



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2LSP / pdb_00002lsp
BMRB ID : 18439
Title : solution structures of BRD4 second bromodomain with NF-kB-K310ac peptide
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He, J.; Zhou, M.-M.
Deposited on : 2012-05-03

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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)
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

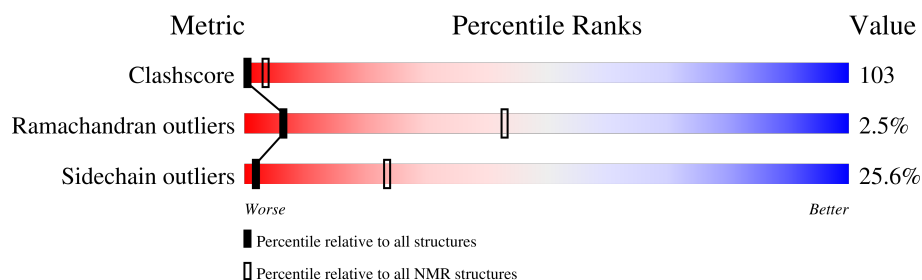
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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	13	100%
2	B	128	14% 48% 18% 20%

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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	B:353-B:454 (102)	0.17	17

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 4 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2294 atoms, of which 1141 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NF-kB-K310ac peptide.

Mol	Chain	Residues	Atoms						Trace
1	A	13	Total	C	H	N	O	S	0
			239	74	123	19	22	1	

- Molecule 2 is a protein called Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms						Trace
2	B	128	Total	C	H	N	O	S	0
			2055	658	1018	175	193	11	

4 Residue-property plots

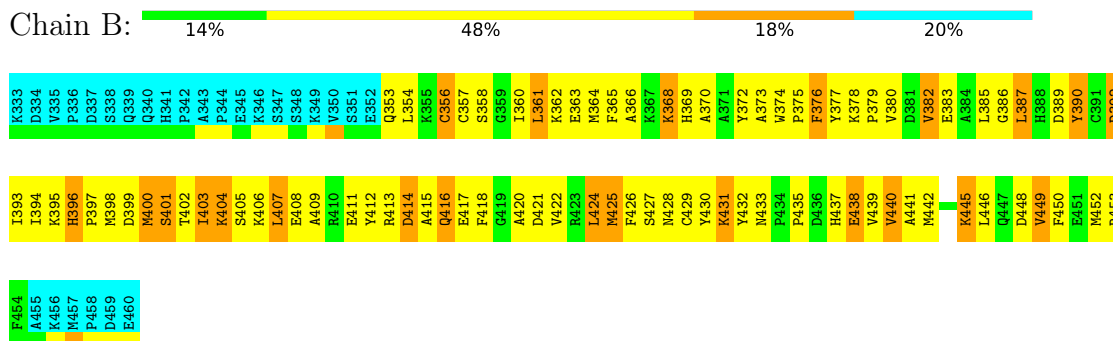
4.1 Average score per residue in the NMR ensemble

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: NF-kB-K310ac peptide



- Molecule 2: Bromodomain-containing protein 4

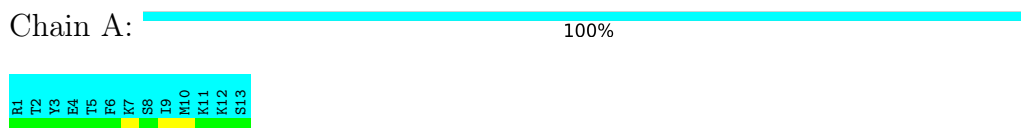


4.2 Scores per residue for each member of the ensemble

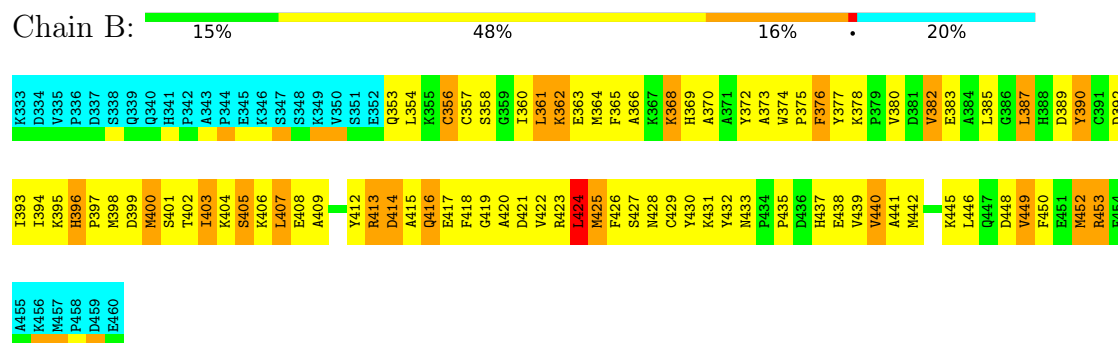
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: NF-kB-K310ac peptide

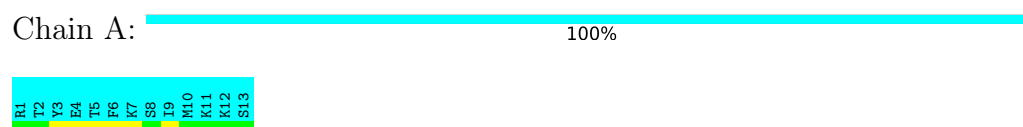


- Molecule 2: Bromodomain-containing protein 4

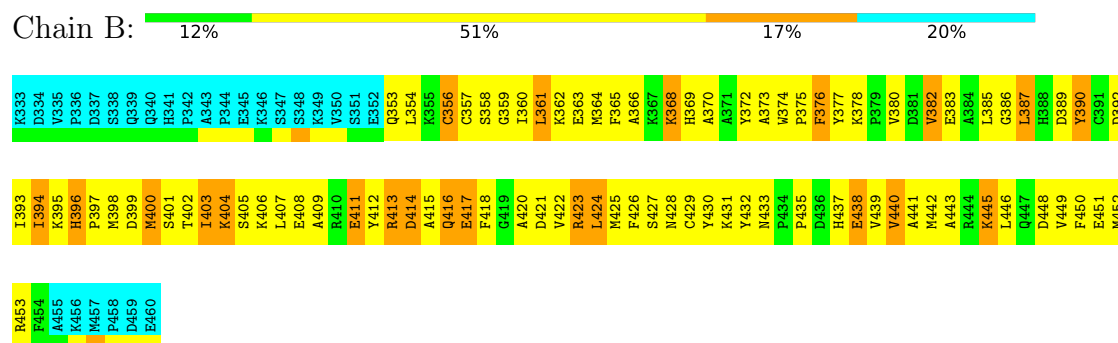


4.2.2 Score per residue for model 2

- Molecule 1: NF-kB-K310ac peptide

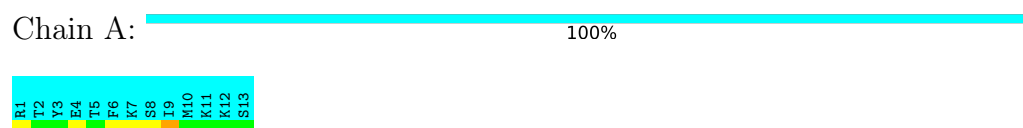


- Molecule 2: Bromodomain-containing protein 4

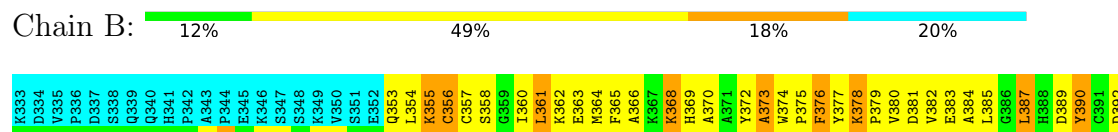


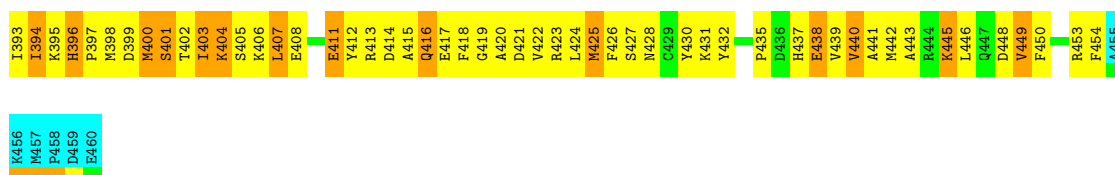
4.2.3 Score per residue for model 3

- Molecule 1: NF-kB-K310ac peptide



- Molecule 2: Bromodomain-containing protein 4



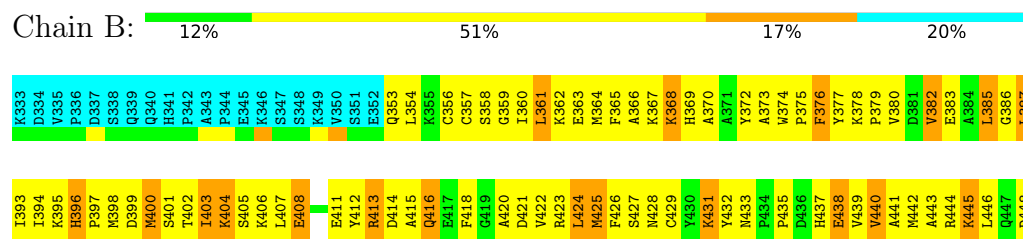


4.2.4 Score per residue for model 4

- Molecule 1: NF-kB-K310ac peptide

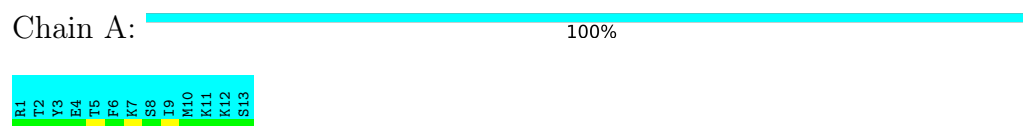


- Molecule 2: Bromodomain-containing protein 4

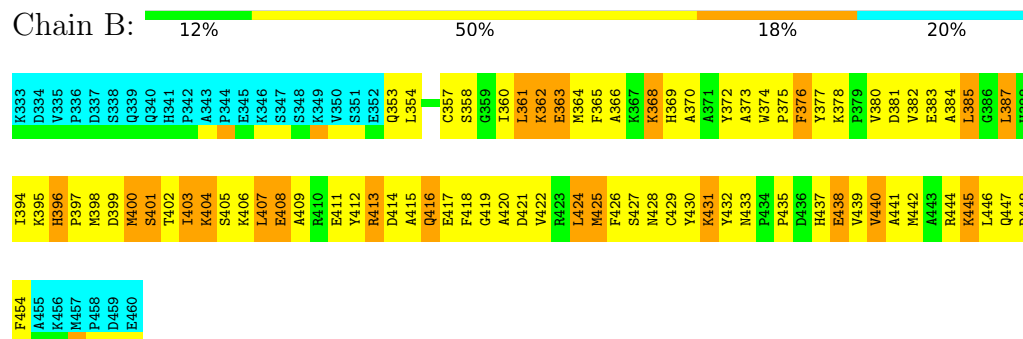


4.2.5 Score per residue for model 5

- Molecule 1: NF-kB-K310ac peptide

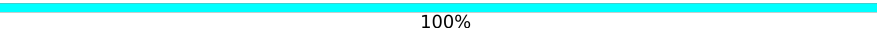


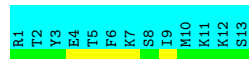
- Molecule 2: Bromodomain-containing protein 4



4.2.6 Score per residue for model 6

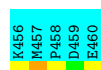
- Molecule 1: NF-kB-K310ac peptide

Chain A:  100%



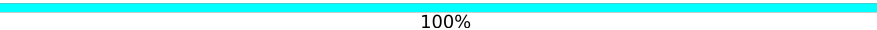
- Molecule 2: Bromodomain-containing protein 4

Chain B:  14% 48% 17% 20%



4.2.7 Score per residue for model 7

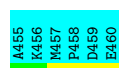
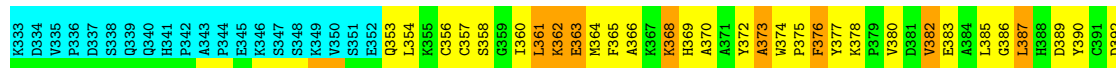
- Molecule 1: NF-kB-K310ac peptide

Chain A:  100%



- Molecule 2: Bromodomain-containing protein 4

Chain B:  17% 46% 16% 20%



4.2.8 Score per residue for model 8

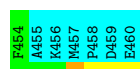
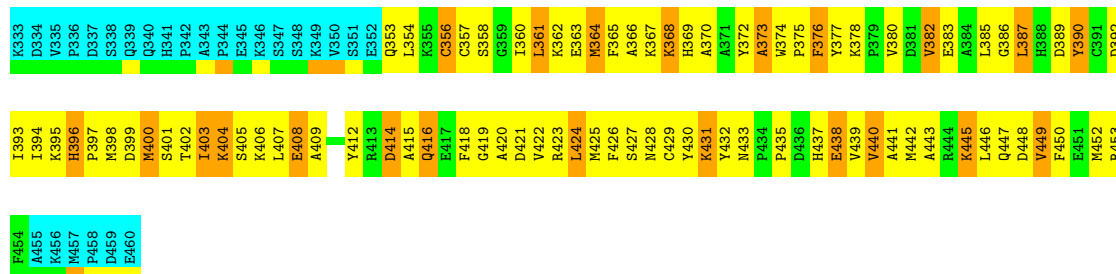
- Molecule 1: NF-kB-K310ac peptide

Chain A:  100%



- Molecule 2: Bromodomain-containing protein 4

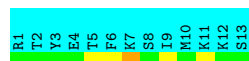
Chain B:  13% 49% 17% 20%



4.2.9 Score per residue for model 9

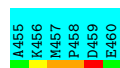
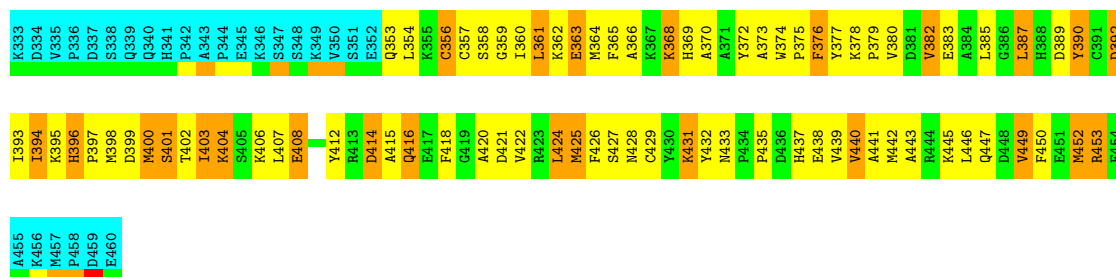
- Molecule 1: NF-kB-K310ac peptide

Chain A:  100%



- Molecule 2: Bromodomain-containing protein 4

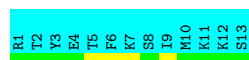
Chain B:  18% 42% 20% 20%



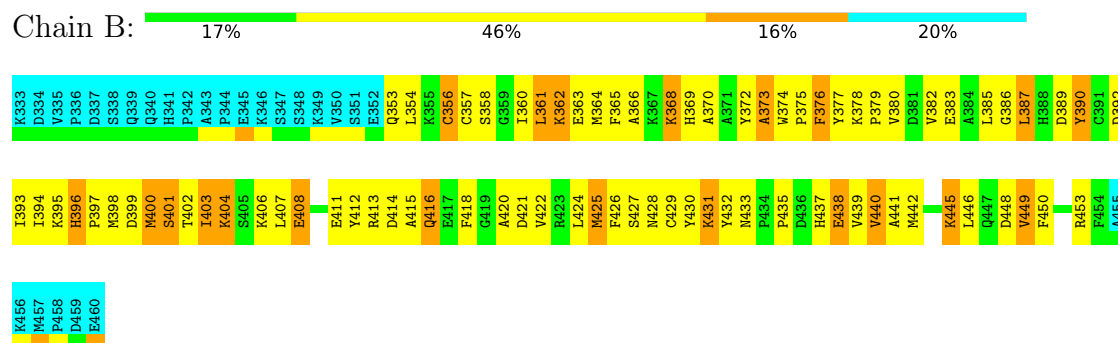
4.2.10 Score per residue for model 10

- Molecule 1: NF-kB-K310ac peptide

Chain A:  100%

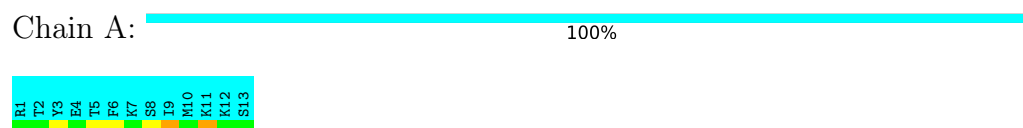


- Molecule 2: Bromodomain-containing protein 4

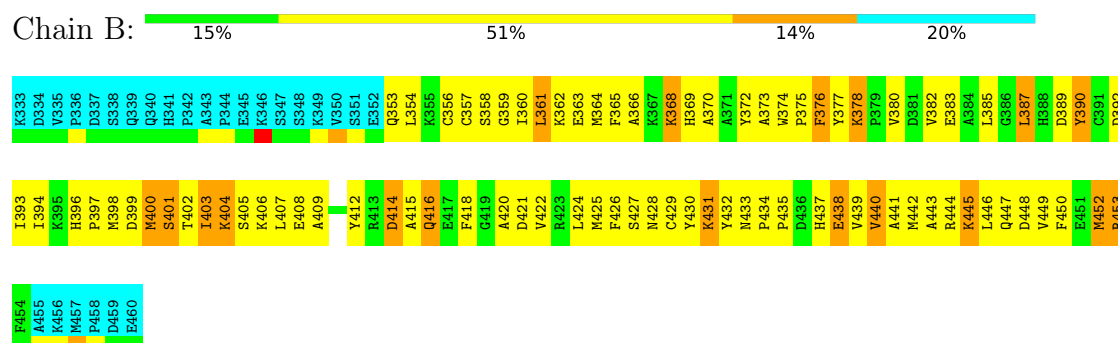


4.2.11 Score per residue for model 11

- Molecule 1: NF-kB-K310ac peptide

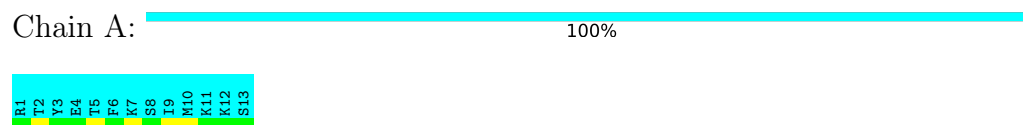


- Molecule 2: Bromodomain-containing protein 4

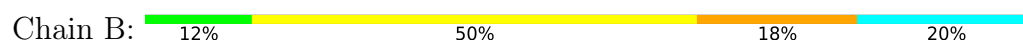


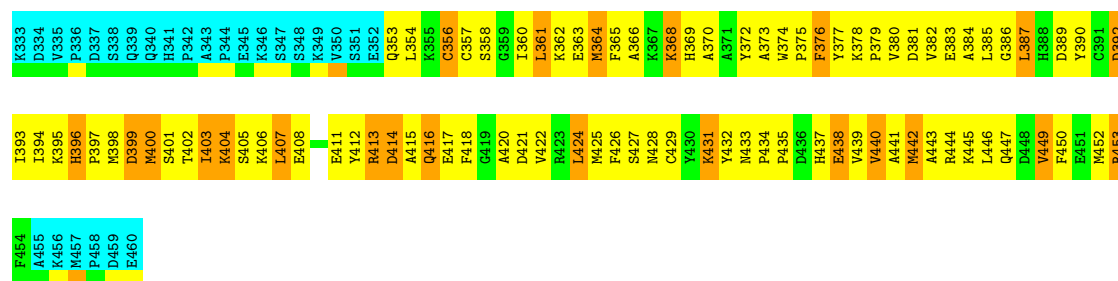
4.2.12 Score per residue for model 12

- Molecule 1: NF-kB-K310ac peptide



- Molecule 2: Bromodomain-containing protein 4

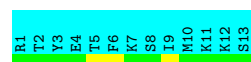




4.2.13 Score per residue for model 13

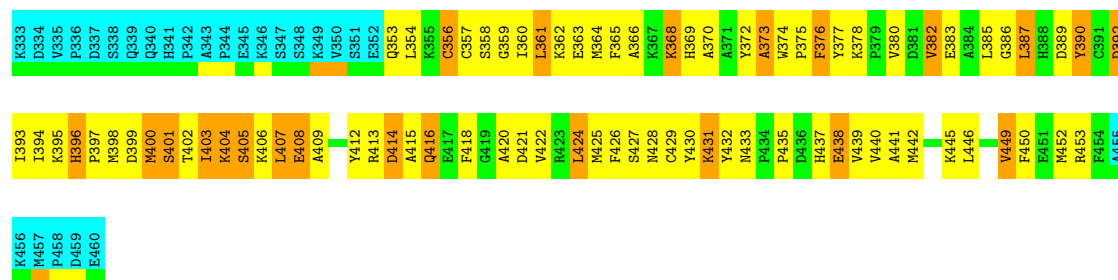
- Molecule 1: NF-kB-K310ac peptide

Chain A: 100%



- Molecule 2: Bromodomain-containing protein 4

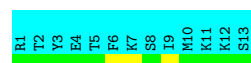
Chain B: 16% 45% 18% 20%



4.2.14 Score per residue for model 14

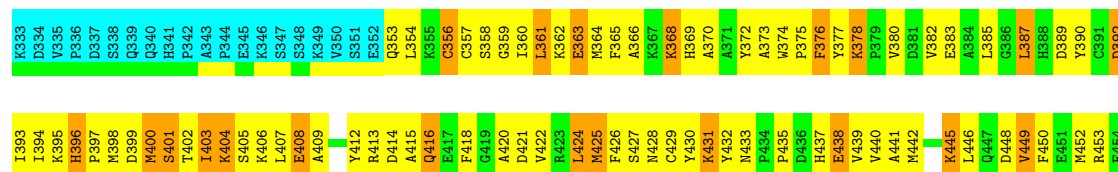
- Molecule 1: NF-kB-K310ac peptide

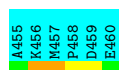
Chain A: 100%



- Molecule 2: Bromodomain-containing protein 4

Chain B: 16% 47% 16% 20%

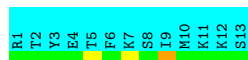




4.2.15 Score per residue for model 15

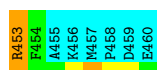
- Molecule 1: NF-kB-K310ac peptide

Chain A: 100%



- Molecule 2: Bromodomain-containing protein 4

Chain B: 12% 45% 22% 20%



4.2.16 Score per residue for model 16

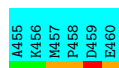
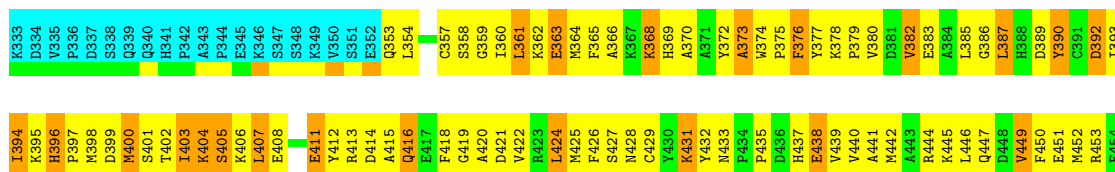
- Molecule 1: NF-kB-K310ac peptide

Chain A: 100%



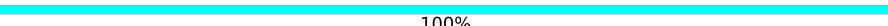
- Molecule 2: Bromodomain-containing protein 4

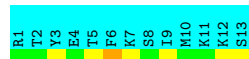
Chain B: 14% 48% 17% 20%



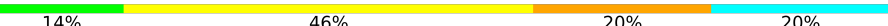
4.2.17 Score per residue for model 17 (medoid)

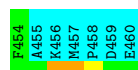
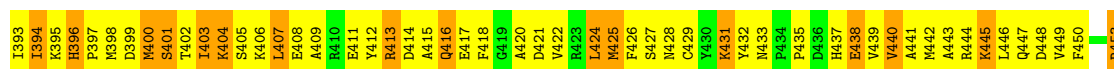
- Molecule 1: NF-kB-K310ac peptide

Chain A:  100%



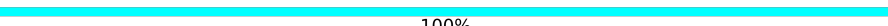
- Molecule 2: Bromodomain-containing protein 4

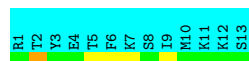
Chain B:  14% 46% 20% 20%



4.2.18 Score per residue for model 18

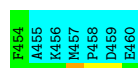
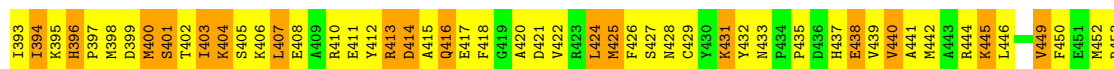
- Molecule 1: NF-kB-K310ac peptide

Chain A:  100%



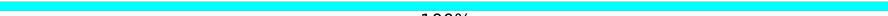
- Molecule 2: Bromodomain-containing protein 4

Chain B:  16% 44% 20% 20%



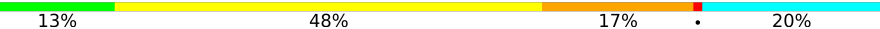
4.2.19 Score per residue for model 19

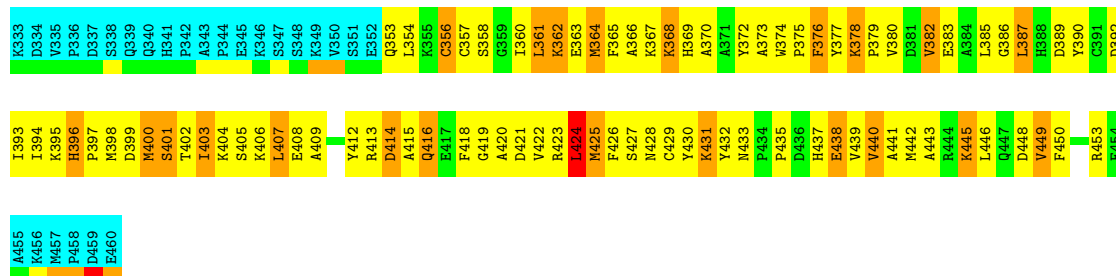
- Molecule 1: NF-kB-K310ac peptide

Chain A:  100%



- Molecule 2: Bromodomain-containing protein 4

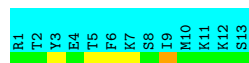
Chain B:  13% 48% 17% 20%



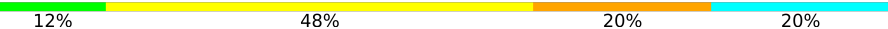
4.2.20 Score per residue for model 20

- Molecule 1: NF-kB-K310ac peptide

Chain A:  100%



- Molecule 2: Bromodomain-containing protein 4

Chain B:  12% 48% 20% 20%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	refinement	2.3
TALOS	geometry optimization	3.70F1
CNS	structure solution	1.21
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1435
Number of shifts mapped to atoms	1435
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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: ALY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
2	B	1.21±0.01	1±0/860 (0.1± 0.1%)	1.23±0.01	1±1/1157 (0.1± 0.1%)
All	All	1.21	11/17200 (0.1%)	1.23	22/23140 (0.1%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	407	LEU	N-CA	-5.23	1.40	1.46	17	11

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	B	411	GLU	N-CA-C	-5.73	105.17	111.82	2	10
2	B	394	ILE	N-CA-CB	-5.40	106.83	112.06	9	9
2	B	413	ARG	N-CA-C	-5.19	105.74	111.71	4	1
2	B	424	LEU	N-CA-C	-5.12	105.40	111.69	19	2

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	0	0	0	0±0
2	B	837	825	821	171±7
All	All	16740	16500	16420	3412

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 103.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:373:ALA:HB2	2:B:446:LEU:HD21	1.11	1.22	16	20
2:B:372:TYR:HA	2:B:442:MET:SD	0.92	2.03	17	20
2:B:372:TYR:CG	2:B:445:LYS:HD2	0.92	1.98	8	7
2:B:372:TYR:CD2	2:B:445:LYS:HG2	0.91	2.00	12	4
2:B:357:CYS:HB3	2:B:418:PHE:CD1	0.91	2.01	5	20
2:B:377:TYR:O	2:B:401:SER:HB2	0.88	1.67	1	14
2:B:377:TYR:O	2:B:401:SER:HB3	0.87	1.70	8	6
2:B:358:SER:N	2:B:407:LEU:HD21	0.84	1.87	19	20
2:B:354:LEU:HD21	2:B:414:ASP:HA	0.79	1.52	20	20
2:B:376:PHE:HD2	2:B:425:MET:SD	0.79	2.01	6	17
2:B:412:TYR:CE2	2:B:418:PHE:HA	0.78	2.13	15	20
2:B:398:MET:HE3	2:B:403:ILE:HG22	0.78	1.53	12	4
2:B:357:CYS:HB2	2:B:407:LEU:HD11	0.76	1.56	9	3
2:B:353:GLN:HB3	2:B:415:ALA:HB2	0.76	1.55	11	20
2:B:428:ASN:HA	2:B:431:LYS:CG	0.76	2.09	14	18
2:B:355:LYS:O	2:B:355:LYS:HE3	0.76	1.79	3	1
2:B:422:VAL:O	2:B:425:MET:HG3	0.75	1.81	1	14
2:B:427:SER:O	2:B:431:LYS:HG2	0.75	1.82	13	18
2:B:422:VAL:HA	2:B:425:MET:SD	0.75	2.21	13	2
2:B:364:MET:C	2:B:400:MET:HE1	0.75	2.06	11	20
2:B:422:VAL:O	2:B:425:MET:HB2	0.74	1.82	13	2
2:B:376:PHE:O	2:B:399:ASP:HB2	0.74	1.81	5	19
2:B:404:LYS:O	2:B:407:LEU:HB3	0.74	1.83	6	20
2:B:429:CYS:SG	2:B:440:VAL:HA	0.73	2.24	20	5
2:B:360:ILE:HG23	2:B:453:ARG:CB	0.73	2.14	20	20
2:B:438:GLU:O	2:B:441:ALA:HB3	0.72	1.84	3	20
2:B:370:ALA:HB2	2:B:377:TYR:OH	0.72	1.85	17	20
2:B:373:ALA:HB2	2:B:446:LEU:CD2	0.72	2.11	12	20
2:B:373:ALA:HA	2:B:446:LEU:HD11	0.71	1.63	8	20
2:B:376:PHE:CD2	2:B:425:MET:SD	0.71	2.84	6	17
2:B:357:CYS:HB3	2:B:418:PHE:CG	0.70	2.22	20	20
2:B:412:TYR:CD1	2:B:417:GLU:HG2	0.70	2.21	12	4
2:B:364:MET:HE3	2:B:400:MET:SD	0.70	2.26	4	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:360:ILE:HG23	2:B:453:ARG:HB3	0.70	1.63	12	20
2:B:403:ILE:HA	2:B:412:TYR:OH	0.70	1.86	12	20
2:B:403:ILE:O	2:B:407:LEU:HB2	0.69	1.88	13	20
2:B:361:LEU:HD13	2:B:404:LYS:HB2	0.69	1.64	6	20
2:B:404:LYS:O	2:B:408:GLU:HG3	0.69	1.88	17	20
2:B:377:TYR:CD1	2:B:400:MET:HE2	0.68	2.22	11	20
2:B:372:TYR:O	2:B:442:MET:HB3	0.68	1.88	5	20
2:B:403:ILE:CD1	2:B:422:VAL:HG22	0.68	2.19	11	20
2:B:403:ILE:HD11	2:B:422:VAL:HG22	0.68	1.66	11	20
2:B:407:LEU:HD22	2:B:418:PHE:CD1	0.68	2.23	19	20
2:B:361:LEU:HD11	2:B:403:ILE:HG12	0.68	1.65	16	20
2:B:362:LYS:HA	2:B:365:PHE:HB2	0.68	1.65	20	20
2:B:398:MET:HE2	2:B:421:ASP:HB3	0.67	1.65	3	20
2:B:372:TYR:C	2:B:442:MET:HB3	0.67	2.15	8	8
2:B:422:VAL:HG13	2:B:425:MET:HE3	0.67	1.67	1	7
2:B:403:ILE:HD12	2:B:425:MET:SD	0.67	2.29	11	2
2:B:365:PHE:HA	2:B:377:TYR:CE1	0.66	2.25	2	20
2:B:425:MET:HA	2:B:428:ASN:ND2	0.66	2.05	7	3
2:B:376:PHE:CZ	2:B:442:MET:HB2	0.66	2.25	15	20
2:B:361:LEU:HD11	2:B:403:ILE:CD1	0.66	2.21	13	20
2:B:390:TYR:CD1	2:B:394:ILE:HB	0.66	2.26	13	20
2:B:398:MET:CE	2:B:403:ILE:HG22	0.66	2.21	13	20
2:B:415:ALA:O	2:B:418:PHE:HB3	0.66	1.91	4	20
2:B:437:HIS:ND1	2:B:439:VAL:HG22	0.65	2.06	12	20
2:B:398:MET:H	2:B:428:ASN:ND2	0.65	1.90	11	12
2:B:428:ASN:HA	2:B:431:LYS:CD	0.65	2.22	19	18
2:B:382:VAL:HG12	2:B:387:LEU:HD12	0.64	1.69	11	20
2:B:393:ILE:HD13	2:B:432:TYR:CE2	0.64	2.28	16	20
2:B:363:GLU:O	2:B:369:HIS:HD2	0.63	1.74	11	18
2:B:353:GLN:CB	2:B:415:ALA:HB2	0.63	2.23	4	6
2:B:422:VAL:O	2:B:425:MET:HB3	0.63	1.94	2	4
2:B:358:SER:O	2:B:362:LYS:HB3	0.63	1.94	7	17
2:B:364:MET:O	2:B:369:HIS:HB2	0.62	1.94	17	20
2:B:444:ARG:O	2:B:447:GLN:HG2	0.62	1.94	20	1
2:B:382:VAL:HG11	2:B:390:TYR:CG	0.62	2.29	16	20
2:B:390:TYR:OH	2:B:397:PRO:HG3	0.62	1.94	9	20
2:B:361:LEU:CD1	2:B:403:ILE:HG12	0.62	2.25	16	20
2:B:364:MET:HA	2:B:369:HIS:CD2	0.62	2.30	3	7
2:B:446:LEU:O	2:B:450:PHE:HB3	0.62	1.95	20	20
2:B:450:PHE:O	2:B:453:ARG:HB2	0.62	1.94	4	20
2:B:452:MET:HA	2:B:452:MET:HE3	0.62	1.71	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:372:TYR:CB	2:B:445:LYS:HD2	0.61	2.24	14	7
2:B:354:LEU:HD21	2:B:414:ASP:CA	0.61	2.25	20	20
2:B:376:PHE:N	2:B:376:PHE:CD1	0.61	2.68	6	8
2:B:403:ILE:CD1	2:B:425:MET:SD	0.61	2.89	13	3
2:B:376:PHE:CD1	2:B:376:PHE:N	0.60	2.68	13	12
2:B:390:TYR:CE1	2:B:394:ILE:HB	0.60	2.31	13	20
2:B:398:MET:HE2	2:B:403:ILE:HG22	0.60	1.73	19	17
2:B:363:GLU:O	2:B:369:HIS:CD2	0.60	2.54	18	20
2:B:433:ASN:HB3	2:B:437:HIS:CD2	0.60	2.31	20	19
2:B:413:ARG:HD2	2:B:417:GLU:OE1	0.60	1.96	3	2
2:B:398:MET:O	2:B:425:MET:HA	0.60	1.97	12	5
2:B:364:MET:SD	2:B:450:PHE:HB2	0.60	2.36	8	20
2:B:372:TYR:O	2:B:446:LEU:HG	0.60	1.95	5	20
2:B:416:GLN:O	2:B:420:ALA:HB2	0.60	1.96	2	20
2:B:354:LEU:HA	2:B:357:CYS:SG	0.60	2.36	5	11
2:B:357:CYS:SG	2:B:415:ALA:HA	0.60	2.37	5	14
2:B:361:LEU:HD13	2:B:404:LYS:CB	0.59	2.26	5	20
2:B:364:MET:CB	2:B:400:MET:HE1	0.59	2.26	16	20
2:B:376:PHE:HB3	2:B:400:MET:HG2	0.59	1.74	12	20
2:B:377:TYR:C	2:B:378:LYS:HG2	0.59	2.22	17	11
2:B:360:ILE:CG2	2:B:453:ARG:HB3	0.59	2.26	12	20
2:B:373:ALA:HB1	2:B:400:MET:SD	0.59	2.37	11	15
2:B:419:GLY:O	2:B:423:ARG:HD2	0.59	1.97	19	2
2:B:412:TYR:N	2:B:412:TYR:CD1	0.59	2.70	10	12
2:B:437:HIS:CE1	2:B:439:VAL:HG22	0.59	2.32	20	19
2:B:407:LEU:HD22	2:B:418:PHE:CE1	0.59	2.32	4	20
2:B:428:ASN:HA	2:B:431:LYS:HD3	0.58	1.76	20	18
2:B:406:LYS:HB2	2:B:412:TYR:CE1	0.58	2.33	15	1
2:B:393:ILE:O	2:B:431:LYS:HE3	0.58	1.99	3	2
2:B:413:ARG:HG3	2:B:417:GLU:OE1	0.58	1.99	12	1
2:B:394:ILE:HD12	2:B:428:ASN:HB3	0.58	1.76	10	16
2:B:361:LEU:HD11	2:B:403:ILE:CG1	0.58	2.29	16	20
2:B:376:PHE:HB3	2:B:425:MET:SD	0.58	2.39	18	12
2:B:403:ILE:HD12	2:B:422:VAL:HA	0.58	1.76	6	20
2:B:389:ASP:O	2:B:392:ASP:HB2	0.58	1.99	12	10
2:B:437:HIS:HB3	2:B:440:VAL:HG13	0.58	1.76	18	20
2:B:398:MET:HE1	2:B:402:THR:HG22	0.57	1.77	2	20
2:B:404:LYS:C	2:B:404:LYS:HE3	0.57	2.23	5	9
2:B:379:PRO:HA	2:B:399:ASP:CG	0.57	2.24	12	1
2:B:412:TYR:CD1	2:B:412:TYR:N	0.57	2.72	16	8
2:B:376:PHE:N	2:B:376:PHE:HD1	0.57	1.98	19	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:398:MET:HE1	2:B:402:THR:CG2	0.57	2.30	11	18
2:B:403:ILE:HB	2:B:412:TYR:OH	0.57	1.98	11	19
2:B:435:PRO:HA	2:B:440:VAL:HG21	0.57	1.77	20	19
2:B:446:LEU:HA	2:B:449:VAL:CG1	0.57	2.30	17	20
2:B:402:THR:O	2:B:406:LYS:HG2	0.57	2.00	15	1
2:B:399:ASP:O	2:B:403:ILE:HG23	0.57	2.00	6	17
2:B:445:LYS:O	2:B:448:ASP:HB3	0.56	2.00	20	11
2:B:374:TRP:CG	2:B:375:PRO:HD3	0.56	2.36	8	20
2:B:380:VAL:CG2	2:B:387:LEU:HD11	0.56	2.29	19	20
2:B:421:ASP:O	2:B:425:MET:HB2	0.56	2.00	6	4
2:B:452:MET:HE3	2:B:452:MET:HA	0.56	1.76	15	2
2:B:372:TYR:CG	2:B:445:LYS:HG2	0.56	2.34	18	4
2:B:402:THR:O	2:B:406:LYS:HG3	0.56	2.01	19	19
2:B:353:GLN:O	2:B:356:CYS:HB3	0.56	2.00	7	1
2:B:400:MET:N	2:B:425:MET:SD	0.56	2.78	8	1
2:B:366:ALA:CB	2:B:368:LYS:HD3	0.56	2.30	2	20
2:B:412:TYR:CD2	2:B:418:PHE:HA	0.56	2.36	3	15
2:B:395:LYS:HB2	2:B:396:HIS:CD2	0.56	2.36	12	14
2:B:360:ILE:O	2:B:363:GLU:HB3	0.55	2.01	17	18
2:B:404:LYS:HE3	2:B:404:LYS:C	0.55	2.27	4	7
2:B:377:TYR:CE1	2:B:400:MET:HE2	0.55	2.36	18	20
2:B:400:MET:SD	2:B:425:MET:HE1	0.55	2.42	3	8
2:B:437:HIS:O	2:B:440:VAL:HG22	0.55	2.02	9	10
2:B:358:SER:CA	2:B:407:LEU:HD21	0.55	2.32	20	16
2:B:437:HIS:CE1	2:B:438:GLU:HG2	0.55	2.37	1	2
2:B:376:PHE:CZ	2:B:429:CYS:SG	0.55	2.95	13	9
2:B:372:TYR:CD1	2:B:445:LYS:CG	0.54	2.90	11	9
2:B:418:PHE:O	2:B:422:VAL:HG23	0.54	2.03	3	20
2:B:372:TYR:CD1	2:B:445:LYS:HG3	0.54	2.38	20	9
2:B:400:MET:HG2	2:B:425:MET:HE3	0.54	1.78	11	2
2:B:398:MET:HG2	2:B:424:LEU:HD13	0.54	1.79	2	20
2:B:369:HIS:HA	2:B:372:TYR:CE1	0.54	2.38	8	11
2:B:353:GLN:O	2:B:357:CYS:N	0.54	2.40	4	17
2:B:357:CYS:O	2:B:360:ILE:HB	0.54	2.02	7	20
2:B:441:ALA:O	2:B:444:ARG:HG2	0.54	2.02	4	2
2:B:403:ILE:HG21	2:B:421:ASP:C	0.53	2.28	7	17
2:B:441:ALA:O	2:B:445:LYS:HD2	0.53	2.04	2	9
2:B:395:LYS:HB2	2:B:396:HIS:CE1	0.53	2.39	13	12
2:B:413:ARG:HD2	2:B:417:GLU:OE2	0.53	2.03	1	2
2:B:387:LEU:HD22	2:B:432:TYR:CZ	0.53	2.39	3	19
2:B:353:GLN:O	2:B:357:CYS:SG	0.53	2.67	3	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:372:TYR:CD2	2:B:445:LYS:HD2	0.52	2.40	1	7
2:B:374:TRP:N	2:B:375:PRO:CD	0.52	2.72	15	20
2:B:435:PRO:C	2:B:440:VAL:HG21	0.52	2.29	2	18
2:B:373:ALA:O	2:B:376:PHE:HB2	0.52	2.05	10	20
2:B:364:MET:CE	2:B:425:MET:HE1	0.52	2.34	6	1
2:B:425:MET:HE3	2:B:426:PHE:CE1	0.52	2.39	7	8
2:B:370:ALA:HB2	2:B:377:TYR:CZ	0.52	2.40	12	20
2:B:376:PHE:CZ	2:B:439:VAL:O	0.52	2.63	16	20
2:B:412:TYR:N	2:B:412:TYR:HD1	0.52	2.01	5	20
2:B:422:VAL:HG12	2:B:426:PHE:CZ	0.52	2.40	8	7
2:B:376:PHE:O	2:B:400:MET:N	0.52	2.43	11	20
2:B:378:LYS:HE2	2:B:379:PRO:HD3	0.52	1.80	4	1
2:B:445:LYS:O	2:B:448:ASP:HB2	0.52	2.05	15	1
2:B:354:LEU:O	2:B:357:CYS:HB2	0.51	2.05	5	14
2:B:378:LYS:HB3	2:B:379:PRO:CD	0.51	2.35	18	9
2:B:400:MET:HA	2:B:425:MET:SD	0.51	2.45	8	1
2:B:424:LEU:HD22	2:B:428:ASN:ND2	0.51	2.20	13	8
2:B:413:ARG:HD3	2:B:417:GLU:OE2	0.51	2.05	17	2
2:B:358:SER:O	2:B:362:LYS:HB2	0.51	2.05	17	1
2:B:401:SER:O	2:B:405:SER:HB2	0.51	2.06	15	12
2:B:372:TYR:CB	2:B:445:LYS:HE2	0.51	2.36	10	2
2:B:382:VAL:HG11	2:B:390:TYR:CD1	0.51	2.40	3	20
2:B:387:LEU:C	2:B:389:ASP:H	0.51	2.14	2	19
2:B:394:ILE:HD12	2:B:428:ASN:HB2	0.51	1.82	11	1
2:B:382:VAL:HA	2:B:387:LEU:HG	0.50	1.82	9	20
2:B:424:LEU:HD22	2:B:428:ASN:HD21	0.50	1.66	16	8
2:B:357:CYS:SG	2:B:415:ALA:CB	0.50	2.99	7	1
2:B:376:PHE:HZ	2:B:439:VAL:O	0.50	1.88	1	10
2:B:406:LYS:CB	2:B:412:TYR:CE1	0.50	2.95	15	1
2:B:369:HIS:HA	2:B:372:TYR:CZ	0.50	2.42	18	13
2:B:404:LYS:C	2:B:404:LYS:HE2	0.50	2.32	15	1
2:B:357:CYS:HB3	2:B:418:PHE:CE1	0.49	2.42	3	10
2:B:374:TRP:H	2:B:374:TRP:CD1	0.49	2.25	16	17
2:B:374:TRP:CD1	2:B:375:PRO:HD3	0.49	2.41	8	10
2:B:376:PHE:CB	2:B:400:MET:HG2	0.49	2.37	12	14
2:B:363:GLU:HG2	2:B:453:ARG:NE	0.49	2.21	19	10
2:B:406:LYS:HB2	2:B:412:TYR:CZ	0.49	2.42	15	1
2:B:378:LYS:CB	2:B:379:PRO:CD	0.49	2.91	19	9
2:B:372:TYR:CB	2:B:445:LYS:HE3	0.49	2.38	12	2
2:B:382:VAL:HA	2:B:387:LEU:CG	0.49	2.37	9	20
2:B:429:CYS:SG	2:B:443:ALA:HB2	0.49	2.48	9	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:394:ILE:HG22	2:B:397:PRO:HD3	0.49	1.83	13	20
2:B:376:PHE:C	2:B:400:MET:HG3	0.49	2.32	11	13
2:B:378:LYS:HE2	2:B:379:PRO:CD	0.49	2.37	4	1
2:B:399:ASP:C	2:B:425:MET:SD	0.49	2.95	8	1
2:B:428:ASN:HA	2:B:431:LYS:HG3	0.49	1.82	11	1
2:B:361:LEU:CD1	2:B:404:LYS:CA	0.49	2.91	8	20
2:B:405:SER:O	2:B:409:ALA:N	0.49	2.45	8	13
2:B:426:PHE:HA	2:B:429:CYS:SG	0.49	2.47	2	2
2:B:377:TYR:N	2:B:400:MET:HG3	0.49	2.22	11	13
2:B:359:GLY:HA2	2:B:362:LYS:HE3	0.48	1.84	13	7
2:B:382:VAL:CG1	2:B:387:LEU:HD12	0.48	2.38	14	20
2:B:424:LEU:HD23	2:B:424:LEU:O	0.48	2.08	10	6
2:B:357:CYS:C	2:B:407:LEU:HD21	0.48	2.33	20	3
2:B:425:MET:HE3	2:B:426:PHE:HE1	0.48	1.68	7	4
2:B:372:TYR:HB2	2:B:442:MET:HA	0.48	1.85	11	16
2:B:358:SER:OG	2:B:407:LEU:HG	0.48	2.09	9	5
2:B:444:ARG:O	2:B:447:GLN:HB3	0.48	2.09	16	5
2:B:372:TYR:HB2	2:B:445:LYS:HD3	0.48	1.85	3	9
2:B:372:TYR:CA	2:B:442:MET:SD	0.48	2.95	2	8
2:B:397:PRO:HA	2:B:428:ASN:ND2	0.48	2.23	3	2
2:B:394:ILE:CG2	2:B:397:PRO:HB3	0.48	2.39	12	16
2:B:355:LYS:HE3	2:B:355:LYS:C	0.48	2.34	3	1
2:B:358:SER:C	2:B:362:LYS:HE3	0.48	2.33	19	2
2:B:372:TYR:CG	2:B:445:LYS:CD	0.47	2.90	6	6
2:B:394:ILE:HG22	2:B:397:PRO:CD	0.47	2.39	13	20
2:B:449:VAL:O	2:B:453:ARG:HG2	0.47	2.09	12	11
2:B:366:ALA:C	2:B:368:LYS:H	0.47	2.17	19	20
2:B:398:MET:C	2:B:425:MET:HB3	0.47	2.34	3	5
2:B:372:TYR:CD2	2:B:445:LYS:CG	0.47	2.92	10	2
2:B:447:GLN:O	2:B:451:GLU:HB2	0.47	2.09	20	2
2:B:419:GLY:HA2	2:B:450:PHE:CZ	0.47	2.44	19	8
2:B:404:LYS:HE3	2:B:405:SER:N	0.47	2.24	6	2
2:B:373:ALA:CA	2:B:446:LEU:HD11	0.47	2.39	10	20
2:B:415:ALA:HB3	2:B:416:GLN:HE21	0.47	1.69	4	1
2:B:437:HIS:ND1	2:B:438:GLU:HG2	0.47	2.24	9	1
2:B:374:TRP:CD1	2:B:374:TRP:H	0.47	2.27	5	3
2:B:422:VAL:HG11	2:B:450:PHE:CD1	0.47	2.45	16	18
2:B:389:ASP:O	2:B:393:ILE:HD12	0.46	2.09	7	20
2:B:382:VAL:CB	2:B:387:LEU:HD12	0.46	2.41	17	19
2:B:390:TYR:CE1	2:B:394:ILE:CG2	0.46	2.98	8	11
2:B:354:LEU:O	2:B:407:LEU:HD11	0.46	2.10	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:357:CYS:HB2	2:B:407:LEU:CD1	0.46	2.35	9	2
2:B:365:PHE:CE2	2:B:400:MET:HB2	0.46	2.45	11	1
2:B:399:ASP:HA	2:B:425:MET:HG2	0.46	1.87	13	2
2:B:422:VAL:O	2:B:426:PHE:CD1	0.46	2.68	4	8
2:B:360:ILE:CG1	2:B:453:ARG:HB3	0.46	2.40	16	12
2:B:399:ASP:C	2:B:425:MET:HG3	0.46	2.36	16	4
2:B:426:PHE:CZ	2:B:446:LEU:HB3	0.46	2.46	11	5
2:B:369:HIS:CE1	2:B:449:VAL:HG21	0.46	2.45	15	11
2:B:373:ALA:O	2:B:377:TYR:N	0.46	2.48	8	20
2:B:397:PRO:HA	2:B:428:ASN:CG	0.46	2.36	6	5
2:B:452:MET:HG3	2:B:453:ARG:N	0.46	2.26	11	2
2:B:364:MET:HE1	2:B:426:PHE:CE1	0.46	2.46	4	4
2:B:369:HIS:O	2:B:373:ALA:N	0.45	2.49	3	20
2:B:372:TYR:CD1	2:B:445:LYS:HG2	0.45	2.46	11	6
2:B:399:ASP:HA	2:B:425:MET:CG	0.45	2.40	16	3
2:B:366:ALA:HB3	2:B:368:LYS:HD3	0.45	1.86	3	1
2:B:400:MET:HA	2:B:403:ILE:HD13	0.45	1.86	6	14
2:B:377:TYR:HA	2:B:400:MET:HB2	0.45	1.88	12	7
2:B:398:MET:CG	2:B:424:LEU:HD13	0.45	2.41	5	10
2:B:360:ILE:HA	2:B:453:ARG:HD2	0.45	1.88	20	3
2:B:394:ILE:HG23	2:B:428:ASN:OD1	0.45	2.12	16	8
2:B:413:ARG:HD3	2:B:417:GLU:OE1	0.45	2.10	15	1
2:B:375:PRO:CG	2:B:442:MET:HE3	0.45	2.42	17	2
2:B:379:PRO:HA	2:B:399:ASP:OD2	0.45	2.11	12	1
2:B:370:ALA:O	2:B:374:TRP:CD1	0.45	2.70	16	20
2:B:427:SER:O	2:B:431:LYS:HB2	0.45	2.12	3	2
2:B:394:ILE:HD11	2:B:432:TYR:HB2	0.45	1.88	9	6
2:B:372:TYR:HB3	2:B:445:LYS:HE2	0.45	1.89	10	2
2:B:446:LEU:HA	2:B:449:VAL:HG12	0.45	1.88	17	7
2:B:396:HIS:CD2	2:B:396:HIS:N	0.45	2.85	3	9
2:B:412:TYR:CE1	2:B:417:GLU:HG2	0.45	2.46	15	2
2:B:430:TYR:CD1	2:B:440:VAL:HB	0.44	2.47	19	13
2:B:420:ALA:O	2:B:424:LEU:HB2	0.44	2.12	16	2
2:B:380:VAL:HG22	2:B:387:LEU:HD11	0.44	1.89	9	3
2:B:365:PHE:CD2	2:B:400:MET:HE3	0.44	2.48	12	12
2:B:437:HIS:O	2:B:441:ALA:HB2	0.44	2.12	8	5
2:B:354:LEU:HB3	2:B:407:LEU:CD1	0.44	2.41	12	6
2:B:443:ALA:O	2:B:447:GLN:HB2	0.44	2.11	9	2
2:B:365:PHE:N	2:B:400:MET:HE1	0.44	2.28	14	10
2:B:413:ARG:HD2	2:B:417:GLU:CD	0.44	2.38	6	1
2:B:382:VAL:HA	2:B:387:LEU:CD1	0.44	2.43	20	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:421:ASP:O	2:B:425:MET:CB	0.44	2.66	6	3
2:B:361:LEU:O	2:B:364:MET:HB2	0.44	2.13	12	6
2:B:372:TYR:CG	2:B:445:LYS:HG3	0.44	2.48	17	3
2:B:437:HIS:ND1	2:B:438:GLU:N	0.44	2.65	17	2
2:B:400:MET:HA	2:B:425:MET:HE2	0.44	1.89	3	3
2:B:357:CYS:SG	2:B:418:PHE:CB	0.44	3.06	5	1
2:B:400:MET:O	2:B:404:LYS:HB2	0.44	2.12	15	5
2:B:375:PRO:C	2:B:376:PHE:HD1	0.43	2.21	12	5
2:B:428:ASN:HA	2:B:431:LYS:HG2	0.43	1.86	8	3
2:B:358:SER:HB2	2:B:362:LYS:HD3	0.43	1.90	17	1
2:B:377:TYR:O	2:B:401:SER:CB	0.43	2.66	7	3
2:B:390:TYR:O	2:B:394:ILE:N	0.43	2.49	13	2
2:B:400:MET:CA	2:B:425:MET:SD	0.43	3.06	8	1
2:B:425:MET:SD	2:B:426:PHE:CD1	0.43	3.10	12	4
2:B:400:MET:O	2:B:404:LYS:N	0.43	2.51	11	8
2:B:403:ILE:HG21	2:B:421:ASP:O	0.43	2.14	12	2
2:B:421:ASP:O	2:B:425:MET:CG	0.43	2.66	8	1
2:B:382:VAL:HG11	2:B:390:TYR:CD2	0.43	2.48	16	4
2:B:364:MET:SD	2:B:446:LEU:HB3	0.43	2.53	16	1
2:B:415:ALA:HA	2:B:418:PHE:HB3	0.43	1.89	19	1
2:B:430:TYR:CE1	2:B:443:ALA:HB3	0.43	2.48	3	2
2:B:376:PHE:CB	2:B:400:MET:CG	0.43	2.97	12	1
2:B:364:MET:HE1	2:B:422:VAL:CG1	0.43	2.44	17	3
2:B:425:MET:O	2:B:429:CYS:SG	0.43	2.77	8	2
2:B:439:VAL:O	2:B:442:MET:HG2	0.43	2.13	17	1
2:B:399:ASP:O	2:B:400:MET:C	0.42	2.62	12	1
2:B:393:ILE:C	2:B:431:LYS:HE3	0.42	2.40	2	2
2:B:442:MET:SD	2:B:442:MET:N	0.42	2.93	20	2
2:B:434:PRO:O	2:B:437:HIS:HB2	0.42	2.14	11	3
2:B:435:PRO:CA	2:B:440:VAL:HG21	0.42	2.44	20	4
2:B:393:ILE:HG22	2:B:431:LYS:HE3	0.42	1.90	16	2
2:B:354:LEU:CA	2:B:407:LEU:HD11	0.42	2.43	3	1
2:B:414:ASP:OD1	2:B:416:GLN:HB2	0.42	2.14	19	1
2:B:403:ILE:HG22	2:B:421:ASP:HB3	0.42	1.90	15	4
2:B:398:MET:HB3	2:B:425:MET:HB3	0.42	1.90	7	7
2:B:442:MET:O	2:B:446:LEU:N	0.42	2.44	9	4
2:B:360:ILE:HG12	2:B:453:ARG:HB3	0.42	1.91	20	1
2:B:382:VAL:CG1	2:B:390:TYR:CD1	0.42	3.02	3	13
2:B:441:ALA:O	2:B:445:LYS:HB3	0.42	2.15	10	3
2:B:452:MET:HE3	2:B:452:MET:CA	0.42	2.44	13	1
2:B:446:LEU:O	2:B:450:PHE:CB	0.42	2.67	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:399:ASP:CA	2:B:425:MET:HG3	0.42	2.45	2	1
2:B:381:ASP:O	2:B:384:ALA:HB3	0.42	2.14	3	2
2:B:381:ASP:HB2	2:B:384:ALA:HB3	0.42	1.92	5	1
2:B:374:TRP:CD2	2:B:375:PRO:HD3	0.42	2.49	8	4
2:B:372:TYR:HB3	2:B:445:LYS:HE3	0.42	1.91	12	1
2:B:356:CYS:O	2:B:360:ILE:HG13	0.42	2.15	20	1
2:B:429:CYS:SG	2:B:443:ALA:CB	0.41	3.08	11	1
2:B:382:VAL:CG1	2:B:390:TYR:CG	0.41	3.03	16	3
2:B:415:ALA:HA	2:B:418:PHE:CB	0.41	2.45	19	1
2:B:412:TYR:C	2:B:414:ASP:N	0.41	2.78	12	6
2:B:361:LEU:CD1	2:B:404:LYS:HA	0.41	2.45	8	2
2:B:448:ASP:O	2:B:452:MET:HB3	0.41	2.14	1	1
2:B:361:LEU:O	2:B:365:PHE:N	0.41	2.52	8	2
2:B:445:LYS:HA	2:B:448:ASP:OD2	0.41	2.15	8	1
2:B:413:ARG:O	2:B:414:ASP:HB3	0.41	2.16	12	2
2:B:390:TYR:HA	2:B:432:TYR:HE2	0.41	1.75	20	6
2:B:361:LEU:HB2	2:B:418:PHE:CE1	0.41	2.51	5	2
2:B:400:MET:HE3	2:B:400:MET:HB3	0.41	1.75	6	2
2:B:404:LYS:O	2:B:408:GLU:CG	0.41	2.68	6	1
2:B:394:ILE:HG21	2:B:397:PRO:HB3	0.41	1.91	12	1
2:B:422:VAL:C	2:B:425:MET:HG3	0.41	2.41	8	1
2:B:403:ILE:CA	2:B:412:TYR:OH	0.41	2.65	12	1
2:B:418:PHE:CE2	2:B:450:PHE:HE1	0.41	2.33	19	1
2:B:363:GLU:O	2:B:366:ALA:CB	0.40	2.70	2	2
2:B:376:PHE:C	2:B:378:LYS:N	0.40	2.77	4	1
2:B:441:ALA:O	2:B:445:LYS:HB2	0.40	2.16	9	1
2:B:433:ASN:HB3	2:B:437:HIS:CG	0.40	2.52	8	1
2:B:423:ARG:HD3	2:B:450:PHE:CE2	0.40	2.52	2	1
2:B:449:VAL:HG13	2:B:450:PHE:H	0.40	1.77	3	3
2:B:357:CYS:CB	2:B:418:PHE:CG	0.40	3.02	20	1
2:B:362:LYS:CA	2:B:365:PHE:HB2	0.40	2.44	6	1
2:B:366:ALA:C	2:B:368:LYS:N	0.40	2.80	18	2
2:B:360:ILE:HG12	2:B:453:ARG:HD3	0.40	1.93	2	1
2:B:429:CYS:O	2:B:440:VAL:HG12	0.40	2.16	2	1
2:B:413:ARG:HG3	2:B:417:GLU:OE2	0.40	2.17	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	0	-	-	-	-	
2	B	102/128 (80%)	85±1 (83±1%)	15±1 (15±1%)	3±1 (3±1%)	6	43
All	All	2040/2820 (72%)	1691 (83%)	297 (15%)	52 (3%)	6	43

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	387	LEU	20
2	B	390	TYR	12
2	B	414	ASP	12
2	B	373	ALA	7
2	B	367	LYS	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	0	-	-	-	
2	B	89/113 (79%)	66±2 (74±2%)	23±2 (26±2%)	2	23
All	All	1780/2500 (71%)	1324 (74%)	456 (26%)	2	23

All 42 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)
2	B	361	LEU	20
2	B	368	LYS	20
2	B	376	PHE	20

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Mol	Chain	Res	Type	Models (Total)
2	B	383	GLU	20
2	B	385	LEU	20
2	B	392	ASP	20
2	B	396	HIS	20
2	B	400	MET	20
2	B	403	ILE	20
2	B	416	GLN	19
2	B	438	GLU	18
2	B	424	LEU	17
2	B	440	VAL	17
2	B	431	LYS	17
2	B	413	ARG	16
2	B	449	VAL	16
2	B	356	CYS	15
2	B	404	LYS	15
2	B	445	LYS	14
2	B	382	VAL	12
2	B	425	MET	12
2	B	401	SER	11
2	B	452	MET	9
2	B	453	ARG	9
2	B	408	GLU	9
2	B	378	LYS	8
2	B	362	LYS	7
2	B	405	SER	6
2	B	411	GLU	5
2	B	363	GLU	5
2	B	423	ARG	4
2	B	364	MET	3
2	B	367	LYS	2
2	B	442	MET	2
2	B	417	GLU	1
2	B	451	GLU	1
2	B	355	LYS	1
2	B	399	ASP	1
2	B	406	LYS	1
2	B	410	ARG	1
2	B	444	ARG	1
2	B	414	ASP	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
1	ALY	A	7	1	10,11,12	0.61±0.04	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
1	ALY	A	7	1	7,12,14	0.94±0.03	0±0 (0±3%)

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
1	ALY	A	7	1	-	0±0,9,10,12	-

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)	Models	
								Worst	Total
1	A	7	ALY	CH3-CH-NZ	2.03	119.59	116.12	9	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 74% 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 [i](#)

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	1435
Number of shifts mapped to atoms	1435
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	19

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	127	-0.45 ± 0.26	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	123	0.33 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	10	—	None (insufficient data)
^{15}N	114	0.41 ± 0.37	None needed (< 0.5 ppm)

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 79%, i.e. 1131 atoms were assigned a chemical shift out of a possible 1435. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	400/503 (80%)	195/202 (97%)	110/204 (54%)	95/97 (98%)
Sidechain	644/774 (83%)	428/502 (85%)	214/242 (88%)	2/30 (7%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	87/158 (55%)	44/76 (58%)	42/73 (58%)	1/9 (11%)
Overall	1131/1435 (79%)	667/780 (86%)	366/519 (71%)	98/136 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 1432 atoms were assigned a chemical shift out of a possible 1936. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	508/685 (74%)	257/274 (94%)	137/280 (49%)	114/131 (87%)
Sidechain	830/1066 (78%)	564/688 (82%)	264/337 (78%)	2/41 (5%)
Aromatic	94/185 (51%)	50/89 (56%)	43/85 (51%)	1/11 (9%)
Overall	1432/1936 (74%)	871/1051 (83%)	444/702 (63%)	117/183 (64%)

7.1.4 Statistically unusual chemical shifts ⓘ

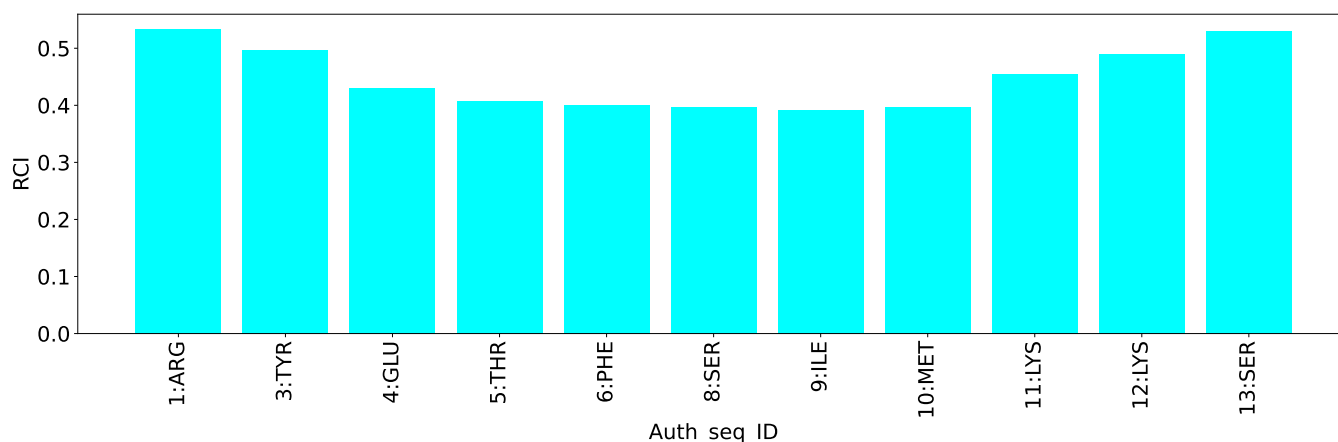
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	347	SER	C	8.45	166.15 – 183.14	-97.8
1	B	386	GLY	C	7.90	164.92 – 182.89	-92.4
1	B	385	LEU	C	7.48	167.56 – 186.66	-88.8
1	B	346	LYS	C	8.51	167.28 – 186.22	-88.8
1	B	447	GLN	C	11.57	166.94 – 185.80	-87.4
1	B	430	TYR	C	7.61	165.86 – 185.23	-86.7
1	B	388	HIS	C	8.30	165.57 – 184.97	-86.1
1	B	437	HIS	C	9.41	165.57 – 184.97	-85.5
1	B	384	ALA	C	7.86	167.61 – 188.05	-83.2
1	B	366	ALA	C	9.11	167.61 – 188.05	-82.5
1	B	375	PRO	HG2	-0.72	0.41 – 3.45	-8.7
1	B	447	GLN	HB2	0.07	0.80 – 3.29	-8.0
1	B	375	PRO	HB2	-0.35	0.37 – 3.78	-7.1
1	B	357	CYS	HB2	0.35	0.81 – 5.11	-6.1
1	B	375	PRO	HD2	1.62	1.93 – 5.38	-5.9
1	B	422	VAL	HG11	-0.67	-0.48 – 2.12	-5.7
1	B	422	VAL	HG12	-0.67	-0.48 – 2.12	-5.7
1	B	422	VAL	HG13	-0.67	-0.48 – 2.12	-5.7
1	B	439	VAL	H	11.70	4.98 – 11.56	5.2

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:



Random coil index (RCI) for chain B:

