



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 08:21 pm BST

PDB ID : 1R9K
Title : Representative solution structure of the catalytic domain of SopE2
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Deposited on : 2003-10-30

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 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
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

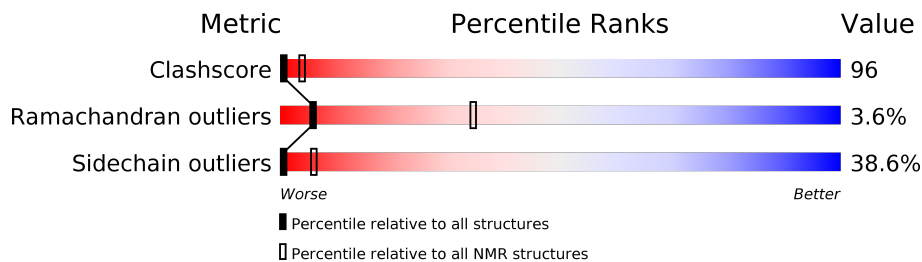
1 Overall quality at a glance

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	172	

2 Ensemble composition and analysis

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2589 atoms, of which 1308 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TypeIII-secreted protein effector: invasion-associated protein.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	168	2589	816	1308	217	241	7	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: TypeIII-secreted protein effector: invasion-associated protein



5 Refinement protocol and experimental data overview i

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

Of the 100 calculated structures, 1 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with the least restraint violations, structures with the lowest energy*.

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

Software name	Classification	Version
XPLOR-NIH	structure solution	2.06
XPLOR-NIH	refinement	2.06

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 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	1281	1308	1308	248
All	All	1281	1308	1308	248

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 96.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:130:LEU:HD22	1:A:135:VAL:HG11	1.00	1.26
1:A:143:GLU:CB	1:A:231:ILE:HG21	0.92	1.94
1:A:186:HIS:HA	1:A:189:ILE:HD12	0.89	1.41
1:A:183:LYS:HG2	1:A:184:TYR:CD2	0.89	2.02
1:A:114:ILE:HG21	1:A:213:PHE:CZ	0.86	2.06
1:A:144:ILE:HG22	1:A:228:ILE:HG12	0.85	1.46
1:A:205:VAL:O	1:A:209:VAL:HG22	0.83	1.72
1:A:130:LEU:CD2	1:A:135:VAL:HG11	0.83	2.02
1:A:130:LEU:HD22	1:A:135:VAL:CG1	0.83	2.04
1:A:83:VAL:HG22	1:A:184:TYR:CD2	0.82	2.09

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:144:ILE:HG22	1:A:228:ILE:CG1	0.81	2.05
1:A:96:ILE:HG23	1:A:172:PHE:CE1	0.81	2.11
1:A:135:VAL:HG13	1:A:136:SER:N	0.79	1.91
1:A:115:LEU:O	1:A:118:VAL:HG22	0.77	1.78
1:A:96:ILE:HG22	1:A:212:LEU:HD11	0.77	1.55
1:A:122:ASN:ND2	1:A:228:ILE:HG23	0.77	1.95
1:A:143:GLU:HB3	1:A:231:ILE:HG21	0.77	1.55
1:A:140:PHE:HD1	1:A:231:ILE:HG22	0.77	1.39
1:A:122:ASN:CG	1:A:228:ILE:HG23	0.75	2.02
1:A:144:ILE:CG2	1:A:228:ILE:HG12	0.74	2.13
1:A:78:LEU:O	1:A:82:THR:HG22	0.74	1.83
1:A:225:GLN:O	1:A:228:ILE:HG22	0.74	1.82
1:A:145:GLY:HA2	1:A:148:ALA:HB3	0.72	1.61
1:A:96:ILE:CG2	1:A:212:LEU:HD11	0.72	2.14
1:A:206:MET:HA	1:A:209:VAL:CG2	0.71	2.15
1:A:119:TYR:HA	1:A:228:ILE:HD11	0.70	1.64
1:A:99:ASN:HB2	1:A:106:TYR:CE1	0.69	2.22
1:A:129:LEU:CD2	1:A:236:LEU:HD12	0.68	2.19
1:A:83:VAL:HG22	1:A:184:TYR:CG	0.67	2.24
1:A:232:ALA:O	1:A:236:LEU:HB2	0.66	1.91
1:A:148:ALA:HB1	1:A:164:PRO:HB3	0.65	1.67
1:A:114:ILE:HG21	1:A:213:PHE:HZ	0.64	1.52
1:A:96:ILE:HG12	1:A:172:PHE:CD1	0.64	2.27
1:A:127:CYS:HA	1:A:130:LEU:HB2	0.61	1.72
1:A:129:LEU:HG	1:A:130:LEU:N	0.61	2.10
1:A:84:LYS:CG	1:A:200:TYR:CE1	0.61	2.83
1:A:135:VAL:CG1	1:A:136:SER:N	0.61	2.61
1:A:140:PHE:CE2	1:A:144:ILE:CD1	0.61	2.84
1:A:140:PHE:CZ	1:A:144:ILE:CD1	0.60	2.84
1:A:90:LYS:O	1:A:94:LEU:N	0.60	2.35
1:A:164:PRO:HG2	1:A:167:ALA:HB2	0.60	1.73
1:A:110:THR:CG2	1:A:172:PHE:CE1	0.59	2.85
1:A:228:ILE:CG2	1:A:229:GLU:N	0.59	2.65
1:A:143:GLU:HB2	1:A:231:ILE:HG21	0.59	1.70
1:A:84:LYS:O	1:A:88:LEU:HB2	0.59	1.98
1:A:141:LEU:HA	1:A:144:ILE:HD11	0.59	1.74
1:A:147:ALA:HB1	1:A:224:PHE:CE1	0.59	2.33
1:A:115:LEU:O	1:A:118:VAL:CG2	0.59	2.50
1:A:145:GLY:O	1:A:162:PHE:CE1	0.58	2.56
1:A:210:THR:N	1:A:211:PRO:HD2	0.58	2.13
1:A:186:HIS:CA	1:A:189:ILE:HD12	0.58	2.23
1:A:110:THR:HG21	1:A:172:PHE:CE1	0.58	2.33

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:212:LEU:HD23	1:A:212:LEU:N	0.58	2.13
1:A:83:VAL:O	1:A:87:MET:N	0.57	2.25
1:A:84:LYS:HG3	1:A:200:TYR:CE1	0.57	2.34
1:A:138:THR:N	1:A:139:PRO:HD2	0.57	2.15
1:A:162:PHE:C	1:A:162:PHE:CD1	0.57	2.77
1:A:121:ASN:O	1:A:125:GLN:HB3	0.57	2.00
1:A:114:ILE:HG21	1:A:213:PHE:CE1	0.57	2.35
1:A:139:PRO:O	1:A:142:LYS:HB3	0.56	2.01
1:A:151:ALA:HB2	1:A:224:PHE:CE1	0.56	2.34
1:A:99:ASN:HB2	1:A:106:TYR:CZ	0.56	2.35
1:A:156:GLU:CB	1:A:163:THR:HB	0.56	2.30
1:A:96:ILE:HG23	1:A:172:PHE:CZ	0.56	2.35
1:A:122:ASN:OD1	1:A:228:ILE:HG23	0.56	2.00
1:A:129:LEU:HD11	1:A:236:LEU:HA	0.56	1.78
1:A:205:VAL:C	1:A:209:VAL:HG22	0.55	2.22
1:A:130:LEU:HD13	1:A:135:VAL:HG11	0.55	1.77
1:A:191:HIS:CD2	1:A:191:HIS:C	0.55	2.78
1:A:129:LEU:HD12	1:A:133:LYS:HE3	0.54	1.78
1:A:77:VAL:C	1:A:78:LEU:HG	0.54	2.22
1:A:177:ILE:CD1	1:A:197:PHE:HB3	0.54	2.33
1:A:126:CYS:SG	1:A:232:ALA:HA	0.54	2.42
1:A:110:THR:HG23	1:A:171:PRO:CG	0.54	2.33
1:A:120:SER:HA	1:A:123:LYS:HD2	0.54	1.78
1:A:176:LEU:HD23	1:A:177:ILE:HG12	0.54	1.78
1:A:114:ILE:O	1:A:117:ALA:HB3	0.54	2.02
1:A:175:PRO:HA	1:A:178:ALA:HB3	0.54	1.80
1:A:91:LEU:HD11	1:A:205:VAL:HA	0.54	1.79
1:A:125:GLN:HG2	1:A:126:CYS:N	0.54	2.16
1:A:80:SER:O	1:A:81:LYS:HB3	0.54	2.02
1:A:206:MET:HA	1:A:209:VAL:HG22	0.54	1.80
1:A:140:PHE:CD1	1:A:231:ILE:HG22	0.54	2.29
1:A:156:GLU:HB3	1:A:163:THR:HB	0.53	1.80
1:A:233:ASN:HA	1:A:236:LEU:CB	0.53	2.33
1:A:234:LYS:O	1:A:234:LYS:NZ	0.53	2.39
1:A:135:VAL:HG13	1:A:136:SER:H	0.53	1.59
1:A:186:HIS:HA	1:A:189:ILE:CD1	0.53	2.27
1:A:213:PHE:N	1:A:213:PHE:CD1	0.53	2.74
1:A:86:PHE:CZ	1:A:183:LYS:HD2	0.53	2.38
1:A:110:THR:CG2	1:A:172:PHE:CZ	0.53	2.91
1:A:213:PHE:CD2	1:A:221:PRO:HD3	0.53	2.39
1:A:176:LEU:HD23	1:A:177:ILE:N	0.53	2.19
1:A:81:LYS:CG	1:A:81:LYS:O	0.53	2.56

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:110:THR:HG23	1:A:171:PRO:HG2	0.53	1.80
1:A:130:LEU:CG	1:A:135:VAL:HG11	0.53	2.33
1:A:103:ASP:CB	1:A:106:TYR:CB	0.53	2.87
1:A:238:ASN:O	1:A:239:ALA:HB3	0.52	2.02
1:A:103:ASP:HB3	1:A:106:TYR:HB2	0.52	1.80
1:A:112:GLU:O	1:A:116:SER:HB3	0.52	2.04
1:A:119:TYR:CA	1:A:228:ILE:HD11	0.52	2.34
1:A:110:THR:HG22	1:A:172:PHE:CZ	0.52	2.39
1:A:110:THR:CG2	1:A:171:PRO:HG2	0.52	2.33
1:A:172:PHE:CE2	1:A:209:VAL:HG12	0.52	2.40
1:A:206:MET:CA	1:A:209:VAL:HG22	0.52	2.35
1:A:107:ALA:O	1:A:111:CYS:HB2	0.52	2.05
1:A:145:GLY:CA	1:A:148:ALA:HB3	0.52	2.31
1:A:209:VAL:O	1:A:212:LEU:HG	0.52	2.05
1:A:202:GLU:O	1:A:205:VAL:HG22	0.52	2.05
1:A:232:ALA:O	1:A:236:LEU:N	0.52	2.43
1:A:198:LYS:HA	1:A:201:ALA:HB3	0.51	1.82
1:A:115:LEU:C	1:A:118:VAL:HG22	0.51	2.26
1:A:86:PHE:CE1	1:A:183:LYS:HD2	0.51	2.41
1:A:103:ASP:HB3	1:A:106:TYR:CB	0.51	2.35
1:A:81:LYS:O	1:A:85:ASP:HB2	0.51	2.06
1:A:173:VAL:HA	1:A:176:LEU:HB3	0.51	1.83
1:A:112:GLU:HB3	1:A:153:LEU:HB3	0.50	1.82
1:A:187:MET:HB3	1:A:197:PHE:CE2	0.50	2.41
1:A:233:ASN:HA	1:A:236:LEU:HB2	0.50	1.82
1:A:120:SER:O	1:A:123:LYS:HD3	0.50	2.05
1:A:207:LYS:HG3	1:A:208:GLU:N	0.50	2.21
1:A:114:ILE:CG2	1:A:213:PHE:CZ	0.50	2.90
1:A:123:LYS:O	1:A:127:CYS:CB	0.50	2.59
1:A:124:ASP:O	1:A:128:LYS:HB2	0.50	2.05
1:A:90:LYS:HA	1:A:90:LYS:CE	0.50	2.36
1:A:130:LEU:CD1	1:A:135:VAL:HG11	0.50	2.37
1:A:221:PRO:O	1:A:225:GLN:CB	0.50	2.60
1:A:123:LYS:O	1:A:127:CYS:HB3	0.50	2.07
1:A:141:LEU:HA	1:A:144:ILE:CG1	0.50	2.37
1:A:174:VAL:HB	1:A:175:PRO:HD3	0.49	1.85
1:A:113:ALA:HA	1:A:116:SER:CB	0.49	2.37
1:A:195:VAL:HA	1:A:198:LYS:HD3	0.49	1.84
1:A:121:ASN:O	1:A:125:GLN:N	0.49	2.33
1:A:176:LEU:CD2	1:A:201:ALA:HB1	0.49	2.36
1:A:90:LYS:O	1:A:94:LEU:HB3	0.49	2.07
1:A:224:PHE:CE2	1:A:228:ILE:HD12	0.49	2.43

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:140:PHE:HD1	1:A:231:ILE:CG2	0.48	2.17
1:A:141:LEU:HA	1:A:144:ILE:CD1	0.48	2.36
1:A:81:LYS:HG2	1:A:81:LYS:O	0.48	2.08
1:A:173:VAL:HG11	1:A:198:LYS:HB2	0.48	1.84
1:A:157:ILE:HG12	1:A:161:VAL:O	0.48	2.08
1:A:179:SER:O	1:A:183:LYS:N	0.48	2.43
1:A:228:ILE:HA	1:A:231:ILE:HD12	0.48	1.83
1:A:180:ALA:HB1	1:A:188:PHE:CZ	0.48	2.43
1:A:107:ALA:O	1:A:111:CYS:SG	0.48	2.72
1:A:173:VAL:CG1	1:A:198:LYS:HB2	0.48	2.38
1:A:118:VAL:HG23	1:A:228:ILE:CD1	0.48	2.39
1:A:228:ILE:HG22	1:A:229:GLU:N	0.48	2.24
1:A:84:LYS:HG2	1:A:200:TYR:CE1	0.47	2.43
1:A:123:LYS:O	1:A:123:LYS:HG2	0.47	2.09
1:A:129:LEU:HD22	1:A:236:LEU:HD12	0.47	1.86
1:A:86:PHE:CD2	1:A:183:LYS:HD3	0.47	2.44
1:A:103:ASP:CB	1:A:106:TYR:HB2	0.47	2.39
1:A:130:LEU:HD11	1:A:235:TYR:HB3	0.47	1.86
1:A:153:LEU:O	1:A:164:PRO:HA	0.47	2.09
1:A:106:TYR:CD1	1:A:106:TYR:C	0.47	2.87
1:A:130:LEU:HD13	1:A:135:VAL:CG1	0.47	2.39
1:A:86:PHE:CD2	1:A:184:TYR:HE2	0.47	2.27
1:A:94:LEU:CD2	1:A:96:ILE:HG13	0.47	2.40
1:A:141:LEU:O	1:A:144:ILE:HG12	0.47	2.10
1:A:80:SER:O	1:A:81:LYS:CB	0.46	2.62
1:A:145:GLY:O	1:A:149:GLN:N	0.46	2.49
1:A:96:ILE:O	1:A:106:TYR:CE1	0.46	2.69
1:A:130:LEU:HD22	1:A:135:VAL:CB	0.46	2.41
1:A:228:ILE:HG22	1:A:229:GLU:H	0.46	1.70
1:A:113:ALA:HA	1:A:116:SER:HB3	0.46	1.87
1:A:158:LYS:HB2	1:A:161:VAL:HG12	0.46	1.88
1:A:86:PHE:CG	1:A:183:LYS:HD3	0.46	2.45
1:A:83:VAL:O	1:A:84:LYS:C	0.46	2.54
1:A:114:ILE:O	1:A:114:ILE:HD12	0.45	2.11
1:A:143:GLU:CB	1:A:231:ILE:CG2	0.45	2.83
1:A:172:PHE:CE2	1:A:209:VAL:CG1	0.45	3.00
1:A:184:TYR:O	1:A:188:PHE:CD1	0.45	2.69
1:A:133:LYS:NZ	1:A:237:GLN:O	0.45	2.49
1:A:187:MET:HB3	1:A:197:PHE:CZ	0.45	2.46
1:A:188:PHE:CD2	1:A:194:GLN:HB2	0.45	2.45
1:A:129:LEU:HD22	1:A:236:LEU:CD1	0.45	2.42
1:A:137:ILE:O	1:A:141:LEU:N	0.44	2.35

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:140:PHE:CZ	1:A:144:ILE:HD13	0.44	2.47
1:A:143:GLU:HB3	1:A:231:ILE:HD13	0.44	1.88
1:A:130:LEU:HD21	1:A:235:TYR:O	0.44	2.11
1:A:111:CYS:O	1:A:114:ILE:CG2	0.44	2.65
1:A:138:THR:N	1:A:139:PRO:CD	0.44	2.80
1:A:157:ILE:HA	1:A:162:PHE:HA	0.44	1.88
1:A:147:ALA:HA	1:A:150:ASN:ND2	0.44	2.27
1:A:86:PHE:HE2	1:A:180:ALA:HB2	0.44	1.71
1:A:119:TYR:CE1	1:A:144:ILE:HG13	0.44	2.47
1:A:86:PHE:HE2	1:A:180:ALA:CB	0.44	2.26
1:A:129:LEU:HD21	1:A:236:LEU:HD12	0.44	1.89
1:A:180:ALA:CB	1:A:188:PHE:CZ	0.44	3.01
1:A:133:LYS:NZ	1:A:236:LEU:O	0.44	2.37
1:A:99:ASN:HB2	1:A:106:TYR:CD1	0.44	2.48
1:A:210:THR:N	1:A:211:PRO:CD	0.44	2.80
1:A:89:GLN:O	1:A:93:SER:HB3	0.44	2.13
1:A:147:ALA:O	1:A:151:ALA:CB	0.43	2.66
1:A:84:LYS:HG3	1:A:200:TYR:CZ	0.43	2.48
1:A:112:GLU:HG2	1:A:153:LEU:HB3	0.43	1.89
1:A:119:TYR:HA	1:A:228:ILE:CD1	0.43	2.40
1:A:170:ASN:HB3	1:A:173:VAL:HB	0.43	1.90
1:A:212:LEU:N	1:A:212:LEU:CD2	0.43	2.76
1:A:188:PHE:N	1:A:188:PHE:CD1	0.43	2.86
1:A:140:PHE:CD1	1:A:231:ILE:CG2	0.43	3.00
1:A:233:ASN:O	1:A:236:LEU:HB3	0.43	2.14
1:A:119:TYR:CE2	1:A:164:PRO:CG	0.43	3.02
1:A:88:LEU:O	1:A:91:LEU:HB3	0.43	2.14
1:A:82:THR:OG1	1:A:83:VAL:N	0.42	2.50
1:A:140:PHE:CE1	1:A:144:ILE:HD13	0.42	2.49
1:A:183:LYS:HD3	1:A:184:TYR:CE2	0.42	2.50
1:A:114:ILE:C	1:A:114:ILE:HD12	0.42	2.34
1:A:113:ALA:HA	1:A:116:SER:OG	0.42	2.13
1:A:199:ALA:O	1:A:202:GLU:HG3	0.42	2.14
1:A:107:ALA:O	1:A:111:CYS:CB	0.42	2.68
1:A:225:GLN:O	1:A:229:GLU:HB2	0.42	2.14
1:A:130:LEU:HD23	1:A:130:LEU:HA	0.42	1.67
1:A:176:LEU:CD2	1:A:177:ILE:HG12	0.42	2.44
1:A:229:GLU:O	1:A:233:ASN:HB2	0.42	2.14
1:A:115:LEU:HA	1:A:118:VAL:HG22	0.42	1.90
1:A:174:VAL:CB	1:A:175:PRO:HD3	0.42	2.45
1:A:197:PHE:HD1	1:A:200:TYR:CE2	0.42	2.33
1:A:220:THR:OG1	1:A:223:GLN:HB3	0.42	2.15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:206:MET:CA	1:A:209:VAL:CG2	0.42	2.94
1:A:169:ALA:O	1:A:170:ASN:CB	0.42	2.67
1:A:223:GLN:CG	1:A:224:PHE:N	0.42	2.82
1:A:86:PHE:CD2	1:A:184:TYR:CE2	0.41	3.07
1:A:140:PHE:HB2	1:A:235:TYR:CD2	0.41	2.50
1:A:99:ASN:O	1:A:103:ASP:N	0.41	2.43
1:A:116:SER:HA	1:A:119:TYR:HB3	0.41	1.90
1:A:210:THR:HA	1:A:213:PHE:CD2	0.41	2.49
1:A:127:CYS:CA	1:A:130:LEU:HB2	0.41	2.45
1:A:209:VAL:C	1:A:211:PRO:HD2	0.41	2.36
1:A:116:SER:O	1:A:119:TYR:HB3	0.41	2.16
1:A:117:ALA:O	1:A:121:ASN:ND2	0.41	2.53
1:A:125:GLN:O	1:A:129:LEU:HD23	0.41	2.16
1:A:153:LEU:O	1:A:164:PRO:CA	0.41	2.69
1:A:179:SER:O	1:A:183:LYS:HB3	0.41	2.15
1:A:205:VAL:O	1:A:208:GLU:N	0.41	2.52
1:A:238:ASN:O	1:A:240:SER:N	0.41	2.51
1:A:157:ILE:HA	1:A:161:VAL:O	0.41	2.16
1:A:164:PRO:HG2	1:A:167:ALA:CB	0.41	2.45
1:A:201:ALA:O	1:A:204:ILE:HG13	0.41	2.16
1:A:97:LYS:O	1:A:101:SER:N	0.41	2.54
1:A:143:GLU:O	1:A:146:GLU:CB	0.40	2.69
1:A:113:ALA:O	1:A:117:ALA:N	0.40	2.54
1:A:144:ILE:HG22	1:A:228:ILE:HG13	0.40	1.90
1:A:111:CYS:SG	1:A:212:LEU:CB	0.40	3.10
1:A:122:ASN:HB3	1:A:140:PHE:CZ	0.40	2.52
1:A:224:PHE:O	1:A:228:ILE:HB	0.40	2.16
1:A:97:LYS:CG	1:A:98:GLY:N	0.40	2.84

5.2 Torsion angles [i](#)

5.2.1 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	166/172 (97%)	144 (87%)	16 (10%)	6 (4%)	6	34
All	All	166/172 (97%)	144 (87%)	16 (10%)	6 (4%)	6	34

All 6 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	165	GLY
1	A	135	VAL
1	A	78	LEU
1	A	237	GLN
1	A	159	ASN
1	A	170	ASN

5.2.2 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	140/142 (99%)	86 (61%)	54 (39%)	0 6
All	All	140/142 (99%)	86 (61%)	54 (39%)	0 6

All 54 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	153	LEU
1	A	123	LYS
1	A	230	ASN
1	A	80	SER
1	A	196	SER
1	A	135	VAL
1	A	206	MET
1	A	220	THR
1	A	212	LEU
1	A	158	LYS
1	A	191	HIS
1	A	234	LYS
1	A	114	ILE
1	A	240	SER
1	A	176	LEU
1	A	144	ILE
1	A	128	LYS
1	A	202	GLU

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Mol	Chain	Res	Type
1	A	73	GLU
1	A	215	LYS
1	A	156	GLU
1	A	225	GLN
1	A	235	TYR
1	A	110	THR
1	A	89	GLN
1	A	226	LEU
1	A	183	LYS
1	A	157	ILE
1	A	182	ILE
1	A	223	GLN
1	A	207	LYS
1	A	93	SER
1	A	189	ILE
1	A	237	GLN
1	A	195	VAL
1	A	122	ASN
1	A	143	GLU
1	A	125	GLN
1	A	86	PHE
1	A	194	GLN
1	A	136	SER
1	A	129	LEU
1	A	90	LYS
1	A	218	MET
1	A	81	LYS
1	A	111	CYS
1	A	162	PHE
1	A	88	LEU
1	A	116	SER
1	A	142	LYS
1	A	150	ASN
1	A	141	LEU
1	A	94	LEU
1	A	197	PHE

5.2.3 RNA

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

No chemical shift data were provided