Full wwPDB NMR Structure Validation Report (i)

Feb 19, 2022 – 02:07 PM EST

PDB ID	:	1S6D
Title	:	Structure in solution of a methionine-rich 2S Albumin protein from Sunflower Seed
Authors	:	Pantoja-Uceda, D.; Bruix, M.; Shewry, P.R.; Santoro, J.; Rico, M.
Deposited on	:	2004-01-23

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

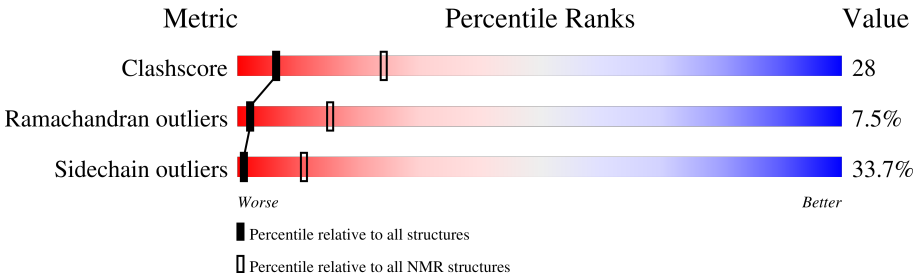
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	103	28% 32% 12% 28%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 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:11-A:31, A:49-A:101 (74)	0.33	15

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1634 atoms, of which 806 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Albumin 8.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	103	1634	502	806	149	153	24	0

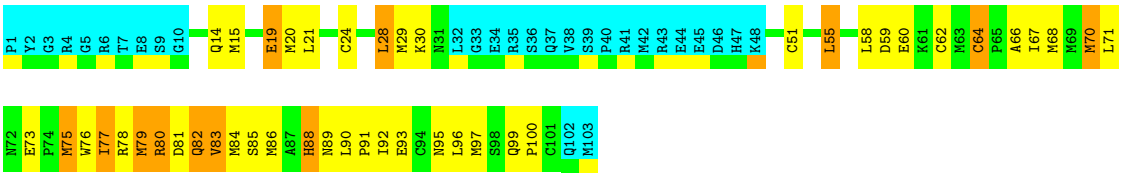
4 Residue-property plots (i)

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: Albumin 8

Chain A: 28% 32% 12% 28%



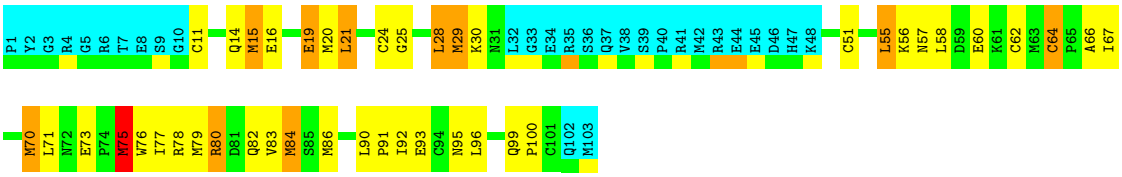
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Albumin 8

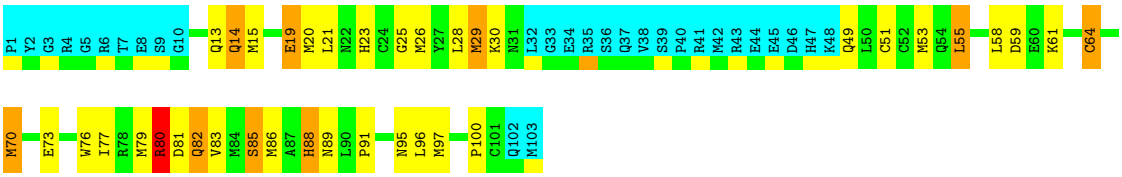
Chain A: 30% 31% 10% • 28%



4.2.2 Score per residue for model 2

• Molecule 1: Albumin 8

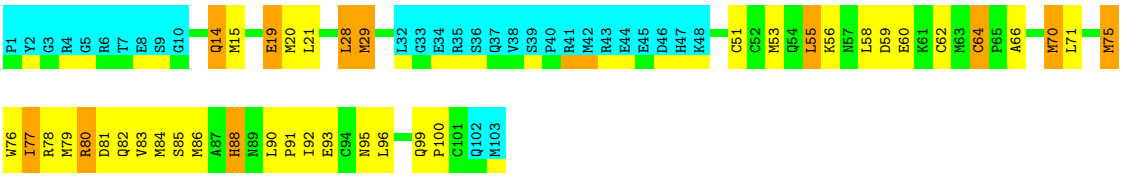
Chain A: 35% 27% 9% • 28%



4.2.3 Score per residue for model 3

- Molecule 1: Albumin 8

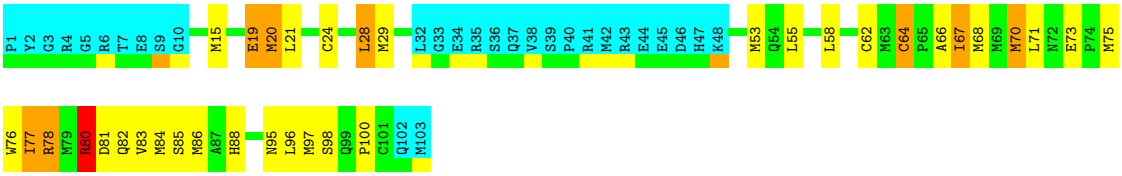
Chain A: 33% 28% 11% 28%



4.2.4 Score per residue for model 4

- Molecule 1: Albumin 8

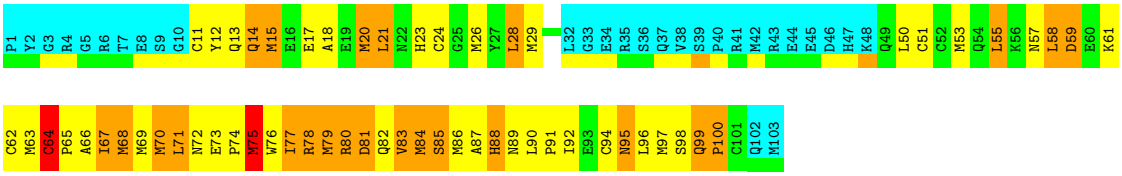
Chain A: 38% 25% 8% • 28%



4.2.5 Score per residue for model 5

- Molecule 1: Albumin 8

Chain A: 14% 33% 23% • 28%



4.2.6 Score per residue for model 6

- Molecule 1: Albumin 8

Chain A: 29% 30% 12% • 28%

P1 Y2 G3 R4 G5 R6 T7 E8 S9 G10 C11 Q14 M15 E19 M20 L21 N22 L28 M29 K30 N31 L32 G33 E34 R35 S36 Q37 V38 S39 P40 R41 M42 R43 E44 E45 D46 H47 K48 C51 L55 L58 D59 E60 K61 C62 M63 C64 P65 A66 I67 M68 M69 M70 L71

M75 W76 I77 R78 M79 R80 D81 Q82 V83 M84 S85 M86 A87 H88 N89 L90 P91 I92 N95 L96 M97 S98 Q99 P100 C101 Q102 M103

4.2.7 Score per residue for model 7

- Molecule 1: Albumin 8

Chain A: 30% 26% 13% • 28%

P1 Y2 G3 R4 G5 R6 T7 E8 S9 G10 C11 Q14 E17 A18 E19 M20 L21 C24 G25 M26 Y27 L28 M29 K30 N31 L32 G33 E34 R35 S36 Q37 V38 S39 P40 R41 M42 R43 E44 E45 D46 H47 K48 C51 C52 H53 Q54 L55 L58 D59 E60 K61 C62 M63 C64 P65

A66 I67 M70 L71 N72 E73 P74 M75 W76 I77 R78 M79 R80 D81 Q82 V83 M86 A87 H88 N89 L90 P91 I92 N95 L96 M97 P100 C101 Q102 M103

4.2.8 Score per residue for model 8

- Molecule 1: Albumin 8

Chain A: 33% 28% 10% • 28%

P1 Y2 G3 R4 G5 R6 T7 E8 S9 G10 Q14 M15 E19 M20 L21 N22 H23 M26 Y27 L28 M29 K30 N31 L32 G33 E34 R35 S36 Q37 V38 S39 P40 R41 M42 R43 E44 E45 D46 H47 K48 C51 L55 D59 E60 K61 C64 P65 A66 I67 M70 L71 N72

E73 P74 M75 W76 I77 R78 M79 R80 D81 Q82 V83 M84 S85 M86 A87 H88 N89 L90 P91 I92 E93 C94 N95 L96 Q99 P100 C101 Q102 M103

4.2.9 Score per residue for model 9

- Molecule 1: Albumin 8

Chain A: 26% 32% 12% • 28%

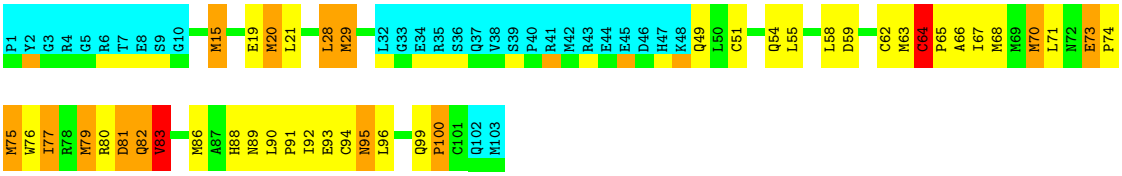
P1 Y2 G3 R4 G5 R6 T7 E8 S9 G10 Q14 M15 E19 M20 L21 C24 G25 M26 Y27 L28 M29 K30 N31 L32 G33 E34 R35 S36 Q37 V38 S39 P40 R41 M42 R43 E44 E45 D46 H47 K48 Q49 L50 L55 L58 D59 E60 K61 C62 M63 C64 P65 A66 I67 M68 M69

M70 L71 N72 E73 P74 M75 W76 I77 R78 M79 R80 D81 Q82 V83 M84 S85 M86 A87 H88 N89 L90 P91 I92 N95 L96 Q99 P100 C101 Q102 M103

4.2.10 Score per residue for model 10

- Molecule 1: Albumin 8

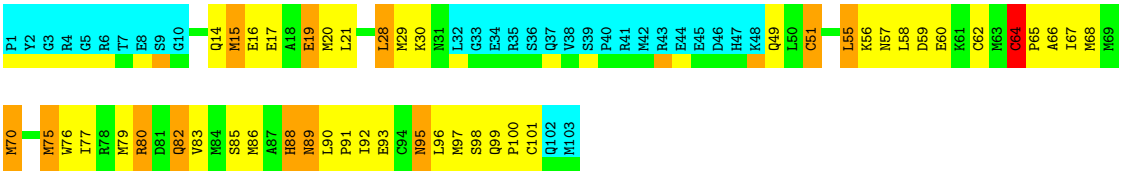
Chain A: 30% 27% 13% • 28%



4.2.11 Score per residue for model 11

- Molecule 1: Albumin 8

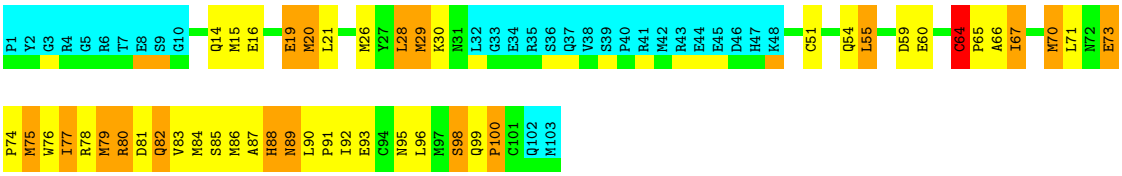
Chain A: 26% 33% 12% • 28%



4.2.12 Score per residue for model 12

- Molecule 1: Albumin 8

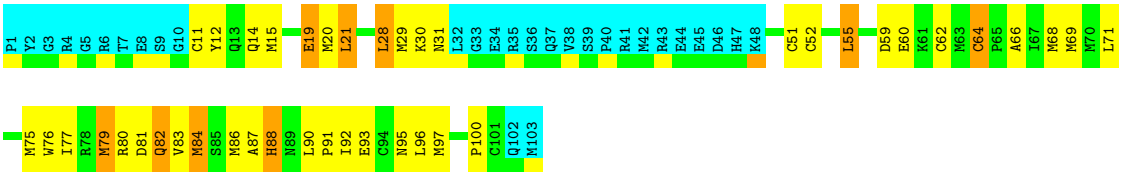
Chain A: 26% 28% 17% • 28%



4.2.13 Score per residue for model 13

- Molecule 1: Albumin 8

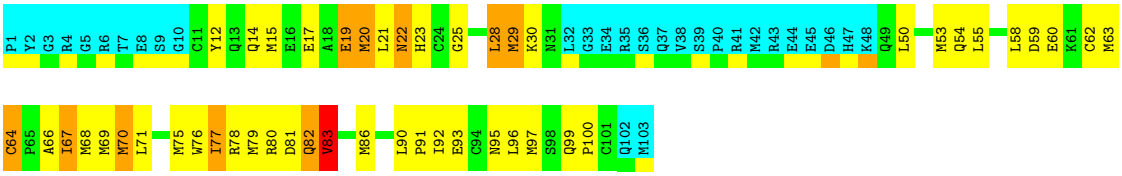
Chain A: 31% 32% 9% 28%



4.2.14 Score per residue for model 14

- Molecule 1: Albumin 8

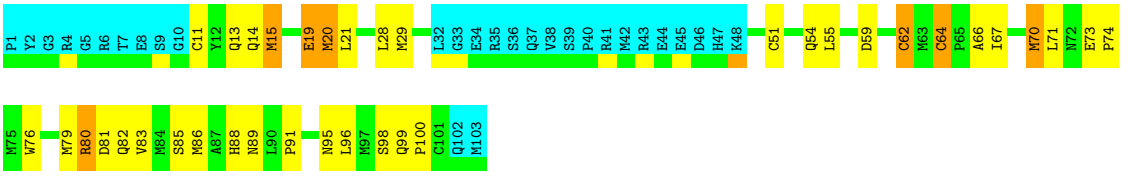
Chain A: 25% 36% 10% • 28%



4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Albumin 8

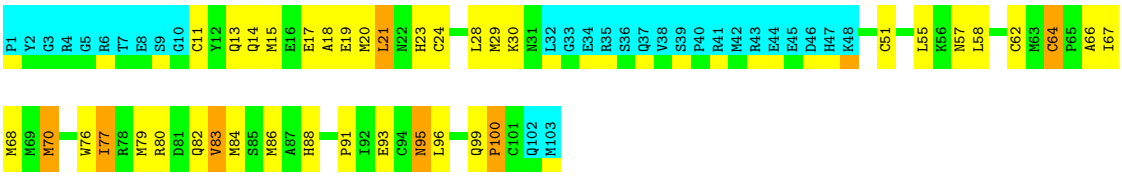
Chain A: 36% 29% 7% 28%



4.2.16 Score per residue for model 16

- Molecule 1: Albumin 8

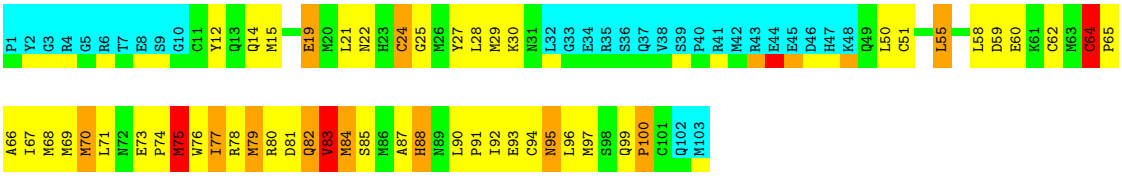
Chain A: 34% 31% 7% 28%



4.2.17 Score per residue for model 17

- Molecule 1: Albumin 8

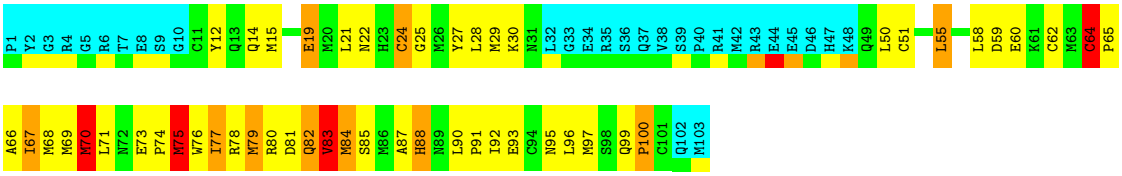
Chain A: 21% 37% 11% • 28%



4.2.18 Score per residue for model 18

- Molecule 1: Albumin 8

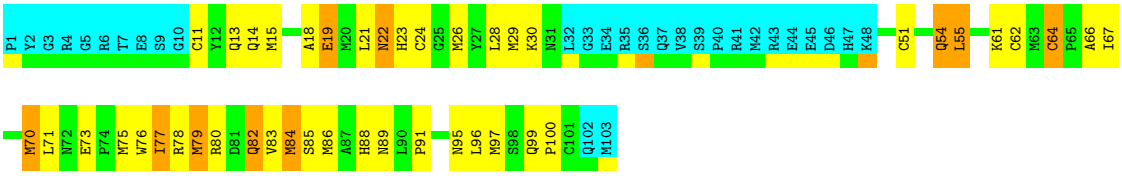
Chain A: 22% 36% 10% • 28%



4.2.19 Score per residue for model 19

- Molecule 1: Albumin 8

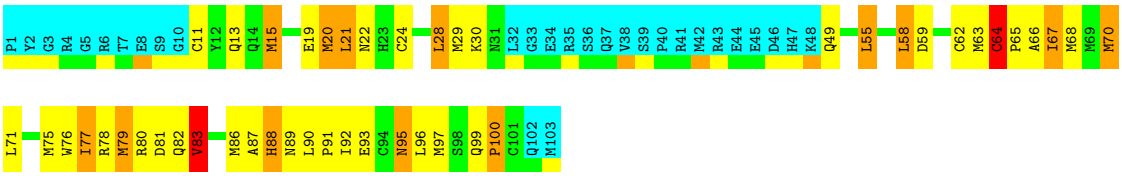
Chain A: 29% 33% 10% 28%



4.2.20 Score per residue for model 20

- Molecule 1: Albumin 8

Chain A: 27% 30% 13% • 28%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing combined with molecular dynamics in torsion angle space followed by a final minimization.*.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *The submitted conformer models are the 20 structures with the lowest target function.*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
Amber	refinement	7

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.67±0.06	0±0/603 (0.0± 0.0%)	0.93±0.12	0±1/807 (0.1± 0.1%)
All	All	0.67	0/12060 (0.0%)	0.94	10/16140 (0.1%)

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	0.1±0.3
All	All	0	2

There are no bond-length outliers.

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	19	GLU	OE1-CD-OE2	7.34	132.11	123.30	19	2
1	A	80	ARG	NE-CZ-NH1	6.68	123.64	120.30	15	3
1	A	81	ASP	CB-CG-OD2	-5.59	113.27	118.30	15	1
1	A	19	GLU	O-C-N	-5.46	113.96	122.70	7	1
1	A	11	CYS	CA-CB-SG	5.40	123.72	114.00	15	1
1	A	15	MET	CG-SD-CE	-5.24	91.82	100.20	15	1
1	A	62	CYS	CA-CB-SG	5.22	123.40	114.00	15	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	22	ASN	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	70	MET	Mainchain	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	593	581	579	33±10
All	All	11860	11620	11580	668

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:LEU:HD22	1:A:96:LEU:HD13	1.09	1.24	1	17
1:A:55:LEU:HD13	1:A:96:LEU:CD1	0.89	1.96	10	16
1:A:21:LEU:CD2	1:A:55:LEU:HD11	0.89	1.98	1	2
1:A:91:PRO:HA	1:A:96:LEU:HD12	0.87	1.46	11	15
1:A:55:LEU:HD13	1:A:96:LEU:HD13	0.86	1.43	20	8
1:A:21:LEU:HD21	1:A:55:LEU:HD11	0.86	1.45	1	2
1:A:71:LEU:HD21	1:A:87:ALA:HB3	0.85	1.49	20	2
1:A:55:LEU:CD2	1:A:96:LEU:HD13	0.83	2.01	12	13
1:A:20:MET:SD	1:A:58:LEU:HD12	0.82	2.14	11	7
1:A:15:MET:SD	1:A:66:ALA:HB1	0.81	2.15	8	10
1:A:21:LEU:HD22	1:A:70:MET:HE3	0.80	1.53	12	3
1:A:76:TRP:C	1:A:77:ILE:HD12	0.78	1.99	17	8
1:A:55:LEU:HD12	1:A:96:LEU:HD13	0.78	1.55	16	2
1:A:28:LEU:HD11	1:A:90:LEU:CD1	0.77	2.09	17	3
1:A:51:CYS:O	1:A:55:LEU:HD12	0.75	1.81	5	12
1:A:28:LEU:HD22	1:A:86:MET:HB3	0.75	1.59	12	17
1:A:21:LEU:HD13	1:A:70:MET:SD	0.74	2.23	17	6
1:A:21:LEU:HB3	1:A:70:MET:HE1	0.74	1.58	3	2
1:A:15:MET:CE	1:A:66:ALA:HB1	0.74	2.13	5	10
1:A:76:TRP:CE3	1:A:79:MET:CE	0.73	2.71	5	6
1:A:28:LEU:HD22	1:A:86:MET:CB	0.72	2.15	13	12
1:A:55:LEU:CD1	1:A:96:LEU:HD13	0.72	2.15	16	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:TRP:CZ3	1:A:83:VAL:HG11	0.71	2.20	11	11
1:A:20:MET:CE	1:A:21:LEU:HD12	0.71	2.15	8	3
1:A:21:LEU:HD13	1:A:76:TRP:CE2	0.69	2.21	9	2
1:A:21:LEU:HD21	1:A:55:LEU:HD21	0.69	1.64	14	4
1:A:20:MET:SD	1:A:55:LEU:HD22	0.69	2.27	16	1
1:A:24:CYS:O	1:A:28:LEU:HD12	0.68	1.87	17	2
1:A:28:LEU:HD22	1:A:86:MET:HB2	0.68	1.65	13	1
1:A:77:ILE:HG22	1:A:78:ARG:N	0.68	2.04	5	5
1:A:80:ARG:HA	1:A:83:VAL:HG22	0.68	1.66	5	13
1:A:80:ARG:HA	1:A:83:VAL:HG13	0.67	1.64	10	6
1:A:71:LEU:HD11	1:A:87:ALA:CB	0.67	2.19	17	3
1:A:76:TRP:C	1:A:77:ILE:HD13	0.66	2.10	20	8
1:A:55:LEU:HD22	1:A:96:LEU:CD1	0.66	2.13	12	7
1:A:21:LEU:HD22	1:A:70:MET:SD	0.65	2.31	8	5
1:A:55:LEU:HD13	1:A:96:LEU:HD11	0.65	1.68	10	4
1:A:20:MET:HG2	1:A:21:LEU:HD13	0.65	1.69	20	3
1:A:28:LEU:HD21	1:A:90:LEU:HD11	0.65	1.67	13	5
1:A:21:LEU:HD12	1:A:70:MET:HE3	0.65	1.68	10	4
1:A:70:MET:CE	1:A:71:LEU:HD21	0.65	2.22	12	5
1:A:67:ILE:O	1:A:71:LEU:HD12	0.64	1.92	20	4
1:A:28:LEU:HD11	1:A:90:LEU:HD12	0.64	1.70	13	1
1:A:21:LEU:CD1	1:A:70:MET:HE3	0.64	2.23	10	1
1:A:21:LEU:HD22	1:A:70:MET:CE	0.64	2.23	12	5
1:A:15:MET:HE3	1:A:66:ALA:O	0.62	1.93	11	1
1:A:55:LEU:HB3	1:A:96:LEU:HD22	0.62	1.71	20	4
1:A:21:LEU:HD13	1:A:70:MET:HG2	0.62	1.70	11	1
1:A:70:MET:HE2	1:A:71:LEU:HD21	0.61	1.71	6	3
1:A:21:LEU:HD12	1:A:70:MET:HE1	0.61	1.72	1	2
1:A:20:MET:CE	1:A:58:LEU:HD12	0.61	2.25	5	2
1:A:15:MET:HE1	1:A:66:ALA:O	0.60	1.96	19	2
1:A:21:LEU:HD12	1:A:70:MET:CE	0.60	2.25	1	3
1:A:91:PRO:CA	1:A:96:LEU:HD12	0.59	2.26	8	8
1:A:20:MET:HE1	1:A:58:LEU:HD12	0.59	1.75	5	1
1:A:21:LEU:HD23	1:A:51:CYS:SG	0.59	2.38	19	1
1:A:11:CYS:HB3	1:A:66:ALA:HB2	0.58	1.74	19	6
1:A:90:LEU:HD23	1:A:93:GLU:OE2	0.58	1.98	11	1
1:A:51:CYS:C	1:A:55:LEU:HD12	0.58	2.18	1	8
1:A:75:MET:O	1:A:76:TRP:CG	0.58	2.57	5	4
1:A:71:LEU:HD21	1:A:87:ALA:CB	0.58	2.28	5	2
1:A:63:MET:SD	1:A:96:LEU:HD22	0.58	2.39	10	2
1:A:80:ARG:CA	1:A:83:VAL:HG22	0.57	2.29	6	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:ILE:HD12	1:A:77:ILE:N	0.57	2.14	5	6
1:A:14:GLN:NE2	1:A:58:LEU:HD22	0.57	2.15	2	3
1:A:84:MET:O	1:A:88:HIS:CE1	0.57	2.58	17	2
1:A:67:ILE:HG23	1:A:70:MET:SD	0.57	2.40	7	5
1:A:21:LEU:HD22	1:A:25:GLY:CA	0.56	2.30	9	1
1:A:73:GLU:CB	1:A:74:PRO:CD	0.56	2.83	17	5
1:A:77:ILE:N	1:A:77:ILE:CD1	0.56	2.67	5	1
1:A:55:LEU:CG	1:A:96:LEU:HD13	0.56	2.30	16	8
1:A:63:MET:HE3	1:A:96:LEU:HA	0.56	1.78	14	5
1:A:20:MET:SD	1:A:21:LEU:HD12	0.56	2.41	12	2
1:A:18:ALA:O	1:A:20:MET:HE2	0.56	2.01	7	1
1:A:15:MET:HE2	1:A:66:ALA:HB1	0.56	1.77	13	1
1:A:71:LEU:CD2	1:A:87:ALA:HB3	0.55	2.27	20	1
1:A:21:LEU:HD13	1:A:70:MET:CB	0.55	2.31	3	1
1:A:76:TRP:HA	1:A:79:MET:HE2	0.55	1.78	16	2
1:A:21:LEU:HD22	1:A:70:MET:HE1	0.54	1.79	18	2
1:A:99:GLN:N	1:A:100:PRO:HD3	0.54	2.18	5	7
1:A:70:MET:HE1	1:A:71:LEU:HD11	0.54	1.78	10	2
1:A:76:TRP:HZ3	1:A:83:VAL:HG11	0.54	1.62	11	7
1:A:51:CYS:O	1:A:55:LEU:HD23	0.54	2.02	16	1
1:A:24:CYS:SG	1:A:90:LEU:HD13	0.54	2.43	9	1
1:A:21:LEU:H	1:A:21:LEU:HD22	0.53	1.63	5	2
1:A:77:ILE:HD13	1:A:77:ILE:N	0.53	2.16	20	2
1:A:21:LEU:HD11	1:A:67:ILE:HG12	0.53	1.80	11	1
1:A:80:ARG:CD	1:A:83:VAL:HG22	0.53	2.34	20	1
1:A:11:CYS:CB	1:A:66:ALA:HB2	0.53	2.34	5	5
1:A:62:CYS:O	1:A:66:ALA:HB3	0.53	2.04	20	17
1:A:21:LEU:HD23	1:A:70:MET:HB2	0.52	1.82	16	1
1:A:21:LEU:HD23	1:A:70:MET:CG	0.52	2.35	16	1
1:A:22:ASN:ND2	1:A:23:HIS:CD2	0.52	2.78	14	2
1:A:21:LEU:HG	1:A:70:MET:SD	0.52	2.45	15	4
1:A:80:ARG:HD3	1:A:84:MET:HE2	0.52	1.82	5	1
1:A:70:MET:HE1	1:A:71:LEU:HD21	0.51	1.80	12	1
1:A:55:LEU:HD22	1:A:58:LEU:HD12	0.51	1.82	9	1
1:A:28:LEU:HD11	1:A:90:LEU:HD11	0.51	1.77	17	2
1:A:71:LEU:CD2	1:A:83:VAL:CG2	0.51	2.88	14	1
1:A:21:LEU:HD23	1:A:70:MET:HG3	0.51	1.83	16	1
1:A:71:LEU:HD21	1:A:83:VAL:HG21	0.51	1.82	10	1
1:A:76:TRP:CZ3	1:A:83:VAL:HG21	0.51	2.41	9	2
1:A:77:ILE:CG2	1:A:78:ARG:N	0.51	2.74	5	1
1:A:76:TRP:O	1:A:77:ILE:HD13	0.50	2.05	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:N	1:A:91:PRO:CD	0.50	2.74	5	8
1:A:20:MET:HE2	1:A:21:LEU:HD12	0.50	1.81	8	3
1:A:76:TRP:CE3	1:A:80:ARG:NE	0.50	2.79	20	1
1:A:21:LEU:CD2	1:A:55:LEU:HD21	0.50	2.36	4	2
1:A:76:TRP:CE3	1:A:83:VAL:HG21	0.50	2.42	5	5
1:A:20:MET:CG	1:A:21:LEU:HD13	0.50	2.36	5	2
1:A:15:MET:SD	1:A:20:MET:HE2	0.49	2.47	11	1
1:A:21:LEU:HD22	1:A:25:GLY:HA3	0.49	1.83	9	1
1:A:70:MET:CE	1:A:87:ALA:HB1	0.49	2.38	12	2
1:A:28:LEU:HB2	1:A:83:VAL:HG12	0.49	1.83	19	4
1:A:20:MET:SD	1:A:58:LEU:HD11	0.49	2.47	14	1
1:A:70:MET:HE2	1:A:71:LEU:CD2	0.48	2.38	6	1
1:A:85:SER:O	1:A:88:HIS:CD2	0.48	2.66	12	6
1:A:76:TRP:CD2	1:A:80:ARG:CZ	0.48	2.96	20	1
1:A:15:MET:CG	1:A:20:MET:SD	0.48	3.02	12	2
1:A:28:LEU:HD21	1:A:90:LEU:CD1	0.48	2.36	13	1
1:A:71:LEU:CD2	1:A:83:VAL:HG23	0.48	2.38	15	3
1:A:73:GLU:CB	1:A:74:PRO:HD2	0.48	2.37	17	3
1:A:77:ILE:HG22	1:A:78:ARG:H	0.47	1.69	5	1
1:A:14:GLN:CG	1:A:58:LEU:HD21	0.47	2.40	3	3
1:A:29:MET:SD	1:A:76:TRP:CZ3	0.47	3.07	12	1
1:A:80:ARG:HD3	1:A:83:VAL:HG22	0.47	1.85	20	1
1:A:12:TYR:CD1	1:A:69:MET:HB3	0.47	2.45	5	3
1:A:80:ARG:O	1:A:84:MET:N	0.47	2.47	5	1
1:A:15:MET:HE1	1:A:66:ALA:HB1	0.47	1.87	20	2
1:A:25:GLY:HA2	1:A:28:LEU:HD12	0.47	1.86	14	1
1:A:94:CYS:O	1:A:95:ASN:CB	0.47	2.63	5	3
1:A:71:LEU:HD23	1:A:80:ARG:HD2	0.47	1.85	20	1
1:A:71:LEU:CD1	1:A:83:VAL:CG2	0.47	2.93	7	1
1:A:76:TRP:CE3	1:A:79:MET:HE1	0.47	2.45	20	3
1:A:14:GLN:HB3	1:A:58:LEU:HD21	0.46	1.86	5	1
1:A:80:ARG:CD	1:A:80:ARG:C	0.46	2.82	5	1
1:A:15:MET:HE2	1:A:66:ALA:O	0.46	2.09	12	4
1:A:67:ILE:CD1	1:A:91:PRO:CB	0.46	2.93	12	2
1:A:28:LEU:CD2	1:A:86:MET:CB	0.46	2.92	13	1
1:A:20:MET:HG2	1:A:21:LEU:HD23	0.46	1.86	15	1
1:A:79:MET:O	1:A:83:VAL:HG13	0.46	2.11	5	1
1:A:20:MET:HE2	1:A:55:LEU:N	0.46	2.25	20	1
1:A:70:MET:O	1:A:76:TRP:CD1	0.46	2.68	12	2
1:A:21:LEU:CB	1:A:70:MET:HG3	0.46	2.40	6	7
1:A:75:MET:O	1:A:79:MET:CE	0.46	2.64	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:SER:C	1:A:88:HIS:CD2	0.45	2.90	5	1
1:A:75:MET:O	1:A:76:TRP:CD2	0.45	2.68	17	6
1:A:84:MET:HG3	1:A:85:SER:N	0.45	2.26	9	1
1:A:15:MET:SD	1:A:20:MET:CE	0.45	3.05	1	1
1:A:88:HIS:CD2	1:A:89:ASN:N	0.45	2.85	6	4
1:A:76:TRP:CE3	1:A:80:ARG:CZ	0.45	2.99	20	1
1:A:12:TYR:CD2	1:A:69:MET:HB3	0.45	2.47	13	2
1:A:21:LEU:HD23	1:A:70:MET:CB	0.45	2.40	16	1
1:A:99:GLN:N	1:A:100:PRO:CD	0.45	2.79	5	1
1:A:20:MET:HE3	1:A:21:LEU:HD12	0.45	1.85	8	1
1:A:20:MET:CG	1:A:21:LEU:HD12	0.45	2.42	12	1
1:A:64:CYS:SG	1:A:65:PRO:HD3	0.44	2.52	11	1
1:A:88:HIS:CE1	1:A:89:ASN:ND2	0.44	2.85	7	4
1:A:21:LEU:HD13	1:A:76:TRP:CZ2	0.44	2.47	9	1
1:A:84:MET:C	1:A:88:HIS:CE1	0.44	2.91	13	1
1:A:25:GLY:HA3	1:A:76:TRP:CZ2	0.44	2.48	17	4
1:A:21:LEU:CB	1:A:70:MET:SD	0.44	3.06	2	2
1:A:18:ALA:O	1:A:20:MET:N	0.44	2.51	16	2
1:A:21:LEU:CD2	1:A:55:LEU:CD1	0.44	2.86	1	1
1:A:15:MET:CE	1:A:66:ALA:O	0.44	2.65	10	1
1:A:15:MET:HA	1:A:20:MET:HE1	0.44	1.88	4	1
1:A:21:LEU:HD13	1:A:70:MET:CG	0.43	2.43	3	1
1:A:64:CYS:N	1:A:65:PRO:CD	0.43	2.81	5	1
1:A:70:MET:HE2	1:A:71:LEU:HD11	0.43	1.90	17	2
1:A:29:MET:HG3	1:A:76:TRP:CZ3	0.43	2.49	10	1
1:A:68:MET:O	1:A:72:ASN:ND2	0.43	2.52	5	1
1:A:21:LEU:HB3	1:A:70:MET:HG3	0.43	1.91	15	2
1:A:64:CYS:CB	1:A:65:PRO:HD3	0.43	2.44	12	9
1:A:78:ARG:O	1:A:81:ASP:N	0.43	2.51	5	1
1:A:55:LEU:CD2	1:A:58:LEU:HD12	0.43	2.44	20	1
1:A:70:MET:HG2	1:A:71:LEU:N	0.43	2.29	20	1
1:A:15:MET:CG	1:A:20:MET:HE3	0.43	2.43	8	1
1:A:97:MET:O	1:A:98:SER:C	0.43	2.57	5	1
1:A:87:ALA:O	1:A:91:PRO:CG	0.43	2.67	5	2
1:A:15:MET:HG3	1:A:20:MET:HE3	0.42	1.90	12	1
1:A:21:LEU:HB3	1:A:70:MET:CE	0.42	2.44	14	3
1:A:15:MET:HE3	1:A:66:ALA:HB1	0.42	1.91	13	1
1:A:75:MET:O	1:A:79:MET:HE2	0.42	2.14	7	2
1:A:14:GLN:CG	1:A:58:LEU:CD2	0.42	2.98	17	2
1:A:80:ARG:C	1:A:82:GLN:N	0.42	2.72	5	1
1:A:11:CYS:HA	1:A:14:GLN:NE2	0.42	2.29	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:MET:CG	1:A:20:MET:CE	0.42	2.97	8	1
1:A:21:LEU:HB3	1:A:70:MET:HE3	0.42	1.91	8	1
1:A:71:LEU:HD22	1:A:83:VAL:HG23	0.42	1.90	12	1
1:A:20:MET:SD	1:A:58:LEU:CD1	0.42	3.07	3	2
1:A:21:LEU:HA	1:A:24:CYS:SG	0.42	2.55	19	1
1:A:70:MET:HE3	1:A:87:ALA:HB1	0.42	1.91	9	1
1:A:80:ARG:O	1:A:81:ASP:C	0.42	2.57	10	1
1:A:18:ALA:HB1	1:A:54:GLN:HG2	0.42	1.91	19	1
1:A:70:MET:HE1	1:A:87:ALA:CB	0.42	2.45	12	1
1:A:71:LEU:HD12	1:A:84:MET:CE	0.42	2.45	19	1
1:A:21:LEU:HD11	1:A:55:LEU:HD21	0.41	1.91	12	1
1:A:27:TYR:CD1	1:A:27:TYR:C	0.41	2.93	17	2
1:A:71:LEU:HD22	1:A:80:ARG:HB2	0.41	1.92	13	1
1:A:23:HIS:CD2	1:A:23:HIS:N	0.41	2.88	16	1
1:A:15:MET:HE2	1:A:66:ALA:C	0.41	2.35	3	1
1:A:21:LEU:HD13	1:A:70:MET:HB2	0.41	1.93	3	1
1:A:21:LEU:CD1	1:A:70:MET:CE	0.41	2.95	10	1
1:A:80:ARG:CZ	1:A:84:MET:CE	0.41	2.99	1	1
1:A:71:LEU:HD21	1:A:83:VAL:CG2	0.41	2.44	10	1
1:A:20:MET:HE1	1:A:58:LEU:CD1	0.41	2.46	11	1
1:A:20:MET:HG2	1:A:21:LEU:CD1	0.41	2.43	5	1
1:A:70:MET:HE1	1:A:87:ALA:HB1	0.41	1.93	5	1
1:A:15:MET:HE3	1:A:66:ALA:C	0.41	2.35	1	1
1:A:58:LEU:HD23	1:A:58:LEU:HA	0.41	1.81	17	1
1:A:14:GLN:CB	1:A:58:LEU:HD21	0.41	2.46	5	1
1:A:80:ARG:O	1:A:82:GLN:N	0.41	2.55	5	1
1:A:15:MET:HA	1:A:20:MET:CE	0.41	2.46	14	1
1:A:55:LEU:HG	1:A:96:LEU:HD13	0.41	1.93	16	1
1:A:64:CYS:HB3	1:A:65:PRO:HD3	0.40	1.93	9	1
1:A:88:HIS:CD2	1:A:88:HIS:N	0.40	2.89	18	2
1:A:71:LEU:HD23	1:A:83:VAL:HG23	0.40	1.92	1	1
1:A:70:MET:CE	1:A:87:ALA:CB	0.40	2.99	12	1
1:A:63:MET:SD	1:A:96:LEU:CD2	0.40	3.09	10	1
1:A:29:MET:CE	1:A:79:MET:HB2	0.40	2.47	15	1
1:A:76:TRP:CZ3	1:A:79:MET:HE3	0.40	2.51	1	1
1:A:15:MET:SD	1:A:70:MET:CB	0.40	3.10	2	1
1:A:71:LEU:HB3	1:A:80:ARG:CD	0.40	2.47	17	1
1:A:80:ARG:HA	1:A:83:VAL:CG1	0.40	2.45	17	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	74/103 (72%)	54±3 (73±4%)	14±2 (19±3%)	6±1 (8±2%)	2 15
All	All	1480/2060 (72%)	1087 (73%)	282 (19%)	111 (8%)	2 15

All 15 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	64	CYS	20
1	A	100	PRO	20
1	A	19	GLU	18
1	A	77	ILE	17
1	A	75	MET	12
1	A	83	VAL	6
1	A	81	ASP	3
1	A	98	SER	3
1	A	95	ASN	3
1	A	58	LEU	2
1	A	84	MET	2
1	A	85	SER	2
1	A	59	ASP	1
1	A	74	PRO	1
1	A	11	CYS	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	70/95 (74%)	46±3 (66±5%)	24±3 (34±5%)	1 11
All	All	1400/1900 (74%)	928 (66%)	472 (34%)	1 11

All 51 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	64	CYS	20
1	A	95	ASN	20
1	A	70	MET	19
1	A	88	HIS	17
1	A	14	GLN	15
1	A	19	GLU	15
1	A	29	MET	15
1	A	30	LYS	15
1	A	92	ILE	15
1	A	55	LEU	14
1	A	59	ASP	14
1	A	67	ILE	14
1	A	75	MET	13
1	A	28	LEU	12
1	A	79	MET	12
1	A	82	GLN	12
1	A	68	MET	12
1	A	60	GLU	11
1	A	93	GLU	11
1	A	20	MET	11
1	A	73	GLU	10
1	A	78	ARG	10
1	A	80	ARG	10
1	A	84	MET	10
1	A	81	ASP	10
1	A	97	MET	10
1	A	24	CYS	9
1	A	99	GLN	9
1	A	83	VAL	9
1	A	15	MET	8
1	A	89	ASN	8
1	A	21	LEU	7
1	A	26	MET	7
1	A	85	SER	7
1	A	53	MET	6
1	A	61	LYS	6
1	A	13	GLN	5
1	A	17	GLU	5
1	A	54	GLN	5
1	A	22	ASN	5
1	A	57	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	49	GLN	4
1	A	51	CYS	4
1	A	16	GLU	3
1	A	56	LYS	3
1	A	98	SER	3
1	A	71	LEU	2
1	A	50	LEU	2
1	A	31	ASN	2
1	A	101	CYS	1
1	A	52	CYS	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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided