Full wwPDB NMR Structure Validation Report (i)

Mar 5, 2022 – 08:04 AM EST

PDB ID	:	2K0G
Title	:	Solution Structure of a Bacterial Cyclic Nucleotide-Activated K+ Channel Binding Domain in Complex with cAMP
Authors	:	Schunke, S.; Stoldt, M.; Willbold, D.
Deposited on	:	2008-02-02

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

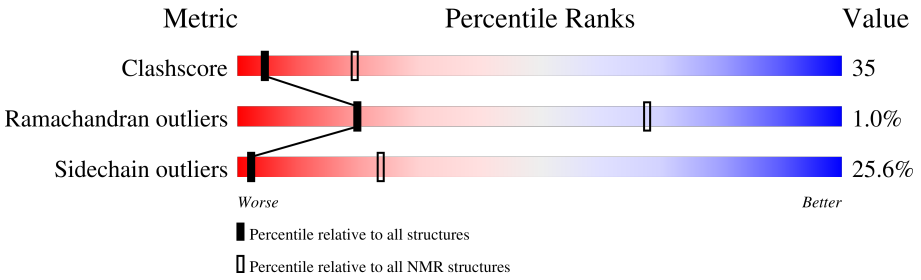
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	142	36% 43% 8% 13%

2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 2 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 and fewest violations*.

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:349 (123)	0.16	2

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 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 5, 7, 9, 12, 13, 14, 15
2	8, 10
3	3, 11
Single-model clusters	6

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2170 atoms, of which 1097 are hydrogens and 0 are deuteriums.

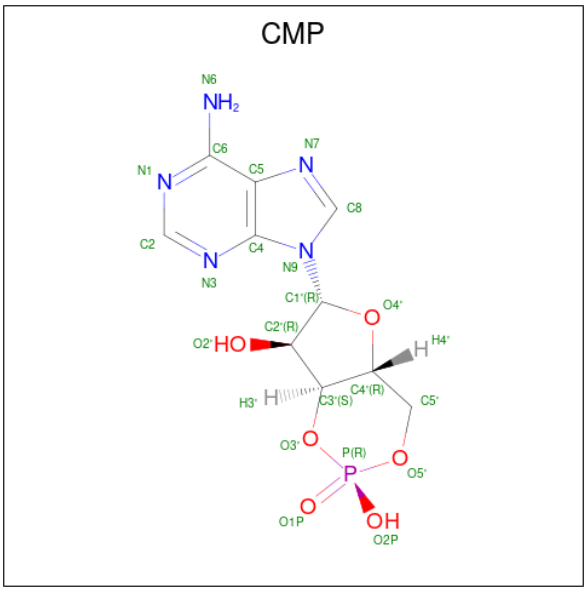
- Molecule 1 is a protein called Mll3241 protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	142	2137	664	1086	189	193	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	GLY	-	expression tag	UNP Q98GN8
A	215	SER	-	expression tag	UNP Q98GN8

- Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: $C_{10}H_{12}N_5O_6P$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
2	A	1	33	10	11	5	6	1

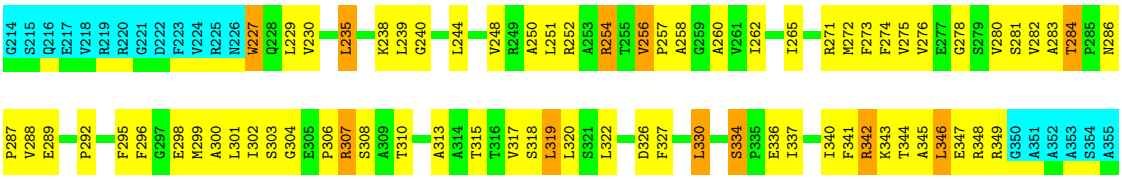
4 Residue-property plots (i)

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: Mll3241 protein

Chain A: 36% 43% 8% 13%



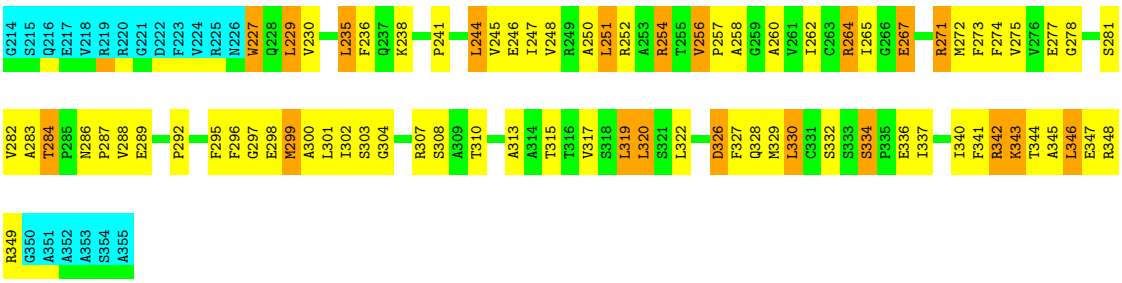
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Mll3241 protein

Chain A: 32% 41% 14% 13%



4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Mll3241 protein

Chain A: 37% 39% 11% 13%

G214 S215 Q216 E217 V218 R219 R220 G221 D222 F223 V224 R225 N226 W227 Q228 L229 V230 L235 L239 G240 P241 L244 V245 V248 R249 A250 L251 R252 A253 R254 T255 V256 P257 A258 I262 C263 R264 D270 R271 M272 F273 F274 V275 V276 E277 G278 S281 V282 A283 T284 P285 N286 P287

V288 E289 P292 F295 F296 G297 E298 M299 A300 L301 I302 S303 G304 R307 S308 A309 T310 A314 T315 T316 V317 S318 L319 L320 S321 L322 D326 F327 L330 S334 I337 A338 E339 I340 F341 R342 K343 T344 A345 L346 E347 R348 R349 G350 A351 A352 A353 S354 A355

4.2.3 Score per residue for model 3

- Molecule 1: Mll3241 protein

Chain A: 35% 42% 9% • 13%

G214 S215 Q216 E217 V218 R219 R220 G221 D222 F223 V224 R225 N226 W227 Q228 L229 V230 L235 G240 L244 V245 E246 I247 V248 R249 A250 L251 R252 A253 R254 T255 V256 P257 A258 G259 A260 V261 I262 I265 R271 M272 F273 F274 V275 V276 E277 G278 S279 V280 S281 V282 A283 T284 P285 N286

P287 V288 E289 P292 F295 F296 G297 E298 M299 A300 L301 I302 S303 G304 E305 P306 R307 S308 A309 T310 A313 A314 T315 T316 V317 S318 L319 L320 S321 L322 H323 S324 A325 D326 F327 L330 S333 S334 P335 E336 I337 I340 F341 R342 K343 T344 A345 L346 E347 R348 R349 G350 A351 A352

A353 S354 A355

4.2.4 Score per residue for model 4

- Molecule 1: Mll3241 protein

Chain A: 35% 43% 8% 13%

G214 S215 Q216 E217 V218 R219 R220 G221 D222 F223 V224 R225 N226 W227 Q228 L229 V230 L235 K238 L239 G240 P241 L244 V245 E246 I247 V248 L251 R252 A253 R254 T255 V256 P257 A258 I262 R271 M272 F273 F274 V275 V276 E277 G278 S279 V280 S281 V282 A283 T284 P285 N286 P287 V288

E289 L290 G291 P292 F295 F296 G297 E298 M299 A300 L301 I302 S303 G304 R307 S308 A309 T310 A313 A314 T315 T316 V317 S318 L319 L320 F327 Q328 M329 L330 C331 S334 P335 E336 I337 A338 E339 I340 F341 R342 K343 T344 A345 L346 E347 R348 R349 G350 A351 A352 A353 S354 A355

4.2.5 Score per residue for model 5

- Molecule 1: Mll3241 protein

Chain A: 41% 38% 7% • 13%

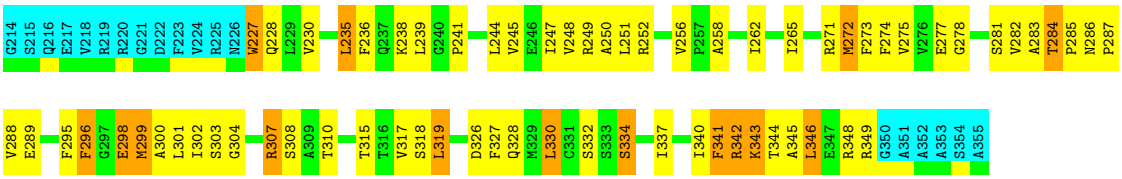
G214 S215 Q216 E217 V218 R219 R220 G221 D222 F223 V224 R225 N226 W227 Q228 L229 L235 K238 L239 G240 L244 V248 R249 A250 L251 R252 A253 R254 T255 V256 P257 A258 I265 R271 M272 F273 F274 V275 V276 E277 G278 S281 V282 A283 T284 P285 N286 P287 V288 E289 P292

F295 F296 G297 E298 M299 A300 L301 I302 S303 G304 E305 P306 R307 S308 A309 T310 T315 T316 V317 S318 L319 L320 S321 L322 D326 F327 L330 C331 S332 S333 S334 P335 E336 I337 I340 F341 R342 K343 T344 A345 L346 E347 G350 A351 A352 A353 S354 A355

4.2.6 Score per residue for model 6

- Molecule 1: Mll3241 protein

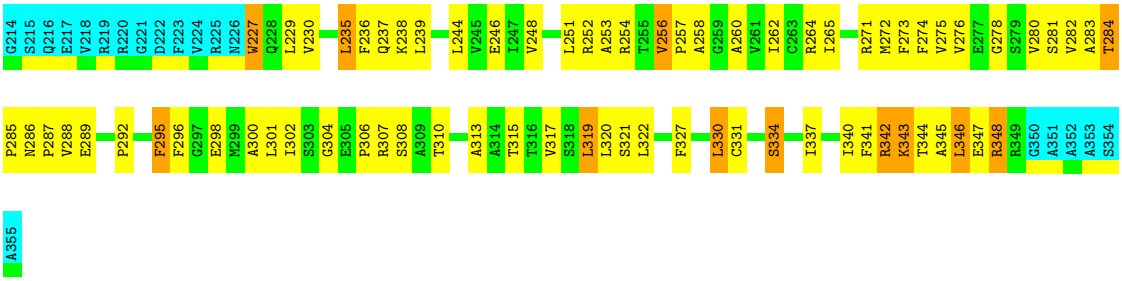
Chain A: 39% 37% 11% 13%



4.2.7 Score per residue for model 7

- Molecule 1: Mll3241 protein

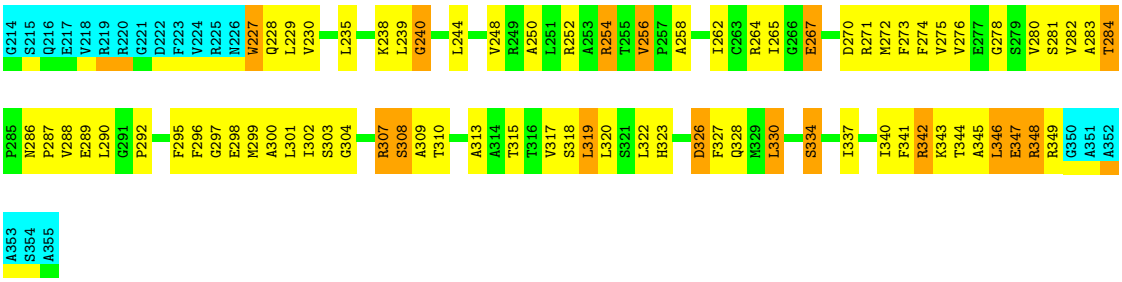
Chain A: 36% 42% 8% 13%



4.2.8 Score per residue for model 8

- Molecule 1: Mll3241 protein

Chain A: 33% 42% 11% 13%



4.2.9 Score per residue for model 9

- Molecule 1: Mll3241 protein

Chain A: 34% 42% 10% • 13%

G214 S215 Q216 E217 V218 R219 R220 G221 D222 F223 V224 R225 N226 W227 Q228 L229 V230 L235 F236 Q237 K238 L239 G240 L244 V245 E246 I247 V248 R249 A250 L251 R252 A253 R254 T255 V256 P257 A258 I262 C263 R264 I265 M272 F273 F274 V275 V276 E277 G278 S279 V280 S281 V282 A283 T284 P285

N286 P287 V288 E289 L290 F295 F296 M299 A300 L301 I302 S303 G304 E305 P306 R307 S308 A309 T310 A313 A314 T315 T316 V317 S318 L319 L320 S321 L322 H323 D326 F327 Q328 M329 L330 C331 S332 S333 S334 P335 E336 I337 A338 E339 I340 F341 R342 K343 T344 A345 L346 E347 G350 A351 A352

A353 S354 A355

4.2.10 Score per residue for model 10

- Molecule 1: Mll3241 protein

Chain A: 35% 42% 9% • 13%

G214 S215 Q216 E217 V218 R219 R220 G221 D222 F223 V224 R225 N226 W227 V230 L235 F236 Q237 K238 L239 G240 P241 A242 V243 L244 V245 E246 I247 V248 R252 A253 R254 T255 V256 P257 A258 G259 A260 V261 I262 I265 R271 M272 F273 F274 V275 V276 E277 G278 S281 V282 A283 T284 P285

N286 P287 V288 E289 P292 F295 F296 G297 E298 L301 I302 E305 P306 R307 S308 A309 T310 A313 A314 T315 T316 V317 S318 L319 L320 S321 L322 H323 S324 A325 D326 F327 Q328 M329 L330 S333 S334 I337 I340 F341 R342 K343 T344 A345 L346 E347 R348 R349 G350 A351 A352 A353

S354 A355

4.2.11 Score per residue for model 11

- Molecule 1: Mll3241 protein

Chain A: 38% 39% 8% • 13%

G214 S215 Q216 E217 V218 R219 R220 G221 D222 F223 V224 R225 N226 W227 Q228 L229 V230 L235 P241 L244 V245 E246 I247 V248 R249 A250 L251 R252 A253 R254 T255 V256 P257 A258 I262 I265 R271 M272 F273 F274 V275 V276 E277 G278 S279 V280 S281 V282 A283 T284 P285 N286 P287 V288

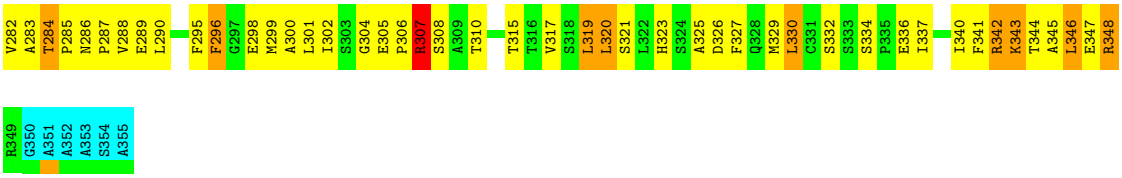
E289 L290 G291 P292 F296 G297 E298 M299 A300 L301 I302 S303 G304 E305 P306 R307 S308 A309 T310 A313 A314 T315 T316 V317 S318 L319 L322 D326 F327 L330 S334 P335 E336 I337 I340 F341 R342 K343 T344 A345 L346 E347 R348 R349 G350 A351 A352 A353 A354 A355

4.2.12 Score per residue for model 12

- Molecule 1: Mll3241 protein

Chain A: 32% 42% 12% • 13%

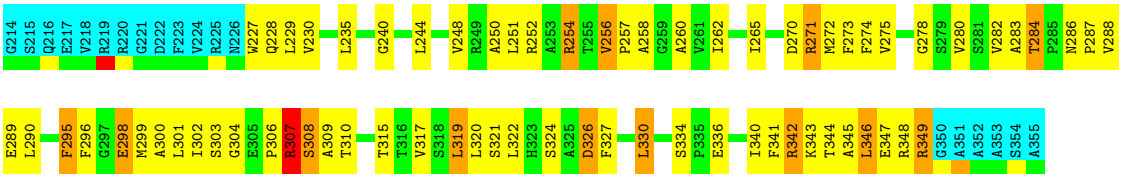
G214 S215 Q216 E217 V218 R219 R220 G221 D222 F223 V224 R225 N226 W227 Q228 L229 V230 L235 K238 L239 G240 L244 V245 E246 I247 V248 R249 A250 L251 R252 A253 R254 T255 V256 P257 A258 G259 A260 V261 I262 C263 R264 I265 G266 E267 P268 R271 M272 F273 F274 V275 G278 S279 V280 S281



4.2.13 Score per residue for model 13

- Molecule 1: Mll3241 protein

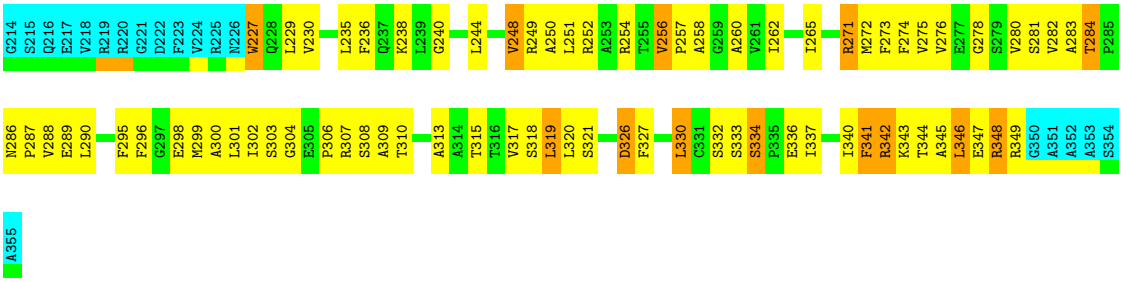
Chain A: 37% 39% 9% • 13%



4.2.14 Score per residue for model 14

- Molecule 1: Mll3241 protein

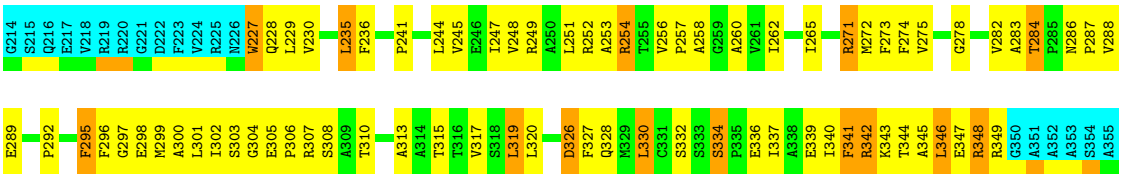
Chain A: 33% 44% 9% 13%



4.2.15 Score per residue for model 15

- Molecule 1: Mll3241 protein

Chain A: 34% 43% 10% 13%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *15 structures with the lowest energy*.

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

Software name	Classification	Version
ATNOS/CANDID	structure solution	1.1
ATNOS/CANDID	refinement	1.1
CYANA	structure solution	1.1
CYANA	refinement	1.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CMP

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	915	955	943	64±8
2	A	22	11	11	3±1
All	All	14055	14490	14310	981

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:370:CMP:H2	2:A:370:CMP:C2	1.53	0.97	8	15
1:A:229:LEU:HD23	1:A:320:LEU:HD21	1.08	1.14	14	1
1:A:230:VAL:HG21	1:A:248:VAL:HG23	1.06	1.21	14	1
1:A:230:VAL:HG21	1:A:248:VAL:HG22	0.92	1.37	15	9
1:A:230:VAL:CG2	1:A:248:VAL:HG23	0.91	1.96	14	1
1:A:317:VAL:HG23	1:A:319:LEU:CD2	0.89	1.97	7	2
1:A:251:LEU:O	1:A:251:LEU:HD13	0.89	1.68	12	1
1:A:244:LEU:O	1:A:248:VAL:HG23	0.87	1.70	8	12
1:A:229:LEU:HD23	1:A:320:LEU:CD2	0.87	1.98	14	1
1:A:317:VAL:HG23	1:A:319:LEU:HD21	0.87	1.45	7	2
1:A:230:VAL:HG11	1:A:244:LEU:HD21	0.85	1.45	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:302:ILE:HD13	1:A:345:ALA:HB2	0.84	1.50	4	13
1:A:251:LEU:HD13	1:A:320:LEU:HD12	0.84	1.46	7	1
1:A:334:SER:CB	1:A:337:ILE:HD12	0.82	2.05	6	11
1:A:282:VAL:HG12	1:A:284:THR:CG2	0.81	2.05	7	15
1:A:317:VAL:HG23	1:A:319:LEU:HD11	0.80	1.53	6	2
1:A:344:THR:HG22	1:A:348:ARG:HD3	0.79	1.54	14	12
1:A:262:ILE:HG23	1:A:273:PHE:CE2	0.78	2.14	12	11
1:A:250:ALA:HB1	1:A:326:ASP:OD1	0.78	1.78	12	3
1:A:271:ARG:C	1:A:301:LEU:HD11	0.78	1.99	7	9
1:A:319:LEU:N	1:A:319:LEU:HD13	0.78	1.94	14	7
1:A:251:LEU:CD1	1:A:320:LEU:HD12	0.77	2.09	7	1
1:A:283:ALA:HB3	1:A:310:THR:HB	0.77	1.57	2	13
1:A:248:VAL:HA	1:A:251:LEU:HD12	0.75	1.58	12	1
1:A:256:VAL:HG21	1:A:319:LEU:HD21	0.75	1.57	12	4
1:A:318:SER:C	1:A:319:LEU:HD13	0.74	2.02	6	4
1:A:322:LEU:HD21	1:A:330:LEU:CD2	0.74	2.11	1	4
1:A:256:VAL:CG2	1:A:319:LEU:HD11	0.74	2.12	7	5
1:A:265:ILE:HG22	1:A:310:THR:OG1	0.74	1.83	10	12
1:A:280:VAL:HG13	1:A:290:LEU:HB2	0.72	1.60	12	5
1:A:265:ILE:HD12	1:A:309:ALA:HA	0.72	1.61	10	7
1:A:250:ALA:HB1	1:A:326:ASP:OD2	0.71	1.85	13	1
1:A:256:VAL:HG21	1:A:319:LEU:HD11	0.71	1.62	7	2
1:A:256:VAL:CG2	1:A:319:LEU:HD21	0.71	2.16	12	3
1:A:283:ALA:C	1:A:284:THR:HG22	0.71	2.06	7	15
1:A:343:LYS:HA	1:A:346:LEU:HD23	0.71	1.63	7	12
1:A:298:GLU:O	1:A:302:ILE:HD12	0.70	1.86	2	6
1:A:327:PHE:CE2	1:A:341:PHE:CZ	0.70	2.79	8	7
1:A:235:LEU:HD23	1:A:236:PHE:CE1	0.70	2.22	9	5
1:A:334:SER:HB3	1:A:337:ILE:HD12	0.69	1.63	5	8
1:A:258:ALA:HB2	1:A:315:THR:HA	0.69	1.64	5	15
1:A:244:LEU:HD23	1:A:244:LEU:O	0.69	1.87	7	3
1:A:227:TRP:CH2	1:A:244:LEU:HD22	0.69	2.23	6	7
1:A:251:LEU:HD22	1:A:252:ARG:N	0.68	2.02	12	1
1:A:272:MET:HG2	1:A:301:LEU:HD12	0.68	1.65	7	10
1:A:323:HIS:CD2	1:A:325:ALA:HB3	0.67	2.24	3	2
1:A:334:SER:HB2	1:A:337:ILE:HD12	0.67	1.64	6	8
1:A:317:VAL:HG23	1:A:319:LEU:CD1	0.67	2.20	4	7
1:A:327:PHE:CE2	1:A:341:PHE:CE2	0.67	2.82	3	4
1:A:308:SER:OG	2:A:370:CMP:H3'	0.67	1.90	3	14
1:A:238:LYS:HB2	1:A:337:ILE:HD11	0.66	1.68	12	8
1:A:262:ILE:HD11	1:A:313:ALA:HB2	0.66	1.67	14	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:241:PRO:O	1:A:245:VAL:HG23	0.65	1.91	4	7
1:A:262:ILE:CG2	1:A:273:PHE:CD2	0.65	2.79	1	8
1:A:278:GLY:HA3	1:A:317:VAL:HG12	0.65	1.65	6	15
1:A:262:ILE:CG2	1:A:273:PHE:CE2	0.65	2.80	15	11
1:A:253:ALA:HB2	1:A:320:LEU:HD23	0.65	1.66	9	3
1:A:238:LYS:HB3	1:A:337:ILE:HD11	0.65	1.69	9	1
1:A:250:ALA:HB1	1:A:326:ASP:CG	0.64	2.13	12	3
1:A:238:LYS:CB	1:A:337:ILE:HD11	0.63	2.23	5	10
1:A:327:PHE:HA	1:A:330:LEU:HD23	0.63	1.69	15	7
1:A:254:ARG:O	1:A:319:LEU:HD22	0.63	1.94	14	6
1:A:295:PHE:CE2	1:A:344:THR:HG21	0.63	2.29	8	3
1:A:302:ILE:CD1	1:A:345:ALA:HB2	0.62	2.25	12	9
1:A:344:THR:HG22	1:A:348:ARG:CD	0.62	2.24	13	5
1:A:244:LEU:O	1:A:244:LEU:HD23	0.62	1.95	11	2
1:A:298:GLU:C	1:A:302:ILE:HD12	0.62	2.14	14	7
1:A:254:ARG:O	1:A:319:LEU:HD12	0.62	1.94	12	5
1:A:330:LEU:HD11	1:A:337:ILE:HG21	0.61	1.72	4	4
1:A:230:VAL:HG11	1:A:244:LEU:CD1	0.61	2.25	9	6
1:A:283:ALA:C	1:A:284:THR:CG2	0.61	2.69	6	15
1:A:299:MET:HG2	1:A:345:ALA:HB1	0.61	1.73	3	4
1:A:317:VAL:CG2	1:A:319:LEU:HD11	0.61	2.24	6	1
1:A:229:LEU:HG	1:A:276:VAL:HG11	0.60	1.72	5	9
1:A:229:LEU:HB3	1:A:320:LEU:HD11	0.60	1.70	13	1
1:A:250:ALA:HB3	1:A:326:ASP:OD2	0.60	1.97	1	3
1:A:251:LEU:HD13	1:A:251:LEU:C	0.60	2.16	12	1
1:A:229:LEU:CG	1:A:276:VAL:HG11	0.60	2.27	4	4
1:A:251:LEU:HG	1:A:322:LEU:HD13	0.60	1.73	13	1
1:A:346:LEU:HD12	1:A:347:GLU:N	0.60	2.12	10	1
1:A:247:ILE:HG23	1:A:251:LEU:HD12	0.59	1.74	6	1
1:A:275:VAL:HG12	1:A:292:PRO:HA	0.59	1.74	2	10
1:A:330:LEU:CD1	1:A:337:ILE:HG21	0.59	2.26	4	5
1:A:239:LEU:HD21	1:A:330:LEU:HD12	0.59	1.73	6	1
1:A:247:ILE:HD12	1:A:326:ASP:OD2	0.59	1.97	15	2
1:A:330:LEU:HD12	1:A:330:LEU:C	0.58	2.18	11	5
1:A:319:LEU:HD22	1:A:319:LEU:N	0.58	2.14	6	1
1:A:283:ALA:O	1:A:284:THR:HG22	0.58	1.98	6	15
1:A:322:LEU:HD21	1:A:330:LEU:HD23	0.57	1.75	1	2
1:A:296:PHE:CD1	1:A:296:PHE:N	0.57	2.72	12	8
1:A:322:LEU:HD21	1:A:330:LEU:HD21	0.57	1.75	5	1
1:A:274:PHE:HB2	1:A:320:LEU:HD12	0.57	1.77	12	1
1:A:272:MET:SD	1:A:274:PHE:CZ	0.57	2.98	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:271:ARG:CA	1:A:301:LEU:HD11	0.56	2.30	2	11
1:A:276:VAL:HG21	1:A:320:LEU:HD23	0.56	1.76	14	1
1:A:295:PHE:N	1:A:295:PHE:CD1	0.56	2.74	7	10
1:A:319:LEU:N	1:A:319:LEU:CD1	0.56	2.69	5	7
1:A:229:LEU:CD1	1:A:276:VAL:HG11	0.56	2.31	11	2
1:A:280:VAL:HG22	1:A:290:LEU:HB2	0.56	1.77	4	1
1:A:331:CYS:SG	1:A:338:ALA:HB2	0.55	2.41	9	1
1:A:235:LEU:CD2	1:A:337:ILE:HG23	0.55	2.31	11	1
1:A:322:LEU:HD12	1:A:323:HIS:N	0.55	2.16	8	1
1:A:317:VAL:HG23	1:A:319:LEU:HD12	0.55	1.78	2	6
1:A:300:ALA:HB2	1:A:307:ARG:HH12	0.55	1.60	8	4
1:A:230:VAL:HG11	1:A:244:LEU:HD11	0.55	1.78	9	5
1:A:235:LEU:HD11	1:A:341:PHE:CE2	0.55	2.35	9	1
1:A:244:LEU:HD23	1:A:248:VAL:HG23	0.55	1.78	7	5
1:A:239:LEU:HD21	1:A:330:LEU:CD1	0.54	2.33	6	1
1:A:227:TRP:CZ3	1:A:244:LEU:HD22	0.54	2.37	10	4
1:A:283:ALA:HB3	1:A:310:THR:CB	0.54	2.33	13	4
1:A:327:PHE:CE1	1:A:341:PHE:CZ	0.54	2.95	13	5
1:A:273:PHE:CB	1:A:296:PHE:CE1	0.54	2.91	5	1
1:A:272:MET:SD	1:A:274:PHE:CE1	0.54	3.01	4	1
1:A:244:LEU:CD2	1:A:248:VAL:HG23	0.53	2.32	15	5
1:A:276:VAL:CG2	1:A:320:LEU:HD11	0.53	2.34	4	1
1:A:279:SER:CB	1:A:290:LEU:O	0.52	2.57	4	2
1:A:243:VAL:HG21	1:A:333:SER:OG	0.52	2.03	10	1
1:A:272:MET:SD	1:A:274:PHE:CE2	0.52	3.03	9	2
1:A:307:ARG:NH2	2:A:370:CMP:O2P	0.52	2.43	9	5
1:A:323:HIS:HD2	1:A:325:ALA:HB3	0.52	1.62	3	2
1:A:251:LEU:C	1:A:251:LEU:HD12	0.52	2.25	9	3
1:A:262:ILE:HG22	1:A:273:PHE:CE2	0.51	2.40	4	2
1:A:265:ILE:CG2	1:A:310:THR:OG1	0.51	2.58	14	7
1:A:229:LEU:HD11	1:A:276:VAL:HG11	0.51	1.81	4	2
1:A:342:ARG:C	1:A:342:ARG:CD	0.51	2.78	12	3
1:A:229:LEU:HB3	1:A:320:LEU:HD21	0.51	1.81	1	3
1:A:253:ALA:HB2	1:A:320:LEU:CD2	0.51	2.36	9	1
1:A:241:PRO:O	1:A:245:VAL:CG2	0.51	2.58	15	4
1:A:239:LEU:HD11	1:A:330:LEU:HD13	0.51	1.83	6	2
1:A:288:VAL:CG1	1:A:289:GLU:N	0.51	2.74	6	15
1:A:327:PHE:CZ	1:A:341:PHE:CE2	0.50	2.99	8	2
1:A:295:PHE:CD1	1:A:295:PHE:N	0.50	2.79	15	2
1:A:331:CYS:SG	1:A:338:ALA:CB	0.50	3.00	9	1
1:A:247:ILE:CD1	1:A:326:ASP:OD2	0.50	2.58	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:319:LEU:HD22	1:A:319:LEU:H	0.50	1.66	6	1
1:A:307:ARG:NE	2:A:370:CMP:O5'	0.50	2.44	7	3
1:A:348:ARG:HG3	2:A:370:CMP:C4	0.50	2.41	11	1
1:A:251:LEU:HD22	1:A:251:LEU:C	0.50	2.26	12	1
1:A:273:PHE:HB3	1:A:296:PHE:CZ	0.50	2.42	3	12
1:A:322:LEU:CD1	1:A:326:ASP:OD1	0.49	2.60	3	1
1:A:235:LEU:HD23	1:A:236:PHE:CD1	0.49	2.42	6	3
1:A:253:ALA:HA	1:A:320:LEU:HD13	0.49	1.84	7	1
1:A:334:SER:CB	1:A:337:ILE:CD1	0.49	2.90	1	1
1:A:236:PHE:CZ	1:A:251:LEU:HD11	0.49	2.42	14	1
1:A:257:PRO:O	1:A:260:ALA:CB	0.49	2.61	7	8
1:A:307:ARG:NH1	2:A:370:CMP:O2P	0.49	2.45	8	4
1:A:239:LEU:CD2	1:A:330:LEU:O	0.49	2.60	10	1
1:A:244:LEU:O	1:A:244:LEU:CD2	0.49	2.61	11	5
1:A:298:GLU:O	1:A:302:ILE:CG1	0.49	2.61	15	2
1:A:251:LEU:HD13	1:A:320:LEU:HD22	0.49	1.84	5	2
1:A:271:ARG:HG3	1:A:273:PHE:CE1	0.49	2.42	7	2
1:A:300:ALA:O	1:A:304:GLY:N	0.49	2.46	5	12
1:A:297:GLY:CA	1:A:307:ARG:NH2	0.49	2.76	2	2
1:A:235:LEU:CD1	1:A:337:ILE:HG23	0.48	2.38	15	3
1:A:244:LEU:HD12	1:A:248:VAL:HG23	0.48	1.85	4	1
1:A:264:ARG:O	1:A:267:GLU:CG	0.48	2.61	1	3
1:A:274:PHE:CD1	1:A:274:PHE:N	0.48	2.81	13	6
1:A:302:ILE:HD11	1:A:341:PHE:HB3	0.48	1.84	11	1
1:A:272:MET:HE1	1:A:295:PHE:HB2	0.48	1.85	13	2
1:A:345:ALA:O	1:A:349:ARG:CG	0.48	2.62	11	1
1:A:300:ALA:HB2	1:A:307:ARG:NH1	0.48	2.24	8	2
1:A:250:ALA:CB	1:A:326:ASP:OD1	0.48	2.61	8	1
1:A:229:LEU:CD2	1:A:320:LEU:HD21	0.47	2.09	14	1
1:A:230:VAL:CG1	1:A:244:LEU:CD1	0.47	2.92	9	2
1:A:275:VAL:HG23	1:A:296:PHE:HE1	0.47	1.69	15	12
1:A:298:GLU:O	1:A:302:ILE:N	0.47	2.48	15	8
1:A:344:THR:O	1:A:348:ARG:CD	0.47	2.63	13	4
1:A:230:VAL:CG1	1:A:244:LEU:HD21	0.47	2.36	6	1
1:A:319:LEU:HD13	1:A:319:LEU:N	0.47	2.24	6	1
1:A:251:LEU:HD12	1:A:251:LEU:O	0.47	2.10	9	1
1:A:301:LEU:HD22	1:A:324:SER:HA	0.47	1.87	10	1
1:A:317:VAL:CG2	1:A:319:LEU:HD21	0.46	2.30	7	2
1:A:272:MET:HB3	1:A:274:PHE:CZ	0.46	2.45	9	1
1:A:274:PHE:O	1:A:319:LEU:CB	0.46	2.63	15	3
1:A:276:VAL:CG2	1:A:320:LEU:HD23	0.46	2.40	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:264:ARG:HA	1:A:310:THR:HG23	0.46	1.86	2	1
1:A:281:SER:HB2	1:A:314:ALA:HB2	0.46	1.87	2	1
1:A:272:MET:HB3	1:A:274:PHE:CE1	0.46	2.45	10	8
1:A:327:PHE:CZ	1:A:341:PHE:CD2	0.46	3.03	3	1
1:A:282:VAL:HG12	1:A:284:THR:HG22	0.45	1.85	7	15
1:A:265:ILE:HG22	1:A:310:THR:HG1	0.45	1.71	14	3
1:A:273:PHE:CB	1:A:296:PHE:CE2	0.45	2.99	3	2
1:A:302:ILE:HD13	1:A:345:ALA:CB	0.45	2.35	4	1
1:A:237:GLN:NE2	1:A:244:LEU:HD11	0.45	2.26	7	1
1:A:250:ALA:HB3	1:A:326:ASP:OD1	0.45	2.11	8	2
1:A:299:MET:SD	1:A:345:ALA:HB1	0.45	2.51	6	2
1:A:251:LEU:HD13	1:A:320:LEU:HB3	0.45	1.89	1	1
1:A:244:LEU:O	1:A:248:VAL:CG2	0.45	2.60	12	3
1:A:272:MET:C	1:A:273:PHE:CD1	0.45	2.90	1	1
1:A:286:ASN:N	1:A:287:PRO:HD3	0.45	2.27	11	15
1:A:306:PRO:O	1:A:307:ARG:C	0.44	2.54	7	9
1:A:250:ALA:CB	1:A:326:ASP:CG	0.44	2.85	12	1
1:A:342:ARG:HG3	1:A:343:LYS:N	0.44	2.27	15	9
1:A:301:LEU:CD2	1:A:324:SER:CB	0.44	2.95	10	2
1:A:253:ALA:CB	1:A:320:LEU:HD23	0.44	2.41	9	1
1:A:247:ILE:HD12	1:A:326:ASP:OD1	0.44	2.13	10	1
1:A:275:VAL:HG23	1:A:296:PHE:HE2	0.44	1.73	5	1
1:A:227:TRP:HA	1:A:227:TRP:CE3	0.43	2.47	14	9
1:A:275:VAL:HG23	1:A:296:PHE:CE1	0.43	2.48	9	5
1:A:229:LEU:CD2	1:A:276:VAL:HG11	0.43	2.43	2	1
1:A:227:TRP:CE3	1:A:227:TRP:HA	0.43	2.48	3	1
1:A:235:LEU:HD11	1:A:341:PHE:CZ	0.43	2.48	9	1
1:A:251:LEU:HD23	1:A:320:LEU:HB3	0.43	1.90	12	1
1:A:334:SER:HB3	1:A:337:ILE:CD1	0.43	2.43	1	1
1:A:337:ILE:CG2	1:A:341:PHE:CE2	0.43	3.02	2	1
1:A:323:HIS:CD2	1:A:325:ALA:CB	0.43	3.01	3	2
1:A:235:LEU:HD23	1:A:337:ILE:HG23	0.43	1.90	11	1
1:A:345:ALA:O	1:A:349:ARG:CB	0.43	2.67	1	1
1:A:322:LEU:HD12	1:A:323:HIS:H	0.43	1.74	8	1
1:A:287:PRO:O	1:A:288:VAL:HG23	0.42	2.13	12	12
1:A:262:ILE:HG22	1:A:273:PHE:CD2	0.42	2.48	1	1
1:A:322:LEU:HD23	1:A:323:HIS:O	0.42	2.14	9	1
1:A:244:LEU:O	1:A:244:LEU:HD12	0.42	2.14	4	1
1:A:272:MET:SD	1:A:297:GLY:C	0.42	2.98	8	3
1:A:280:VAL:CG1	1:A:281:SER:N	0.42	2.83	7	2
1:A:307:ARG:NH1	2:A:370:CMP:O5'	0.42	2.53	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:250:ALA:CB	1:A:326:ASP:OD2	0.42	2.66	1	3
1:A:239:LEU:HD21	1:A:330:LEU:O	0.42	2.15	8	1
1:A:337:ILE:O	1:A:341:PHE:CD2	0.41	2.73	2	1
1:A:342:ARG:CD	1:A:342:ARG:C	0.41	2.88	5	2
1:A:329:MET:CG	1:A:330:LEU:N	0.41	2.84	12	1
1:A:327:PHE:CZ	1:A:341:PHE:CZ	0.41	3.08	8	1
1:A:308:SER:HG	2:A:370:CMP:H3'	0.41	1.73	10	1
1:A:307:ARG:CZ	2:A:370:CMP:O5'	0.41	2.69	6	1
1:A:288:VAL:HG12	1:A:289:GLU:N	0.41	2.30	7	2
1:A:229:LEU:HG	1:A:276:VAL:CG1	0.41	2.46	4	1
1:A:253:ALA:CA	1:A:320:LEU:HD13	0.41	2.45	7	1
1:A:230:VAL:CG1	1:A:244:LEU:HD11	0.41	2.46	9	2
1:A:246:GLU:O	1:A:250:ALA:HB2	0.41	2.16	9	1
1:A:284:THR:OG1	1:A:285:PRO:HD2	0.41	2.15	7	6
1:A:273:PHE:HB3	1:A:296:PHE:CE1	0.41	2.50	5	1
1:A:282:VAL:O	1:A:287:PRO:CB	0.41	2.69	11	2
1:A:251:LEU:C	1:A:251:LEU:CD1	0.41	2.86	12	1
1:A:329:MET:SD	1:A:329:MET:C	0.41	2.99	10	2
1:A:322:LEU:HD21	1:A:326:ASP:HB2	0.41	1.91	9	1
1:A:247:ILE:HD11	1:A:330:LEU:HB3	0.41	1.92	11	1
1:A:274:PHE:O	1:A:319:LEU:HA	0.41	2.16	15	1
1:A:239:LEU:O	1:A:240:GLY:O	0.41	2.39	4	5
1:A:298:GLU:O	1:A:302:ILE:CB	0.41	2.69	15	1
1:A:322:LEU:CD1	1:A:326:ASP:HB3	0.40	2.45	8	1
1:A:322:LEU:HD11	1:A:326:ASP:HB3	0.40	1.92	10	1
1:A:262:ILE:HG22	1:A:263:CYS:SG	0.40	2.56	12	1
1:A:267:GLU:OE1	1:A:268:PRO:O	0.40	2.39	12	1
1:A:348:ARG:CG	2:A:370:CMP:H2'	0.40	2.47	14	1
1:A:329:MET:C	1:A:329:MET:SD	0.40	3.00	4	1
1:A:275:VAL:HA	1:A:319:LEU:HD12	0.40	1.93	6	1
1:A:298:GLU:OE2	1:A:348:ARG:NH1	0.40	2.54	7	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	123/142 (87%)	114±1 (93±1%)	8±1 (6±1%)	1±1 (1±1%)	20 68
All	All	1845/2130 (87%)	1714 (93%)	113 (6%)	18 (1%)	20 68

All 3 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	240	GLY	9
1	A	307	ARG	7
1	A	304	GLY	2

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	98/110 (89%)	73±2 (74±2%)	25±2 (26±2%)	2 24
All	All	1470/1650 (89%)	1093 (74%)	377 (26%)	2 24

All 53 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	227	TRP	15
1	A	235	LEU	15
1	A	256	VAL	15
1	A	284	THR	15
1	A	319	LEU	15
1	A	340	ILE	15
1	A	342	ARG	15
1	A	346	LEU	14
1	A	252	ARG	13
1	A	254	ARG	13
1	A	281	SER	12
1	A	307	ARG	12
1	A	330	LEU	12
1	A	334	SER	12
1	A	299	MET	11

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Mol	Chain	Res	Type	Models (Total)
1	A	271	ARG	10
1	A	336	GLU	10
1	A	303	SER	9
1	A	326	ASP	8
1	A	348	ARG	8
1	A	249	ARG	7
1	A	318	SER	7
1	A	321	SER	7
1	A	277	GLU	6
1	A	328	GLN	6
1	A	332	SER	6
1	A	343	LYS	6
1	A	298	GLU	6
1	A	244	LEU	5
1	A	246	GLU	5
1	A	320	LEU	5
1	A	228	GLN	5
1	A	272	MET	5
1	A	339	GLU	4
1	A	308	SER	4
1	A	333	SER	4
1	A	341	PHE	4
1	A	295	PHE	4
1	A	264	ARG	3
1	A	267	GLU	3
1	A	347	GLU	3
1	A	270	ASP	3
1	A	331	CYS	3
1	A	305	GLU	3
1	A	251	LEU	2
1	A	322	LEU	2
1	A	296	PHE	2
1	A	237	GLN	2
1	A	349	ARG	2
1	A	229	LEU	1
1	A	302	ILE	1
1	A	323	HIS	1
1	A	248	VAL	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	CMP	A	370	-	22,25,25	1.45±0.01	4±0 (18±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	CMP	A	370	-	24,39,39	1.73±0.01	5±0 (20±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CMP	A	370	-	-	0±0,0,31,31	0±0,4,4,4

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
2	A	370	CMP	P-O5'	3.01	1.61	1.57	6	15
2	A	370	CMP	O4'-C1'	2.97	1.45	1.41	6	15
2	A	370	CMP	P-O3'	2.56	1.62	1.57	9	15
2	A	370	CMP	C8-N7	2.30	1.30	1.34	15	15

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	370	CMP	O3'-C3'-C4'	4.55	107.27	110.71	6	15
2	A	370	CMP	N3-C2-N1	4.02	122.40	128.68	10	15
2	A	370	CMP	O5'-P-O3'	3.86	110.99	105.68	12	15
2	A	370	CMP	C4-C5-N7	2.26	107.05	109.40	12	15
2	A	370	CMP	C5'-C4'-C3'	2.12	108.19	112.49	5	15

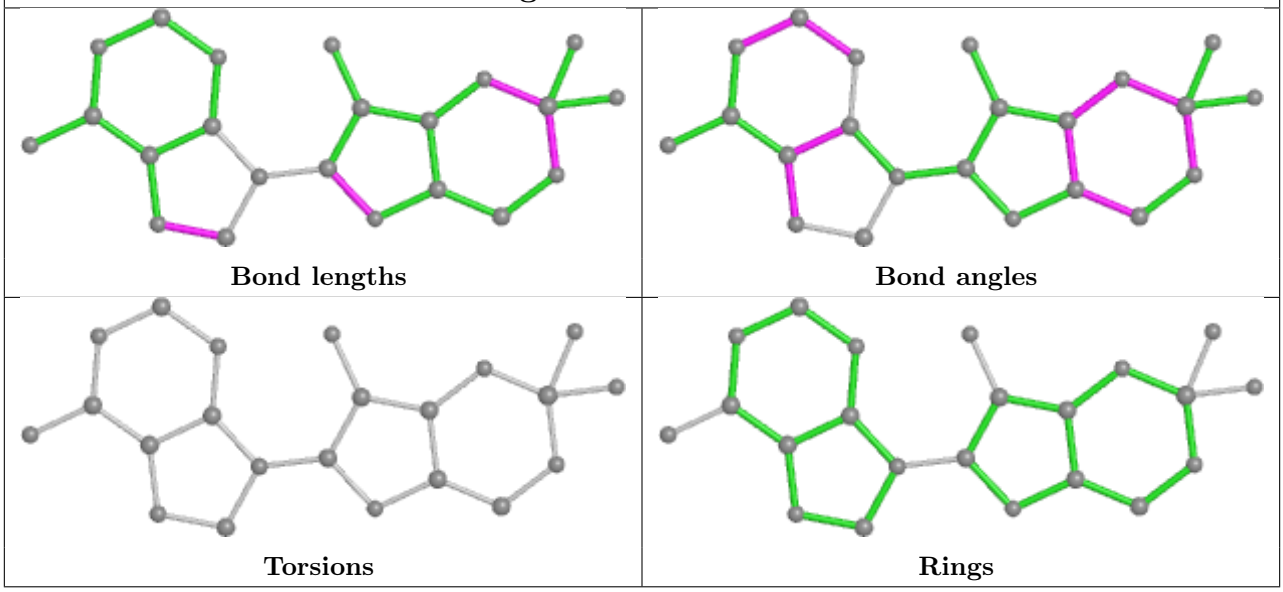
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CMP A 370



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 (i)

No chemical shift data were provided