



Full wwPDB NMR Structure Validation Report i

Apr 16, 2023 – 09:00 AM EDT

PDB ID : 8F4V
BMRB ID : 31058
Title : Alpha7 nicotinic acetylcholine receptor intracellular and transmembrane domains bound to ivermectin in a desensitized state
Authors : Bondarenko, V.; Chen, Q.; Tang, P.
Deposited on : 2022-11-11

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

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

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

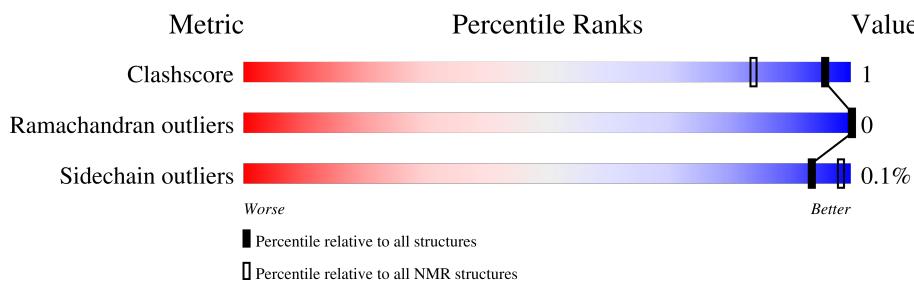
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

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 12%.

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



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

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



2 Ensemble composition and analysis [\(i\)](#)

This entry contains 15 models. Model 11 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:209-A:472, B:209-B:472, C:209-C:472, D:209-D:472, E:209-E:472 (1320)	1.08	11

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 21090 atoms, of which 10680 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Neuronal acetylcholine receptor subunit alpha-7.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	264	4082	1300	2062	340	359	21	0
1	B	264	4082	1300	2062	340	359	21	0
1	C	264	4082	1300	2062	340	359	21	0
1	D	264	4082	1300	2062	340	359	21	0
1	E	264	4082	1300	2062	340	359	21	0

There are 50 discrepancies between the modelled and reference sequences:

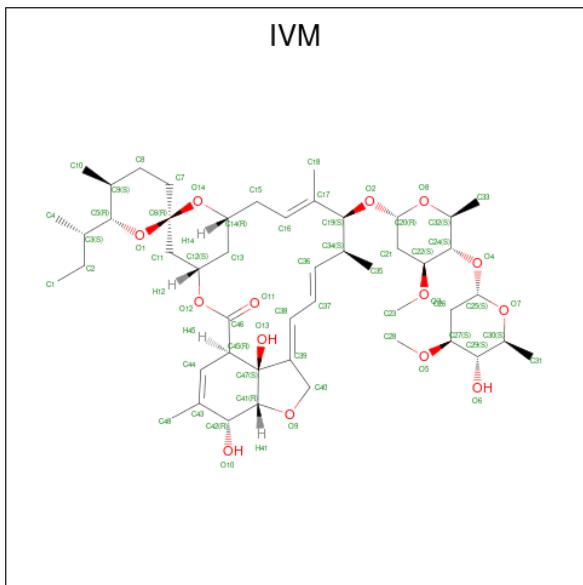
Chain	Residue	Modelled	Actual	Comment	Reference
A	203	SER	-	expression tag	UNP P36544
A	204	ASN	-	expression tag	UNP P36544
A	205	ALA	-	expression tag	UNP P36544
A	206	GLU	-	expression tag	UNP P36544
A	207	GLU	-	expression tag	UNP P36544
A	208	GLU	-	expression tag	UNP P36544
A	263	SER	ALA	engineered mutation	UNP P36544
A	268	SER	VAL	engineered mutation	UNP P36544
A	270	SER	LEU	engineered mutation	UNP P36544
A	474	GLU	ALA	engineered mutation	UNP P36544
B	203	SER	-	expression tag	UNP P36544
B	204	ASN	-	expression tag	UNP P36544
B	205	ALA	-	expression tag	UNP P36544
B	206	GLU	-	expression tag	UNP P36544
B	207	GLU	-	expression tag	UNP P36544
B	208	GLU	-	expression tag	UNP P36544
B	263	SER	ALA	engineered mutation	UNP P36544
B	268	SER	VAL	engineered mutation	UNP P36544
B	270	SER	LEU	engineered mutation	UNP P36544
B	474	GLU	ALA	engineered mutation	UNP P36544
C	203	SER	-	expression tag	UNP P36544
C	204	ASN	-	expression tag	UNP P36544
C	205	ALA	-	expression tag	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
C	206	GLU	-	expression tag	UNP P36544
C	207	GLU	-	expression tag	UNP P36544
C	208	GLU	-	expression tag	UNP P36544
C	263	SER	ALA	engineered mutation	UNP P36544
C	268	SER	VAL	engineered mutation	UNP P36544
C	270	SER	LEU	engineered mutation	UNP P36544
C	474	GLU	ALA	engineered mutation	UNP P36544
D	203	SER	-	expression tag	UNP P36544
D	204	ASN	-	expression tag	UNP P36544
D	205	ALA	-	expression tag	UNP P36544
D	206	GLU	-	expression tag	UNP P36544
D	207	GLU	-	expression tag	UNP P36544
D	208	GLU	-	expression tag	UNP P36544
D	263	SER	ALA	engineered mutation	UNP P36544
D	268	SER	VAL	engineered mutation	UNP P36544
D	270	SER	LEU	engineered mutation	UNP P36544
D	474	GLU	ALA	engineered mutation	UNP P36544
E	203	SER	-	expression tag	UNP P36544
E	204	ASN	-	expression tag	UNP P36544
E	205	ALA	-	expression tag	UNP P36544
E	206	GLU	-	expression tag	UNP P36544
E	207	GLU	-	expression tag	UNP P36544
E	208	GLU	-	expression tag	UNP P36544
E	263	SER	ALA	engineered mutation	UNP P36544
E	268	SER	VAL	engineered mutation	UNP P36544
E	270	SER	LEU	engineered mutation	UNP P36544
E	474	GLU	ALA	engineered mutation	UNP P36544

- Molecule 2 is (2aE,4E,5'S,6S,6'R,7S,8E,11R,13R,15S,17aR,20R,20aR,20bS)-6'-[(2S)-butan-2-yl]-20,20b-dihydroxy-5',6,8,19-tetramethyl-17'-oxo-3',4',5',6,6',10,11,14,15,17,17a,20,20a,20b-tetradecahydro-2H,7H-spiro[11,15-methanofuro[4,3,2-pq][2,6]benzodioxacyclooctadecine-1,3,2'-pyran]-7-yl 2,6-dideoxy-4-O-(2,6-dideoxy-3-O-methyl-alpha-L-arabino-hexopyranosyl)-3-O-methyl-alpha-L-arabino-hexopyranoside (three-letter code: IVM) (formula: C₄₈H₇₄O₁₄) (labeled as "Ligand of Interest" by depositor).



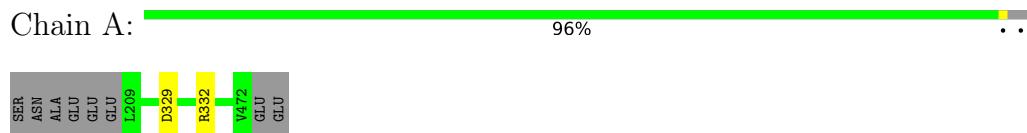
Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	O
			136	48	74	14
2	A	1	Total	C	H	O
			136	48	74	14
2	B	1	Total	C	H	O
			136	48	74	14
2	C	1	Total	C	H	O
			136	48	74	14
2	D	1	Total	C	H	O
			136	48	74	14

4 Residue-property plots

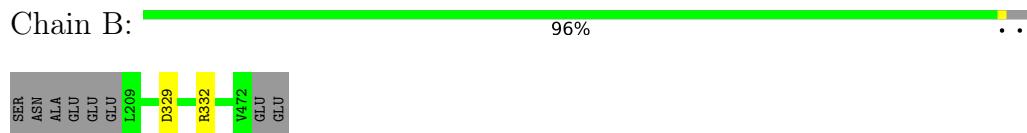
4.1 Average score per residue in the NMR ensemble

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.

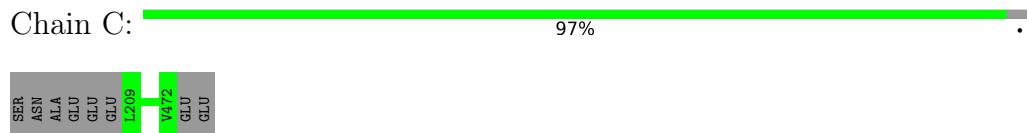
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



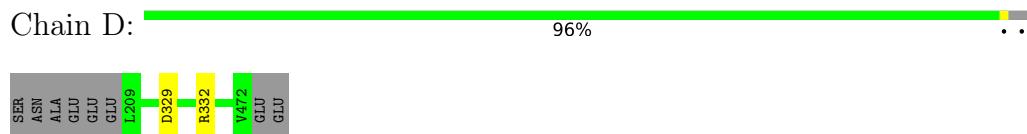
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



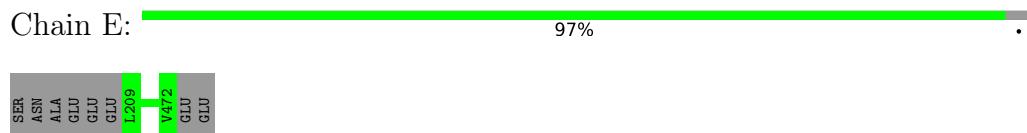
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



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- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

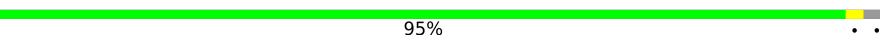


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

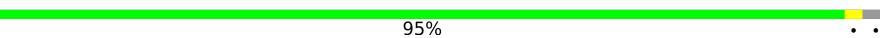
4.2.1 Score per residue for model 1

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain A:  95%



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain B:  95%



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain C:  94%



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain D:  94%



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain E:  95%



4.2.2 Score per residue for model 2

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain A:  96%



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain B: 94%



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain C: 96%



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain D: 95%



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain E: 94%



4.2.3 Score per residue for model 3

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain A: 96%

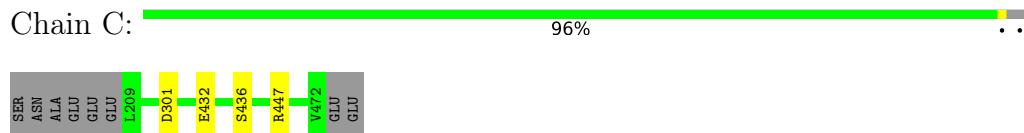


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

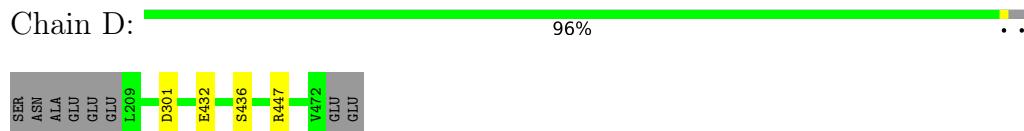
Chain B: 95%



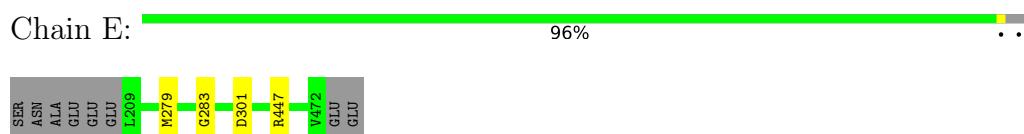
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

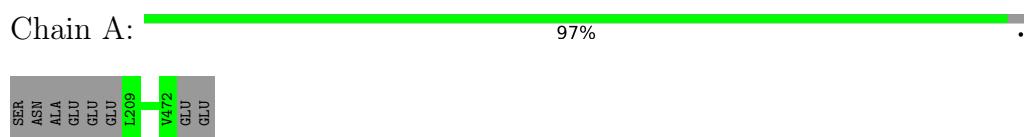


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

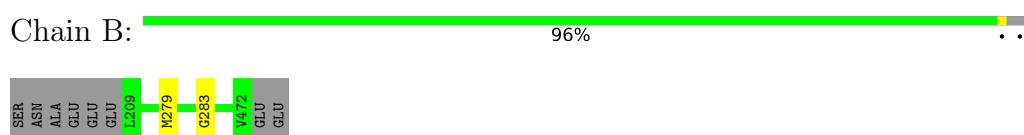


4.2.4 Score per residue for model 4

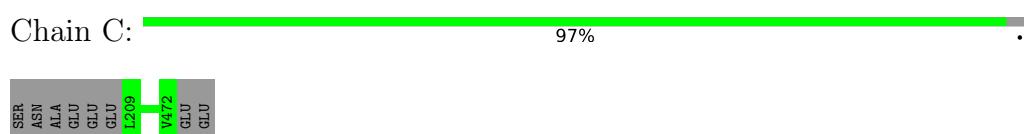
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



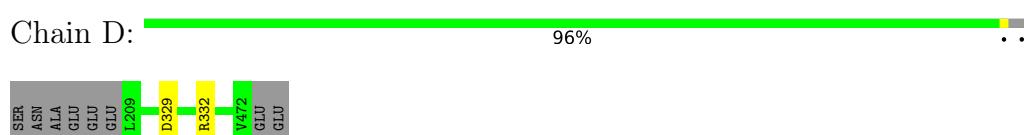
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



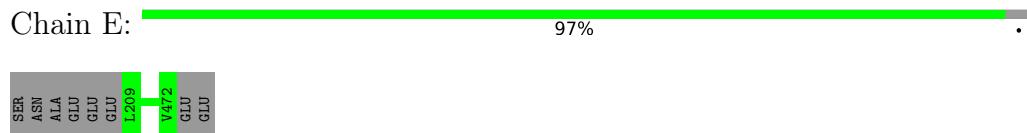
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

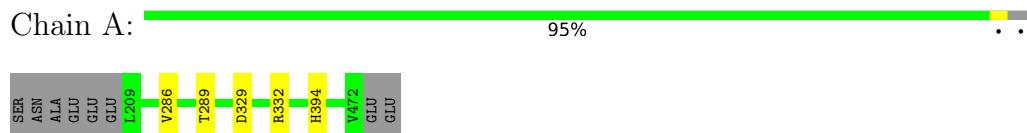


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

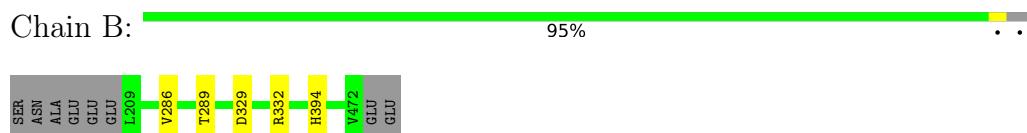


4.2.5 Score per residue for model 5

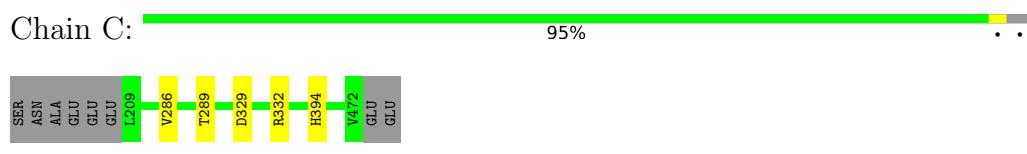
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



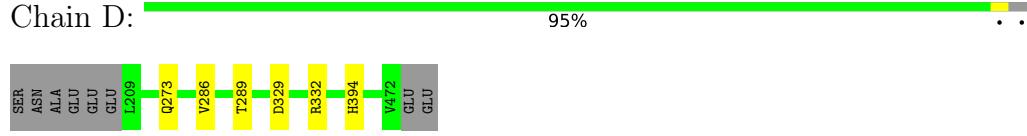
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



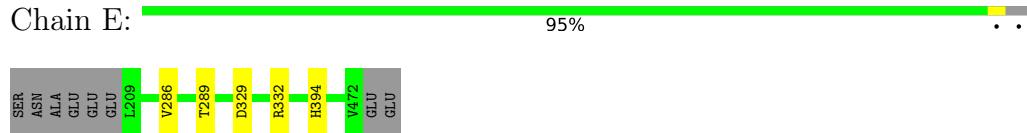
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



4.2.6 Score per residue for model 6

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7





- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain B: 96% ..



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain C: 96% ..



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain D: 96% ..



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain E: 97% ..



4.2.7 Score per residue for model 7

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain A: 96% ..

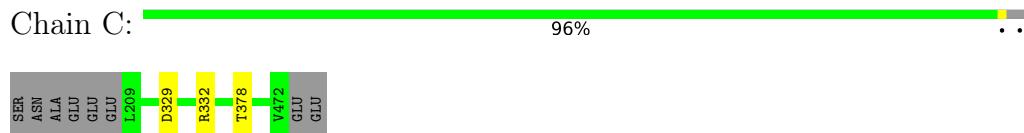


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

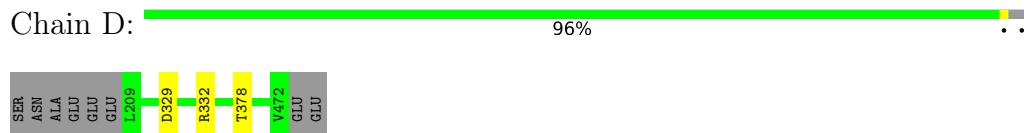
Chain B: 95% ..



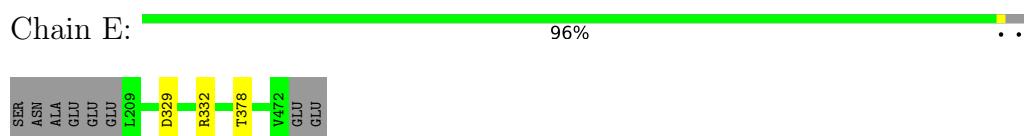
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

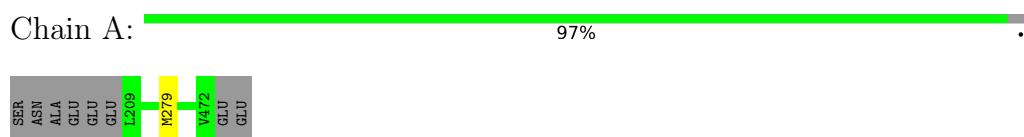


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

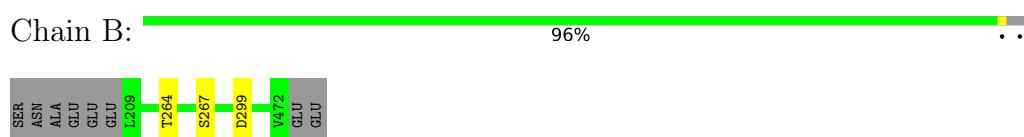


4.2.8 Score per residue for model 8

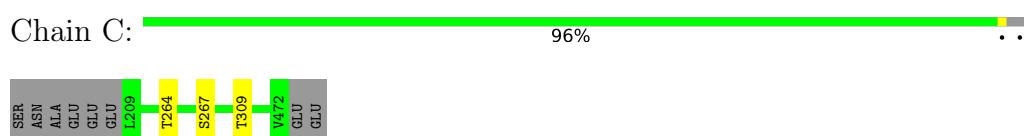
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



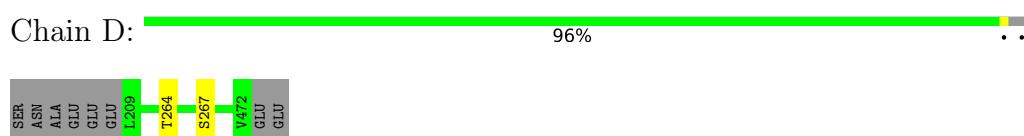
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



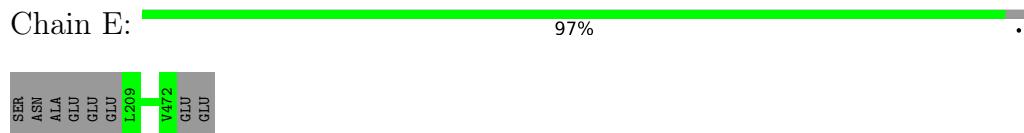
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

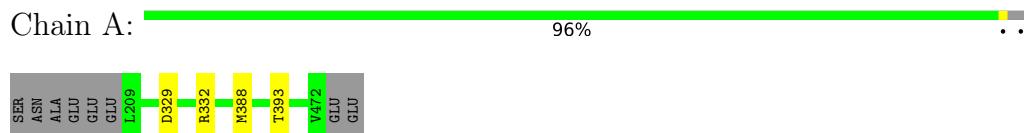


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

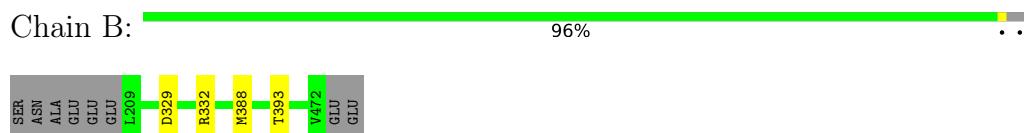


4.2.9 Score per residue for model 9

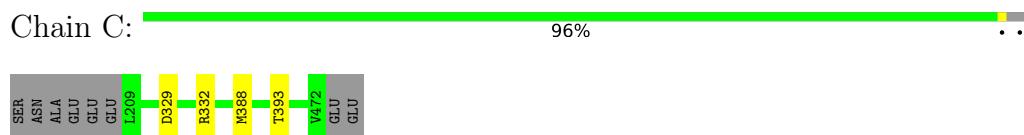
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



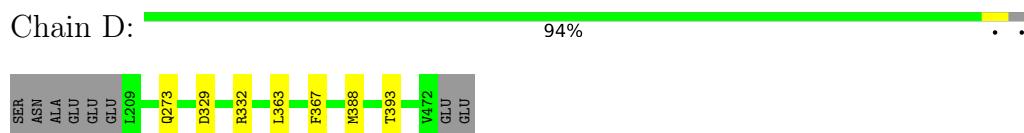
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



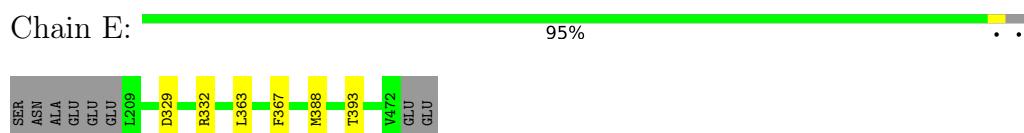
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



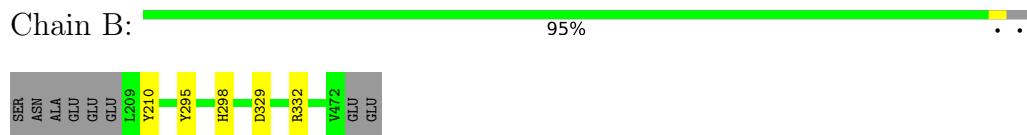
4.2.10 Score per residue for model 10

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

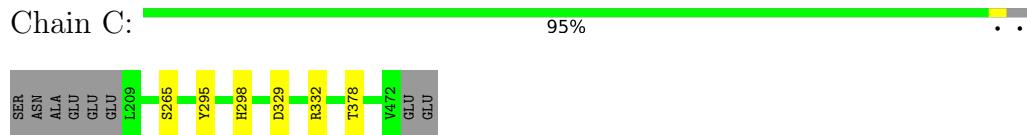




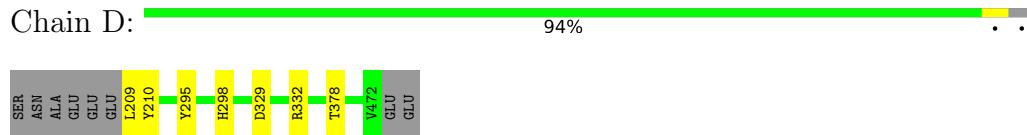
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



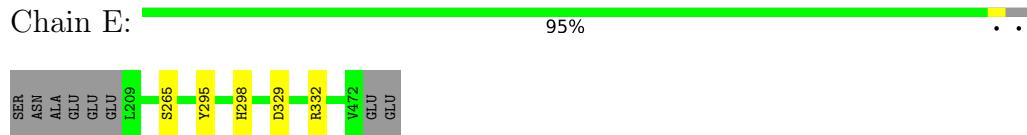
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

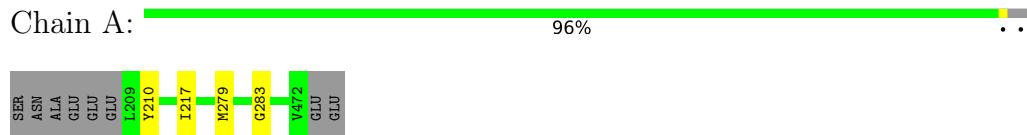


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

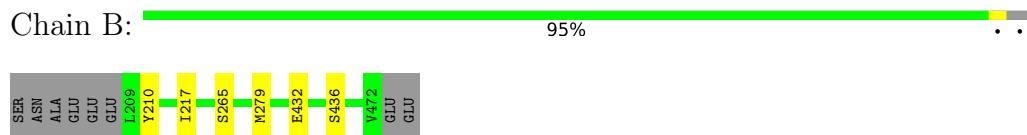


4.2.11 Score per residue for model 11 (medoid)

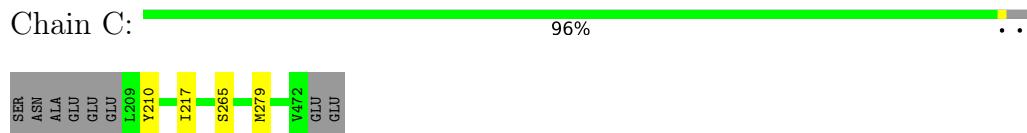
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



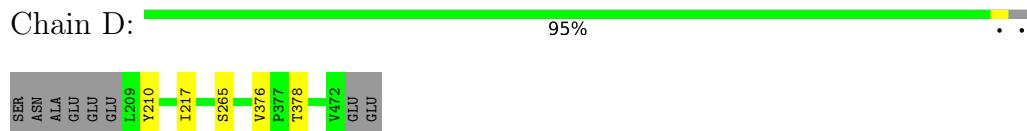
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



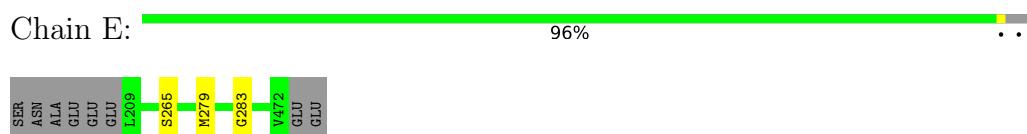
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

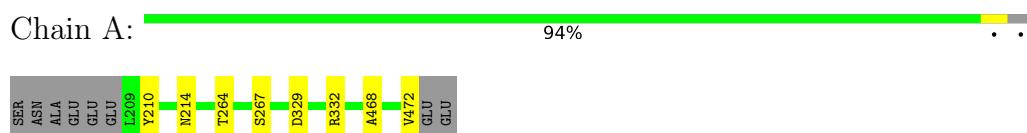


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

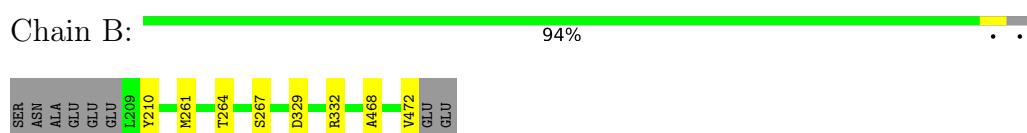


4.2.12 Score per residue for model 12

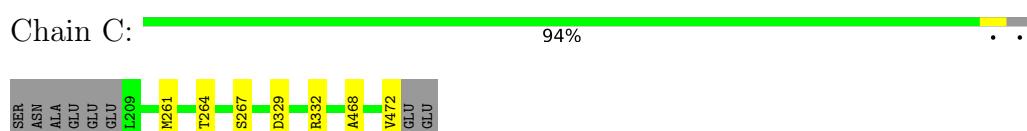
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



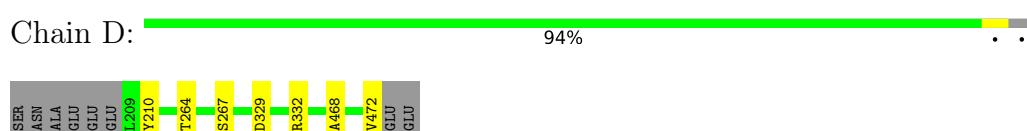
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



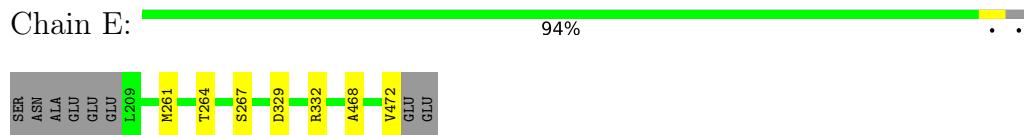
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

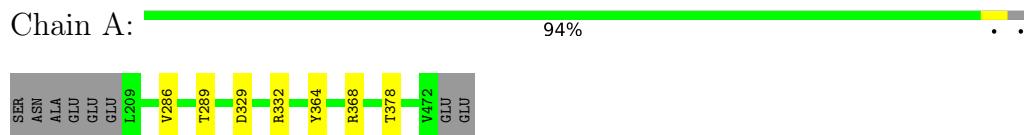


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

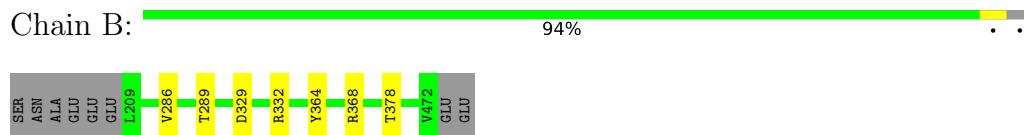


4.2.13 Score per residue for model 13

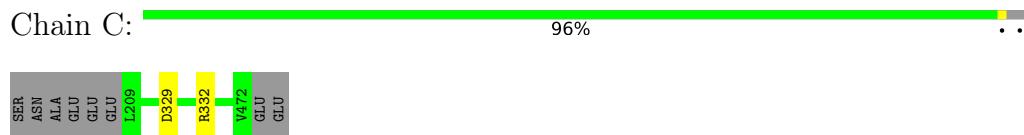
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



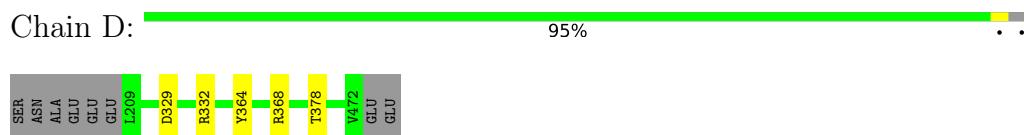
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



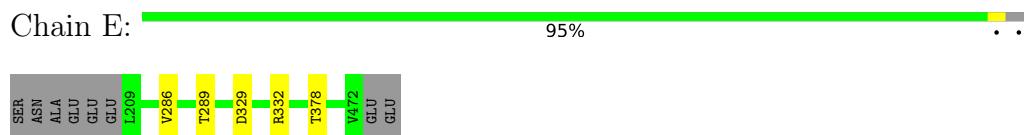
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



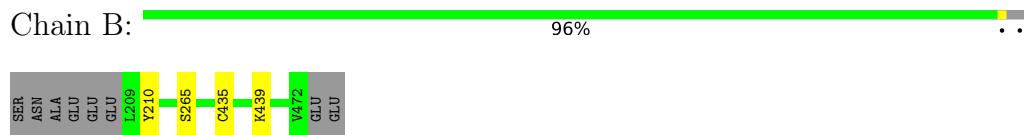
4.2.14 Score per residue for model 14

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

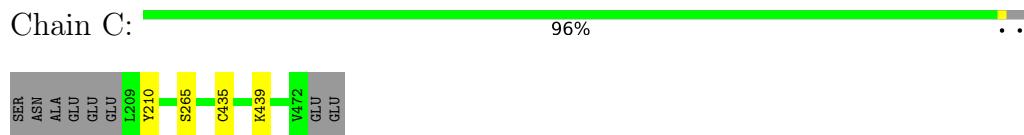




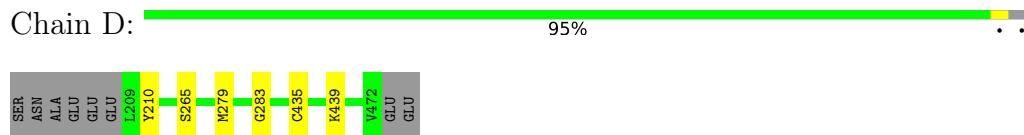
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



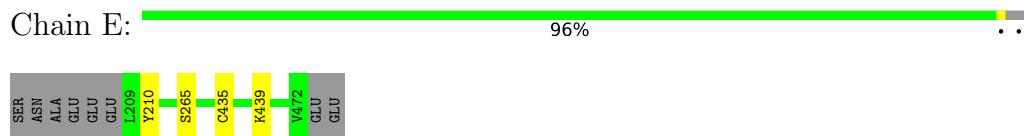
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

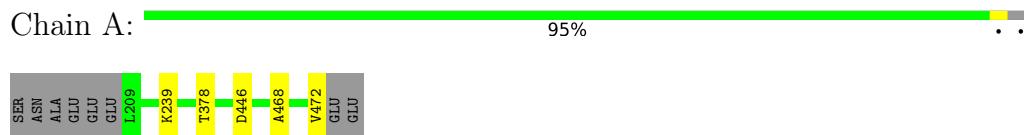


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

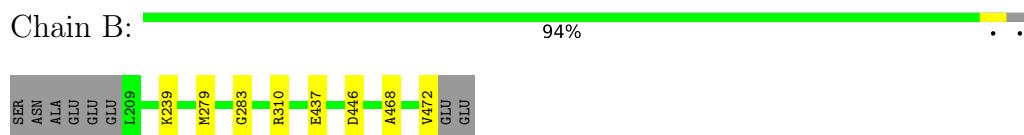


4.2.15 Score per residue for model 15

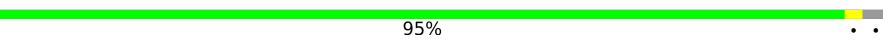
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

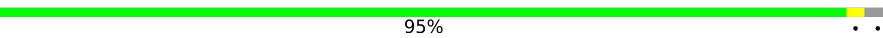


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain C:  95%

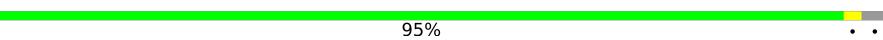


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain D:  95%



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain E:  95%



5 Refinement protocol and experimental data overview i

The models were refined using the following method: *na, na*.

Of the 1000 calculated structures, 15 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
CS-ROSETTA	structure calculation	3.17
Rosetta	structure calculation	3.7
Rosetta	refinement	3.7
MolProbity	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	2107
Number of shifts mapped to atoms	2107
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	12%

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: IVM

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2020	2062	2054	2±1
1	B	2020	2062	2054	3±1
1	C	2020	2062	2054	2±1
1	D	2020	2062	2054	3±1
1	E	2020	2062	2054	2±1
2	A	124	148	148	3±1
2	B	62	74	74	2±1
2	C	62	74	74	2±1
2	D	62	74	74	2±1
All	All	156150	160200	159600	292

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:501:IVM:O9	2:A:501:IVM:C40	1.45	1.65	8	7
2:A:502:IVM:C40	2:A:502:IVM:O9	1.45	1.64	4	15
2:D:501:IVM:C40	2:D:501:IVM:O9	1.45	1.65	8	7
2:D:501:IVM:O9	2:D:501:IVM:C40	1.45	1.64	15	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:501:IVM:C40	2:C:501:IVM:O9	1.44	1.65	1	15
2:A:501:IVM:C40	2:A:501:IVM:O9	1.43	1.64	1	8
2:B:501:IVM:C40	2:B:501:IVM:O9	1.43	1.65	5	15
1:D:264:THR:OG1	1:D:267:SER:O	0.75	2.04	12	2
1:E:264:THR:OG1	1:E:267:SER:O	0.75	2.04	12	1
1:B:264:THR:OG1	1:B:267:SER:O	0.74	2.04	12	2
1:A:264:THR:OG1	1:A:267:SER:O	0.71	2.09	12	1
1:E:239:LYS:NZ	1:E:446:ASP:OD1	0.70	2.25	15	1
1:D:239:LYS:NZ	1:D:446:ASP:OD1	0.69	2.25	15	1
1:C:264:THR:OG1	1:C:267:SER:O	0.68	2.07	12	2
1:B:239:LYS:NZ	1:B:446:ASP:OD1	0.67	2.27	15	1
1:C:239:LYS:NZ	1:C:446:ASP:OD1	0.66	2.28	15	1
1:A:432:GLU:OE2	1:A:439:LYS:NZ	0.61	2.27	2	1
2:D:501:IVM:H38	2:D:501:IVM:C46	0.60	2.26	6	1
1:C:432:GLU:OE2	1:C:439:LYS:NZ	0.59	2.33	2	1
1:C:432:GLU:O	1:C:436:SER:N	0.59	2.36	2	2
1:B:432:GLU:OE2	1:B:439:LYS:NZ	0.59	2.30	2	1
1:E:432:GLU:O	1:E:436:SER:N	0.58	2.36	2	1
1:A:432:GLU:O	1:A:436:SER:N	0.58	2.36	2	2
2:A:502:IVM:C46	2:A:502:IVM:H38	0.58	2.28	3	3
1:C:447:ARG:NH1	1:D:301:ASP:OD2	0.58	2.37	3	1
1:D:432:GLU:O	1:D:436:SER:N	0.57	2.37	2	2
2:A:501:IVM:H38	2:A:501:IVM:C46	0.57	2.28	10	3
2:C:501:IVM:C46	2:C:501:IVM:H38	0.57	2.29	9	3
1:B:432:GLU:O	1:B:436:SER:N	0.57	2.38	2	4
1:B:329:ASP:O	1:B:332:ARG:NE	0.56	2.38	1	8
1:E:329:ASP:O	1:E:332:ARG:NE	0.56	2.38	1	7
1:D:329:ASP:O	1:D:332:ARG:NE	0.56	2.38	1	9
1:A:447:ARG:NH1	1:B:301:ASP:OD2	0.56	2.36	3	1
1:C:329:ASP:O	1:C:332:ARG:NE	0.56	2.39	1	7
1:A:301:ASP:OD2	1:E:447:ARG:NH1	0.55	2.37	3	1
1:A:329:ASP:O	1:A:332:ARG:NE	0.55	2.40	13	8
2:D:501:IVM:C46	2:D:501:IVM:H38	0.55	2.32	10	3
1:D:447:ARG:NH1	1:E:301:ASP:OD2	0.55	2.36	3	1
1:E:432:GLU:OE2	1:E:439:LYS:NZ	0.54	2.30	2	1
1:D:432:GLU:OE2	1:D:439:LYS:NZ	0.54	2.31	2	1
1:B:447:ARG:NH1	1:C:301:ASP:OD2	0.54	2.37	3	1
1:A:239:LYS:NZ	1:A:446:ASP:OD1	0.54	2.35	15	1
2:B:501:IVM:C46	2:B:501:IVM:H38	0.54	2.33	1	4
2:B:501:IVM:H38	2:B:501:IVM:C46	0.54	2.33	6	1
1:C:210:TYR:N	1:D:265:SER:O	0.54	2.41	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:502:IVM:H38	2:A:502:IVM:C46	0.54	2.33	6	1
1:A:265:SER:O	1:E:210:TYR:N	0.54	2.39	14	1
2:B:501:IVM:H38	2:B:501:IVM:O12	0.53	2.03	6	1
1:A:286:VAL:O	1:A:289:THR:OG1	0.52	2.23	5	2
1:D:286:VAL:O	1:D:289:THR:OG1	0.52	2.25	5	1
1:C:286:VAL:O	1:C:289:THR:OG1	0.52	2.26	5	1
2:C:501:IVM:H38	2:C:501:IVM:C46	0.52	2.35	6	1
1:B:210:TYR:N	1:C:265:SER:O	0.51	2.43	11	4
1:A:295:TYR:O	1:A:298:HIS:ND1	0.51	2.44	10	1
1:D:210:TYR:N	1:E:265:SER:O	0.51	2.43	14	4
1:C:295:TYR:O	1:C:298:HIS:ND1	0.51	2.44	10	1
1:E:295:TYR:O	1:E:298:HIS:ND1	0.51	2.44	10	1
1:B:217:ILE:HG23	2:B:501:IVM:H4B	0.51	1.82	11	1
1:D:295:TYR:O	1:D:298:HIS:ND1	0.51	2.43	10	1
1:A:210:TYR:N	1:B:265:SER:O	0.50	2.45	14	3
1:B:295:TYR:O	1:B:298:HIS:ND1	0.50	2.44	10	1
1:B:286:VAL:O	1:B:289:THR:OG1	0.50	2.26	5	2
2:D:501:IVM:C46	2:D:501:IVM:C38	0.50	2.90	6	3
1:C:217:ILE:HG23	2:C:501:IVM:H4B	0.50	1.83	11	1
1:E:286:VAL:O	1:E:289:THR:OG1	0.50	2.29	5	2
1:B:388:MET:SD	1:B:393:THR:OG1	0.49	2.66	1	2
1:A:217:ILE:HG23	2:A:502:IVM:H4B	0.49	1.84	11	1
1:D:217:ILE:HG23	2:D:501:IVM:H4B	0.49	1.85	11	1
2:C:501:IVM:C38	2:C:501:IVM:C46	0.48	2.91	13	2
1:D:388:MET:SD	1:D:393:THR:OG1	0.48	2.67	9	2
2:B:501:IVM:C46	2:B:501:IVM:C38	0.48	2.92	7	4
1:B:210:TYR:OH	1:C:261:MET:SD	0.48	2.65	12	1
1:E:388:MET:SD	1:E:393:THR:OG1	0.48	2.66	9	2
2:A:502:IVM:C46	2:A:502:IVM:C38	0.48	2.92	13	4
1:E:394:HIS:ND1	1:E:394:HIS:O	0.48	2.47	5	1
1:A:468:ALA:O	1:A:472:VAL:N	0.48	2.47	15	3
1:C:388:MET:SD	1:C:393:THR:OG1	0.47	2.68	9	2
1:A:210:TYR:OH	1:B:261:MET:SD	0.47	2.70	12	1
2:D:501:IVM:C44	1:E:279:MET:CE	0.47	2.92	11	1
1:C:435:CYS:O	1:C:439:LYS:N	0.47	2.45	14	1
1:D:435:CYS:O	1:D:439:LYS:N	0.47	2.46	14	1
1:B:394:HIS:O	1:B:394:HIS:ND1	0.47	2.47	5	1
2:A:501:IVM:C46	2:A:501:IVM:C38	0.47	2.93	15	3
1:B:435:CYS:O	1:B:439:LYS:N	0.47	2.45	14	1
1:C:394:HIS:O	1:C:394:HIS:ND1	0.47	2.48	5	1
2:D:501:IVM:C38	2:D:501:IVM:C46	0.47	2.92	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:394:HIS:O	1:D:394:HIS:ND1	0.47	2.48	5	1
1:B:468:ALA:O	1:B:472:VAL:N	0.47	2.48	15	3
1:A:388:MET:SD	1:A:393:THR:OG1	0.47	2.68	9	2
1:A:394:HIS:ND1	1:A:394:HIS:O	0.46	2.47	5	1
2:C:501:IVM:C46	2:C:501:IVM:C38	0.46	2.92	6	3
1:C:468:ALA:O	1:C:472:VAL:N	0.46	2.49	15	3
1:E:279:MET:O	1:E:283:GLY:N	0.45	2.48	11	2
2:C:501:IVM:H18	1:D:273:GLN:OE1	0.45	2.12	9	2
1:A:210:TYR:O	1:A:214:ASN:ND2	0.45	2.49	12	1
1:E:468:ALA:O	1:E:472:VAL:N	0.45	2.49	15	2
1:D:276:ALA:HB2	2:D:501:IVM:H37	0.45	1.88	2	1
1:D:468:ALA:O	1:D:472:VAL:N	0.45	2.49	15	2
2:A:501:IVM:C38	2:A:501:IVM:C46	0.45	2.94	13	1
2:C:501:IVM:H18	1:D:273:GLN:HG3	0.45	1.89	5	1
1:A:364:TYR:O	1:A:368:ARG:N	0.45	2.48	13	1
2:D:501:IVM:H38	2:D:501:IVM:O12	0.44	2.12	6	1
1:A:435:CYS:O	1:A:439:LYS:N	0.44	2.46	14	1
2:B:501:IVM:C44	1:C:279:MET:CE	0.44	2.96	11	1
1:A:279:MET:O	1:A:283:GLY:N	0.44	2.50	11	1
2:C:501:IVM:H48	1:D:279:MET:SD	0.43	2.52	1	1
2:A:502:IVM:H38	2:A:502:IVM:O12	0.43	2.13	3	1
1:D:364:TYR:O	1:D:368:ARG:N	0.43	2.49	13	1
2:A:501:IVM:C46	2:A:501:IVM:H38	0.43	2.43	13	1
1:E:378:THR:N	1:E:379:PRO:CD	0.43	2.81	2	1
1:D:382:GLY:O	1:D:386:GLY:N	0.43	2.52	2	1
1:E:435:CYS:O	1:E:439:LYS:N	0.42	2.46	14	1
1:B:382:GLY:O	1:B:386:GLY:N	0.42	2.53	2	1
2:B:501:IVM:H18	1:C:273:GLN:OE1	0.42	2.15	15	1
2:B:501:IVM:H48	1:C:279:MET:SD	0.41	2.55	1	1
1:E:400:HIS:N	1:E:403:GLN:O	0.41	2.51	2	1
1:B:310:ARG:NH1	1:B:437:GLU:OE1	0.41	2.53	15	1
2:D:501:IVM:H18	1:E:273:GLN:OE1	0.41	2.15	15	1
1:B:279:MET:O	1:B:283:GLY:N	0.41	2.46	4	2
1:B:364:TYR:O	1:B:368:ARG:N	0.41	2.52	13	1
1:D:376:VAL:O	1:D:378:THR:N	0.41	2.54	11	1
1:E:363:LEU:O	1:E:367:PHE:N	0.41	2.53	9	1
1:D:209:LEU:N	1:E:265:SER:O	0.40	2.54	10	1
1:D:210:TYR:OH	1:E:261:MET:SD	0.40	2.75	12	1
1:D:279:MET:O	1:D:283:GLY:N	0.40	2.49	14	1
1:B:376:VAL:HG12	1:B:378:THR:HG23	0.40	1.93	2	1
1:D:363:LEU:O	1:D:367:PHE:N	0.40	2.53	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:502:IVM:C44	1:B:279:MET:CE	0.40	2.99	11	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	262/272 (96%)	259±1 (99±1%)	3±1 (1±1%)	0±0 (0±0%)	100 100
1	B	262/272 (96%)	259±1 (99±1%)	3±1 (1±1%)	0±0 (0±0%)	100 100
1	C	262/272 (96%)	259±1 (99±0%)	3±1 (1±0%)	0±0 (0±0%)	100 100
1	D	262/272 (96%)	259±1 (99±1%)	3±1 (1±1%)	0±0 (0±0%)	100 100
1	E	262/272 (96%)	259±1 (99±0%)	3±1 (1±0%)	0±0 (0±0%)	100 100
All	All	19650/20400 (96%)	19443 (99%)	207 (1%)	0 (0%)	100 100

There are no Ramachandran outliers.

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	227/234 (97%)	227±0 (100±0%)	0±0 (0±0%)	93 98
1	B	227/234 (97%)	227±0 (100±0%)	0±0 (0±0%)	93 98
1	C	227/234 (97%)	227±0 (100±0%)	0±0 (0±0%)	93 98
1	D	227/234 (97%)	227±0 (100±0%)	0±0 (0±0%)	93 98
1	E	227/234 (97%)	227±0 (100±0%)	0±0 (0±0%)	93 98
All	All	17025/17550 (97%)	17007 (100%)	18 (0%)	93 98

All 8 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	D	378	THR	4
1	A	378	THR	3
1	C	378	THR	3
1	E	378	THR	3
1	B	378	THR	2
1	A	279	MET	1
1	B	299	ASP	1
1	C	309	THR	1

6.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [\(i\)](#)

5 ligands are 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	IVM	A	501	-	65,68,68	3.79 ± 0.04	22 ± 0 ($34 \pm 0\%$)
2	IVM	A	502	-	65,68,68	3.80 ± 0.03	22 ± 0 ($34 \pm 0\%$)
2	IVM	D	501	-	65,68,68	3.80 ± 0.03	22 ± 1 ($34 \pm 0\%$)

Mol	Type	Chain	Res	Link	Counts	Bond lengths		
						RMSZ	#Z>2	
2	IVM	B	501	-	65,68,68	3.81±0.04	22±1 (34±1%)	
2	IVM	C	501	-	65,68,68	3.80±0.03	22±1 (34±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	Counts	Bond angles		
						RMSZ	#Z>2	
2	IVM	A	501	-	82,102,102	2.13±0.04	18±2 (21±2%)	
2	IVM	A	502	-	82,102,102	2.12±0.04	17±2 (21±2%)	
2	IVM	D	501	-	82,102,102	2.12±0.04	17±2 (20±2%)	
2	IVM	B	501	-	82,102,102	2.12±0.05	18±2 (21±2%)	
2	IVM	C	501	-	82,102,102	2.12±0.04	17±2 (20±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	IVM	B	501	-	-	0±0,45,141,141	1±0,6,7,7
2	IVM	A	501	-	-	0±0,45,141,141	1±0,6,7,7
2	IVM	C	501	-	-	0±0,45,141,141	1±0,6,7,7
2	IVM	D	501	-	-	0±0,45,141,141	1±0,6,7,7
2	IVM	A	502	-	-	0±0,45,141,141	1±0,6,7,7

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	D	501	IVM	C38-C39	17.53	1.56	1.33	7	15
2	B	501	IVM	C38-C39	17.40	1.56	1.33	3	15
2	C	501	IVM	C38-C39	17.38	1.56	1.33	10	15
2	A	502	IVM	C38-C39	17.35	1.56	1.33	10	15
2	A	501	IVM	C38-C39	17.35	1.56	1.33	14	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	D	501	IVM	O9-C40	13.79	1.65	1.43	7	15
2	A	501	IVM	O9-C40	13.75	1.65	1.43	9	15
2	B	501	IVM	O9-C40	13.74	1.65	1.43	3	15
2	A	502	IVM	O9-C40	13.74	1.65	1.43	12	15
2	C	501	IVM	O9-C40	13.73	1.65	1.43	3	15
2	B	501	IVM	C44-C43	13.01	1.49	1.33	1	15
2	A	501	IVM	C44-C43	13.00	1.49	1.33	3	15
2	C	501	IVM	C44-C43	12.99	1.49	1.33	8	15
2	A	502	IVM	C44-C43	12.93	1.49	1.33	3	15
2	D	501	IVM	C44-C43	12.93	1.49	1.33	10	15
2	A	501	IVM	C40-C39	6.25	1.61	1.50	3	15
2	C	501	IVM	C40-C39	6.20	1.61	1.50	14	15
2	B	501	IVM	C40-C39	6.19	1.61	1.50	4	15
2	A	502	IVM	C40-C39	6.16	1.61	1.50	10	15
2	D	501	IVM	C40-C39	6.16	1.61	1.50	4	15
2	D	501	IVM	C37-C36	5.53	1.55	1.33	5	15
2	A	502	IVM	C37-C36	5.52	1.55	1.33	12	15
2	A	501	IVM	C37-C36	5.52	1.55	1.33	2	15
2	B	501	IVM	C37-C36	5.51	1.55	1.33	12	15
2	C	501	IVM	C37-C36	5.50	1.55	1.33	10	15
2	A	502	IVM	C11-C6	5.20	1.60	1.52	6	15
2	C	501	IVM	C11-C6	5.19	1.60	1.52	3	15
2	D	501	IVM	C11-C6	5.17	1.60	1.52	3	15
2	B	501	IVM	C11-C6	5.13	1.59	1.52	9	15
2	A	501	IVM	C11-C6	5.09	1.59	1.52	5	15
2	B	501	IVM	O12-C46	4.88	1.45	1.34	13	15
2	A	502	IVM	O12-C46	4.76	1.45	1.34	7	15
2	C	501	IVM	O12-C46	4.76	1.45	1.34	5	15
2	A	501	IVM	O12-C46	4.74	1.45	1.34	10	15
2	D	501	IVM	O12-C46	4.74	1.45	1.34	13	15
2	B	501	IVM	C45-C44	4.33	1.56	1.51	10	15
2	D	501	IVM	C45-C44	4.21	1.55	1.51	10	15
2	A	501	IVM	C45-C44	4.20	1.55	1.51	10	15
2	C	501	IVM	C45-C44	4.17	1.55	1.51	1	15
2	D	501	IVM	C16-C17	4.13	1.38	1.33	2	15
2	A	502	IVM	C16-C17	4.09	1.38	1.33	8	15
2	A	502	IVM	C45-C44	4.06	1.55	1.51	3	15
2	D	501	IVM	C42-C43	4.06	1.62	1.50	13	15
2	A	501	IVM	C16-C17	4.05	1.38	1.33	7	15
2	C	501	IVM	C16-C17	4.05	1.38	1.33	8	15
2	A	501	IVM	C42-C43	4.02	1.62	1.50	2	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	501	IVM	C16-C17	4.02	1.38	1.33	5	15
2	C	501	IVM	C37-C38	4.00	1.55	1.43	14	15
2	A	502	IVM	C37-C38	4.00	1.55	1.43	10	15
2	A	502	IVM	C42-C43	4.00	1.62	1.50	15	15
2	B	501	IVM	C42-C43	3.97	1.61	1.50	8	15
2	C	501	IVM	C42-C43	3.96	1.61	1.50	10	15
2	A	501	IVM	C37-C38	3.96	1.55	1.43	8	15
2	B	501	IVM	C37-C38	3.96	1.55	1.43	5	15
2	D	501	IVM	C37-C38	3.95	1.55	1.43	5	15
2	A	502	IVM	C21-C20	3.94	1.59	1.51	7	15
2	C	501	IVM	C21-C20	3.92	1.59	1.51	7	15
2	A	501	IVM	C21-C20	3.91	1.59	1.51	6	15
2	D	501	IVM	C21-C20	3.90	1.59	1.51	7	15
2	B	501	IVM	C21-C20	3.87	1.59	1.51	4	15
2	D	501	IVM	C41-C42	3.70	1.45	1.51	10	15
2	A	501	IVM	C41-C42	3.70	1.45	1.51	10	15
2	B	501	IVM	C41-C42	3.69	1.45	1.51	1	15
2	C	501	IVM	C41-C42	3.67	1.45	1.51	1	15
2	D	501	IVM	C15-C16	3.66	1.57	1.50	6	15
2	C	501	IVM	C15-C16	3.63	1.57	1.50	6	15
2	A	502	IVM	C41-C42	3.62	1.45	1.51	3	15
2	A	501	IVM	C15-C16	3.59	1.57	1.50	12	15
2	A	502	IVM	C15-C16	3.59	1.57	1.50	8	15
2	B	501	IVM	C15-C16	3.54	1.57	1.50	6	15
2	C	501	IVM	C21-C22	3.15	1.58	1.52	12	15
2	A	501	IVM	C21-C22	3.14	1.58	1.52	7	15
2	A	502	IVM	C21-C22	3.14	1.58	1.52	10	15
2	D	501	IVM	C21-C22	3.13	1.57	1.52	2	15
2	B	501	IVM	C21-C22	3.11	1.57	1.52	8	15
2	A	501	IVM	C48-C43	2.97	1.56	1.50	1	15
2	C	501	IVM	C48-C43	2.95	1.56	1.50	5	15
2	B	501	IVM	C48-C43	2.95	1.56	1.50	10	15
2	A	502	IVM	C48-C43	2.94	1.56	1.50	8	15
2	D	501	IVM	C48-C43	2.92	1.56	1.50	12	15
2	B	501	IVM	C26-C25	2.90	1.57	1.51	9	15
2	A	501	IVM	C26-C25	2.89	1.57	1.51	3	15
2	A	502	IVM	C26-C25	2.89	1.57	1.51	12	15
2	D	501	IVM	C26-C25	2.87	1.57	1.51	4	15
2	C	501	IVM	C26-C25	2.86	1.57	1.51	9	15
2	C	501	IVM	C18-C17	2.83	1.55	1.50	10	15
2	A	501	IVM	C18-C17	2.81	1.55	1.50	3	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	501	IVM	C18-C17	2.80	1.55	1.50	13	15
2	A	502	IVM	C18-C17	2.79	1.55	1.50	8	15
2	D	501	IVM	C18-C17	2.78	1.55	1.50	8	15
2	D	501	IVM	O9-C41	2.70	1.48	1.44	7	15
2	B	501	IVM	O9-C41	2.70	1.48	1.44	3	15
2	B	501	IVM	C11-C12	2.56	1.56	1.51	10	15
2	C	501	IVM	C11-C12	2.56	1.56	1.51	14	15
2	C	501	IVM	O9-C41	2.56	1.48	1.44	13	15
2	A	501	IVM	C19-C17	2.55	1.55	1.51	7	15
2	C	501	IVM	C19-C17	2.55	1.55	1.51	12	15
2	D	501	IVM	C11-C12	2.54	1.56	1.51	12	15
2	A	502	IVM	C11-C12	2.53	1.56	1.51	5	15
2	A	501	IVM	O9-C41	2.52	1.48	1.44	14	15
2	D	501	IVM	C19-C17	2.52	1.55	1.51	15	15
2	A	501	IVM	C11-C12	2.51	1.56	1.51	8	15
2	A	501	IVM	C47-C41	2.50	1.51	1.54	3	7
2	B	501	IVM	C19-C17	2.50	1.55	1.51	15	15
2	A	502	IVM	O9-C41	2.47	1.48	1.44	4	15
2	A	502	IVM	C19-C17	2.46	1.55	1.51	4	15
2	B	501	IVM	C47-C41	2.44	1.51	1.54	1	6
2	C	501	IVM	C47-C41	2.40	1.51	1.54	1	5
2	A	502	IVM	C47-C41	2.38	1.51	1.54	8	7
2	D	501	IVM	C47-C41	2.32	1.51	1.54	10	8
2	A	502	IVM	O12-C12	2.13	1.41	1.46	2	15
2	C	501	IVM	O12-C12	2.13	1.41	1.46	14	14
2	A	501	IVM	O12-C12	2.11	1.41	1.46	8	15
2	D	501	IVM	O12-C12	2.10	1.41	1.46	4	13
2	B	501	IVM	O12-C12	2.10	1.41	1.46	4	13

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	501	IVM	O1-C6-C11	7.56	95.26	106.26	14	15
2	A	501	IVM	O1-C6-C11	7.52	95.31	106.26	14	15
2	A	502	IVM	O1-C6-C11	7.46	95.40	106.26	14	15
2	C	501	IVM	O1-C6-C11	7.39	95.51	106.26	12	15
2	D	501	IVM	O1-C6-C11	7.29	95.65	106.26	8	15
2	B	501	IVM	C34-C36-C37	7.09	111.24	126.16	15	15
2	C	501	IVM	C34-C36-C37	7.09	111.24	126.16	15	15
2	B	501	IVM	O12-C46-C45	7.08	121.22	110.97	14	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	501	IVM	C34-C36-C37	7.07	111.28	126.16	7	15
2	D	501	IVM	C34-C36-C37	7.07	111.28	126.16	15	15
2	A	502	IVM	C34-C36-C37	7.06	111.31	126.16	5	15
2	D	501	IVM	O12-C46-C45	7.04	121.16	110.97	14	15
2	A	502	IVM	O12-C46-C45	6.95	121.03	110.97	14	15
2	A	501	IVM	O12-C46-C45	6.81	120.83	110.97	14	15
2	C	501	IVM	O12-C46-C45	6.56	120.47	110.97	5	15
2	A	501	IVM	C37-C38-C39	6.07	110.88	130.07	7	15
2	D	501	IVM	C37-C38-C39	6.02	111.03	130.07	13	15
2	C	501	IVM	C37-C38-C39	5.98	111.17	130.07	12	15
2	B	501	IVM	C37-C38-C39	5.97	111.20	130.07	15	15
2	A	502	IVM	C37-C38-C39	5.93	111.31	130.07	1	15
2	A	502	IVM	O14-C6-C7	5.43	122.91	107.37	4	15
2	C	501	IVM	O14-C6-C7	5.37	122.76	107.37	4	15
2	B	501	IVM	O14-C6-C7	5.35	122.70	107.37	4	15
2	D	501	IVM	O14-C6-C7	5.34	122.65	107.37	14	15
2	A	501	IVM	O14-C6-C7	5.31	122.59	107.37	7	15
2	D	501	IVM	C38-C37-C36	5.24	111.82	124.53	6	15
2	A	501	IVM	C38-C37-C36	5.23	111.84	124.53	10	15
2	B	501	IVM	C38-C37-C36	5.19	111.93	124.53	6	15
2	C	501	IVM	C38-C37-C36	5.13	112.09	124.53	6	15
2	A	502	IVM	C38-C37-C36	5.06	112.26	124.53	3	15
2	C	501	IVM	C40-O9-C41	4.94	97.04	107.88	14	15
2	A	502	IVM	O14-C6-O1	4.89	98.47	109.88	4	15
2	C	501	IVM	O14-C6-O1	4.81	98.67	109.88	4	15
2	B	501	IVM	O14-C6-O1	4.80	98.67	109.88	4	15
2	D	501	IVM	O14-C6-O1	4.80	98.69	109.88	4	15
2	A	501	IVM	C3-C5-C9	4.78	107.95	116.50	10	15
2	A	501	IVM	O14-C6-O1	4.73	98.85	109.88	2	15
2	A	501	IVM	C40-O9-C41	4.73	97.50	107.88	12	15
2	D	501	IVM	C3-C5-C9	4.72	108.06	116.50	10	15
2	C	501	IVM	C3-C5-C9	4.71	108.08	116.50	6	15
2	A	502	IVM	C40-O9-C41	4.70	97.57	107.88	12	15
2	D	501	IVM	C40-O9-C41	4.70	97.57	107.88	12	15
2	A	502	IVM	C3-C5-C9	4.68	108.13	116.50	6	15
2	B	501	IVM	C40-O9-C41	4.68	97.61	107.88	1	15
2	B	501	IVM	C3-C5-C9	4.65	108.19	116.50	1	15
2	D	501	IVM	O9-C40-C39	3.83	102.19	105.73	7	5
2	B	501	IVM	O9-C40-C39	3.61	102.40	105.73	3	7
2	B	501	IVM	O11-C46-C45	3.48	119.10	125.05	14	15
2	D	501	IVM	O1-C5-C3	3.46	111.40	106.12	3	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	D	501	IVM	O11-C46-C45	3.44	119.16	125.05	14	15
2	C	501	IVM	O1-C5-C3	3.44	111.36	106.12	3	15
2	A	502	IVM	O11-C46-C45	3.43	119.17	125.05	14	15
2	A	502	IVM	O1-C5-C3	3.38	111.27	106.12	3	15
2	B	501	IVM	O1-C5-C3	3.37	111.26	106.12	3	15
2	A	501	IVM	O11-C46-C45	3.36	119.30	125.05	14	15
2	A	501	IVM	O1-C5-C3	3.36	111.24	106.12	5	15
2	C	501	IVM	O11-C46-C45	3.22	119.54	125.05	14	15
2	D	501	IVM	O14-C14-C15	3.19	108.89	105.82	3	8
2	B	501	IVM	O14-C14-C15	3.17	108.88	105.82	5	10
2	C	501	IVM	C42-C43-C44	3.02	114.93	120.46	4	3
2	A	502	IVM	C42-C43-C44	3.01	114.94	120.46	4	4
2	A	501	IVM	C42-C43-C44	2.99	114.98	120.46	14	6
2	D	501	IVM	C42-C43-C44	2.97	115.01	120.46	1	2
2	C	501	IVM	O14-C14-C15	2.91	108.63	105.82	3	8
2	A	502	IVM	O14-C14-C15	2.83	108.55	105.82	3	11
2	A	502	IVM	C13-C14-C15	2.78	109.48	113.21	8	12
2	D	501	IVM	C13-C14-C15	2.76	109.51	113.21	8	11
2	A	501	IVM	O14-C14-C15	2.76	108.48	105.82	5	10
2	B	501	IVM	C42-C43-C44	2.74	115.43	120.46	2	3
2	A	501	IVM	C13-C14-C15	2.72	109.56	113.21	7	12
2	B	501	IVM	C12-O12-C46	2.72	113.24	117.69	14	3
2	C	501	IVM	C13-C14-C15	2.71	109.58	113.21	8	11
2	A	502	IVM	O9-C40-C39	2.61	103.32	105.73	14	5
2	A	502	IVM	C12-O12-C46	2.60	113.44	117.69	14	2
2	B	501	IVM	C13-C14-C15	2.58	109.76	113.21	14	12
2	A	502	IVM	C6-O1-C5	2.57	110.71	114.27	4	1
2	C	501	IVM	C48-C43-C42	2.56	121.48	116.81	5	3
2	A	501	IVM	O9-C40-C39	2.54	103.38	105.73	11	5
2	D	501	IVM	C12-O12-C46	2.52	113.55	117.69	14	2
2	A	501	IVM	C48-C43-C42	2.52	121.39	116.81	4	6
2	C	501	IVM	O9-C40-C39	2.51	103.41	105.73	5	5
2	C	501	IVM	C34-C19-C17	2.51	108.89	113.89	5	12
2	A	501	IVM	C12-O12-C46	2.49	113.60	117.69	14	4
2	B	501	IVM	C48-C43-C42	2.47	121.30	116.81	11	3
2	C	501	IVM	C6-O1-C5	2.46	110.86	114.27	4	4
2	D	501	IVM	C48-C43-C42	2.44	121.25	116.81	11	3
2	B	501	IVM	C34-C19-C17	2.43	109.04	113.89	2	14
2	D	501	IVM	C34-C19-C17	2.43	109.05	113.89	1	11
2	A	501	IVM	C34-C19-C17	2.42	109.06	113.89	1	13
2	A	502	IVM	C48-C43-C42	2.42	121.21	116.81	11	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	502	IVM	C34-C19-C17	2.40	109.10	113.89	3	13
2	B	501	IVM	C33-C32-C24	2.31	109.89	113.41	8	15
2	C	501	IVM	C33-C32-C24	2.30	109.90	113.41	5	13
2	A	501	IVM	C33-C32-C24	2.29	109.91	113.41	1	14
2	D	501	IVM	O12-C46-O11	2.28	119.68	123.94	14	5
2	B	501	IVM	O12-C46-O11	2.28	119.68	123.94	14	4
2	D	501	IVM	C33-C32-C24	2.27	109.94	113.41	1	14
2	B	501	IVM	C6-O1-C5	2.23	111.18	114.27	4	3
2	A	502	IVM	C33-C32-C24	2.22	110.03	113.41	6	14
2	A	502	IVM	O12-C46-O11	2.21	119.80	123.94	14	6
2	D	501	IVM	C7-C8-C9	2.21	108.00	112.30	6	8
2	A	502	IVM	C7-C8-C9	2.20	108.02	112.30	5	8
2	D	501	IVM	C6-O1-C5	2.20	111.22	114.27	4	2
2	B	501	IVM	C7-C8-C9	2.19	108.04	112.30	6	9
2	C	501	IVM	C7-C8-C9	2.18	108.06	112.30	1	7
2	A	501	IVM	O12-C46-O11	2.18	119.87	123.94	14	9
2	A	501	IVM	C7-C8-C9	2.17	108.09	112.30	9	10
2	A	501	IVM	C31-C30-C29	2.15	109.10	113.07	5	15
2	A	502	IVM	C31-C30-C29	2.14	109.11	113.07	2	15
2	C	501	IVM	C31-C30-C29	2.14	109.11	113.07	8	15
2	B	501	IVM	C31-C30-C29	2.14	109.12	113.07	4	15
2	D	501	IVM	C31-C30-C29	2.13	109.13	113.07	9	15
2	C	501	IVM	O12-C46-O11	2.13	119.95	123.94	5	5
2	C	501	IVM	C12-O12-C46	2.11	114.23	117.69	14	2
2	A	501	IVM	C6-O1-C5	2.04	111.45	114.27	7	1
2	A	502	IVM	O13-C47-C41	2.02	107.00	111.74	1	1

There are no chirality outliers.

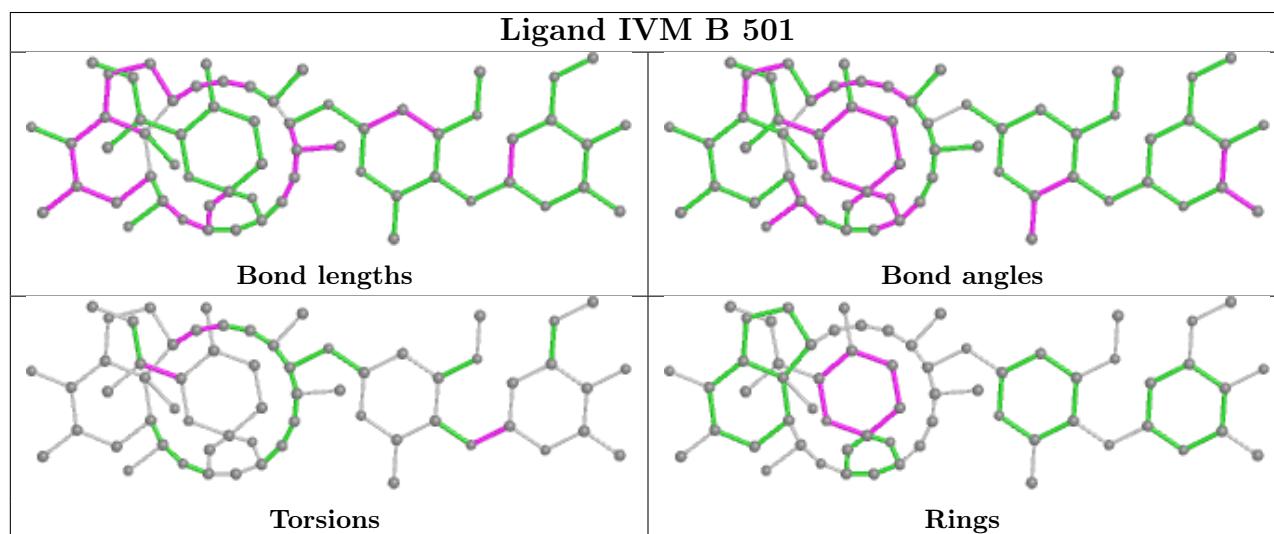
All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

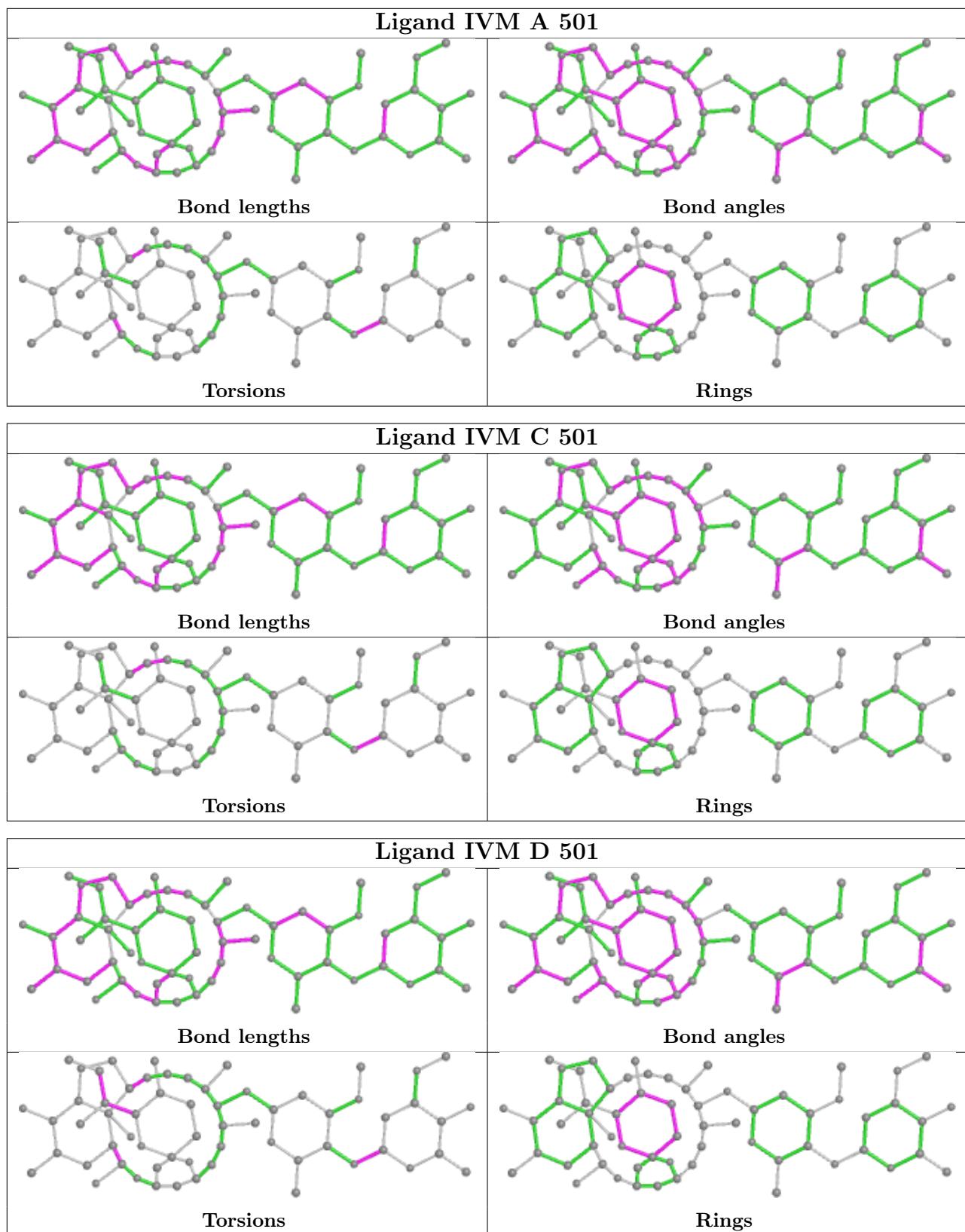
Mol	Chain	Res	Type	Atoms	Models (Total)
2	D	501	IVM	C37-C38-C39-C40	4
2	A	502	IVM	C37-C38-C39-C40	3
2	B	501	IVM	C37-C38-C39-C40	3
2	C	501	IVM	C37-C38-C39-C40	2
2	A	501	IVM	C37-C38-C39-C40	1

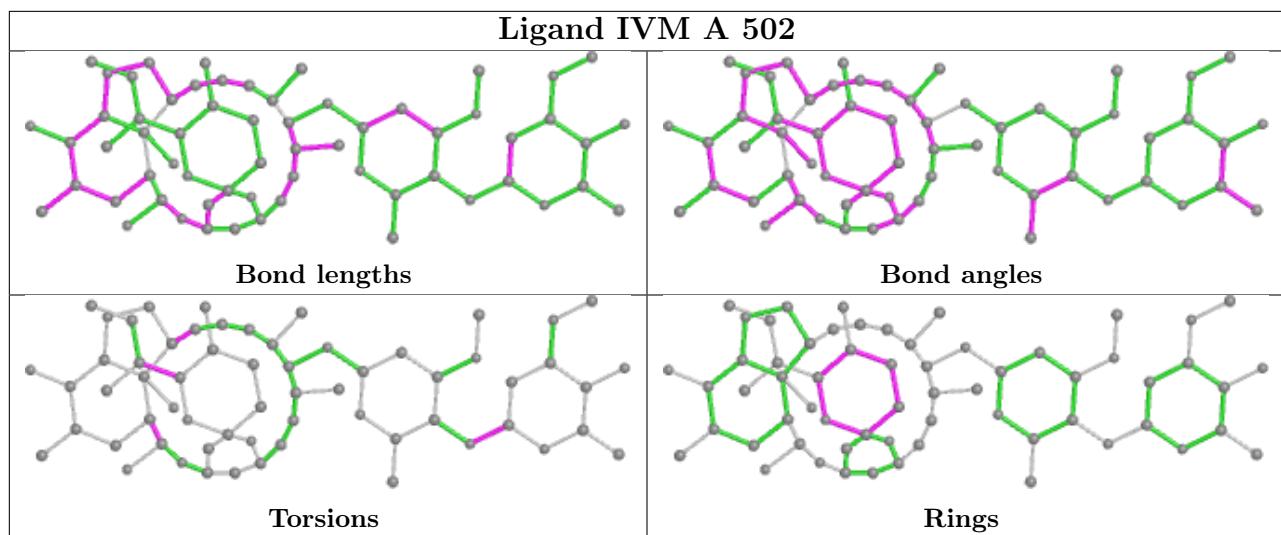
All unique ring outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	501	IVM	C5-C6-C7-C8-C9-O1	15
2	A	502	IVM	C5-C6-C7-C8-C9-O1	15
2	B	501	IVM	C5-C6-C7-C8-C9-O1	15
2	C	501	IVM	C5-C6-C7-C8-C9-O1	15
2	D	501	IVM	C5-C6-C7-C8-C9-O1	15

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 i

The completeness of assignment taking into account all chemical shift lists is 12% for the well-defined parts and 12% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

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	2107
Number of shifts mapped to atoms	2107
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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
$^{13}\text{C}_\alpha$	259	-0.51 \pm 0.12	Should be checked
$^{13}\text{C}_\beta$	170	0.25 \pm 0.03	None needed (< 0.5 ppm)
$^{13}\text{C}'$	200	-0.09 \pm 0.07	None needed (< 0.5 ppm)
^{15}N	231	0.33 \pm 0.08	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 12%, i.e. 2107 atoms were assigned a chemical shift out of a possible 17880. 0 out of 285 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1155/6505 (18%)	465/2635 (18%)	459/2640 (17%)	231/1230 (19%)
Sidechain	904/10045 (9%)	612/6665 (9%)	288/3100 (9%)	4/280 (1%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	48/1330 (4%)	27/650 (4%)	17/580 (3%)	4/100 (4%)
Overall	2107/17880 (12%)	1104/9950 (11%)	764/6320 (12%)	239/1610 (15%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 12%, i.e. 2107 atoms were assigned a chemical shift out of a possible 17880. 0 out of 285 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	1155/6505 (18%)	465/2635 (18%)	459/2640 (17%)	231/1230 (19%)
Sidechain	904/10045 (9%)	612/6665 (9%)	288/3100 (9%)	4/280 (1%)
Aromatic	48/1330 (4%)	27/650 (4%)	17/580 (3%)	4/100 (4%)
Overall	2107/17880 (12%)	1104/9950 (11%)	764/6320 (12%)	239/1610 (15%)

7.1.4 Statistically unusual chemical shifts [\(i\)](#)

There are no statistically unusual chemical shifts.

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:

