



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:04 pm BST

PDB ID : 2L5G
Title : Co-ordinates and 1H, 13C and 15N chemical shift assignments for the complex of GPS2 53-90 and SMRT 167-207
Authors : Oberoi, J.; Yang, J.; Neuhaus, D.; Schwabe, J.W.R.
Deposited on : 2010-11-01

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 ⓘ 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
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

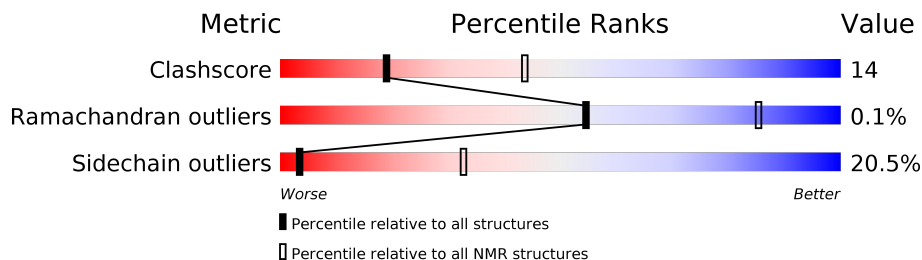
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	38	 61% 16% 24%
2	B	42	 52% 29% 5% 14%

2 Ensemble composition and analysis i

This entry contains 35 models. Model 20 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:62-A:90, B:166-B:201 (65)	0.43	20

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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 8, 9, 10, 13, 16, 19, 20, 21, 22, 24, 26, 27, 28, 29, 30, 32
2	5, 11, 12, 15, 17, 23, 25, 35
3	3, 6, 7, 18, 31
4	4, 33
Single-model clusters	14; 34

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1377 atoms, of which 706 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called G protein pathway suppressor 2.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	38	673	207	346	53	65	2	0

- Molecule 2 is a protein called Putative uncharacterized protein NCOR2.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
2	B	42	704	210	360	61	71	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	166	GLY	-	EXPRESSION TAG	UNP C9JQE8

4 Residue-property plots [i](#)

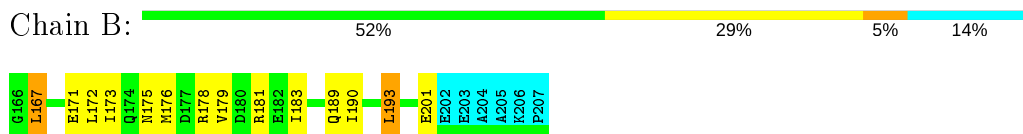
4.1 Average score per residue in the NMR ensemble

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: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2



4.2 Scores per residue for each member of the ensemble

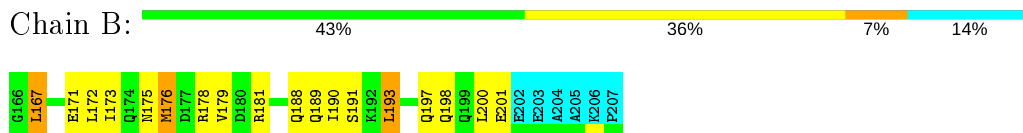
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

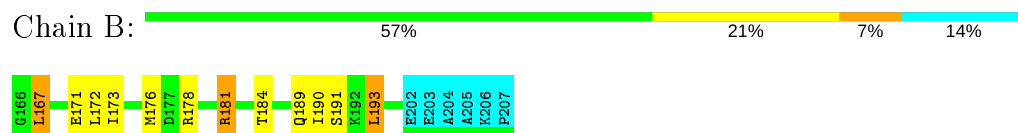


4.2.2 Score per residue for model 2

- Molecule 1: G protein pathway suppressor 2

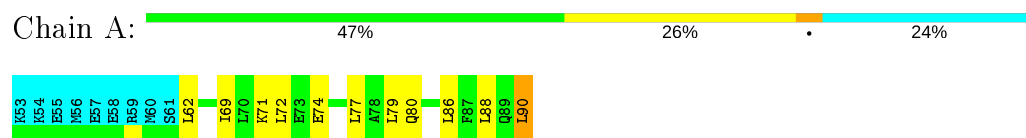


- Molecule 2: Putative uncharacterized protein NCOR2

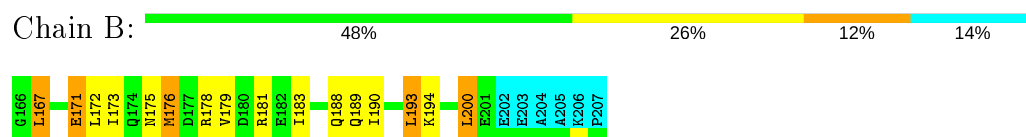


4.2.3 Score per residue for model 3

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

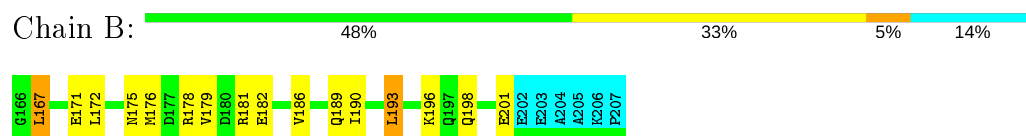


4.2.4 Score per residue for model 4

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

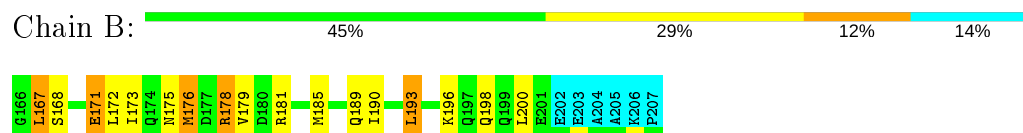


4.2.5 Score per residue for model 5

- Molecule 1: G protein pathway suppressor 2

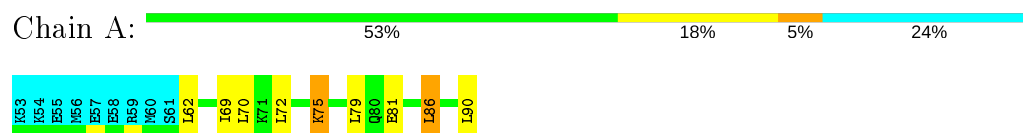


- Molecule 2: Putative uncharacterized protein NCOR2

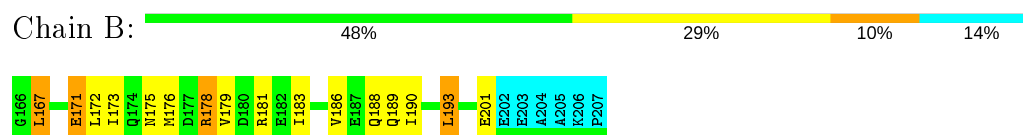


4.2.6 Score per residue for model 6

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

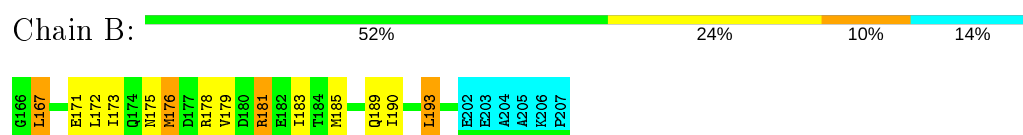


4.2.7 Score per residue for model 7

- Molecule 1: G protein pathway suppressor 2

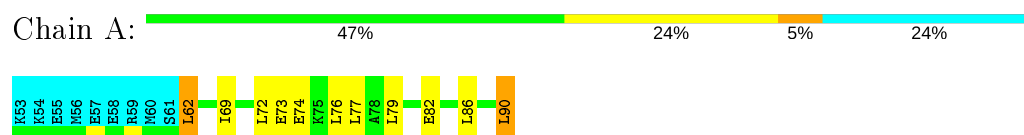


- Molecule 2: Putative uncharacterized protein NCOR2

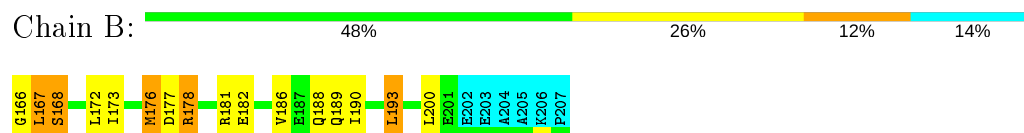


4.2.8 Score per residue for model 8

- Molecule 1: G protein pathway suppressor 2

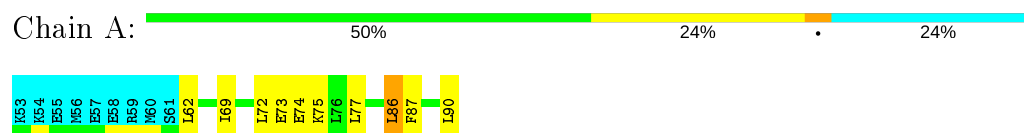


- Molecule 2: Putative uncharacterized protein NCOR2

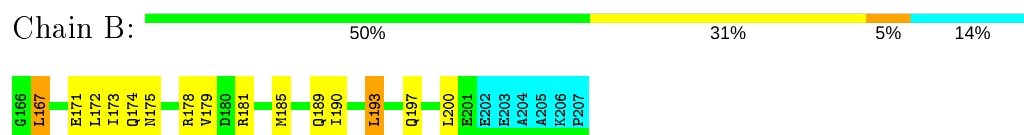


4.2.9 Score per residue for model 9

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

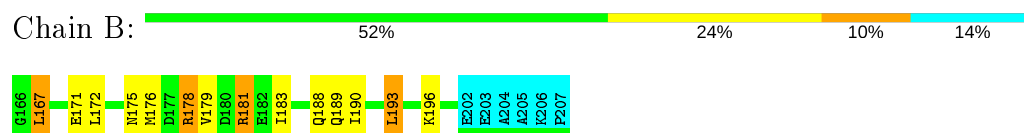


4.2.10 Score per residue for model 10

- Molecule 1: G protein pathway suppressor 2

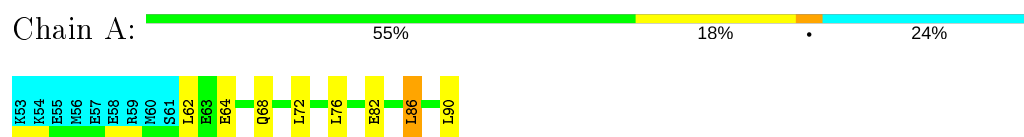


- Molecule 2: Putative uncharacterized protein NCOR2

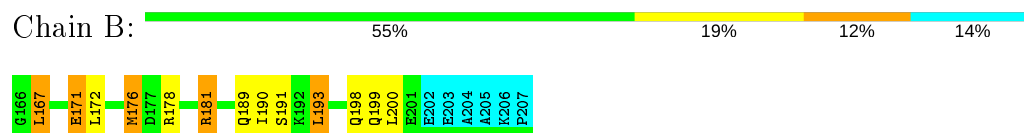


4.2.11 Score per residue for model 11

- Molecule 1: G protein pathway suppressor 2

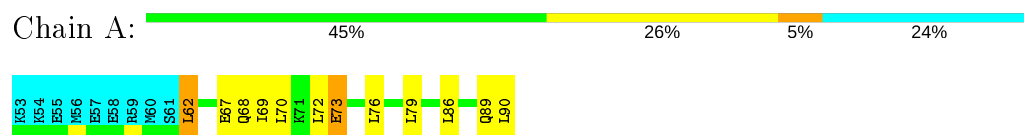


- Molecule 2: Putative uncharacterized protein NCOR2

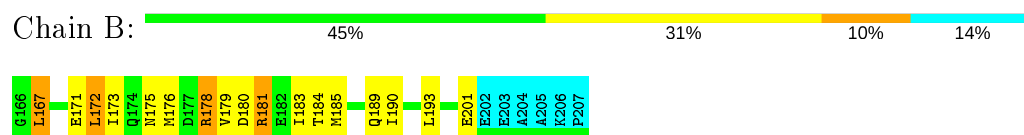


4.2.12 Score per residue for model 12

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

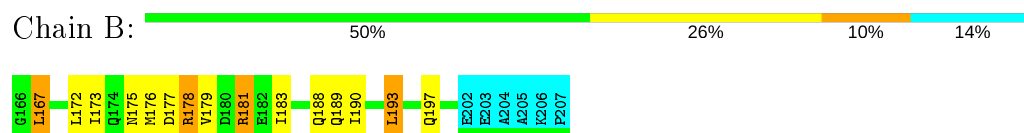


4.2.13 Score per residue for model 13

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

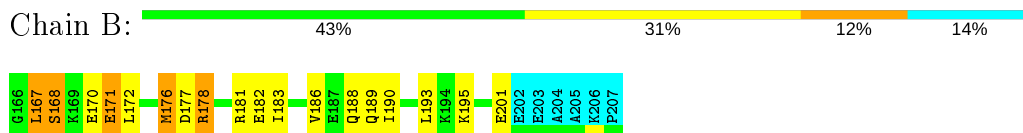


4.2.14 Score per residue for model 14

- Molecule 1: G protein pathway suppressor 2

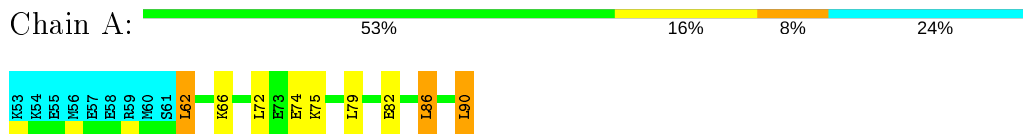


- Molecule 2: Putative uncharacterized protein NCOR2

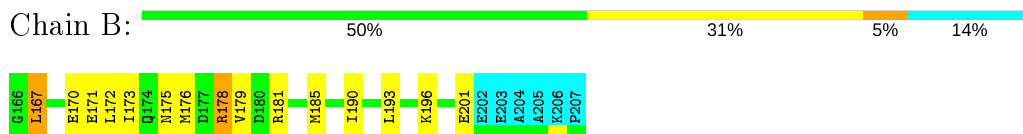


4.2.15 Score per residue for model 15

- Molecule 1: G protein pathway suppressor 2

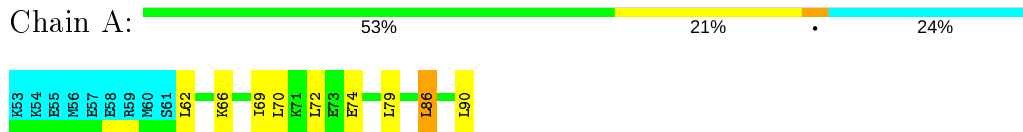


- Molecule 2: Putative uncharacterized protein NCOR2

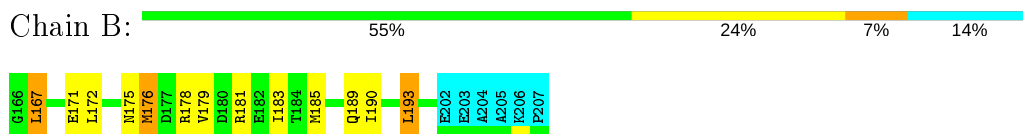


4.2.16 Score per residue for model 16

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

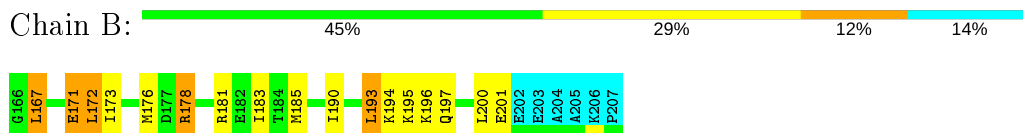


4.2.17 Score per residue for model 17

- Molecule 1: G protein pathway suppressor 2

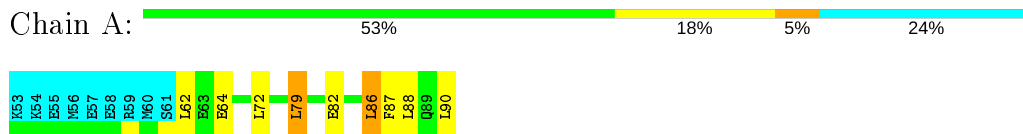


- Molecule 2: Putative uncharacterized protein NCOR2

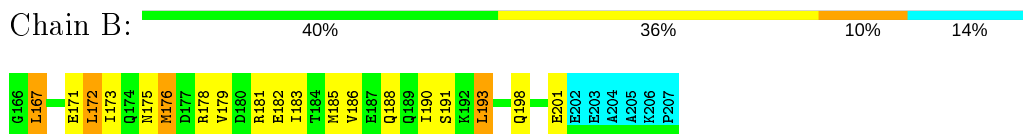


4.2.18 Score per residue for model 18

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

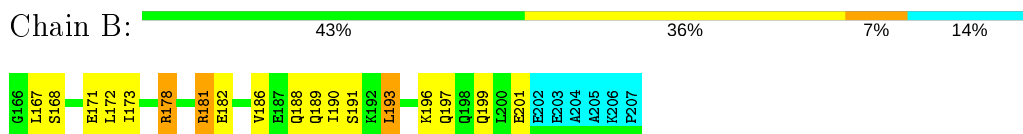


4.2.19 Score per residue for model 19

- Molecule 1: G protein pathway suppressor 2

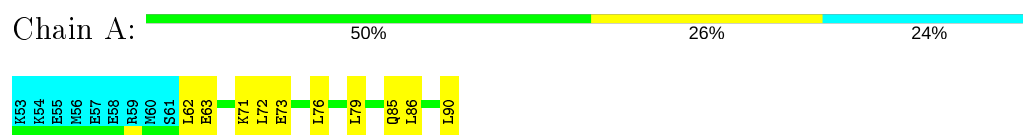


- Molecule 2: Putative uncharacterized protein NCOR2

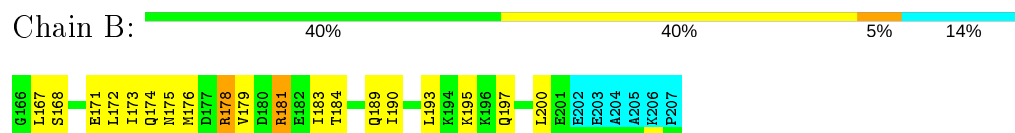


4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

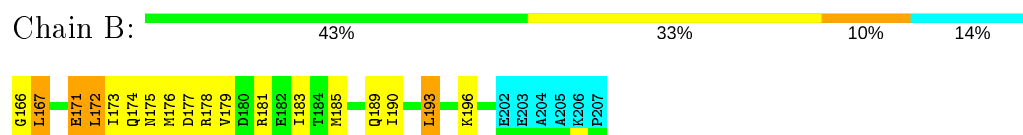


4.2.21 Score per residue for model 21

- Molecule 1: G protein pathway suppressor 2

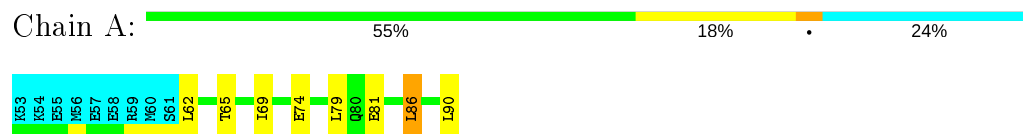


- Molecule 2: Putative uncharacterized protein NCOR2

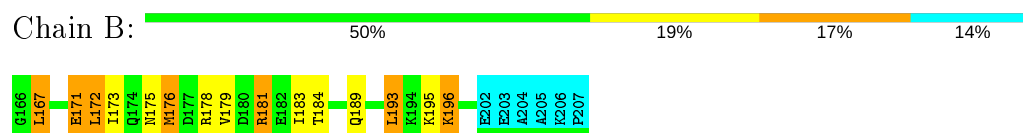


4.2.22 Score per residue for model 22

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

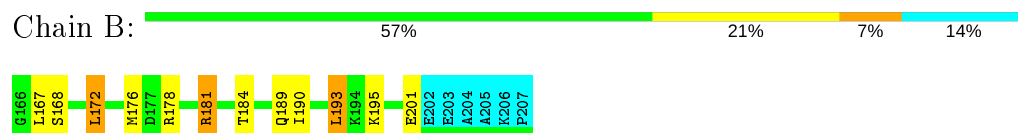


4.2.23 Score per residue for model 23

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

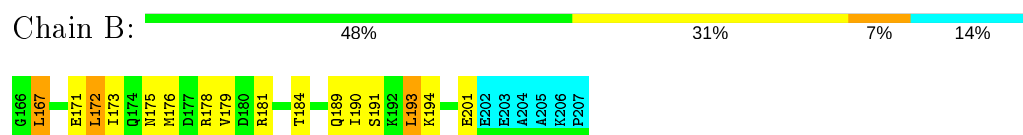


4.2.24 Score per residue for model 24

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

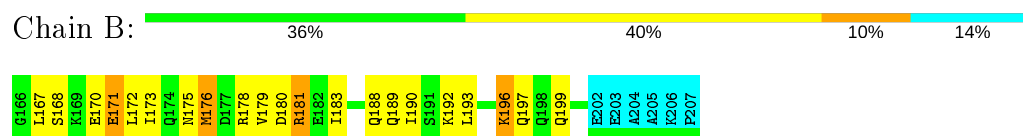


4.2.25 Score per residue for model 25

- Molecule 1: G protein pathway suppressor 2

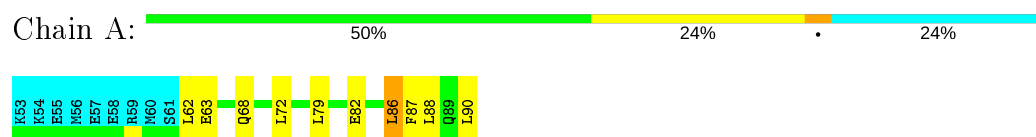


- Molecule 2: Putative uncharacterized protein NCOR2

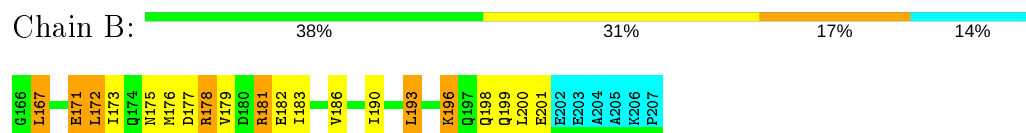


4.2.26 Score per residue for model 26

- Molecule 1: G protein pathway suppressor 2

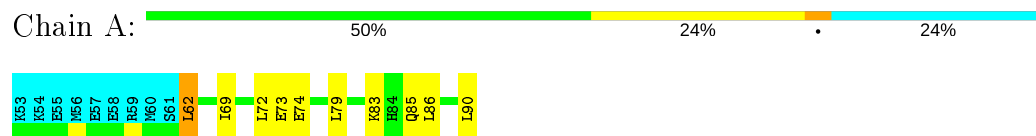


- Molecule 2: Putative uncharacterized protein NCOR2

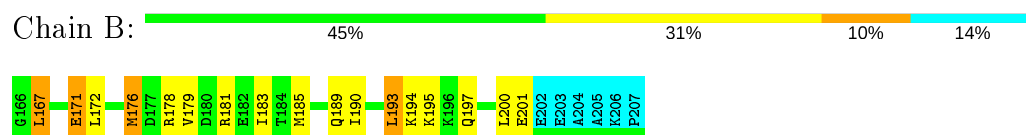


4.2.27 Score per residue for model 27

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

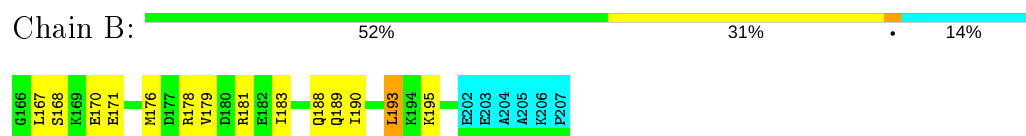


4.2.28 Score per residue for model 28

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

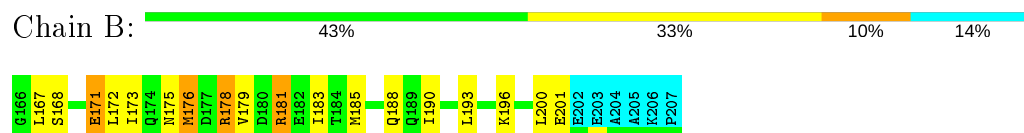


4.2.29 Score per residue for model 29

- Molecule 1: G protein pathway suppressor 2

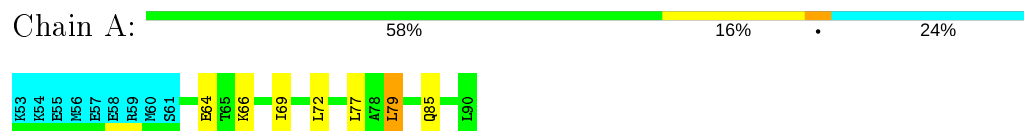


- Molecule 2: Putative uncharacterized protein NCOR2



4.2.30 Score per residue for model 30

- Molecule 1: G protein pathway suppressor 2

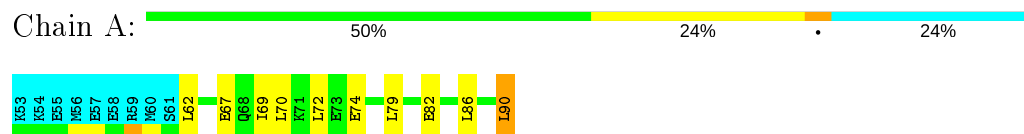


- Molecule 2: Putative uncharacterized protein NCOR2

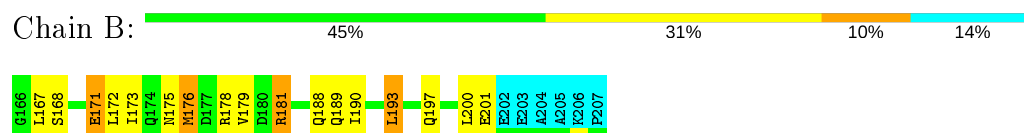


4.2.31 Score per residue for model 31

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

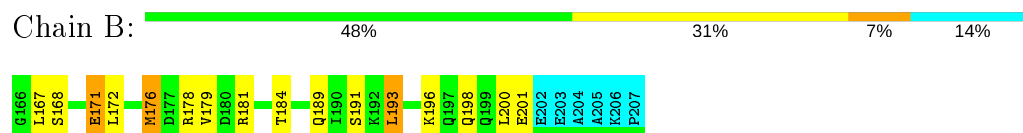


4.2.32 Score per residue for model 32

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2

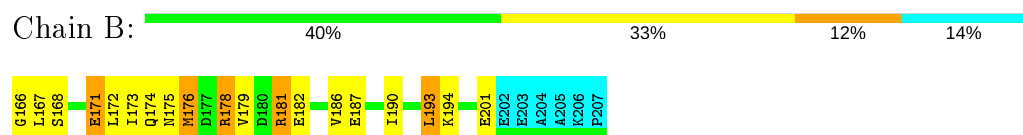


4.2.33 Score per residue for model 33

- Molecule 1: G protein pathway suppressor 2

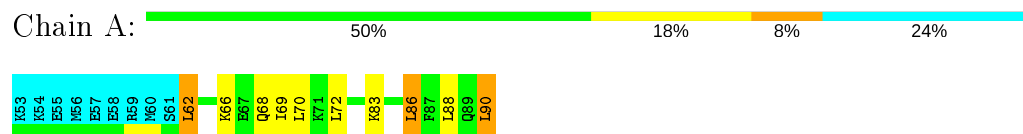


- Molecule 2: Putative uncharacterized protein NCOR2

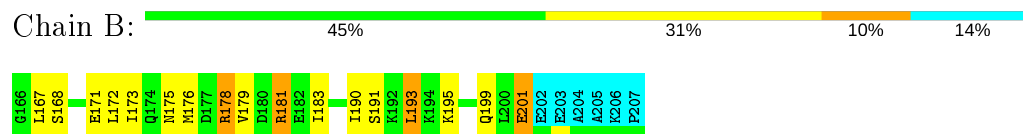


4.2.34 Score per residue for model 34

- Molecule 1: G protein pathway suppressor 2

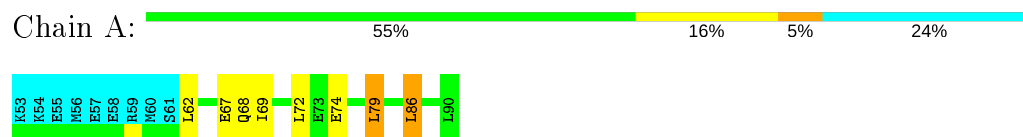


- Molecule 2: Putative uncharacterized protein NCOR2

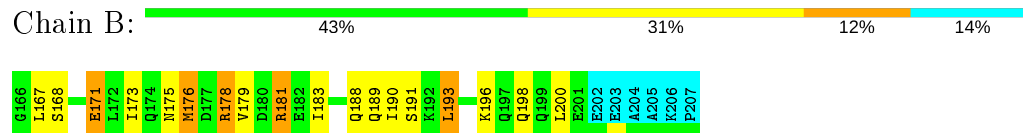


4.2.35 Score per residue for model 35

- Molecule 1: G protein pathway suppressor 2



- Molecule 2: Putative uncharacterized protein NCOR2



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 35 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
X-PLOR NIH	structure solution	2.19
X-PLOR NIH	refinement	2.19

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 [i](#)

6.1 Standard geometry [i](#)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
2	B	0.0±0.0	2.0±0.0
All	All	0	70

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	178	ARG	Sidechain	35
2	B	181	ARG	Sidechain	35

6.2 Too-close contacts [i](#)

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	249	264	264	9±3
2	B	299	318	315	16±4
All	All	19180	20370	20265	563

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:HD23	2:B:176:MET:HE3	0.95	1.36	7	6
2:B:167:LEU:HD21	2:B:172:LEU:HD13	0.90	1.41	10	4
2:B:167:LEU:HD21	2:B:172:LEU:HD12	0.85	1.48	2	9
1:A:76:LEU:HD13	2:B:190:ILE:HD12	0.78	1.53	11	5
2:B:167:LEU:HD13	2:B:171:GLU:CB	0.78	2.09	26	4
1:A:72:LEU:HD13	2:B:193:LEU:HD13	0.77	1.54	2	2
1:A:62:LEU:HD22	2:B:200:LEU:HD23	0.77	1.56	9	2
1:A:72:LEU:HD23	2:B:190:ILE:HD13	0.77	1.56	3	2
2:B:167:LEU:CD2	2:B:172:LEU:HD13	0.75	2.11	10	3
1:A:72:LEU:CD1	2:B:193:LEU:HD13	0.74	2.12	2	9
1:A:62:LEU:HD12	2:B:200:LEU:HD23	0.74	1.60	26	7
1:A:79:LEU:HD12	2:B:183:ILE:CG1	0.73	2.14	14	5
2:B:167:LEU:CD2	2:B:172:LEU:HD12	0.72	2.14	2	9
2:B:175:ASN:O	2:B:179:VAL:HG23	0.71	1.85	3	24
1:A:86:LEU:HD23	2:B:172:LEU:HD21	0.70	1.63	15	10
1:A:90:LEU:HD11	2:B:173:ILE:CD1	0.70	2.16	1	17
1:A:69:ILE:HG12	2:B:193:LEU:HD23	0.69	1.63	16	8
2:B:167:LEU:HD11	2:B:172:LEU:N	0.68	2.04	15	16
2:B:172:LEU:O	2:B:172:LEU:HD23	0.67	1.89	13	5
1:A:72:LEU:HD22	2:B:190:ILE:HG12	0.67	1.67	14	23
2:B:167:LEU:HD11	2:B:171:GLU:CB	0.67	2.19	33	8
1:A:90:LEU:HD11	2:B:173:ILE:HD11	0.66	1.68	24	9
2:B:167:LEU:HD12	2:B:168:SER:N	0.66	2.06	19	14
2:B:167:LEU:HD21	2:B:172:LEU:CD1	0.65	2.21	10	9
1:A:72:LEU:HD12	2:B:190:ILE:HG12	0.65	1.67	30	4
1:A:72:LEU:HD22	2:B:193:LEU:CD1	0.65	2.22	33	2
1:A:72:LEU:HD12	2:B:193:LEU:HD22	0.65	1.66	16	1
1:A:90:LEU:HD23	2:B:176:MET:CE	0.65	2.19	7	4
2:B:167:LEU:HD11	2:B:172:LEU:HG	0.65	1.69	17	4
1:A:79:LEU:HD12	2:B:183:ILE:HG12	0.64	1.66	18	7
1:A:90:LEU:HD23	2:B:176:MET:HE2	0.64	1.68	24	1
1:A:72:LEU:HD11	2:B:193:LEU:HD13	0.64	1.69	19	10
1:A:62:LEU:HD11	2:B:201:GLU:HG2	0.64	1.68	24	11
1:A:90:LEU:HD13	2:B:176:MET:HE1	0.63	1.70	6	2
2:B:172:LEU:HD23	2:B:172:LEU:O	0.63	1.93	11	8
1:A:90:LEU:HD13	2:B:176:MET:HE3	0.62	1.69	27	4
1:A:76:LEU:O	1:A:76:LEU:HD13	0.62	1.94	17	2
1:A:72:LEU:HD22	2:B:190:ILE:HD13	0.61	1.69	18	3
1:A:90:LEU:HD12	2:B:172:LEU:HD22	0.61	1.71	4	2
1:A:86:LEU:HD11	2:B:175:ASN:HB3	0.61	1.73	26	1
1:A:90:LEU:HA	2:B:172:LEU:HD13	0.60	1.74	13	5
1:A:90:LEU:HD13	2:B:176:MET:CE	0.60	2.26	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:ILE:HG12	2:B:193:LEU:HD22	0.60	1.74	27	10
1:A:69:ILE:CG1	2:B:193:LEU:HD23	0.59	2.27	16	3
1:A:62:LEU:HD11	2:B:201:GLU:CG	0.59	2.27	32	7
1:A:79:LEU:HD23	2:B:183:ILE:HA	0.59	1.75	12	13
1:A:86:LEU:HD22	2:B:176:MET:HG3	0.59	1.73	32	6
2:B:173:ILE:HD12	2:B:173:ILE:N	0.58	2.14	25	6
2:B:182:GLU:O	2:B:186:VAL:HG23	0.58	1.97	33	7
1:A:62:LEU:HD11	2:B:197:GLN:NE2	0.58	2.13	17	1
1:A:90:LEU:HD22	2:B:172:LEU:HD22	0.58	1.75	7	2
2:B:167:LEU:HD13	2:B:171:GLU:HB3	0.58	1.76	22	7
1:A:90:LEU:HD21	2:B:173:ILE:HD13	0.58	1.76	34	5
1:A:83:LYS:HG3	2:B:183:ILE:HD11	0.57	1.76	34	1
2:B:173:ILE:N	2:B:173:ILE:HD12	0.57	2.15	29	3
2:B:167:LEU:HD12	2:B:168:SER:H	0.57	1.60	8	2
1:A:72:LEU:HD12	2:B:190:ILE:CG1	0.56	2.29	30	4
2:B:167:LEU:HD11	2:B:172:LEU:CG	0.56	2.30	27	3
1:A:83:LYS:CG	2:B:183:ILE:HD11	0.56	2.31	34	1
1:A:79:LEU:HD12	2:B:183:ILE:HG13	0.56	1.77	14	1
1:A:72:LEU:HD22	2:B:190:ILE:CG1	0.56	2.31	35	14
1:A:86:LEU:HD22	2:B:176:MET:CG	0.55	2.32	22	5
1:A:72:LEU:HD22	2:B:190:ILE:CD1	0.55	2.32	16	2
2:B:167:LEU:HD12	2:B:168:SER:CB	0.55	2.31	33	9
2:B:167:LEU:HD11	2:B:172:LEU:HD23	0.55	1.79	24	2
2:B:167:LEU:HD13	2:B:171:GLU:HB2	0.54	1.78	14	3
1:A:62:LEU:CD1	2:B:200:LEU:HD23	0.54	2.31	3	1
1:A:90:LEU:CD2	2:B:173:ILE:HD11	0.54	2.33	15	1
2:B:167:LEU:HD22	2:B:171:GLU:OE1	0.53	2.03	26	1
1:A:86:LEU:CD2	2:B:172:LEU:HD21	0.53	2.33	15	3
2:B:167:LEU:HD11	2:B:172:LEU:H	0.53	1.64	10	2
2:B:167:LEU:HD22	2:B:171:GLU:HB3	0.53	1.80	21	7
1:A:73:GLU:O	1:A:77:LEU:HD13	0.53	2.03	10	3
2:B:167:LEU:HD13	2:B:172:LEU:N	0.52	2.19	18	5
1:A:65:THR:HG21	2:B:196:LYS:NZ	0.52	2.20	25	1
1:A:90:LEU:HA	2:B:172:LEU:HD23	0.52	1.80	10	4
2:B:167:LEU:HD11	2:B:171:GLU:HB2	0.52	1.80	33	4
2:B:166:GLY:HA3	2:B:172:LEU:HD13	0.52	1.82	33	1
2:B:167:LEU:HD21	2:B:172:LEU:HB2	0.52	1.80	10	2
2:B:167:LEU:N	2:B:167:LEU:HD12	0.52	2.20	24	1
1:A:62:LEU:HG	2:B:200:LEU:HD23	0.51	1.82	5	2
2:B:167:LEU:HD12	2:B:168:SER:HB3	0.51	1.83	30	3
1:A:72:LEU:HD22	2:B:193:LEU:HD13	0.51	1.81	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:167:LEU:HD12	2:B:168:SER:HB2	0.51	1.82	32	2
1:A:62:LEU:HD11	2:B:197:GLN:OE1	0.50	2.06	25	1
1:A:86:LEU:HD23	2:B:172:LEU:CD1	0.50	2.37	24	1
2:B:166:GLY:HA2	2:B:172:LEU:HD22	0.50	1.82	8	1
2:B:167:LEU:HD12	2:B:167:LEU:N	0.50	2.21	26	2
1:A:79:LEU:HD21	2:B:186:VAL:HG21	0.49	1.84	6	1
1:A:72:LEU:HD22	2:B:193:LEU:HD12	0.49	1.84	33	1
2:B:167:LEU:HD12	2:B:171:GLU:HB2	0.49	1.83	2	12
1:A:75:LYS:O	1:A:79:LEU:HD13	0.49	2.08	6	1
2:B:167:LEU:HD11	2:B:172:LEU:CD2	0.49	2.38	24	2
2:B:193:LEU:HD23	2:B:196:LYS:HE2	0.48	1.85	26	2
2:B:167:LEU:HD21	2:B:172:LEU:CG	0.48	2.37	1	6
1:A:69:ILE:CD1	2:B:193:LEU:HD22	0.48	2.39	30	1
1:A:76:LEU:HD13	2:B:190:ILE:CD1	0.48	2.32	11	2
2:B:167:LEU:HD11	2:B:172:LEU:HB2	0.48	1.86	2	10
1:A:90:LEU:CD1	2:B:172:LEU:HD22	0.47	2.39	4	1
1:A:86:LEU:CD1	2:B:179:VAL:HG21	0.47	2.39	28	2
1:A:72:LEU:CD2	2:B:193:LEU:HD12	0.47	2.40	33	1
2:B:167:LEU:HD21	2:B:172:LEU:CB	0.47	2.40	20	3
2:B:176:MET:O	2:B:179:VAL:HG22	0.47	2.09	27	1
1:A:72:LEU:CD2	2:B:190:ILE:HD13	0.47	2.35	3	1
1:A:72:LEU:HD13	2:B:190:ILE:HG12	0.47	1.86	35	1
1:A:62:LEU:HD22	2:B:200:LEU:CD2	0.46	2.39	17	1
1:A:70:LEU:O	1:A:70:LEU:HD23	0.46	2.10	31	1
2:B:166:GLY:HA2	2:B:172:LEU:HD12	0.46	1.88	21	1
2:B:166:GLY:CA	2:B:172:LEU:HD13	0.45	2.41	33	1
1:A:62:LEU:HD21	2:B:201:GLU:HG2	0.45	1.89	12	2
1:A:86:LEU:HD23	2:B:172:LEU:CD2	0.45	2.40	12	2
1:A:76:LEU:HD13	2:B:187:GLU:HA	0.45	1.88	33	1
2:B:167:LEU:HD11	2:B:171:GLU:HB3	0.45	1.87	33	1
1:A:62:LEU:HD21	2:B:201:GLU:OE2	0.45	2.11	12	1
1:A:72:LEU:CD1	2:B:193:LEU:HD22	0.44	2.39	16	1
1:A:86:LEU:HD22	2:B:176:MET:HG2	0.44	1.90	35	1
1:A:77:LEU:HD23	1:A:77:LEU:O	0.44	2.12	23	1
2:B:173:ILE:N	2:B:173:ILE:CD1	0.44	2.81	2	4
2:B:173:ILE:CD1	2:B:173:ILE:N	0.44	2.80	25	5
1:A:69:ILE:HD12	2:B:197:GLN:NE2	0.44	2.28	9	1
1:A:62:LEU:CD2	2:B:200:LEU:HD23	0.44	2.38	9	1
2:B:167:LEU:HD12	2:B:167:LEU:H	0.44	1.72	27	1
1:A:62:LEU:HD11	2:B:201:GLU:HA	0.43	1.90	4	1
1:A:83:LYS:CE	2:B:179:VAL:HG13	0.43	2.43	34	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:167:LEU:HD12	2:B:171:GLU:CB	0.43	2.44	3	2
1:A:70:LEU:C	1:A:70:LEU:HD23	0.42	2.34	31	3
1:A:89:GLN:O	2:B:172:LEU:HD13	0.42	2.15	21	1
1:A:90:LEU:HD22	2:B:176:MET:CE	0.42	2.44	18	3
1:A:70:LEU:HD23	1:A:70:LEU:C	0.41	2.36	10	1
2:B:167:LEU:CD1	2:B:171:GLU:CB	0.41	2.99	34	6
1:A:86:LEU:HD23	2:B:172:LEU:HD11	0.41	1.91	24	1
2:B:167:LEU:CD1	2:B:172:LEU:HD23	0.41	2.46	24	1
1:A:86:LEU:HD21	2:B:175:ASN:HB3	0.41	1.91	34	1
1:A:72:LEU:HD23	2:B:190:ILE:CD1	0.41	2.39	3	1
1:A:69:ILE:HG22	1:A:73:GLU:OE2	0.41	2.15	12	1
2:B:167:LEU:H	2:B:167:LEU:HD12	0.41	1.76	26	1
1:A:90:LEU:HD11	2:B:173:ILE:HD13	0.41	1.90	5	1
2:B:167:LEU:HD23	2:B:172:LEU:HD12	0.40	1.94	29	1
1:A:90:LEU:O	1:A:90:LEU:HD13	0.40	2.16	1	1
1:A:72:LEU:CG	2:B:190:ILE:CD1	0.40	2.99	3	1
2:B:180:ASP:O	2:B:184:THR:OG1	0.40	2.39	12	1
1:A:90:LEU:CD1	2:B:173:ILE:CD1	0.40	3.00	18	1
2:B:167:LEU:CD1	2:B:172:LEU:N	0.40	2.84	22	3
1:A:65:THR:HG23	2:B:196:LYS:NZ	0.40	2.32	22	1
1:A:69:ILE:CD1	2:B:197:GLN:NE2	0.40	2.85	19	2
1:A:86:LEU:CD2	2:B:172:LEU:CD2	0.40	3.00	14	1
2:B:188:GLN:O	2:B:191:SER:OG	0.40	2.39	1	1
1:A:69:ILE:CD1	2:B:197:GLN:CG	0.40	3.00	27	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	28/38 (74%)	28±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
2	B	35/42 (83%)	32±1 (91±2%)	3±1 (8±2%)	0±0 (0±1%)	50	82
All	All	2205/2800 (79%)	2099 (95%)	104 (5%)	2 (0%)	54	85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
2	B	168	SER	2

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	28/37 (76%)	23±2 (83±5%)	5±2 (17±5%)	5	40
2	B	35/39 (90%)	27±2 (77±5%)	8±2 (23±5%)	3	28
All	All	2205/2660 (83%)	1752 (79%)	453 (21%)	3	33

All 52 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	193	LEU	35
2	B	176	MET	30
2	B	189	GLN	27
2	B	167	LEU	23
1	A	86	LEU	23
2	B	171	GLU	19
2	B	178	ARG	17
2	B	181	ARG	17
1	A	79	LEU	17
2	B	188	GLN	13
1	A	62	LEU	13
1	A	74	GLU	13
2	B	196	LYS	12
1	A	82	GLU	12
2	B	185	MET	11
2	B	195	LYS	9
2	B	172	LEU	9
2	B	198	GLN	8
2	B	191	SER	8
1	A	90	LEU	8
1	A	77	LEU	7
1	A	71	LYS	7
2	B	184	THR	7
1	A	85	GLN	6

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Mol	Chain	Res	Type	Models (Total)
1	A	68	GLN	6
1	A	70	LEU	6
2	B	194	LYS	6
1	A	75	LYS	6
2	B	177	ASP	6
1	A	66	LYS	6
1	A	88	LEU	5
1	A	73	GLU	5
2	B	201	GLU	5
1	A	87	PHE	5
1	A	81	GLU	5
2	B	199	GLN	5
2	B	170	GLU	4
2	B	174	GLN	4
2	B	200	LEU	4
1	A	89	GLN	3
1	A	64	GLU	3
2	B	197	GLN	3
1	A	67	GLU	3
1	A	76	LEU	2
1	A	83	LYS	2
1	A	63	GLU	2
2	B	168	SER	1
1	A	80	GLN	1
2	B	182	GLU	1
2	B	180	ASP	1
1	A	72	LEU	1
2	B	192	LYS	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