



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:30 PM BST

PDB ID : 1F5X
Title : NMR STRUCTURE OF THE Y174 AUTOINHIBITED DBL HOMOLOGY DOMAIN
Authors : Aghazadeh, B.; Rosen, M.K.; Lowry, W.E.; Huang, X.Y.
Deposited on : 2000-06-18

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

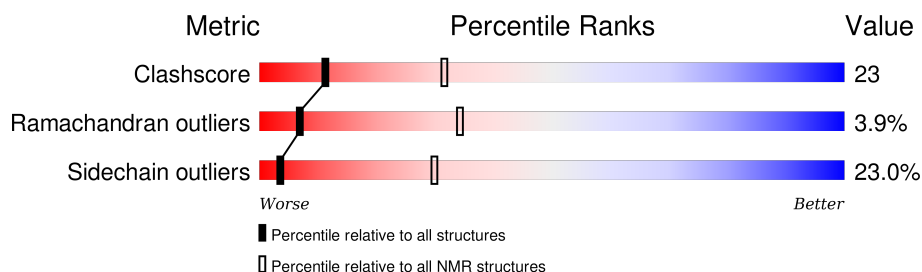
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	208	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 16 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:10, A:30-A:206 (185)	0.47	12

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 5 clusters and 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3440 atoms, of which 1730 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RHO-GEF VAV.

Mol	Chain	Residues	Atoms						Trace
1	A	208	Total	C	H	N	O	S	0
			3440	1076	1730	298	321	15	

There are 2 discrepancies between the modelled and reference sequences:

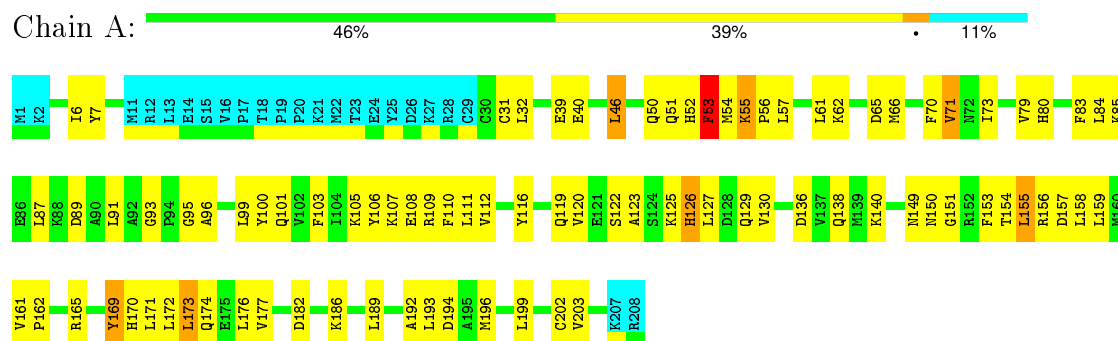
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	ALA	CONFLICT	UNP P27870
A	2	LYS	GLU	CONFLICT	UNP P27870

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: RHO-GEF VAV

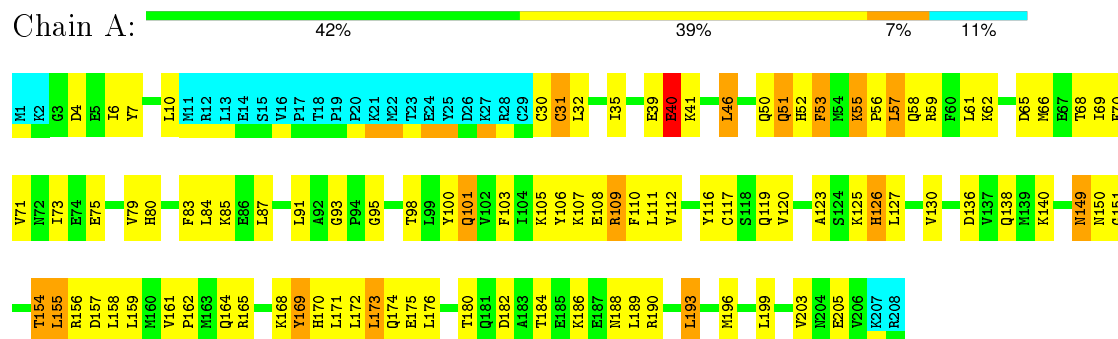


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: RHO-GEF VAV



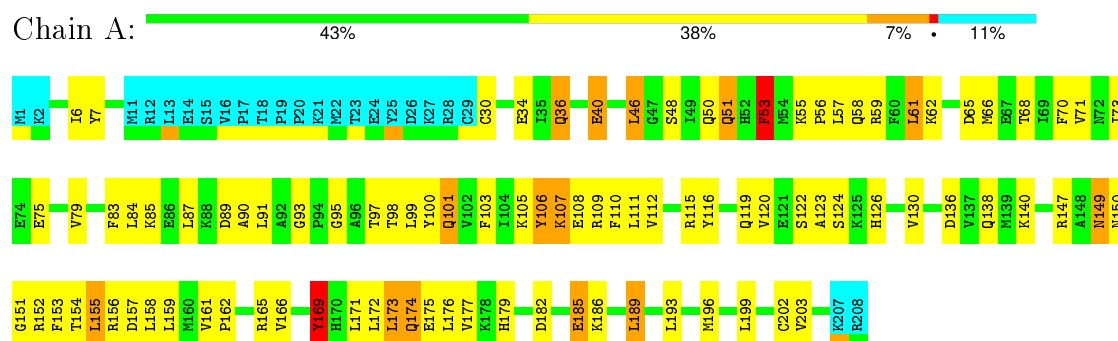
4.2.2 Score per residue for model 2

- Molecule 1: RHO-GEF VAV



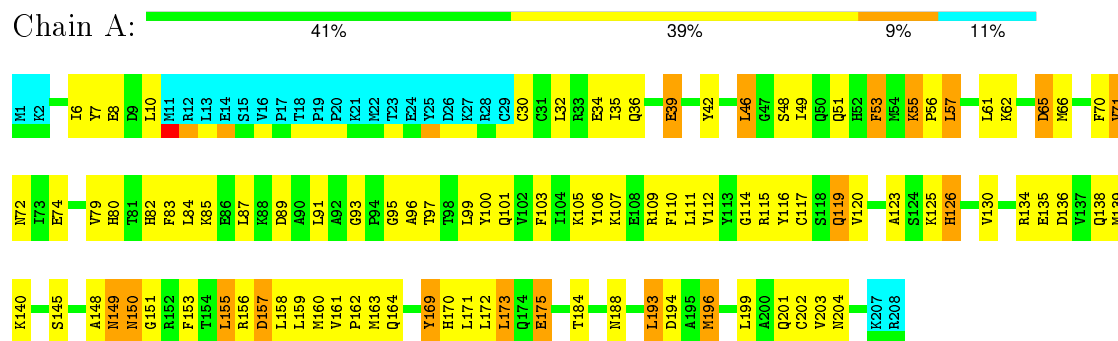
4.2.3 Score per residue for model 3

- Molecule 1: RHO-GEF VAV



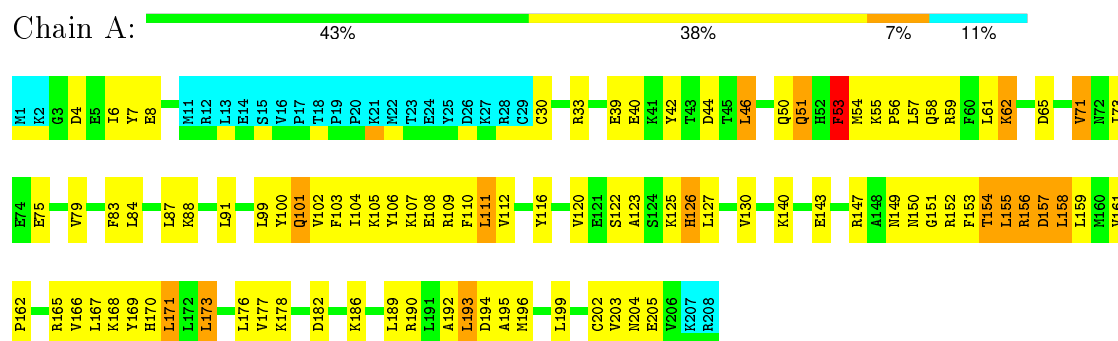
4.2.4 Score per residue for model 4

- Molecule 1: RHO-GEF VAV



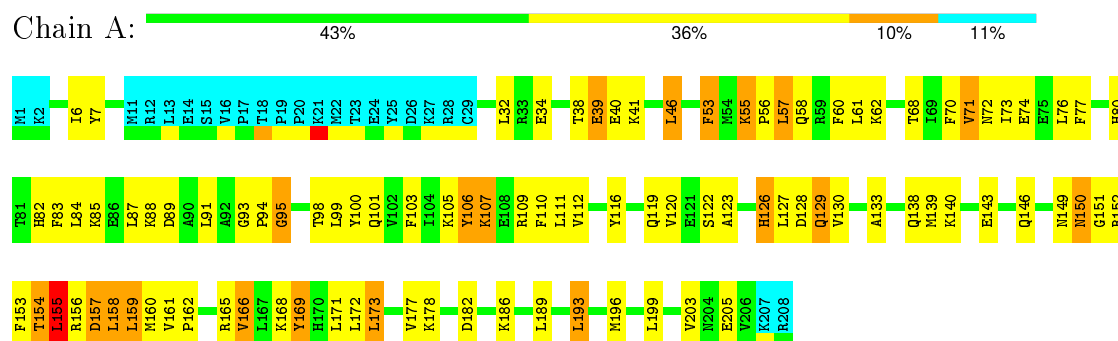
4.2.5 Score per residue for model 5

- Molecule 1: RHO-GEF VAV



4.2.8 Score per residue for model 8

- Molecule 1: RHO-GEF VAV



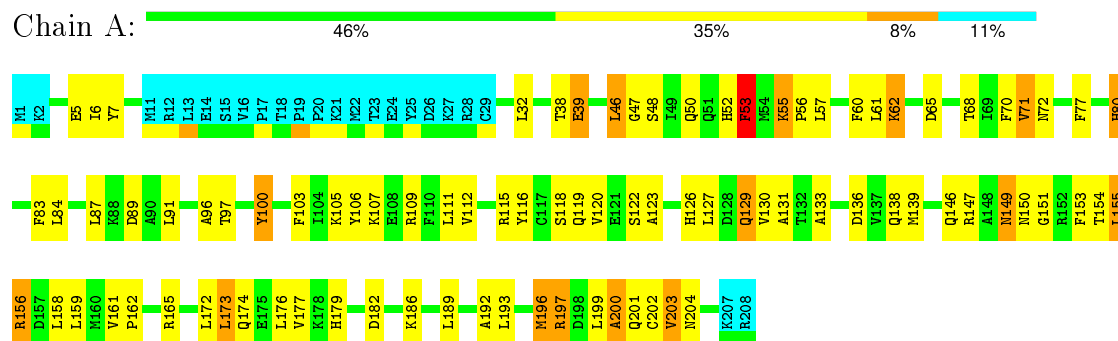
4.2.9 Score per residue for model 9

- Molecule 1: RHO-GEF VAV



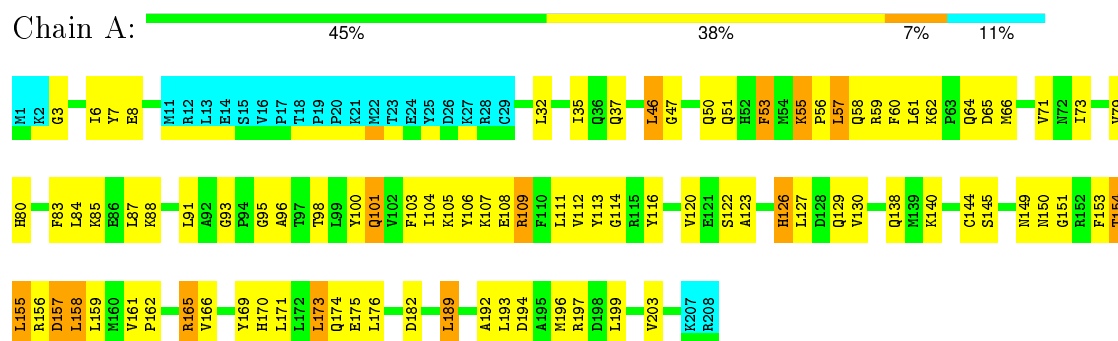
4.2.10 Score per residue for model 10

- Molecule 1: RHO-GEF VAV



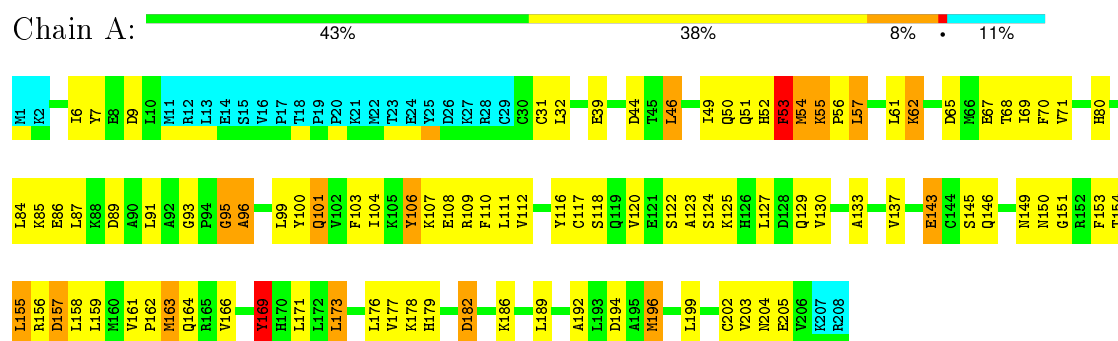
4.2.11 Score per residue for model 11

- Molecule 1: RHO-GEF VAV



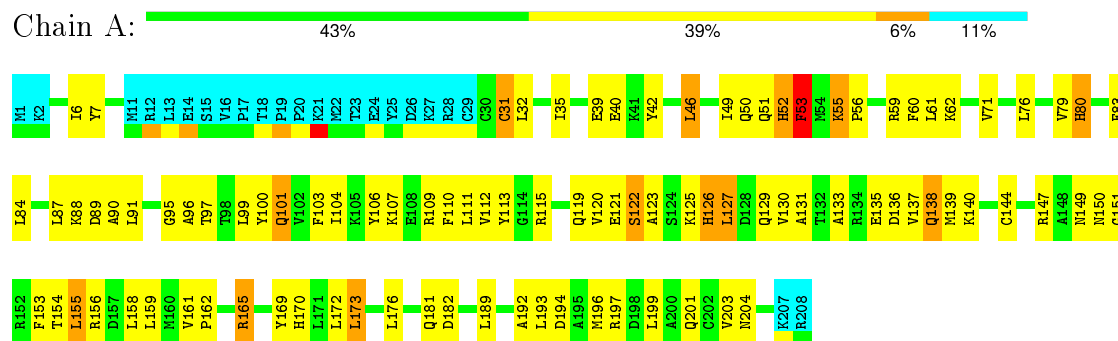
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: RHO-GEF VAV



4.2.13 Score per residue for model 13

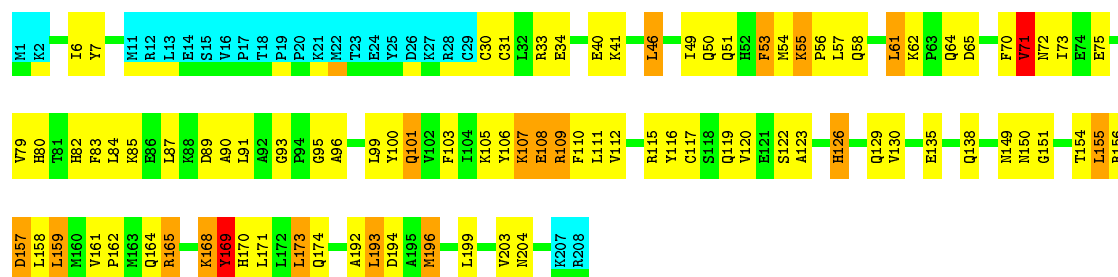
- Molecule 1: RHO-GEF VAV



4.2.14 Score per residue for model 14

- Molecule 1: RHO-GEF VAV

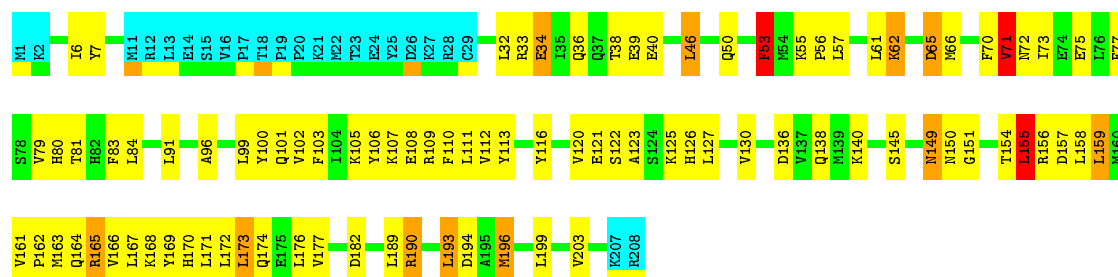
Chain A:  46% 34% 8% 11%



4.2.15 Score per residue for model 15

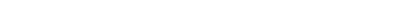
- Molecule 1: RHO-GEF VAV

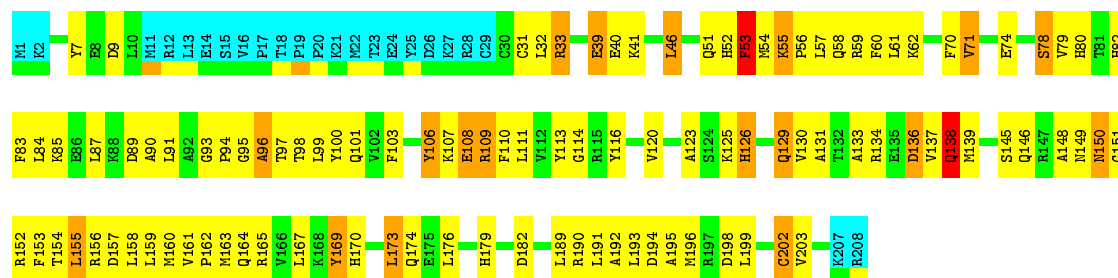
Chain A:  45% 38% 5% • 11%



4.2.16 Score per residue for model 16

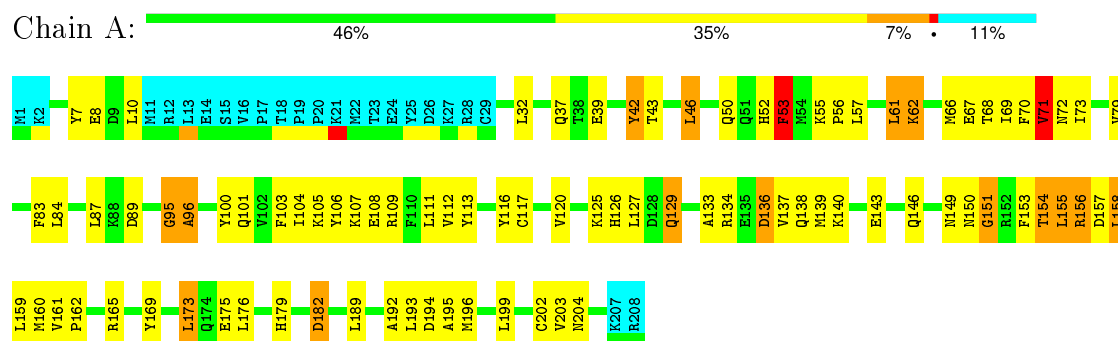
- Molecule 1: RHO-GEF VAV

Chain A:  38% 42% 9% • 11%



4.2.17 Score per residue for model 17

- Molecule 1: RHO-GEF VAV



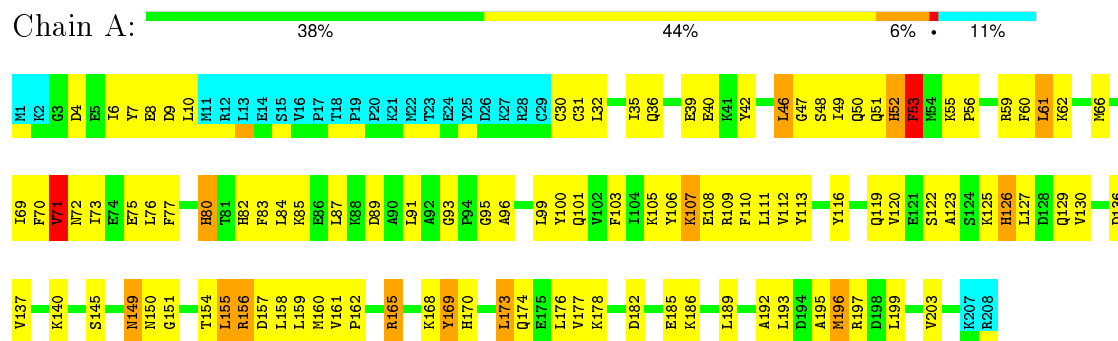
4.2.18 Score per residue for model 18

- Molecule 1: RHO-GEF VAV



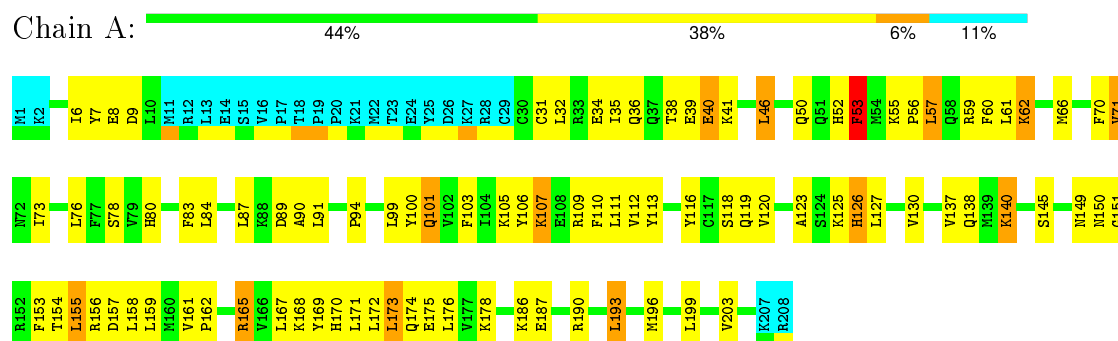
4.2.19 Score per residue for model 19

- Molecule 1: RHO-GEF VAV



4.2.20 Score per residue for model 20

● Molecule 1: RHO-GEF VAV



5 Refinement protocol and experimental data overview ⓘ

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CNS	structure solution	0.3
ARIA	refinement	1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1516	1520	1514	71±8
All	All	30320	30400	30280	1423

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:70:PHE:CE1	1:A:155:LEU:HD21	0.93	1.98	20	9
1:A:61:LEU:HD21	1:A:69:ILE:HD13	0.89	1.43	17	1
1:A:7:TYR:CD1	1:A:161:VAL:HG11	0.89	2.02	7	3
1:A:7:TYR:CE1	1:A:161:VAL:HG21	0.88	2.03	4	3
1:A:199:LEU:O	1:A:203:VAL:HG23	0.87	1.70	7	19
1:A:71:VAL:CG2	1:A:73:ILE:HD12	0.86	2.00	6	1
1:A:126:HIS:O	1:A:130:VAL:HG23	0.85	1.72	15	18
1:A:153:PHE:O	1:A:158:LEU:HD13	0.84	1.72	8	8
1:A:32:LEU:HD21	1:A:96:ALA:CB	0.84	2.03	19	4
1:A:7:TYR:CE2	1:A:161:VAL:HG11	0.84	2.08	17	1
1:A:61:LEU:HD13	1:A:62:LYS:N	0.83	1.87	8	14
1:A:155:LEU:O	1:A:159:LEU:HD12	0.83	1.74	2	20
1:A:157:ASP:O	1:A:161:VAL:HG23	0.82	1.74	9	16
1:A:7:TYR:CG	1:A:161:VAL:HG11	0.81	2.10	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:PHE:CZ	1:A:87:LEU:HD11	0.81	2.10	8	10
1:A:90:ALA:HB1	1:A:99:LEU:HD23	0.80	1.52	20	1
1:A:79:VAL:HG22	1:A:109:ARG:HB3	0.80	1.54	6	12
1:A:71:VAL:HG22	1:A:73:ILE:HD12	0.80	1.53	6	1
1:A:195:ALA:O	1:A:199:LEU:HD12	0.79	1.76	19	7
1:A:127:LEU:HD21	1:A:155:LEU:HD13	0.79	1.54	7	4
1:A:6:ILE:HG23	1:A:153:PHE:CG	0.78	2.13	6	7
1:A:173:LEU:HD23	1:A:196:MET:CE	0.77	2.10	14	3
1:A:32:LEU:HD11	1:A:91:LEU:HD21	0.77	1.56	10	6
1:A:131:ALA:HB1	1:A:138:GLN:HG2	0.76	1.56	13	4
1:A:83:PHE:CE2	1:A:87:LEU:HD11	0.76	2.16	16	11
1:A:39:GLU:HG2	1:A:84:LEU:HD21	0.75	1.57	20	1
1:A:91:LEU:HD11	1:A:99:LEU:HD21	0.75	1.57	6	3
1:A:177:VAL:HG22	1:A:189:LEU:HG	0.75	1.57	10	1
1:A:70:PHE:O	1:A:71:VAL:HG22	0.74	1.82	15	1
1:A:7:TYR:CZ	1:A:161:VAL:HG12	0.74	2.18	20	13
1:A:6:ILE:HD12	1:A:161:VAL:HG22	0.74	1.59	6	7
1:A:95:GLY:O	1:A:98:THR:HG22	0.73	1.84	1	3
1:A:185:GLU:O	1:A:189:LEU:HD23	0.73	1.84	19	1
1:A:73:ILE:HD11	1:A:159:LEU:HD23	0.73	1.59	9	8
1:A:131:ALA:HB1	1:A:138:GLN:CG	0.73	2.13	13	3
1:A:10:LEU:HD13	1:A:10:LEU:O	0.73	1.84	2	1
1:A:32:LEU:HD11	1:A:91:LEU:HD22	0.72	1.61	16	4
1:A:32:LEU:HD21	1:A:96:ALA:HB2	0.72	1.59	7	1
1:A:7:TYR:CZ	1:A:161:VAL:HG11	0.71	2.20	17	2
1:A:7:TYR:CD1	1:A:10:LEU:HD22	0.71	2.21	17	1
1:A:120:VAL:HG22	1:A:159:LEU:HB3	0.71	1.61	15	1
1:A:191:LEU:HD12	1:A:191:LEU:O	0.70	1.86	18	1
1:A:91:LEU:CD1	1:A:99:LEU:HD21	0.70	2.16	6	4
1:A:107:LYS:O	1:A:111:LEU:HD22	0.70	1.86	5	1
1:A:32:LEU:HD21	1:A:91:LEU:HD23	0.69	1.63	2	1
1:A:6:ILE:HG23	1:A:153:PHE:CD2	0.68	2.23	3	6
1:A:184:THR:HG22	1:A:188:ASN:OD1	0.68	1.88	4	1
1:A:7:TYR:CE1	1:A:161:VAL:HG11	0.68	2.23	7	6
1:A:166:VAL:HG13	1:A:167:LEU:HD12	0.68	1.66	5	1
1:A:80:HIS:O	1:A:84:LEU:HD12	0.68	1.87	8	10
1:A:32:LEU:HD11	1:A:91:LEU:CD2	0.67	2.19	20	6
1:A:108:GLU:HA	1:A:111:LEU:HD12	0.67	1.66	16	4
1:A:46:LEU:O	1:A:46:LEU:HD13	0.66	1.90	13	9
1:A:91:LEU:HD23	1:A:96:ALA:HB1	0.66	1.66	11	2
1:A:32:LEU:HD21	1:A:96:ALA:HB1	0.66	1.68	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:VAL:HG23	1:A:72:ASN:N	0.65	2.06	15	2
1:A:193:LEU:HD23	1:A:193:LEU:N	0.65	2.06	14	4
1:A:76:LEU:HD22	1:A:112:VAL:HG12	0.65	1.67	6	1
1:A:91:LEU:HD23	1:A:99:LEU:HD11	0.65	1.68	8	1
1:A:71:VAL:HG22	1:A:72:ASN:N	0.65	2.07	14	2
1:A:116:TYR:CD2	1:A:120:VAL:HG21	0.65	2.26	10	3
1:A:166:VAL:HG21	1:A:203:VAL:HG21	0.65	1.68	2	5
1:A:70:PHE:CE2	1:A:155:LEU:HD21	0.65	2.26	9	2
1:A:155:LEU:N	1:A:158:LEU:HD22	0.65	2.07	7	8
1:A:32:LEU:HD21	1:A:99:LEU:HD11	0.65	1.67	16	1
1:A:173:LEU:HD23	1:A:196:MET:HE2	0.65	1.69	14	1
1:A:100:TYR:HB3	1:A:192:ALA:HB2	0.64	1.70	10	1
1:A:177:VAL:HG22	1:A:189:LEU:HD23	0.64	1.70	5	1
1:A:96:ALA:O	1:A:99:LEU:HD13	0.64	1.93	18	2
1:A:90:ALA:CB	1:A:99:LEU:HD23	0.64	2.22	20	2
1:A:173:LEU:HD12	1:A:193:LEU:HD11	0.64	1.68	16	1
1:A:91:LEU:HD21	1:A:99:LEU:HD21	0.63	1.70	7	2
1:A:68:THR:O	1:A:123:ALA:HB2	0.63	1.94	8	4
1:A:49:ILE:HD11	1:A:158:LEU:HD13	0.62	1.70	13	5
1:A:103:PHE:CE2	1:A:173:LEU:HD23	0.62	2.29	16	1
1:A:46:LEU:HD13	1:A:46:LEU:O	0.62	1.95	4	9
1:A:127:LEU:HD21	1:A:155:LEU:HD23	0.62	1.71	15	2
1:A:91:LEU:CD2	1:A:99:LEU:HD11	0.61	2.26	8	2
1:A:57:LEU:HD22	1:A:70:PHE:CE2	0.61	2.30	2	1
1:A:69:ILE:HG23	1:A:127:LEU:HD11	0.61	1.71	1	3
1:A:189:LEU:O	1:A:193:LEU:HD12	0.61	1.96	13	5
1:A:131:ALA:HB1	1:A:138:GLN:HG3	0.61	1.73	10	2
1:A:73:ILE:HD11	1:A:159:LEU:CD2	0.61	2.26	9	2
1:A:7:TYR:CD2	1:A:161:VAL:HG11	0.61	2.30	17	2
1:A:71:VAL:HG11	1:A:119:GLN:HB3	0.60	1.74	2	1
1:A:177:VAL:HG22	1:A:189:LEU:HB3	0.60	1.73	9	7
1:A:32:LEU:CD2	1:A:35:ILE:HD12	0.60	2.27	20	1
1:A:158:LEU:O	1:A:161:VAL:HG23	0.60	1.97	13	5
1:A:103:PHE:CE2	1:A:173:LEU:HD21	0.60	2.32	4	13
1:A:39:GLU:HB3	1:A:84:LEU:HD11	0.59	1.72	6	10
1:A:126:HIS:C	1:A:130:VAL:HG23	0.59	2.15	13	3
1:A:83:PHE:CD1	1:A:106:TYR:CE2	0.59	2.90	16	1
1:A:35:ILE:HG12	1:A:172:LEU:HD23	0.59	1.72	13	1
1:A:106:TYR:CE2	1:A:110:PHE:CE1	0.59	2.90	16	1
1:A:123:ALA:O	1:A:127:LEU:HD12	0.59	1.97	10	9
1:A:49:ILE:CD1	1:A:158:LEU:HD13	0.59	2.26	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:HA	1:A:35:ILE:HD12	0.59	1.75	1	1
1:A:10:LEU:O	1:A:10:LEU:HD13	0.59	1.98	1	2
1:A:32:LEU:HB2	1:A:176:LEU:HD21	0.58	1.74	15	2
1:A:91:LEU:CD2	1:A:99:LEU:HD21	0.58	2.28	7	3
1:A:6:ILE:HG23	1:A:153:PHE:CD1	0.58	2.34	13	3
1:A:39:GLU:CG	1:A:84:LEU:HD21	0.57	2.29	20	1
1:A:106:TYR:CD1	1:A:110:PHE:CE1	0.57	2.92	12	1
1:A:166:VAL:HG23	1:A:199:LEU:HD12	0.57	1.75	3	1
1:A:110:PHE:CZ	1:A:169:TYR:CZ	0.57	2.93	2	4
1:A:42:TYR:CD2	1:A:80:HIS:CE1	0.57	2.92	19	1
1:A:84:LEU:HD23	1:A:84:LEU:N	0.57	2.13	18	2
1:A:7:TYR:CE2	1:A:42:TYR:CE2	0.57	2.92	7	3
1:A:79:VAL:HG22	1:A:109:ARG:CB	0.57	2.30	11	7
1:A:129:GLN:O	1:A:133:ALA:HB2	0.57	2.00	9	3
1:A:73:ILE:HD11	1:A:116:TYR:OH	0.57	2.00	5	3
1:A:109:ARG:HA	1:A:112:VAL:HG23	0.56	1.75	7	14
1:A:7:TYR:CE2	1:A:161:VAL:HG12	0.56	2.35	3	4
1:A:107:LYS:O	1:A:111:LEU:HD12	0.56	2.01	2	16
1:A:10:LEU:HD13	1:A:10:LEU:C	0.56	2.21	1	2
1:A:174:GLN:HG2	1:A:193:LEU:HD13	0.56	1.76	15	3
1:A:10:LEU:C	1:A:10:LEU:HD13	0.56	2.21	2	1
1:A:87:LEU:HA	1:A:90:ALA:HB3	0.56	1.76	2	6
1:A:103:PHE:CZ	1:A:173:LEU:HD23	0.56	2.36	16	1
1:A:35:ILE:HD11	1:A:176:LEU:HD11	0.55	1.78	7	2
1:A:177:VAL:HG22	1:A:189:LEU:CG	0.55	2.31	10	1
1:A:173:LEU:HA	1:A:176:LEU:HD13	0.55	1.78	3	15
1:A:83:PHE:CE1	1:A:106:TYR:CZ	0.55	2.94	16	1
1:A:191:LEU:O	1:A:191:LEU:HD12	0.55	2.02	16	1
1:A:155:LEU:C	1:A:159:LEU:HD12	0.55	2.21	17	20
1:A:70:PHE:HE1	1:A:155:LEU:HD21	0.55	1.61	7	2
1:A:199:LEU:C	1:A:203:VAL:HG23	0.55	2.21	13	18
1:A:70:PHE:C	1:A:71:VAL:HG13	0.55	2.21	15	1
1:A:103:PHE:CD2	1:A:192:ALA:HB1	0.55	2.37	16	1
1:A:96:ALA:HB1	1:A:99:LEU:HD12	0.55	1.77	4	1
1:A:61:LEU:HD11	1:A:65:ASP:HB2	0.55	1.78	2	1
1:A:173:LEU:O	1:A:173:LEU:HD13	0.55	2.02	16	1
1:A:96:ALA:HB1	1:A:99:LEU:CD1	0.54	2.32	4	2
1:A:40:GLU:HG2	1:A:84:LEU:HD13	0.54	1.79	18	4
1:A:103:PHE:CE2	1:A:173:LEU:CD2	0.54	2.90	5	19
1:A:70:PHE:C	1:A:71:VAL:HG23	0.54	2.23	20	3
1:A:7:TYR:CZ	1:A:161:VAL:CG1	0.54	2.91	8	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:HD21	1:A:96:ALA:HB3	0.54	1.79	11	1
1:A:91:LEU:HD21	1:A:99:LEU:HD11	0.54	1.80	9	1
1:A:114:GLY:N	1:A:203:VAL:HG13	0.54	2.18	9	2
1:A:40:GLU:HG2	1:A:84:LEU:HD22	0.54	1.79	9	4
1:A:66:MET:HE2	1:A:70:PHE:CD1	0.54	2.37	18	1
1:A:32:LEU:HD21	1:A:91:LEU:CD2	0.54	2.32	8	1
1:A:70:PHE:CD1	1:A:155:LEU:HD21	0.54	2.36	20	2
1:A:83:PHE:CE2	1:A:87:LEU:HD22	0.54	2.38	11	1
1:A:172:LEU:O	1:A:176:LEU:HD12	0.54	2.03	15	4
1:A:169:TYR:CE2	1:A:196:MET:HE2	0.54	2.38	20	3
1:A:116:TYR:O	1:A:120:VAL:HG23	0.53	2.03	2	14
1:A:61:LEU:HD11	1:A:65:ASP:HB3	0.53	1.79	12	3
1:A:136:ASP:OD1	1:A:137:VAL:HG23	0.53	2.03	18	2
1:A:7:TYR:CE1	1:A:161:VAL:CG1	0.53	2.92	11	10
1:A:60:PHE:CE1	1:A:137:VAL:CG2	0.53	2.91	7	2
1:A:71:VAL:HG11	1:A:120:VAL:HG23	0.53	1.80	6	1
1:A:173:LEU:O	1:A:173:LEU:HD12	0.53	2.03	1	9
1:A:107:LYS:C	1:A:111:LEU:HD12	0.53	2.24	17	5
1:A:32:LEU:HD11	1:A:99:LEU:CD1	0.53	2.33	13	1
1:A:100:TYR:CD1	1:A:101:GLN:N	0.53	2.77	9	3
1:A:49:ILE:CD1	1:A:158:LEU:HD23	0.53	2.33	9	1
1:A:87:LEU:HD22	1:A:99:LEU:CD2	0.53	2.34	6	3
1:A:104:ILE:HD11	1:A:192:ALA:HA	0.53	1.79	13	7
1:A:70:PHE:CZ	1:A:155:LEU:HD21	0.53	2.38	14	3
1:A:106:TYR:CG	1:A:110:PHE:CE1	0.52	2.97	12	1
1:A:66:MET:CE	1:A:70:PHE:CD1	0.52	2.92	18	1
1:A:116:TYR:OH	1:A:159:LEU:HD23	0.52	2.04	7	3
1:A:32:LEU:HD23	1:A:176:LEU:HD21	0.52	1.79	16	1
1:A:61:LEU:HD13	1:A:62:LYS:O	0.52	2.04	13	3
1:A:39:GLU:HB3	1:A:84:LEU:HD21	0.52	1.80	9	2
1:A:7:TYR:CE2	1:A:165:ARG:NH1	0.52	2.78	3	1
1:A:32:LEU:CD2	1:A:96:ALA:HB1	0.52	2.35	18	2
1:A:169:TYR:CE2	1:A:196:MET:CE	0.52	2.92	13	3
1:A:60:PHE:CD1	1:A:140:LYS:CD	0.52	2.93	8	2
1:A:177:VAL:HG11	1:A:190:ARG:HD3	0.52	1.80	2	1
1:A:91:LEU:HA	1:A:96:ALA:HB2	0.52	1.82	19	1
1:A:193:LEU:N	1:A:193:LEU:HD23	0.52	2.19	8	1
1:A:49:ILE:HD11	1:A:158:LEU:CG	0.52	2.35	9	1
1:A:70:PHE:CE1	1:A:155:LEU:CD2	0.52	2.92	4	1
1:A:76:LEU:HD23	1:A:116:TYR:CE1	0.52	2.40	18	2
1:A:80:HIS:CG	1:A:165:ARG:NH2	0.52	2.77	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:TYR:CE1	1:A:80:HIS:CE1	0.52	2.98	4	1
1:A:173:LEU:HD12	1:A:173:LEU:O	0.52	2.05	4	8
1:A:46:LEU:CD2	1:A:80:HIS:CE1	0.51	2.93	20	1
1:A:169:TYR:CD1	1:A:170:HIS:N	0.51	2.77	15	2
1:A:91:LEU:HG	1:A:99:LEU:HD21	0.51	1.82	16	2
1:A:42:TYR:CZ	1:A:161:VAL:HG11	0.51	2.40	19	1
1:A:36:GLN:HG3	1:A:84:LEU:HD23	0.51	1.82	19	1
1:A:87:LEU:HD22	1:A:99:LEU:HD22	0.51	1.83	19	2
1:A:65:ASP:O	1:A:68:THR:HG22	0.51	2.05	3	1
1:A:170:HIS:CD2	1:A:171:LEU:N	0.51	2.79	5	3
1:A:110:PHE:CE2	1:A:169:TYR:CE2	0.51	2.99	12	3
1:A:127:LEU:HD23	1:A:141:LEU:HD21	0.51	1.82	9	1
1:A:110:PHE:HB3	1:A:199:LEU:HD22	0.51	1.82	1	6
1:A:7:TYR:CD2	1:A:42:TYR:CE2	0.51	2.99	13	3
1:A:32:LEU:HD22	1:A:35:ILE:HD12	0.51	1.83	20	1
1:A:46:LEU:HD23	1:A:80:HIS:CD2	0.51	2.41	14	2
1:A:90:ALA:HB1	1:A:99:LEU:HG	0.51	1.80	14	1
1:A:83:PHE:CE2	1:A:87:LEU:CD1	0.50	2.92	4	4
1:A:39:GLU:CG	1:A:84:LEU:HD11	0.50	2.35	2	2
1:A:60:PHE:CZ	1:A:137:VAL:CG2	0.50	2.95	7	1
1:A:66:MET:HE1	1:A:70:PHE:CE2	0.50	2.42	6	1
1:A:83:PHE:CE2	1:A:87:LEU:HD21	0.50	2.41	13	1
1:A:69:ILE:CG1	1:A:127:LEU:HD11	0.50	2.36	17	1
1:A:171:LEU:HD12	1:A:174:GLN:OE1	0.50	2.06	15	1
1:A:170:HIS:CG	1:A:196:MET:CB	0.50	2.95	19	1
1:A:196:MET:HA	1:A:196:MET:HE3	0.50	1.83	15	1
1:A:100:TYR:CG	1:A:101:GLN:N	0.50	2.79	4	17
1:A:116:TYR:CE2	1:A:162:PRO:CG	0.50	2.95	6	1
1:A:87:LEU:HD22	1:A:99:LEU:HD23	0.50	1.83	6	1
1:A:180:THR:HG21	1:A:185:GLU:HB3	0.50	1.83	18	1
1:A:100:TYR:CB	1:A:192:ALA:HB2	0.50	2.37	10	1
1:A:42:TYR:CD2	1:A:80:HIS:NE2	0.49	2.79	19	1
1:A:70:PHE:O	1:A:71:VAL:CG2	0.49	2.60	15	1
1:A:71:VAL:CG2	1:A:72:ASN:N	0.49	2.76	15	1
1:A:100:TYR:CD1	1:A:100:TYR:N	0.49	2.79	10	1
1:A:170:HIS:CG	1:A:196:MET:HB3	0.49	2.41	19	1
1:A:49:ILE:HG22	1:A:70:PHE:CE2	0.49	2.43	14	2
1:A:71:VAL:HG12	1:A:119:GLN:HB3	0.49	1.83	6	1
1:A:70:PHE:O	1:A:71:VAL:HG13	0.49	2.07	15	1
1:A:60:PHE:HB3	1:A:137:VAL:HG22	0.49	1.83	19	3
1:A:161:VAL:N	1:A:162:PRO:CD	0.49	2.76	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:GLY:CA	1:A:203:VAL:HG13	0.48	2.37	11	3
1:A:55:LYS:N	1:A:56:PRO:CD	0.48	2.76	16	2
1:A:66:MET:CE	1:A:70:PHE:CD2	0.48	2.96	6	1
1:A:7:TYR:CE1	1:A:161:VAL:HG12	0.48	2.43	9	2
1:A:7:TYR:CD1	1:A:161:VAL:HG21	0.48	2.41	4	1
1:A:55:LYS:CB	1:A:56:PRO:CD	0.48	2.91	17	18
1:A:40:GLU:N	1:A:84:LEU:HD21	0.48	2.24	13	5
1:A:57:LEU:HD22	1:A:70:PHE:CZ	0.48	2.43	2	1
1:A:161:VAL:N	1:A:162:PRO:HD2	0.48	2.23	2	16
1:A:6:ILE:HG21	1:A:161:VAL:HG22	0.48	1.86	1	1
1:A:32:LEU:CD2	1:A:96:ALA:CB	0.48	2.92	17	2
1:A:174:GLN:HA	1:A:193:LEU:HD21	0.48	1.85	11	3
1:A:108:GLU:CA	1:A:111:LEU:HD12	0.48	2.37	14	4
1:A:103:PHE:CD1	1:A:196:MET:CE	0.48	2.97	4	2
1:A:52:HIS:O	1:A:53:PHE:CD2	0.48	2.67	13	9
1:A:6:ILE:HD11	1:A:157:ASP:OD1	0.48	2.08	11	1
1:A:116:TYR:CE2	1:A:120:VAL:HG21	0.48	2.43	3	4
1:A:61:LEU:HD13	1:A:62:LYS:H	0.48	1.64	8	1
1:A:193:LEU:CD2	1:A:193:LEU:N	0.48	2.77	5	2
1:A:32:LEU:CD1	1:A:91:LEU:CD2	0.48	2.92	2	1
1:A:191:LEU:C	1:A:191:LEU:HD12	0.48	2.27	18	1
1:A:40:GLU:CG	1:A:84:LEU:CD2	0.48	2.92	15	2
1:A:95:GLY:O	1:A:96:ALA:HB2	0.48	2.09	16	5
1:A:166:VAL:O	1:A:169:TYR:CE2	0.48	2.66	9	1
1:A:152:ARG:O	1:A:153:PHE:CD1	0.47	2.67	8	5
1:A:97:THR:O	1:A:100:TYR:CD2	0.47	2.67	10	1
1:A:110:PHE:O	1:A:113:TYR:CD2	0.47	2.67	16	2
1:A:106:TYR:OH	1:A:110:PHE:CZ	0.47	2.67	16	1
1:A:57:LEU:HD12	1:A:57:LEU:O	0.47	2.09	12	1
1:A:43:THR:OG1	1:A:84:LEU:HD13	0.47	2.10	17	1
1:A:32:LEU:C	1:A:32:LEU:HD13	0.47	2.30	12	3
1:A:110:PHE:CD2	1:A:196:MET:HE1	0.47	2.45	12	1
1:A:173:LEU:HD12	1:A:193:LEU:CD1	0.47	2.37	16	1
1:A:71:VAL:HG23	1:A:116:TYR:CE1	0.47	2.45	2	1
1:A:163:MET:CE	1:A:203:VAL:HG12	0.47	2.40	7	1
1:A:110:PHE:CZ	1:A:169:TYR:CE2	0.47	3.03	12	2
1:A:170:HIS:CE1	1:A:192:ALA:HB1	0.47	2.45	19	1
1:A:53:PHE:O	1:A:70:PHE:CZ	0.47	2.68	17	1
1:A:7:TYR:CE2	1:A:161:VAL:CG1	0.47	2.98	5	3
1:A:170:HIS:CE1	1:A:192:ALA:O	0.47	2.68	19	1
1:A:170:HIS:ND1	1:A:171:LEU:N	0.47	2.63	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:PHE:CE1	1:A:169:TYR:OH	0.47	2.68	14	2
1:A:77:PHE:CE1	1:A:81:THR:OG1	0.46	2.68	15	1
1:A:130:VAL:HG12	1:A:137:VAL:HG11	0.46	1.87	20	2
1:A:60:PHE:CE2	1:A:136:ASP:CB	0.46	2.98	16	1
1:A:39:GLU:OE2	1:A:83:PHE:CD2	0.46	2.68	4	1
1:A:90:ALA:O	1:A:98:THR:HG22	0.46	2.10	16	1
1:A:60:PHE:CE1	1:A:137:VAL:HG22	0.46	2.45	16	2
1:A:32:LEU:HD13	1:A:32:LEU:C	0.46	2.31	4	1
1:A:170:HIS:NE2	1:A:197:ARG:CG	0.46	2.78	13	1
1:A:76:LEU:HD22	1:A:112:VAL:CG1	0.46	2.40	6	1
1:A:170:HIS:CB	1:A:196:MET:CB	0.46	2.93	19	1
1:A:59:ARG:O	1:A:60:PHE:CD1	0.46	2.68	19	2
1:A:91:LEU:CD1	1:A:91:LEU:N	0.46	2.79	19	2
1:A:167:LEU:O	1:A:170:HIS:CD2	0.46	2.68	16	1
1:A:100:TYR:HA	1:A:192:ALA:HB2	0.46	1.86	16	1
1:A:36:GLN:OE1	1:A:91:LEU:HD12	0.46	2.10	3	1
1:A:76:LEU:CD2	1:A:116:TYR:CE2	0.46	2.98	20	1
1:A:117:CYS:SG	1:A:163:MET:HE2	0.46	2.51	6	1
1:A:196:MET:HG3	1:A:197:ARG:N	0.46	2.26	19	1
1:A:135:GLU:CG	1:A:136:ASP:N	0.46	2.79	4	1
1:A:149:ASN:O	1:A:151:GLY:N	0.45	2.49	16	20
1:A:116:TYR:CD2	1:A:120:VAL:CG2	0.45	2.98	10	1
1:A:80:HIS:CD2	1:A:165:ARG:CZ	0.45	2.99	13	1
1:A:87:LEU:CD2	1:A:102:VAL:HG11	0.45	2.42	5	2
1:A:168:LYS:HG2	1:A:172:LEU:HD13	0.45	1.88	6	1
1:A:107:LYS:O	1:A:111:LEU:CD1	0.45	2.65	19	16
1:A:60:PHE:CZ	1:A:140:LYS:HD2	0.45	2.47	2	2
1:A:106:TYR:CE1	1:A:109:ARG:CG	0.45	2.99	6	2
1:A:70:PHE:O	1:A:73:ILE:CG1	0.45	2.64	8	2
1:A:77:PHE:O	1:A:77:PHE:CD1	0.45	2.69	2	1
1:A:170:HIS:CD2	1:A:196:MET:HB2	0.45	2.47	19	1
1:A:91:LEU:HD12	1:A:99:LEU:HD21	0.45	1.85	5	1
1:A:109:ARG:O	1:A:112:VAL:N	0.45	2.50	6	19
1:A:127:LEU:HD23	1:A:127:LEU:N	0.45	2.27	13	1
1:A:32:LEU:HD21	1:A:99:LEU:CD1	0.45	2.41	16	1
1:A:177:VAL:HG11	1:A:190:ARG:HG2	0.45	1.89	15	1
1:A:83:PHE:CE2	1:A:87:LEU:CD2	0.45	3.00	13	2
1:A:71:VAL:HG13	1:A:116:TYR:CE1	0.45	2.47	19	1
1:A:7:TYR:CD1	1:A:161:VAL:CG1	0.45	2.92	4	3
1:A:196:MET:O	1:A:199:LEU:HD12	0.45	2.11	9	1
1:A:103:PHE:CD2	1:A:196:MET:SD	0.45	3.10	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:HIS:HB2	1:A:196:MET:CB	0.45	2.42	19	1
1:A:7:TYR:OH	1:A:42:TYR:CE1	0.45	2.67	17	1
1:A:32:LEU:CD2	1:A:96:ALA:HB3	0.45	2.42	11	1
1:A:173:LEU:HD11	1:A:189:LEU:HD11	0.45	1.87	10	1
1:A:47:GLY:CA	1:A:77:PHE:CE1	0.45	3.00	10	1
1:A:170:HIS:HE1	1:A:192:ALA:HB1	0.45	1.72	19	1
1:A:199:LEU:O	1:A:202:CYS:N	0.45	2.49	10	7
1:A:32:LEU:HD13	1:A:33:ARG:N	0.45	2.27	16	1
1:A:174:GLN:NE2	1:A:193:LEU:HD22	0.44	2.27	10	1
1:A:73:ILE:HD13	1:A:116:TYR:CE1	0.44	2.47	15	1
1:A:87:LEU:HG	1:A:99:LEU:HD21	0.44	1.89	12	1
1:A:6:ILE:HG21	1:A:161:VAL:CG2	0.44	2.43	18	2
1:A:96:ALA:HB1	1:A:99:LEU:HD11	0.44	1.89	14	1
1:A:32:LEU:CG	1:A:91:LEU:CD2	0.44	2.95	2	1
1:A:173:LEU:O	1:A:177:VAL:HG23	0.44	2.13	9	1
1:A:169:TYR:CD2	1:A:196:MET:HE1	0.44	2.47	8	1
1:A:193:LEU:H	1:A:193:LEU:HD12	0.44	1.73	19	2
1:A:55:LYS:N	1:A:56:PRO:HD2	0.44	2.27	16	1
1:A:73:ILE:HD13	1:A:116:TYR:HE1	0.44	1.72	15	1
1:A:173:LEU:O	1:A:173:LEU:CD1	0.44	2.65	16	8
1:A:199:LEU:O	1:A:201:GLN:N	0.44	2.51	10	1
1:A:60:PHE:CE2	1:A:136:ASP:HB3	0.44	2.47	16	1
1:A:46:LEU:HD12	1:A:77:PHE:HA	0.44	1.88	2	5
1:A:67:GLU:CG	1:A:68:THR:N	0.44	2.81	7	1
1:A:174:GLN:HB2	1:A:193:LEU:HD21	0.44	1.89	19	1
1:A:154:THR:O	1:A:156:ARG:N	0.44	2.51	1	19
1:A:173:LEU:CD1	1:A:173:LEU:O	0.44	2.66	4	9
1:A:57:LEU:HD22	1:A:140:LYS:HE2	0.44	1.90	8	1
1:A:39:GLU:CB	1:A:84:LEU:HD21	0.44	2.41	9	1
1:A:116:TYR:O	1:A:120:VAL:CG2	0.44	2.66	18	13
1:A:32:LEU:HD12	1:A:35:ILE:HD12	0.44	1.90	7	2
1:A:51:GLN:CG	1:A:52:HIS:N	0.44	2.81	1	1
1:A:71:VAL:HG21	1:A:116:TYR:CE1	0.43	2.47	15	2
1:A:155:LEU:O	1:A:158:LEU:N	0.43	2.51	3	16
1:A:6:ILE:HG23	1:A:153:PHE:CE2	0.43	2.48	8	1
1:A:46:LEU:CD1	1:A:46:LEU:O	0.43	2.66	17	5
1:A:158:LEU:O	1:A:162:PRO:CD	0.43	2.67	12	4
1:A:83:PHE:CE1	1:A:87:LEU:HD21	0.43	2.48	16	2
1:A:176:LEU:O	1:A:180:THR:N	0.43	2.50	1	1
1:A:61:LEU:CD1	1:A:62:LYS:O	0.43	2.67	15	2
1:A:60:PHE:CE1	1:A:140:LYS:HD3	0.43	2.48	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:193:LEU:O	1:A:196:MET:N	0.43	2.52	10	1
1:A:119:GLN:O	1:A:123:ALA:N	0.43	2.51	7	5
1:A:113:TYR:OH	1:A:165:ARG:NE	0.43	2.52	13	4
1:A:54:MET:HG3	1:A:70:PHE:CD2	0.43	2.49	2	1
1:A:193:LEU:O	1:A:197:ARG:CG	0.43	2.66	10	1
1:A:106:TYR:CE1	1:A:109:ARG:HG3	0.43	2.49	6	1
1:A:169:TYR:C	1:A:169:TYR:CD1	0.43	2.92	15	2
1:A:47:GLY:O	1:A:50:GLN:CG	0.43	2.67	11	1
1:A:50:GLN:O	1:A:54:MET:CB	0.43	2.67	12	3
1:A:110:PHE:HB3	1:A:199:LEU:CD1	0.43	2.43	3	2
1:A:60:PHE:CE1	1:A:140:LYS:CD	0.43	3.01	2	1
1:A:47:GLY:HA3	1:A:77:PHE:CE1	0.43	2.49	10	2
1:A:60:PHE:CZ	1:A:140:LYS:CD	0.43	3.02	18	1
1:A:30:CYS:O	1:A:34:GLU:CB	0.43	2.67	4	1
1:A:110:PHE:CB	1:A:199:LEU:HD22	0.43	2.44	5	1
1:A:6:ILE:HG21	1:A:161:VAL:HG21	0.43	1.89	15	1
1:A:176:LEU:N	1:A:176:LEU:HD12	0.43	2.29	11	1
1:A:200:ALA:O	1:A:204:ASN:CB	0.43	2.66	10	1
1:A:121:GLU:O	1:A:125:LYS:CD	0.43	2.67	13	1
1:A:170:HIS:HB2	1:A:196:MET:CG	0.43	2.43	19	1
1:A:162:PRO:O	1:A:165:ARG:N	0.43	2.52	13	2
1:A:60:PHE:CD1	1:A:60:PHE:C	0.43	2.91	7	1
1:A:192:ALA:O	1:A:196:MET:CG	0.43	2.67	5	4
1:A:42:TYR:CD1	1:A:42:TYR:O	0.43	2.72	9	1
1:A:73:ILE:CD1	1:A:116:TYR:OH	0.43	2.67	2	4
1:A:57:LEU:O	1:A:57:LEU:CD1	0.43	2.67	1	2
1:A:120:VAL:O	1:A:123:ALA:N	0.43	2.52	7	15
1:A:68:THR:O	1:A:123:ALA:CB	0.43	2.67	7	6
1:A:3:GLY:HA2	1:A:6:ILE:HD12	0.43	1.91	11	1
1:A:199:LEU:HD23	1:A:203:VAL:HG21	0.43	1.91	10	1
1:A:153:PHE:O	1:A:158:LEU:N	0.43	2.51	6	1
1:A:168:LYS:CG	1:A:172:LEU:HD13	0.43	2.44	6	1
1:A:152:ARG:O	1:A:153:PHE:CG	0.43	2.72	16	1
1:A:146:GLN:CG	1:A:150:ASN:OD1	0.43	2.67	16	1
1:A:78:SER:O	1:A:82:HIS:N	0.43	2.52	16	1
1:A:145:SER:O	1:A:149:ASN:N	0.42	2.52	20	7
1:A:49:ILE:HD11	1:A:158:LEU:HD23	0.42	1.90	9	1
1:A:70:PHE:CE2	1:A:155:LEU:CD2	0.42	3.00	9	1
1:A:123:ALA:O	1:A:126:HIS:N	0.42	2.52	5	4
1:A:129:GLN:O	1:A:133:ALA:CB	0.42	2.67	9	3
1:A:107:LYS:C	1:A:111:LEU:HD22	0.42	2.32	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:LYS:O	1:A:66:MET:N	0.42	2.52	17	1
1:A:40:GLU:HG2	1:A:84:LEU:CD2	0.42	2.44	6	3
1:A:7:TYR:CE2	1:A:42:TYR:CZ	0.42	3.07	7	2
1:A:6:ILE:O	1:A:10:LEU:CB	0.42	2.67	9	3
1:A:70:PHE:O	1:A:71:VAL:HB	0.42	2.15	4	1
1:A:61:LEU:C	1:A:61:LEU:HD13	0.42	2.34	4	1
1:A:121:GLU:O	1:A:125:LYS:CB	0.42	2.68	15	1
1:A:57:LEU:CD1	1:A:57:LEU:O	0.42	2.67	12	3
1:A:163:MET:O	1:A:166:VAL:HG12	0.42	2.13	12	1
1:A:143:GLU:O	1:A:146:GLN:CG	0.42	2.68	12	1
1:A:71:VAL:HG13	1:A:72:ASN:H	0.42	1.75	10	2
1:A:87:LEU:HD23	1:A:102:VAL:HG11	0.42	1.89	6	1
1:A:100:TYR:CZ	1:A:101:GLN:HG3	0.42	2.49	17	1
1:A:129:GLN:O	1:A:133:ALA:N	0.42	2.52	12	6
1:A:6:ILE:CD1	1:A:157:ASP:OD2	0.42	2.67	2	1
1:A:76:LEU:CD1	1:A:76:LEU:O	0.42	2.67	6	1
1:A:70:PHE:O	1:A:71:VAL:CB	0.42	2.68	9	4
1:A:154:THR:O	1:A:155:LEU:C	0.42	2.58	5	12
1:A:65:ASP:OD1	1:A:69:ILE:HD11	0.42	2.14	12	1
1:A:76:LEU:CD2	1:A:116:TYR:CE1	0.42	3.03	8	1
1:A:60:PHE:CD1	1:A:137:VAL:HG22	0.42	2.49	16	1
1:A:34:GLU:O	1:A:38:THR:CB	0.42	2.68	15	3
1:A:173:LEU:HD23	1:A:196:MET:HE1	0.42	1.91	20	1
1:A:6:ILE:CD1	1:A:157:ASP:OD1	0.42	2.68	7	2
1:A:199:LEU:O	1:A:203:VAL:N	0.42	2.52	10	1
1:A:32:LEU:O	1:A:35:ILE:N	0.42	2.53	4	1
1:A:169:TYR:CG	1:A:170:HIS:N	0.42	2.87	11	1
1:A:76:LEU:CD2	1:A:116:TYR:CD1	0.42	3.03	8	1
1:A:143:GLU:O	1:A:146:GLN:CB	0.42	2.68	8	2
1:A:51:GLN:O	1:A:53:PHE:N	0.42	2.52	5	4
1:A:110:PHE:CE2	1:A:196:MET:CE	0.42	3.02	1	1
1:A:35:ILE:O	1:A:39:GLU:CG	0.42	2.68	19	1
1:A:113:TYR:CE1	1:A:162:PRO:HB2	0.42	2.49	17	1
1:A:40:GLU:HA	1:A:84:LEU:HD11	0.42	1.90	18	1
1:A:84:LEU:N	1:A:84:LEU:CD2	0.42	2.83	18	1
1:A:102:VAL:HG12	1:A:102:VAL:O	0.42	2.15	15	1
1:A:157:ASP:O	1:A:161:VAL:CG2	0.42	2.67	6	3
1:A:103:PHE:O	1:A:196:MET:CE	0.42	2.68	7	1
1:A:165:ARG:O	1:A:168:LYS:N	0.42	2.52	14	1
1:A:83:PHE:CZ	1:A:87:LEU:HD21	0.42	2.49	16	1
1:A:90:ALA:O	1:A:98:THR:CG2	0.42	2.68	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:TYR:CE2	1:A:120:VAL:CG2	0.42	3.02	19	1
1:A:168:LYS:O	1:A:171:LEU:N	0.42	2.53	15	1
1:A:167:LEU:HA	1:A:170:HIS:CD2	0.42	2.50	15	2
1:A:153:PHE:O	1:A:158:LEU:CD2	0.42	2.68	16	1
1:A:110:PHE:CE1	1:A:169:TYR:CE2	0.42	3.08	18	1
1:A:53:PHE:CZ	1:A:145:SER:CB	0.42	3.03	15	1
1:A:57:LEU:HG	1:A:70:PHE:CZ	0.42	2.50	8	1
1:A:39:GLU:HG3	1:A:84:LEU:HD11	0.42	1.91	2	1
1:A:113:TYR:OH	1:A:165:ARG:CG	0.42	2.68	13	1
1:A:122:SER:O	1:A:126:HIS:N	0.42	2.52	13	1
1:A:83:PHE:CE2	1:A:169:TYR:OH	0.42	2.71	16	1
1:A:67:GLU:O	1:A:71:VAL:N	0.42	2.53	17	1
1:A:136:ASP:OD1	1:A:137:VAL:N	0.42	2.53	18	1
1:A:60:PHE:CE1	1:A:140:LYS:HG3	0.41	2.50	11	1
1:A:93:GLY:O	1:A:95:GLY:N	0.41	2.52	16	4
1:A:189:LEU:O	1:A:193:LEU:CD1	0.41	2.68	13	3
1:A:80:HIS:O	1:A:84:LEU:CD1	0.41	2.67	2	1
1:A:140:LYS:O	1:A:144:CYS:N	0.41	2.53	2	1
1:A:87:LEU:HB3	1:A:91:LEU:HD12	0.41	1.92	13	1
1:A:145:SER:O	1:A:148:ALA:N	0.41	2.53	4	2
1:A:36:GLN:O	1:A:40:GLU:N	0.41	2.53	3	1
1:A:76:LEU:HD11	1:A:165:ARG:NH2	0.41	2.28	19	1
1:A:7:TYR:OH	1:A:42:TYR:CE2	0.41	2.67	5	1
1:A:39:GLU:OE2	1:A:83:PHE:CE2	0.41	2.72	5	1
1:A:173:LEU:HG	1:A:193:LEU:CD2	0.41	2.45	5	1
1:A:69:ILE:CG1	1:A:127:LEU:CD1	0.41	2.98	17	1
1:A:150:ASN:N	1:A:150:ASN:OD1	0.41	2.53	8	1
1:A:177:VAL:CG2	1:A:193:LEU:HD11	0.41	2.45	10	1
1:A:107:LYS:O	1:A:111:LEU:CG	0.41	2.69	13	1
1:A:110:PHE:CD2	1:A:196:MET:HE2	0.41	2.50	1	1
1:A:173:LEU:HD11	1:A:189:LEU:HG	0.41	1.93	1	1
1:A:96:ALA:O	1:A:99:LEU:CD1	0.41	2.67	18	1
1:A:46:LEU:HD21	1:A:80:HIS:CE1	0.41	2.51	12	1
1:A:106:TYR:HB3	1:A:110:PHE:CZ	0.41	2.51	3	2
1:A:47:GLY:CA	1:A:77:PHE:CD1	0.41	3.03	9	1
1:A:173:LEU:CD1	1:A:189:LEU:HD11	0.41	2.45	10	1
1:A:116:TYR:CD1	1:A:120:VAL:CG2	0.41	3.03	6	1
1:A:103:PHE:CD1	1:A:196:MET:HE1	0.41	2.51	4	1
1:A:123:ALA:O	1:A:127:LEU:CD1	0.41	2.68	15	1
1:A:39:GLU:OE1	1:A:39:GLU:N	0.41	2.53	9	2
1:A:113:TYR:CD2	1:A:166:VAL:HB	0.41	2.51	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:VAL:HG22	1:A:189:LEU:CB	0.41	2.46	12	1
1:A:76:LEU:HD23	1:A:116:TYR:CZ	0.41	2.50	9	1
1:A:96:ALA:CA	1:A:99:LEU:CD1	0.41	2.98	14	1
1:A:173:LEU:HD12	1:A:177:VAL:HG23	0.41	1.93	2	1
1:A:103:PHE:CD1	1:A:196:MET:SD	0.41	3.13	1	1
1:A:71:VAL:HG12	1:A:72:ASN:N	0.41	2.31	7	1
1:A:114:GLY:CA	1:A:206:VAL:HG21	0.41	2.46	7	1
1:A:130:VAL:CG1	1:A:137:VAL:HG11	0.41	2.46	12	1
1:A:103:PHE:CG	1:A:196:MET:HE2	0.41	2.51	10	1
1:A:111:LEU:HG	1:A:199:LEU:HD21	0.41	1.91	13	2
1:A:158:LEU:O	1:A:162:PRO:HD2	0.41	2.16	3	2
1:A:79:VAL:CG2	1:A:109:ARG:HB3	0.41	2.46	16	1
1:A:106:TYR:HB3	1:A:110:PHE:CE1	0.41	2.51	6	1
1:A:172:LEU:O	1:A:175:GLU:N	0.41	2.53	4	2
1:A:57:LEU:HG	1:A:70:PHE:CE2	0.40	2.51	8	1
1:A:184:THR:O	1:A:188:ASN:N	0.40	2.53	1	1
1:A:46:LEU:HG	1:A:80:HIS:CD2	0.40	2.51	4	1
1:A:39:GLU:CD	1:A:83:PHE:CD2	0.40	2.95	20	1
1:A:39:GLU:OE1	1:A:83:PHE:CE2	0.40	2.74	20	1
1:A:7:TYR:CE2	1:A:42:TYR:CD2	0.40	3.09	7	1
1:A:50:GLN:O	1:A:54:MET:CG	0.40	2.69	9	1
1:A:148:ALA:O	1:A:149:ASN:ND2	0.40	2.54	2	1
1:A:199:LEU:HD23	1:A:203:VAL:CG2	0.40	2.45	10	1
1:A:155:LEU:H	1:A:155:LEU:HD13	0.40	1.75	8	2
1:A:177:VAL:HG11	1:A:190:ARG:CD	0.40	2.46	6	1
1:A:161:VAL:HB	1:A:162:PRO:CD	0.40	2.46	1	2
1:A:71:VAL:HG22	1:A:72:ASN:CG	0.40	2.37	19	1
1:A:170:HIS:CG	1:A:171:LEU:N	0.40	2.88	4	1
1:A:113:TYR:OH	1:A:165:ARG:CZ	0.40	2.70	13	1
1:A:71:VAL:HG13	1:A:116:TYR:HE1	0.40	1.76	19	1
1:A:155:LEU:HB3	1:A:159:LEU:HD11	0.40	1.94	17	1
1:A:172:LEU:O	1:A:175:GLU:CG	0.40	2.69	4	1
1:A:196:MET:N	1:A:196:MET:SD	0.40	2.95	15	1
1:A:65:ASP:OD1	1:A:65:ASP:N	0.40	2.55	15	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	185/208 (89%)	147±5 (80±3%)	31±4 (16±2%)	7±2 (4±1%)	7	34
All	All	3700/4160 (89%)	2946 (80%)	610 (16%)	144 (4%)	7	34

All 23 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	150	ASN	20
1	A	155	LEU	20
1	A	71	VAL	20
1	A	53	PHE	20
1	A	169	TYR	9
1	A	154	THR	9
1	A	95	GLY	9
1	A	93	GLY	7
1	A	96	ALA	7
1	A	182	ASP	4
1	A	94	PRO	3
1	A	3	GLY	2
1	A	165	ARG	2
1	A	52	HIS	2
1	A	40	GLU	2
1	A	166	VAL	1
1	A	185	GLU	1
1	A	138	GLN	1
1	A	200	ALA	1
1	A	143	GLU	1
1	A	31	CYS	1
1	A	74	GLU	1
1	A	151	GLY	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	168/191 (88%)	129±4 (77±2%)	39±4 (23±2%)	3	30
All	All	3360/3820 (88%)	2587 (77%)	773 (23%)	3	30

All 122 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	46	LEU	20
1	A	53	PHE	20
1	A	173	LEU	20
1	A	106	TYR	20
1	A	57	LEU	18
1	A	182	ASP	16
1	A	105	LYS	15
1	A	89	ASP	15
1	A	138	GLN	15
1	A	165	ARG	14
1	A	140	LYS	14
1	A	55	LYS	14
1	A	126	HIS	13
1	A	122	SER	13
1	A	85	LYS	12
1	A	125	LYS	12
1	A	50	GLN	12
1	A	194	ASP	12
1	A	186	LYS	11
1	A	101	GLN	11
1	A	169	TYR	11
1	A	51	GLN	11
1	A	108	GLU	11
1	A	62	LYS	11
1	A	157	ASP	11
1	A	136	ASP	10
1	A	129	GLN	10
1	A	196	MET	10
1	A	58	GLN	9
1	A	66	MET	9
1	A	139	MET	9
1	A	158	LEU	8
1	A	115	ARG	8
1	A	119	GLN	8
1	A	61	LEU	8
1	A	39	GLU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	75	GLU	8
1	A	31	CYS	8
1	A	204	ASN	8
1	A	168	LYS	7
1	A	109	ARG	7
1	A	59	ARG	7
1	A	178	LYS	7
1	A	65	ASP	7
1	A	175	GLU	7
1	A	149	ASN	7
1	A	107	LYS	7
1	A	156	ARG	7
1	A	117	CYS	7
1	A	193	LEU	7
1	A	171	LEU	6
1	A	97	THR	6
1	A	54	MET	6
1	A	41	LYS	6
1	A	71	VAL	6
1	A	164	GLN	6
1	A	36	GLN	6
1	A	8	GLU	6
1	A	179	HIS	6
1	A	30	CYS	5
1	A	118	SER	5
1	A	202	CYS	5
1	A	9	ASP	5
1	A	205	GLU	5
1	A	34	GLU	5
1	A	159	LEU	5
1	A	190	ARG	5
1	A	144	CYS	5
1	A	88	LYS	5
1	A	160	MET	5
1	A	155	LEU	4
1	A	48	SER	4
1	A	33	ARG	4
1	A	4	ASP	4
1	A	80	HIS	4
1	A	78	SER	4
1	A	143	GLU	4
1	A	82	HIS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	44	ASP	4
1	A	40	GLU	4
1	A	147	ARG	4
1	A	163	MET	4
1	A	134	ARG	4
1	A	187	GLU	3
1	A	124	SER	3
1	A	201	GLN	3
1	A	172	LEU	3
1	A	174	GLN	3
1	A	64	GLN	3
1	A	37	GLN	3
1	A	76	LEU	3
1	A	135	GLU	2
1	A	5	GLU	2
1	A	52	HIS	2
1	A	74	GLU	2
1	A	146	GLN	2
1	A	197	ARG	2
1	A	189	LEU	2
1	A	191	LEU	1
1	A	121	GLU	1
1	A	67	GLU	1
1	A	128	ASP	1
1	A	181	GLN	1
1	A	198	ASP	1
1	A	111	LEU	1
1	A	150	ASN	1
1	A	152	ARG	1
1	A	100	TYR	1
1	A	91	LEU	1
1	A	42	TYR	1
1	A	188	ASN	1
1	A	83	PHE	1
1	A	127	LEU	1
1	A	86	GLU	1
1	A	98	THR	1
1	A	73	ILE	1
1	A	116	TYR	1
1	A	68	THR	1
1	A	185	GLU	1
1	A	72	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	60	PHE	1
1	A	203	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided