

Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	6D6S
Title	:	Solution structure of Trigger Factor dimer
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Deposited on	:	2018-04-22

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 following versions of software and data (see references (1)) were used in the production of this report:

Cyrange	:	Kirchner and Güntert (2011)
$\operatorname{NmrClust}$:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	$v_1n_1_5_13_A$ (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
${ m ShiftChecker}$:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

Sidechain outliers

1 Overall quality at a glance (i)

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.



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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 <=5%

11428

Mol	Chain	Length	Quality of chain				
1	А	443	91%	6% ••			
1	В	443	92%	• • •			



2 Ensemble composition and analysis (i)

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 ran	ge (total)	Backbone RMSD (Å)	Medoid model			
1	A:2-A:111,	B:109-B:429	0.88	5			
	(431)						
2	A:112-A:430,	B:2-B:108	0.87	5			
	(426)						

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, 17, 18
2	3,11,13,14,16,19
3	8, 12, 20



3 Entry composition (i)

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	1 1	420	Total	С	Η	Ν	Ο	S	0
	432	6789	2119	3403	582	674	11	0	
1	1 D	D 420	Total	С	Η	Ν	Ο	S	0
I B	432	6789	2119	3403	582	674	11	0	

There are 22 discrepancies between the modelled and reference sequences:

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



4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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



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





L394 N397 N397 A407 A407 T422 T422 Q430 Q431 Q432 Q432

• Molecule 1: Trigger factor



4.2.2 Score per residue for model 2

• Molecule 1: Trigger factor



L394 A407 A407 B411 E419 E419 L427 L427 A432

• Molecule 1: Trigger factor



4.2.3 Score per residue for model 3





• Molecule 1: Trigger factor



4.2.4 Score per residue for model 4

• Molecule 1: Trigger factor



4.2.5 Score per residue for model 5 (medoid)





K206 MET P218 LYS R232 HIS R232 HIS R246 HIS R256 HIS R246 HIS R256 R46 R272 NB2 R272 NB2 R273 NB2 R274 NB2 R273 NB2 R274 NB2 R288 NB2 R291 NB3 R293 NB3 R294 L117 R394 L144 R394 L144 R394 L144 R394 L144 R394 L166 L390 R166 R394 L166 L390 R196 R384 L166</td

K392 E393 L394 K395 N395 N395 N397 V411 K416 K416 K416

• Molecule 1: Trigger factor



4.2.6 Score per residue for model 6

• Molecule 1: Trigger factor



4.2.7 Score per residue for model 7



193 MET 196 H.S. 196 H.S. 196 H.S. 196 H.S. 196 H.S. 215 H.S. 216 H.S. 217 H.S. 216 H.S. 217 H.S. 218 H.S. 219 K.46 216 K.29 217 H.S. 218 K.81 219 K.46 214 K.33 216 K.46 217 H.46 218 K.46 219 K.46 214 K.46 217 H.46 <tr/td>

L394 M395 E405 L412 V417 V417 V417

• Molecule 1: Trigger factor



4.2.8 Score per residue for model 8

• Molecule 1: Trigger factor

Chain A:	80%	16% ••
MET ASN LYS LYS LYS HITS HITS HITS HITS HITS CO 00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	118 153 153 153 153 153 153 154 154 154 179 179 179 179 179 179 179 179 179 179	8106 1117 1117 1117 1121 1121 1121 1125 1132 1132 1132 1132
1166 E176 M193 M193 F198 F198 T216 N225 A230	K239 R243 F245 F245 F246 F247 F252 F252 F252 F256 R247 F252 F256 R273 R27 F269 R273 R27 F269 R278 R278 F269 R278 R287	1291 P303 P303 P303 E331 P333 P333 P333 P333 P333 P333 P33
L360 K361 K361 L362 K361 L371 L371 L385 L338 L386 L386 L394 L394 K395	1420 4407 1412 1412 1412 1417 1427 1427 1427 1433	

• Molecule 1: Trigger factor



4.2.9 Score per residue for model 9







Score per residue for model 11 4.2.11

• Molecule 1: Trigger factor



• Molecule 1: Trigger factor



Score per residue for model 12 4.2.12

• Molecule 1: Trigger factor

Chain A:	81%	16% ••
MET ASN ASN ASN VAL VAL VAL HIS HIS HIS HIS HIS HIS CO CO CO CO CO CO CO CO CO CO CO CO CO	V66 V66 R73 R73 F75 176 176 176 176 176 176 127 1123 1123	V132 138 6139 0140 1141 1144 1144 1144 1145 1165
1166 E177 E177 E177 E177 E177 E178 E178 E249 E244 E244 E244 E244 E244 E244 E244	N254 V258 L266 K272 K279 K279 K376 K372 K373 K371 K373 K321 K334	43 44 A3 44 K3 42 K3 42 K3 42 K3 42 K3 42 K3 82 K3 82 K3 82 K3 82 K3 92 K3 92
E333 L394 M395 M395 R395 R399 R406 A407 R413 R413 R413 R413 R413 R413 R413 R413		
• Molecule 1: Trigger factor		
Chain B:	85%	11%
MET ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	L141 F177 F198 F198 F198 F198 F198 F198 F241 F241 F241 F245 F246 F246 F246 F246 F248 F246 F248 F248 F248 F248 F248 F248 F248 F248	L266 L266 R271 L278 K279 K279 K279 K283 L283
P303 R321 R321 R321 R324 R325 R325 R325 R325 R325 R325 R325 R325	2389 V384 K390 K396 K396 K396 V411 L412 L412 V417 V417 L427	0430 0431 A432



4.2.13 Score per residue for model 13

• Molecule 1: Trigger factor





4.2.14 Score per residue for model 14

• Molecule 1: Trigger factor

MET ASN HIS LYS LYS VAL HIS HIS HIS HIS



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



4.2.17 Score per residue for model 17

• Molecule 1: Trigger factor



• Molecule 1: Trigger factor



4.2.18 Score per residue for model 18

• Molecule 1: Trigger factor

 Chain A:
 89%
 7%

 Image: State of the stat



4.2.19 Score per residue for model 19

• Molecule 1: Trigger factor

Chain A: 87% 9% •• MET ASN HIS LYS LYS HIS HIS HIS HIS HIS HIS HIS V41 L41

• Molecule 1: Trigger factor



- 4.2.20 Score per residue for model 20
- Molecule 1: Trigger factor







5 Refinement protocol and experimental data overview (i)

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 6 of this report.

Chemical shift file(s)	input_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)	12%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	А	3363	3381	3379	21 ± 5
1	В	3354	3373	2581	18 ± 4
All	All	134340	135080	119200	761

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.



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A 4 1			D1 (8)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	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:A:189:MET:SD	1:A:243:ARG:HG3	0.58	2.39	8	7	
1:B:125:VAL:HB	1:B:417:VAL:HA	0.58	1.75	10	8	
1:A:207:ALA:HB2	1:A:240:VAL:HG23	0.58	1.75	6	4	
1:B:253:ILE:HG23	1:B:266:LEU:HB2	0.57	1.75	15	7	
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: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	
1:B:409:GLU:HA	1:B:412:LEU:HB2	0.56	1.76	16	1	
1:A:303:PRO:HB2	1:A:306:LEU:HD13	0.56	1.78	10	7	
1:A:125:VAL:HB	1:A:417:VAL:HA	0.56	1.77	7	11	
1:B:291:ILE:HG23	1:B:347:VAL:HG21	0.56	1.76	4	3	
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:253:ILE:HG23	1:A:266:LEU:HB2	0.55	1.79	15	6	
1:A:36:ALA:HB1	1:A:42:ASP:HA	0.55	1.78	9	2	
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: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	



Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models		
7100m 1	1100111 =			Worst	Total	
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: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: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:98:LYS:HD2	1:A:101:GLU:HB2	0.52	1.80	20	2	
1:B:121:GLU:HA	1:B:415:ALA:HA	0.52	1.82	10	3	
1:A:126:GLU:HB3	1:A:289:GLN:HG3	0.52	1.82	5	1	
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	
1:B:165:THR:HB	1:B:239:LYS:HB2	0.51	1.82	1	7	
1:A:172:VAL:HA	1:A:231:ALA:HA	0.51	1.82	16	1	
1:B:124:GLU:HG3	1:B:289:GLN:NE2	0.51	2.21	7	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:80:ILE:HD13	1:B:384:VAL:HA	0.50	1.82	12	2	
1:A:22:ASP:HA	1:A:25:GLU:HB3	0.50	1.82	7	1	
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:B:338:GLU:HA	1:B:341:ALA:HB3	0.50	1.82	7	1	
1:A:3:VAL:HG12	1:A:17:ILE:HG23	0.50	1.84	11	2	
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:A:225:ASN:HB2	1:A:331:GLU:HG2	0.50	1.84	8	2	
1:B:362:ALA:HB2	1:B:399:ARG:HG3	0.50	1.82	7	2	
1:B:284:ASN:HB3	1:B:285:ARG:HH21	0.50	1.66	3	1	
1:A:2:GLN:HB2	1:A:18:THR:HB	0.50	1.84	8	2	
1:A:161:GLU:HA	1:A:189:MET:SD	0.49	2.47	10	1	
1:B:224:GLU:HA	1:B:227:LYS:HG2	0.49	1.83	6	2	
1:A:41:ILE:HG21	1:B:336:LEU:HD13	0.49	1.84	4	1	
1:A:398:MET:HA	1:A:401:VAL:HG22	0.49	1.84	14	2	



A 4 1		(1,1,(3))		Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
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: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:128:PRO:HG2	1:B:285:ARG:HG2	0.49	1.83	18	1	
1:B:364:GLU:HA	1:B:367:VAL:HG12	0.49	1.85	9	1	
1:A:352:GLY:O	1:A:355:ILE:HG12	0.49	2.08	15	1	
1:A:117:LEU:HD23	1:A:117:LEU:H	0.49	1.67	3	2	
1:A:355:ILE:HG23	1:A:407:ALA:HB2	0.49	1.85	1	5	
1:A:144:LEU:HD21	1:A:256:PHE:HZ	0.49	1.67	13	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:B:189:MET:SD	1:B:243:ARG:NE	0.49	2.86	3	1	
1:B:364:GLU:HG2	1:B:368:LYS:HE3	0.48	1.84	8	1	
1:B:145:ARG:HB3	1:B:248:LEU:HD13	0.48	1.85	1	1	
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:218:PRO:HG2	1:A:221:TYR:HB2	0.48	1.86	17	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:320:GLN:HA	1:A:324:GLY:HA2	0.48	1.86	9	3	
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: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:159:GLU:HA	1:B:203:LYS:HZ3	0.48	1.68	2	1	
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:172:VAL:HG21	1:A:226:LEU:HD22	0.47	1.86	11	3	
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:338:GLU:HA	1:A:341:ALA:HB3	0.47	1.86	7	1	
1:A:53:ILE:HD12	1:B:185:PHE:HA	0.47	1.86	2	1	
1:B:110:GLU:HB2	1:B:303:PRO:HB3	0.47	1.86	17	2	
1:A:194:MET:SD	1:A:198:PHE:CD2	0.47	3.08	8	3	
1:A:62:VAL:HG23	1:B:321:ARG:NH2	0.47	2.24	1	2	
1:B:352:GLY:O	1:B:355:ILE:HG12	0.47	2.09	15	1	
1:B:216:THR:HA	1:B:230:ALA:HA	0.47	1.85	8	2	
1:A:216:THR:HA	1:A:230:ALA:HA	0.47	1.86	10	3	
1:A:25:GLU:HG3	1:A:29:LYS:NZ	0.47	2.24	7	1	
1:A:172:VAL:HG11	1:A:226:LEU:HA	0.47	1.87	11	1	



				Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
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:A:123:ILE:HD13	1:A:294:LEU:HD22	0.47	1.84	17	2	
1:A:302:VAL:HG21	1:A:345:VAL:HG23	0.47	1.86	14	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:311:ILE:HD11	1:A:338:GLU:HA	0.47	1.86	10	1	
1:B:408:VAL:O	1:B:412:LEU:HB2	0.47	2.10	20	2	
1:B:270:VAL:HG12	1:B:274:MET:SD	0.47	2.49	9	1	
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	
1:B:364:GLU:O	1:B:368:LYS:HB2	0.46	2.11	3	1	
1:B:117:LEU:H	1:B:117:LEU:HD23	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:159:GLU:HG3	1:A:161:GLU:H	0.46	1.70	3	1	
1:A:194:MET:HB2	1:A:199:GLU:HB2	0.46	1.86	17	1	
1:A:148:GLN:HE21	1:A:148:GLN:HA	0.46	1.71	7	1	
1:A:362:ALA:HB2	1:A:399:ARG:HG3	0.46	1.88	20	1	
1:A:352:GLY:O	1:A:356:ARG:HG2	0.46	2.11	15	1	
1:A:190:GLY:HA3	1:A:243:ARG:HH22	0.46	1.70	1	1	
1:B:321:ARG:HB2	1:B:321:ARG:HH11	0.46	1.71	1	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:A:294:LEU:HB3	1:A:350:LEU:HD13	0.45	1.86	7	1	
1:B:360:LEU:HB3	1:B:406:GLN:HE22	0.45	1.71	4	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:B:276:ARG:HH11	1:B:377:ALA:HB2	0.45	1.71	19	1	
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:375:ALA:HA	1:B:378:TYR:HD2	0.45	1.70	20	2	
1:B:302:VAL:HG23	1:B:307:ILE:HD11	0.45	1.87	8	4	
1:A:149:ALA:HB1	1:A:246:PRO:HD2	0.45	1.88	2	3	
1:B:333:PRO:O	1:B:336:LEU:HG	0.45	2.12	8	4	



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	1		D1 (8)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:274:MET:O	1:A:278:LEU:HB2	0.45	2.11	2	6	
1:A:48:LYS:HB2	1:B:194:MET:HB2	0.45	1.89	20	1	
1:B:321:ARG:NH1	1:B:321:ARG:HB2	0.45	2.26	1	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:H	1:A:392:LYS:HD2	0.45	1.72	5	1	
1:B:300:ILE:HD11	1:B:346:VAL:HA	0.45	1.88	5	2	
1:A:317:GLN:NE2	1:A:321:ARG:HH12	0.45	2.09	18	1	
1:A:315:ARG:HG2	1:A:329:ALA:HB1	0.45	1.88	3	2	
1:B:317:GLN:O	1:B:321:ARG:HD3	0.45	2.12	3	1	
1:A:172:VAL:HG12	1:A:229:LYS:HB3	0.45	1.88	16	1	
1:A:110:GLU:HG3	1:A:305:ALA:H	0.45	1.70	1	1	
1:B:145:ARG:NH1	1:B:247:GLU:HA	0.44	2.27	19	1	
1:A:93:VAL:HB	1:A:106:SER:HB3	0.44	1.89	4	2	
1:A:342:LYS:O	1:A:346:VAL:HG23	0.44	2.12	12	5	
1:B:125:VAL:HG11	1:B:412:LEU:HD11	0.44	1.88	5	2	
1:B:201:GLY:HA3	1:B:213:ILE:HG21	0.44	1.90	5	2	
1:A:76:ILE:HD11	1:B:394:LEU:HD11	0.44	1.88	3	1	
1:A:119:GLY:O	1:A:123:ILE:HG13	0.44	2.13	14	2	
1:B:152:LYS:HE3	1:B:244:GLU:HG3	0.44	1.87	14	1	
1:B:158:VAL:HG11	1:B:202:ILE:HG22	0.44	1.88	8	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: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:B:344:ARG:HH21	1:B:345:VAL:HG12	0.44	1.73	2	1	
1:B:311:ILE:HD11	1:B:338:GLU:HA	0.44	1.89	16	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: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: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:B:355:ILE:HA	1:B:360:LEU:HB2	0.44	1.89	7	1	
1:A:81:LYS:NZ	1:A:81:LYS:HA	0.44	2.28	15	1	
1:A:339:GLU:O	1:A:343:ARG:HG2	0.43	2.13	20	2	



			D ! (8)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:B:294:LEU:HD11	1:B:411:VAL:HG21	0.43	1.90	5	2	
1:A:319:ALA:HB2	1:A:329:ALA:HB2	0.43	1.90	13	1	
1:A:83:LYS:HA	1:A:83:LYS:HE2	0.43	1.88	6	1	
1:A:56:GLN:HE22	1:A:100:GLY:HA3	0.43	1.73	12	1	
1:B:339:GLU:O	1:B:343:ARG:HD3	0.43	2.13	7	1	
1:A:57:ARG:HD2	1:B:183:SER:O	0.43	2.12	14	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:SD	1:A:428:MET:N	0.43	2.91	9	1	
1:A:28:VAL:HG22	1:A:66:VAL:HG21	0.43	1.91	2	1	
1:B:178:GLU:HB2	1:B:323:GLY:HA2	0.43	1.89	10	1	
1:A:272:LYS:HE3	1:A:272:LYS:HA	0.43	1.91	17	1	
1:A:12:GLY:HA2	1:A:110:GLU:HG2	0.43	1.91	4	1	
1:B:172:VAL:HG21	1:B:226:LEU:HD22	0.43	1.90	14	2	
1:B:179:GLY:HA3	1:B:323:GLY:HA2	0.43	1.89	16	1	
1:A:141:LEU:HD22	1:A:144:LEU:HD11	0.43	1.91	12	1	
1:B:149:ALA:HB1	1:B:246:PRO:HD2	0.43	1.91	2	1	
1:B:347:VAL:HG13	1:B:351:LEU:HD12	0.43	1.90	20	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:147:GLN:HA	1:A:243:ARG:NH2	0.43	2.29	4	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:62:VAL:HG23	1:B:321:ARG:HH21	0.43	1.74	1	1	
1:A:321:ARG:CZ	1:A:321:ARG:HA	0.43	2.44	14	1	
1:A:285:ARG:HA	1:A:285:ARG:NE	0.43	2.29	16	1	
1:A:51:MET:N	1:A:51:MET:SD	0.43	2.91	16	1	
1:B:207:ALA:HB2	1:B:240:VAL:HG23	0.43	1.89	6	1	
1:A:163:ARG:HA	1:A:187:LEU:O	0.43	2.14	1	1	
1:A:380:ASP:O	1:A:384:VAL:HG23	0.42	2.14	15	2	
1:B:363:ASP:HB2	1:B:366:ARG:HB2	0.42	1.91	10	1	
1:A:172:VAL:HG23	1:A:177:PHE:CD1	0.42	2.49	16	1	
1:B:113:PRO:HG2	1:B:303:PRO:HD3	0.42	1.90	12	1	
1:A:382:LYS:H	1:A:382:LYS:HD3	0.42	1.73	11	1	
1:B:428:MET:SD	1:B:428:MET:N	0.42	2.92	17	1	
1:A:287:LYS:O	1:A:291:ILE:HG12	0.42	2.15	5	4	
1:B:119:GLY:HA3	1:B:297:ALA:HB1	0.42	1.92	14	1	
1:A:130:VAL:HG12	1:A:422:THR:HB	0.42	1.91	18	1	
1:A:427:LEU:HB3	1:A:428:MET:SD	0.42	2.54	9	1	
1:B:311:ILE:HG12	1:B:334:ARG:HB2	0.42	1.91	7	1	
1:A:151:TRP:CZ3	1:A:243:ARG:HG2	0.42	2.49	15	1	



				Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:206:LYS:O	1:A:209:GLU:HG2	0.42	2.14	14	3
1:A:67:LEU:HD23	1:A:70:LEU:HD12	0.42	1.90	10	1
1:A:137:VAL:HG13	1:A:270:VAL:HG11	0.42	1.90	6	1
1:A:343:ARG:O	1:A:347:VAL:HG23	0.42	2.15	12	2
1:B:287:LYS:O	1:B:291:ILE:HG12	0.42	2.14	7	4
1:A:40:ARG:HD3	1:B:340:GLN:HB2	0.42	1.90	11	1
1:B:225:ASN:HB2	1:B:331:GLU:HB3	0.42	1.92	17	2
1:A:127:LYS:HE3	1:A:286:VAL:HG21	0.42	1.90	13	1
1:A:292:GLU:HG3	1:A:343:ARG:HH12	0.42	1.74	16	1
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:B:117:LEU:HD23	1:B:117:LEU:H	0.42	1.74	13	1
1:A:198:PHE:H	1:A:215:VAL:HG11	0.42	1.75	7	1
1:A:48:LYS:HD3	1:A:49:VAL:H	0.42	1.75	1	1
1:B:372:GLU:HG2	1:B:385:ILE:HD13	0.42	1.92	1	1
1:B:118:GLN:O	1:B:297:ALA:HB1	0.42	2.15	17	1
1:A:319:ALA:HB1	1:A:325:ASN:O	0.42	2.14	14	1
1:A:80:ILE:HD12	1:B:384:VAL:HA	0.42	1.92	14	1
1:A:300:ILE:HD11	1:A:346:VAL:HA	0.42	1.91	10	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:B:317:GLN:O	1:B:321:ARG:HG2	0.42	2.14	15	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:290:ALA:HB2	1:A:412:LEU:HD13	0.42	1.90	7	1
1:A:137:VAL:O	1:A:141:LEU:HB2	0.42	2.14	20	1
1:A:382:LYS:HA	1:A:382:LYS:HE3	0.42	1.91	10	1
1:A:32:LEU:HD23	1:B:321:ARG:HH21	0.42	1.75	2	1
1:A:90:PRO:HG2	1:A:92:TYR:CZ	0.42	2.50	20	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:B:320:GLN:HE21	1:B:321:ARG:NH1	0.42	2.13	13	1
1:B:428:MET:N	1:B:428:MET:SD	0.41	2.93	13	1
1:A:258:VAL:HG12	1:A:261:GLY:H	0.41	1.74	1	2
1:B:194:MET:SD	1:B:198:PHE:CE1	0.41	3.13	19	1
1:B:315:ARG:NH2	1:B:334:ARG:HB3	0.41	2.30	18	1
1:B:320:GLN:HG2	1:B:321:ARG:NH2	0.41	2.30	15	1
1:B:147:GLN:HE21	1:B:190:GLY:HA3	0.41	1.75	15	1
1:B:120:LEU:O	1:B:415:ALA:HA	0.41	2.16	19	1
1:B:137:VAL:O	1:B:141:LEU:HB2	0.41	2.15	15	4
1:B:364:GLU:O	1:B:368:LYS:HB3	0.41	2.15	16	1



	1 5		Distance(Å)	Models		
Atom-1	Atom-2	Clash(A)		Worst	Total	
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: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: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:88:GLY:HA3	1:A:306:LEU:HD11	0.41	1.91	14	1	
1:A:355:ILE:HA	1:A:360:LEU:HB2	0.41	1.92	8	1	
1:B:115:VAL:HG13	1:B:353:GLU:HG3	0.41	1.93	3	1	
1:A:110:GLU:HG3	1:A:305:ALA:N	0.41	2.31	1	1	
1:B:154:LYS:HB2	1:B:242:GLU:HB2	0.41	1.93	4	1	
1:A:150:THR:HG23	1:A:252:PHE:HB2	0.41	1.93	8	1	
1:B:191:GLN:HA	1:B:191:GLN:HE21	0.41	1.75	10	1	
1:A:177:PHE:HE2	1:A:181:LYS:HB3	0.41	1.75	16	1	
1:B:366:ARG:HE	1:B:405:GLU:HB3	0.41	1.75	4	1	
1:B:194:MET:HB3	1:B:199:GLU:HB2	0.41	1.93	15	1	
1:A:167:ASP:HB3	1:A:184:ASP:H	0.41	1.76	1	1	
1:B:307:ILE:HD13	1:B:307:ILE:H	0.41	1.76	19	1	
1:A:408:VAL:O	1:A:412:LEU:HB2	0.41	2.15	10	1	
1:A:51:MET:SD	1:A:51:MET:N	0.41	2.94	10	1	
1:A:38:LYS:HE2	1:A:38:LYS:HA	0.41	1.92	16	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:B:267:ARG:O	1:B:271:ARG:HG2	0.41	2.16	12	1	
1:A:258:VAL:HG21	1:A:266:LEU:HA	0.41	1.91	12	1	
1:A:136:ASP:HB3	1:A:424:PHE:HB3	0.41	1.93	18	1	
1:A:307:ILE:HD11	1:A:345:VAL:HG21	0.41	1.93	7	1	
1:A:48:LYS:HE2	1:B:188:ALA:HB3	0.41	1.92	7	1	
1:B:375:ALA:HA	1:B:378:TYR:CD2	0.41	2.51	4	1	
1:A:128:PRO:HD2	1:A:282:ILE:HG23	0.41	1.93	2	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:328:GLN:O	1:A:331:GLU:HB3	0.41	2.16	3	1	
1:A:317:GLN:O	1:A:321:ARG:HD3	0.41	2.16	3	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:B:121:GLU:HG2	1:B:414:LYS:HB3	0.41	1.91	17	1	
1:B:166:ILE:HG22	1:B:237:LEU:HA	0.41	1.93	6	1	
1:A:19:ILE:HG12	1:A:74:ASN:HD22	0.41	1.76	12	1	
1:B:264:GLU:HA	1:B:267:ARG:HE	0.41	1.76	11	1	
1:A:158:VAL:HB	1:A:203:LYS:HA	0.41	1.92	1	1	



Atom 1	Atom 2	$Cleat (\lambda)$	\mathbf{D} :stores($\hat{\mathbf{A}}$)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:B:254:LYS:HD3	1:B:259:GLU:HA	0.40	1.92	10	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: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:A:325:ASN:HB2	1:A:328:GLN:HG2	0.40	1.92	14	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: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: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:B:399:ARG:O	1:B:403:LEU:HB2	0.40	2.16	13	1	
1:B:315:ARG:HG2	1:B:329:ALA:HB1	0.40	1.91	6	1	
1:A:126:GLU:H	1:A:289:GLN:HG2	0.40	1.76	3	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:127:LYS:HB2	1:A:419:GLU:HA	0.40	1.93	11	1	
1:A:19:ILE:HG12	1:A:74:ASN:ND2	0.40	2.31	20	1	
1:A:39:VAL:HG11	1:B:318:ALA:HB2	0.40	1.94	15	1	
1:A:124:GLU:HG2	1:A:416:LYS:HD2	0.40	1.93	17	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	

5.2 Torsion angles (i)

5.2.1 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	А	429/443~(97%)	384 ± 6 (89 $\pm1\%$)	$40\pm 6 (9\pm 1\%)$	$5\pm2~(1\pm0\%)$	17 64
1	В	330/443~(74%)	$302 \pm 4 \ (92 \pm 1\%)$	$26 \pm 4 \ (8 \pm 1\%)$	2±1 (1±0%)	26 73
All	All	15180/17720~(86%)	13711 (90%)	1321 (9%)	148 (1%)	20 68

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



occurrence in the ensemble.

Mol	Chain	\mathbf{Res}	Type	Models (Total)
1	А	10	GLY	15
1	В	246	PRO	13
1	А	246	PRO	12
1	В	362	ALA	12
1	А	362	ALA	9
1	А	49	VAL	9
1	А	430	GLN	7
1	В	234	ALA	4
1	А	45	ARG	4
1	А	81	LYS	4
1	А	43	GLY	4
1	А	48	LYS	3
1	А	44	PHE	2
1	В	323	GLY	2
1	А	196	PRO	2
1	А	94	PRO	2
1	А	192	GLY	2
1	А	248	LEU	2
1	А	2	GLN	2
1	В	248	LEU	2
1	А	46	LYS	2
1	А	95	GLY	1
1	А	47	GLY	1
1	А	113	PRO	1
1	A	303	PRO	1
1	A	178	GLU	1
1	В	123	ILE	1
1	A	386	GLU	1
1	A	117	LEU	1
1	A	198	PHE	1
1	A	156	GLY	1
1	В	102	ASP	1
1	В	379	GLU	1
1	В	192	GLY	1
1	В	198	PHE	1
1	A	123	ILE	1
1	A	166	ILE	1
1	A	247	GLU	1
1	В	178	GLU	1
1	В	237	LEU	1
1	A	50	PRO	1
$ 1^{-}$	B	113	PRO	1



Mol	Chain	Res	Type	Models (Total)
1	А	99	LEU	1
1	А	419	GLU	1
1	В	170	GLY	1
1	А	323	GLY	1
1	А	132	VAL	1
1	В	156	GLY	1
1	А	102	ASP	1
1	В	193	ARG	1
1	В	333	PRO	1
1	А	193	ARG	1
1	В	285	ARG	1
1	А	96	GLU	1
1	В	303	PRO	1

5.2.2 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	Perce	entiles
1	А	357/370~(96%)	$335 \pm 4 \ (94 \pm 1\%)$	$22 \pm 4 \ (6 \pm 1\%)$	22	71
1	В	275/370~(74%)	256 ± 3 (93 $\pm1\%$)	$19\pm3~(7\pm1\%)$	19	68
All	All	12640/14800~(85%)	11826 (94%)	814 (6%)	21	70

All 247 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	В	141	LEU	16
1	В	105	TYR	15
1	А	121	GLU	15
1	В	121	GLU	14
1	А	141	LEU	14
1	В	243	ARG	11
1	А	340	GLN	10
1	В	366	ARG	10
1	А	177	PHE	10
1	А	9	GLN	10
1	В	382	LYS	9



Mol	Chain	\mathbf{Res}	Type	Models (Total)
1	В	177	PHE	9
1	А	382	LYS	9
1	А	81	LYS	9
1	А	73	ARG	8
1	В	419	GLU	8
1	А	272	LYS	8
1	А	243	ARG	8
1	В	193	ARG	8
1	А	193	ARG	8
1	А	244	GLU	8
1	В	255	ARG	8
1	В	285	ARG	8
1	В	421	GLU	7
1	В	272	LYS	7
1	А	145	ARG	7
1	В	395	MET	7
1	В	244	GLU	7
1	В	278	LEU	7
1	В	340	GLN	7
1	А	394	LEU	7
1	В	344	ARG	7
1	А	344	ARG	7
1	А	176	GLU	6
1	А	255	ARG	6
1	В	176	GLU	6
1	А	45	ARG	6
1	А	283	ARG	6
1	А	419	GLU	6
1	В	373	GLU	6
1	А	327	LYS	6
1	A	310	GLU	6
1	В	316	ARG	6
1	A	273	ASN	5
1	A	279	LYS	5
1	В	394	LEU	5
1	А	278	LEU	5
1	А	321	ARG	5
1	А	421	GLU	5
1	А	57	ARG	5
1	В	117	LEU	5
1	В	416	LYS	5
1	В	310	GLU	5



Mol	Chain	Res	Type	Models (Total)
1	А	316	ARG	5
1	В	406	GLN	5
1	А	395	MET	5
1	А	285	ARG	5
1	В	279	LYS	5
1	А	366	ARG	5
1	A	416	LYS	5
1	А	63	ARG	5
1	В	152	LYS	5
1	В	372	GLU	5
1	A	144	LEU	4
1	A	117	LEU	4
1	A	397	ASN	4
1	A	276	ARG	4
1	В	334	ARG	4
1	A	405	GLU	4
1	В	145	ARG	4
1	В	428	MET	4
1	В	148	GLN	4
1	В	203	LYS	4
1	A	114	GLU	4
1	В	124	GLU	4
1	В	321	ARG	4
1	A	96	GLU	4
1	A	373	GLU	4
1	A	148	GLN	4
1	В	283	ARG	4
1	В	327	LYS	4
1	A	203	LYS	3
1	A	403	LEU	3
1	A	85	ASN	3
1	А	414	LYS	3
1	A	356	ARG	3
1	В	107	VAL	3
1	A	430	GLN	3
1	А	400	ASN	3
1	А	334	ARG	3
1	В	355	ILE	3
1	A	199	GLU	3
1	A	328	GLN	3
1	A	37	LYS	3
1	В	422	THR	3



Mol	Chain	\mathbf{Res}	Type	Models (Total)
1	В	273	ASN	3
1	А	224	GLU	3
1	В	403	LEU	3
1	В	247	GLU	3
1	А	353	GLU	3
1	В	114	GLU	3
1	А	269	GLU	3
1	В	229	LYS	3
1	В	276	ARG	3
1	А	206	LYS	3
1	А	392	LYS	3
1	А	64	GLN	3
1	А	368	LYS	3
1	В	296	LYS	3
1	A	404	GLU	3
1	A	390	LYS	3
1	В	269	GLU	3
1	В	326	GLU	3
1	В	215	VAL	2
1	А	152	LYS	2
1	В	287	LYS	2
1	А	267	ARG	2
1	В	374	MET	2
1	А	428	MET	2
1	В	342	LYS	2
1	А	355	ILE	2
1	А	52	ASN	2
1	А	374	MET	2
1	А	393	GLU	2
1	В	356	ARG	2
1	В	320	GLN	2
1	В	254	LYS	2
1	В	328	GLN	2
1	В	126	GLU	2
1	В	259	GLU	2
1	В	206	LYS	2
1	А	292	GLU	2
1	А	342	LYS	2
1	А	406	GLN	2
1	В	392	LYS	2
1	А	275	GLU	2
1	В	339	GLU	2

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Mol	Chain	\mathbf{Res}	Type	Models (Total)
1	В	409	GLU	2
1	А	254	LYS	2
1	А	229	LYS	2
1	А	287	LYS	2
1	В	364	GLU	2
1	А	38	LYS	2
1	А	74	ASN	2
1	В	292	GLU	2
1	В	147	GLN	2
1	А	191	GLN	2
1	А	320	GLN	2
1	А	298	ASN	2
1	А	181	LYS	2
1	А	147	GLN	2
1	В	120	LEU	2
1	В	191	GLN	2
1	В	390	LYS	2
1	В	353	GLU	2
1	А	420	LYS	2
1	В	400	ASN	2
1	А	46	LYS	2
1	В	414	LYS	2
1	А	98	LYS	2
1	А	175	GLU	2
1	В	399	ARG	2
1	В	429	ASN	1
1	А	386	GLU	1
1	А	289	GLN	1
1	В	241	GLU	1
1	В	335	GLU	1
1	A	214	ASP	1
1	В	144	LEU	1
1	В	189	MET	1
1	В	425	ASN	1
1	A	308	ASP	1
1	В	266	LEU	1
1	A	146	LYS	1
1	В	199	GLU	1
1	A	338	GLU	1
1	A	264	GLU	1
1	A	247	GLU	1
1	A	101	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	А	396	ASP	1
1	В	289	GLN	1
1	А	118	GLN	1
1	А	186	VAL	1
1	В	181	LYS	1
1	В	128	PRO	1
1	А	361	LYS	1
1	А	427	LEU	1
1	В	167	ASP	1
1	В	219	GLU	1
1	В	194	MET	1
1	А	99	LEU	1
1	А	364	GLU	1
1	А	120	LEU	1
1	А	138	ASP	1
1	В	101	GLU	1
1	В	361	LYS	1
1	В	307	ILE	1
1	В	368	LYS	1
1	В	404	GLU	1
1	А	219	GLU	1
1	В	225	ASN	1
1	А	48	LYS	1
1	В	267	ARG	1
1	А	133	THR	1
1	В	251	GLU	1
1	А	225	ASN	1
1	А	266	LEU	1
1	В	397	ASN	1
1	А	372	GLU	1
1	А	383	GLU	1
1	В	159	GLU	1
1	А	25	GLU	1
1	В	311	ILE	1
1	A	303	PRO	1
1	А	307	ILE	1
1	А	241	GLU	1
1	А	31	GLU	1
1	А	215	VAL	1
1	В	214	ASP	1
1	В	224	GLU	1
1	В	405	GLU	1

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Mol	Chain	\mathbf{Res}	Type	Models (Total)
1	А	56	GLN	1
1	В	427	LEU	1
1	А	217	PHE	1
1	А	343	ARG	1
1	В	275	GLU	1
1	А	126	GLU	1
1	А	232	LYS	1
1	А	159	GLU	1
1	В	146	LYS	1
1	В	238	LYS	1
1	А	379	GLU	1
1	А	296	LYS	1
1	В	134	ASP	1
1	В	420	LYS	1
1	А	294	LEU	1
1	В	325	ASN	1
1	А	358	ASN	1
1	А	317	GLN	1
1	А	399	ARG	1
1	А	339	GLU	1
1	А	422	THR	1
1	А	2	GLN	1
1	А	65	ASP	1
1	В	343	ARG	1
1	А	326	GLU	1
1	В	308	ASP	1

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5.2.3 RNA (i)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains (i)

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

5.4 Carbohydrates (i)

There are no carbohydrates in this entry.



5.5 Ligand geometry (i)

There are no ligands in this entry.

5.6 Other polymers (i)

There are no such molecules in this entry.

5.7 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 12% for the well-defined parts and 11% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

 $Chemical \ shift \ list \ name: \ starch-3let.str$

6.1.1 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

6.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	${\bf Correction}\pm{\bf precision},ppm$	Suggested action
$^{13}C_{\alpha}$	0		None (insufficient data)
$^{13}C_{\beta}$	41	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	0		None (insufficient data)
¹⁵ N	331	-0.42 ± 0.20	None needed (< 0.5 ppm)

6.1.3 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. 1216 atoms were assigned a chemical shift out of a possible 10565. 72 out of 146 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	658/4237~(16%)	329/1690 (19%)	0/1714~(0%)	329/833~(39%)
Sidechain	440/5838~(8%)	220/3386~(6%)	220/2165~(10%)	0/287~(0%)



Continueu from previous page						
	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	15 N		
Aromatic	118/490~(24%)	62/262~(24%)	56/218~(26%)	0/10~(0%)		
Overall	1216/10565~(12%)	611/5338 (11%)	276/4097 (7%)	329/1130 (29%		

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 1224 atoms were assigned a chemical shift out of a possible 10650. 72 out of 146 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	662/4272~(15%)	331/1704~(19%)	0/1728~(0%)	331/840~(39%)
Sidechain	444/5888 (8%)	222/3416~(6%)	222/2182~(10%)	0/290~(0%)
Aromatic	118/490~(24%)	62/262~(24%)	56/218~(26%)	0/10~(0%)
Overall	1224/10650~(11%)	615/5382~(11%)	278/4128~(7%)	331/1140~(29%)

6.1.4 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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	А	109	PHE	CE2	137.12	136.81 - 124.71	5.3

6.1.5 Random Coil Index (RCI) plots ()

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.

Random coil index (RCI) for chain A:



