



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2MCY / pdb_00002mcy
BMRB ID : 19458
Title : CR1 Sushi domains 2 and 3
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Deposited on : 2013-08-27

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

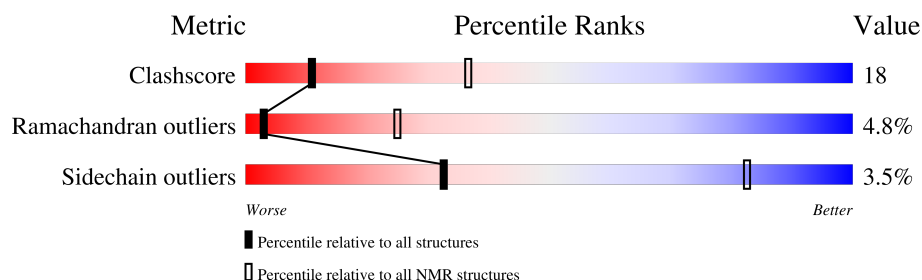
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 28%.

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	136	

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:61-A:192 (132)	1.70	4

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 7, 9, 10, 11, 12, 14, 16, 17, 18, 20
2	6, 19
Single-model clusters	8; 13; 15

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1957 atoms, of which 960 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Complement receptor type 1.

Mol	Chain	Residues	Atoms						Trace
1	A	132	Total	C	H	N	O	S	0
			1957	623	960	172	193	9	

There are 5 discrepancies between the modelled and reference sequences:

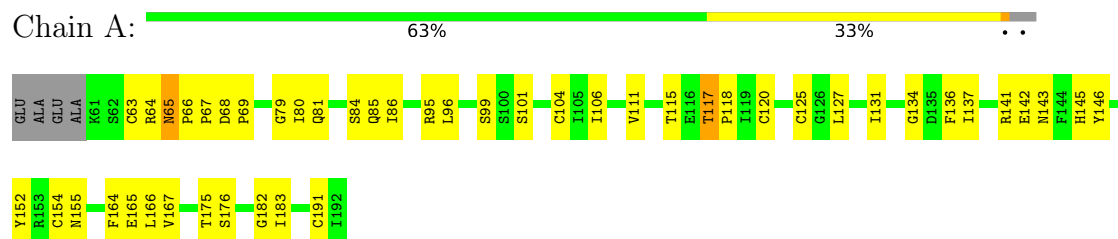
Chain	Residue	Modelled	Actual	Comment	Reference
A	57	GLU	-	expression tag	UNP P17927
A	58	ALA	-	expression tag	UNP P17927
A	59	GLU	-	expression tag	UNP P17927
A	60	ALA	-	expression tag	UNP P17927
A	115	THR	ASN	conflict	UNP P17927

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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: Complement receptor type 1

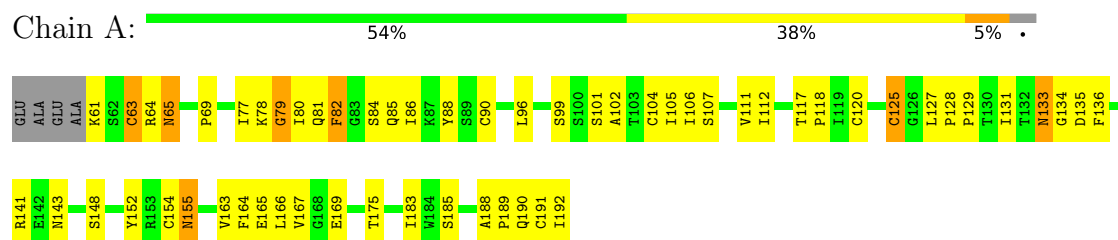


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

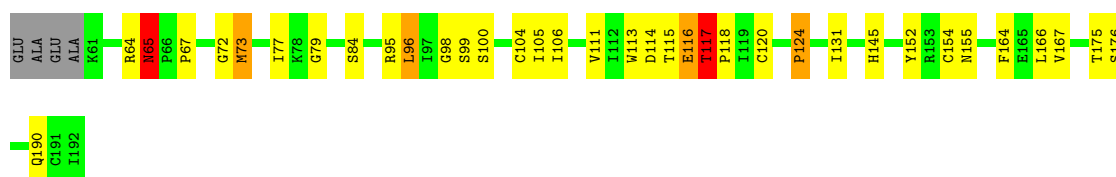
- Molecule 1: Complement receptor type 1



4.2.2 Score per residue for model 2

- Molecule 1: Complement receptor type 1

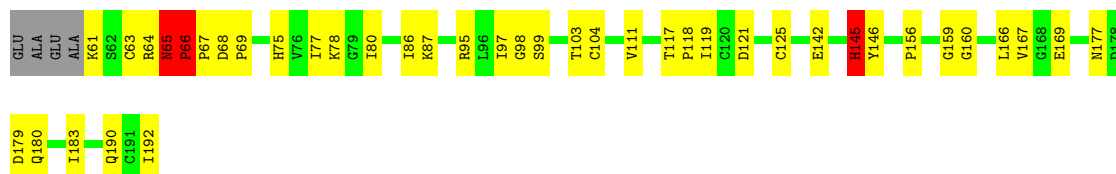




4.2.3 Score per residue for model 3

- Molecule 1: Complement receptor type 1

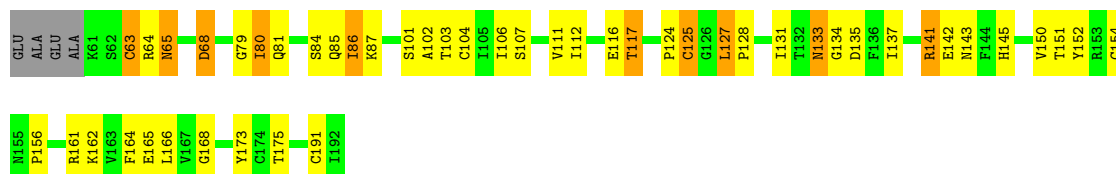
Chain A: 67% 28% . .



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Complement receptor type 1

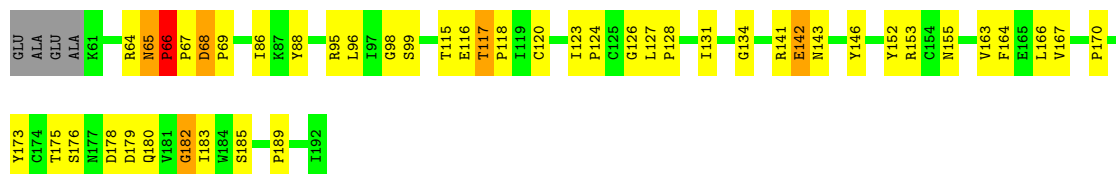
Chain A: 62% 28% 7% .



4.2.5 Score per residue for model 5

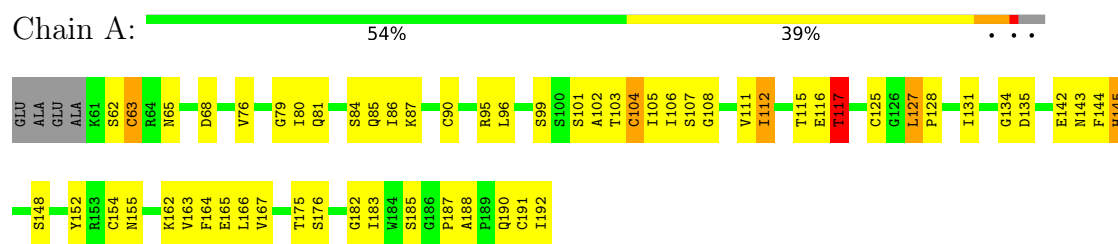
- Molecule 1: Complement receptor type 1

Chain A: 63% 29% . . .



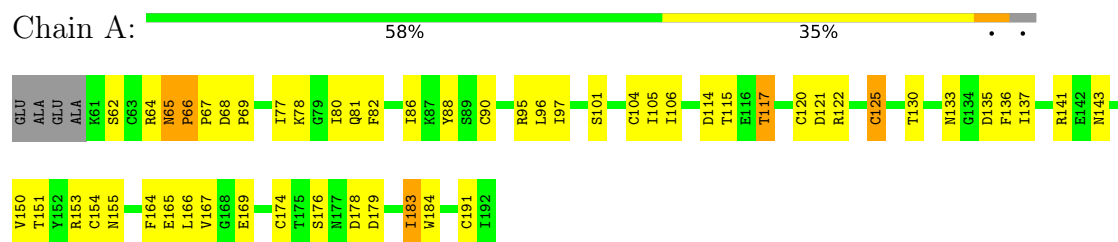
4.2.6 Score per residue for model 6

- Molecule 1: Complement receptor type 1



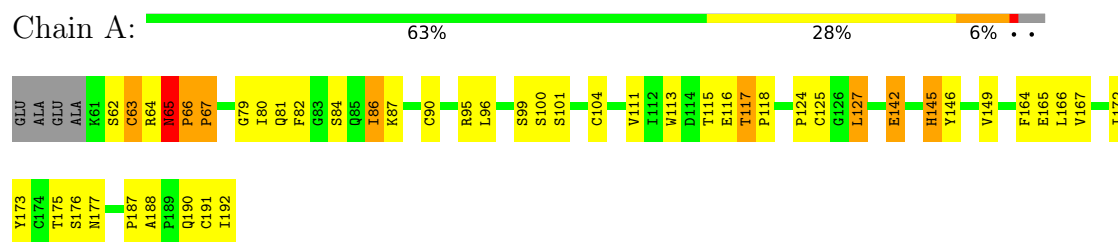
4.2.7 Score per residue for model 7

- Molecule 1: Complement receptor type 1



4.2.8 Score per residue for model 8

- Molecule 1: Complement receptor type 1



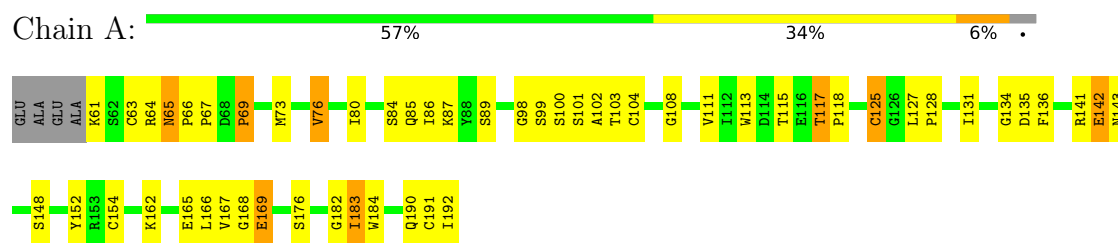
4.2.9 Score per residue for model 9

- Molecule 1: Complement receptor type 1



4.2.10 Score per residue for model 10

- Molecule 1: Complement receptor type 1



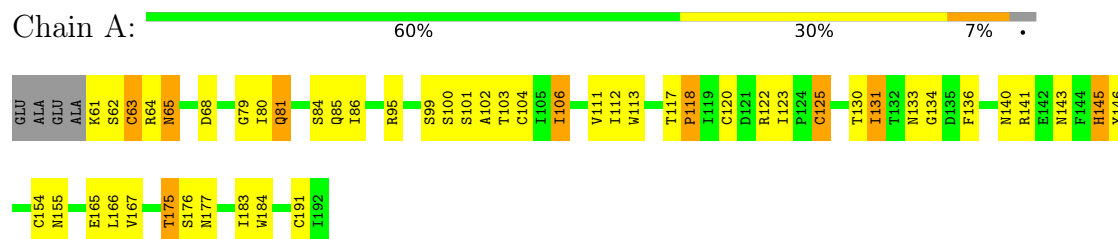
4.2.11 Score per residue for model 11

- Molecule 1: Complement receptor type 1



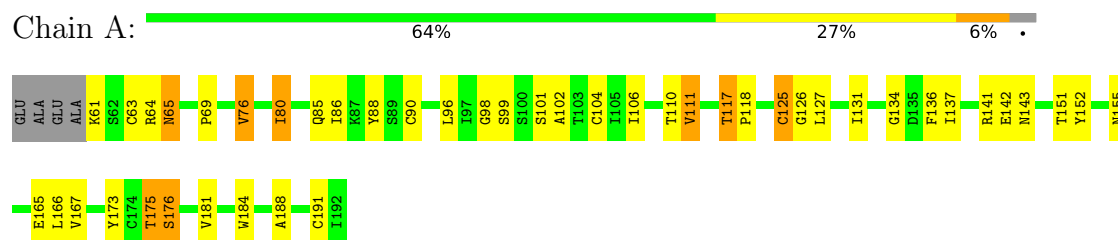
4.2.12 Score per residue for model 12

- Molecule 1: Complement receptor type 1



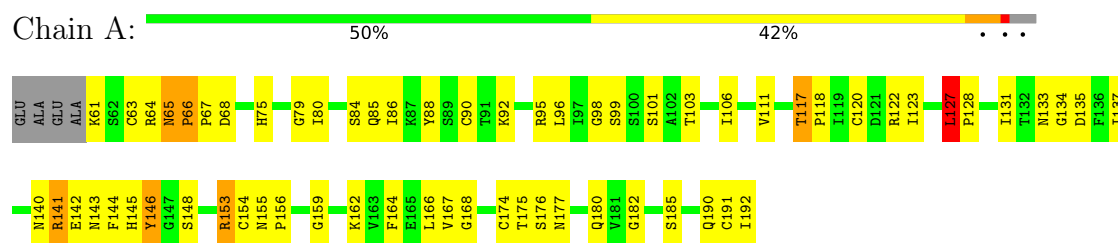
4.2.13 Score per residue for model 13

- Molecule 1: Complement receptor type 1



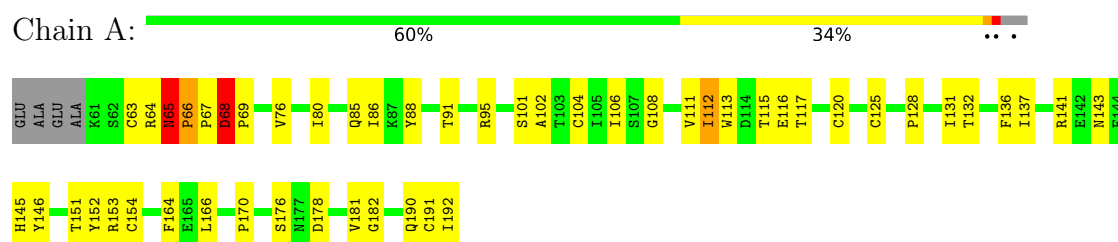
4.2.14 Score per residue for model 14

- Molecule 1: Complement receptor type 1



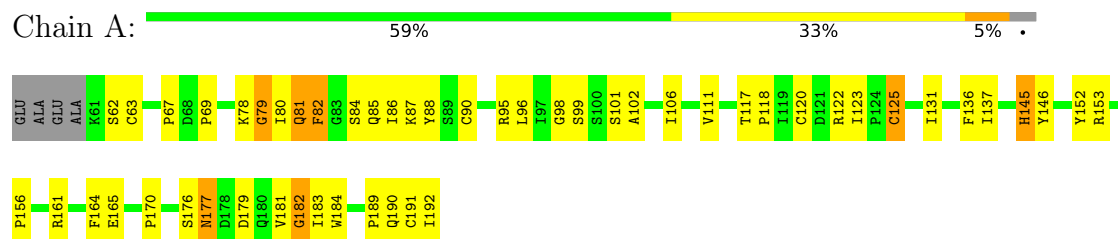
4.2.15 Score per residue for model 15

- Molecule 1: Complement receptor type 1



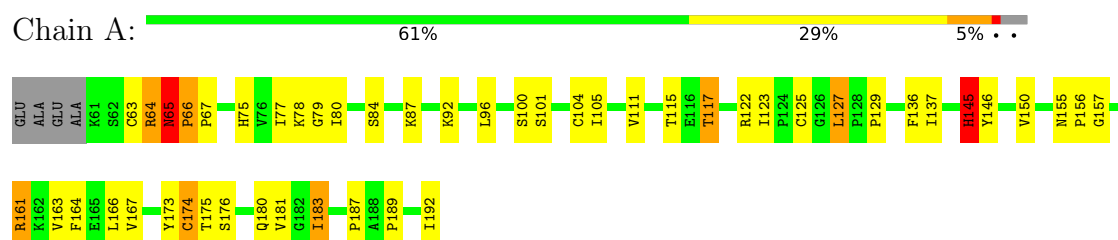
4.2.16 Score per residue for model 16

- Molecule 1: Complement receptor type 1



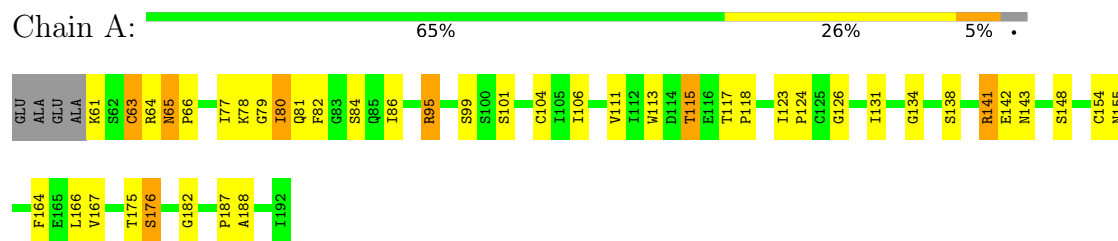
4.2.17 Score per residue for model 17

- Molecule 1: Complement receptor type 1



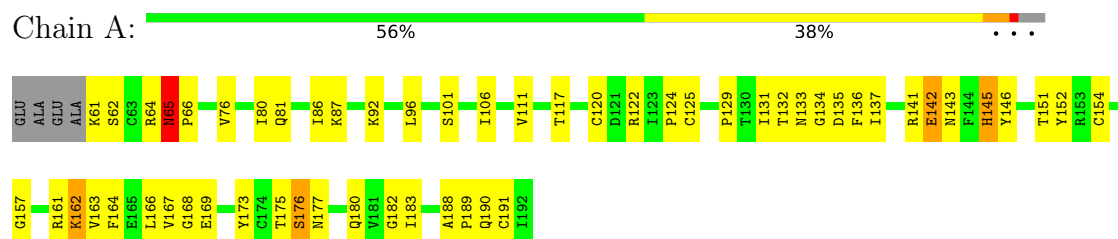
4.2.18 Score per residue for model 18

- Molecule 1: Complement receptor type 1



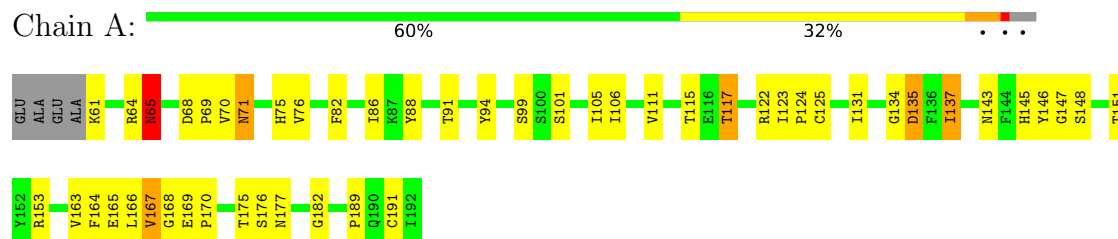
4.2.19 Score per residue for model 19

- Molecule 1: Complement receptor type 1



4.2.20 Score per residue for model 20

- Molecule 1: Complement receptor type 1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	486
Number of shifts mapped to atoms	485
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	28%

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	1.16±0.06	1±1/1022 (0.1± 0.1%)	1.09±0.04	3±2/1392 (0.2± 0.1%)
All	All	1.16	29/20440 (0.1%)	1.09	55/27840 (0.2%)

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	0.0±0.0	0.2±0.4
All	All	0	4

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	189	PRO	C-N	-7.80	1.24	1.33	19	2
1	A	79	GLY	C-N	-7.32	1.26	1.34	16	1
1	A	68	ASP	CA-C	6.53	1.61	1.52	15	1
1	A	137	ILE	N-CA	-6.53	1.38	1.46	20	1
1	A	135	ASP	C-N	-6.41	1.25	1.33	20	1
1	A	137	ILE	C-N	-6.33	1.25	1.33	17	1
1	A	115	THR	N-CA	-6.14	1.39	1.46	17	2
1	A	66	PRO	CA-C	6.05	1.57	1.52	11	4
1	A	162	LYS	C-N	-6.01	1.27	1.33	14	3
1	A	146	TYR	C-N	-5.93	1.24	1.33	14	1
1	A	96	LEU	C-N	-5.75	1.26	1.33	5	1
1	A	131	ILE	N-CA	-5.61	1.39	1.46	12	1
1	A	124	PRO	C-N	-5.51	1.26	1.33	2	1
1	A	175	THR	C-N	-5.44	1.25	1.33	9	1
1	A	178	ASP	CA-C	5.40	1.59	1.52	15	1
1	A	103	THR	N-CA	-5.25	1.39	1.46	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	118	PRO	C-N	-5.21	1.26	1.33	12	1
1	A	145	HIS	N-CA	5.21	1.52	1.45	6	1
1	A	123	ILE	CA-C	-5.17	1.47	1.52	9	1
1	A	130	THR	C-N	-5.14	1.27	1.33	12	1
1	A	98	GLY	CA-C	-5.05	1.48	1.51	11	1
1	A	64	ARG	N-CA	-5.03	1.40	1.46	17	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	144	PHE	N-CA-C	7.41	119.44	111.36	6	1
1	A	82	PHE	CA-CB-CG	7.29	121.09	113.80	1	1
1	A	66	PRO	N-CA-C	7.07	119.32	110.70	3	2
1	A	80	ILE	N-CA-C	-6.95	105.95	112.83	16	4
1	A	69	PRO	CB-CA-C	-6.83	102.65	111.46	10	1
1	A	177	ASN	N-CA-C	6.60	118.47	111.28	20	2
1	A	65	ASN	CA-C-N	6.21	126.78	120.38	3	3
1	A	65	ASN	C-N-CA	6.21	126.78	120.38	3	3
1	A	66	PRO	CA-C-N	6.14	125.86	119.05	5	3
1	A	66	PRO	C-N-CA	6.14	125.86	119.05	5	3
1	A	178	ASP	N-CA-C	5.96	117.86	111.36	5	1
1	A	155	ASN	CA-C-N	5.91	125.53	119.56	9	1
1	A	155	ASN	C-N-CA	5.91	125.53	119.56	9	1
1	A	104	CYS	CB-CA-C	-5.66	99.49	109.62	9	2
1	A	106	ILE	CB-CA-C	-5.63	103.27	110.98	12	1
1	A	117	THR	CA-C-N	5.62	125.59	120.03	6	6
1	A	117	THR	C-N-CA	5.62	125.59	120.03	6	6
1	A	138	SER	N-CA-C	5.47	117.24	111.28	18	1
1	A	133	ASN	N-CA-C	5.46	118.06	111.40	1	2
1	A	76	VAL	N-CA-C	5.31	116.03	110.62	11	1
1	A	188	ALA	CA-C-N	5.28	125.26	120.03	13	1
1	A	188	ALA	C-N-CA	5.28	125.26	120.03	13	1
1	A	145	HIS	CA-C-N	5.28	128.21	120.71	17	1
1	A	145	HIS	C-N-CA	5.28	128.21	120.71	17	1
1	A	80	ILE	CB-CA-C	-5.21	104.33	110.84	18	1
1	A	145	HIS	N-CA-C	5.15	116.63	108.96	6	1
1	A	77	ILE	N-CA-C	5.11	115.88	110.72	17	1
1	A	183	ILE	CB-CA-C	-5.07	103.32	110.82	6	1
1	A	147	GLY	N-CA-C	-5.03	108.18	115.27	20	1
1	A	125	CYS	CB-CA-C	5.01	117.98	111.42	13	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	153	ARG	Sidechain	3
1	A	95	ARG	Sidechain	1

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	997	960	959	36±7
All	All	19940	19200	19180	718

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:ARG:HB3	1:A:145:HIS:CE1	0.90	2.01	12	3
1:A:106:ILE:HG12	1:A:111:VAL:HG22	0.89	1.45	18	5
1:A:64:ARG:O	1:A:65:ASN:HB3	0.79	1.77	2	11
1:A:67:PRO:CG	1:A:117:THR:HG21	0.78	2.08	5	1
1:A:166:LEU:HD21	1:A:170:PRO:HB3	0.78	1.54	15	1
1:A:131:ILE:HG21	1:A:134:GLY:C	0.78	2.02	5	5
1:A:156:PRO:HA	1:A:161:ARG:O	0.77	1.78	17	4
1:A:146:TYR:HA	1:A:174:CYS:CB	0.74	2.13	14	2
1:A:131:ILE:HG21	1:A:134:GLY:O	0.72	1.84	5	5
1:A:161:ARG:HG2	1:A:162:LYS:H	0.72	1.44	19	1
1:A:127:LEU:HD12	1:A:128:PRO:HD2	0.71	1.59	5	1
1:A:127:LEU:HD13	1:A:142:GLU:HA	0.71	1.60	5	1
1:A:84:SER:O	1:A:103:THR:HA	0.71	1.85	10	4
1:A:61:LYS:HZ3	1:A:110:THR:N	0.71	1.84	13	1
1:A:86:ILE:O	1:A:101:SER:HA	0.70	1.86	6	16
1:A:176:SER:HB2	1:A:181:VAL:O	0.70	1.85	9	2
1:A:122:ARG:HD2	1:A:145:HIS:NE2	0.70	2.02	11	2
1:A:63:CYS:HB2	1:A:80:ILE:O	0.70	1.86	18	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:TYR:CD2	1:A:175:THR:HG22	0.70	2.21	5	5
1:A:133:ASN:OD1	1:A:154:CYS:HA	0.70	1.86	9	3
1:A:137:ILE:HA	1:A:153:ARG:NH1	0.70	2.01	14	1
1:A:122:ARG:HD2	1:A:145:HIS:CE1	0.69	2.22	17	1
1:A:154:CYS:SG	1:A:166:LEU:HB2	0.69	2.26	19	4
1:A:99:SER:O	1:A:118:PRO:HG2	0.69	1.87	5	1
1:A:61:LYS:O	1:A:111:VAL:HB	0.69	1.86	18	1
1:A:176:SER:OG	1:A:182:GLY:HA2	0.69	1.86	18	1
1:A:123:ILE:O	1:A:145:HIS:HA	0.69	1.87	14	3
1:A:63:CYS:SG	1:A:111:VAL:HG12	0.69	2.28	12	3
1:A:79:GLY:O	1:A:84:SER:HB2	0.69	1.87	12	2
1:A:91:THR:HG23	1:A:94:TYR:CD2	0.68	2.23	20	1
1:A:104:CYS:SG	1:A:111:VAL:HG22	0.68	2.28	8	4
1:A:141:ARG:HG2	1:A:142:GLU:H	0.68	1.48	14	1
1:A:67:PRO:HG3	1:A:117:THR:HG21	0.68	1.66	5	1
1:A:129:PRO:HG2	1:A:187:PRO:O	0.68	1.88	17	1
1:A:154:CYS:SG	1:A:166:LEU:HD12	0.68	2.29	6	7
1:A:61:LYS:NZ	1:A:106:ILE:HG23	0.68	2.04	13	1
1:A:88:TYR:HE2	1:A:120:CYS:SG	0.67	2.12	5	3
1:A:137:ILE:N	1:A:153:ARG:HH12	0.67	1.85	16	1
1:A:85:GLN:HA	1:A:102:ALA:O	0.67	1.90	10	10
1:A:175:THR:HG21	1:A:185:SER:HA	0.66	1.67	14	1
1:A:131:ILE:HG23	1:A:134:GLY:H	0.66	1.50	9	6
1:A:88:TYR:HE1	1:A:120:CYS:SG	0.66	2.13	7	1
1:A:179:ASP:HB2	1:A:183:ILE:HD13	0.66	1.66	3	1
1:A:87:LYS:HA	1:A:100:SER:O	0.66	1.91	10	1
1:A:137:ILE:HD12	1:A:153:ARG:HE	0.66	1.51	11	1
1:A:131:ILE:HG21	1:A:135:ASP:N	0.66	2.06	14	1
1:A:67:PRO:O	1:A:69:PRO:HD3	0.66	1.90	16	1
1:A:155:ASN:O	1:A:163:VAL:HG22	0.65	1.91	6	2
1:A:183:ILE:HD12	1:A:184:TRP:O	0.65	1.92	10	3
1:A:67:PRO:HB3	1:A:88:TYR:CZ	0.65	2.27	15	1
1:A:99:SER:HB2	1:A:115:THR:HG21	0.64	1.70	10	1
1:A:125:CYS:SG	1:A:146:TYR:HA	0.63	2.33	15	3
1:A:97:ILE:HG12	1:A:119:ILE:O	0.63	1.92	3	2
1:A:176:SER:CB	1:A:182:GLY:H	0.63	2.06	5	3
1:A:106:ILE:HG12	1:A:111:VAL:CG2	0.63	2.23	15	3
1:A:143:ASN:HB3	1:A:148:SER:OG	0.63	1.93	20	1
1:A:61:LYS:HD3	1:A:111:VAL:HG23	0.63	1.70	13	3
1:A:98:GLY:H	1:A:118:PRO:HB3	0.63	1.53	3	8
1:A:84:SER:HB3	1:A:104:CYS:SG	0.63	2.34	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:ILE:HD13	1:A:181:VAL:O	0.63	1.94	17	1
1:A:82:PHE:HA	1:A:104:CYS:HB2	0.63	1.70	9	2
1:A:123:ILE:HD13	1:A:182:GLY:HA3	0.63	1.69	9	1
1:A:113:TRP:HB3	1:A:115:THR:O	0.62	1.94	18	1
1:A:106:ILE:CD1	1:A:111:VAL:HG22	0.62	2.24	20	3
1:A:146:TYR:HA	1:A:174:CYS:HB3	0.62	1.70	14	1
1:A:97:ILE:HD11	1:A:121:ASP:HB3	0.62	1.72	11	2
1:A:64:ARG:O	1:A:65:ASN:HB2	0.62	1.94	1	4
1:A:87:LYS:HG2	1:A:101:SER:OG	0.62	1.95	16	3
1:A:157:GLY:CA	1:A:163:VAL:HG13	0.62	2.25	19	1
1:A:136:PHE:HZ	1:A:141:ARG:O	0.61	1.78	10	5
1:A:91:THR:HG23	1:A:94:TYR:HD2	0.61	1.52	20	1
1:A:123:ILE:HG21	1:A:182:GLY:HA2	0.60	1.72	5	1
1:A:69:PRO:HD2	1:A:88:TYR:OH	0.60	1.95	20	1
1:A:99:SER:N	1:A:118:PRO:HG3	0.60	2.11	3	6
1:A:131:ILE:HG21	1:A:135:ASP:O	0.60	1.96	19	2
1:A:87:LYS:HB3	1:A:101:SER:OG	0.60	1.96	10	1
1:A:81:GLN:O	1:A:104:CYS:HB3	0.60	1.96	4	2
1:A:127:LEU:HD12	1:A:142:GLU:OE1	0.60	1.97	9	1
1:A:95:ARG:O	1:A:120:CYS:HA	0.59	1.97	14	6
1:A:62:SER:OG	1:A:81:GLN:HG3	0.59	1.98	16	1
1:A:136:PHE:CZ	1:A:141:ARG:O	0.59	2.55	9	2
1:A:154:CYS:HB2	1:A:164:PHE:CD1	0.59	2.33	2	2
1:A:143:ASN:ND2	1:A:148:SER:HB3	0.59	2.13	14	1
1:A:122:ARG:O	1:A:124:PRO:HD3	0.59	1.97	20	3
1:A:166:LEU:HD23	1:A:167:VAL:N	0.59	2.12	7	11
1:A:176:SER:HB3	1:A:181:VAL:C	0.59	2.22	17	1
1:A:145:HIS:CE1	1:A:146:TYR:HB3	0.59	2.32	17	2
1:A:122:ARG:HG2	1:A:145:HIS:NE2	0.58	2.13	16	1
1:A:124:PRO:HA	1:A:145:HIS:CD2	0.58	2.34	8	2
1:A:90:CYS:SG	1:A:96:LEU:HD13	0.58	2.38	8	6
1:A:104:CYS:SG	1:A:111:VAL:CG1	0.58	2.91	13	3
1:A:161:ARG:HG2	1:A:162:LYS:N	0.58	2.12	19	1
1:A:173:TYR:CE2	1:A:175:THR:HG22	0.58	2.33	19	2
1:A:127:LEU:HD11	1:A:142:GLU:HB3	0.58	1.75	6	1
1:A:79:GLY:CA	1:A:84:SER:HB3	0.58	2.29	4	2
1:A:79:GLY:HA2	1:A:84:SER:HB3	0.58	1.76	4	4
1:A:127:LEU:HD12	1:A:128:PRO:CD	0.58	2.29	5	1
1:A:125:CYS:SG	1:A:184:TRP:CE2	0.58	2.97	13	5
1:A:106:ILE:HD13	1:A:111:VAL:HG22	0.58	1.74	20	3
1:A:166:LEU:HD23	1:A:167:VAL:O	0.58	1.99	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:SER:HB3	1:A:115:THR:HG21	0.57	1.76	2	1
1:A:99:SER:O	1:A:115:THR:HG21	0.57	2.00	6	1
1:A:115:THR:O	1:A:116:GLU:HG2	0.57	2.00	8	2
1:A:82:PHE:HZ	1:A:106:ILE:HD11	0.56	1.59	1	1
1:A:123:ILE:HD13	1:A:182:GLY:CA	0.56	2.30	9	1
1:A:87:LYS:HD3	1:A:101:SER:OG	0.56	2.00	4	1
1:A:66:PRO:HG3	1:A:86:ILE:HG21	0.56	1.76	8	1
1:A:73:MET:HG2	1:A:89:SER:HB2	0.56	1.78	10	1
1:A:82:PHE:HA	1:A:104:CYS:HB3	0.56	1.77	8	1
1:A:175:THR:CG2	1:A:185:SER:HA	0.56	2.31	14	3
1:A:67:PRO:C	1:A:69:PRO:HD2	0.56	2.24	3	1
1:A:66:PRO:HA	1:A:86:ILE:CD1	0.56	2.31	15	1
1:A:125:CYS:HB3	1:A:143:ASN:OD1	0.55	2.01	1	1
1:A:137:ILE:CG2	1:A:151:THR:HB	0.55	2.32	7	4
1:A:153:ARG:HH11	1:A:153:ARG:HG3	0.55	1.61	16	1
1:A:63:CYS:HB3	1:A:113:TRP:CE2	0.55	2.37	18	3
1:A:179:ASP:O	1:A:180:GLN:HG2	0.55	2.02	5	1
1:A:122:ARG:HB3	1:A:145:HIS:ND1	0.55	2.17	17	1
1:A:176:SER:HB3	1:A:182:GLY:H	0.55	1.62	19	3
1:A:66:PRO:HD3	1:A:80:ILE:CG2	0.55	2.31	15	2
1:A:176:SER:O	1:A:177:ASN:HB2	0.55	2.02	16	1
1:A:122:ARG:HB3	1:A:145:HIS:NE2	0.55	2.17	20	2
1:A:136:PHE:HB3	1:A:152:TYR:CE1	0.55	2.37	16	2
1:A:99:SER:O	1:A:118:PRO:HG3	0.54	2.02	1	2
1:A:137:ILE:HD12	1:A:151:THR:HB	0.54	1.79	4	1
1:A:131:ILE:HD11	1:A:189:PRO:O	0.54	2.01	9	1
1:A:145:HIS:CG	1:A:146:TYR:N	0.54	2.76	17	5
1:A:176:SER:HB2	1:A:182:GLY:H	0.54	1.61	10	2
1:A:167:VAL:HG12	1:A:192:ILE:HD12	0.54	1.78	17	1
1:A:96:LEU:HD13	1:A:120:CYS:SG	0.54	2.43	19	1
1:A:95:ARG:HD2	1:A:96:LEU:O	0.54	2.02	16	2
1:A:131:ILE:HB	1:A:152:TYR:CD1	0.53	2.37	15	8
1:A:99:SER:H	1:A:118:PRO:HG3	0.53	1.63	5	1
1:A:137:ILE:HB	1:A:153:ARG:NH1	0.53	2.18	16	1
1:A:167:VAL:HG13	1:A:190:GLN:O	0.53	2.03	2	1
1:A:61:LYS:HZ2	1:A:106:ILE:HG23	0.53	1.63	13	1
1:A:173:TYR:O	1:A:175:THR:HG23	0.53	2.03	5	1
1:A:133:ASN:HA	1:A:155:ASN:OD1	0.53	2.03	12	1
1:A:165:GLU:O	1:A:191:CYS:HA	0.53	2.04	6	10
1:A:154:CYS:HB3	1:A:164:PHE:HB2	0.53	1.80	9	3
1:A:76:VAL:HG21	1:A:86:ILE:HG22	0.53	1.80	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:GLY:O	1:A:143:ASN:HB3	0.53	2.04	5	1
1:A:163:VAL:HG23	1:A:164:PHE:CD2	0.53	2.39	17	4
1:A:62:SER:HB2	1:A:81:GLN:CD	0.53	2.29	19	1
1:A:128:PRO:CD	1:A:142:GLU:HG3	0.53	2.34	10	1
1:A:155:ASN:HB2	1:A:164:PHE:CZ	0.53	2.39	6	1
1:A:128:PRO:HD3	1:A:142:GLU:HG3	0.53	1.81	10	1
1:A:140:ASN:O	1:A:141:ARG:HB2	0.53	2.04	14	1
1:A:67:PRO:HB3	1:A:88:TYR:CE1	0.53	2.39	15	1
1:A:77:ILE:HG23	1:A:78:LYS:H	0.52	1.63	3	4
1:A:145:HIS:ND1	1:A:146:TYR:N	0.52	2.57	12	1
1:A:166:LEU:HG	1:A:167:VAL:N	0.52	2.19	9	4
1:A:126:GLY:HA3	1:A:143:ASN:O	0.52	2.04	13	1
1:A:176:SER:CB	1:A:183:ILE:H	0.52	2.18	17	1
1:A:133:ASN:HB3	1:A:155:ASN:ND2	0.52	2.20	14	2
1:A:65:ASN:CG	1:A:66:PRO:HD2	0.52	2.29	3	1
1:A:143:ASN:ND2	1:A:150:VAL:HG13	0.52	2.20	4	1
1:A:82:PHE:CZ	1:A:106:ILE:HD11	0.52	2.40	1	1
1:A:129:PRO:HB2	1:A:188:ALA:HB2	0.52	1.80	1	3
1:A:98:GLY:N	1:A:118:PRO:HB3	0.52	2.19	3	3
1:A:190:GLN:HG3	1:A:192:ILE:HG12	0.51	1.81	15	4
1:A:127:LEU:HD21	1:A:142:GLU:HG2	0.51	1.82	8	1
1:A:67:PRO:HD3	1:A:86:ILE:HD12	0.51	1.82	3	2
1:A:130:THR:OG1	1:A:135:ASP:HA	0.51	2.04	7	1
1:A:173:TYR:CE2	1:A:175:THR:HB	0.51	2.41	17	2
1:A:77:ILE:O	1:A:78:LYS:HG3	0.51	2.05	9	1
1:A:157:GLY:HA3	1:A:163:VAL:CG1	0.51	2.36	17	1
1:A:95:ARG:HE	1:A:124:PRO:HD2	0.51	1.66	8	1
1:A:95:ARG:NH2	1:A:182:GLY:HA3	0.51	2.21	6	2
1:A:157:GLY:HA2	1:A:163:VAL:HG13	0.50	1.81	19	1
1:A:68:ASP:N	1:A:69:PRO:CD	0.50	2.74	15	3
1:A:110:THR:HG23	1:A:111:VAL:N	0.50	2.21	9	1
1:A:99:SER:C	1:A:118:PRO:HG3	0.50	2.31	1	2
1:A:95:ARG:HE	1:A:123:ILE:HG23	0.50	1.65	18	1
1:A:175:THR:O	1:A:175:THR:HG23	0.50	2.06	9	4
1:A:162:LYS:O	1:A:162:LYS:HD3	0.50	2.06	10	1
1:A:162:LYS:HG2	1:A:164:PHE:O	0.50	2.06	6	1
1:A:176:SER:HB2	1:A:181:VAL:C	0.50	2.32	9	2
1:A:133:ASN:ND2	1:A:191:CYS:SG	0.50	2.84	1	2
1:A:137:ILE:HD12	1:A:151:THR:HG22	0.50	1.83	15	2
1:A:66:PRO:HA	1:A:86:ILE:HD13	0.50	1.83	15	1
1:A:107:SER:HB3	1:A:112:ILE:HD11	0.50	1.84	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:ILE:CG1	1:A:111:VAL:HG22	0.50	2.30	18	2
1:A:81:GLN:HB2	1:A:84:SER:OG	0.49	2.06	8	1
1:A:176:SER:HB2	1:A:183:ILE:O	0.49	2.07	17	1
1:A:141:ARG:CG	1:A:142:GLU:H	0.49	2.14	14	1
1:A:77:ILE:HG23	1:A:78:LYS:N	0.49	2.22	7	1
1:A:154:CYS:HB3	1:A:164:PHE:CB	0.49	2.37	9	2
1:A:136:PHE:HB2	1:A:150:VAL:CG1	0.49	2.37	17	1
1:A:62:SER:OG	1:A:80:ILE:HG13	0.49	2.08	19	1
1:A:190:GLN:HG3	1:A:192:ILE:HG13	0.49	1.83	10	1
1:A:67:PRO:HD2	1:A:117:THR:OG1	0.49	2.08	14	1
1:A:80:ILE:O	1:A:104:CYS:SG	0.49	2.71	6	2
1:A:106:ILE:HD13	1:A:111:VAL:CG2	0.49	2.38	12	1
1:A:141:ARG:HG2	1:A:142:GLU:N	0.49	2.19	14	1
1:A:176:SER:HB2	1:A:183:ILE:H	0.48	1.67	17	2
1:A:161:ARG:CG	1:A:162:LYS:H	0.48	2.18	19	1
1:A:82:PHE:CE1	1:A:105:ILE:HA	0.48	2.43	7	1
1:A:104:CYS:SG	1:A:113:TRP:CZ3	0.48	3.06	10	2
1:A:90:CYS:SG	1:A:96:LEU:CD1	0.48	3.01	1	4
1:A:62:SER:OG	1:A:81:GLN:HG2	0.48	2.07	6	1
1:A:61:LYS:CD	1:A:111:VAL:HG23	0.48	2.38	13	1
1:A:127:LEU:CD1	1:A:142:GLU:HB3	0.48	2.38	6	1
1:A:61:LYS:O	1:A:111:VAL:HG21	0.48	2.08	20	1
1:A:99:SER:C	1:A:118:PRO:HG2	0.48	2.33	5	1
1:A:76:VAL:O	1:A:78:LYS:N	0.48	2.47	11	1
1:A:190:GLN:HB2	1:A:192:ILE:HG13	0.48	1.85	8	2
1:A:81:GLN:O	1:A:104:CYS:HB2	0.48	2.09	11	2
1:A:164:PHE:HB3	1:A:191:CYS:HB3	0.48	1.85	19	3
1:A:128:PRO:HD3	1:A:143:ASN:OD1	0.48	2.08	15	1
1:A:175:THR:HG22	1:A:185:SER:HA	0.48	1.84	1	1
1:A:79:GLY:O	1:A:84:SER:HB3	0.48	2.09	14	2
1:A:162:LYS:HD3	1:A:162:LYS:C	0.48	2.34	10	1
1:A:63:CYS:HA	1:A:111:VAL:HG12	0.48	1.85	6	1
1:A:62:SER:HA	1:A:81:GLN:HA	0.48	1.86	9	3
1:A:66:PRO:HD3	1:A:80:ILE:HG21	0.48	1.85	15	1
1:A:107:SER:HB2	1:A:112:ILE:HD12	0.47	1.86	6	1
1:A:157:GLY:HA2	1:A:163:VAL:CG1	0.47	2.39	19	1
1:A:176:SER:HA	1:A:183:ILE:O	0.47	2.09	19	1
1:A:104:CYS:SG	1:A:111:VAL:CG2	0.47	3.02	8	1
1:A:63:CYS:SG	1:A:111:VAL:HG22	0.47	2.49	16	1
1:A:64:ARG:O	1:A:65:ASN:CB	0.47	2.62	7	9
1:A:104:CYS:SG	1:A:111:VAL:HG13	0.47	2.49	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:CYS:HB3	1:A:113:TRP:CZ2	0.47	2.43	8	1
1:A:181:VAL:O	1:A:183:ILE:HG23	0.47	2.10	16	1
1:A:96:LEU:HD12	1:A:118:PRO:HG2	0.47	1.86	2	1
1:A:115:THR:O	1:A:116:GLU:HB2	0.47	2.08	2	3
1:A:166:LEU:HA	1:A:190:GLN:O	0.47	2.08	8	2
1:A:85:GLN:HE22	1:A:103:THR:CB	0.47	2.22	14	1
1:A:122:ARG:HG2	1:A:145:HIS:CD2	0.47	2.44	16	1
1:A:66:PRO:CG	1:A:76:VAL:HG21	0.47	2.40	10	1
1:A:76:VAL:O	1:A:76:VAL:HG22	0.47	2.09	10	1
1:A:146:TYR:HA	1:A:174:CYS:HB2	0.47	1.82	14	1
1:A:69:PRO:HG3	1:A:88:TYR:CE2	0.47	2.44	15	1
1:A:156:PRO:O	1:A:161:ARG:HG2	0.47	2.10	17	1
1:A:133:ASN:HD22	1:A:154:CYS:HA	0.47	1.69	1	1
1:A:79:GLY:HA2	1:A:84:SER:CB	0.47	2.40	16	2
1:A:134:GLY:HA3	1:A:153:ARG:O	0.47	2.09	14	1
1:A:166:LEU:HD23	1:A:168:GLY:H	0.46	1.70	4	1
1:A:137:ILE:HG22	1:A:151:THR:O	0.46	2.10	19	2
1:A:164:PHE:O	1:A:191:CYS:HB3	0.46	2.09	8	1
1:A:170:PRO:HA	1:A:189:PRO:HG3	0.46	1.87	20	1
1:A:68:ASP:N	1:A:69:PRO:HD3	0.46	2.25	9	2
1:A:82:PHE:HA	1:A:104:CYS:CB	0.46	2.40	7	1
1:A:187:PRO:O	1:A:188:ALA:C	0.46	2.58	6	3
1:A:82:PHE:CD1	1:A:105:ILE:HA	0.46	2.46	7	1
1:A:157:GLY:HA3	1:A:163:VAL:HG13	0.46	1.88	19	1
1:A:128:PRO:HG2	1:A:136:PHE:CZ	0.46	2.45	1	1
1:A:175:THR:C	1:A:177:ASN:H	0.46	2.19	12	1
1:A:161:ARG:CG	1:A:162:LYS:N	0.46	2.77	19	1
1:A:137:ILE:HD12	1:A:151:THR:CG2	0.46	2.40	15	3
1:A:107:SER:OG	1:A:112:ILE:HD11	0.46	2.10	11	1
1:A:66:PRO:HB2	1:A:67:PRO:CD	0.46	2.41	15	1
1:A:95:ARG:NE	1:A:124:PRO:HD2	0.46	2.26	2	1
1:A:123:ILE:HB	1:A:146:TYR:HB2	0.46	1.86	16	2
1:A:62:SER:O	1:A:111:VAL:HB	0.46	2.11	12	1
1:A:99:SER:O	1:A:118:PRO:HD3	0.46	2.11	18	4
1:A:137:ILE:HD12	1:A:153:ARG:NE	0.46	2.25	11	1
1:A:88:TYR:CZ	1:A:120:CYS:SG	0.46	3.09	1	1
1:A:99:SER:H	1:A:118:PRO:CG	0.46	2.24	5	1
1:A:79:GLY:C	1:A:84:SER:HB2	0.46	2.36	16	2
1:A:145:HIS:CD2	1:A:146:TYR:H	0.46	2.29	16	1
1:A:170:PRO:HA	1:A:189:PRO:HG2	0.45	1.88	5	2
1:A:82:PHE:CD1	1:A:106:ILE:HG13	0.45	2.46	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:LEU:HG	1:A:100:SER:HB2	0.45	1.86	8	1
1:A:96:LEU:HG	1:A:100:SER:CB	0.45	2.41	17	1
1:A:141:ARG:O	1:A:142:GLU:HB2	0.45	2.11	4	3
1:A:82:PHE:CE1	1:A:106:ILE:HG12	0.45	2.46	16	1
1:A:67:PRO:HB3	1:A:117:THR:HG23	0.45	1.88	8	1
1:A:131:ILE:HB	1:A:152:TYR:CD2	0.45	2.45	9	1
1:A:137:ILE:CG1	1:A:153:ARG:HG2	0.45	2.41	15	1
1:A:133:ASN:HB3	1:A:155:ASN:HD21	0.45	1.71	1	1
1:A:95:ARG:NE	1:A:123:ILE:HG23	0.45	2.26	18	1
1:A:63:CYS:O	1:A:80:ILE:HD12	0.45	2.10	15	1
1:A:175:THR:HG21	1:A:185:SER:HB3	0.45	1.87	5	1
1:A:131:ILE:HD13	1:A:152:TYR:HB3	0.45	1.88	2	1
1:A:67:PRO:HG3	1:A:117:THR:OG1	0.45	2.12	17	1
1:A:69:PRO:HG2	1:A:88:TYR:CZ	0.45	2.47	13	1
1:A:179:ASP:HB2	1:A:183:ILE:HG12	0.45	1.88	16	1
1:A:104:CYS:SG	1:A:111:VAL:HG12	0.45	2.51	18	1
1:A:125:CYS:O	1:A:143:ASN:HB2	0.45	2.12	19	1
1:A:143:ASN:HD21	1:A:148:SER:CB	0.45	2.25	1	1
1:A:88:TYR:CE2	1:A:120:CYS:SG	0.45	3.03	5	5
1:A:66:PRO:HD3	1:A:80:ILE:HG22	0.45	1.88	7	3
1:A:99:SER:HB2	1:A:115:THR:CG2	0.45	2.42	20	1
1:A:128:PRO:HB2	1:A:152:TYR:OH	0.44	2.12	5	1
1:A:62:SER:HB3	1:A:81:GLN:NE2	0.44	2.27	8	1
1:A:61:LYS:HB3	1:A:111:VAL:CG2	0.44	2.42	18	2
1:A:92:LYS:HG3	1:A:177:ASN:HD21	0.44	1.72	19	1
1:A:61:LYS:HB3	1:A:111:VAL:CG1	0.44	2.42	3	1
1:A:133:ASN:CG	1:A:154:CYS:HA	0.44	2.37	12	1
1:A:132:THR:HG21	1:A:191:CYS:HB2	0.44	1.88	19	1
1:A:143:ASN:HD21	1:A:148:SER:HB3	0.44	1.73	6	2
1:A:69:PRO:HG3	1:A:88:TYR:CE1	0.44	2.48	1	1
1:A:149:VAL:HG23	1:A:172:ILE:O	0.44	2.13	8	1
1:A:178:ASP:CG	1:A:179:ASP:H	0.44	2.20	7	1
1:A:79:GLY:CA	1:A:84:SER:CB	0.44	2.95	16	1
1:A:97:ILE:HG22	1:A:97:ILE:O	0.44	2.13	7	1
1:A:98:GLY:H	1:A:118:PRO:CB	0.43	2.26	2	1
1:A:154:CYS:SG	1:A:166:LEU:HD13	0.43	2.53	15	1
1:A:167:VAL:HG23	1:A:190:GLN:O	0.43	2.12	1	1
1:A:105:ILE:HG12	1:A:114:ASP:HB3	0.43	1.88	2	1
1:A:131:ILE:CG2	1:A:134:GLY:C	0.43	2.91	10	2
1:A:127:LEU:HD13	1:A:142:GLU:CB	0.43	2.44	9	1
1:A:61:LYS:HB2	1:A:111:VAL:CG2	0.43	2.43	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:HIS:CG	1:A:146:TYR:H	0.43	2.28	14	2
1:A:164:PHE:CB	1:A:191:CYS:HB3	0.43	2.43	19	1
1:A:104:CYS:HB2	1:A:113:TRP:CE3	0.43	2.48	2	1
1:A:128:PRO:HB3	1:A:184:TRP:CE2	0.43	2.48	10	1
1:A:141:ARG:O	1:A:141:ARG:HG2	0.43	2.12	18	1
1:A:137:ILE:HD12	1:A:151:THR:CB	0.43	2.43	4	1
1:A:105:ILE:CG1	1:A:114:ASP:HB2	0.43	2.44	7	1
1:A:133:ASN:HB3	1:A:155:ASN:HB3	0.43	1.91	7	1
1:A:87:LYS:HG3	1:A:101:SER:OG	0.43	2.13	8	2
1:A:99:SER:O	1:A:118:PRO:CG	0.43	2.66	14	1
1:A:179:ASP:O	1:A:183:ILE:HG12	0.43	2.14	7	1
1:A:141:ARG:O	1:A:142:GLU:HG3	0.43	2.14	9	1
1:A:95:ARG:NH1	1:A:97:ILE:HA	0.43	2.29	11	1
1:A:69:PRO:HB2	1:A:88:TYR:OH	0.43	2.14	16	1
1:A:143:ASN:HD21	1:A:148:SER:HB2	0.43	1.74	18	1
1:A:140:ASN:O	1:A:141:ARG:CB	0.43	2.67	14	1
1:A:67:PRO:HG2	1:A:117:THR:HG21	0.43	1.90	2	1
1:A:72:GLY:O	1:A:73:MET:HB3	0.43	2.14	2	1
1:A:67:PRO:O	1:A:68:ASP:HB3	0.43	2.14	5	1
1:A:90:CYS:SG	1:A:96:LEU:HD22	0.43	2.54	6	3
1:A:67:PRO:O	1:A:69:PRO:HD2	0.43	2.14	10	1
1:A:66:PRO:HB3	1:A:86:ILE:HD13	0.43	1.90	19	1
1:A:137:ILE:HG22	1:A:151:THR:HB	0.43	1.91	20	1
1:A:81:GLN:HG3	1:A:82:PHE:N	0.42	2.28	9	1
1:A:81:GLN:HG2	1:A:82:PHE:N	0.42	2.29	18	1
1:A:82:PHE:CZ	1:A:106:ILE:CD1	0.42	3.03	1	1
1:A:96:LEU:HD22	1:A:96:LEU:N	0.42	2.29	1	2
1:A:110:THR:CG2	1:A:111:VAL:N	0.42	2.83	9	1
1:A:137:ILE:HG13	1:A:153:ARG:NH1	0.42	2.29	14	1
1:A:62:SER:HB2	1:A:80:ILE:HG13	0.42	1.91	9	1
1:A:67:PRO:C	1:A:69:PRO:HD3	0.42	2.39	7	1
1:A:73:MET:HG2	1:A:89:SER:CB	0.42	2.43	10	1
1:A:176:SER:CB	1:A:181:VAL:C	0.42	2.93	17	1
1:A:143:ASN:HD21	1:A:150:VAL:HG13	0.42	1.73	4	1
1:A:105:ILE:HG12	1:A:114:ASP:HB2	0.42	1.91	7	1
1:A:85:GLN:HE22	1:A:103:THR:CG2	0.42	2.28	14	1
1:A:123:ILE:N	1:A:145:HIS:HE1	0.42	2.12	20	1
1:A:154:CYS:HB3	1:A:164:PHE:CD1	0.42	2.50	15	1
1:A:181:VAL:O	1:A:182:GLY:C	0.42	2.63	16	1
1:A:106:ILE:HD13	1:A:111:VAL:HG23	0.42	1.91	4	1
1:A:87:LYS:N	1:A:87:LYS:HD2	0.42	2.28	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:CYS:HA	1:A:111:VAL:O	0.42	2.14	12	1
1:A:124:PRO:C	1:A:126:GLY:H	0.42	2.22	18	2
1:A:86:ILE:O	1:A:86:ILE:HG13	0.42	2.15	14	3
1:A:146:TYR:CD1	1:A:174:CYS:HB3	0.42	2.49	17	1
1:A:167:VAL:HG21	1:A:189:PRO:HB3	0.42	1.92	17	1
1:A:190:GLN:NE2	1:A:192:ILE:HG13	0.42	2.29	6	1
1:A:88:TYR:CE1	1:A:120:CYS:SG	0.42	3.04	7	1
1:A:143:ASN:ND2	1:A:184:TRP:HH2	0.42	2.12	7	1
1:A:127:LEU:HB3	1:A:142:GLU:OE1	0.42	2.15	9	1
1:A:167:VAL:O	1:A:169:GLU:N	0.42	2.53	10	2
1:A:92:LYS:HG3	1:A:177:ASN:OD1	0.42	2.15	14	1
1:A:70:VAL:O	1:A:71:ASN:HB2	0.42	2.15	20	1
1:A:95:ARG:HH21	1:A:182:GLY:CA	0.41	2.28	6	1
1:A:66:PRO:HB2	1:A:67:PRO:HD2	0.41	1.90	8	1
1:A:166:LEU:HA	1:A:191:CYS:HA	0.41	1.90	15	1
1:A:82:PHE:CD1	1:A:106:ILE:HG12	0.41	2.49	16	2
1:A:66:PRO:CB	1:A:86:ILE:HD12	0.41	2.46	8	1
1:A:69:PRO:HG2	1:A:72:GLY:CA	0.41	2.45	11	1
1:A:85:GLN:NE2	1:A:103:THR:OG1	0.41	2.52	14	1
1:A:154:CYS:O	1:A:155:ASN:HB2	0.41	2.15	18	1
1:A:136:PHE:HB3	1:A:152:TYR:CE2	0.41	2.51	1	1
1:A:95:ARG:NH1	1:A:97:ILE:HD13	0.41	2.29	3	1
1:A:66:PRO:HB3	1:A:86:ILE:CD1	0.41	2.45	10	1
1:A:143:ASN:HB2	1:A:148:SER:HB3	0.41	1.92	10	1
1:A:127:LEU:HD23	1:A:128:PRO:HD2	0.41	1.91	14	1
1:A:66:PRO:CB	1:A:67:PRO:CD	0.41	2.98	15	1
1:A:156:PRO:HB3	1:A:160:GLY:H	0.41	1.76	3	1
1:A:165:GLU:O	1:A:191:CYS:CA	0.41	2.68	1	1
1:A:125:CYS:SG	1:A:145:HIS:O	0.41	2.79	3	1
1:A:107:SER:HB2	1:A:112:ILE:CG1	0.41	2.44	4	1
1:A:77:ILE:CG2	1:A:78:LYS:H	0.41	2.28	7	1
1:A:131:ILE:HG13	1:A:132:THR:N	0.41	2.30	15	1
1:A:62:SER:HB2	1:A:81:GLN:NE2	0.41	2.30	19	1
1:A:77:ILE:HG22	1:A:78:LYS:HG3	0.41	1.92	1	1
1:A:175:THR:HG22	1:A:185:SER:CA	0.41	2.45	6	1
1:A:127:LEU:HD23	1:A:142:GLU:HB3	0.41	1.92	13	1
1:A:61:LYS:HG2	1:A:111:VAL:HG23	0.41	1.91	14	1
1:A:75:HIS:O	1:A:75:HIS:CG	0.41	2.73	20	2
1:A:163:VAL:HB	1:A:164:PHE:CD2	0.41	2.51	20	1
1:A:99:SER:HB2	1:A:115:THR:HG23	0.41	1.93	6	1
1:A:95:ARG:HH11	1:A:97:ILE:HD13	0.41	1.74	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:PRO:HB2	1:A:159:GLY:O	0.41	2.16	14	1
1:A:125:CYS:SG	1:A:184:TRP:CZ2	0.41	3.14	11	1
1:A:131:ILE:HG23	1:A:134:GLY:N	0.41	2.31	12	1
1:A:122:ARG:HG2	1:A:145:HIS:CE1	0.41	2.50	14	1
1:A:116:GLU:O	1:A:117:THR:HB	0.41	2.16	4	1
1:A:128:PRO:HD3	1:A:143:ASN:H	0.41	1.75	4	1
1:A:143:ASN:HD21	1:A:150:VAL:CG1	0.41	2.29	7	1
1:A:166:LEU:HG	1:A:167:VAL:H	0.41	1.74	9	1
1:A:140:ASN:HB3	1:A:143:ASN:HD21	0.41	1.76	12	1
1:A:136:PHE:CZ	1:A:141:ARG:HA	0.41	2.50	13	1
1:A:92:LYS:HE3	1:A:146:TYR:OH	0.41	2.16	17	1
1:A:167:VAL:CG2	1:A:189:PRO:HB3	0.41	2.46	17	1
1:A:123:ILE:CG2	1:A:182:GLY:HA2	0.41	2.45	5	1
1:A:133:ASN:ND2	1:A:191:CYS:HB2	0.40	2.31	4	1
1:A:121:ASP:OD1	1:A:122:ARG:N	0.40	2.54	7	1
1:A:131:ILE:HD13	1:A:152:TYR:CD1	0.40	2.51	19	1
1:A:142:GLU:HG3	1:A:144:PHE:CE2	0.40	2.51	14	1
1:A:153:ARG:HA	1:A:166:LEU:CD1	0.40	2.47	20	1
1:A:128:PRO:HG3	1:A:143:ASN:H	0.40	1.76	6	1
1:A:112:ILE:HD13	1:A:112:ILE:H	0.40	1.75	15	1
1:A:66:PRO:HG3	1:A:76:VAL:HG11	0.40	1.93	15	1
1:A:176:SER:HB3	1:A:181:VAL:O	0.40	2.17	17	1
1:A:162:LYS:HG3	1:A:164:PHE:O	0.40	2.16	19	1
1:A:169:GLU:O	1:A:169:GLU:HG2	0.40	2.16	19	1

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	130/136 (96%)	113±2 (87±1%)	11±2 (8±2%)	6±2 (5±1%)	3	25
All	All	2600/2720 (96%)	2262 (87%)	212 (8%)	126 (5%)	3	25

All 34 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	117	THR	20
1	A	65	ASN	16
1	A	145	HIS	8
1	A	176	SER	8
1	A	66	PRO	7
1	A	68	ASP	7
1	A	127	LEU	6
1	A	142	GLU	5
1	A	135	ASP	4
1	A	180	GLN	4
1	A	168	GLY	4
1	A	125	CYS	3
1	A	141	ARG	3
1	A	108	GLY	3
1	A	78	LYS	3
1	A	79	GLY	2
1	A	77	ILE	2
1	A	75	HIS	2
1	A	177	ASN	2
1	A	182	GLY	2
1	A	76	VAL	2
1	A	73	MET	1
1	A	116	GLU	1
1	A	87	LYS	1
1	A	159	GLY	1
1	A	67	PRO	1
1	A	165	GLU	1
1	A	179	ASP	1
1	A	134	GLY	1
1	A	81	GLN	1
1	A	104	CYS	1
1	A	82	PHE	1
1	A	161	ARG	1
1	A	71	ASN	1

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	115/117 (98%)	111±2 (97±2%)	4±2 (3±2%)	32	82
All	All	2300/2340 (98%)	2220 (97%)	80 (3%)	32	82

All 28 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	125	CYS	10
1	A	63	CYS	8
1	A	65	ASN	7
1	A	105	ILE	4
1	A	155	ASN	4
1	A	169	GLU	4
1	A	183	ILE	4
1	A	175	THR	4
1	A	127	LEU	4
1	A	66	PRO	3
1	A	68	ASP	3
1	A	112	ILE	3
1	A	174	CYS	3
1	A	100	SER	2
1	A	145	HIS	2
1	A	86	ILE	2
1	A	76	VAL	2
1	A	96	LEU	1
1	A	117	THR	1
1	A	115	THR	1
1	A	110	THR	1
1	A	173	TYR	1
1	A	142	GLU	1
1	A	137	ILE	1
1	A	111	VAL	1
1	A	91	THR	1
1	A	81	GLN	1
1	A	167	VAL	1

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 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

The completeness of assignment taking into account all chemical shift lists is 28% for the well-defined parts and 28% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	486
Number of shifts mapped to atoms	485
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	101

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	120	CYS	HG	1.7	.	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	75	0.51 ± 0.59	None needed (imprecise)
$^{13}\text{C}_\beta$	58	-2.40 ± 0.66	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	67	-1.09 ± 1.11	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 28%, i.e. 470 atoms were assigned a chemical shift out of a possible 1684. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	256/653 (39%)	122/268 (46%)	75/264 (28%)	59/121 (49%)
Sidechain	201/908 (22%)	130/591 (22%)	71/283 (25%)	0/34 (0%)
Aromatic	13/123 (11%)	9/60 (15%)	4/59 (7%)	0/4 (0%)
Overall	470/1684 (28%)	261/919 (28%)	150/606 (25%)	59/159 (37%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 28%, i.e. 470 atoms were assigned a chemical shift out of a possible 1684. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	256/653 (39%)	122/268 (46%)	75/264 (28%)	59/121 (49%)
Sidechain	201/908 (22%)	130/591 (22%)	71/283 (25%)	0/34 (0%)
Aromatic	13/123 (11%)	9/60 (15%)	4/59 (7%)	0/4 (0%)
Overall	470/1684 (28%)	261/919 (28%)	150/606 (25%)	59/159 (37%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	180	GLN	CD	50.89	173.59 – 185.85	-105.1
1	A	136	PHE	CD2	13.65	125.53 – 137.61	-97.6
1	A	136	PHE	CD1	13.65	125.33 – 137.83	-94.3
1	A	152	TYR	CD1	25.83	125.84 – 139.60	-77.7
1	A	152	TYR	CD2	25.83	125.28 – 140.14	-71.9
1	A	143	ASN	CG	25.14	164.52 – 188.90	-62.2
1	A	184	TRP	CG	25.21	101.31 – 120.62	-44.4
1	A	152	TYR	CG	27.97	112.42 – 146.96	-29.4
1	A	118	PRO	CB	65.42	26.06 – 37.61	29.1
1	A	188	ALA	CB	68.71	10.19 – 27.75	28.3
1	A	156	PRO	CB	64.01	26.06 – 37.61	27.9
1	A	158	SER	CB	24.48	56.28 – 71.32	-26.1
1	A	178	ASP	CG	27.50	149.18 – 208.82	-25.4
1	A	127	LEU	HD11	7.39	-0.61 – 2.12	24.3

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	127	LEU	HD12	7.39	-0.61 – 2.12	24.3
1	A	127	LEU	HD13	7.39	-0.61 – 2.12	24.3
1	A	132	THR	CB	31.32	61.12 – 78.27	-22.4
1	A	129	PRO	CG	51.66	21.69 – 32.72	22.2
1	A	152	TYR	HD1	0.55	5.49 – 8.39	-22.0
1	A	152	TYR	HD2	0.55	5.48 – 8.39	-21.9
1	A	127	LEU	HD21	6.79	-0.65 – 2.13	21.8
1	A	127	LEU	HD22	6.79	-0.65 – 2.13	21.8
1	A	127	LEU	HD23	6.79	-0.65 – 2.13	21.8
1	A	192	ILE	HD11	6.75	-0.72 – 2.09	21.6
1	A	192	ILE	HD12	6.75	-0.72 – 2.09	21.6
1	A	192	ILE	HD13	6.75	-0.72 – 2.09	21.6
1	A	151	THR	CB	33.35	61.12 – 78.27	-21.2
1	A	148	SER	CB	31.97	56.28 – 71.32	-21.2
1	A	185	SER	CB	32.02	56.28 – 71.32	-21.1
1	A	117	THR	CB	34.04	61.12 – 78.27	-20.8
1	A	130	THR	CB	34.72	61.12 – 78.27	-20.4
1	A	136	PHE	HD2	0.90	5.52 – 8.61	-19.9
1	A	136	PHE	HD1	0.90	5.51 – 8.60	-19.9
1	A	163	VAL	CB	63.74	23.86 – 41.50	17.6
1	A	145	HIS	CB	65.99	19.76 – 40.75	17.0
1	A	175	THR	CB	41.19	61.12 – 78.27	-16.6
1	A	138	SER	CB	39.43	56.28 – 71.32	-16.2
1	A	166	LEU	CB	71.06	33.11 – 51.34	15.8
1	A	140	ASN	CB	64.05	30.50 – 46.89	15.5
1	A	155	ASN	CB	64.01	30.50 – 46.89	15.4
1	A	126	GLY	CA	64.67	38.93 – 51.79	15.0
1	A	176	SER	CB	41.23	56.28 – 71.32	-15.0
1	A	173	TYR	CB	70.02	28.67 – 49.81	14.6
1	A	184	TRP	HD1	2.43	5.46 – 8.81	-14.1
1	A	114	ASP	CB	19.10	32.98 – 48.76	-13.8
1	A	147	GLY	CA	62.92	38.93 – 51.79	13.7
1	A	186	GLY	CA	61.92	38.93 – 51.79	12.9
1	A	159	GLY	CA	61.27	38.93 – 51.79	12.4
1	A	143	ASN	HD21	1.62	4.94 – 9.72	-11.9
1	A	143	ASN	HD22	1.62	4.69 – 9.61	-11.2
1	A	168	GLY	CA	59.77	38.93 – 51.79	11.2
1	A	128	PRO	CA	46.89	55.85 – 70.84	-11.0
1	A	153	ARG	HD2	0.80	1.97 – 4.26	-10.1
1	A	161	ARG	HD2	0.87	1.97 – 4.26	-9.8
1	A	184	TRP	HB3	-0.38	1.31 – 4.93	-9.7
1	A	187	PRO	HD2	0.48	1.93 – 5.38	-9.2

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	158	SER	HB2	1.56	2.61 – 5.13	-9.2
1	A	157	GLY	CA	56.89	38.93 – 51.79	9.0
1	A	153	ARG	HD3	0.80	1.81 – 4.39	-8.9
1	A	181	VAL	CB	48.06	23.86 – 41.50	8.7
1	A	161	ARG	HD3	0.87	1.81 – 4.39	-8.7
1	A	158	SER	HB3	1.56	2.49 – 5.20	-8.4
1	A	187	PRO	HD3	0.48	1.76 – 5.48	-8.4
1	A	142	GLU	HG3	0.49	1.20 – 3.30	-8.4
1	A	148	SER	HB2	1.75	2.61 – 5.13	-8.4
1	A	185	SER	HB3	1.57	2.49 – 5.20	-8.4
1	A	187	PRO	CB	41.52	26.06 – 37.61	8.4
1	A	134	GLY	CA	55.83	38.93 – 51.79	8.1
1	A	142	GLU	HG2	0.64	1.24 – 3.30	-7.9
1	A	122	ARG	CD	50.39	38.57 – 47.75	7.9
1	A	148	SER	HB3	1.71	2.49 – 5.20	-7.9
1	A	175	THR	HB	1.70	2.57 – 5.77	-7.7
1	A	160	GLY	CA	55.23	38.93 – 51.79	7.7
1	A	130	THR	HB	1.78	2.57 – 5.77	-7.4
1	A	183	ILE	CD1	25.25	5.18 – 21.60	7.2
1	A	139	THR	CA	44.39	49.41 – 75.05	-7.0
1	A	170	PRO	CB	39.83	26.06 – 37.61	6.9
1	A	124	PRO	CA	53.08	55.85 – 70.84	-6.8
1	A	184	TRP	HB2	0.89	1.51 – 4.87	-6.8
1	A	132	THR	HB	2.01	2.57 – 5.77	-6.8
1	A	185	SER	HB2	2.18	2.61 – 5.13	-6.7
1	A	149	VAL	CA	43.62	48.38 – 76.73	-6.7
1	A	156	PRO	HB2	4.31	0.37 – 3.78	6.5
1	A	169	GLU	HB2	3.36	1.00 – 3.05	6.5
1	A	161	ARG	CB	42.21	21.74 – 39.52	6.5
1	A	142	GLU	CB	40.88	21.56 – 38.37	6.5
1	A	178	ASP	CB	30.65	32.98 – 48.76	-6.5
1	A	116	GLU	CB	19.41	21.56 – 38.37	-6.3
1	A	141	ARG	CG	34.72	21.24 – 33.19	6.3
1	A	129	PRO	CA	54.41	55.85 – 70.84	-6.0
1	A	162	LYS	HD2	0.40	0.58 – 2.64	-5.8
1	A	128	PRO	N	104.64	108.67 – 162.11	-5.8
1	A	162	LYS	HD3	0.40	0.54 – 2.65	-5.7
1	A	189	PRO	CA	55.11	55.85 – 70.84	-5.5
1	A	156	PRO	HB3	3.90	0.25 – 3.76	5.4
1	A	114	ASP	HB2	1.32	1.41 – 4.01	-5.3
1	A	176	SER	HB3	2.41	2.49 – 5.20	-5.3
1	A	188	ALA	CA	63.21	43.52 – 62.81	5.2

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	169	GLU	HB3	3.09	0.95 – 3.05	5.2
1	A	170	PRO	CA	55.80	55.85 – 70.84	-5.0
1	A	171	SER	CB	71.38	56.28 – 71.32	5.0

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

