WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:19 PM BST

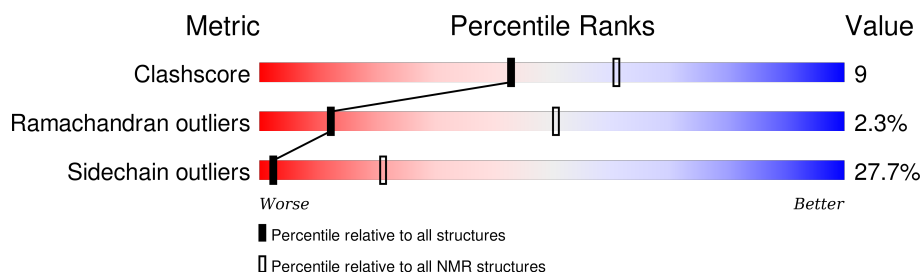|		
PDB ID	:	2JQY
Title	:	Outer Membrane Protein G
Authors	:	Liang, B.; Tamm, L.K.
Deposited on	:	2007-06-15

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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	Percentile Ranks	Value
Clashscore		9
Ramachandran outliers		2.3%
Sidechain outliers		27.7%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	280	31% 29% 40%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 6 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:5-A:14, A:33-A:52, A:68-A:95, A:106-A:139, A:148-A:176, A:189-A:211, A:236-A:243, A:248-A:254, A:273-A:280 (167)	0.81	6

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 6, 8, 10
2	5, 7, 9
Single-model clusters	4

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 4402 atoms, of which 2074 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Outer membrane protein G.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	280	4402	1477	2074	387	459	5	0

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: Outer membrane protein G
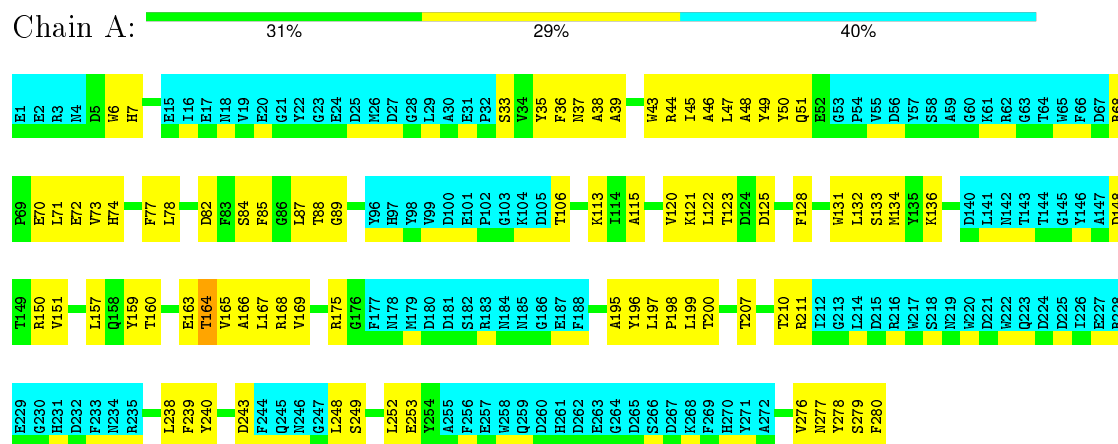
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Outer membrane protein G
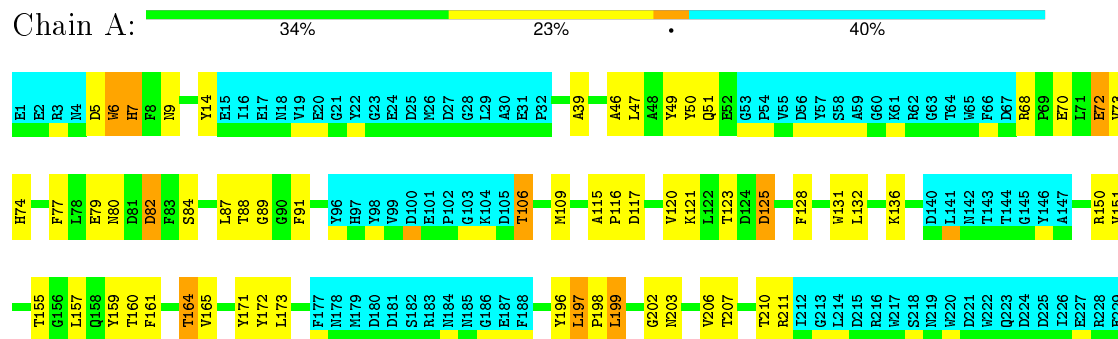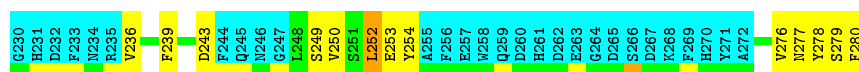
4.2.2 Score per residue for model 2

• Molecule 1: Outer membrane protein G

4.2.3 Score per residue for model 3

• Molecule 1: Outer membrane protein G
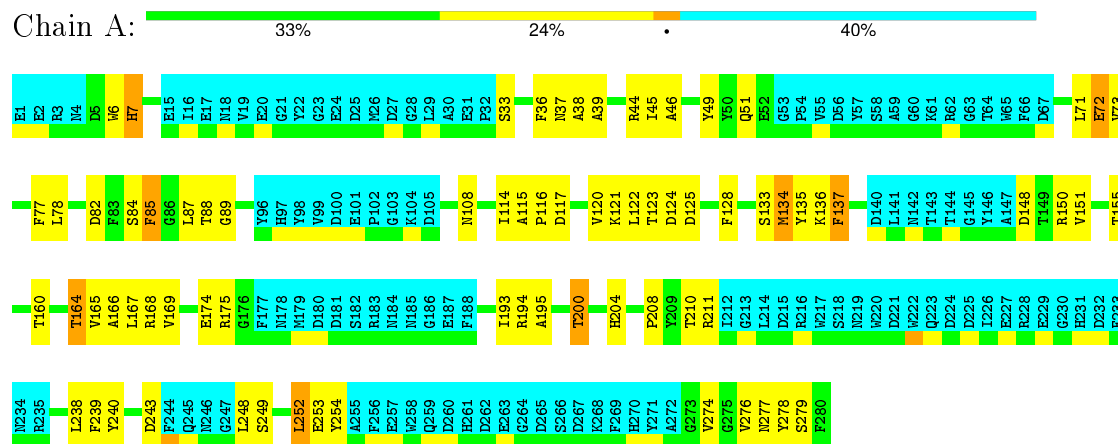
4.2.4 Score per residue for model 4

• Molecule 1: Outer membrane protein G
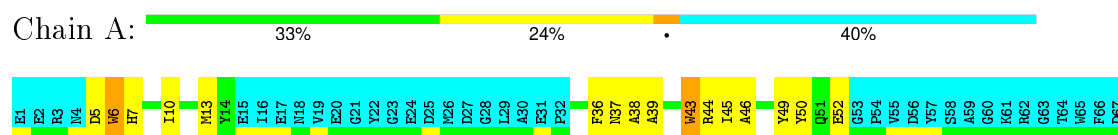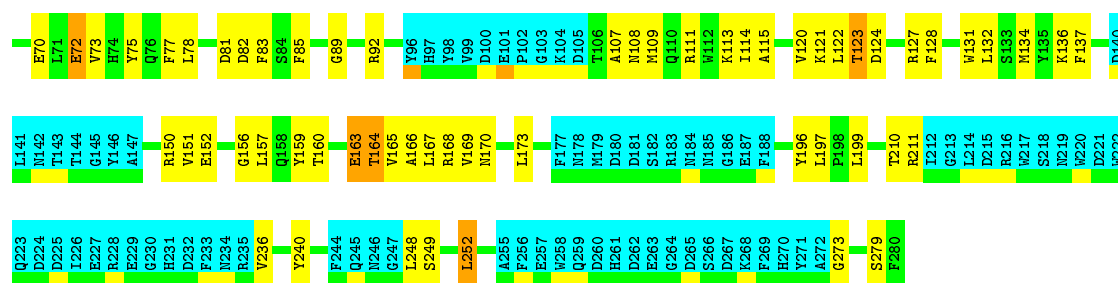
4.2.5 Score per residue for model 5

- Molecule 1: Outer membrane protein G
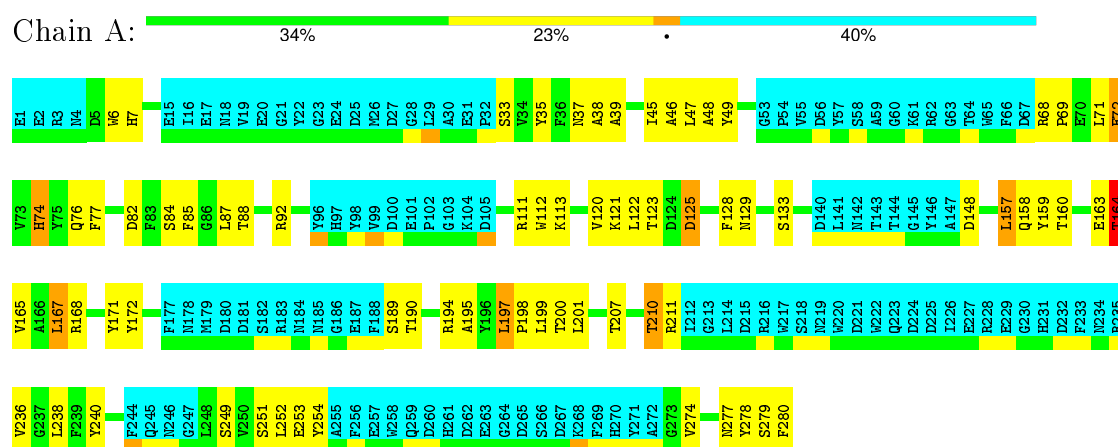
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Outer membrane protein G
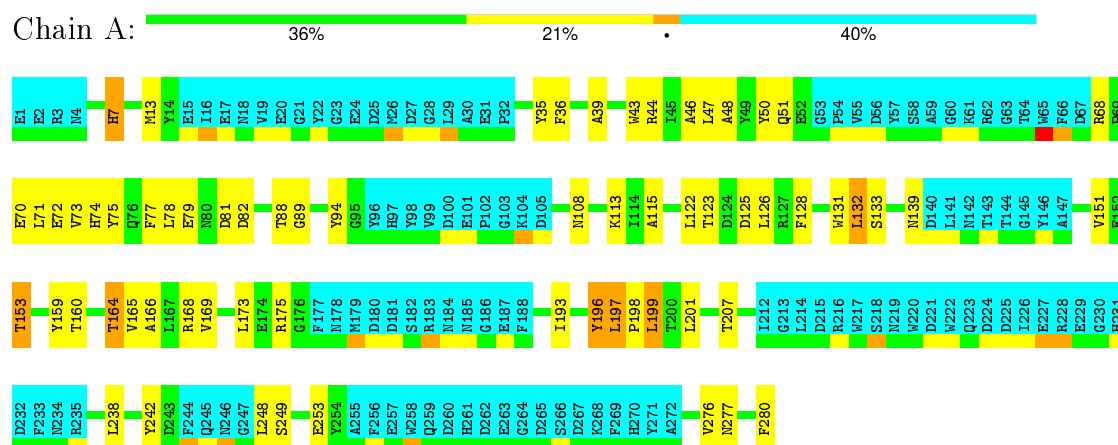
4.2.7 Score per residue for model 7

• Molecule 1: Outer membrane protein G

Chain A:
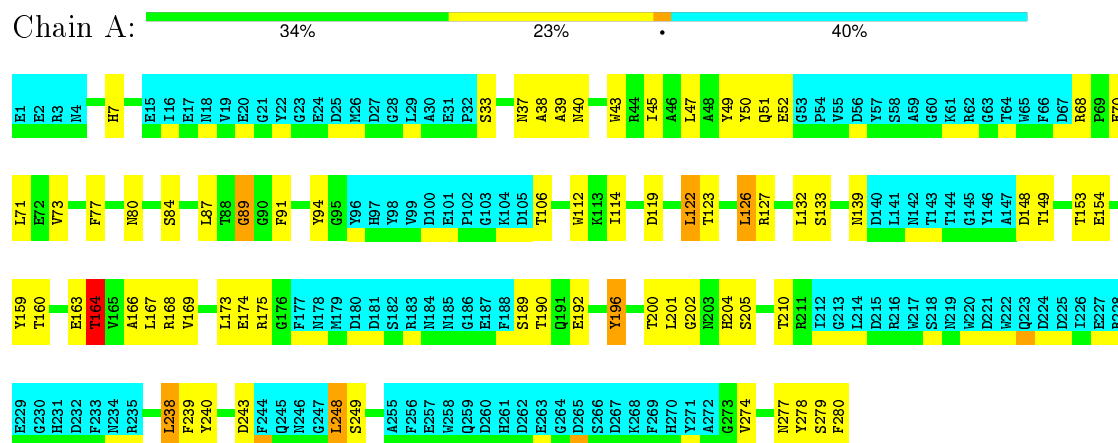
4.2.8 Score per residue for model 8

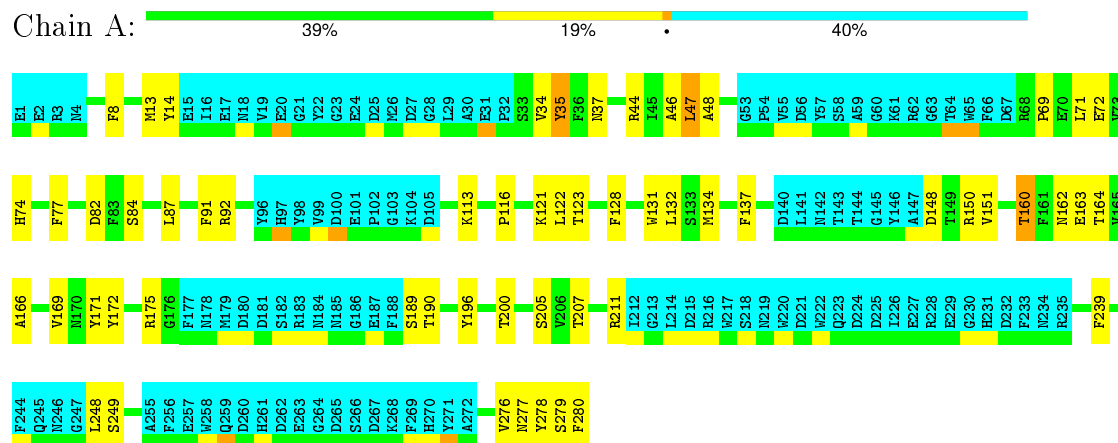• Molecule 1: Outer membrane protein G

Chain A:
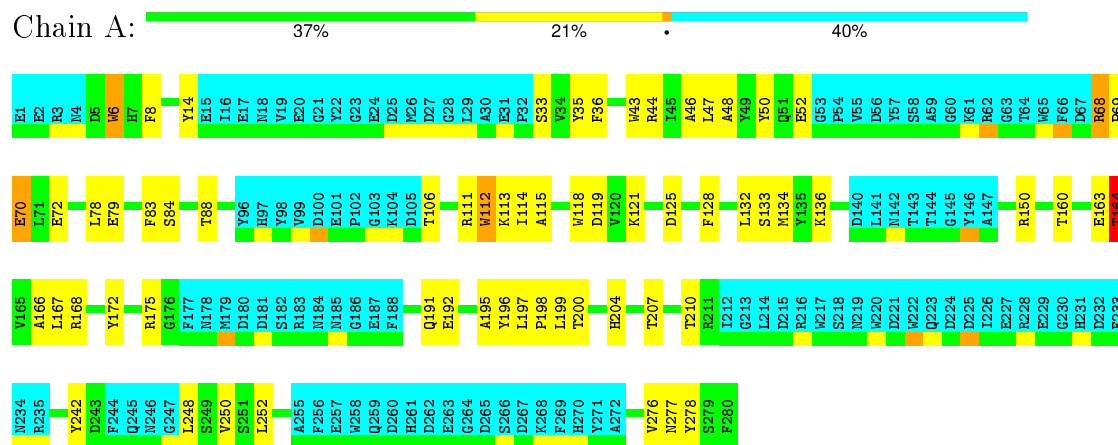
4.2.9 Score per residue for model 9

• Molecule 1: Outer membrane protein G

Chain A:
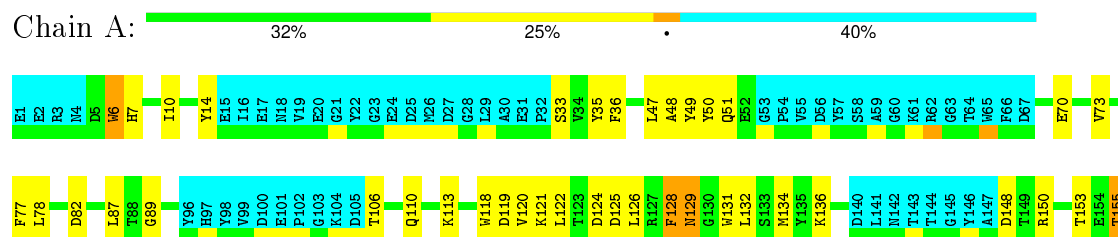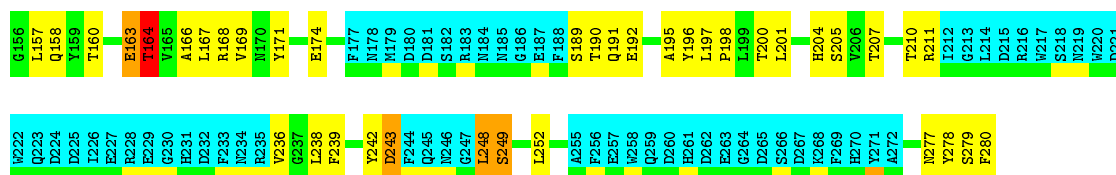
4.2.10 Score per residue for model 10

• Molecule 1: Outer membrane protein G

Chain A:
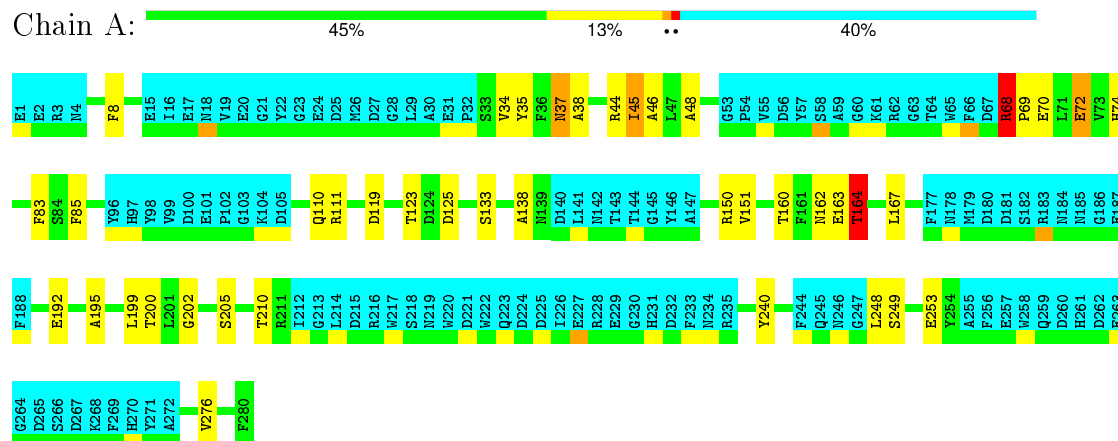
5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 10 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	

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.

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 (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	1388	1291	1288	23±5
All	All	13880	12910	12880	231

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:160:THR:HG23	1:A:166:ALA:HB2	0.89	1.45	2	6
1:A:115:ALA:HB3	1:A:132:LEU:O	0.82	1.74	4	1
1:A:87:LEU:HD21	1:A:114:ILE:HG23	0.82	1.49	3	1
1:A:238:LEU:HD22	1:A:240:TYR:CZ	0.79	2.12	7	1
1:A:73:VAL:HG12	1:A:89:GLY:O	0.74	1.82	7	2
1:A:7:HIS:HB2	1:A:39:ALA:HB3	0.73	1.60	5	6
1:A:82:ASP:O	1:A:120:VAL:HG23	0.72	1.84	1	3
1:A:200:THR:HG23	1:A:204:HIS:O	0.72	1.85	8	2
1:A:46:ALA:HB3	1:A:72:GLU:HB3	0.72	1.62	4	6
1:A:73:VAL:HG22	1:A:89:GLY:O	0.71	1.85	3	3
1:A:88:THR:CG2	1:A:115:ALA:HB3	0.71	2.14	1	1
1:A:46:ALA:HB3	1:A:72:GLU:HB2	0.70	1.64	6	2
1:A:160:THR:CG2	1:A:166:ALA:HB2	0.70	2.16	2	7
1:A:88:THR:HG22	1:A:115:ALA:HB3	0.70	1.61	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:LEU:HD12	1:A:199:LEU:HD11	0.69	1.64	1	1
1:A:160:THR:HG22	1:A:166:ALA:HB2	0.69	1.64	4	1
1:A:198:PRO:HA	1:A:207:THR:HG22	0.67	1.67	6	4
1:A:128:PHE:CE1	1:A:155:THR:HG22	0.67	2.25	9	1
1:A:134:MET:HG3	1:A:151:VAL:HG12	0.66	1.67	4	1
1:A:249:SER:O	1:A:276:VAL:HG13	0.65	1.91	6	3
1:A:112:TRP:CE3	1:A:114:ILE:HD11	0.65	2.26	8	1
1:A:200:THR:HG22	1:A:205:SER:HA	0.64	1.68	2	2
1:A:48:ALA:HB3	1:A:70:GLU:HB3	0.63	1.69	9	2
1:A:195:ALA:HB3	1:A:210:THR:HB	0.63	1.71	8	4
1:A:114:ILE:HG22	1:A:116:PRO:HD3	0.63	1.70	3	1
1:A:38:ALA:HB3	1:A:45:ILE:CG2	0.62	2.23	10	3
1:A:156:GLY:C	1:A:157:LEU:HD22	0.62	2.15	4	1
1:A:38:ALA:HB3	1:A:45:ILE:HB	0.61	1.73	3	2
1:A:200:THR:HG22	1:A:204:HIS:O	0.60	1.96	3	2
1:A:163:GLU:O	1:A:164:THR:HG23	0.60	1.97	9	4
1:A:132:LEU:HD11	1:A:153:THR:HG23	0.60	1.73	6	1
1:A:48:ALA:HB3	1:A:70:GLU:CG	0.59	2.27	8	1
1:A:132:LEU:CD1	1:A:153:THR:HG23	0.59	2.27	6	2
1:A:89:GLY:HA2	1:A:114:ILE:HG22	0.59	1.72	7	2
1:A:248:LEU:HD13	1:A:278:TYR:HB2	0.59	1.74	2	1
1:A:37:ASN:ND2	1:A:46:ALA:HB2	0.58	2.14	10	1
1:A:248:LEU:N	1:A:248:LEU:HD12	0.58	2.14	9	1
1:A:77:PHE:HB3	1:A:78:LEU:HD12	0.58	1.73	4	1
1:A:87:LEU:O	1:A:87:LEU:HD12	0.57	1.99	2	1
1:A:196:TYR:O	1:A:197:LEU:HD23	0.57	1.99	4	1
1:A:248:LEU:O	1:A:248:LEU:HD12	0.57	1.98	6	1
1:A:46:ALA:HB3	1:A:72:GLU:CB	0.57	2.28	4	3
1:A:169:VAL:HG13	1:A:169:VAL:O	0.56	2.00	3	2
1:A:7:HIS:CB	1:A:39:ALA:HB3	0.56	2.30	5	1
1:A:120:VAL:O	1:A:120:VAL:HG13	0.56	2.01	3	1
1:A:198:PRO:CA	1:A:207:THR:HG23	0.55	2.32	8	1
1:A:198:PRO:HA	1:A:207:THR:HG23	0.55	1.77	8	1
1:A:200:THR:O	1:A:201:LEU:HD12	0.54	2.02	9	1
1:A:122:LEU:HD12	1:A:123:THR:OG1	0.54	2.03	5	1
1:A:88:THR:HB	1:A:115:ALA:HB3	0.54	1.78	3	1
1:A:48:ALA:HB3	1:A:70:GLU:HB2	0.53	1.79	6	1
1:A:210:THR:HG22	1:A:236:VAL:HG12	0.53	1.79	9	1
1:A:236:VAL:O	1:A:236:VAL:HG22	0.53	2.03	4	1
1:A:122:LEU:HD12	1:A:123:THR:N	0.53	2.19	5	1
1:A:120:VAL:HG13	1:A:120:VAL:O	0.53	2.03	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:VAL:CG1	1:A:123:THR:HG21	0.53	2.34	4	1
1:A:206:VAL:HG13	1:A:206:VAL:O	0.53	2.04	1	1
1:A:159:TYR:O	1:A:167:LEU:HD12	0.53	2.04	4	1
1:A:169:VAL:HG23	1:A:169:VAL:O	0.53	2.04	9	1
1:A:208:PRO:HB3	1:A:238:LEU:HD23	0.53	1.80	3	1
1:A:126:LEU:HD12	1:A:159:TYR:CD1	0.52	2.39	7	1
1:A:134:MET:CG	1:A:151:VAL:HG12	0.52	2.35	4	1
1:A:159:TYR:OH	1:A:167:LEU:HD11	0.52	2.05	5	1
1:A:120:VAL:HG23	1:A:128:PHE:HB2	0.52	1.81	5	1
1:A:151:VAL:O	1:A:151:VAL:HG13	0.52	2.04	6	2
1:A:167:LEU:HD12	1:A:167:LEU:N	0.52	2.19	10	1
1:A:199:LEU:HD23	1:A:200:THR:N	0.51	2.20	5	1
1:A:48:ALA:HB3	1:A:70:GLU:HG3	0.51	1.81	8	1
1:A:250:VAL:HG12	1:A:276:VAL:HG12	0.51	1.82	8	1
1:A:10:ILE:HG23	1:A:36:PHE:CE1	0.51	2.40	4	1
1:A:89:GLY:CA	1:A:114:ILE:HG22	0.50	2.35	4	2
1:A:128:PHE:CZ	1:A:157:LEU:HD11	0.50	2.41	9	1
1:A:193:ILE:O	1:A:193:ILE:HG23	0.50	2.06	6	2
1:A:169:VAL:O	1:A:169:VAL:HG13	0.50	2.05	7	1
1:A:165:VAL:HG13	1:A:165:VAL:O	0.50	2.06	5	1
1:A:45:ILE:HG22	1:A:47:LEU:HD23	0.49	1.83	5	1
1:A:134:MET:HG3	1:A:151:VAL:HG22	0.49	1.84	2	1
1:A:47:LEU:HD23	1:A:48:ALA:N	0.49	2.22	2	1
1:A:132:LEU:HG	1:A:153:THR:HG23	0.49	1.84	9	2
1:A:128:PHE:CD1	1:A:157:LEU:HD22	0.49	2.43	5	1
1:A:242:TYR:H	1:A:250:VAL:HG23	0.49	1.67	8	1
1:A:43:TRP:CZ2	1:A:75:TYR:CE1	0.49	3.00	6	1
1:A:88:THR:OG1	1:A:115:ALA:HB3	0.49	2.07	8	2
1:A:195:ALA:HB3	1:A:210:THR:OG1	0.49	2.08	9	1
1:A:134:MET:HG2	1:A:151:VAL:HG12	0.49	1.83	3	1
1:A:110:GLN:HB3	1:A:138:ALA:HB3	0.49	1.84	10	1
1:A:248:LEU:HD23	1:A:278:TYR:HD1	0.48	1.67	9	1
1:A:159:TYR:CZ	1:A:167:LEU:HD11	0.48	2.44	5	1
1:A:165:VAL:O	1:A:165:VAL:HG23	0.48	2.08	3	2
1:A:165:VAL:HG23	1:A:165:VAL:O	0.47	2.09	4	1
1:A:88:THR:O	1:A:88:THR:HG23	0.47	2.09	1	1
1:A:115:ALA:HB3	1:A:132:LEU:C	0.47	2.29	4	1
1:A:238:LEU:HD22	1:A:240:TYR:OH	0.47	2.10	7	1
1:A:248:LEU:C	1:A:248:LEU:HD12	0.47	2.30	6	1
1:A:196:TYR:N	1:A:196:TYR:CD1	0.47	2.82	7	2
1:A:169:VAL:O	1:A:169:VAL:HG23	0.46	2.10	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:74:HIS:CD2	1:A:88:THR:HG23	0.46	2.46	5	1
1:A:74:HIS:CD2	1:A:74:HIS:N	0.46	2.83	1	1
1:A:151:VAL:HG23	1:A:151:VAL:O	0.46	2.09	10	1
1:A:120:VAL:HG12	1:A:123:THR:OG1	0.46	2.11	4	1
1:A:249:SER:CB	1:A:277:ASN:O	0.46	2.64	5	5
1:A:165:VAL:HG13	1:A:199:LEU:HG	0.46	1.88	6	1
1:A:128:PHE:CG	1:A:157:LEU:HD22	0.45	2.47	5	1
1:A:248:LEU:HD11	1:A:276:VAL:HG11	0.45	1.89	3	1
1:A:278:TYR:CD1	1:A:279:SER:N	0.45	2.85	7	3
1:A:197:LEU:HD12	1:A:199:LEU:CD1	0.45	2.42	6	1
1:A:68:ARG:CB	1:A:69:PRO:CD	0.45	2.94	8	2
1:A:160:THR:HG22	1:A:166:ALA:CB	0.45	2.38	4	1
1:A:128:PHE:CZ	1:A:157:LEU:CD1	0.45	3.00	9	1
1:A:112:TRP:CZ3	1:A:114:ILE:HD11	0.45	2.46	8	1
1:A:199:LEU:HD12	1:A:206:VAL:O	0.45	2.12	1	1
1:A:10:ILE:CD1	1:A:36:PHE:CE2	0.45	2.99	9	1
1:A:252:LEU:CD2	1:A:254:TYR:CE2	0.45	3.00	3	1
1:A:196:TYR:CD1	1:A:196:TYR:N	0.44	2.85	6	1
1:A:163:GLU:C	1:A:164:THR:HG22	0.44	2.33	8	1
1:A:240:TYR:N	1:A:240:TYR:CD1	0.44	2.85	7	1
1:A:252:LEU:HD23	1:A:273:GLY:O	0.44	2.12	4	1
1:A:35:TYR:CD1	1:A:35:TYR:N	0.44	2.85	8	1
1:A:38:ALA:HB3	1:A:45:ILE:HG23	0.44	1.89	10	1
1:A:129:ASN:ND2	1:A:131:TRP:CE2	0.44	2.85	9	1
1:A:250:VAL:HA	1:A:276:VAL:HG12	0.44	1.89	1	1
1:A:128:PHE:CD2	1:A:157:LEU:CD1	0.43	3.00	1	1
1:A:195:ALA:HB3	1:A:210:THR:CB	0.43	2.43	5	1
1:A:82:ASP:HB3	1:A:120:VAL:HG13	0.43	1.89	4	1
1:A:83:PHE:O	1:A:83:PHE:CD1	0.43	2.72	10	1
1:A:91:PHE:N	1:A:91:PHE:CD1	0.43	2.86	7	1
1:A:159:TYR:N	1:A:159:TYR:CD1	0.43	2.87	1	1
1:A:73:VAL:O	1:A:73:VAL:HG13	0.43	2.14	6	1
1:A:248:LEU:HD12	1:A:276:VAL:HG11	0.43	1.89	2	1
1:A:128:PHE:CZ	1:A:155:THR:CG2	0.42	3.01	1	1
1:A:114:ILE:O	1:A:115:ALA:HB2	0.42	2.15	4	1
1:A:249:SER:O	1:A:277:ASN:N	0.42	2.52	9	1
1:A:6:TRP:O	1:A:6:TRP:CG	0.42	2.72	8	1
1:A:249:SER:O	1:A:277:ASN:HB3	0.42	2.14	9	1
1:A:114:ILE:HD12	1:A:114:ILE:O	0.42	2.15	4	1
1:A:120:VAL:HG13	1:A:128:PHE:HB2	0.42	1.90	3	1
1:A:126:LEU:CD1	1:A:159:TYR:CD1	0.42	3.03	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:167:LEU:CB	1:A:197:LEU:HD11	0.42	2.45	5	1
1:A:128:PHE:CE1	1:A:155:THR:HG23	0.42	2.49	1	1
1:A:68:ARG:CB	1:A:69:PRO:HD3	0.42	2.44	10	1
1:A:248:LEU:HD12	1:A:248:LEU:H	0.42	1.73	9	1
1:A:277:ASN:O	1:A:278:TYR:CD1	0.41	2.73	9	1
1:A:68:ARG:N	1:A:69:PRO:CD	0.41	2.83	5	1
1:A:120:VAL:CG1	1:A:123:THR:CG2	0.41	2.98	4	1
1:A:14:TYR:N	1:A:14:TYR:CD1	0.41	2.89	8	1
1:A:40:ASN:O	1:A:43:TRP:CD1	0.41	2.73	7	1
1:A:43:TRP:CZ3	1:A:75:TYR:CE1	0.41	3.09	4	1
1:A:248:LEU:HD22	1:A:278:TYR:CG	0.41	2.50	2	1
1:A:35:TYR:CE1	1:A:48:ALA:HB2	0.41	2.51	5	1
1:A:73:VAL:HG23	1:A:89:GLY:HA3	0.41	1.92	4	1
1:A:242:TYR:CE2	1:A:243:ASP:O	0.41	2.74	9	1
1:A:123:THR:HG22	1:A:123:THR:O	0.41	2.16	7	1
1:A:252:LEU:HD13	1:A:253:GLU:H	0.41	1.76	1	1
1:A:252:LEU:CD2	1:A:274:VAL:HG12	0.40	2.46	5	1
1:A:34:VAL:HG12	1:A:35:TYR:N	0.40	2.32	2	2
1:A:128:PHE:HE1	1:A:155:THR:HG22	0.40	1.72	9	1
1:A:249:SER:O	1:A:276:VAL:HA	0.40	2.16	1	1
1:A:278:TYR:CD1	1:A:278:TYR:C	0.40	2.94	5	1
1:A:200:THR:HG22	1:A:205:SER:OG	0.40	2.17	10	1
1:A:207:THR:O	1:A:207:THR:HG23	0.40	2.16	2	1
1:A:122:LEU:HD12	1:A:123:THR:CB	0.40	2.46	5	1
1:A:128:PHE:N	1:A:128:PHE:CD1	0.40	2.89	6	1
1:A:159:TYR:CD1	1:A:159:TYR:O	0.40	2.75	6	1
1:A:35:TYR:O	1:A:36:PHE:CD1	0.40	2.74	6	1
1:A:85:PHE:CD1	1:A:117:ASP:O	0.40	2.75	3	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	166/280 (59%)	148±3 (89±2%)	14±3 (9±2%)	4±2 (2±1%)	12	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1660/2800 (59%)	1478 (89%)	144 (9%)	38 (2%)	12	51

All 16 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	164	THR	10
1	A	125	ASP	5
1	A	6	TRP	4
1	A	202	GLY	3
1	A	236	VAL	2
1	A	211	ARG	2
1	A	116	PRO	2
1	A	83	PHE	2
1	A	124	ASP	1
1	A	243	ASP	1
1	A	89	GLY	1
1	A	122	LEU	1
1	A	68	ARG	1
1	A	163	GLU	1
1	A	162	ASN	1
1	A	69	PRO	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	143/238 (60%)	103±7 (72±5%)	40±7 (28±5%)	2	21
All	All	1430/2380 (60%)	1034 (72%)	396 (28%)	2	21

All 114 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	164	THR	9
1	A	168	ARG	7
1	A	77	PHE	7

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Mol	Chain	Res	Type	Models (Total)
1	A	121	LYS	7
1	A	150	ARG	7
1	A	123	THR	6
1	A	133	SER	6
1	A	44	ARG	6
1	A	49	TYR	6
1	A	84	SER	6
1	A	47	LEU	6
1	A	50	TYR	6
1	A	113	LYS	6
1	A	122	LEU	6
1	A	37	ASN	6
1	A	280	PHE	6
1	A	196	TYR	5
1	A	71	LEU	5
1	A	167	LEU	5
1	A	136	LYS	5
1	A	248	LEU	5
1	A	148	ASP	5
1	A	197	LEU	5
1	A	72	GLU	5
1	A	252	LEU	5
1	A	6	TRP	5
1	A	199	LEU	5
1	A	33	SER	5
1	A	175	ARG	5
1	A	239	PHE	5
1	A	68	ARG	5
1	A	51	GLN	5
1	A	87	LEU	4
1	A	70	GLU	4
1	A	210	THR	4
1	A	192	GLU	4
1	A	171	TYR	4
1	A	211	ARG	4
1	A	238	LEU	4
1	A	128	PHE	4
1	A	74	HIS	4
1	A	279	SER	4
1	A	160	THR	4
1	A	253	GLU	4
1	A	82	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	111	ARG	4
1	A	172	TYR	4
1	A	132	LEU	4
1	A	85	PHE	4
1	A	173	LEU	4
1	A	78	LEU	4
1	A	131	TRP	4
1	A	240	TYR	4
1	A	119	ASP	4
1	A	7	HIS	4
1	A	189	SER	4
1	A	125	ASP	4
1	A	190	THR	4
1	A	14	TYR	3
1	A	106	THR	3
1	A	112	TRP	3
1	A	126	LEU	3
1	A	134	MET	3
1	A	243	ASP	3
1	A	163	GLU	3
1	A	79	GLU	3
1	A	108	ASN	3
1	A	52	GLU	3
1	A	174	GLU	3
1	A	137	PHE	3
1	A	201	LEU	3
1	A	92	ARG	3
1	A	13	MET	3
1	A	8	PHE	3
1	A	124	ASP	2
1	A	277	ASN	2
1	A	80	ASN	2
1	A	191	GLN	2
1	A	194	ARG	2
1	A	155	THR	2
1	A	109	MET	2
1	A	94	TYR	2
1	A	158	GLN	2
1	A	5	ASP	2
1	A	81	ASP	2
1	A	127	ARG	2
1	A	36	PHE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	43	TRP	2
1	A	118	TRP	2
1	A	249	SER	2
1	A	91	PHE	2
1	A	35	TYR	2
1	A	129	ASN	2
1	A	254	TYR	2
1	A	139	ASN	2
1	A	153	THR	1
1	A	135	TYR	1
1	A	117	ASP	1
1	A	200	THR	1
1	A	9	ASN	1
1	A	203	ASN	1
1	A	45	ILE	1
1	A	205	SER	1
1	A	157	LEU	1
1	A	154	GLU	1
1	A	242	TYR	1
1	A	152	GLU	1
1	A	170	ASN	1
1	A	76	GLN	1
1	A	149	THR	1
1	A	162	ASN	1
1	A	110	GLN	1
1	A	161	PHE	1
1	A	251	SER	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 (i)

No chemical shift data were provided