



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 07:32 PM UTC

PDB ID : 2P03 / pdb_00002p03
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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

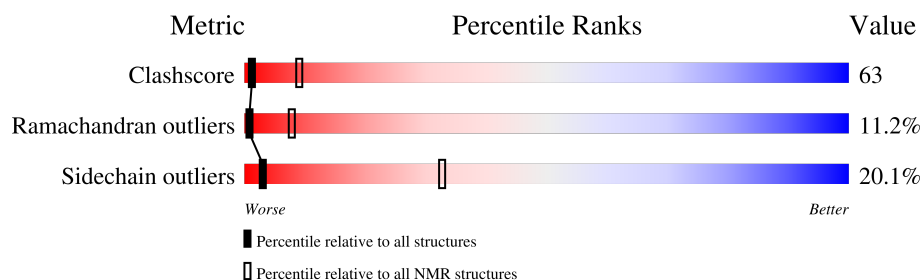
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	34% 43% 22% .

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.

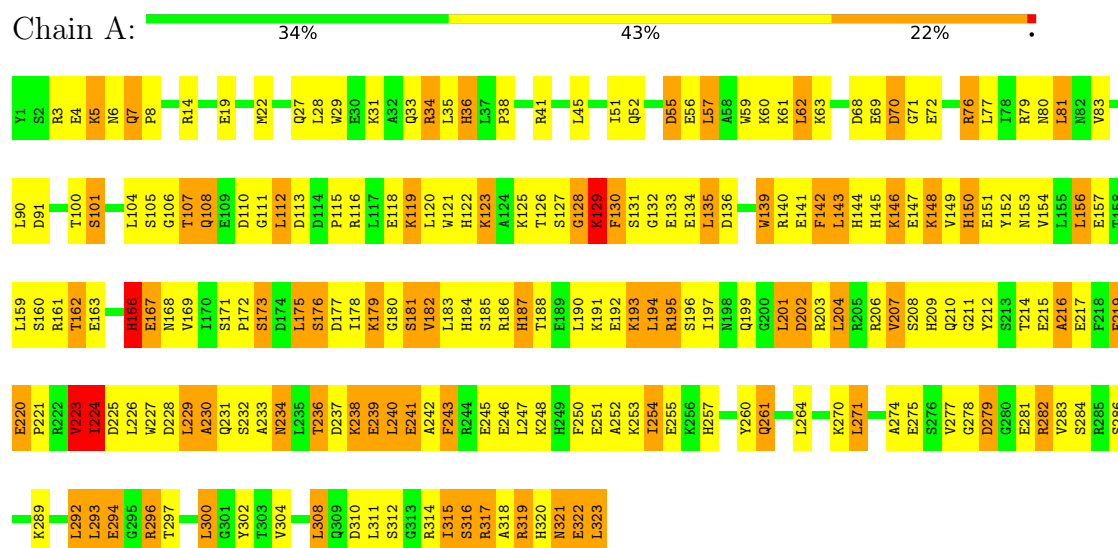
- Molecule 1 is a protein called Alpha-2-macroglobulin receptor-associated protein.

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, DNA and oligosaccharide 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.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.63	0/2713 (0.0%)	1.07	1/3636 (0.0%)
All	All	0.63	0/2713 (0.0%)	1.07	1/3636 (0.0%)

There are no bond-length outliers.

All angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	HIS	CA-CB-CG	-5.12	108.68	113.80

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	2666	2659	2661	334
All	All	2666	2659	2661	334

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 63.

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:156:LEU:C	1:A:156:LEU:HD12	0.82	2.00
1:A:323:LEU:C	1:A:323:LEU:HD23	0.81	2.00
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:141:GLU:CD	1:A:204:LEU:HD21	0.80	2.01
1:A:194:LEU:HD12	1:A:194:LEU:C	0.80	2.01
1:A:223:VAL:HG11	1:A:308:LEU:CD2	0.76	2.11
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
1:A:121:TRP:CE2	1:A:135:LEU:HD13	0.74	2.18
1:A:29:TRP:NE1	1:A:33:GLN:NE2	0.73	2.36
1:A:145:HIS:O	1:A:149:VAL:HG22	0.73	1.82
1:A:282:ARG:H	1:A:282:ARG:NE	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:187:HIS:ND1	1:A:187:HIS:C	0.70	2.48
1:A:201:LEU:C	1:A:201:LEU:HD12	0.70	2.11
1:A:195:ARG:HH11	1:A:199:GLN:NE2	0.70	1.85
1:A:243:PHE:CD1	1:A:243:PHE:C	0.70	2.69
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:55:ASP:CG	1:A:56:GLU:N	0.69	2.50
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:79:ARG:O	1:A:83:VAL:HG23	0.68	1.88
1:A:139:TRP:O	1:A:143:LEU:CD2	0.68	2.42
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:147:GLU:CD	1:A:148:LYS:N	0.67	2.53
1:A:292:LEU:HD12	1:A:292:LEU:C	0.67	2.14
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:257:HIS:NE2	1:A:261:GLN:OE1	0.66	2.27
1:A:62:LEU:HD12	1:A:62:LEU:C	0.66	2.16
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: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:202:ASP:OD1	1:A:202:ASP:C	0.64	2.40
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:N	1:A:112:LEU:CD2	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:251:GLU:CD	1:A:252:ALA:N	0.63	2.56
1:A:292:LEU:HD12	1:A:292:LEU:O	0.63	1.94
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:145:HIS:O	1:A:149:VAL:CG1	0.62	2.47
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:240:LEU:O	1:A:241:GLU:C	0.62	2.43
1:A:254:ILE:HG23	1:A:255:GLU:N	0.61	2.10
1:A:229:LEU:C	1:A:229:LEU:HD12	0.61	2.20
1:A:14:ARG:N	1:A:14:ARG:NE	0.60	2.49
1:A:134:GLU:CD	1:A:134:GLU:H	0.60	2.04
1:A:179:LYS:NZ	1:A:179:LYS:CB	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:159:LEU:HD12	1:A:159:LEU:C	0.59	2.22
1:A:69:GLU:C	1:A:71:GLY:H	0.59	2.05
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:314:ARG:O	1:A:315:ILE:C	0.59	2.44
1:A:251:GLU:C	1:A:251:GLU:OE1	0.59	2.46
1:A:132:GLY:O	1:A:136:ASP:CG	0.59	2.46

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:112:LEU:O	1:A:118:GLU:CD	0.58	2.46
1:A:147:GLU:O	1:A:150:HIS:CD2	0.58	2.55
1:A:182:VAL:C	1:A:184:HIS:H	0.58	2.05
1:A:206:ARG:O	1:A:210:GLN:N	0.58	2.37
1:A:104:LEU:C	1:A:104:LEU:HD23	0.58	2.23
1:A:69:GLU:C	1:A:71:GLY:N	0.58	2.58
1:A:214:THR:CG2	1:A:215:GLU:H	0.58	2.12
1:A:168:ASN:CG	1:A:169:VAL:H	0.57	2.06
1:A:282:ARG:HE	1:A:283:VAL:N	0.57	1.97
1:A:315:ILE:O	1:A:316:SER:C	0.57	2.46
1:A:62:LEU:CD1	1:A:68:ASP:N	0.57	2.67
1:A:156:LEU:C	1:A:156:LEU:CD1	0.57	2.69
1:A:214:THR:CG2	1:A:215:GLU:N	0.57	2.67
1:A:147:GLU:OE1	1:A:147:GLU:C	0.57	2.46
1:A:282:ARG:NE	1:A:282:ARG:N	0.57	2.52
1:A:106:GLY:O	1:A:107:THR:O	0.57	2.22
1:A:14:ARG:H	1:A:14:ARG:HE	0.56	1.43
1:A:282:ARG:O	1:A:286:SER:OG	0.56	2.22
1:A:56:GLU:CG	1:A:57:LEU:N	0.56	2.67
1:A:239:GLU:OE1	1:A:320:HIS:O	0.56	2.22
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
1:A:14:ARG:NE	1:A:14:ARG:H	0.56	1.98
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:187:HIS:CE1	1:A:188:THR:OG1	0.56	2.58
1:A:210:GLN:C	1:A:212:TYR:H	0.56	2.08
1:A:296:ARG:C	1:A:296:ARG:CD	0.56	2.79
1:A:57:LEU:C	1:A:57:LEU:CD1	0.56	2.78
1:A:223:VAL:HG23	1:A:224:ILE:H	0.56	1.60
1:A:271:LEU:C	1:A:271:LEU:HD12	0.56	2.26
1:A:100:THR:O	1:A:101:SER:O	0.56	2.23
1:A:292:LEU:C	1:A:292:LEU:CD1	0.56	2.78
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:55:ASP:OD1	1:A:55:ASP:C	0.55	2.48
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:175:LEU:O	1:A:176:SER:O	0.55	2.23
1:A:229:LEU:O	1:A:230:ALA:C	0.55	2.50
1:A:233:ALA:O	1:A:234:ASN:C	0.55	2.50
1:A:150:HIS:CD2	1:A:150:HIS:C	0.55	2.85
1:A:316:SER:O	1:A:318:ALA:N	0.55	2.39
1:A:294:GLU:OE1	1:A:294:GLU:O	0.54	2.25
1:A:323:LEU:C	1:A:323:LEU:CD2	0.54	2.69
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:168:ASN:O	1:A:169:VAL:CG2	0.54	2.55
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:194:LEU:C	1:A:194:LEU:CD1	0.54	2.70
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:O	1:A:150:HIS:HD2	0.53	1.87
1:A:81:LEU:HD13	1:A:81:LEU:O	0.53	2.04
1:A:236:THR:O	1:A:237:ASP:C	0.52	2.52
1:A:62:LEU:HD12	1:A:62:LEU:O	0.52	2.05
1:A:62:LEU:C	1:A:62:LEU:CD1	0.52	2.81
1:A:184:HIS:CG	1:A:185:SER:N	0.52	2.78
1:A:81:LEU:CD1	1:A:81:LEU:C	0.52	2.82
1:A:115:PRO:O	1:A:119:LYS:CG	0.52	2.57
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:195:ARG:NH1	1:A:199:GLN:CD	0.51	2.68
1:A:257:HIS:NE2	1:A:261:GLN:CG	0.51	2.73
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:57:LEU:C	1:A:57:LEU:HD13	0.51	2.30
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:172:PRO:O	1:A:173:SER:OG	0.50	2.26
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:22:MET:CE	1:A:56:GLU:OE2	0.50	2.59
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:166:HIS:O	1:A:167:GLU:HG2	0.50	2.07
1:A:90:LEU:N	1:A:90:LEU:CD1	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:41:ARG:O	1:A:45:LEU:CB	0.49	2.60
1:A:260:TYR:CD1	1:A:293:LEU:HD11	0.49	2.43
1:A:14:ARG:N	1:A:14:ARG:CD	0.49	2.76
1:A:81:LEU:HD13	1:A:81:LEU:C	0.49	2.32
1:A:111:GLY:C	1:A:112:LEU:HD22	0.49	2.32
1:A:192:GLU:O	1:A:196:SER:OG	0.49	2.29
1:A:51:ILE:HD13	1:A:51:ILE:N	0.49	2.23
1:A:156:LEU:HG	1:A:157:GLU:N	0.49	2.23
1:A:254:ILE:CG2	1:A:255:GLU:N	0.49	2.76
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: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:182:VAL:C	1:A:184:HIS:N	0.48	2.71
1:A:201:LEU:C	1:A:201:LEU:CD1	0.48	2.77
1:A:14:ARG:N	1:A:14:ARG:HE	0.48	2.04
1:A:250:PHE:O	1:A:253:LYS:N	0.48	2.45
1:A:139:TRP:O	1:A:140:ARG:C	0.48	2.55
1:A:220:GLU:O	1:A:220:GLU:CD	0.48	2.56
1:A:126:THR:C	1:A:128:GLY:N	0.48	2.70
1:A:199:GLN:O	1:A:202:ASP:CG	0.48	2.57
1:A:139:TRP:CZ3	1:A:142:PHE:CD2	0.48	3.02
1:A:314:ARG:O	1:A:323:LEU:HD11	0.48	2.09
1:A:156:LEU:O	1:A:160:SER:OG	0.47	2.30
1:A:260:TYR:CE1	1:A:293:LEU:HD11	0.47	2.44
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:223:VAL:C	1:A:225:ASP:N	0.47	2.71
1:A:279:ASP:OD1	1:A:279:ASP:C	0.47	2.56
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:57:LEU:HD13	1:A:57:LEU:O	0.47	2.10
1:A:62:LEU:HG	1:A:63:LYS:N	0.47	2.24
1:A:243:PHE:O	1:A:247:LEU:HD23	0.47	2.09
1:A:220:GLU:CD	1:A:220:GLU:C	0.47	2.82

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:251:GLU:OE1	1:A:252:ALA:N	0.47	2.47
1:A:202:ASP:OD1	1:A:203:ARG:N	0.47	2.48
1:A:320:HIS:O	1:A:322:GLU:N	0.47	2.45
1:A:271:LEU:HD12	1:A:271:LEU:O	0.46	2.10
1:A:57:LEU:O	1:A:60:LYS:CG	0.46	2.63
1:A:121:TRP:CD1	1:A:121:TRP:C	0.46	2.93
1:A:149:VAL:CG2	1:A:150:HIS:N	0.46	2.77
1:A:210:GLN:C	1:A:212:TYR:N	0.46	2.73
1:A:152:TYR:CE1	1:A:193:LYS:HE2	0.46	2.44
1:A:229:LEU:C	1:A:231:GLN:N	0.46	2.71
1:A:29:TRP:NE1	1:A:33:GLN:CD	0.46	2.73
1:A:90:LEU:N	1:A:90:LEU:HD12	0.46	2.25
1:A:260:TYR:O	1:A:264:LEU:CB	0.46	2.64
1:A:60:LYS:HG3	1:A:61:LYS:N	0.46	2.26
1:A:34:ARG:O	1:A:34:ARG:CD	0.46	2.64
1:A:152:TYR:CE1	1:A:193:LYS:HE3	0.46	2.45
1:A:184:HIS:HA	1:A:187:HIS:CD2	0.46	2.45
1:A:104:LEU:C	1:A:104:LEU:CD2	0.46	2.88
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:4:GLU:O	1:A:6:ASN:N	0.46	2.49
1:A:139:TRP:C	1:A:143:LEU:CD2	0.46	2.89
1:A:168:ASN:OD1	1:A:169:VAL:N	0.46	2.48
1:A:238:LYS:O	1:A:239:GLU:C	0.46	2.59
1:A:161:ARG:C	1:A:163:GLU:N	0.45	2.74
1:A:121:TRP:CE2	1:A:135:LEU:CD1	0.45	2.95
1:A:179:LYS:NZ	1:A:179:LYS:HB2	0.45	2.26
1:A:229:LEU:C	1:A:229:LEU:CD1	0.45	2.85
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:192:GLU:O	1:A:195:ARG:HG3	0.45	2.11
1:A:239:GLU:OE2	1:A:239:GLU:N	0.45	2.49
1:A:139:TRP:CE3	1:A:139:TRP:HA	0.45	2.45
1:A:281:GLU:N	1:A:282:ARG:HH21	0.45	2.04
1:A:194:LEU:HD12	1:A:194:LEU:O	0.45	2.12
1:A:227:TRP:N	1:A:227:TRP:CD1	0.45	2.78
1:A:250:PHE:O	1:A:251:GLU:C	0.45	2.59
1:A:107:THR:CG2	1:A:108:GLN:N	0.45	2.78
1:A:247:LEU:O	1:A:248:LYS:C	0.45	2.59
1:A:257:HIS:O	1:A:261:GLN:CG	0.45	2.65
1:A:76:ARG:C	1:A:76:ARG:CD	0.45	2.90

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:129:LYS:C	1:A:131:SER:N	0.45	2.75
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:186:ARG:O	1:A:190:LEU:HD23	0.44	2.11
1:A:257:HIS:NE2	1:A:261:GLN:CD	0.44	2.74
1:A:100:THR:C	1:A:101:SER:O	0.44	2.61
1:A:106:GLY:C	1:A:107:THR:O	0.44	2.61
1:A:161:ARG:C	1:A:163:GLU:H	0.44	2.17
1:A:312:SER:C	1:A:314:ARG:N	0.44	2.76
1:A:70:ASP:C	1:A:72:GLU:H	0.44	2.20
1:A:130:PHE:O	1:A:135:LEU:HG	0.44	2.12
1:A:223:VAL:O	1:A:225:ASP:N	0.44	2.50
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: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:294:GLU:O	1:A:294:GLU:CD	0.44	2.61
1:A:3:ARG:C	1:A:5:LYS:H	0.43	2.21
1:A:182:VAL:O	1:A:184:HIS:N	0.43	2.51
1:A:146:LYS:HZ2	1:A:146:LYS:HB3	0.43	1.73
1:A:27:GLN:HG3	1:A:28:LEU:N	0.43	2.28
1:A:147:GLU:HA	1:A:150:HIS:NE2	0.43	2.28
1:A:168:ASN:CG	1:A:169:VAL:N	0.43	2.74
1:A:223:VAL:O	1:A:224:ILE:C	0.43	2.61
1:A:257:HIS:NE2	1:A:261:GLN:HG3	0.43	2.29
1:A:320:HIS:C	1:A:322:GLU:H	0.43	2.20
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:144:HIS:O	1:A:147:GLU:CD	0.43	2.61
1:A:237:ASP:O	1:A:238:LYS:C	0.43	2.62
1:A:294:GLU:CD	1:A:294:GLU:C	0.43	2.86
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:59:TRP:HA	1:A:62:LEU:HD23	0.42	1.90
1:A:130:PHE:CD2	1:A:134:GLU:HB3	0.42	2.48
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:250:PHE:CD1	1:A:250:PHE:C	0.42	2.97
1:A:271:LEU:C	1:A:271:LEU:CD1	0.42	2.88

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:70:ASP:C	1:A:72:GLU:N	0.42	2.76
1:A:105:SER:OG	1:A:151:GLU:CD	0.42	2.63
1:A:126:THR:O	1:A:127:SER:C	0.42	2.63
1:A:175:LEU:HD11	1:A:183:LEU:CD2	0.42	2.45
1:A:179:LYS:CB	1:A:179:LYS:HZ3	0.42	2.28
1:A:274:ALA:O	1:A:277:VAL:HG12	0.42	2.15
1:A:302:TYR:CD2	1:A:302:TYR:C	0.42	2.96
1:A:168:ASN:C	1:A:169:VAL:HG23	0.41	2.39
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: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:207:VAL:C	1:A:211:GLY:H	0.41	2.24
1:A:52:GLN:O	1:A:55:ASP:OD2	0.41	2.39
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:156:LEU:CG	1:A:157:GLU:N	0.41	2.82
1:A:130:PHE:O	1:A:135:LEU:CG	0.41	2.68
1:A:147:GLU:O	1:A:151:GLU:HB2	0.41	2.16
1:A:184:HIS:CD2	1:A:184:HIS:N	0.41	2.89
1:A:187:HIS:CG	1:A:188:THR:N	0.41	2.87
1:A:206:ARG:O	1:A:210:GLN:CB	0.41	2.68
1:A:223:VAL:O	1:A:226:LEU:N	0.41	2.54
1:A:229:LEU:HG	1:A:230:ALA:N	0.41	2.31
1:A:296:ARG:HG3	1:A:297:THR:N	0.41	2.31
1:A:310:ASP:O	1:A:311:LEU:C	0.41	2.63
1:A:123:LYS:O	1:A:127:SER:HB2	0.41	2.15
1:A:133:GLU:CD	1:A:133:GLU:N	0.40	2.78
1:A:159:LEU:HD12	1:A:160:SER:CA	0.40	2.45
1:A:191:LYS:O	1:A:195:ARG:CB	0.40	2.69
1:A:202:ASP:CG	1:A:203:ARG:N	0.40	2.78
1:A:121:TRP:HB2	1:A:139:TRP:CH2	0.40	2.52
1:A:149:VAL:O	1:A:153:ASN:CG	0.40	2.64
1:A:227:TRP:O	1:A:243:PHE:CE2	0.40	2.75
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

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	5	LYS
1	A	36	HIS
1	A	38	PRO
1	A	70	ASP
1	A	91	ASP
1	A	101	SER
1	A	107	THR
1	A	108	GLN
1	A	110	ASP
1	A	128	GLY
1	A	129	LYS
1	A	130	PHE
1	A	162	THR
1	A	166	HIS
1	A	173	SER
1	A	176	SER
1	A	177	ASP
1	A	180	GLY
1	A	181	SER
1	A	216	ALA
1	A	219	GLU
1	A	223	VAL
1	A	224	ILE
1	A	230	ALA
1	A	234	ASN
1	A	238	LYS
1	A	240	LEU

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Mol	Chain	Res	Type
1	A	241	GLU
1	A	279	ASP
1	A	284	SER
1	A	315	ILE
1	A	316	SER
1	A	317	ARG
1	A	319	ARG
1	A	321	ASN
1	A	322	GLU

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%)	231 (80%)	58 (20%)	3	33
All	All	289/289 (100%)	231 (80%)	58 (20%)	3	33

All 58 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	7	GLN
1	A	34	ARG
1	A	55	ASP
1	A	57	LEU
1	A	62	LEU
1	A	76	ARG
1	A	81	LEU
1	A	112	LEU
1	A	116	ARG
1	A	119	LYS
1	A	123	LYS
1	A	129	LYS
1	A	135	LEU
1	A	139	TRP
1	A	142	PHE
1	A	143	LEU

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Mol	Chain	Res	Type
1	A	146	LYS
1	A	148	LYS
1	A	156	LEU
1	A	166	HIS
1	A	167	GLU
1	A	171	SER
1	A	175	LEU
1	A	179	LYS
1	A	182	VAL
1	A	187	HIS
1	A	193	LYS
1	A	194	LEU
1	A	195	ARG
1	A	201	LEU
1	A	202	ASP
1	A	204	LEU
1	A	207	VAL
1	A	208	SER
1	A	209	HIS
1	A	220	GLU
1	A	223	VAL
1	A	224	ILE
1	A	228	ASP
1	A	229	LEU
1	A	236	THR
1	A	239	GLU
1	A	243	PHE
1	A	254	ILE
1	A	261	GLN
1	A	270	LYS
1	A	271	LEU
1	A	282	ARG
1	A	289	LYS
1	A	292	LEU
1	A	293	LEU
1	A	294	GLU
1	A	296	ARG
1	A	300	LEU
1	A	304	VAL
1	A	308	LEU
1	A	319	ARG
1	A	323	LEU

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 oligosaccharides 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