Full wwPDB NMR Structure Validation Report (i)

Feb 8, 2022 – 05:03 PM EST

PDB ID	:	1CKR
Title	:	HIGH RESOLUTION SOLUTION STRUCTURE OF THE HEAT SHOCK COGNATE-70 KD SUBSTRATE BINDING DOMAIN OBTAINED BY MULTIDIMENSIONAL NMR TECHNIQUES
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Deposited on	:	1999-04-22

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

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

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

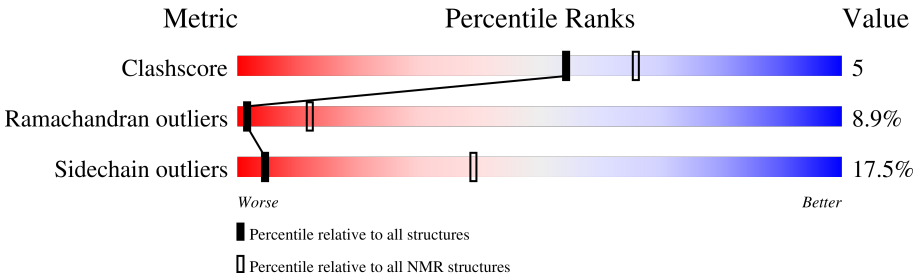
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

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	159	58% 25% 8% • 8%

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 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:392-A:503, A:507-A:540 (146)	0.31	12

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 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2482 atoms, of which 1252 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	159	2482	762	1252	209	256	3	0

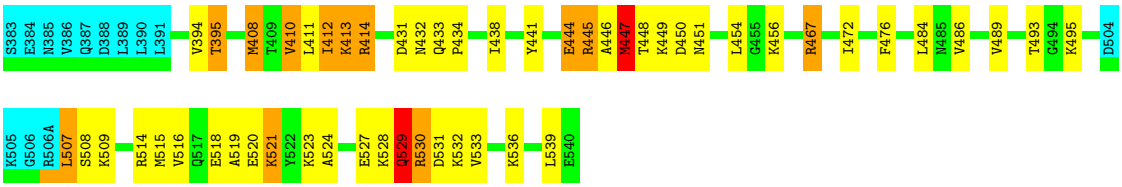
4 Residue-property plots (i)

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: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

Chain A: 



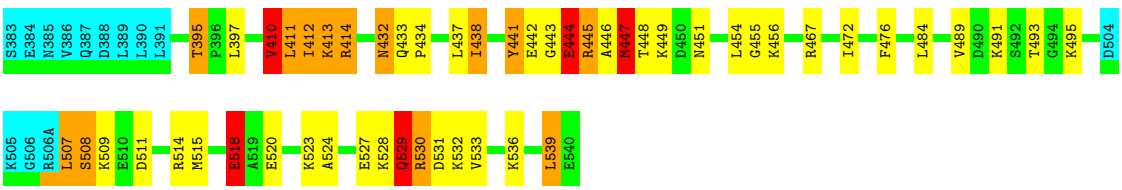
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

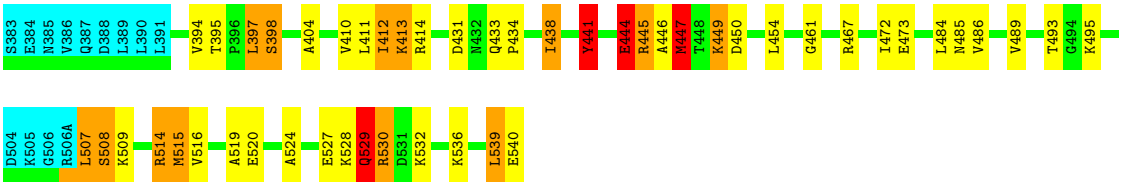
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

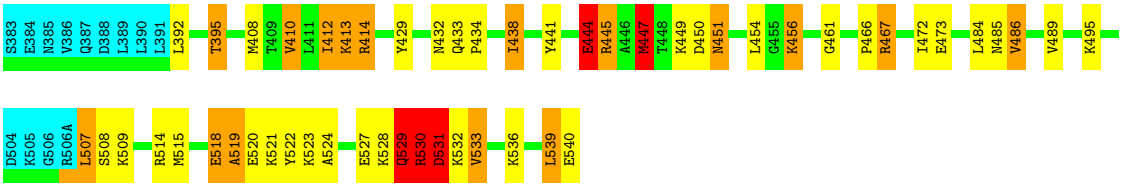
Chain A: 



4.2.3 Score per residue for model 3

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

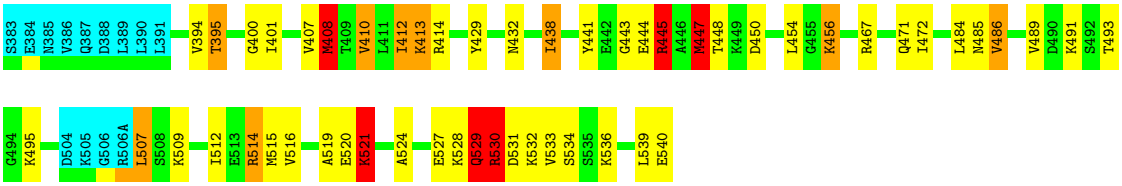
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

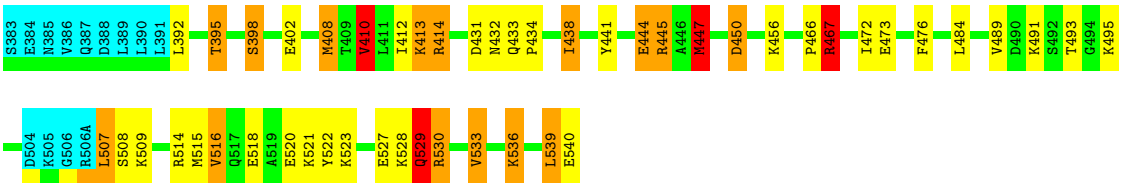
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

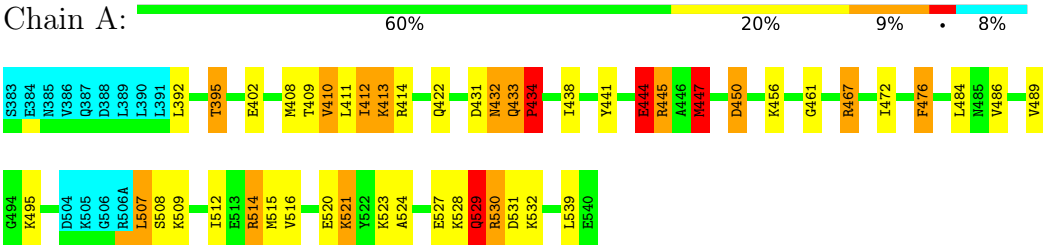
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

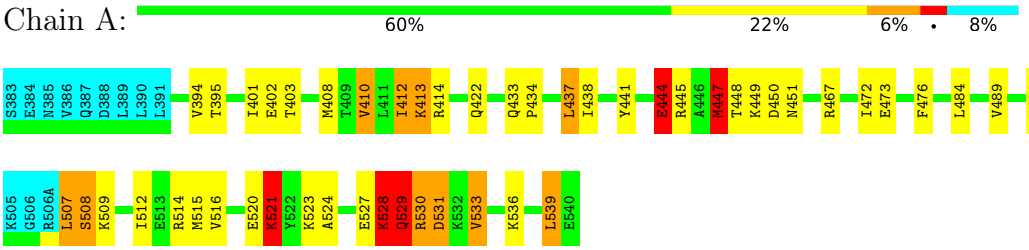
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

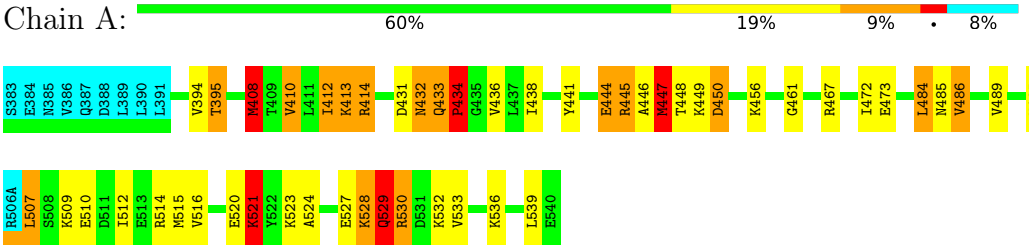
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

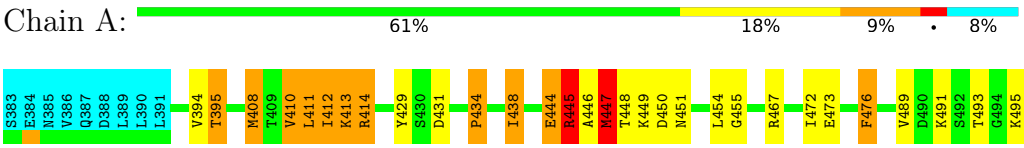
Chain A:



4.2.9 Score per residue for model 9

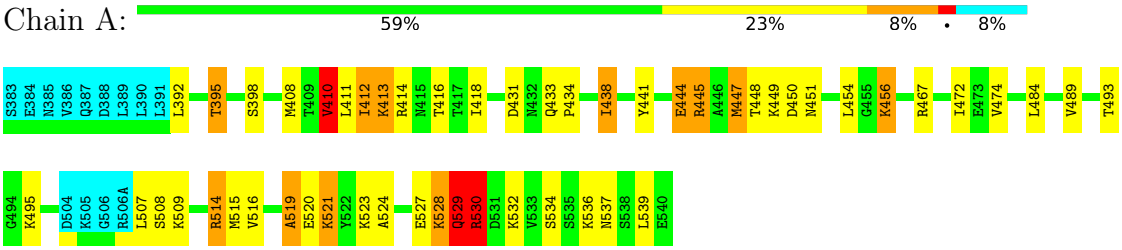
• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

Chain A:



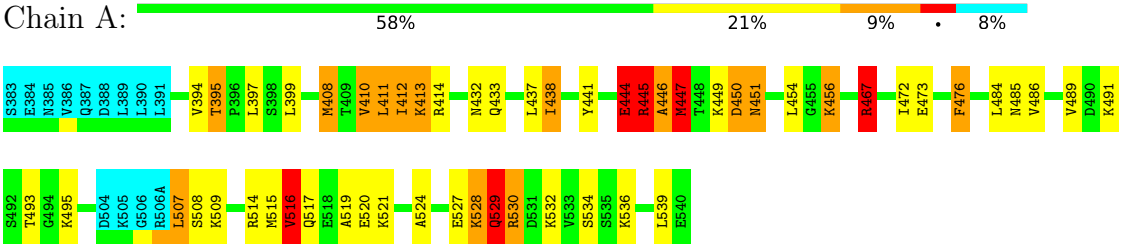
4.2.10 Score per residue for model 10

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70



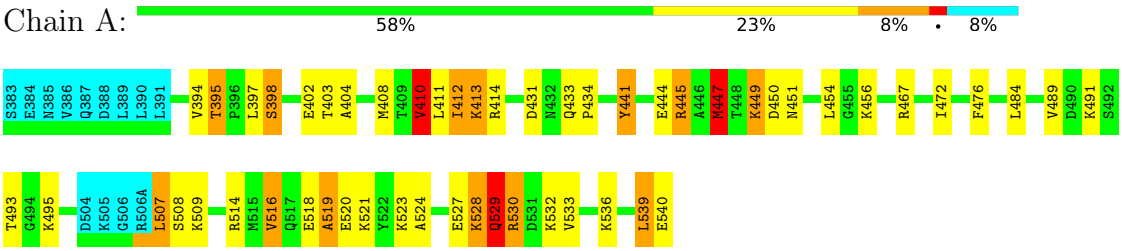
4.2.11 Score per residue for model 11

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70



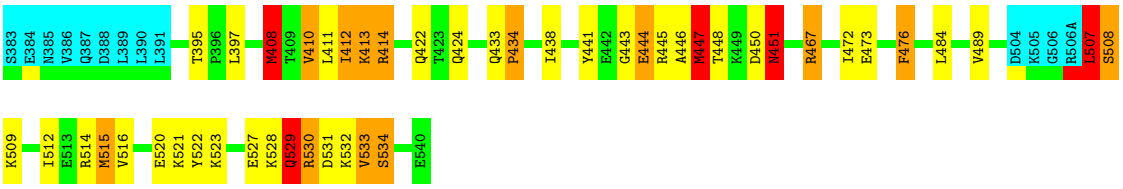
4.2.12 Score per residue for model 12 (medoid)

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70



4.2.13 Score per residue for model 13

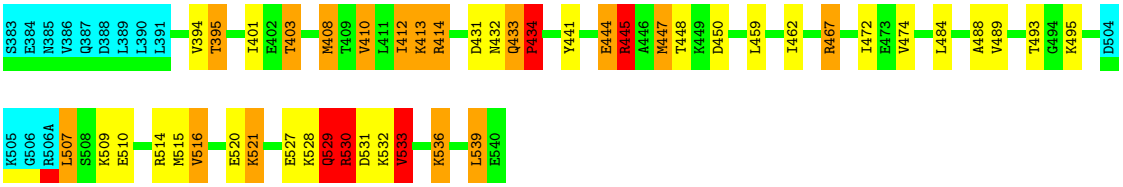
• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70



4.2.14 Score per residue for model 14

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

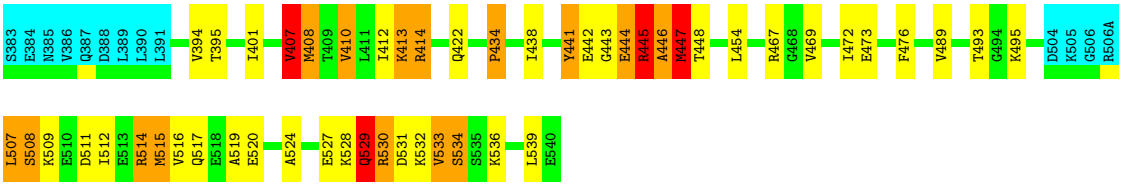
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

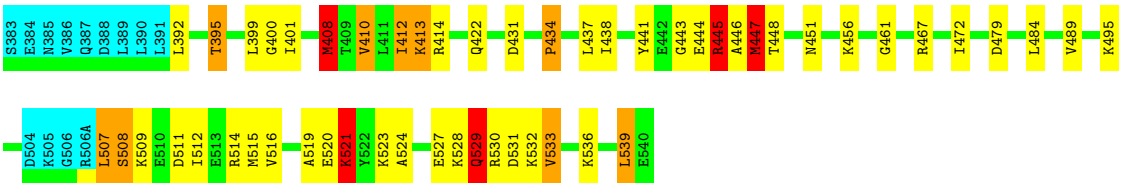
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

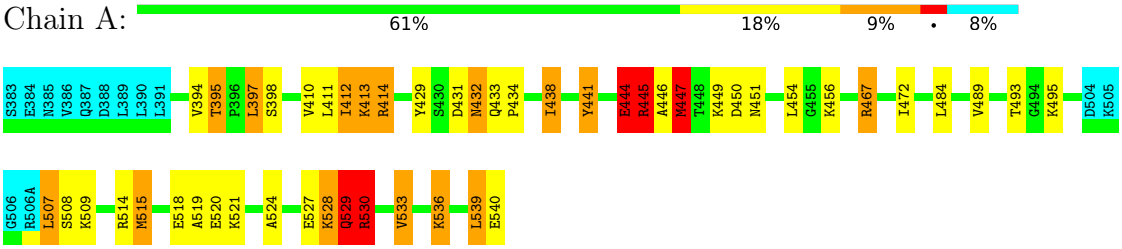
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

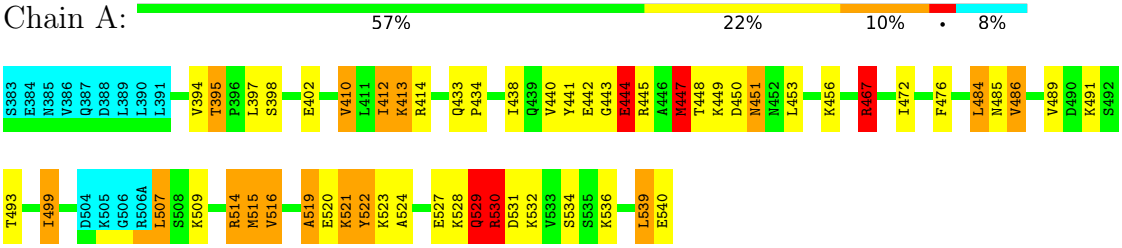
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

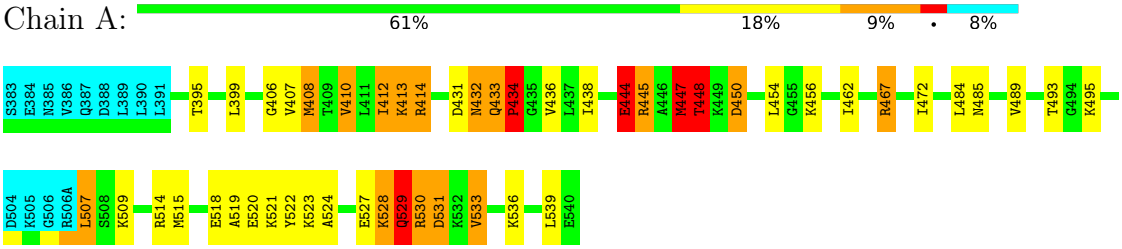
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

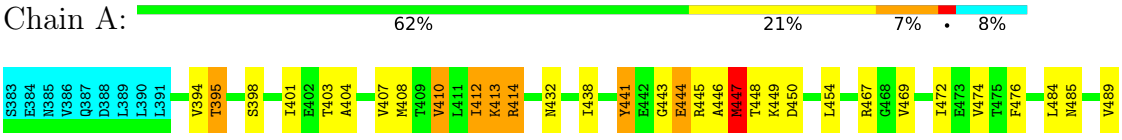
Chain A:

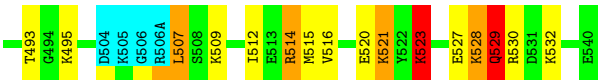


4.2.20 Score per residue for model 20

• Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

Chain A:




T493
G494
K495
D504
K505
G506
R506A
L507
S508
K509
I512
E513
R514
M515
V516
E520
K521
Y522
K523
E527
K528
Q529
R530
D531
K532
E540

5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY, SIMULATE ANNEALING*.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *LOWEST TOTAL ENERGY*.

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

Software name	Classification	Version
Discover	refinement	
Felix	structure solution	
MSI INSIGHT	structure solution	INSIGHT
MSI DISCOVER	structure solution	DISCOVER

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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	1.12±0.01	0±0/1139 (0.0± 0.0%)	1.84±0.03	33±3/1539 (2.1± 0.2%)
All	All	1.12	0/22780 (0.0%)	1.84	655/30780 (2.1%)

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	1.9±1.1
All	All	0	38

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	447	MET	N-CA-C	14.26	149.49	111.00	20	15
1	A	408	MET	CA-CB-CG	12.95	135.32	113.30	8	6
1	A	447	MET	CB-CA-C	11.83	134.06	110.40	15	5
1	A	447	MET	N-CA-CB	-11.59	89.73	110.60	20	20
1	A	514	ARG	NE-CZ-NH1	10.75	125.67	120.30	13	20
1	A	528	LYS	CB-CA-C	10.55	131.50	110.40	19	20
1	A	467	ARG	NE-CZ-NH1	10.50	125.55	120.30	8	20
1	A	444	GLU	N-CA-CB	-10.36	91.96	110.60	10	13
1	A	414	ARG	NE-CZ-NH1	9.39	124.99	120.30	8	20
1	A	445	ARG	NE-CZ-NH1	9.34	124.97	120.30	2	20
1	A	524	ALA	CB-CA-C	8.84	123.36	110.10	1	16
1	A	529	GLN	N-CA-CB	-8.81	94.74	110.60	5	18
1	A	443	GLY	N-CA-C	8.78	135.04	113.10	20	4
1	A	446	ALA	C-N-CA	8.54	143.05	121.70	15	3
1	A	444	GLU	N-CA-C	8.50	133.94	111.00	10	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	441	TYR	CB-CG-CD2	-8.33	116.00	121.00	2	12
1	A	446	ALA	CA-C-N	-8.27	99.01	117.20	15	4
1	A	530	ARG	NE-CZ-NH1	8.12	124.36	120.30	3	20
1	A	514	ARG	NE-CZ-NH2	-8.07	116.26	120.30	13	12
1	A	529	GLN	CB-CG-CD	8.05	132.54	111.60	16	4
1	A	445	ARG	NE-CZ-NH2	-7.98	116.31	120.30	14	13
1	A	524	ALA	N-CA-CB	-7.82	99.16	110.10	1	5
1	A	447	MET	CG-SD-CE	7.80	112.68	100.20	4	4
1	A	441	TYR	CB-CG-CD1	7.75	125.65	121.00	14	11
1	A	519	ALA	N-CA-CB	-7.73	99.28	110.10	3	3
1	A	450	ASP	N-CA-CB	-7.54	97.04	110.60	9	9
1	A	523	LYS	CB-CA-C	7.39	125.19	110.40	20	1
1	A	531	ASP	CA-C-N	-7.35	101.02	117.20	19	2
1	A	523	LYS	N-CA-CB	-7.33	97.40	110.60	12	12
1	A	529	GLN	CA-CB-CG	7.33	129.52	113.40	15	12
1	A	398	SER	N-CA-CB	-7.29	99.57	110.50	18	4
1	A	519	ALA	CB-CA-C	7.26	120.99	110.10	10	5
1	A	486	VAL	CA-CB-CG1	7.21	121.71	110.90	18	1
1	A	429	TYR	CB-CG-CD2	-7.08	116.75	121.00	9	4
1	A	533	VAL	N-CA-CB	-7.01	96.07	111.50	19	5
1	A	529	GLN	CB-CA-C	6.88	124.16	110.40	3	5
1	A	521	LYS	N-CA-CB	-6.74	98.47	110.60	10	10
1	A	493	THR	CA-CB-CG2	6.64	121.69	112.40	2	16
1	A	447	MET	CA-C-N	-6.62	102.64	117.20	13	7
1	A	410	VAL	CA-CB-CG1	6.62	120.82	110.90	17	20
1	A	447	MET	C-N-CA	6.60	138.19	121.70	13	4
1	A	528	LYS	N-CA-CB	-6.52	98.86	110.60	19	2
1	A	407	VAL	CA-CB-CG1	6.37	120.45	110.90	15	1
1	A	451	ASN	N-CA-CB	-6.30	99.25	110.60	10	2
1	A	489	VAL	CA-CB-CG2	6.28	120.32	110.90	9	20
1	A	443	GLY	CA-C-N	6.26	130.98	117.20	20	1
1	A	410	VAL	CG1-CB-CG2	-6.20	100.98	110.90	17	12
1	A	515	MET	CA-CB-CG	6.17	123.80	113.30	2	2
1	A	444	GLU	C-N-CA	6.14	137.04	121.70	3	2
1	A	529	GLN	CA-C-N	-6.05	103.89	117.20	13	12
1	A	530	ARG	NE-CZ-NH2	-5.96	117.32	120.30	8	8
1	A	467	ARG	NE-CZ-NH2	-5.95	117.32	120.30	10	14
1	A	444	GLU	CA-CB-CG	5.92	126.41	113.40	1	2
1	A	451	ASN	CB-CA-C	5.88	122.16	110.40	11	4
1	A	446	ALA	N-CA-CB	-5.84	101.93	110.10	2	1
1	A	445	ARG	CA-C-N	5.77	129.90	117.20	16	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	445	ARG	N-CA-CB	-5.77	100.22	110.60	18	3
1	A	536	LYS	CB-CA-C	5.75	121.90	110.40	3	3
1	A	407	VAL	CG1-CB-CG2	-5.73	101.72	110.90	15	1
1	A	533	VAL	CB-CA-C	5.73	122.28	111.40	19	4
1	A	451	ASN	CA-CB-CG	5.69	125.92	113.40	11	2
1	A	450	ASP	CA-CB-CG	5.66	125.86	113.40	17	1
1	A	495	LYS	N-CA-CB	-5.64	100.44	110.60	9	15
1	A	456	LYS	CA-CB-CG	5.54	125.58	113.40	10	5
1	A	408	MET	CB-CA-C	-5.54	99.33	110.40	11	5
1	A	414	ARG	NE-CZ-NH2	-5.53	117.53	120.30	16	3
1	A	539	LEU	CA-CB-CG	5.51	127.97	115.30	1	3
1	A	395	THR	CA-CB-CG2	5.49	120.08	112.40	18	15
1	A	440	VAL	CG1-CB-CG2	-5.47	102.14	110.90	18	1
1	A	434	PRO	N-CA-C	5.45	126.26	112.10	14	4
1	A	410	VAL	CA-C-N	-5.44	105.24	117.20	10	6
1	A	394	VAL	CA-CB-CG2	5.42	119.03	110.90	17	12
1	A	519	ALA	CA-C-N	5.42	129.12	117.20	16	2
1	A	516	VAL	CA-CB-CG1	5.42	119.02	110.90	5	4
1	A	484	LEU	CB-CG-CD1	5.40	120.19	111.00	13	7
1	A	429	TYR	CB-CG-CD1	5.34	124.20	121.00	9	1
1	A	533	VAL	CA-CB-CG1	5.32	118.88	110.90	17	1
1	A	446	ALA	CA-C-O	5.30	131.24	120.10	15	1
1	A	534	SER	CB-CA-C	5.28	120.14	110.10	13	1
1	A	469	VAL	CA-C-N	5.28	131.88	117.10	15	2
1	A	433	GLN	N-CA-C	5.28	125.25	111.00	11	4
1	A	444	GLU	CB-CG-CD	5.26	128.40	114.20	9	2
1	A	508	SER	N-CA-CB	-5.25	102.62	110.50	15	6
1	A	444	GLU	O-C-N	-5.24	114.31	122.70	10	1
1	A	433	GLN	CA-C-N	5.23	131.74	117.10	6	4
1	A	403	THR	CA-CB-CG2	5.22	119.70	112.40	14	1
1	A	528	LYS	C-N-CA	5.21	134.74	121.70	7	4
1	A	453	LEU	CB-CG-CD1	5.20	119.84	111.00	18	1
1	A	522	TYR	N-CA-CB	-5.20	101.25	110.60	9	1
1	A	402	GLU	CA-CB-CG	5.17	124.78	113.40	5	1
1	A	518	GLU	N-CA-CB	5.17	119.91	110.60	1	2
1	A	508	SER	CB-CA-C	5.17	119.92	110.10	12	6
1	A	486	VAL	CA-CB-CG2	5.17	118.66	110.90	3	3
1	A	399	LEU	CB-CG-CD2	5.17	119.79	111.00	19	2
1	A	522	TYR	CB-CG-CD1	-5.17	117.90	121.00	18	1
1	A	539	LEU	CB-CG-CD1	5.16	119.77	111.00	14	2
1	A	402	GLU	N-CA-CB	-5.16	101.32	110.60	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	532	LYS	CA-CB-CG	5.15	124.73	113.40	9	1
1	A	516	VAL	CA-CB-CG2	5.14	118.61	110.90	11	1
1	A	450	ASP	CB-CG-OD1	5.13	122.92	118.30	8	1
1	A	517	GLN	CB-CA-C	5.13	120.66	110.40	11	1
1	A	408	MET	N-CA-CB	-5.09	101.44	110.60	8	1
1	A	443	GLY	CA-C-O	-5.07	111.47	120.60	20	1
1	A	493	THR	N-CA-CB	-5.04	100.71	110.30	11	3
1	A	443	GLY	C-N-CA	5.01	134.23	121.70	18	1
1	A	507	LEU	CB-CG-CD1	5.01	119.51	111.00	13	1
1	A	442	GLU	CB-CA-C	5.00	120.40	110.40	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	441	TYR	Sidechain	10
1	A	476	PHE	Sidechain	10
1	A	445	ARG	Sidechain	8
1	A	530	ARG	Sidechain	2
1	A	522	TYR	Sidechain	2
1	A	447	MET	Mainchain	2
1	A	450	ASP	Mainchain	1
1	A	528	LYS	Mainchain	1
1	A	467	ARG	Sidechain	1
1	A	514	ARG	Sidechain	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	1127	1146	1146	12±4
All	All	22540	22920	22919	247

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:408:MET:HB3	1:A:447:MET:SD	0.86	2.10	4	3
1:A:444:GLU:HB2	1:A:447:MET:SD	0.69	2.27	15	3
1:A:444:GLU:CB	1:A:447:MET:SD	0.66	2.84	20	5
1:A:408:MET:HB2	1:A:447:MET:SD	0.65	2.32	15	3
1:A:408:MET:HB2	1:A:447:MET:HG3	0.64	1.69	14	2
1:A:401:ILE:HD12	1:A:403:THR:HG21	0.64	1.69	7	1
1:A:529:GLN:HG2	1:A:530:ARG:H	0.63	1.52	4	11
1:A:400:GLY:HA3	1:A:408:MET:SD	0.63	2.33	16	2
1:A:438:ILE:HD12	1:A:539:LEU:HD11	0.63	1.70	4	5
1:A:408:MET:CG	1:A:447:MET:SD	0.62	2.87	8	2
1:A:447:MET:SD	1:A:448:THR:N	0.62	2.72	19	1
1:A:407:VAL:HB	1:A:447:MET:HB3	0.62	1.71	4	1
1:A:507:LEU:H	1:A:507:LEU:HD23	0.61	1.55	9	10
1:A:398:SER:OG	1:A:410:VAL:HG21	0.61	1.95	5	2
1:A:444:GLU:CD	1:A:447:MET:SD	0.61	2.79	19	4
1:A:412:ILE:HG22	1:A:413:LYS:H	0.61	1.55	2	20
1:A:444:GLU:HB3	1:A:447:MET:SD	0.61	2.36	8	9
1:A:408:MET:CB	1:A:447:MET:SD	0.61	2.89	8	2
1:A:438:ILE:HD12	1:A:539:LEU:HD21	0.60	1.71	2	3
1:A:447:MET:SD	1:A:447:MET:C	0.60	2.79	6	5
1:A:438:ILE:CD1	1:A:539:LEU:HD21	0.60	2.27	5	2
1:A:408:MET:HG2	1:A:447:MET:SD	0.60	2.37	8	2
1:A:529:GLN:CG	1:A:530:ARG:H	0.58	2.10	3	16
1:A:523:LYS:HG2	1:A:529:GLN:HG3	0.58	1.73	9	3
1:A:408:MET:HB2	1:A:447:MET:CG	0.57	2.30	14	2
1:A:408:MET:HB3	1:A:447:MET:CE	0.56	2.31	16	2
1:A:444:GLU:C	1:A:519:ALA:HB1	0.56	2.21	10	1
1:A:523:LYS:CG	1:A:529:GLN:HG3	0.56	2.31	16	1
1:A:397:LEU:HD11	1:A:515:MET:SD	0.54	2.43	17	1
1:A:451:ASN:OD1	1:A:515:MET:SD	0.54	2.66	13	1
1:A:407:VAL:HG23	1:A:408:MET:H	0.54	1.63	15	1
1:A:450:ASP:O	1:A:515:MET:SD	0.53	2.66	5	9
1:A:408:MET:CB	1:A:447:MET:HG3	0.53	2.33	14	1
1:A:444:GLU:OE1	1:A:515:MET:SD	0.53	2.67	17	1
1:A:516:VAL:HG23	1:A:520:GLU:CG	0.52	2.35	14	2
1:A:401:ILE:O	1:A:408:MET:HA	0.51	2.06	15	4
1:A:531:ASP:O	1:A:533:VAL:HG12	0.51	2.06	13	6
1:A:408:MET:HB3	1:A:447:MET:CG	0.50	2.35	8	2
1:A:407:VAL:HG12	1:A:447:MET:O	0.50	2.06	20	1
1:A:410:VAL:HG21	1:A:444:GLU:OE1	0.50	2.06	10	1
1:A:529:GLN:CD	1:A:530:ARG:H	0.50	2.10	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:444:GLU:CG	1:A:447:MET:SD	0.49	3.00	18	2
1:A:512:ILE:O	1:A:516:VAL:HG12	0.49	2.08	4	6
1:A:407:VAL:HG21	1:A:530:ARG:CB	0.49	2.37	19	1
1:A:401:ILE:HD12	1:A:403:THR:CG2	0.49	2.38	7	2
1:A:408:MET:H	1:A:447:MET:HG3	0.49	1.67	16	2
1:A:539:LEU:O	1:A:539:LEU:HD22	0.48	2.08	5	2
1:A:446:ALA:HB2	1:A:529:GLN:HB2	0.48	1.84	17	3
1:A:437:LEU:O	1:A:539:LEU:HD11	0.48	2.08	7	1
1:A:408:MET:SD	1:A:447:MET:HE2	0.48	2.49	12	4
1:A:400:GLY:CA	1:A:408:MET:SD	0.47	3.03	16	2
1:A:397:LEU:HD11	1:A:443:GLY:HA2	0.47	1.87	1	1
1:A:445:ARG:O	1:A:447:MET:HB3	0.47	2.10	11	2
1:A:401:ILE:HD13	1:A:474:VAL:HG11	0.46	1.86	20	2
1:A:507:LEU:H	1:A:507:LEU:CD2	0.46	2.23	9	3
1:A:408:MET:HB2	1:A:447:MET:HE3	0.46	1.88	7	1
1:A:410:VAL:HB	1:A:523:LYS:HE3	0.46	1.86	1	1
1:A:518:GLU:O	1:A:522:TYR:HB3	0.46	2.11	19	2
1:A:444:GLU:O	1:A:523:LYS:HD2	0.46	2.11	1	1
1:A:407:VAL:HB	1:A:447:MET:CB	0.46	2.41	4	1
1:A:507:LEU:CD1	1:A:508:SER:H	0.45	2.24	5	2
1:A:516:VAL:HG23	1:A:520:GLU:HB2	0.45	1.88	5	1
1:A:511:ASP:O	1:A:515:MET:SD	0.45	2.74	16	2
1:A:408:MET:HB2	1:A:447:MET:CE	0.45	2.42	7	4
1:A:528:LYS:HB3	1:A:531:ASP:CB	0.45	2.42	7	2
1:A:397:LEU:HD12	1:A:516:VAL:HG11	0.45	1.88	11	1
1:A:486:VAL:HG13	1:A:499:ILE:HG23	0.44	1.89	18	1
1:A:398:SER:OG	1:A:444:GLU:OE1	0.44	2.33	10	1
1:A:447:MET:SD	1:A:447:MET:O	0.43	2.76	18	2
1:A:411:LEU:HD22	1:A:424:GLN:HB2	0.43	1.89	13	1
1:A:403:THR:HG22	1:A:539:LEU:HD22	0.43	1.90	7	1
1:A:438:ILE:HG21	1:A:474:VAL:HG11	0.43	1.91	10	1
1:A:408:MET:H	1:A:447:MET:CG	0.43	2.27	16	1
1:A:398:SER:OG	1:A:410:VAL:HG11	0.43	2.14	12	2
1:A:484:LEU:HD22	1:A:486:VAL:HB	0.43	1.90	18	1
1:A:444:GLU:HG2	1:A:450:ASP:H	0.43	1.73	5	1
1:A:397:LEU:HD21	1:A:515:MET:SD	0.43	2.54	13	1
1:A:512:ILE:HG23	1:A:516:VAL:CG1	0.42	2.44	15	2
1:A:444:GLU:HG3	1:A:450:ASP:H	0.42	1.73	14	2
1:A:407:VAL:CB	1:A:447:MET:HB3	0.42	2.42	4	1
1:A:411:LEU:HD21	1:A:476:PHE:CE1	0.42	2.49	1	5
1:A:459:LEU:HG	1:A:488:ALA:HB3	0.42	1.91	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:447:MET:HE3	1:A:447:MET:O	0.42	2.15	9	1
1:A:408:MET:CB	1:A:447:MET:CG	0.41	2.97	15	1
1:A:414:ARG:HD2	1:A:516:VAL:HG13	0.41	1.92	8	1
1:A:397:LEU:HD23	1:A:398:SER:H	0.41	1.76	2	1
1:A:444:GLU:HG3	1:A:449:LYS:HB3	0.41	1.91	8	2
1:A:533:VAL:HG13	1:A:534:SER:H	0.41	1.74	15	1
1:A:443:GLY:O	1:A:515:MET:SD	0.41	2.79	4	1
1:A:484:LEU:HG	1:A:486:VAL:HG22	0.41	1.91	8	1
1:A:408:MET:CG	1:A:444:GLU:HG3	0.41	2.46	10	1
1:A:408:MET:CB	1:A:447:MET:CE	0.41	2.98	16	1
1:A:416:THR:HG23	1:A:418:ILE:HG23	0.40	1.94	10	1
1:A:523:LYS:HG3	1:A:529:GLN:HG3	0.40	1.94	16	1
1:A:411:LEU:HD22	1:A:424:GLN:CB	0.40	2.46	13	1
1:A:529:GLN:HG2	1:A:530:ARG:N	0.40	2.31	8	1
1:A:444:GLU:HG2	1:A:447:MET:SD	0.40	2.55	18	1
1:A:512:ILE:HG23	1:A:516:VAL:HG11	0.40	1.93	6	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	145/159 (91%)	110±3 (76±2%)	22±3 (15±2%)	13±3 (9±2%)	1	12
All	All	2900/3180 (91%)	2202 (76%)	440 (15%)	258 (9%)	1	12

All 32 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	527	GLU	20
1	A	529	GLN	20
1	A	412	ILE	18
1	A	434	PRO	16
1	A	521	LYS	14
1	A	433	GLN	13

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Mol	Chain	Res	Type	Models (Total)
1	A	533	VAL	12
1	A	456	LYS	12
1	A	444	GLU	11
1	A	445	ARG	11
1	A	508	SER	10
1	A	449	LYS	9
1	A	519	ALA	8
1	A	467	ARG	8
1	A	448	THR	8
1	A	432	ASN	7
1	A	536	LYS	7
1	A	507	LEU	7
1	A	534	SER	6
1	A	518	GLU	5
1	A	461	GLY	5
1	A	516	VAL	5
1	A	447	MET	5
1	A	446	ALA	4
1	A	404	ALA	3
1	A	531	ASP	3
1	A	431	ASP	3
1	A	455	GLY	2
1	A	466	PRO	2
1	A	450	ASP	2
1	A	407	VAL	1
1	A	406	GLY	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	129/141 (91%)	106±2 (82±2%)	23±2 (18±2%)	4 39
All	All	2580/2820 (91%)	2128 (82%)	452 (18%)	4 39

All 63 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	395	THR	20
1	A	413	LYS	20
1	A	472	ILE	20
1	A	507	LEU	20
1	A	509	LYS	20
1	A	410	VAL	18
1	A	529	GLN	18
1	A	438	ILE	17
1	A	520	GLU	17
1	A	447	MET	16
1	A	532	LYS	16
1	A	539	LEU	13
1	A	454	LEU	12
1	A	484	LEU	11
1	A	414	ARG	10
1	A	432	ASN	9
1	A	536	LYS	9
1	A	473	GLU	9
1	A	434	PRO	9
1	A	445	ARG	8
1	A	491	LYS	8
1	A	431	ASP	8
1	A	485	ASN	8
1	A	451	ASN	8
1	A	411	LEU	7
1	A	515	MET	7
1	A	540	GLU	7
1	A	448	THR	6
1	A	514	ARG	6
1	A	530	ARG	6
1	A	521	LYS	6
1	A	528	LYS	6
1	A	486	VAL	5
1	A	392	LEU	5
1	A	408	MET	5
1	A	422	GLN	5
1	A	437	LEU	4
1	A	397	LEU	4
1	A	444	GLU	4
1	A	441	TYR	3
1	A	518	GLU	3
1	A	531	ASP	3
1	A	495	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	467	ARG	3
1	A	402	GLU	3
1	A	449	LYS	3
1	A	442	GLU	2
1	A	398	SER	2
1	A	436	VAL	2
1	A	510	GLU	2
1	A	537	ASN	2
1	A	403	THR	2
1	A	462	ILE	2
1	A	511	ASP	1
1	A	471	GLN	1
1	A	522	TYR	1
1	A	409	THR	1
1	A	399	LEU	1
1	A	516	VAL	1
1	A	517	GLN	1
1	A	479	ASP	1
1	A	499	ILE	1
1	A	523	LYS	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

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