Full wwPDB NMR Structure Validation Report (i)

Jun 16, 2024 – 07:11 AM EDT

PDB ID	:	1SVR
Title	:	STRUCTURE OF SEVERIN DOMAIN 2 IN SOLUTION
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Deposited on	:	1994-10-12

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 (i) 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 (i)) were used in the production of this report:

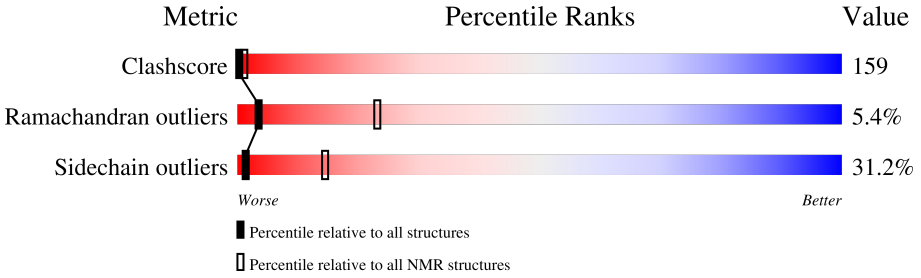
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	114	10% 45% 25% • 18%

2 Ensemble composition and analysis (i)

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 1430 atoms, of which 713 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SEVERIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	94	1430	453	713	121	141	2	0

4 Residue-property plots (i)

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: SEVERIN

Chain A: 10% 45% 25% • 18%

SER GLY PHE ASN HIS VAL LYS PRO THR E158 Y159 K160 P161 R162 L163 L164 H165 I166 S167 G168 D169 K170 N171 A172 K173 V174 A175 E176 V177 P178 L179 A180 T181 S182 S183 L184 N185 S186 G187 D188 C189 F190 L191 L192 D193 A194 G195 L196 T197 I198 Y199 Q200 F201 N202 G203 S204 K205 S206 S207 P208

Q209 E210 K211 N212 K213 A214 V217 A218 R219 A220 I221 D222 A223 E224 R225 K226 G227 L228 P229 E232 V233 F234 C235 E236 T237 D238 S239 D240 I241 P242 A243 E244 F245 W246 K247 L248 L249 G250 G251 LYS GLY ALA ILE ALA ALA LYS HIS GLU THR ALA

5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 1 were deposited, based on the following criterion: *?*.

The authors did not provide any information on software used for structure solution, optimization or refinement.

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	1.57	13/730 (1.8%)	1.35	8/985 (0.8%)
All	All	1.57	13/730 (1.8%)	1.35	8/985 (0.8%)

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
1	A	0	3
All	All	0	3

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	GLU	C-N	-9.13	1.13	1.34
1	A	158	GLU	N-CA	-8.07	1.30	1.46
1	A	159	TYR	N-CA	-7.56	1.31	1.46
1	A	159	TYR	C-N	-7.39	1.17	1.34
1	A	158	GLU	CA-C	-6.79	1.35	1.52
1	A	160	LYS	N-CA	-6.54	1.33	1.46
1	A	158	GLU	CA-CB	-6.41	1.39	1.53
1	A	219	ARG	NE-CZ	-5.95	1.25	1.33
1	A	187	GLY	C-O	-5.67	1.14	1.23
1	A	206	SER	C-N	-5.66	1.21	1.34
1	A	250	GLY	N-CA	5.65	1.54	1.46
1	A	161	PRO	N-CA	-5.60	1.37	1.47
1	A	160	LYS	CA-CB	-5.46	1.42	1.53

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	207	SER	N-CA-CB	-7.75	98.87	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	158	GLU	N-CA-C	-7.20	91.56	111.00
1	A	246	TRP	CA-CB-CG	-6.52	101.31	113.70
1	A	251	GLY	N-CA-C	-6.51	96.82	113.10
1	A	159	TYR	CB-CA-C	6.38	123.16	110.40
1	A	219	ARG	CA-CB-CG	-6.19	99.79	113.40
1	A	159	TYR	CA-CB-CG	-5.70	102.57	113.40
1	A	219	ARG	CG-CD-NE	-5.26	100.76	111.80

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	162	ARG	Sidechain
1	A	219	ARG	Sidechain
1	A	225	ARG	Sidechain

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	717	713	709	227
All	All	717	713	709	227

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 159.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:207:SER:HB2	1:A:208:PRO:HD2	1.04	1.25
1:A:163:LEU:HD11	1:A:249:LEU:HD22	1.03	1.04
1:A:241:ILE:HG23	1:A:246:TRP:CD2	1.01	1.89
1:A:245:PHE:HE1	1:A:249:LEU:HD23	0.99	1.16
1:A:207:SER:CB	1:A:208:PRO:HD2	0.92	1.94
1:A:200:GLN:CB	1:A:233:VAL:HG12	0.92	1.92
1:A:163:LEU:CD1	1:A:249:LEU:HD22	0.90	1.94
1:A:192:LEU:HD12	1:A:192:LEU:C	0.89	1.88

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:187:GLY:CA	1:A:205:LYS:HB2	0.87	2.00
1:A:187:GLY:HA2	1:A:205:LYS:HB2	0.87	1.47
1:A:163:LEU:HG	1:A:179:LEU:HA	0.86	1.48
1:A:172:ALA:HB2	1:A:209:GLN:HB3	0.85	1.46
1:A:202:ASN:C	1:A:235:CYS:HA	0.85	1.90
1:A:163:LEU:O	1:A:177:VAL:HG13	0.84	1.72
1:A:164:LEU:HD13	1:A:165:HIS:N	0.84	1.88
1:A:199:TYR:CD2	1:A:232:GLU:CG	0.84	2.61
1:A:164:LEU:HD12	1:A:166:ILE:HD11	0.83	1.50
1:A:207:SER:CB	1:A:208:PRO:CD	0.83	2.57
1:A:207:SER:HB2	1:A:208:PRO:CD	0.81	2.04
1:A:181:THR:HG21	1:A:250:GLY:HA3	0.81	1.50
1:A:181:THR:HG22	1:A:246:TRP:CE3	0.81	2.10
1:A:200:GLN:HB2	1:A:233:VAL:HG12	0.81	1.51
1:A:245:PHE:CE1	1:A:249:LEU:HD23	0.81	2.08
1:A:174:VAL:HG11	1:A:213:LYS:HG3	0.80	1.53
1:A:202:ASN:HB3	1:A:235:CYS:CB	0.80	2.06
1:A:179:LEU:HD12	1:A:180:ALA:N	0.79	1.92
1:A:199:TYR:CD2	1:A:232:GLU:HG3	0.78	2.13
1:A:249:LEU:HD12	1:A:249:LEU:O	0.78	1.77
1:A:203:GLY:N	1:A:235:CYS:SG	0.77	2.57
1:A:241:ILE:HG23	1:A:246:TRP:CG	0.77	2.15
1:A:163:LEU:HD11	1:A:249:LEU:CD2	0.76	1.99
1:A:164:LEU:HD12	1:A:166:ILE:CD1	0.75	2.10
1:A:187:GLY:O	1:A:206:SER:CB	0.75	2.35
1:A:202:ASN:HB2	1:A:234:PHE:C	0.75	2.01
1:A:166:ILE:HD13	1:A:166:ILE:N	0.75	1.97
1:A:165:HIS:HB2	1:A:177:VAL:HG11	0.74	1.59
1:A:202:ASN:HB3	1:A:235:CYS:SG	0.74	2.22
1:A:180:ALA:O	1:A:184:LEU:HD12	0.74	1.82
1:A:189:CYS:HA	1:A:202:ASN:HA	0.74	1.58
1:A:165:HIS:C	1:A:166:ILE:HD13	0.74	2.03
1:A:201:PHE:CZ	1:A:240:ASP:HB2	0.72	2.20
1:A:202:ASN:HB3	1:A:235:CYS:CA	0.71	2.16
1:A:249:LEU:HD12	1:A:249:LEU:C	0.70	2.06
1:A:200:GLN:NE2	1:A:214:ALA:HB1	0.69	2.01
1:A:166:ILE:HD12	1:A:174:VAL:HG23	0.69	1.63
1:A:199:TYR:CD2	1:A:232:GLU:HG2	0.68	2.22
1:A:164:LEU:CD1	1:A:166:ILE:CD1	0.68	2.71
1:A:167:SER:CB	1:A:188:ASP:CB	0.68	2.71
1:A:241:ILE:HA	1:A:246:TRP:NE1	0.67	2.03
1:A:189:CYS:SG	1:A:202:ASN:CG	0.66	2.73

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:225:ARG:HD3	1:A:229:PRO:HG3	0.66	1.68
1:A:192:LEU:HD12	1:A:192:LEU:O	0.66	1.90
1:A:162:ARG:C	1:A:163:LEU:HD22	0.66	2.10
1:A:205:LYS:HG3	1:A:237:THR:CG2	0.66	2.20
1:A:179:LEU:HD12	1:A:179:LEU:C	0.66	2.10
1:A:192:LEU:C	1:A:192:LEU:CD1	0.66	2.63
1:A:167:SER:HB2	1:A:188:ASP:CB	0.65	2.21
1:A:243:ALA:O	1:A:247:LYS:CB	0.65	2.45
1:A:166:ILE:HG21	1:A:214:ALA:HB2	0.65	1.66
1:A:188:ASP:HA	1:A:206:SER:OG	0.64	1.92
1:A:200:GLN:HB3	1:A:233:VAL:HG12	0.64	1.67
1:A:181:THR:OG1	1:A:250:GLY:CA	0.64	2.46
1:A:166:ILE:HD12	1:A:174:VAL:CG2	0.63	2.22
1:A:241:ILE:HG23	1:A:246:TRP:CE2	0.63	2.28
1:A:245:PHE:CD1	1:A:245:PHE:C	0.63	2.71
1:A:243:ALA:O	1:A:247:LYS:HB2	0.62	1.94
1:A:200:GLN:HE21	1:A:214:ALA:HB1	0.62	1.54
1:A:163:LEU:CG	1:A:179:LEU:HA	0.62	2.22
1:A:181:THR:CG2	1:A:250:GLY:HA3	0.62	2.24
1:A:225:ARG:HB3	1:A:229:PRO:HD3	0.62	1.71
1:A:202:ASN:CB	1:A:235:CYS:CA	0.62	2.78
1:A:225:ARG:CD	1:A:229:PRO:HG3	0.61	2.25
1:A:187:GLY:O	1:A:206:SER:HB3	0.61	1.95
1:A:228:LEU:HB3	1:A:229:PRO:HD3	0.60	1.73
1:A:165:HIS:CB	1:A:177:VAL:HG11	0.60	2.25
1:A:191:LEU:CD1	1:A:198:ILE:CG2	0.60	2.80
1:A:205:LYS:CG	1:A:237:THR:HG21	0.60	2.26
1:A:165:HIS:NE2	1:A:185:ASN:ND2	0.59	2.50
1:A:191:LEU:CD1	1:A:198:ILE:HG23	0.59	2.27
1:A:163:LEU:HG	1:A:179:LEU:CA	0.59	2.25
1:A:163:LEU:HB3	1:A:177:VAL:HG22	0.59	1.75
1:A:187:GLY:O	1:A:206:SER:N	0.59	2.36
1:A:205:LYS:HG3	1:A:237:THR:HG21	0.58	1.72
1:A:181:THR:OG1	1:A:250:GLY:HA2	0.58	1.98
1:A:213:LYS:O	1:A:217:VAL:HG23	0.58	1.99
1:A:228:LEU:N	1:A:229:PRO:CD	0.58	2.66
1:A:166:ILE:CD1	1:A:166:ILE:N	0.58	2.66
1:A:241:ILE:CG2	1:A:246:TRP:CG	0.57	2.85
1:A:159:TYR:HB3	1:A:195:GLY:CA	0.57	2.29
1:A:167:SER:HB2	1:A:188:ASP:CG	0.57	2.20
1:A:202:ASN:CB	1:A:235:CYS:HA	0.57	2.29
1:A:246:TRP:O	1:A:251:GLY:N	0.57	2.38

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:174:VAL:HG11	1:A:213:LYS:CG	0.57	2.28
1:A:226:LYS:HD2	1:A:226:LYS:N	0.56	2.16
1:A:205:LYS:N	1:A:237:THR:CG2	0.56	2.69
1:A:225:ARG:HB3	1:A:229:PRO:CD	0.56	2.31
1:A:171:ASN:O	1:A:173:LYS:CG	0.56	2.53
1:A:226:LYS:N	1:A:226:LYS:CD	0.56	2.68
1:A:206:SER:OG	1:A:210:GLU:CG	0.56	2.54
1:A:228:LEU:N	1:A:229:PRO:HD2	0.55	2.16
1:A:165:HIS:NE2	1:A:167:SER:OG	0.55	2.40
1:A:167:SER:HB3	1:A:188:ASP:HB2	0.55	1.78
1:A:187:GLY:HA2	1:A:205:LYS:CB	0.55	2.29
1:A:233:VAL:C	1:A:234:PHE:HD1	0.55	2.05
1:A:165:HIS:CE1	1:A:167:SER:HG	0.55	2.20
1:A:174:VAL:CG1	1:A:213:LYS:CG	0.55	2.85
1:A:201:PHE:CE1	1:A:240:ASP:HB2	0.55	2.37
1:A:165:HIS:O	1:A:174:VAL:HG23	0.55	2.01
1:A:199:TYR:CE2	1:A:232:GLU:HG3	0.55	2.37
1:A:171:ASN:O	1:A:173:LYS:HG2	0.55	2.01
1:A:234:PHE:CD1	1:A:234:PHE:N	0.55	2.75
1:A:246:TRP:N	1:A:246:TRP:CD1	0.55	2.75
1:A:202:ASN:CB	1:A:235:CYS:SG	0.54	2.95
1:A:166:ILE:HG21	1:A:210:GLU:O	0.54	2.03
1:A:233:VAL:C	1:A:234:PHE:CD1	0.54	2.81
1:A:172:ALA:C	1:A:173:LYS:HG2	0.54	2.21
1:A:247:LYS:HA	1:A:251:GLY:H	0.54	1.63
1:A:187:GLY:HA3	1:A:205:LYS:HB2	0.54	1.78
1:A:181:THR:N	1:A:249:LEU:HD11	0.53	2.18
1:A:196:LEU:O	1:A:229:PRO:CB	0.53	2.57
1:A:161:PRO:HA	1:A:193:ASP:O	0.53	2.03
1:A:162:ARG:O	1:A:163:LEU:HD22	0.52	2.04
1:A:174:VAL:CG1	1:A:213:LYS:HG3	0.52	2.32
1:A:202:ASN:O	1:A:235:CYS:HA	0.52	2.03
1:A:179:LEU:C	1:A:179:LEU:CD1	0.52	2.76
1:A:166:ILE:HG21	1:A:214:ALA:N	0.52	2.20
1:A:166:ILE:HG21	1:A:214:ALA:CB	0.52	2.35
1:A:205:LYS:N	1:A:237:THR:HG21	0.52	2.20
1:A:167:SER:HB3	1:A:188:ASP:CB	0.51	2.34
1:A:217:VAL:HG12	1:A:221:ILE:HD11	0.51	1.82
1:A:196:LEU:O	1:A:229:PRO:HB2	0.51	2.05
1:A:189:CYS:SG	1:A:202:ASN:CB	0.51	2.99
1:A:167:SER:O	1:A:173:LYS:O	0.51	2.29
1:A:189:CYS:SG	1:A:202:ASN:ND2	0.50	2.84

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:163:LEU:HB2	1:A:178:PRO:O	0.50	2.06
1:A:166:ILE:HG13	1:A:214:ALA:HA	0.50	1.82
1:A:166:ILE:HG22	1:A:210:GLU:HA	0.50	1.82
1:A:164:LEU:CD2	1:A:176:GLU:HA	0.50	2.37
1:A:204:SER:N	1:A:237:THR:HG23	0.50	2.21
1:A:245:PHE:CD1	1:A:245:PHE:O	0.50	2.65
1:A:206:SER:OG	1:A:210:GLU:CD	0.49	2.51
1:A:163:LEU:N	1:A:163:LEU:CD2	0.49	2.75
1:A:166:ILE:HB	1:A:189:CYS:O	0.49	2.07
1:A:184:LEU:HD21	1:A:201:PHE:HD2	0.49	1.68
1:A:174:VAL:HG21	1:A:217:VAL:HG21	0.48	1.85
1:A:246:TRP:O	1:A:250:GLY:CA	0.48	2.61
1:A:223:ALA:O	1:A:226:LYS:HE3	0.48	2.07
1:A:159:TYR:CD1	1:A:159:TYR:N	0.48	2.73
1:A:165:HIS:C	1:A:166:ILE:CD1	0.48	2.80
1:A:206:SER:CB	1:A:210:GLU:CD	0.48	2.82
1:A:187:GLY:O	1:A:206:SER:OG	0.48	2.31
1:A:188:ASP:O	1:A:203:GLY:N	0.48	2.46
1:A:197:THR:C	1:A:198:ILE:HD12	0.48	2.29
1:A:206:SER:OG	1:A:210:GLU:HG3	0.48	2.09
1:A:164:LEU:O	1:A:190:PHE:CD1	0.48	2.66
1:A:166:ILE:O	1:A:210:GLU:CB	0.48	2.62
1:A:191:LEU:HA	1:A:200:GLN:HA	0.48	1.85
1:A:236:GLU:HG3	1:A:237:THR:N	0.48	2.24
1:A:166:ILE:HG22	1:A:210:GLU:CA	0.47	2.40
1:A:192:LEU:HD23	1:A:245:PHE:CD1	0.47	2.44
1:A:163:LEU:CB	1:A:177:VAL:HG22	0.47	2.40
1:A:168:GLY:O	1:A:169:ASP:C	0.47	2.53
1:A:164:LEU:HD22	1:A:175:ALA:O	0.47	2.10
1:A:210:GLU:CD	1:A:210:GLU:H	0.47	2.13
1:A:191:LEU:O	1:A:191:LEU:HG	0.47	2.10
1:A:166:ILE:HG13	1:A:214:ALA:CB	0.46	2.41
1:A:176:GLU:HG2	1:A:177:VAL:N	0.46	2.25
1:A:206:SER:HB2	1:A:210:GLU:CD	0.46	2.31
1:A:202:ASN:HB2	1:A:234:PHE:O	0.46	2.11
1:A:202:ASN:CA	1:A:235:CYS:HA	0.46	2.41
1:A:193:ASP:HA	1:A:198:ILE:HG13	0.46	1.86
1:A:163:LEU:O	1:A:177:VAL:N	0.46	2.48
1:A:164:LEU:O	1:A:190:PHE:CE1	0.46	2.69
1:A:166:ILE:CG1	1:A:214:ALA:HB2	0.46	2.40
1:A:181:THR:HG22	1:A:246:TRP:HE3	0.45	1.63
1:A:199:TYR:HD2	1:A:232:GLU:CG	0.45	2.18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:164:LEU:HD22	1:A:176:GLU:HA	0.45	1.89
1:A:163:LEU:CD2	1:A:179:LEU:HA	0.45	2.42
1:A:207:SER:O	1:A:211:LYS:HB2	0.45	2.11
1:A:159:TYR:HB3	1:A:195:GLY:HA2	0.45	1.88
1:A:191:LEU:HD11	1:A:198:ILE:CG2	0.45	2.42
1:A:202:ASN:C	1:A:235:CYS:SG	0.45	2.95
1:A:166:ILE:HG13	1:A:214:ALA:CA	0.45	2.42
1:A:191:LEU:HD11	1:A:198:ILE:HG23	0.44	1.88
1:A:201:PHE:CE1	1:A:202:ASN:O	0.44	2.70
1:A:163:LEU:HB2	1:A:177:VAL:O	0.44	2.13
1:A:165:HIS:CE1	1:A:167:SER:OG	0.44	2.71
1:A:179:LEU:HD13	1:A:249:LEU:CD1	0.44	2.42
1:A:164:LEU:HD13	1:A:164:LEU:C	0.44	2.31
1:A:190:PHE:O	1:A:201:PHE:N	0.44	2.50
1:A:162:ARG:C	1:A:163:LEU:CD2	0.44	2.83
1:A:179:LEU:HD12	1:A:180:ALA:CA	0.44	2.42
1:A:163:LEU:CB	1:A:178:PRO:O	0.43	2.66
1:A:241:ILE:HA	1:A:246:TRP:CD1	0.43	2.48
1:A:217:VAL:O	1:A:221:ILE:HG13	0.43	2.12
1:A:225:ARG:CB	1:A:229:PRO:CD	0.43	2.96
1:A:166:ILE:CG2	1:A:213:LYS:HB3	0.43	2.43
1:A:175:ALA:O	1:A:177:VAL:HG12	0.43	2.14
1:A:202:ASN:CB	1:A:235:CYS:N	0.43	2.82
1:A:247:LYS:HA	1:A:251:GLY:N	0.43	2.28
1:A:247:LYS:O	1:A:251:GLY:C	0.43	2.57
1:A:165:HIS:NE2	1:A:185:ASN:CG	0.43	2.71
1:A:210:GLU:HG2	1:A:211:LYS:N	0.43	2.29
1:A:164:LEU:HD11	1:A:174:VAL:CG2	0.43	2.44
1:A:205:LYS:H	1:A:237:THR:CG2	0.43	2.26
1:A:187:GLY:O	1:A:203:GLY:O	0.43	2.36
1:A:203:GLY:HA2	1:A:236:GLU:O	0.43	2.13
1:A:179:LEU:HD13	1:A:249:LEU:HD12	0.43	1.91
1:A:180:ALA:HB1	1:A:183:SER:HB3	0.43	1.91
1:A:200:GLN:OE1	1:A:218:ALA:HB2	0.43	2.13
1:A:246:TRP:O	1:A:250:GLY:N	0.43	2.51
1:A:242:PRO:O	1:A:244:GLU:N	0.42	2.52
1:A:159:TYR:CB	1:A:195:GLY:CA	0.42	2.97
1:A:172:ALA:CB	1:A:209:GLN:HB3	0.42	2.32
1:A:239:SER:C	1:A:241:ILE:H	0.42	2.18
1:A:200:GLN:OE1	1:A:233:VAL:CG1	0.42	2.68
1:A:245:PHE:CE1	1:A:249:LEU:CD2	0.41	2.94
1:A:202:ASN:HB2	1:A:235:CYS:N	0.41	2.30

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:242:PRO:HD2	1:A:246:TRP:NE1	0.41	2.31
1:A:164:LEU:HD22	1:A:175:ALA:C	0.41	2.36
1:A:165:HIS:CD2	1:A:166:ILE:N	0.41	2.89
1:A:166:ILE:CG2	1:A:214:ALA:HB2	0.41	2.39
1:A:165:HIS:CD2	1:A:185:ASN:ND2	0.41	2.89
1:A:242:PRO:O	1:A:243:ALA:C	0.41	2.57
1:A:199:TYR:HD2	1:A:232:GLU:HG3	0.40	1.68
1:A:245:PHE:CD2	1:A:246:TRP:NE1	0.40	2.89
1:A:192:LEU:HD12	1:A:193:ASP:N	0.40	2.27

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	92/114 (81%)	77 (84%)	10 (11%)	5 (5%)	3 23
All	All	92/114 (81%)	77 (84%)	10 (11%)	5 (5%)	3 23

All 5 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	168	GLY
1	A	184	LEU
1	A	207	SER
1	A	240	ASP
1	A	243	ALA

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	77/91 (85%)	53 (69%)	24 (31%)	1 14
All	All	77/91 (85%)	53 (69%)	24 (31%)	1 14

All 24 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	166	ILE
1	A	170	LYS
1	A	173	LYS
1	A	177	VAL
1	A	179	LEU
1	A	181	THR
1	A	182	SER
1	A	184	LEU
1	A	188	ASP
1	A	192	LEU
1	A	204	SER
1	A	207	SER
1	A	209	GLN
1	A	225	ARG
1	A	226	LYS
1	A	228	LEU
1	A	232	GLU
1	A	234	PHE
1	A	235	CYS
1	A	238	ASP
1	A	244	GLU
1	A	245	PHE
1	A	248	LEU
1	A	249	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 monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	159:TYR	C	160:LYS	N	1.17
1	A	158:GLU	C	159:TYR	N	1.13

7 Chemical shift validation (i)

No chemical shift data were provided