Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 08:29 pm BST

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 following versions of software and data (see references (1)) were used in the production of this report:

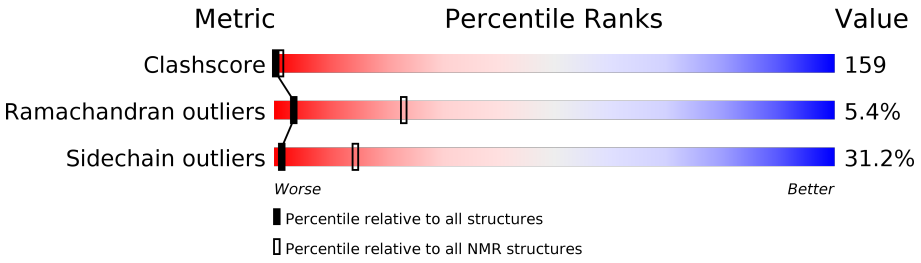
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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.

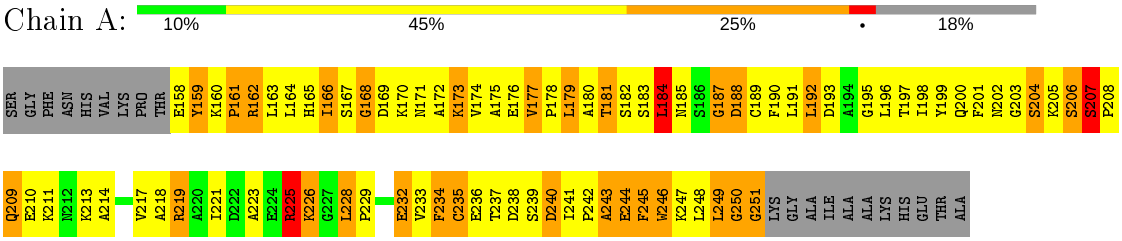
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	94	1430	453	713	121	141	2	0

4 Residue-property plots (i)

These plots are provided for all protein, RNA 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: SEVERIN

Chain A:



5 Refinement protocol and experimental data overview

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. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	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:C	1:A:192:LEU:HD12	0.89	1.88
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:O	1:A:249:LEU:HD12	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:202:ASN:HB2	1:A:234:PHE:C	0.75	2.01
1:A:187:GLY:O	1:A:206:SER:CB	0.75	2.35
1:A:166:ILE:N	1:A:166:ILE:HD13	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:C	1:A:249:LEU:HD12	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
1:A:225:ARG:HD3	1:A:229:PRO:HG3	0.66	1.68
1:A:192:LEU:O	1:A:192:LEU:HD12	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:C	1:A:179:LEU:HD12	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:C	1:A:245:PHE:CD1	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:225:ARG:HB3	1:A:229:PRO:HD3	0.62	1.71
1:A:181:THR:CG2	1:A:250:GLY:HA3	0.62	2.24
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:N	1:A:166:ILE:CD1	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
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:CD	1:A:226:LYS:N	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:N	1:A:234:PHE:CD1	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:CD1	1:A:179:LEU:C	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
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:O	1:A:245:PHE:CD1	0.50	2.65
1:A:206:SER:OG	1:A:210:GLU:CD	0.49	2.51
1:A:163:LEU:CD2	1:A:163:LEU:N	0.49	2.75
1:A:166:ILE:HB	1:A:189:CYS:O	0.49	2.07

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:N	1:A:159:TYR:CD1	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:197:THR:C	1:A:198:ILE:HD12	0.48	2.29
1:A:188:ASP:O	1:A:203:GLY:N	0.48	2.46
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:HG	1:A:191:LEU:O	0.47	2.10
1:A:176:GLU:HG2	1:A:177:VAL:N	0.46	2.25
1:A:166:ILE:HG13	1:A:214:ALA:CB	0.46	2.41
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:166:ILE:CG1	1:A:214:ALA:HB2	0.46	2.40
1:A:164:LEU:O	1:A:190:PHE:CE1	0.46	2.69
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:165:HIS:CE1	1:A:167:SER:OG	0.44	2.71
1:A:163:LEU:HB2	1:A:177:VAL:O	0.44	2.13
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:O	1:A:251:GLY:C	0.43	2.57
1:A:247:LYS:HA	1:A:251:GLY:N	0.43	2.28
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: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:179:LEU:HD13	1:A:249:LEU:HD12	0.43	1.91
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
1:A:242:PRO:HD2	1:A:246:TRP:NE1	0.41	2.31
1:A:165:HIS:CD2	1:A:166:ILE:N	0.41	2.89
1:A:164:LEU:HD22	1:A:175:ALA:C	0.41	2.36
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

5.2 Torsion angles

5.2.1 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	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	207	SER
1	A	184	LEU
1	A	240	ASP
1	A	168	GLY
1	A	243	ALA

5.2.2 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	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	245	PHE
1	A	235	CYS
1	A	209	GLN
1	A	184	LEU
1	A	182	SER

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Mol	Chain	Res	Type
1	A	192	LEU
1	A	232	GLU
1	A	226	LYS
1	A	238	ASP
1	A	228	LEU
1	A	170	LYS
1	A	173	LYS
1	A	177	VAL
1	A	207	SER
1	A	204	SER
1	A	225	ARG
1	A	234	PHE
1	A	181	THR
1	A	188	ASP
1	A	166	ILE
1	A	249	LEU
1	A	179	LEU
1	A	244	GLU
1	A	248	LEU

5.2.3 RNA

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.4 Carbohydrates

There are no carbohydrates in this entry.

5.5 Ligand geometry

There are no ligands in this entry.

5.6 Other polymers

There are no such molecules in this entry.

5.7 Polymer linkage issues

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

6 Chemical shift validation

No chemical shift data were provided