



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:23 PM UTC

PDB ID : 1CKR / pdb_00001ckr
Title : HIGH RESOLUTION SOLUTION STRUCTURE OF THE HEAT SHOCK COGNATE-70 KD SUBSTRATE BINDING DOMAIN OBTAINED BY MULTIDIMENSIONAL NMR TECHNIQUES
Authors : Morshauser, R.C.; Hu, W.; Wang, H.; Pang, Y.; Flynn, G.C.; Zuiderweg, E.R.P.
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

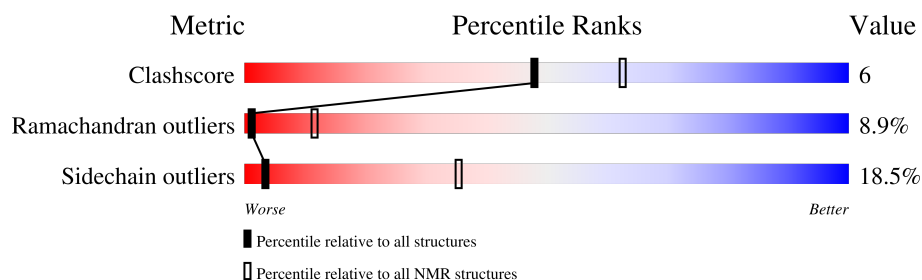
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	159	

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)	0.54	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.

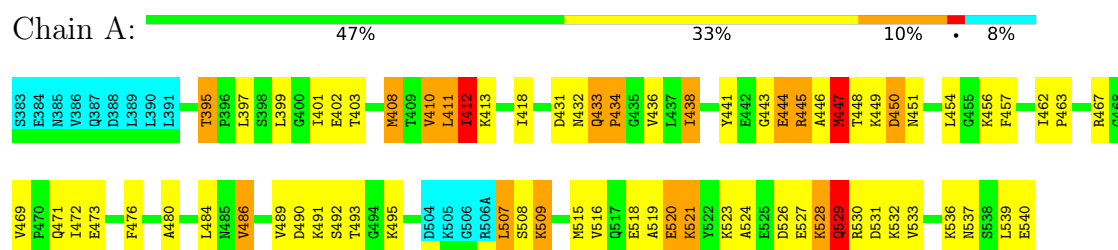
Mol	Chain	Residues	Atoms						Trace
1	A	159	Total	C	H	N	O	S	0
			2482	762	1252	209	256	3	

4 Residue-property plots

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

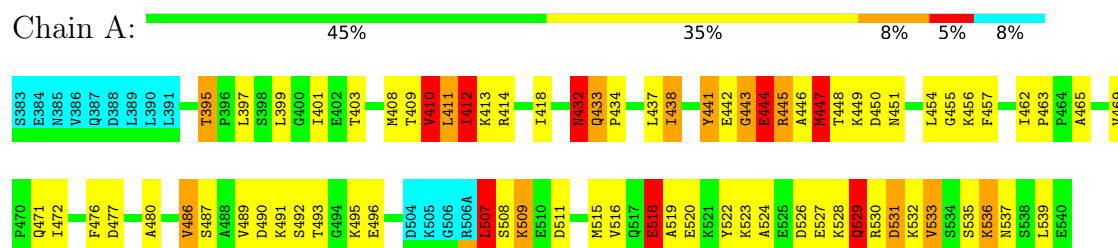


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

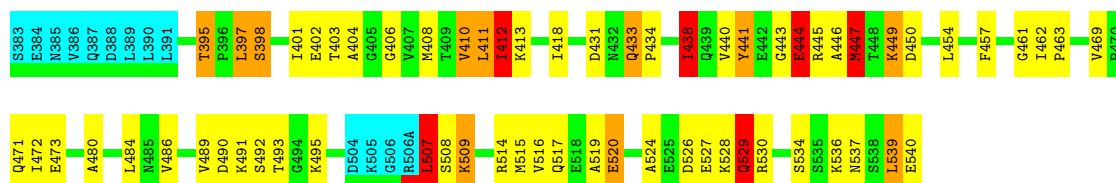
- Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70



4.2.2 Score per residue for model 2

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

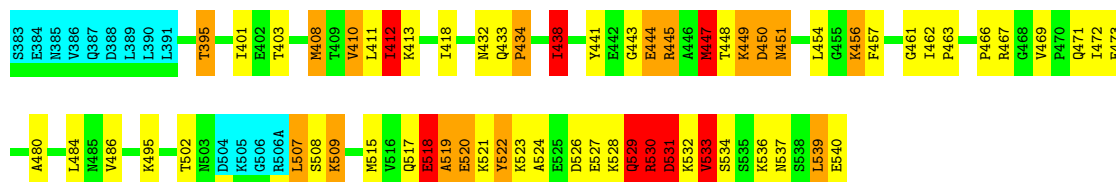




4.2.3 Score per residue for model 3

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

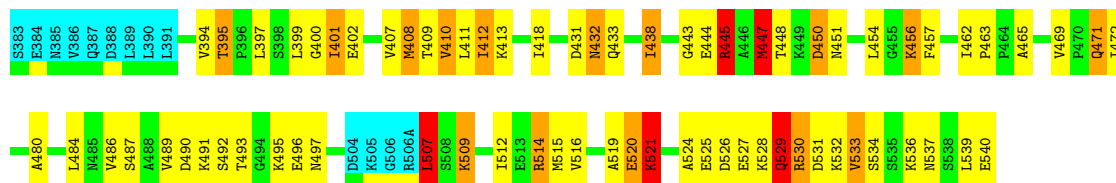
Chain A:



4.2.4 Score per residue for model 4

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

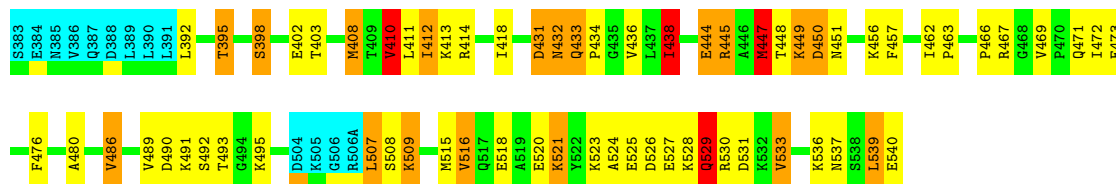
Chain A:



4.2.5 Score per residue for model 5

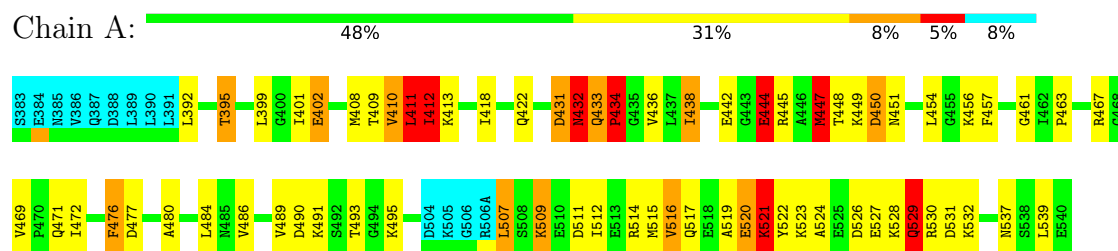
- Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

Chain A:



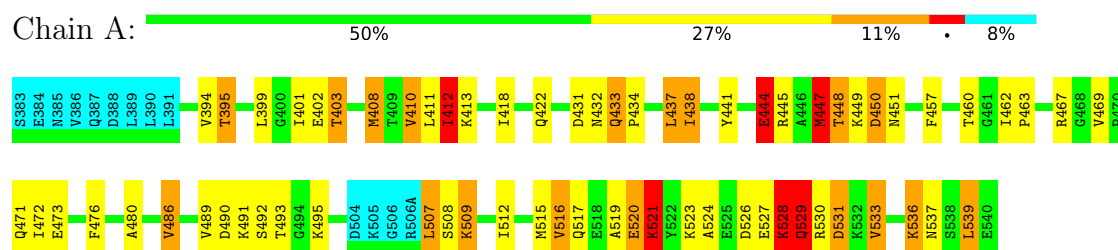
4.2.6 Score per residue for model 6

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



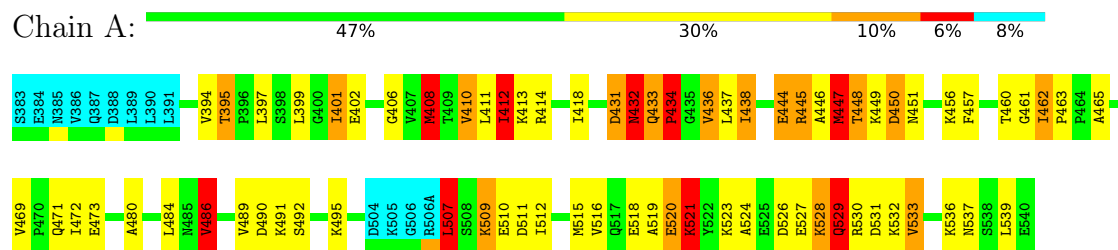
4.2.7 Score per residue for model 7

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



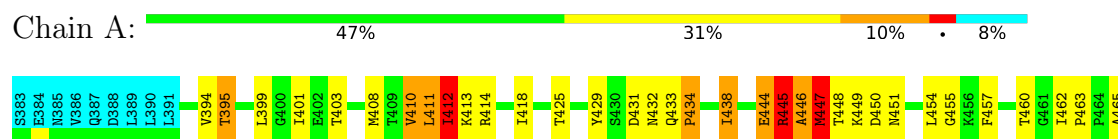
4.2.8 Score per residue for model 8

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



4.2.9 Score per residue for model 9

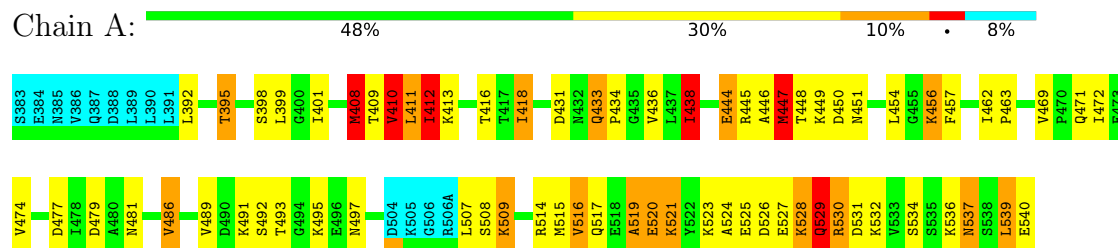
- Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70





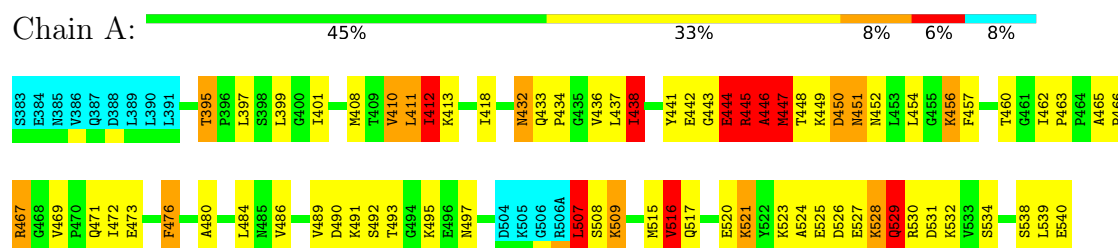
4.2.10 Score per residue for model 10

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



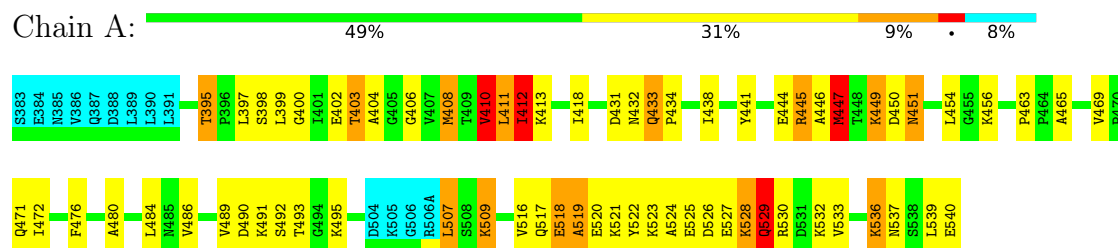
4.2.11 Score per residue for model 11

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



4.2.12 Score per residue for model 12 (medoid)

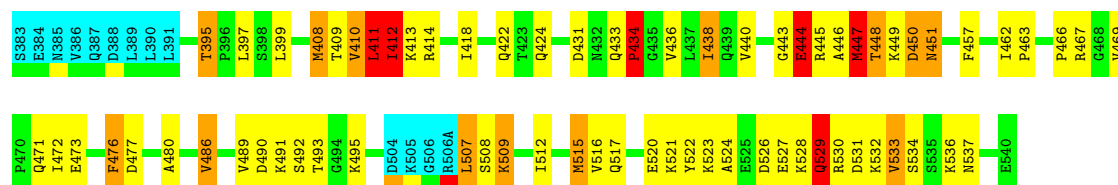
- Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70



4.2.13 Score per residue for model 13

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

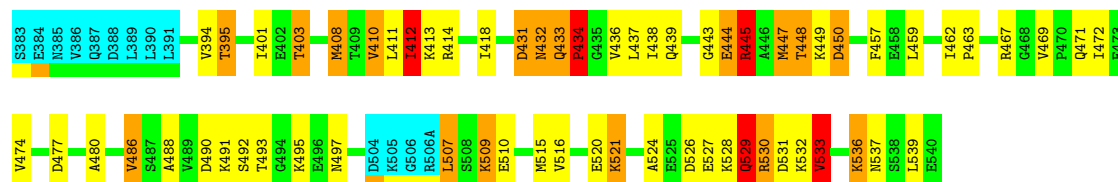




4.2.14 Score per residue for model 14

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

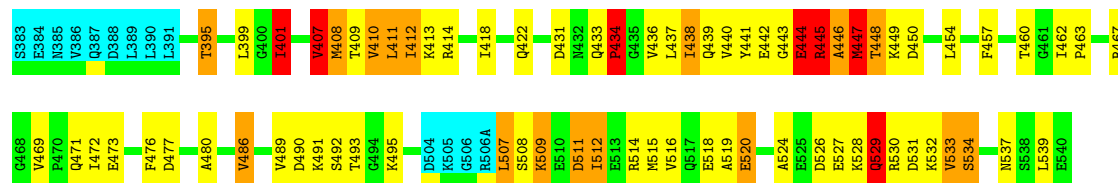
Chain A: 52% 26% 11% 8%



4.2.15 Score per residue for model 15

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

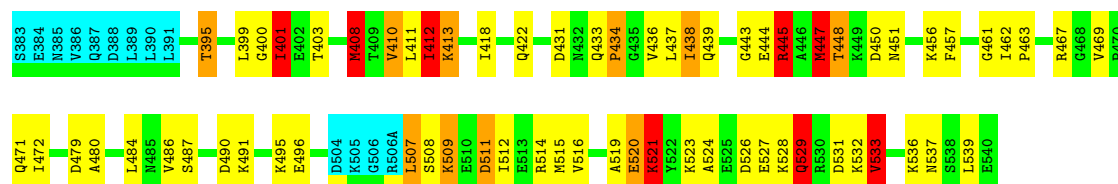
Chain A: 45% 32% 10% 8%



4.2.16 Score per residue for model 16

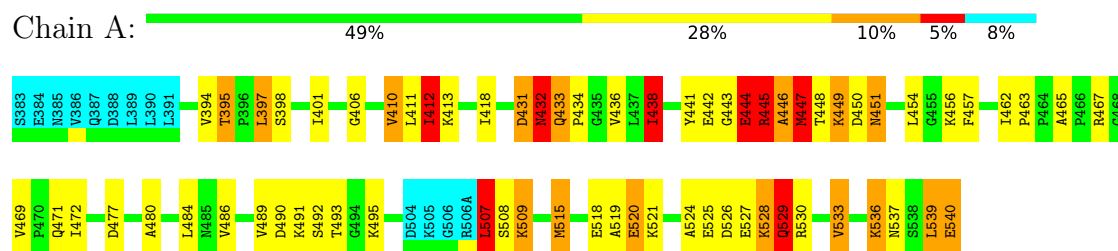
- Molecule 1: HEAT SHOCK SUBSTRATE BINDING DOMAIN OF HSC-70

Chain A: 50% 31% 6% 5% 8%



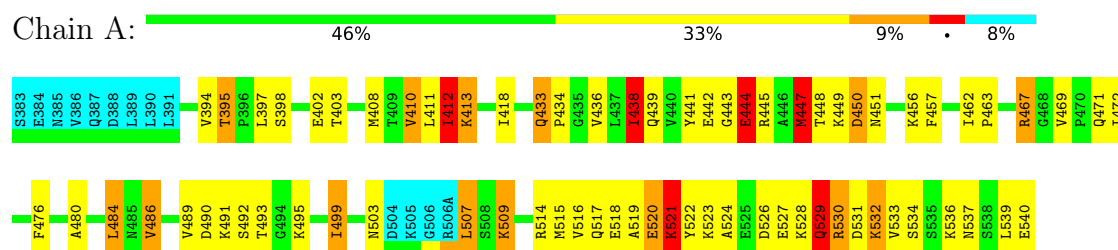
4.2.17 Score per residue for model 17

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



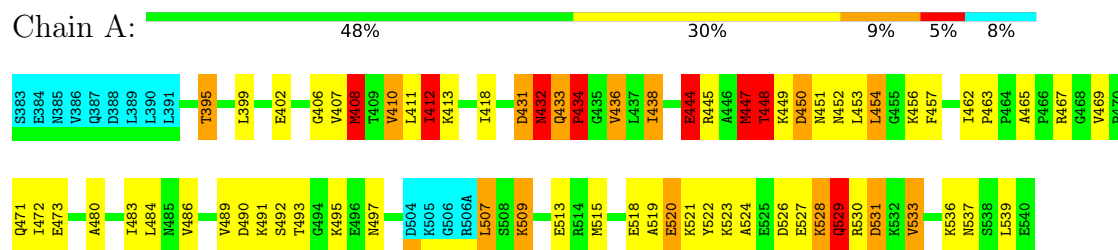
4.2.18 Score per residue for model 18

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



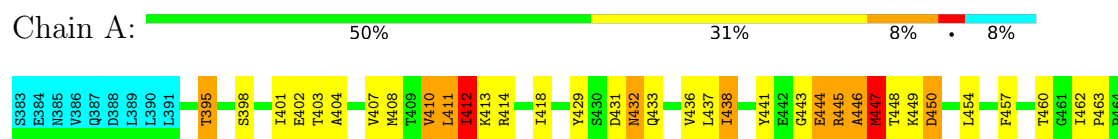
4.2.19 Score per residue for model 19

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



4.2.20 Score per residue for model 20

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





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	1.81±0.02	15±3/1139 (1.3± 0.2%)	2.21±0.05	53±5/1539 (3.5± 0.3%)
All	All	1.81	306/22780 (1.3%)	2.21	1065/30780 (3.5%)

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

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	526	ASP	CA-C	8.35	1.64	1.52	11	20
1	A	447	MET	CA-C	8.18	1.63	1.52	19	12
1	A	418	ILE	CA-C	8.00	1.61	1.52	10	20
1	A	446	ALA	CA-C	7.19	1.62	1.52	15	6
1	A	463	PRO	CA-C	7.11	1.58	1.52	20	20
1	A	524	ALA	CA-C	7.05	1.62	1.52	11	20
1	A	444	GLU	CA-C	7.05	1.62	1.52	9	8
1	A	519	ALA	CA-C	6.99	1.56	1.52	8	2
1	A	448	THR	CA-C	6.83	1.61	1.52	19	11
1	A	469	VAL	CA-C	6.82	1.60	1.52	15	20
1	A	403	THR	CA-C	6.71	1.57	1.53	3	4
1	A	433	GLN	CA-C	6.38	1.60	1.52	20	17
1	A	520	GLU	N-CA	6.30	1.54	1.46	16	10
1	A	451	ASN	N-CA	6.25	1.50	1.46	1	1
1	A	451	ASN	CA-C	6.21	1.57	1.53	1	1
1	A	526	ASP	N-CA	6.05	1.54	1.46	5	19

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	450	ASP	CA-C	5.93	1.59	1.53	16	1
1	A	528	LYS	CA-C	5.93	1.59	1.53	15	10
1	A	412	ILE	CA-C	5.84	1.60	1.52	13	19
1	A	525	GLU	CA-C	5.76	1.60	1.52	11	7
1	A	531	ASP	CA-C	5.68	1.60	1.52	11	5
1	A	445	ARG	CA-C	5.64	1.60	1.52	3	3
1	A	447	MET	N-CA	5.63	1.53	1.46	11	3
1	A	411	LEU	CA-C	5.57	1.60	1.52	15	10
1	A	534	SER	CA-C	5.52	1.58	1.52	2	1
1	A	446	ALA	N-CA	5.48	1.53	1.46	15	2
1	A	469	VAL	C-N	5.44	1.40	1.33	15	1
1	A	492	SER	CA-C	5.43	1.60	1.52	19	17
1	A	465	ALA	CA-C	5.35	1.58	1.52	17	7
1	A	462	ILE	CA-C	5.28	1.58	1.52	9	3
1	A	493	THR	CA-C	5.28	1.59	1.52	2	10
1	A	532	LYS	CA-C	5.25	1.59	1.52	9	2
1	A	445	ARG	N-CA	5.24	1.52	1.46	11	4
1	A	449	LYS	CA-C	5.21	1.59	1.52	6	4
1	A	536	LYS	CA-C	5.18	1.57	1.52	12	1
1	A	535	SER	CA-C	5.13	1.56	1.52	1	1
1	A	466	PRO	CA-C	5.08	1.58	1.53	13	2
1	A	517	GLN	CA-C	5.06	1.57	1.52	11	1
1	A	518	GLU	CA-C	5.05	1.59	1.52	18	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	447	MET	N-CA-C	28.36	149.49	110.35	20	15
1	A	447	MET	N-CA-CB	-14.96	89.73	110.38	20	20
1	A	451	ASN	CA-CB-CG	13.32	125.92	112.60	11	11
1	A	450	ASP	CA-CB-CG	13.26	125.86	112.60	17	20
1	A	528	LYS	CB-CA-C	12.36	131.50	111.36	19	20
1	A	447	MET	CB-CA-C	11.88	134.06	110.42	15	7
1	A	529	GLN	CB-CG-CD	11.73	132.54	112.60	16	6
1	A	446	ALA	CA-C-N	11.26	143.05	121.54	15	3
1	A	446	ALA	C-N-CA	11.26	143.05	121.54	15	3
1	A	432	ASN	CA-CB-CG	11.25	123.85	112.60	6	13
1	A	537	ASN	CA-CB-CG	11.07	123.67	112.60	2	18
1	A	444	GLU	N-CA-CB	-10.96	91.96	110.49	10	13
1	A	444	GLU	N-CA-C	10.86	133.94	110.80	10	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	519	ALA	CA-C-O	-10.78	112.98	119.55	8	5
1	A	408	MET	CA-CB-CG	10.61	135.32	114.10	8	6
1	A	523	LYS	CB-CA-C	9.62	125.19	110.08	20	3
1	A	408	MET	N-CA-C	9.35	123.07	109.14	8	15
1	A	529	GLN	N-CA-CB	-9.32	94.74	110.49	5	18
1	A	444	GLU	CB-CG-CD	9.29	128.40	112.60	9	7
1	A	443	GLY	N-CA-C	9.22	135.04	113.18	20	6
1	A	533	VAL	N-CA-CB	-9.19	96.07	111.23	19	10
1	A	528	LYS	N-CA-CB	-8.74	98.86	112.41	19	6
1	A	447	MET	CA-C-N	8.72	138.19	121.54	13	8
1	A	447	MET	C-N-CA	8.72	138.19	121.54	13	8
1	A	431	ASP	CA-CB-CG	8.47	121.07	112.60	8	9
1	A	497	ASN	CA-CB-CG	8.28	120.88	112.60	4	5
1	A	450	ASP	N-CA-CB	-8.25	97.53	111.96	10	10
1	A	444	GLU	CA-C-N	8.12	137.04	121.54	3	7
1	A	444	GLU	C-N-CA	8.12	137.04	121.54	3	7
1	A	538	SER	N-CA-C	8.11	121.05	110.43	9	1
1	A	438	ILE	N-CA-CB	8.08	120.68	110.99	20	13
1	A	480	ALA	N-CA-C	8.02	122.01	111.75	3	19
1	A	410	VAL	CA-C-O	7.96	128.11	120.31	6	20
1	A	528	LYS	N-CA-C	-7.96	101.60	110.91	15	13
1	A	445	ARG	N-CA-C	7.90	121.14	108.41	17	4
1	A	451	ASN	OD1-CG-ND2	-7.79	114.81	122.60	1	10
1	A	523	LYS	N-CA-CB	-7.76	98.03	110.14	10	12
1	A	529	GLN	CA-CB-CG	7.71	129.52	114.10	15	13
1	A	451	ASN	CB-CA-C	7.53	122.16	109.80	11	4
1	A	446	ALA	CA-C-O	7.50	131.24	120.51	15	3
1	A	509	LYS	N-CA-C	7.39	120.28	111.33	7	20
1	A	436	VAL	N-CA-C	7.20	118.66	108.36	16	12
1	A	447	MET	CA-C-O	7.13	128.53	121.05	18	13
1	A	521	LYS	N-CA-CB	-7.12	98.47	110.49	10	11
1	A	448	THR	CA-C-N	7.00	131.39	120.89	13	1
1	A	448	THR	C-N-CA	7.00	131.39	120.89	13	1
1	A	433	GLN	N-CA-C	6.99	125.25	109.81	11	16
1	A	531	ASP	CA-CB-CG	6.98	119.58	112.60	19	2
1	A	401	ILE	N-CA-C	6.92	118.70	108.45	9	11
1	A	528	LYS	CA-C-N	6.91	134.74	121.54	7	18
1	A	528	LYS	C-N-CA	6.91	134.74	121.54	7	18
1	A	529	GLN	CB-CA-C	6.90	124.16	110.42	3	5
1	A	531	ASP	CA-C-O	6.89	129.90	121.56	19	2
1	A	402	GLU	CB-CG-CD	6.89	124.31	112.60	4	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	507	LEU	N-CA-C	6.88	119.65	111.33	1	6
1	A	526	ASP	CA-CB-CG	6.75	119.35	112.60	2	5
1	A	533	VAL	CB-CA-C	6.70	122.28	111.29	19	4
1	A	406	GLY	N-CA-C	6.69	124.58	114.61	12	4
1	A	434	PRO	N-CA-C	6.69	126.26	112.47	14	4
1	A	431	ASP	N-CA-C	6.68	121.03	112.34	20	4
1	A	486	VAL	CA-CB-CG1	6.65	121.71	110.40	18	1
1	A	451	ASN	N-CA-CB	-6.65	99.25	110.49	10	5
1	A	443	GLY	CA-C-N	6.64	134.23	121.54	18	5
1	A	443	GLY	C-N-CA	6.64	134.23	121.54	18	5
1	A	519	ALA	N-CA-CB	-6.63	99.28	110.49	3	3
1	A	493	THR	CA-CB-CG2	6.58	121.69	110.50	2	16
1	A	524	ALA	N-CA-CB	-6.57	99.16	110.32	1	4
1	A	457	PHE	CA-CB-CG	6.57	120.36	113.80	11	19
1	A	471	GLN	N-CA-C	6.56	118.83	108.79	14	20
1	A	398	SER	N-CA-CB	-6.56	99.57	110.39	18	3
1	A	408	MET	CB-CA-C	-6.50	99.64	110.29	5	11
1	A	454	LEU	CA-C-O	6.48	128.25	120.99	19	1
1	A	434	PRO	N-CA-CB	6.43	106.52	102.92	11	2
1	A	477	ASP	CA-CB-CG	6.43	119.03	112.60	1	7
1	A	446	ALA	N-CA-CB	-6.40	101.93	110.57	2	3
1	A	495	LYS	N-CA-CB	-6.40	100.92	110.71	15	17
1	A	403	THR	N-CA-C	6.38	119.12	109.23	7	8
1	A	490	ASP	CA-CB-CG	6.37	118.97	112.60	19	10
1	A	517	GLN	CB-CA-C	6.37	119.21	109.34	18	7
1	A	524	ALA	CA-C-N	6.36	131.50	120.68	19	14
1	A	524	ALA	C-N-CA	6.36	131.50	120.68	19	14
1	A	408	MET	N-CA-CB	-6.29	101.44	111.62	8	1
1	A	536	LYS	CB-CA-C	6.27	121.90	112.31	3	3
1	A	486	VAL	N-CA-CB	6.23	118.10	111.00	8	8
1	A	444	GLU	O-C-N	-6.22	114.31	122.59	10	1
1	A	493	THR	N-CA-CB	-6.21	100.71	110.46	11	15
1	A	524	ALA	CB-CA-C	6.18	123.36	110.32	1	3
1	A	469	VAL	CA-C-O	-6.17	111.69	119.95	20	6
1	A	444	GLU	CA-CB-CG	6.16	126.41	114.10	1	2
1	A	465	ALA	O-C-N	-6.14	116.72	121.14	4	1
1	A	410	VAL	CA-CB-CG1	6.13	120.82	110.40	17	16
1	A	445	ARG	CA-C-O	-6.11	111.77	120.51	16	2
1	A	491	LYS	N-CA-C	6.09	118.00	111.36	7	10
1	A	445	ARG	N-CA-CB	-6.08	100.22	110.49	18	4
1	A	526	ASP	CA-C-N	6.05	133.10	121.54	18	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	526	ASP	C-N-CA	6.05	133.10	121.54	18	20
1	A	401	ILE	CA-C-N	6.04	130.70	122.19	8	1
1	A	401	ILE	C-N-CA	6.04	130.70	122.19	8	1
1	A	530	ARG	CA-C-O	-6.00	112.54	119.14	3	1
1	A	517	GLN	N-CA-C	-5.96	106.05	113.55	18	3
1	A	518	GLU	CB-CG-CD	5.94	122.70	112.60	8	3
1	A	407	VAL	CA-CB-CG1	5.91	120.45	110.40	15	1
1	A	520	GLU	N-CA-C	5.89	118.45	111.33	10	6
1	A	433	GLN	CA-C-O	-5.86	112.14	120.16	19	4
1	A	395	THR	N-CA-C	-5.85	102.40	109.72	10	1
1	A	516	VAL	N-CA-C	5.84	121.49	109.34	10	4
1	A	489	VAL	CA-CB-CG2	5.84	120.32	110.40	9	17
1	A	439	GLN	OE1-CD-NE2	-5.84	116.76	122.60	14	4
1	A	443	GLY	CA-C-O	-5.83	118.43	122.22	3	3
1	A	446	ALA	N-CA-C	5.79	123.14	110.80	15	1
1	A	529	GLN	CA-C-O	5.79	128.79	120.51	13	5
1	A	456	LYS	CA-CB-CG	5.74	125.58	114.10	10	5
1	A	401	ILE	O-C-N	5.73	129.05	123.03	8	1
1	A	449	LYS	N-CA-C	5.72	122.99	110.80	19	2
1	A	462	ILE	CA-CB-CG1	5.71	120.11	110.40	20	11
1	A	514	ARG	N-CA-C	5.71	117.30	111.14	16	2
1	A	511	ASP	CA-CB-CG	5.69	118.29	112.60	16	4
1	A	516	VAL	CB-CA-C	5.68	120.61	111.29	1	1
1	A	452	ASN	CA-CB-CG	5.66	118.26	112.60	11	2
1	A	395	THR	CA-CB-CG2	5.64	120.08	110.50	18	20
1	A	490	ASP	N-CA-C	-5.62	98.79	108.56	4	8
1	A	533	VAL	N-CA-C	5.61	117.49	108.85	18	1
1	A	517	GLN	CB-CG-CD	5.61	122.13	112.60	6	2
1	A	467	ARG	N-CA-C	5.61	118.94	110.64	9	4
1	A	518	GLU	N-CA-CB	5.57	119.91	110.49	1	4
1	A	451	ASN	CB-CG-ND2	5.53	124.70	116.40	13	2
1	A	522	TYR	N-CA-CB	-5.47	101.25	110.49	9	3
1	A	439	GLN	CB-CG-CD	5.46	121.88	112.60	15	3
1	A	403	THR	CA-CB-CG2	5.42	119.70	110.50	14	2
1	A	479	ASP	CA-CB-CG	5.40	118.00	112.60	10	1
1	A	517	GLN	CA-C-N	5.39	131.83	121.54	12	2
1	A	517	GLN	C-N-CA	5.39	131.83	121.54	12	2
1	A	438	ILE	CA-CB-CG1	5.37	119.53	110.40	10	4
1	A	395	THR	CB-CA-C	5.37	116.43	108.87	12	1
1	A	434	PRO	CB-CA-C	5.36	120.41	111.56	15	2
1	A	447	MET	CG-SD-CE	5.35	112.68	100.90	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	503	ASN	CA-CB-CG	5.34	117.94	112.60	18	1
1	A	402	GLU	CA-CB-CG	5.34	124.78	114.10	5	1
1	A	522	TYR	N-CA-C	5.32	119.25	112.34	12	2
1	A	532	LYS	CA-CB-CG	5.32	124.73	114.10	9	1
1	A	418	ILE	O-C-N	-5.30	115.06	121.10	6	2
1	A	409	THR	N-CA-CB	5.29	119.08	110.77	13	2
1	A	429	TYR	N-CA-C	5.28	118.88	112.23	20	1
1	A	450	ASP	N-CA-C	5.27	122.02	110.80	1	3
1	A	402	GLU	N-CA-CB	-5.27	101.32	110.17	12	2
1	A	437	LEU	N-CA-CB	-5.26	101.29	109.87	14	1
1	A	483	ILE	CB-CA-C	5.25	118.17	110.98	19	1
1	A	397	LEU	N-CA-CB	-5.23	102.73	111.20	8	2
1	A	434	PRO	CA-N-CD	-5.22	104.70	112.00	13	1
1	A	534	SER	N-CA-C	5.21	116.96	111.28	3	1
1	A	449	LYS	N-CA-CB	-5.20	101.70	110.49	3	1
1	A	409	THR	N-CA-C	-5.20	100.77	109.24	4	1
1	A	536	LYS	N-CA-C	-5.20	99.73	110.80	1	1
1	A	442	GLU	CB-CA-C	5.19	120.40	111.68	15	2
1	A	491	LYS	N-CA-CB	-5.19	102.47	110.20	13	1
1	A	540	GLU	CB-CG-CD	5.19	121.42	112.60	10	2
1	A	448	THR	CA-CB-OG1	5.19	117.38	109.60	7	1
1	A	465	ALA	N-CA-CB	-5.19	103.81	109.72	20	1
1	A	445	ARG	O-C-N	-5.18	115.70	122.59	3	1
1	A	410	VAL	CA-C-N	5.17	130.76	121.66	10	4
1	A	410	VAL	C-N-CA	5.17	130.76	121.66	10	4
1	A	519	ALA	N-CA-C	5.13	121.74	110.80	1	1
1	A	460	THR	CA-CB-CG2	5.12	119.20	110.50	15	4
1	A	529	GLN	OE1-CD-NE2	-5.11	117.49	122.60	20	1
1	A	539	LEU	CB-CA-C	5.11	119.64	110.81	10	1
1	A	394	VAL	CA-CB-CG2	5.08	119.03	110.40	17	7
1	A	531	ASP	N-CA-C	-5.08	105.40	111.03	1	1
1	A	516	VAL	CA-CB-CG1	5.07	119.02	110.40	5	1
1	A	518	GLU	N-CA-C	-5.06	100.02	110.80	1	2
1	A	481	ASN	CA-CB-CG	5.06	117.66	112.60	10	1
1	A	490	ASP	CB-CA-C	5.03	120.14	111.68	9	1
1	A	462	ILE	N-CA-CB	-5.03	104.17	111.21	8	1
1	A	485	ASN	CA-CB-CG	5.02	117.62	112.60	9	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 ⓘ

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	14±4
All	All	22540	22920	22920	270

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 6.

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:444:GLU:CD	1:A:447:MET:SD	0.66	2.79	19	5
1:A:408:MET:HB2	1:A:447:MET:SD	0.65	2.32	15	3
1:A:447:MET:SD	1:A:447:MET:C	0.65	2.79	6	8
1:A:408:MET:HB2	1:A:447:MET:HG3	0.64	1.69	14	2
1:A:408:MET:CB	1:A:447:MET:HE2	0.64	2.22	16	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	9
1:A:398:SER:OG	1:A:410:VAL:HG21	0.61	1.95	5	2
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:444:GLU:C	1:A:519:ALA:HB1	0.61	2.21	10	3
1:A:438:ILE:HD12	1:A:539:LEU:HD21	0.60	1.71	2	3
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:507:LEU:HD23	1:A:507:LEU:H	0.59	1.57	16	1
1:A:529:GLN:CG	1:A:530:ARG:H	0.58	2.10	3	16
1:A:447:MET:HE3	1:A:447:MET:O	0.58	1.99	10	5
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:523:LYS:CG	1:A:529:GLN:HG3	0.56	2.31	16	1
1:A:529:GLN:CD	1:A:530:ARG:H	0.54	2.10	14	3
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:HB3	1:A:447:MET:HE2	0.53	1.78	16	1
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:444:GLU:OE1	1:A:447:MET:HE3	0.51	2.06	15	1
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: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:400:GLY:CA	1:A:408:MET:SD	0.47	3.03	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:400:GLY:HA3	1:A:408:MET:HE3	0.46	1.87	12	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:425:THR:OG1	1:A:473:GLU:OE2	0.45	2.35	9	1
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:444:GLU:C	1:A:447:MET:SD	0.43	3.02	20	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:408:MET:SD	1:A:447:MET:HE2	0.42	2.53	3	2
1:A:538:SER:OG	1:A:540:GLU:O	0.42	2.37	11	1
1:A:407:VAL:HG12	1:A:447:MET:C	0.42	2.39	20	1
1:A:408:MET:HB2	1:A:447:MET:HE3	0.42	1.92	7	1
1:A:459:LEU:HG	1:A:488:ALA:HB3	0.42	1.91	14	1
1:A:444:GLU:HB2	1:A:447:MET:HE1	0.42	1.92	16	1
1:A:429:TYR:H	1:A:540:GLU:CD	0.42	2.23	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:487:SER:OG	1:A:496:GLU:OE1	0.41	2.38	16	3
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: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:407:VAL:O	1:A:447:MET:HE2	0.40	2.17	15	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 ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	145/159 (91%)	110±3 (76±2%)	22±3 (15±2%)	13±3 (9±2%)	1	11
All	All	2900/3180 (91%)	2202 (76%)	440 (15%)	258 (9%)	1	11

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
1	A	533	VAL	12
1	A	456	LYS	12

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Mol	Chain	Res	Type	Models (Total)
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%)	105±2 (81±2%)	24±2 (19±2%)	3	35
All	All	2580/2820 (91%)	2102 (81%)	478 (19%)	3	35

All 66 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

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Mol	Chain	Res	Type	Models (Total)
1	A	410	VAL	20
1	A	472	ILE	20
1	A	507	LEU	20
1	A	509	LYS	20
1	A	486	VAL	19
1	A	438	ILE	18
1	A	529	GLN	18
1	A	411	LEU	17
1	A	520	GLU	17
1	A	447	MET	16
1	A	532	LYS	14
1	A	399	LEU	13
1	A	454	LEU	13
1	A	539	LEU	13
1	A	484	LEU	11
1	A	445	ARG	10
1	A	473	GLU	10
1	A	432	ASN	9
1	A	434	PRO	9
1	A	521	LYS	9
1	A	491	LYS	8
1	A	536	LYS	8
1	A	540	GLU	8
1	A	414	ARG	7
1	A	437	LEU	7
1	A	528	LYS	7
1	A	448	THR	6
1	A	515	MET	6
1	A	431	ASP	6
1	A	449	LYS	6
1	A	514	ARG	5
1	A	530	ARG	5
1	A	422	GLN	5
1	A	462	ILE	5
1	A	442	GLU	4
1	A	397	LEU	4
1	A	402	GLU	4
1	A	444	GLU	4
1	A	451	ASN	4
1	A	408	MET	4
1	A	409	THR	3
1	A	518	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	531	ASP	3
1	A	440	VAL	3
1	A	495	LYS	3
1	A	392	LEU	3
1	A	401	ILE	3
1	A	436	VAL	3
1	A	441	TYR	2
1	A	398	SER	2
1	A	460	THR	2
1	A	510	GLU	2
1	A	537	ASN	2
1	A	467	ARG	2
1	A	403	THR	2
1	A	413	LYS	2
1	A	511	ASP	1
1	A	471	GLN	1
1	A	516	VAL	1
1	A	512	ILE	1
1	A	479	ASP	1
1	A	499	ILE	1
1	A	453	LEU	1
1	A	513	GLU	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 oligosaccharides 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

No chemical shift data were provided