



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:49 AM UTC

PDB ID : 2K31 / pdb_00002k31
BMRB ID : 15734
Title : Solution Structure of cGMP-binding GAF domain of Phosphodiesterase 5
Authors : Heikaus, C.C.; Stout, J.R.; Sekharan, M.R.; Eakin, C.M.; Rajagopal, P.; Brzovic, P.S.; Beavo, J.A.; Klevit, R.E.
Deposited on : 2008-04-16

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
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

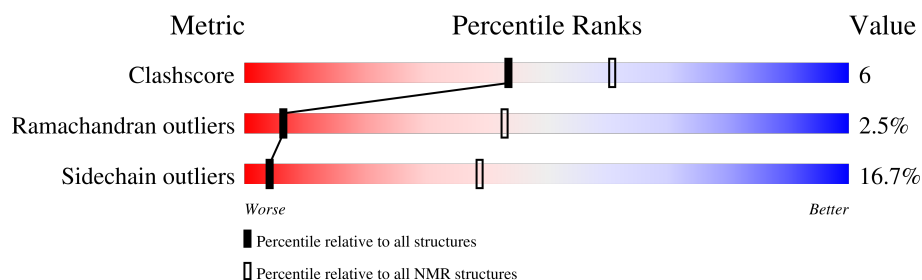
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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	176	

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:157-A:263, A:268-A:277, A:285-A:302 (135)	0.43	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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2342 atoms, of which 1151 are hydrogens and 0 are deuteriums.

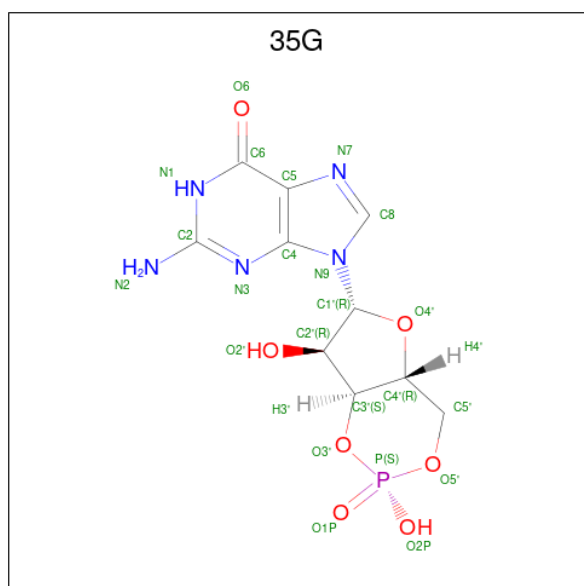
- Molecule 1 is a protein called Phosphodiesterase 5A, cGMP-specific.

Mol	Chain	Residues	Atoms						Trace
1	A	149	Total	C	H	N	O	S	0
			2308	738	1140	197	227	6	

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	MET	-	initiating methionine	UNP Q0VBW0
A	295	GLU	ALA	engineered mutation	UNP Q0VBW0
A	302	GLU	ILE	engineered mutation	UNP Q0VBW0
A	321	LEU	-	expression tag	UNP Q0VBW0
A	322	GLU	-	expression tag	UNP Q0VBW0
A	323	HIS	-	expression tag	UNP Q0VBW0
A	324	HIS	-	expression tag	UNP Q0VBW0
A	325	HIS	-	expression tag	UNP Q0VBW0
A	326	HIS	-	expression tag	UNP Q0VBW0
A	327	HIS	-	expression tag	UNP Q0VBW0
A	328	HIS	-	expression tag	UNP Q0VBW0

- Molecule 2 is GUANOSINE-3',5'-MONOPHOSPHATE (CCD ID: 35G) (formula: $C_{10}H_{12}N_5O_7P$).



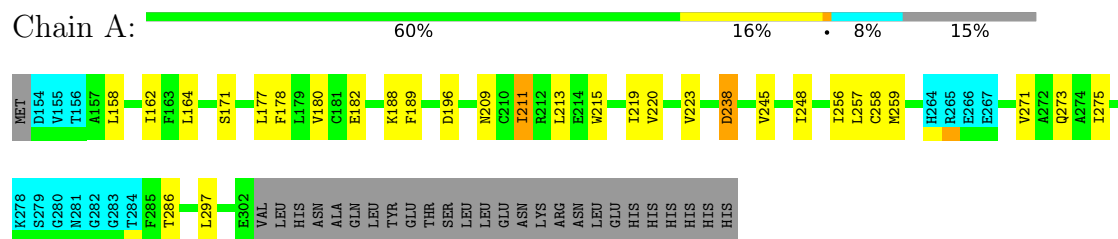
Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
2	A	1	34	10	11	5	7	1

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: Phosphodiesterase 5A, cGMP-specific

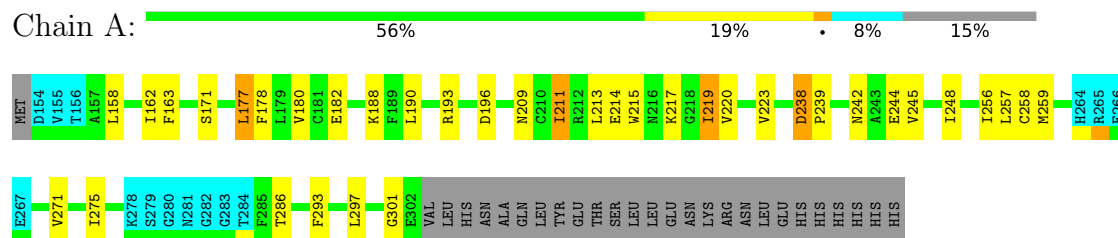


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

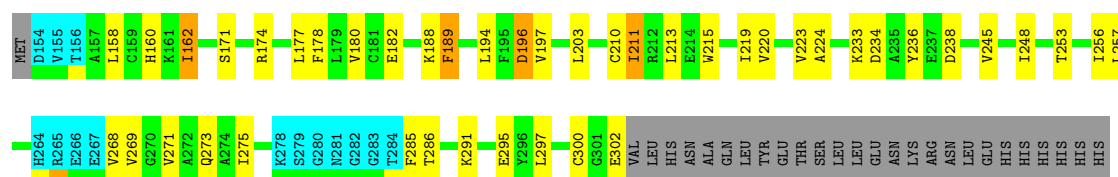
- Molecule 1: Phosphodiesterase 5A, cGMP-specific



4.2.2 Score per residue for model 2

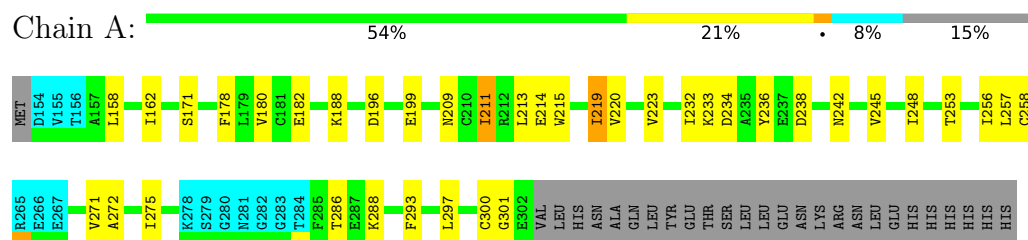
- Molecule 1: Phosphodiesterase 5A, cGMP-specific





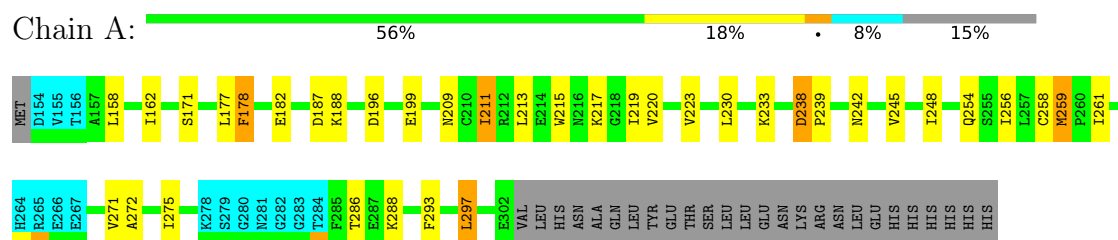
4.2.3 Score per residue for model 3

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



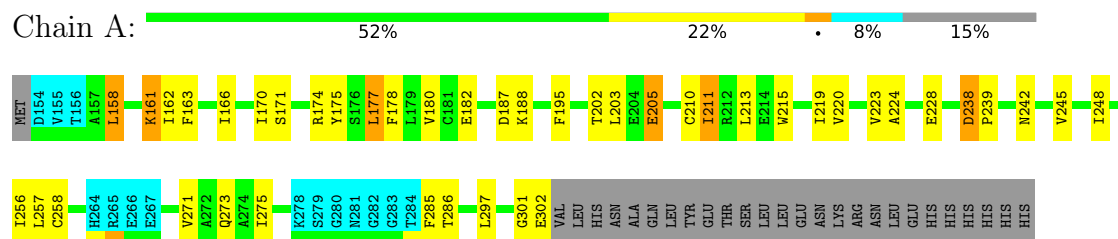
4.2.4 Score per residue for model 4

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



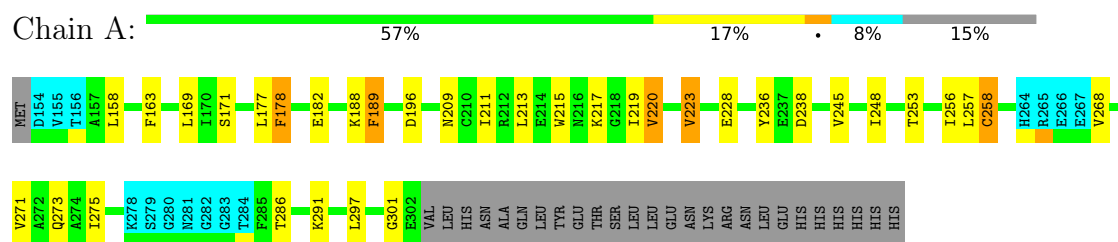
4.2.5 Score per residue for model 5

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



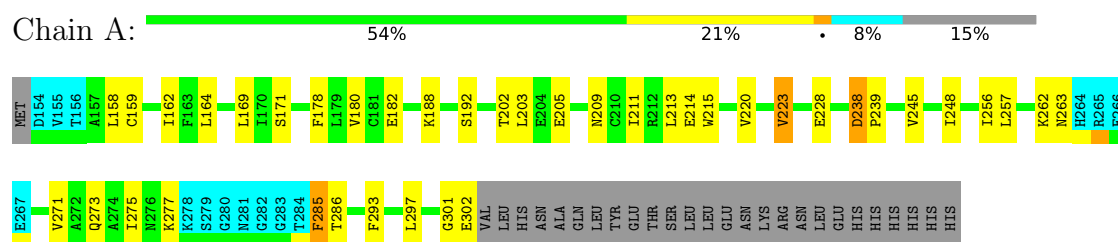
4.2.6 Score per residue for model 6

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



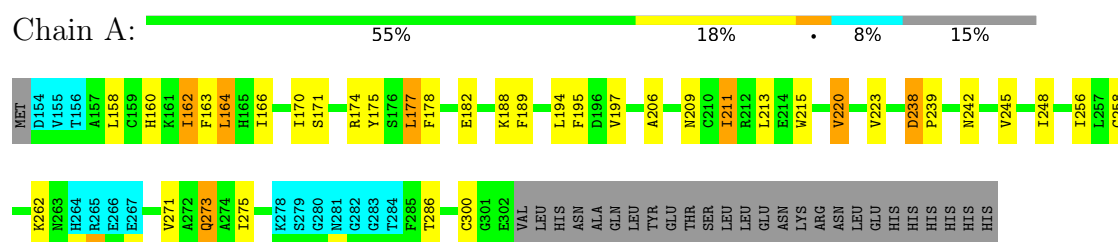
4.2.7 Score per residue for model 7

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



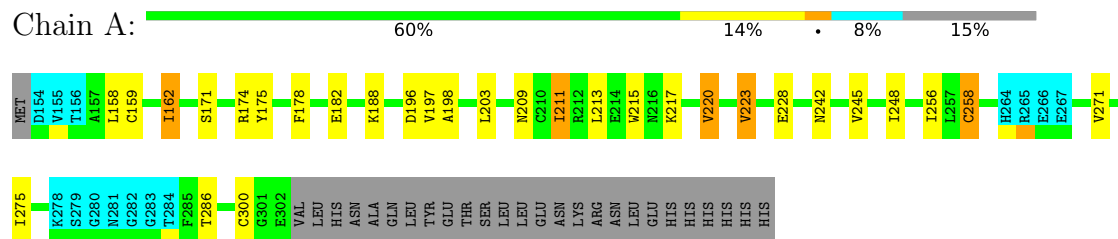
4.2.8 Score per residue for model 8

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



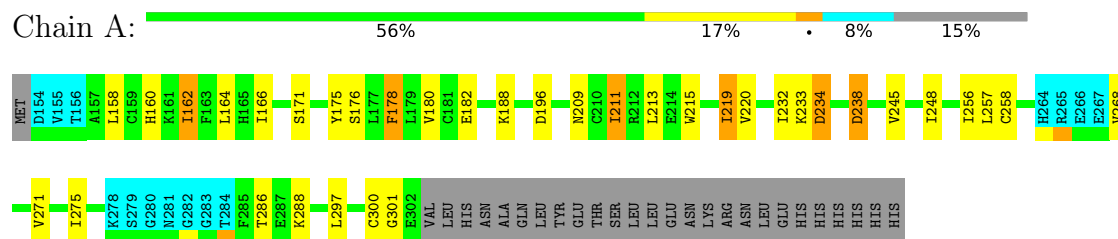
4.2.9 Score per residue for model 9

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



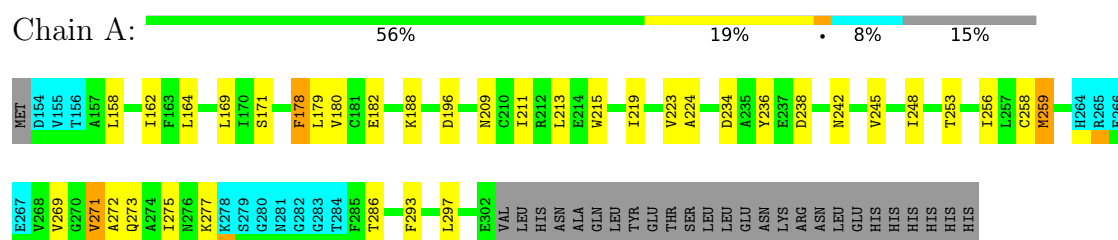
4.2.10 Score per residue for model 10

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



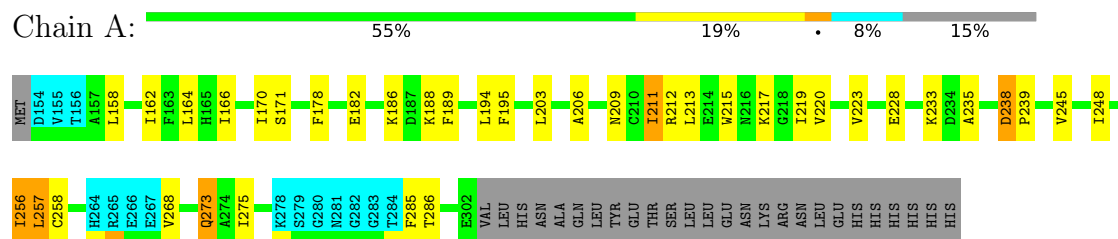
4.2.11 Score per residue for model 11

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



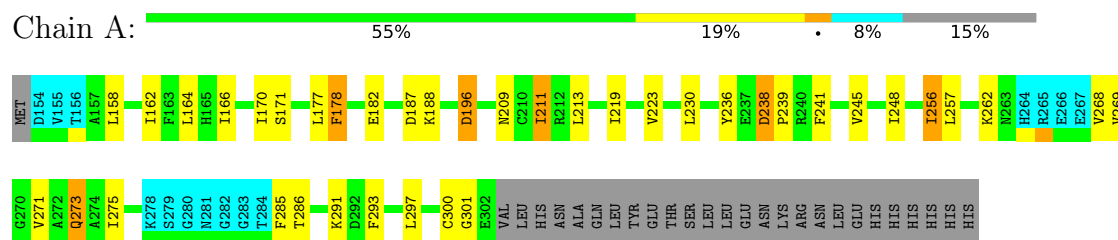
4.2.12 Score per residue for model 12

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



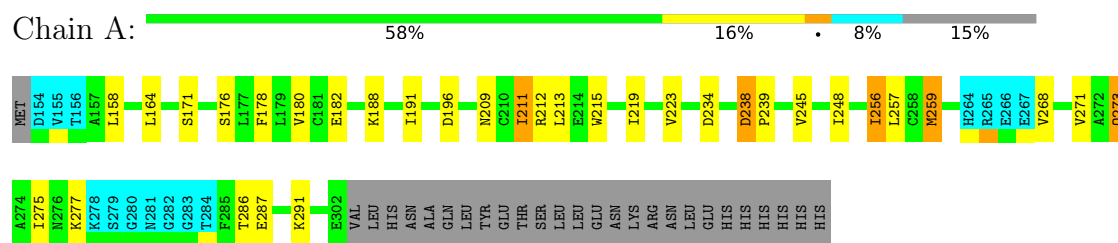
4.2.13 Score per residue for model 13

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



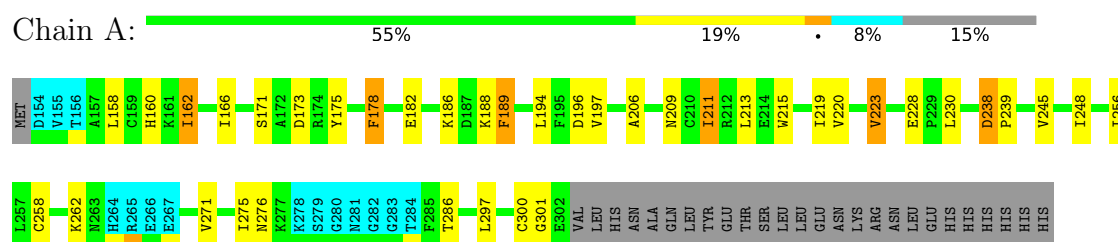
4.2.14 Score per residue for model 14

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



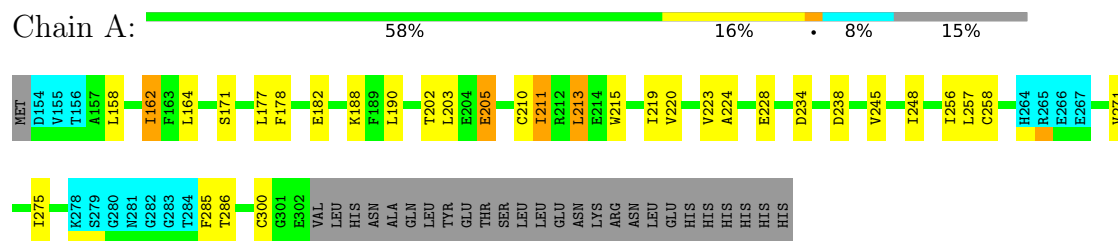
4.2.15 Score per residue for model 15

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



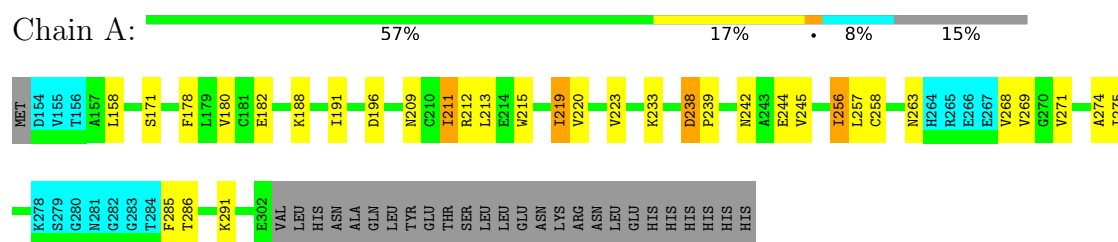
4.2.16 Score per residue for model 16

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



4.2.17 Score per residue for model 17

- Molecule 1: Phosphodiesterase 5A, cGMP-specific



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
CNS	structure solution	1.1
CYANA	structure solution	2.0
CYANA	refinement	2.0

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	1765
Number of shifts mapped to atoms	1675
Number of unparsed shifts	0
Number of shifts with mapping errors	90
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 35G

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 ⓘ

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	1065	1047	1043	14±3
2	A	23	11	11	2±1
All	All	21760	21160	21080	278

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:273:GLN:HE22	2:A:1:35G:H2'	0.71	1.45	14	2
1:A:297:LEU:HA	1:A:300:CYS:SG	0.67	2.30	13	2
1:A:158:LEU:O	1:A:161:LYS:HG3	0.65	1.92	5	1
1:A:273:GLN:HE22	2:A:1:35G:H3'	0.62	1.55	8	2
1:A:256:ILE:HG12	1:A:257:LEU:N	0.62	2.09	17	2
1:A:256:ILE:HD11	1:A:273:GLN:HG2	0.61	1.73	14	2
1:A:162:ILE:HG21	1:A:300:CYS:SG	0.59	2.37	10	3
1:A:162:ILE:HD13	1:A:300:CYS:SG	0.59	2.36	10	3
1:A:219:ILE:HD12	1:A:258:CYS:SG	0.59	2.37	12	8
1:A:161:LYS:HD2	1:A:162:ILE:N	0.57	2.14	5	1
1:A:211:ILE:HG21	1:A:245:VAL:HG13	0.55	1.78	5	19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:256:ILE:HG13	1:A:274:ALA:O	0.55	2.01	19	2
1:A:230:LEU:HB3	1:A:258:CYS:SG	0.54	2.42	20	4
1:A:191:ILE:HG23	1:A:212:ARG:HG2	0.54	1.79	17	2
1:A:161:LYS:HD2	1:A:161:LYS:C	0.53	2.28	5	1
1:A:162:ILE:HG12	1:A:300:CYS:SG	0.53	2.44	9	2
1:A:188:LYS:HE3	1:A:215:TRP:CD1	0.52	2.40	7	18
1:A:273:GLN:NE2	2:A:1:35G:H2'	0.51	2.20	14	2
1:A:178:PHE:CE2	1:A:211:ILE:HD11	0.50	2.41	11	1
1:A:223:VAL:HG21	1:A:258:CYS:SG	0.50	2.46	5	1
1:A:223:VAL:HG12	1:A:228:GLU:O	0.50	2.07	9	6
1:A:273:GLN:OE1	2:A:1:35G:H2'	0.50	2.06	12	1
1:A:245:VAL:HG21	2:A:1:35G:O4'	0.50	2.06	8	13
1:A:202:THR:OG1	1:A:205:GLU:HB2	0.50	2.07	7	3
1:A:173:ASP:N	1:A:276:ASN:HD22	0.50	2.05	20	2
1:A:219:ILE:HD11	1:A:273:GLN:NE2	0.49	2.22	20	2
1:A:188:LYS:HE3	1:A:215:TRP:NE1	0.49	2.22	15	15
1:A:219:ILE:HD11	1:A:273:GLN:HE22	0.49	1.67	5	2
1:A:194:LEU:HD21	1:A:203:LEU:HD12	0.49	1.83	12	1
1:A:258:CYS:HA	1:A:273:GLN:OE1	0.48	2.08	6	1
1:A:259:MET:SD	1:A:272:ALA:HB3	0.48	2.49	18	3
1:A:178:PHE:CE2	2:A:1:35G:H8	0.48	2.43	19	4
1:A:256:ILE:HD13	1:A:257:LEU:N	0.47	2.24	13	1
1:A:180:VAL:HG12	1:A:269:VAL:O	0.47	2.09	19	3
1:A:232:ILE:HG12	1:A:258:CYS:SG	0.47	2.50	10	2
1:A:257:LEU:HB2	1:A:285:PHE:CE2	0.47	2.45	20	2
1:A:194:LEU:HD11	1:A:203:LEU:HD11	0.47	1.86	2	1
1:A:220:VAL:HA	1:A:258:CYS:SG	0.47	2.49	8	3
1:A:235:ALA:HA	1:A:238:ASP:OD2	0.47	2.08	18	1
1:A:182:GLU:OE1	1:A:188:LYS:HE3	0.47	2.09	5	1
1:A:163:PHE:CE2	1:A:177:LEU:HD11	0.47	2.45	6	1
1:A:257:LEU:O	1:A:259:MET:HE3	0.47	2.10	14	1
1:A:273:GLN:OE1	2:A:1:35G:H3'	0.47	2.10	2	2
1:A:257:LEU:HB2	1:A:285:PHE:CZ	0.47	2.45	5	3
1:A:166:ILE:HD12	1:A:175:TYR:CZ	0.46	2.46	5	5
1:A:234:ASP:O	1:A:238:ASP:HB2	0.46	2.09	16	7
1:A:259:MET:SD	1:A:297:LEU:HD11	0.46	2.51	3	1
1:A:238:ASP:OD2	1:A:239:PRO:HD2	0.46	2.11	5	10
1:A:293:PHE:O	1:A:297:LEU:HG	0.46	2.11	19	6
1:A:215:TRP:CH2	1:A:224:ALA:HB1	0.46	2.46	11	5
1:A:236:TYR:CD2	1:A:253:THR:HG22	0.46	2.46	6	4
1:A:194:LEU:HA	1:A:206:ALA:O	0.45	2.11	15	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:261:ILE:HD11	1:A:272:ALA:HB2	0.45	1.88	3	2
1:A:178:PHE:CD1	1:A:178:PHE:N	0.45	2.85	4	2
1:A:189:PHE:CD1	1:A:189:PHE:N	0.45	2.84	15	5
1:A:215:TRP:CD1	1:A:216:ASN:HD22	0.45	2.30	19	1
1:A:163:PHE:CZ	1:A:177:LEU:HD22	0.45	2.46	5	3
1:A:297:LEU:O	1:A:301:GLY:N	0.45	2.50	3	9
1:A:214:GLU:OE1	1:A:217:LYS:HG2	0.44	2.12	1	1
1:A:160:HIS:O	1:A:164:LEU:HD12	0.44	2.11	8	1
1:A:178:PHE:HE2	1:A:211:ILE:HD11	0.44	1.70	11	1
1:A:243:ALA:O	1:A:247:GLN:HG3	0.44	2.12	18	1
1:A:257:LEU:HD13	1:A:285:PHE:CG	0.44	2.47	20	1
1:A:173:ASP:HB2	1:A:276:ASN:OD1	0.44	2.12	18	1
1:A:263:ASN:HB2	1:A:269:VAL:HG13	0.44	1.90	17	1
1:A:167:HIS:CE1	1:A:199:GLU:HB2	0.43	2.48	20	1
1:A:257:LEU:HD13	1:A:285:PHE:CD1	0.43	2.49	2	1
1:A:178:PHE:CE1	1:A:211:ILE:HD11	0.43	2.49	6	1
1:A:160:HIS:NE2	1:A:197:VAL:HG13	0.43	2.28	8	2
1:A:257:LEU:HD23	1:A:285:PHE:CD1	0.43	2.48	12	1
1:A:232:ILE:HB	1:A:256:ILE:O	0.43	2.13	20	1
1:A:190:LEU:HD13	1:A:213:LEU:HD12	0.43	1.90	20	2
1:A:180:VAL:HG13	1:A:215:TRP:CZ3	0.43	2.49	10	9
1:A:195:PHE:CE1	1:A:211:ILE:HG12	0.43	2.48	5	3
1:A:174:ARG:NH1	1:A:198:ALA:HB2	0.43	2.28	9	1
1:A:235:ALA:HB2	1:A:256:ILE:HG21	0.43	1.90	12	1
1:A:233:LYS:O	1:A:254:GLN:O	0.43	2.37	4	1
1:A:245:VAL:HG11	2:A:1:35G:C1'	0.43	2.43	17	5
1:A:166:ILE:O	1:A:170:ILE:HG13	0.42	2.14	19	5
1:A:262:LYS:HA	1:A:269:VAL:HG22	0.42	1.91	13	1
1:A:160:HIS:CE1	1:A:197:VAL:HG13	0.42	2.50	20	2
1:A:223:VAL:HG13	1:A:228:GLU:O	0.42	2.15	16	3
1:A:287:GLU:O	1:A:291:LYS:HG2	0.42	2.15	14	1
1:A:219:ILE:O	1:A:223:VAL:HG23	0.41	2.16	2	1
1:A:159:CYS:O	1:A:162:ILE:HG13	0.41	2.16	7	1
1:A:263:ASN:OD1	1:A:302:GLU:HA	0.41	2.15	7	1
1:A:176:SER:OG	1:A:273:GLN:HB3	0.41	2.16	14	1
1:A:174:ARG:HD2	1:A:196:ASP:OD2	0.41	2.14	2	1
1:A:176:SER:CB	2:A:1:35G:N7	0.41	2.84	20	1
1:A:159:CYS:SG	1:A:300:CYS:SG	0.41	3.16	9	1
1:A:190:LEU:HD12	1:A:214:GLU:O	0.40	2.16	1	1
1:A:175:TYR:O	1:A:197:VAL:HG23	0.40	2.16	9	1
1:A:189:PHE:N	1:A:189:PHE:CD1	0.40	2.89	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:291:LYS:O	1:A:295:GLU:HG3	0.40	2.16	2	1
1:A:271:VAL:HG12	1:A:273:GLN:HE22	0.40	1.76	11	1
1:A:236:TYR:HA	1:A:241:PHE:CD2	0.40	2.52	13	1
1:A:230:LEU:C	1:A:258:CYS:HG	0.40	2.24	15	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	134/176 (76%)	124±2 (92±2%)	7±2 (5±1%)	3±1 (2±1%)	6	43
All	All	2680/3520 (76%)	2477 (92%)	136 (5%)	67 (2%)	6	43

All 7 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	171	SER	20
1	A	209	ASN	17
1	A	196	ASP	15
1	A	268	VAL	8
1	A	210	CYS	3
1	A	285	PHE	3
1	A	234	ASP	1

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	115/152 (76%)	96±2 (83±2%)	19±2 (17±2%)	4	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2300/3040 (76%)	1916 (83%)	384 (17%)	4 39

All 54 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	158	LEU	20
1	A	178	PHE	20
1	A	213	LEU	20
1	A	256	ILE	20
1	A	275	ILE	20
1	A	286	THR	20
1	A	182	GLU	19
1	A	248	ILE	19
1	A	271	VAL	19
1	A	211	ILE	17
1	A	220	VAL	16
1	A	223	VAL	15
1	A	162	ILE	14
1	A	238	ASP	12
1	A	164	LEU	11
1	A	219	ILE	10
1	A	242	ASN	10
1	A	177	LEU	8
1	A	189	PHE	7
1	A	257	LEU	6
1	A	259	MET	6
1	A	297	LEU	5
1	A	203	LEU	5
1	A	273	GLN	5
1	A	217	LYS	4
1	A	169	LEU	4
1	A	291	LYS	4
1	A	244	GLU	3
1	A	233	LYS	3
1	A	302	GLU	3
1	A	199	GLU	3
1	A	214	GLU	3
1	A	288	LYS	3
1	A	187	ASP	3
1	A	174	ARG	3
1	A	205	GLU	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	258	CYS	2
1	A	277	LYS	2
1	A	179	LEU	2
1	A	186	LYS	2
1	A	193	ARG	1
1	A	261	ILE	1
1	A	161	LYS	1
1	A	192	SER	1
1	A	160	HIS	1
1	A	176	SER	1
1	A	293	PHE	1
1	A	212	ARG	1
1	A	188	LYS	1
1	A	196	ASP	1
1	A	230	LEU	1
1	A	234	ASP	1
1	A	240	ARG	1
1	A	190	LEU	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 oligosaccharides 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	Counts	Bond lengths	
						RMSZ	#Z>2
2	35G	A	1	-	26,26,26	4.02±0.01	13±0 (49±1%)

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	Counts	Bond angles	
						RMSZ	#Z>2
2	35G	A	1	-	39,41,41	2.89±0.01	16±1 (41±2%)

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	35G	A	1	-	-	0±0,4,31,31	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	1	35G	C6-N1	9.58	1.56	1.38	13	20
2	A	1	35G	P-O5'	9.29	1.68	1.57	15	20
2	A	1	35G	C4-N3	8.38	1.53	1.34	15	20
2	A	1	35G	C2-N3	6.46	1.48	1.33	6	20
2	A	1	35G	C2-N1	4.91	1.49	1.37	13	20
2	A	1	35G	P-O3'	4.80	1.65	1.57	14	20
2	A	1	35G	O4'-C4'	4.37	1.35	1.45	7	20
2	A	1	35G	C5'-C4'	4.15	1.58	1.51	4	20
2	A	1	35G	O3'-C3'	4.11	1.50	1.44	13	20
2	A	1	35G	C5-C4	3.62	1.48	1.38	17	20
2	A	1	35G	C5-C6	3.13	1.56	1.44	10	20
2	A	1	35G	C4-N9	2.48	1.31	1.38	4	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	1	35G	O5'-C5'	2.28	1.49	1.46	15	18

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
2	A	1	35G	C2-N3-C4	7.58	125.36	112.30	10	20
2	A	1	35G	O5'-P-O3'	7.36	95.85	105.70	15	20
2	A	1	35G	N1-C2-N3	6.19	112.00	123.32	10	20
2	A	1	35G	C6-C5-N7	5.87	140.97	130.29	10	20
2	A	1	35G	C6-C5-C4	4.76	111.67	118.83	10	20
2	A	1	35G	O2P-P-O1P	4.27	121.68	108.56	4	20
2	A	1	35G	N2-C2-N1	3.72	124.62	116.76	3	20
2	A	1	35G	C5-C6-N1	3.40	121.92	113.25	4	20
2	A	1	35G	O4'-C4'-C5'	3.08	121.69	112.38	15	20
2	A	1	35G	O3'-C3'-C2'	2.73	118.28	115.61	14	19
2	A	1	35G	C4'-O4'-C1'	2.63	103.65	109.47	9	20
2	A	1	35G	O6-C6-C5	2.51	119.92	126.53	20	20
2	A	1	35G	C5-C4-N3	2.44	124.50	128.39	11	20
2	A	1	35G	C1'-N9-C4	2.42	119.34	126.49	10	20
2	A	1	35G	O3'-C3'-C4'	2.30	108.97	110.71	7	17
2	A	1	35G	C4-C5-N7	2.09	107.35	110.67	10	16
2	A	1	35G	N9-C8-N7	2.06	109.58	113.40	4	6
2	A	1	35G	C8-N9-C4	2.02	109.80	106.03	7	1
2	A	1	35G	C2'-C3'-C4'	2.01	99.72	103.24	14	4

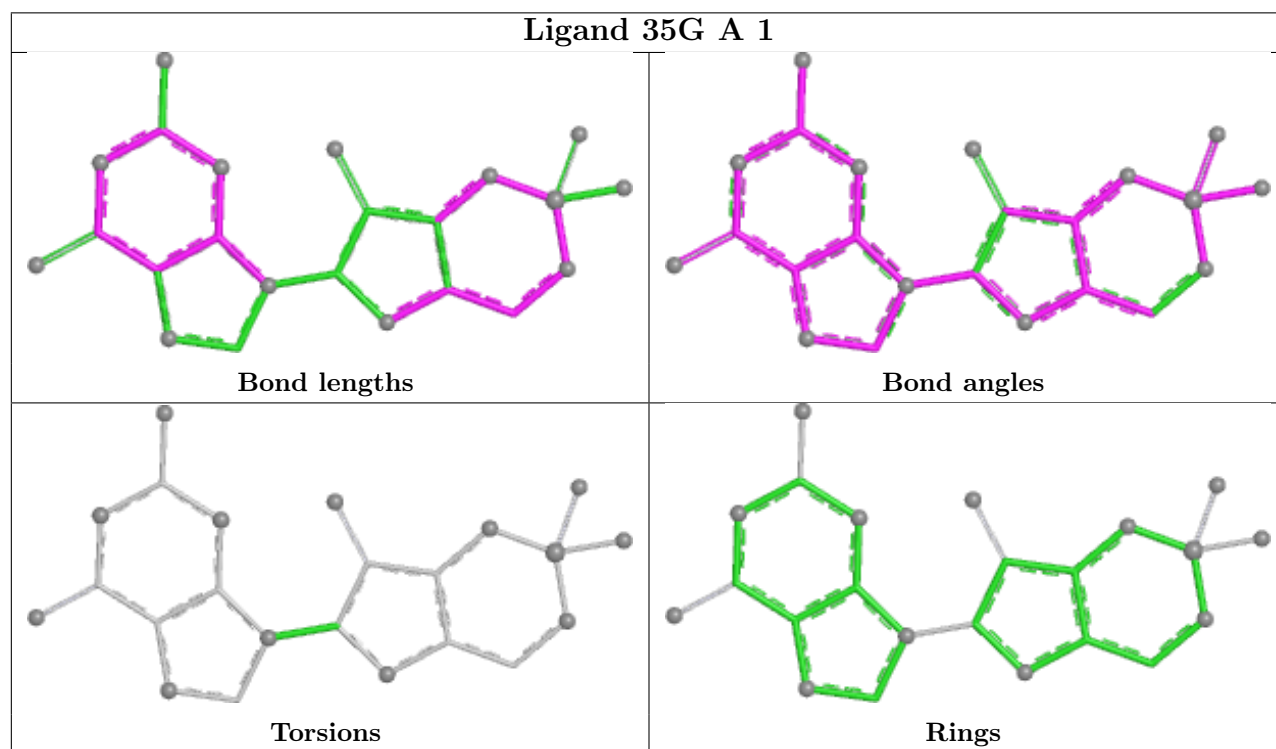
There are no chirality outliers.

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 than 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.



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 84% for the well-defined parts and 84% 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	1765
Number of shifts mapped to atoms	1675
Number of unparsed shifts	0
Number of shifts with mapping errors	90
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- No matching atom found in the structure. All 90 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	304	LEU	CA	53.8	0.5	1
1	A	304	LEU	CB	42.4	0.5	1
1	A	304	LEU	CD1	23.1	0.5	1
1	A	304	LEU	CD2	23.1	0.5	1
1	A	304	LEU	CG	24.7	0.5	1
1	A	305	HIS	H	8.09	0.05	1
1	A	305	HIS	HA	4.572	0.05	1
1	A	305	HIS	HB2	2.992	0.05	2
1	A	305	HIS	HB3	3.032	0.05	2
1	A	305	HIS	HD2	6.932	0.05	4
1	A	305	HIS	HE1	7.852	0.05	4
1	A	305	HIS	CA	56.3	0.5	1
1	A	305	HIS	CB	31.0	0.5	1
1	A	305	HIS	N	120.9	0.5	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	307	ALA	HA	4.272	0.05	1
1	A	307	ALA	HB1	1.532	0.05	1
1	A	307	ALA	HB2	1.532	0.05	1
1	A	307	ALA	HB3	1.532	0.05	1
1	A	307	ALA	C	178.7	0.5	1
1	A	307	ALA	CA	54.402	0.5	1
1	A	307	ALA	CB	19.3	0.5	1
1	A	308	GLN	H	7.99	0.05	1
1	A	308	GLN	HA	4.252	0.05	1
1	A	308	GLN	HB2	2.162	0.05	2
1	A	308	GLN	HB3	2.162	0.05	2
1	A	308	GLN	HG2	2.48	0.05	2
1	A	308	GLN	HG3	2.38	0.05	2
1	A	308	GLN	CA	57.651	0.5	1
1	A	308	GLN	CB	28.7	0.5	1
1	A	308	GLN	CG	34.0	0.5	1
1	A	308	GLN	N	117.384	0.5	1
1	A	309	LEU	H	7.88	0.05	1
1	A	309	LEU	HA	4.182	0.05	1
1	A	309	LEU	CA	55.0	0.5	1
1	A	309	LEU	CB	42.1	0.5	1
1	A	309	LEU	CD1	26.3	0.5	1
1	A	309	LEU	CD2	23.9	0.5	1
1	A	309	LEU	CG	27.2	0.5	1
1	A	309	LEU	N	120.125	0.5	1
1	A	310	TYR	CA	54.2	0.5	1
1	A	310	TYR	CB	38.2	0.5	1
1	A	311	GLU	C	177.8	0.5	1
1	A	311	GLU	CA	57.8	0.5	1
1	A	311	GLU	CB	30.1	0.5	1
1	A	311	GLU	N	117.6	0.5	1
1	A	312	THR	H	8.14	0.05	1
1	A	312	THR	HA	4.244	0.05	1
1	A	312	THR	HB	4.312	0.05	1
1	A	312	THR	HG21	1.27	0.05	1
1	A	312	THR	HG22	1.27	0.05	1
1	A	312	THR	HG23	1.27	0.05	1
1	A	312	THR	CA	63.874	0.5	1
1	A	312	THR	CB	69.5	0.5	1
1	A	312	THR	CG2	21.9	0.5	1
1	A	312	THR	N	113.933	0.5	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	313	SER	H	8.15	0.05	1
1	A	313	SER	HA	4.282	0.05	1
1	A	313	SER	HB2	3.952	0.05	2
1	A	313	SER	HB3	4.432	0.05	2
1	A	313	SER	HG	3.96	0.05	1
1	A	313	SER	C	175.2	0.5	1
1	A	313	SER	CA	59.947	0.5	1
1	A	313	SER	CB	63.5	0.5	1
1	A	313	SER	N	117.711	0.5	1
1	A	314	LEU	H	7.89	0.05	1
1	A	314	LEU	HA	4.262	0.05	1
1	A	314	LEU	CA	56.332	0.5	1
1	A	314	LEU	CB	41.698	0.5	1
1	A	314	LEU	CD1	25.2	0.5	1
1	A	314	LEU	CD2	23.6	0.5	1
1	A	314	LEU	CG	27.0	0.5	1
1	A	314	LEU	N	122.666	0.5	1
1	A	315	LEU	H	7.82	0.05	1
1	A	315	LEU	HA	4.262	0.05	1
1	A	315	LEU	HD11	0.922	0.05	2
1	A	315	LEU	HD12	0.922	0.05	2
1	A	315	LEU	HD13	0.922	0.05	2
1	A	315	LEU	HD21	0.852	0.05	2
1	A	315	LEU	HD22	0.852	0.05	2
1	A	315	LEU	HD23	0.852	0.05	2
1	A	315	LEU	CA	55.964	0.5	1
1	A	315	LEU	CB	41.851	0.5	1
1	A	315	LEU	CD1	25.3	0.5	1
1	A	315	LEU	CD2	23.8	0.5	1
1	A	315	LEU	CG	26.9	0.5	1
1	A	315	LEU	N	120.047	0.5	1
1	A	316	GLU	H	8.08	0.05	1
1	A	316	GLU	CA	57.169	0.5	1
1	A	316	GLU	CB	30.097	0.5	1
1	A	316	GLU	N	119.575	0.5	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, <i>ppm</i>	Suggested action
$^{13}\text{C}_\alpha$	161	-0.09 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	150	-0.11 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	124	0.10 ± 0.10	None needed (< 0.5 ppm)
^{15}N	150	0.75 ± 0.34	Should be applied

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 84%, i.e. 1545 atoms were assigned a chemical shift out of a possible 1829. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	644/677 (95%)	270/275 (98%)	245/270 (91%)	129/132 (98%)
Sidechain	843/982 (86%)	568/638 (89%)	275/312 (88%)	0/32 (0%)
Aromatic	58/170 (34%)	30/83 (36%)	27/78 (35%)	1/9 (11%)
Overall	1545/1829 (84%)	868/996 (87%)	547/660 (83%)	130/173 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1675 atoms were assigned a chemical shift out of a possible 1994. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	709/750 (95%)	298/306 (97%)	270/298 (91%)	141/146 (97%)
Sidechain	906/1066 (85%)	609/690 (88%)	297/339 (88%)	0/37 (0%)
Aromatic	60/178 (34%)	31/87 (36%)	28/80 (35%)	1/11 (9%)
Overall	1675/1994 (84%)	938/1083 (87%)	595/717 (83%)	142/194 (73%)

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, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
1	A	188	LYS	HB2	0.52	0.58 – 2.97	-5.3
1	A	188	LYS	HD2	0.55	0.58 – 2.64	-5.1
1	A	232	ILE	CG2	10.90	10.93 – 24.12	-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:

