



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:21 AM BST

PDB ID : 2P03
Title : The structure of receptor-associated protein(RAP)
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Deposited on : 2007-02-28

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

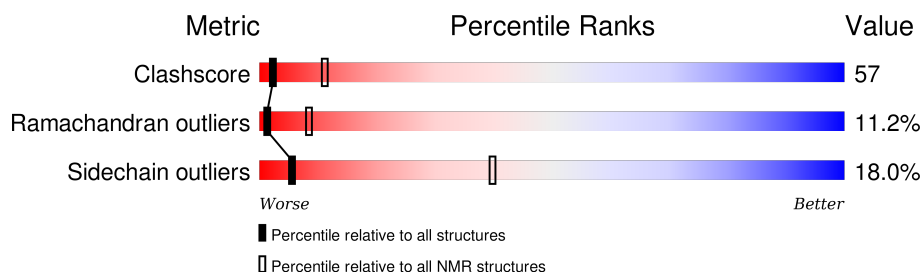
1 Overall quality at a glance

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	323	<div> <div>37%</div> <div>42%</div> <div>20%</div> <div>.</div> </div>

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 5325 atoms, of which 2659 are hydrogens and 0 are deuteriums.

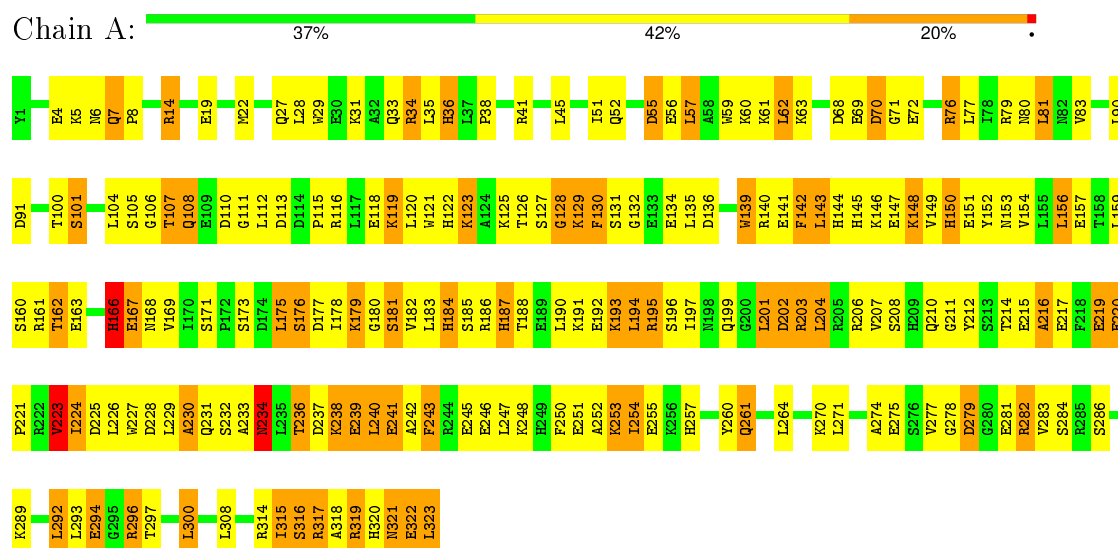
- Molecule 1 is a protein called Alpha-2-macroglobulin receptor-associated protein.

Mol	Chain	Residues	Atoms						Trace
1	A	323	Total	C	H	N	O	S	0
			5325	1655	2659	501	509	1	

4 Residue-property plots

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: Alpha-2-macroglobulin receptor-associated protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *RG refinement*.

Of the 1 calculated structures, 1 were deposited, based on the following criterion: *energy minimized average structure*.

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

Software name	Classification	Version
CYANA	structure solution	2.1.4
X-PLOR	refinement	3

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	2666	2659	2661	306
All	All	2666	2659	2661	306

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:159:LEU:HD12	1:A:160:SER:N	0.92	1.80
1:A:145:HIS:O	1:A:149:VAL:HG13	0.87	1.70
1:A:112:LEU:N	1:A:112:LEU:HD22	0.86	1.84
1:A:120:LEU:HD22	1:A:142:PHE:CZ	0.85	2.07
1:A:150:HIS:O	1:A:154:VAL:HG23	0.85	1.69
1:A:121:TRP:CE3	1:A:135:LEU:HD22	0.81	2.09
1:A:187:HIS:ND1	1:A:188:THR:N	0.81	2.28
1:A:156:LEU:HD12	1:A:156:LEU:C	0.78	2.00
1:A:323:LEU:HD23	1:A:323:LEU:C	0.76	2.00
1:A:223:VAL:HG11	1:A:308:LEU:CD2	0.76	2.11
1:A:194:LEU:C	1:A:194:LEU:HD12	0.75	2.01
1:A:141:GLU:CD	1:A:204:LEU:HD21	0.75	2.01
1:A:214:THR:HG23	1:A:215:GLU:H	0.75	1.42
1:A:214:THR:HG23	1:A:215:GLU:N	0.75	1.97
1:A:140:ARG:O	1:A:144:HIS:CG	0.74	2.40

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:121:TRP:CE2	1:A:135:LEU:HD13	0.74	2.18
1:A:145:HIS:O	1:A:149:VAL:HG22	0.73	1.82
1:A:29:TRP:NE1	1:A:33:GLN:NE2	0.73	2.36
1:A:282:ARG:NE	1:A:282:ARG:H	0.72	1.81
1:A:120:LEU:HD22	1:A:142:PHE:CE1	0.71	2.21
1:A:207:VAL:O	1:A:211:GLY:N	0.71	2.24
1:A:195:ARG:NH1	1:A:199:GLN:NE2	0.71	2.38
1:A:118:GLU:O	1:A:122:HIS:CD2	0.70	2.44
1:A:129:LYS:O	1:A:131:SER:N	0.70	2.24
1:A:195:ARG:HH11	1:A:199:GLN:NE2	0.70	1.85
1:A:168:ASN:O	1:A:169:VAL:HG23	0.70	1.85
1:A:184:HIS:CD2	1:A:185:SER:H	0.70	2.05
1:A:240:LEU:O	1:A:243:PHE:N	0.68	2.26
1:A:147:GLU:OE1	1:A:148:LYS:N	0.68	2.27
1:A:139:TRP:O	1:A:143:LEU:CD2	0.68	2.42
1:A:79:ARG:O	1:A:83:VAL:HG23	0.68	1.88
1:A:55:ASP:OD1	1:A:56:GLU:N	0.68	2.27
1:A:281:GLU:H	1:A:282:ARG:NH2	0.67	1.86
1:A:176:SER:O	1:A:178:ILE:N	0.67	2.28
1:A:62:LEU:HD11	1:A:68:ASP:CB	0.67	2.19
1:A:150:HIS:CD2	1:A:151:GLU:N	0.67	2.63
1:A:22:MET:SD	1:A:56:GLU:OE2	0.66	2.54
1:A:281:GLU:N	1:A:282:ARG:NH2	0.66	2.43
1:A:147:GLU:O	1:A:151:GLU:CG	0.66	2.44
1:A:257:HIS:NE2	1:A:261:GLN:OE1	0.66	2.27
1:A:201:LEU:HD12	1:A:201:LEU:C	0.66	2.11
1:A:187:HIS:ND1	1:A:187:HIS:C	0.66	2.48
1:A:161:ARG:O	1:A:163:GLU:N	0.65	2.26
1:A:296:ARG:NH1	1:A:300:LEU:HD23	0.65	2.05
1:A:19:GLU:OE1	1:A:29:TRP:NE1	0.65	2.30
1:A:243:PHE:C	1:A:243:PHE:CD1	0.65	2.69
1:A:181:SER:O	1:A:184:HIS:NE2	0.65	2.29
1:A:76:ARG:NE	1:A:80:ASN:ND2	0.65	2.44
1:A:55:ASP:CG	1:A:56:GLU:N	0.65	2.50
1:A:76:ARG:HE	1:A:80:ASN:HD21	0.64	1.35
1:A:183:LEU:O	1:A:183:LEU:HD23	0.64	1.92
1:A:145:HIS:CE1	1:A:197:ILE:HG23	0.64	2.27
1:A:296:ARG:NH1	1:A:300:LEU:CD2	0.64	2.60
1:A:112:LEU:CD2	1:A:112:LEU:N	0.64	2.58
1:A:69:GLU:O	1:A:71:GLY:N	0.64	2.31
1:A:178:ILE:HG22	1:A:179:LYS:N	0.64	2.06
1:A:292:LEU:HD12	1:A:292:LEU:O	0.63	1.94

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:152:TYR:CE1	1:A:193:LYS:CE	0.62	2.81
1:A:62:LEU:HD11	1:A:68:ASP:HB2	0.62	1.71
1:A:147:GLU:CD	1:A:148:LYS:N	0.62	2.53
1:A:145:HIS:O	1:A:149:VAL:CG1	0.62	2.47
1:A:292:LEU:HD12	1:A:292:LEU:C	0.62	2.14
1:A:121:TRP:CZ2	1:A:135:LEU:HD13	0.62	2.29
1:A:281:GLU:H	1:A:282:ARG:HH21	0.62	1.37
1:A:76:ARG:NE	1:A:80:ASN:HD21	0.62	1.93
1:A:206:ARG:NH2	1:A:210:GLN:HE22	0.62	1.92
1:A:323:LEU:HD23	1:A:323:LEU:O	0.62	1.93
1:A:199:GLN:O	1:A:202:ASP:OD2	0.62	2.17
1:A:254:ILE:HG23	1:A:255:GLU:N	0.61	2.10
1:A:62:LEU:HD12	1:A:62:LEU:C	0.61	2.16
1:A:14:ARG:NE	1:A:14:ARG:N	0.60	2.49
1:A:179:LYS:CB	1:A:179:LYS:NZ	0.60	2.63
1:A:149:VAL:HG23	1:A:150:HIS:N	0.60	2.11
1:A:107:THR:HG22	1:A:108:GLN:N	0.60	2.12
1:A:202:ASP:OD1	1:A:202:ASP:C	0.60	2.40
1:A:260:TYR:CE2	1:A:296:ARG:NH2	0.59	2.70
1:A:207:VAL:O	1:A:211:GLY:CA	0.59	2.49
1:A:141:GLU:OE2	1:A:204:LEU:HD21	0.59	1.96
1:A:251:GLU:CD	1:A:252:ALA:N	0.59	2.56
1:A:7:GLN:N	1:A:8:PRO:CD	0.58	2.66
1:A:123:LYS:O	1:A:127:SER:CB	0.58	2.51
1:A:147:GLU:O	1:A:150:HIS:CD2	0.58	2.55
1:A:206:ARG:O	1:A:210:GLN:N	0.58	2.37
1:A:214:THR:CG2	1:A:215:GLU:H	0.58	2.12
1:A:282:ARG:HE	1:A:283:VAL:N	0.57	1.97
1:A:214:THR:CG2	1:A:215:GLU:N	0.57	2.67
1:A:62:LEU:CD1	1:A:68:ASP:N	0.57	2.67
1:A:194:LEU:CD1	1:A:194:LEU:C	0.57	2.70
1:A:240:LEU:O	1:A:241:GLU:C	0.57	2.43
1:A:282:ARG:N	1:A:282:ARG:NE	0.57	2.52
1:A:69:GLU:C	1:A:71:GLY:N	0.57	2.58
1:A:106:GLY:O	1:A:107:THR:O	0.57	2.22
1:A:14:ARG:HE	1:A:14:ARG:H	0.56	1.43
1:A:229:LEU:C	1:A:229:LEU:HD12	0.56	2.20
1:A:239:GLU:OE1	1:A:320:HIS:O	0.56	2.22
1:A:56:GLU:CG	1:A:57:LEU:N	0.56	2.67
1:A:112:LEU:O	1:A:118:GLU:OE1	0.56	2.24
1:A:191:LYS:O	1:A:195:ARG:CG	0.56	2.54
1:A:293:LEU:O	1:A:297:THR:OG1	0.56	2.21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:187:HIS:CE1	1:A:188:THR:OG1	0.56	2.58
1:A:29:TRP:HE1	1:A:33:GLN:NE2	0.56	1.96
1:A:178:ILE:CG2	1:A:179:LYS:N	0.56	2.67
1:A:14:ARG:H	1:A:14:ARG:NE	0.56	1.98
1:A:134:GLU:H	1:A:134:GLU:CD	0.56	2.04
1:A:223:VAL:HG23	1:A:224:ILE:H	0.56	1.60
1:A:100:THR:O	1:A:101:SER:O	0.56	2.23
1:A:156:LEU:HD12	1:A:156:LEU:O	0.56	2.01
1:A:219:GLU:O	1:A:224:ILE:HD13	0.56	2.01
1:A:229:LEU:O	1:A:231:GLN:N	0.55	2.40
1:A:167:GLU:CG	1:A:167:GLU:O	0.55	2.55
1:A:113:ASP:O	1:A:118:GLU:OE2	0.55	2.23
1:A:175:LEU:O	1:A:176:SER:O	0.55	2.23
1:A:159:LEU:HD12	1:A:159:LEU:C	0.55	2.22
1:A:316:SER:O	1:A:318:ALA:N	0.55	2.39
1:A:314:ARG:O	1:A:315:ILE:C	0.54	2.44
1:A:251:GLU:OE1	1:A:251:GLU:C	0.54	2.46
1:A:294:GLU:OE1	1:A:294:GLU:O	0.54	2.25
1:A:315:ILE:O	1:A:316:SER:O	0.54	2.25
1:A:321:ASN:O	1:A:323:LEU:N	0.54	2.40
1:A:132:GLY:O	1:A:136:ASP:CG	0.54	2.46
1:A:282:ARG:O	1:A:286:SER:OG	0.54	2.22
1:A:168:ASN:O	1:A:169:VAL:CG2	0.54	2.55
1:A:69:GLU:C	1:A:71:GLY:H	0.54	2.05
1:A:120:LEU:CD2	1:A:142:PHE:CE1	0.54	2.91
1:A:145:HIS:O	1:A:149:VAL:CG2	0.54	2.55
1:A:112:LEU:O	1:A:118:GLU:CD	0.54	2.46
1:A:182:VAL:C	1:A:184:HIS:H	0.54	2.05
1:A:104:LEU:HD23	1:A:104:LEU:C	0.53	2.23
1:A:139:TRP:O	1:A:143:LEU:HD23	0.53	2.02
1:A:144:HIS:O	1:A:147:GLU:OE2	0.53	2.26
1:A:104:LEU:HD23	1:A:105:SER:N	0.53	2.17
1:A:147:GLU:OE1	1:A:147:GLU:C	0.53	2.46
1:A:147:GLU:O	1:A:150:HIS:HD2	0.53	1.87
1:A:168:ASN:CG	1:A:169:VAL:H	0.53	2.06
1:A:315:ILE:O	1:A:316:SER:C	0.53	2.46
1:A:81:LEU:O	1:A:81:LEU:HD13	0.53	2.04
1:A:323:LEU:CD2	1:A:323:LEU:C	0.52	2.69
1:A:62:LEU:HD12	1:A:62:LEU:O	0.52	2.05
1:A:184:HIS:CG	1:A:185:SER:N	0.52	2.78
1:A:57:LEU:CD1	1:A:57:LEU:C	0.52	2.78
1:A:115:PRO:O	1:A:119:LYS:CG	0.52	2.57

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:34:ARG:O	1:A:36:HIS:CE1	0.52	2.63
1:A:121:TRP:HE1	1:A:125:LYS:CE	0.52	2.18
1:A:152:TYR:O	1:A:190:LEU:HD12	0.52	2.05
1:A:271:LEU:HD12	1:A:271:LEU:C	0.52	2.26
1:A:210:GLN:C	1:A:212:TYR:H	0.51	2.08
1:A:257:HIS:NE2	1:A:261:GLN:CG	0.51	2.73
1:A:296:ARG:C	1:A:296:ARG:CD	0.51	2.79
1:A:194:LEU:HG	1:A:195:ARG:N	0.51	2.20
1:A:184:HIS:CD2	1:A:185:SER:N	0.51	2.79
1:A:292:LEU:C	1:A:292:LEU:CD1	0.51	2.78
1:A:55:ASP:C	1:A:55:ASP:OD1	0.51	2.48
1:A:277:VAL:HG13	1:A:278:GLY:N	0.51	2.20
1:A:62:LEU:CD1	1:A:68:ASP:H	0.51	2.19
1:A:201:LEU:HD12	1:A:201:LEU:O	0.50	2.06
1:A:201:LEU:HG	1:A:202:ASP:N	0.50	2.20
1:A:229:LEU:O	1:A:230:ALA:C	0.50	2.50
1:A:233:ALA:O	1:A:234:ASN:C	0.50	2.50
1:A:120:LEU:CD2	1:A:142:PHE:CZ	0.50	2.90
1:A:145:HIS:CE1	1:A:197:ILE:CG2	0.50	2.93
1:A:22:MET:CE	1:A:56:GLU:OE2	0.50	2.59
1:A:79:ARG:O	1:A:83:VAL:CG2	0.50	2.60
1:A:159:LEU:CD1	1:A:160:SER:N	0.50	2.66
1:A:150:HIS:C	1:A:150:HIS:CD2	0.50	2.85
1:A:166:HIS:O	1:A:167:GLU:HG2	0.50	2.07
1:A:90:LEU:CD1	1:A:90:LEU:N	0.50	2.73
1:A:216:ALA:O	1:A:217:GLU:CG	0.49	2.59
1:A:240:LEU:O	1:A:242:ALA:N	0.49	2.45
1:A:206:ARG:CZ	1:A:210:GLN:HE22	0.49	2.21
1:A:260:TYR:CD1	1:A:293:LEU:HD11	0.49	2.43
1:A:41:ARG:O	1:A:45:LEU:CB	0.49	2.60
1:A:14:ARG:CD	1:A:14:ARG:N	0.49	2.76
1:A:156:LEU:HG	1:A:157:GLU:N	0.49	2.23
1:A:275:GLU:OE2	1:A:283:VAL:HG13	0.49	2.08
1:A:296:ARG:HH11	1:A:300:LEU:HD23	0.49	1.65
1:A:254:ILE:CG2	1:A:255:GLU:N	0.49	2.76
1:A:51:ILE:HD13	1:A:51:ILE:N	0.49	2.23
1:A:52:GLN:NE2	1:A:81:LEU:HD22	0.49	2.23
1:A:127:SER:O	1:A:212:TYR:CE1	0.48	2.66
1:A:162:THR:O	1:A:162:THR:HG22	0.48	2.08
1:A:14:ARG:HE	1:A:14:ARG:N	0.48	2.04
1:A:250:PHE:O	1:A:253:LYS:N	0.48	2.45
1:A:139:TRP:CZ3	1:A:142:PHE:CD2	0.48	3.02

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:314:ARG:O	1:A:323:LEU:HD11	0.48	2.09
1:A:236:THR:O	1:A:237:ASP:C	0.48	2.52
1:A:62:LEU:C	1:A:62:LEU:CD1	0.47	2.81
1:A:260:TYR:CE1	1:A:293:LEU:HD11	0.47	2.44
1:A:81:LEU:CD1	1:A:81:LEU:C	0.47	2.82
1:A:7:GLN:N	1:A:8:PRO:HD2	0.47	2.24
1:A:122:HIS:CD2	1:A:122:HIS:N	0.47	2.83
1:A:55:ASP:OD1	1:A:77:LEU:HD13	0.47	2.08
1:A:147:GLU:O	1:A:151:GLU:CB	0.47	2.63
1:A:194:LEU:CG	1:A:195:ARG:N	0.47	2.78
1:A:243:PHE:O	1:A:247:LEU:HD23	0.47	2.09
1:A:57:LEU:O	1:A:57:LEU:HD13	0.47	2.10
1:A:62:LEU:HG	1:A:63:LYS:N	0.47	2.24
1:A:251:GLU:OE1	1:A:252:ALA:N	0.47	2.47
1:A:320:HIS:O	1:A:322:GLU:N	0.47	2.45
1:A:202:ASP:OD1	1:A:203:ARG:N	0.47	2.48
1:A:192:GLU:O	1:A:196:SER:OG	0.46	2.29
1:A:271:LEU:HD12	1:A:271:LEU:O	0.46	2.10
1:A:149:VAL:CG2	1:A:150:HIS:N	0.46	2.77
1:A:57:LEU:O	1:A:60:LYS:CG	0.46	2.63
1:A:152:TYR:CE1	1:A:193:LYS:HE2	0.46	2.44
1:A:156:LEU:CD1	1:A:156:LEU:C	0.46	2.69
1:A:195:ARG:NH1	1:A:199:GLN:CD	0.46	2.68
1:A:57:LEU:HD13	1:A:57:LEU:C	0.46	2.30
1:A:260:TYR:O	1:A:264:LEU:CB	0.46	2.64
1:A:90:LEU:HD12	1:A:90:LEU:N	0.46	2.25
1:A:60:LYS:HG3	1:A:61:LYS:N	0.46	2.26
1:A:184:HIS:HA	1:A:187:HIS:CD2	0.46	2.45
1:A:152:TYR:CE1	1:A:193:LYS:HE3	0.46	2.45
1:A:34:ARG:CD	1:A:34:ARG:O	0.46	2.64
1:A:105:SER:OG	1:A:151:GLU:OE2	0.46	2.33
1:A:239:GLU:OE1	1:A:322:GLU:N	0.46	2.48
1:A:31:LYS:O	1:A:35:LEU:HD13	0.46	2.10
1:A:168:ASN:OD1	1:A:169:VAL:N	0.46	2.48
1:A:4:GLU:O	1:A:6:ASN:N	0.46	2.49
1:A:121:TRP:CE2	1:A:135:LEU:CD1	0.45	2.95
1:A:179:LYS:HB2	1:A:179:LYS:NZ	0.45	2.26
1:A:257:HIS:CD2	1:A:261:GLN:CG	0.45	3.00
1:A:140:ARG:O	1:A:144:HIS:CB	0.45	2.63
1:A:239:GLU:OE2	1:A:239:GLU:N	0.45	2.49
1:A:192:GLU:O	1:A:195:ARG:HG3	0.45	2.11
1:A:139:TRP:HA	1:A:139:TRP:CE3	0.45	2.45

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:281:GLU:N	1:A:282:ARG:HH21	0.45	2.04
1:A:194:LEU:O	1:A:194:LEU:HD12	0.45	2.12
1:A:227:TRP:CD1	1:A:227:TRP:N	0.45	2.78
1:A:257:HIS:O	1:A:261:GLN:CG	0.45	2.65
1:A:107:THR:CG2	1:A:108:GLN:N	0.45	2.78
1:A:107:THR:HG22	1:A:108:GLN:H	0.44	1.72
1:A:232:SER:O	1:A:234:ASN:N	0.44	2.47
1:A:121:TRP:NE1	1:A:125:LYS:HE3	0.44	2.28
1:A:111:GLY:C	1:A:112:LEU:HD22	0.44	2.32
1:A:186:ARG:O	1:A:190:LEU:HD23	0.44	2.11
1:A:130:PHE:O	1:A:135:LEU:HG	0.44	2.12
1:A:236:THR:OG1	1:A:239:GLU:CG	0.44	2.65
1:A:317:ARG:O	1:A:318:ALA:HB3	0.44	2.13
1:A:223:VAL:O	1:A:225:ASP:N	0.44	2.50
1:A:279:ASP:OD1	1:A:279:ASP:C	0.44	2.56
1:A:201:LEU:C	1:A:201:LEU:CD1	0.44	2.77
1:A:181:SER:O	1:A:184:HIS:CD2	0.44	2.71
1:A:247:LEU:O	1:A:250:PHE:N	0.44	2.51
1:A:81:LEU:C	1:A:81:LEU:HD13	0.44	2.32
1:A:182:VAL:C	1:A:184:HIS:N	0.43	2.71
1:A:139:TRP:O	1:A:140:ARG:C	0.43	2.55
1:A:223:VAL:C	1:A:225:ASP:N	0.43	2.71
1:A:182:VAL:O	1:A:184:HIS:N	0.43	2.51
1:A:220:GLU:CD	1:A:220:GLU:O	0.43	2.56
1:A:199:GLN:O	1:A:202:ASP:CG	0.43	2.57
1:A:229:LEU:C	1:A:231:GLN:N	0.43	2.71
1:A:126:THR:C	1:A:128:GLY:N	0.43	2.70
1:A:147:GLU:HA	1:A:150:HIS:NE2	0.43	2.28
1:A:257:HIS:NE2	1:A:261:GLN:HG3	0.43	2.29
1:A:27:GLN:HG3	1:A:28:LEU:N	0.43	2.28
1:A:121:TRP:CD2	1:A:135:LEU:HD22	0.43	2.47
1:A:126:THR:O	1:A:128:GLY:N	0.43	2.52
1:A:150:HIS:O	1:A:154:VAL:CG2	0.43	2.56
1:A:178:ILE:CG2	1:A:179:LYS:H	0.42	2.27
1:A:254:ILE:HG23	1:A:255:GLU:H	0.42	1.72
1:A:130:PHE:CD2	1:A:134:GLU:HB3	0.42	2.48
1:A:59:TRP:HA	1:A:62:LEU:HD23	0.42	1.90
1:A:127:SER:O	1:A:212:TYR:CZ	0.42	2.72
1:A:245:GLU:HG3	1:A:246:GLU:N	0.42	2.30
1:A:121:TRP:CD1	1:A:125:LYS:HE3	0.42	2.50
1:A:175:LEU:HD11	1:A:183:LEU:CD2	0.42	2.45
1:A:104:LEU:C	1:A:104:LEU:CD2	0.42	2.88

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:121:TRP:CD1	1:A:121:TRP:C	0.42	2.93
1:A:179:LYS:HZ3	1:A:179:LYS:CB	0.42	2.28
1:A:210:GLN:C	1:A:212:TYR:N	0.42	2.73
1:A:274:ALA:O	1:A:277:VAL:HG12	0.42	2.15
1:A:139:TRP:O	1:A:143:LEU:CG	0.41	2.68
1:A:147:GLU:HA	1:A:150:HIS:CD2	0.41	2.50
1:A:29:TRP:NE1	1:A:33:GLN:CD	0.41	2.73
1:A:220:GLU:N	1:A:221:PRO:CD	0.41	2.82
1:A:140:ARG:O	1:A:144:HIS:HB2	0.41	2.15
1:A:282:ARG:O	1:A:286:SER:CB	0.41	2.67
1:A:139:TRP:O	1:A:143:LEU:HG	0.41	2.15
1:A:322:GLU:O	1:A:323:LEU:O	0.41	2.39
1:A:52:GLN:O	1:A:55:ASP:OD2	0.41	2.39
1:A:156:LEU:CG	1:A:157:GLU:N	0.41	2.82
1:A:238:LYS:O	1:A:239:GLU:C	0.41	2.59
1:A:130:PHE:O	1:A:135:LEU:CG	0.41	2.68
1:A:139:TRP:C	1:A:143:LEU:CD2	0.41	2.89
1:A:147:GLU:O	1:A:151:GLU:HB2	0.41	2.16
1:A:187:HIS:CG	1:A:188:THR:N	0.41	2.87
1:A:184:HIS:CD2	1:A:184:HIS:N	0.41	2.89
1:A:223:VAL:O	1:A:226:LEU:N	0.41	2.54
1:A:296:ARG:HG3	1:A:297:THR:N	0.41	2.31
1:A:161:ARG:C	1:A:163:GLU:N	0.41	2.74
1:A:206:ARG:O	1:A:210:GLN:CB	0.41	2.68
1:A:229:LEU:HG	1:A:230:ALA:N	0.41	2.31
1:A:123:LYS:O	1:A:127:SER:HB2	0.41	2.15
1:A:229:LEU:CD1	1:A:229:LEU:C	0.41	2.85
1:A:159:LEU:HD12	1:A:160:SER:CA	0.40	2.45
1:A:168:ASN:CG	1:A:169:VAL:N	0.40	2.74
1:A:292:LEU:HG	1:A:293:LEU:N	0.40	2.31
1:A:191:LYS:O	1:A:195:ARG:CB	0.40	2.69
1:A:121:TRP:HB2	1:A:139:TRP:CH2	0.40	2.52
1:A:227:TRP:O	1:A:243:PHE:CE2	0.40	2.75
1:A:250:PHE:O	1:A:251:GLU:C	0.40	2.59
1:A:247:LEU:O	1:A:248:LYS:C	0.40	2.59
1:A:27:GLN:CG	1:A:28:LEU:N	0.40	2.84
1:A:227:TRP:O	1:A:243:PHE:CZ	0.40	2.75
1:A:70:ASP:C	1:A:72:GLU:H	0.40	2.20
1:A:153:ASN:ND2	1:A:153:ASN:N	0.40	2.70

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	321/323 (99%)	223 (69%)	62 (19%)	36 (11%)	1	8
All	All	321/323 (99%)	223 (69%)	62 (19%)	36 (11%)	1	8

All 36 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	128	GLY
1	A	316	SER
1	A	5	LYS
1	A	129	LYS
1	A	108	GLN
1	A	38	PRO
1	A	216	ALA
1	A	173	SER
1	A	130	PHE
1	A	70	ASP
1	A	234	ASN
1	A	279	ASP
1	A	238	LYS
1	A	223	VAL
1	A	177	ASP
1	A	241	GLU
1	A	36	HIS
1	A	240	LEU
1	A	319	ARG
1	A	181	SER
1	A	180	GLY
1	A	101	SER
1	A	166	HIS
1	A	219	GLU
1	A	284	SER
1	A	315	ILE
1	A	317	ARG

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Mol	Chain	Res	Type
1	A	224	ILE
1	A	107	THR
1	A	176	SER
1	A	110	ASP
1	A	321	ASN
1	A	230	ALA
1	A	162	THR
1	A	322	GLU
1	A	91	ASP

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	289/289 (100%)	237 (82%)	52 (18%)	5	40
All	All	289/289 (100%)	237 (82%)	52 (18%)	5	40

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

Mol	Chain	Res	Type
1	A	292	LEU
1	A	62	LEU
1	A	184	HIS
1	A	167	GLU
1	A	179	LYS
1	A	282	ARG
1	A	254	ILE
1	A	146	LYS
1	A	253	LYS
1	A	203	ARG
1	A	239	GLU
1	A	261	GLN
1	A	171	SER
1	A	14	ARG
1	A	148	LYS
1	A	7	GLN

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Mol	Chain	Res	Type
1	A	296	ARG
1	A	194	LEU
1	A	220	GLU
1	A	175	LEU
1	A	300	LEU
1	A	270	LYS
1	A	123	LYS
1	A	234	ASN
1	A	208	SER
1	A	195	ARG
1	A	204	LEU
1	A	228	ASP
1	A	294	GLU
1	A	319	ARG
1	A	187	HIS
1	A	223	VAL
1	A	323	LEU
1	A	166	HIS
1	A	289	LYS
1	A	81	LEU
1	A	34	ARG
1	A	193	LYS
1	A	76	ARG
1	A	116	ARG
1	A	201	LEU
1	A	139	TRP
1	A	142	PHE
1	A	156	LEU
1	A	202	ASP
1	A	55	ASP
1	A	236	THR
1	A	143	LEU
1	A	243	PHE
1	A	57	LEU
1	A	150	HIS
1	A	119	LYS

6.3.3 RNA ⓘ

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