



Full wwPDB NMR Structure Validation Report ⓘ

Apr 28, 2016 – 10:17 PM EDT

PDB ID : 4BHP
Title : A structural model of CAP mutant (T127L and S128I) in cGMP-bound state
Authors : Tzeng, S.R.; Kalodimos, C.G.
Deposited on : 2013-04-04

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
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

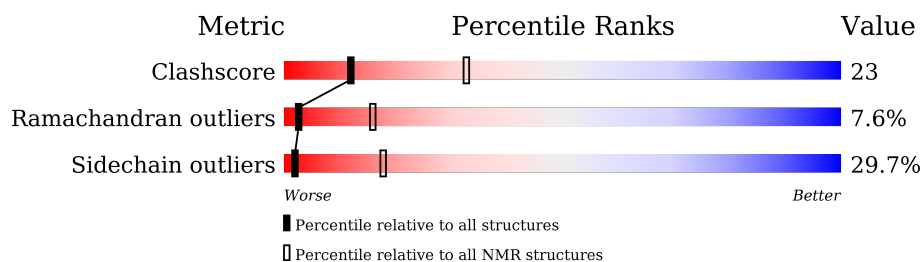
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 13%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	209	

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:7-A:31, A:37-A:51, A:58-A:75, A:82-A:126, A:130-A:209 (183)	0.55	18

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 2 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3182 atoms, of which 1530 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CAMP RECEPTOR PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	209	Total	C	H	N	O	S	0
			3182	1049	1530	290	304	9	

There are 2 discrepancies between the modelled and reference sequences:

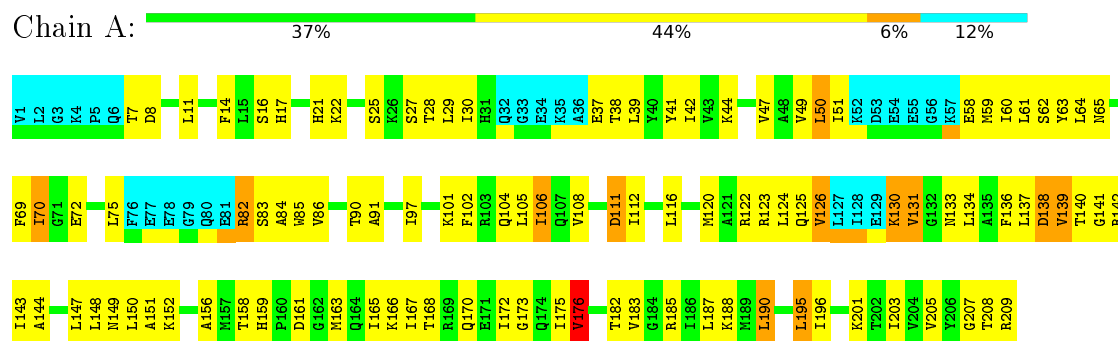
Chain	Residue	Modelled	Actual	Comment	Reference
A	127	LEU	THR	ENGINEERED MUTATION	UNP P0ACJ8
A	128	ILE	SER	ENGINEERED MUTATION	UNP P0ACJ8

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: CAMP RECEPTOR PROTEIN

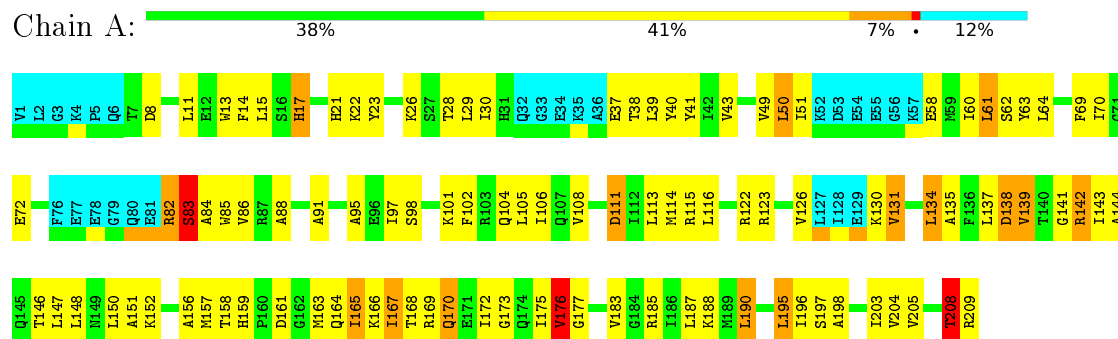


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

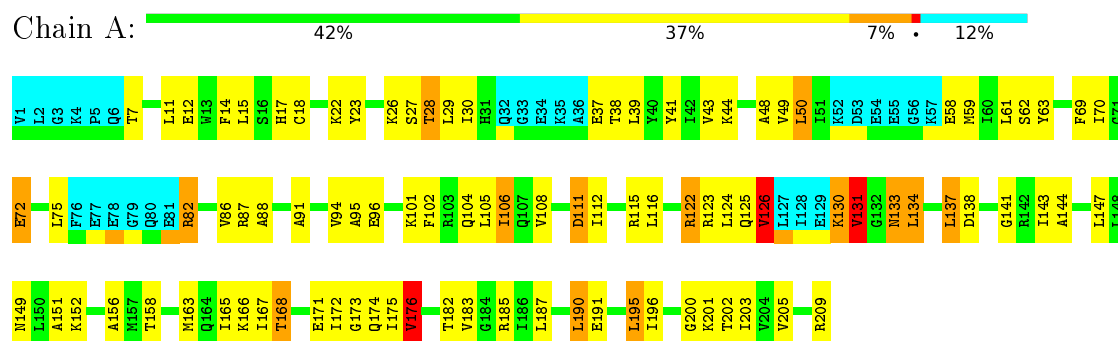
4.2.1 Score per residue for model 1

• Molecule 1: CAMP RECEPTOR PROTEIN



4.2.2 Score per residue for model 2

• Molecule 1: CAMP RECEPTOR PROTEIN



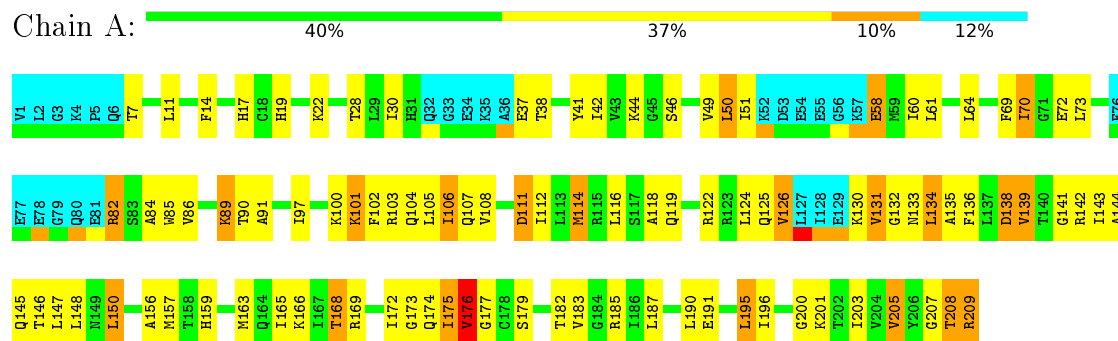
4.2.3 Score per residue for model 3

• Molecule 1: CAMP RECEPTOR PROTEIN



4.2.4 Score per residue for model 4

• Molecule 1: CAMP RECEPTOR PROTEIN



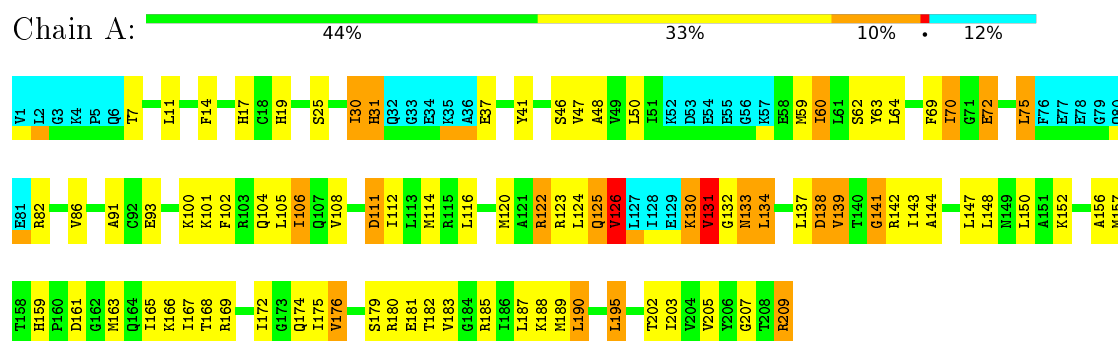
4.2.5 Score per residue for model 5

• Molecule 1: CAMP RECEPTOR PROTEIN



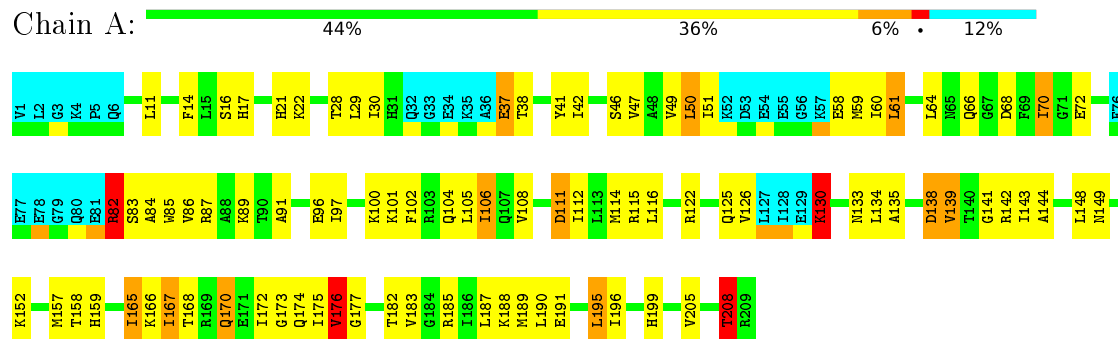
4.2.6 Score per residue for model 6

• Molecule 1: CAMP RECEPTOR PROTEIN



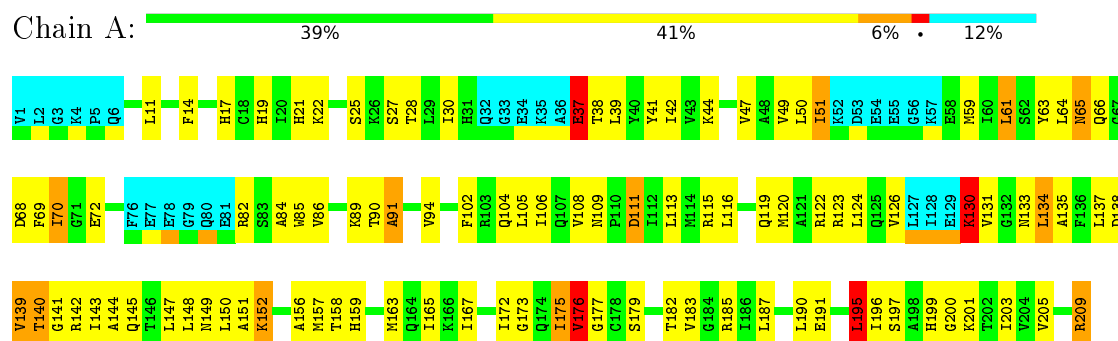
4.2.7 Score per residue for model 7

• Molecule 1: CAMP RECEPTOR PROTEIN



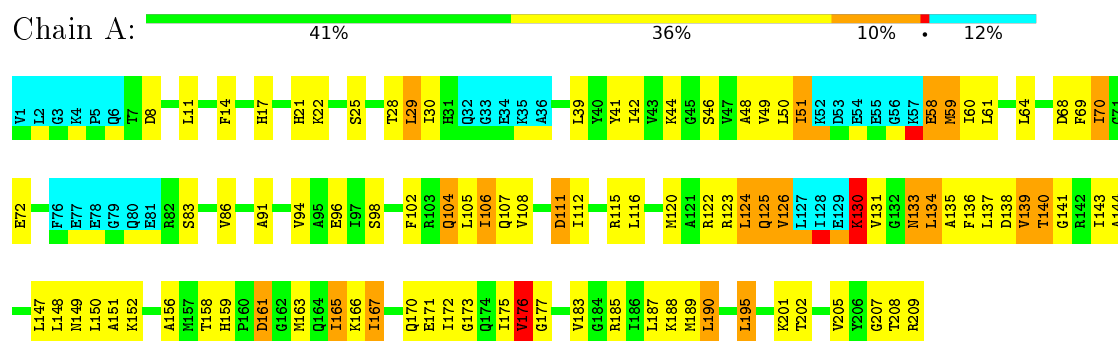
4.2.8 Score per residue for model 8

• Molecule 1: CAMP RECEPTOR PROTEIN



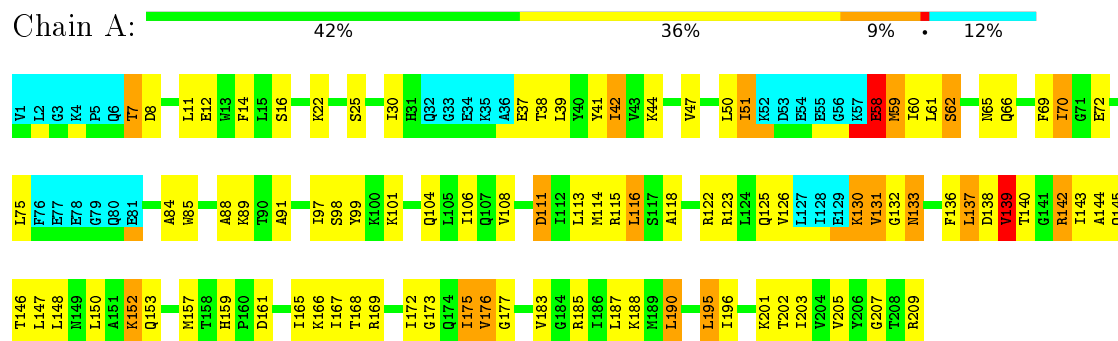
4.2.9 Score per residue for model 9

• Molecule 1: CAMP RECEPTOR PROTEIN



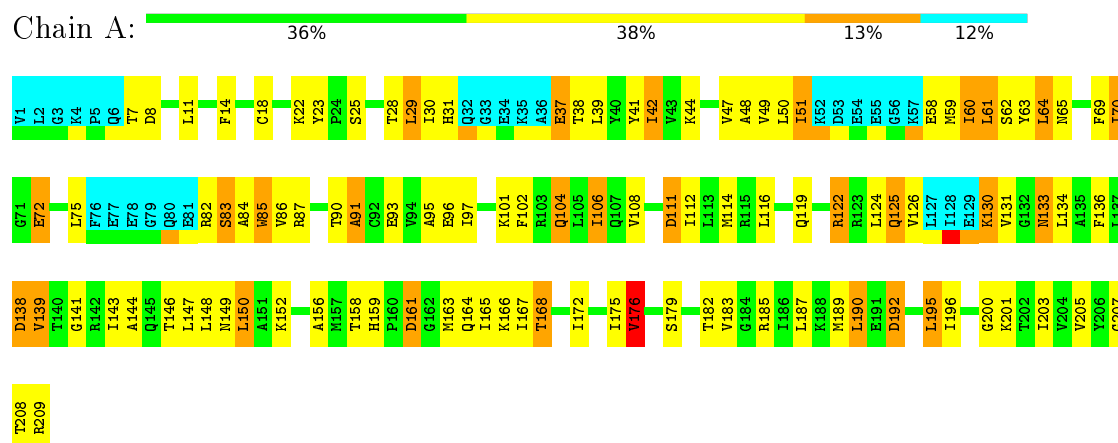
4.2.10 Score per residue for model 10

• Molecule 1: CAMP RECEPTOR PROTEIN



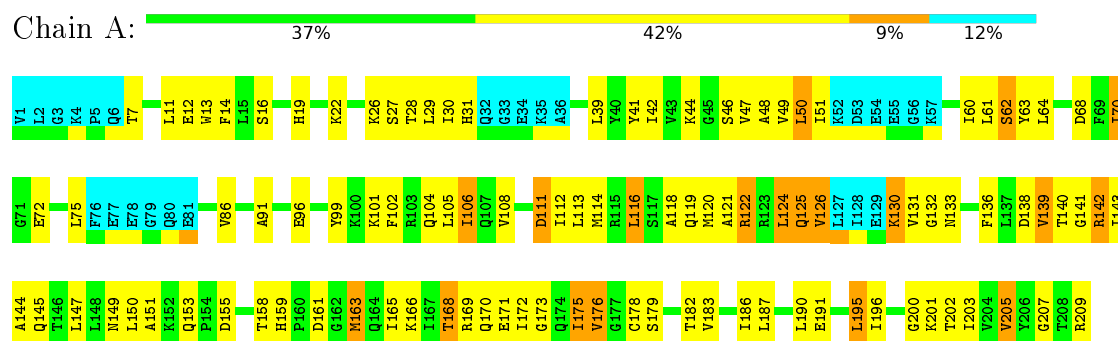
4.2.11 Score per residue for model 11

• Molecule 1: CAMP RECEPTOR PROTEIN



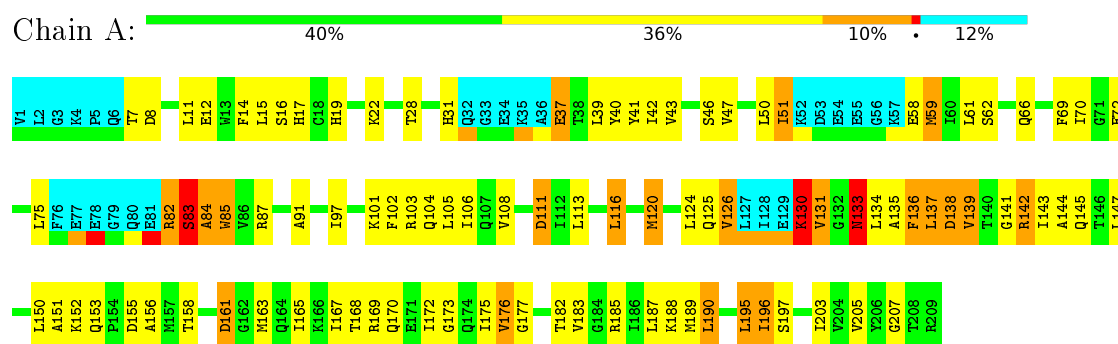
4.2.12 Score per residue for model 12

• Molecule 1: CAMP RECEPTOR PROTEIN



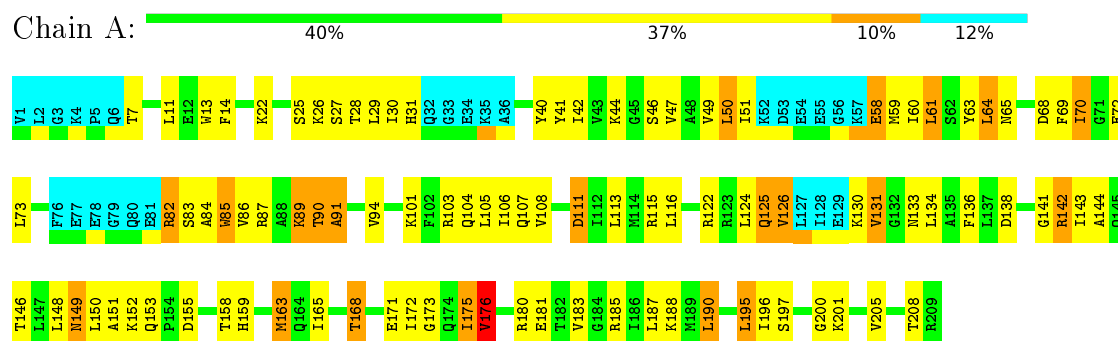
4.2.13 Score per residue for model 13

• Molecule 1: CAMP RECEPTOR PROTEIN



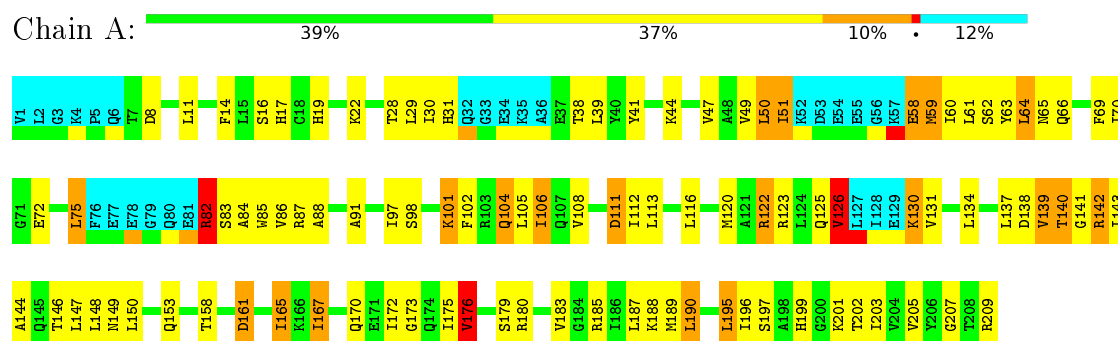
4.2.14 Score per residue for model 14

• Molecule 1: CAMP RECEPTOR PROTEIN



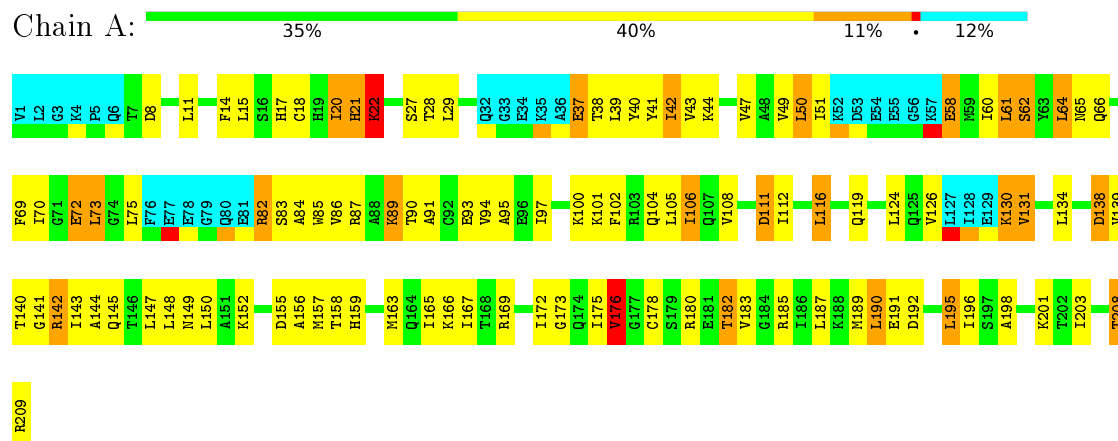
4.2.15 Score per residue for model 15

• Molecule 1: CAMP RECEPTOR PROTEIN



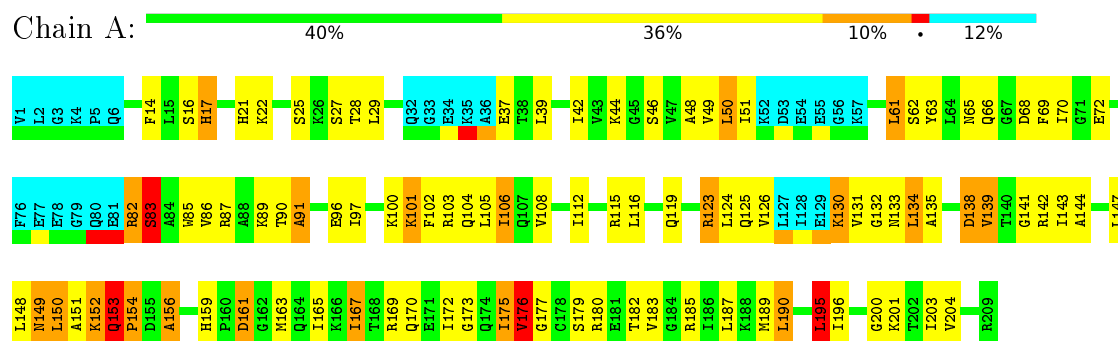
4.2.16 Score per residue for model 16

• Molecule 1: CAMP RECEPTOR PROTEIN



4.2.17 Score per residue for model 17

• Molecule 1: CAMP RECEPTOR PROTEIN



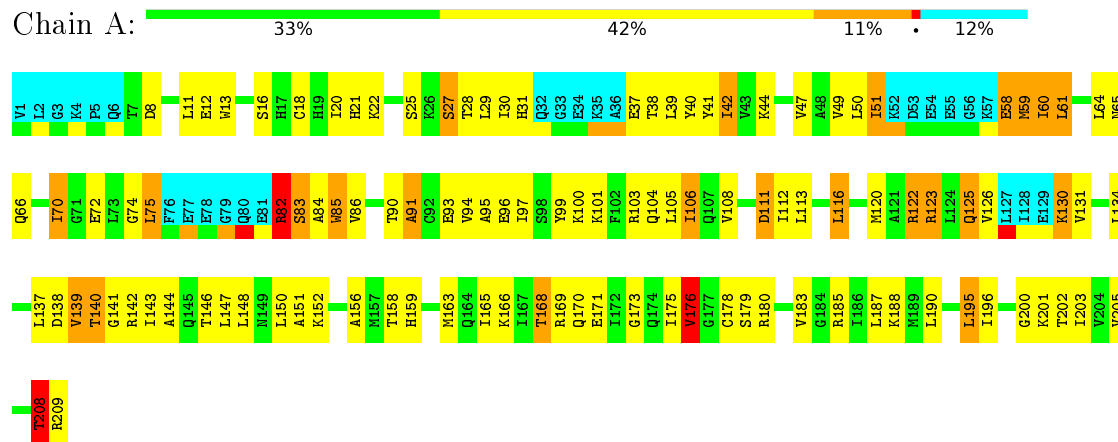
4.2.18 Score per residue for model 18 (medoid)

• Molecule 1: CAMP RECEPTOR PROTEIN



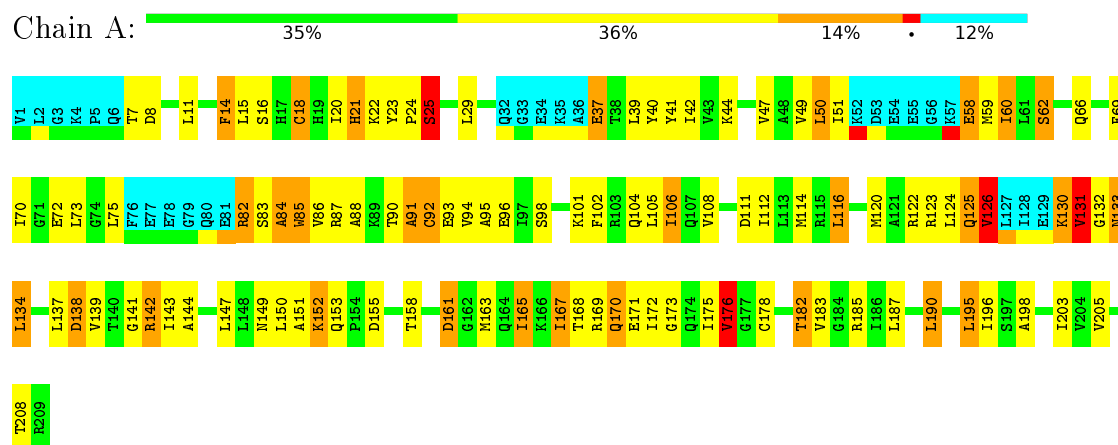
4.2.19 Score per residue for model 19

• Molecule 1: CAMP RECEPTOR PROTEIN



4.2.20 Score per residue for model 20

• Molecule 1: CAMP RECEPTOR PROTEIN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *NTORSION ANGLE DYNAMICS, SIMULATED SIMULATED*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *STRUCTURES WITH THE LEAST RESTRAINT VIOLATIONS*.

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

Software name	Classification	Version
CNS	refinement	
CARA; NMRPIPE; CYANA	structure solution	
HADDOCK	structure solution	

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

Chemical shift file(s)	4bhp_cs.cif
Number of chemical shift lists	1
Total number of shifts	369
Number of shifts mapped to atoms	369
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	13%

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	1448	1344	1507	67±11
All	All	28960	26880	30140	1333

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LEU:HD23	1:A:131:VAL:HG12	1.04	1.30	14	1
1:A:187:LEU:HD13	1:A:190:LEU:HD11	1.02	1.30	17	20
1:A:61:LEU:HD23	1:A:131:VAL:HG11	1.02	1.26	8	2
1:A:150:LEU:HD13	1:A:165:ILE:HD13	0.96	1.33	4	3
1:A:49:VAL:HG13	1:A:85:TRP:CB	0.87	2.00	14	1
1:A:122:ARG:O	1:A:126:VAL:N	0.86	2.07	15	6
1:A:29:LEU:HD13	1:A:86:VAL:HG12	0.81	1.51	17	9
1:A:29:LEU:HD11	1:A:88:ALA:HB2	0.80	1.54	18	6
1:A:143:ILE:HD12	1:A:144:ALA:N	0.80	1.91	9	20
1:A:49:VAL:C	1:A:50:LEU:HD13	0.80	1.96	4	8
1:A:143:ILE:HG22	1:A:183:VAL:HG13	0.77	1.56	10	8
1:A:50:LEU:HD22	1:A:85:TRP:O	0.76	1.80	16	5
1:A:150:LEU:HD22	1:A:165:ILE:HG23	0.76	1.56	19	3
1:A:31:HIS:NE2	1:A:84:ALA:HB3	0.76	1.95	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:GLY:HA2	1:A:183:VAL:HG21	0.76	1.58	10	18
1:A:151:ALA:HB2	1:A:205:VAL:HG21	0.75	1.57	1	10
1:A:20:ILE:HG23	1:A:95:ALA:HB2	0.75	1.57	16	1
1:A:106:ILE:HD12	1:A:113:LEU:HD13	0.74	1.60	13	8
1:A:124:LEU:O	1:A:125:GLN:CB	0.74	2.36	12	1
1:A:142:ARG:HB3	1:A:176:VAL:HG13	0.73	1.57	13	12
1:A:106:ILE:HD12	1:A:113:LEU:HD22	0.72	1.60	12	1
1:A:130:LYS:HG2	1:A:130:LYS:O	0.72	1.83	17	1
1:A:70:ILE:HG21	1:A:86:VAL:HG21	0.72	1.62	19	6
1:A:137:LEU:HD23	1:A:138:ASP:N	0.72	2.00	10	1
1:A:51:ILE:CG2	1:A:61:LEU:HD12	0.71	2.14	3	5
1:A:61:LEU:CD2	1:A:131:VAL:HG11	0.71	2.15	3	2
1:A:130:LYS:O	1:A:134:LEU:HD11	0.71	1.85	20	4
1:A:51:ILE:HD13	1:A:61:LEU:HD12	0.71	1.61	9	6
1:A:130:LYS:HD2	1:A:175:ILE:HG21	0.70	1.61	1	2
1:A:39:LEU:HD13	1:A:72:GLU:CD	0.70	2.06	19	1
1:A:70:ILE:CG2	1:A:86:VAL:HG21	0.70	2.16	9	1
1:A:142:ARG:CB	1:A:176:VAL:HG13	0.70	2.16	13	7
1:A:134:LEU:HD22	1:A:134:LEU:C	0.69	2.08	17	1
1:A:72:GLU:CG	1:A:116:LEU:HD11	0.69	2.18	8	8
1:A:23:TYR:CE1	1:A:29:LEU:HD21	0.68	2.23	5	1
1:A:49:VAL:HG13	1:A:85:TRP:HB2	0.68	1.63	14	1
1:A:142:ARG:HD2	1:A:176:VAL:HG12	0.68	1.64	6	1
1:A:146:THR:CG2	1:A:175:ILE:HD12	0.68	2.18	1	4
1:A:147:LEU:HD13	1:A:196:ILE:HG21	0.68	1.66	17	1
1:A:61:LEU:HD22	1:A:131:VAL:HG12	0.68	1.65	19	4
1:A:39:LEU:HD12	1:A:40:TYR:N	0.68	2.02	19	1
1:A:146:THR:HG23	1:A:175:ILE:HD12	0.68	1.65	1	6
1:A:142:ARG:HG2	1:A:176:VAL:HG12	0.68	1.64	12	1
1:A:123:ARG:O	1:A:131:VAL:HG21	0.68	1.88	17	3
1:A:82:ARG:O	1:A:83:SER:C	0.67	2.33	17	3
1:A:47:VAL:HG13	1:A:92:CYS:SG	0.67	2.29	5	1
1:A:104:GLN:O	1:A:108:VAL:HG13	0.67	1.89	4	1
1:A:168:THR:HG23	1:A:200:GLY:C	0.67	2.10	19	8
1:A:50:LEU:HD13	1:A:50:LEU:N	0.67	2.04	3	4
1:A:148:LEU:HD22	1:A:208:THR:HG22	0.67	1.64	19	3
1:A:49:VAL:HG13	1:A:84:ALA:HB1	0.67	1.66	4	4
1:A:134:LEU:HD12	1:A:135:ALA:N	0.67	2.05	13	7
1:A:90:THR:O	1:A:91:ALA:C	0.67	2.33	20	9
1:A:196:ILE:HG21	1:A:205:VAL:HG12	0.66	1.67	5	8
1:A:150:LEU:CD1	1:A:167:ILE:HD11	0.66	2.20	6	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:LYS:O	1:A:134:LEU:HD21	0.66	1.90	19	3
1:A:140:THR:HG22	1:A:186:ILE:HD11	0.66	1.65	12	1
1:A:196:ILE:CG2	1:A:205:VAL:HG12	0.66	2.21	7	9
1:A:47:VAL:HG12	1:A:88:ALA:HA	0.66	1.67	5	3
1:A:104:GLN:O	1:A:108:VAL:HG23	0.66	1.91	17	19
1:A:39:LEU:HD22	1:A:102:PHE:CE2	0.66	2.25	12	7
1:A:150:LEU:HD11	1:A:167:ILE:HD11	0.66	1.66	16	3
1:A:20:ILE:O	1:A:21:HIS:CB	0.66	2.43	20	2
1:A:143:ILE:CG2	1:A:183:VAL:HG13	0.65	2.21	19	9
1:A:51:ILE:O	1:A:59:MET:HB3	0.65	1.92	18	6
1:A:39:LEU:HD22	1:A:102:PHE:CD2	0.65	2.27	2	6
1:A:50:LEU:N	1:A:50:LEU:HD13	0.65	2.06	4	3
1:A:72:GLU:CB	1:A:116:LEU:HD11	0.65	2.22	4	16
1:A:50:LEU:HD22	1:A:50:LEU:H	0.65	1.50	14	5
1:A:51:ILE:O	1:A:58:GLU:HA	0.65	1.92	14	4
1:A:31:HIS:CD2	1:A:84:ALA:HB3	0.64	2.28	18	1
1:A:30:ILE:HD11	1:A:40:TYR:CG	0.64	2.28	18	1
1:A:63:TYR:CE2	1:A:150:LEU:HD21	0.64	2.28	17	1
1:A:72:GLU:CD	1:A:116:LEU:HD21	0.64	2.12	1	1
1:A:187:LEU:CD1	1:A:190:LEU:HD11	0.64	2.21	1	17
1:A:137:LEU:HD23	1:A:137:LEU:C	0.64	2.12	10	1
1:A:72:GLU:OE2	1:A:116:LEU:HD22	0.64	1.92	19	1
1:A:29:LEU:HD13	1:A:86:VAL:CG1	0.64	2.22	20	2
1:A:150:LEU:HD22	1:A:165:ILE:CG2	0.64	2.23	16	4
1:A:142:ARG:CG	1:A:176:VAL:HG12	0.63	2.23	12	1
1:A:50:LEU:HD12	1:A:60:ILE:HG23	0.63	1.69	14	6
1:A:139:VAL:O	1:A:140:THR:HG22	0.63	1.93	10	5
1:A:15:LEU:O	1:A:20:ILE:HD11	0.63	1.94	16	1
1:A:42:ILE:CG1	1:A:70:ILE:HD11	0.63	2.23	9	5
1:A:119:GLN:O	1:A:124:LEU:HD11	0.63	1.94	12	1
1:A:49:VAL:CG1	1:A:84:ALA:HB1	0.63	2.23	4	5
1:A:50:LEU:N	1:A:50:LEU:HD22	0.63	2.09	14	4
1:A:120:MET:CG	1:A:124:LEU:HD21	0.63	2.24	9	1
1:A:150:LEU:CB	1:A:165:ILE:HD13	0.63	2.24	20	3
1:A:123:ARG:O	1:A:131:VAL:HG11	0.63	1.93	6	4
1:A:39:LEU:HD13	1:A:102:PHE:CE2	0.62	2.29	20	1
1:A:150:LEU:HD22	1:A:167:ILE:HD13	0.62	1.70	18	1
1:A:142:ARG:HG2	1:A:176:VAL:HG13	0.62	1.72	5	2
1:A:29:LEU:HD12	1:A:86:VAL:O	0.62	1.94	11	1
1:A:51:ILE:O	1:A:59:MET:CB	0.62	2.48	9	5
1:A:165:ILE:HD12	1:A:203:ILE:HB	0.62	1.72	17	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ILE:HA	1:A:85:TRP:CE3	0.62	2.30	14	1
1:A:196:ILE:CG2	1:A:205:VAL:HG13	0.62	2.25	4	2
1:A:150:LEU:HD13	1:A:167:ILE:HD11	0.62	1.71	13	5
1:A:62:SER:HB2	1:A:131:VAL:HG12	0.62	1.71	2	1
1:A:50:LEU:HD21	1:A:87:ARG:CB	0.62	2.24	14	1
1:A:196:ILE:HD11	1:A:209:ARG:C	0.61	2.16	18	2
1:A:63:TYR:O	1:A:64:LEU:HD23	0.61	1.94	3	3
1:A:64:LEU:HD22	1:A:68:ASP:HB3	0.61	1.71	7	4
1:A:51:ILE:HG21	1:A:61:LEU:HD12	0.61	1.71	18	2
1:A:11:LEU:HD11	1:A:41:TYR:CZ	0.61	2.29	12	9
1:A:102:PHE:HA	1:A:105:LEU:HD12	0.61	1.71	1	11
1:A:147:LEU:HA	1:A:150:LEU:HD12	0.61	1.71	20	3
1:A:147:LEU:HD22	1:A:203:ILE:HG21	0.61	1.72	3	12
1:A:142:ARG:HB2	1:A:176:VAL:HG13	0.61	1.72	4	1
1:A:82:ARG:HD3	1:A:84:ALA:HB3	0.61	1.72	4	1
1:A:120:MET:HG2	1:A:124:LEU:HD21	0.61	1.69	9	2
1:A:75:LEU:HD13	1:A:102:PHE:CD2	0.61	2.31	20	2
1:A:156:ALA:HB1	1:A:163:MET:CG	0.60	2.26	8	10
1:A:61:LEU:CD2	1:A:131:VAL:HG12	0.60	2.26	19	3
1:A:72:GLU:HB3	1:A:116:LEU:HD11	0.60	1.72	16	5
1:A:61:LEU:O	1:A:131:VAL:HG13	0.60	1.96	18	4
1:A:29:LEU:CD1	1:A:88:ALA:HB2	0.60	2.26	18	2
1:A:196:ILE:CG1	1:A:205:VAL:HG12	0.60	2.26	8	1
1:A:165:ILE:CG2	1:A:167:ILE:HD12	0.60	2.26	17	7
1:A:126:VAL:HB	1:A:131:VAL:HG22	0.60	1.72	12	1
1:A:50:LEU:HD13	1:A:60:ILE:HA	0.60	1.74	6	5
1:A:150:LEU:CD1	1:A:165:ILE:HD13	0.60	2.27	12	1
1:A:29:LEU:HD22	1:A:94:VAL:HG21	0.59	1.74	9	2
1:A:69:PHE:CB	1:A:116:LEU:HD13	0.59	2.27	20	14
1:A:151:ALA:HB1	1:A:163:MET:CE	0.59	2.27	3	7
1:A:49:VAL:HG22	1:A:86:VAL:HG22	0.59	1.74	3	4
1:A:11:LEU:HD11	1:A:41:TYR:CE2	0.59	2.31	20	2
1:A:84:ALA:O	1:A:86:VAL:N	0.59	2.36	11	2
1:A:125:GLN:O	1:A:126:VAL:C	0.59	2.41	18	12
1:A:20:ILE:HG23	1:A:95:ALA:CB	0.59	2.27	16	1
1:A:147:LEU:HD23	1:A:172:ILE:CD1	0.58	2.27	8	12
1:A:130:LYS:HE2	1:A:175:ILE:HG21	0.58	1.73	19	1
1:A:148:LEU:HD13	1:A:208:THR:CG2	0.58	2.28	11	2
1:A:50:LEU:HD22	1:A:50:LEU:N	0.58	2.12	12	4
1:A:139:VAL:N	1:A:142:ARG:CZ	0.58	2.66	12	1
1:A:143:ILE:HG23	1:A:176:VAL:HG11	0.58	1.74	9	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:VAL:HG13	1:A:85:TRP:HB3	0.58	1.74	14	1
1:A:38:THR:HG23	1:A:97:ILE:C	0.58	2.19	18	9
1:A:11:LEU:HD11	1:A:41:TYR:OH	0.58	1.98	1	10
1:A:126:VAL:HG21	1:A:152:LYS:CD	0.58	2.28	18	1
1:A:150:LEU:O	1:A:156:ALA:HB3	0.58	1.99	19	2
1:A:150:LEU:HB3	1:A:165:ILE:HD13	0.58	1.73	20	2
1:A:61:LEU:O	1:A:131:VAL:HG12	0.58	1.98	17	3
1:A:30:ILE:HD12	1:A:86:VAL:HG21	0.58	1.76	14	5
1:A:59:MET:CE	1:A:134:LEU:HD23	0.58	2.29	18	1
1:A:126:VAL:HG11	1:A:152:LYS:NZ	0.58	2.14	5	2
1:A:130:LYS:HG2	1:A:134:LEU:HD23	0.57	1.76	13	1
1:A:126:VAL:HG12	1:A:131:VAL:CG2	0.57	2.28	13	1
1:A:152:LYS:HG2	1:A:152:LYS:O	0.57	1.98	17	1
1:A:64:LEU:HD22	1:A:68:ASP:OD1	0.57	1.98	3	1
1:A:146:THR:O	1:A:150:LEU:HD12	0.57	1.99	15	2
1:A:70:ILE:HG21	1:A:86:VAL:CG2	0.57	2.29	19	1
1:A:51:ILE:HG22	1:A:85:TRP:CE3	0.57	2.33	14	1
1:A:11:LEU:HD21	1:A:41:TYR:OH	0.57	1.98	4	10
1:A:23:TYR:CG	1:A:29:LEU:HD23	0.57	2.33	11	1
1:A:143:ILE:CG2	1:A:183:VAL:HG22	0.57	2.29	14	12
1:A:69:PHE:CG	1:A:116:LEU:HD13	0.57	2.35	1	11
1:A:15:LEU:HD22	1:A:20:ILE:CG1	0.57	2.29	20	1
1:A:15:LEU:HD21	1:A:43:VAL:HG22	0.57	1.75	3	4
1:A:130:LYS:C	1:A:134:LEU:HD21	0.57	2.19	19	1
1:A:18:CYS:SG	1:A:95:ALA:HB1	0.57	2.39	16	1
1:A:195:LEU:C	1:A:196:ILE:HD12	0.57	2.19	8	2
1:A:39:LEU:HD13	1:A:72:GLU:CG	0.57	2.30	19	1
1:A:47:VAL:HG22	1:A:64:LEU:HB2	0.56	1.76	19	5
1:A:148:LEU:HB3	1:A:208:THR:HG23	0.56	1.77	9	3
1:A:163:MET:O	1:A:204:VAL:HG22	0.56	1.99	17	1
1:A:151:ALA:HB2	1:A:205:VAL:CG2	0.56	2.30	20	6
1:A:130:LYS:NZ	1:A:175:ILE:HD13	0.56	2.15	19	2
1:A:191:GLU:HG2	1:A:198:ALA:HB3	0.56	1.75	16	1
1:A:72:GLU:OE2	1:A:73:LEU:HD23	0.56	2.00	5	1
1:A:140:THR:O	1:A:140:THR:HG23	0.56	1.98	15	2
1:A:196:ILE:HG13	1:A:205:VAL:HG12	0.56	1.77	8	1
1:A:176:VAL:HG12	1:A:177:GLY:H	0.56	1.60	13	8
1:A:83:SER:O	1:A:84:ALA:HB2	0.56	2.01	13	1
1:A:51:ILE:HG22	1:A:61:LEU:HD12	0.56	1.77	8	1
1:A:20:ILE:HG21	1:A:43:VAL:HG21	0.56	1.78	16	1
1:A:7:THR:HG21	1:A:11:LEU:HD23	0.56	1.77	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:ILE:O	1:A:176:VAL:HG23	0.56	2.00	13	14
1:A:49:VAL:CG2	1:A:64:LEU:HD11	0.55	2.30	16	4
1:A:150:LEU:HD22	1:A:165:ILE:HG21	0.55	1.78	1	2
1:A:24:PRO:O	1:A:25:SER:CB	0.55	2.54	20	1
1:A:130:LYS:HD3	1:A:175:ILE:HG22	0.55	1.76	12	1
1:A:196:ILE:HG21	1:A:205:VAL:HG13	0.55	1.77	4	2
1:A:20:ILE:HG21	1:A:43:VAL:CG2	0.55	2.32	16	1
1:A:124:LEU:HA	1:A:131:VAL:HG23	0.54	1.77	9	2
1:A:124:LEU:O	1:A:125:GLN:HB2	0.54	2.02	12	1
1:A:143:ILE:HG22	1:A:176:VAL:HG21	0.54	1.79	11	8
1:A:137:LEU:O	1:A:176:VAL:HG12	0.54	2.02	10	1
1:A:18:CYS:HB2	1:A:95:ALA:HB1	0.54	1.79	2	5
1:A:137:LEU:HD23	1:A:141:GLY:HA3	0.54	1.78	6	1
1:A:39:LEU:HD22	1:A:102:PHE:CZ	0.54	2.38	20	3
1:A:30:ILE:HD11	1:A:40:TYR:CD2	0.54	2.37	3	2
1:A:106:ILE:HG22	1:A:112:ILE:CG2	0.54	2.32	16	13
1:A:130:LYS:O	1:A:130:LYS:CG	0.54	2.55	17	2
1:A:48:ALA:HB2	1:A:63:TYR:CE1	0.54	2.37	2	6
1:A:143:ILE:HA	1:A:176:VAL:HG11	0.54	1.79	6	2
1:A:30:ILE:CD1	1:A:86:VAL:HG21	0.54	2.33	14	1
1:A:147:LEU:HD23	1:A:172:ILE:HD12	0.54	1.79	18	5
1:A:17:HIS:CB	1:A:105:LEU:HD11	0.54	2.32	17	2
1:A:30:ILE:HD12	1:A:70:ILE:HG22	0.54	1.78	9	1
1:A:130:LYS:CD	1:A:175:ILE:HG21	0.54	2.33	4	2
1:A:59:MET:HG3	1:A:59:MET:O	0.54	2.03	10	1
1:A:23:TYR:CD2	1:A:29:LEU:HD23	0.54	2.37	11	3
1:A:114:MET:O	1:A:118:ALA:HB2	0.54	2.02	10	3
1:A:51:ILE:HD13	1:A:61:LEU:CD1	0.54	2.31	9	6
1:A:50:LEU:O	1:A:85:TRP:N	0.53	2.41	13	7
1:A:196:ILE:HD11	1:A:209:ARG:HG3	0.53	1.80	11	1
1:A:134:LEU:HD22	1:A:135:ALA:N	0.53	2.18	17	1
1:A:147:LEU:HB3	1:A:205:VAL:HG11	0.53	1.80	13	2
1:A:140:THR:HG22	1:A:186:ILE:CD1	0.53	2.34	12	1
1:A:75:LEU:O	1:A:75:LEU:HD12	0.53	2.03	6	2
1:A:14:PHE:HB2	1:A:105:LEU:HD13	0.53	1.81	3	1
1:A:156:ALA:HB1	1:A:163:MET:HG2	0.53	1.79	8	3
1:A:21:HIS:O	1:A:22:LYS:HB3	0.53	2.04	16	1
1:A:126:VAL:HG21	1:A:152:LYS:NZ	0.53	2.17	8	1
1:A:147:LEU:HD12	1:A:196:ILE:HD12	0.53	1.79	3	1
1:A:150:LEU:HB3	1:A:165:ILE:HD12	0.53	1.79	14	1
1:A:126:VAL:HG12	1:A:131:VAL:HG22	0.53	1.81	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LEU:HD21	1:A:94:VAL:HG21	0.53	1.80	20	1
1:A:106:ILE:CD1	1:A:113:LEU:HD13	0.53	2.30	3	5
1:A:143:ILE:HD12	1:A:144:ALA:H	0.53	1.63	15	18
1:A:151:ALA:HB1	1:A:163:MET:HE2	0.53	1.81	8	2
1:A:62:SER:HB3	1:A:131:VAL:HG12	0.53	1.79	20	2
1:A:124:LEU:HA	1:A:131:VAL:HG11	0.53	1.80	11	2
1:A:161:ASP:OD2	1:A:204:VAL:HG11	0.53	2.04	1	1
1:A:106:ILE:HG22	1:A:112:ILE:HG23	0.53	1.81	4	6
1:A:148:LEU:HD21	1:A:209:ARG:HG3	0.53	1.81	4	1
1:A:21:HIS:HA	1:A:93:GLU:HA	0.53	1.81	20	2
1:A:50:LEU:HD21	1:A:87:ARG:HB3	0.53	1.81	14	2
1:A:153:GLN:H	1:A:154:PRO:HD2	0.53	1.64	17	1
1:A:148:LEU:HD21	1:A:209:ARG:C	0.52	2.25	6	1
1:A:42:ILE:N	1:A:94:VAL:HG13	0.52	2.19	8	1
1:A:49:VAL:HG22	1:A:85:TRP:O	0.52	2.04	14	1
1:A:148:LEU:HB3	1:A:208:THR:HG22	0.52	1.80	7	1
1:A:116:LEU:O	1:A:116:LEU:HD12	0.52	2.04	12	4
1:A:140:THR:HG23	1:A:140:THR:O	0.52	2.04	8	2
1:A:17:HIS:CD2	1:A:105:LEU:HD21	0.52	2.39	17	1
1:A:97:ILE:HD11	1:A:101:LYS:HB3	0.52	1.82	4	5
1:A:131:VAL:HG23	1:A:132:GLY:H	0.52	1.64	20	2
1:A:39:LEU:HD22	1:A:102:PHE:CE1	0.52	2.40	20	1
1:A:195:LEU:O	1:A:196:ILE:HD12	0.52	2.05	17	2
1:A:134:LEU:H	1:A:134:LEU:HD22	0.52	1.65	5	2
1:A:133:ASN:O	1:A:136:PHE:CD1	0.52	2.62	13	1
1:A:72:GLU:HG2	1:A:116:LEU:HD11	0.52	1.80	1	1
1:A:31:HIS:HA	1:A:85:TRP:CD1	0.51	2.41	13	1
1:A:73:LEU:HD23	1:A:120:MET:SD	0.51	2.45	20	1
1:A:73:LEU:HD12	1:A:83:SER:HB3	0.51	1.82	14	1
1:A:122:ARG:O	1:A:126:VAL:HB	0.51	2.05	14	9
1:A:60:ILE:O	1:A:175:ILE:HG23	0.51	2.05	14	2
1:A:62:SER:HB2	1:A:131:VAL:HG13	0.51	1.82	10	2
1:A:106:ILE:HD11	1:A:113:LEU:HD22	0.51	1.82	8	2
1:A:17:HIS:CG	1:A:105:LEU:HD11	0.51	2.41	17	1
1:A:50:LEU:CD1	1:A:60:ILE:HG23	0.51	2.35	20	3
1:A:30:ILE:HD12	1:A:86:VAL:CG2	0.51	2.36	4	4
1:A:64:LEU:CD1	1:A:70:ILE:HG23	0.51	2.35	7	2
1:A:42:ILE:HG12	1:A:70:ILE:HD11	0.51	1.82	9	1
1:A:82:ARG:O	1:A:83:SER:CB	0.51	2.59	1	1
1:A:84:ALA:O	1:A:86:VAL:HG23	0.51	2.05	14	3
1:A:97:ILE:HD11	1:A:101:LYS:HG2	0.51	1.83	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LEU:HD22	1:A:102:PHE:CE2	0.51	2.41	11	2
1:A:134:LEU:HD22	1:A:134:LEU:H	0.51	1.66	20	2
1:A:165:ILE:HG21	1:A:167:ILE:HD12	0.50	1.82	17	1
1:A:75:LEU:HD13	1:A:102:PHE:CE2	0.50	2.41	20	2
1:A:191:GLU:CG	1:A:198:ALA:HB3	0.50	2.37	16	1
1:A:61:LEU:HD23	1:A:131:VAL:HG21	0.50	1.84	9	1
1:A:139:VAL:HG21	1:A:182:THR:HG23	0.50	1.83	16	2
1:A:142:ARG:HG2	1:A:176:VAL:CG1	0.50	2.35	12	1
1:A:29:LEU:CD2	1:A:94:VAL:HG21	0.50	2.37	16	2
1:A:42:ILE:HD11	1:A:47:VAL:HG22	0.50	1.82	7	4
1:A:136:PHE:CD1	1:A:137:LEU:N	0.50	2.79	13	1
1:A:203:ILE:HG22	1:A:205:VAL:HG13	0.50	1.83	13	1
1:A:42:ILE:CD1	1:A:47:VAL:HG22	0.50	2.37	7	5
1:A:50:LEU:N	1:A:50:LEU:CD1	0.50	2.75	16	2
1:A:50:LEU:H	1:A:50:LEU:HD22	0.50	1.65	12	4
1:A:126:VAL:HG11	1:A:130:LYS:HB2	0.50	1.84	9	1
1:A:23:TYR:HB2	1:A:29:LEU:HD21	0.49	1.83	18	1
1:A:27:SER:O	1:A:29:LEU:HD12	0.49	2.07	19	3
1:A:153:GLN:CB	1:A:154:PRO:CD	0.49	2.90	17	1
1:A:198:ALA:HB1	1:A:203:ILE:HD12	0.49	1.84	20	3
1:A:60:ILE:HB	1:A:175:ILE:HG23	0.49	1.85	12	5
1:A:90:THR:O	1:A:92:CYS:N	0.49	2.45	5	1
1:A:30:ILE:HD13	1:A:82:ARG:HD2	0.49	1.83	4	1
1:A:15:LEU:HD22	1:A:20:ILE:HG12	0.49	1.85	16	1
1:A:130:LYS:HA	1:A:133:ASN:OD1	0.49	2.07	10	1
1:A:139:VAL:O	1:A:140:THR:CG2	0.49	2.60	10	1
1:A:142:ARG:CD	1:A:176:VAL:HG12	0.49	2.36	6	1
1:A:72:GLU:OE2	1:A:73:LEU:HD22	0.49	2.07	16	1
1:A:75:LEU:HD11	1:A:103:ARG:HG2	0.49	1.84	13	1
1:A:143:ILE:CG2	1:A:176:VAL:HG11	0.49	2.37	12	1
1:A:50:LEU:O	1:A:51:ILE:HG22	0.49	2.08	13	2
1:A:133:ASN:OD1	1:A:133:ASN:C	0.49	2.50	10	2
1:A:39:LEU:HD23	1:A:102:PHE:CD1	0.49	2.43	3	5
1:A:50:LEU:C	1:A:51:ILE:CG2	0.49	2.80	13	5
1:A:148:LEU:HD22	1:A:209:ARG:N	0.49	2.23	9	3
1:A:37:GLU:O	1:A:37:GLU:CG	0.49	2.60	19	1
1:A:138:ASP:O	1:A:139:VAL:C	0.48	2.51	6	8
1:A:147:LEU:HB3	1:A:203:ILE:HG21	0.48	1.86	17	1
1:A:15:LEU:HD21	1:A:43:VAL:CG2	0.48	2.38	3	2
1:A:192:ASP:O	1:A:192:ASP:CG	0.48	2.50	11	1
1:A:137:LEU:HD12	1:A:138:ASP:N	0.48	2.23	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LEU:HD13	1:A:99:TYR:CD1	0.48	2.44	12	2
1:A:49:VAL:O	1:A:61:LEU:N	0.48	2.46	1	10
1:A:116:LEU:HD12	1:A:116:LEU:O	0.48	2.08	1	5
1:A:61:LEU:HD22	1:A:124:LEU:CD2	0.48	2.39	13	1
1:A:51:ILE:HG23	1:A:61:LEU:HB2	0.48	1.86	17	2
1:A:124:LEU:HD22	1:A:125:GLN:N	0.48	2.24	5	1
1:A:70:ILE:CG2	1:A:86:VAL:HG22	0.48	2.39	14	1
1:A:89:LYS:O	1:A:90:THR:HG23	0.48	2.08	16	3
1:A:190:LEU:HD12	1:A:191:GLU:N	0.48	2.23	8	3
1:A:61:LEU:O	1:A:61:LEU:HD23	0.48	2.09	10	2
1:A:72:GLU:HG3	1:A:116:LEU:HD11	0.48	1.85	8	1
1:A:47:VAL:CG2	1:A:64:LEU:HD12	0.48	2.39	14	6
1:A:143:ILE:CA	1:A:176:VAL:HG11	0.48	2.38	6	1
1:A:49:VAL:CG2	1:A:64:LEU:HD21	0.48	2.38	19	2
1:A:75:LEU:HD21	1:A:116:LEU:HD21	0.47	1.85	15	1
1:A:30:ILE:CG2	1:A:31:HIS:N	0.47	2.77	11	1
1:A:126:VAL:HG22	1:A:152:LYS:HG3	0.47	1.85	10	1
1:A:150:LEU:HB2	1:A:165:ILE:HD13	0.47	1.86	9	3
1:A:61:LEU:HD22	1:A:124:LEU:HD23	0.47	1.86	13	1
1:A:49:VAL:O	1:A:50:LEU:HD13	0.47	2.08	9	1
1:A:134:LEU:HD12	1:A:135:ALA:H	0.47	1.69	8	4
1:A:30:ILE:HG22	1:A:31:HIS:N	0.47	2.25	18	2
1:A:149:ASN:OD1	1:A:150:LEU:HD12	0.47	2.09	17	1
1:A:23:TYR:CZ	1:A:29:LEU:HD23	0.47	2.45	20	1
1:A:150:LEU:HD11	1:A:175:ILE:CD1	0.47	2.40	11	1
1:A:47:VAL:HG21	1:A:64:LEU:HD12	0.47	1.85	14	3
1:A:148:LEU:O	1:A:152:LYS:HD2	0.47	2.09	17	1
1:A:13:TRP:CZ2	1:A:105:LEU:HD23	0.47	2.43	1	1
1:A:126:VAL:CB	1:A:131:VAL:HG22	0.47	2.40	12	1
1:A:62:SER:CB	1:A:131:VAL:HG12	0.47	2.40	6	2
1:A:14:PHE:CE1	1:A:97:ILE:HD13	0.47	2.45	16	1
1:A:40:TYR:HB3	1:A:94:VAL:CG1	0.47	2.39	20	2
1:A:130:LYS:C	1:A:134:LEU:HD23	0.47	2.30	11	1
1:A:31:HIS:CD2	1:A:83:SER:HA	0.47	2.44	11	1
1:A:75:LEU:HD11	1:A:103:ARG:CG	0.47	2.39	13	1
1:A:134:LEU:C	1:A:134:LEU:CD2	0.47	2.80	17	1
1:A:30:ILE:HG22	1:A:84:ALA:CB	0.47	2.39	14	1
1:A:63:TYR:OH	1:A:175:ILE:HD11	0.47	2.10	8	1
1:A:20:ILE:HG23	1:A:95:ALA:CA	0.47	2.39	16	1
1:A:126:VAL:HG11	1:A:130:LYS:CG	0.47	2.40	8	1
1:A:152:LYS:CG	1:A:152:LYS:O	0.47	2.63	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:ARG:O	1:A:131:VAL:CG2	0.46	2.64	19	1
1:A:30:ILE:HD11	1:A:40:TYR:CB	0.46	2.40	18	1
1:A:148:LEU:HD13	1:A:208:THR:HG23	0.46	1.87	11	1
1:A:106:ILE:HD12	1:A:113:LEU:HB2	0.46	1.86	10	2
1:A:137:LEU:C	1:A:137:LEU:CD2	0.46	2.82	10	1
1:A:50:LEU:CD1	1:A:50:LEU:N	0.46	2.75	4	2
1:A:62:SER:CB	1:A:131:VAL:HG13	0.46	2.41	10	2
1:A:72:GLU:CD	1:A:116:LEU:HD22	0.46	2.31	19	1
1:A:39:LEU:HD22	1:A:102:PHE:CG	0.46	2.46	9	1
1:A:149:ASN:O	1:A:153:GLN:HB2	0.46	2.10	17	1
1:A:136:PHE:O	1:A:137:LEU:CB	0.46	2.62	13	1
1:A:198:ALA:HB1	1:A:203:ILE:CD1	0.46	2.41	16	3
1:A:124:LEU:HD13	1:A:124:LEU:H	0.46	1.70	5	1
1:A:23:TYR:HE1	1:A:29:LEU:HD21	0.46	1.67	5	1
1:A:150:LEU:O	1:A:156:ALA:HB2	0.46	2.10	17	1
1:A:85:TRP:CD2	1:A:85:TRP:N	0.46	2.82	14	1
1:A:59:MET:HE2	1:A:134:LEU:HD23	0.45	1.87	18	1
1:A:167:ILE:O	1:A:167:ILE:HD13	0.45	2.10	17	1
1:A:150:LEU:HD13	1:A:165:ILE:CD1	0.45	2.24	4	1
1:A:130:LYS:NZ	1:A:175:ILE:HG23	0.45	2.27	11	1
1:A:72:GLU:HB2	1:A:116:LEU:HD21	0.45	1.88	8	2
1:A:84:ALA:O	1:A:85:TRP:C	0.45	2.55	18	1
1:A:50:LEU:C	1:A:51:ILE:HG22	0.45	2.32	13	1
1:A:124:LEU:N	1:A:124:LEU:HD13	0.45	2.26	5	1
1:A:168:THR:O	1:A:172:ILE:N	0.45	2.48	3	3
1:A:50:LEU:HD21	1:A:87:ARG:HB2	0.45	1.89	14	2
1:A:140:THR:HA	1:A:143:ILE:HD11	0.45	1.88	10	1
1:A:11:LEU:O	1:A:15:LEU:HD12	0.45	2.11	3	1
1:A:148:LEU:HD22	1:A:208:THR:CG2	0.45	2.42	16	1
1:A:69:PHE:HB2	1:A:116:LEU:HD13	0.45	1.87	20	2
1:A:20:ILE:O	1:A:21:HIS:HB3	0.45	2.11	20	2
1:A:61:LEU:HD22	1:A:131:VAL:CG1	0.45	2.42	4	1
1:A:196:ILE:HD13	1:A:205:VAL:HG12	0.45	1.87	14	1
1:A:29:LEU:N	1:A:29:LEU:HD12	0.45	2.27	14	1
1:A:48:ALA:HB2	1:A:63:TYR:CD1	0.45	2.46	12	1
1:A:151:ALA:HB1	1:A:163:MET:HG3	0.45	1.87	17	1
1:A:28:THR:HG23	1:A:87:ARG:HG2	0.45	1.89	2	1
1:A:73:LEU:HD12	1:A:83:SER:CB	0.45	2.42	14	1
1:A:134:LEU:HD13	1:A:134:LEU:N	0.45	2.27	20	1
1:A:131:VAL:CG2	1:A:132:GLY:N	0.45	2.80	12	1
1:A:173:GLY:O	1:A:178:CYS:O	0.44	2.35	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ILE:HG22	1:A:31:HIS:H	0.44	1.72	6	1
1:A:133:ASN:C	1:A:133:ASN:OD1	0.44	2.55	5	1
1:A:65:ASN:O	1:A:66:GLN:C	0.44	2.56	3	4
1:A:41:TYR:C	1:A:94:VAL:HG13	0.44	2.32	8	1
1:A:42:ILE:HD11	1:A:47:VAL:CG2	0.44	2.42	7	4
1:A:7:THR:HG21	1:A:11:LEU:CD2	0.44	2.42	3	2
1:A:130:LYS:O	1:A:131:VAL:C	0.44	2.55	13	3
1:A:142:ARG:CG	1:A:176:VAL:HG13	0.44	2.43	7	1
1:A:172:ILE:HG22	1:A:183:VAL:HG11	0.44	1.88	12	1
1:A:134:LEU:CD1	1:A:135:ALA:N	0.44	2.80	9	1
1:A:143:ILE:HG21	1:A:183:VAL:HG13	0.44	1.89	13	2
1:A:106:ILE:HA	1:A:112:ILE:HG22	0.44	1.89	5	3
1:A:49:VAL:HG21	1:A:64:LEU:HD21	0.44	1.89	5	2
1:A:173:GLY:HA2	1:A:176:VAL:HG23	0.44	1.89	12	1
1:A:126:VAL:HG21	1:A:152:LYS:HD3	0.44	1.89	18	1
1:A:13:TRP:CZ2	1:A:105:LEU:HD22	0.44	2.48	19	3
1:A:130:LYS:CE	1:A:175:ILE:HG22	0.44	2.43	12	1
1:A:126:VAL:CG1	1:A:130:LYS:HB2	0.44	2.42	9	1
1:A:60:ILE:HD12	1:A:175:ILE:HG12	0.43	1.90	3	1
1:A:153:GLN:HB3	1:A:154:PRO:HD3	0.43	1.90	17	1
1:A:168:THR:HG23	1:A:170:GLN:H	0.43	1.73	7	3
1:A:120:MET:O	1:A:124:LEU:HD12	0.43	2.14	18	1
1:A:29:LEU:CD1	1:A:86:VAL:HG12	0.43	2.42	11	1
1:A:126:VAL:HG11	1:A:130:LYS:HG3	0.43	1.90	8	1
1:A:75:LEU:CD2	1:A:116:LEU:HD21	0.43	2.44	19	1
1:A:134:LEU:N	1:A:134:LEU:HD13	0.43	2.27	17	1
1:A:49:VAL:O	1:A:49:VAL:HG12	0.43	2.12	14	1
1:A:151:ALA:HB2	1:A:163:MET:SD	0.43	2.53	12	1
1:A:125:GLN:O	1:A:125:GLN:CG	0.43	2.67	12	1
1:A:142:ARG:O	1:A:145:GLN:N	0.43	2.50	12	1
1:A:126:VAL:HG21	1:A:152:LYS:CE	0.43	2.44	8	1
1:A:134:LEU:N	1:A:134:LEU:CD1	0.43	2.80	17	1
1:A:130:LYS:CD	1:A:175:ILE:HG22	0.43	2.42	12	1
1:A:151:ALA:HB1	1:A:163:MET:HE3	0.43	1.91	3	2
1:A:140:THR:O	1:A:140:THR:CG2	0.43	2.67	15	1
1:A:51:ILE:HG22	1:A:84:ALA:HA	0.43	1.90	10	2
1:A:196:ILE:HG23	1:A:205:VAL:HG12	0.43	1.86	7	1
1:A:145:GLN:HA	1:A:148:LEU:HD12	0.43	1.90	10	1
1:A:137:LEU:HD23	1:A:139:VAL:O	0.43	2.14	3	1
1:A:38:THR:HG23	1:A:97:ILE:O	0.43	2.14	16	1
1:A:23:TYR:CD1	1:A:29:LEU:HD23	0.43	2.48	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:GLU:CD	1:A:116:LEU:HD11	0.43	2.34	8	1
1:A:122:ARG:O	1:A:126:VAL:CA	0.43	2.67	5	3
1:A:73:LEU:HD23	1:A:82:ARG:NH2	0.43	2.29	4	1
1:A:144:ALA:HB3	1:A:145:GLN:NE2	0.43	2.28	8	1
1:A:70:ILE:CD1	1:A:94:VAL:HG11	0.43	2.43	14	1
1:A:150:LEU:HD11	1:A:172:ILE:CD1	0.43	2.44	9	1
1:A:42:ILE:HG12	1:A:94:VAL:HG22	0.43	1.91	19	3
1:A:39:LEU:HD12	1:A:40:TYR:H	0.43	1.74	13	1
1:A:83:SER:O	1:A:84:ALA:CB	0.43	2.66	13	1
1:A:39:LEU:HD13	1:A:72:GLU:HG2	0.42	1.89	19	1
1:A:75:LEU:HB2	1:A:99:TYR:CE1	0.42	2.49	19	1
1:A:134:LEU:HD12	1:A:134:LEU:N	0.42	2.28	18	2
1:A:168:THR:HG23	1:A:169:ARG:N	0.42	2.29	10	4
1:A:148:LEU:HD22	1:A:208:THR:HA	0.42	1.91	18	1
1:A:24:PRO:HA	1:A:91:ALA:HA	0.42	1.89	5	1
1:A:126:VAL:HG11	1:A:152:LYS:HZ1	0.42	1.73	14	1
1:A:88:ALA:HB1	1:A:92:CYS:SG	0.42	2.55	20	1
1:A:172:ILE:O	1:A:176:VAL:HG22	0.42	2.15	12	1
1:A:14:PHE:HD1	1:A:105:LEU:HD12	0.42	1.74	16	1
1:A:42:ILE:HG22	1:A:66:GLN:HA	0.42	1.91	17	1
1:A:150:LEU:HD13	1:A:167:ILE:CD1	0.42	2.44	18	2
1:A:136:PHE:O	1:A:137:LEU:HD12	0.42	2.14	5	1
1:A:59:MET:CE	1:A:134:LEU:HD13	0.42	2.45	19	1
1:A:72:GLU:OE2	1:A:116:LEU:HD21	0.42	2.14	1	1
1:A:17:HIS:CD2	1:A:105:LEU:HD11	0.42	2.49	1	1
1:A:30:ILE:CD1	1:A:70:ILE:HG22	0.42	2.44	9	2
1:A:138:ASP:O	1:A:139:VAL:O	0.42	2.36	12	1
1:A:60:ILE:HG22	1:A:130:LYS:CE	0.42	2.45	16	1
1:A:64:LEU:HD12	1:A:70:ILE:HG23	0.42	1.90	8	1
1:A:15:LEU:HD21	1:A:41:TYR:HD2	0.42	1.74	16	1
1:A:196:ILE:HG12	1:A:205:VAL:HG12	0.42	1.92	20	1
1:A:41:TYR:HB3	1:A:95:ALA:HB3	0.42	1.92	20	1
1:A:50:LEU:HB2	1:A:85:TRP:HB2	0.42	1.91	18	2
1:A:75:LEU:HB2	1:A:99:TYR:CD1	0.42	2.50	19	1
1:A:131:VAL:HG23	1:A:132:GLY:N	0.42	2.30	17	2
1:A:39:LEU:HD13	1:A:72:GLU:HA	0.42	1.92	10	1
1:A:196:ILE:HD11	1:A:209:ARG:O	0.42	2.14	16	1
1:A:20:ILE:HG22	1:A:93:GLU:O	0.42	2.15	16	1
1:A:18:CYS:CB	1:A:95:ALA:HB1	0.42	2.45	11	1
1:A:130:LYS:CE	1:A:175:ILE:HG21	0.42	2.44	19	1
1:A:40:TYR:HA	1:A:95:ALA:O	0.42	2.15	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:MET:HB2	1:A:124:LEU:HD12	0.41	1.90	13	1
1:A:59:MET:O	1:A:59:MET:HG3	0.41	2.14	13	1
1:A:42:ILE:HD12	1:A:68:ASP:HB2	0.41	1.91	5	2
1:A:122:ARG:O	1:A:126:VAL:HG12	0.41	2.15	19	1
1:A:124:LEU:O	1:A:125:GLN:HB3	0.41	2.13	12	1
1:A:51:ILE:HA	1:A:85:TRP:CZ3	0.41	2.50	14	1
1:A:116:LEU:C	1:A:116:LEU:HD12	0.41	2.36	20	1
1:A:29:LEU:HD22	1:A:94:VAL:CG2	0.41	2.44	9	1
1:A:23:TYR:O	1:A:91:ALA:HA	0.41	2.15	20	1
1:A:130:LYS:O	1:A:134:LEU:HD23	0.41	2.16	9	1
1:A:61:LEU:CD2	1:A:131:VAL:HG21	0.41	2.45	9	1
1:A:75:LEU:HD22	1:A:102:PHE:HE2	0.41	1.74	11	1
1:A:51:ILE:HG22	1:A:85:TRP:CZ3	0.41	2.51	14	1
1:A:75:LEU:HD22	1:A:102:PHE:CD2	0.41	2.51	16	1
1:A:130:LYS:HG3	1:A:175:ILE:HG22	0.41	1.93	17	1
1:A:49:VAL:HA	1:A:85:TRP:O	0.41	2.15	17	1
1:A:42:ILE:HD12	1:A:68:ASP:HB3	0.41	1.92	17	1
1:A:143:ILE:CG2	1:A:176:VAL:HG21	0.41	2.46	8	1
1:A:30:ILE:HD11	1:A:40:TYR:CE2	0.41	2.50	14	1
1:A:120:MET:CB	1:A:124:LEU:HD12	0.41	2.45	13	1
1:A:51:ILE:HA	1:A:85:TRP:HE3	0.41	1.74	14	1
1:A:49:VAL:HG12	1:A:61:LEU:CB	0.41	2.45	14	1
1:A:14:PHE:CD1	1:A:112:ILE:HD11	0.41	2.50	20	1
1:A:48:ALA:O	1:A:50:LEU:HD22	0.41	2.15	9	1
1:A:146:THR:HG23	1:A:175:ILE:HG21	0.41	1.93	11	1
1:A:106:ILE:HG22	1:A:112:ILE:HG21	0.41	1.93	19	1
1:A:30:ILE:HD12	1:A:70:ILE:HB	0.40	1.93	18	1
1:A:50:LEU:O	1:A:85:TRP:HE3	0.40	1.99	11	1
1:A:139:VAL:O	1:A:140:THR:CB	0.40	2.69	8	1
1:A:124:LEU:CD2	1:A:124:LEU:C	0.40	2.90	5	1
1:A:121:ALA:O	1:A:122:ARG:HB3	0.40	2.16	12	1
1:A:60:ILE:HD11	1:A:171:GLU:OE2	0.40	2.16	3	1
1:A:143:ILE:HG22	1:A:183:VAL:HG22	0.40	1.93	9	1
1:A:126:VAL:CG1	1:A:131:VAL:HG21	0.40	2.46	2	1
1:A:187:LEU:HD13	1:A:190:LEU:CD1	0.40	2.35	8	1
1:A:102:PHE:O	1:A:106:ILE:HG23	0.40	2.17	16	1
1:A:124:LEU:C	1:A:131:VAL:HG21	0.40	2.36	11	1
1:A:167:ILE:HD11	1:A:172:ILE:HD11	0.40	1.93	2	1
1:A:42:ILE:HG23	1:A:92:CYS:SG	0.40	2.57	5	1
1:A:22:LYS:HA	1:A:93:GLU:HA	0.40	1.92	5	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	182/209 (87%)	141±3 (78±2%)	27±3 (15±2%)	14±3 (8±1%)	2	16
All	All	3640/4180 (87%)	2823 (78%)	539 (15%)	278 (8%)	2	16

All 36 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	195	LEU	20
1	A	111	ASP	19
1	A	141	GLY	19
1	A	91	ALA	18
1	A	176	VAL	18
1	A	138	ASP	17
1	A	58	GLU	14
1	A	139	VAL	13
1	A	207	GLY	11
1	A	82	ARG	11
1	A	126	VAL	10
1	A	161	ASP	9
1	A	130	LYS	8
1	A	133	ASN	8
1	A	83	SER	8
1	A	37	GLU	7
1	A	42	ILE	7
1	A	208	THR	7
1	A	136	PHE	7
1	A	85	TRP	6
1	A	25	SER	6
1	A	7	THR	5
1	A	84	ALA	5
1	A	131	VAL	4
1	A	137	LEU	4
1	A	60	ILE	3
1	A	22	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	21	HIS	2
1	A	156	ALA	2
1	A	200	GLY	2
1	A	62	SER	1
1	A	20	ILE	1
1	A	153	GLN	1
1	A	154	PRO	1
1	A	122	ARG	1
1	A	125	GLN	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	159/180 (88%)	112±5 (70±3%)	47±5 (30±3%)	2	18
All	All	3180/3600 (88%)	2235 (70%)	945 (30%)	2	18

All 120 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	70	ILE	20
1	A	195	LEU	20
1	A	176	VAL	18
1	A	185	ARG	18
1	A	14	PHE	18
1	A	111	ASP	18
1	A	175	ILE	17
1	A	44	LYS	16
1	A	28	THR	16
1	A	130	LYS	16
1	A	22	LYS	16
1	A	158	THR	16
1	A	159	HIS	15
1	A	152	LYS	15
1	A	190	LEU	15
1	A	201	LYS	14

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Mol	Chain	Res	Type	Models (Total)
1	A	101	LYS	14
1	A	166	LYS	13
1	A	125	GLN	13
1	A	59	MET	13
1	A	82	ARG	13
1	A	124	LEU	13
1	A	106	ILE	13
1	A	182	THR	12
1	A	134	LEU	12
1	A	8	ASP	12
1	A	50	LEU	12
1	A	149	ASN	12
1	A	161	ASP	12
1	A	188	LYS	12
1	A	17	HIS	11
1	A	131	VAL	11
1	A	16	SER	11
1	A	209	ARG	11
1	A	61	LEU	11
1	A	170	GLN	10
1	A	202	THR	10
1	A	62	SER	10
1	A	157	MET	10
1	A	115	ARG	10
1	A	180	ARG	9
1	A	37	GLU	9
1	A	189	MET	9
1	A	96	GLU	9
1	A	46	SER	9
1	A	126	VAL	9
1	A	179	SER	9
1	A	51	ILE	9
1	A	27	SER	9
1	A	142	ARG	9
1	A	120	MET	8
1	A	123	ARG	8
1	A	137	LEU	8
1	A	65	ASN	8
1	A	168	THR	8
1	A	171	GLU	8
1	A	114	MET	7
1	A	21	HIS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	19	HIS	7
1	A	167	ILE	7
1	A	89	LYS	7
1	A	155	ASP	7
1	A	133	ASN	7
1	A	83	SER	7
1	A	87	ARG	7
1	A	153	GLN	7
1	A	122	ARG	7
1	A	72	GLU	6
1	A	119	GLN	6
1	A	197	SER	6
1	A	169	ARG	6
1	A	12	GLU	6
1	A	100	LYS	6
1	A	116	LEU	6
1	A	7	THR	5
1	A	138	ASP	5
1	A	25	SER	5
1	A	103	ARG	5
1	A	66	GLN	5
1	A	165	ILE	5
1	A	98	SER	5
1	A	140	THR	5
1	A	208	THR	5
1	A	26	LYS	5
1	A	163	MET	5
1	A	58	GLU	5
1	A	64	LEU	5
1	A	38	THR	4
1	A	174	GLN	4
1	A	104	GLN	4
1	A	60	ILE	4
1	A	199	HIS	4
1	A	191	GLU	3
1	A	145	GLN	3
1	A	178	CYS	3
1	A	93	GLU	3
1	A	150	LEU	3
1	A	75	LEU	3
1	A	31	HIS	3
1	A	205	VAL	3

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Mol	Chain	Res	Type	Models (Total)
1	A	107	GLN	3
1	A	18	CYS	2
1	A	92	CYS	2
1	A	196	ILE	2
1	A	136	PHE	2
1	A	181	GLU	2
1	A	29	LEU	2
1	A	192	ASP	2
1	A	164	GLN	2
1	A	23	TYR	1
1	A	113	LEU	1
1	A	20	ILE	1
1	A	30	ILE	1
1	A	139	VAL	1
1	A	193	GLN	1
1	A	63	TYR	1
1	A	73	LEU	1
1	A	85	TRP	1
1	A	90	THR	1
1	A	109	ASN	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 [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

The completeness of assignment taking into account all chemical shift lists is 13% for the well-defined parts and 14% for the entire structure.

7.1 Chemical shift list 1

File name: 4bhp_cs.cif

Chemical shift list name: *T127128N_cGMP_1.str.csh*

7.1.1 Bookkeeping

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

Total number of shifts	369
Number of shifts mapped to atoms	369
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	108	0.02 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	83	1.28 ± 0.11	Should be applied
$^{13}\text{C}'$	60	-0.23 ± 0.16	None needed (< 0.5 ppm)
^{15}N	118	0.09 ± 0.30	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 13%, i.e. 301 atoms were assigned a chemical shift out of a possible 2310. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	232/905 (26%)	0/361 (0%)	138/366 (38%)	94/178 (53%)
Sidechain	69/1255 (5%)	0/732 (0%)	69/463 (15%)	0/60 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/150 (0%)	0/80 (0%)	0/62 (0%)	0/8 (0%)
Overall	301/2310 (13%)	0/1173 (0%)	207/891 (23%)	94/246 (38%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 14%, i.e. 369 atoms were assigned a chemical shift out of a possible 2629. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	286/1033 (28%)	0/412 (0%)	168/418 (40%)	118/203 (58%)
Sidechain	83/1437 (6%)	0/839 (0%)	83/531 (16%)	0/67 (0%)
Aromatic	0/159 (0%)	0/85 (0%)	0/66 (0%)	0/8 (0%)
Overall	369/2629 (14%)	0/1336 (0%)	251/1015 (25%)	118/278 (42%)

7.1.4 Statistically unusual chemical shifts ⓘ

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	124	LEU	CB	31.24	51.69 – 32.89	-5.9

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

