



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 08:38 AM UTC

PDB ID : 2L3Q / pdb_00002l3q
Title : Structure of the prolyl trans isomer of the Crk Protein
Authors : Kalodimos, C.; Sarkar, P.; Saleh, T.; Tzeng, S.; Birge, R.
Deposited on : 2010-09-21

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

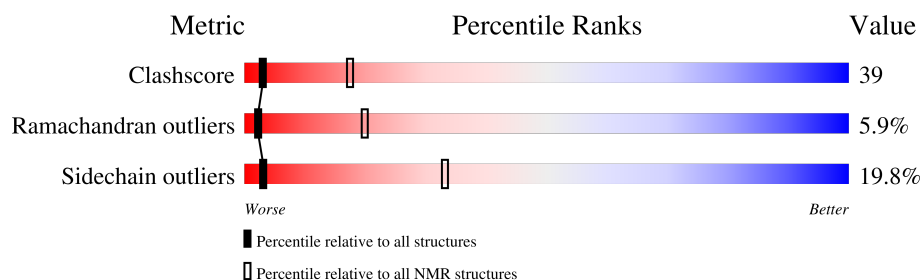
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	78	26% 58% 8% 9%

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:227-A:297 (71)	0.79	1

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 5 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1234 atoms, of which 618 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Trans isomer of Crk protein.

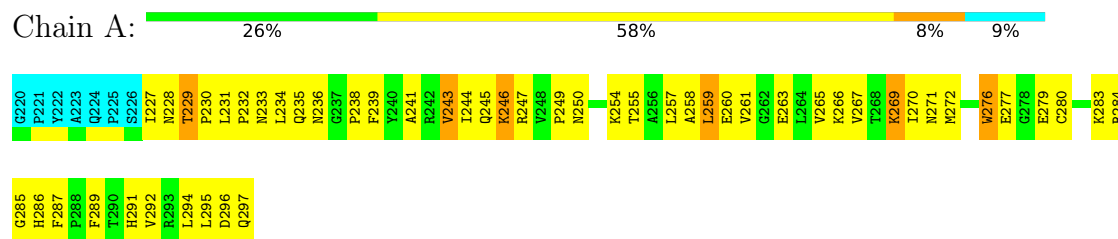
Mol	Chain	Residues	Atoms						Trace
1	A	78	Total	C	H	N	O	S	0
			1234	392	618	111	111	2	

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: Trans isomer of Crk protein

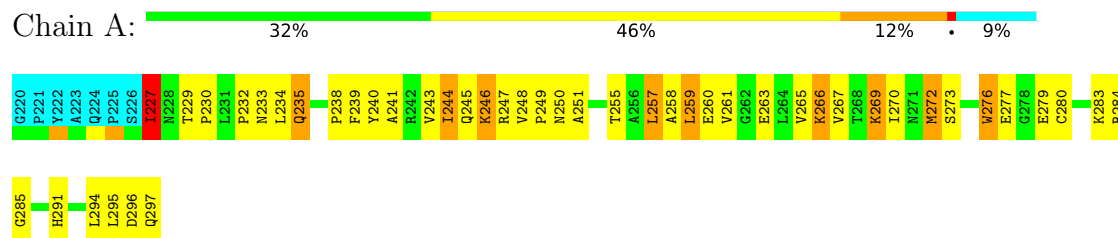


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

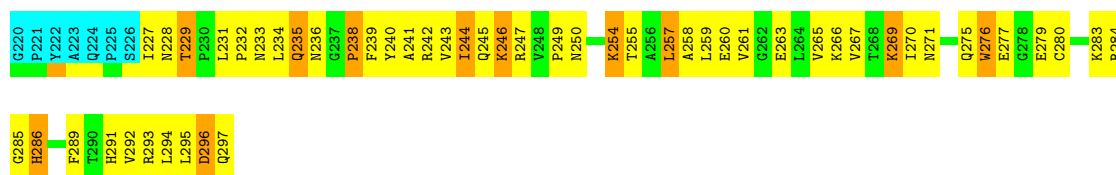
- Molecule 1: Trans isomer of Crk protein



4.2.2 Score per residue for model 2

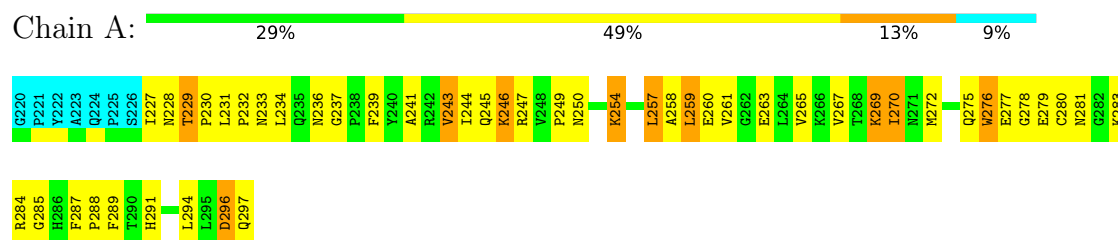
- Molecule 1: Trans isomer of Crk protein





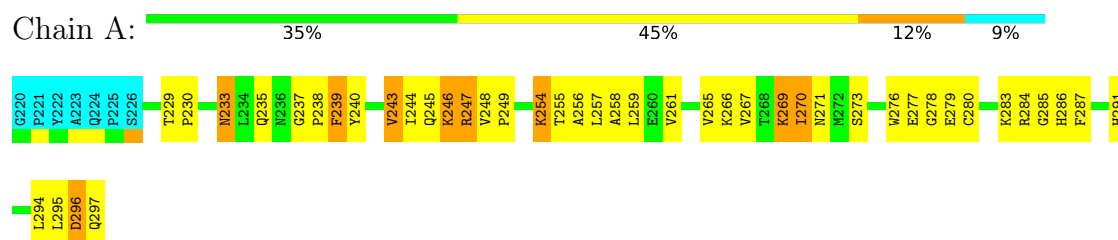
4.2.3 Score per residue for model 3

- Molecule 1: Trans isomer of Crk protein



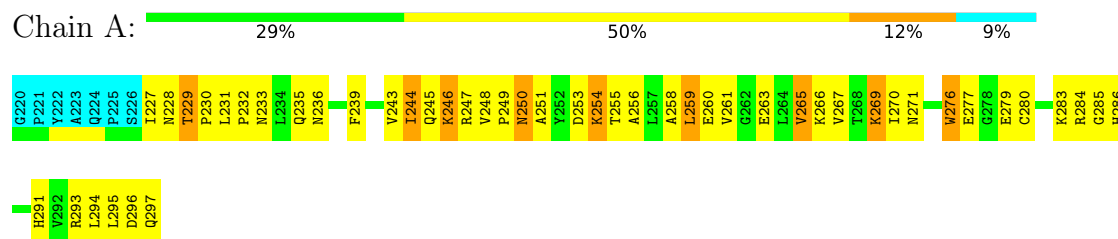
4.2.4 Score per residue for model 4

- Molecule 1: Trans isomer of Crk protein



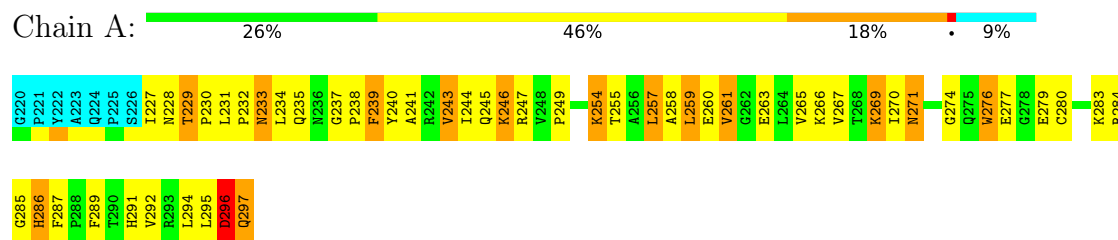
4.2.5 Score per residue for model 5

- Molecule 1: Trans isomer of Crk protein



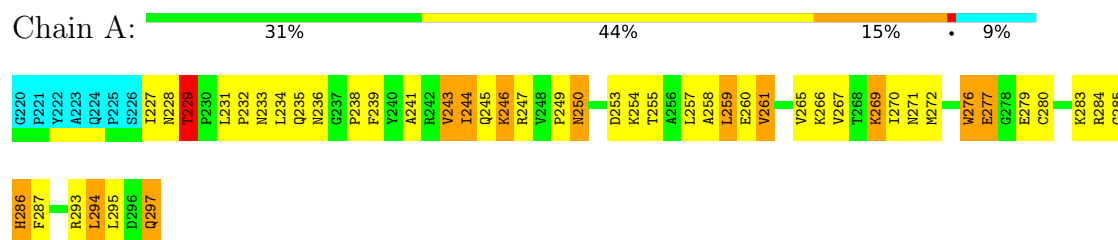
4.2.6 Score per residue for model 6

- Molecule 1: Trans isomer of Crk protein



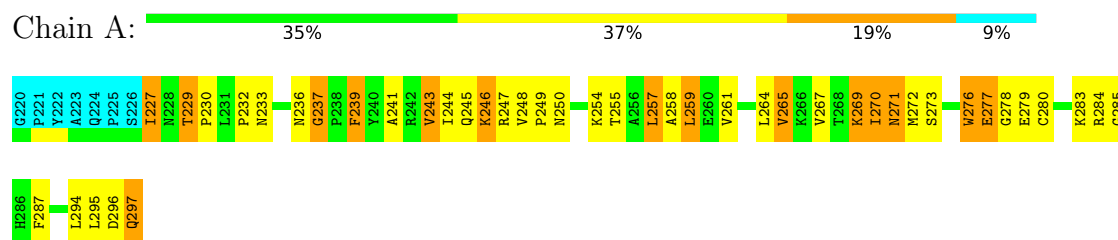
4.2.7 Score per residue for model 7

- Molecule 1: Trans isomer of Crk protein



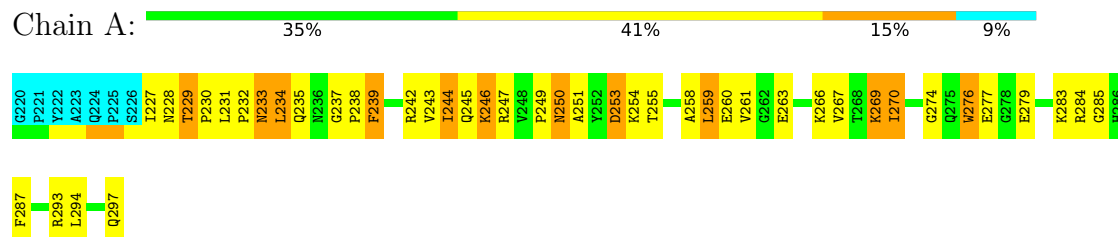
4.2.8 Score per residue for model 8

- Molecule 1: Trans isomer of Crk protein



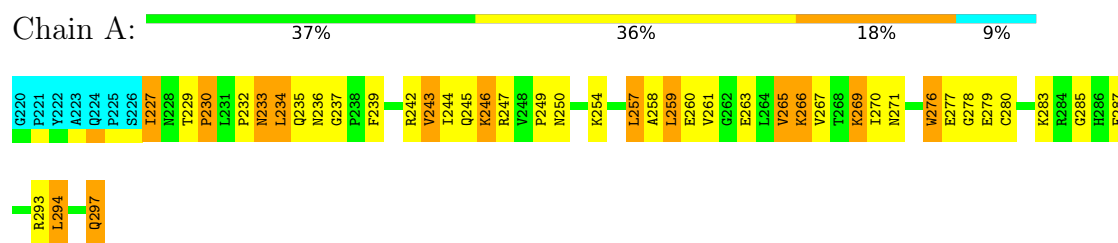
4.2.9 Score per residue for model 9

- Molecule 1: Trans isomer of Crk protein



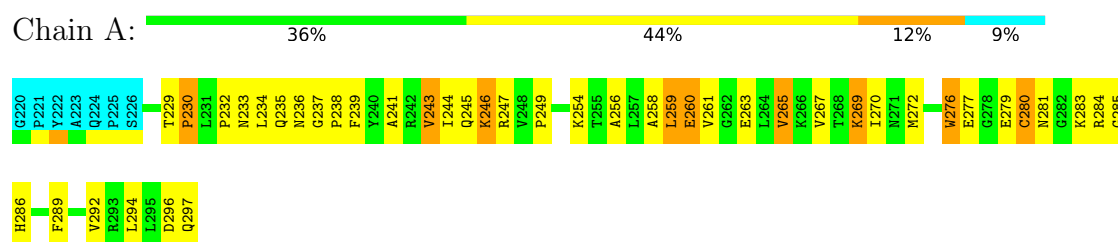
4.2.10 Score per residue for model 10

- Molecule 1: Trans isomer of Crk protein



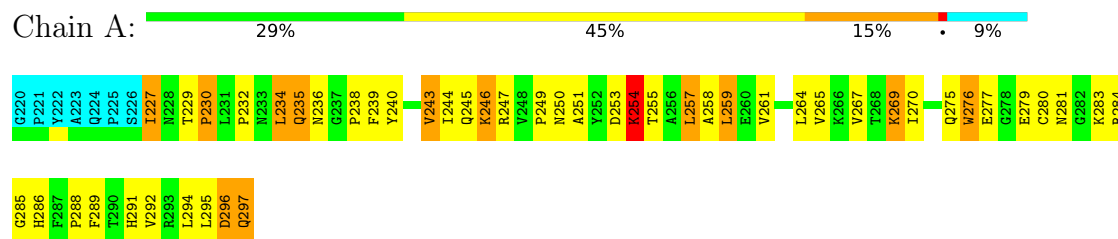
4.2.11 Score per residue for model 11

- Molecule 1: Trans isomer of Crk protein



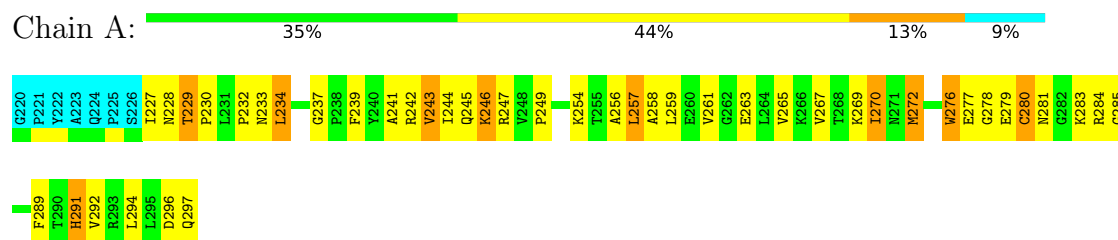
4.2.12 Score per residue for model 12

- Molecule 1: Trans isomer of Crk protein



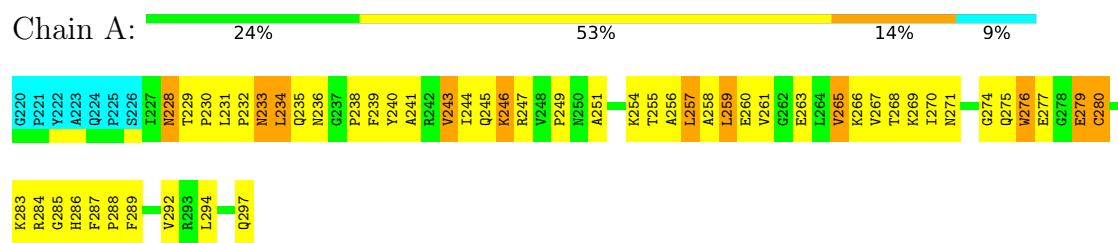
4.2.13 Score per residue for model 13

- Molecule 1: Trans isomer of Crk protein



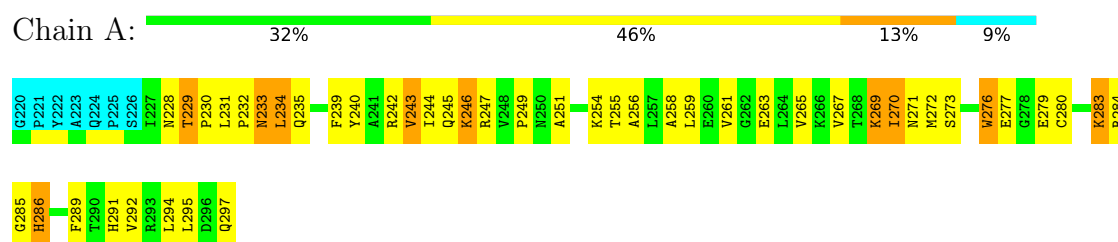
4.2.14 Score per residue for model 14

- Molecule 1: Trans isomer of Crk protein



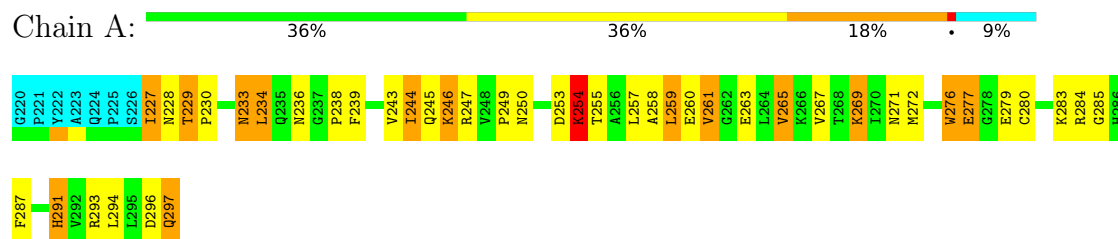
4.2.15 Score per residue for model 15

- Molecule 1: Trans isomer of Crk protein



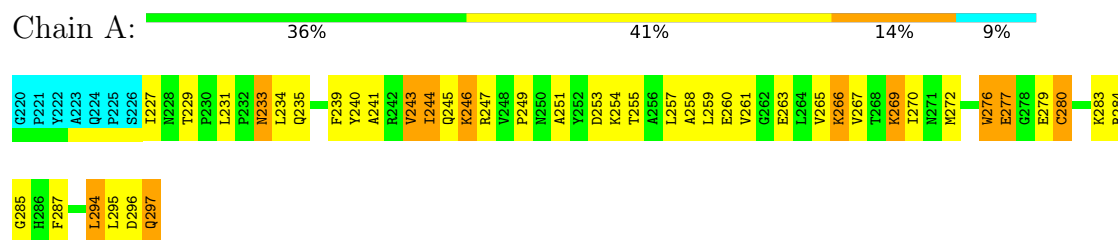
4.2.16 Score per residue for model 16

- Molecule 1: Trans isomer of Crk protein



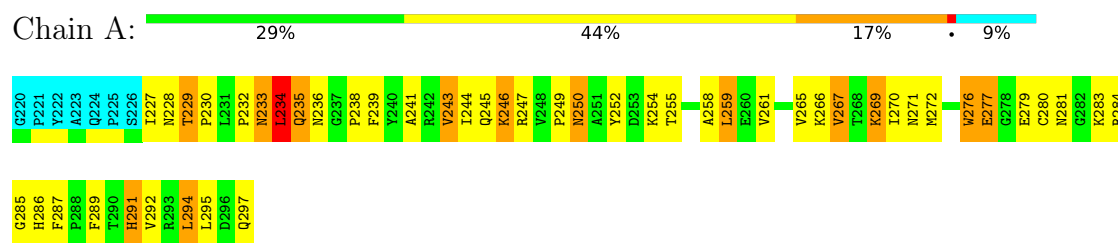
4.2.17 Score per residue for model 17

- Molecule 1: Trans isomer of Crk protein



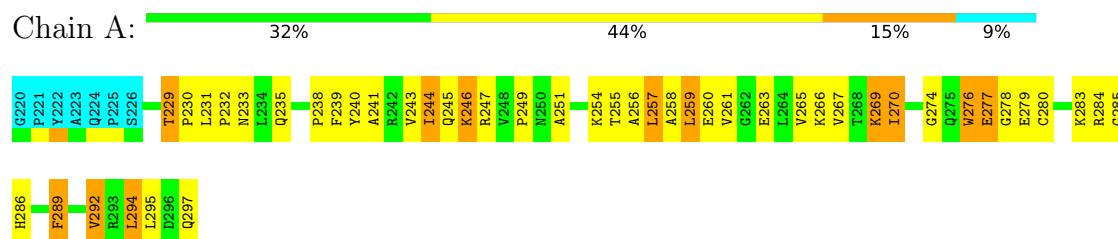
4.2.18 Score per residue for model 18

- Molecule 1: Trans isomer of Crk protein



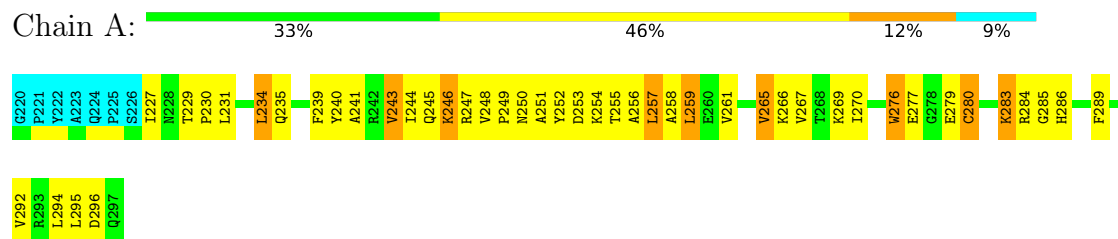
4.2.19 Score per residue for model 19

- Molecule 1: Trans isomer of Crk protein



4.2.20 Score per residue for model 20

- Molecule 1: Trans isomer of Crk protein



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *torsion angle dynamics*.

Of the 20 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
ARIA	refinement	1.2

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.74±0.03	0±0/579 (0.0± 0.0%)	0.94±0.03	0±0/783 (0.0± 0.1%)
All	All	0.74	0/11580 (0.0%)	0.94	5/15660 (0.0%)

There are no bond-length outliers.

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	235	GLN	N-CA-C	-5.64	106.53	113.41	12	1
1	A	256	ALA	N-CA-C	5.48	118.02	110.35	11	4

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	566	572	570	44±5
All	All	11320	11440	11400	882

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:227:ILE:HD13	1:A:296:ASP:HB2	0.98	1.32	20	2
1:A:243:VAL:HG21	1:A:246:LYS:HB2	0.92	1.41	2	20
1:A:232:PRO:HA	1:A:270:ILE:HG13	0.90	1.40	15	5
1:A:232:PRO:HA	1:A:270:ILE:HG12	0.88	1.44	8	9
1:A:260:GLU:H	1:A:263:GLU:HG3	0.88	1.29	19	8
1:A:265:VAL:HG23	1:A:280:CYS:HB2	0.86	1.46	10	13
1:A:236:ASN:HD21	1:A:297:GLN:HB2	0.85	1.31	16	1
1:A:239:PHE:CE1	1:A:267:VAL:HB	0.83	2.08	2	10
1:A:249:PRO:HD2	1:A:258:ALA:HA	0.81	1.51	12	20
1:A:227:ILE:HG21	1:A:270:ILE:HB	0.81	1.50	17	3
1:A:239:PHE:CE2	1:A:267:VAL:HB	0.81	2.10	4	9
1:A:260:GLU:HG3	1:A:261:VAL:N	0.80	1.89	11	6
1:A:247:ARG:O	1:A:249:PRO:HD3	0.80	1.77	4	20
1:A:241:ALA:HB2	1:A:294:LEU:HD12	0.79	1.52	8	6
1:A:244:ILE:C	1:A:261:VAL:HB	0.78	2.03	6	3
1:A:227:ILE:CG1	1:A:236:ASN:HB2	0.77	2.09	7	1
1:A:239:PHE:HD2	1:A:294:LEU:HD11	0.77	1.40	8	8
1:A:239:PHE:CZ	1:A:270:ILE:HG23	0.75	2.16	4	6
1:A:239:PHE:CD1	1:A:294:LEU:HD11	0.74	2.17	1	4
1:A:239:PHE:CD2	1:A:294:LEU:HD11	0.74	2.16	8	5
1:A:228:ASN:C	1:A:230:PRO:HD3	0.74	2.06	3	5
1:A:229:THR:HA	1:A:272:MET:HA	0.72	1.60	15	2
1:A:227:ILE:HD11	1:A:297:GLN:HG2	0.71	1.63	3	1
1:A:289:PHE:HA	1:A:292:VAL:HG23	0.71	1.62	19	1
1:A:244:ILE:O	1:A:261:VAL:HB	0.70	1.85	7	3
1:A:258:ALA:C	1:A:259:LEU:HD13	0.70	2.12	20	1
1:A:236:ASN:HB3	1:A:297:GLN:HB2	0.69	1.64	8	2
1:A:239:PHE:CD1	1:A:294:LEU:HD21	0.69	2.22	16	6
1:A:229:THR:N	1:A:230:PRO:HD3	0.69	2.03	11	11
1:A:243:VAL:CG2	1:A:246:LYS:HB2	0.69	2.17	13	19
1:A:279:GLU:HA	1:A:283:LYS:O	0.68	1.89	18	20
1:A:297:GLN:HE21	1:A:297:GLN:HA	0.67	1.50	17	1
1:A:230:PRO:HB2	1:A:270:ILE:HD12	0.67	1.65	4	1
1:A:245:GLN:HA	1:A:261:VAL:HG22	0.66	1.67	9	17
1:A:239:PHE:HE1	1:A:267:VAL:HB	0.66	1.50	2	7
1:A:280:CYS:HB3	1:A:283:LYS:HG2	0.66	1.68	11	7
1:A:239:PHE:CE1	1:A:270:ILE:HG23	0.65	2.26	8	1
1:A:239:PHE:CE1	1:A:270:ILE:HG22	0.65	2.26	6	3
1:A:280:CYS:HB3	1:A:283:LYS:CG	0.65	2.21	11	7
1:A:241:ALA:HB3	1:A:265:VAL:HG12	0.64	1.67	19	4
1:A:280:CYS:O	1:A:283:LYS:HG2	0.64	1.91	17	7
1:A:289:PHE:HA	1:A:292:VAL:CG2	0.64	2.22	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:239:PHE:CZ	1:A:270:ILE:HG22	0.64	2.27	6	8
1:A:236:ASN:ND2	1:A:297:GLN:HB2	0.63	2.08	16	1
1:A:227:ILE:HG23	1:A:230:PRO:HG3	0.63	1.70	1	3
1:A:227:ILE:HG13	1:A:235:GLN:NE2	0.63	2.08	12	1
1:A:236:ASN:HB3	1:A:297:GLN:HB3	0.63	1.71	11	1
1:A:271:ASN:ND2	1:A:276:TRP:HA	0.63	2.09	15	3
1:A:228:ASN:C	1:A:230:PRO:HD2	0.63	2.19	5	4
1:A:238:PRO:O	1:A:297:GLN:HB2	0.62	1.93	11	5
1:A:233:ASN:HA	1:A:237:GLY:HA2	0.62	1.70	3	1
1:A:269:LYS:HG2	1:A:277:GLU:OE1	0.62	1.94	15	3
1:A:255:THR:OG1	1:A:285:GLY:HA2	0.61	1.95	20	9
1:A:229:THR:HB	1:A:230:PRO:HD3	0.61	1.72	13	1
1:A:260:GLU:HG3	1:A:261:VAL:H	0.61	1.53	10	2
1:A:236:ASN:HD22	1:A:297:GLN:HG3	0.61	1.54	12	1
1:A:265:VAL:HG23	1:A:280:CYS:SG	0.61	2.36	20	3
1:A:276:TRP:CH2	1:A:294:LEU:HD22	0.61	2.31	20	2
1:A:269:LYS:HE2	1:A:271:ASN:HB3	0.60	1.71	5	4
1:A:269:LYS:HD3	1:A:269:LYS:C	0.60	2.21	7	6
1:A:271:ASN:OD1	1:A:276:TRP:HA	0.60	1.97	8	1
1:A:276:TRP:H	1:A:276:TRP:CD1	0.59	2.15	20	5
1:A:250:ASN:O	1:A:253:ASP:HB2	0.59	1.98	9	2
1:A:227:ILE:HG23	1:A:230:PRO:CG	0.59	2.28	16	3
1:A:227:ILE:HG12	1:A:236:ASN:HB2	0.59	1.75	7	1
1:A:234:LEU:HD21	1:A:238:PRO:HG3	0.59	1.75	16	1
1:A:254:LYS:HE2	1:A:254:LYS:N	0.58	2.13	6	2
1:A:277:GLU:HG2	1:A:286:HIS:HB3	0.58	1.74	6	5
1:A:231:LEU:HB3	1:A:232:PRO:HD2	0.58	1.74	3	5
1:A:265:VAL:CG2	1:A:280:CYS:HB2	0.58	2.27	5	2
1:A:234:LEU:CD2	1:A:235:GLN:H	0.57	2.12	20	1
1:A:284:ARG:HG3	1:A:285:GLY:N	0.57	2.15	9	19
1:A:269:LYS:HG2	1:A:277:GLU:OE2	0.57	1.99	8	3
1:A:271:ASN:HD22	1:A:276:TRP:HA	0.57	1.58	15	1
1:A:228:ASN:O	1:A:230:PRO:HD3	0.57	2.00	6	1
1:A:244:ILE:HD13	1:A:244:ILE:H	0.57	1.59	16	8
1:A:233:ASN:H	1:A:270:ILE:HG12	0.57	1.60	17	3
1:A:280:CYS:HB3	1:A:283:LYS:HE2	0.57	1.77	7	1
1:A:257:LEU:HB3	1:A:259:LEU:HD11	0.57	1.77	20	1
1:A:244:ILE:O	1:A:261:VAL:HG13	0.56	2.01	2	17
1:A:239:PHE:CE1	1:A:267:VAL:HG22	0.56	2.35	18	1
1:A:227:ILE:HG12	1:A:239:PHE:HE2	0.56	1.59	10	2
1:A:232:PRO:HA	1:A:270:ILE:CG1	0.56	2.31	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:239:PHE:CB	1:A:296:ASP:HA	0.56	2.29	20	1
1:A:269:LYS:HG3	1:A:277:GLU:OE2	0.55	2.02	4	1
1:A:243:VAL:HG21	1:A:246:LYS:HD3	0.55	1.78	16	2
1:A:267:VAL:HG11	1:A:276:TRP:CG	0.55	2.37	19	6
1:A:269:LYS:CB	1:A:277:GLU:HB2	0.55	2.31	19	20
1:A:246:LYS:HE2	1:A:287:PHE:CG	0.55	2.36	17	7
1:A:266:LYS:NZ	1:A:266:LYS:HB3	0.55	2.16	17	2
1:A:249:PRO:HG2	1:A:256:ALA:HB1	0.55	1.77	20	3
1:A:239:PHE:CE2	1:A:270:ILE:HG23	0.55	2.36	19	1
1:A:254:LYS:HE2	1:A:254:LYS:H	0.55	1.59	6	3
1:A:294:LEU:HG	1:A:296:ASP:H	0.55	1.61	6	2
1:A:239:PHE:HB3	1:A:296:ASP:C	0.55	2.27	3	1
1:A:227:ILE:HG13	1:A:235:GLN:HE22	0.55	1.60	12	1
1:A:238:PRO:O	1:A:297:GLN:HA	0.55	2.01	2	3
1:A:239:PHE:CG	1:A:294:LEU:HD11	0.55	2.37	18	4
1:A:258:ALA:HB3	1:A:283:LYS:HE2	0.55	1.78	20	2
1:A:231:LEU:H	1:A:231:LEU:HD23	0.55	1.61	2	3
1:A:239:PHE:CE2	1:A:270:ILE:HG22	0.55	2.37	2	3
1:A:239:PHE:HE1	1:A:270:ILE:HD12	0.54	1.62	8	1
1:A:294:LEU:CD2	1:A:296:ASP:HB3	0.54	2.33	20	1
1:A:255:THR:HB	1:A:285:GLY:HA2	0.54	1.79	8	3
1:A:238:PRO:CB	1:A:266:LYS:HE3	0.54	2.33	14	1
1:A:230:PRO:HD2	1:A:272:MET:HA	0.54	1.77	18	1
1:A:251:ALA:O	1:A:255:THR:HA	0.54	2.03	1	6
1:A:246:LYS:HB3	1:A:259:LEU:O	0.54	2.02	7	1
1:A:227:ILE:HG22	1:A:270:ILE:HG21	0.54	1.79	13	1
1:A:229:THR:HB	1:A:230:PRO:CD	0.54	2.33	15	1
1:A:247:ARG:CG	1:A:249:PRO:HG3	0.54	2.33	2	2
1:A:244:ILE:O	1:A:245:GLN:HG3	0.54	2.03	6	5
1:A:241:ALA:HB3	1:A:265:VAL:CG1	0.54	2.33	6	4
1:A:269:LYS:HB3	1:A:277:GLU:HB2	0.53	1.81	15	18
1:A:269:LYS:HD3	1:A:269:LYS:O	0.53	2.03	17	4
1:A:257:LEU:HD11	1:A:278:GLY:C	0.53	2.28	4	1
1:A:234:LEU:O	1:A:234:LEU:HD12	0.53	2.03	15	4
1:A:260:GLU:CG	1:A:261:VAL:N	0.53	2.68	11	2
1:A:239:PHE:CD1	1:A:239:PHE:N	0.53	2.77	12	7
1:A:250:ASN:ND2	1:A:252:TYR:HB3	0.53	2.19	20	1
1:A:257:LEU:HD21	1:A:278:GLY:CA	0.52	2.34	19	4
1:A:246:LYS:HG2	1:A:259:LEU:CD1	0.52	2.35	10	13
1:A:228:ASN:O	1:A:230:PRO:HD2	0.52	2.04	15	2
1:A:275:GLN:HA	1:A:288:PRO:HA	0.52	1.82	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:257:LEU:HB3	1:A:259:LEU:HD21	0.52	1.80	20	1
1:A:233:ASN:HA	1:A:268:THR:O	0.52	2.05	14	1
1:A:266:LYS:O	1:A:266:LYS:HD2	0.51	2.05	19	5
1:A:280:CYS:HB3	1:A:283:LYS:CE	0.51	2.35	7	1
1:A:271:ASN:OD1	1:A:274:GLY:HA2	0.51	2.06	6	1
1:A:227:ILE:HG12	1:A:239:PHE:CE2	0.51	2.39	10	2
1:A:241:ALA:HB2	1:A:294:LEU:HD22	0.51	1.83	17	2
1:A:247:ARG:HG2	1:A:248:VAL:N	0.51	2.20	20	1
1:A:237:GLY:O	1:A:297:GLN:HG2	0.51	2.05	10	1
1:A:227:ILE:CD1	1:A:296:ASP:HB2	0.51	2.22	20	2
1:A:243:VAL:HG23	1:A:246:LYS:HD3	0.51	1.81	14	4
1:A:249:PRO:O	1:A:258:ALA:HB2	0.51	2.05	20	9
1:A:241:ALA:HB2	1:A:294:LEU:CD1	0.51	2.34	2	2
1:A:280:CYS:O	1:A:283:LYS:HD2	0.51	2.05	4	1
1:A:238:PRO:O	1:A:297:GLN:HB3	0.51	2.07	4	1
1:A:243:VAL:CG2	1:A:246:LYS:HD3	0.50	2.36	16	3
1:A:227:ILE:HG13	1:A:236:ASN:HB2	0.50	1.83	7	1
1:A:232:PRO:O	1:A:233:ASN:HB2	0.50	2.05	14	1
1:A:259:LEU:HD12	1:A:280:CYS:SG	0.50	2.46	20	1
1:A:272:MET:HG3	1:A:273:SER:N	0.50	2.22	8	2
1:A:244:ILE:HD12	1:A:293:ARG:HG2	0.50	1.82	9	5
1:A:255:THR:CB	1:A:285:GLY:HA2	0.50	2.36	8	4
1:A:233:ASN:H	1:A:270:ILE:HD11	0.50	1.67	9	1
1:A:247:ARG:HB3	1:A:249:PRO:HG3	0.50	1.83	3	1
1:A:233:ASN:O	1:A:234:LEU:HB2	0.49	2.06	16	1
1:A:228:ASN:O	1:A:229:THR:HB	0.49	2.07	3	1
1:A:250:ASN:OD1	1:A:252:TYR:HB3	0.49	2.08	18	1
1:A:240:TYR:HB2	1:A:295:LEU:HB2	0.49	1.83	2	5
1:A:294:LEU:HD23	1:A:296:ASP:HB3	0.49	1.84	20	1
1:A:238:PRO:HB3	1:A:266:LYS:HE3	0.49	1.85	14	1
1:A:269:LYS:HD2	1:A:270:ILE:N	0.49	2.22	4	1
1:A:234:LEU:HD13	1:A:234:LEU:N	0.48	2.23	20	1
1:A:277:GLU:HA	1:A:285:GLY:O	0.48	2.08	9	7
1:A:232:PRO:HG3	1:A:269:LYS:HA	0.48	1.83	7	1
1:A:270:ILE:HD12	1:A:270:ILE:C	0.48	2.33	12	3
1:A:242:ARG:HD3	1:A:263:GLU:O	0.48	2.09	13	3
1:A:275:GLN:HE22	1:A:288:PRO:HG3	0.48	1.68	3	1
1:A:259:LEU:HD22	1:A:259:LEU:N	0.48	2.23	20	1
1:A:267:VAL:HG12	1:A:269:LYS:O	0.48	2.07	11	3
1:A:241:ALA:HA	1:A:294:LEU:HA	0.48	1.86	14	1
1:A:229:THR:N	1:A:230:PRO:CD	0.48	2.76	18	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:230:PRO:O	1:A:270:ILE:HB	0.48	2.09	13	1
1:A:241:ALA:HB2	1:A:294:LEU:CD2	0.48	2.38	17	2
1:A:289:PHE:HE1	1:A:294:LEU:HD22	0.48	1.69	14	1
1:A:234:LEU:HD23	1:A:235:GLN:H	0.47	1.69	20	1
1:A:227:ILE:CG2	1:A:270:ILE:HB	0.47	2.36	5	2
1:A:244:ILE:C	1:A:245:GLN:HG3	0.47	2.34	16	1
1:A:274:GLY:O	1:A:289:PHE:HB3	0.47	2.09	19	1
1:A:231:LEU:HB2	1:A:232:PRO:CD	0.47	2.39	2	1
1:A:244:ILE:CD1	1:A:293:ARG:HG2	0.47	2.39	9	2
1:A:264:LEU:HD11	1:A:295:LEU:HD22	0.47	1.86	12	2
1:A:233:ASN:O	1:A:234:LEU:HB3	0.47	2.09	18	1
1:A:242:ARG:HG2	1:A:263:GLU:O	0.47	2.10	9	2
1:A:267:VAL:HG13	1:A:277:GLU:O	0.47	2.09	10	6
1:A:257:LEU:HD22	1:A:285:GLY:CA	0.47	2.39	8	11
1:A:276:TRP:CD1	1:A:276:TRP:N	0.47	2.83	6	1
1:A:227:ILE:HG12	1:A:270:ILE:HG21	0.47	1.87	9	1
1:A:239:PHE:CE1	1:A:267:VAL:CG2	0.47	2.98	18	1
1:A:276:TRP:CZ2	1:A:289:PHE:HD2	0.46	2.28	3	1
1:A:228:ASN:HA	1:A:271:ASN:HD21	0.46	1.70	6	1
1:A:267:VAL:CG1	1:A:276:TRP:HB2	0.46	2.40	3	13
1:A:237:GLY:O	1:A:239:PHE:HD1	0.46	1.93	8	1
1:A:230:PRO:HD2	1:A:270:ILE:HD13	0.46	1.85	14	1
1:A:239:PHE:HB3	1:A:296:ASP:HA	0.46	1.87	20	1
1:A:231:LEU:HB3	1:A:232:PRO:CD	0.46	2.39	7	3
1:A:243:VAL:O	1:A:261:VAL:HA	0.46	2.11	7	2
1:A:240:TYR:HA	1:A:265:VAL:O	0.46	2.11	4	4
1:A:228:ASN:O	1:A:229:THR:CB	0.46	2.64	2	7
1:A:260:GLU:HG2	1:A:261:VAL:O	0.46	2.10	6	2
1:A:247:ARG:NH1	1:A:249:PRO:HB3	0.46	2.26	8	2
1:A:266:LYS:HD2	1:A:266:LYS:C	0.46	2.35	10	1
1:A:230:PRO:O	1:A:271:ASN:HA	0.46	2.10	16	1
1:A:229:THR:H	1:A:272:MET:HA	0.46	1.70	11	2
1:A:229:THR:N	1:A:272:MET:HA	0.46	2.25	7	1
1:A:227:ILE:HG21	1:A:239:PHE:HE2	0.46	1.71	3	2
1:A:277:GLU:HG3	1:A:286:HIS:HB3	0.46	1.86	12	7
1:A:246:LYS:HE2	1:A:287:PHE:CD2	0.46	2.45	14	8
1:A:289:PHE:HA	1:A:292:VAL:HG22	0.46	1.87	6	6
1:A:246:LYS:HE3	1:A:287:PHE:HB3	0.46	1.86	4	1
1:A:258:ALA:N	1:A:283:LYS:HE3	0.46	2.25	5	1
1:A:270:ILE:H	1:A:270:ILE:HD13	0.46	1.70	9	1
1:A:294:LEU:HD13	1:A:295:LEU:N	0.45	2.27	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:250:ASN:ND2	1:A:253:ASP:HB2	0.45	2.27	7	1
1:A:228:ASN:HA	1:A:271:ASN:ND2	0.45	2.26	6	1
1:A:259:LEU:HD23	1:A:280:CYS:SG	0.45	2.52	11	1
1:A:233:ASN:HA	1:A:237:GLY:O	0.45	2.12	4	2
1:A:269:LYS:HD2	1:A:277:GLU:N	0.45	2.25	17	1
1:A:240:TYR:O	1:A:295:LEU:HB2	0.44	2.12	15	3
1:A:232:PRO:CA	1:A:270:ILE:HG12	0.44	2.39	7	2
1:A:242:ARG:HB3	1:A:293:ARG:HB2	0.44	1.88	10	1
1:A:237:GLY:O	1:A:297:GLN:HB2	0.44	2.12	13	1
1:A:272:MET:HG2	1:A:273:SER:N	0.44	2.28	1	1
1:A:227:ILE:HD13	1:A:270:ILE:HG21	0.44	1.90	8	1
1:A:227:ILE:HD12	1:A:227:ILE:N	0.44	2.26	2	2
1:A:227:ILE:HG13	1:A:234:LEU:HG	0.44	1.89	20	1
1:A:269:LYS:HA	1:A:269:LYS:CE	0.44	2.43	3	1
1:A:260:GLU:O	1:A:263:GLU:HG3	0.44	2.13	6	2
1:A:236:ASN:ND2	1:A:297:GLN:HG3	0.44	2.27	12	1
1:A:239:PHE:HA	1:A:296:ASP:O	0.44	2.13	12	1
1:A:276:TRP:HZ2	1:A:289:PHE:CD2	0.44	2.31	19	1
1:A:244:ILE:HD13	1:A:244:ILE:N	0.43	2.28	9	2
1:A:269:LYS:O	1:A:276:TRP:CB	0.43	2.66	19	2
1:A:227:ILE:HG23	1:A:270:ILE:HD12	0.43	1.89	7	1
1:A:234:LEU:CD2	1:A:238:PRO:HG3	0.43	2.43	12	1
1:A:297:GLN:H	1:A:297:GLN:CD	0.43	2.21	12	1
1:A:227:ILE:HG22	1:A:227:ILE:O	0.43	2.13	17	1
1:A:248:VAL:HG13	1:A:248:VAL:O	0.43	2.14	1	4
1:A:269:LYS:HD2	1:A:269:LYS:C	0.43	2.38	4	1
1:A:247:ARG:HG3	1:A:249:PRO:HG3	0.42	1.89	9	1
1:A:253:ASP:C	1:A:254:LYS:HE3	0.42	2.38	12	1
1:A:247:ARG:C	1:A:249:PRO:HD3	0.42	2.38	3	2
1:A:249:PRO:HB2	1:A:256:ALA:HB3	0.42	1.91	15	1
1:A:276:TRP:CD1	1:A:276:TRP:H	0.42	2.31	18	1
1:A:243:VAL:HA	1:A:292:VAL:HG13	0.42	1.91	19	1
1:A:269:LYS:HD2	1:A:277:GLU:OE1	0.42	2.14	20	1
1:A:236:ASN:CB	1:A:297:GLN:HB3	0.42	2.43	11	1
1:A:251:ALA:HA	1:A:255:THR:C	0.42	2.40	20	3
1:A:257:LEU:HD21	1:A:278:GLY:N	0.42	2.30	19	1
1:A:231:LEU:HD12	1:A:232:PRO:HD2	0.42	1.91	14	1
1:A:266:LYS:HG3	1:A:279:GLU:O	0.42	2.15	5	1
1:A:232:PRO:HB3	1:A:269:LYS:HE2	0.42	1.92	12	1
1:A:239:PHE:CZ	1:A:267:VAL:HB	0.42	2.49	12	1
1:A:289:PHE:HD1	1:A:292:VAL:HG23	0.42	1.74	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:283:LYS:HA	1:A:283:LYS:HE3	0.42	1.91	20	1
1:A:227:ILE:HD11	1:A:235:GLN:HB3	0.42	1.91	2	1
1:A:227:ILE:HG22	1:A:294:LEU:HD21	0.42	1.91	9	1
1:A:239:PHE:HB2	1:A:296:ASP:HA	0.41	1.91	20	1
1:A:257:LEU:HD21	1:A:278:GLY:H	0.41	1.75	19	3
1:A:242:ARG:C	1:A:242:ARG:HD2	0.41	2.40	9	1
1:A:240:TYR:O	1:A:294:LEU:HD12	0.41	2.15	12	2
1:A:269:LYS:O	1:A:276:TRP:HB3	0.41	2.15	10	1
1:A:235:GLN:O	1:A:297:GLN:HG3	0.41	2.15	7	1
1:A:267:VAL:HG11	1:A:276:TRP:HB2	0.41	1.91	20	2
1:A:245:GLN:HB2	1:A:291:HIS:HB2	0.41	1.93	16	1
1:A:247:ARG:HH22	1:A:253:ASP:CG	0.41	2.24	17	1
1:A:236:ASN:HB3	1:A:297:GLN:C	0.41	2.40	18	1
1:A:239:PHE:CE1	1:A:294:LEU:HD11	0.41	2.51	2	1
1:A:247:ARG:CZ	1:A:249:PRO:HB3	0.41	2.45	2	1
1:A:243:VAL:CG1	1:A:263:GLU:HB2	0.41	2.46	11	2
1:A:238:PRO:O	1:A:297:GLN:HG3	0.41	2.16	14	1
1:A:257:LEU:HD21	1:A:278:GLY:HA3	0.41	1.91	19	1
1:A:266:LYS:HE3	1:A:279:GLU:HB3	0.41	1.92	2	1
1:A:236:ASN:HB3	1:A:297:GLN:O	0.41	2.15	18	1
1:A:233:ASN:HB3	1:A:236:ASN:OD1	0.41	2.14	7	1
1:A:228:ASN:OD1	1:A:274:GLY:HA2	0.41	2.15	9	1
1:A:227:ILE:HG12	1:A:239:PHE:CD1	0.41	2.50	12	1
1:A:280:CYS:O	1:A:281:ASN:C	0.41	2.63	18	2
1:A:234:LEU:HD13	1:A:238:PRO:HD3	0.41	1.93	12	1
1:A:274:GLY:HA3	1:A:289:PHE:HB2	0.40	1.93	14	1
1:A:280:CYS:HB3	1:A:283:LYS:HD2	0.40	1.92	8	1
1:A:276:TRP:CZ2	1:A:289:PHE:HD1	0.40	2.34	14	1
1:A:232:PRO:HG3	1:A:269:LYS:HG2	0.40	1.93	5	1
1:A:253:ASP:C	1:A:254:LYS:HE2	0.40	2.42	16	1
1:A:227:ILE:HD12	1:A:296:ASP:OD1	0.40	2.17	1	1
1:A:233:ASN:OD1	1:A:234:LEU:HG	0.40	2.16	10	1
1:A:249:PRO:HD2	1:A:257:LEU:O	0.40	2.17	17	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	70/78 (90%)	56±2 (80±3%)	10±3 (15±4%)	4±1 (6±2%)	2	20
All	All	1400/1560 (90%)	1113 (80%)	205 (15%)	82 (6%)	2	20

All 11 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	254	LYS	19
1	A	233	ASN	15
1	A	234	LEU	12
1	A	229	THR	11
1	A	296	ASP	8
1	A	227	ILE	6
1	A	237	GLY	3
1	A	230	PRO	3
1	A	238	PRO	2
1	A	291	HIS	2
1	A	256	ALA	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	61/66 (92%)	49±2 (80±3%)	12±2 (20±3%)	3	33
All	All	1220/1320 (92%)	978 (80%)	242 (20%)	3	33

All 41 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	246	LYS	20
1	A	259	LEU	20
1	A	276	TRP	20
1	A	269	LYS	17
1	A	243	VAL	14
1	A	250	ASN	11

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Mol	Chain	Res	Type	Models (Total)
1	A	257	LEU	11
1	A	291	HIS	11
1	A	266	LYS	9
1	A	297	GLN	9
1	A	244	ILE	8
1	A	270	ILE	8
1	A	265	VAL	8
1	A	277	GLU	6
1	A	234	LEU	5
1	A	294	LEU	5
1	A	280	CYS	5
1	A	235	GLN	4
1	A	272	MET	4
1	A	286	HIS	4
1	A	254	LYS	4
1	A	239	PHE	4
1	A	271	ASN	4
1	A	296	ASP	4
1	A	281	ASN	3
1	A	261	VAL	3
1	A	229	THR	3
1	A	228	ASN	2
1	A	260	GLU	2
1	A	253	ASP	2
1	A	283	LYS	2
1	A	227	ILE	1
1	A	275	GLN	1
1	A	247	ARG	1
1	A	273	SER	1
1	A	231	LEU	1
1	A	279	GLU	1
1	A	233	ASN	1
1	A	267	VAL	1
1	A	289	PHE	1
1	A	292	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

No chemical shift data were provided