



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 10:41 AM UTC

PDB ID : 2BBN / pdb_00002bbn
Title : SOLUTION STRUCTURE OF A CALMODULIN-TARGET PEPTIDE
COMPLEX BY MULTIDIMENSIONAL NMR
Authors : Clore, G.M.; Bax, A.; Ikura, M.; Gronenborn, A.M.
Deposited on : 1992-07-16

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 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

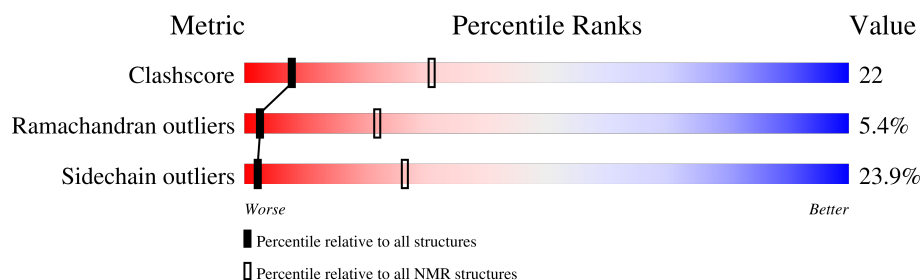
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	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	148	
2	B	26	

2 Ensemble composition and analysis

This entry contains 21 models. Model 17 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:5-A:74, A:81-A:145, B:3-B:21 (154)	1.15	17

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

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

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

Cluster number	Models
1	1, 2, 3, 5, 7, 9, 10, 11, 15, 17, 20
2	8, 12, 13, 18
3	4, 19, 21
Single-model clusters	6; 14; 16

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2704 atoms, of which 1326 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CALMODULIN.

Mol	Chain	Residues	Atoms						Trace
1	A	148	Total	C	H	N	O	S	0
			2259	713	1095	187	255	9	

- Molecule 2 is a protein called MYOSIN LIGHT CHAIN KINASE.

Mol	Chain	Residues	Atoms					Trace
2	B	26	Total	C	H	N	O	0
			441	134	231	43	33	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
3	A	4	Total	Ca
			4	4

4 Residue-property plots [i](#)

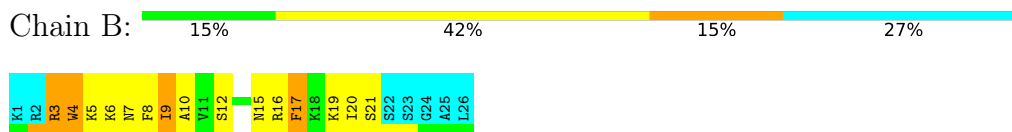
4.1 Average score per residue in the NMR ensemble

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: CALMODULIN



• Molecule 2: MYOSIN LIGHT CHAIN KINASE

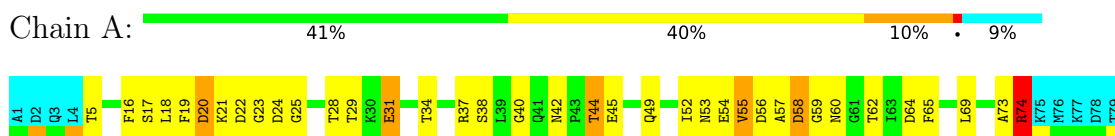


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: CALMODULIN



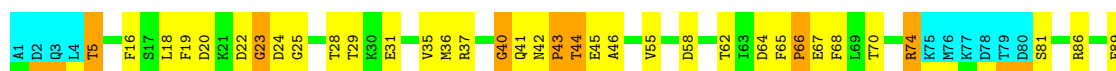


• Molecule 2: MYOSIN LIGHT CHAIN KINASE



4.2.2 Score per residue for model 2

• Molecule 1: CALMODULIN

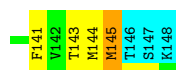
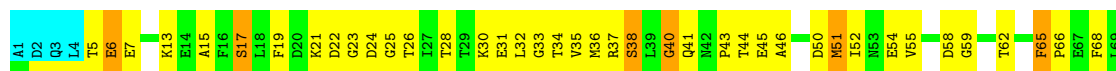


• Molecule 2: MYOSIN LIGHT CHAIN KINASE



4.2.3 Score per residue for model 3

• Molecule 1: CALMODULIN



• Molecule 2: MYOSIN LIGHT CHAIN KINASE

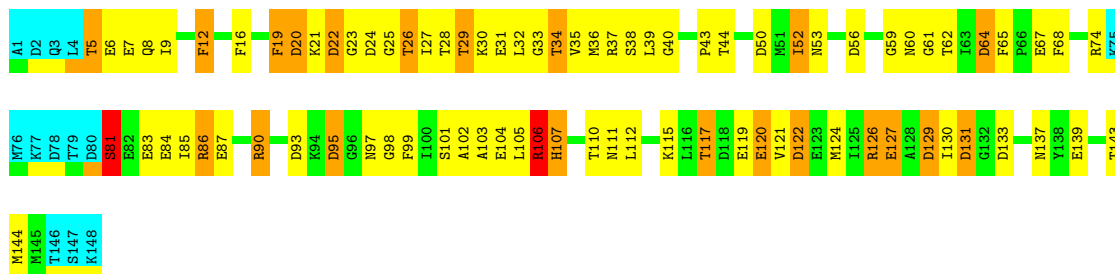




4.2.4 Score per residue for model 4

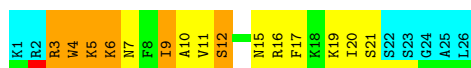
- Molecule 1: CALMODULIN

Chain A: 35% 41% 14% 9%



- Molecule 2: MYOSIN LIGHT CHAIN KINASE

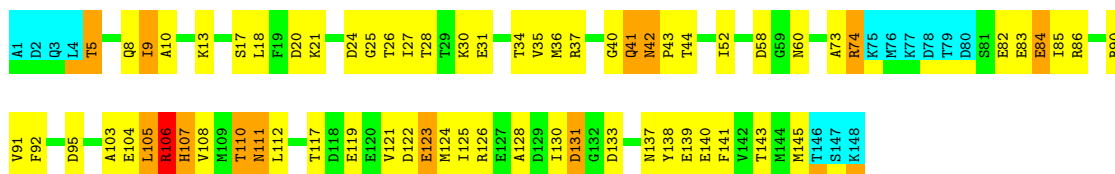
Chain B: 15% 35% 23% 27%



4.2.5 Score per residue for model 5

- Molecule 1: CALMODULIN

Chain A: 46% 36% 8% 9%



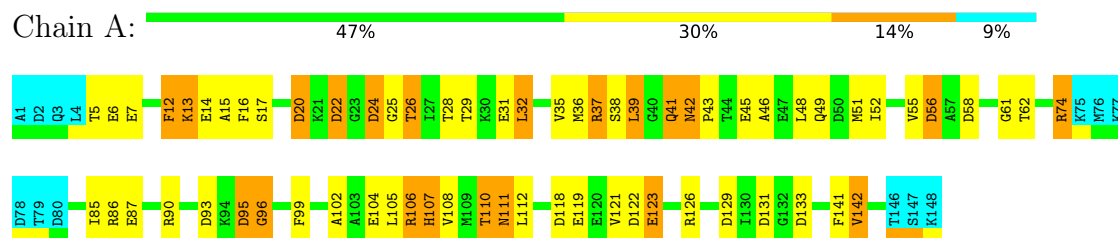
- Molecule 2: MYOSIN LIGHT CHAIN KINASE

Chain B: 27% 31% 15% 27%

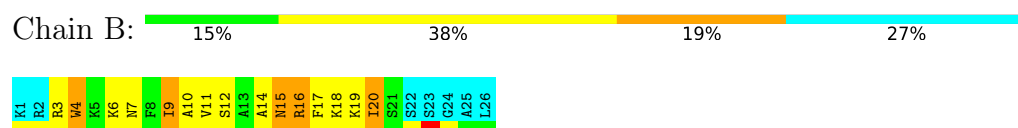


4.2.6 Score per residue for model 6

- Molecule 1: CALMODULIN

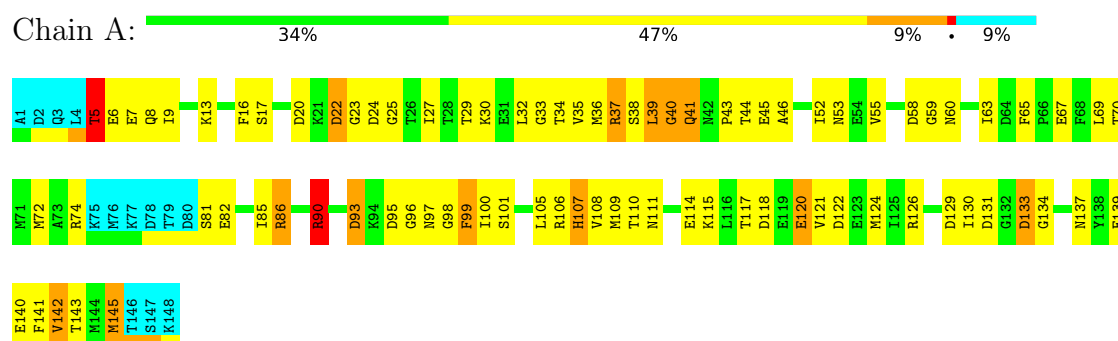


• Molecule 2: MYOSIN LIGHT CHAIN KINASE

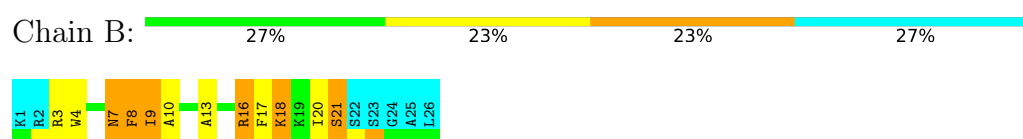


4.2.7 Score per residue for model 7

• Molecule 1: CALMODULIN

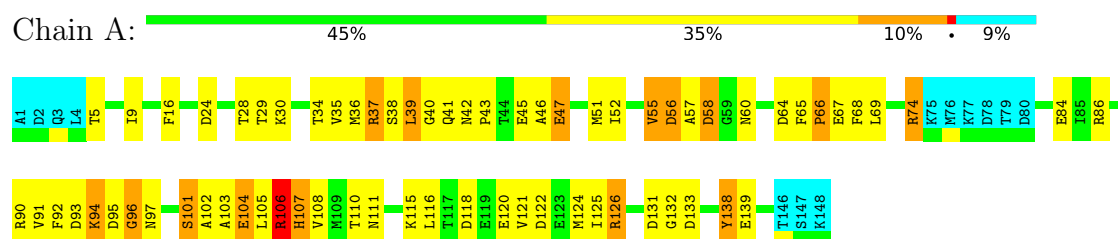


• Molecule 2: MYOSIN LIGHT CHAIN KINASE



4.2.8 Score per residue for model 8

• Molecule 1: CALMODULIN



Category	Color	Relative Length (approx.)
K1	Cyan	1.0
R2	Orange	1.0
R3	Orange	1.0
W4	Yellow	1.0
K5	Yellow	1.0
K6	Yellow	1.0
I9	Orange	1.0
A10	Yellow	1.0
N15	Yellow	1.0
R16	Orange	1.0
F17	Red	1.0
K18	Green	1.0
K19	Yellow	1.0
I20	Orange	1.0
S21	Orange	1.0
S22	Cyan	1.0
S23	Cyan	1.0
G24	Cyan	1.0
A25	Cyan	1.0
L26	Cyan	1.0

T146	R74	A1
S147	M75	D2
K148	K76	Q3
	K77	L4
	D78	T5
	T79	E6
	D80	E7
	S81	
		E14
	E84	A15
	I85	F16
	R86	
	E87	
		D20
	R90	K21
		D22
		G23
	K94	D24
	D95	G25
		T26
	F99	I27
	I100	T28
	S101	T29
	A102	K30
	A103	E31
	E104	
	L105	T34
	R106	V35
	H107	M36
	V108	R37
	M109	
	T110	G40
	L112	Q41
		N42
		P43
	K115	T44
	L116	E45
	T117	A46
	D118	E47
	E119	L48
	E120	Q49
	V121	D50
	D122	M51
	E123	I52
	M124	N53
	R125	E54
	K126	V55
	D129	G59
	I130	N60
	D133	D64
	G134	F65
		P66
	N137	E67
	E138	F68
	E139	L69
	E140	T70
	F141	M71
		M72
		E73

K1	R2	R3	W4	K5	K6	N7	F8	I9	A10	V11	S12		R16	F17	K18	K19	I20	S21	S22	S23	G24	A25	L26
----	----	----	----	----	----	----	----	----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

M144	M145	T146	S147	K148	T70	M71	R74	K75	M76	K77	D78	T79	D80	S81	E82	I85	R86	E87	A88	F89	R90	D93	K94	D95	G96	N97	G98	F99	A103	E104	L105	R106	H107	V108	A103	E104	L112	L116	T117	D118	E119	E120	V121	D122	E123	M124	I125	R126	D131	G132	D133	G134	N137	V138	F141	V142	T143											
M1	A1	D2	Q3	L4							Q8	I9	A10	E11			E14	A15	F16	S17	L18	F19	D20	K21	D22	G23	D24			T27	T28	T29	K30	E31	L32	G33	T34	V35	M36	R37	S38	L39	G40	Q41	N42	P43	T44	E45	A46	E47	L48			M51	I52	N53	E54	V55	D56	A57			M60	G61	T62	I63	D64	F65

Chain B:



4.2.11 Score per residue for model 11

- Molecule 1: CALMODULIN

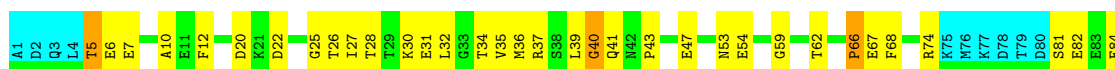


- Molecule 2: MYOSIN LIGHT CHAIN KINASE

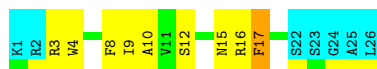


4.2.12 Score per residue for model 12

- Molecule 1: CALMODULIN



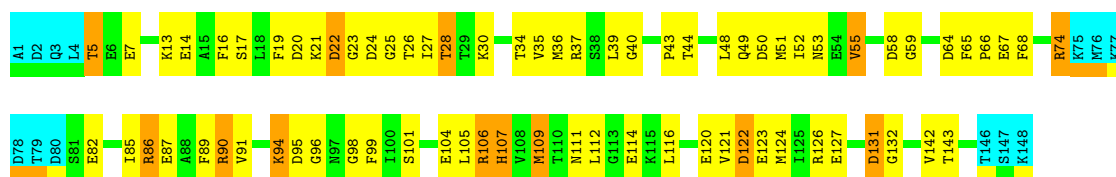
- Molecule 2: MYOSIN LIGHT CHAIN KINASE



4.2.13 Score per residue for model 13

- Molecule 1: CALMODULIN





• Molecule 2: MYOSIN LIGHT CHAIN KINASE

Chain B: 27% 23% 23% 27%



4.2.14 Score per residue for model 14

• Molecule 1: CALMODULIN

Chain A: 39% 40% 11% 9%



• Molecule 2: MYOSIN LIGHT CHAIN KINASE

Chain B: 27% 31% 15% 27%



4.2.15 Score per residue for model 15

• Molecule 1: CALMODULIN

Chain A: 41% 38% 11% 9%



• Molecule 2: MYOSIN LIGHT CHAIN KINASE

Chain B: 27% 31% 15% 27%

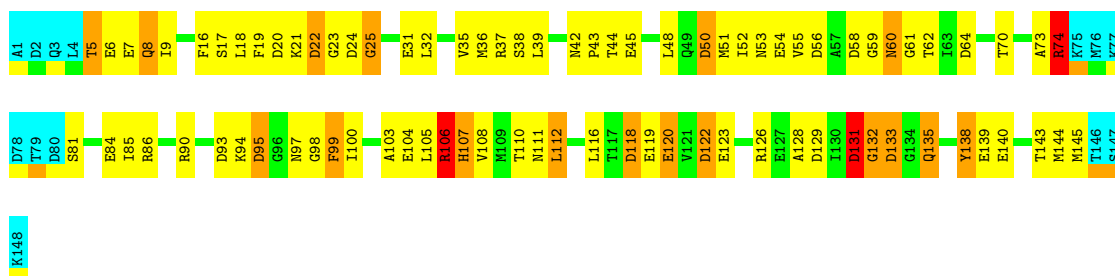




4.2.16 Score per residue for model 16

- Molecule 1: CALMODULIN

Chain A: 35% 43% 11% 9%



- Molecule 2: MYOSIN LIGHT CHAIN KINASE

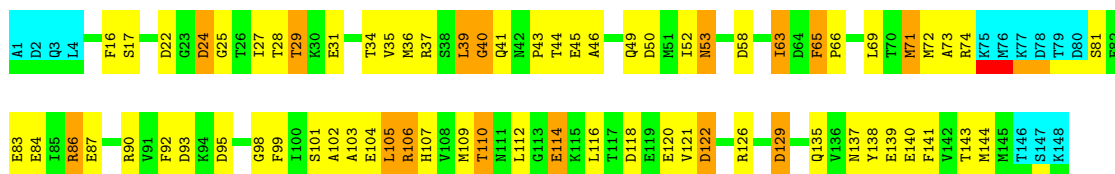
Chain B: 23% 27% 19% 27%



4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: CALMODULIN

Chain A: 44% 37% 10% 9%



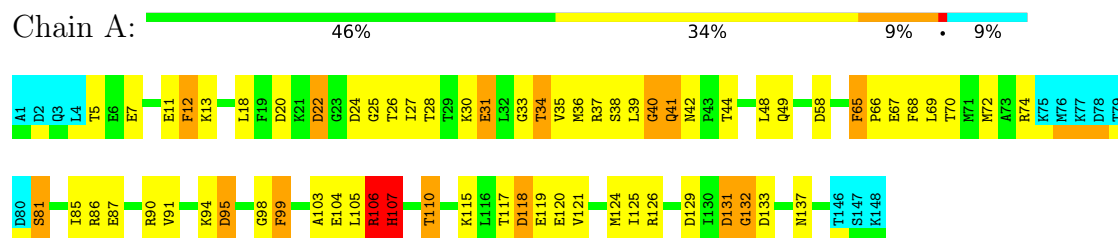
- Molecule 2: MYOSIN LIGHT CHAIN KINASE

Chain B: 12% 35% 23% 27%

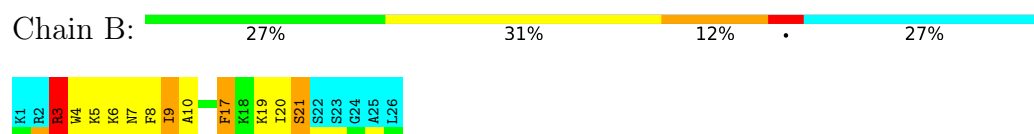


4.2.18 Score per residue for model 18

- Molecule 1: CALMODULIN

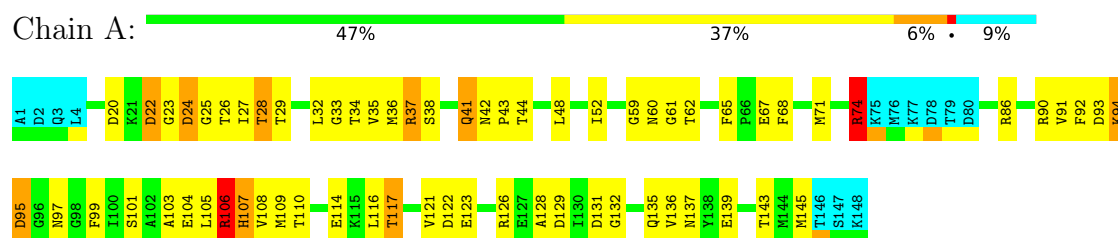


• Molecule 2: MYOSIN LIGHT CHAIN KINASE

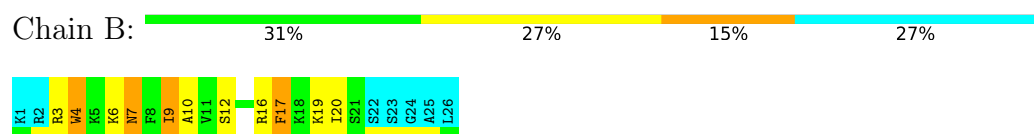


4.2.19 Score per residue for model 19

• Molecule 1: CALMODULIN

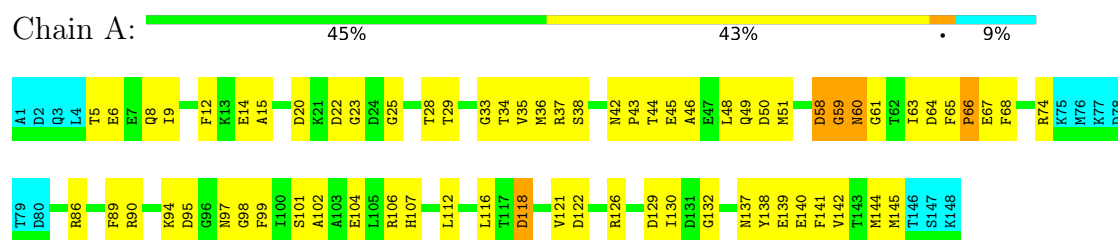


• Molecule 2: MYOSIN LIGHT CHAIN KINASE



4.2.20 Score per residue for model 20

• Molecule 1: CALMODULIN



• Molecule 2: MYOSIN LIGHT CHAIN KINASE





4.2.21 Score per residue for model 21

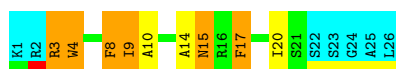
- Molecule 1: CALMODULIN

Chain A: 42% 41% 7% 9%



- Molecule 2: MYOSIN LIGHT CHAIN KINASE

Chain B: 38% 12% 23% 27%



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: ?.

Of the ? calculated structures, 21 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	1.54±0.01	2±1/1075 (0.2± 0.1%)	1.34±0.01	1±1/1446 (0.1± 0.0%)
2	B	1.52±0.02	1±0/164 (0.6± 0.0%)	1.47±0.02	3±1/218 (1.2± 0.3%)
All	All	1.54	59/26019 (0.2%)	1.36	81/34944 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	5.7±0.5
2	B	0.0±0.0	1.9±0.3
All	All	0	159

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	107	HIS	CG-ND1	-11.41	1.25	1.38	4	21
1	A	5	THR	N-CA	6.30	1.50	1.46	16	1
2	B	4	TRP	CG-CD2	-6.09	1.32	1.43	4	21
1	A	137	ASN	N-CA	5.75	1.49	1.46	3	1
1	A	131	ASP	N-CA	5.46	1.49	1.46	13	1
1	A	107	HIS	ND1-CE1	-5.13	1.27	1.32	8	13
1	A	64	ASP	N-CA	5.07	1.49	1.46	11	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($^{\circ}$)	Ideal($^{\circ}$)	Models	
								Worst	Total
1	A	107	HIS	CE1-NE2-CD2	-7.25	101.75	109.00	3	21
2	B	17	PHE	CA-CB-CG	-6.95	106.86	113.80	15	12
2	B	4	TRP	NE1-CE2-CZ2	6.16	139.34	130.10	4	21
2	B	4	TRP	NE1-CE2-CD2	-5.42	100.35	107.40	4	15
2	B	8	PHE	CA-CB-CG	-5.35	108.45	113.80	5	7
1	A	137	ASN	CB-CA-C	-5.32	109.41	117.07	3	1
1	A	64	ASP	CB-CA-C	-5.22	109.56	117.07	11	1
1	A	131	ASP	CB-CA-C	-5.21	109.57	117.07	13	1
1	A	64	ASP	CA-C-O	5.19	120.95	117.94	11	1
1	A	5	THR	CB-CA-C	-5.01	109.86	117.07	4	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	37	ARG	Sidechain	21
2	B	3	ARG	Sidechain	21
1	A	86	ARG	Sidechain	20
1	A	90	ARG	Sidechain	20
1	A	126	ARG	Sidechain	20
1	A	74	ARG	Sidechain	19
1	A	106	ARG	Sidechain	19
2	B	16	ARG	Sidechain	19

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	1062	990	990	48 $\pm$ 8
2	B	160	174	174	8 $\pm$ 3
3	A	4	0	0	0 $\pm$ 0
All	All	25746	24444	24441	1127

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ILE:H	1:A:85:ILE:HD12	0.75	1.39	6	1
1:A:27:ILE:HG21	2:B:17:PHE:CE2	0.73	2.17	9	8
1:A:28:THR:HG22	1:A:29:THR:H	0.71	1.45	8	6
1:A:85:ILE:HD12	1:A:85:ILE:N	0.68	2.03	6	5
1:A:117:THR:HG23	1:A:118:ASP:N	0.67	2.05	1	2
1:A:69:LEU:O	1:A:73:ALA:HB3	0.67	1.90	17	1
1:A:105:LEU:HD22	2:B:4:TRP:CH2	0.67	2.25	14	1
1:A:124:MET:HE2	2:B:4:TRP:CD1	0.66	2.24	8	1
1:A:5:THR:HG23	1:A:6:GLU:H	0.66	1.50	20	2
1:A:22:ASP:OD2	3:A:181:CA:CA	0.65	1.73	19	1
1:A:28:THR:HG22	1:A:29:THR:N	0.65	2.07	8	8
1:A:65:PHE:CD1	1:A:65:PHE:N	0.65	2.65	17	2
1:A:5:THR:HG23	1:A:6:GLU:N	0.65	2.06	16	3
1:A:30:LYS:O	1:A:34:THR:HG23	0.64	1.92	13	5
1:A:99:PHE:CD1	1:A:99:PHE:N	0.63	2.66	1	4
1:A:117:THR:HG23	1:A:118:ASP:H	0.63	1.53	9	1
1:A:137:ASN:HD22	1:A:137:ASN:N	0.62	1.92	3	1
1:A:97:ASN:ND2	1:A:98:GLY:N	0.62	2.47	7	1
1:A:137:ASN:ND2	1:A:138:TYR:N	0.62	2.48	21	2
1:A:29:THR:HG23	1:A:52:ILE:HD12	0.61	1.71	4	1
1:A:42:ASN:ND2	2:B:18:LYS:NZ	0.61	2.48	16	1
1:A:97:ASN:ND2	1:A:99:PHE:N	0.61	2.48	7	1
1:A:36:MET:HE2	2:B:14:ALA:HB1	0.61	1.71	17	2
1:A:99:PHE:CZ	1:A:137:ASN:ND2	0.61	2.69	17	1
1:A:124:MET:SD	2:B:4:TRP:CE2	0.60	2.95	9	1
1:A:65:PHE:N	1:A:66:PRO:CD	0.60	2.64	13	6
1:A:48:LEU:HD12	1:A:48:LEU:N	0.60	2.12	10	1
2:B:6:LYS:CB	2:B:6:LYS:NZ	0.59	2.65	4	1
1:A:42:ASN:HD21	2:B:18:LYS:NZ	0.59	1.95	16	1
1:A:91:VAL:HG23	1:A:92:PHE:N	0.59	2.12	8	1
1:A:85:ILE:H	1:A:85:ILE:CD1	0.59	2.11	6	1
1:A:7:GLU:O	1:A:10:ALA:HB3	0.59	1.98	12	1
1:A:145:MET:SD	1:A:145:MET:N	0.59	2.75	20	2
1:A:141:PHE:CD1	1:A:145:MET:SD	0.59	2.96	21	1
1:A:12:PHE:CD1	1:A:12:PHE:N	0.58	2.69	4	1
1:A:89:PHE:CD2	1:A:138:TYR:CZ	0.57	2.91	3	1
1:A:135:GLN:H	1:A:135:GLN:NE2	0.57	1.97	17	1
1:A:65:PHE:C	1:A:65:PHE:CD1	0.56	2.83	10	1
1:A:32:LEU:HD11	2:B:17:PHE:CG	0.56	2.34	12	1
1:A:20:ASP:CG	1:A:25:GLY:H	0.56	2.08	20	7
1:A:31:GLU:H	1:A:31:GLU:CD	0.56	2.09	2	2
1:A:89:PHE:CD2	1:A:138:TYR:CE1	0.56	2.94	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:15:ASN:OD1	2:B:16:ARG:N	0.56	2.38	16	1
1:A:24:ASP:OD1	1:A:24:ASP:N	0.56	2.39	4	9
1:A:137:ASN:ND2	1:A:138:TYR:H	0.56	1.98	21	1
1:A:84:GLU:H	1:A:84:GLU:CD	0.56	2.08	5	1
1:A:144:MET:SD	1:A:145:MET:SD	0.56	3.03	2	2
1:A:97:ASN:ND2	1:A:99:PHE:CD2	0.56	2.74	7	1
1:A:12:PHE:CG	1:A:13:LYS:N	0.55	2.75	6	2
1:A:106:ARG:O	1:A:110:THR:HG23	0.55	2.01	3	2
1:A:97:ASN:HD22	1:A:99:PHE:H	0.55	1.44	7	2
1:A:64:ASP:CG	1:A:65:PHE:H	0.55	2.10	9	5
1:A:141:PHE:CZ	1:A:145:MET:SD	0.55	2.99	3	1
1:A:25:GLY:O	1:A:26:THR:HG23	0.55	2.02	12	3
1:A:135:GLN:NE2	1:A:135:GLN:N	0.55	2.54	17	1
1:A:22:ASP:CG	1:A:23:GLY:N	0.55	2.63	4	4
1:A:69:LEU:O	1:A:73:ALA:N	0.54	2.40	9	2
1:A:141:PHE:CE1	1:A:145:MET:SD	0.54	3.00	21	2
1:A:99:PHE:N	1:A:99:PHE:CD1	0.54	2.73	7	1
1:A:16:PHE:CZ	1:A:64:ASP:O	0.54	2.61	13	1
1:A:31:GLU:CD	1:A:31:GLU:N	0.54	2.66	18	2
1:A:12:PHE:CD1	1:A:68:PHE:CE2	0.54	2.95	20	1
1:A:36:MET:O	1:A:40:GLY:N	0.54	2.40	2	10
1:A:22:ASP:OD1	1:A:23:GLY:N	0.54	2.40	4	1
1:A:105:LEU:HD21	1:A:109:MET:SD	0.54	2.43	13	1
1:A:60:ASN:H	1:A:60:ASN:ND2	0.54	2.01	21	1
1:A:137:ASN:CG	1:A:138:TYR:N	0.54	2.65	21	4
1:A:60:ASN:N	1:A:60:ASN:ND2	0.54	2.54	16	1
1:A:105:LEU:O	1:A:107:HIS:N	0.54	2.41	9	5
1:A:135:GLN:H	1:A:135:GLN:CD	0.54	2.11	21	1
1:A:126:ARG:C	1:A:128:ALA:N	0.53	2.66	14	1
1:A:41:GLN:HE22	1:A:42:ASN:ND2	0.53	2.02	2	1
1:A:32:LEU:HD11	1:A:36:MET:SD	0.53	2.43	4	1
1:A:22:ASP:N	1:A:22:ASP:OD1	0.53	2.42	16	1
1:A:60:ASN:ND2	1:A:62:THR:H	0.53	2.01	10	1
1:A:141:PHE:CE2	1:A:145:MET:HE2	0.53	2.38	11	1
2:B:13:ALA:O	2:B:17:PHE:CD2	0.53	2.61	14	2
1:A:31:GLU:CD	1:A:31:GLU:H	0.53	2.11	18	1
1:A:64:ASP:CG	1:A:65:PHE:N	0.53	2.66	13	5
1:A:16:PHE:CD2	1:A:25:GLY:O	0.53	2.61	17	2
1:A:135:GLN:CD	1:A:135:GLN:N	0.53	2.66	15	2
1:A:98:GLY:O	1:A:99:PHE:CD2	0.53	2.62	10	2
1:A:95:ASP:CG	1:A:96:GLY:N	0.53	2.67	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:PHE:CE2	1:A:145:MET:SD	0.53	3.02	12	1
1:A:98:GLY:C	1:A:99:PHE:CG	0.52	2.86	1	2
1:A:59:GLY:O	1:A:61:GLY:N	0.52	2.42	20	5
1:A:123:GLU:OE1	1:A:123:GLU:N	0.52	2.42	6	2
1:A:116:LEU:O	1:A:117:THR:C	0.52	2.52	11	1
1:A:137:ASN:ND2	1:A:139:GLU:H	0.52	2.02	11	1
1:A:28:THR:OG1	1:A:29:THR:N	0.52	2.42	20	3
1:A:63:ILE:HD11	2:B:17:PHE:CZ	0.52	2.40	15	1
1:A:16:PHE:O	1:A:20:ASP:N	0.52	2.43	16	2
1:A:56:ASP:OD1	1:A:59:GLY:N	0.52	2.42	4	1
1:A:32:LEU:HD11	1:A:36:MET:HE2	0.52	1.81	3	1
1:A:107:HIS:O	1:A:111:ASN:ND2	0.52	2.43	7	2
1:A:90:ARG:O	1:A:94:LYS:N	0.52	2.42	21	1
1:A:133:ASP:CG	1:A:134:GLY:N	0.52	2.68	21	2
1:A:53:ASN:O	1:A:53:ASN:ND2	0.52	2.42	17	1
1:A:41:GLN:NE2	1:A:42:ASN:ND2	0.52	2.56	2	1
1:A:64:ASP:OD1	1:A:65:PHE:CD2	0.52	2.62	9	1
1:A:137:ASN:HD21	1:A:139:GLU:H	0.52	1.45	11	1
1:A:72:MET:SD	1:A:72:MET:N	0.52	2.81	15	1
2:B:19:LYS:CB	2:B:19:LYS:NZ	0.52	2.73	17	1
2:B:16:ARG:C	2:B:18:LYS:N	0.52	2.65	17	5
1:A:42:ASN:HD21	2:B:18:LYS:HZ3	0.52	1.44	16	1
1:A:16:PHE:CD2	1:A:65:PHE:CE1	0.52	2.98	8	2
1:A:53:ASN:O	1:A:55:VAL:N	0.52	2.43	11	1
1:A:58:ASP:CG	1:A:59:GLY:N	0.52	2.66	13	1
1:A:95:ASP:O	1:A:97:ASN:N	0.52	2.42	14	1
1:A:105:LEU:HD11	1:A:109:MET:SD	0.52	2.44	14	2
1:A:14:GLU:OE2	2:B:6:LYS:NZ	0.52	2.42	9	1
1:A:98:GLY:O	1:A:99:PHE:CD1	0.52	2.63	11	2
1:A:36:MET:SD	2:B:18:LYS:NZ	0.52	2.76	16	1
1:A:106:ARG:O	1:A:110:THR:N	0.52	2.43	17	1
1:A:40:GLY:O	1:A:41:GLN:CB	0.51	2.57	7	4
1:A:137:ASN:OD1	1:A:139:GLU:N	0.51	2.42	5	1
1:A:12:PHE:CE2	1:A:69:LEU:HD11	0.51	2.40	18	1
1:A:59:GLY:C	1:A:61:GLY:N	0.51	2.67	21	6
1:A:122:ASP:CG	1:A:123:GLU:N	0.51	2.68	16	1
1:A:99:PHE:O	1:A:99:PHE:CG	0.51	2.62	19	1
1:A:64:ASP:N	1:A:64:ASP:OD1	0.51	2.42	21	1
1:A:58:ASP:OD1	1:A:59:GLY:N	0.51	2.43	3	1
1:A:81:SER:OG	1:A:82:GLU:N	0.51	2.42	14	2
1:A:45:GLU:CD	1:A:45:GLU:N	0.51	2.69	21	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:THR:OG1	1:A:6:GLU:N	0.51	2.41	4	5
1:A:58:ASP:N	1:A:58:ASP:OD1	0.51	2.42	6	2
1:A:55:VAL:HG13	1:A:56:ASP:N	0.51	2.21	10	1
1:A:64:ASP:OD1	1:A:65:PHE:CE2	0.51	2.63	13	1
1:A:6:GLU:OE1	1:A:9:ILE:HD12	0.51	2.06	21	1
1:A:117:THR:CG2	1:A:118:ASP:N	0.51	2.74	18	3
1:A:65:PHE:H	1:A:66:PRO:CD	0.51	2.17	13	2
1:A:126:ARG:O	1:A:128:ALA:N	0.51	2.43	14	1
2:B:5:LYS:O	2:B:7:ASN:N	0.51	2.44	1	3
2:B:16:ARG:O	2:B:18:LYS:N	0.51	2.44	17	2
1:A:53:ASN:C	1:A:55:VAL:N	0.51	2.67	11	5
1:A:137:ASN:OD1	1:A:138:TYR:N	0.51	2.44	5	1
1:A:97:ASN:N	1:A:97:ASN:OD1	0.50	2.44	2	1
1:A:5:THR:C	1:A:7:GLU:N	0.50	2.69	12	7
1:A:48:LEU:N	1:A:48:LEU:CD1	0.50	2.74	10	1
1:A:82:GLU:C	1:A:84:GLU:N	0.50	2.67	14	1
1:A:84:GLU:CD	1:A:84:GLU:N	0.50	2.69	5	1
1:A:139:GLU:O	1:A:141:PHE:N	0.50	2.45	20	2
1:A:28:THR:CG2	1:A:29:THR:H	0.50	2.19	8	2
1:A:105:LEU:C	1:A:107:HIS:N	0.50	2.66	12	6
1:A:133:ASP:OD1	1:A:134:GLY:N	0.50	2.45	7	2
1:A:99:PHE:CE2	1:A:137:ASN:OD1	0.50	2.65	3	1
1:A:141:PHE:CD1	1:A:141:PHE:C	0.50	2.88	17	5
1:A:64:ASP:OD2	1:A:65:PHE:CD2	0.50	2.64	13	1
1:A:117:THR:OG1	1:A:118:ASP:N	0.50	2.42	9	1
1:A:97:ASN:HD22	1:A:97:ASN:N	0.50	2.04	12	1
1:A:121:VAL:O	1:A:124:MET:N	0.50	2.45	15	7
1:A:138:TYR:O	1:A:142:VAL:HG23	0.50	2.07	15	1
1:A:60:ASN:ND2	1:A:60:ASN:H	0.50	2.03	20	1
1:A:106:ARG:O	1:A:110:THR:HG22	0.50	2.07	7	2
1:A:141:PHE:O	1:A:145:MET:SD	0.50	2.70	11	2
1:A:12:PHE:CE1	1:A:68:PHE:CD1	0.50	3.00	12	1
1:A:20:ASP:OD2	1:A:23:GLY:N	0.49	2.44	1	1
1:A:51:MET:SD	2:B:17:PHE:O	0.49	2.70	21	5
1:A:94:LYS:O	1:A:96:GLY:N	0.49	2.45	14	2
1:A:12:PHE:CE1	1:A:68:PHE:CD2	0.49	2.99	14	1
1:A:92:PHE:O	1:A:108:VAL:HG21	0.49	2.06	15	1
1:A:5:THR:C	1:A:7:GLU:H	0.49	2.15	11	5
1:A:24:ASP:OD1	1:A:25:GLY:N	0.49	2.44	3	3
1:A:9:ILE:CG2	1:A:10:ALA:N	0.49	2.75	5	1
2:B:7:ASN:CG	2:B:8:PHE:N	0.49	2.70	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:ILE:O	1:A:128:ALA:HB3	0.49	2.08	5	1
1:A:64:ASP:OD1	1:A:65:PHE:CZ	0.49	2.66	13	1
1:A:5:THR:O	1:A:6:GLU:CG	0.49	2.61	15	1
1:A:9:ILE:HG23	1:A:10:ALA:N	0.49	2.23	5	1
1:A:86:ARG:HE	1:A:90:ARG:NH2	0.49	2.05	7	1
1:A:50:ASP:CG	1:A:51:MET:N	0.49	2.69	16	2
1:A:53:ASN:C	1:A:55:VAL:H	0.49	2.15	1	7
1:A:55:VAL:CG1	1:A:56:ASP:N	0.49	2.75	10	1
1:A:16:PHE:CE1	1:A:25:GLY:O	0.49	2.66	2	1
1:A:28:THR:CG2	1:A:29:THR:N	0.49	2.76	1	7
1:A:70:THR:O	1:A:74:ARG:N	0.49	2.46	21	5
1:A:19:PHE:O	1:A:21:LYS:N	0.49	2.45	1	1
1:A:84:GLU:N	1:A:84:GLU:OE1	0.49	2.46	8	1
1:A:142:VAL:O	1:A:142:VAL:HG12	0.49	2.08	20	2
1:A:71:MET:C	1:A:72:MET:SD	0.49	2.96	15	1
2:B:6:LYS:CG	2:B:7:ASN:N	0.49	2.76	19	1
1:A:64:ASP:OD1	1:A:65:PHE:N	0.49	2.45	1	2
1:A:52:ILE:C	1:A:54:GLU:N	0.49	2.70	3	1
1:A:121:VAL:O	1:A:122:ASP:C	0.48	2.56	5	16
1:A:16:PHE:CE2	1:A:25:GLY:O	0.48	2.65	7	1
1:A:16:PHE:CE2	1:A:65:PHE:CE1	0.48	3.00	8	1
1:A:42:ASN:ND2	1:A:42:ASN:C	0.48	2.70	5	1
1:A:97:ASN:ND2	1:A:99:PHE:H	0.48	2.05	7	1
1:A:117:THR:CG2	1:A:118:ASP:H	0.48	2.17	9	1
1:A:50:ASP:C	1:A:52:ILE:N	0.48	2.70	3	2
1:A:65:PHE:CE1	1:A:69:LEU:HD11	0.48	2.43	7	1
1:A:113:GLY:C	1:A:115:LYS:N	0.48	2.69	12	1
1:A:94:LYS:CB	1:A:94:LYS:NZ	0.48	2.76	13	2
1:A:114:GLU:CD	1:A:114:GLU:N	0.48	2.72	7	2
1:A:34:THR:CG2	1:A:35:VAL:N	0.48	2.76	12	3
1:A:16:PHE:O	1:A:19:PHE:N	0.48	2.47	10	1
1:A:95:ASP:OD1	1:A:96:GLY:N	0.48	2.46	1	2
1:A:98:GLY:C	1:A:99:PHE:CD1	0.48	2.92	13	4
2:B:5:LYS:C	2:B:7:ASN:N	0.48	2.69	1	3
1:A:137:ASN:OD1	1:A:137:ASN:N	0.48	2.46	4	1
1:A:14:GLU:CD	2:B:6:LYS:HZ1	0.48	2.17	9	1
1:A:141:PHE:CZ	1:A:145:MET:HE2	0.48	2.43	11	1
2:B:3:ARG:O	2:B:6:LYS:NZ	0.48	2.46	11	1
1:A:71:MET:HE1	2:B:20:ILE:HD11	0.48	1.84	17	1
1:A:71:MET:SD	1:A:71:MET:O	0.48	2.71	9	1
1:A:120:GLU:N	1:A:120:GLU:OE1	0.48	2.47	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ASP:N	1:A:131:ASP:OD1	0.48	2.44	18	1
1:A:101:SER:OG	1:A:102:ALA:N	0.48	2.42	20	1
1:A:105:LEU:O	1:A:106:ARG:C	0.48	2.56	5	20
1:A:137:ASN:N	1:A:137:ASN:ND2	0.48	2.60	3	1
1:A:93:ASP:OD1	1:A:96:GLY:N	0.48	2.47	11	2
1:A:93:ASP:OD2	1:A:98:GLY:CA	0.48	2.62	3	2
1:A:20:ASP:OD2	1:A:25:GLY:N	0.48	2.47	5	2
1:A:105:LEU:HD22	1:A:109:MET:SD	0.48	2.48	17	1
1:A:35:VAL:O	1:A:38:SER:N	0.48	2.47	20	5
1:A:35:VAL:C	1:A:37:ARG:N	0.48	2.71	11	2
1:A:94:LYS:O	1:A:94:LYS:CG	0.48	2.62	12	1
1:A:95:ASP:CG	1:A:96:GLY:H	0.47	2.17	11	2
1:A:131:ASP:OD1	1:A:131:ASP:N	0.47	2.47	10	1
1:A:97:ASN:N	1:A:97:ASN:ND2	0.47	2.61	12	1
1:A:87:GLU:O	1:A:91:VAL:HG23	0.47	2.08	18	1
1:A:45:GLU:N	1:A:45:GLU:OE2	0.47	2.47	21	2
1:A:141:PHE:CE2	1:A:145:MET:CE	0.47	2.97	3	1
1:A:28:THR:C	1:A:30:LYS:N	0.47	2.71	10	4
2:B:19:LYS:C	2:B:21:SER:N	0.47	2.67	17	3
1:A:51:MET:C	1:A:51:MET:SD	0.47	2.97	3	1
1:A:56:ASP:OD2	1:A:60:ASN:N	0.47	2.47	10	1
1:A:113:GLY:O	1:A:115:LYS:N	0.47	2.46	12	1
1:A:99:PHE:O	1:A:99:PHE:CD1	0.47	2.67	19	1
1:A:12:PHE:CD1	1:A:12:PHE:C	0.47	2.88	20	1
1:A:85:ILE:N	1:A:85:ILE:CD1	0.47	2.77	10	4
1:A:18:LEU:O	1:A:21:LYS:NZ	0.47	2.43	5	1
1:A:37:ARG:C	1:A:39:LEU:N	0.47	2.73	8	4
1:A:137:ASN:CG	1:A:138:TYR:H	0.47	2.17	20	1
1:A:86:ARG:O	1:A:89:PHE:N	0.47	2.48	10	3
2:B:5:LYS:O	2:B:6:LYS:C	0.47	2.57	10	8
1:A:22:ASP:OD1	1:A:22:ASP:N	0.47	2.47	7	5
1:A:126:ARG:CG	1:A:126:ARG:HH11	0.47	2.22	3	1
2:B:9:ILE:O	2:B:12:SER:N	0.47	2.47	5	5
2:B:9:ILE:O	2:B:12:SER:CB	0.47	2.63	4	3
1:A:117:THR:C	1:A:119:GLU:H	0.47	2.16	21	2
2:B:16:ARG:C	2:B:18:LYS:H	0.47	2.16	17	2
1:A:45:GLU:CG	1:A:46:ALA:N	0.47	2.77	20	2
1:A:55:VAL:O	1:A:57:ALA:N	0.47	2.47	8	1
2:B:4:TRP:O	2:B:5:LYS:C	0.47	2.58	9	4
2:B:19:LYS:CB	2:B:19:LYS:HZ3	0.47	2.23	17	1
2:B:18:LYS:CD	2:B:18:LYS:C	0.47	2.88	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:THR:HG23	1:A:62:THR:HG22	0.47	1.86	1	2
1:A:139:GLU:C	1:A:141:PHE:N	0.47	2.70	20	5
1:A:28:THR:OG1	1:A:62:THR:CG2	0.47	2.62	2	2
1:A:14:GLU:CD	2:B:6:LYS:NZ	0.47	2.73	9	1
1:A:28:THR:O	1:A:30:LYS:N	0.47	2.48	10	1
1:A:94:LYS:C	1:A:96:GLY:N	0.47	2.70	13	1
1:A:20:ASP:C	1:A:22:ASP:N	0.46	2.72	12	3
1:A:82:GLU:O	1:A:84:GLU:N	0.46	2.48	14	1
1:A:126:ARG:C	1:A:128:ALA:H	0.46	2.18	14	1
1:A:93:ASP:OD2	1:A:98:GLY:N	0.46	2.48	17	1
2:B:19:LYS:O	2:B:21:SER:N	0.46	2.48	17	2
1:A:105:LEU:O	1:A:109:MET:N	0.46	2.49	1	1
1:A:91:VAL:CG2	1:A:92:PHE:N	0.46	2.78	8	1
1:A:37:ARG:N	1:A:42:ASN:OD1	0.46	2.48	10	1
1:A:114:GLU:CD	1:A:114:GLU:H	0.46	2.17	17	2
1:A:44:THR:O	1:A:48:LEU:CD1	0.46	2.63	9	1
1:A:87:GLU:OE1	1:A:88:ALA:N	0.46	2.48	15	1
1:A:31:GLU:N	1:A:31:GLU:OE1	0.46	2.48	2	1
1:A:12:PHE:CD1	1:A:13:LYS:N	0.46	2.84	6	1
1:A:47:GLU:CD	1:A:47:GLU:C	0.46	2.82	12	1
1:A:117:THR:HG22	1:A:118:ASP:N	0.46	2.24	18	1
1:A:129:ASP:OD1	1:A:130:ILE:N	0.46	2.49	20	1
1:A:15:ALA:C	1:A:17:SER:N	0.46	2.73	3	2
2:B:6:LYS:CB	2:B:6:LYS:HZ2	0.46	2.24	4	1
1:A:110:THR:CG2	1:A:111:ASN:N	0.46	2.79	8	1
2:B:4:TRP:CD1	2:B:4:TRP:N	0.46	2.84	6	5
1:A:106:ARG:O	1:A:110:THR:CG2	0.46	2.64	8	3
1:A:126:ARG:O	1:A:129:ASP:N	0.46	2.49	4	1
1:A:54:GLU:CG	1:A:54:GLU:O	0.46	2.63	16	1
1:A:23:GLY:O	1:A:24:ASP:C	0.46	2.59	4	3
1:A:42:ASN:ND2	1:A:42:ASN:H	0.46	2.08	2	1
1:A:97:ASN:OD1	1:A:97:ASN:N	0.46	2.47	20	2
1:A:5:THR:O	1:A:6:GLU:CB	0.46	2.63	15	1
1:A:135:GLN:N	1:A:135:GLN:OE1	0.46	2.48	19	1
1:A:99:PHE:CD1	1:A:99:PHE:C	0.46	2.94	4	1
1:A:93:ASP:C	1:A:95:ASP:H	0.46	2.18	12	1
1:A:105:LEU:O	1:A:108:VAL:N	0.46	2.48	5	4
1:A:35:VAL:O	1:A:37:ARG:N	0.46	2.48	11	2
2:B:3:ARG:H	2:B:6:LYS:NZ	0.46	2.07	17	1
1:A:44:THR:O	1:A:48:LEU:HD13	0.46	2.11	20	1
1:A:94:LYS:CG	1:A:95:ASP:N	0.46	2.79	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ASP:CG	1:A:132:GLY:N	0.46	2.73	13	1
1:A:32:LEU:HD22	1:A:36:MET:SD	0.45	2.52	7	1
1:A:36:MET:CG	1:A:42:ASN:HD21	0.45	2.25	20	1
1:A:99:PHE:CZ	1:A:137:ASN:OD1	0.45	2.69	20	2
1:A:84:GLU:OE2	2:B:16:ARG:NH1	0.45	2.49	9	1
2:B:4:TRP:CD1	2:B:4:TRP:H	0.45	2.29	9	1
1:A:93:ASP:O	1:A:94:LYS:C	0.45	2.60	14	8
1:A:56:ASP:OD2	1:A:60:ASN:ND2	0.45	2.49	16	1
1:A:120:GLU:OE1	1:A:120:GLU:CA	0.45	2.64	16	1
1:A:35:VAL:O	1:A:36:MET:C	0.45	2.60	13	17
1:A:67:GLU:O	1:A:68:PHE:C	0.45	2.59	21	9
1:A:33:GLY:O	1:A:34:THR:C	0.45	2.60	11	8
1:A:8:GLN:H	1:A:8:GLN:HE21	0.45	1.52	16	1
1:A:56:ASP:OD1	1:A:60:ASN:N	0.45	2.49	4	1
1:A:81:SER:C	1:A:83:GLU:H	0.45	2.20	4	2
1:A:65:PHE:CD1	1:A:65:PHE:C	0.45	2.94	7	1
2:B:5:LYS:HG2	2:B:9:ILE:HD12	0.45	1.87	10	1
1:A:20:ASP:C	1:A:22:ASP:H	0.45	2.19	18	2
1:A:43:PRO:O	1:A:44:THR:O	0.45	2.35	9	2
1:A:66:PRO:O	1:A:67:GLU:C	0.45	2.60	14	5
1:A:56:ASP:OD2	1:A:62:THR:N	0.45	2.50	4	3
2:B:7:ASN:OD1	2:B:7:ASN:C	0.45	2.60	7	1
1:A:22:ASP:OD1	1:A:31:GLU:CD	0.45	2.60	4	2
1:A:139:GLU:O	1:A:140:GLU:C	0.45	2.59	7	3
1:A:26:THR:O	1:A:31:GLU:OE1	0.45	2.35	3	5
1:A:59:GLY:C	1:A:61:GLY:H	0.45	2.19	4	2
1:A:32:LEU:CD1	2:B:17:PHE:CD1	0.45	2.99	19	1
1:A:9:ILE:HD12	1:A:9:ILE:N	0.45	2.27	4	1
2:B:4:TRP:O	2:B:7:ASN:N	0.45	2.50	9	1
1:A:5:THR:CG2	1:A:6:GLU:H	0.45	2.18	16	1
1:A:41:GLN:CG	1:A:42:ASN:N	0.45	2.79	18	1
1:A:37:ARG:C	1:A:39:LEU:H	0.45	2.20	8	4
1:A:65:PHE:CZ	1:A:69:LEU:HD11	0.45	2.47	7	1
1:A:64:ASP:CG	1:A:65:PHE:CD2	0.45	2.95	13	1
2:B:9:ILE:O	2:B:10:ALA:C	0.45	2.60	6	15
1:A:99:PHE:CD1	1:A:99:PHE:O	0.45	2.70	4	1
1:A:25:GLY:C	1:A:26:THR:OG1	0.45	2.60	6	2
1:A:39:LEU:HD12	1:A:39:LEU:N	0.45	2.27	11	1
1:A:110:THR:C	1:A:112:LEU:H	0.45	2.19	16	2
1:A:93:ASP:OD2	1:A:95:ASP:O	0.45	2.35	19	1
2:B:20:ILE:O	2:B:21:SER:C	0.44	2.60	1	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ARG:O	1:A:127:GLU:C	0.44	2.60	4	1
1:A:130:ILE:O	1:A:130:ILE:HG22	0.44	2.11	9	2
1:A:56:ASP:OD1	1:A:57:ALA:N	0.44	2.50	10	1
1:A:97:ASN:OD1	1:A:97:ASN:C	0.44	2.61	10	1
1:A:36:MET:O	1:A:39:LEU:N	0.44	2.49	12	2
1:A:16:PHE:C	1:A:18:LEU:N	0.44	2.73	16	2
1:A:120:GLU:O	1:A:121:VAL:C	0.44	2.60	13	9
1:A:103:ALA:O	1:A:104:GLU:C	0.44	2.61	4	14
1:A:30:LYS:O	1:A:34:THR:OG1	0.44	2.34	4	1
1:A:73:ALA:O	1:A:74:ARG:C	0.44	2.61	17	4
1:A:138:TYR:O	1:A:139:GLU:C	0.44	2.60	16	6
1:A:48:LEU:C	1:A:50:ASP:N	0.44	2.74	9	1
1:A:5:THR:O	1:A:7:GLU:N	0.44	2.50	12	3
1:A:9:ILE:N	1:A:9:ILE:CD1	0.44	2.80	4	1
1:A:131:ASP:OD1	1:A:132:GLY:N	0.44	2.50	14	2
1:A:24:ASP:CG	1:A:25:GLY:N	0.44	2.76	1	2
1:A:45:GLU:CD	1:A:45:GLU:H	0.44	2.21	2	1
1:A:89:PHE:CZ	1:A:98:GLY:O	0.44	2.70	2	1
1:A:95:ASP:CG	1:A:97:ASN:OD1	0.44	2.61	11	2
1:A:114:GLU:C	1:A:116:LEU:H	0.44	2.21	19	1
1:A:60:ASN:C	1:A:62:THR:H	0.44	2.21	1	3
1:A:93:ASP:O	1:A:93:ASP:CG	0.44	2.61	2	1
1:A:99:PHE:CE2	1:A:137:ASN:ND2	0.44	2.86	17	1
1:A:6:GLU:CD	1:A:6:GLU:N	0.44	2.74	21	1
1:A:60:ASN:OD1	1:A:62:THR:O	0.44	2.36	10	1
1:A:87:GLU:OE1	1:A:87:GLU:CA	0.44	2.65	10	1
1:A:24:ASP:CG	1:A:25:GLY:H	0.44	2.21	13	1
1:A:68:PHE:CZ	1:A:72:MET:SD	0.44	3.10	3	1
2:B:3:ARG:C	2:B:5:LYS:N	0.44	2.71	8	2
1:A:24:ASP:CG	1:A:26:THR:OG1	0.44	2.61	6	1
1:A:56:ASP:OD1	1:A:56:ASP:O	0.44	2.36	4	1
1:A:93:ASP:O	1:A:93:ASP:OD1	0.44	2.36	12	2
1:A:139:GLU:O	1:A:143:THR:N	0.44	2.50	5	1
1:A:24:ASP:OD1	1:A:24:ASP:C	0.44	2.61	6	1
1:A:48:LEU:HD13	1:A:51:MET:SD	0.44	2.53	6	1
1:A:101:SER:O	1:A:102:ALA:C	0.44	2.61	8	2
1:A:90:ARG:O	1:A:91:VAL:C	0.44	2.61	13	1
1:A:138:TYR:C	1:A:140:GLU:N	0.44	2.74	14	1
1:A:128:ALA:O	1:A:140:GLU:OE1	0.44	2.36	16	1
1:A:130:ILE:C	1:A:132:GLY:H	0.44	2.20	20	1
1:A:110:THR:O	1:A:111:ASN:C	0.44	2.61	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:ASP:OD2	1:A:97:ASN:OD1	0.44	2.36	11	3
2:B:18:LYS:C	2:B:20:ILE:N	0.44	2.73	7	1
2:B:20:ILE:O	2:B:21:SER:O	0.44	2.36	7	2
1:A:55:VAL:O	1:A:56:ASP:C	0.44	2.59	8	2
1:A:111:ASN:ND2	1:A:111:ASN:C	0.44	2.74	9	1
1:A:89:PHE:CG	1:A:138:TYR:CE1	0.44	3.06	20	1
1:A:45:GLU:O	1:A:46:ALA:C	0.43	2.61	6	8
1:A:56:ASP:OD2	1:A:62:THR:O	0.43	2.36	4	1
1:A:107:HIS:O	1:A:110:THR:OG1	0.43	2.36	18	1
1:A:95:ASP:O	1:A:96:GLY:C	0.43	2.60	14	4
1:A:55:VAL:O	1:A:67:GLU:OE2	0.43	2.36	2	1
1:A:91:VAL:O	1:A:92:PHE:C	0.43	2.61	19	5
1:A:130:ILE:CG2	1:A:131:ASP:N	0.43	2.80	7	1
1:A:22:ASP:OD2	1:A:31:GLU:OE1	0.43	2.35	14	1
1:A:22:ASP:OD2	1:A:31:GLU:OE2	0.43	2.36	15	1
1:A:63:ILE:HD13	2:B:17:PHE:CZ	0.43	2.47	20	1
1:A:117:THR:OG1	1:A:120:GLU:OE1	0.43	2.36	2	1
2:B:19:LYS:O	2:B:20:ILE:C	0.43	2.61	17	4
1:A:8:GLN:O	1:A:9:ILE:C	0.43	2.61	10	6
1:A:43:PRO:O	1:A:45:GLU:OE2	0.43	2.37	7	1
1:A:85:ILE:O	1:A:86:ARG:C	0.43	2.61	7	3
2:B:17:PHE:HA	2:B:20:ILE:HD12	0.43	1.90	7	2
1:A:68:PHE:O	1:A:69:LEU:C	0.43	2.60	8	2
1:A:20:ASP:OD1	1:A:22:ASP:OD1	0.43	2.37	10	1
1:A:83:GLU:O	1:A:87:GLU:OE1	0.43	2.37	11	1
1:A:129:ASP:OD1	1:A:140:GLU:OE1	0.43	2.36	17	1
1:A:62:THR:O	1:A:67:GLU:OE2	0.43	2.35	21	1
1:A:16:PHE:O	1:A:17:SER:C	0.43	2.61	1	4
1:A:58:ASP:OD2	1:A:60:ASN:OD1	0.43	2.37	20	2
1:A:50:ASP:O	1:A:52:ILE:N	0.43	2.51	3	1
1:A:125:ILE:O	1:A:126:ARG:C	0.43	2.61	3	1
2:B:16:ARG:O	2:B:17:PHE:C	0.43	2.61	5	2
1:A:20:ASP:OD2	1:A:24:ASP:OD1	0.43	2.36	6	1
1:A:95:ASP:OD1	1:A:104:GLU:CD	0.43	2.62	6	1
1:A:32:LEU:O	1:A:33:GLY:C	0.43	2.61	21	2
1:A:137:ASN:O	1:A:138:TYR:C	0.43	2.61	9	1
1:A:66:PRO:C	1:A:68:PHE:N	0.43	2.75	12	1
1:A:27:ILE:HG21	2:B:17:PHE:CD2	0.43	2.47	14	1
1:A:19:PHE:O	1:A:31:GLU:OE1	0.43	2.36	16	1
1:A:69:LEU:O	1:A:73:ALA:CB	0.43	2.65	17	1
1:A:84:GLU:O	1:A:85:ILE:C	0.43	2.62	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:ALA:O	1:A:11:GLU:C	0.43	2.62	10	1
1:A:66:PRO:O	1:A:68:PHE:N	0.43	2.51	12	1
1:A:58:ASP:OD2	1:A:67:GLU:OE1	0.43	2.37	2	1
1:A:114:GLU:C	1:A:114:GLU:CD	0.43	2.87	3	1
1:A:106:ARG:O	1:A:110:THR:OG1	0.43	2.35	18	2
1:A:105:LEU:HD23	1:A:105:LEU:O	0.43	2.14	7	1
1:A:129:ASP:OD2	1:A:133:ASP:N	0.43	2.50	7	2
1:A:126:ARG:O	1:A:129:ASP:O	0.43	2.37	9	1
1:A:43:PRO:O	1:A:44:THR:C	0.43	2.60	9	2
1:A:20:ASP:OD1	1:A:22:ASP:CG	0.43	2.62	9	1
1:A:28:THR:O	1:A:29:THR:C	0.43	2.62	10	1
1:A:13:LYS:O	1:A:14:GLU:C	0.43	2.62	13	2
2:B:4:TRP:O	2:B:7:ASN:OD1	0.43	2.36	11	2
1:A:94:LYS:C	1:A:96:GLY:H	0.43	2.22	13	1
1:A:110:THR:C	1:A:112:LEU:N	0.43	2.77	16	1
1:A:20:ASP:OD1	1:A:24:ASP:N	0.43	2.52	4	1
1:A:20:ASP:OD1	1:A:31:GLU:OE2	0.43	2.37	12	2
1:A:59:GLY:O	1:A:60:ASN:C	0.43	2.62	14	5
1:A:82:GLU:OE2	1:A:82:GLU:N	0.43	2.52	10	1
1:A:22:ASP:OD2	1:A:24:ASP:CG	0.43	2.62	11	1
1:A:118:ASP:OD1	1:A:122:ASP:OD2	0.43	2.37	11	2
1:A:95:ASP:C	1:A:97:ASN:H	0.43	2.21	19	1
1:A:107:HIS:O	1:A:111:ASN:CG	0.43	2.62	21	1
1:A:86:ARG:O	1:A:87:GLU:C	0.43	2.62	1	5
1:A:119:GLU:O	1:A:120:GLU:C	0.43	2.62	2	2
1:A:52:ILE:C	1:A:54:GLU:H	0.43	2.21	3	1
1:A:82:GLU:O	1:A:82:GLU:CD	0.43	2.62	5	1
1:A:14:GLU:O	1:A:15:ALA:C	0.43	2.61	10	3
1:A:119:GLU:O	1:A:123:GLU:OE2	0.43	2.37	6	1
1:A:105:LEU:HD23	1:A:105:LEU:C	0.43	2.39	7	1
1:A:58:ASP:OD2	1:A:60:ASN:CG	0.43	2.62	8	1
1:A:56:ASP:OD1	1:A:56:ASP:C	0.43	2.61	10	1
2:B:5:LYS:CB	2:B:5:LYS:NZ	0.43	2.82	13	1
1:A:133:ASP:OD1	1:A:135:GLN:O	0.43	2.37	16	1
1:A:118:ASP:O	1:A:118:ASP:OD1	0.43	2.37	21	1
1:A:21:LYS:CB	1:A:21:LYS:NZ	0.43	2.82	14	2
1:A:50:ASP:C	1:A:52:ILE:H	0.43	2.22	9	1
1:A:95:ASP:OD1	1:A:97:ASN:OD1	0.43	2.37	11	1
1:A:94:LYS:O	1:A:95:ASP:O	0.43	2.36	18	1
1:A:42:ASN:O	1:A:42:ASN:CG	0.42	2.62	1	1
2:B:15:ASN:OD1	2:B:15:ASN:C	0.42	2.61	21	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:MET:SD	2:B:16:ARG:NH1	0.42	2.92	17	1
1:A:45:GLU:C	1:A:47:GLU:N	0.42	2.75	21	1
1:A:117:THR:OG1	1:A:120:GLU:CD	0.42	2.62	2	1
1:A:129:ASP:OD2	1:A:133:ASP:OD1	0.42	2.37	16	3
1:A:67:GLU:O	1:A:70:THR:OG1	0.42	2.37	7	1
1:A:65:PHE:CB	1:A:66:PRO:CD	0.42	2.96	8	1
1:A:120:GLU:O	1:A:120:GLU:OE1	0.42	2.37	9	1
1:A:95:ASP:OD1	1:A:95:ASP:N	0.42	2.52	11	2
1:A:104:GLU:O	1:A:105:LEU:C	0.42	2.62	18	3
1:A:107:HIS:CD2	1:A:107:HIS:N	0.42	2.86	16	1
2:B:8:PHE:CD2	2:B:8:PHE:C	0.42	2.97	21	2
1:A:12:PHE:CD2	1:A:13:LYS:N	0.42	2.87	18	1
1:A:117:THR:O	1:A:118:ASP:OD2	0.42	2.36	21	1
1:A:93:ASP:OD1	1:A:104:GLU:OE1	0.42	2.37	2	1
1:A:111:ASN:C	1:A:113:GLY:H	0.42	2.21	2	1
1:A:26:THR:O	1:A:31:GLU:CD	0.42	2.62	5	1
1:A:97:ASN:ND2	1:A:98:GLY:H	0.42	2.11	7	1
1:A:25:GLY:O	1:A:26:THR:CG2	0.42	2.67	12	1
1:A:22:ASP:OD2	1:A:24:ASP:OD1	0.42	2.37	14	2
1:A:95:ASP:OD2	1:A:104:GLU:OE1	0.42	2.36	18	1
1:A:18:LEU:O	1:A:19:PHE:C	0.42	2.62	2	2
2:B:8:PHE:O	2:B:12:SER:OG	0.42	2.37	12	1
1:A:22:ASP:OD2	1:A:24:ASP:OD2	0.42	2.37	19	1
1:A:95:ASP:OD1	1:A:95:ASP:C	0.42	2.62	1	3
1:A:129:ASP:O	1:A:130:ILE:C	0.42	2.62	1	1
1:A:13:LYS:O	1:A:17:SER:OG	0.42	2.37	3	1
1:A:56:ASP:OD2	1:A:61:GLY:C	0.42	2.62	6	1
1:A:40:GLY:O	1:A:41:GLN:O	0.42	2.37	9	1
1:A:138:TYR:O	1:A:141:PHE:N	0.42	2.52	12	2
1:A:130:ILE:C	1:A:132:GLY:N	0.42	2.77	20	1
1:A:98:GLY:C	1:A:99:PHE:CD2	0.42	2.98	16	1
1:A:136:VAL:HG12	1:A:137:ASN:N	0.42	2.28	19	1
1:A:65:PHE:N	1:A:66:PRO:HD2	0.42	2.30	18	3
1:A:19:PHE:CZ	1:A:35:VAL:HG11	0.42	2.49	4	1
1:A:145:MET:N	1:A:145:MET:SD	0.42	2.92	7	1
1:A:68:PHE:C	1:A:68:PHE:CD1	0.42	2.97	9	1
1:A:53:ASN:O	1:A:54:GLU:C	0.42	2.63	12	2
1:A:113:GLY:O	1:A:114:GLU:C	0.42	2.61	12	1
1:A:5:THR:CG2	1:A:6:GLU:N	0.42	2.82	3	1
1:A:108:VAL:O	1:A:109:MET:C	0.42	2.63	3	1
1:A:139:GLU:O	1:A:143:THR:OG1	0.42	2.36	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:9:ILE:HG22	2:B:10:ALA:N	0.42	2.29	16	6
1:A:93:ASP:OD2	1:A:95:ASP:OD1	0.42	2.37	10	1
1:A:131:ASP:CG	1:A:132:GLY:H	0.42	2.22	18	1
1:A:49:GLN:OE1	1:A:49:GLN:O	0.42	2.37	20	1
1:A:45:GLU:N	1:A:45:GLU:OE1	0.42	2.52	1	1
1:A:58:ASP:OD1	1:A:58:ASP:N	0.42	2.52	3	1
2:B:3:ARG:O	2:B:4:TRP:C	0.42	2.61	4	1
1:A:123:GLU:OE1	1:A:123:GLU:CA	0.42	2.65	10	2
1:A:129:ASP:OD1	1:A:131:ASP:OD1	0.42	2.38	7	1
1:A:82:GLU:C	1:A:82:GLU:CD	0.42	2.87	10	1
1:A:33:GLY:O	1:A:37:ARG:CB	0.42	2.68	11	2
1:A:50:ASP:O	1:A:51:MET:C	0.42	2.62	3	1
1:A:131:ASP:OD1	1:A:133:ASP:OD1	0.42	2.37	5	2
1:A:34:THR:OG1	1:A:35:VAL:N	0.42	2.53	5	1
1:A:87:GLU:OE1	1:A:87:GLU:N	0.42	2.53	10	1
1:A:137:ASN:OD1	1:A:137:ASN:C	0.42	2.63	10	1
1:A:137:ASN:ND2	1:A:137:ASN:N	0.42	2.68	12	1
1:A:42:ASN:C	1:A:44:THR:N	0.42	2.78	15	1
1:A:19:PHE:CE2	2:B:13:ALA:HB3	0.41	2.50	3	1
1:A:141:PHE:CD2	1:A:142:VAL:N	0.41	2.88	6	1
1:A:64:ASP:O	1:A:65:PHE:C	0.41	2.63	10	1
1:A:118:ASP:CG	1:A:119:GLU:N	0.41	2.78	2	1
1:A:89:PHE:CE2	1:A:138:TYR:CE1	0.41	3.09	3	1
1:A:95:ASP:OD2	1:A:104:GLU:OE2	0.41	2.37	4	1
1:A:107:HIS:CD2	1:A:107:HIS:C	0.41	2.98	6	1
1:A:22:ASP:CG	1:A:24:ASP:H	0.41	2.23	11	1
2:B:5:LYS:HB2	2:B:5:LYS:HZ2	0.41	1.75	13	1
1:A:142:VAL:O	1:A:142:VAL:CG1	0.41	2.68	20	1
1:A:117:THR:HG1	1:A:120:GLU:CD	0.41	2.22	2	1
1:A:41:GLN:C	1:A:42:ASN:CG	0.41	2.88	6	1
1:A:139:GLU:C	1:A:143:THR:HG1	0.41	2.20	7	1
1:A:101:SER:O	1:A:103:ALA:N	0.41	2.54	8	1
1:A:118:ASP:O	1:A:119:GLU:C	0.41	2.62	12	3
1:A:134:GLY:C	1:A:135:GLN:OE1	0.41	2.62	14	1
1:A:92:PHE:CZ	2:B:7:ASN:OD1	0.41	2.73	17	1
1:A:44:THR:C	1:A:45:GLU:OE1	0.41	2.63	1	1
2:B:10:ALA:O	2:B:13:ALA:HB3	0.41	2.15	7	1
1:A:91:VAL:HG23	1:A:92:PHE:H	0.41	1.73	8	1
1:A:125:ILE:O	1:A:129:ASP:CB	0.41	2.68	9	1
1:A:130:ILE:O	1:A:130:ILE:CG2	0.41	2.68	9	1
1:A:95:ASP:OD2	1:A:97:ASN:CG	0.41	2.63	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:ALA:O	1:A:129:ASP:C	0.41	2.63	19	1
1:A:117:THR:OG1	1:A:120:GLU:OE2	0.41	2.38	2	1
1:A:47:GLU:OE2	1:A:47:GLU:O	0.41	2.37	8	1
1:A:101:SER:C	1:A:103:ALA:N	0.41	2.78	8	1
1:A:97:ASN:O	1:A:98:GLY:O	0.41	2.38	10	1
1:A:12:PHE:O	1:A:12:PHE:CD1	0.41	2.73	12	1
1:A:42:ASN:C	1:A:44:THR:H	0.41	2.22	15	1
1:A:22:ASP:C	1:A:22:ASP:OD1	0.41	2.63	17	1
2:B:8:PHE:CD1	2:B:8:PHE:C	0.41	2.97	18	1
1:A:20:ASP:CG	1:A:22:ASP:OD2	0.41	2.63	19	1
1:A:20:ASP:OD2	1:A:22:ASP:OD2	0.41	2.39	2	2
2:B:7:ASN:O	2:B:11:VAL:HG23	0.41	2.15	6	1
1:A:130:ILE:HG23	1:A:131:ASP:N	0.41	2.30	7	1
1:A:115:LYS:O	1:A:116:LEU:C	0.41	2.63	8	1
1:A:31:GLU:O	1:A:34:THR:OG1	0.41	2.37	17	2
1:A:93:ASP:CG	1:A:95:ASP:OD1	0.41	2.64	10	1
1:A:84:GLU:O	2:B:15:ASN:ND2	0.41	2.54	12	1
1:A:93:ASP:OD1	1:A:93:ASP:C	0.41	2.62	15	1
1:A:95:ASP:OD1	1:A:104:GLU:OE2	0.41	2.38	1	1
1:A:129:ASP:OD1	1:A:135:GLN:O	0.41	2.39	1	1
1:A:52:ILE:O	1:A:55:VAL:HG22	0.41	2.16	3	1
2:B:10:ALA:O	2:B:11:VAL:C	0.41	2.63	4	2
1:A:132:GLY:O	1:A:133:ASP:C	0.41	2.64	14	1
1:A:20:ASP:OD1	1:A:22:ASP:OD2	0.41	2.39	9	1
1:A:63:ILE:N	1:A:63:ILE:HD13	0.41	2.31	11	1
1:A:18:LEU:C	1:A:20:ASP:H	0.41	2.22	18	1
1:A:107:HIS:O	1:A:111:ASN:OD1	0.41	2.38	16	2
1:A:117:THR:C	1:A:119:GLU:N	0.41	2.77	21	2
1:A:22:ASP:OD1	1:A:22:ASP:C	0.41	2.62	11	1
1:A:123:GLU:O	1:A:127:GLU:OE1	0.41	2.39	14	1
1:A:48:LEU:N	1:A:48:LEU:HD12	0.41	2.31	20	1
1:A:52:ILE:O	1:A:56:ASP:N	0.41	2.54	1	1
1:A:93:ASP:OD2	1:A:98:GLY:C	0.41	2.64	3	1
1:A:25:GLY:C	1:A:26:THR:CG2	0.41	2.94	4	1
1:A:95:ASP:O	1:A:97:ASN:OD1	0.41	2.38	8	1
1:A:89:PHE:CE1	1:A:141:PHE:CG	0.41	3.09	10	1
1:A:137:ASN:ND2	1:A:139:GLU:N	0.41	2.69	11	1
1:A:63:ILE:HD13	1:A:63:ILE:N	0.41	2.31	17	1
1:A:36:MET:CE	2:B:14:ALA:O	0.41	2.69	21	1
1:A:93:ASP:C	1:A:95:ASP:N	0.40	2.76	2	2
2:B:14:ALA:O	2:B:15:ASN:C	0.40	2.64	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:16:ARG:O	2:B:20:ILE:N	0.40	2.54	9	1
1:A:26:THR:CG2	1:A:62:THR:OG1	0.40	2.69	15	1
1:A:16:PHE:O	1:A:18:LEU:N	0.40	2.54	16	1
1:A:94:LYS:HB2	1:A:94:LYS:HZ3	0.40	1.76	20	1
1:A:97:ASN:OD1	1:A:104:GLU:OE2	0.40	2.39	12	1
1:A:56:ASP:O	1:A:57:ALA:C	0.40	2.65	1	1
1:A:82:GLU:CD	1:A:82:GLU:C	0.40	2.89	5	1
1:A:39:LEU:N	1:A:39:LEU:CD1	0.40	2.85	11	1
1:A:93:ASP:OD1	1:A:95:ASP:OD2	0.40	2.39	12	1
1:A:13:LYS:O	1:A:16:PHE:N	0.40	2.54	13	1
1:A:124:MET:O	1:A:125:ILE:C	0.40	2.64	18	1
1:A:32:LEU:HD13	2:B:17:PHE:CD2	0.40	2.51	21	1
1:A:32:LEU:HD23	1:A:48:LEU:CD1	0.40	2.47	6	1
1:A:97:ASN:CG	1:A:98:GLY:N	0.40	2.79	7	1
1:A:82:GLU:O	1:A:83:GLU:C	0.40	2.65	14	1
1:A:133:ASP:C	1:A:135:GLN:H	0.40	2.24	14	1
1:A:84:GLU:OE1	2:B:16:ARG:NH1	0.40	2.53	16	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	135/148 (91%)	93±22 (69±16%)	27±8 (20±6%)	7±3 (5±2%)	2	22
2	B	19/26 (73%)	14±4 (76±19%)	3±2 (14±8%)	1±1 (3±4%)	5	35
All	All	3031/3654 (83%)	2250 (74%)	617 (20%)	164 (5%)	2	22

All 54 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	43	PRO	13
1	A	40	GLY	12
1	A	23	GLY	8
1	A	41	GLN	8

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Mol	Chain	Res	Type	Models (Total)
1	A	95	ASP	7
1	A	112	LEU	6
1	A	117	THR	5
2	B	21	SER	5
1	A	5	THR	5
1	A	55	VAL	4
1	A	58	ASP	4
1	A	59	GLY	4
1	A	74	ARG	4
2	B	5	LYS	4
1	A	66	PRO	4
1	A	64	ASP	4
1	A	81	SER	4
1	A	96	GLY	4
1	A	131	ASP	4
1	A	132	GLY	4
1	A	104	GLU	4
1	A	106	ARG	3
1	A	54	GLU	2
1	A	113	GLY	2
1	A	44	THR	2
1	A	98	GLY	2
1	A	102	ALA	2
1	A	6	GLU	2
1	A	94	LYS	2
1	A	139	GLU	2
1	A	116	LEU	2
1	A	114	GLU	2
2	B	3	ARG	2
1	A	60	ASN	2
1	A	20	ASP	1
1	A	84	GLU	1
1	A	115	LYS	1
2	B	6	LYS	1
1	A	133	ASP	1
1	A	93	ASP	1
1	A	56	ASP	1
1	A	29	THR	1
1	A	34	THR	1
1	A	57	ALA	1
1	A	99	PHE	1
1	A	35	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	36	MET	1
1	A	127	GLU	1
1	A	25	GLY	1
1	A	24	ASP	1
1	A	122	ASP	1
2	B	17	PHE	1
1	A	118	ASP	1
1	A	140	GLU	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	115/127 (91%)	75±30 (65±26%)	22±10 (19±8%)	3	34
2	B	16/21 (76%)	10±4 (62±22%)	4±2 (26±12%)	2	23
All	All	2331/3108 (75%)	1775 (76%)	556 (24%)	2	26

All 113 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	9	ILE	17
2	B	20	ILE	16
1	A	44	THR	15
1	A	143	THR	13
1	A	52	ILE	13
1	A	39	LEU	12
1	A	118	ASP	11
1	A	22	ASP	11
1	A	101	SER	10
1	A	109	MET	10
1	A	38	SER	9
1	A	110	THR	9
1	A	112	LEU	9
1	A	131	ASP	9
1	A	87	GLU	8
1	A	99	PHE	8

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Mol	Chain	Res	Type	Models (Total)
1	A	111	ASN	8
2	B	6	LYS	8
2	B	19	LYS	8
1	A	133	ASP	7
2	B	7	ASN	7
2	B	12	SER	7
2	B	15	ASN	7
1	A	17	SER	7
1	A	41	GLN	7
1	A	105	LEU	7
1	A	42	ASN	7
1	A	123	GLU	7
1	A	24	ASP	7
1	A	34	THR	6
1	A	49	GLN	6
1	A	107	HIS	6
1	A	122	ASP	6
1	A	137	ASN	6
1	A	28	THR	6
1	A	65	PHE	6
1	A	144	MET	6
1	A	106	ARG	6
1	A	58	ASP	6
1	A	95	ASP	6
1	A	74	ARG	5
2	B	3	ARG	5
1	A	145	MET	5
1	A	26	THR	5
1	A	29	THR	5
1	A	50	ASP	5
1	A	117	THR	5
1	A	127	GLU	5
1	A	60	ASN	5
1	A	71	MET	5
1	A	31	GLU	4
1	A	94	LYS	4
1	A	21	LYS	4
1	A	97	ASN	4
1	A	116	LEU	4
1	A	126	ARG	4
1	A	138	TYR	4
1	A	8	GLN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	19	PHE	4
1	A	20	ASP	4
1	A	27	ILE	4
1	A	115	LYS	4
1	A	120	GLU	4
1	A	129	ASP	4
1	A	139	GLU	4
1	A	5	THR	4
2	B	17	PHE	4
1	A	32	LEU	4
1	A	55	VAL	4
1	A	108	VAL	4
1	A	7	GLU	4
1	A	125	ILE	4
1	A	48	LEU	4
1	A	142	VAL	3
2	B	18	LYS	3
1	A	12	PHE	3
1	A	53	ASN	3
1	A	81	SER	3
1	A	90	ARG	3
1	A	13	LYS	3
1	A	63	ILE	3
1	A	72	MET	3
1	A	70	THR	3
1	A	6	GLU	2
1	A	62	THR	2
1	A	104	GLU	2
1	A	114	GLU	2
2	B	21	SER	2
1	A	9	ILE	2
1	A	84	GLU	2
1	A	130	ILE	2
1	A	100	ILE	2
1	A	16	PHE	2
1	A	119	GLU	2
2	B	16	ARG	2
1	A	86	ARG	2
1	A	135	GLN	2
1	A	51	MET	1
1	A	89	PHE	1
1	A	36	MET	1

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Mol	Chain	Res	Type	Models (Total)
1	A	83	GLU	1
1	A	56	ASP	1
1	A	93	ASP	1
1	A	47	GLU	1
1	A	69	LEU	1
1	A	82	GLU	1
1	A	124	MET	1
1	A	45	GLU	1
1	A	136	VAL	1
2	B	5	LYS	1
1	A	54	GLU	1
1	A	11	GLU	1
1	A	30	LYS	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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