



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 3, 2022 – 01:02 PM EST

PDB ID : 2JND  
Title : 3D NMR structure of ECD1 of mCRF-R2b in complex with Astressin  
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Deposited on : 2007-01-08

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

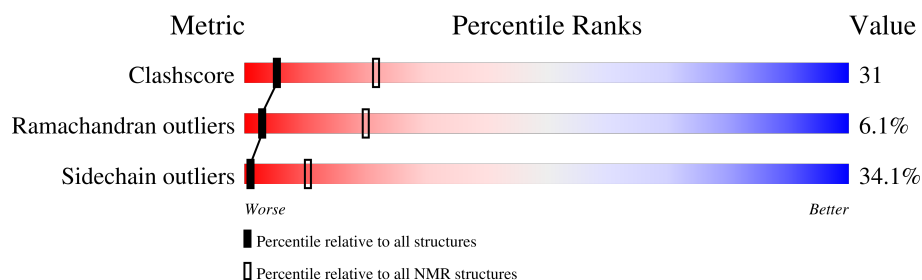
# 1 Overall quality at a glance

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  $\geq 3$ , 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	119	
2	B	31	

## 2 Ensemble composition and analysis

This entry contains 19 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*.

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:59-A:121, B:230-B:237, B:239-B:241 (74)	0.56	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 2 clusters and 4 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1471 atoms, of which 716 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Corticotropin-releasing factor receptor 2.

Mol	Chain	Residues	Atoms						Trace
1	A	79	Total	C	H	N	O	S	0
			1212	396	580	110	120	6	

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	cloning artifact	UNP Q60748
A	16	SER	-	cloning artifact	UNP Q60748
A	17	GLY	-	cloning artifact	UNP Q60748
A	18	MET	-	cloning artifact	UNP Q60748
A	19	LYS	-	cloning artifact	UNP Q60748
A	20	GLU	-	cloning artifact	UNP Q60748
A	21	THR	-	cloning artifact	UNP Q60748
A	22	ALA	-	cloning artifact	UNP Q60748
A	23	ALA	-	cloning artifact	UNP Q60748
A	24	ALA	-	cloning artifact	UNP Q60748
A	25	LYS	-	cloning artifact	UNP Q60748
A	26	PHE	-	cloning artifact	UNP Q60748
A	27	GLU	-	cloning artifact	UNP Q60748
A	28	ARG	-	cloning artifact	UNP Q60748
A	29	GLN	-	cloning artifact	UNP Q60748
A	30	HIS	-	cloning artifact	UNP Q60748
A	31	MET	-	cloning artifact	UNP Q60748
A	32	ASP	-	cloning artifact	UNP Q60748
A	33	SER	-	cloning artifact	UNP Q60748
A	34	PRO	-	cloning artifact	UNP Q60748
A	35	ASP	-	cloning artifact	UNP Q60748
A	36	LEU	-	cloning artifact	UNP Q60748
A	37	GLY	-	cloning artifact	UNP Q60748
A	38	THR	-	cloning artifact	UNP Q60748

- Molecule 2 is a protein called ASTRESSIN.

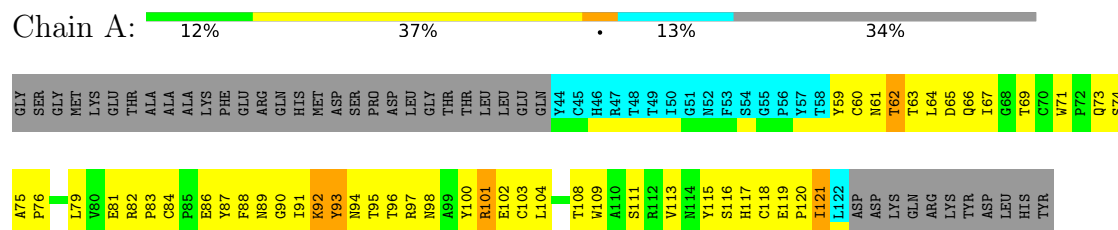
Mol	Chain	Residues	Atoms						Trace
2	B	15	Total	C	H	N	O		0
			259	79	136	24	20		

## 4 Residue-property plots [i](#)

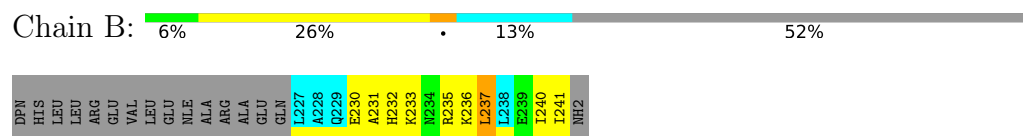
### 4.1 Average score per residue in the NMR ensemble

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: Corticotropin-releasing factor receptor 2



- Molecule 2: ASTRESSIN

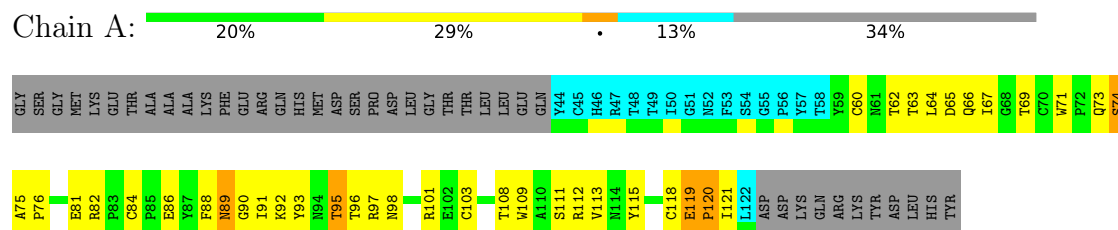


### 4.2 Scores per residue for each member of the ensemble

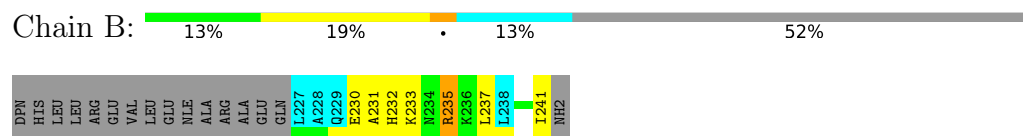
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Corticotropin-releasing factor receptor 2

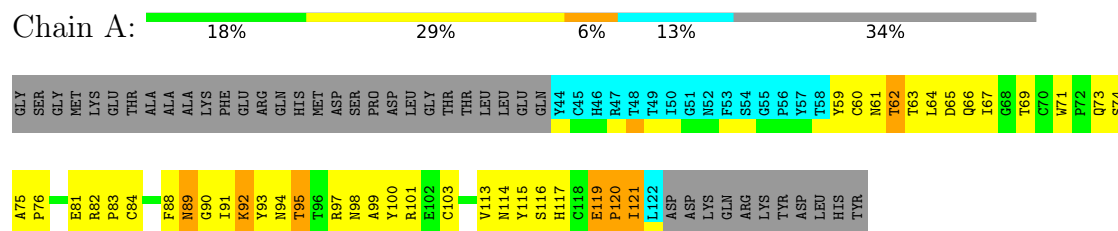


- Molecule 2: ASTRESSIN

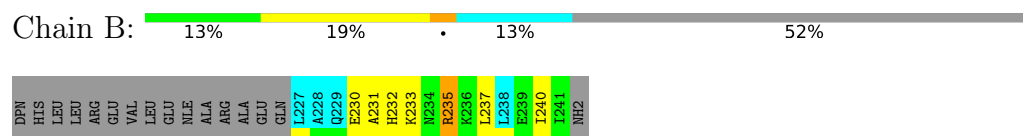


#### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Corticotropin-releasing factor receptor 2

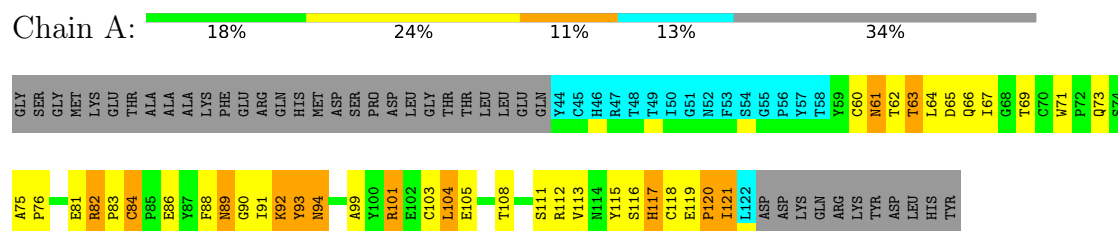


- Molecule 2: ASTRESSIN

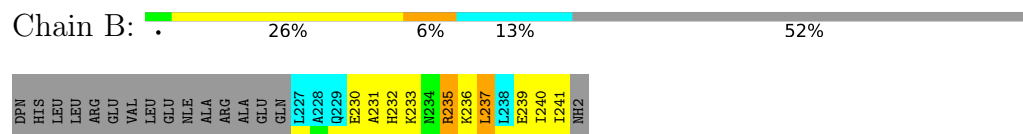


#### 4.2.3 Score per residue for model 3

- Molecule 1: Corticotropin-releasing factor receptor 2

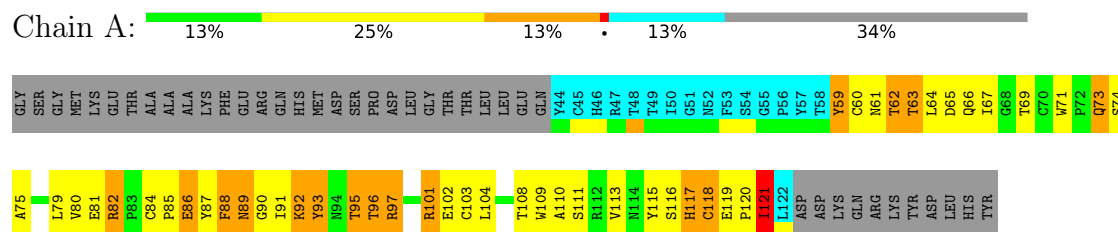


- Molecule 2: ASTRESSIN

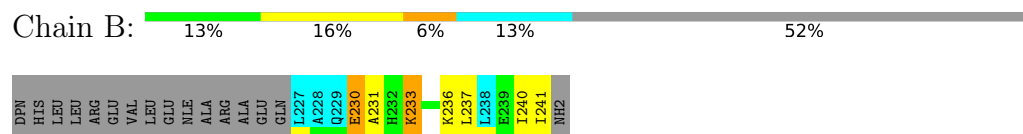


#### 4.2.4 Score per residue for model 4

- Molecule 1: Corticotropin-releasing factor receptor 2

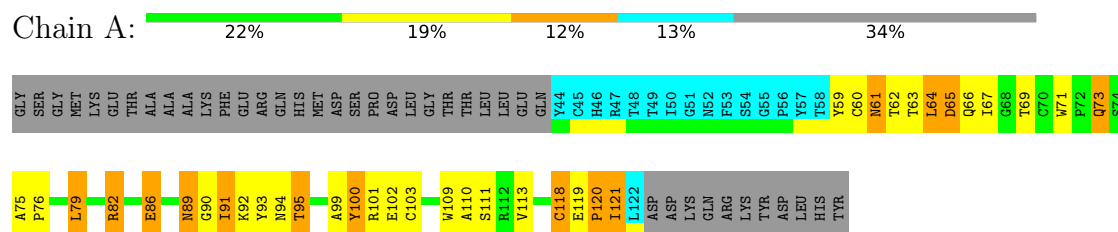


• Molecule 2: ASTRESSIN

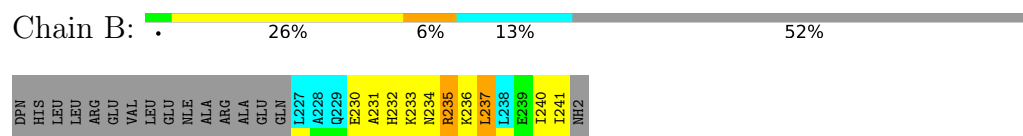


#### 4.2.5 Score per residue for model 5

• Molecule 1: Corticotropin-releasing factor receptor 2

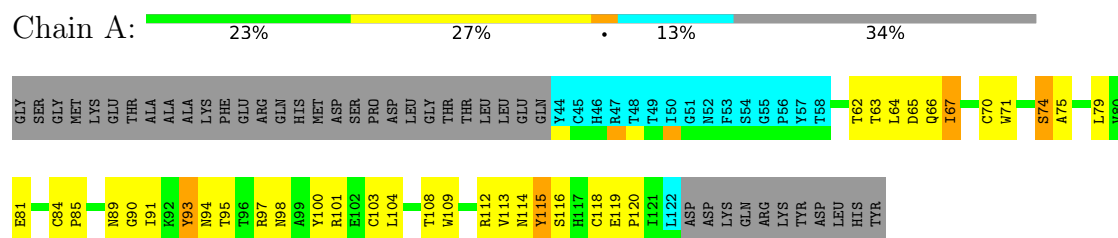


• Molecule 2: ASTRESSIN

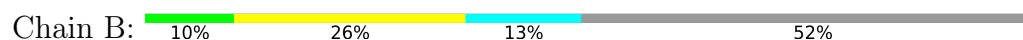


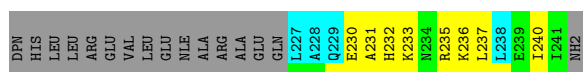
#### 4.2.6 Score per residue for model 6

• Molecule 1: Corticotropin-releasing factor receptor 2



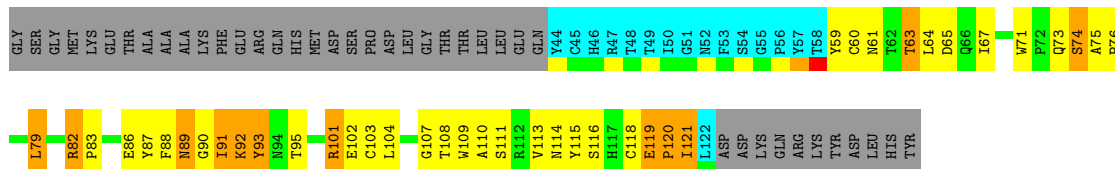
• Molecule 2: ASTRESSIN



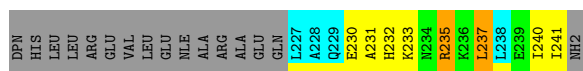
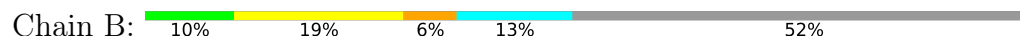


#### 4.2.7 Score per residue for model 7

- Molecule 1: Corticotropin-releasing factor receptor 2

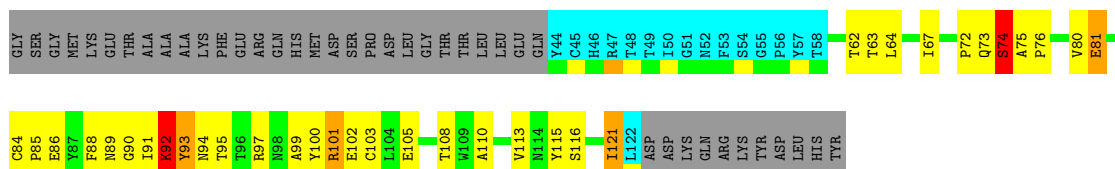


- Molecule 2: ASTRESSIN

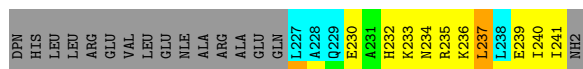
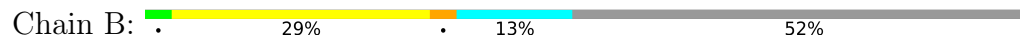


#### 4.2.8 Score per residue for model 8

- Molecule 1: Corticotropin-releasing factor receptor 2



- Molecule 2: ASTRESSIN

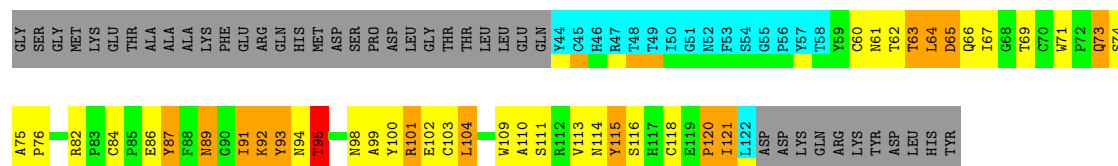


#### 4.2.9 Score per residue for model 9

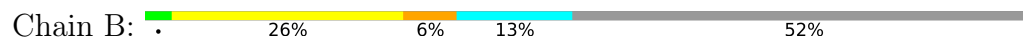
- Molecule 1: Corticotropin-releasing factor receptor 2







### • Molecule 2: ASTRESSIN

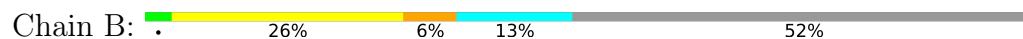


## 4.2.10 Score per residue for model 10

### • Molecule 1: Corticotropin-releasing factor receptor 2



### • Molecule 2: ASTRESSIN

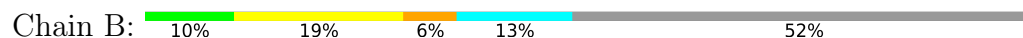


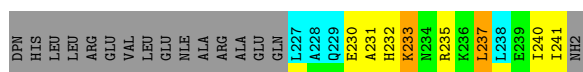
## 4.2.11 Score per residue for model 11

### • Molecule 1: Corticotropin-releasing factor receptor 2



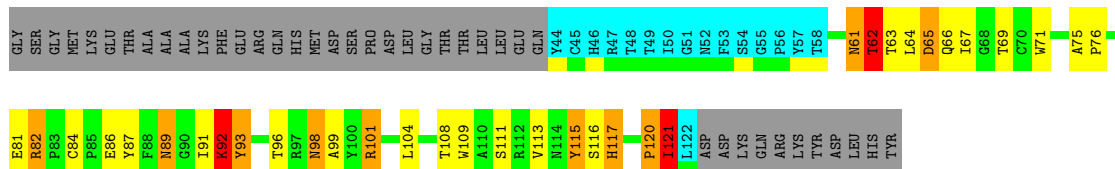
### • Molecule 2: ASTRESSIN



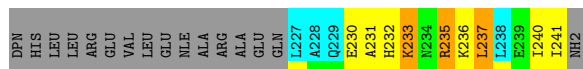
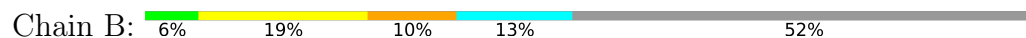


#### 4.2.12 Score per residue for model 12

- Molecule 1: Corticotropin-releasing factor receptor 2

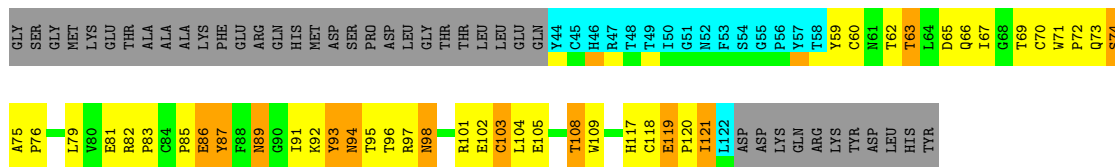


- Molecule 2: ASTRESSIN

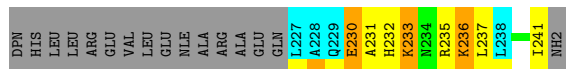
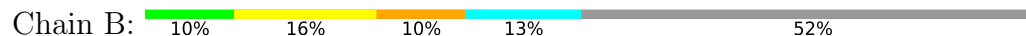


#### 4.2.13 Score per residue for model 13

- Molecule 1: Corticotropin-releasing factor receptor 2



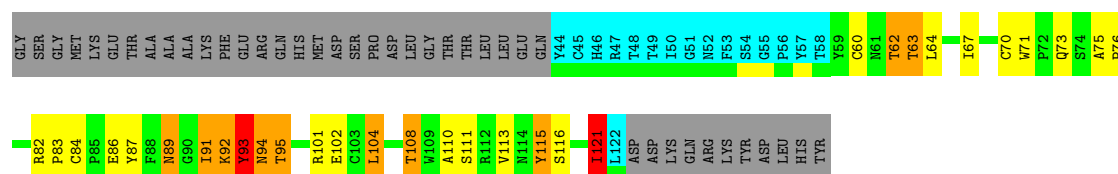
- Molecule 2: ASTRESSIN



#### 4.2.14 Score per residue for model 14

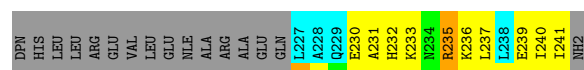
- Molecule 1: Corticotropin-releasing factor receptor 2





### • Molecule 2: ASTRESSIN

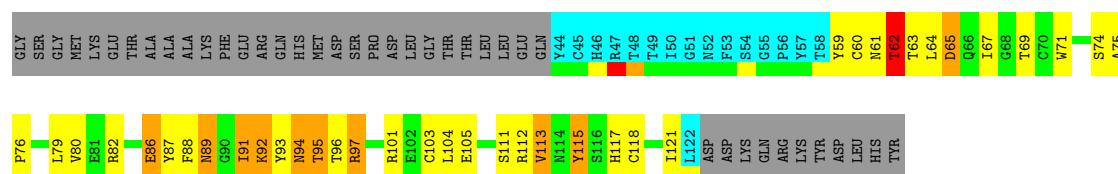
Chain B: 29% 13% 52%



## 4.2.15 Score per residue for model 15

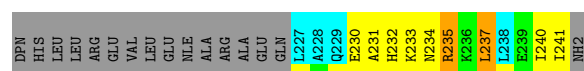
### • Molecule 1: Corticotropin-releasing factor receptor 2

Chain A: 21% 23% 8% 13% 34%



### • Molecule 2: ASTRESSIN

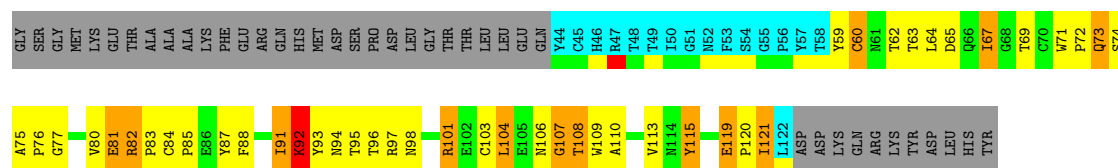
Chain B: 6% 23% 6% 13% 52%



## 4.2.16 Score per residue for model 16

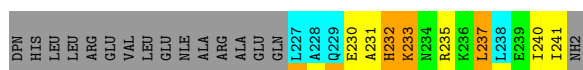
### • Molecule 1: Corticotropin-releasing factor receptor 2

Chain A: 16% 25% 11% 13% 34%



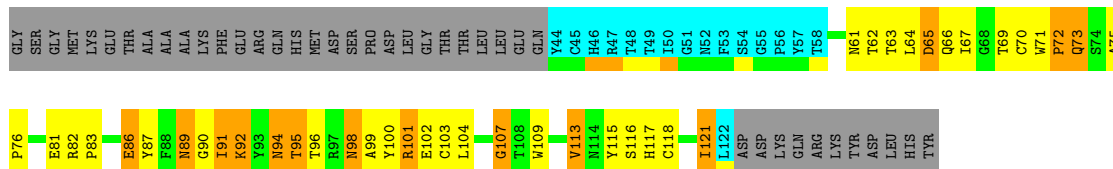
### • Molecule 2: ASTRESSIN

Chain B: 10% 16% 10% 13% 52%

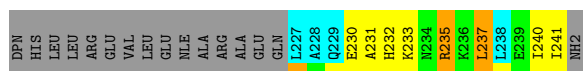
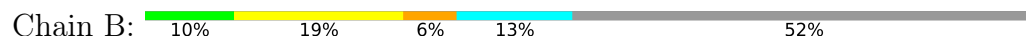


#### 4.2.17 Score per residue for model 17

- Molecule 1: Corticotropin-releasing factor receptor 2

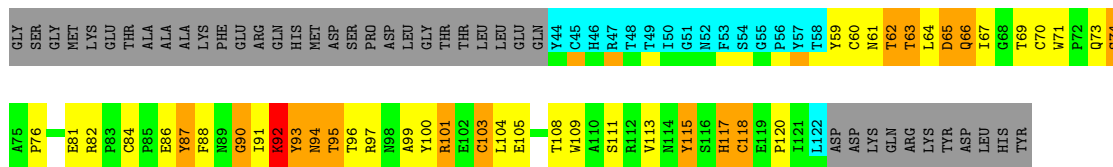


- Molecule 2: ASTRESSIN

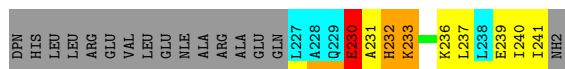
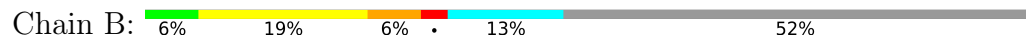


#### 4.2.18 Score per residue for model 18

- Molecule 1: Corticotropin-releasing factor receptor 2

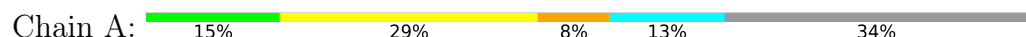


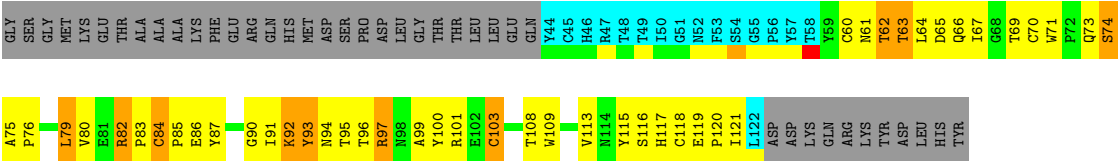
- Molecule 2: ASTRESSIN



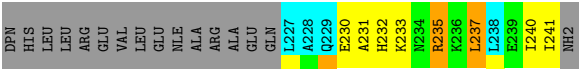
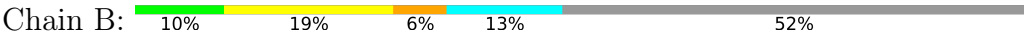
#### 4.2.19 Score per residue for model 19

- Molecule 1: Corticotropin-releasing factor receptor 2





● Molecule 2: ASTRESSIN



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 19 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	1.0.6
CNS	refinement	

No chemical shift data was provided.

## 6 Model quality

### 6.1 Standard geometry

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

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	504	461	460	31±7
2	B	93	101	102	11±3
All	All	11343	10678	10678	693

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:230:GLU:CD	2:B:233:LYS:HZ1	1.03	1.55	9	14
2:B:230:GLU:CD	2:B:233:LYS:HZ3	1.03	1.57	19	10
1:A:92:LYS:HA	1:A:121:ILE:HD12	0.99	1.29	12	6
1:A:91:ILE:HD13	2:B:231:ALA:HB2	0.98	1.34	1	3
2:B:237:LEU:HD13	2:B:240:ILE:HD12	0.93	1.36	12	11
2:B:230:GLU:CD	2:B:233:LYS:HZ2	0.93	1.67	17	11
2:B:230:GLU:CD	2:B:233:LYS:NZ	0.90	2.25	11	19
1:A:92:LYS:HE2	1:A:95:THR:HG22	0.89	1.40	14	1
1:A:75:ALA:HB1	1:A:76:PRO:HD2	0.86	1.48	17	16
1:A:92:LYS:CE	1:A:95:THR:HG22	0.84	2.02	14	1
1:A:82:ARG:O	1:A:99:ALA:HB3	0.82	1.75	5	2

*Continued on next page...*

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:LYS:HE3	1:A:95:THR:HG23	0.81	1.50	2	3
1:A:91:ILE:HG21	2:B:231:ALA:HB2	0.79	1.51	19	13
1:A:91:ILE:HD13	2:B:231:ALA:CB	0.79	2.08	1	2
1:A:84:CYS:HB3	1:A:99:ALA:HB2	0.79	1.55	9	2
1:A:63:THR:HG22	1:A:71:TRP:HB2	0.78	1.54	14	5
1:A:65:ASP:OD1	2:B:241:ILE:HG23	0.78	1.78	10	3
2:B:237:LEU:CD1	2:B:240:ILE:HD12	0.78	2.09	12	7
1:A:91:ILE:HG21	2:B:231:ALA:CB	0.77	2.09	15	8
1:A:67:ILE:HG13	2:B:241:ILE:HD11	0.77	1.57	5	12
1:A:91:ILE:HG12	2:B:231:ALA:HB2	0.75	1.57	10	2
1:A:101:ARG:HD2	1:A:113:VAL:HG22	0.74	1.59	4	1
1:A:91:ILE:HD11	2:B:230:GLU:HB3	0.74	1.59	9	1
2:B:237:LEU:HD12	2:B:240:ILE:HD12	0.74	1.56	14	6
1:A:84:CYS:SG	1:A:86:GLU:HG3	0.73	2.24	1	1
1:A:91:ILE:HG23	1:A:92:LYS:HG3	0.72	1.62	4	1
1:A:63:THR:HG21	1:A:109:TRP:CD1	0.72	2.20	10	2
1:A:91:ILE:HG13	2:B:231:ALA:HB2	0.71	1.62	5	2
1:A:101:ARG:HD3	1:A:113:VAL:HG22	0.67	1.66	14	1
1:A:115:TYR:CE2	2:B:239:GLU:HA	0.67	2.25	10	2
2:B:237:LEU:HD12	2:B:240:ILE:CD1	0.66	2.20	10	1
2:B:237:LEU:HA	2:B:240:ILE:HD12	0.66	1.67	10	1
1:A:71:TRP:CH2	1:A:101:ARG:HG2	0.65	2.27	3	1
1:A:62:THR:HG22	1:A:72:PRO:HA	0.65	1.67	17	3
1:A:92:LYS:CE	1:A:95:THR:HG23	0.65	2.21	13	3
1:A:101:ARG:CG	1:A:113:VAL:HG13	0.64	2.23	14	3
1:A:91:ILE:HG23	1:A:92:LYS:N	0.64	2.08	14	1
1:A:71:TRP:CE2	1:A:101:ARG:HD2	0.64	2.28	19	1
1:A:65:ASP:HB2	1:A:69:THR:HB	0.63	1.70	18	8
1:A:101:ARG:HG3	1:A:113:VAL:HG13	0.63	1.68	7	3
1:A:101:ARG:HG2	1:A:113:VAL:HG13	0.62	1.70	14	1
1:A:101:ARG:HD3	1:A:113:VAL:HG11	0.62	1.69	17	1
1:A:92:LYS:HG2	1:A:95:THR:HG23	0.62	1.69	17	1
1:A:67:ILE:HG23	1:A:88:PHE:CE2	0.62	2.29	11	2
1:A:121:ILE:N	1:A:121:ILE:HD13	0.62	2.10	12	2
1:A:101:ARG:HD2	1:A:113:VAL:CG1	0.62	2.25	18	1
1:A:92:LYS:NZ	1:A:119:GLU:O	0.62	2.29	1	3
1:A:91:ILE:CG1	2:B:231:ALA:HB2	0.61	2.25	10	2
1:A:67:ILE:CG1	2:B:241:ILE:HD11	0.61	2.25	14	8
1:A:92:LYS:HE3	1:A:95:THR:CG2	0.61	2.25	15	2
1:A:71:TRP:CZ3	1:A:80:VAL:HG13	0.60	2.30	4	1
2:B:230:GLU:HA	2:B:233:LYS:HZ3	0.60	1.55	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:TYR:N	1:A:87:TYR:CD1	0.59	2.70	18	7
1:A:71:TRP:CZ2	1:A:101:ARG:NE	0.59	2.70	18	1
1:A:92:LYS:HE2	1:A:95:THR:HG23	0.59	1.71	1	1
1:A:71:TRP:CZ2	1:A:101:ARG:HD3	0.59	2.32	1	7
2:B:235:ARG:N	2:B:235:ARG:HD3	0.59	2.12	1	1
1:A:101:ARG:N	1:A:101:ARG:HD3	0.59	2.13	18	1
1:A:67:ILE:CG1	2:B:237:LEU:HD12	0.59	2.28	19	1
1:A:113:VAL:HB	1:A:115:TYR:CE1	0.59	2.33	7	4
1:A:74:SER:OG	1:A:80:VAL:HG21	0.58	1.97	8	4
1:A:101:ARG:HG3	1:A:113:VAL:HG22	0.58	1.74	9	1
1:A:93:TYR:HD1	1:A:121:ILE:HG21	0.58	1.59	19	1
1:A:121:ILE:H	1:A:121:ILE:HD13	0.58	1.58	3	6
1:A:86:GLU:HB2	1:A:118:CYS:SG	0.57	2.39	4	2
1:A:93:TYR:CD1	1:A:93:TYR:N	0.57	2.72	9	8
1:A:81:GLU:HB2	1:A:98:ASN:ND2	0.57	2.14	6	2
1:A:67:ILE:HG12	2:B:237:LEU:HD22	0.57	1.75	11	1
1:A:71:TRP:CZ2	1:A:101:ARG:HG3	0.57	2.35	17	1
1:A:86:GLU:HG2	1:A:92:LYS:NZ	0.57	2.14	12	1
1:A:101:ARG:NH1	1:A:113:VAL:HG11	0.57	2.15	18	1
1:A:99:ALA:HB1	1:A:113:VAL:HG12	0.57	1.76	3	1
1:A:86:GLU:HG3	1:A:118:CYS:HB3	0.57	1.76	4	1
1:A:101:ARG:HD3	1:A:109:TRP:CE3	0.56	2.34	19	1
1:A:92:LYS:HD3	1:A:120:PRO:HA	0.56	1.76	18	1
1:A:61:ASN:HA	1:A:73:GLN:HA	0.56	1.77	10	4
1:A:90:GLY:O	1:A:91:ILE:HD13	0.56	2.00	2	1
1:A:101:ARG:HB3	1:A:113:VAL:HG13	0.56	1.78	3	1
1:A:86:GLU:HG2	1:A:118:CYS:SG	0.56	2.41	5	1
1:A:92:LYS:NZ	1:A:95:THR:HG23	0.56	2.16	13	1
1:A:92:LYS:N	1:A:92:LYS:HD2	0.56	2.15	12	1
1:A:92:LYS:CD	1:A:95:THR:HG22	0.56	2.31	7	1
1:A:93:TYR:CD1	1:A:121:ILE:HG21	0.56	2.36	19	1
1:A:102:GLU:O	1:A:110:ALA:HB2	0.56	2.01	8	1
1:A:61:ASN:HA	1:A:73:GLN:CG	0.55	2.31	18	2
1:A:101:ARG:HD3	1:A:113:VAL:CG1	0.55	2.30	17	1
1:A:101:ARG:NH1	1:A:110:ALA:O	0.55	2.40	14	4
1:A:79:LEU:HD21	1:A:100:TYR:HB3	0.55	1.77	10	1
1:A:93:TYR:CD2	1:A:121:ILE:HD11	0.55	2.37	16	1
1:A:92:LYS:HE3	1:A:120:PRO:HA	0.55	1.78	9	1
1:A:93:TYR:CD2	1:A:120:PRO:HB3	0.55	2.36	10	1
1:A:91:ILE:O	1:A:92:LYS:HB3	0.55	2.02	11	1
1:A:67:ILE:HG12	2:B:237:LEU:HG	0.55	1.79	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:ASN:O	1:A:117:HIS:NE2	0.55	2.34	17	2
1:A:119:GLU:HB2	1:A:120:PRO:HD2	0.54	1.79	2	4
1:A:118:CYS:O	2:B:235:ARG:NH1	0.54	2.40	3	1
1:A:101:ARG:HG2	1:A:113:VAL:HG11	0.54	1.78	17	1
1:A:113:VAL:HG21	2:B:241:ILE:HG22	0.54	1.77	10	1
1:A:71:TRP:CE2	1:A:101:ARG:HD3	0.54	2.38	15	6
1:A:82:ARG:HD3	1:A:83:PRO:HD2	0.54	1.80	2	1
1:A:92:LYS:CG	1:A:120:PRO:HB3	0.54	2.33	4	1
1:A:67:ILE:HG22	1:A:67:ILE:O	0.54	2.03	2	5
1:A:121:ILE:O	1:A:121:ILE:HG23	0.54	2.02	7	2
1:A:119:GLU:HB2	1:A:120:PRO:CD	0.54	2.33	19	2
1:A:92:LYS:HA	1:A:121:ILE:HB	0.54	1.80	1	1
1:A:62:THR:HA	1:A:71:TRP:O	0.54	2.03	11	10
1:A:120:PRO:HB3	2:B:235:ARG:NH2	0.54	2.18	12	2
1:A:92:LYS:O	1:A:121:ILE:HD12	0.53	2.03	3	1
1:A:92:LYS:HD2	1:A:120:PRO:HA	0.53	1.81	19	1
1:A:101:ARG:HD2	1:A:113:VAL:CG2	0.53	2.31	4	1
1:A:71:TRP:HB3	1:A:109:TRP:CH2	0.53	2.38	9	7
1:A:87:TYR:CE1	1:A:92:LYS:HB3	0.53	2.38	19	2
1:A:92:LYS:C	1:A:93:TYR:CD1	0.53	2.82	15	4
1:A:92:LYS:HD2	1:A:95:THR:HG22	0.53	1.79	7	1
1:A:101:ARG:CD	1:A:113:VAL:HG11	0.53	2.34	17	1
1:A:87:TYR:CD1	1:A:92:LYS:HB2	0.52	2.38	16	2
1:A:92:LYS:CE	1:A:120:PRO:HA	0.52	2.34	9	1
1:A:67:ILE:CG1	2:B:237:LEU:HG	0.52	2.33	6	1
1:A:120:PRO:HB2	1:A:121:ILE:HD13	0.52	1.81	12	1
1:A:121:ILE:N	1:A:121:ILE:CD1	0.52	2.72	12	1
1:A:113:VAL:HB	1:A:115:TYR:CD2	0.52	2.38	6	5
1:A:101:ARG:NH2	1:A:109:TRP:HB3	0.52	2.20	16	2
1:A:101:ARG:HD2	1:A:113:VAL:HG13	0.52	1.82	4	1
2:B:230:GLU:HA	2:B:233:LYS:NZ	0.52	2.19	9	2
1:A:121:ILE:O	1:A:121:ILE:HG12	0.51	2.06	2	2
1:A:101:ARG:HB2	1:A:113:VAL:HG13	0.51	1.82	15	2
1:A:91:ILE:O	1:A:92:LYS:HB2	0.51	2.05	9	3
1:A:74:SER:OG	1:A:75:ALA:N	0.51	2.44	6	3
1:A:87:TYR:CD1	1:A:92:LYS:CB	0.51	2.94	9	1
1:A:71:TRP:CH2	1:A:82:ARG:HD2	0.51	2.41	12	1
1:A:86:GLU:CB	1:A:92:LYS:HE2	0.51	2.36	13	1
1:A:101:ARG:CG	1:A:113:VAL:HG11	0.51	2.36	17	1
1:A:65:ASP:CG	2:B:241:ILE:HG23	0.51	2.25	9	2
1:A:63:THR:OG1	1:A:109:TRP:NE1	0.51	2.43	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ASN:HA	1:A:73:GLN:HG2	0.51	1.82	17	3
1:A:119:GLU:HA	2:B:235:ARG:NH1	0.51	2.21	2	1
1:A:75:ALA:HB1	1:A:76:PRO:CD	0.51	2.30	17	3
1:A:65:ASP:CB	1:A:69:THR:HB	0.51	2.35	18	1
1:A:86:GLU:HG3	1:A:118:CYS:SG	0.50	2.46	15	1
1:A:91:ILE:CG2	1:A:92:LYS:N	0.50	2.75	9	2
1:A:92:LYS:HD2	1:A:95:THR:HG23	0.50	1.83	9	1
1:A:97:ARG:HB2	1:A:117:HIS:HB3	0.50	1.83	15	1
2:B:241:ILE:N	2:B:241:ILE:HD13	0.50	2.20	10	2
1:A:97:ARG:CZ	1:A:119:GLU:HG3	0.50	2.37	19	1
1:A:67:ILE:HD12	2:B:241:ILE:CG1	0.50	2.37	19	3
1:A:63:THR:O	1:A:71:TRP:N	0.50	2.44	7	4
1:A:89:ASN:HD21	1:A:91:ILE:HD13	0.50	1.67	15	1
1:A:74:SER:HB3	1:A:103:CYS:SG	0.50	2.46	4	1
1:A:92:LYS:HE2	2:B:231:ALA:HB1	0.50	1.82	4	1
1:A:61:ASN:O	1:A:62:THR:C	0.50	2.51	10	4
1:A:67:ILE:HG21	1:A:85:PRO:HB2	0.49	1.84	8	1
1:A:101:ARG:O	1:A:101:ARG:HG3	0.49	2.07	3	1
1:A:86:GLU:HG2	1:A:92:LYS:HB2	0.49	1.83	7	1
1:A:101:ARG:NH2	1:A:102:GLU:O	0.49	2.42	7	1
1:A:104:LEU:HD12	1:A:108:THR:HB	0.49	1.83	16	1
1:A:71:TRP:CH2	1:A:101:ARG:HG3	0.49	2.42	17	1
1:A:97:ARG:HG2	1:A:117:HIS:CD2	0.49	2.42	4	1
2:B:230:GLU:HA	2:B:233:LYS:HD3	0.49	1.85	7	1
1:A:59:TYR:N	1:A:59:TYR:CD1	0.49	2.80	4	1
1:A:69:THR:HG21	1:A:71:TRP:CZ2	0.49	2.42	17	1
1:A:79:LEU:HD21	1:A:100:TYR:CD2	0.49	2.43	19	1
1:A:89:ASN:ND2	1:A:91:ILE:HD13	0.49	2.22	15	1
1:A:113:VAL:CG1	2:B:241:ILE:HG22	0.49	2.38	1	1
1:A:88:PHE:CE2	2:B:237:LEU:HD23	0.49	2.42	2	2
1:A:115:TYR:OH	2:B:241:ILE:HB	0.49	2.07	3	1
1:A:80:VAL:HG12	1:A:101:ARG:HB3	0.49	1.84	4	1
1:A:113:VAL:HB	1:A:115:TYR:CE2	0.49	2.42	15	4
1:A:67:ILE:HD11	2:B:237:LEU:C	0.49	2.28	19	1
1:A:101:ARG:NH2	2:B:241:ILE:O	0.49	2.43	9	1
1:A:87:TYR:CE1	1:A:92:LYS:CB	0.49	2.96	19	1
1:A:101:ARG:HD3	1:A:113:VAL:HG21	0.48	1.86	17	1
1:A:96:THR:HG23	1:A:97:ARG:HG2	0.48	1.84	18	1
1:A:86:GLU:OE2	1:A:92:LYS:HE3	0.48	2.08	8	1
1:A:92:LYS:HA	1:A:121:ILE:CD1	0.48	2.19	12	3
1:A:93:TYR:O	1:A:94:ASN:HB2	0.48	2.07	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:ARG:O	1:A:99:ALA:N	0.48	2.42	17	1
1:A:71:TRP:CH2	1:A:82:ARG:CD	0.48	2.97	18	1
1:A:67:ILE:HG21	1:A:85:PRO:HG2	0.48	1.85	13	2
1:A:67:ILE:HD11	2:B:237:LEU:O	0.48	2.09	19	1
1:A:71:TRP:CH2	1:A:82:ARG:HB2	0.48	2.44	13	2
1:A:95:THR:N	1:A:119:GLU:O	0.47	2.44	4	1
1:A:62:THR:HA	1:A:72:PRO:HA	0.47	1.85	16	1
1:A:67:ILE:HG21	1:A:85:PRO:HG3	0.47	1.84	16	1
1:A:113:VAL:HG12	1:A:113:VAL:O	0.47	2.10	3	1
1:A:79:LEU:HD23	1:A:102:GLU:HB2	0.47	1.85	11	1
1:A:96:THR:O	1:A:97:ARG:HD3	0.47	2.09	4	1
1:A:118:CYS:O	2:B:235:ARG:NH2	0.47	2.45	17	1
1:A:71:TRP:CH2	1:A:82:ARG:HB3	0.47	2.44	18	1
1:A:71:TRP:CZ3	1:A:82:ARG:HB2	0.47	2.44	19	4
1:A:91:ILE:CG2	2:B:231:ALA:HB2	0.47	2.35	15	3
1:A:91:ILE:CD1	2:B:231:ALA:HB2	0.47	2.24	1	1
1:A:100:TYR:HB2	1:A:114:ASN:HB2	0.47	1.85	9	2
1:A:82:ARG:HG3	1:A:83:PRO:HD2	0.47	1.86	7	4
1:A:86:GLU:CG	1:A:118:CYS:SG	0.47	3.03	5	1
1:A:87:TYR:CE1	1:A:92:LYS:HE2	0.47	2.44	11	1
1:A:60:CYS:N	1:A:74:SER:O	0.47	2.43	13	1
1:A:92:LYS:O	1:A:121:ILE:HD13	0.47	2.10	14	1
1:A:66:GLN:HG2	2:B:240:ILE:CG2	0.47	2.40	18	1
1:A:101:ARG:N	1:A:101:ARG:CD	0.47	2.78	18	1
1:A:92:LYS:C	1:A:93:TYR:CG	0.47	2.89	3	1
1:A:91:ILE:CB	2:B:231:ALA:HB2	0.47	2.39	6	1
1:A:76:PRO:HB2	1:A:105:GLU:HA	0.47	1.87	13	1
1:A:66:GLN:HG2	2:B:240:ILE:HG21	0.47	1.87	9	2
1:A:86:GLU:HG3	1:A:118:CYS:CB	0.47	2.40	4	1
1:A:86:GLU:CG	1:A:92:LYS:HB2	0.47	2.39	7	1
1:A:86:GLU:HG2	2:B:235:ARG:HG3	0.47	1.86	8	1
1:A:66:GLN:HB3	2:B:241:ILE:CD1	0.47	2.40	10	1
1:A:59:TYR:O	1:A:107:GLY:HA2	0.47	2.10	16	1
2:B:236:LYS:C	2:B:236:LYS:CD	0.46	2.83	13	1
1:A:79:LEU:HA	1:A:102:GLU:HA	0.46	1.85	4	1
1:A:71:TRP:HZ2	1:A:101:ARG:CZ	0.46	2.23	18	1
1:A:91:ILE:HD13	1:A:91:ILE:N	0.46	2.25	19	1
1:A:60:CYS:HB2	1:A:75:ALA:N	0.46	2.25	7	1
1:A:71:TRP:CH2	1:A:101:ARG:HB2	0.46	2.45	13	3
1:A:91:ILE:C	1:A:92:LYS:HD2	0.46	2.30	12	1
1:A:83:PRO:HA	1:A:98:ASN:HA	0.46	1.88	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:GLU:CG	2:B:235:ARG:HD2	0.46	2.40	17	1
1:A:60:CYS:HB3	1:A:109:TRP:CE2	0.46	2.45	4	1
1:A:97:ARG:NH2	1:A:119:GLU:OE2	0.46	2.37	6	1
1:A:67:ILE:CG1	2:B:237:LEU:HD22	0.46	2.39	11	1
1:A:92:LYS:HG2	1:A:93:TYR:N	0.46	2.25	12	1
2:B:230:GLU:CG	2:B:233:LYS:HZ2	0.46	2.23	18	1
1:A:67:ILE:CG2	1:A:85:PRO:HG3	0.46	2.40	6	1
1:A:97:ARG:HD2	1:A:117:HIS:CD2	0.46	2.45	13	1
1:A:104:LEU:N	1:A:108:THR:O	0.46	2.49	13	4
1:A:60:CYS:O	1:A:74:SER:N	0.46	2.39	1	4
1:A:118:CYS:O	2:B:235:ARG:HD3	0.46	2.11	6	2
1:A:86:GLU:CG	2:B:235:ARG:NH2	0.46	2.79	14	1
1:A:91:ILE:N	1:A:91:ILE:HD12	0.46	2.26	18	1
2:B:230:GLU:O	2:B:233:LYS:HG2	0.46	2.11	14	3
1:A:67:ILE:HG21	1:A:85:PRO:CG	0.46	2.40	4	1
1:A:92:LYS:HD2	1:A:95:THR:CG2	0.46	2.41	7	1
1:A:79:LEU:C	1:A:79:LEU:HD13	0.46	2.31	11	1
1:A:87:TYR:HB3	1:A:91:ILE:HB	0.46	1.88	16	1
1:A:103:CYS:SG	1:A:109:TRP:CD2	0.46	3.09	16	1
1:A:60:CYS:O	1:A:73:GLN:HG2	0.45	2.12	3	1
1:A:104:LEU:HB2	1:A:108:THR:O	0.45	2.10	3	2
1:A:86:GLU:HG2	1:A:92:LYS:HE2	0.45	1.88	13	1
1:A:69:THR:HG22	1:A:71:TRP:NE1	0.45	2.26	16	1
1:A:100:TYR:O	1:A:113:VAL:HG12	0.45	2.10	17	1
1:A:63:THR:HB	1:A:71:TRP:HB2	0.45	1.88	12	2
1:A:101:ARG:HD3	1:A:113:VAL:CG2	0.45	2.41	17	1
1:A:60:CYS:O	1:A:73:GLN:HA	0.45	2.12	4	1
1:A:67:ILE:HG12	2:B:237:LEU:HD12	0.45	1.87	19	2
1:A:79:LEU:HD11	1:A:100:TYR:CD2	0.45	2.46	5	1
1:A:93:TYR:H	1:A:121:ILE:HD13	0.45	1.70	7	1
1:A:88:PHE:HB2	2:B:234:ASN:ND2	0.45	2.27	15	1
1:A:71:TRP:CZ3	1:A:82:ARG:HD2	0.45	2.46	18	1
1:A:91:ILE:HG22	1:A:91:ILE:O	0.45	2.11	6	1
1:A:81:GLU:HG2	1:A:100:TYR:CD2	0.45	2.47	18	1
1:A:113:VAL:HG11	1:A:115:TYR:CE1	0.45	2.47	2	1
1:A:82:ARG:HB2	1:A:83:PRO:HD2	0.45	1.88	11	1
1:A:93:TYR:CE2	1:A:121:ILE:HG13	0.45	2.45	9	1
1:A:86:GLU:CD	2:B:235:ARG:NE	0.45	2.70	15	1
1:A:67:ILE:HB	2:B:241:ILE:HD11	0.45	1.89	16	1
1:A:74:SER:HB2	1:A:109:TRP:CZ2	0.45	2.47	19	1
1:A:92:LYS:O	1:A:121:ILE:HG21	0.45	2.12	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:PHE:CZ	2:B:234:ASN:HA	0.45	2.46	8	1
1:A:101:ARG:NH1	1:A:111:SER:O	0.45	2.46	9	1
1:A:88:PHE:HB3	2:B:234:ASN:ND2	0.44	2.27	10	1
1:A:92:LYS:HG3	1:A:120:PRO:O	0.44	2.13	5	1
1:A:87:TYR:CD1	1:A:92:LYS:CE	0.44	3.00	12	1
1:A:91:ILE:HG22	1:A:92:LYS:H	0.44	1.73	3	1
1:A:94:ASN:N	1:A:121:ILE:HG23	0.44	2.27	10	1
1:A:93:TYR:O	1:A:94:ASN:C	0.44	2.55	10	1
1:A:88:PHE:CE2	2:B:237:LEU:HD13	0.44	2.47	11	1
1:A:118:CYS:O	2:B:235:ARG:HD2	0.44	2.13	7	1
1:A:101:ARG:HH11	1:A:113:VAL:HG11	0.44	1.71	18	1
1:A:117:HIS:O	1:A:118:CYS:CB	0.44	2.65	18	1
1:A:71:TRP:HB3	1:A:109:TRP:CZ2	0.44	2.48	9	2
1:A:101:ARG:HH11	1:A:113:VAL:HG22	0.44	1.71	2	1
1:A:118:CYS:HB3	2:B:235:ARG:NH2	0.44	2.28	10	1
1:A:81:GLU:HA	1:A:99:ALA:O	0.44	2.12	12	1
1:A:71:TRP:CD2	1:A:101:ARG:HD2	0.44	2.48	19	1
1:A:101:ARG:NH1	1:A:113:VAL:HG22	0.44	2.28	2	1
1:A:84:CYS:O	1:A:86:GLU:N	0.44	2.50	12	3
1:A:76:PRO:HA	1:A:103:CYS:HB3	0.44	1.90	18	2
1:A:67:ILE:HG13	2:B:237:LEU:HD12	0.44	1.88	19	1
1:A:101:ARG:NH2	1:A:110:ALA:O	0.44	2.49	5	1
1:A:86:GLU:HG2	2:B:235:ARG:CZ	0.44	2.43	14	1
1:A:101:ARG:CZ	2:B:241:ILE:HG21	0.44	2.43	17	1
1:A:67:ILE:HG13	2:B:237:LEU:HG	0.43	1.89	6	1
2:B:237:LEU:CD2	2:B:240:ILE:HD12	0.43	2.42	11	1
1:A:86:GLU:HG3	2:B:235:ARG:NE	0.43	2.28	12	1
1:A:71:TRP:CZ2	1:A:101:ARG:HB2	0.43	2.48	13	1
1:A:60:CYS:HB3	1:A:74:SER:OG	0.43	2.13	7	1
1:A:59:TYR:O	1:A:60:CYS:HB2	0.43	2.14	15	1
1:A:101:ARG:HD2	1:A:113:VAL:HG11	0.43	1.89	18	1
1:A:92:LYS:O	1:A:93:TYR:CD2	0.43	2.71	3	1
1:A:115:TYR:CZ	2:B:241:ILE:HB	0.43	2.49	3	1
1:A:67:ILE:O	1:A:67:ILE:HG22	0.43	2.13	5	1
1:A:65:ASP:HB2	2:B:241:ILE:HG23	0.43	1.89	16	1
1:A:121:ILE:HD13	1:A:121:ILE:N	0.43	2.28	3	1
1:A:92:LYS:HG2	1:A:120:PRO:HB3	0.43	1.88	4	1
1:A:108:THR:OG1	1:A:109:TRP:N	0.43	2.50	4	1
1:A:91:ILE:O	1:A:92:LYS:CB	0.43	2.66	11	1
1:A:91:ILE:O	1:A:92:LYS:HD2	0.43	2.13	14	1
1:A:67:ILE:HD13	1:A:85:PRO:HG2	0.43	1.91	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:GLY:C	1:A:91:ILE:HD13	0.43	2.34	2	2
2:B:233:LYS:HG2	2:B:234:ASN:N	0.43	2.28	10	1
1:A:86:GLU:CG	1:A:118:CYS:HB3	0.43	2.44	1	1
1:A:63:THR:HG22	1:A:71:TRP:CB	0.43	2.34	14	1
1:A:71:TRP:CZ3	1:A:82:ARG:HB3	0.43	2.49	18	1
1:A:90:GLY:C	1:A:91:ILE:HD12	0.43	2.34	18	1
1:A:71:TRP:CD2	1:A:101:ARG:HD3	0.43	2.48	2	1
1:A:99:ALA:HB1	1:A:115:TYR:HE1	0.43	1.73	2	1
1:A:75:ALA:O	1:A:103:CYS:HB2	0.43	2.14	4	1
1:A:87:TYR:CD1	1:A:92:LYS:HE2	0.43	2.49	12	1
1:A:91:ILE:HB	1:A:92:LYS:NZ	0.43	2.29	19	1
1:A:87:TYR:CD1	1:A:87:TYR:N	0.43	2.87	11	2
1:A:82:ARG:HD3	1:A:83:PRO:O	0.43	2.14	11	1
1:A:74:SER:O	1:A:75:ALA:HB2	0.43	2.13	15	1
1:A:82:ARG:CG	1:A:83:PRO:HD2	0.43	2.44	16	1
1:A:71:TRP:CZ2	1:A:101:ARG:CZ	0.43	3.02	18	1
1:A:93:TYR:CE2	1:A:121:ILE:HD11	0.42	2.49	14	1
1:A:84:CYS:HB3	1:A:86:GLU:OE1	0.42	2.14	3	1
1:A:65:ASP:HB2	1:A:69:THR:O	0.42	2.14	17	1
1:A:92:LYS:CD	1:A:95:THR:HG23	0.42	2.44	5	1
1:A:86:GLU:CD	1:A:93:TYR:HB2	0.42	2.35	10	1
1:A:67:ILE:HG23	1:A:88:PHE:CZ	0.42	2.49	3	1
2:B:231:ALA:HB1	2:B:235:ARG:HH12	0.42	1.74	5	1
1:A:104:LEU:HD23	1:A:108:THR:CB	0.42	2.45	14	1
1:A:120:PRO:O	1:A:121:ILE:C	0.42	2.58	4	1
1:A:75:ALA:CB	1:A:76:PRO:HD2	0.42	2.41	10	2
1:A:81:GLU:O	1:A:82:ARG:NE	0.42	2.42	16	1
1:A:120:PRO:O	1:A:121:ILE:HB	0.42	2.15	7	1
1:A:92:LYS:HE2	1:A:121:ILE:HG23	0.42	1.92	9	1
1:A:63:THR:CB	1:A:109:TRP:CD1	0.42	3.03	19	1
1:A:67:ILE:O	1:A:67:ILE:CG2	0.42	2.67	2	4
1:A:92:LYS:HD3	1:A:93:TYR:N	0.42	2.29	14	1
1:A:80:VAL:HB	1:A:101:ARG:O	0.42	2.15	15	1
1:A:97:ARG:NH1	1:A:119:GLU:OE2	0.41	2.50	2	1
1:A:100:TYR:O	1:A:114:ASN:HB2	0.41	2.14	6	1
2:B:236:LYS:O	2:B:239:GLU:HG3	0.41	2.15	8	1
1:A:89:ASN:ND2	2:B:230:GLU:HB3	0.41	2.30	13	1
1:A:104:LEU:HD12	1:A:108:THR:HG23	0.41	1.91	4	1
1:A:71:TRP:CE3	1:A:82:ARG:HD2	0.41	2.50	16	1
1:A:81:GLU:HB3	1:A:100:TYR:CD1	0.41	2.50	17	1
1:A:60:CYS:HB2	1:A:74:SER:C	0.41	2.36	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:TYR:CD1	1:A:100:TYR:N	0.41	2.88	18	2
1:A:101:ARG:CB	1:A:113:VAL:HG13	0.41	2.46	16	2
1:A:69:THR:HG22	1:A:71:TRP:CE2	0.41	2.50	3	1
1:A:101:ARG:HH12	1:A:110:ALA:HB3	0.41	1.75	7	1
1:A:86:GLU:CG	1:A:92:LYS:HE2	0.41	2.46	13	1
1:A:117:HIS:O	1:A:118:CYS:HB2	0.41	2.15	18	2
1:A:97:ARG:NH2	1:A:120:PRO:O	0.41	2.47	19	1
1:A:103:CYS:SG	1:A:108:THR:C	0.41	2.99	19	1
1:A:98:ASN:OD1	1:A:98:ASN:N	0.41	2.53	9	1
1:A:92:LYS:HA	1:A:121:ILE:HD13	0.41	1.92	14	1
1:A:97:ARG:CB	1:A:117:HIS:HB3	0.41	2.45	15	1
1:A:63:THR:HB	1:A:109:TRP:CD1	0.41	2.51	18	1
1:A:99:ALA:HB1	1:A:115:TYR:CE1	0.41	2.51	2	1
1:A:71:TRP:CE3	1:A:80:VAL:HG13	0.41	2.51	4	1
1:A:79:LEU:HA	1:A:102:GLU:HG3	0.41	1.92	7	1
1:A:81:GLU:HA	1:A:100:TYR:HA	0.41	1.93	8	1
2:B:231:ALA:HB1	2:B:235:ARG:NH2	0.41	2.30	9	1
1:A:63:THR:N	1:A:71:TRP:O	0.41	2.48	14	1
1:A:92:LYS:CD	1:A:120:PRO:HA	0.41	2.45	18	1
2:B:234:ASN:O	2:B:237:LEU:HB2	0.41	2.15	5	1
1:A:120:PRO:O	1:A:121:ILE:HG23	0.41	2.15	12	1
1:A:93:TYR:HA	1:A:121:ILE:HG12	0.41	1.93	10	1
1:A:77:GLY:N	1:A:104:LEU:O	0.41	2.54	16	1
1:A:85:PRO:HB2	1:A:88:PHE:CE2	0.41	2.50	16	1
1:A:87:TYR:N	1:A:87:TYR:HD1	0.41	2.12	18	1
1:A:71:TRP:CE2	1:A:101:ARG:NE	0.40	2.89	3	1
1:A:120:PRO:O	1:A:121:ILE:CG2	0.40	2.69	12	1
2:B:231:ALA:O	2:B:235:ARG:NH1	0.40	2.54	12	1
2:B:230:GLU:HA	2:B:233:LYS:HG2	0.40	1.92	15	1
1:A:60:CYS:HB3	1:A:109:TRP:CD1	0.40	2.51	19	1
1:A:69:THR:HG21	1:A:115:TYR:OH	0.40	2.16	1	1
1:A:71:TRP:CE3	1:A:80:VAL:CG1	0.40	3.03	4	1
2:B:237:LEU:O	2:B:240:ILE:HB	0.40	2.15	9	1
1:A:76:PRO:HA	1:A:103:CYS:O	0.40	2.15	10	1
1:A:82:ARG:HD2	1:A:83:PRO:HD2	0.40	1.93	13	1
1:A:82:ARG:HG2	1:A:83:PRO:HD2	0.40	1.92	19	1
1:A:99:ALA:CB	1:A:115:TYR:CD1	0.40	3.04	19	1
1:A:71:TRP:CZ2	1:A:101:ARG:HG2	0.40	2.51	18	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	63/119 (53%)	47±3 (75±4%)	12±2 (18±4%)	4±1 (7±2%)	2	17
2	B	10/31 (32%)	9±1 (93±8%)	1±1 (6±7%)	0±0 (1±3%)	18	66
All	All	1387/2850 (49%)	1070 (77%)	232 (17%)	85 (6%)	3	20

All 19 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	94	ASN	14
1	A	89	ASN	12
1	A	90	GLY	10
1	A	120	PRO	8
1	A	92	LYS	7
1	A	121	ILE	5
1	A	74	SER	4
1	A	62	THR	4
1	A	107	GLY	3
1	A	95	THR	3
1	A	104	LEU	3
1	A	60	CYS	2
1	A	73	GLN	2
1	A	118	CYS	2
2	B	230	GLU	2
1	A	117	HIS	1
1	A	93	TYR	1
1	A	72	PRO	1
1	A	83	PRO	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	55/103 (53%)	36±2 (66±4%)	19±2 (34±4%)	1	10
2	B	10/23 (43%)	7±1 (66±10%)	3±1 (34±10%)	1	10
All	All	1235/2394 (52%)	814 (66%)	421 (34%)	1	10

All 55 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	64	LEU	18
2	B	232	HIS	18
1	A	63	THR	16
1	A	103	CYS	15
1	A	89	ASN	13
1	A	95	THR	13
2	B	237	LEU	13
1	A	92	LYS	13
1	A	121	ILE	13
1	A	82	ARG	12
1	A	93	TYR	12
1	A	66	GLN	11
2	B	235	ARG	11
1	A	116	SER	11
1	A	101	ARG	11
1	A	65	ASP	10
1	A	73	GLN	10
1	A	111	SER	10
1	A	96	THR	9
2	B	236	LYS	9
1	A	115	TYR	9
1	A	97	ARG	8
1	A	62	THR	8
1	A	91	ILE	8
1	A	59	TYR	7
1	A	117	HIS	7
2	B	233	LYS	7
1	A	79	LEU	7
1	A	102	GLU	7
1	A	81	GLU	6
1	A	88	PHE	6
1	A	98	ASN	6
1	A	108	THR	6
1	A	112	ARG	6

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Mol	Chain	Res	Type	Models (Total)
1	A	61	ASN	6
1	A	86	GLU	6
1	A	70	CYS	6
1	A	87	TYR	6
1	A	119	GLU	5
1	A	84	CYS	5
1	A	94	ASN	5
1	A	104	LEU	5
1	A	105	GLU	5
1	A	74	SER	4
2	B	230	GLU	4
2	B	239	GLU	3
1	A	118	CYS	3
1	A	67	ILE	3
1	A	60	CYS	2
1	A	113	VAL	2
1	A	100	TYR	1
1	A	114	ASN	1
1	A	69	THR	1
1	A	80	VAL	1
1	A	120	PRO	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	NLE	B	238	2	6,7,8	0.43±0.02	0±0 (0±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	NLE	B	238	2	2,7,9	0.35±0.02	0±0 (0±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	NLE	B	238	2	-	0±0,5,6,8	-

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates [i](#)

There are no monosaccharides 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 ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided