Full wwPDB NMR Structure Validation Report (i)

Jun 2, 2020 – 03:09 pm BST

PDB ID	:	5ZC6
Title	:	Solution structure of H-RasT35S mutant protein in complex with KBFM123
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Deposited on	:	2018-02-15

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

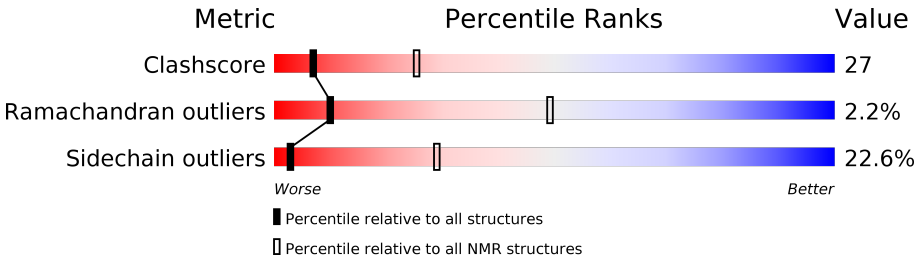
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 0%.

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	166	37% 51% · 8%

2 Ensemble composition and analysis

This entry contains 15 models. Model 11 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:2-A:29, A:39-A:60, A:65-A:166 (152)	0.29	11

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15

3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2701 atoms, of which 1327 are hydrogens and 0 are deuteriums.

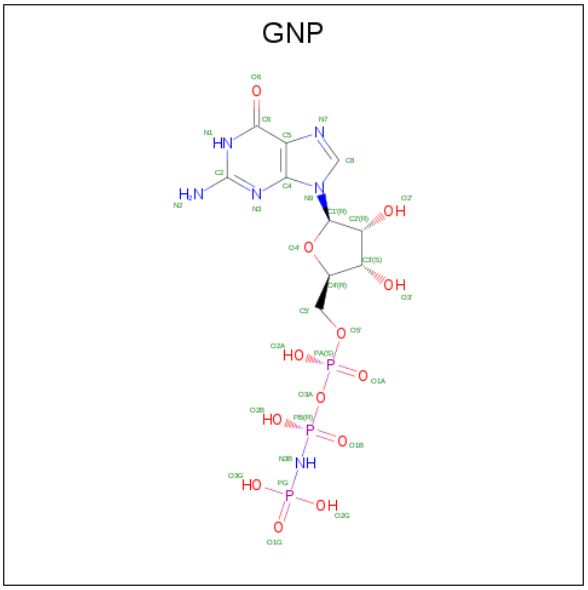
- Molecule 1 is a protein called GTPase HRas.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	166	2618	823	1297	228	263	7	0

There is a discrepancy between the modelled and reference sequences:

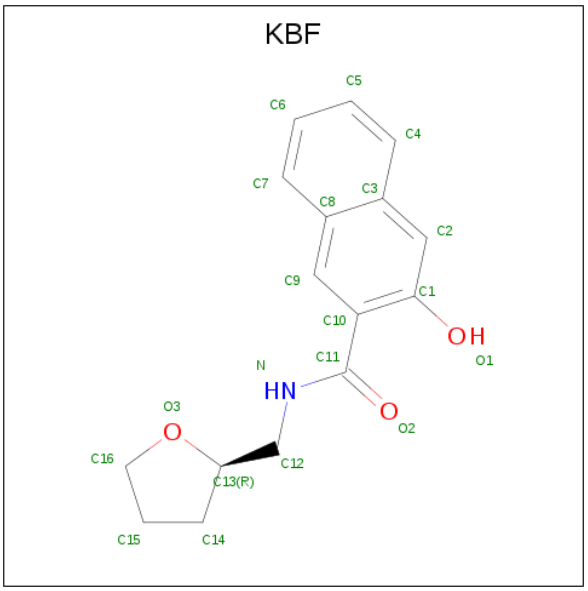
Chain	Residue	Modelled	Actual	Comment	Reference
A	35	SER	THR	engineered mutation	UNP P01112

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
2	A	1	45	10	13	6	13	3

- Molecule 3 is 3-oxidanyl- {N}-[[(2 {R})-oxolan-2-yl]methyl]naphthalene-2-carboxamide (three-letter code: KBF) (formula: $C_{16}H_{17}NO_3$).



Mol	Chain	Residues	Atoms				
3	A	1	Total	C	H	N	O
			37	16	17	1	3

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
4	A	1	Total	Mg
			1	1

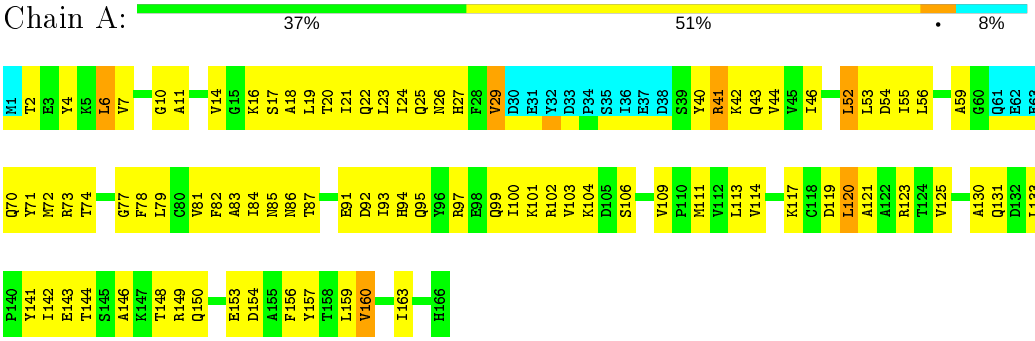
4 Residue-property plots

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: GTPase HRas

Chain A:



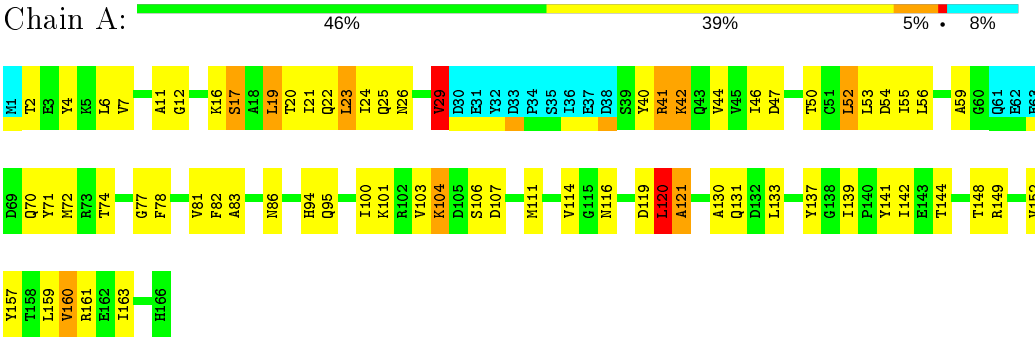
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: GTPase HRas

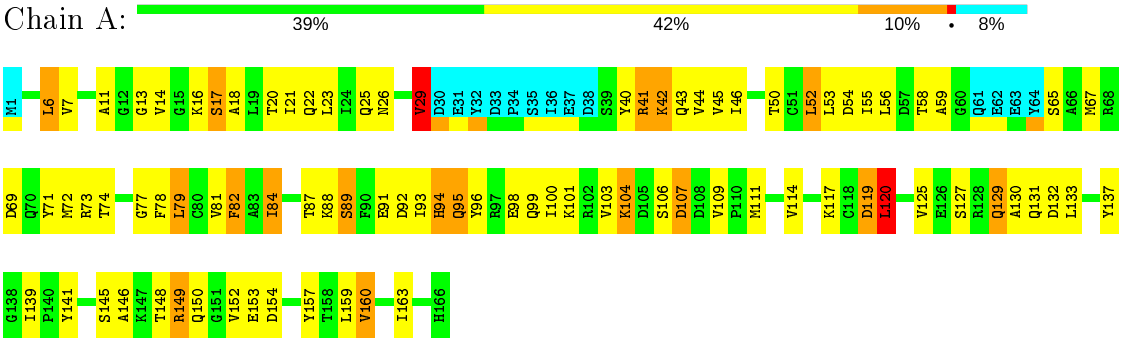
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: GTPase HRas

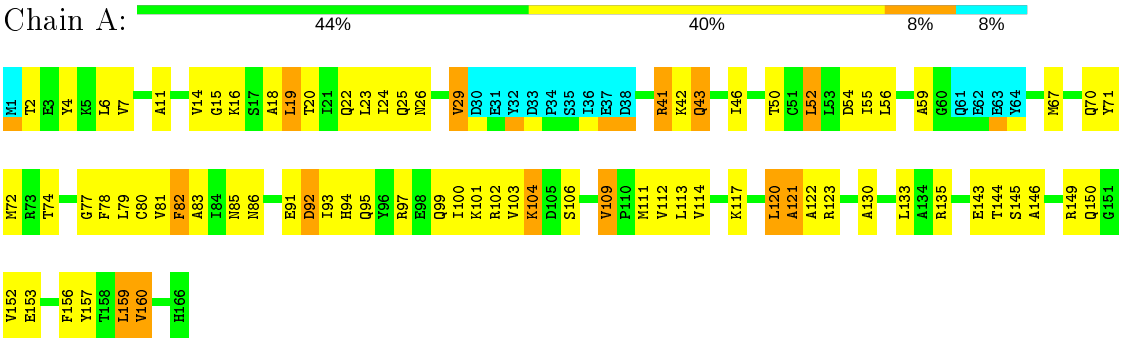
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: GTPase HRas

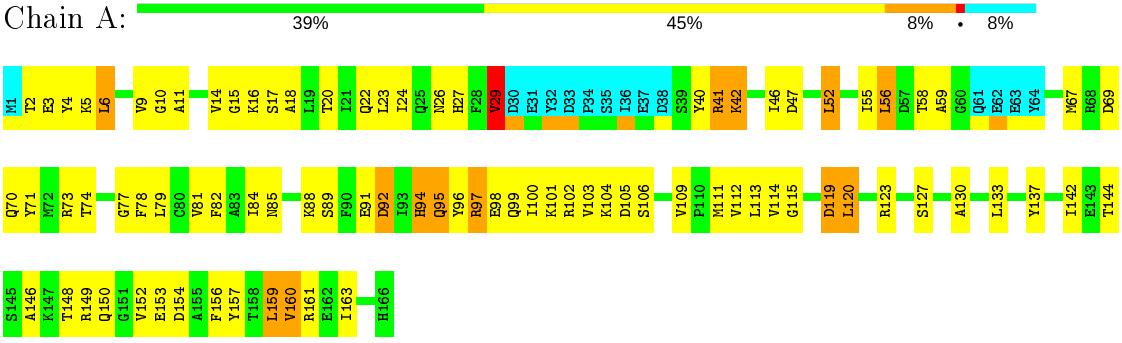
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: GTPase HRas

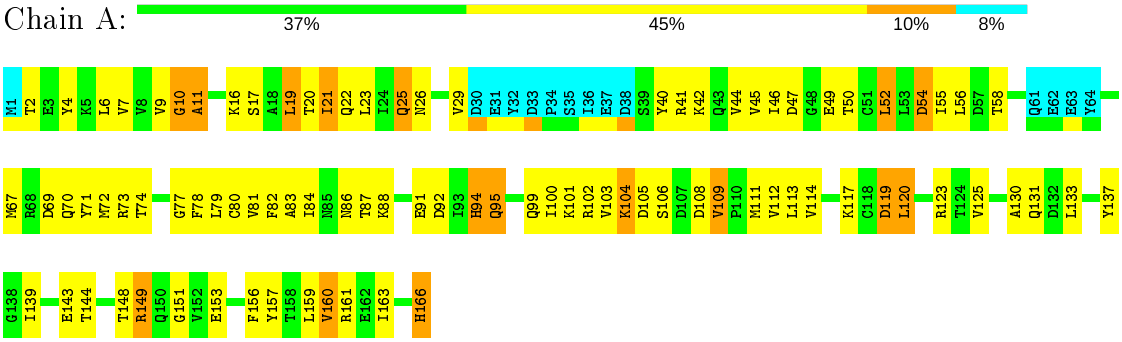
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: GTPase HRas

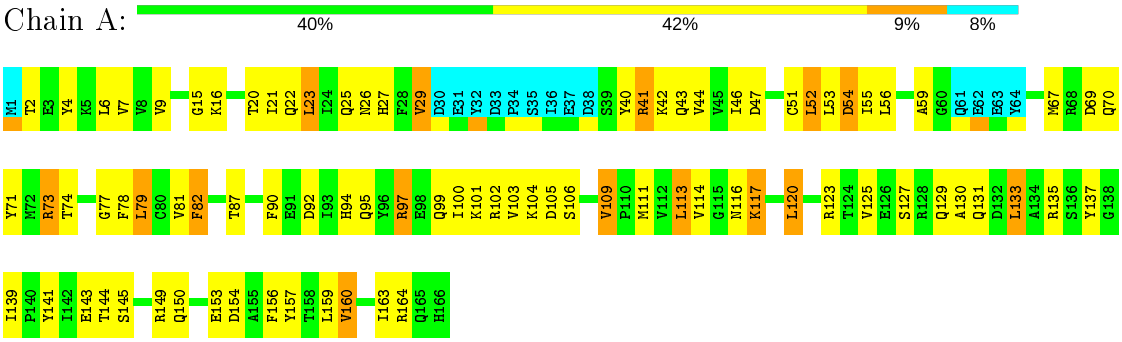
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: GTPase HRas

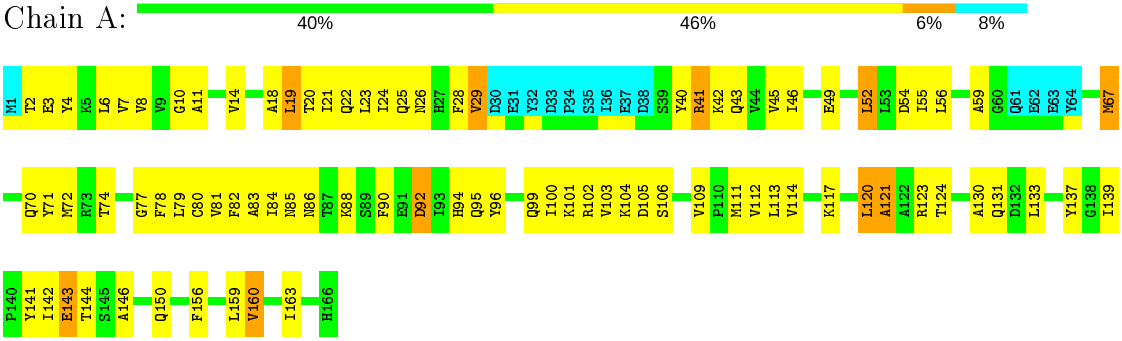
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: GTPase HRas

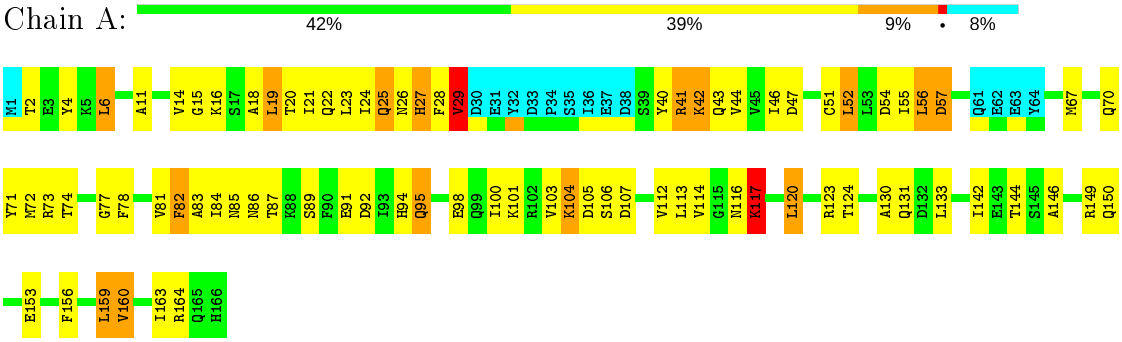
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: GTPase HRas

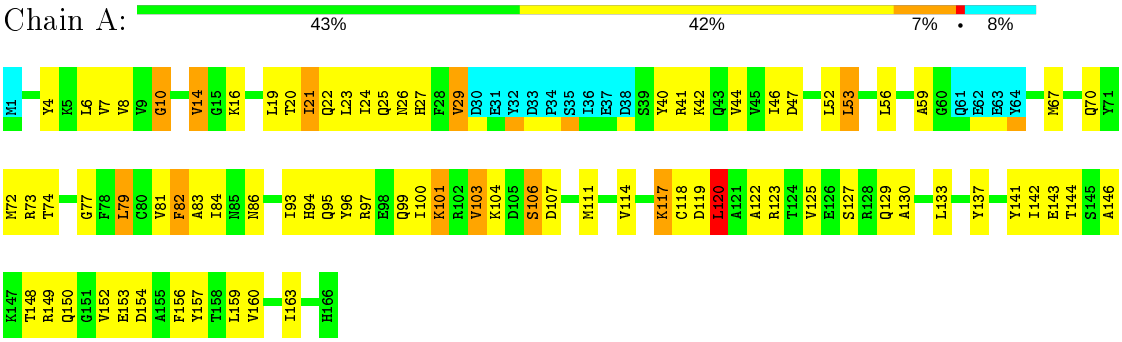
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: GTPase HRas

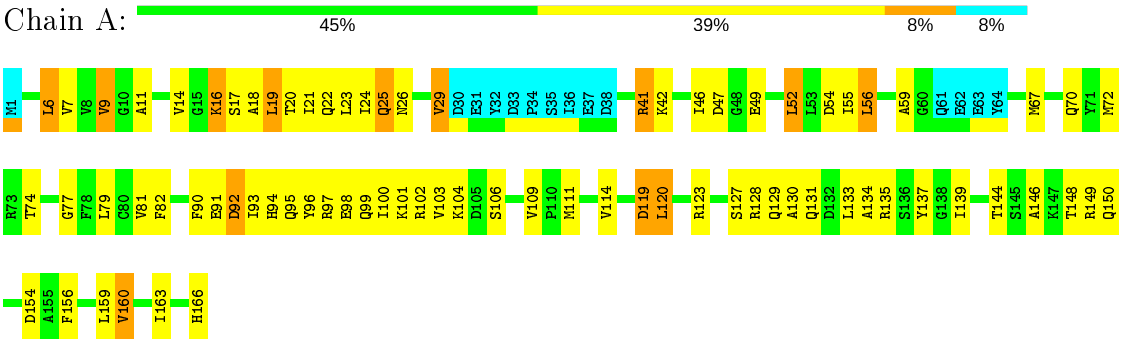
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: GTPase HRas

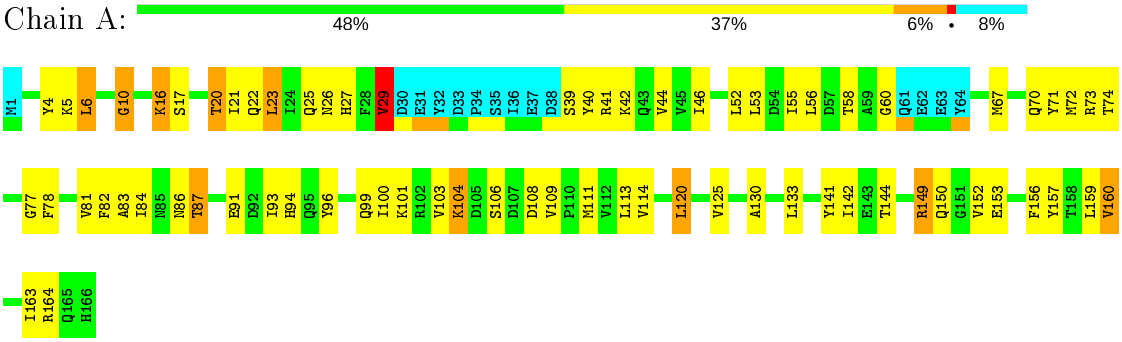
Chain A:



4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: GTPase HRas

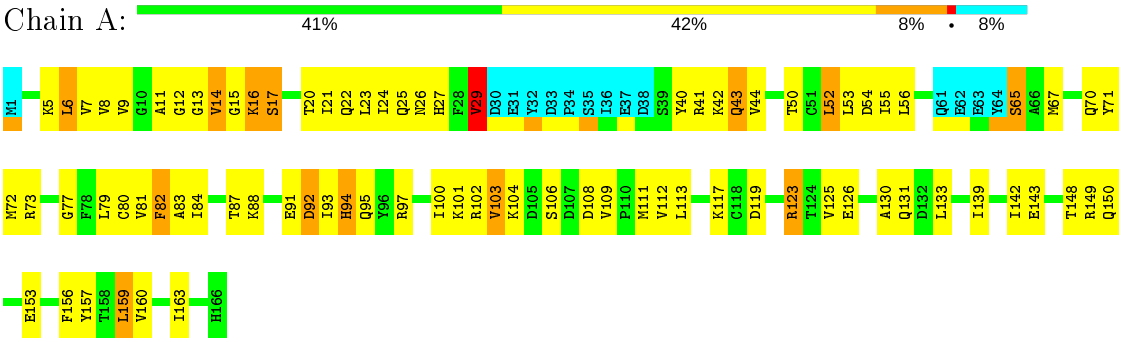
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: GTPase HRas

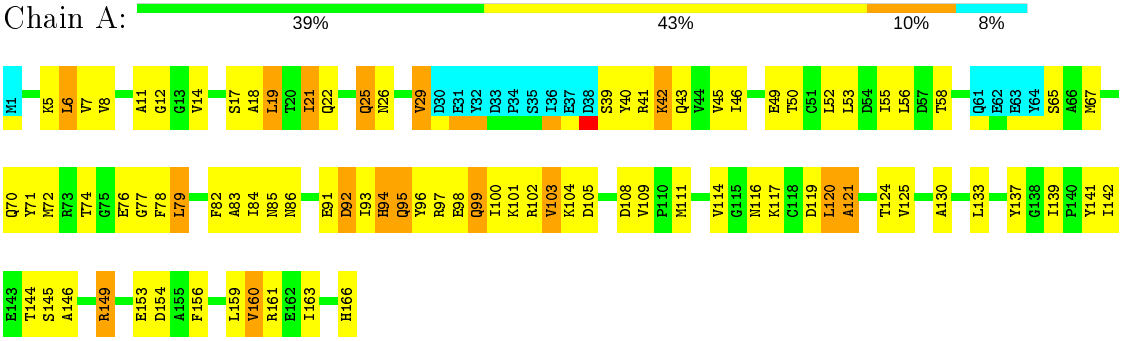
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: GTPase HRas

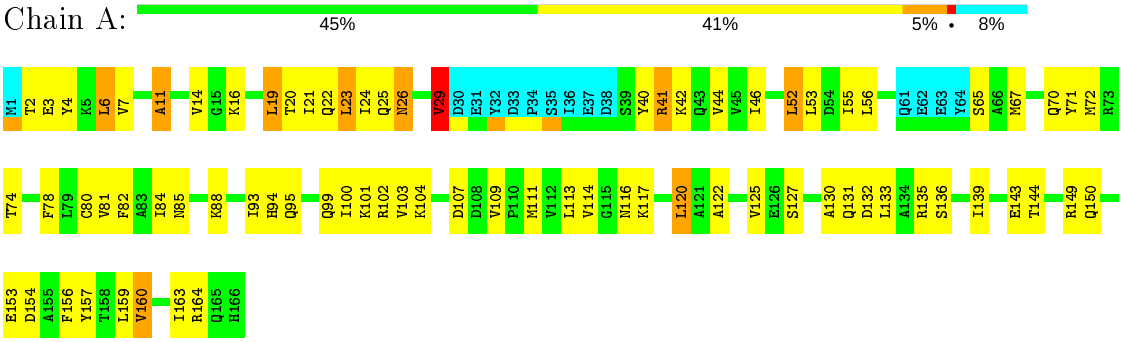
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: GTPase HRas

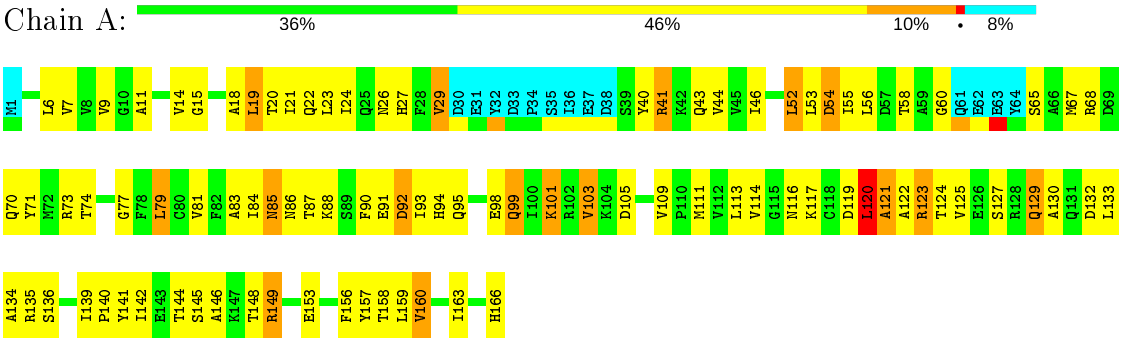
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: GTPase HRas

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 15 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
CNS	refinement	

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	28
Number of shifts mapped to atoms	28
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, KBF, MG

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	1199	1201	1197	66±5
2	A	32	13	13	1±1
3	A	20	17	0	2±1
All	All	18780	18465	18150	1000

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD23	1:A:159:LEU:HD12	1.01	1.31	2	11
1:A:6:LEU:HD13	1:A:55:ILE:HD13	0.99	1.35	2	7
1:A:7:VAL:HG22	1:A:56:LEU:HD23	0.93	1.39	12	8
1:A:113:LEU:HD22	1:A:133:LEU:HD22	0.87	1.47	12	2
1:A:81:VAL:HG12	1:A:114:VAL:CG1	0.87	2.00	7	9
1:A:20:THR:HG21	1:A:57:ASP:OD1	0.84	1.72	8	1
1:A:23:LEU:HD22	1:A:156:PHE:CD1	0.83	2.08	9	4
1:A:24:ILE:HD11	1:A:55:ILE:CG1	0.81	2.05	12	9
1:A:90:PHE:CE2	1:A:133:LEU:HD12	0.81	2.10	6	2
1:A:46:ILE:HD12	1:A:160:VAL:HG11	0.80	1.52	14	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:VAL:HG12	1:A:114:VAL:HG13	0.79	1.52	8	9
1:A:70:GLN:O	1:A:74:THR:HG22	0.78	1.79	4	13
1:A:93:ILE:HG21	1:A:133:LEU:HD21	0.77	1.56	14	6
1:A:100:ILE:HG21	1:A:111:MET:CE	0.77	2.09	6	10
1:A:72:MET:HB2	1:A:103:VAL:HG21	0.76	1.58	3	7
1:A:23:LEU:HD22	1:A:156:PHE:CG	0.76	2.15	15	7
1:A:23:LEU:HD22	1:A:156:PHE:CD2	0.75	2.15	8	6
1:A:72:MET:CB	1:A:103:VAL:HG21	0.74	2.12	10	6
1:A:24:ILE:HD11	1:A:55:ILE:HG12	0.74	1.59	12	9
1:A:44:VAL:HG23	1:A:46:ILE:HD11	0.72	1.59	9	1
1:A:19:LEU:HD13	1:A:116:ASN:ND2	0.72	1.98	15	2
1:A:20:THR:HG23	1:A:55:ILE:CG2	0.72	2.14	3	10
1:A:56:LEU:HD11	1:A:71:TYR:CE1	0.72	2.19	2	1
1:A:41:ARG:HG2	1:A:52:LEU:HD11	0.72	1.59	5	10
1:A:80:CYS:SG	1:A:93:ILE:HD12	0.72	2.24	14	1
1:A:6:LEU:CD2	1:A:159:LEU:HD12	0.71	2.15	4	7
1:A:44:VAL:HG11	1:A:157:TYR:OH	0.71	1.86	5	5
1:A:93:ILE:CG2	1:A:133:LEU:HD21	0.71	2.14	2	5
1:A:80:CYS:SG	1:A:93:ILE:HG23	0.71	2.26	14	1
1:A:6:LEU:HD12	1:A:55:ILE:HD13	0.71	1.63	4	3
1:A:19:LEU:HD12	1:A:156:PHE:CZ	0.71	2.21	5	2
1:A:83:ALA:HB3	1:A:86:ASN:HB3	0.70	1.62	8	9
1:A:11:ALA:HB2	1:A:92:ASP:OD1	0.70	1.87	4	1
1:A:46:ILE:HG21	1:A:157:TYR:O	0.70	1.86	9	1
1:A:100:ILE:HG21	1:A:111:MET:HE2	0.70	1.64	2	11
1:A:14:VAL:HG11	1:A:89:SER:OG	0.70	1.86	2	2
1:A:44:VAL:HG23	1:A:46:ILE:CD1	0.70	2.17	9	1
1:A:58:THR:HG22	1:A:71:TYR:CD1	0.69	2.22	2	3
1:A:6:LEU:HD12	1:A:54:ASP:O	0.69	1.86	2	9
1:A:81:VAL:HG13	1:A:114:VAL:HG13	0.69	1.62	3	2
1:A:6:LEU:CD1	1:A:55:ILE:HD13	0.69	2.18	4	4
1:A:20:THR:HG23	1:A:55:ILE:HG21	0.68	1.66	12	9
1:A:125:VAL:HG13	1:A:129:GLN:NE2	0.68	2.03	9	1
1:A:6:LEU:HD12	1:A:55:ILE:CD1	0.68	2.18	14	2
1:A:52:LEU:HD12	1:A:54:ASP:OD1	0.67	1.89	3	4
1:A:6:LEU:HD23	1:A:159:LEU:CD1	0.67	2.19	6	7
1:A:7:VAL:HG22	1:A:56:LEU:CD2	0.67	2.18	13	2
1:A:78:PHE:CE2	1:A:100:ILE:HG23	0.67	2.25	11	3
1:A:56:LEU:HD11	3:A:202:KBF:C5	0.67	2.20	14	7
1:A:87:THR:HG23	1:A:125:VAL:HG22	0.67	1.64	2	5
1:A:11:ALA:O	1:A:14:VAL:HG22	0.67	1.89	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:VAL:HG22	1:A:114:VAL:CG1	0.66	2.20	3	2
1:A:119:ASP:CG	1:A:148:THR:HG21	0.66	2.09	2	7
1:A:23:LEU:HD23	1:A:55:ILE:HG13	0.66	1.66	3	2
1:A:87:THR:HG23	1:A:125:VAL:CG2	0.66	2.19	2	2
1:A:24:ILE:HG23	1:A:41:ARG:O	0.66	1.90	7	2
1:A:85:ASN:CG	1:A:120:LEU:HD23	0.65	2.11	14	1
1:A:23:LEU:HD21	1:A:42:LYS:NZ	0.65	2.06	1	3
1:A:84:ILE:HG21	1:A:118:CYS:SG	0.65	2.31	9	1
1:A:111:MET:HB2	1:A:139:ILE:HG21	0.65	1.68	5	9
1:A:6:LEU:HD22	1:A:159:LEU:HD12	0.65	1.66	14	3
1:A:20:THR:HG21	1:A:40:TYR:CD1	0.64	2.27	1	4
1:A:6:LEU:HD23	1:A:159:LEU:HG	0.64	1.70	5	1
1:A:44:VAL:CG2	1:A:46:ILE:HD11	0.64	2.22	9	1
1:A:11:ALA:O	1:A:14:VAL:HG13	0.64	1.91	15	2
1:A:120:LEU:HD12	2:A:201:GNP:N2	0.64	2.08	13	1
1:A:9:VAL:O	1:A:81:VAL:HG12	0.64	1.93	5	2
1:A:104:LYS:HE3	1:A:109:VAL:HG11	0.64	1.70	3	4
1:A:117:LYS:HD3	1:A:120:LEU:HD12	0.64	1.70	7	1
1:A:94:HIS:CE1	1:A:133:LEU:HD12	0.64	2.28	12	1
1:A:56:LEU:HD21	1:A:71:TYR:CD1	0.63	2.27	3	1
1:A:74:THR:HG21	3:A:202:KBF:C7	0.63	2.24	13	10
1:A:117:LYS:HB3	1:A:120:LEU:HD21	0.63	1.71	2	2
1:A:9:VAL:O	1:A:81:VAL:HG22	0.63	1.93	4	3
1:A:19:LEU:HD23	1:A:116:ASN:ND2	0.63	2.09	14	1
1:A:42:LYS:O	1:A:52:LEU:HD23	0.63	1.93	13	3
1:A:82:PHE:CZ	1:A:130:ALA:HB2	0.63	2.29	9	10
1:A:21:ILE:HG13	1:A:29:VAL:HG23	0.63	1.69	1	6
1:A:21:ILE:HG12	1:A:29:VAL:HG23	0.62	1.68	14	2
1:A:6:LEU:HD13	1:A:55:ILE:CD1	0.62	2.22	8	4
1:A:80:CYS:O	1:A:113:LEU:HD12	0.62	1.94	7	4
1:A:93:ILE:HB	1:A:133:LEU:HD11	0.62	1.71	10	3
1:A:77:GLY:HA3	1:A:159:LEU:HD11	0.62	1.72	9	13
1:A:7:VAL:CG2	1:A:56:LEU:HD23	0.62	2.21	12	2
1:A:159:LEU:CD1	1:A:163:ILE:HD11	0.62	2.25	6	11
1:A:55:ILE:HG21	1:A:156:PHE:CE1	0.62	2.29	1	1
1:A:113:LEU:HD22	1:A:133:LEU:CD2	0.62	2.23	12	1
1:A:43:GLN:NE2	1:A:50:THR:HG23	0.62	2.10	12	1
1:A:113:LEU:HD12	1:A:141:TYR:CE1	0.61	2.30	6	1
1:A:130:ALA:HB1	1:A:141:TYR:CE1	0.61	2.30	6	3
1:A:78:PHE:CE1	1:A:100:ILE:HG23	0.61	2.30	14	4
1:A:82:PHE:HB3	1:A:93:ILE:HD11	0.61	1.72	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LYS:O	1:A:117:LYS:CG	0.61	2.49	6	1
1:A:21:ILE:HG22	1:A:27:HIS:O	0.61	1.95	8	2
1:A:114:VAL:HG23	1:A:144:THR:HG23	0.61	1.73	14	13
1:A:119:ASP:OD1	1:A:148:THR:HG21	0.61	1.96	5	2
1:A:24:ILE:HG21	1:A:40:TYR:HB3	0.60	1.73	12	4
1:A:22:GLN:O	1:A:26:ASN:HA	0.60	1.97	7	15
1:A:117:LYS:HB2	1:A:120:LEU:HD21	0.60	1.74	9	1
1:A:79:LEU:HD12	1:A:159:LEU:HB2	0.59	1.72	2	3
1:A:58:THR:HG22	1:A:71:TYR:CD2	0.59	2.32	5	3
1:A:100:ILE:HG21	1:A:111:MET:HE3	0.59	1.74	12	1
1:A:149:ARG:HD2	1:A:152:VAL:HG21	0.59	1.73	9	1
1:A:17:SER:HB2	1:A:29:VAL:HG21	0.59	1.75	12	3
1:A:56:LEU:HD21	1:A:71:TYR:CG	0.59	2.33	13	1
1:A:85:ASN:OD1	1:A:120:LEU:HD23	0.59	1.97	14	1
1:A:2:THR:HG21	1:A:4:TYR:CZ	0.59	2.33	1	8
1:A:18:ALA:HB1	1:A:146:ALA:HB1	0.59	1.74	3	5
1:A:79:LEU:HD12	1:A:112:VAL:HB	0.59	1.75	5	2
1:A:78:PHE:CD1	1:A:100:ILE:HG23	0.59	2.33	2	1
1:A:11:ALA:HB2	1:A:92:ASP:CG	0.58	2.18	4	5
1:A:8:VAL:HG12	1:A:79:LEU:HB3	0.58	1.74	7	2
1:A:19:LEU:HD12	1:A:146:ALA:HB2	0.58	1.73	10	1
1:A:20:THR:HG21	1:A:40:TYR:CD2	0.58	2.33	4	3
1:A:46:ILE:HD13	1:A:160:VAL:HG11	0.58	1.75	9	2
1:A:21:ILE:HG23	1:A:25:GLN:HB2	0.58	1.76	9	1
1:A:159:LEU:HD13	1:A:159:LEU:O	0.58	1.98	1	8
1:A:45:VAL:HG23	1:A:49:GLU:C	0.58	2.18	13	2
1:A:18:ALA:CB	1:A:146:ALA:HB1	0.58	2.29	13	6
1:A:104:LYS:HD3	1:A:109:VAL:HG11	0.57	1.75	14	1
1:A:82:PHE:CE1	1:A:130:ALA:HB2	0.57	2.35	12	1
1:A:109:VAL:HG23	1:A:111:MET:HE3	0.57	1.76	3	1
1:A:24:ILE:HG22	1:A:25:GLN:OE1	0.57	1.99	9	2
1:A:92:ASP:OD2	1:A:93:ILE:HD13	0.57	2.00	10	1
1:A:90:PHE:CD2	1:A:133:LEU:HD12	0.57	2.34	6	2
1:A:46:ILE:HD12	1:A:160:VAL:CG1	0.57	2.29	7	6
1:A:117:LYS:HE3	1:A:120:LEU:HD22	0.56	1.77	3	1
1:A:20:THR:HG21	1:A:57:ASP:CG	0.56	2.20	8	1
1:A:41:ARG:NH1	1:A:52:LEU:HD21	0.56	2.15	10	1
1:A:114:VAL:HG23	1:A:142:ILE:O	0.56	2.01	7	8
1:A:23:LEU:HD12	1:A:153:GLU:HG3	0.56	1.78	12	2
1:A:120:LEU:C	1:A:120:LEU:HD22	0.56	2.21	6	1
1:A:4:TYR:O	1:A:6:LEU:HD12	0.56	2.00	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:PHE:CE2	1:A:130:ALA:HB2	0.56	2.36	6	1
1:A:93:ILE:HG21	1:A:133:LEU:CD2	0.56	2.31	2	2
1:A:134:ALA:HB1	1:A:139:ILE:O	0.56	2.01	15	2
1:A:104:LYS:HE2	1:A:109:VAL:HG11	0.55	1.77	11	3
1:A:44:VAL:HG22	1:A:53:LEU:HD23	0.55	1.79	14	3
1:A:29:VAL:HG11	2:A:201:GNP:O2B	0.55	2.01	9	1
1:A:5:LYS:HE3	1:A:56:LEU:HD12	0.55	1.79	11	1
1:A:97:ARG:HA	1:A:100:ILE:HD12	0.54	1.79	6	4
1:A:149:ARG:HD3	1:A:152:VAL:HG21	0.54	1.78	2	2
1:A:23:LEU:HD13	1:A:156:PHE:CB	0.54	2.32	6	2
1:A:159:LEU:O	1:A:159:LEU:HD13	0.54	2.03	6	6
1:A:78:PHE:CG	1:A:100:ILE:HD13	0.54	2.38	13	4
1:A:125:VAL:HG13	1:A:125:VAL:O	0.53	2.03	13	1
1:A:120:LEU:O	1:A:121:ALA:HB2	0.53	2.03	7	4
1:A:113:LEU:HD13	1:A:114:VAL:N	0.53	2.18	4	1
1:A:11:ALA:HB2	1:A:92:ASP:CB	0.53	2.33	3	1
1:A:7:VAL:HG22	1:A:56:LEU:HD13	0.53	1.79	9	3
1:A:18:ALA:HB1	1:A:28:PHE:CE1	0.53	2.37	7	1
1:A:58:THR:HG22	1:A:71:TYR:HD1	0.53	1.63	4	2
1:A:21:ILE:CG1	1:A:29:VAL:HG23	0.53	2.32	2	4
1:A:82:PHE:CE1	1:A:113:LEU:HD21	0.53	2.37	3	1
1:A:19:LEU:HD12	1:A:156:PHE:CE2	0.53	2.39	7	2
1:A:23:LEU:HD23	1:A:55:ILE:CG1	0.53	2.33	3	1
1:A:85:ASN:OD1	1:A:122:ALA:HB3	0.53	2.04	14	1
1:A:6:LEU:HD23	1:A:159:LEU:CG	0.53	2.33	5	1
1:A:77:GLY:HA3	1:A:163:ILE:HD11	0.53	1.79	5	1
1:A:79:LEU:HD21	1:A:114:VAL:HG11	0.53	1.81	6	2
1:A:6:LEU:HD12	1:A:54:ASP:C	0.53	2.24	8	1
1:A:24:ILE:HD11	1:A:55:ILE:HG13	0.53	1.79	12	2
1:A:82:PHE:CZ	1:A:113:LEU:HD21	0.53	2.39	3	1
1:A:82:PHE:CZ	1:A:130:ALA:HB1	0.52	2.40	3	2
1:A:100:ILE:HG22	1:A:104:LYS:HG3	0.52	1.81	5	2
1:A:23:LEU:HD13	1:A:156:PHE:CG	0.52	2.39	6	2
1:A:46:ILE:HD13	1:A:53:LEU:HD21	0.52	1.79	9	1
2:A:201:GNP:H8	2:A:201:GNP:H5'2	0.52	1.80	11	1
1:A:45:VAL:HG22	1:A:50:THR:OG1	0.52	2.05	2	2
1:A:56:LEU:HD11	1:A:71:TYR:CD1	0.52	2.39	2	1
1:A:19:LEU:HB3	1:A:146:ALA:HB2	0.52	1.80	8	2
1:A:45:VAL:O	1:A:45:VAL:HG13	0.52	2.05	13	2
1:A:159:LEU:HD12	1:A:163:ILE:HD11	0.52	1.82	6	3
1:A:84:ILE:HD12	1:A:123:ARG:HB3	0.52	1.82	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:LEU:HG	1:A:146:ALA:HB2	0.52	1.81	9	1
1:A:78:PHE:CD2	1:A:100:ILE:HG23	0.52	2.40	11	1
1:A:14:VAL:HA	1:A:83:ALA:HB2	0.51	1.81	13	4
1:A:109:VAL:HG23	1:A:111:MET:CE	0.51	2.35	3	2
1:A:56:LEU:HD21	3:A:202:KBF:C5	0.51	2.35	9	2
1:A:93:ILE:CB	1:A:133:LEU:HD21	0.51	2.35	14	4
1:A:16:LYS:CB	1:A:81:VAL:HG21	0.51	2.36	10	1
1:A:99:GLN:O	1:A:103:VAL:HG22	0.51	2.05	3	3
1:A:84:ILE:HD12	1:A:123:ARG:CB	0.51	2.36	15	3
1:A:104:LYS:HD3	1:A:109:VAL:HG21	0.51	1.81	6	3
1:A:119:ASP:CB	1:A:148:THR:HG21	0.51	2.36	5	2
1:A:55:ILE:HG21	1:A:156:PHE:HE1	0.51	1.65	1	1
1:A:41:ARG:CG	1:A:52:LEU:HD11	0.51	2.35	2	5
1:A:43:GLN:OE1	1:A:50:THR:HG23	0.51	2.04	3	1
1:A:94:HIS:CE1	1:A:133:LEU:HD13	0.51	2.41	14	3
1:A:23:LEU:CD2	1:A:55:ILE:HD11	0.51	2.36	3	1
1:A:5:LYS:HZ3	1:A:56:LEU:HD13	0.50	1.66	4	1
1:A:24:ILE:HD13	1:A:42:LYS:HD3	0.50	1.82	8	1
1:A:23:LEU:HD11	1:A:157:TYR:CE1	0.50	2.42	5	1
1:A:82:PHE:HE1	1:A:133:LEU:HD23	0.50	1.67	3	1
1:A:74:THR:HG21	3:A:202:KBF:C6	0.50	2.37	8	5
1:A:78:PHE:CD1	1:A:100:ILE:HD13	0.50	2.42	7	1
1:A:78:PHE:CD2	1:A:78:PHE:N	0.50	2.79	14	2
1:A:119:ASP:OD2	1:A:148:THR:HG21	0.50	2.07	12	1
1:A:23:LEU:HD21	1:A:42:LYS:HE2	0.50	1.83	10	2
1:A:23:LEU:HD12	1:A:153:GLU:HA	0.50	1.83	1	1
1:A:46:ILE:CD1	1:A:53:LEU:HD21	0.49	2.36	1	2
1:A:15:GLY:HA3	2:A:201:GNP:H8	0.49	1.82	6	1
1:A:78:PHE:CD1	1:A:78:PHE:N	0.49	2.79	6	2
1:A:112:VAL:HG23	1:A:159:LEU:HD22	0.49	1.84	8	4
1:A:53:LEU:CD2	1:A:160:VAL:HG21	0.49	2.38	13	1
1:A:23:LEU:HD21	1:A:42:LYS:CE	0.49	2.37	6	1
1:A:113:LEU:HD12	1:A:141:TYR:CD2	0.49	2.42	15	1
1:A:23:LEU:HD13	1:A:156:PHE:HB2	0.49	1.85	6	2
1:A:84:ILE:HD11	1:A:117:LYS:O	0.49	2.08	2	3
1:A:92:ASP:O	1:A:95:GLN:HG3	0.49	2.08	8	3
1:A:6:LEU:N	1:A:6:LEU:HD23	0.49	2.23	11	1
1:A:23:LEU:HD22	1:A:156:PHE:HD2	0.48	1.64	6	1
1:A:20:THR:CG2	1:A:40:TYR:CD1	0.48	2.96	2	4
1:A:56:LEU:HD21	1:A:71:TYR:HD1	0.48	1.66	3	1
1:A:8:VAL:HG12	1:A:16:LYS:HG3	0.48	1.84	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:LYS:HD2	1:A:101:LYS:N	0.48	2.23	9	1
1:A:81:VAL:HG23	1:A:114:VAL:HG13	0.48	1.85	2	1
1:A:141:TYR:HH	1:A:143:GLU:CD	0.48	2.11	7	1
1:A:125:VAL:HG13	1:A:129:GLN:HE21	0.48	1.68	15	2
1:A:82:PHE:CE1	1:A:113:LEU:HD11	0.48	2.44	3	1
1:A:133:LEU:O	1:A:133:LEU:HD23	0.48	2.08	10	4
1:A:21:ILE:O	1:A:25:GLN:N	0.48	2.43	8	3
1:A:93:ILE:HB	1:A:133:LEU:HD21	0.48	1.86	3	1
1:A:130:ALA:HB1	1:A:141:TYR:HE1	0.48	1.66	6	1
1:A:133:LEU:CD2	1:A:137:TYR:CE2	0.48	2.97	7	6
1:A:120:LEU:HD13	1:A:120:LEU:H	0.48	1.69	11	1
1:A:46:ILE:HG22	1:A:47:ASP:OD1	0.48	2.09	4	1
1:A:6:LEU:HD23	1:A:163:ILE:HD11	0.48	1.84	4	1
1:A:56:LEU:CD2	1:A:71:TYR:CD1	0.47	2.97	4	3
1:A:114:VAL:CG2	1:A:144:THR:HG23	0.47	2.37	13	1
1:A:90:PHE:CE1	1:A:133:LEU:HD22	0.47	2.45	15	1
1:A:52:LEU:HD12	1:A:54:ASP:CG	0.47	2.29	3	3
1:A:133:LEU:HD22	1:A:137:TYR:CE2	0.47	2.44	6	1
1:A:23:LEU:HB2	1:A:152:VAL:HG12	0.47	1.87	1	2
1:A:100:ILE:HG21	1:A:111:MET:HE1	0.47	1.86	11	2
1:A:78:PHE:CZ	1:A:100:ILE:HG23	0.47	2.45	13	4
1:A:133:LEU:HD21	1:A:137:TYR:OH	0.47	2.10	13	3
1:A:130:ALA:HB1	1:A:141:TYR:CE2	0.47	2.45	15	1
1:A:23:LEU:HD11	1:A:42:LYS:NZ	0.47	2.24	10	3
1:A:82:PHE:CZ	1:A:113:LEU:HD11	0.47	2.45	3	1
1:A:120:LEU:CD2	2:A:201:GNP:N2	0.47	2.77	15	1
1:A:6:LEU:HD23	1:A:163:ILE:CD1	0.46	2.40	12	2
1:A:81:VAL:HG23	1:A:81:VAL:O	0.46	2.10	11	1
1:A:95:GLN:NE2	1:A:96:TYR:CE2	0.46	2.84	4	1
1:A:91:GLU:HA	1:A:94:HIS:CD2	0.46	2.45	13	9
1:A:90:PHE:CE1	1:A:133:LEU:HD12	0.46	2.45	7	1
1:A:72:MET:HA	1:A:78:PHE:CZ	0.46	2.45	2	3
1:A:82:PHE:CZ	1:A:130:ALA:CB	0.46	2.98	13	1
1:A:41:ARG:NE	1:A:52:LEU:HD21	0.46	2.25	5	1
1:A:56:LEU:HD21	1:A:71:TYR:CD2	0.46	2.46	5	1
1:A:157:TYR:O	1:A:160:VAL:HG12	0.46	2.09	9	1
1:A:10:GLY:O	1:A:11:ALA:HB2	0.46	2.10	5	1
1:A:41:ARG:HG2	1:A:52:LEU:CD1	0.46	2.41	2	1
1:A:9:VAL:HG22	1:A:79:LEU:O	0.46	2.11	15	1
1:A:44:VAL:CG2	1:A:53:LEU:HD23	0.46	2.41	11	3
1:A:148:THR:O	1:A:149:ARG:CB	0.46	2.64	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:THR:HG22	1:A:151:GLY:HA3	0.46	1.88	5	1
1:A:113:LEU:HD12	1:A:114:VAL:N	0.46	2.25	14	1
1:A:85:ASN:HA	1:A:124:THR:HG23	0.46	1.87	15	4
1:A:23:LEU:HD13	1:A:156:PHE:HD2	0.46	1.70	4	2
1:A:21:ILE:CD1	1:A:21:ILE:N	0.46	2.78	9	1
1:A:18:ALA:HB1	1:A:28:PHE:HE1	0.46	1.69	7	1
1:A:21:ILE:HG23	1:A:25:GLN:HG3	0.46	1.88	8	1
1:A:109:VAL:CG2	1:A:111:MET:HE2	0.46	2.41	10	1
1:A:2:THR:CG2	1:A:4:TYR:CZ	0.45	2.99	5	5
1:A:23:LEU:HD22	1:A:156:PHE:HD1	0.45	1.67	11	1
1:A:7:VAL:HG21	1:A:71:TYR:O	0.45	2.11	3	2
1:A:17:SER:HB2	1:A:29:VAL:HG11	0.45	1.88	2	1
1:A:18:ALA:HB1	1:A:28:PHE:CE2	0.45	2.46	8	1
1:A:95:GLN:NE2	1:A:96:TYR:CD1	0.45	2.84	13	1
1:A:133:LEU:CD1	1:A:137:TYR:CE2	0.45	3.00	2	1
2:A:201:GNP:O2A	2:A:201:GNP:N3B	0.45	2.50	2	1
1:A:130:ALA:CB	1:A:141:TYR:CZ	0.45	2.99	15	1
1:A:81:VAL:CG1	1:A:114:VAL:HG13	0.45	2.41	15	1
1:A:23:LEU:HD21	1:A:42:LYS:HZ2	0.45	1.68	1	1
1:A:21:ILE:HG23	1:A:25:GLN:CG	0.45	2.41	5	3
1:A:78:PHE:CD2	1:A:100:ILE:HD13	0.45	2.47	8	1
1:A:78:PHE:N	1:A:78:PHE:CD1	0.45	2.83	4	2
1:A:125:VAL:HG12	1:A:129:GLN:HB2	0.45	1.87	6	1
1:A:43:GLN:O	1:A:44:VAL:HG13	0.45	2.12	15	1
1:A:19:LEU:HD12	1:A:156:PHE:HZ	0.45	1.72	14	1
1:A:94:HIS:CE1	1:A:133:LEU:CD1	0.45	3.00	8	1
1:A:45:VAL:HG23	1:A:50:THR:N	0.45	2.27	13	1
1:A:46:ILE:HD13	1:A:157:TYR:HA	0.45	1.89	6	2
1:A:20:THR:CG2	1:A:40:TYR:CD2	0.45	3.00	4	2
1:A:67:MET:CE	1:A:71:TYR:CE2	0.45	3.00	7	1
1:A:84:ILE:HD12	1:A:123:ARG:CA	0.45	2.41	15	1
1:A:100:ILE:HD12	1:A:111:MET:HE1	0.44	1.89	1	2
1:A:20:THR:HG21	1:A:40:TYR:CE1	0.44	2.47	2	2
1:A:116:ASN:O	1:A:117:LYS:HB2	0.44	2.12	8	1
1:A:82:PHE:CE1	1:A:130:ALA:CB	0.44	2.99	12	1
1:A:101:LYS:CD	1:A:101:LYS:N	0.44	2.80	9	1
1:A:82:PHE:CE2	1:A:113:LEU:HD11	0.44	2.46	4	2
1:A:120:LEU:N	1:A:120:LEU:CD1	0.44	2.81	6	1
1:A:120:LEU:HD22	1:A:120:LEU:N	0.44	2.28	11	1
1:A:82:PHE:CE2	1:A:113:LEU:HD21	0.44	2.47	8	1
1:A:73:ARG:HG3	1:A:103:VAL:HG12	0.44	1.89	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:PHE:HZ	1:A:130:ALA:HB1	0.44	1.73	3	1
1:A:106:SER:O	1:A:107:ASP:CB	0.44	2.65	2	2
1:A:55:ILE:HD12	1:A:156:PHE:CD2	0.44	2.48	14	2
1:A:137:TYR:CD1	1:A:137:TYR:N	0.44	2.83	5	2
1:A:21:ILE:HD11	1:A:40:TYR:OH	0.44	2.12	2	1
1:A:133:LEU:CD2	1:A:137:TYR:CZ	0.44	3.01	13	2
1:A:100:ILE:HD13	1:A:111:MET:SD	0.44	2.53	4	1
1:A:77:GLY:C	1:A:159:LEU:HD21	0.43	2.34	5	1
1:A:56:LEU:HD11	3:A:202:KBF:C4	0.43	2.43	5	1
1:A:53:LEU:CD1	1:A:160:VAL:CG2	0.43	2.97	6	3
1:A:82:PHE:CE2	1:A:115:GLY:CA	0.43	3.01	4	1
1:A:15:GLY:HA2	2:A:201:GNP:H8	0.43	1.89	15	1
1:A:81:VAL:O	1:A:81:VAL:HG23	0.43	2.12	9	1
1:A:149:ARG:O	1:A:149:ARG:CD	0.43	2.67	15	1
1:A:116:ASN:O	1:A:117:LYS:CB	0.43	2.66	8	2
1:A:14:VAL:HG12	1:A:83:ALA:N	0.43	2.28	9	1
1:A:19:LEU:CD1	1:A:156:PHE:CZ	0.43	3.02	8	1
1:A:14:VAL:HG23	1:A:15:GLY:N	0.43	2.29	12	4
1:A:67:MET:O	1:A:71:TYR:CD1	0.43	2.72	14	2
1:A:159:LEU:C	1:A:159:LEU:HD13	0.43	2.34	9	2
1:A:103:VAL:HG23	1:A:104:LYS:N	0.43	2.29	8	2
1:A:120:LEU:CD1	2:A:201:GNP:N2	0.43	2.82	10	2
1:A:149:ARG:CG	1:A:149:ARG:O	0.43	2.66	13	2
1:A:116:ASN:OD1	1:A:117:LYS:N	0.43	2.51	15	1
1:A:21:ILE:N	1:A:21:ILE:CD1	0.43	2.82	13	2
1:A:83:ALA:HB1	1:A:117:LYS:NZ	0.43	2.27	8	1
1:A:142:ILE:HD12	1:A:142:ILE:N	0.43	2.29	12	1
1:A:56:LEU:HD23	1:A:71:TYR:CD1	0.43	2.49	4	1
1:A:72:MET:CE	1:A:99:GLN:CG	0.42	2.97	10	1
1:A:92:ASP:O	1:A:96:TYR:CD2	0.42	2.71	10	1
1:A:77:GLY:CA	1:A:159:LEU:HD11	0.42	2.44	6	2
1:A:137:TYR:N	1:A:137:TYR:CD2	0.42	2.87	4	1
1:A:16:LYS:HB3	1:A:81:VAL:HG21	0.42	1.90	4	1
1:A:153:GLU:O	1:A:157:TYR:CG	0.42	2.72	5	7
1:A:159:LEU:O	1:A:159:LEU:HD12	0.42	2.14	5	1
1:A:163:ILE:O	1:A:166:HIS:CG	0.42	2.72	5	1
1:A:24:ILE:HD13	1:A:42:LYS:HB2	0.42	1.91	4	2
1:A:101:LYS:HZ3	1:A:109:VAL:HG22	0.42	1.73	15	1
1:A:113:LEU:CB	1:A:134:ALA:HB2	0.42	2.43	15	1
1:A:83:ALA:HB1	1:A:117:LYS:HZ3	0.42	1.75	13	1
1:A:120:LEU:HD12	1:A:122:ALA:HB3	0.42	1.92	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:SER:HB2	1:A:109:VAL:HG13	0.42	1.92	3	1
1:A:85:ASN:ND2	1:A:122:ALA:HB3	0.42	2.29	3	1
1:A:120:LEU:O	1:A:121:ALA:CB	0.42	2.67	13	2
1:A:92:ASP:OD2	1:A:96:TYR:CD2	0.42	2.72	7	1
1:A:4:TYR:CD2	1:A:160:VAL:HG22	0.42	2.50	8	1
1:A:69:ASP:O	1:A:73:ARG:CG	0.42	2.67	6	1
1:A:159:LEU:HD13	1:A:159:LEU:C	0.42	2.35	7	2
1:A:81:VAL:CG1	1:A:114:VAL:CG1	0.42	2.98	15	1
1:A:140:PRO:CG	1:A:158:THR:CG2	0.42	2.97	15	1
1:A:23:LEU:HD13	1:A:153:GLU:HA	0.42	1.90	8	2
1:A:82:PHE:CE1	1:A:133:LEU:HD23	0.42	2.49	3	1
1:A:53:LEU:HD21	1:A:160:VAL:HG21	0.42	1.90	13	1
1:A:130:ALA:HB1	1:A:141:TYR:CZ	0.42	2.50	1	3
1:A:20:THR:CG2	1:A:21:ILE:N	0.42	2.83	11	1
1:A:23:LEU:HD13	1:A:156:PHE:CD2	0.42	2.49	4	1
1:A:153:GLU:O	1:A:157:TYR:CD1	0.42	2.73	12	2
1:A:133:LEU:HD11	1:A:137:TYR:CE2	0.42	2.49	2	1
1:A:22:GLN:HB2	1:A:152:VAL:HG21	0.42	1.92	3	1
1:A:58:THR:HG22	1:A:71:TYR:HD2	0.42	1.68	5	1
1:A:133:LEU:O	1:A:137:TYR:CD2	0.42	2.73	4	1
1:A:92:ASP:HB2	1:A:96:TYR:CE1	0.42	2.50	4	1
1:A:117:LYS:O	1:A:120:LEU:HD12	0.41	2.15	8	1
1:A:42:LYS:HE2	1:A:44:VAL:HG13	0.41	1.91	1	2
1:A:41:ARG:HH11	1:A:52:LEU:HD21	0.41	1.74	10	1
1:A:44:VAL:CG2	1:A:53:LEU:CD2	0.41	2.98	12	1
1:A:8:VAL:HG22	1:A:56:LEU:O	0.41	2.14	9	1
1:A:16:LYS:CG	1:A:81:VAL:CG2	0.41	2.98	11	1
1:A:18:ALA:O	1:A:22:GLN:CG	0.41	2.68	2	1
1:A:23:LEU:O	1:A:42:LYS:CE	0.41	2.68	14	1
1:A:116:ASN:O	1:A:117:LYS:HG2	0.41	2.15	6	1
1:A:113:LEU:CD2	1:A:133:LEU:HD22	0.41	2.32	12	1
1:A:10:GLY:HA3	1:A:14:VAL:HG21	0.41	1.91	7	1
1:A:23:LEU:HD21	1:A:42:LYS:HZ3	0.41	1.73	1	1
1:A:117:LYS:O	1:A:117:LYS:HG2	0.41	2.13	6	1
1:A:133:LEU:HD11	1:A:137:TYR:OH	0.41	2.15	9	1
1:A:109:VAL:CG2	1:A:111:MET:CE	0.41	2.98	10	2
1:A:84:ILE:O	1:A:124:THR:N	0.41	2.53	7	1
2:A:201:GNP:H5'1	2:A:201:GNP:O2B	0.41	2.16	10	1
1:A:92:ASP:OD1	1:A:96:TYR:CZ	0.41	2.74	13	2
1:A:6:LEU:HD23	1:A:6:LEU:N	0.41	2.30	13	1
1:A:153:GLU:O	1:A:157:TYR:CD2	0.41	2.73	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:MET:HB3	1:A:71:TYR:CE2	0.41	2.50	12	1
1:A:72:MET:HB2	1:A:103:VAL:HG11	0.41	1.92	2	1
1:A:26:ASN:O	1:A:27:HIS:CD2	0.41	2.74	9	1
1:A:10:GLY:O	1:A:96:TYR:CE1	0.41	2.74	11	2
1:A:4:TYR:CD1	1:A:160:VAL:HG22	0.41	2.50	11	1
1:A:10:GLY:N	1:A:16:LYS:CE	0.41	2.84	4	1
1:A:69:ASP:OD1	1:A:70:GLN:N	0.41	2.54	4	1
1:A:73:ARG:CG	1:A:103:VAL:HB	0.41	2.45	8	1
1:A:69:ASP:O	1:A:73:ARG:HG2	0.41	2.16	5	1
1:A:83:ALA:HB1	1:A:117:LYS:HD2	0.41	1.93	9	1
1:A:19:LEU:CD1	1:A:156:PHE:CE2	0.41	3.04	7	1
1:A:84:ILE:HD11	1:A:120:LEU:CD2	0.41	2.45	11	1
1:A:42:LYS:O	1:A:53:LEU:N	0.41	2.51	2	1
1:A:120:LEU:CD1	1:A:121:ALA:N	0.41	2.83	15	1
1:A:8:VAL:HG13	1:A:8:VAL:O	0.41	2.16	13	1
1:A:53:LEU:HD13	1:A:160:VAL:CG2	0.41	2.46	6	1
1:A:20:THR:HG21	1:A:40:TYR:CE2	0.41	2.51	14	1
1:A:113:LEU:HD12	1:A:141:TYR:CD1	0.41	2.51	6	1
1:A:113:LEU:C	1:A:113:LEU:HD13	0.41	2.37	4	1
1:A:5:LYS:NZ	1:A:74:THR:HG23	0.41	2.31	4	1
1:A:13:GLY:O	1:A:14:VAL:CG2	0.41	2.68	2	1
1:A:92:ASP:OD2	1:A:96:TYR:CZ	0.41	2.74	2	1
1:A:82:PHE:CE2	1:A:130:ALA:CB	0.41	3.04	2	1
2:A:201:GNP:H5'2	2:A:201:GNP:H8	0.41	1.92	3	1
1:A:23:LEU:CD2	1:A:55:ILE:CD1	0.41	2.99	3	1
1:A:19:LEU:CD1	1:A:116:ASN:ND2	0.41	2.84	1	1
1:A:159:LEU:CD1	1:A:163:ILE:CD1	0.41	2.99	10	1
1:A:100:ILE:CG2	1:A:111:MET:CE	0.41	2.99	12	1
1:A:82:PHE:HE2	1:A:141:TYR:HH	0.41	1.54	1	1
1:A:120:LEU:HD12	2:A:201:GNP:C2	0.40	2.45	13	1
1:A:43:GLN:NE2	1:A:44:VAL:N	0.40	2.69	12	1
1:A:95:GLN:O	1:A:98:GLU:CG	0.40	2.69	2	1
1:A:78:PHE:CE1	1:A:104:LYS:CE	0.40	3.04	5	1
1:A:91:GLU:O	1:A:94:HIS:CD2	0.40	2.74	4	1
1:A:160:VAL:CG1	1:A:161:ARG:N	0.40	2.83	1	1
1:A:20:THR:CG2	1:A:40:TYR:CE2	0.40	3.05	14	1
1:A:149:ARG:CD	1:A:149:ARG:O	0.40	2.70	5	1
1:A:21:ILE:CD1	1:A:40:TYR:CE2	0.40	3.05	15	1
1:A:109:VAL:CG2	1:A:111:MET:HE3	0.40	2.46	3	1
1:A:19:LEU:HD21	1:A:144:THR:OG1	0.40	2.17	3	1
1:A:104:LYS:CE	1:A:109:VAL:HG11	0.40	2.46	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ALA:CB	1:A:146:ALA:CB	0.40	3.00	13	1
1:A:84:ILE:CG1	1:A:117:LYS:O	0.40	2.70	12	1
1:A:123:ARG:NH2	1:A:127:SER:N	0.40	2.69	9	1
1:A:113:LEU:HD21	1:A:133:LEU:HD23	0.40	1.94	11	1
1:A:6:LEU:CD1	1:A:55:ILE:CD1	0.40	3.00	11	1
1:A:53:LEU:CD1	1:A:160:VAL:HG23	0.40	2.47	15	1
1:A:46:ILE:HD12	1:A:53:LEU:HD21	0.40	1.94	1	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	151/166 (91%)	140±2 (93±1%)	8±2 (5±1%)	3±1 (2±1%)	10	49
All	All	2265/2490 (91%)	2097 (93%)	118 (5%)	50 (2%)	10	49

All 13 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	29	VAL	14
1	A	120	LEU	8
1	A	121	ALA	5
1	A	65	SER	5
1	A	11	ALA	4
1	A	12	GLY	3
1	A	10	GLY	3
1	A	117	LYS	2
1	A	60	GLY	2
1	A	14	VAL	1
1	A	107	ASP	1
1	A	122	ALA	1
1	A	13	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	130/144 (90%)	101±6 (77±5%)	29±6 (23±5%)	3 29
All	All	1950/2160 (90%)	1509 (77%)	441 (23%)	3 29

All 83 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	101	LYS	15
1	A	95	GLN	14
1	A	41	ARG	14
1	A	160	VAL	13
1	A	67	MET	12
1	A	52	LEU	12
1	A	149	ARG	12
1	A	120	LEU	11
1	A	150	GLN	11
1	A	16	LYS	11
1	A	106	SER	10
1	A	99	GLN	10
1	A	131	GLN	9
1	A	79	LEU	9
1	A	94	HIS	9
1	A	25	GLN	9
1	A	19	LEU	9
1	A	102	ARG	9
1	A	154	ASP	8
1	A	6	LEU	8
1	A	123	ARG	8
1	A	104	LYS	8
1	A	92	ASP	8
1	A	17	SER	8
1	A	105	ASP	7
1	A	88	LYS	7
1	A	43	GLN	7
1	A	42	LYS	7
1	A	103	VAL	7

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Mol	Chain	Res	Type	Models (Total)
1	A	29	VAL	7
1	A	143	GLU	7
1	A	82	PHE	6
1	A	127	SER	6
1	A	47	ASP	6
1	A	27	HIS	6
1	A	135	ARG	5
1	A	145	SER	5
1	A	119	ASP	5
1	A	98	GLU	5
1	A	73	ARG	5
1	A	97	ARG	5
1	A	164	ARG	4
1	A	166	HIS	4
1	A	54	ASP	4
1	A	23	LEU	4
1	A	108	ASP	4
1	A	72	MET	4
1	A	159	LEU	4
1	A	84	ILE	3
1	A	87	THR	3
1	A	107	ASP	3
1	A	161	ARG	3
1	A	132	ASP	3
1	A	129	GLN	3
1	A	109	VAL	3
1	A	3	GLU	3
1	A	56	LEU	3
1	A	21	ILE	3
1	A	89	SER	2
1	A	39	SER	2
1	A	5	LYS	2
1	A	117	LYS	2
1	A	49	GLU	2
1	A	85	ASN	2
1	A	136	SER	2
1	A	51	CYS	2
1	A	9	VAL	1
1	A	57	ASP	1
1	A	76	GLU	1
1	A	113	LEU	1
1	A	128	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	153	GLU	1
1	A	14	VAL	1
1	A	133	LEU	1
1	A	69	ASP	1
1	A	26	ASN	1
1	A	68	ARG	1
1	A	70	GLN	1
1	A	53	LEU	1
1	A	20	THR	1
1	A	74	THR	1
1	A	126	GLU	1
1	A	125	VAL	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

LIGAND-GEOMETRY INFOmissingINFO

6.6 Other polymers

There are no such molecules in this entry.

6.7 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *kbfm123_starfile.tbl*

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	28
Number of shifts mapped to atoms	28
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

No chemical shift referencing corrections were calculated (not enough data).

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 0%, i.e. 9 atoms were assigned a chemical shift out of a possible 1879. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/756 (0%)	0/302 (0%)	0/304 (0%)	0/150 (0%)
Sidechain	9/998 (1%)	5/579 (1%)	4/364 (1%)	0/55 (0%)
Aromatic	0/125 (0%)	0/65 (0%)	0/54 (0%)	0/6 (0%)
Overall	9/1879 (0%)	5/946 (1%)	4/722 (1%)	0/211 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 9 atoms were assigned a chemical shift out of a possible 2048. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/824 (0%)	0/329 (0%)	0/332 (0%)	0/163 (0%)
Sidechain	9/1083 (1%)	5/629 (1%)	4/398 (1%)	0/56 (0%)
Aromatic	0/141 (0%)	0/73 (0%)	0/62 (0%)	0/6 (0%)
Overall	9/2048 (0%)	5/1031 (0%)	4/792 (1%)	0/225 (0%)

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	74	THR	CG2	55.06	27.15 – 15.95	29.9

7.1.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (kbfm123_starfile.tbl). RCI is only applicable to proteins.