



Full wwPDB NMR Structure Validation Report ⓘ

Mar 23, 2026 – 11:47 AM UTC

PDB ID : 6D6S / pdb_00006d6s
BMRB ID : 30456
Title : Solution structure of Trigger Factor dimer
Authors : Saio, T.; Kawagoe, S.; Ishimori, K.; Kalodimos, C.G.
Deposited on : 2018-04-22

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
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

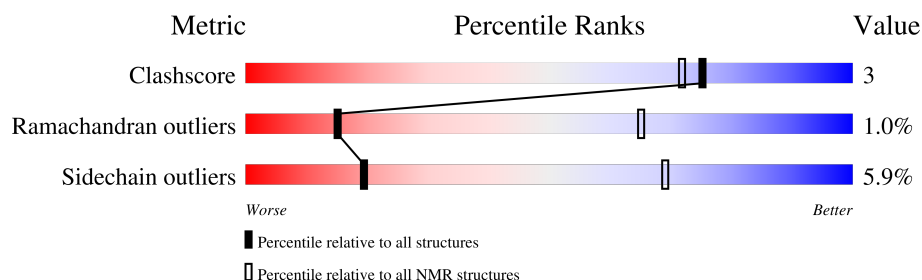
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

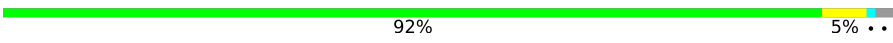
The overall completeness of chemical shifts assignment is 14%.

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	443	 91% 6% ..
1	B	443	 92% 5% ..

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:2-A:111, B:109-B:429 (431)	1.53	5
2	A:112-A:430, B:2-B:108 (426)	1.51	5

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13578 atoms, of which 6806 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms						Trace
1	A	432	Total	C	H	N	O	S	0
			6789	2119	3403	582	674	11	
1	B	432	Total	C	H	N	O	S	0
			6789	2119	3403	582	674	11	

There are 22 discrepancies between the modelled and reference sequences:

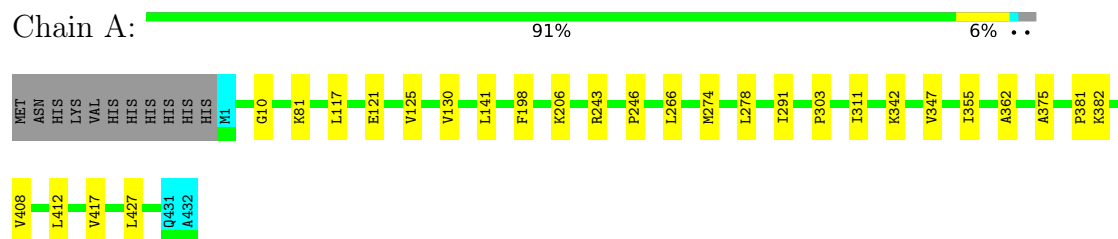
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP P0A850
A	-9	ASN	-	expression tag	UNP P0A850
A	-8	HIS	-	expression tag	UNP P0A850
A	-7	LYS	-	expression tag	UNP P0A850
A	-6	VAL	-	expression tag	UNP P0A850
A	-5	HIS	-	expression tag	UNP P0A850
A	-4	HIS	-	expression tag	UNP P0A850
A	-3	HIS	-	expression tag	UNP P0A850
A	-2	HIS	-	expression tag	UNP P0A850
A	-1	HIS	-	expression tag	UNP P0A850
A	0	HIS	-	expression tag	UNP P0A850
B	-10	MET	-	initiating methionine	UNP P0A850
B	-9	ASN	-	expression tag	UNP P0A850
B	-8	HIS	-	expression tag	UNP P0A850
B	-7	LYS	-	expression tag	UNP P0A850
B	-6	VAL	-	expression tag	UNP P0A850
B	-5	HIS	-	expression tag	UNP P0A850
B	-4	HIS	-	expression tag	UNP P0A850
B	-3	HIS	-	expression tag	UNP P0A850
B	-2	HIS	-	expression tag	UNP P0A850
B	-1	HIS	-	expression tag	UNP P0A850
B	0	HIS	-	expression tag	UNP P0A850

4 Residue-property plots

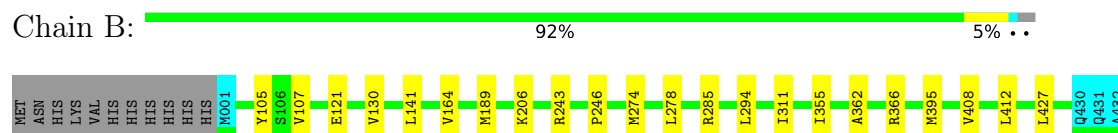
4.1 Average score per residue in the NMR ensemble

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: Trigger factor



- Molecule 1: Trigger factor

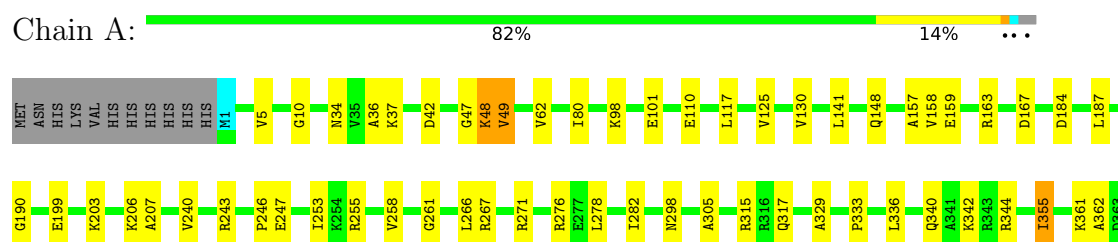


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

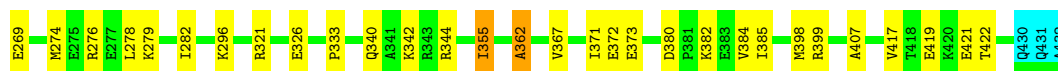
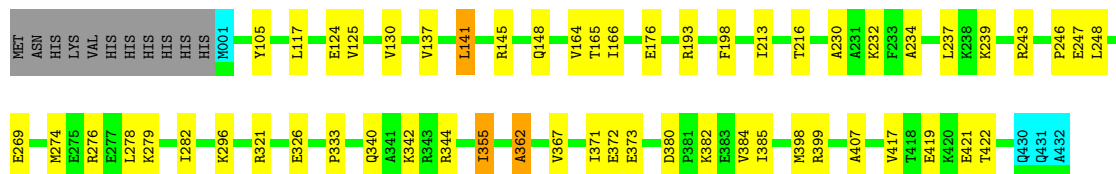
- Molecule 1: Trigger factor





- Molecule 1: Trigger factor

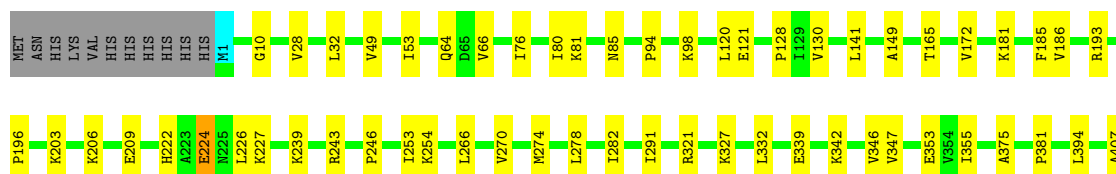
Chain B: 84% 12% ..



4.2.2 Score per residue for model 2

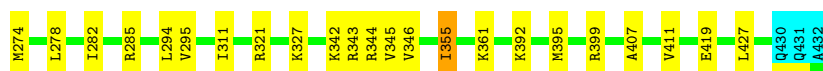
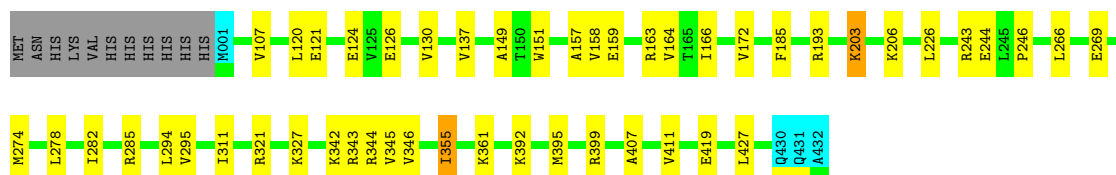
- Molecule 1: Trigger factor

Chain A: 83% 13% ..



- Molecule 1: Trigger factor

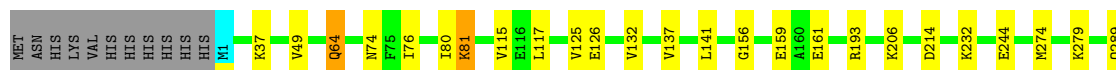
Chain B: 86% 11% ..



4.2.3 Score per residue for model 3

- Molecule 1: Trigger factor

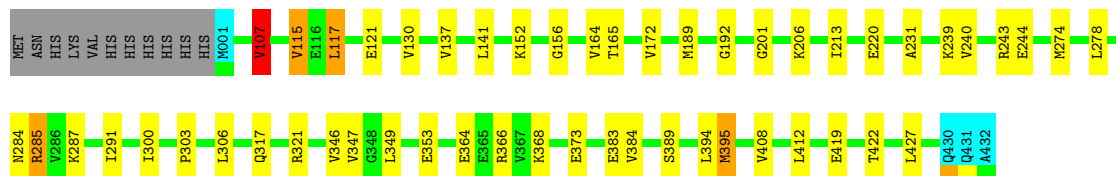
Chain A: 86% 10% ..





- Molecule 1: Trigger factor

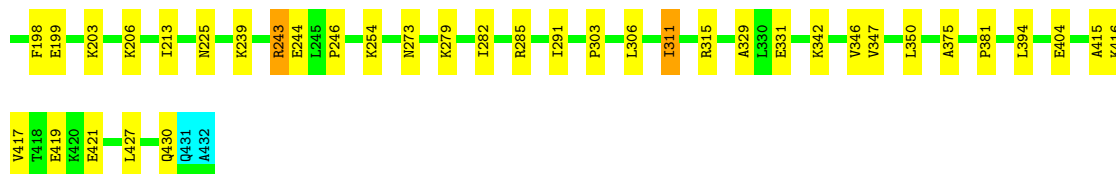
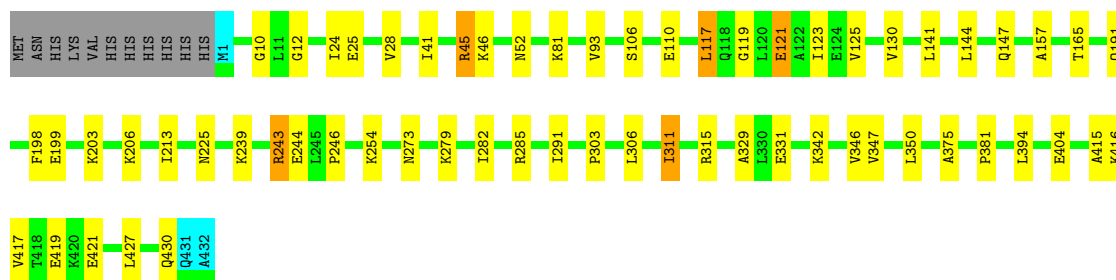
Chain B: 85% 11% ...



4.2.4 Score per residue for model 4

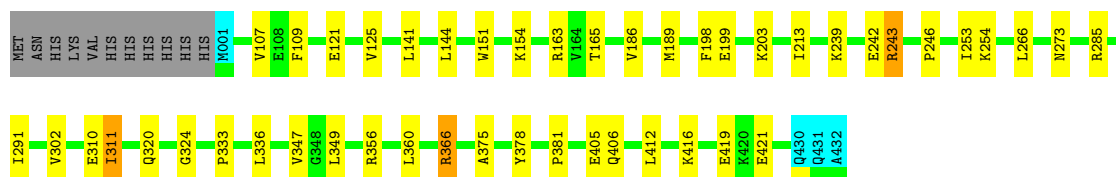
- Molecule 1: Trigger factor

Chain A: 83% 13% ...



- Molecule 1: Trigger factor

Chain B: 86% 10% ...

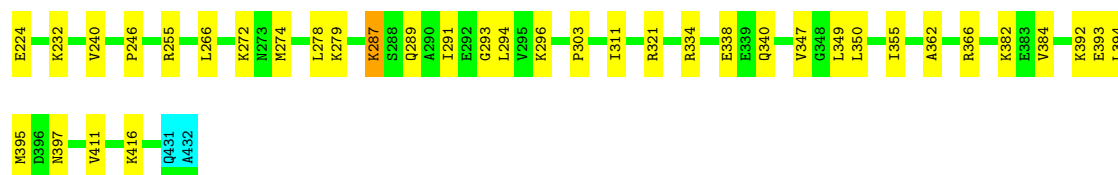


4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Trigger factor

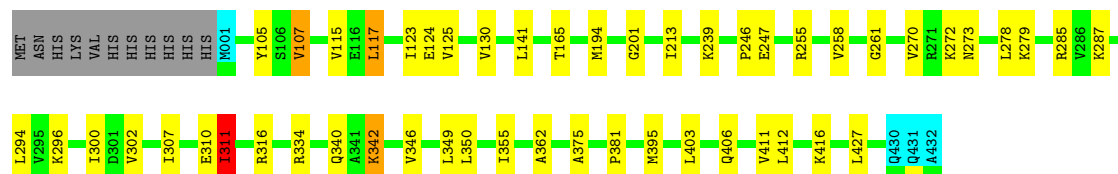
Chain A: 83% 14% ...





- Molecule 1: Trigger factor

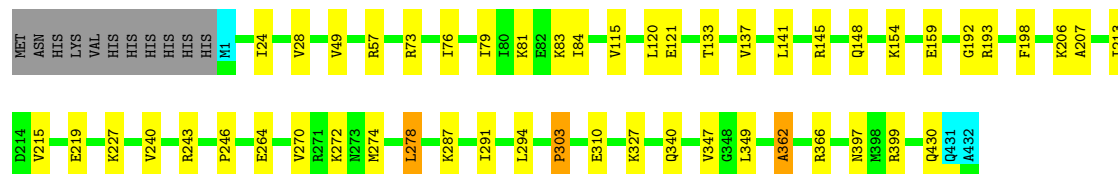
Chain B: 85% 11% ...



4.2.6 Score per residue for model 6

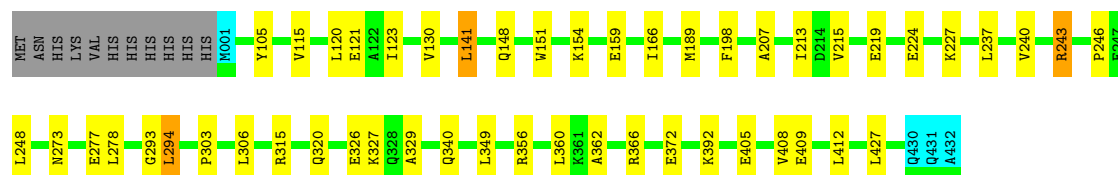
- Molecule 1: Trigger factor

Chain A: 85% 11% ...



- Molecule 1: Trigger factor

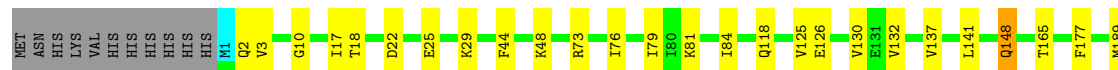
Chain B: 85% 11% ...

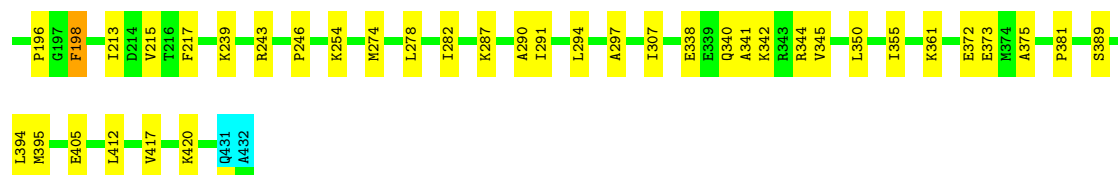


4.2.7 Score per residue for model 7

- Molecule 1: Trigger factor

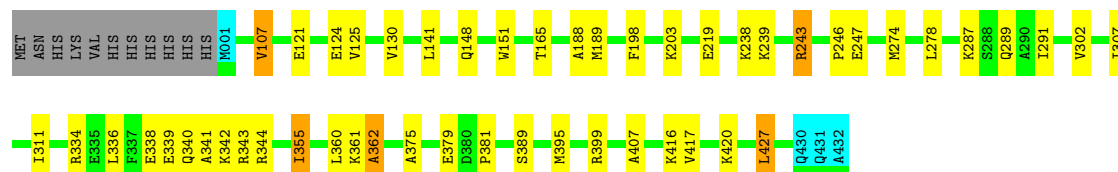
Chain A: 82% 14% ...





- Molecule 1: Trigger factor

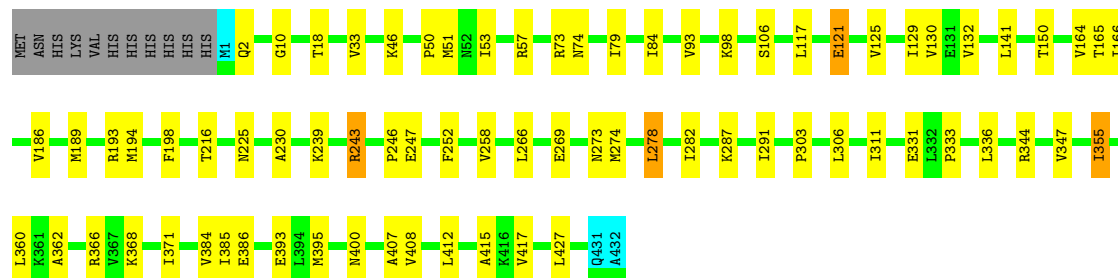
Chain B: 85% 10% ...



4.2.8 Score per residue for model 8

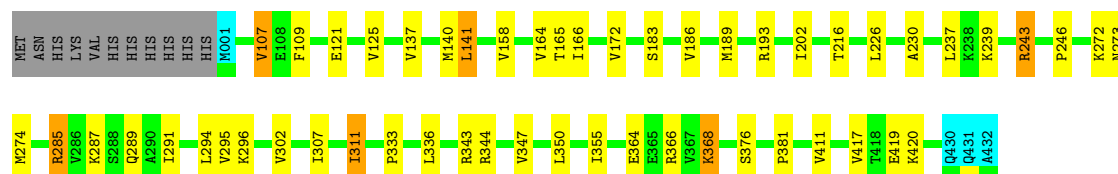
- Molecule 1: Trigger factor

Chain A: 80% 16% ...



- Molecule 1: Trigger factor

Chain B: 85% 11% ...

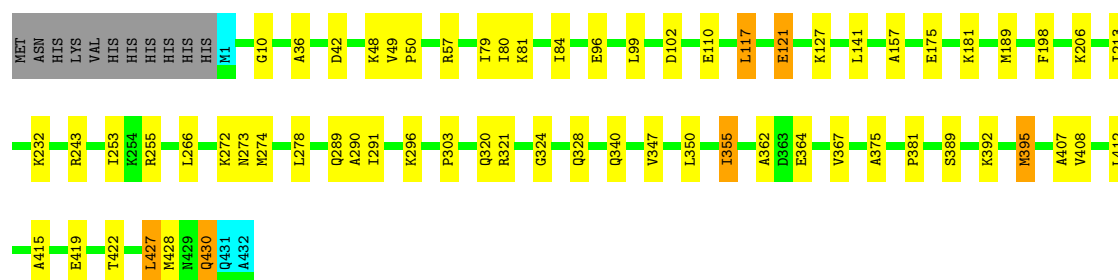


4.2.9 Score per residue for model 9

- Molecule 1: Trigger factor

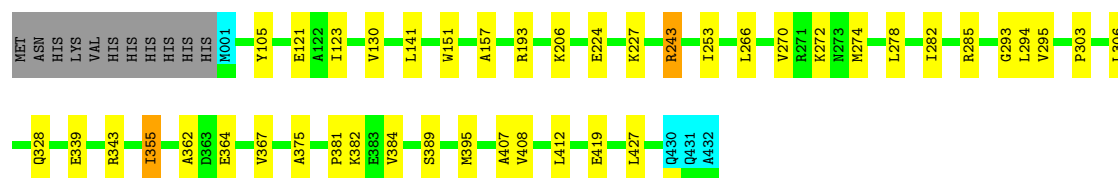
Chain A: 82% 13% ...





- Molecule 1: Trigger factor

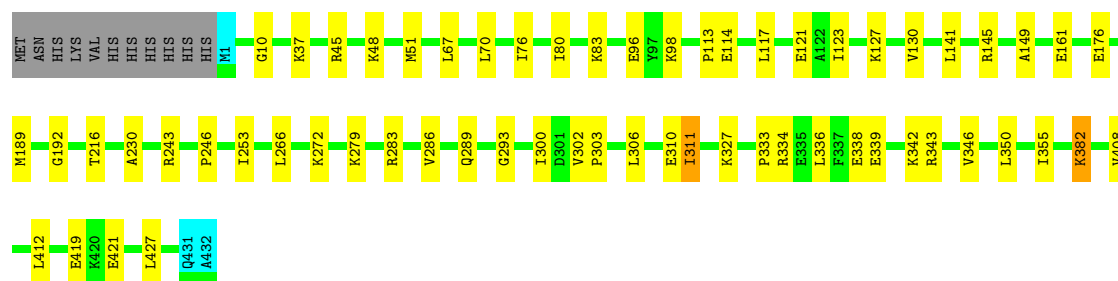
Chain B: 87% 9% ..



4.2.10 Score per residue for model 10

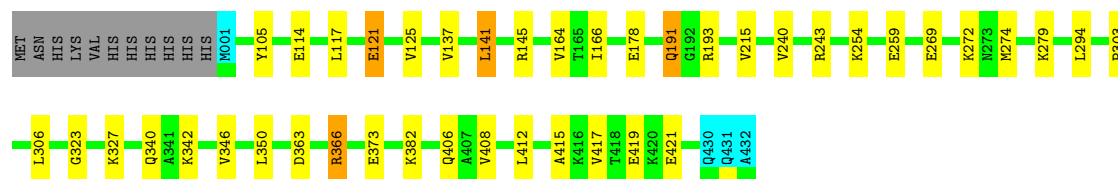
- Molecule 1: Trigger factor

Chain A: 83% 13% ..



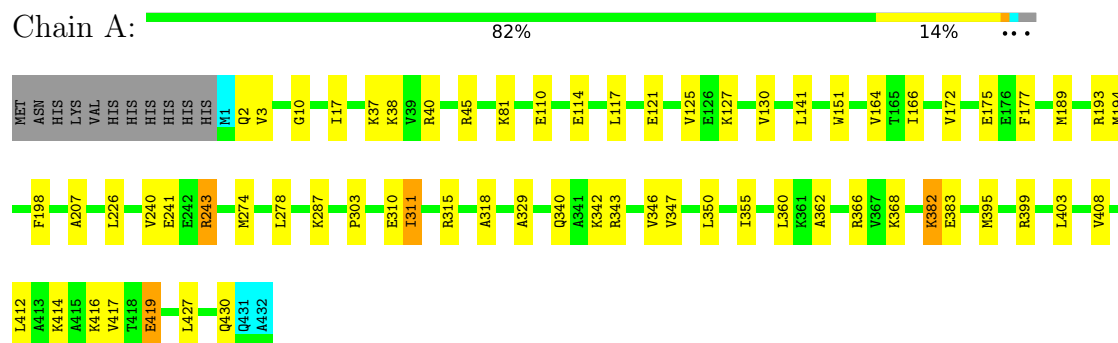
- Molecule 1: Trigger factor

Chain B: 87% 9% ..

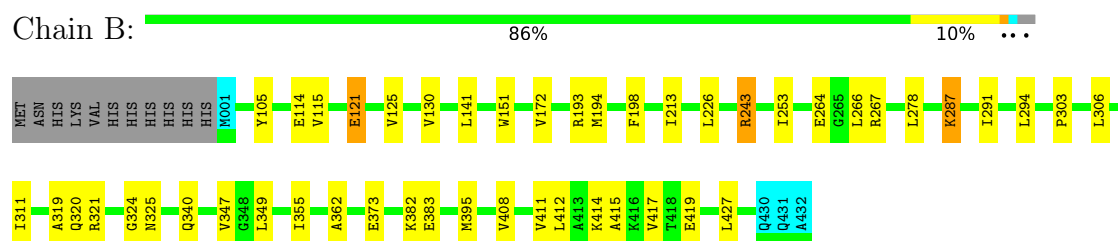


4.2.11 Score per residue for model 11

- Molecule 1: Trigger factor

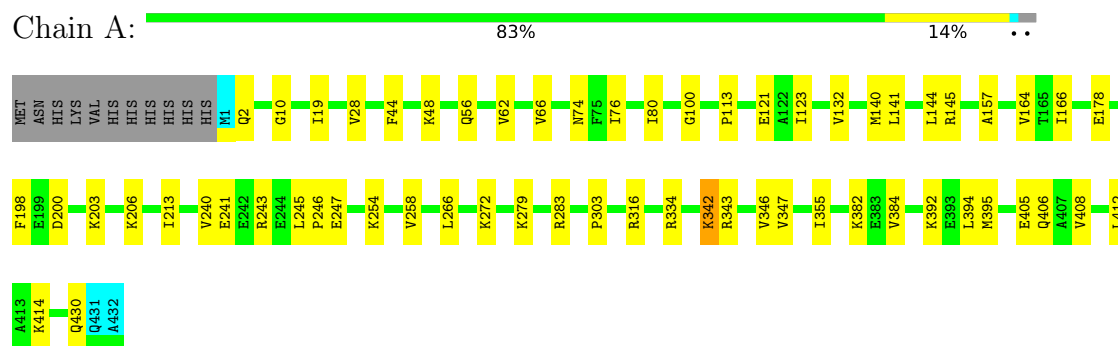


- Molecule 1: Trigger factor

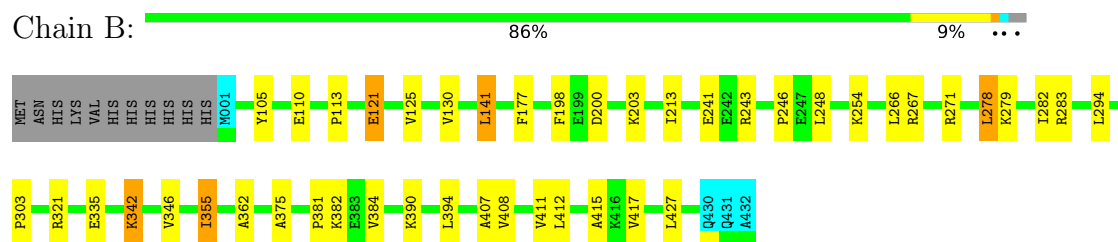


4.2.12 Score per residue for model 12

- Molecule 1: Trigger factor

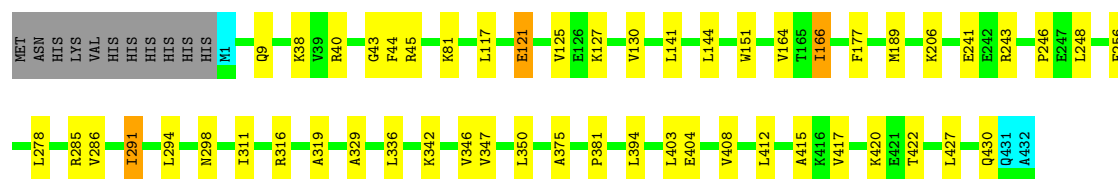


- Molecule 1: Trigger factor

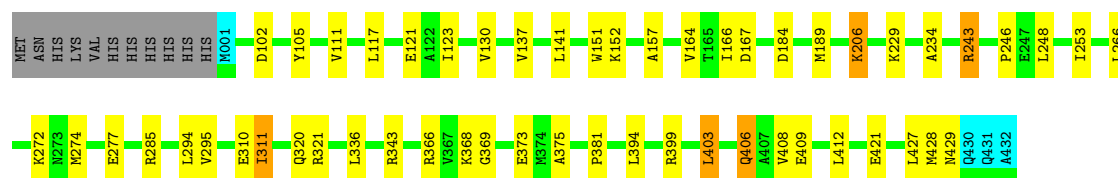


4.2.13 Score per residue for model 13

- Molecule 1: Trigger factor

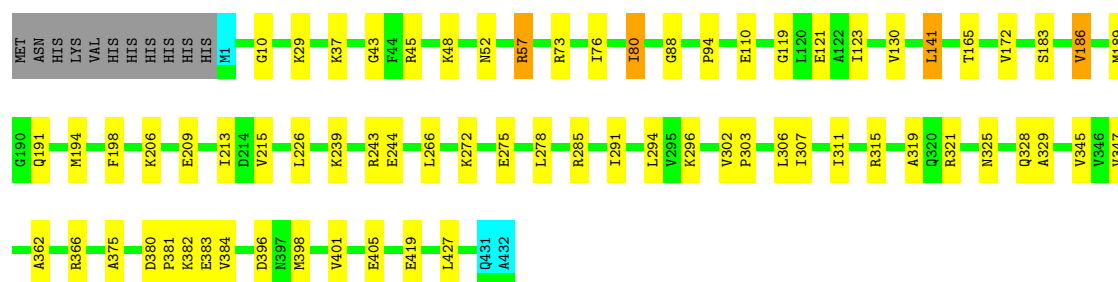
Chain A: 

- Molecule 1: Trigger factor

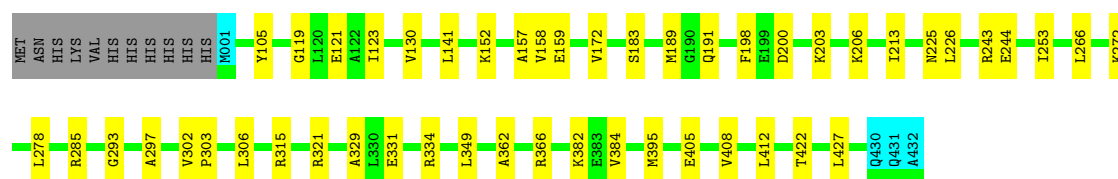
Chain B: 

4.2.14 Score per residue for model 14

- Molecule 1: Trigger factor

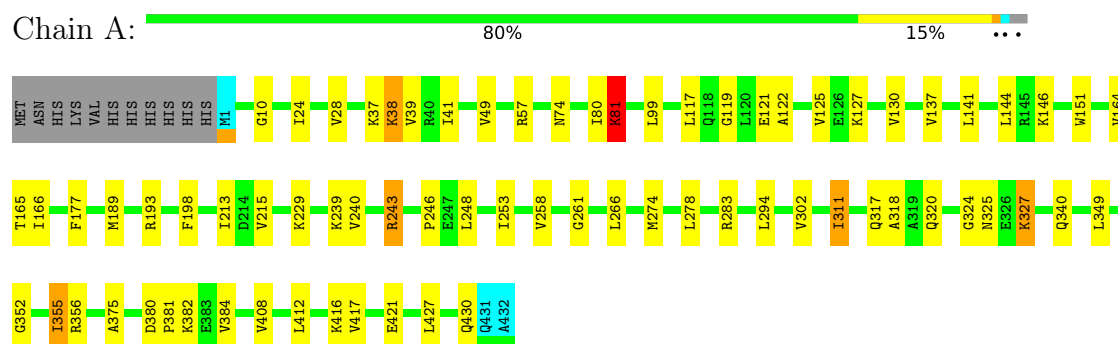
Chain A: 

- Molecule 1: Trigger factor

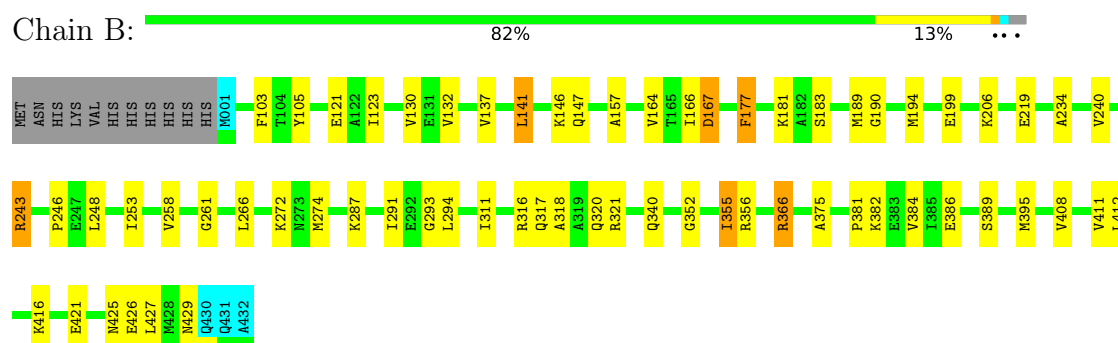
Chain B: 

4.2.15 Score per residue for model 15

- Molecule 1: Trigger factor

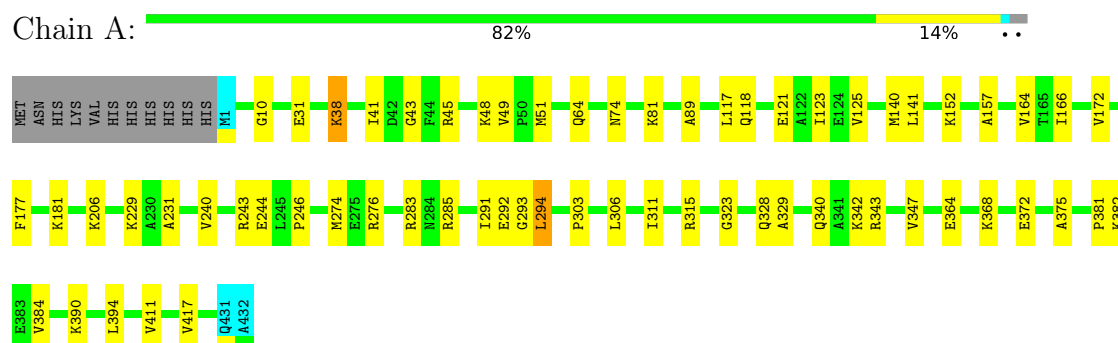


- Molecule 1: Trigger factor

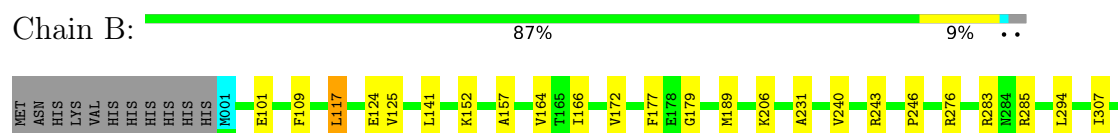


4.2.16 Score per residue for model 16

- Molecule 1: Trigger factor



- Molecule 1: Trigger factor

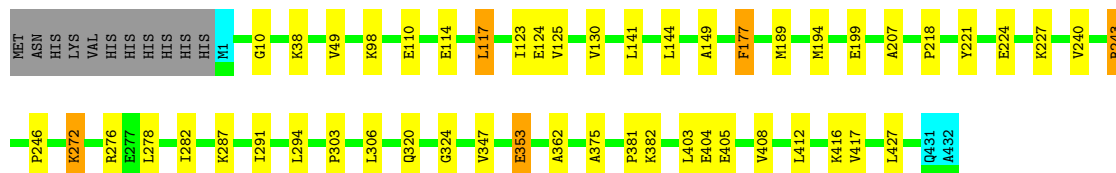




4.2.17 Score per residue for model 17

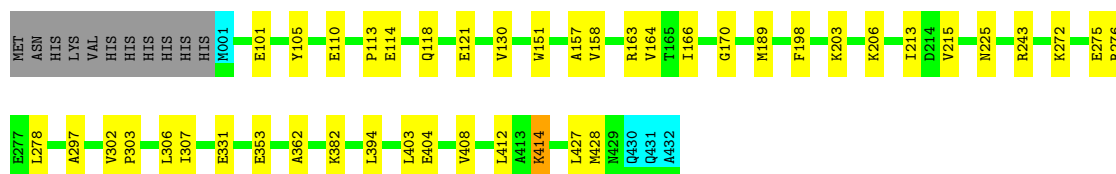
- Molecule 1: Trigger factor

Chain A: 85% 10% ..



- Molecule 1: Trigger factor

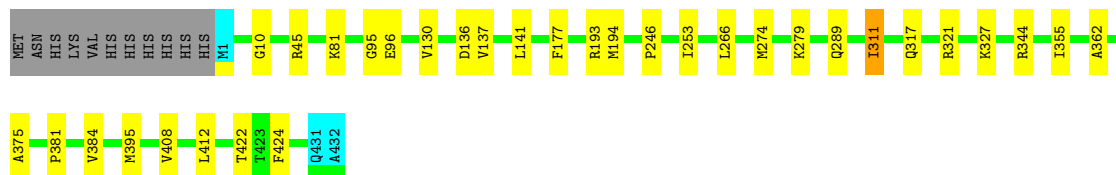
Chain B: 87% 10% ..



4.2.18 Score per residue for model 18

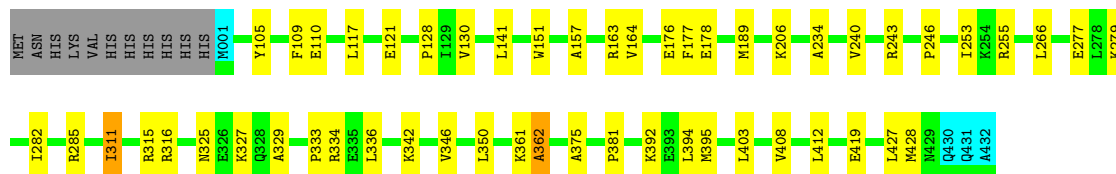
- Molecule 1: Trigger factor

Chain A: 89% 7% ..



- Molecule 1: Trigger factor

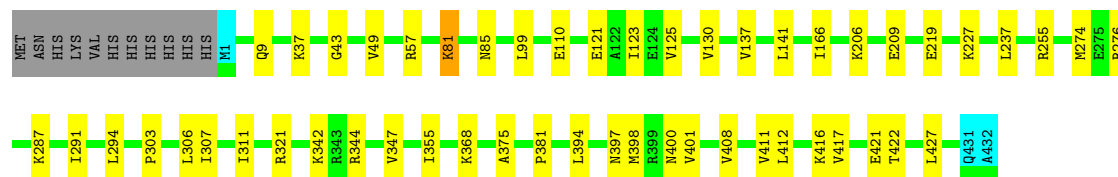
Chain B: 85% 12% ..



4.2.19 Score per residue for model 19

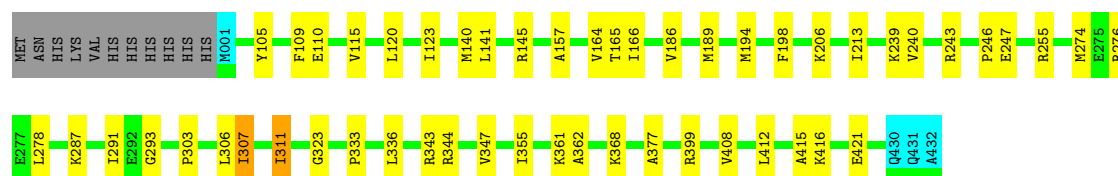
- Molecule 1: Trigger factor

Chain A:  85% 12% ..



- Molecule 1: Trigger factor

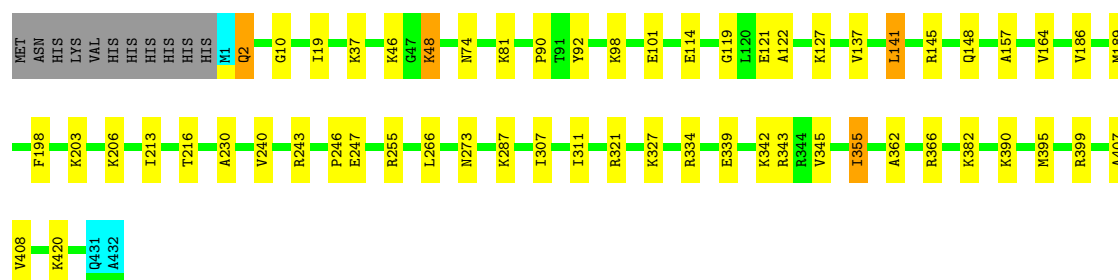
Chain B:  85% 11% ..



4.2.20 Score per residue for model 20

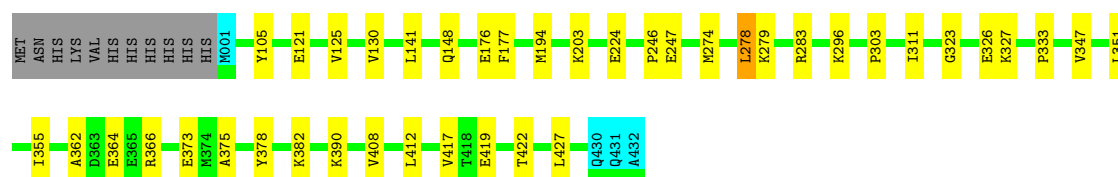
- Molecule 1: Trigger factor

Chain A:  84% 12% ...



- Molecule 1: Trigger factor

Chain B:  87% 9% ..



5 Refinement protocol and experimental data overview

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

Of the 800 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure calculation	

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	1674
Number of shifts mapped to atoms	1674
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	14%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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
1	A	1.25±0.02	1±1/3404 (0.0± 0.0%)	1.01±0.01	0±0/4579 (0.0± 0.0%)
1	B	1.23±0.02	1±1/2637 (0.0± 0.0%)	1.01±0.01	0±0/3543 (0.0± 0.0%)
All	All	1.24	37/120820 (0.0%)	1.01	2/162440 (0.0%)

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
1	A	311	ILE	CA-CB	6.70	1.61	1.54	20	11
1	A	5	VAL	CA-CB	6.24	1.60	1.53	1	1
1	B	107	VAL	CA-CB	6.16	1.61	1.53	5	2
1	B	311	ILE	CA-CB	6.14	1.61	1.54	16	11
1	A	186	VAL	CA-CB	5.52	1.59	1.53	14	2
1	A	44	PHE	CA-C	5.50	1.55	1.52	12	1
1	A	80	ILE	CA-CB	5.48	1.60	1.54	14	1
1	A	41	ILE	CA-CB	5.47	1.59	1.53	15	2
1	B	346	VAL	CA-CB	5.35	1.60	1.54	10	1
1	A	129	ILE	CA-CB	5.12	1.58	1.53	8	1
1	A	291	ILE	CA-CB	5.11	1.60	1.54	13	1
1	B	123	ILE	CA-CB	5.10	1.59	1.54	13	1
1	A	89	ALA	C-N	5.05	1.38	1.33	16	1
1	A	302	VAL	CA-CB	5.02	1.58	1.54	10	1

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
1	B	177	PHE	CA-CB-CG	5.12	118.92	113.80	15	1
1	A	177	PHE	CA-CB-CG	5.01	118.81	113.80	17	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	3363	3381	3379	22±5
1	B	3354	3373	2581	19±4
All	All	134340	135080	119200	782

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:MET:SD	1:A:199:GLU:HB2	0.66	2.30	5	1
1:A:132:VAL:HG11	1:A:274:MET:SD	0.64	2.33	8	3
1:A:79:ILE:HB	1:A:84:ILE:HB	0.62	1.70	9	4
1:B:189:MET:SD	1:B:243:ARG:HG3	0.61	2.36	13	12
1:A:110:GLU:HB2	1:A:303:PRO:HB3	0.61	1.70	19	6
1:A:389:SER:HA	1:A:395:MET:SD	0.61	2.35	9	2
1:B:130:VAL:HG21	1:B:427:LEU:HD22	0.60	1.73	15	11
1:A:80:ILE:HD13	1:B:384:VAL:HG22	0.59	1.73	3	3
1:A:291:ILE:HG23	1:A:347:VAL:HG21	0.59	1.74	19	10
1:B:158:VAL:HB	1:B:203:LYS:HA	0.59	1.74	2	3
1:A:117:LEU:HB3	1:A:350:LEU:HD22	0.58	1.75	5	6
1:A:224:GLU:HA	1:A:227:LYS:HG2	0.58	1.73	17	2
1:B:320:GLN:HA	1:B:324:GLY:HA2	0.58	1.74	4	2
1:B:125:VAL:HB	1:B:417:VAL:HA	0.58	1.75	10	8
1:A:189:MET:SD	1:A:243:ARG:HG3	0.58	2.39	8	7
1:A:207:ALA:HB2	1:A:240:VAL:HG23	0.58	1.75	6	4
1:A:165:THR:HB	1:A:239:LYS:HB2	0.57	1.74	8	6
1:B:389:SER:HA	1:B:395:MET:SD	0.57	2.39	9	4
1:B:253:ILE:HG23	1:B:266:LEU:HB2	0.57	1.75	15	7
1:A:287:LYS:HE3	1:A:408:VAL:HG21	0.57	1.76	20	1
1:B:117:LEU:HB3	1:B:350:LEU:HD22	0.57	1.75	5	4
1:B:303:PRO:HB2	1:B:306:LEU:HD13	0.57	1.76	9	8
1:A:375:ALA:HB1	1:A:381:PRO:HA	0.56	1.76	17	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:409:GLU:HA	1:B:412:LEU:HB2	0.56	1.76	16	1
1:A:125:VAL:HB	1:A:417:VAL:HA	0.56	1.77	7	11
1:A:303:PRO:HB2	1:A:306:LEU:HD13	0.56	1.78	10	7
1:B:291:ILE:HG23	1:B:347:VAL:HG21	0.56	1.76	4	3
1:B:137:VAL:HA	1:B:274:MET:HE1	0.56	1.78	13	4
1:A:258:VAL:HG22	1:A:269:GLU:HG3	0.56	1.76	8	1
1:A:198:PHE:HA	1:A:213:ILE:HD12	0.56	1.76	14	8
1:B:302:VAL:HG12	1:B:349:LEU:HD12	0.55	1.77	14	2
1:A:130:VAL:HG21	1:A:427:LEU:HD22	0.55	1.79	17	8
1:A:164:VAL:HG23	1:A:240:VAL:HG22	0.55	1.79	12	5
1:A:36:ALA:HB1	1:A:42:ASP:HA	0.55	1.78	9	2
1:A:253:ILE:HG23	1:A:266:LEU:HB2	0.55	1.79	15	6
1:B:130:VAL:HG21	1:B:427:LEU:HD12	0.55	1.78	7	1
1:B:167:ASP:HB3	1:B:183:SER:HA	0.54	1.79	15	1
1:A:302:VAL:HG23	1:A:307:ILE:HD11	0.54	1.77	14	1
1:A:140:MET:HE2	1:A:274:MET:SD	0.54	2.42	16	1
1:A:130:VAL:HG22	1:A:282:ILE:HD11	0.54	1.78	1	6
1:B:157:ALA:HA	1:B:206:LYS:HA	0.54	1.79	13	9
1:B:172:VAL:HA	1:B:231:ALA:HA	0.54	1.78	3	2
1:A:81:LYS:HD2	1:B:383:GLU:HG3	0.53	1.80	11	1
1:A:302:VAL:HB	1:A:307:ILE:HD11	0.53	1.80	3	1
1:A:50:PRO:HD2	1:A:53:ILE:HD12	0.53	1.80	8	1
1:A:121:GLU:HA	1:A:415:ALA:HA	0.53	1.81	4	4
1:B:141:LEU:HD11	1:B:248:LEU:HD22	0.53	1.81	6	2
1:B:140:MET:HE2	1:B:274:MET:SD	0.53	2.43	8	2
1:B:219:GLU:HA	1:B:227:LYS:HD2	0.53	1.81	6	1
1:A:189:MET:SD	1:A:243:ARG:NE	0.52	2.82	7	2
1:B:166:ILE:HG21	1:B:237:LEU:HD23	0.52	1.81	8	1
1:B:115:VAL:HG11	1:B:349:LEU:HB3	0.52	1.81	3	4
1:A:355:ILE:HG22	1:A:360:LEU:HD23	0.52	1.81	11	1
1:B:426:GLU:HA	1:B:429:ASN:HB3	0.52	1.81	15	1
1:A:127:LYS:HB3	1:A:419:GLU:HA	0.52	1.82	9	1
1:A:98:LYS:HD2	1:A:101:GLU:HB2	0.52	1.80	20	2
1:A:157:ALA:HA	1:A:206:LYS:HA	0.52	1.80	4	7
1:B:172:VAL:HG11	1:B:226:LEU:HA	0.52	1.81	2	2
1:A:126:GLU:HB3	1:A:289:GLN:HG3	0.52	1.82	5	1
1:B:121:GLU:HA	1:B:415:ALA:HA	0.52	1.82	10	3
1:B:164:VAL:HG23	1:B:240:VAL:HG22	0.52	1.81	16	6
1:A:76:ILE:HD12	1:A:79:ILE:HD11	0.51	1.82	7	2
1:B:355:ILE:HG23	1:B:407:ALA:HB2	0.51	1.81	9	5
1:A:214:ASP:HB3	1:A:232:LYS:HG2	0.51	1.82	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:165:THR:HB	1:B:239:LYS:HB2	0.51	1.82	1	7
1:B:124:GLU:HG3	1:B:289:GLN:NE2	0.51	2.21	7	1
1:A:172:VAL:HA	1:A:231:ALA:HA	0.51	1.82	16	1
1:B:130:VAL:HG22	1:B:282:ILE:HD11	0.51	1.82	18	4
1:B:382:LYS:HA	1:B:385:ILE:HD12	0.51	1.82	1	1
1:B:198:PHE:HA	1:B:213:ILE:HD12	0.50	1.83	12	8
1:A:22:ASP:HA	1:A:25:GLU:HB3	0.50	1.82	7	1
1:A:80:ILE:HD13	1:B:384:VAL:HA	0.50	1.82	12	2
1:B:164:VAL:HG22	1:B:166:ILE:HG23	0.50	1.81	1	9
1:A:164:VAL:HG22	1:A:166:ILE:HG23	0.50	1.83	5	7
1:A:3:VAL:HG12	1:A:17:ILE:HG23	0.50	1.84	11	2
1:B:338:GLU:HA	1:B:341:ALA:HB3	0.50	1.82	7	1
1:B:375:ALA:HB1	1:B:381:PRO:HA	0.50	1.82	4	9
1:B:315:ARG:HB3	1:B:329:ALA:HB1	0.50	1.84	18	2
1:B:362:ALA:HB2	1:B:399:ARG:HG3	0.50	1.82	7	2
1:A:137:VAL:HA	1:A:274:MET:HE1	0.50	1.84	19	5
1:B:284:ASN:HB3	1:B:285:ARG:HH21	0.50	1.66	3	1
1:A:225:ASN:HB2	1:A:331:GLU:HG2	0.50	1.84	8	2
1:A:2:GLN:HB2	1:A:18:THR:HB	0.50	1.84	8	2
1:A:41:ILE:HG21	1:B:336:LEU:HD13	0.49	1.84	4	1
1:B:224:GLU:HA	1:B:227:LYS:HG2	0.49	1.83	6	2
1:A:161:GLU:HA	1:A:189:MET:SD	0.49	2.47	10	1
1:B:294:LEU:HD21	1:B:411:VAL:HG11	0.49	1.83	15	3
1:A:140:MET:SD	1:A:144:LEU:HD23	0.49	2.47	12	1
1:A:398:MET:HA	1:A:401:VAL:HG22	0.49	1.84	14	2
1:B:295:VAL:HG11	1:B:343:ARG:HG2	0.49	1.83	2	2
1:A:151:TRP:HB3	1:A:241:GLU:HB3	0.49	1.85	11	2
1:B:364:GLU:HA	1:B:367:VAL:HG12	0.49	1.85	9	1
1:B:128:PRO:HG2	1:B:285:ARG:HG2	0.49	1.83	18	1
1:B:159:GLU:HA	1:B:203:LYS:HZ3	0.49	1.66	2	1
1:A:117:LEU:H	1:A:117:LEU:HD23	0.49	1.67	3	2
1:A:127:LYS:HZ1	1:A:419:GLU:HB3	0.49	1.68	10	1
1:A:352:GLY:O	1:A:355:ILE:HG12	0.49	2.08	15	1
1:A:355:ILE:HG23	1:A:407:ALA:HB2	0.49	1.85	1	5
1:B:189:MET:SD	1:B:243:ARG:NE	0.49	2.86	3	1
1:B:151:TRP:CZ3	1:B:243:ARG:HG2	0.49	2.43	4	6
1:A:37:LYS:O	1:A:40:ARG:HD2	0.49	2.07	11	1
1:A:144:LEU:HD21	1:A:256:PHE:HZ	0.49	1.67	13	1
1:B:277:GLU:HB3	1:B:428:MET:HE1	0.48	1.83	18	1
1:B:145:ARG:HB3	1:B:248:LEU:HD13	0.48	1.85	1	1
1:B:364:GLU:HG2	1:B:368:LYS:HE3	0.48	1.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:VAL:HG11	1:A:349:LEU:HB3	0.48	1.85	3	3
1:A:29:LYS:HE3	1:A:52:ASN:HB2	0.48	1.83	14	1
1:A:123:ILE:HG23	1:A:293:GLY:HA3	0.48	1.83	16	3
1:A:364:GLU:O	1:A:368:LYS:HB3	0.48	2.09	16	1
1:A:218:PRO:HG2	1:A:221:TYR:HB2	0.48	1.86	17	1
1:A:315:ARG:HB3	1:A:329:ALA:HB1	0.48	1.84	16	4
1:A:125:VAL:HG22	1:A:412:LEU:HD12	0.48	1.86	7	1
1:A:320:GLN:HA	1:A:324:GLY:HA2	0.48	1.86	9	3
1:A:154:LYS:HE2	1:A:159:GLU:HG2	0.48	1.85	6	1
1:B:151:TRP:CZ3	1:B:163:ARG:HB2	0.48	2.44	2	4
1:B:408:VAL:O	1:B:412:LEU:HG	0.47	2.09	18	11
1:A:130:VAL:HG11	1:A:427:LEU:HB2	0.47	1.85	11	3
1:A:53:ILE:HD12	1:B:185:PHE:HA	0.47	1.86	2	1
1:A:172:VAL:HG21	1:A:226:LEU:HD22	0.47	1.86	11	3
1:A:338:GLU:HA	1:A:341:ALA:HB3	0.47	1.86	7	1
1:A:283:ARG:HH21	1:A:286:VAL:HG13	0.47	1.68	10	1
1:A:200:ASP:HA	1:A:203:LYS:HE2	0.47	1.86	12	1
1:A:62:VAL:HG23	1:B:321:ARG:NH2	0.47	2.24	1	2
1:A:194:MET:SD	1:A:198:PHE:CD2	0.47	3.08	8	3
1:B:352:GLY:O	1:B:355:ILE:HG12	0.47	2.09	15	1
1:B:110:GLU:HB2	1:B:303:PRO:HB3	0.47	1.86	17	2
1:B:216:THR:HA	1:B:230:ALA:HA	0.47	1.85	8	2
1:A:25:GLU:HG3	1:A:29:LYS:NZ	0.47	2.24	7	1
1:A:216:THR:HA	1:A:230:ALA:HA	0.47	1.86	10	3
1:A:172:VAL:HG11	1:A:226:LEU:HA	0.47	1.87	11	1
1:A:371:ILE:HG22	1:A:385:ILE:HG12	0.47	1.86	8	1
1:A:253:ILE:HD12	1:A:266:LEU:HG	0.47	1.85	9	1
1:A:364:GLU:HA	1:A:367:VAL:HG12	0.47	1.86	9	1
1:B:274:MET:O	1:B:278:LEU:HB2	0.47	2.09	3	6
1:A:76:ILE:O	1:A:80:ILE:HG13	0.47	2.10	12	3
1:B:291:ILE:HD12	1:B:347:VAL:HG11	0.47	1.85	3	1
1:A:302:VAL:HG21	1:A:345:VAL:HG23	0.47	1.86	14	1
1:A:123:ILE:HD13	1:A:294:LEU:HD22	0.47	1.84	17	2
1:A:311:ILE:HD11	1:A:338:GLU:HA	0.47	1.86	10	1
1:B:270:VAL:HG12	1:B:274:MET:SD	0.47	2.49	9	1
1:B:408:VAL:O	1:B:412:LEU:HB2	0.47	2.10	20	2
1:A:117:LEU:HD21	1:A:353:GLU:HB3	0.47	1.86	17	1
1:B:294:LEU:HD21	1:B:411:VAL:HG21	0.46	1.86	11	1
1:A:38:LYS:HA	1:B:340:GLN:HG3	0.46	1.86	15	1
1:A:408:VAL:O	1:A:412:LEU:HG	0.46	2.09	13	10
1:B:130:VAL:HG11	1:B:427:LEU:HB2	0.46	1.85	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:364:GLU:O	1:B:368:LYS:HB2	0.46	2.11	3	1
1:A:34:ASN:HA	1:A:37:LYS:HZ2	0.46	1.70	1	1
1:B:117:LEU:H	1:B:117:LEU:HD23	0.46	1.70	3	2
1:A:159:GLU:HG3	1:A:161:GLU:H	0.46	1.70	3	1
1:A:291:ILE:HD12	1:A:347:VAL:HG11	0.46	1.87	6	2
1:B:194:MET:SD	1:B:198:PHE:CD2	0.46	3.09	11	1
1:A:190:GLY:HA3	1:A:243:ARG:HH22	0.46	1.70	1	1
1:B:321:ARG:HH11	1:B:321:ARG:HB2	0.46	1.71	1	1
1:A:148:GLN:HE21	1:A:148:GLN:HA	0.46	1.71	7	1
1:A:352:GLY:O	1:A:356:ARG:HG2	0.46	2.11	15	1
1:A:194:MET:HB2	1:A:199:GLU:HB2	0.46	1.86	17	1
1:A:362:ALA:HB2	1:A:399:ARG:HG3	0.46	1.88	20	1
1:B:200:ASP:HA	1:B:203:LYS:HE2	0.46	1.88	14	2
1:B:167:ASP:HB3	1:B:184:ASP:H	0.46	1.71	13	1
1:B:366:ARG:HA	1:B:366:ARG:HE	0.46	1.71	15	1
1:B:360:LEU:HB3	1:B:406:GLN:HE22	0.45	1.71	4	1
1:A:294:LEU:HB3	1:A:350:LEU:HD13	0.45	1.86	7	1
1:A:33:VAL:HA	1:A:51:MET:HE3	0.45	1.87	8	1
1:B:343:ARG:O	1:B:347:VAL:HG23	0.45	2.11	8	1
1:B:123:ILE:HG23	1:B:293:GLY:HA3	0.45	1.89	9	5
1:A:28:VAL:HA	1:A:66:VAL:HG21	0.45	1.88	12	1
1:A:302:VAL:HG12	1:A:349:LEU:HD12	0.45	1.87	15	1
1:B:276:ARG:HH11	1:B:377:ALA:HB2	0.45	1.71	19	1
1:B:375:ALA:HA	1:B:378:TYR:HD2	0.45	1.70	20	2
1:B:321:ARG:HB2	1:B:321:ARG:NH1	0.45	2.26	1	1
1:A:149:ALA:HB1	1:A:246:PRO:HD2	0.45	1.88	2	3
1:A:274:MET:O	1:A:278:LEU:HB2	0.45	2.11	2	6
1:B:333:PRO:O	1:B:336:LEU:HG	0.45	2.12	8	4
1:B:302:VAL:HG23	1:B:307:ILE:HD11	0.45	1.87	8	4
1:B:132:VAL:HG13	1:B:274:MET:HE2	0.45	1.88	15	1
1:A:48:LYS:HB2	1:B:194:MET:HB2	0.45	1.89	20	1
1:A:219:GLU:HA	1:A:227:LYS:HD2	0.45	1.88	19	2
1:A:372:GLU:HA	1:A:375:ALA:HB3	0.45	1.88	7	1
1:A:342:LYS:HA	1:A:345:VAL:HG22	0.45	1.89	20	1
1:A:294:LEU:HD21	1:A:411:VAL:HG11	0.45	1.87	5	3
1:B:361:LYS:HD3	1:B:362:ALA:N	0.45	2.26	18	1
1:A:392:LYS:HD2	1:A:392:LYS:H	0.45	1.72	5	1
1:A:315:ARG:HG2	1:A:329:ALA:HB1	0.45	1.88	3	2
1:B:300:ILE:HD11	1:B:346:VAL:HA	0.45	1.88	5	2
1:B:317:GLN:O	1:B:321:ARG:HD3	0.45	2.12	3	1
1:A:317:GLN:NE2	1:A:321:ARG:HH12	0.45	2.09	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:GLU:HG3	1:A:305:ALA:H	0.45	1.70	1	1
1:A:172:VAL:HG12	1:A:229:LYS:HB3	0.45	1.88	16	1
1:A:342:LYS:O	1:A:346:VAL:HG23	0.44	2.12	12	5
1:A:93:VAL:HB	1:A:106:SER:HB3	0.44	1.89	4	2
1:B:145:ARG:NH1	1:B:247:GLU:HA	0.44	2.27	19	1
1:A:76:ILE:HD11	1:B:394:LEU:HD11	0.44	1.88	3	1
1:B:201:GLY:HA3	1:B:213:ILE:HG21	0.44	1.90	5	2
1:B:125:VAL:HG11	1:B:412:LEU:HD11	0.44	1.88	5	2
1:A:119:GLY:O	1:A:123:ILE:HG13	0.44	2.13	14	2
1:B:158:VAL:HG11	1:B:202:ILE:HG22	0.44	1.88	8	1
1:B:152:LYS:HE3	1:B:244:GLU:HG3	0.44	1.87	14	1
1:B:307:ILE:HD11	1:B:345:VAL:HG21	0.44	1.89	16	1
1:B:224:GLU:H	1:B:333:PRO:HD3	0.44	1.72	20	1
1:A:333:PRO:O	1:A:336:LEU:HG	0.44	2.12	1	3
1:A:325:ASN:ND2	1:A:327:LYS:HD2	0.44	2.28	15	1
1:B:344:ARG:HH21	1:B:345:VAL:HG12	0.44	1.73	2	1
1:B:406:GLN:HA	1:B:409:GLU:HB3	0.44	1.90	13	1
1:B:189:MET:SD	1:B:243:ARG:CZ	0.44	3.06	18	1
1:A:130:VAL:HG23	1:A:278:LEU:HD11	0.44	1.90	5	1
1:A:137:VAL:HG22	1:A:274:MET:SD	0.44	2.53	5	1
1:B:311:ILE:HD11	1:B:338:GLU:HA	0.44	1.89	16	1
1:B:342:LYS:O	1:B:346:VAL:HG23	0.44	2.12	5	4
1:A:24:ILE:O	1:A:28:VAL:HG23	0.44	2.11	6	3
1:A:141:LEU:HD21	1:A:266:LEU:HD11	0.44	1.88	5	2
1:A:311:ILE:HG12	1:A:334:ARG:HG3	0.44	1.87	5	1
1:B:355:ILE:HA	1:B:360:LEU:HB2	0.44	1.89	7	1
1:A:81:LYS:HA	1:A:81:LYS:NZ	0.44	2.28	15	1
1:B:294:LEU:HD11	1:B:411:VAL:HG21	0.43	1.90	5	2
1:A:339:GLU:O	1:A:343:ARG:HG2	0.43	2.13	20	2
1:B:371:ILE:HG12	1:B:398:MET:HE2	0.43	1.89	1	1
1:A:83:LYS:HA	1:A:83:LYS:HE2	0.43	1.88	6	1
1:B:339:GLU:O	1:B:343:ARG:HD3	0.43	2.13	7	1
1:A:56:GLN:HE22	1:A:100:GLY:HA3	0.43	1.73	12	1
1:A:319:ALA:HB2	1:A:329:ALA:HB2	0.43	1.90	13	1
1:A:28:VAL:HG22	1:A:66:VAL:HG21	0.43	1.91	2	1
1:B:258:VAL:HG12	1:B:261:GLY:H	0.43	1.73	5	2
1:B:154:LYS:HE2	1:B:159:GLU:HG2	0.43	1.90	6	1
1:A:428:MET:N	1:A:428:MET:SD	0.43	2.91	9	1
1:A:57:ARG:HD2	1:B:183:SER:O	0.43	2.12	14	1
1:B:178:GLU:HB2	1:B:323:GLY:HA2	0.43	1.89	10	1
1:A:272:LYS:HA	1:A:272:LYS:HE3	0.43	1.91	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:GLY:HA2	1:A:110:GLU:HG2	0.43	1.91	4	1
1:B:149:ALA:HB1	1:B:246:PRO:HD2	0.43	1.91	2	1
1:B:172:VAL:HG21	1:B:226:LEU:HD22	0.43	1.90	14	2
1:A:141:LEU:HD22	1:A:144:LEU:HD11	0.43	1.91	12	1
1:B:179:GLY:HA3	1:B:323:GLY:HA2	0.43	1.89	16	1
1:B:347:VAL:HG13	1:B:351:LEU:HD12	0.43	1.90	20	1
1:A:147:GLN:HA	1:A:243:ARG:NH2	0.43	2.29	4	1
1:B:141:LEU:HD23	1:B:270:VAL:HG21	0.43	1.91	5	1
1:A:145:ARG:NH1	1:A:247:GLU:HA	0.43	2.28	12	1
1:A:62:VAL:HG23	1:B:321:ARG:HH21	0.43	1.74	1	1
1:B:294:LEU:HB3	1:B:350:LEU:HD13	0.43	1.91	8	3
1:B:319:ALA:HB1	1:B:325:ASN:O	0.43	2.14	11	1
1:A:163:ARG:HA	1:A:187:LEU:O	0.43	2.14	1	1
1:B:207:ALA:HB2	1:B:240:VAL:HG23	0.43	1.89	6	1
1:A:321:ARG:CZ	1:A:321:ARG:HA	0.43	2.44	14	1
1:A:51:MET:SD	1:A:51:MET:N	0.43	2.91	16	1
1:A:285:ARG:NE	1:A:285:ARG:HA	0.43	2.29	16	1
1:B:363:ASP:HB2	1:B:366:ARG:HB2	0.42	1.91	10	1
1:A:382:LYS:HD3	1:A:382:LYS:H	0.42	1.73	11	1
1:B:113:PRO:HG2	1:B:303:PRO:HD3	0.42	1.90	12	1
1:A:380:ASP:O	1:A:384:VAL:HG23	0.42	2.14	15	2
1:A:172:VAL:HG23	1:A:177:PHE:CD1	0.42	2.49	16	1
1:A:287:LYS:O	1:A:291:ILE:HG12	0.42	2.15	5	4
1:B:311:ILE:HG12	1:B:334:ARG:HB2	0.42	1.91	7	1
1:A:427:LEU:HB3	1:A:428:MET:SD	0.42	2.54	9	1
1:B:428:MET:N	1:B:428:MET:SD	0.42	2.92	17	2
1:B:119:GLY:HA3	1:B:297:ALA:HB1	0.42	1.92	14	1
1:A:151:TRP:CZ3	1:A:243:ARG:HG2	0.42	2.49	15	1
1:A:130:VAL:HG12	1:A:422:THR:HB	0.42	1.91	18	1
1:A:206:LYS:O	1:A:209:GLU:HG2	0.42	2.14	14	3
1:B:287:LYS:O	1:B:291:ILE:HG12	0.42	2.14	7	4
1:A:137:VAL:HG13	1:A:270:VAL:HG11	0.42	1.90	6	1
1:A:67:LEU:HD23	1:A:70:LEU:HD12	0.42	1.90	10	1
1:A:40:ARG:HD3	1:B:340:GLN:HB2	0.42	1.90	11	1
1:A:343:ARG:O	1:A:347:VAL:HG23	0.42	2.15	12	2
1:B:273:ASN:O	1:B:277:GLU:HG2	0.42	2.14	6	1
1:A:243:ARG:HD2	1:A:245:LEU:HD21	0.42	1.92	12	1
1:A:127:LYS:HE3	1:A:286:VAL:HG21	0.42	1.90	13	1
1:B:225:ASN:HB2	1:B:331:GLU:HB3	0.42	1.92	17	2
1:A:292:GLU:HG3	1:A:343:ARG:HH12	0.42	1.74	16	1
1:A:48:LYS:HD3	1:A:49:VAL:H	0.42	1.75	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:372:GLU:HG2	1:B:385:ILE:HD13	0.42	1.92	1	1
1:A:198:PHE:H	1:A:215:VAL:HG11	0.42	1.75	7	1
1:A:362:ALA:HB3	1:A:399:ARG:HH11	0.42	1.73	6	1
1:A:290:ALA:HB2	1:A:412:LEU:HD21	0.42	1.92	9	1
1:A:300:ILE:HD11	1:A:346:VAL:HA	0.42	1.91	10	1
1:A:80:ILE:HD12	1:B:384:VAL:HA	0.42	1.92	14	1
1:A:319:ALA:HB1	1:A:325:ASN:O	0.42	2.14	14	1
1:B:118:GLN:O	1:B:297:ALA:HB1	0.42	2.15	17	1
1:B:317:GLN:O	1:B:321:ARG:HG2	0.42	2.14	15	1
1:A:290:ALA:HB2	1:A:412:LEU:HD13	0.42	1.90	7	1
1:B:376:SER:HA	1:B:381:PRO:HG3	0.42	1.92	8	1
1:B:369:GLY:O	1:B:373:GLU:HG3	0.42	2.14	13	1
1:A:137:VAL:O	1:A:141:LEU:HB2	0.42	2.14	20	1
1:A:32:LEU:HD23	1:B:321:ARG:HH21	0.42	1.75	2	1
1:B:189:MET:SD	1:B:189:MET:C	0.42	3.02	3	1
1:A:382:LYS:HE3	1:A:382:LYS:HA	0.42	1.91	10	1
1:A:90:PRO:HG2	1:A:92:TYR:CZ	0.42	2.50	20	1
1:B:320:GLN:HE21	1:B:321:ARG:NH1	0.42	2.13	13	1
1:A:76:ILE:O	1:A:80:ILE:HG12	0.42	2.15	14	1
1:A:166:ILE:HG22	1:A:237:LEU:HA	0.42	1.92	19	1
1:A:258:VAL:HG12	1:A:261:GLY:H	0.41	1.74	1	2
1:B:320:GLN:HG2	1:B:321:ARG:NH2	0.41	2.30	15	1
1:B:315:ARG:NH2	1:B:334:ARG:HB3	0.41	2.30	18	1
1:B:194:MET:SD	1:B:198:PHE:CE1	0.41	3.13	19	1
1:B:147:GLN:HE21	1:B:190:GLY:HA3	0.41	1.75	15	1
1:B:137:VAL:O	1:B:141:LEU:HB2	0.41	2.15	15	4
1:A:120:LEU:HD22	1:A:411:VAL:HG23	0.41	1.92	2	1
1:A:141:LEU:HD21	1:A:270:VAL:HG11	0.41	1.92	2	1
1:B:123:ILE:HD13	1:B:294:LEU:HD22	0.41	1.92	6	2
1:A:362:ALA:HB3	1:A:399:ARG:HG2	0.41	1.92	11	1
1:B:364:GLU:O	1:B:368:LYS:HB3	0.41	2.15	16	1
1:B:120:LEU:O	1:B:415:ALA:HA	0.41	2.16	19	1
1:B:403:LEU:HD23	1:B:406:GLN:NE2	0.41	2.30	5	1
1:A:113:PRO:HG2	1:A:303:PRO:HD3	0.41	1.91	12	1
1:A:110:GLU:HG3	1:A:305:ALA:N	0.41	2.31	1	1
1:B:115:VAL:HG13	1:B:353:GLU:HG3	0.41	1.93	3	1
1:A:355:ILE:HA	1:A:360:LEU:HB2	0.41	1.92	8	1
1:A:88:GLY:HA3	1:A:306:LEU:HD11	0.41	1.91	14	1
1:B:154:LYS:HB2	1:B:242:GLU:HB2	0.41	1.93	4	1
1:A:167:ASP:HB3	1:A:184:ASP:H	0.41	1.76	1	1
1:B:366:ARG:HE	1:B:405:GLU:HB3	0.41	1.75	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:THR:HG23	1:A:252:PHE:HB2	0.41	1.93	8	1
1:B:191:GLN:HE21	1:B:191:GLN:HA	0.41	1.75	10	1
1:B:194:MET:HB3	1:B:199:GLU:HB2	0.41	1.93	15	1
1:A:177:PHE:HE2	1:A:181:LYS:HB3	0.41	1.75	16	1
1:A:267:ARG:O	1:A:271:ARG:HG2	0.41	2.16	1	1
1:B:367:VAL:O	1:B:371:ILE:HG13	0.41	2.15	1	1
1:A:128:PRO:HD2	1:A:282:ILE:HG23	0.41	1.93	2	1
1:A:317:GLN:O	1:A:321:ARG:HD3	0.41	2.16	3	1
1:A:328:GLN:O	1:A:331:GLU:HB3	0.41	2.16	3	1
1:B:375:ALA:HA	1:B:378:TYR:CD2	0.41	2.51	4	1
1:B:403:LEU:HD23	1:B:406:GLN:HE21	0.41	1.76	5	1
1:B:405:GLU:O	1:B:409:GLU:HG2	0.41	2.15	6	1
1:A:48:LYS:HE2	1:B:188:ALA:HB3	0.41	1.92	7	1
1:A:307:ILE:HD11	1:A:345:VAL:HG21	0.41	1.93	7	1
1:A:51:MET:N	1:A:51:MET:SD	0.41	2.94	10	1
1:A:408:VAL:O	1:A:412:LEU:HB2	0.41	2.15	10	1
1:A:258:VAL:HG21	1:A:266:LEU:HA	0.41	1.91	12	1
1:B:267:ARG:O	1:B:271:ARG:HG2	0.41	2.16	12	1
1:A:119:GLY:HA2	1:A:122:ALA:HB3	0.41	1.92	20	2
1:B:352:GLY:O	1:B:356:ARG:HG2	0.41	2.16	15	1
1:A:38:LYS:HA	1:A:38:LYS:HE2	0.41	1.92	16	1
1:A:136:ASP:HB3	1:A:424:PHE:HB3	0.41	1.93	18	1
1:B:307:ILE:H	1:B:307:ILE:HD13	0.41	1.76	19	1
1:A:158:VAL:HB	1:A:203:LYS:HA	0.41	1.92	1	1
1:B:166:ILE:HG22	1:B:237:LEU:HA	0.41	1.93	6	1
1:B:264:GLU:HA	1:B:267:ARG:HE	0.41	1.76	11	1
1:A:19:ILE:HG12	1:A:74:ASN:HD22	0.41	1.76	12	1
1:B:121:GLU:HG2	1:B:414:LYS:HB3	0.41	1.91	17	1
1:A:222:HIS:O	1:A:332:LEU:HG	0.40	2.16	2	1
1:B:395:MET:O	1:B:399:ARG:HG3	0.40	2.16	2	1
1:B:311:ILE:HG12	1:B:334:ARG:HE	0.40	1.76	5	1
1:A:118:GLN:O	1:A:297:ALA:HB1	0.40	2.15	7	1
1:B:254:LYS:HD3	1:B:259:GLU:HA	0.40	1.92	10	1
1:A:364:GLU:O	1:A:368:LYS:HB2	0.40	2.16	1	1
1:B:380:ASP:O	1:B:384:VAL:HG23	0.40	2.17	1	1
1:A:64:GLN:HE21	1:A:64:GLN:HA	0.40	1.76	3	1
1:A:80:ILE:HG23	1:B:383:GLU:HB2	0.40	1.92	3	1
1:A:130:VAL:HG21	1:A:278:LEU:HD21	0.40	1.91	5	1
1:A:196:PRO:HD2	1:A:218:PRO:HD3	0.40	1.93	5	1
1:A:325:ASN:HB2	1:A:328:GLN:HG2	0.40	1.92	14	1
1:A:126:GLU:H	1:A:289:GLN:HG2	0.40	1.76	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:315:ARG:HG2	1:B:329:ALA:HB1	0.40	1.91	6	1
1:B:399:ARG:O	1:B:403:LEU:HB2	0.40	2.16	13	1
1:A:81:LYS:HA	1:A:81:LYS:HZ3	0.40	1.76	15	1
1:A:127:LYS:HB2	1:A:419:GLU:HA	0.40	1.93	11	1
1:A:40:ARG:HH11	1:B:336:LEU:HA	0.40	1.77	13	1
1:B:295:VAL:HG21	1:B:343:ARG:HD2	0.40	1.93	13	1
1:A:39:VAL:HG11	1:B:318:ALA:HB2	0.40	1.94	15	1
1:A:19:ILE:HG12	1:A:74:ASN:ND2	0.40	2.31	20	1
1:A:57:ARG:HD3	1:B:183:SER:O	0.40	2.17	8	1
1:B:291:ILE:O	1:B:295:VAL:HG23	0.40	2.16	8	1
1:B:278:LEU:O	1:B:282:ILE:HG12	0.40	2.16	12	1
1:A:124:GLU:HG2	1:A:416:LYS:HD2	0.40	1.93	17	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/443 (97%)	384±6 (89±1%)	40±6 (9±1%)	5±2 (1±0%)	13	61
1	B	330/443 (74%)	302±4 (92±1%)	26±4 (8±1%)	2±1 (1±0%)	20	70
All	All	15180/17720 (86%)	13711 (90%)	1321 (9%)	148 (1%)	15	65

All 55 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	10	GLY	15
1	B	246	PRO	13
1	A	246	PRO	12
1	B	362	ALA	12
1	A	49	VAL	9
1	A	362	ALA	9
1	A	430	GLN	7
1	B	234	ALA	4
1	A	81	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	45	ARG	4
1	A	43	GLY	4
1	A	48	LYS	3
1	A	94	PRO	2
1	A	196	PRO	2
1	A	46	LYS	2
1	A	192	GLY	2
1	A	44	PHE	2
1	A	2	GLN	2
1	A	248	LEU	2
1	B	248	LEU	2
1	B	323	GLY	2
1	A	47	GLY	1
1	B	237	LEU	1
1	B	333	PRO	1
1	A	419	GLU	1
1	A	156	GLY	1
1	A	193	ARG	1
1	A	386	GLU	1
1	B	156	GLY	1
1	B	192	GLY	1
1	B	123	ILE	1
1	A	303	PRO	1
1	A	198	PHE	1
1	B	198	PHE	1
1	B	379	GLU	1
1	A	247	GLU	1
1	B	285	ARG	1
1	A	50	PRO	1
1	A	99	LEU	1
1	A	102	ASP	1
1	B	193	ARG	1
1	A	96	GLU	1
1	A	113	PRO	1
1	A	123	ILE	1
1	A	132	VAL	1
1	A	178	GLU	1
1	A	166	ILE	1
1	B	102	ASP	1
1	A	323	GLY	1
1	A	117	LEU	1
1	B	113	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	B	170	GLY	1
1	A	95	GLY	1
1	B	178	GLU	1
1	B	303	PRO	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/370 (96%)	337±4 (94±1%)	20±4 (6±1%)	21	70
1	B	275/370 (74%)	257±3 (94±1%)	18±3 (6±1%)	18	67
All	All	12640/14800 (85%)	11892 (94%)	748 (6%)	19	69

All 218 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	141	LEU	17
1	B	141	LEU	17
1	B	121	GLU	15
1	A	121	GLU	14
1	B	105	TYR	13
1	B	243	ARG	12
1	A	355	ILE	11
1	B	355	ILE	11
1	A	81	LYS	11
1	B	419	GLU	10
1	A	243	ARG	9
1	B	366	ARG	9
1	A	382	LYS	9
1	B	382	LYS	9
1	A	394	LEU	8
1	B	278	LEU	8
1	B	285	ARG	8
1	B	272	LYS	8
1	A	278	LEU	7
1	A	193	ARG	7

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Mol	Chain	Res	Type	Models (Total)
1	A	366	ARG	7
1	B	311	ILE	7
1	A	272	LYS	7
1	A	395	MET	7
1	A	340	GLN	6
1	A	342	LYS	6
1	A	344	ARG	6
1	B	279	LYS	6
1	B	342	LYS	6
1	B	421	GLU	6
1	A	327	LYS	6
1	B	107	VAL	6
1	A	37	LYS	6
1	A	279	LYS	6
1	B	395	MET	6
1	A	57	ARG	6
1	A	177	PHE	6
1	A	117	LEU	5
1	A	255	ARG	5
1	A	422	THR	5
1	B	193	ARG	5
1	B	340	GLN	5
1	B	373	GLU	5
1	B	327	LYS	5
1	A	416	LYS	5
1	B	416	LYS	5
1	A	73	ARG	5
1	A	294	LEU	5
1	A	38	LYS	5
1	B	177	PHE	5
1	B	394	LEU	5
1	A	48	LYS	4
1	A	148	GLN	4
1	A	276	ARG	4
1	A	368	LYS	4
1	A	397	ASN	4
1	B	117	LEU	4
1	B	124	GLU	4
1	B	148	GLN	4
1	B	247	GLU	4
1	B	296	LYS	4
1	B	344	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	B	422	THR	4
1	A	98	LYS	4
1	A	254	LYS	4
1	B	203	LYS	4
1	A	244	GLU	4
1	A	420	LYS	4
1	A	45	ARG	4
1	A	273	ASN	4
1	A	311	ILE	4
1	A	421	GLU	4
1	B	310	GLU	4
1	A	287	LYS	4
1	B	287	LYS	4
1	A	405	GLU	4
1	A	114	GLU	4
1	B	176	GLU	3
1	B	269	GLU	3
1	B	276	ARG	3
1	B	326	GLU	3
1	A	64	GLN	3
1	A	85	ASN	3
1	A	203	LYS	3
1	B	361	LYS	3
1	B	392	LYS	3
1	A	206	LYS	3
1	A	390	LYS	3
1	A	392	LYS	3
1	B	152	LYS	3
1	A	144	LEU	3
1	A	285	ARG	3
1	A	404	GLU	3
1	A	419	GLU	3
1	B	186	VAL	3
1	B	273	ASN	3
1	A	296	LYS	3
1	B	255	ARG	3
1	B	316	ARG	3
1	A	145	ARG	3
1	A	215	VAL	3
1	A	310	GLU	3
1	B	215	VAL	3
1	B	294	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	B	368	LYS	3
1	A	289	GLN	3
1	A	334	ARG	3
1	B	114	GLU	3
1	A	403	LEU	3
1	B	321	ARG	3
1	A	283	ARG	3
1	B	283	ARG	3
1	B	390	LYS	3
1	B	403	LEU	3
1	A	199	GLU	2
1	A	247	GLU	2
1	A	298	ASN	2
1	A	361	LYS	2
1	A	430	GLN	2
1	A	181	LYS	2
1	A	224	GLU	2
1	A	353	GLU	2
1	B	120	LEU	2
1	B	244	GLU	2
1	B	266	LEU	2
1	A	373	GLU	2
1	B	115	VAL	2
1	B	206	LYS	2
1	A	52	ASN	2
1	A	191	GLN	2
1	B	254	LYS	2
1	B	356	ARG	2
1	A	46	LYS	2
1	A	176	GLU	2
1	A	232	LYS	2
1	A	393	GLU	2
1	B	219	GLU	2
1	B	420	LYS	2
1	A	74	ASN	2
1	A	186	VAL	2
1	A	266	LEU	2
1	A	400	ASN	2
1	A	96	GLU	2
1	A	175	GLU	2
1	A	328	GLN	2
1	B	191	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	B	406	GLN	2
1	A	414	LYS	2
1	B	414	LYS	2
1	A	316	ARG	2
1	A	9	GLN	2
1	A	99	LEU	2
1	A	127	LYS	2
1	A	307	ILE	2
1	A	159	GLU	1
1	B	232	LYS	1
1	B	126	GLU	1
1	B	220	GLU	1
1	A	25	GLU	1
1	B	144	LEU	1
1	B	199	GLU	1
1	A	338	GLU	1
1	B	194	MET	1
1	A	120	LEU	1
1	A	133	THR	1
1	A	264	GLU	1
1	A	303	PRO	1
1	B	320	GLN	1
1	B	360	LEU	1
1	B	372	GLU	1
1	A	126	GLU	1
1	A	217	PHE	1
1	B	238	LYS	1
1	B	336	LEU	1
1	B	427	LEU	1
1	A	386	GLU	1
1	B	289	GLN	1
1	A	321	ARG	1
1	A	427	LEU	1
1	B	328	GLN	1
1	B	339	GLU	1
1	A	83	LYS	1
1	B	145	ARG	1
1	A	2	GLN	1
1	A	241	GLU	1
1	A	406	GLN	1
1	B	241	GLU	1
1	B	335	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	B	229	LYS	1
1	B	277	GLU	1
1	B	429	ASN	1
1	A	275	GLU	1
1	A	383	GLU	1
1	A	396	ASP	1
1	B	159	GLU	1
1	B	334	ARG	1
1	B	405	GLU	1
1	A	146	LYS	1
1	A	229	LYS	1
1	A	317	GLN	1
1	B	146	LYS	1
1	B	167	ASP	1
1	B	181	LYS	1
1	B	386	GLU	1
1	B	425	ASN	1
1	A	31	GLU	1
1	A	118	GLN	1
1	A	152	LYS	1
1	A	372	GLU	1
1	B	101	GLU	1
1	B	275	GLU	1
1	B	353	GLU	1
1	B	404	GLU	1
1	B	325	ASN	1
1	B	307	ILE	1
1	B	343	ARG	1
1	B	399	ARG	1
1	B	364	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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 14% for the well-defined parts and 14% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch-3let.str*

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	1674
Number of shifts mapped to atoms	1674
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	41	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	331	-0.42 ± 0.19	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 14%, i.e. 1662 atoms were assigned a chemical shift out of a possible 11739. 0 out of 146 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	658/4301 (15%)	329/1754 (19%)	0/1714 (0%)	329/833 (39%)
Sidechain	880/6898 (13%)	660/4446 (15%)	220/2165 (10%)	0/287 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	124/540 (23%)	62/262 (24%)	62/268 (23%)	0/10 (0%)
Overall	1662/11739 (14%)	1051/6462 (16%)	282/4147 (7%)	329/1130 (29%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 14%, i.e. 1674 atoms were assigned a chemical shift out of a possible 11832. 0 out of 146 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	662/4336 (15%)	331/1768 (19%)	0/1728 (0%)	331/840 (39%)
Sidechain	888/6956 (13%)	666/4484 (15%)	222/2182 (10%)	0/290 (0%)
Aromatic	124/540 (23%)	62/262 (24%)	62/268 (23%)	0/10 (0%)
Overall	1674/11832 (14%)	1059/6514 (16%)	284/4178 (7%)	331/1140 (29%)

7.1.4 Statistically unusual chemical shifts [i](#)

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

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	109	PHE	CE2	137.12	124.80 – 136.72	5.3

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:

