



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:26 AM BST

PDB ID : 2L2E
Title : Solution NMR structure of myristoylated NCS1p in apo form
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Deposited on : 2010-08-17

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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

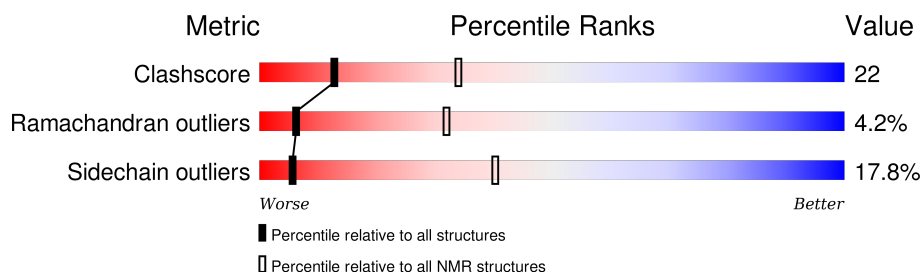
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	190	

2 Ensemble composition and analysis

This entry contains 15 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:9-A:138, A:145-A:190 (176)	0.72	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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 5, 6, 7, 8, 9, 13, 14
2	3, 10, 12, 15
Single-model clusters	11

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3088 atoms, of which 1530 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calcium-binding protein NCS-1.

Mol	Chain	Residues	Atoms						Trace
1	A	190	Total	C	H	N	O	S	0
			3088	1002	1530	249	299	8	

There is a discrepancy between the modelled and reference sequences:

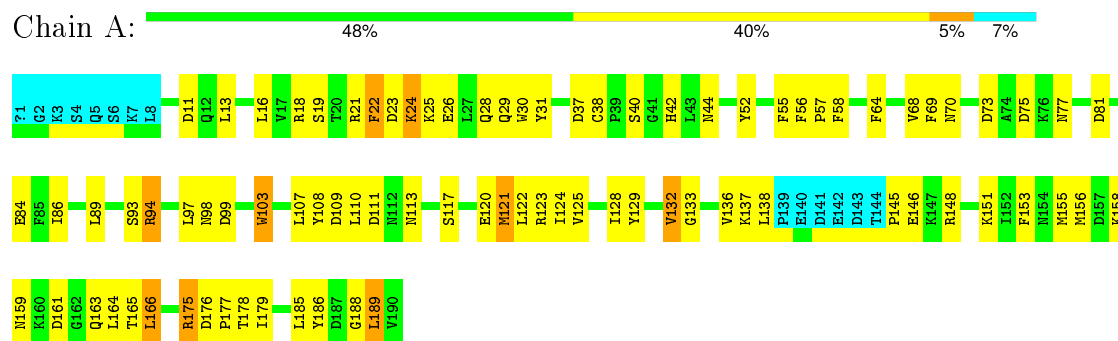
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MYR	-	INSERTION	UNP Q09711

4 Residue-property plots

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: Calcium-binding protein NCS-1

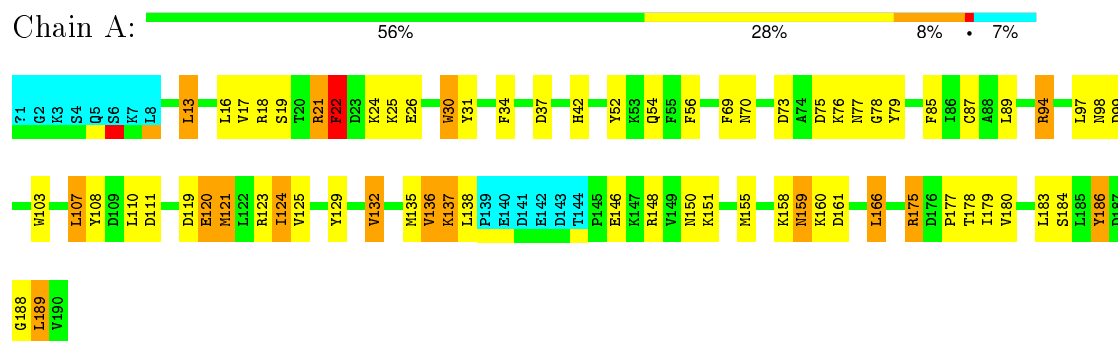


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

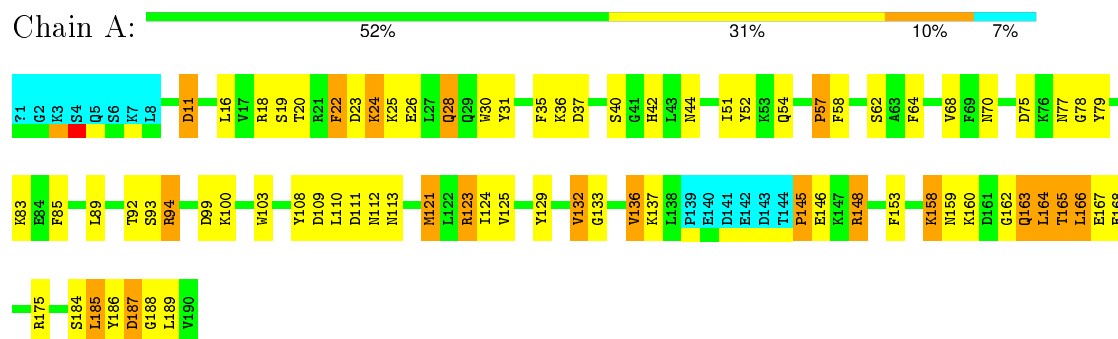
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Calcium-binding protein NCS-1



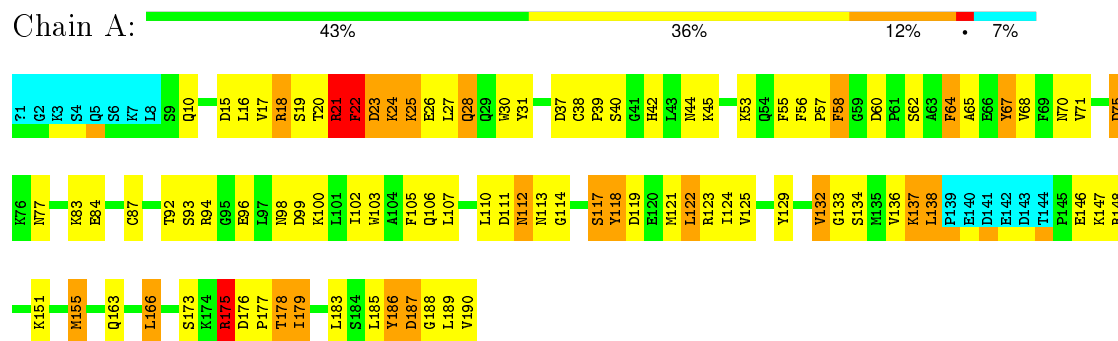
4.2.2 Score per residue for model 2

- Molecule 1: Calcium-binding protein NCS-1



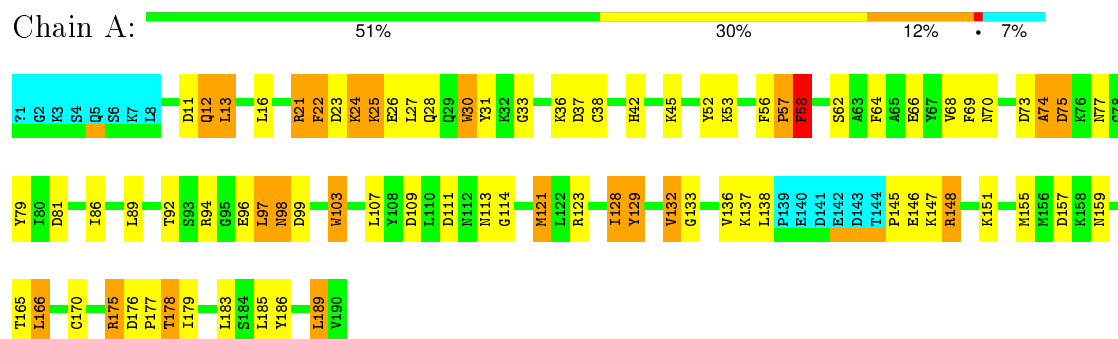
4.2.3 Score per residue for model 3

- Molecule 1: Calcium-binding protein NCS-1



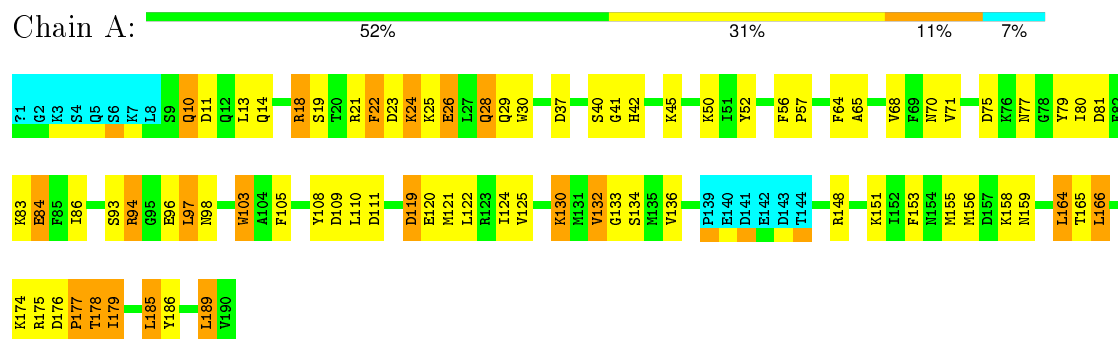
4.2.4 Score per residue for model 4

- Molecule 1: Calcium-binding protein NCS-1



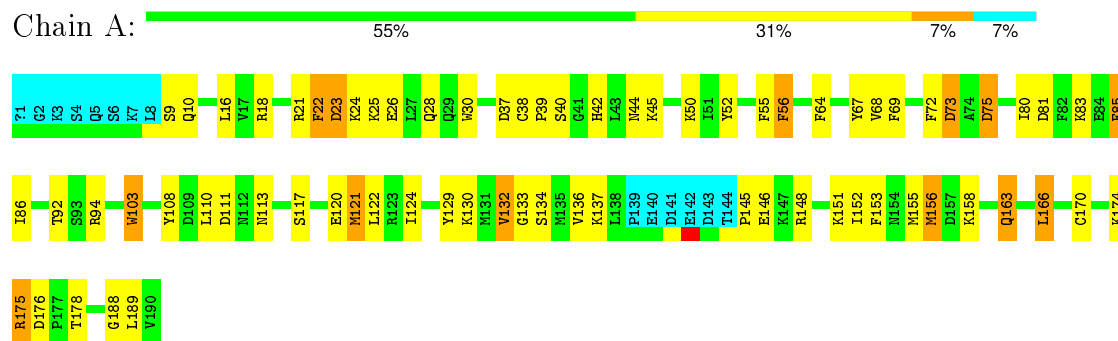
4.2.5 Score per residue for model 5

- Molecule 1: Calcium-binding protein NCS-1



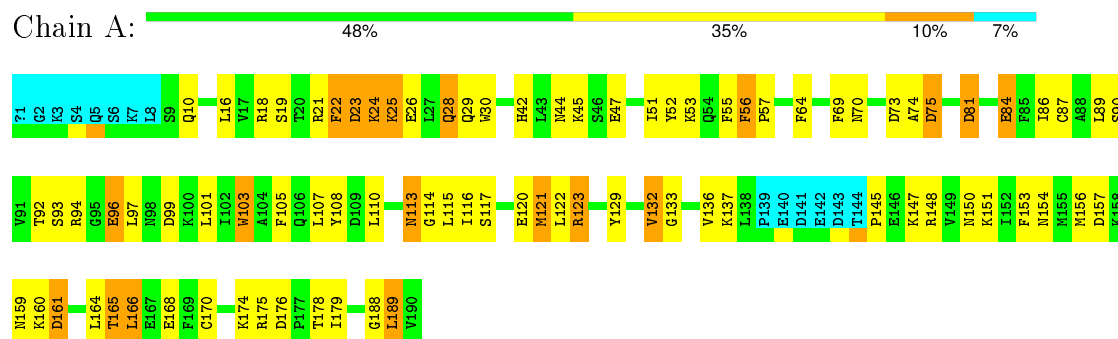
4.2.6 Score per residue for model 6

- Molecule 1: Calcium-binding protein NCS-1



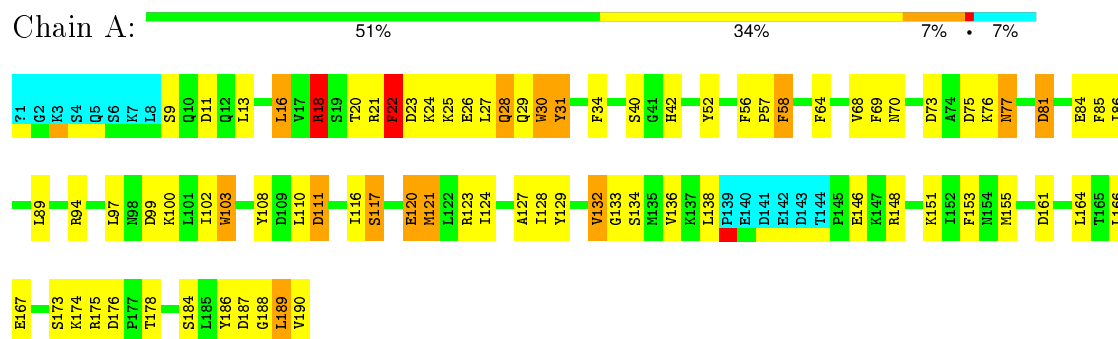
4.2.7 Score per residue for model 7

- Molecule 1: Calcium-binding protein NCS-1



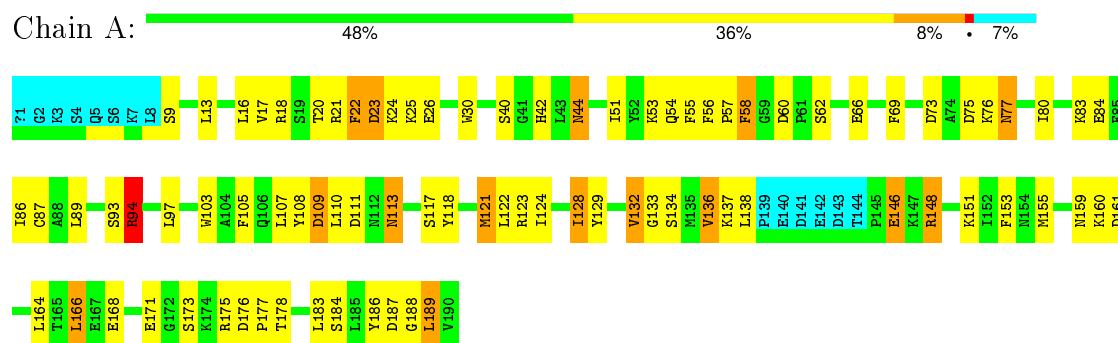
4.2.8 Score per residue for model 8

- Molecule 1: Calcium-binding protein NCS-1



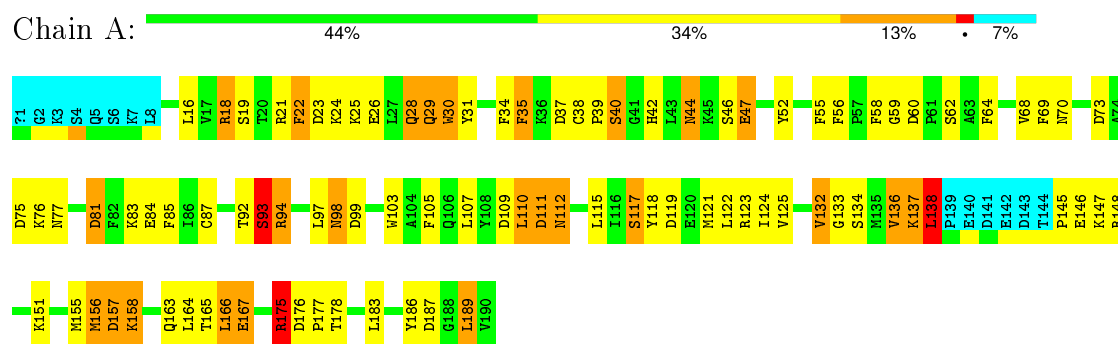
4.2.9 Score per residue for model 9

- Molecule 1: Calcium-binding protein NCS-1



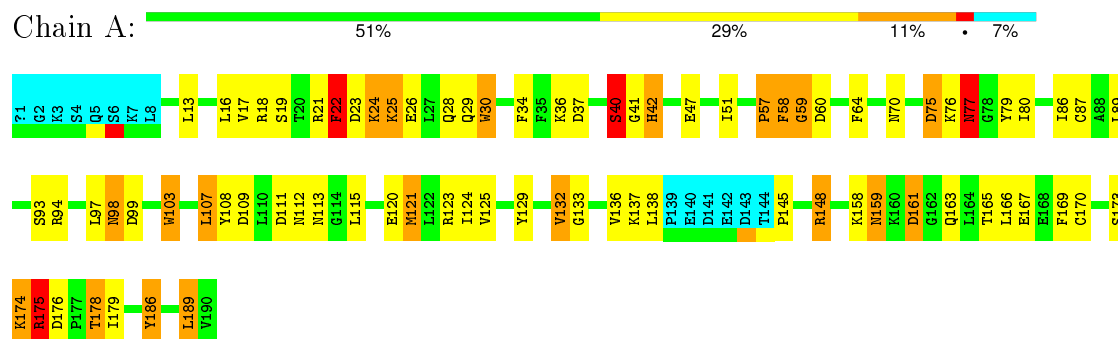
4.2.10 Score per residue for model 10

- Molecule 1: Calcium-binding protein NCS-1



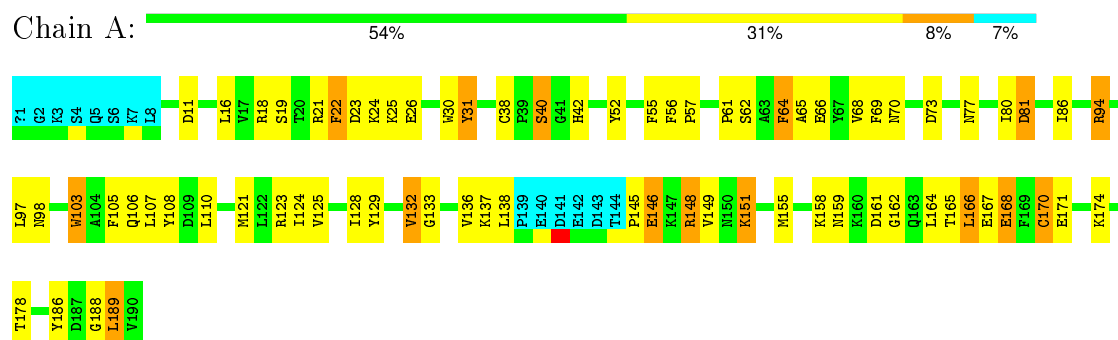
4.2.11 Score per residue for model 11

- Molecule 1: Calcium-binding protein NCS-1



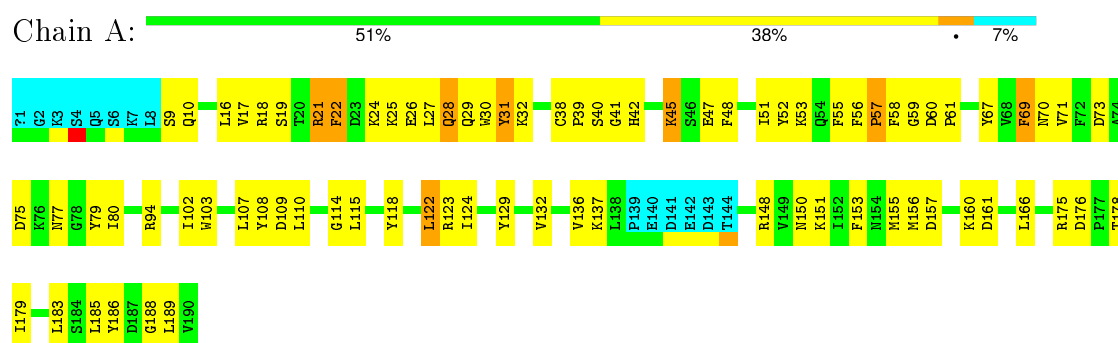
4.2.12 Score per residue for model 12

- Molecule 1: Calcium-binding protein NCS-1



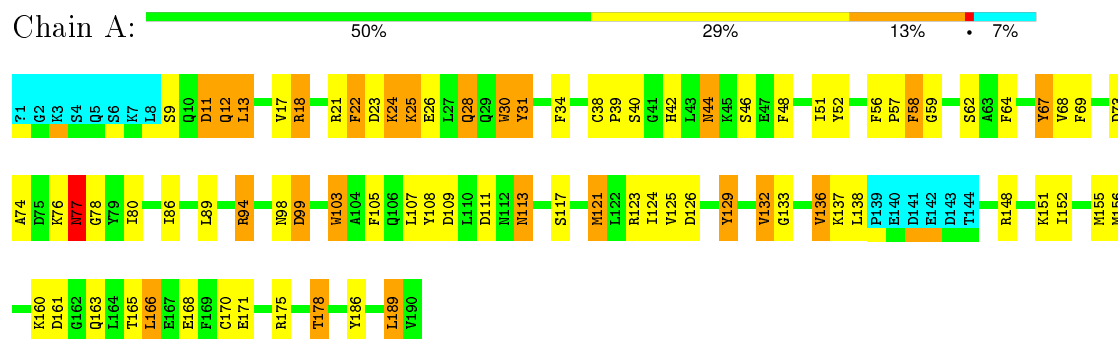
4.2.13 Score per residue for model 13

- Molecule 1: Calcium-binding protein NCS-1



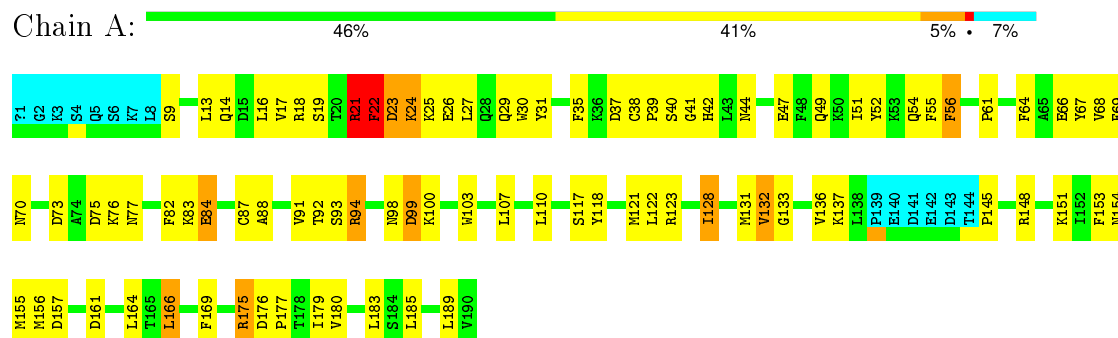
4.2.14 Score per residue for model 14

- Molecule 1: Calcium-binding protein NCS-1



4.2.15 Score per residue for model 15

- Molecule 1: Calcium-binding protein NCS-1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 40 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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

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

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	0.98±0.00	3±0/1476 (0.2±0.0%)	1.21±0.00	13±1/1982 (0.7±0.0%)
All	All	0.98	45/22140 (0.2%)	1.21	199/29730 (0.7%)

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	5.3±0.6
All	All	0	80

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	103	TRP	CG-CD2	-7.42	1.31	1.43	11	15
1	A	30	TRP	CG-CD2	-7.31	1.31	1.43	6	15
1	A	42	HIS	CG-ND1	-6.21	1.25	1.38	3	15

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	103	TRP	NE1-CE2-CZ2	9.38	140.72	130.40	11	15
1	A	30	TRP	NE1-CE2-CZ2	9.11	140.42	130.40	8	15
1	A	103	TRP	NE1-CE2-CD2	-7.74	99.56	107.30	15	15
1	A	30	TRP	NE1-CE2-CD2	-7.59	99.71	107.30	8	15
1	A	30	TRP	CG-CD1-NE1	-6.55	103.55	110.10	6	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	103	TRP	CG-CD1-NE1	-6.52	103.58	110.10	13	15
1	A	103	TRP	CG-CD2-CE3	-6.26	128.26	133.90	11	15
1	A	30	TRP	CD1-CG-CD2	6.24	111.29	106.30	13	15
1	A	103	TRP	CD1-CG-CD2	6.19	111.25	106.30	11	15
1	A	30	TRP	CG-CD2-CE3	-5.95	128.54	133.90	8	14
1	A	30	TRP	CD1-NE1-CE2	5.77	114.19	109.00	15	15
1	A	103	TRP	CD1-NE1-CE2	5.75	114.17	109.00	15	15
1	A	103	TRP	CE2-CD2-CG	5.44	111.65	107.30	3	15
1	A	30	TRP	CE2-CD2-CG	5.14	111.42	107.30	8	5

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	148	ARG	Sidechain	14
1	A	94	ARG	Sidechain	14
1	A	21	ARG	Sidechain	13
1	A	175	ARG	Sidechain	13
1	A	123	ARG	Sidechain	13
1	A	18	ARG	Sidechain	13

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	1444	1411	1411	62±9
All	All	21660	21165	21165	931

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:87:CYS:SG	1:A:107:LEU:HD13	0.85	2.10	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:TYR:CE1	1:A:56:PHE:CG	0.78	2.70	14	1
1:A:98:ASN:ND2	1:A:99:ASP:N	0.77	2.33	4	4
1:A:27:LEU:CD1	1:A:55:PHE:CE2	0.76	2.68	3	1
1:A:115:LEU:HD13	1:A:115:LEU:C	0.75	2.02	7	1
1:A:58:PHE:CD2	1:A:59:GLY:N	0.75	2.54	14	2
1:A:16:LEU:O	1:A:16:LEU:HD13	0.73	1.83	6	2
1:A:22:PHE:CD1	1:A:23:ASP:N	0.72	2.57	3	2
1:A:86:ILE:HG22	1:A:103:TRP:HE1	0.72	1.43	6	8
1:A:156:MET:SD	1:A:175:ARG:NH1	0.72	2.63	13	1
1:A:163:GLN:N	1:A:163:GLN:NE2	0.71	2.37	6	2
1:A:153:PHE:CZ	1:A:164:LEU:HD12	0.70	2.21	8	2
1:A:185:LEU:HD23	1:A:185:LEU:O	0.70	1.86	15	1
1:A:118:TYR:CE1	1:A:122:LEU:HD23	0.69	2.22	3	1
1:A:153:PHE:CZ	1:A:164:LEU:HD11	0.69	2.22	9	2
1:A:163:GLN:N	1:A:163:GLN:HE21	0.69	1.85	6	1
1:A:94:ARG:CD	1:A:94:ARG:H	0.69	2.01	10	1
1:A:52:TYR:CE2	1:A:56:PHE:CZ	0.68	2.81	1	1
1:A:67:TYR:O	1:A:71:VAL:HG23	0.68	1.89	3	1
1:A:12:GLN:HE21	1:A:12:GLN:N	0.68	1.86	14	1
1:A:73:ASP:OD1	1:A:74:ALA:N	0.68	2.27	14	1
1:A:185:LEU:HD12	1:A:185:LEU:C	0.68	2.08	4	1
1:A:183:LEU:HD23	1:A:183:LEU:O	0.67	1.88	3	1
1:A:88:ALA:O	1:A:91:VAL:HG22	0.67	1.89	15	1
1:A:27:LEU:HD12	1:A:55:PHE:CZ	0.67	2.24	15	2
1:A:22:PHE:CG	1:A:23:ASP:N	0.67	2.61	11	7
1:A:56:PHE:CD1	1:A:56:PHE:N	0.67	2.59	15	3
1:A:132:VAL:CG2	1:A:133:GLY:N	0.66	2.58	9	1
1:A:166:LEU:HD13	1:A:167:GLU:N	0.66	2.04	8	2
1:A:13:LEU:HD11	1:A:186:TYR:OH	0.66	1.90	4	1
1:A:152:ILE:HG22	1:A:156:MET:SD	0.66	2.31	6	2
1:A:30:TRP:CZ2	1:A:34:PHE:CG	0.66	2.83	8	1
1:A:58:PHE:CG	1:A:59:GLY:N	0.66	2.64	14	1
1:A:129:TYR:CD1	1:A:129:TYR:C	0.65	2.69	14	4
1:A:12:GLN:HE21	1:A:12:GLN:CA	0.65	2.04	14	1
1:A:22:PHE:C	1:A:22:PHE:CD1	0.65	2.70	5	8
1:A:31:TYR:CD1	1:A:31:TYR:C	0.65	2.69	13	3
1:A:136:VAL:HG22	1:A:137:LYS:N	0.65	2.07	15	8
1:A:16:LEU:HD13	1:A:16:LEU:C	0.65	2.12	1	2
1:A:156:MET:CG	1:A:157:ASP:N	0.64	2.59	10	1
1:A:64:PHE:O	1:A:68:VAL:HG23	0.64	1.92	3	8
1:A:83:LYS:CG	1:A:84:GLU:N	0.64	2.60	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:ASP:O	1:A:74:ALA:HB3	0.64	1.93	14	1
1:A:84:GLU:OE1	1:A:127:ALA:HB2	0.64	1.92	8	1
1:A:94:ARG:NE	1:A:94:ARG:C	0.64	2.51	9	1
1:A:132:VAL:CG1	1:A:138:LEU:HD21	0.64	2.23	14	2
1:A:113:ASN:ND2	1:A:113:ASN:H	0.64	1.89	9	1
1:A:98:ASN:CG	1:A:99:ASP:N	0.64	2.50	10	2
1:A:136:VAL:CG2	1:A:137:LYS:N	0.63	2.62	12	12
1:A:16:LEU:O	1:A:20:THR:HG23	0.63	1.94	3	2
1:A:108:TYR:CD2	1:A:120:GLU:CD	0.62	2.72	1	1
1:A:185:LEU:HD12	1:A:186:TYR:N	0.62	2.09	4	1
1:A:129:TYR:CE2	1:A:138:LEU:HD22	0.62	2.29	14	2
1:A:31:TYR:CE1	1:A:35:PHE:CE1	0.62	2.87	15	1
1:A:22:PHE:CD1	1:A:22:PHE:C	0.62	2.71	8	6
1:A:153:PHE:CE1	1:A:164:LEU:HD11	0.62	2.29	9	2
1:A:69:PHE:CG	1:A:73:ASP:OD2	0.62	2.53	14	1
1:A:146:GLU:CG	1:A:147:LYS:N	0.62	2.63	3	2
1:A:108:TYR:CE2	1:A:120:GLU:OE2	0.62	2.53	1	1
1:A:167:GLU:CD	1:A:167:GLU:H	0.61	1.95	10	1
1:A:166:LEU:C	1:A:166:LEU:HD13	0.61	2.15	8	2
1:A:175:ARG:CG	1:A:175:ARG:HH11	0.61	2.07	10	1
1:A:93:SER:OG	1:A:94:ARG:N	0.61	2.33	5	3
1:A:117:SER:N	1:A:120:GLU:OE1	0.61	2.34	6	1
1:A:69:PHE:CE2	1:A:73:ASP:OD2	0.61	2.53	1	2
1:A:98:ASN:ND2	1:A:99:ASP:OD2	0.61	2.33	4	1
1:A:108:TYR:CE1	1:A:120:GLU:OE1	0.61	2.54	7	1
1:A:98:ASN:ND2	1:A:99:ASP:CG	0.61	2.54	4	1
1:A:187:ASP:OD1	1:A:187:ASP:N	0.60	2.33	3	4
1:A:13:LEU:O	1:A:17:VAL:HG23	0.60	1.95	15	4
1:A:30:TRP:CH2	1:A:34:PHE:CD2	0.60	2.89	1	1
1:A:81:ASP:N	1:A:81:ASP:OD1	0.60	2.34	8	2
1:A:107:LEU:O	1:A:107:LEU:HD23	0.60	1.96	13	2
1:A:167:GLU:CD	1:A:167:GLU:N	0.59	2.56	10	1
1:A:69:PHE:CD2	1:A:73:ASP:OD2	0.59	2.55	1	3
1:A:16:LEU:C	1:A:16:LEU:HD13	0.59	2.18	3	1
1:A:163:GLN:H	1:A:163:GLN:HE21	0.59	1.38	6	1
1:A:52:TYR:C	1:A:52:TYR:CD1	0.59	2.75	5	4
1:A:21:ARG:O	1:A:22:PHE:CG	0.59	2.56	1	1
1:A:98:ASN:HD22	1:A:99:ASP:N	0.59	1.95	11	2
1:A:19:SER:CB	1:A:64:PHE:CE1	0.59	2.86	11	1
1:A:105:PHE:CE2	1:A:166:LEU:N	0.59	2.71	14	1
1:A:129:TYR:CZ	1:A:138:LEU:CD2	0.59	2.85	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ASP:CG	1:A:12:GLN:N	0.58	2.57	4	1
1:A:30:TRP:CH2	1:A:34:PHE:CG	0.58	2.91	10	3
1:A:58:PHE:CD1	1:A:58:PHE:N	0.58	2.65	4	1
1:A:23:ASP:N	1:A:23:ASP:OD1	0.58	2.35	6	2
1:A:184:SER:OG	1:A:185:LEU:N	0.58	2.35	2	1
1:A:11:ASP:OD1	1:A:11:ASP:N	0.58	2.36	2	1
1:A:111:ASP:OD1	1:A:111:ASP:N	0.58	2.36	8	1
1:A:24:LYS:CG	1:A:25:LYS:N	0.58	2.67	5	5
1:A:24:LYS:CG	1:A:25:LYS:H	0.58	2.11	1	5
1:A:22:PHE:CE1	1:A:23:ASP:O	0.58	2.57	15	4
1:A:185:LEU:C	1:A:185:LEU:HD12	0.58	2.19	3	1
1:A:96:GLU:CD	1:A:96:GLU:H	0.58	2.02	3	2
1:A:52:TYR:CZ	1:A:56:PHE:CG	0.57	2.92	4	2
1:A:132:VAL:CG1	1:A:133:GLY:N	0.57	2.67	10	12
1:A:75:ASP:CG	1:A:77:ASN:ND2	0.57	2.57	8	1
1:A:189:LEU:HD12	1:A:189:LEU:C	0.57	2.19	15	8
1:A:60:ASP:N	1:A:60:ASP:OD1	0.57	2.37	10	1
1:A:52:TYR:CD1	1:A:52:TYR:C	0.57	2.78	13	1
1:A:79:TYR:C	1:A:79:TYR:CD1	0.57	2.77	4	2
1:A:55:PHE:C	1:A:56:PHE:CD1	0.57	2.78	9	2
1:A:16:LEU:HD13	1:A:16:LEU:O	0.56	2.00	1	1
1:A:163:GLN:CD	1:A:163:GLN:N	0.56	2.58	3	1
1:A:86:ILE:HG22	1:A:103:TRP:NE1	0.56	2.15	6	3
1:A:58:PHE:O	1:A:58:PHE:CG	0.56	2.58	8	2
1:A:186:TYR:O	1:A:186:TYR:CG	0.56	2.58	5	1
1:A:121:MET:C	1:A:121:MET:SD	0.56	2.84	2	4
1:A:58:PHE:O	1:A:58:PHE:CD2	0.56	2.59	3	1
1:A:73:ASP:OD1	1:A:80:ILE:CG2	0.56	2.53	6	1
1:A:128:ILE:HD12	1:A:128:ILE:N	0.56	2.16	12	1
1:A:119:ASP:OD1	1:A:120:GLU:N	0.56	2.38	1	2
1:A:189:LEU:HD12	1:A:189:LEU:O	0.56	2.01	13	2
1:A:22:PHE:CE2	1:A:89:LEU:CD2	0.56	2.89	14	1
1:A:31:TYR:CD2	1:A:86:ILE:CD1	0.56	2.89	12	1
1:A:21:ARG:O	1:A:22:PHE:CD2	0.56	2.58	15	1
1:A:115:LEU:HD13	1:A:116:ILE:N	0.55	2.16	7	1
1:A:162:GLY:C	1:A:163:GLN:HE21	0.55	2.05	2	1
1:A:44:ASN:N	1:A:44:ASN:OD1	0.55	2.39	2	2
1:A:118:TYR:CD1	1:A:118:TYR:C	0.55	2.80	9	2
1:A:115:LEU:CD1	1:A:115:LEU:C	0.55	2.74	7	1
1:A:121:MET:CE	1:A:169:PHE:CE1	0.55	2.90	15	1
1:A:75:ASP:O	1:A:77:ASN:N	0.55	2.40	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:PHE:CE2	1:A:23:ASP:O	0.55	2.60	14	11
1:A:10:GLN:CD	1:A:10:GLN:N	0.55	2.60	13	1
1:A:189:LEU:O	1:A:189:LEU:HD12	0.55	2.02	3	1
1:A:55:PHE:O	1:A:56:PHE:CG	0.54	2.61	10	3
1:A:22:PHE:CD2	1:A:23:ASP:O	0.54	2.61	3	6
1:A:79:TYR:CD1	1:A:79:TYR:N	0.54	2.76	11	1
1:A:166:LEU:CD2	1:A:166:LEU:C	0.54	2.75	6	4
1:A:189:LEU:C	1:A:189:LEU:HD12	0.54	2.23	13	6
1:A:38:CYS:C	1:A:40:SER:H	0.54	2.05	3	7
1:A:52:TYR:CE1	1:A:56:PHE:CD1	0.54	2.96	14	1
1:A:58:PHE:O	1:A:60:ASP:N	0.54	2.41	11	1
1:A:108:TYR:CD2	1:A:124:ILE:CG1	0.54	2.90	2	2
1:A:113:ASN:CG	1:A:114:GLY:N	0.54	2.61	7	1
1:A:52:TYR:CD1	1:A:56:PHE:CD1	0.54	2.95	14	1
1:A:52:TYR:CD1	1:A:52:TYR:O	0.54	2.61	15	3
1:A:113:ASN:OD1	1:A:114:GLY:N	0.54	2.41	4	2
1:A:75:ASP:OD1	1:A:75:ASP:N	0.54	2.41	6	1
1:A:128:ILE:HD13	1:A:128:ILE:N	0.54	2.18	15	3
1:A:186:TYR:CG	1:A:186:TYR:O	0.54	2.60	13	5
1:A:19:SER:O	1:A:56:PHE:CE1	0.54	2.61	10	1
1:A:31:TYR:C	1:A:31:TYR:CD1	0.54	2.79	8	1
1:A:186:TYR:CD2	1:A:186:TYR:O	0.54	2.61	10	6
1:A:109:ASP:C	1:A:111:ASP:H	0.54	2.05	5	3
1:A:166:LEU:C	1:A:166:LEU:CD2	0.54	2.77	14	8
1:A:98:ASN:HD21	1:A:99:ASP:CG	0.54	2.06	4	1
1:A:17:VAL:HG21	1:A:186:TYR:OH	0.53	2.03	3	1
1:A:129:TYR:C	1:A:129:TYR:CD1	0.53	2.81	7	3
1:A:146:GLU:N	1:A:146:GLU:OE1	0.53	2.42	9	1
1:A:176:ASP:O	1:A:178:THR:N	0.53	2.42	13	7
1:A:40:SER:O	1:A:42:HIS:N	0.53	2.41	11	1
1:A:124:ILE:HG22	1:A:125:VAL:N	0.53	2.18	1	8
1:A:73:ASP:O	1:A:75:ASP:N	0.53	2.41	4	1
1:A:75:ASP:O	1:A:77:ASN:ND2	0.53	2.41	15	1
1:A:56:PHE:O	1:A:58:PHE:N	0.53	2.42	13	1
1:A:21:ARG:O	1:A:22:PHE:CB	0.53	2.57	1	2
1:A:81:ASP:OD1	1:A:81:ASP:N	0.53	2.39	7	2
1:A:98:ASN:OD1	1:A:99:ASP:N	0.53	2.42	15	3
1:A:22:PHE:CD1	1:A:23:ASP:O	0.53	2.62	15	1
1:A:28:GLN:C	1:A:28:GLN:CD	0.53	2.67	13	5
1:A:186:TYR:CE1	1:A:189:LEU:HD21	0.53	2.39	10	1
1:A:69:PHE:O	1:A:73:ASP:N	0.53	2.41	13	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ASP:OD2	1:A:115:LEU:N	0.53	2.41	13	1
1:A:24:LYS:O	1:A:27:LEU:N	0.53	2.41	3	5
1:A:111:ASP:OD2	1:A:113:ASN:ND2	0.53	2.42	11	1
1:A:96:GLU:N	1:A:96:GLU:CD	0.53	2.62	5	2
1:A:27:LEU:CD1	1:A:55:PHE:CZ	0.53	2.92	3	1
1:A:159:ASN:C	1:A:161:ASP:H	0.53	2.08	7	3
1:A:73:ASP:O	1:A:74:ALA:CB	0.53	2.57	14	1
1:A:11:ASP:OD1	1:A:12:GLN:N	0.53	2.42	4	1
1:A:24:LYS:O	1:A:26:GLU:N	0.52	2.42	12	14
1:A:24:LYS:C	1:A:26:GLU:N	0.52	2.62	3	15
1:A:108:TYR:CE1	1:A:124:ILE:CG1	0.52	2.92	11	3
1:A:49:GLN:NE2	1:A:61:PRO:O	0.52	2.42	15	1
1:A:107:LEU:HD23	1:A:107:LEU:C	0.52	2.24	13	4
1:A:56:PHE:C	1:A:58:PHE:H	0.52	2.07	13	2
1:A:159:ASN:O	1:A:161:ASP:N	0.52	2.42	1	3
1:A:151:LYS:O	1:A:155:MET:N	0.52	2.42	15	12
1:A:96:GLU:OE1	1:A:96:GLU:N	0.52	2.43	7	1
1:A:108:TYR:CE2	1:A:120:GLU:CD	0.52	2.82	1	1
1:A:19:SER:O	1:A:56:PHE:CE2	0.52	2.63	15	1
1:A:155:MET:SD	1:A:176:ASP:OD1	0.52	2.67	15	1
1:A:22:PHE:CZ	1:A:23:ASP:O	0.52	2.62	6	5
1:A:52:TYR:CE1	1:A:56:PHE:CD2	0.52	2.98	14	1
1:A:129:TYR:CD1	1:A:129:TYR:O	0.52	2.62	8	1
1:A:177:PRO:O	1:A:180:VAL:N	0.52	2.42	15	2
1:A:31:TYR:CD1	1:A:32:LYS:N	0.52	2.78	13	1
1:A:185:LEU:C	1:A:185:LEU:CD1	0.52	2.78	4	2
1:A:18:ARG:CZ	1:A:18:ARG:CB	0.52	2.88	8	1
1:A:44:ASN:OD1	1:A:44:ASN:N	0.52	2.43	14	1
1:A:159:ASN:C	1:A:161:ASP:N	0.51	2.63	1	4
1:A:73:ASP:C	1:A:75:ASP:N	0.51	2.63	4	1
1:A:45:LYS:NZ	1:A:65:ALA:HB1	0.51	2.20	5	1
1:A:173:SER:C	1:A:175:ARG:H	0.51	2.09	11	2
1:A:86:ILE:CG2	1:A:103:TRP:HE1	0.51	2.17	8	2
1:A:27:LEU:O	1:A:31:TYR:N	0.51	2.41	3	1
1:A:22:PHE:O	1:A:22:PHE:CD1	0.51	2.64	13	1
1:A:112:ASN:N	1:A:112:ASN:ND2	0.51	2.59	10	1
1:A:121:MET:O	1:A:121:MET:SD	0.51	2.69	2	5
1:A:31:TYR:O	1:A:31:TYR:CD1	0.51	2.63	1	2
1:A:74:ALA:O	1:A:75:ASP:CB	0.51	2.59	4	2
1:A:175:ARG:NH1	1:A:175:ARG:CG	0.51	2.73	10	1
1:A:105:PHE:CE1	1:A:166:LEU:N	0.51	2.79	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:ASP:O	1:A:163:GLN:NE2	0.51	2.44	14	1
1:A:96:GLU:O	1:A:98:ASN:N	0.51	2.43	5	1
1:A:94:ARG:CD	1:A:94:ARG:N	0.51	2.68	10	1
1:A:184:SER:C	1:A:186:TYR:H	0.51	2.09	8	4
1:A:118:TYR:CE1	1:A:122:LEU:CD2	0.51	2.94	3	1
1:A:28:GLN:CD	1:A:28:GLN:C	0.51	2.69	14	1
1:A:31:TYR:OH	1:A:110:LEU:HD13	0.51	2.06	10	2
1:A:165:THR:OG1	1:A:168:GLU:CG	0.51	2.59	7	1
1:A:22:PHE:CZ	1:A:89:LEU:HD21	0.51	2.41	11	5
1:A:56:PHE:N	1:A:57:PRO:HD3	0.50	2.21	9	4
1:A:19:SER:O	1:A:56:PHE:CD1	0.50	2.63	12	2
1:A:62:SER:O	1:A:65:ALA:HB3	0.50	2.06	3	1
1:A:28:GLN:NE2	1:A:28:GLN:O	0.50	2.44	3	1
1:A:119:ASP:CG	1:A:120:GLU:N	0.50	2.64	5	1
1:A:117:SER:O	1:A:119:ASP:N	0.50	2.44	3	2
1:A:75:ASP:C	1:A:77:ASN:N	0.50	2.65	15	4
1:A:96:GLU:CD	1:A:96:GLU:N	0.50	2.63	3	1
1:A:72:PHE:C	1:A:73:ASP:OD1	0.50	2.50	6	1
1:A:120:GLU:CD	1:A:120:GLU:N	0.50	2.64	11	1
1:A:52:TYR:CD2	1:A:56:PHE:CE1	0.50	2.99	15	1
1:A:60:ASP:N	1:A:61:PRO:HD3	0.50	2.22	13	1
1:A:176:ASP:C	1:A:178:THR:H	0.50	2.10	10	2
1:A:113:ASN:ND2	1:A:114:GLY:H	0.50	2.03	7	1
1:A:129:TYR:CE2	1:A:138:LEU:CD2	0.50	2.95	3	3
1:A:77:ASN:N	1:A:77:ASN:OD1	0.50	2.42	14	1
1:A:86:ILE:HD12	1:A:86:ILE:N	0.50	2.22	9	1
1:A:110:LEU:CD1	1:A:110:LEU:N	0.50	2.75	9	1
1:A:52:TYR:CE2	1:A:56:PHE:CE2	0.50	3.00	1	1
1:A:176:ASP:HB3	1:A:179:ILE:HD11	0.49	1.84	5	1
1:A:47:GLU:O	1:A:51:ILE:HD13	0.49	2.06	11	4
1:A:111:ASP:N	1:A:111:ASP:OD1	0.49	2.45	10	3
1:A:40:SER:C	1:A:42:HIS:N	0.49	2.65	11	1
1:A:111:ASP:O	1:A:113:ASN:ND2	0.49	2.44	2	3
1:A:128:ILE:H	1:A:128:ILE:HD12	0.49	1.67	12	1
1:A:163:GLN:N	1:A:163:GLN:OE1	0.49	2.45	10	1
1:A:158:LYS:NZ	1:A:168:GLU:OE1	0.49	2.44	2	1
1:A:108:TYR:C	1:A:109:ASP:OD1	0.49	2.51	9	1
1:A:121:MET:SD	1:A:121:MET:O	0.49	2.70	9	2
1:A:96:GLU:H	1:A:96:GLU:CD	0.49	2.11	5	1
1:A:48:PHE:CD1	1:A:48:PHE:C	0.49	2.86	14	2
1:A:99:ASP:OD1	1:A:99:ASP:N	0.49	2.46	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:ASP:C	1:A:75:ASP:H	0.49	2.11	4	1
1:A:58:PHE:CD2	1:A:58:PHE:O	0.49	2.66	8	1
1:A:99:ASP:HA	1:A:102:ILE:HD12	0.49	1.84	8	1
1:A:30:TRP:CZ2	1:A:34:PHE:CD1	0.49	3.01	10	2
1:A:52:TYR:CE1	1:A:56:PHE:CB	0.49	2.96	4	1
1:A:120:GLU:OE1	1:A:120:GLU:N	0.49	2.46	8	1
1:A:105:PHE:CD1	1:A:105:PHE:C	0.49	2.86	5	2
1:A:173:SER:O	1:A:176:ASP:N	0.49	2.42	8	1
1:A:173:SER:C	1:A:175:ARG:N	0.48	2.65	11	2
1:A:21:ARG:O	1:A:22:PHE:CD1	0.48	2.66	1	1
1:A:176:ASP:CB	1:A:179:ILE:HD12	0.48	2.38	15	1
1:A:84:GLU:OE1	1:A:84:GLU:N	0.48	2.46	5	3
1:A:186:TYR:CE1	1:A:189:LEU:CD2	0.48	2.96	10	1
1:A:18:ARG:NH2	1:A:58:PHE:O	0.48	2.46	10	1
1:A:173:SER:O	1:A:175:ARG:N	0.48	2.47	11	2
1:A:79:TYR:O	1:A:79:TYR:CD1	0.48	2.66	1	1
1:A:105:PHE:C	1:A:107:LEU:N	0.48	2.67	10	1
1:A:108:TYR:CE2	1:A:124:ILE:CG1	0.48	2.96	8	3
1:A:118:TYR:CZ	1:A:122:LEU:HD23	0.48	2.43	13	1
1:A:109:ASP:C	1:A:109:ASP:OD1	0.48	2.50	10	2
1:A:109:ASP:OD1	1:A:113:ASN:N	0.48	2.44	14	1
1:A:40:SER:OG	1:A:41:GLY:N	0.48	2.46	13	3
1:A:84:GLU:N	1:A:84:GLU:CD	0.48	2.67	10	1
1:A:186:TYR:C	1:A:186:TYR:CD1	0.48	2.86	11	1
1:A:112:ASN:HD22	1:A:112:ASN:N	0.48	2.06	10	1
1:A:87:CYS:SG	1:A:107:LEU:HD22	0.48	2.49	7	1
1:A:153:PHE:CZ	1:A:164:LEU:CD1	0.48	2.95	8	3
1:A:57:PRO:C	1:A:58:PHE:CG	0.48	2.86	4	1
1:A:60:ASP:OD1	1:A:60:ASP:N	0.47	2.45	3	1
1:A:51:ILE:HD13	1:A:51:ILE:N	0.47	2.22	9	2
1:A:25:LYS:NZ	1:A:25:LYS:CB	0.47	2.77	4	1
1:A:91:VAL:HG23	1:A:92:THR:HG23	0.47	1.86	15	1
1:A:158:LYS:NZ	1:A:163:GLN:O	0.47	2.47	10	1
1:A:163:GLN:OE1	1:A:163:GLN:N	0.47	2.47	14	1
1:A:98:ASN:HD22	1:A:99:ASP:H	0.47	1.51	4	1
1:A:77:ASN:HD22	1:A:77:ASN:N	0.47	2.07	4	1
1:A:52:TYR:CZ	1:A:56:PHE:CD2	0.47	3.02	4	1
1:A:146:GLU:HG3	1:A:147:LYS:N	0.47	2.24	4	2
1:A:38:CYS:O	1:A:38:CYS:SG	0.47	2.72	13	2
1:A:137:LYS:O	1:A:138:LEU:C	0.47	2.53	10	2
1:A:38:CYS:O	1:A:40:SER:N	0.47	2.47	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:MET:HG3	1:A:157:ASP:N	0.47	2.24	10	1
1:A:59:GLY:C	1:A:60:ASP:OD1	0.47	2.53	11	2
1:A:44:ASN:ND2	1:A:47:GLU:OE2	0.47	2.45	10	1
1:A:184:SER:OG	1:A:187:ASP:OD1	0.47	2.33	2	1
1:A:163:GLN:HE21	1:A:163:GLN:N	0.47	2.07	2	1
1:A:73:ASP:C	1:A:73:ASP:OD1	0.47	2.52	14	1
1:A:121:MET:CE	1:A:169:PHE:CE2	0.47	2.98	11	1
1:A:10:GLN:CG	1:A:11:ASP:N	0.47	2.78	5	1
1:A:153:PHE:CZ	1:A:164:LEU:HD23	0.47	2.45	2	2
1:A:109:ASP:OD1	1:A:114:GLY:N	0.47	2.47	13	1
1:A:89:LEU:O	1:A:92:THR:N	0.47	2.45	7	1
1:A:121:MET:HE3	1:A:169:PHE:CE1	0.47	2.45	15	1
1:A:190:VAL:HG22	1:A:190:VAL:OXT	0.47	2.10	8	1
1:A:161:ASP:OD1	1:A:161:ASP:C	0.47	2.53	13	1
1:A:108:TYR:CD2	1:A:124:ILE:HG12	0.47	2.45	2	1
1:A:183:LEU:N	1:A:183:LEU:CD2	0.47	2.78	9	1
1:A:55:PHE:HB3	1:A:56:PHE:CD2	0.46	2.45	7	2
1:A:78:GLY:C	1:A:79:TYR:CG	0.46	2.89	2	1
1:A:184:SER:C	1:A:186:TYR:N	0.46	2.68	8	1
1:A:101:LEU:HD13	1:A:170:CYS:SG	0.46	2.50	7	1
1:A:28:GLN:O	1:A:28:GLN:NE2	0.46	2.48	14	1
1:A:132:VAL:O	1:A:134:SER:N	0.46	2.49	9	1
1:A:94:ARG:HD3	1:A:94:ARG:H	0.46	1.68	10	1
1:A:49:GLN:HE22	1:A:61:PRO:C	0.46	2.14	15	1
1:A:96:GLU:C	1:A:98:ASN:H	0.46	2.13	5	1
1:A:119:ASP:C	1:A:119:ASP:OD1	0.46	2.53	5	1
1:A:22:PHE:CE2	1:A:89:LEU:HD23	0.46	2.45	14	1
1:A:189:LEU:CD1	1:A:189:LEU:C	0.46	2.84	4	3
1:A:84:GLU:OE1	1:A:127:ALA:CB	0.46	2.61	8	1
1:A:73:ASP:N	1:A:73:ASP:OD1	0.46	2.48	6	1
1:A:129:TYR:O	1:A:129:TYR:CD1	0.46	2.68	6	2
1:A:164:LEU:HD13	1:A:165:THR:N	0.46	2.24	5	2
1:A:178:THR:CG2	1:A:179:ILE:N	0.46	2.79	13	5
1:A:44:ASN:CG	1:A:45:LYS:N	0.46	2.69	6	3
1:A:56:PHE:N	1:A:57:PRO:CD	0.46	2.79	9	1
1:A:129:TYR:O	1:A:129:TYR:CG	0.46	2.68	8	2
1:A:166:LEU:CD1	1:A:167:GLU:N	0.46	2.76	8	1
1:A:10:GLN:CD	1:A:11:ASP:N	0.46	2.69	5	1
1:A:55:PHE:C	1:A:56:PHE:CG	0.46	2.89	10	2
1:A:60:ASP:OD1	1:A:62:SER:OG	0.46	2.33	9	1
1:A:117:SER:C	1:A:119:ASP:N	0.45	2.70	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:TYR:C	1:A:187:ASP:OD1	0.45	2.55	3	2
1:A:51:ILE:N	1:A:51:ILE:HD13	0.45	2.27	2	1
1:A:22:PHE:CE2	1:A:89:LEU:HD21	0.45	2.46	7	2
1:A:168:GLU:O	1:A:171:GLU:N	0.45	2.49	9	2
1:A:98:ASN:ND2	1:A:98:ASN:C	0.45	2.69	4	1
1:A:56:PHE:N	1:A:56:PHE:CD1	0.45	2.83	3	2
1:A:73:ASP:OD1	1:A:73:ASP:C	0.45	2.55	15	1
1:A:24:LYS:HG3	1:A:25:LYS:N	0.45	2.27	1	3
1:A:122:LEU:CD2	1:A:122:LEU:N	0.45	2.80	5	1
1:A:115:LEU:HD21	1:A:165:THR:HG22	0.45	1.88	10	1
1:A:102:ILE:CG2	1:A:106:GLN:NE2	0.45	2.80	3	1
1:A:108:TYR:CE1	1:A:124:ILE:HG13	0.45	2.46	1	5
1:A:67:TYR:CE2	1:A:134:SER:OG	0.45	2.70	3	1
1:A:21:ARG:C	1:A:22:PHE:CD1	0.45	2.90	1	1
1:A:52:TYR:CE1	1:A:56:PHE:O	0.45	2.69	6	1
1:A:19:SER:HB2	1:A:64:PHE:CE1	0.45	2.46	11	1
1:A:30:TRP:O	1:A:33:GLY:N	0.45	2.50	4	1
1:A:97:LEU:HD23	1:A:97:LEU:O	0.45	2.12	5	2
1:A:94:ARG:HD3	1:A:94:ARG:N	0.45	2.26	10	1
1:A:38:CYS:C	1:A:40:SER:N	0.45	2.70	3	4
1:A:52:TYR:CE1	1:A:64:PHE:CD2	0.45	3.05	12	1
1:A:108:TYR:CE1	1:A:124:ILE:HG12	0.45	2.46	11	1
1:A:59:GLY:C	1:A:60:ASP:CG	0.44	2.75	13	1
1:A:153:PHE:O	1:A:157:ASP:N	0.44	2.50	13	1
1:A:55:PHE:O	1:A:56:PHE:CD1	0.44	2.70	9	2
1:A:146:GLU:CG	1:A:147:LYS:H	0.44	2.24	4	2
1:A:190:VAL:HG22	1:A:190:VAL:O	0.44	2.12	3	1
1:A:30:TRP:CE3	1:A:30:TRP:C	0.44	2.90	8	1
1:A:19:SER:HB3	1:A:64:PHE:CE1	0.44	2.46	11	2
1:A:92:THR:O	1:A:93:SER:CB	0.44	2.65	2	2
1:A:28:GLN:HG3	1:A:29:GLN:N	0.44	2.27	7	3
1:A:166:LEU:HD23	1:A:166:LEU:C	0.44	2.32	6	5
1:A:86:ILE:CD1	1:A:86:ILE:N	0.44	2.81	9	1
1:A:109:ASP:C	1:A:111:ASP:N	0.44	2.71	5	1
1:A:130:LYS:HZ2	1:A:130:LYS:HB3	0.44	1.72	6	1
1:A:18:ARG:CG	1:A:18:ARG:HH11	0.44	2.26	14	1
1:A:75:ASP:O	1:A:75:ASP:CG	0.44	2.56	7	1
1:A:159:ASN:O	1:A:162:GLY:N	0.44	2.50	12	1
1:A:158:LYS:HB3	1:A:158:LYS:HZ3	0.44	1.72	1	1
1:A:108:TYR:CD1	1:A:124:ILE:CG1	0.44	3.01	11	1
1:A:189:LEU:C	1:A:189:LEU:CD1	0.44	2.86	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:VAL:O	1:A:138:LEU:N	0.44	2.51	10	1
1:A:158:LYS:CE	1:A:163:GLN:O	0.44	2.66	10	1
1:A:120:GLU:CD	1:A:120:GLU:H	0.44	2.16	6	1
1:A:158:LYS:O	1:A:159:ASN:ND2	0.44	2.46	11	1
1:A:52:TYR:CE1	1:A:56:PHE:HB2	0.44	2.48	4	2
1:A:132:VAL:HG22	1:A:133:GLY:N	0.44	2.27	9	1
1:A:129:TYR:CZ	1:A:138:LEU:HD22	0.44	2.48	8	3
1:A:118:TYR:CD1	1:A:153:PHE:CE2	0.44	3.06	15	1
1:A:166:LEU:C	1:A:166:LEU:CD1	0.44	2.86	8	1
1:A:17:VAL:C	1:A:19:SER:N	0.44	2.70	11	3
1:A:79:TYR:N	1:A:79:TYR:CD1	0.44	2.85	2	1
1:A:64:PHE:O	1:A:67:TYR:N	0.44	2.49	14	1
1:A:69:PHE:C	1:A:71:VAL:N	0.43	2.71	13	1
1:A:83:LYS:C	1:A:85:PHE:N	0.43	2.70	6	2
1:A:69:PHE:CD1	1:A:73:ASP:OD2	0.43	2.71	14	1
1:A:148:ARG:O	1:A:151:LYS:N	0.43	2.51	4	1
1:A:84:GLU:OE1	1:A:84:GLU:CA	0.43	2.66	5	1
1:A:94:ARG:HD2	1:A:94:ARG:H	0.43	1.71	10	1
1:A:156:MET:HG2	1:A:157:ASP:N	0.43	2.27	10	1
1:A:84:GLU:H	1:A:84:GLU:CD	0.43	2.17	10	1
1:A:108:TYR:CE2	1:A:124:ILE:HG13	0.43	2.48	6	1
1:A:162:GLY:C	1:A:163:GLN:NE2	0.43	2.71	2	1
1:A:130:LYS:HB3	1:A:130:LYS:HZ3	0.43	1.72	5	1
1:A:45:LYS:NZ	1:A:48:PHE:CG	0.43	2.85	13	1
1:A:27:LEU:HD11	1:A:55:PHE:CE2	0.43	2.48	3	1
1:A:176:ASP:HB2	1:A:179:ILE:HD12	0.43	1.89	15	1
1:A:167:GLU:CG	1:A:168:GLU:N	0.43	2.81	12	1
1:A:185:LEU:O	1:A:185:LEU:HD23	0.43	2.14	5	1
1:A:98:ASN:CG	1:A:99:ASP:H	0.43	2.16	3	2
1:A:83:LYS:HG3	1:A:84:GLU:N	0.43	2.29	9	2
1:A:31:TYR:CD2	1:A:86:ILE:HD11	0.43	2.49	12	1
1:A:184:SER:O	1:A:186:TYR:N	0.43	2.51	8	2
1:A:52:TYR:CE2	1:A:64:PHE:CG	0.43	3.07	7	1
1:A:16:LEU:C	1:A:16:LEU:CD1	0.43	2.84	1	1
1:A:69:PHE:CD2	1:A:73:ASP:CG	0.43	2.92	4	1
1:A:24:LYS:O	1:A:25:LYS:C	0.43	2.57	11	11
1:A:105:PHE:C	1:A:105:PHE:CD1	0.43	2.92	3	1
1:A:132:VAL:C	1:A:134:SER:N	0.43	2.70	9	1
1:A:31:TYR:OH	1:A:110:LEU:CD1	0.43	2.67	12	1
1:A:56:PHE:C	1:A:58:PHE:N	0.42	2.72	13	1
1:A:107:LEU:C	1:A:107:LEU:HD23	0.42	2.34	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ASP:N	1:A:61:PRO:CD	0.42	2.81	13	1
1:A:118:TYR:OH	1:A:146:GLU:CD	0.42	2.57	10	1
1:A:111:ASP:O	1:A:112:ASN:CB	0.42	2.67	3	1
1:A:170:CYS:SG	1:A:171:GLU:N	0.42	2.92	12	1
1:A:56:PHE:CG	1:A:56:PHE:O	0.42	2.71	1	1
1:A:98:ASN:ND2	1:A:99:ASP:H	0.42	2.11	11	1
1:A:179:ILE:O	1:A:179:ILE:CG2	0.42	2.67	11	1
1:A:121:MET:HE1	1:A:169:PHE:CE1	0.42	2.49	15	1
1:A:117:SER:OG	1:A:120:GLU:OE2	0.42	2.37	8	1
1:A:128:ILE:HD12	1:A:128:ILE:H	0.42	1.74	8	1
1:A:35:PHE:CZ	1:A:83:LYS:HG2	0.42	2.49	2	1
1:A:183:LEU:C	1:A:185:LEU:H	0.42	2.17	4	1
1:A:169:PHE:C	1:A:169:PHE:CD1	0.42	2.92	15	1
1:A:167:GLU:OE1	1:A:167:GLU:CA	0.42	2.62	10	1
1:A:28:GLN:HG2	1:A:29:GLN:N	0.42	2.30	10	2
1:A:166:LEU:C	1:A:166:LEU:HD23	0.42	2.35	7	2
1:A:31:TYR:CE1	1:A:35:PHE:CZ	0.42	3.08	15	1
1:A:71:VAL:CG1	1:A:134:SER:OG	0.42	2.66	5	1
1:A:77:ASN:HB2	1:A:79:TYR:CZ	0.42	2.49	5	1
1:A:107:LEU:HD23	1:A:107:LEU:O	0.42	2.14	10	2
1:A:167:GLU:OE1	1:A:167:GLU:N	0.42	2.45	2	1
1:A:67:TYR:O	1:A:68:VAL:C	0.42	2.58	15	2
1:A:157:ASP:OD2	1:A:164:LEU:CD1	0.42	2.67	10	1
1:A:55:PHE:HB3	1:A:56:PHE:CE2	0.42	2.49	7	1
1:A:87:CYS:SG	1:A:107:LEU:CD1	0.42	2.98	1	1
1:A:85:PHE:CE1	1:A:89:LEU:HD13	0.42	2.49	1	1
1:A:86:ILE:CG2	1:A:103:TRP:NE1	0.42	2.82	8	1
1:A:122:LEU:HD21	1:A:146:GLU:OE1	0.42	2.15	10	1
1:A:105:PHE:C	1:A:107:LEU:H	0.42	2.18	10	1
1:A:105:PHE:CE2	1:A:166:LEU:CA	0.42	3.03	14	1
1:A:31:TYR:CG	1:A:32:LYS:N	0.42	2.88	13	1
1:A:45:LYS:HD3	1:A:69:PHE:CD1	0.42	2.49	13	1
1:A:113:ASN:N	1:A:113:ASN:HD22	0.42	2.13	7	1
1:A:113:ASN:CG	1:A:114:GLY:H	0.42	2.18	7	1
1:A:18:ARG:CG	1:A:18:ARG:NH1	0.42	2.81	14	1
1:A:145:PRO:O	1:A:146:GLU:C	0.42	2.58	12	1
1:A:148:ARG:HG3	1:A:149:VAL:N	0.42	2.30	12	1
1:A:129:TYR:CE1	1:A:138:LEU:HD22	0.42	2.50	11	2
1:A:108:TYR:CD1	1:A:120:GLU:OE1	0.42	2.73	5	1
1:A:159:ASN:H	1:A:159:ASN:ND2	0.42	2.13	5	1
1:A:165:THR:OG1	1:A:168:GLU:OE2	0.42	2.37	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:CYS:N	1:A:107:LEU:HD11	0.42	2.30	11	2
1:A:118:TYR:O	1:A:118:TYR:CD1	0.42	2.73	3	1
1:A:146:GLU:C	1:A:146:GLU:OE1	0.42	2.58	2	1
1:A:57:PRO:O	1:A:58:PHE:CG	0.42	2.73	2	1
1:A:110:LEU:HD12	1:A:110:LEU:N	0.42	2.29	9	1
1:A:40:SER:C	1:A:42:HIS:H	0.42	2.18	11	1
1:A:183:LEU:C	1:A:185:LEU:N	0.42	2.74	4	1
1:A:109:ASP:OD1	1:A:109:ASP:N	0.41	2.53	9	1
1:A:167:GLU:HG3	1:A:168:GLU:N	0.41	2.30	12	1
1:A:75:ASP:C	1:A:77:ASN:H	0.41	2.18	15	1
1:A:24:LYS:C	1:A:26:GLU:H	0.41	2.19	9	1
1:A:73:ASP:O	1:A:73:ASP:CG	0.41	2.57	15	1
1:A:102:ILE:N	1:A:102:ILE:HD12	0.41	2.30	13	1
1:A:186:TYR:O	1:A:186:TYR:CD2	0.41	2.73	2	1
1:A:15:ASP:O	1:A:19:SER:N	0.41	2.53	3	1
1:A:69:PHE:CA	1:A:73:ASP:OD1	0.41	2.68	14	1
1:A:148:ARG:CB	1:A:148:ARG:CZ	0.41	2.97	9	1
1:A:69:PHE:O	1:A:73:ASP:CG	0.41	2.58	15	1
1:A:107:LEU:CD2	1:A:107:LEU:C	0.41	2.88	15	1
1:A:69:PHE:O	1:A:71:VAL:N	0.41	2.54	13	1
1:A:31:TYR:CE1	1:A:35:PHE:CD1	0.41	3.08	10	1
1:A:19:SER:HB2	1:A:64:PHE:CD1	0.41	2.51	2	1
1:A:22:PHE:CG	1:A:56:PHE:CZ	0.41	3.08	13	1
1:A:16:LEU:CD1	1:A:16:LEU:C	0.41	2.89	3	1
1:A:117:SER:O	1:A:118:TYR:C	0.41	2.59	3	1
1:A:9:SER:OG	1:A:10:GLN:N	0.41	2.53	6	2
1:A:19:SER:OG	1:A:64:PHE:CE1	0.41	2.69	7	1
1:A:105:PHE:CD2	1:A:166:LEU:HG	0.41	2.51	12	1
1:A:24:LYS:NZ	1:A:24:LYS:CB	0.41	2.84	5	1
1:A:176:ASP:N	1:A:177:PRO:HD3	0.41	2.31	5	1
1:A:22:PHE:HB3	1:A:56:PHE:CZ	0.41	2.51	13	1
1:A:118:TYR:C	1:A:118:TYR:CD1	0.41	2.93	13	1
1:A:44:ASN:ND2	1:A:45:LYS:H	0.41	2.14	6	1
1:A:108:TYR:CE2	1:A:124:ILE:HG12	0.41	2.51	2	3
1:A:94:ARG:C	1:A:94:ARG:CD	0.41	2.89	1	1
1:A:111:ASP:O	1:A:112:ASN:CG	0.41	2.59	11	1
1:A:11:ASP:CG	1:A:12:GLN:H	0.41	2.17	4	1
1:A:128:ILE:N	1:A:128:ILE:HD12	0.41	2.30	8	1
1:A:85:PHE:CD1	1:A:85:PHE:C	0.41	2.94	8	1
1:A:186:TYR:CZ	1:A:189:LEU:CD1	0.41	3.04	10	1
1:A:176:ASP:C	1:A:178:THR:N	0.41	2.74	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:PHE:O	1:A:73:ASP:C	0.41	2.59	7	1
1:A:76:LYS:O	1:A:77:ASN:C	0.41	2.60	9	1
1:A:61:PRO:O	1:A:65:ALA:HB2	0.41	2.16	12	1
1:A:115:LEU:CD2	1:A:165:THR:HG22	0.41	2.46	11	1
1:A:156:MET:O	1:A:157:ASP:C	0.40	2.59	7	1
1:A:57:PRO:C	1:A:58:PHE:CD1	0.40	2.94	11	1
1:A:132:VAL:HG11	1:A:138:LEU:HD21	0.40	1.90	14	1
1:A:166:LEU:O	1:A:167:GLU:C	0.40	2.60	12	1
1:A:81:ASP:C	1:A:83:LYS:N	0.40	2.75	10	1
1:A:89:LEU:O	1:A:90:SER:C	0.40	2.60	7	1
1:A:9:SER:OG	1:A:11:ASP:OD1	0.40	2.35	14	1
1:A:55:PHE:C	1:A:56:PHE:CD2	0.40	2.95	12	1
1:A:109:ASP:CG	1:A:109:ASP:O	0.40	2.60	11	1
1:A:45:LYS:NZ	1:A:48:PHE:HB3	0.40	2.32	13	1
1:A:83:LYS:HG2	1:A:84:GLU:N	0.40	2.29	3	1
1:A:156:MET:O	1:A:157:ASP:CG	0.40	2.60	7	1
1:A:113:ASN:N	1:A:113:ASN:ND2	0.40	2.66	9	1
1:A:136:VAL:CG2	1:A:137:LYS:H	0.40	2.29	15	1
1:A:100:LYS:CD	1:A:183:LEU:HD21	0.40	2.46	15	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	175/190 (92%)	142±3 (81±2%)	25±2 (15±1%)	7±3 (4±2%)	6	32
All	All	2625/2850 (92%)	2132 (81%)	382 (15%)	111 (4%)	6	32

All 34 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	188	GLY	9
1	A	57	PRO	8
1	A	75	ASP	7

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Mol	Chain	Res	Type	Models (Total)
1	A	25	LYS	7
1	A	39	PRO	6
1	A	77	ASN	6
1	A	178	THR	6
1	A	177	PRO	5
1	A	58	PHE	5
1	A	22	PHE	5
1	A	40	SER	4
1	A	145	PRO	4
1	A	76	LYS	4
1	A	93	SER	4
1	A	157	ASP	3
1	A	161	ASP	3
1	A	160	LYS	3
1	A	158	LYS	2
1	A	23	ASP	2
1	A	78	GLY	2
1	A	138	LEU	2
1	A	186	TYR	2
1	A	189	LEU	1
1	A	156	MET	1
1	A	21	ARG	1
1	A	118	TYR	1
1	A	110	LEU	1
1	A	41	GLY	1
1	A	137	LYS	1
1	A	174	LYS	1
1	A	159	ASN	1
1	A	187	ASP	1
1	A	74	ALA	1
1	A	59	GLY	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	159/171 (93%)	131±4 (82±2%)	28±4 (18±2%)	6 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2385/2565 (93%)	1961 (82%)	424 (18%)	6 40

All 116 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	132	VAL	15
1	A	22	PHE	15
1	A	121	MET	13
1	A	166	LEU	13
1	A	70	ASN	12
1	A	28	GLN	11
1	A	16	LEU	10
1	A	37	ASP	9
1	A	189	LEU	9
1	A	97	LEU	9
1	A	110	LEU	8
1	A	24	LYS	8
1	A	136	VAL	8
1	A	81	ASP	7
1	A	117	SER	7
1	A	175	ARG	7
1	A	77	ASN	6
1	A	122	LEU	6
1	A	174	LYS	6
1	A	31	TYR	6
1	A	80	ILE	6
1	A	13	LEU	6
1	A	21	ARG	5
1	A	170	CYS	5
1	A	53	LYS	5
1	A	165	THR	5
1	A	62	SER	5
1	A	107	LEU	5
1	A	94	ARG	4
1	A	18	ARG	4
1	A	98	ASN	4
1	A	87	CYS	4
1	A	66	GLU	4
1	A	11	ASP	4
1	A	75	ASP	4
1	A	67	TYR	4

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Mol	Chain	Res	Type	Models (Total)
1	A	54	GLN	4
1	A	44	ASN	4
1	A	40	SER	3
1	A	158	LYS	3
1	A	134	SER	3
1	A	112	ASN	3
1	A	164	LEU	3
1	A	84	GLU	3
1	A	183	LEU	3
1	A	150	ASN	3
1	A	113	ASN	3
1	A	111	ASP	3
1	A	128	ILE	3
1	A	178	THR	3
1	A	179	ILE	3
1	A	148	ARG	3
1	A	9	SER	3
1	A	10	GLN	3
1	A	163	GLN	3
1	A	36	LYS	3
1	A	100	LYS	3
1	A	92	THR	3
1	A	160	LYS	3
1	A	56	PHE	3
1	A	156	MET	3
1	A	185	LEU	3
1	A	23	ASP	3
1	A	159	ASN	3
1	A	99	ASP	3
1	A	29	GLN	3
1	A	129	TYR	2
1	A	83	LYS	2
1	A	123	ARG	2
1	A	161	ASP	2
1	A	120	GLU	2
1	A	138	LEU	2
1	A	14	GLN	2
1	A	85	PHE	2
1	A	12	GLN	2
1	A	147	LYS	2
1	A	146	GLU	2
1	A	50	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	20	THR	2
1	A	93	SER	2
1	A	137	LYS	2
1	A	187	ASP	2
1	A	45	LYS	2
1	A	76	LYS	2
1	A	151	LYS	2
1	A	46	SER	2
1	A	154	ASN	2
1	A	58	PHE	2
1	A	64	PHE	2
1	A	25	LYS	1
1	A	73	ASP	1
1	A	131	MET	1
1	A	96	GLU	1
1	A	135	MET	1
1	A	168	GLU	1
1	A	35	PHE	1
1	A	47	GLU	1
1	A	155	MET	1
1	A	109	ASP	1
1	A	38	CYS	1
1	A	26	GLU	1
1	A	145	PRO	1
1	A	79	TYR	1
1	A	116	ILE	1
1	A	119	ASP	1
1	A	82	PHE	1
1	A	153	PHE	1
1	A	126	ASP	1
1	A	68	VAL	1
1	A	106	GLN	1
1	A	124	ILE	1
1	A	130	LYS	1
1	A	69	PHE	1
1	A	167	GLU	1
1	A	186	TYR	1
1	A	173	SER	1

6.3.3 RNA ⓘ

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