:117:MET:HG3	0.41	1.93	30	1
1:A:104:LEU:O	1:A:108:VAL:HG23	0.41	2.16	2	2
1:A:140:TYR:HB3	1:A:145:MET:SD	0.41	2.56	11	1
1:A:196:LEU:O	1:A:199:TYR:HB3	0.41	2.16	30	1
1:A:142:VAL:HG22	1:A:164:ARG:HH11	0.40	1.76	3	1
1:A:129:MET:HE3	1:A:130:GLY:HA2	0.40	1.92	7	1
1:A:116:ALA:HB2	1:A:183:PRO:HB3	0.40	1.93	9	2
1:A:77:ILE:HA	1:A:109:MET:HG3	0.40	1.91	19	1
1:A:164:ARG:HE	1:A:165:ASN:HD21	0.40	1.59	30	1
1:A:138:VAL:O	1:A:142:VAL:HG23	0.40	2.17	3	1
1:A:77:ILE:HG12	1:A:109:MET:HB3	0.40	1.93	4	1
1:A:150:SER:HA	1:A:157:LYS:HG2	0.40	1.93	23	1
1:A:16:LEU:HD13	1:A:16:LEU:O	0.40	2.17	15	1
1:A:105:ASN:O	1:A:109:MET:HG2	0.40	2.16	2	1
1:A:74:ILE:HD13	1:A:74:ILE:O	0.40	2.17	12	1
1:A:87:LEU:HD22	1:A:141:LEU:HD22	0.40	1.93	21	1
1:A:70:VAL:HB	1:A:71:PRO:HD3	0.40	1.94	30	1
1:A:98:PHE:O	1:A:102:ILE:HG12	0.40	2.17	12	1
1:A:209:GLY:HA2	1:A:212:ALA:HB3	0.40	1.94	23	1
1:A:74:ILE:CG2	1:A:75:ASP:N	0.40	2.84	28	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	210/247 (85%)	198±2 (94±1%)	10±1 (5±1%)	2±1 (1±1%)	20 68
All	All	6300/7410 (85%)	5947 (94%)	291 (5%)	62 (1%)	20 68

All 9 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	64	ALA	30
1	A	186	ALA	11
1	A	113	PHE	4
1	A	181	GLY	4
1	A	182	PRO	4
1	A	183	PRO	4
1	A	3	GLY	2
1	A	143	GLY	2
1	A	185	VAL	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	161/189 (85%)	151±2 (94±1%)	10±2 (6±1%)	22 71
All	All	4830/5670 (85%)	4532 (94%)	298 (6%)	22 71

All 51 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	74	ILE	30
1	A	129	MET	28
1	A	105	ASN	27
1	A	165	ASN	26
1	A	16	LEU	18
1	A	170	LEU	17
1	A	113	PHE	16
1	A	208	PHE	13

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Mol	Chain	Res	Type	Models (Total)
1	A	179	LEU	13
1	A	43	ILE	13
1	A	210	PHE	10
1	A	70	VAL	9
1	A	15	MET	7
1	A	97	GLU	6
1	A	201	ASP	6
1	A	135	ILE	5
1	A	82	LEU	4
1	A	164	ARG	4
1	A	78	LEU	3
1	A	107	VAL	3
1	A	166	LEU	3
1	A	104	LEU	2
1	A	126	LEU	2
1	A	202	LEU	2
1	A	176	PHE	2
1	A	117	MET	2
1	A	4	LEU	2
1	A	196	LEU	2
1	A	169	VAL	1
1	A	65	GLU	1
1	A	109	MET	1
1	A	66	ARG	1
1	A	123	ARG	1
1	A	152	ARG	1
1	A	24	TRP	1
1	A	58	VAL	1
1	A	141	LEU	1
1	A	180	LEU	1
1	A	185	VAL	1
1	A	211	ILE	1
1	A	20	LEU	1
1	A	40	LEU	1
1	A	206	VAL	1
1	A	49	VAL	1
1	A	161	VAL	1
1	A	72	ARG	1
1	A	98	PHE	1
1	A	159	LEU	1
1	A	183	PRO	1
1	A	188	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	218	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 monosaccharides in this entry.

6.6 Ligand geometry

1 ligand 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	Bond lengths		
					Counts	RMSZ	#Z>2
2	RET	A	301	1	20,20,21	1.77±0.03	4±0 (20±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	Bond angles		
					Counts	RMSZ	#Z>2
2	RET	A	301	1	27,27,28	1.23±0.02	4±0 (14±0%)

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	RET	A	301	1	-	0±0,13,30,31	0±0,1,1,1

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	A	301	RET	C1-C6	5.54	1.60	1.53	13	30
2	A	301	RET	C5-C6	3.44	1.40	1.34	13	30
2	A	301	RET	C14-C13	2.71	1.35	1.33	23	30
2	A	301	RET	C15-C14	2.58	1.39	1.49	26	30

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	301	RET	C2-C1-C6	2.78	114.47	110.44	19	30
2	A	301	RET	C1-C6-C7	2.69	122.95	115.65	10	30
2	A	301	RET	C8-C7-C6	2.65	134.06	127.00	10	30
2	A	301	RET	C1-C6-C5	2.60	119.08	122.64	3	30

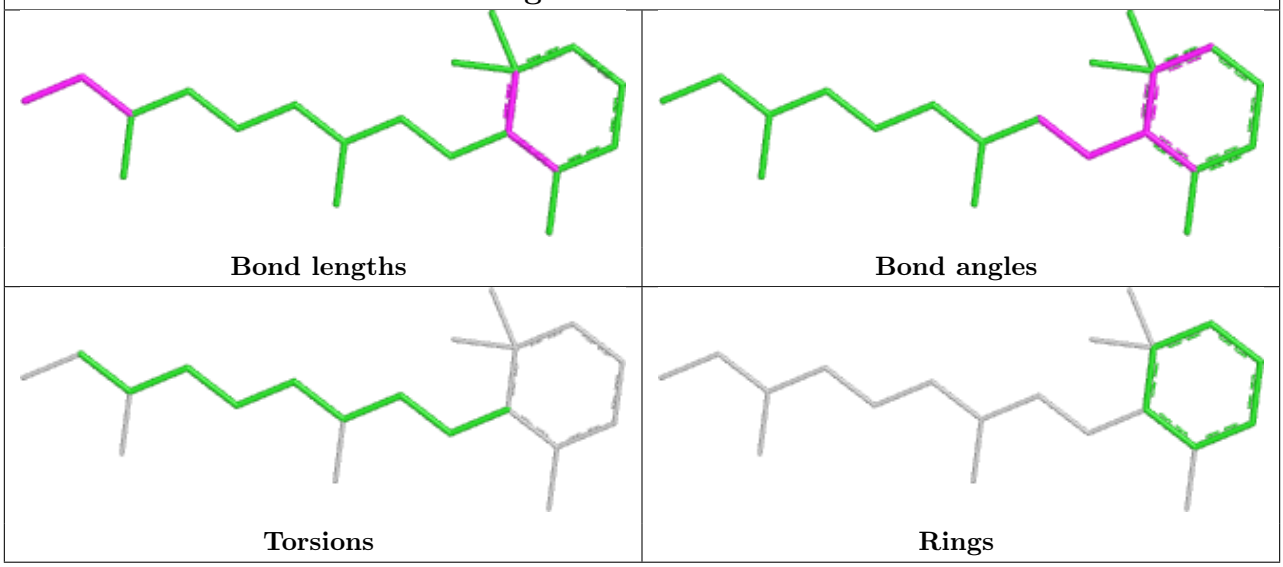
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand RET A 301



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