



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:53 pm BST

PDB ID : 2L5P
Title : Solution NMR structure of protein lipocalin 12 from rat epididymis
Authors : Peng, Y.; Lin, D.
Deposited on : 2010-11-03

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 ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
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_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

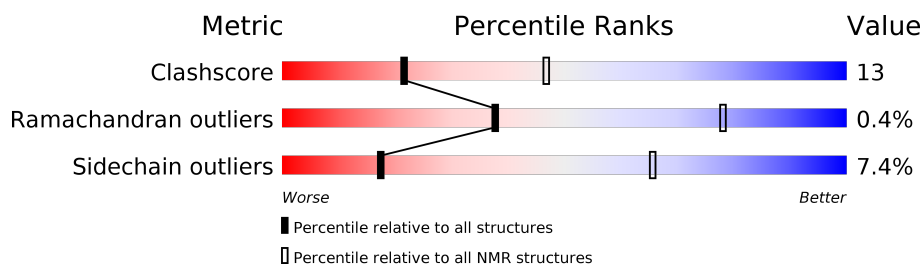
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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	184	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:33-A:118, A:125-A:192 (154)	0.49	1

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

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

The models can be grouped into 3 clusters and 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2828 atoms, of which 1411 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lipocalin 12.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	175	2828	898	1411	252	262	5	0

There are 10 discrepancies between the modelled and reference sequences:

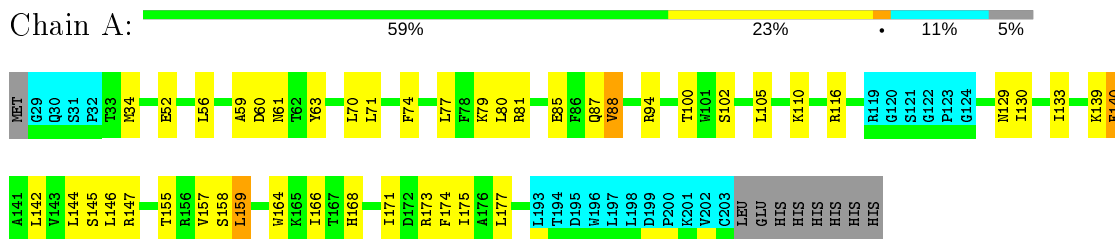
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	EXPRESSION TAG	UNP B3EY83
A	176	ALA	CYS	ENGINEERED MUTATION	UNP B3EY83
A	204	LEU	-	EXPRESSION TAG	UNP B3EY83
A	205	GLU	-	EXPRESSION TAG	UNP B3EY83
A	206	HIS	-	EXPRESSION TAG	UNP B3EY83
A	207	HIS	-	EXPRESSION TAG	UNP B3EY83
A	208	HIS	-	EXPRESSION TAG	UNP B3EY83
A	209	HIS	-	EXPRESSION TAG	UNP B3EY83
A	210	HIS	-	EXPRESSION TAG	UNP B3EY83
A	211	HIS	-	EXPRESSION TAG	UNP B3EY83

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: Lipocalin 12

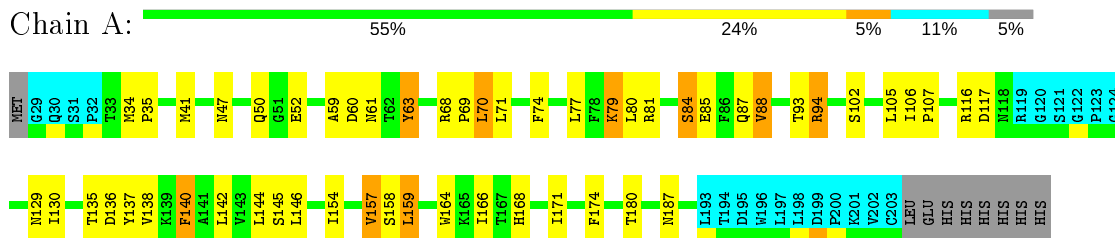


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

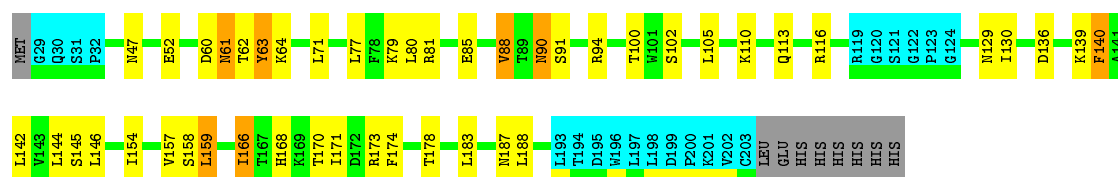
- Molecule 1: Lipocalin 12



4.2.2 Score per residue for model 2

- Molecule 1: Lipocalin 12

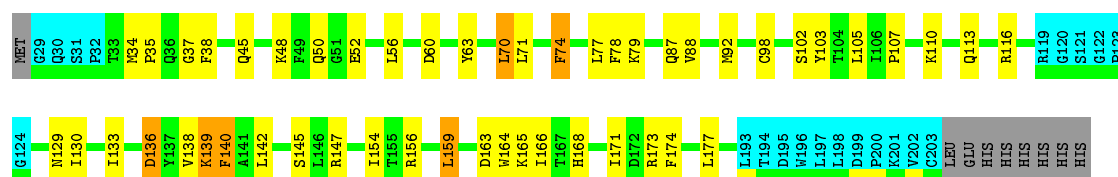




4.2.3 Score per residue for model 3

- Molecule 1: Lipocalin 12

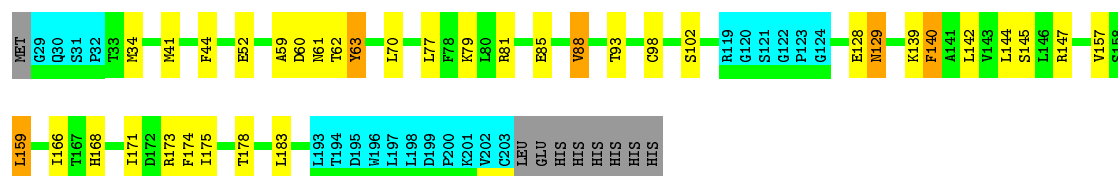
Chain A: 57% 24% 11% 5%



4.2.4 Score per residue for model 4

- Molecule 1: Lipocalin 12

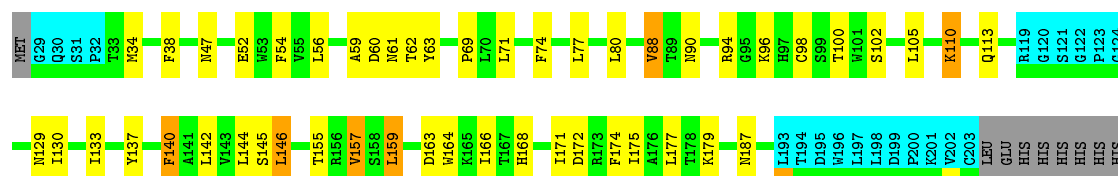
Chain A: 64% 17% 11% 5%



4.2.5 Score per residue for model 5

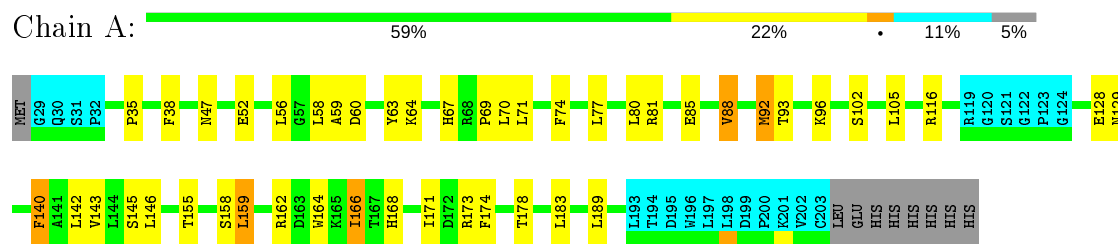
- Molecule 1: Lipocalin 12

Chain A: 57% 23% 11% 5%



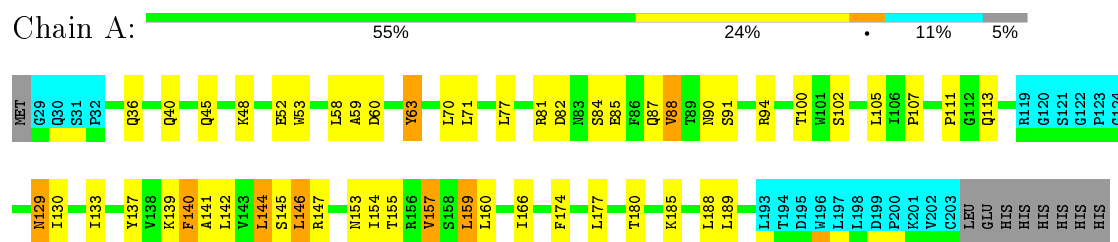
4.2.6 Score per residue for model 6

- Molecule 1: Lipocalin 12



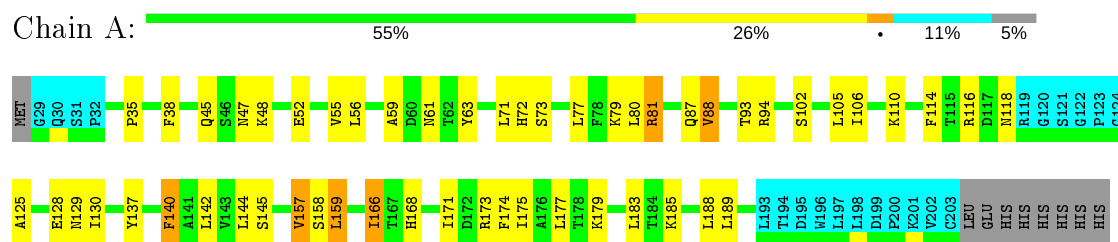
4.2.7 Score per residue for model 7

- Molecule 1: Lipocalin 12



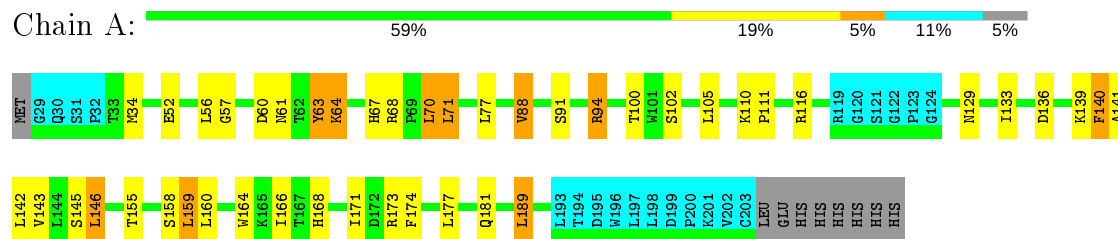
4.2.8 Score per residue for model 8

- Molecule 1: Lipocalin 12



4.2.9 Score per residue for model 9

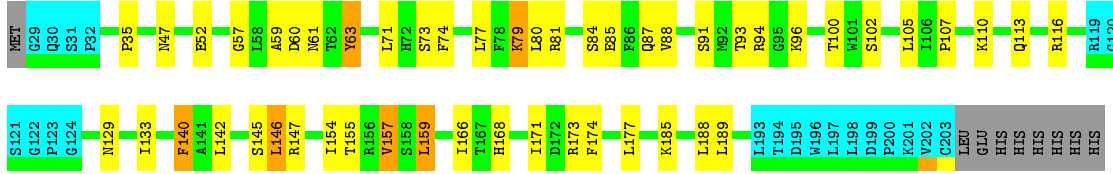
- Molecule 1: Lipocalin 12



4.2.10 Score per residue for model 10

- Molecule 1: Lipocalin 12

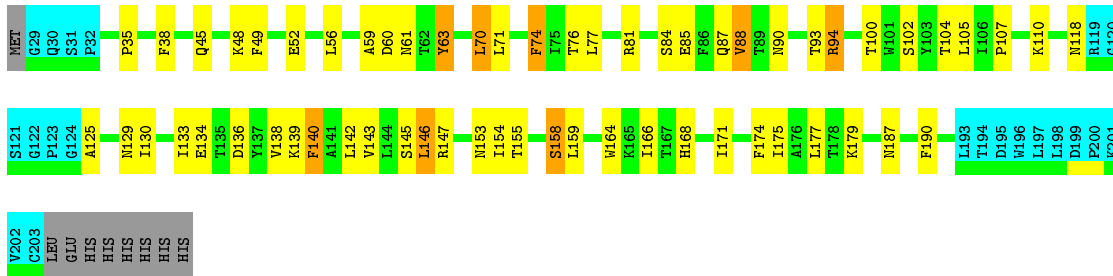
Chain A: 



4.2.11 Score per residue for model 11

- Molecule 1: Lipocalin 12

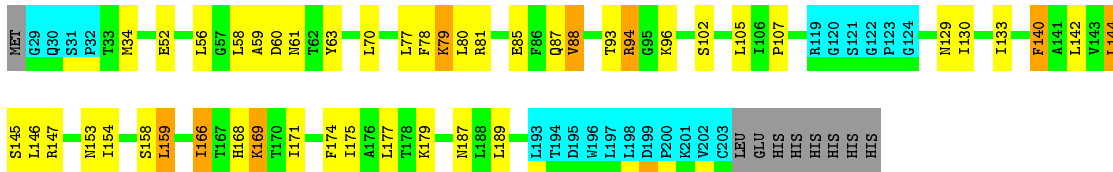
Chain A: 



4.2.12 Score per residue for model 12

- Molecule 1: Lipocalin 12

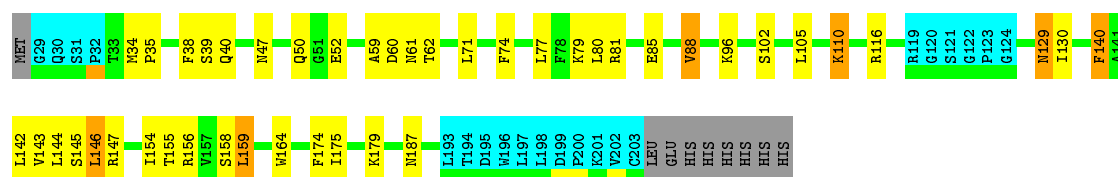
Chain A: 



4.2.13 Score per residue for model 13

- Molecule 1: Lipocalin 12

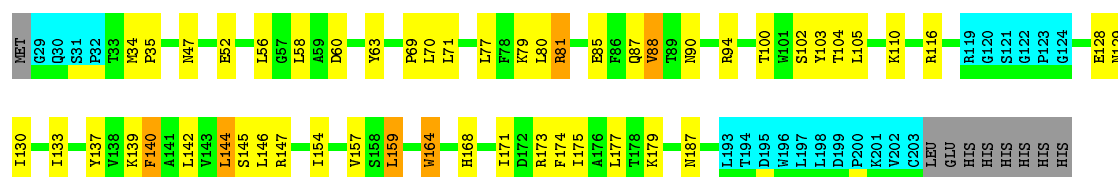
Chain A: 



4.2.14 Score per residue for model 14

- Molecule 1: Lipocalin 12

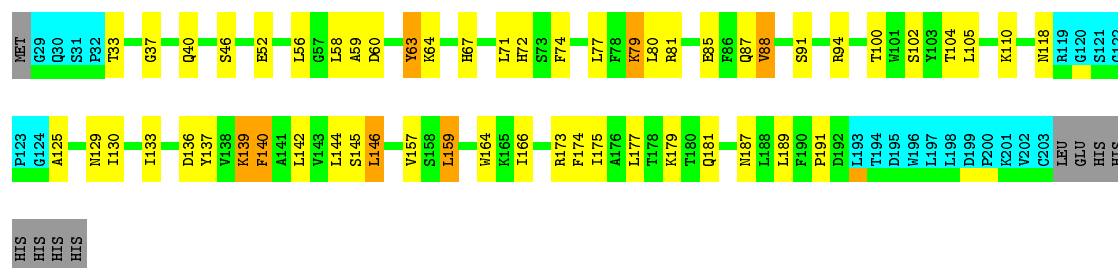
Chain A: 56% 24% 11% 5%



4.2.15 Score per residue for model 15

- Molecule 1: Lipocalin 12

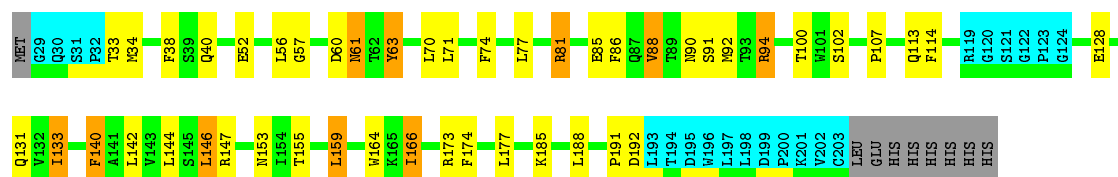
Chain A: 54% 26% 11% 5%



4.2.16 Score per residue for model 16

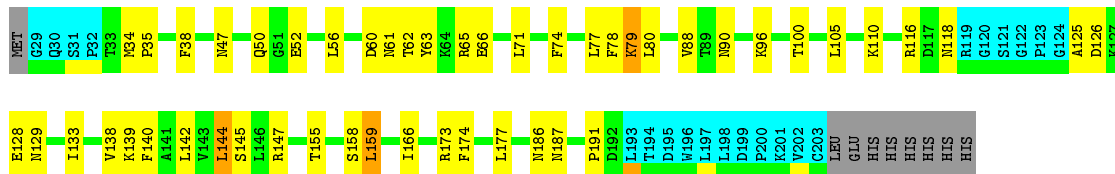
- Molecule 1: Lipocalin 12

Chain A: 58% 20% 5% 11% 5%



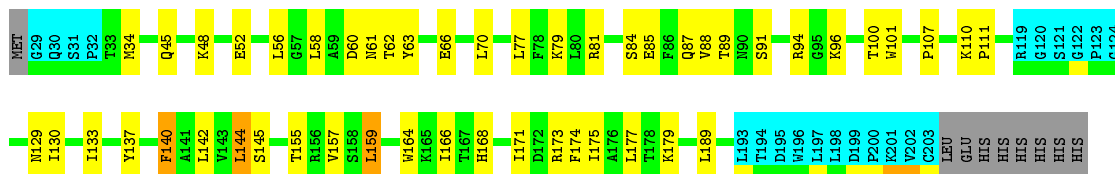
4.2.17 Score per residue for model 17

- Molecule 1: Lipocalin 12

Chain A: 

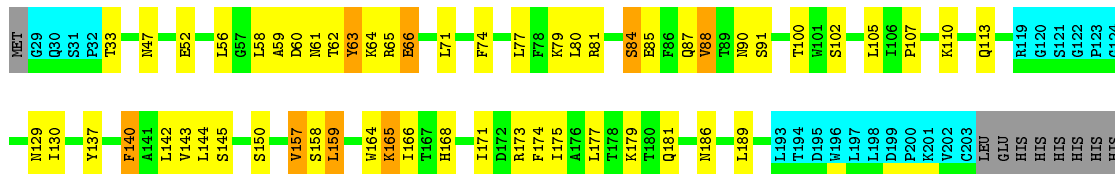
4.2.18 Score per residue for model 18

- Molecule 1: Lipocalin 12

Chain A: 

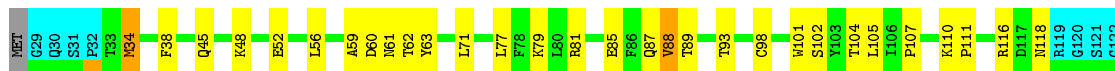
4.2.19 Score per residue for model 19

- Molecule 1: Lipocalin 12

Chain A: 

4.2.20 Score per residue for model 20

- Molecule 1: Lipocalin 12

Chain A: 

V202	P123	P191	M186
C203	G124	D192	M187
LEU	A125	L193	
GLU		T194	
HIS	I130	D195	
HIS	I133	W196	
HIS		L197	
HIS	K139	L198	
HIS	F140	D199	
HIS	A141	P200	
HIS	L142	K201	
	W143		
	L144		
	S145		
	L146		
	R147		
	S150		
	M153		
	I154		
	T155		
	R156		
	V157		
	S158		
	L159		
	I166		
	T167		
	H168		
	I171		
	D172		
	R173		
	F174		
	I175		
	A176		
	L177		
	T178		
	K179		
	T180		
	Q181		
	N182		
	L183		
	M186		
	M187		
	P191		
	D192		
	L193		
	T194		
	D195		
	W196		
	L197		
	L198		
	D199		
	P200		
	K201		

5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 320 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	1.2

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1265	1263	1259	33±5
All	All	25300	25260	25180	655

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ASP:HB3	1:A:63:TYR:HB2	0.91	1.43	11	15
1:A:146:LEU:HD12	1:A:155:THR:HA	0.84	1.50	9	5
1:A:159:LEU:HG	1:A:174:PHE:HB2	0.84	1.48	14	20
1:A:70:LEU:HD12	1:A:71:LEU:HG	0.81	1.50	9	3
1:A:59:ALA:HB3	1:A:157:VAL:HG23	0.79	1.54	8	6
1:A:138:VAL:HG23	1:A:139:LYS:HG2	0.79	1.55	3	2
1:A:185:LYS:HA	1:A:188:LEU:HD13	0.77	1.54	10	4
1:A:47:ASN:HA	1:A:80:LEU:HD11	0.76	1.57	13	10
1:A:81:ARG:HB2	1:A:85:GLU:HB2	0.75	1.58	15	9
1:A:71:LEU:HD23	1:A:74:PHE:HB3	0.75	1.57	5	8
1:A:72:HIS:HA	1:A:189:LEU:HD21	0.75	1.58	8	1
1:A:142:LEU:HD11	1:A:173:ARG:HB3	0.74	1.59	2	14
1:A:118:ASN:HB2	1:A:125:ALA:HB1	0.73	1.58	8	1
1:A:52:GLU:HA	1:A:77:LEU:HD22	0.73	1.59	3	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:LEU:HD23	1:A:157:VAL:HG22	0.72	1.59	20	1
1:A:140:PHE:CE2	1:A:142:LEU:HG	0.71	2.20	6	16
1:A:81:ARG:HD3	1:A:87:GLN:HB2	0.71	1.61	11	9
1:A:81:ARG:HB3	1:A:85:GLU:HB2	0.69	1.64	4	6
1:A:91:SER:HA	1:A:100:THR:HG22	0.69	1.62	10	8
1:A:178:THR:HA	1:A:183:LEU:HD12	0.68	1.66	6	3
1:A:84:SER:HB2	1:A:107:PRO:HG3	0.68	1.64	18	2
1:A:84:SER:HB3	1:A:107:PRO:HG3	0.67	1.67	19	4
1:A:79:LYS:HB2	1:A:87:GLN:HB3	0.66	1.68	10	6
1:A:71:LEU:HD13	1:A:94:ARG:HG3	0.66	1.68	5	4
1:A:133:ILE:HG21	1:A:177:LEU:HD21	0.66	1.67	17	13
1:A:81:ARG:HG3	1:A:104:THR:HG23	0.66	1.68	11	4
1:A:56:LEU:HD11	1:A:164:TRP:HA	0.66	1.66	14	8
1:A:129:ASN:O	1:A:145:SER:HA	0.66	1.90	11	18
1:A:143:VAL:HG13	1:A:158:SER:HB2	0.65	1.67	9	4
1:A:70:LEU:HD13	1:A:94:ARG:HD3	0.65	1.68	18	2
1:A:70:LEU:HD13	1:A:94:ARG:HD2	0.65	1.69	11	3
1:A:71:LEU:HD11	1:A:93:THR:H	0.64	1.53	8	1
1:A:175:ILE:HD11	1:A:190:PHE:HZ	0.63	1.53	11	1
1:A:136:ASP:OD1	1:A:139:LYS:HG3	0.62	1.95	3	1
1:A:157:VAL:HB	1:A:174:PHE:HE1	0.61	1.55	1	3
1:A:110:LYS:HB2	1:A:113:GLN:HB3	0.61	1.73	10	3
1:A:146:LEU:H	1:A:146:LEU:HD22	0.61	1.55	16	1
1:A:85:GLU:HG3	1:A:107:PRO:HD2	0.61	1.72	16	3
1:A:155:THR:HG21	1:A:181:GLN:HB3	0.61	1.72	20	1
1:A:142:LEU:HD23	1:A:159:LEU:HD23	0.61	1.71	11	16
1:A:52:GLU:HG3	1:A:77:LEU:HD22	0.60	1.72	4	13
1:A:136:ASP:HB2	1:A:139:LYS:HB2	0.60	1.74	2	2
1:A:159:LEU:HB2	1:A:174:PHE:CD1	0.60	2.32	9	5
1:A:157:VAL:HB	1:A:174:PHE:CE1	0.59	2.32	1	6
1:A:33:THR:HB	1:A:146:LEU:HG	0.59	1.74	15	1
1:A:55:VAL:O	1:A:73:SER:HA	0.59	1.97	8	1
1:A:35:PRO:HG2	1:A:38:PHE:HB2	0.59	1.72	13	4
1:A:147:ARG:HB3	1:A:154:ILE:HB	0.59	1.73	12	7
1:A:58:LEU:HB2	1:A:189:LEU:HB3	0.59	1.73	19	2
1:A:64:LYS:HB3	1:A:66:GLU:OE1	0.58	1.98	19	1
1:A:146:LEU:HA	1:A:154:ILE:O	0.58	1.98	7	7
1:A:63:TYR:CD1	1:A:187:ASN:HA	0.58	2.34	17	2
1:A:146:LEU:N	1:A:146:LEU:HD13	0.57	2.14	5	1
1:A:105:LEU:CD2	1:A:116:ARG:HG2	0.57	2.29	17	8
1:A:88:VAL:O	1:A:102:SER:HA	0.57	1.99	15	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:LEU:HD22	1:A:93:THR:H	0.57	1.60	11	2
1:A:71:LEU:H	1:A:71:LEU:HD23	0.56	1.61	3	1
1:A:38:PHE:HB3	1:A:133:ILE:HG23	0.56	1.76	17	4
1:A:69:PRO:HB2	1:A:74:PHE:HZ	0.56	1.59	6	1
1:A:59:ALA:HA	1:A:187:ASN:O	0.56	1.99	5	7
1:A:64:LYS:HB2	1:A:67:HIS:HB2	0.56	1.76	9	3
1:A:68:ARG:HD3	1:A:189:LEU:HD21	0.56	1.77	9	1
1:A:60:ASP:HB2	1:A:63:TYR:HB2	0.56	1.76	9	2
1:A:110:LYS:HZ2	1:A:110:LYS:HB3	0.56	1.60	5	1
1:A:93:THR:HA	1:A:98:CYS:HA	0.55	1.77	4	2
1:A:60:ASP:HB3	1:A:63:TYR:CB	0.55	2.31	3	1
1:A:60:ASP:OD1	1:A:154:ILE:HG23	0.54	2.02	2	1
1:A:34:MET:CE	1:A:34:MET:HA	0.54	2.32	16	1
1:A:107:PRO:HA	1:A:113:GLN:O	0.54	2.02	16	3
1:A:77:LEU:O	1:A:88:VAL:HA	0.54	2.02	12	7
1:A:54:PHE:CD2	1:A:163:ASP:HA	0.54	2.36	5	1
1:A:40:GLN:HE22	1:A:110:LYS:HD3	0.54	1.63	13	1
1:A:61:ASN:ND2	1:A:155:THR:H	0.54	1.99	18	2
1:A:128:GLU:HG3	1:A:147:ARG:HB2	0.54	1.78	17	1
1:A:140:PHE:HD2	1:A:159:LEU:HD21	0.54	1.63	11	16
1:A:34:MET:HA	1:A:34:MET:HE2	0.53	1.81	16	1
1:A:126:ASP:OD2	1:A:147:ARG:HD3	0.53	2.04	17	1
1:A:166:ILE:HG23	1:A:170:THR:HB	0.53	1.81	2	1
1:A:45:GLN:HB3	1:A:48:LYS:HG3	0.53	1.81	3	2
1:A:45:GLN:OE1	1:A:48:LYS:HG3	0.53	2.04	11	3
1:A:70:LEU:HD11	1:A:92:MET:SD	0.53	2.43	16	1
1:A:105:LEU:HD13	1:A:130:ILE:HG21	0.52	1.81	3	10
1:A:77:LEU:HB2	1:A:79:LYS:HE3	0.52	1.81	1	1
1:A:159:LEU:HB2	1:A:174:PHE:CG	0.52	2.39	11	9
1:A:139:LYS:HE2	1:A:140:PHE:CE1	0.52	2.39	11	2
1:A:58:LEU:HB3	1:A:189:LEU:HB3	0.52	1.81	6	2
1:A:140:PHE:HE2	1:A:142:LEU:HG	0.52	1.62	6	3
1:A:118:ASN:HB3	1:A:125:ALA:HB1	0.52	1.81	15	4
1:A:143:VAL:HG13	1:A:158:SER:CB	0.52	2.35	13	1
1:A:65:ARG:HD3	1:A:186:ASN:OD1	0.52	2.05	17	1
1:A:168:HIS:HA	1:A:171:ILE:HB	0.51	1.82	18	15
1:A:130:ILE:HG13	1:A:145:SER:OG	0.51	2.06	14	4
1:A:146:LEU:HD13	1:A:146:LEU:N	0.51	2.19	15	1
1:A:133:ILE:HD13	1:A:144:LEU:HB2	0.51	1.82	18	5
1:A:71:LEU:HD12	1:A:92:MET:HB2	0.51	1.80	6	1
1:A:59:ALA:HB1	1:A:183:LEU:HD13	0.51	1.82	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:PRO:HB3	1:A:74:PHE:HZ	0.51	1.64	1	1
1:A:146:LEU:HB3	1:A:153:ASN:OD1	0.51	2.06	11	2
1:A:159:LEU:HG	1:A:174:PHE:CB	0.50	2.36	13	13
1:A:72:HIS:CE1	1:A:191:PRO:HA	0.50	2.41	15	1
1:A:145:SER:C	1:A:146:LEU:HD12	0.50	2.27	2	2
1:A:138:VAL:HG23	1:A:139:LYS:CG	0.50	2.35	3	1
1:A:175:ILE:O	1:A:179:LYS:HG2	0.50	2.07	14	10
1:A:49:PHE:CE1	1:A:136:ASP:HA	0.50	2.42	11	1
1:A:157:VAL:HG11	1:A:177:LEU:HB3	0.49	1.84	19	2
1:A:106:ILE:CG1	1:A:117:ASP:HB2	0.49	2.37	1	1
1:A:136:ASP:HB3	1:A:139:LYS:HG2	0.49	1.83	11	1
1:A:163:ASP:OD1	1:A:165:LYS:HG2	0.49	2.06	3	1
1:A:76:THR:HB	1:A:90:ASN:OD1	0.49	2.08	11	1
1:A:58:LEU:HB2	1:A:189:LEU:CB	0.49	2.38	19	1
1:A:40:GLN:HG3	1:A:110:LYS:HD2	0.49	1.85	15	1
1:A:155:THR:CG2	1:A:181:GLN:HB3	0.49	2.36	20	1
1:A:34:MET:HB2	1:A:35:PRO:HD2	0.48	1.85	14	4
1:A:90:ASN:O	1:A:100:THR:HA	0.48	2.08	17	7
1:A:110:LYS:NZ	1:A:113:GLN:HB2	0.48	2.24	5	1
1:A:141:ALA:HB3	1:A:160:LEU:HB2	0.48	1.84	9	2
1:A:63:TYR:CE2	1:A:189:LEU:HB2	0.48	2.43	18	3
1:A:40:GLN:NE2	1:A:131:GLN:HE21	0.48	2.06	16	1
1:A:46:SER:HB2	1:A:80:LEU:HD21	0.48	1.84	15	1
1:A:145:SER:O	1:A:156:ARG:HB3	0.48	2.08	13	1
1:A:128:GLU:HA	1:A:147:ARG:HA	0.48	1.86	14	4
1:A:34:MET:CE	1:A:39:SER:HA	0.47	2.39	13	1
1:A:85:GLU:HA	1:A:105:LEU:O	0.47	2.09	1	2
1:A:45:GLN:HB3	1:A:48:LYS:CG	0.47	2.39	3	1
1:A:142:LEU:HB3	1:A:177:LEU:HD11	0.47	1.85	17	3
1:A:52:GLU:HG3	1:A:77:LEU:CD2	0.47	2.39	5	2
1:A:136:ASP:HB2	1:A:139:LYS:CG	0.47	2.40	15	1
1:A:146:LEU:HB3	1:A:153:ASN:HD21	0.47	1.68	20	2
1:A:159:LEU:CG	1:A:174:PHE:HB2	0.47	2.33	14	1
1:A:143:VAL:HG13	1:A:158:SER:HB3	0.47	1.85	19	1
1:A:50:GLN:CD	1:A:80:LEU:HG	0.46	2.30	17	3
1:A:58:LEU:HB3	1:A:189:LEU:HD23	0.46	1.87	18	1
1:A:89:THR:HA	1:A:101:TRP:O	0.46	2.11	20	2
1:A:40:GLN:NE2	1:A:110:LYS:HD3	0.46	2.25	13	1
1:A:71:LEU:HD13	1:A:94:ARG:HG2	0.45	1.86	2	1
1:A:110:LYS:HB3	1:A:113:GLN:CB	0.45	2.41	5	1
1:A:34:MET:HE1	1:A:39:SER:HA	0.45	1.87	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:178:THR:HG21	1:A:188:LEU:HD11	0.45	1.87	2	1
1:A:56:LEU:HD21	1:A:164:TRP:HA	0.45	1.87	11	2
1:A:68:ARG:HB2	1:A:69:PRO:CD	0.45	2.40	1	1
1:A:72:HIS:HB3	1:A:189:LEU:HD11	0.45	1.88	8	1
1:A:38:PHE:CB	1:A:133:ILE:HG23	0.45	2.42	3	1
1:A:71:LEU:HB2	1:A:74:PHE:CE1	0.45	2.45	6	1
1:A:56:LEU:CD2	1:A:166:ILE:HB	0.45	2.42	12	1
1:A:45:GLN:HB2	1:A:48:LYS:CG	0.45	2.42	20	1
1:A:60:ASP:HA	1:A:155:THR:O	0.45	2.12	17	3
1:A:71:LEU:HD12	1:A:92:MET:HA	0.45	1.89	3	1
1:A:69:PRO:HB3	1:A:74:PHE:CZ	0.45	2.46	1	1
1:A:56:LEU:HD12	1:A:166:ILE:HD12	0.45	1.89	6	1
1:A:139:LYS:HG3	1:A:140:PHE:HD1	0.45	1.71	20	2
1:A:60:ASP:OD1	1:A:62:THR:HG22	0.45	2.12	5	4
1:A:140:PHE:CD2	1:A:159:LEU:HD21	0.45	2.46	12	1
1:A:146:LEU:HD22	1:A:146:LEU:N	0.45	2.26	16	1
1:A:78:PHE:C	1:A:79:LYS:HD2	0.45	2.31	12	2
1:A:80:LEU:HA	1:A:85:GLU:O	0.45	2.12	12	1
1:A:41:MET:CE	1:A:44:PHE:HD1	0.44	2.26	4	1
1:A:136:ASP:HB3	1:A:139:LYS:CG	0.44	2.42	11	1
1:A:77:LEU:HB3	1:A:79:LYS:HE3	0.44	1.89	17	1
1:A:140:PHE:HB3	1:A:166:ILE:HD11	0.44	1.90	20	1
1:A:146:LEU:HB3	1:A:155:THR:HA	0.44	1.90	5	1
1:A:128:GLU:HG2	1:A:145:SER:OG	0.44	2.13	17	1
1:A:34:MET:HE3	1:A:34:MET:HA	0.44	1.89	20	1
1:A:36:GLN:H	1:A:180:THR:HG21	0.44	1.73	7	1
1:A:169:LYS:HD2	1:A:169:LYS:C	0.44	2.32	12	1
1:A:60:ASP:OD2	1:A:156:ARG:HD3	0.44	2.13	3	1
1:A:57:GLY:HA2	1:A:189:LEU:O	0.44	2.13	10	1
1:A:56:LEU:CD2	1:A:164:TRP:HA	0.44	2.42	11	1
1:A:34:MET:HA	1:A:34:MET:CE	0.44	2.43	5	1
1:A:58:LEU:HD23	1:A:69:PRO:HG3	0.44	1.90	14	1
1:A:116:ARG:HG3	1:A:128:GLU:HB3	0.43	1.89	6	1
1:A:144:LEU:HD22	1:A:145:SER:N	0.43	2.28	20	1
1:A:60:ASP:OD1	1:A:61:ASN:N	0.43	2.51	2	2
1:A:116:ARG:HD3	1:A:128:GLU:HB3	0.43	1.90	8	1
1:A:157:VAL:CG2	1:A:183:LEU:HD12	0.43	2.43	8	1
1:A:63:TYR:CD2	1:A:187:ASN:HA	0.43	2.48	2	1
1:A:87:GLN:HA	1:A:103:TYR:O	0.43	2.12	3	2
1:A:63:TYR:CE2	1:A:69:PRO:HD2	0.43	2.48	5	1
1:A:146:LEU:HB2	1:A:153:ASN:HD21	0.43	1.72	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:LYS:HG3	1:A:140:PHE:CD1	0.43	2.48	20	1
1:A:50:GLN:HB2	1:A:78:PHE:O	0.43	2.12	3	1
1:A:146:LEU:HD11	1:A:155:THR:HG23	0.43	1.91	6	1
1:A:71:LEU:HD21	1:A:94:ARG:HA	0.43	1.90	1	1
1:A:110:LYS:HE2	1:A:111:PRO:HD2	0.43	1.90	20	3
1:A:81:ARG:HA	1:A:81:ARG:NE	0.43	2.29	19	1
1:A:70:LEU:HD12	1:A:71:LEU:N	0.43	2.29	3	1
1:A:129:ASN:N	1:A:129:ASN:HD22	0.43	2.11	4	1
1:A:56:LEU:O	1:A:191:PRO:HD3	0.42	2.14	17	1
1:A:146:LEU:HG	1:A:155:THR:HA	0.42	1.90	6	1
1:A:165:LYS:HD3	1:A:165:LYS:H	0.42	1.75	19	1
1:A:41:MET:SD	1:A:135:THR:HG22	0.42	2.54	1	1
1:A:146:LEU:CB	1:A:153:ASN:HD21	0.42	2.28	7	1
1:A:105:LEU:HD22	1:A:130:ILE:HD13	0.42	1.90	12	2
1:A:71:LEU:HB3	1:A:94:ARG:HG3	0.42	1.91	9	1
1:A:81:ARG:HD2	1:A:87:GLN:HB2	0.42	1.91	19	1
1:A:53:TRP:CH2	1:A:137:TYR:HA	0.41	2.50	7	1
1:A:56:LEU:HD13	1:A:166:ILE:HB	0.41	1.91	16	1
1:A:40:GLN:NE2	1:A:111:PRO:HD2	0.41	2.30	7	1
1:A:143:VAL:CG1	1:A:158:SER:HB3	0.41	2.45	19	1
1:A:136:ASP:OD1	1:A:138:VAL:HG22	0.41	2.15	11	2
1:A:139:LYS:HE2	1:A:140:PHE:CD1	0.41	2.50	7	1
1:A:63:TYR:OH	1:A:189:LEU:HD13	0.41	2.15	8	1
1:A:64:LYS:HD2	1:A:64:LYS:N	0.41	2.31	9	1
1:A:157:VAL:CG2	1:A:183:LEU:HD11	0.41	2.45	2	1
1:A:105:LEU:HD23	1:A:116:ARG:HG3	0.41	1.91	13	1
1:A:65:ARG:HB3	1:A:186:ASN:O	0.41	2.16	19	1
1:A:105:LEU:CD2	1:A:116:ARG:HG3	0.41	2.46	2	2
1:A:57:GLY:HA3	1:A:159:LEU:HB3	0.41	1.92	16	2
1:A:33:THR:HG22	1:A:181:GLN:HA	0.41	1.93	19	1
1:A:106:ILE:O	1:A:114:PHE:HA	0.41	2.16	8	1
1:A:146:LEU:HD12	1:A:155:THR:HG23	0.41	1.92	16	1
1:A:86:PHE:HD2	1:A:114:PHE:CE2	0.41	2.34	16	1
1:A:35:PRO:HA	1:A:180:THR:CB	0.40	2.46	1	1
1:A:171:ILE:O	1:A:175:ILE:HG12	0.40	2.17	8	2
1:A:82:ASP:HB2	1:A:85:GLU:OE1	0.40	2.16	7	1
1:A:56:LEU:HD22	1:A:166:ILE:HB	0.40	1.92	8	1
1:A:56:LEU:HA	1:A:191:PRO:HG2	0.40	1.93	16	1
1:A:35:PRO:HG3	1:A:177:LEU:CD2	0.40	2.46	10	1
1:A:71:LEU:HD21	1:A:74:PHE:CD2	0.40	2.51	3	1
1:A:60:ASP:OD2	1:A:62:THR:HG22	0.40	2.17	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:VAL:CG1	1:A:158:SER:HB2	0.40	2.46	6	1
1:A:58:LEU:HD23	1:A:189:LEU:HD23	0.40	1.93	7	1
1:A:142:LEU:CD2	1:A:159:LEU:HD23	0.40	2.45	11	1
1:A:56:LEU:HB3	1:A:191:PRO:HG3	0.40	1.94	20	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	154/184 (84%)	140±2 (91±1%)	13±2 (9±1%)	1±1 (0±0%)	38	78
All	All	3080/3680 (84%)	2802 (91%)	266 (9%)	12 (0%)	38	78

All 7 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	81	ARG	3
1	A	37	GLY	2
1	A	84	SER	2
1	A	150	SER	2
1	A	64	LYS	1
1	A	73	SER	1
1	A	63	TYR	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	143/169 (85%)	132±2 (93±1%)	11±2 (7±1%)	17	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2860/3380 (85%)	2649 (93%)	211 (7%)	17 65

All 38 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	140	PHE	20
1	A	159	LEU	19
1	A	88	VAL	18
1	A	166	ILE	18
1	A	144	LEU	14
1	A	61	ASN	13
1	A	79	LYS	11
1	A	157	VAL	10
1	A	63	TYR	9
1	A	146	LEU	8
1	A	110	LYS	7
1	A	137	TYR	7
1	A	94	ARG	7
1	A	158	SER	6
1	A	70	LEU	6
1	A	34	MET	4
1	A	62	THR	3
1	A	129	ASN	3
1	A	66	GLU	3
1	A	139	LYS	3
1	A	164	TRP	2
1	A	74	PHE	2
1	A	90	ASN	2
1	A	181	GLN	2
1	A	64	LYS	1
1	A	96	LYS	1
1	A	172	ASP	1
1	A	162	ARG	1
1	A	92	MET	1
1	A	189	LEU	1
1	A	134	GLU	1
1	A	33	THR	1
1	A	136	ASP	1
1	A	186	ASN	1
1	A	169	LYS	1
1	A	133	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	165	LYS	1
1	A	71	LEU	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 carbohydrates 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

No chemical shift data were provided