



Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 06:34 PM UTC

PDB ID : 2GW6 / pdb_00002gw6
Title : NMR structure of the human tRNA endonuclease SEN15 subunit
Authors : Song, J.; Markley, J.L.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2006-05-03

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

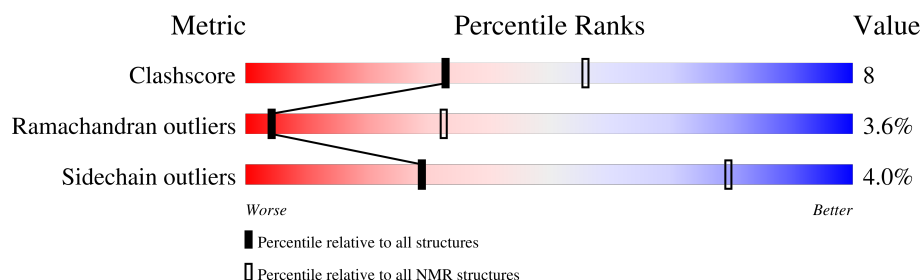
1 Overall quality at a glance

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	123	
1	B	123	

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:8-A:123, B:308-B:423 (232)	1.38	9

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 4 clusters and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3857 atoms, of which 1928 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called tRNA-splicing endonuclease subunit Sen15.

Mol	Chain	Residues	Atoms						Trace
1	A	123	Total	C	H	N	O	S	0
			1929	616	965	151	190	7	
1	B	123	Total	C	H	N	O	S	0
			1928	616	963	151	191	7	

There are 2 discrepancies between the modelled and reference sequences:

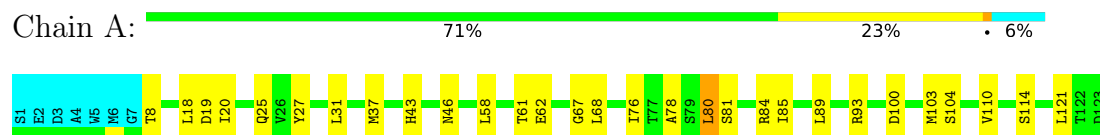
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	cloning artifact	UNP Q8WW01
B	301	SER	-	cloning artifact	UNP Q8WW01

4 Residue-property plots

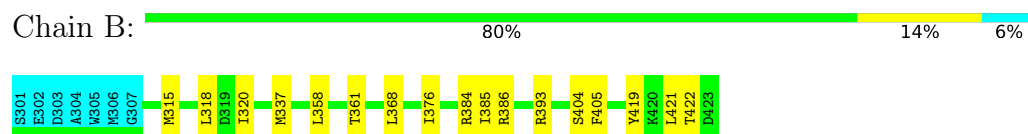
4.1 Average score per residue in the NMR ensemble

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: tRNA-splicing endonuclease subunit Sen15



- Molecule 1: tRNA-splicing endonuclease subunit Sen15

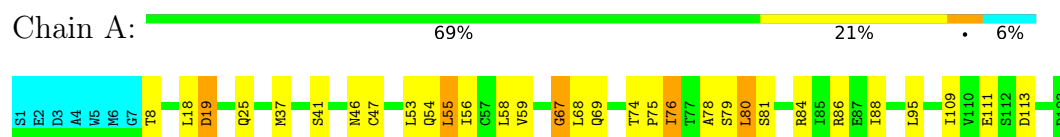


4.2 Scores per residue for each member of the ensemble

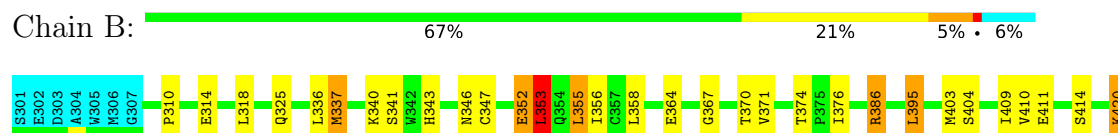
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: tRNA-splicing endonuclease subunit Sen15



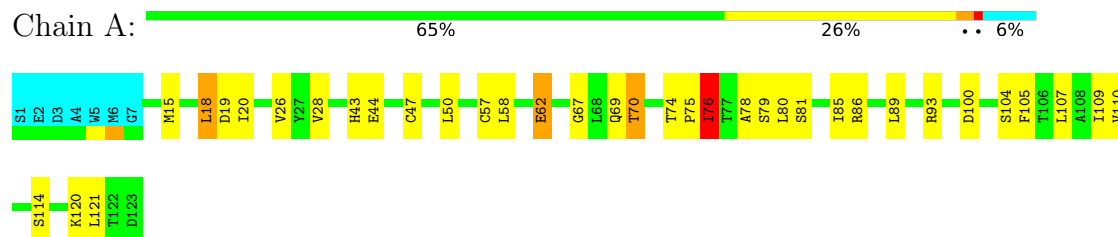
- Molecule 1: tRNA-splicing endonuclease subunit Sen15



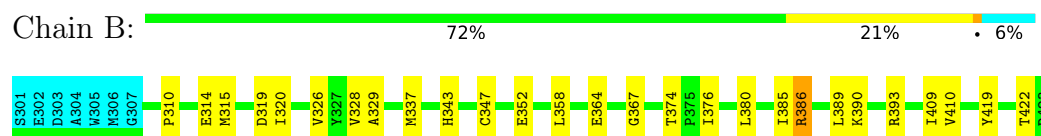


4.2.2 Score per residue for model 2

- Molecule 1: tRNA-splicing endonuclease subunit Sen15

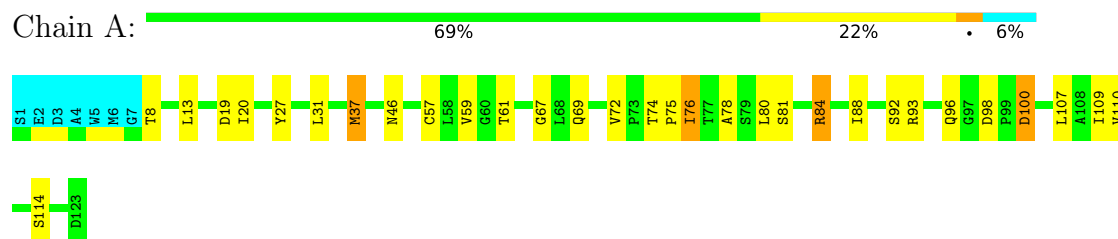


- Molecule 1: tRNA-splicing endonuclease subunit Sen15

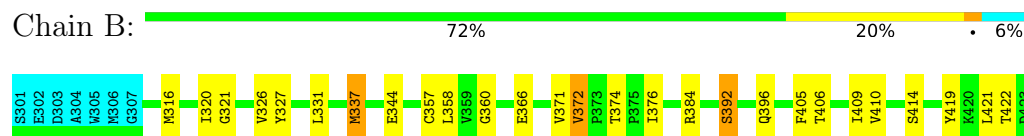


4.2.3 Score per residue for model 3

- Molecule 1: tRNA-splicing endonuclease subunit Sen15



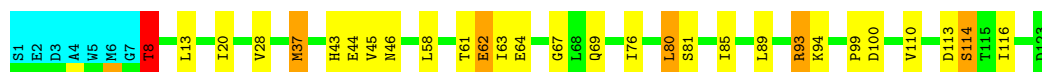
- Molecule 1: tRNA-splicing endonuclease subunit Sen15



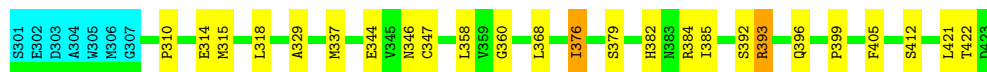
4.2.4 Score per residue for model 4

- Molecule 1: tRNA-splicing endonuclease subunit Sen15





- Molecule 1: tRNA-splicing endonuclease subunit Sen15



4.2.5 Score per residue for model 5

- Molecule 1: tRNA-splicing endonuclease subunit Sen15

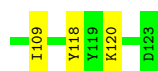


- Molecule 1: tRNA-splicing endonuclease subunit Sen15



4.2.6 Score per residue for model 6

- Molecule 1: tRNA-splicing endonuclease subunit Sen15



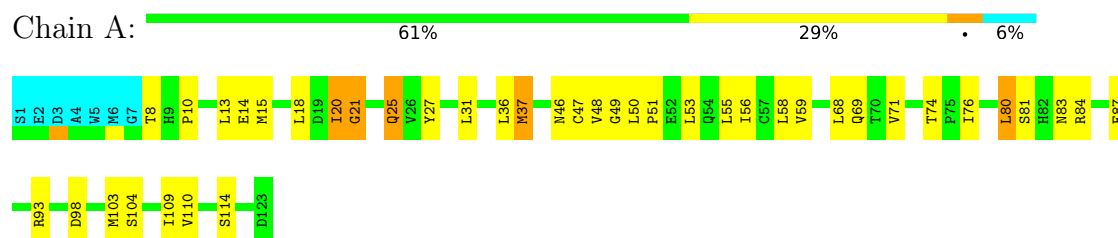
- Molecule 1: tRNA-splicing endonuclease subunit Sen15



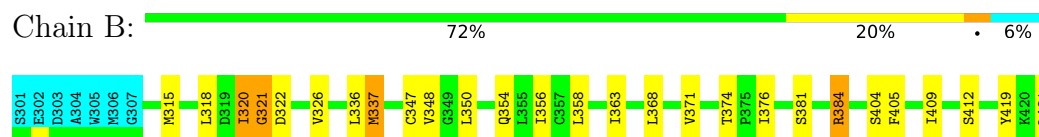


4.2.7 Score per residue for model 7

- Molecule 1: tRNA-splicing endonuclease subunit Sen15

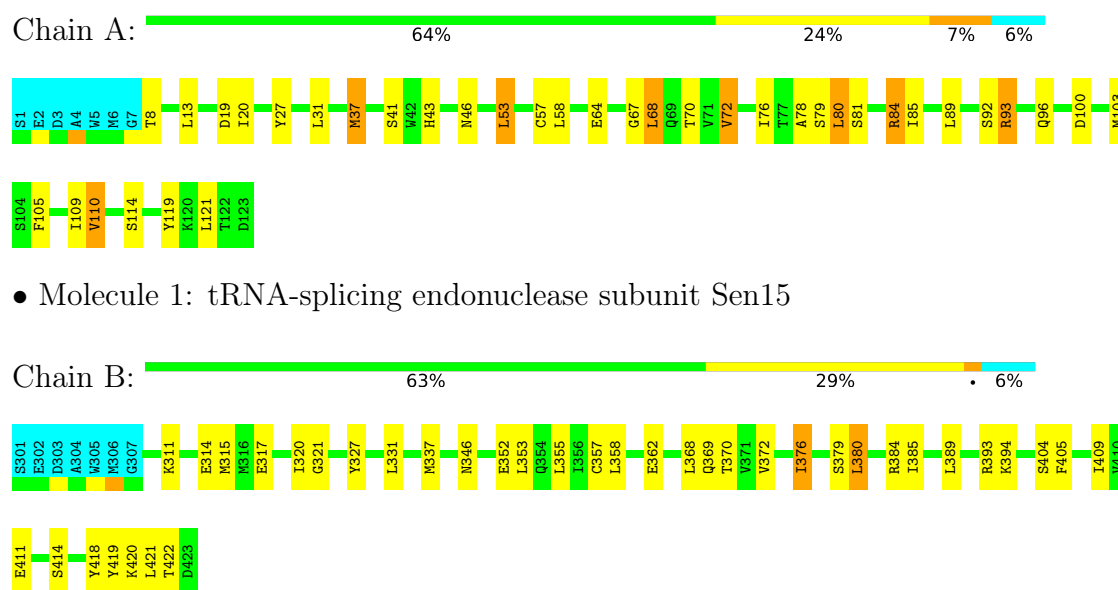


- Molecule 1: tRNA-splicing endonuclease subunit Sen15



4.2.8 Score per residue for model 8

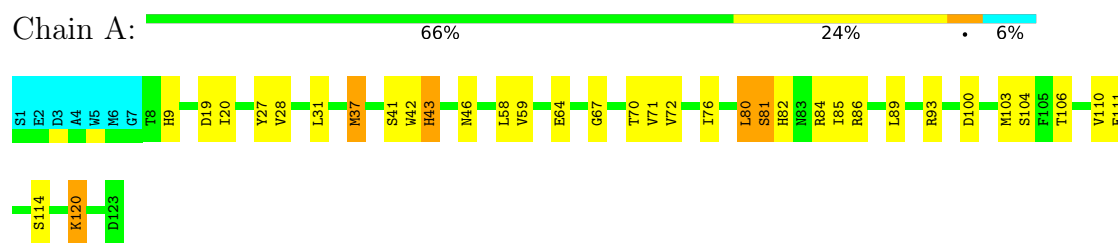
- Molecule 1: tRNA-splicing endonuclease subunit Sen15



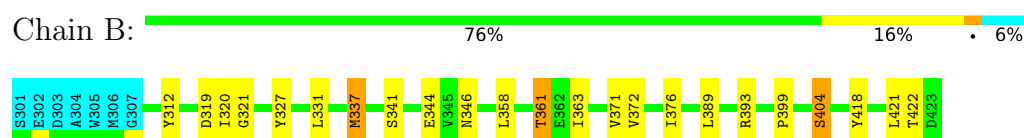
- Molecule 1: tRNA-splicing endonuclease subunit Sen15

4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: tRNA-splicing endonuclease subunit Sen15

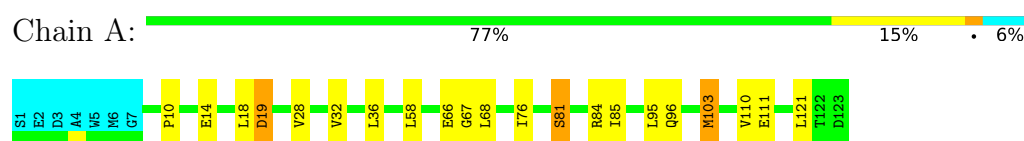


- Molecule 1: tRNA-splicing endonuclease subunit Sen15

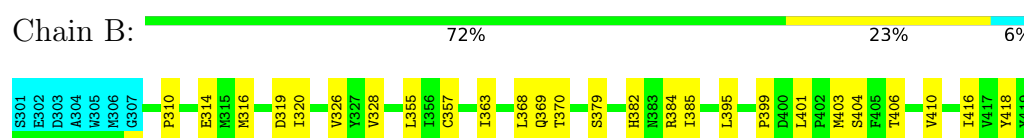


4.2.10 Score per residue for model 10

- Molecule 1: tRNA-splicing endonuclease subunit Sen15

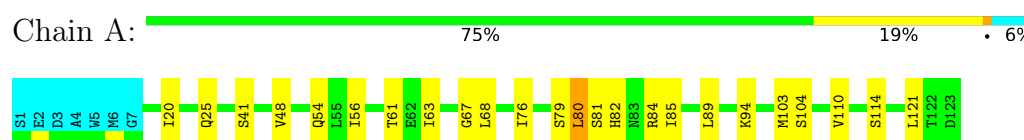


- Molecule 1: tRNA-splicing endonuclease subunit Sen15

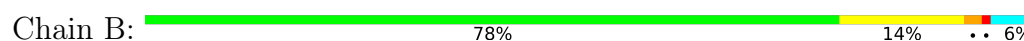


4.2.11 Score per residue for model 11

- Molecule 1: tRNA-splicing endonuclease subunit Sen15



- Molecule 1: tRNA-splicing endonuclease subunit Sen15

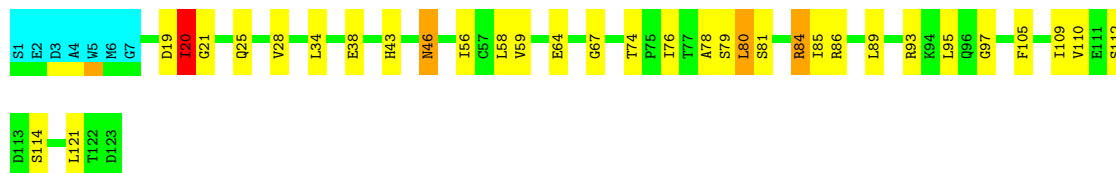




4.2.12 Score per residue for model 12

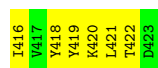
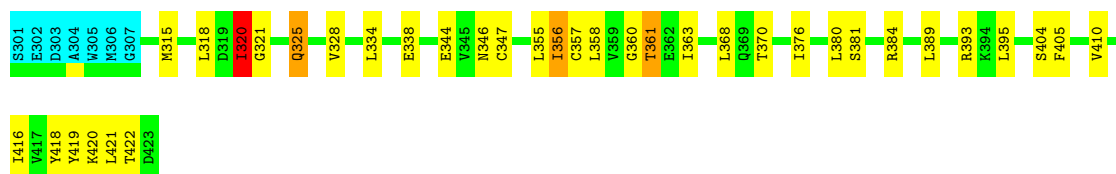
- Molecule 1: tRNA-splicing endonuclease subunit Sen15

Chain A: 67% 24% 6%



- Molecule 1: tRNA-splicing endonuclease subunit Sen15

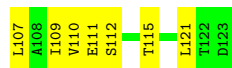
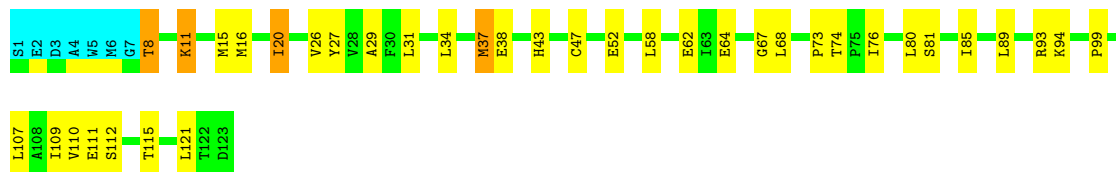
Chain B: 65% 26% 6%



4.2.13 Score per residue for model 13

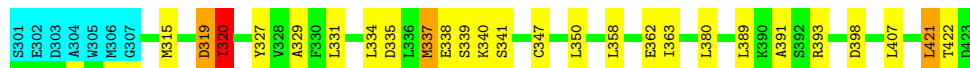
- Molecule 1: tRNA-splicing endonuclease subunit Sen15

Chain A: 64% 27% 6%



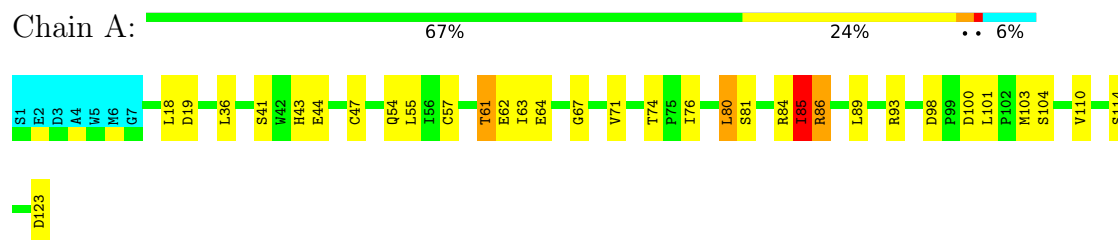
- Molecule 1: tRNA-splicing endonuclease subunit Sen15

Chain B: 73% 18% 6%

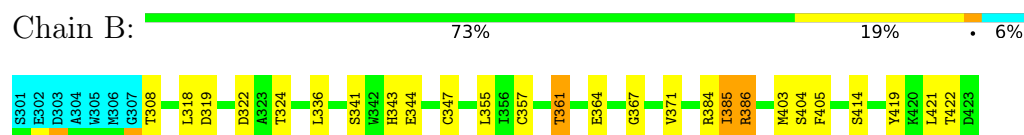


4.2.14 Score per residue for model 14

- Molecule 1: tRNA-splicing endonuclease subunit Sen15

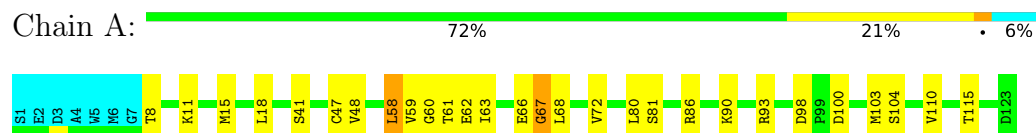


- Molecule 1: tRNA-splicing endonuclease subunit Sen15

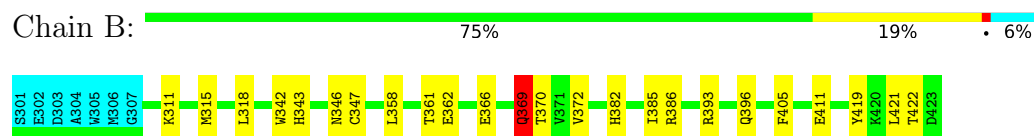


4.2.15 Score per residue for model 15

- Molecule 1: tRNA-splicing endonuclease subunit Sen15

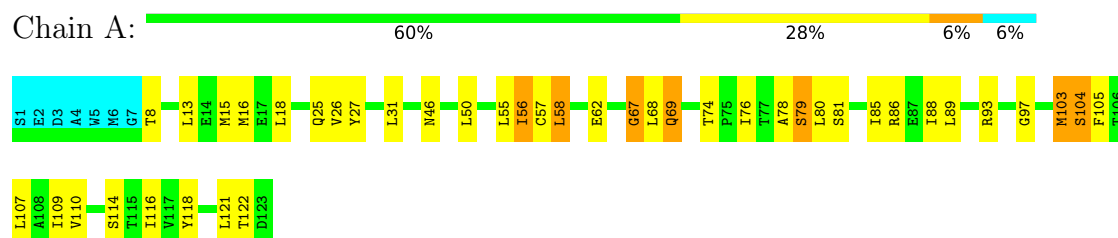


- Molecule 1: tRNA-splicing endonuclease subunit Sen15



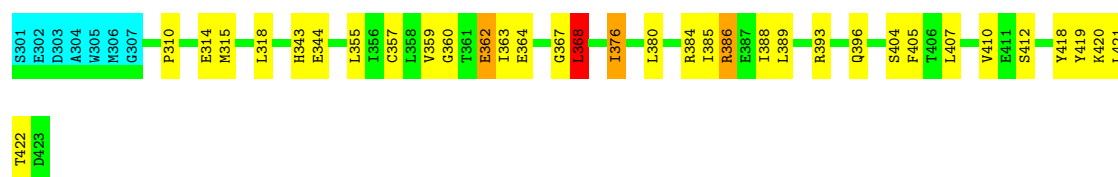
4.2.16 Score per residue for model 16

- Molecule 1: tRNA-splicing endonuclease subunit Sen15



- Molecule 1: tRNA-splicing endonuclease subunit Sen15

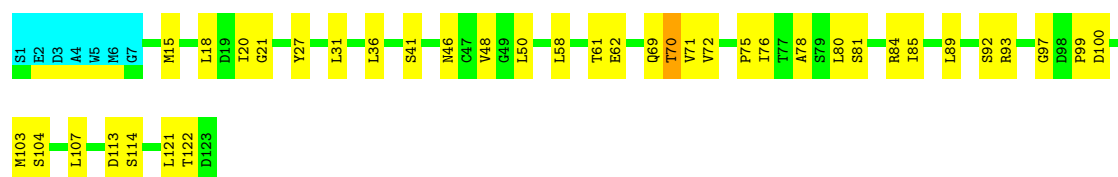




4.2.17 Score per residue for model 17

- Molecule 1: tRNA-splicing endonuclease subunit Sen15

Chain A: 63% 30% 6%



- Molecule 1: tRNA-splicing endonuclease subunit Sen15

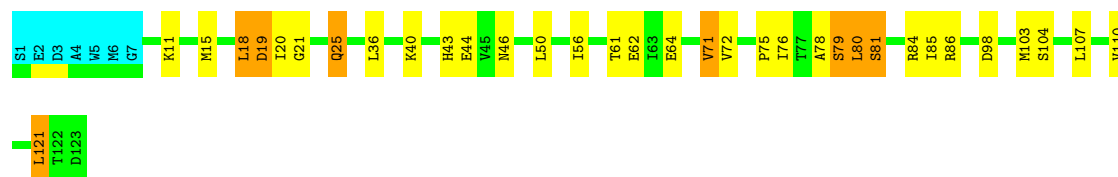
Chain B: 68% 24% 6%



4.2.18 Score per residue for model 18

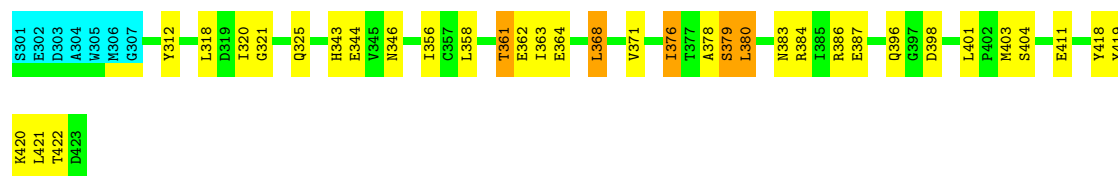
- Molecule 1: tRNA-splicing endonuclease subunit Sen15

Chain A: 67% 21% 7% 6%



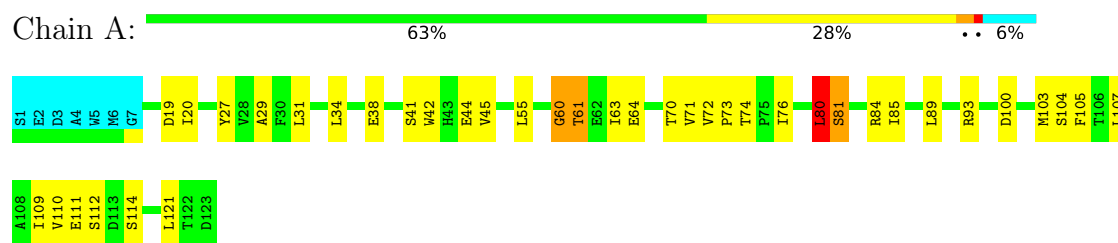
- Molecule 1: tRNA-splicing endonuclease subunit Sen15

Chain B: 66% 24% 6%

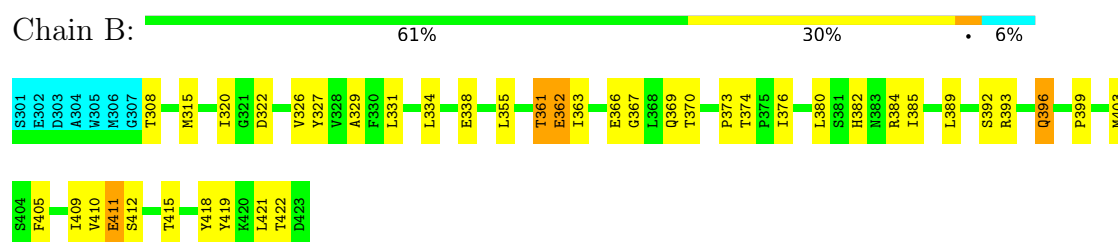


4.2.19 Score per residue for model 19

- Molecule 1: tRNA-splicing endonuclease subunit Sen15

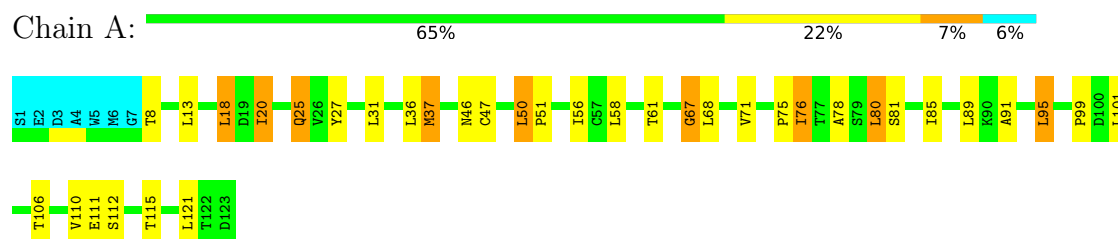


- Molecule 1: tRNA-splicing endonuclease subunit Sen15

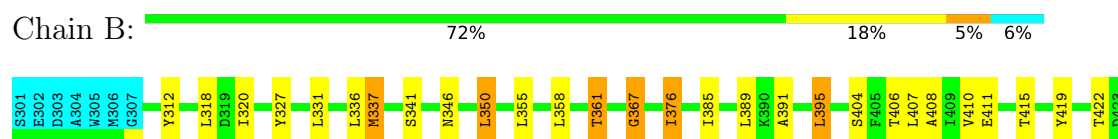


4.2.20 Score per residue for model 20

- Molecule 1: tRNA-splicing endonuclease subunit Sen15



- Molecule 1: tRNA-splicing endonuclease subunit Sen15



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing, distance geometry*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
Xplor-NIH	refinement	2.9.8

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	1.27±0.05	3±2/927 (0.3± 0.2%)	1.08±0.05	2±2/1262 (0.2± 0.2%)
1	B	1.25±0.08	3±2/928 (0.3± 0.2%)	1.07±0.04	1±1/1262 (0.1± 0.1%)
All	All	1.26	121/37100 (0.3%)	1.08	59/50480 (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	B	0.0±0.0	0.1±0.3
All	All	0	2

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	19	ASP	CA-C	-8.48	1.44	1.53	6	1
1	A	48	VAL	C-N	-8.18	1.29	1.33	17	4
1	A	97	GLY	C-N	-8.16	1.27	1.33	16	1
1	A	20	ILE	C-N	-8.02	1.21	1.33	4	3
1	B	319	ASP	C-N	-7.72	1.23	1.33	6	2
1	A	80	LEU	C-O	-7.68	1.14	1.23	8	5
1	B	379	SER	N-CA	7.58	1.54	1.46	8	2
1	A	61	THR	N-CA	-7.18	1.37	1.46	15	7
1	A	60	GLY	N-CA	-7.17	1.38	1.45	19	2
1	B	372	VAL	N-CA	-6.97	1.40	1.46	9	3
1	A	72	VAL	N-CA	-6.93	1.40	1.46	9	5
1	A	80	LEU	N-CA	-6.89	1.37	1.45	19	1
1	A	70	THR	C-N	-6.80	1.25	1.33	17	1
1	B	361	THR	N-CA	-6.79	1.38	1.46	19	8
1	A	80	LEU	C-N	-6.69	1.24	1.33	4	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	369	GLN	C-N	-6.65	1.24	1.33	8	4
1	B	370	THR	N-CA	-6.54	1.38	1.46	8	6
1	A	69	GLN	C-N	-6.50	1.25	1.33	2	2
1	B	380	LEU	C-O	6.47	1.31	1.23	16	3
1	A	79	SER	N-CA	-6.34	1.38	1.46	2	4
1	A	81	SER	CA-C	-6.22	1.45	1.52	6	3
1	B	421	LEU	C-N	-6.16	1.24	1.33	6	3
1	B	368	LEU	C-N	-6.15	1.24	1.33	8	1
1	B	320	ILE	C-N	-6.14	1.24	1.33	19	1
1	B	349	GLY	CA-C	-6.11	1.48	1.52	6	1
1	B	380	LEU	C-N	6.01	1.42	1.33	16	1
1	A	103	MET	CA-CB	5.86	1.60	1.53	16	1
1	A	20	ILE	CA-CB	5.84	1.62	1.54	12	1
1	B	320	ILE	CA-CB	5.83	1.62	1.54	12	1
1	B	371	VAL	C-N	-5.79	1.27	1.33	3	2
1	A	59	VAL	C-N	-5.79	1.25	1.33	15	1
1	B	411	GLU	N-CA	-5.76	1.39	1.46	8	1
1	B	404	SER	N-CA	-5.71	1.39	1.46	7	1
1	B	380	LEU	CA-C	-5.56	1.45	1.52	8	1
1	B	405	PHE	C-O	5.54	1.30	1.23	11	1
1	A	70	THR	N-CA	-5.51	1.40	1.46	5	3
1	B	348	VAL	C-N	-5.48	1.30	1.33	7	1
1	A	17	GLU	C-N	-5.42	1.28	1.33	6	1
1	A	63	ILE	N-CA	-5.40	1.40	1.46	11	1
1	B	420	LYS	N-CA	-5.36	1.39	1.46	1	1
1	A	59	VAL	CA-C	-5.33	1.45	1.52	15	1
1	B	406	THR	N-CA	-5.33	1.39	1.46	20	2
1	B	409	ILE	C-N	-5.32	1.26	1.33	8	1
1	B	405	PHE	C-N	-5.30	1.26	1.33	7	3
1	A	60	GLY	C-N	-5.30	1.26	1.33	19	1
1	A	74	THR	N-CA	-5.26	1.41	1.46	13	1
1	B	308	THR	C-N	-5.24	1.28	1.33	5	1
1	B	403	MET	C-N	-5.24	1.27	1.33	19	1
1	A	19	ASP	C-N	-5.23	1.26	1.33	6	1
1	A	76	ILE	CA-C	5.22	1.60	1.52	2	1
1	B	369	GLN	N-CA	-5.22	1.39	1.45	8	1
1	A	8	THR	C-N	-5.16	1.25	1.33	4	1
1	B	398	ASP	C-O	-5.16	1.21	1.25	6	1
1	A	103	MET	C-N	-5.12	1.27	1.33	10	1
1	A	110	VAL	CA-C	-5.08	1.46	1.52	8	1
1	B	343	HIS	C-N	-5.07	1.27	1.33	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	58	LEU	CA-C	-5.07	1.46	1.52	15	1
1	B	320	ILE	CA-C	-5.04	1.46	1.52	6	1
1	A	46	ASN	CA-C	-5.04	1.46	1.52	12	1
1	B	385	ILE	CA-CB	5.02	1.60	1.54	11	1
1	B	356	ILE	C-N	-5.01	1.26	1.33	12	1
1	A	120	LYS	N-CA	-5.01	1.40	1.46	2	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	83	ASN	CA-CB-CG	8.19	120.79	112.60	5	1
1	A	62	GLU	N-CA-C	-6.71	104.05	111.36	13	3
1	A	19	ASP	CA-C-N	-6.55	116.55	122.97	19	2
1	A	19	ASP	C-N-CA	-6.55	116.55	122.97	19	2
1	B	346	ASN	CA-CB-CG	6.25	118.85	112.60	15	1
1	A	46	ASN	CA-CB-CG	6.03	118.63	112.60	5	3
1	A	18	LEU	N-CA-C	6.03	118.45	109.59	10	2
1	A	110	VAL	N-CA-C	6.03	116.29	107.37	8	1
1	A	121	LEU	CA-C-N	-5.95	113.34	122.62	16	2
1	A	121	LEU	C-N-CA	-5.95	113.34	122.62	16	2
1	B	311	LYS	N-CA-CB	5.78	119.20	110.30	5	1
1	B	355	LEU	N-CA-C	5.69	118.82	109.72	1	1
1	B	405	PHE	CA-CB-CG	5.68	119.48	113.80	17	2
1	A	80	LEU	N-CA-C	-5.65	102.09	110.46	11	3
1	A	50	LEU	CA-C-N	5.60	125.71	119.32	20	3
1	A	50	LEU	C-N-CA	5.60	125.71	119.32	20	3
1	B	320	ILE	N-CA-C	-5.60	97.69	109.34	6	1
1	B	355	LEU	N-CA-CB	5.56	120.58	111.08	1	1
1	A	85	ILE	CA-CB-CG1	5.52	119.78	110.40	14	1
1	A	71	VAL	CA-C-N	-5.50	118.06	122.85	19	2
1	A	71	VAL	C-N-CA	-5.50	118.06	122.85	19	2
1	A	98	ASP	CA-C-N	5.43	124.89	119.24	15	2
1	A	98	ASP	C-N-CA	5.43	124.89	119.24	15	2
1	A	20	ILE	N-CA-C	5.40	120.58	109.34	6	1
1	A	95	LEU	N-CA-CB	5.39	119.18	110.40	20	1
1	A	18	LEU	CA-C-N	5.38	131.82	121.54	10	1
1	A	18	LEU	C-N-CA	5.38	131.82	121.54	10	1
1	A	66	GLU	N-CA-C	-5.33	106.54	112.57	6	1
1	B	410	VAL	N-CA-CB	5.29	118.34	111.67	16	1
1	B	382	HIS	CA-CB-CG	5.24	119.04	113.80	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	53	LEU	N-CA-C	-5.22	106.94	113.72	8	1
1	B	353	LEU	N-CA-CB	5.20	118.62	110.46	1	1
1	B	371	VAL	CA-C-N	-5.13	118.38	122.85	18	1
1	B	371	VAL	C-N-CA	-5.13	118.38	122.85	18	1
1	A	19	ASP	N-CA-C	5.13	121.73	110.80	10	1
1	B	362	GLU	N-CA-C	-5.12	105.78	111.36	16	2
1	B	350	LEU	CA-C-N	5.11	124.55	119.24	20	1
1	B	350	LEU	C-N-CA	5.11	124.55	119.24	20	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	B	393	ARG	Sidechain	1
1	B	384	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	910	921	918	19±5
1	B	911	921	918	16±4
All	All	36420	36840	36720	617

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:SER:OG	1:B:422:THR:HB	0.75	1.81	14	4
1:B:318:LEU:HD11	1:B:347:CYS:SG	0.74	2.23	12	4
1:B:325:GLN:CD	1:B:356:ILE:HG13	0.72	2.10	12	1
1:A:25:GLN:NE2	1:A:56:ILE:HG12	0.71	1.99	20	1
1:A:81:SER:HB3	1:B:422:THR:HB	0.70	1.62	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:MET:O	1:A:18:LEU:HG	0.70	1.85	16	3
1:A:89:LEU:O	1:A:93:ARG:HG2	0.69	1.88	6	4
1:A:81:SER:HA	1:B:422:THR:O	0.69	1.88	1	10
1:A:57:CYS:SG	1:A:72:VAL:HB	0.69	2.28	5	2
1:A:37:MET:HA	1:A:37:MET:HE2	0.67	1.66	7	4
1:B:355:LEU:HD13	1:B:357:CYS:SG	0.67	2.30	10	5
1:B:389:LEU:O	1:B:393:ARG:HG2	0.67	1.90	9	3
1:A:43:HIS:CE1	1:A:64:GLU:HB3	0.67	2.25	9	5
1:B:315:MET:O	1:B:318:LEU:HG	0.67	1.90	17	2
1:A:81:SER:HB3	1:B:422:THR:OG1	0.67	1.89	10	1
1:B:337:MET:HA	1:B:337:MET:HE3	0.67	1.67	3	4
1:A:37:MET:HE3	1:A:37:MET:HA	0.66	1.68	9	3
1:B:318:LEU:HG	1:B:319:ASP:O	0.64	1.92	5	1
1:B:334:LEU:O	1:B:338:GLU:HG2	0.64	1.92	19	3
1:A:89:LEU:O	1:A:93:ARG:HG3	0.63	1.93	9	3
1:B:337:MET:HA	1:B:337:MET:HE2	0.63	1.71	9	4
1:A:80:LEU:O	1:B:421:LEU:HA	0.62	1.94	4	10
1:A:43:HIS:CE1	1:A:64:GLU:HB2	0.62	2.29	4	4
1:B:389:LEU:O	1:B:393:ARG:HG3	0.62	1.94	6	4
1:A:25:GLN:NE2	1:A:56:ILE:HG13	0.62	2.10	18	1
1:A:25:GLN:CD	1:A:56:ILE:HG13	0.61	2.20	12	2
1:A:85:ILE:O	1:A:89:LEU:HG	0.61	1.95	8	10
1:A:34:LEU:O	1:A:38:GLU:HG2	0.61	1.95	19	3
1:A:75:PRO:HG2	1:A:78:ALA:HB2	0.61	1.72	2	6
1:B:382:HIS:HA	1:B:385:ILE:CG1	0.60	2.25	15	1
1:B:385:ILE:HG13	1:B:405:PHE:CE2	0.60	2.31	16	2
1:A:80:LEU:HB2	1:B:419:TYR:OH	0.60	1.96	15	1
1:A:15:MET:O	1:A:18:LEU:HB3	0.59	1.97	18	1
1:A:25:GLN:HE22	1:A:56:ILE:HG12	0.59	1.56	20	1
1:B:398:ASP:HB2	1:B:401:LEU:HD13	0.59	1.73	18	1
1:A:18:LEU:HD11	1:A:47:CYS:SG	0.58	2.39	20	2
1:A:81:SER:HB2	1:B:422:THR:HG23	0.58	1.75	18	1
1:A:93:ARG:HB3	1:A:98:ASP:O	0.57	2.00	7	1
1:A:76:ILE:HG12	1:A:110:VAL:O	0.57	2.00	4	10
1:A:82:HIS:O	1:A:85:ILE:HG13	0.57	2.00	11	1
1:A:80:LEU:HD13	1:A:81:SER:N	0.57	2.14	16	4
1:A:80:LEU:HA	1:A:84:ARG:HG3	0.57	1.75	12	1
1:B:404:SER:CB	1:B:422:THR:HA	0.56	2.30	9	2
1:A:76:ILE:HB	1:A:110:VAL:O	0.56	2.00	20	2
1:A:81:SER:O	1:A:85:ILE:HG13	0.56	2.00	18	3
1:B:382:HIS:O	1:B:385:ILE:HG13	0.56	2.00	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:343:HIS:CE1	1:B:364:GLU:HB3	0.56	2.36	18	4
1:A:28:VAL:HG13	1:A:110:VAL:HG11	0.56	1.77	12	5
1:A:15:MET:O	1:A:18:LEU:HD22	0.56	2.01	7	2
1:A:20:ILE:HG21	1:A:51:PRO:HA	0.56	1.77	20	1
1:A:80:LEU:HD22	1:B:419:TYR:CE2	0.55	2.36	8	2
1:A:82:HIS:O	1:A:86:ARG:HG2	0.55	2.01	9	1
1:B:376:ILE:HG12	1:B:410:VAL:O	0.55	2.01	3	3
1:A:93:ARG:HG3	1:A:98:ASP:HB2	0.55	1.78	14	1
1:A:76:ILE:HG23	1:B:418:TYR:O	0.55	2.02	9	6
1:A:75:PRO:HG2	1:A:78:ALA:HB3	0.54	1.79	6	1
1:A:81:SER:HB3	1:B:422:THR:HG23	0.54	1.78	5	1
1:B:315:MET:O	1:B:318:LEU:HD22	0.54	2.02	7	2
1:B:398:ASP:HB2	1:B:401:LEU:HD23	0.54	1.78	17	1
1:B:325:GLN:NE2	1:B:356:ILE:HG12	0.54	2.18	18	1
1:A:81:SER:HB2	1:B:422:THR:OG1	0.53	2.02	9	1
1:B:386:ARG:C	1:B:386:ARG:HD2	0.53	2.28	2	2
1:A:70:THR:O	1:A:105:PHE:HB2	0.53	2.04	8	3
1:A:104:SER:HB3	1:A:121:LEU:O	0.53	2.04	2	1
1:A:49:GLY:O	1:A:51:PRO:HD3	0.53	2.04	7	1
1:A:81:SER:OG	1:A:84:ARG:HB2	0.53	2.03	8	1
1:B:342:TRP:CZ3	1:B:362:GLU:HB2	0.53	2.39	15	1
1:B:325:GLN:NE2	1:B:356:ILE:HB	0.53	2.19	1	1
1:A:25:GLN:HG3	1:A:56:ILE:HG12	0.53	1.81	16	1
1:A:25:GLN:NE2	1:A:56:ILE:HB	0.52	2.19	1	2
1:B:405:PHE:CZ	1:B:421:LEU:HD22	0.52	2.38	19	4
1:A:47:CYS:HA	1:A:58:LEU:HD13	0.52	1.81	7	4
1:B:328:VAL:HG13	1:B:410:VAL:HG11	0.52	1.81	12	4
1:A:107:LEU:HD22	1:B:419:TYR:OH	0.52	2.04	16	5
1:B:318:LEU:HD11	1:B:356:ILE:HD13	0.52	1.82	7	1
1:A:80:LEU:HD21	1:A:121:LEU:CD1	0.52	2.34	17	1
1:B:346:ASN:O	1:B:358:LEU:HA	0.52	2.05	8	6
1:A:80:LEU:HD21	1:B:380:LEU:HD22	0.51	1.81	2	1
1:B:327:TYR:O	1:B:331:LEU:HG	0.51	2.06	17	5
1:A:57:CYS:SG	1:A:72:VAL:HG22	0.51	2.44	8	1
1:B:359:VAL:HG11	1:B:396:GLN:OE1	0.51	2.05	16	1
1:A:43:HIS:ND1	1:A:44:GLU:HG2	0.51	2.20	2	1
1:A:84:ARG:O	1:A:88:ILE:HG13	0.51	2.05	3	2
1:A:27:TYR:O	1:A:31:LEU:HG	0.51	2.06	20	5
1:A:85:ILE:HD13	1:A:86:ARG:N	0.51	2.21	14	1
1:A:59:VAL:HG22	1:A:70:THR:HG23	0.51	1.83	9	1
1:A:93:ARG:HB2	1:A:98:ASP:O	0.51	2.06	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:ALA:O	1:B:420:LYS:HB3	0.51	2.05	18	4
1:B:374:THR:O	1:B:409:ILE:HA	0.50	2.06	3	5
1:A:109:ILE:HG12	1:B:419:TYR:CE1	0.50	2.42	6	3
1:A:121:LEU:C	1:A:121:LEU:HD23	0.50	2.31	11	2
1:B:385:ILE:HD12	1:B:386:ARG:N	0.50	2.21	14	3
1:A:88:ILE:HB	1:A:105:PHE:CE2	0.50	2.42	16	1
1:B:336:LEU:HD11	1:B:371:VAL:HG21	0.50	1.84	14	3
1:B:357:CYS:SG	1:B:372:VAL:HB	0.50	2.46	5	2
1:A:55:LEU:HD13	1:A:57:CYS:SG	0.50	2.46	16	2
1:A:89:LEU:O	1:A:93:ARG:HB3	0.50	2.07	8	1
1:B:385:ILE:O	1:B:389:LEU:HG	0.50	2.07	2	4
1:A:62:GLU:C	1:A:63:ILE:HD12	0.50	2.32	15	4
1:B:376:ILE:O	1:B:376:ILE:HD13	0.50	2.07	18	7
1:B:403:MET:HG2	1:B:404:SER:H	0.49	1.67	17	6
1:A:92:SER:O	1:A:96:GLN:HG2	0.49	2.07	3	1
1:A:81:SER:HB3	1:A:84:ARG:HB2	0.49	1.84	9	1
1:B:361:THR:HG23	1:B:367:GLY:CA	0.49	2.36	20	1
1:A:53:LEU:HG	1:A:55:LEU:HD23	0.49	1.85	1	1
1:A:85:ILE:HG13	1:A:105:PHE:CE2	0.49	2.41	16	2
1:B:371:VAL:HG12	1:B:406:THR:HB	0.49	1.83	6	1
1:B:388:ILE:HB	1:B:405:PHE:CE2	0.49	2.43	16	1
1:A:103:MET:HG2	1:A:104:SER:H	0.49	1.68	19	8
1:A:80:LEU:HD11	1:A:121:LEU:HD22	0.49	1.84	8	1
1:B:315:MET:SD	1:B:329:ALA:HB3	0.49	2.47	4	4
1:B:376:ILE:HD13	1:B:409:ILE:HG22	0.49	1.85	2	1
1:A:101:LEU:H	1:A:101:LEU:HD23	0.49	1.68	20	1
1:A:74:THR:O	1:A:109:ILE:HA	0.48	2.08	19	6
1:B:381:SER:O	1:B:384:ARG:HB3	0.48	2.07	12	2
1:A:37:MET:HA	1:A:37:MET:CE	0.48	2.39	3	2
1:A:93:ARG:C	1:A:93:ARG:HD2	0.48	2.33	4	1
1:B:407:LEU:O	1:B:418:TYR:HA	0.48	2.08	16	1
1:A:46:ASN:HB2	1:A:59:VAL:O	0.48	2.08	12	3
1:B:343:HIS:CD2	1:B:364:GLU:HB2	0.48	2.43	6	1
1:B:325:GLN:NE2	1:B:356:ILE:HG13	0.48	2.23	12	1
1:B:361:THR:HG23	1:B:367:GLY:HA3	0.48	1.84	14	1
1:B:337:MET:HA	1:B:337:MET:CE	0.48	2.39	9	3
1:A:111:GLU:HB3	1:A:115:THR:HB	0.48	1.86	20	2
1:A:36:LEU:HD11	1:A:71:VAL:HG21	0.48	1.85	17	4
1:B:396:GLN:HG3	1:B:403:MET:SD	0.48	2.49	17	1
1:A:20:ILE:HG13	1:A:21:GLY:H	0.48	1.68	7	1
1:A:79:SER:CB	1:B:420:LYS:HD2	0.48	2.39	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:329:ALA:HB2	1:B:373:PRO:HG3	0.48	1.85	19	1
1:A:71:VAL:HG12	1:A:106:THR:HB	0.48	1.85	6	1
1:A:8:THR:H	1:A:13:LEU:CD1	0.48	2.21	16	1
1:A:81:SER:HB2	1:A:84:ARG:H	0.48	1.68	17	1
1:A:25:GLN:HG3	1:A:56:ILE:HD13	0.48	1.86	5	1
1:A:75:PRO:HG2	1:A:78:ALA:CB	0.48	2.39	6	2
1:A:18:LEU:HD12	1:A:19:ASP:N	0.48	2.24	18	1
1:A:107:LEU:HD13	1:B:419:TYR:CE2	0.47	2.44	19	4
1:B:347:CYS:HA	1:B:358:LEU:HD13	0.47	1.86	2	4
1:A:46:ASN:O	1:A:58:LEU:HA	0.47	2.10	12	7
1:B:320:ILE:HG13	1:B:321:GLY:H	0.47	1.69	7	1
1:A:81:SER:O	1:A:84:ARG:HB2	0.47	2.09	11	1
1:A:80:LEU:HD13	1:A:81:SER:H	0.47	1.68	12	2
1:A:76:ILE:HD11	1:A:109:ILE:CG2	0.47	2.39	13	1
1:A:59:VAL:HA	1:A:69:GLN:O	0.47	2.09	7	1
1:B:311:LYS:O	1:B:315:MET:HG3	0.47	2.09	15	1
1:B:315:MET:SD	1:B:326:VAL:HA	0.47	2.50	2	1
1:B:394:LYS:HD3	1:B:394:LYS:C	0.47	2.34	11	1
1:A:80:LEU:HG	1:A:81:SER:N	0.47	2.25	17	2
1:A:76:ILE:CG1	1:A:111:GLU:HA	0.47	2.39	19	1
1:B:393:ARG:HB3	1:B:398:ASP:O	0.47	2.09	6	2
1:B:385:ILE:CD1	1:B:421:LEU:HD11	0.47	2.39	15	1
1:B:405:PHE:CE2	1:B:421:LEU:HD23	0.47	2.44	12	1
1:A:93:ARG:NH2	1:A:101:LEU:HD23	0.47	2.24	14	1
1:A:76:ILE:HD13	1:A:76:ILE:O	0.47	2.10	2	3
1:B:340:LYS:NZ	1:B:340:LYS:HB2	0.47	2.25	5	1
1:B:403:MET:HG2	1:B:404:SER:N	0.47	2.24	10	1
1:B:361:THR:HG22	1:B:363:ILE:O	0.47	2.10	12	1
1:A:11:LYS:HD2	1:A:11:LYS:H	0.47	1.70	13	1
1:A:29:ALA:HB2	1:A:73:PRO:HG3	0.47	1.85	19	2
1:B:382:HIS:HA	1:B:385:ILE:HG12	0.47	1.85	15	1
1:B:404:SER:HB2	1:B:421:LEU:O	0.47	2.09	18	1
1:A:76:ILE:CG2	1:B:418:TYR:HB2	0.47	2.39	8	1
1:A:81:SER:HB3	1:B:422:THR:CB	0.47	2.38	6	1
1:B:362:GLU:C	1:B:363:ILE:HD12	0.47	2.35	16	5
1:A:53:LEU:HD13	1:A:53:LEU:O	0.46	2.10	8	1
1:A:16:MET:SD	1:A:26:VAL:HG21	0.46	2.49	16	2
1:A:11:LYS:O	1:A:15:MET:HG3	0.46	2.10	15	1
1:A:93:ARG:HD3	1:A:100:ASP:HA	0.46	1.86	19	1
1:B:367:GLY:O	1:B:368:LEU:HB2	0.46	2.10	16	1
1:A:121:LEU:CB	1:B:380:LEU:HB3	0.46	2.40	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:346:ASN:O	1:B:358:LEU:HD12	0.46	2.10	18	2
1:B:315:MET:HG2	1:B:347:CYS:SG	0.46	2.50	12	1
1:A:43:HIS:CE1	1:A:44:GLU:HG2	0.46	2.46	2	1
1:B:344:GLU:HB3	1:B:361:THR:OG1	0.46	2.10	18	1
1:B:318:LEU:HD21	1:B:347:CYS:SG	0.46	2.51	14	1
1:A:80:LEU:HD12	1:A:84:ARG:HD2	0.46	1.88	3	1
1:A:27:TYR:O	1:A:31:LEU:HD13	0.46	2.10	8	5
1:A:57:CYS:SG	1:A:70:THR:HG23	0.46	2.51	6	1
1:A:76:ILE:CD1	1:B:418:TYR:HB2	0.46	2.41	6	1
1:A:109:ILE:HG12	1:B:419:TYR:CZ	0.46	2.45	8	1
1:A:68:LEU:O	1:A:68:LEU:HD13	0.46	2.11	13	1
1:B:382:HIS:HA	1:B:385:ILE:HG13	0.46	1.87	15	1
1:B:393:ARG:NH2	1:B:400:ASP:HA	0.46	2.26	17	1
1:A:40:LYS:HD3	1:A:118:TYR:CE2	0.46	2.46	6	1
1:B:316:MET:SD	1:B:326:VAL:HG11	0.46	2.51	3	2
1:A:81:SER:HB3	1:A:84:ARG:CB	0.46	2.41	9	1
1:B:392:SER:O	1:B:396:GLN:HG2	0.45	2.10	4	2
1:A:15:MET:SD	1:A:29:ALA:HB3	0.45	2.51	13	1
1:B:406:THR:OG1	1:B:420:LYS:HG2	0.45	2.12	10	1
1:A:80:LEU:O	1:B:422:THR:N	0.45	2.48	18	4
1:A:85:ILE:HD12	1:A:86:ARG:N	0.45	2.27	5	1
1:A:92:SER:O	1:A:96:GLN:HG3	0.45	2.11	8	1
1:B:327:TYR:O	1:B:331:LEU:HD13	0.45	2.11	6	3
1:B:376:ILE:HD13	1:B:409:ILE:CG2	0.45	2.42	2	3
1:B:410:VAL:HG22	1:B:411:GLU:O	0.45	2.12	1	1
1:B:380:LEU:HD13	1:B:381:SER:N	0.45	2.27	6	1
1:A:119:TYR:CE2	1:B:380:LEU:HD21	0.45	2.46	8	1
1:A:110:VAL:HA	1:A:115:THR:O	0.45	2.12	15	2
1:A:80:LEU:HD21	1:A:121:LEU:HD12	0.45	1.86	18	1
1:B:352:GLU:OE2	1:B:390:LYS:HE3	0.45	2.12	2	1
1:A:37:MET:SD	1:A:45:VAL:HG11	0.45	2.51	4	1
1:B:310:PRO:O	1:B:314:GLU:HG2	0.45	2.11	4	1
1:B:343:HIS:CE1	1:B:364:GLU:HB2	0.45	2.47	16	1
1:A:80:LEU:HG	1:A:81:SER:H	0.45	1.72	17	1
1:A:85:ILE:HD11	1:A:121:LEU:HD11	0.45	1.87	18	1
1:B:344:GLU:O	1:B:360:GLY:HA3	0.45	2.12	4	4
1:A:74:THR:HG21	1:B:419:TYR:OH	0.45	2.12	12	4
1:A:83:ASN:O	1:A:87:GLU:HG3	0.45	2.12	7	1
1:A:79:SER:HA	1:B:420:LYS:HB3	0.45	1.89	8	1
1:B:392:SER:O	1:B:396:GLN:HB2	0.45	2.12	19	1
1:A:81:SER:HB3	1:B:422:THR:CG2	0.45	2.42	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:353:LEU:HG	1:B:355:LEU:HD13	0.45	1.89	5	1
1:A:80:LEU:O	1:B:422:THR:HB	0.45	2.12	12	1
1:A:103:MET:HG2	1:A:104:SER:N	0.45	2.27	17	1
1:A:83:ASN:C	1:A:83:ASN:HD22	0.44	2.20	5	1
1:A:75:PRO:CG	1:A:78:ALA:HB3	0.44	2.41	6	1
1:A:89:LEU:HD22	1:A:103:MET:HB3	0.44	1.88	8	1
1:A:66:GLU:CD	1:A:67:GLY:H	0.44	2.19	10	1
1:B:393:ARG:HG3	1:B:398:ASP:O	0.44	2.12	11	1
1:B:361:THR:HA	1:B:367:GLY:HA2	0.44	1.89	19	1
1:B:310:PRO:O	1:B:314:GLU:HB2	0.44	2.12	1	3
1:A:50:LEU:HD23	1:A:57:CYS:SG	0.44	2.51	2	1
1:A:71:VAL:HA	1:A:106:THR:O	0.44	2.12	20	2
1:A:96:GLN:HG3	1:A:103:MET:HE1	0.44	1.87	10	1
1:A:103:MET:CG	1:A:104:SER:H	0.44	2.25	16	1
1:A:104:SER:OG	1:A:120:LYS:HE2	0.44	2.12	9	1
1:B:362:GLU:O	1:B:366:GLU:HB2	0.44	2.13	19	1
1:A:93:ARG:CZ	1:A:100:ASP:HA	0.44	2.43	3	1
1:A:80:LEU:CD2	1:B:380:LEU:HG	0.44	2.43	8	1
1:A:25:GLN:HB3	1:A:56:ILE:HG12	0.44	1.90	11	1
1:A:42:TRP:CE3	1:A:45:VAL:HG22	0.44	2.47	19	1
1:A:79:SER:HB2	1:B:422:THR:OG1	0.44	2.12	1	1
1:B:384:ARG:O	1:B:388:ILE:HG13	0.44	2.13	6	1
1:B:311:LYS:O	1:B:315:MET:HG2	0.44	2.13	8	1
1:B:382:HIS:O	1:B:385:ILE:HB	0.44	2.13	10	1
1:A:85:ILE:HD12	1:A:121:LEU:CD2	0.44	2.43	20	1
1:A:59:VAL:HG13	1:A:69:GLN:O	0.43	2.13	3	1
1:B:319:ASP:O	1:B:320:ILE:HG23	0.43	2.13	13	2
1:B:380:LEU:HD21	1:B:421:LEU:CD1	0.43	2.43	19	1
1:B:312:TYR:O	1:B:316:MET:HG3	0.43	2.13	5	1
1:A:46:ASN:O	1:A:58:LEU:HD12	0.43	2.13	6	2
1:B:361:THR:HG23	1:B:366:GLU:O	0.43	2.12	15	1
1:A:15:MET:SD	1:A:26:VAL:HA	0.43	2.54	2	2
1:A:80:LEU:HB2	1:B:419:TYR:CE2	0.43	2.49	20	2
1:A:104:SER:OG	1:A:122:THR:HA	0.43	2.13	16	1
1:A:76:ILE:HD11	1:B:417:VAL:HG13	0.43	1.90	17	1
1:A:80:LEU:C	1:B:421:LEU:HA	0.43	2.39	17	1
1:A:75:PRO:CG	1:A:78:ALA:HB2	0.43	2.41	2	1
1:A:81:SER:O	1:A:85:ILE:HG23	0.43	2.14	9	1
1:A:68:LEU:HG	1:A:96:GLN:OE1	0.43	2.13	10	1
1:B:310:PRO:O	1:B:314:GLU:HG3	0.43	2.14	10	1
1:B:315:MET:SD	1:B:326:VAL:HG13	0.43	2.54	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ILE:CG2	1:A:54:GLN:HG3	0.43	2.44	11	1
1:A:79:SER:HB3	1:B:420:LYS:HD2	0.43	1.91	18	1
1:A:67:GLY:C	1:A:68:LEU:HD12	0.43	2.39	1	4
1:A:70:THR:HG21	1:A:92:SER:OG	0.43	2.13	6	1
1:A:68:LEU:HD12	1:A:68:LEU:H	0.43	1.72	8	1
1:A:61:THR:CG2	1:A:64:GLU:HA	0.43	2.43	19	1
1:A:68:LEU:HD12	1:A:68:LEU:O	0.43	2.14	7	1
1:A:93:ARG:HD3	1:A:99:PRO:C	0.43	2.39	13	1
1:B:320:ILE:O	1:B:322:ASP:N	0.43	2.52	6	1
1:B:376:ILE:HB	1:B:410:VAL:O	0.43	2.14	20	1
1:B:382:HIS:O	1:B:385:ILE:HG12	0.42	2.15	4	2
1:A:107:LEU:O	1:A:118:TYR:HA	0.42	2.13	16	1
1:B:410:VAL:HA	1:B:415:THR:O	0.42	2.14	19	1
1:B:391:ALA:O	1:B:395:LEU:HD23	0.42	2.14	20	1
1:A:44:GLU:HB3	1:A:61:THR:OG1	0.42	2.14	18	3
1:B:322:ASP:O	1:B:326:VAL:HG22	0.42	2.14	7	1
1:A:111:GLU:OE1	1:A:113:ASP:HB2	0.42	2.14	1	1
1:A:113:ASP:O	1:A:114:SER:HB2	0.42	2.14	5	2
1:A:80:LEU:HB3	1:B:421:LEU:CB	0.42	2.44	13	1
1:B:322:ASP:OD2	1:B:324:THR:HB	0.42	2.15	14	1
1:B:411:GLU:HB3	1:B:415:THR:HB	0.42	1.90	20	1
1:A:81:SER:O	1:A:85:ILE:HG12	0.42	2.15	6	1
1:B:344:GLU:HB3	1:B:361:THR:HB	0.42	1.90	9	2
1:B:335:ASP:O	1:B:339:SER:HB3	0.42	2.14	13	1
1:A:76:ILE:HD12	1:B:418:TYR:O	0.42	2.14	10	1
1:A:103:MET:O	1:A:123:ASP:HB3	0.42	2.14	14	1
1:B:405:PHE:CE1	1:B:421:LEU:HD21	0.42	2.50	16	1
1:A:80:LEU:HD13	1:B:419:TYR:OH	0.42	2.15	3	1
1:A:70:THR:HG21	1:A:92:SER:HB3	0.42	1.91	17	1
1:A:121:LEU:HD12	1:B:380:LEU:HB2	0.42	1.91	8	1
1:B:325:GLN:HB3	1:B:356:ILE:HG12	0.42	1.90	11	1
1:A:27:TYR:O	1:A:31:LEU:HD23	0.42	2.15	19	1
1:A:79:SER:HA	1:B:420:LYS:O	0.42	2.14	1	1
1:A:10:PRO:O	1:A:14:GLU:HG2	0.42	2.15	7	1
1:A:62:GLU:HG2	1:A:69:GLN:NE2	0.42	2.30	16	1
1:A:79:SER:O	1:A:84:ARG:HG3	0.42	2.15	18	1
1:B:394:LYS:C	1:B:394:LYS:HD2	0.41	2.40	8	1
1:B:407:LEU:HG	1:B:421:LEU:CD2	0.41	2.45	13	1
1:A:25:GLN:CG	1:A:56:ILE:HG12	0.41	2.44	16	1
1:A:107:LEU:HD13	1:B:419:TYR:CZ	0.41	2.50	16	1
1:A:86:ARG:HD2	1:A:86:ARG:C	0.41	2.39	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:342:TRP:CZ3	1:B:369:GLN:HB3	0.41	2.50	15	1
1:A:81:SER:HB2	1:B:422:THR:CG2	0.41	2.44	18	1
1:B:421:LEU:C	1:B:421:LEU:HD23	0.41	2.40	9	2
1:B:350:LEU:CD1	1:B:391:ALA:HB1	0.41	2.46	20	2
1:A:81:SER:HA	1:B:422:THR:H	0.41	1.75	17	1
1:A:83:ASN:O	1:A:87:GLU:HG2	0.41	2.15	6	1
1:B:352:GLU:HB2	1:B:353:LEU:HD12	0.41	1.92	8	1
1:A:121:LEU:CD1	1:B:380:LEU:HD23	0.41	2.45	12	1
1:A:44:GLU:O	1:A:60:GLY:HA3	0.41	2.16	19	1
1:A:67:GLY:C	1:A:68:LEU:HD22	0.41	2.40	20	1
1:B:386:ARG:HD2	1:B:386:ARG:C	0.41	2.41	1	1
1:B:367:GLY:C	1:B:368:LEU:HD12	0.41	2.41	5	1
1:A:81:SER:O	1:A:84:ARG:HB3	0.41	2.16	7	1
1:A:85:ILE:HB	1:A:121:LEU:HD21	0.41	1.92	8	1
1:A:76:ILE:HD13	1:A:110:VAL:C	0.41	2.39	13	1
1:A:97:GLY:O	1:A:99:PRO:HD3	0.41	2.16	17	1
1:B:395:LEU:HD12	1:B:395:LEU:C	0.41	2.41	1	1
1:B:366:GLU:CD	1:B:367:GLY:H	0.41	2.22	5	1
1:B:314:GLU:O	1:B:317:GLU:HB3	0.41	2.15	8	1
1:A:18:LEU:HD21	1:A:47:CYS:SG	0.41	2.56	14	1
1:A:81:SER:HG	1:B:422:THR:HB	0.41	1.74	14	1
1:A:62:GLU:H	1:A:62:GLU:CD	0.41	2.23	2	1
1:B:360:GLY:O	1:B:368:LEU:HD12	0.41	2.15	4	1
1:A:25:GLN:HB3	1:A:56:ILE:CG1	0.41	2.45	11	1
1:A:66:GLU:HG3	1:A:67:GLY:H	0.41	1.75	15	1
1:A:93:ARG:NH2	1:A:100:ASP:HA	0.41	2.30	17	1
1:A:50:LEU:CD1	1:A:91:ALA:HB1	0.41	2.46	20	1
1:A:110:VAL:HG22	1:A:111:GLU:O	0.41	2.16	9	1
1:A:10:PRO:O	1:A:14:GLU:HG3	0.41	2.16	10	1
1:A:32:VAL:O	1:A:36:LEU:HG	0.41	2.16	10	1
1:B:316:MET:SD	1:B:326:VAL:HG21	0.41	2.56	10	1
1:A:111:GLU:CD	1:A:112:SER:H	0.41	2.24	13	1
1:A:90:LYS:HG3	1:A:93:ARG:NH1	0.41	2.31	15	1
1:B:383:ASN:O	1:B:387:GLU:HG2	0.41	2.15	18	1
1:A:36:LEU:HD12	1:A:58:LEU:HD23	0.41	1.93	20	1
1:B:325:GLN:HB3	1:B:356:ILE:CG1	0.41	2.46	11	1
1:A:105:PHE:CE2	1:A:121:LEU:HD23	0.41	2.51	12	1
1:B:352:GLU:OE1	1:B:353:LEU:HD13	0.40	2.16	1	1
1:A:56:ILE:N	1:A:56:ILE:HD12	0.40	2.31	5	1
1:A:53:LEU:HB2	1:A:55:LEU:HG	0.40	1.93	7	1
1:B:407:LEU:HD23	1:B:408:ALA:N	0.40	2.31	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:396:GLN:CG	1:B:403:MET:HE1	0.40	2.47	6	1
1:A:107:LEU:HG	1:A:121:LEU:CD2	0.40	2.46	13	1
1:A:85:ILE:HG21	1:A:121:LEU:HD11	0.40	1.93	19	1
1:B:376:ILE:HB	1:B:411:GLU:HB2	0.40	1.93	19	1
1:A:28:VAL:HG13	1:A:110:VAL:HG21	0.40	1.94	4	1
1:A:81:SER:CB	1:B:422:THR:O	0.40	2.69	8	1
1:B:405:PHE:CE2	1:B:421:LEU:HD22	0.40	2.51	14	1
1:B:322:ASP:O	1:B:326:VAL:HG23	0.40	2.16	19	1
1:A:76:ILE:HD13	1:A:110:VAL:O	0.40	2.15	13	1
1:B:327:TYR:O	1:B:331:LEU:HD23	0.40	2.16	19	1
1:A:80:LEU:O	1:B:422:THR:HG22	0.40	2.17	20	1
1:B:336:LEU:HD12	1:B:358:LEU:HD23	0.40	1.94	20	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	115/123 (93%)	104±2 (90±2%)	7±1 (6±1%)	4±2 (4±2%)	4	30
1	B	115/123 (93%)	103±3 (89±2%)	8±3 (7±2%)	4±1 (3±1%)	5	35
All	All	4600/4920 (93%)	4128 (90%)	305 (7%)	167 (4%)	4	32

All 36 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	67	GLY	13
1	A	114	SER	13
1	B	320	ILE	13
1	A	20	ILE	11
1	A	41	SER	9
1	A	8	THR	8
1	B	414	SER	8
1	A	19	ASP	8
1	A	100	ASP	8

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Mol	Chain	Res	Type	Models (Total)
1	B	321	GLY	8
1	B	341	SER	7
1	B	319	ASP	5
1	B	399	PRO	5
1	B	368	LEU	5
1	B	404	SER	5
1	B	412	SER	4
1	A	21	GLY	4
1	B	363	ILE	4
1	B	367	GLY	3
1	A	99	PRO	3
1	B	379	SER	3
1	A	112	SER	3
1	B	400	ASP	2
1	A	68	LEU	2
1	B	308	THR	2
1	A	78	ALA	1
1	A	42	TRP	1
1	A	43	HIS	1
1	A	97	GLY	1
1	A	104	SER	1
1	A	113	ASP	1
1	B	378	ALA	1
1	A	63	ILE	1
1	B	411	GLU	1
1	A	18	LEU	1
1	B	318	LEU	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	105/110 (95%)	101±2 (96±2%)	4±2 (4±2%)	28	79
1	B	105/110 (95%)	101±2 (96±2%)	4±2 (4±2%)	30	80
All	All	4200/4400 (95%)	4033 (96%)	167 (4%)	29	79

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	B	384	ARG	10
1	B	376	ILE	9
1	A	37	MET	8
1	A	84	ARG	8
1	B	337	MET	7
1	A	76	ILE	6
1	A	86	ARG	6
1	B	386	ARG	6
1	A	95	LEU	4
1	B	395	LEU	4
1	A	94	LYS	4
1	A	69	GLN	3
1	B	340	LYS	3
1	B	355	LEU	3
1	A	18	LEU	3
1	B	393	ARG	3
1	A	11	LYS	3
1	A	25	GLN	3
1	B	396	GLN	3
1	A	54	GLN	2
1	A	55	LEU	2
1	B	353	LEU	2
1	A	62	GLU	2
1	B	366	GLU	2
1	A	93	ARG	2
1	A	116	ILE	2
1	A	72	VAL	2
1	B	394	LYS	2
1	A	13	LEU	2
1	A	40	LYS	2
1	A	120	LYS	2
1	A	50	LEU	2
1	B	350	LEU	2
1	A	58	LEU	2
1	A	81	SER	2
1	B	401	LEU	2
1	B	416	ILE	2
1	B	385	ILE	2
1	A	20	ILE	2
1	A	80	LEU	2
1	B	320	ILE	2
1	B	411	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	B	368	LEU	2
1	A	19	ASP	1
1	B	352	GLU	1
1	B	358	LEU	1
1	B	392	SER	1
1	A	9	HIS	1
1	A	83	ASN	1
1	B	311	LYS	1
1	B	383	ASN	1
1	A	68	LEU	1
1	B	354	GLN	1
1	A	111	GLU	1
1	A	121	LEU	1
1	B	325	GLN	1
1	A	52	GLU	1
1	A	85	ILE	1
1	B	369	GLN	1
1	B	372	VAL	1
1	A	56	ILE	1
1	A	122	THR	1
1	B	422	THR	1
1	B	318	LEU	1
1	B	380	LEU	1
1	B	362	GLU	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