



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 10:48 AM UTC

PDB ID : 1UMS / pdb_00001ums
Title : STROMELYSIN-1 CATALYTIC DOMAIN WITH HYDROPHOBIC INHIBITOR BOUND, PH 7.0, 32OC, 20 MM CACL2, 15% ACETONITRILE; NMR ENSEMBLE OF 20 STRUCTURES
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Deposited on : 1995-10-31

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
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

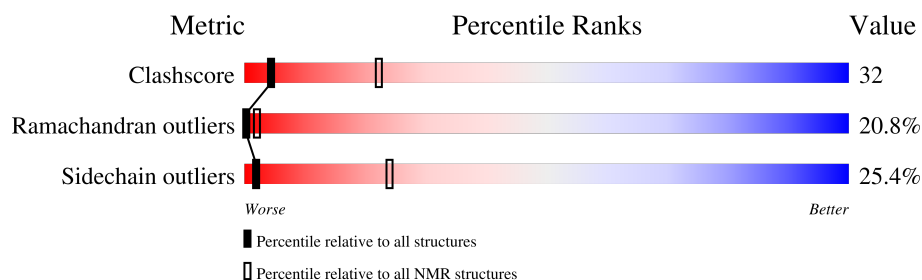
1 Overall quality at a glance

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	174	25% 37% 26% 7% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
4	A	0DS	261	2	-

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:83-A:248 (166)	1.09	6

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2643 atoms, of which 1284 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called STROMELYSIN-1.

Mol	Chain	Residues	Atoms						Trace
1	A	166	Total	C	H	N	O	S	0
			2572	851	1248	221	250	2	

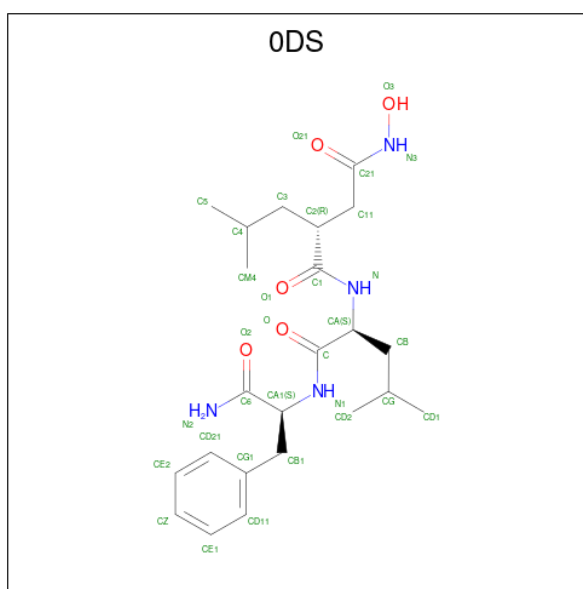
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
3	A	1	Total	Ca
			1	1

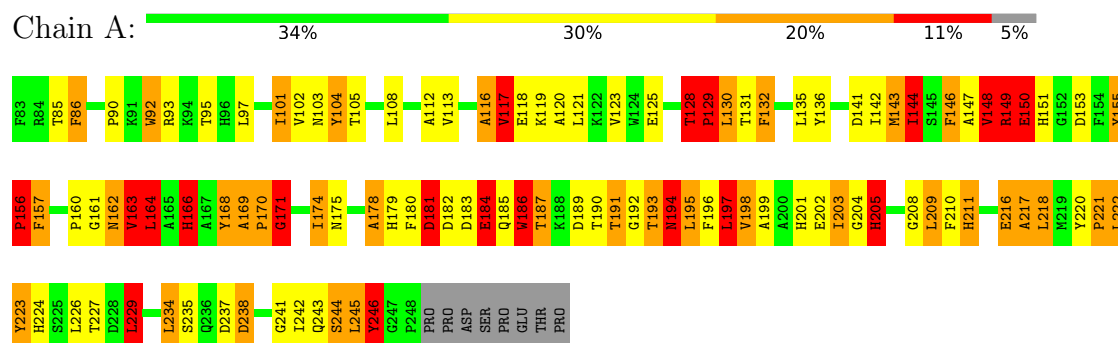
- Molecule 4 is N-{(2R)-2-[2-(hydroxyamino)-2-oxoethyl]-4-methylpentanoyl}-L-leucyl-L-phenylalaninamide (CCD ID: 0DS) (formula: C₂₃H₃₆N₄O₅).



Mol	Chain	Residues	Atoms				
4	A	1	Total	C	H	N	O
			68	23	36	4	5

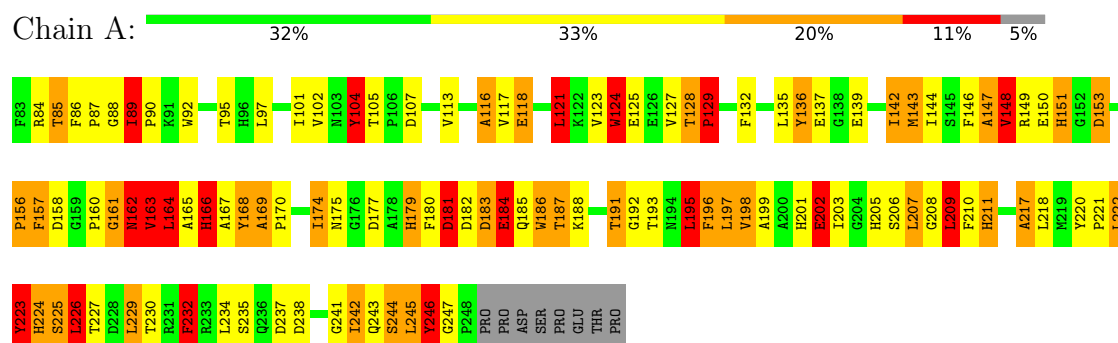
4.2.2 Score per residue for model 2

• Molecule 1: STROMELYSIN-1



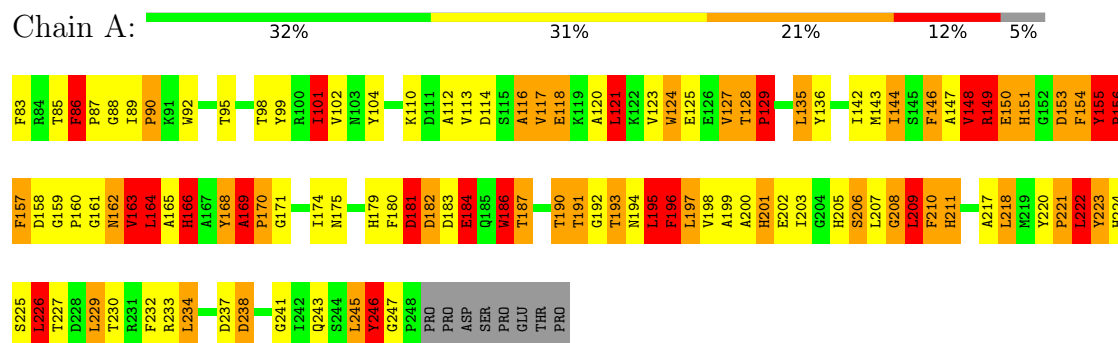
4.2.3 Score per residue for model 3

• Molecule 1: STROMELYSIN-1



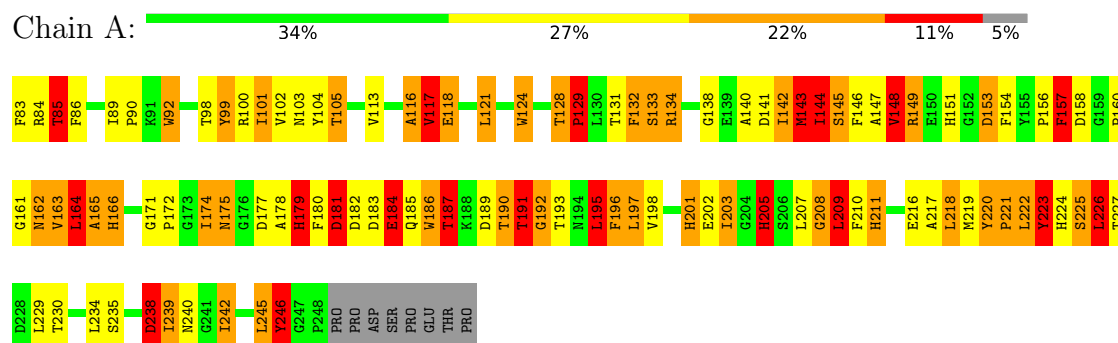
4.2.4 Score per residue for model 4

• Molecule 1: STROMELYSIN-1



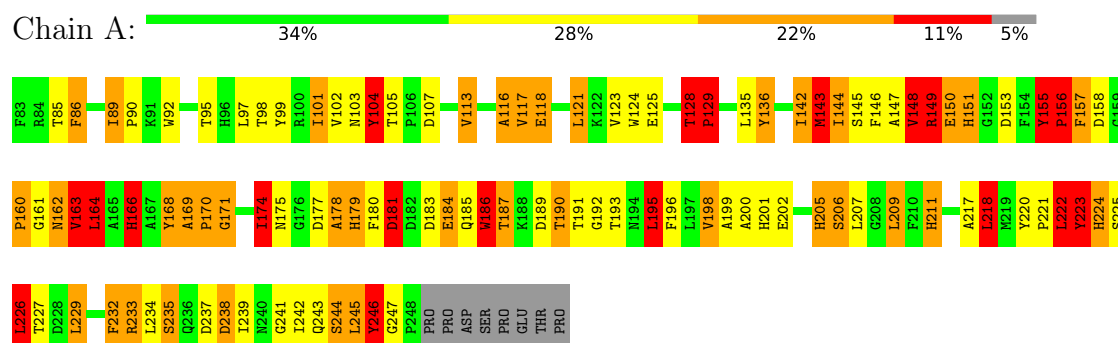
4.2.5 Score per residue for model 5

• Molecule 1: STROMELYSIN-1



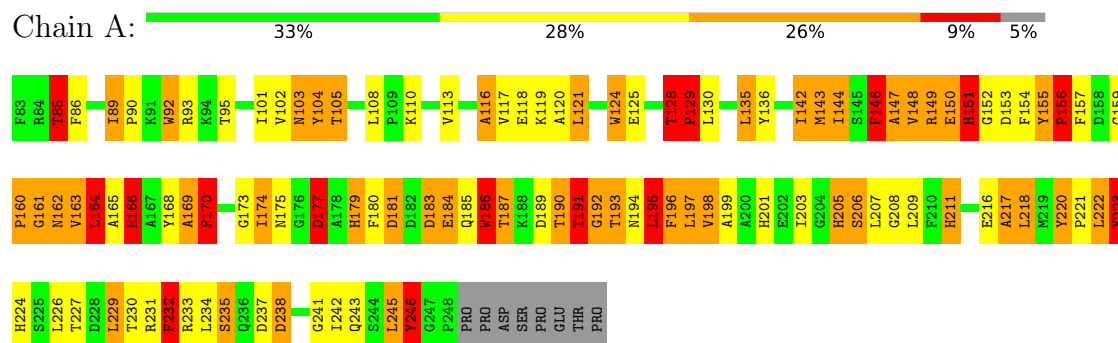
4.2.6 Score per residue for model 6 (medoid)

• Molecule 1: STROMELYSIN-1



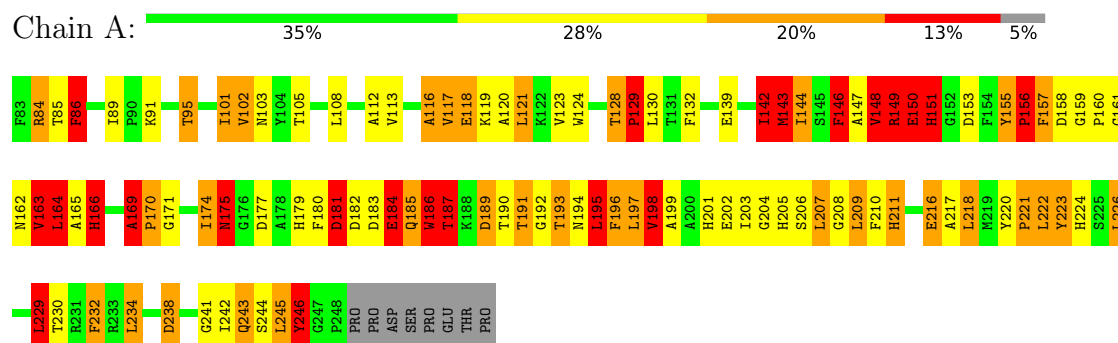
4.2.7 Score per residue for model 7

• Molecule 1: STROMELYSIN-1



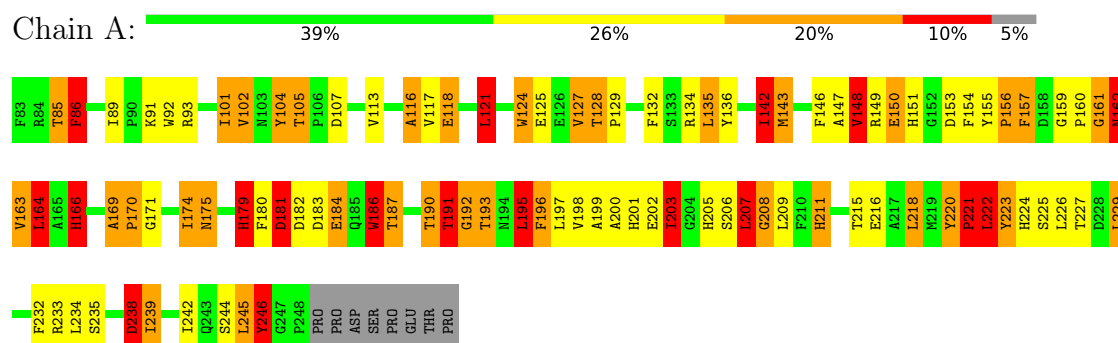
4.2.8 Score per residue for model 8

• Molecule 1: STROMELYSIN-1



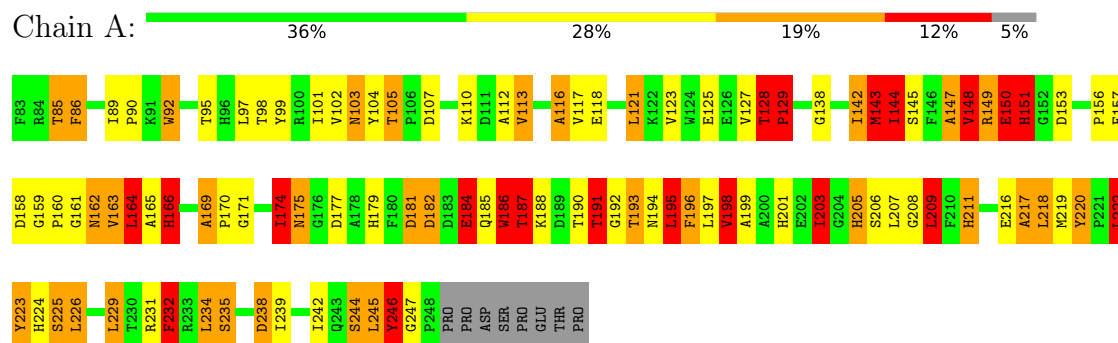
4.2.9 Score per residue for model 9

• Molecule 1: STROMELYSIN-1



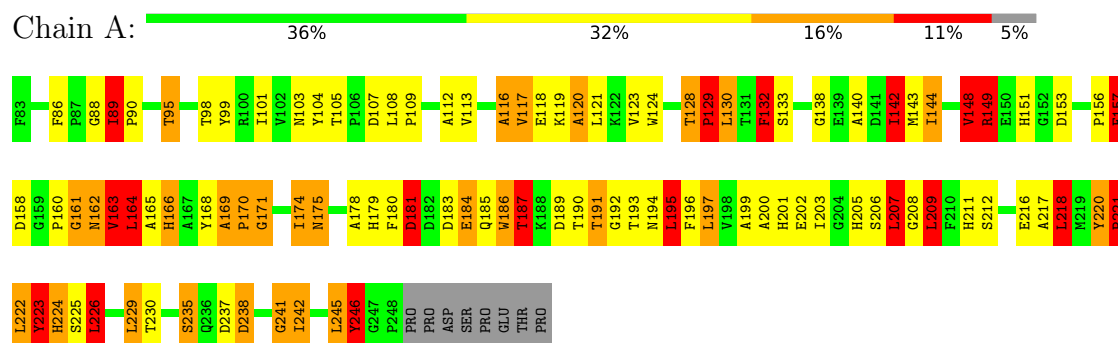
4.2.10 Score per residue for model 10

• Molecule 1: STROMELYSIN-1



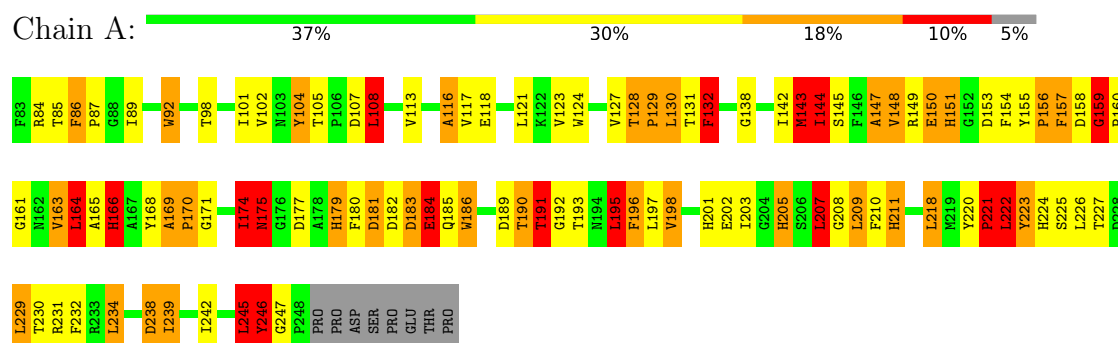
4.2.11 Score per residue for model 11

- Molecule 1: STROMELYSIN-1



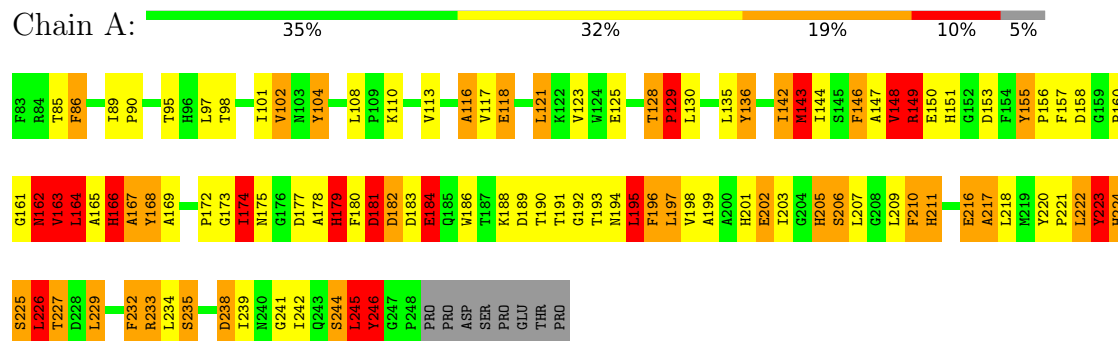
4.2.12 Score per residue for model 12

- Molecule 1: STROMELYSIN-1



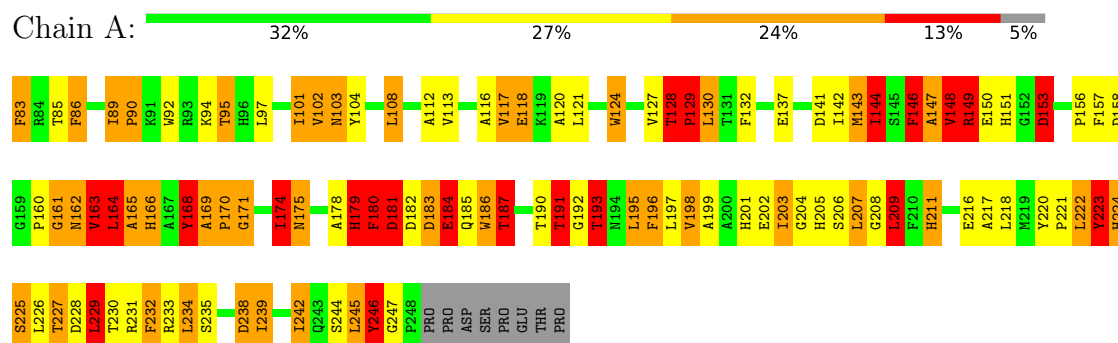
4.2.13 Score per residue for model 13

- Molecule 1: STROMELYSIN-1



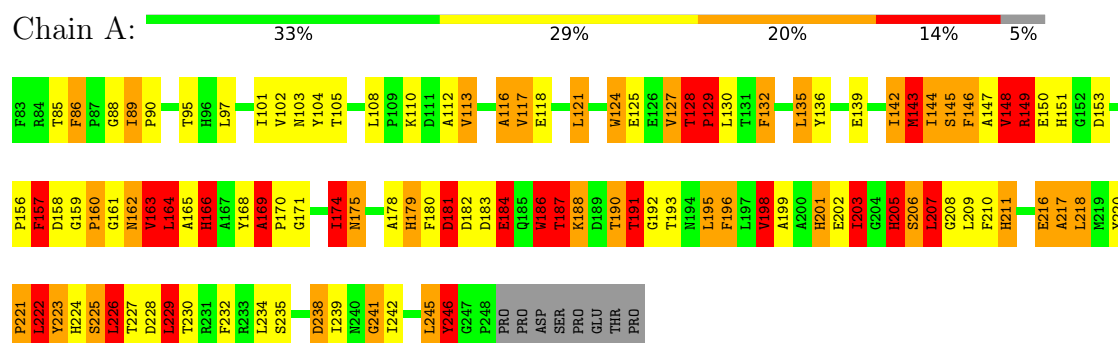
4.2.14 Score per residue for model 14

• Molecule 1: STROMELYSIN-1



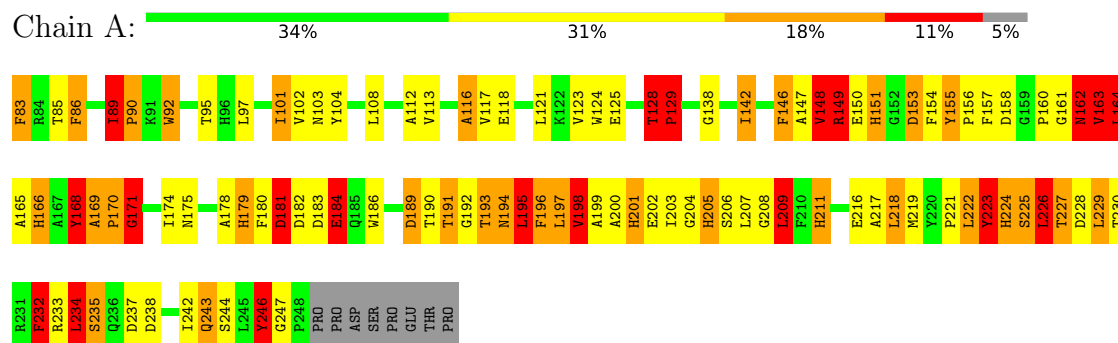
4.2.15 Score per residue for model 15

• Molecule 1: STROMELYSIN-1



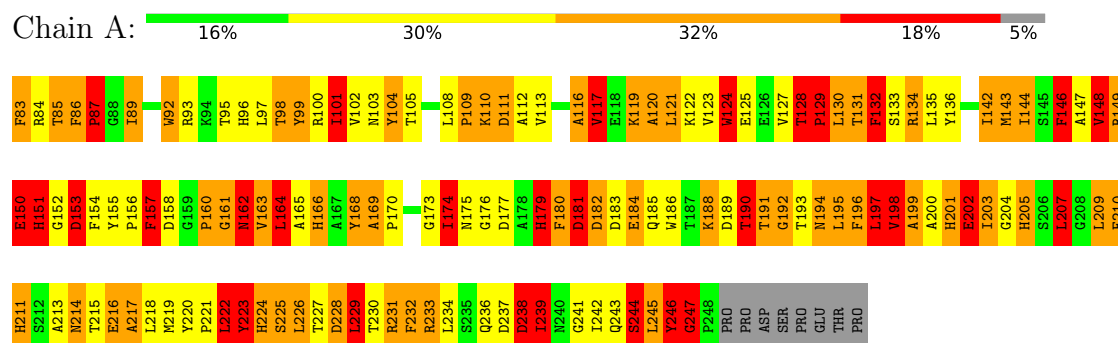
4.2.16 Score per residue for model 16

• Molecule 1: STROMELYSIN-1



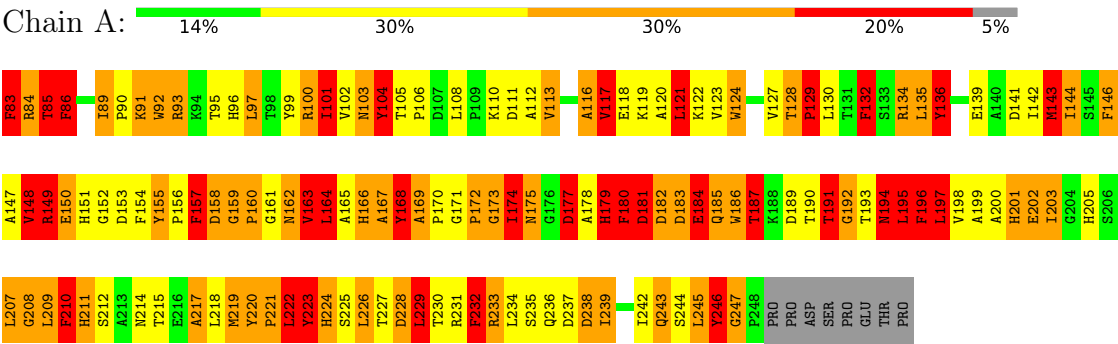
4.2.17 Score per residue for model 17

• Molecule 1: STROMELYSIN-1



4.2.20 Score per residue for model 20

● Molecule 1: STROMELYSIN-1



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 20 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DGII	refinement	
Discover	refinement	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ODS, CA, ZN

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	1.17±0.44	7±14/1366 (0.5± 1.0%)	2.57±0.31	120±38/1864 (6.4± 2.0%)
All	All	1.25	147/27320 (0.5%)	2.59	2393/37280 (6.4%)

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	0.1±0.2	10.8±4.4
All	All	1	215

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	166	HIS	ND1-CE1	9.16	1.41	1.32	18	1
1	A	144	ILE	N-CA	-8.76	1.35	1.46	18	1
1	A	199	ALA	N-CA	-8.60	1.36	1.46	17	1
1	A	154	PHE	N-CA	-8.56	1.38	1.46	18	1
1	A	198	VAL	CA-C	-8.53	1.40	1.52	17	2
1	A	155	TYR	CA-CB	8.41	1.62	1.53	17	1
1	A	234	LEU	CA-C	8.25	1.63	1.52	18	1
1	A	116	ALA	CA-C	8.13	1.62	1.52	17	2
1	A	162	ASN	N-CA	-8.10	1.35	1.46	19	3
1	A	236	GLN	CA-C	8.10	1.64	1.52	19	2
1	A	178	ALA	N-CA	7.61	1.55	1.46	19	1
1	A	198	VAL	CA-CB	-7.60	1.43	1.54	17	1
1	A	159	GLY	CA-C	7.47	1.62	1.51	18	1
1	A	238	ASP	N-CA	-7.30	1.35	1.45	20	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	148	VAL	N-CA	-7.16	1.37	1.46	7	4
1	A	128	THR	N-CA	-7.09	1.35	1.46	17	1
1	A	201	HIS	CB-CG	6.99	1.59	1.50	19	1
1	A	180	PHE	CA-C	-6.92	1.44	1.52	18	1
1	A	211	HIS	CB-CG	6.89	1.59	1.50	18	1
1	A	166	HIS	CA-C	6.73	1.60	1.52	18	1
1	A	160	PRO	CA-C	-6.70	1.44	1.52	17	1
1	A	179	HIS	ND1-CE1	-6.62	1.25	1.32	18	1
1	A	190	THR	N-CA	-6.60	1.37	1.46	19	1
1	A	96	HIS	CG-ND1	6.58	1.45	1.38	19	1
1	A	220	TYR	CA-C	6.52	1.59	1.52	20	2
1	A	191	THR	CA-C	-6.51	1.44	1.52	19	3
1	A	167	ALA	C-O	6.48	1.31	1.23	19	1
1	A	155	TYR	N-CA	6.46	1.55	1.46	18	1
1	A	150	GLU	CA-CB	-6.44	1.45	1.53	18	1
1	A	169	ALA	CA-C	6.40	1.60	1.52	20	1
1	A	164	LEU	CA-C	-6.39	1.44	1.52	17	1
1	A	131	THR	N-CA	-6.38	1.38	1.46	17	1
1	A	240	ASN	CA-CB	-6.37	1.45	1.53	18	1
1	A	201	HIS	ND1-CE1	6.34	1.38	1.32	17	1
1	A	116	ALA	N-CA	-6.32	1.39	1.46	19	1
1	A	156	PRO	N-CD	-6.31	1.39	1.47	18	1
1	A	230	THR	CA-C	6.31	1.60	1.52	18	1
1	A	201	HIS	CE1-NE2	6.30	1.38	1.32	19	1
1	A	223	TYR	N-CA	6.26	1.54	1.46	19	1
1	A	101	ILE	N-CA	-6.25	1.39	1.46	17	2
1	A	225	SER	N-CA	-6.24	1.38	1.46	19	1
1	A	86	PHE	CA-CB	6.23	1.63	1.53	17	1
1	A	230	THR	CB-OG1	-6.21	1.33	1.43	17	1
1	A	202	GLU	C-N	6.21	1.41	1.33	18	1
1	A	148	VAL	CA-C	-6.20	1.44	1.52	18	2
1	A	194	ASN	N-CA	6.17	1.53	1.46	17	1
1	A	124	TRP	N-CA	6.08	1.54	1.46	18	1
1	A	174	ILE	CA-CB	-6.04	1.46	1.54	18	1
1	A	161	GLY	N-CA	-6.04	1.37	1.45	20	2
1	A	103	ASN	CA-C	-6.04	1.50	1.53	17	1
1	A	181	ASP	N-CA	-6.03	1.38	1.46	18	1
1	A	235	SER	CA-C	-6.01	1.44	1.52	19	1
1	A	244	SER	CA-CB	-5.96	1.42	1.54	18	1
1	A	202	GLU	CA-CB	-5.96	1.44	1.53	17	1
1	A	219	MET	CA-C	5.95	1.61	1.52	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	163	VAL	CA-C	-5.92	1.45	1.52	17	3
1	A	235	SER	CA-CB	-5.88	1.43	1.53	19	1
1	A	128	THR	CB-OG1	-5.85	1.34	1.43	19	1
1	A	201	HIS	CG-CD2	5.85	1.42	1.35	17	2
1	A	142	ILE	CA-C	-5.78	1.46	1.53	19	1
1	A	205	HIS	CD2-NE2	5.72	1.44	1.37	18	1
1	A	85	THR	CB-OG1	-5.71	1.34	1.43	20	1
1	A	195	LEU	CA-C	5.69	1.60	1.52	19	1
1	A	89	ILE	CA-C	5.68	1.58	1.52	18	1
1	A	216	GLU	C-N	-5.64	1.25	1.33	17	1
1	A	184	GLU	CA-C	5.64	1.60	1.52	20	1
1	A	173	GLY	C-N	5.62	1.41	1.33	18	1
1	A	123	VAL	CA-CB	-5.59	1.46	1.54	18	2
1	A	233	ARG	CA-C	-5.58	1.45	1.53	19	1
1	A	99	TYR	CA-C	-5.56	1.45	1.52	18	1
1	A	108	LEU	CA-CB	-5.54	1.43	1.52	17	1
1	A	149	ARG	CZ-NH2	-5.51	1.26	1.33	19	1
1	A	153	ASP	N-CA	-5.51	1.39	1.46	17	1
1	A	101	ILE	CA-CB	5.51	1.60	1.53	18	1
1	A	173	GLY	C-O	-5.51	1.17	1.23	17	1
1	A	191	THR	CA-CB	5.51	1.62	1.53	20	1
1	A	126	GLU	N-CA	-5.50	1.39	1.46	19	1
1	A	173	GLY	CA-C	-5.49	1.44	1.51	18	1
1	A	166	HIS	N-CA	-5.48	1.39	1.46	14	1
1	A	233	ARG	CA-CB	5.47	1.62	1.53	17	1
1	A	181	ASP	CA-CB	5.47	1.62	1.53	18	1
1	A	201	HIS	CG-ND1	-5.44	1.32	1.38	17	1
1	A	95	THR	CB-OG1	-5.43	1.35	1.43	19	1
1	A	108	LEU	C-N	5.43	1.40	1.33	17	1
1	A	147	ALA	CA-CB	5.41	1.62	1.53	19	1
1	A	175	ASN	CA-C	-5.39	1.45	1.52	18	1
1	A	163	VAL	C-N	-5.39	1.26	1.33	17	1
1	A	111	ASP	CA-C	5.38	1.59	1.52	20	1
1	A	166	HIS	CA-CB	5.37	1.62	1.53	20	1
1	A	159	GLY	C-N	5.37	1.39	1.33	18	1
1	A	176	GLY	N-CA	-5.35	1.37	1.45	17	1
1	A	198	VAL	N-CA	-5.34	1.39	1.46	19	1
1	A	142	ILE	N-CA	-5.33	1.40	1.46	19	1
1	A	219	MET	N-CA	-5.33	1.39	1.46	20	1
1	A	108	LEU	N-CA	5.32	1.52	1.46	19	1
1	A	186	TRP	CD2-CE3	-5.32	1.31	1.40	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	206	SER	CA-CB	-5.31	1.44	1.53	19	1
1	A	245	LEU	CA-C	-5.31	1.46	1.52	17	1
1	A	93	ARG	N-CA	5.28	1.52	1.46	19	1
1	A	131	THR	C-O	-5.26	1.18	1.23	17	1
1	A	97	LEU	C-N	5.25	1.40	1.33	19	1
1	A	221	PRO	C-O	-5.25	1.17	1.24	17	1
1	A	146	PHE	N-CA	-5.25	1.40	1.46	17	1
1	A	141	ASP	CA-C	-5.23	1.45	1.52	18	1
1	A	151	HIS	CD2-NE2	5.22	1.43	1.37	18	1
1	A	113	VAL	N-CA	-5.22	1.41	1.46	20	1
1	A	100	ARG	C-O	-5.22	1.18	1.24	19	1
1	A	234	LEU	CB-CG	5.21	1.63	1.53	18	1
1	A	224	HIS	C-N	5.21	1.41	1.33	18	1
1	A	245	LEU	N-CA	-5.21	1.40	1.46	18	1
1	A	179	HIS	N-CA	-5.18	1.40	1.46	19	1
1	A	106	PRO	N-CA	-5.17	1.43	1.47	20	1
1	A	108	LEU	CA-C	-5.17	1.46	1.52	19	1
1	A	128	THR	CA-CB	-5.14	1.43	1.52	18	1
1	A	186	TRP	C-O	-5.13	1.17	1.24	19	1
1	A	179	HIS	CG-ND1	5.12	1.43	1.38	18	1
1	A	117	VAL	N-CA	-5.11	1.40	1.46	20	1
1	A	235	SER	C-O	-5.11	1.17	1.24	19	1
1	A	215	THR	C-O	-5.10	1.18	1.24	17	1
1	A	224	HIS	CE1-NE2	5.10	1.37	1.32	17	1
1	A	132	PHE	N-CA	-5.10	1.39	1.46	19	1
1	A	128	THR	CA-C	-5.09	1.46	1.52	19	1
1	A	224	HIS	CB-CG	-5.08	1.43	1.50	20	1
1	A	132	PHE	CA-C	5.07	1.58	1.52	17	1
1	A	206	SER	N-CA	-5.06	1.39	1.46	19	1
1	A	156	PRO	N-CA	-5.06	1.40	1.47	19	1
1	A	183	ASP	N-CA	-5.05	1.39	1.46	20	1
1	A	203	ILE	N-CA	-5.00	1.41	1.46	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	192	GLY	N-CA-C	-25.46	80.80	111.35	17	20
1	A	181	ASP	CA-CB-CG	21.71	134.31	112.60	2	19
1	A	160	PRO	N-CA-CB	21.20	122.03	103.17	20	20
1	A	157	PHE	CA-CB-CG	16.92	130.72	113.80	19	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	238	ASP	N-CA-C	-16.59	93.27	111.36	19	15
1	A	166	HIS	CA-CB-CG	15.97	129.77	113.80	8	17
1	A	151	HIS	ND1-CE1-NE2	15.70	124.10	108.40	18	20
1	A	166	HIS	ND1-CE1-NE2	15.26	123.66	108.40	19	20
1	A	245	LEU	N-CA-C	-14.75	95.29	111.07	20	18
1	A	166	HIS	N-CA-C	-14.69	86.29	109.50	18	11
1	A	232	PHE	CA-CB-CG	14.24	128.04	113.80	18	14
1	A	191	THR	CA-C-N	14.22	149.29	122.56	3	12
1	A	191	THR	C-N-CA	14.22	149.29	122.56	3	12
1	A	163	VAL	N-CA-CB	14.21	132.41	112.52	17	4
1	A	149	ARG	N-CA-C	-13.87	94.76	112.23	19	6
1	A	148	VAL	CA-C-N	13.75	144.12	122.26	12	6
1	A	148	VAL	C-N-CA	13.75	144.12	122.26	12	6
1	A	163	VAL	N-CA-C	-13.69	88.82	108.80	17	5
1	A	238	ASP	CB-CA-C	13.64	134.03	110.85	19	8
1	A	239	ILE	N-CA-C	-13.35	97.23	110.72	20	9
1	A	108	LEU	N-CA-C	-13.03	91.21	110.24	17	10
1	A	166	HIS	CB-CA-C	12.89	133.33	111.41	13	19
1	A	148	VAL	CA-CB-CG1	12.50	131.65	110.40	5	6
1	A	151	HIS	CE1-NE2-CD2	-12.46	96.54	109.00	18	20
1	A	165	ALA	N-CA-C	-12.39	93.03	110.50	19	9
1	A	149	ARG	CA-C-N	12.38	141.63	122.93	18	16
1	A	149	ARG	C-N-CA	12.38	141.63	122.93	18	16
1	A	211	HIS	CA-CB-CG	-12.30	101.50	113.80	20	1
1	A	173	GLY	N-CA-C	-12.16	97.61	112.33	17	3
1	A	105	THR	CA-CB-OG1	-12.06	91.51	109.60	18	1
1	A	224	HIS	N-CA-C	-12.04	94.16	113.19	17	16
1	A	211	HIS	ND1-CE1-NE2	11.73	120.13	108.40	17	20
1	A	146	PHE	CA-CB-CG	11.70	125.50	113.80	14	3
1	A	151	HIS	CA-CB-CG	11.57	125.37	113.80	6	11
1	A	205	HIS	ND1-CE1-NE2	11.56	119.96	108.40	19	20
1	A	173	GLY	CA-C-O	-11.34	114.85	122.22	20	2
1	A	105	THR	CA-CB-CG2	11.33	129.76	110.50	18	2
1	A	166	HIS	CA-C-N	11.29	141.05	122.87	19	10
1	A	166	HIS	C-N-CA	11.29	141.05	122.87	19	10
1	A	182	ASP	CA-CB-CG	11.08	123.68	112.60	20	9
1	A	174	ILE	N-CA-C	-11.08	93.28	108.12	19	18
1	A	183	ASP	N-CA-C	-10.98	98.40	112.23	17	7
1	A	223	TYR	CA-C-N	10.90	142.36	121.54	14	9
1	A	223	TYR	C-N-CA	10.90	142.36	121.54	14	9
1	A	128	THR	CA-C-N	10.86	133.41	119.84	20	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	128	THR	C-N-CA	10.86	133.41	119.84	20	20
1	A	166	HIS	CE1-NE2-CD2	-10.83	98.17	109.00	20	18
1	A	203	ILE	N-CA-C	-10.82	99.00	110.36	18	6
1	A	179	HIS	CA-CB-CG	10.81	124.61	113.80	7	8
1	A	113	VAL	N-CA-C	-10.73	103.14	111.62	20	2
1	A	103	ASN	CA-CB-CG	10.70	123.30	112.60	2	3
1	A	218	LEU	N-CA-C	-10.60	99.75	112.89	8	18
1	A	216	GLU	CA-C-N	10.60	141.78	121.54	17	7
1	A	216	GLU	C-N-CA	10.60	141.78	121.54	17	7
1	A	127	VAL	CB-CA-C	10.57	128.63	111.29	20	1
1	A	173	GLY	CA-C-N	10.42	140.73	121.97	18	1
1	A	173	GLY	C-N-CA	10.42	140.73	121.97	18	1
1	A	128	THR	CA-C-O	-10.39	112.54	119.29	19	1
1	A	163	VAL	O-C-N	10.38	135.55	122.57	18	6
1	A	224	HIS	CA-CB-CG	-10.34	103.46	113.80	17	3
1	A	132	PHE	CA-CB-CG	10.25	124.05	113.80	11	2
1	A	182	ASP	N-CA-C	-10.17	100.89	113.20	19	7
1	A	201	HIS	ND1-CE1-NE2	10.14	118.54	108.40	15	20
1	A	191	THR	CA-CB-CG2	10.13	127.72	110.50	20	5
1	A	195	LEU	N-CA-CB	-10.11	94.64	110.22	18	9
1	A	83	PHE	CA-CB-CG	10.04	123.84	113.80	19	3
1	A	86	PHE	CA-CB-CG	9.99	123.79	113.80	4	4
1	A	123	VAL	CA-C-O	-9.98	109.47	120.25	19	1
1	A	148	VAL	CB-CA-C	-9.91	95.04	111.29	18	5
1	A	238	ASP	N-CA-CB	-9.88	96.12	110.65	20	3
1	A	246	TYR	CA-CB-CG	9.85	131.63	113.90	17	20
1	A	210	PHE	CA-CB-CG	9.82	123.62	113.80	19	5
1	A	158	ASP	N-CA-C	-9.80	102.58	112.97	15	7
1	A	243	GLN	N-CA-C	-9.79	101.97	112.93	17	4
1	A	190	THR	N-CA-C	-9.75	100.51	111.82	6	14
1	A	161	GLY	CA-C-N	9.68	140.03	121.54	5	11
1	A	161	GLY	C-N-CA	9.68	140.03	121.54	5	11
1	A	143	MET	N-CA-C	-9.67	94.25	109.72	19	16
1	A	166	HIS	O-C-N	9.66	134.48	123.28	19	1
1	A	130	LEU	N-CA-CB	9.65	124.16	109.97	20	3
1	A	102	VAL	CA-C-N	9.58	136.87	121.74	2	5
1	A	102	VAL	C-N-CA	9.58	136.87	121.74	2	5
1	A	223	TYR	CA-CB-CG	-9.54	96.73	113.90	20	1
1	A	130	LEU	N-CA-C	-9.53	97.95	110.43	19	3
1	A	109	PRO	N-CA-CB	9.52	111.63	103.25	17	1
1	A	174	ILE	CB-CG1-CD1	9.51	133.77	113.80	18	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	179	HIS	CG-ND1-CE1	-9.50	93.16	109.30	13	2
1	A	144	ILE	N-CA-CB	-9.46	98.42	111.19	18	6
1	A	237	ASP	N-CA-C	-9.44	102.27	113.88	18	8
1	A	163	VAL	CB-CA-C	9.44	123.12	111.13	12	10
1	A	116	ALA	CB-CA-C	9.36	125.37	110.96	17	17
1	A	163	VAL	CA-C-O	-9.35	109.10	120.78	18	1
1	A	174	ILE	N-CA-CB	9.29	121.41	111.46	19	6
1	A	109	PRO	CA-C-N	9.29	133.08	120.54	18	2
1	A	109	PRO	C-N-CA	9.29	133.08	120.54	18	2
1	A	101	ILE	N-CA-C	-9.27	94.82	108.54	19	7
1	A	148	VAL	N-CA-CB	9.24	126.48	111.23	13	14
1	A	179	HIS	N-CA-C	-9.24	95.19	109.52	18	2
1	A	141	ASP	CA-CB-CG	9.23	121.83	112.60	20	3
1	A	209	LEU	CA-C-N	9.23	139.16	121.54	3	13
1	A	209	LEU	C-N-CA	9.23	139.16	121.54	3	13
1	A	131	THR	O-C-N	9.17	133.01	122.19	19	1
1	A	194	ASN	CA-CB-CG	9.11	121.71	112.60	20	2
1	A	150	GLU	CA-C-N	9.06	132.41	120.28	8	10
1	A	150	GLU	C-N-CA	9.06	132.41	120.28	8	10
1	A	164	LEU	N-CA-CB	-9.05	98.96	111.00	7	9
1	A	211	HIS	ND1-CG-CD2	8.98	115.08	106.10	20	19
1	A	231	ARG	NE-CZ-NH2	-8.98	111.11	119.20	17	1
1	A	177	ASP	CB-CA-C	-8.91	93.34	109.38	20	8
1	A	220	TYR	CA-C-N	8.87	130.93	119.84	12	7
1	A	220	TYR	C-N-CA	8.87	130.93	119.84	12	7
1	A	164	LEU	N-CA-C	8.81	129.56	110.80	12	14
1	A	166	HIS	ND1-CG-CD2	8.74	114.84	106.10	17	5
1	A	160	PRO	O-C-N	8.73	133.60	123.03	19	3
1	A	207	LEU	CA-C-N	8.70	138.46	121.41	8	1
1	A	207	LEU	C-N-CA	8.70	138.46	121.41	8	1
1	A	161	GLY	N-CA-C	-8.66	102.00	112.48	12	1
1	A	102	VAL	CB-CA-C	8.60	125.39	111.29	8	5
1	A	185	GLN	N-CA-C	-8.58	97.78	109.54	17	15
1	A	230	THR	N-CA-C	-8.54	101.82	113.18	18	11
1	A	179	HIS	CG-CD2-NE2	-8.54	98.66	107.20	13	1
1	A	129	PRO	N-CA-CB	-8.53	94.30	103.25	18	4
1	A	102	VAL	N-CA-C	-8.50	102.06	110.30	5	11
1	A	111	ASP	CA-CB-CG	8.46	121.06	112.60	17	1
1	A	154	PHE	CA-CB-CG	8.37	122.17	113.80	18	1
1	A	189	ASP	CA-C-N	8.33	137.46	121.54	17	1
1	A	189	ASP	C-N-CA	8.33	137.46	121.54	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	199	ALA	N-CA-C	-8.33	102.28	111.36	9	2
1	A	156	PRO	CB-CA-C	-8.31	97.84	111.56	20	6
1	A	160	PRO	CB-CA-C	-8.31	100.91	111.71	20	5
1	A	205	HIS	CE1-NE2-CD2	-8.30	100.70	109.00	18	20
1	A	177	ASP	CA-CB-CG	8.25	120.85	112.60	20	2
1	A	224	HIS	ND1-CE1-NE2	8.24	116.64	108.40	20	2
1	A	206	SER	CB-CA-C	8.22	124.06	110.17	4	1
1	A	143	MET	CA-CB-CG	8.22	130.53	114.10	6	4
1	A	192	GLY	CA-C-N	-8.16	107.26	123.09	18	3
1	A	192	GLY	C-N-CA	-8.16	107.26	123.09	18	3
1	A	148	VAL	N-CA-C	8.10	126.19	109.34	3	5
1	A	202	GLU	N-CA-C	8.10	119.74	111.07	20	1
1	A	189	ASP	CA-CB-CG	8.06	120.66	112.60	18	1
1	A	105	THR	N-CA-C	-8.03	99.98	109.93	20	3
1	A	161	GLY	O-C-N	7.98	133.07	122.70	19	5
1	A	187	THR	CA-C-N	7.98	136.78	121.54	15	5
1	A	187	THR	C-N-CA	7.98	136.78	121.54	15	5
1	A	217	ALA	N-CA-CB	-7.98	99.44	110.29	2	9
1	A	199	ALA	CA-C-O	-7.97	112.30	121.07	17	2
1	A	198	VAL	N-CA-C	-7.96	101.14	111.09	18	4
1	A	102	VAL	O-C-N	7.96	130.46	121.94	17	1
1	A	201	HIS	CE1-NE2-CD2	-7.93	101.07	109.00	19	18
1	A	210	PHE	CA-C-N	7.91	136.65	121.54	19	2
1	A	210	PHE	C-N-CA	7.91	136.65	121.54	19	2
1	A	143	MET	CB-CA-C	7.88	124.85	109.33	20	7
1	A	211	HIS	CE1-NE2-CD2	-7.87	101.13	109.00	17	19
1	A	105	THR	N-CA-CB	7.86	121.22	110.14	17	1
1	A	244	SER	O-C-N	7.80	131.46	122.25	17	2
1	A	195	LEU	CA-C-N	7.80	130.94	120.65	6	7
1	A	195	LEU	C-N-CA	7.80	130.94	120.65	6	7
1	A	143	MET	N-CA-CB	7.79	122.72	110.56	18	7
1	A	207	LEU	N-CA-C	-7.78	94.24	110.80	4	5
1	A	186	TRP	CZ3-CH2-CZ2	-7.77	111.40	121.50	20	3
1	A	101	ILE	CA-C-N	7.77	130.19	120.72	4	5
1	A	101	ILE	C-N-CA	7.77	130.19	120.72	4	5
1	A	148	VAL	CG1-CB-CG2	7.76	127.88	110.80	17	4
1	A	103	ASN	CA-C-N	7.76	136.36	121.54	14	9
1	A	103	ASN	C-N-CA	7.76	136.36	121.54	14	9
1	A	113	VAL	CB-CA-C	7.75	117.95	111.05	20	3
1	A	223	TYR	O-C-N	7.75	132.90	122.59	20	1
1	A	96	HIS	CA-CB-CG	7.75	121.55	113.80	17	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	149	ARG	O-C-N	7.75	132.89	122.59	18	1
1	A	225	SER	CA-C-N	7.73	136.30	121.54	20	13
1	A	225	SER	C-N-CA	7.73	136.30	121.54	20	13
1	A	222	LEU	CA-C-N	7.73	132.06	120.31	4	8
1	A	222	LEU	C-N-CA	7.73	132.06	120.31	4	8
1	A	186	TRP	N-CA-C	-7.70	100.23	110.24	20	1
1	A	144	ILE	N-CA-C	7.70	118.99	107.75	14	4
1	A	167	ALA	N-CA-C	7.69	121.44	108.90	13	4
1	A	186	TRP	CB-CA-C	7.68	123.37	109.62	14	11
1	A	164	LEU	CB-CG-CD2	7.67	133.71	110.70	15	7
1	A	105	THR	CA-C-O	-7.66	112.42	120.23	17	1
1	A	147	ALA	CA-C-N	7.64	135.72	121.97	7	8
1	A	147	ALA	C-N-CA	7.64	135.72	121.97	7	8
1	A	203	ILE	CB-CG1-CD1	7.64	129.84	113.80	20	6
1	A	235	SER	N-CA-C	7.64	119.66	110.19	6	3
1	A	171	GLY	CA-C-O	-7.64	110.60	121.52	18	1
1	A	203	ILE	CA-CB-CG1	7.62	123.35	110.40	7	14
1	A	201	HIS	ND1-CG-CD2	7.60	113.70	106.10	17	18
1	A	221	PRO	N-CA-C	7.59	123.84	114.35	17	6
1	A	144	ILE	CA-C-O	7.59	129.17	120.67	20	2
1	A	177	ASP	N-CA-C	7.56	121.06	108.73	7	2
1	A	169	ALA	CA-C-N	7.50	126.78	118.97	15	7
1	A	169	ALA	C-N-CA	7.50	126.78	118.97	15	7
1	A	166	HIS	CG-ND1-CE1	-7.50	96.56	109.30	19	18
1	A	221	PRO	CA-N-CD	-7.46	101.55	112.00	12	1
1	A	142	ILE	CB-CA-C	7.44	119.46	111.35	19	2
1	A	116	ALA	N-CA-C	-7.44	102.77	111.03	20	8
1	A	151	HIS	N-CA-CB	-7.42	98.41	111.39	6	6
1	A	112	ALA	CA-C-N	7.38	130.99	123.16	20	10
1	A	112	ALA	C-N-CA	7.38	130.99	123.16	20	10
1	A	230	THR	CA-C-N	7.38	135.63	121.54	7	8
1	A	230	THR	C-N-CA	7.38	135.63	121.54	7	8
1	A	163	VAL	CA-CB-CG1	-7.38	97.86	110.40	8	5
1	A	122	LYS	CA-C-O	-7.35	113.28	121.00	19	4
1	A	193	THR	N-CA-CB	-7.34	98.80	110.77	9	6
1	A	150	GLU	N-CA-CB	-7.33	99.33	110.33	6	2
1	A	124	TRP	N-CA-CB	-7.33	98.11	110.49	17	1
1	A	224	HIS	CE1-NE2-CD2	-7.31	101.69	109.00	18	2
1	A	103	ASN	N-CA-C	7.29	114.76	108.78	17	2
1	A	221	PRO	CA-C-O	-7.28	110.09	118.98	17	1
1	A	196	PHE	CA-CB-CG	7.27	121.07	113.80	20	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	246	TYR	N-CA-CB	-7.27	98.21	110.49	14	12
1	A	128	THR	N-CA-CB	7.26	119.40	110.17	19	1
1	A	174	ILE	CA-C-N	7.26	135.41	121.54	18	1
1	A	174	ILE	C-N-CA	7.26	135.41	121.54	18	1
1	A	205	HIS	CG-ND1-CE1	-7.21	97.05	109.30	20	19
1	A	245	LEU	CA-C-N	7.20	135.28	121.54	5	10
1	A	245	LEU	C-N-CA	7.20	135.28	121.54	5	10
1	A	134	ARG	CB-CA-C	-7.18	96.12	110.42	17	2
1	A	140	ALA	CA-C-N	7.18	135.25	121.54	18	2
1	A	140	ALA	C-N-CA	7.18	135.25	121.54	18	2
1	A	247	GLY	CA-C-O	-7.16	111.28	121.52	19	3
1	A	229	LEU	CA-C-N	7.15	133.02	122.08	7	5
1	A	229	LEU	C-N-CA	7.15	133.02	122.08	7	5
1	A	162	ASN	CA-CB-CG	7.14	119.74	112.60	10	4
1	A	164	LEU	CA-C-N	-7.12	111.32	121.50	14	8
1	A	164	LEU	C-N-CA	-7.12	111.32	121.50	14	8
1	A	179	HIS	CB-CG-CD2	-7.11	121.96	131.20	13	1
1	A	236	GLN	CB-CG-CD	-7.11	100.52	112.60	17	1
1	A	224	HIS	CA-C-N	7.07	135.04	121.54	7	10
1	A	224	HIS	C-N-CA	7.07	135.04	121.54	7	10
1	A	221	PRO	CA-C-N	7.07	135.04	121.54	19	3
1	A	221	PRO	C-N-CA	7.07	135.04	121.54	19	3
1	A	205	HIS	ND1-CG-CD2	7.06	113.16	106.10	20	18
1	A	160	PRO	CA-N-CD	-7.06	102.12	112.00	20	3
1	A	156	PRO	CA-N-CD	-7.06	102.12	112.00	4	4
1	A	122	LYS	CA-C-N	-7.06	109.26	120.55	17	4
1	A	122	LYS	C-N-CA	-7.06	109.26	120.55	17	4
1	A	238	ASP	CA-C-O	-7.05	112.94	120.42	19	1
1	A	143	MET	O-C-N	7.04	132.34	123.19	20	1
1	A	106	PRO	N-CA-CB	7.04	107.52	102.81	20	1
1	A	153	ASP	CA-C-N	7.01	133.60	122.11	19	4
1	A	153	ASP	C-N-CA	7.01	133.60	122.11	19	4
1	A	170	PRO	CA-C-N	7.01	132.87	121.87	17	2
1	A	170	PRO	C-N-CA	7.01	132.87	121.87	17	2
1	A	190	THR	CA-C-N	7.01	134.92	121.54	4	3
1	A	190	THR	C-N-CA	7.01	134.92	121.54	4	3
1	A	90	PRO	N-CA-CB	6.99	110.59	103.25	20	1
1	A	168	TYR	CA-C-N	6.98	138.84	121.80	15	8
1	A	168	TYR	C-N-CA	6.98	138.84	121.80	15	8
1	A	102	VAL	CA-CB-CG1	6.97	122.25	110.40	13	9
1	A	124	TRP	CA-CB-CG	6.97	126.84	113.60	17	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	211	HIS	CG-ND1-CE1	-6.96	97.46	109.30	19	20
1	A	187	THR	N-CA-C	6.96	125.62	110.80	1	5
1	A	170	PRO	CA-N-CD	-6.96	102.26	112.00	19	3
1	A	245	LEU	O-C-N	6.95	129.52	122.08	18	1
1	A	165	ALA	N-CA-CB	6.95	120.72	109.95	14	2
1	A	149	ARG	NE-CZ-NH1	6.95	128.45	121.50	20	2
1	A	197	LEU	CA-C-O	-6.92	111.62	119.79	20	4
1	A	124	TRP	CB-CA-C	-6.92	96.65	110.42	19	1
1	A	198	VAL	CA-CB-CG2	6.89	122.12	110.40	19	5
1	A	91	LYS	CA-C-O	-6.89	113.88	121.87	20	1
1	A	198	VAL	CB-CA-C	-6.88	103.03	112.04	10	6
1	A	176	GLY	CA-C-O	-6.87	111.84	119.88	18	1
1	A	183	ASP	CA-CB-CG	-6.85	105.75	112.60	18	1
1	A	170	PRO	N-CA-CB	6.85	110.44	103.25	17	7
1	A	103	ASN	O-C-N	6.84	131.69	122.59	20	1
1	A	234	LEU	CA-C-N	6.83	134.58	121.54	16	1
1	A	234	LEU	C-N-CA	6.83	134.58	121.54	16	1
1	A	89	ILE	CA-C-N	6.82	128.37	119.84	16	9
1	A	89	ILE	C-N-CA	6.82	128.37	119.84	16	9
1	A	128	THR	N-CA-C	-6.82	101.20	109.72	2	1
1	A	239	ILE	CB-CA-C	-6.81	102.82	112.22	20	1
1	A	136	TYR	CA-CB-CG	6.80	126.14	113.90	18	1
1	A	151	HIS	ND1-CG-CD2	6.79	112.89	106.10	18	18
1	A	223	TYR	CA-C-O	6.79	130.22	120.51	19	1
1	A	90	PRO	O-C-N	6.79	131.80	122.64	18	1
1	A	156	PRO	O-C-N	6.78	131.80	122.64	17	2
1	A	151	HIS	CG-ND1-CE1	-6.75	97.82	109.30	19	19
1	A	198	VAL	N-CA-CB	-6.75	102.03	110.47	14	1
1	A	119	LYS	O-C-N	-6.75	115.01	122.03	17	1
1	A	163	VAL	CG1-CB-CG2	6.75	125.64	110.80	7	4
1	A	128	THR	O-C-N	-6.74	115.77	121.23	18	1
1	A	205	HIS	CA-CB-CG	6.72	120.53	113.80	4	4
1	A	193	THR	O-C-N	-6.69	113.82	122.72	18	1
1	A	102	VAL	CG1-CB-CG2	-6.68	96.09	110.80	8	2
1	A	228	ASP	CA-CB-CG	-6.68	105.92	112.60	20	1
1	A	238	ASP	CA-CB-CG	-6.68	105.92	112.60	19	5
1	A	171	GLY	CA-C-N	6.67	127.06	119.93	2	13
1	A	171	GLY	C-N-CA	6.67	127.06	119.93	2	13
1	A	232	PHE	O-C-N	6.67	130.47	121.74	17	2
1	A	131	THR	CA-C-N	6.65	134.25	121.54	5	2
1	A	131	THR	C-N-CA	6.65	134.25	121.54	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	202	GLU	CA-C-O	-6.64	113.84	120.82	20	2
1	A	148	VAL	CA-C-O	6.64	129.09	120.78	19	2
1	A	196	PHE	O-C-N	-6.64	113.76	122.59	19	1
1	A	91	LYS	N-CA-C	-6.62	105.95	112.97	9	1
1	A	217	ALA	N-CA-C	6.61	118.39	110.19	15	5
1	A	183	ASP	CB-CA-C	-6.61	99.62	110.85	19	1
1	A	246	TYR	CB-CG-CD2	-6.61	110.89	120.80	20	1
1	A	121	LEU	CB-CA-C	-6.60	100.25	110.81	5	5
1	A	169	ALA	N-CA-C	6.60	124.39	109.81	17	2
1	A	160	PRO	N-CA-C	-6.59	101.55	111.57	17	1
1	A	146	PHE	CB-CA-C	6.59	120.57	110.62	17	2
1	A	207	LEU	N-CA-CB	-6.58	103.89	111.79	18	2
1	A	232	PHE	CA-C-N	6.57	132.15	122.82	19	1
1	A	232	PHE	C-N-CA	6.57	132.15	122.82	19	1
1	A	237	ASP	O-C-N	6.57	131.32	122.59	19	3
1	A	156	PRO	N-CA-C	6.56	125.99	112.47	1	1
1	A	156	PRO	CA-C-N	-6.55	112.45	122.08	19	3
1	A	156	PRO	C-N-CA	-6.55	112.45	122.08	19	3
1	A	89	ILE	CA-CB-CG2	6.55	121.63	110.50	20	2
1	A	232	PHE	N-CA-CB	-6.54	101.04	110.45	17	2
1	A	195	LEU	CB-CA-C	6.53	122.72	110.63	18	8
1	A	237	ASP	CB-CA-C	6.53	119.61	109.03	18	1
1	A	221	PRO	CB-CA-C	-6.53	101.67	110.88	17	1
1	A	113	VAL	N-CA-CB	-6.51	100.82	110.58	18	2
1	A	128	THR	CA-CB-OG1	-6.50	99.85	109.60	19	1
1	A	175	ASN	CA-CB-CG	6.50	119.10	112.60	19	1
1	A	98	THR	N-CA-CB	-6.50	100.96	111.22	17	2
1	A	202	GLU	CA-C-N	6.49	128.98	120.60	18	2
1	A	202	GLU	C-N-CA	6.49	128.98	120.60	18	2
1	A	101	ILE	N-CA-CB	6.48	118.21	110.95	19	1
1	A	128	THR	CA-CB-CG2	6.48	121.52	110.50	20	1
1	A	230	THR	CA-C-O	6.48	128.15	119.47	17	1
1	A	144	ILE	CA-C-N	6.47	133.90	121.54	6	4
1	A	144	ILE	C-N-CA	6.47	133.90	121.54	6	4
1	A	137	GLU	N-CA-C	-6.46	99.86	108.19	18	1
1	A	124	TRP	CD2-CE2-CZ2	-6.43	115.97	122.40	17	1
1	A	110	LYS	CA-C-N	6.42	128.88	120.28	19	5
1	A	110	LYS	C-N-CA	6.42	128.88	120.28	19	5
1	A	163	VAL	CA-CB-CG2	6.42	121.31	110.40	17	1
1	A	189	ASP	N-CA-C	-6.42	105.32	112.57	11	7
1	A	179	HIS	ND1-CE1-NE2	6.41	114.81	108.40	19	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	196	PHE	CB-CG-CD1	-6.41	109.81	120.70	20	1
1	A	150	GLU	CB-CG-CD	-6.40	101.71	112.60	18	1
1	A	187	THR	CA-CB-CG2	6.40	121.37	110.50	19	1
1	A	187	THR	CA-CB-OG1	6.39	119.19	109.60	15	1
1	A	219	MET	N-CA-C	-6.38	104.98	112.89	19	2
1	A	85	THR	CA-C-N	6.38	137.37	121.80	9	4
1	A	85	THR	C-N-CA	6.38	137.37	121.80	9	4
1	A	182	ASP	CA-C-N	6.36	128.80	120.28	18	4
1	A	182	ASP	C-N-CA	6.36	128.80	120.28	18	4
1	A	233	ARG	N-CA-C	-6.36	103.47	110.91	16	1
1	A	187	THR	N-CA-CB	-6.35	101.06	110.97	6	7
1	A	180	PHE	O-C-N	6.33	130.37	123.10	20	1
1	A	186	TRP	CE2-CD2-CG	6.31	114.78	107.20	20	1
1	A	179	HIS	CB-CG-ND1	-6.31	113.23	122.70	13	2
1	A	98	THR	CA-CB-OG1	-6.30	100.15	109.60	17	1
1	A	169	ALA	CA-C-O	-6.30	111.53	120.16	20	1
1	A	117	VAL	CA-C-N	6.29	133.56	121.54	17	5
1	A	117	VAL	C-N-CA	6.29	133.56	121.54	17	5
1	A	153	ASP	CA-CB-CG	6.28	118.88	112.60	17	3
1	A	226	LEU	CA-C-N	6.27	133.52	121.54	9	2
1	A	226	LEU	C-N-CA	6.27	133.52	121.54	9	2
1	A	186	TRP	CD2-CE3-CZ3	6.27	126.75	118.60	20	1
1	A	146	PHE	CB-CG-CD2	-6.26	110.05	120.70	15	1
1	A	212	SER	CA-C-O	-6.26	114.61	121.31	19	1
1	A	96	HIS	ND1-CE1-NE2	6.23	114.63	108.40	19	2
1	A	127	VAL	CA-CB-CG2	6.22	120.97	110.40	20	2
1	A	91	LYS	O-C-N	6.22	129.99	122.96	18	1
1	A	193	THR	CA-CB-OG1	-6.22	100.28	109.60	18	1
1	A	209	LEU	N-CA-CB	6.21	119.28	110.46	16	4
1	A	146	PHE	CA-C-N	6.21	133.41	121.54	20	1
1	A	146	PHE	C-N-CA	6.21	133.41	121.54	20	1
1	A	117	VAL	CA-CB-CG1	6.21	120.96	110.40	17	1
1	A	165	ALA	CA-C-O	-6.19	113.93	121.36	18	2
1	A	162	ASN	CA-C-N	-6.18	114.01	122.92	17	3
1	A	162	ASN	C-N-CA	-6.18	114.01	122.92	17	3
1	A	170	PRO	N-CD-CG	6.18	112.48	103.20	19	1
1	A	248	PRO	CA-N-CD	-6.18	103.34	112.00	18	1
1	A	184	GLU	CB-CG-CD	6.18	123.10	112.60	19	1
1	A	233	ARG	CD-NE-CZ	-6.17	115.77	124.40	20	1
1	A	186	TRP	CE2-CD2-CE3	-6.17	112.64	118.80	20	1
1	A	84	ARG	NE-CZ-NH2	-6.16	113.66	119.20	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	119	LYS	CA-C-O	-6.15	114.36	120.70	18	1
1	A	243	GLN	OE1-CD-NE2	-6.15	116.45	122.60	18	1
1	A	114	ASP	N-CA-C	-6.14	104.50	111.14	19	2
1	A	114	ASP	CA-CB-CG	6.13	118.73	112.60	18	1
1	A	163	VAL	CA-C-N	6.12	133.24	121.54	12	1
1	A	163	VAL	C-N-CA	6.12	133.24	121.54	12	1
1	A	206	SER	CA-C-N	-6.12	108.57	121.80	19	1
1	A	206	SER	C-N-CA	-6.12	108.57	121.80	19	1
1	A	100	ARG	NE-CZ-NH2	6.12	124.71	119.20	18	1
1	A	100	ARG	CA-C-N	6.12	130.14	122.43	18	1
1	A	100	ARG	C-N-CA	6.12	130.14	122.43	18	1
1	A	209	LEU	CA-C-O	6.09	129.23	120.51	19	2
1	A	190	THR	CA-CB-OG1	-6.09	100.46	109.60	19	1
1	A	99	TYR	CA-C-N	-6.04	114.25	122.77	17	1
1	A	99	TYR	C-N-CA	-6.04	114.25	122.77	17	1
1	A	202	GLU	CA-CB-CG	-6.03	102.04	114.10	19	1
1	A	164	LEU	CD1-CG-CD2	-6.02	97.55	110.80	20	2
1	A	121	LEU	N-CA-CB	-6.02	100.31	110.49	20	1
1	A	229	LEU	CD1-CG-CD2	-6.01	97.58	110.80	17	2
1	A	85	THR	CA-CB-CG2	5.99	120.69	110.50	3	2
1	A	115	SER	CA-C-O	-5.99	112.24	119.49	18	1
1	A	199	ALA	N-CA-CB	5.99	119.03	110.16	9	2
1	A	105	THR	OG1-CB-CG2	-5.99	97.33	109.30	20	1
1	A	194	ASN	CB-CA-C	5.98	120.80	109.37	1	1
1	A	100	ARG	N-CA-C	5.95	118.19	108.55	20	1
1	A	239	ILE	N-CA-CB	5.94	119.48	110.58	20	1
1	A	191	THR	O-C-N	5.93	130.48	122.59	18	1
1	A	235	SER	CA-CB-OG	-5.92	99.26	111.10	20	1
1	A	197	LEU	N-CA-CB	5.91	120.33	110.41	19	1
1	A	129	PRO	CA-N-CD	-5.90	103.74	112.00	18	15
1	A	154	PHE	N-CA-CB	-5.90	98.30	111.10	18	1
1	A	146	PHE	CB-CG-CD1	-5.89	110.68	120.70	2	2
1	A	234	LEU	CB-CA-C	5.89	122.14	110.42	7	1
1	A	224	HIS	ND1-CG-CD2	5.89	111.99	106.10	20	1
1	A	228	ASP	N-CA-C	-5.89	104.02	110.91	14	1
1	A	164	LEU	CB-CA-C	5.88	122.13	110.42	19	2
1	A	83	PHE	CA-C-O	-5.88	110.80	120.80	17	1
1	A	110	LYS	N-CA-C	-5.88	104.05	111.11	18	1
1	A	128	THR	CB-CA-C	5.87	116.55	109.85	20	1
1	A	144	ILE	O-C-N	5.86	129.69	123.00	17	1
1	A	152	GLY	N-CA-C	-5.86	99.30	113.18	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	222	LEU	N-CA-CB	5.85	120.38	110.49	1	1
1	A	136	TYR	CA-C-N	5.84	132.70	121.54	3	2
1	A	136	TYR	C-N-CA	5.84	132.70	121.54	3	2
1	A	201	HIS	CA-CB-CG	-5.84	107.96	113.80	3	2
1	A	142	ILE	CA-CB-CG1	5.84	120.33	110.40	19	3
1	A	241	GLY	CA-C-N	5.82	129.84	120.30	7	3
1	A	241	GLY	C-N-CA	5.82	129.84	120.30	7	3
1	A	100	ARG	CA-CB-CG	5.82	125.74	114.10	17	1
1	A	85	THR	CB-CA-C	-5.82	98.84	110.42	18	1
1	A	193	THR	CA-C-O	-5.81	113.13	120.28	14	1
1	A	244	SER	CA-C-N	5.80	128.86	120.79	6	2
1	A	244	SER	C-N-CA	5.80	128.86	120.79	6	2
1	A	95	THR	N-CA-C	-5.80	103.45	110.88	18	2
1	A	90	PRO	CA-N-CD	-5.80	103.88	112.00	19	1
1	A	183	ASP	N-CA-CB	5.79	118.64	110.12	18	1
1	A	211	HIS	CB-CG-CD2	-5.79	123.67	131.20	20	1
1	A	151	HIS	CB-CG-CD2	-5.79	123.67	131.20	19	2
1	A	148	VAL	O-C-N	5.79	129.81	122.57	7	2
1	A	96	HIS	CA-C-O	-5.79	114.24	120.09	20	1
1	A	151	HIS	N-CA-C	-5.79	106.84	114.31	20	1
1	A	233	ARG	CA-C-N	5.77	132.56	121.54	14	1
1	A	233	ARG	C-N-CA	5.77	132.56	121.54	14	1
1	A	155	TYR	CA-C-N	5.76	127.04	119.84	9	3
1	A	155	TYR	C-N-CA	5.76	127.04	119.84	9	3
1	A	125	GLU	CA-C-O	5.75	126.45	119.38	17	1
1	A	242	ILE	CA-C-O	5.73	126.88	120.64	19	1
1	A	116	ALA	N-CA-CB	-5.72	101.56	109.91	19	1
1	A	246	TYR	CA-C-N	5.71	125.30	121.13	7	2
1	A	246	TYR	C-N-CA	5.71	125.30	121.13	7	2
1	A	205	HIS	N-CA-CB	5.71	119.01	110.22	17	1
1	A	220	TYR	N-CA-C	5.70	120.24	112.55	20	1
1	A	92	TRP	CA-C-N	5.68	128.16	120.38	7	2
1	A	92	TRP	C-N-CA	5.68	128.16	120.38	7	2
1	A	150	GLU	CB-CA-C	5.67	121.71	110.42	8	1
1	A	217	ALA	CA-C-N	-5.67	111.21	121.14	18	3
1	A	217	ALA	C-N-CA	-5.67	111.21	121.14	18	3
1	A	181	ASP	N-CA-CB	5.67	120.06	110.49	19	1
1	A	236	GLN	N-CA-CB	-5.66	101.17	110.40	20	2
1	A	127	VAL	CA-C-N	5.66	130.66	121.83	20	2
1	A	127	VAL	C-N-CA	5.66	130.66	121.83	20	2
1	A	146	PHE	O-C-N	5.65	130.26	123.36	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	110	LYS	O-C-N	5.65	128.11	122.12	17	1
1	A	184	GLU	CA-C-O	5.63	128.57	120.51	19	1
1	A	88	GLY	CA-C-N	5.61	132.52	122.13	18	3
1	A	88	GLY	C-N-CA	5.61	132.52	122.13	18	3
1	A	162	ASN	OD1-CG-ND2	-5.61	116.99	122.60	17	1
1	A	142	ILE	CA-CB-CG2	-5.60	100.97	110.50	17	1
1	A	201	HIS	CG-ND1-CE1	-5.59	99.79	109.30	1	17
1	A	93	ARG	NE-CZ-NH1	-5.59	115.91	121.50	18	1
1	A	178	ALA	CA-C-O	-5.59	115.10	121.58	18	1
1	A	166	HIS	CB-CG-ND1	-5.58	114.33	122.70	19	1
1	A	203	ILE	O-C-N	5.58	127.35	121.89	20	1
1	A	141	ASP	CA-C-N	-5.57	112.21	121.63	19	1
1	A	141	ASP	C-N-CA	-5.57	112.21	121.63	19	1
1	A	191	THR	N-CA-C	-5.57	98.94	110.80	4	1
1	A	220	TYR	O-C-N	-5.57	114.92	121.32	17	2
1	A	237	ASP	CA-C-N	5.56	128.19	120.29	3	1
1	A	237	ASP	C-N-CA	5.56	128.19	120.29	3	1
1	A	180	PHE	CA-C-O	-5.56	114.83	121.11	18	2
1	A	160	PRO	CA-C-O	-5.55	115.23	122.12	17	1
1	A	144	ILE	CB-CA-C	5.55	120.39	111.29	19	1
1	A	127	VAL	O-C-N	-5.55	115.63	122.57	19	1
1	A	211	HIS	CB-CG-ND1	-5.55	114.38	122.70	19	1
1	A	149	ARG	CA-C-O	5.55	128.44	120.51	20	1
1	A	142	ILE	CA-C-O	5.54	127.58	121.70	18	2
1	A	156	PRO	N-CA-CB	5.54	109.06	103.25	19	3
1	A	155	TYR	O-C-N	-5.54	116.02	121.17	17	2
1	A	134	ARG	CD-NE-CZ	5.53	132.15	124.40	18	1
1	A	178	ALA	N-CA-C	5.53	118.48	108.69	6	1
1	A	214	ASN	CA-CB-CG	5.53	118.13	112.60	17	2
1	A	108	LEU	CA-C-O	-5.53	113.33	121.46	19	1
1	A	207	LEU	CB-CG-CD1	5.53	127.28	110.70	17	1
1	A	234	LEU	N-CA-CB	-5.51	101.17	110.49	18	1
1	A	98	THR	N-CA-C	5.51	117.00	109.18	17	1
1	A	225	SER	O-C-N	5.51	129.91	122.59	17	1
1	A	206	SER	N-CA-C	-5.50	106.57	113.28	3	1
1	A	243	GLN	N-CA-CB	-5.50	102.97	110.56	20	2
1	A	159	GLY	CA-C-O	-5.50	113.66	121.52	7	3
1	A	211	HIS	CA-C-N	5.49	132.02	121.54	11	1
1	A	211	HIS	C-N-CA	5.49	132.02	121.54	11	1
1	A	201	HIS	CA-C-O	-5.48	114.79	120.92	2	3
1	A	187	THR	OG1-CB-CG2	-5.47	98.35	109.30	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	170	PRO	CA-C-O	5.47	130.56	120.60	20	1
1	A	136	TYR	CA-C-O	5.46	130.57	122.32	20	1
1	A	240	ASN	CA-C-N	5.46	132.11	121.41	19	1
1	A	240	ASN	C-N-CA	5.46	132.11	121.41	19	1
1	A	235	SER	CB-CA-C	-5.45	101.67	109.84	20	2
1	A	242	ILE	CB-CA-C	5.43	119.98	112.05	19	2
1	A	191	THR	CB-CA-C	5.43	121.22	110.42	15	1
1	A	150	GLU	CA-CB-CG	5.43	124.96	114.10	18	1
1	A	157	PHE	N-CA-C	5.43	122.36	110.80	17	1
1	A	125	GLU	N-CA-CB	-5.43	101.38	110.39	17	1
1	A	108	LEU	CB-CA-C	5.42	117.23	109.26	14	1
1	A	129	PRO	CA-CB-CG	-5.42	94.20	104.50	20	1
1	A	136	TYR	N-CA-C	-5.41	106.73	113.55	18	1
1	A	198	VAL	CA-CB-CG1	5.41	119.60	110.40	12	4
1	A	178	ALA	CB-CA-C	5.40	118.13	110.24	2	1
1	A	129	PRO	N-CA-C	5.40	123.60	112.47	17	2
1	A	95	THR	CA-C-N	5.40	129.31	121.26	14	2
1	A	95	THR	C-N-CA	5.40	129.31	121.26	14	2
1	A	115	SER	N-CA-C	-5.39	105.80	112.38	19	1
1	A	185	GLN	CA-C-N	5.39	131.84	121.54	11	2
1	A	185	GLN	C-N-CA	5.39	131.84	121.54	11	2
1	A	107	ASP	CA-C-N	-5.38	114.33	122.29	6	2
1	A	107	ASP	C-N-CA	-5.38	114.33	122.29	6	2
1	A	104	TYR	CA-CB-CG	5.38	123.58	113.90	1	3
1	A	147	ALA	N-CA-C	5.37	116.61	108.07	14	1
1	A	137	GLU	O-C-N	5.36	129.38	122.68	18	1
1	A	121	LEU	CD1-CG-CD2	-5.36	99.00	110.80	7	2
1	A	130	LEU	O-C-N	5.36	129.43	122.89	20	1
1	A	201	HIS	CB-CG-ND1	-5.36	114.66	122.70	17	1
1	A	157	PHE	CB-CA-C	-5.35	102.27	109.71	5	1
1	A	142	ILE	N-CA-CB	5.35	117.19	111.46	19	1
1	A	174	ILE	CA-CB-CG1	5.35	119.49	110.40	19	1
1	A	239	ILE	CA-C-O	-5.34	115.50	121.05	17	1
1	A	178	ALA	O-C-N	-5.34	116.43	123.21	19	1
1	A	107	ASP	N-CA-C	-5.33	104.36	111.24	3	2
1	A	91	LYS	CA-C-N	5.33	128.79	121.33	8	1
1	A	91	LYS	C-N-CA	5.33	128.79	121.33	8	1
1	A	87	PRO	N-CD-CG	5.33	110.19	103.80	17	2
1	A	150	GLU	OE1-CD-OE2	5.33	135.69	122.90	18	1
1	A	97	LEU	N-CA-C	5.33	118.38	109.96	20	1
1	A	179	HIS	CB-CA-C	5.32	121.37	109.56	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	126	GLU	N-CA-CB	-5.32	102.08	110.06	19	1
1	A	149	ARG	NE-CZ-NH2	-5.32	114.41	119.20	18	1
1	A	143	MET	CA-C-O	5.31	126.10	120.36	15	2
1	A	244	SER	N-CA-C	-5.31	106.74	113.43	9	1
1	A	108	LEU	O-C-N	5.29	128.32	120.96	19	1
1	A	86	PHE	CA-C-O	-5.29	112.91	120.16	20	1
1	A	88	GLY	N-CA-C	-5.29	108.42	115.40	4	1
1	A	119	LYS	CA-CB-CG	-5.29	103.52	114.10	18	1
1	A	151	HIS	CB-CA-C	5.28	117.89	109.02	20	1
1	A	180	PHE	CA-CB-CG	5.28	119.08	113.80	20	1
1	A	239	ILE	CA-C-N	-5.27	111.48	121.54	19	1
1	A	239	ILE	C-N-CA	-5.27	111.48	121.54	19	1
1	A	219	MET	CA-C-N	-5.25	113.22	120.26	18	1
1	A	219	MET	C-N-CA	-5.25	113.22	120.26	18	1
1	A	202	GLU	CB-CG-CD	5.25	121.53	112.60	16	1
1	A	186	TRP	NE1-CE2-CD2	-5.25	100.57	107.40	19	1
1	A	125	GLU	N-CA-C	5.25	118.94	112.54	17	1
1	A	135	LEU	CB-CA-C	-5.24	99.99	110.42	18	1
1	A	160	PRO	CA-CB-CG	-5.24	94.54	104.50	20	1
1	A	183	ASP	O-C-N	5.24	128.12	122.15	19	1
1	A	86	PHE	CB-CA-C	5.23	120.48	110.17	9	1
1	A	93	ARG	N-CA-C	-5.23	106.21	112.59	19	1
1	A	156	PRO	CA-C-O	-5.22	111.09	120.60	1	1
1	A	195	LEU	N-CA-C	-5.22	106.01	112.38	8	1
1	A	203	ILE	CA-C-N	5.22	125.63	119.94	13	1
1	A	203	ILE	C-N-CA	5.22	125.63	119.94	13	1
1	A	164	LEU	CB-CG-CD1	5.21	126.32	110.70	20	1
1	A	231	ARG	O-C-N	-5.20	115.67	122.59	17	1
1	A	171	GLY	O-C-N	5.20	126.97	121.77	18	1
1	A	194	ASN	CA-C-N	5.20	127.76	120.28	7	2
1	A	194	ASN	C-N-CA	5.20	127.76	120.28	7	2
1	A	175	ASN	OD1-CG-ND2	-5.17	117.43	122.60	19	1
1	A	157	PHE	CA-C-N	-5.17	111.97	122.31	20	1
1	A	157	PHE	C-N-CA	-5.17	111.97	122.31	20	1
1	A	102	VAL	N-CA-CB	-5.17	101.82	110.86	19	1
1	A	106	PRO	CA-N-CD	-5.17	104.77	112.00	20	1
1	A	174	ILE	CB-CA-C	-5.17	102.82	111.29	20	1
1	A	124	TRP	NE1-CE2-CZ2	5.16	137.84	130.10	17	1
1	A	225	SER	CA-CB-OG	5.16	121.43	111.10	18	1
1	A	121	LEU	O-C-N	5.16	129.46	122.59	18	1
1	A	187	THR	CB-CA-C	-5.14	103.26	113.80	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	124	TRP	CE3-CZ3-CH2	-5.13	114.44	121.10	18	1
1	A	191	THR	CA-CB-OG1	5.12	117.28	109.60	15	1
1	A	120	ALA	CA-C-N	5.11	131.29	121.54	11	1
1	A	120	ALA	C-N-CA	5.11	131.29	121.54	11	1
1	A	158	ASP	O-C-N	-5.11	115.60	122.19	18	1
1	A	210	PHE	N-CA-C	5.08	118.35	110.17	17	1
1	A	231	ARG	N-CA-C	-5.08	99.97	110.80	18	1
1	A	233	ARG	O-C-N	5.08	129.34	122.59	17	1
1	A	155	TYR	CB-CA-C	-5.07	103.81	111.27	20	1
1	A	222	LEU	CD1-CG-CD2	5.06	121.93	110.80	20	1
1	A	188	LYS	N-CA-CB	5.03	118.99	110.49	15	1
1	A	85	THR	O-C-N	5.03	129.28	122.59	17	1
1	A	170	PRO	N-CA-C	-5.03	102.12	112.47	7	1
1	A	133	SER	CA-CB-OG	-5.03	101.05	111.10	17	1
1	A	159	GLY	CA-C-N	5.02	125.80	119.98	20	1
1	A	159	GLY	C-N-CA	5.02	125.80	119.98	20	1
1	A	168	TYR	CB-CA-C	-5.02	101.64	109.72	20	1
1	A	144	ILE	CA-CB-CG2	5.02	119.03	110.50	5	1
1	A	208	GLY	O-C-N	5.01	129.21	122.70	18	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	164	LEU	CA	1

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	246	TYR	Sidechain	20
1	A	128	THR	Peptide	19
1	A	223	TYR	Sidechain	19
1	A	196	PHE	Sidechain	15
1	A	146	PHE	Sidechain	14
1	A	168	TYR	Sidechain	12
1	A	166	HIS	Sidechain	11
1	A	136	TYR	Sidechain	10
1	A	220	TYR	Sidechain,Peptide	9
1	A	232	PHE	Sidechain	8
1	A	155	TYR	Sidechain,Peptide	7
1	A	132	PHE	Sidechain	7

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	180	PHE	Sidechain	7
1	A	104	TYR	Sidechain	6
1	A	99	TYR	Sidechain	6
1	A	157	PHE	Sidechain	6
1	A	83	PHE	Sidechain	5
1	A	151	HIS	Sidechain	5
1	A	179	HIS	Sidechain	4
1	A	159	GLY	Peptide	3
1	A	169	ALA	Peptide	3
1	A	89	ILE	Peptide	3
1	A	154	PHE	Sidechain	3
1	A	86	PHE	Sidechain	2
1	A	93	ARG	Sidechain	1
1	A	149	ARG	Sidechain	1
1	A	210	PHE	Sidechain	1
1	A	105	THR	Peptide	1
1	A	100	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	1324	1248	1252	75±10
4	A	32	36	35	14±3
All	All	27180	25680	25740	1668

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 32.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:261:0DS:CD11	4:A:261:0DS:CG1	1.17	1.43	19	1
4:A:261:0DS:HD1	4:A:261:0DS:CD11	1.11	0.97	5	19
4:A:261:0DS:CE2	4:A:261:0DS:CG1	1.11	2.29	18	8
4:A:261:0DS:CD21	4:A:261:0DS:HD2	1.10	0.97	7	20
4:A:261:0DS:CD11	4:A:261:0DS:HD1	1.06	0.97	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:164:LEU:HD23	1:A:198:VAL:HG13	1.05	1.13	15	4
4:A:261:0DS:CE1	4:A:261:0DS:CG1	0.99	2.40	11	11
4:A:261:0DS:CG1	4:A:261:0DS:CE1	0.96	2.42	19	9
4:A:261:0DS:CG1	4:A:261:0DS:CE2	0.96	2.41	11	12
1:A:222:LEU:HD22	1:A:223:TYR:H	0.94	1.21	11	19
1:A:148:VAL:HG12	1:A:181:ASP:HA	0.93	1.35	5	3
1:A:222:LEU:HD22	1:A:223:TYR:N	0.92	1.80	3	17
1:A:163:VAL:C	1:A:164:LEU:HD13	0.85	1.95	16	14
1:A:163:VAL:HG21	4:A:261:0DS:HM42	0.84	1.49	5	2
1:A:163:VAL:O	1:A:164:LEU:HD22	0.84	1.72	19	9
1:A:164:LEU:HD13	1:A:198:VAL:HG13	0.83	1.50	10	2
4:A:261:0DS:CG1	4:A:261:0DS:HD2	0.83	2.04	19	2
1:A:148:VAL:HG12	1:A:166:HIS:CE1	0.83	2.08	13	1
4:A:261:0DS:HD2	4:A:261:0DS:CE2	0.82	2.04	19	19
1:A:163:VAL:HG22	4:A:261:0DS:HD12	0.82	1.49	7	2
1:A:164:LEU:HD11	4:A:261:0DS:HD23	0.81	1.50	13	5
4:A:261:0DS:HD2	4:A:261:0DS:CG1	0.81	2.06	10	18
4:A:261:0DS:HD1	4:A:261:0DS:CE1	0.80	2.06	3	20
1:A:147:ALA:O	1:A:148:VAL:HG13	0.80	1.76	14	9
1:A:148:VAL:HG12	1:A:181:ASP:CA	0.80	2.06	5	2
4:A:261:0DS:HD1	4:A:261:0DS:CG1	0.80	2.06	20	18
1:A:163:VAL:HG21	4:A:261:0DS:HD12	0.80	1.51	12	6
4:A:261:0DS:CG1	4:A:261:0DS:HD1	0.79	2.06	18	2
4:A:261:0DS:CE2	4:A:261:0DS:HD2	0.79	2.06	18	1
1:A:116:ALA:HB1	1:A:196:PHE:N	0.79	1.91	14	20
1:A:164:LEU:CD2	1:A:198:VAL:HG13	0.79	2.03	15	5
1:A:148:VAL:HG12	1:A:166:HIS:CD2	0.79	2.12	4	6
1:A:184:GLU:CD	1:A:193:THR:HG21	0.79	2.02	11	6
1:A:148:VAL:HG11	1:A:181:ASP:OD1	0.79	1.78	15	7
1:A:164:LEU:HD21	4:A:261:0DS:HD21	0.78	1.55	11	1
1:A:118:GLU:HA	1:A:121:LEU:HD23	0.78	1.55	5	9
1:A:164:LEU:HD11	4:A:261:0DS:HG	0.77	1.55	11	1
1:A:164:LEU:HD11	4:A:261:0DS:CG	0.77	2.09	11	1
1:A:164:LEU:HD23	1:A:198:VAL:CG1	0.76	2.11	2	5
1:A:85:THR:HG21	1:A:208:GLY:HA2	0.76	1.58	9	1
1:A:113:VAL:HG13	1:A:195:LEU:HG	0.75	1.57	16	19
1:A:164:LEU:HD21	4:A:261:0DS:HD11	0.75	1.57	5	5
1:A:217:ALA:HB1	1:A:235:SER:CB	0.75	2.12	6	7
1:A:180:PHE:CD1	1:A:198:VAL:HG22	0.74	2.17	4	1
1:A:164:LEU:CD1	1:A:198:VAL:HG13	0.73	2.14	10	2
1:A:209:LEU:HD13	1:A:238:ASP:HB2	0.73	1.59	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:HIS:CE1	1:A:179:HIS:CE1	0.72	2.77	13	1
1:A:202:GLU:CD	1:A:202:GLU:C	0.72	2.57	18	4
1:A:85:THR:HG22	1:A:245:LEU:HD21	0.72	1.60	7	1
1:A:164:LEU:HD23	1:A:198:VAL:HG23	0.71	1.59	12	2
1:A:148:VAL:HG12	1:A:166:HIS:ND1	0.71	1.99	13	1
1:A:222:LEU:HD21	4:A:261:ODS:HB31	0.71	1.62	4	6
1:A:164:LEU:H	1:A:164:LEU:HD22	0.71	1.45	12	2
1:A:222:LEU:HD11	4:A:261:ODS:HA1	0.70	1.61	5	1
1:A:153:ASP:HB2	1:A:166:HIS:CE1	0.70	2.21	3	8
1:A:226:LEU:H	1:A:226:LEU:HD12	0.70	1.46	11	1
1:A:163:VAL:HG21	4:A:261:ODS:HD23	0.70	1.64	1	3
1:A:164:LEU:HD13	1:A:198:VAL:CG1	0.70	2.16	10	2
1:A:174:ILE:HD12	1:A:174:ILE:O	0.68	1.88	8	2
1:A:223:TYR:CD2	1:A:223:TYR:C	0.68	2.72	20	1
1:A:169:ALA:HB1	1:A:170:PRO:HD2	0.68	1.65	1	11
1:A:197:LEU:C	1:A:197:LEU:HD13	0.68	2.13	3	5
1:A:148:VAL:HG13	1:A:181:ASP:HA	0.68	1.63	13	5
1:A:116:ALA:HB1	1:A:196:PHE:CA	0.68	2.18	14	14
1:A:195:LEU:O	1:A:198:VAL:HG23	0.67	1.90	10	5
1:A:196:PHE:O	1:A:199:ALA:HB3	0.67	1.90	10	15
1:A:169:ALA:HB1	1:A:170:PRO:CD	0.67	2.19	14	13
1:A:164:LEU:HD11	4:A:261:ODS:CD1	0.67	2.19	5	4
1:A:163:VAL:HG11	4:A:261:ODS:HA	0.67	1.64	12	2
1:A:178:ALA:HB2	1:A:202:GLU:CD	0.67	2.15	11	5
1:A:148:VAL:CG1	1:A:181:ASP:HA	0.66	2.20	9	12
1:A:153:ASP:HB2	1:A:166:HIS:CD2	0.66	2.23	5	6
1:A:163:VAL:HG11	4:A:261:ODS:C5	0.66	2.20	17	1
1:A:163:VAL:C	1:A:164:LEU:HG	0.66	2.13	10	2
1:A:162:ASN:C	1:A:163:VAL:HG22	0.66	2.15	20	4
1:A:184:GLU:OE2	1:A:193:THR:HG21	0.66	1.91	8	6
1:A:147:ALA:O	1:A:148:VAL:HB	0.66	1.91	9	2
1:A:163:VAL:HG23	1:A:164:LEU:HD13	0.65	1.66	5	1
1:A:226:LEU:N	1:A:226:LEU:HD12	0.65	2.07	1	2
1:A:164:LEU:HD11	4:A:261:ODS:CD2	0.65	2.22	13	7
1:A:197:LEU:HD11	4:A:261:ODS:H51	0.65	1.67	5	3
1:A:120:ALA:HB1	1:A:124:TRP:CZ2	0.64	2.26	1	1
1:A:164:LEU:CG	1:A:198:VAL:HG13	0.64	2.23	10	3
1:A:121:LEU:HD12	1:A:132:PHE:CB	0.64	2.23	12	5
1:A:187:THR:HG23	1:A:193:THR:N	0.64	2.08	10	2
1:A:164:LEU:HD23	1:A:198:VAL:CG2	0.64	2.21	12	1
1:A:101:ILE:HD11	1:A:117:VAL:HG11	0.64	1.67	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:MET:O	1:A:144:ILE:HD12	0.64	1.90	18	1
1:A:162:ASN:HA	4:A:261:ODS:CB1	0.64	2.22	7	9
1:A:144:ILE:HG21	1:A:180:PHE:CE2	0.64	2.27	5	7
1:A:209:LEU:HB2	1:A:238:ASP:HB3	0.64	1.69	9	4
1:A:113:VAL:HG13	1:A:195:LEU:CG	0.64	2.23	9	12
1:A:164:LEU:HD12	1:A:186:TRP:HH2	0.64	1.50	4	3
1:A:222:LEU:HD13	1:A:223:TYR:N	0.64	2.08	6	7
1:A:117:VAL:HG22	1:A:199:ALA:HB2	0.64	1.69	2	6
1:A:200:ALA:O	1:A:201:HIS:C	0.63	2.39	19	5
1:A:217:ALA:HB1	1:A:235:SER:HB2	0.63	1.69	6	1
1:A:124:TRP:CH2	1:A:207:LEU:HD11	0.63	2.28	3	2
1:A:124:TRP:CH2	1:A:209:LEU:HD23	0.63	2.28	7	1
1:A:164:LEU:HD23	1:A:198:VAL:HG12	0.63	1.69	2	2
1:A:164:LEU:HB3	1:A:186:TRP:CH2	0.62	2.29	12	1
1:A:162:ASN:HA	4:A:261:ODS:HB21	0.62	1.70	9	5
1:A:142:ILE:CG2	1:A:206:SER:CB	0.62	2.77	9	8
1:A:164:LEU:HD12	1:A:186:TRP:CH2	0.62	2.30	12	3
1:A:105:THR:CG2	1:A:186:TRP:CD1	0.62	2.82	6	10
1:A:108:LEU:CB	1:A:113:VAL:HG23	0.62	2.25	1	1
1:A:85:THR:HG22	1:A:86:PHE:N	0.62	2.09	9	3
1:A:123:VAL:HG23	1:A:229:LEU:HD13	0.62	1.72	13	6
1:A:222:LEU:HD13	1:A:223:TYR:H	0.61	1.53	8	3
1:A:220:TYR:CD2	1:A:226:LEU:HD11	0.61	2.30	11	1
1:A:165:ALA:N	1:A:198:VAL:HG13	0.61	2.10	14	1
1:A:118:GLU:CA	1:A:121:LEU:HD23	0.61	2.24	5	5
1:A:222:LEU:CD2	1:A:223:TYR:H	0.61	2.07	17	10
1:A:144:ILE:CG1	1:A:178:ALA:HB3	0.61	2.25	2	1
1:A:227:THR:HG23	1:A:232:PHE:CD1	0.61	2.30	16	3
1:A:163:VAL:HA	1:A:164:LEU:HD13	0.61	1.72	4	3
1:A:235:SER:CB	1:A:238:ASP:HB2	0.61	2.26	10	2
1:A:163:VAL:O	1:A:164:LEU:HD13	0.61	1.94	6	1
1:A:209:LEU:CB	1:A:238:ASP:HB3	0.61	2.26	12	1
1:A:164:LEU:HG	1:A:186:TRP:CH2	0.60	2.30	7	4
1:A:148:VAL:CG2	1:A:181:ASP:HA	0.60	2.26	2	6
1:A:184:GLU:HG3	1:A:193:THR:HG21	0.60	1.72	5	1
1:A:119:LYS:O	1:A:229:LEU:HD21	0.60	1.95	7	1
1:A:119:LYS:O	1:A:120:ALA:C	0.60	2.43	17	6
1:A:146:PHE:N	1:A:146:PHE:CD1	0.60	2.68	18	2
1:A:164:LEU:CD2	1:A:198:VAL:CG1	0.60	2.79	2	4
1:A:164:LEU:H	1:A:198:VAL:CG2	0.60	2.09	5	1
1:A:164:LEU:HD12	1:A:164:LEU:H	0.60	1.56	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:LEU:HD12	1:A:132:PHE:CG	0.60	2.32	15	2
1:A:184:GLU:HG2	1:A:193:THR:CB	0.60	2.27	2	9
1:A:164:LEU:HD23	1:A:198:VAL:HB	0.60	1.71	9	1
1:A:124:TRP:CZ2	1:A:218:LEU:HD11	0.59	2.31	4	1
1:A:163:VAL:HA	1:A:164:LEU:HD22	0.59	1.73	15	4
1:A:161:GLY:HA2	1:A:193:THR:HG23	0.59	1.74	2	10
1:A:164:LEU:HD11	4:A:261:0DS:HD11	0.59	1.74	5	1
1:A:113:VAL:HG22	1:A:195:LEU:HG	0.59	1.74	1	12
1:A:164:LEU:H	1:A:164:LEU:CD2	0.59	2.07	12	1
1:A:164:LEU:HD22	1:A:164:LEU:N	0.59	2.13	1	4
1:A:92:TRP:CD1	1:A:97:LEU:HD21	0.59	2.33	6	3
1:A:163:VAL:HG21	4:A:261:0DS:CM4	0.59	2.27	11	2
1:A:196:PHE:CD1	1:A:196:PHE:C	0.58	2.79	17	6
1:A:184:GLU:OE1	1:A:193:THR:HG21	0.58	1.97	11	1
1:A:197:LEU:HD11	4:A:261:0DS:C5	0.58	2.28	3	2
1:A:163:VAL:C	1:A:164:LEU:CD1	0.58	2.73	16	4
1:A:164:LEU:HD12	1:A:193:THR:HG22	0.58	1.76	2	1
1:A:226:LEU:CD1	1:A:227:THR:HG22	0.58	2.29	6	1
1:A:174:ILE:HD13	1:A:177:ASP:HB2	0.58	1.75	13	1
1:A:164:LEU:H	1:A:198:VAL:HG23	0.58	1.59	5	1
1:A:163:VAL:HG12	1:A:198:VAL:CG2	0.58	2.29	14	1
1:A:124:TRP:HB3	1:A:234:LEU:HD21	0.58	1.75	14	1
1:A:164:LEU:HB3	1:A:181:ASP:CG	0.57	2.24	15	1
1:A:184:GLU:CG	1:A:193:THR:HG21	0.57	2.28	5	15
1:A:124:TRP:CH2	1:A:218:LEU:HD11	0.57	2.35	4	4
1:A:148:VAL:HG23	1:A:149:ARG:N	0.57	2.14	17	5
1:A:164:LEU:HD21	4:A:261:0DS:CD1	0.57	2.29	13	1
1:A:164:LEU:HD12	1:A:193:THR:HB	0.57	1.77	1	2
1:A:165:ALA:HB2	1:A:198:VAL:HB	0.57	1.75	7	1
1:A:227:THR:HG21	1:A:232:PHE:CD1	0.57	2.35	12	1
1:A:164:LEU:CD1	4:A:261:0DS:HD23	0.57	2.28	13	2
1:A:235:SER:OG	1:A:238:ASP:OD2	0.57	2.17	19	1
1:A:165:ALA:HB2	1:A:198:VAL:HG23	0.57	1.77	4	1
1:A:161:GLY:CA	1:A:193:THR:HG23	0.57	2.29	2	4
1:A:164:LEU:CD2	1:A:198:VAL:HB	0.57	2.30	9	2
1:A:142:ILE:HG21	1:A:206:SER:CB	0.57	2.30	18	2
1:A:227:THR:HG21	1:A:232:PHE:HA	0.56	1.76	15	1
1:A:194:ASN:HB2	1:A:223:TYR:CE2	0.56	2.35	13	3
1:A:159:GLY:HA2	1:A:183:ASP:CG	0.56	2.25	12	2
1:A:101:ILE:HG22	1:A:146:PHE:CE1	0.56	2.35	4	3
1:A:165:ALA:N	1:A:198:VAL:CG2	0.56	2.68	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:THR:HG23	1:A:193:THR:H	0.56	1.61	7	3
1:A:166:HIS:CE1	1:A:179:HIS:HB2	0.56	2.36	19	2
4:A:261:0DS:H1	4:A:261:0DS:HD22	0.56	1.61	11	1
1:A:128:THR:O	1:A:130:LEU:N	0.56	2.37	18	2
1:A:142:ILE:HG22	1:A:176:GLY:HA3	0.56	1.78	19	1
1:A:148:VAL:CG2	1:A:183:ASP:HB2	0.56	2.31	2	9
1:A:148:VAL:HG23	1:A:183:ASP:HB2	0.56	1.78	11	6
1:A:163:VAL:HG21	4:A:261:0DS:CD1	0.56	2.30	8	6
1:A:191:THR:HG23	1:A:223:TYR:O	0.56	2.01	17	1
1:A:218:LEU:HD13	1:A:234:LEU:HD23	0.56	1.76	10	1
1:A:186:TRP:CZ3	1:A:193:THR:HB	0.56	2.36	20	10
1:A:190:THR:O	1:A:191:THR:HG23	0.56	2.00	19	3
1:A:148:VAL:HA	1:A:166:HIS:CE1	0.56	2.36	11	1
1:A:121:LEU:HD12	1:A:132:PHE:HB3	0.56	1.78	12	1
1:A:101:ILE:HD13	1:A:101:ILE:N	0.56	2.16	20	2
1:A:97:LEU:HD22	1:A:130:LEU:HD21	0.56	1.78	2	1
1:A:226:LEU:HD13	1:A:227:THR:HG22	0.56	1.77	5	6
1:A:105:THR:HG21	1:A:186:TRP:CD1	0.56	2.36	6	5
1:A:190:THR:HG22	1:A:190:THR:O	0.56	2.00	7	3
1:A:218:LEU:HD21	1:A:232:PHE:CE2	0.56	2.36	16	2
1:A:86:PHE:CB	1:A:244:SER:HB3	0.56	2.31	13	8
1:A:209:LEU:N	1:A:209:LEU:HD23	0.55	2.16	12	3
1:A:226:LEU:HD12	1:A:226:LEU:H	0.55	1.59	1	1
1:A:148:VAL:HG23	1:A:151:HIS:N	0.55	2.17	7	2
1:A:222:LEU:CD1	1:A:223:TYR:H	0.55	2.15	8	2
1:A:143:MET:C	1:A:144:ILE:HD12	0.55	2.26	19	3
1:A:164:LEU:CD1	1:A:193:THR:HG22	0.55	2.32	2	1
1:A:163:VAL:HG11	4:A:261:0DS:H52	0.55	1.79	17	1
1:A:191:THR:HG22	1:A:192:GLY:O	0.55	2.00	17	1
1:A:163:VAL:CG2	4:A:261:0DS:HD23	0.55	2.31	1	2
1:A:163:VAL:CA	1:A:164:LEU:HD13	0.55	2.32	4	3
1:A:129:PRO:CD	1:A:246:TYR:HA	0.55	2.32	9	1
1:A:164:LEU:CD2	1:A:164:LEU:N	0.54	2.69	1	3
1:A:148:VAL:HG22	1:A:157:PHE:HB3	0.54	1.78	3	1
1:A:156:PRO:HG3	1:A:163:VAL:HG23	0.54	1.79	7	1
1:A:101:ILE:HD13	1:A:101:ILE:H	0.54	1.62	20	1
1:A:180:PHE:O	1:A:182:ASP:N	0.54	2.40	18	6
1:A:197:LEU:HD13	1:A:223:TYR:CD1	0.54	2.37	10	3
1:A:178:ALA:CB	1:A:202:GLU:CG	0.54	2.85	14	2
1:A:187:THR:N	1:A:193:THR:O	0.54	2.39	19	3
1:A:197:LEU:HD11	4:A:261:0DS:HM41	0.54	1.78	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:TRP:CD2	1:A:195:LEU:HD23	0.54	2.38	9	4
1:A:144:ILE:HG13	1:A:178:ALA:HB3	0.54	1.80	19	2
1:A:222:LEU:CG	1:A:223:TYR:H	0.54	2.15	17	7
1:A:121:LEU:HD22	1:A:121:LEU:H	0.54	1.61	14	3
1:A:163:VAL:O	1:A:164:LEU:CD2	0.54	2.55	5	8
1:A:160:PRO:HA	1:A:184:GLU:CD	0.54	2.27	15	4
1:A:161:GLY:HA2	1:A:193:THR:CG2	0.54	2.32	17	3
1:A:186:TRP:CE3	1:A:195:LEU:N	0.54	2.76	6	9
1:A:153:ASP:CB	1:A:166:HIS:CD2	0.54	2.90	13	3
1:A:124:TRP:CH2	1:A:204:GLY:HA3	0.54	2.37	16	1
4:A:261:0DS:H52	4:A:261:0DS:N	0.54	2.18	16	2
1:A:101:ILE:H	1:A:101:ILE:HD13	0.54	1.61	17	1
1:A:123:VAL:H	1:A:229:LEU:HD11	0.54	1.63	17	5
1:A:182:ASP:O	1:A:182:ASP:OD1	0.54	2.26	17	1
1:A:162:ASN:O	1:A:164:LEU:HD13	0.54	2.03	1	1
1:A:166:HIS:ND1	1:A:179:HIS:HB2	0.53	2.18	11	1
1:A:163:VAL:CG2	4:A:261:0DS:HD12	0.53	2.33	2	4
1:A:124:TRP:CZ3	1:A:234:LEU:CD2	0.53	2.91	8	2
1:A:117:VAL:HG12	1:A:121:LEU:CD2	0.53	2.34	8	1
1:A:164:LEU:HB2	1:A:198:VAL:CG1	0.53	2.32	8	1
1:A:189:ASP:C	1:A:191:THR:H	0.53	2.12	19	4
1:A:148:VAL:HG11	1:A:166:HIS:CE1	0.53	2.39	19	1
1:A:181:ASP:C	1:A:183:ASP:N	0.53	2.65	19	11
1:A:164:LEU:HD11	4:A:261:0DS:HD12	0.53	1.80	16	2
1:A:148:VAL:HG21	1:A:181:ASP:CG	0.53	2.29	10	3
1:A:165:ALA:N	1:A:198:VAL:HG12	0.53	2.18	8	3
1:A:178:ALA:HB2	1:A:202:GLU:CG	0.53	2.34	6	2
1:A:143:MET:HE3	1:A:174:ILE:CD1	0.53	2.33	10	2
1:A:164:LEU:HG	1:A:198:VAL:CG1	0.53	2.34	2	2
1:A:165:ALA:HB2	1:A:180:PHE:CE1	0.53	2.38	5	1
1:A:164:LEU:HD12	1:A:164:LEU:N	0.53	2.18	10	2
1:A:127:VAL:HG11	1:A:234:LEU:HD13	0.53	1.80	12	1
1:A:179:HIS:CD2	1:A:179:HIS:H	0.53	2.20	14	1
1:A:153:ASP:HB2	1:A:166:HIS:ND1	0.53	2.19	20	3
1:A:162:ASN:N	1:A:193:THR:HG22	0.53	2.18	5	1
1:A:186:TRP:O	1:A:187:THR:HB	0.53	2.02	20	1
1:A:191:THR:HG21	1:A:223:TYR:O	0.52	2.03	1	1
1:A:123:VAL:HG11	1:A:232:PHE:H	0.52	1.63	3	1
1:A:234:LEU:H	1:A:234:LEU:HD12	0.52	1.63	4	5
1:A:164:LEU:CD1	1:A:164:LEU:N	0.52	2.71	10	4
1:A:163:VAL:HG22	4:A:261:0DS:CD1	0.52	2.27	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:TRP:CZ3	1:A:242:ILE:HD11	0.52	2.39	11	1
1:A:134:ARG:O	1:A:135:LEU:C	0.52	2.53	20	1
1:A:197:LEU:CD1	4:A:261:0DS:HM41	0.52	2.35	5	1
1:A:85:THR:HG22	1:A:86:PHE:H	0.52	1.64	9	1
1:A:164:LEU:HD22	1:A:186:TRP:CH2	0.52	2.39	10	1
1:A:85:THR:CG2	1:A:86:PHE:H	0.52	2.17	3	2
1:A:155:TYR:CD2	4:A:261:0DS:HD11	0.52	2.38	12	1
1:A:120:ALA:HA	1:A:229:LEU:HD13	0.52	1.82	14	1
1:A:197:LEU:HB2	1:A:223:TYR:CE2	0.52	2.39	1	1
1:A:184:GLU:HG2	1:A:193:THR:OG1	0.52	2.04	19	6
1:A:165:ALA:HB2	1:A:198:VAL:CG2	0.52	2.34	12	2
1:A:186:TRP:CE2	1:A:195:LEU:HD23	0.52	2.39	4	4
1:A:218:LEU:HD22	1:A:234:LEU:HD23	0.52	1.80	8	1
1:A:162:ASN:OD1	1:A:222:LEU:HD13	0.52	2.05	5	1
1:A:243:GLN:HG3	1:A:246:TYR:CZ	0.52	2.40	20	1
1:A:85:THR:H	1:A:208:GLY:HA3	0.52	1.65	4	1
1:A:165:ALA:HB1	1:A:202:GLU:HG3	0.52	1.82	4	1
1:A:143:MET:CE	1:A:174:ILE:HD12	0.52	2.35	5	3
1:A:184:GLU:HG2	1:A:193:THR:HB	0.52	1.82	14	1
1:A:144:ILE:HG23	1:A:180:PHE:CD1	0.51	2.41	14	1
1:A:99:TYR:CE1	1:A:117:VAL:HG11	0.51	2.40	5	1
1:A:153:ASP:HB2	1:A:166:HIS:NE2	0.51	2.21	14	1
1:A:158:ASP:CG	1:A:158:ASP:O	0.51	2.53	20	2
1:A:99:TYR:CZ	1:A:144:ILE:HD11	0.51	2.40	5	1
1:A:222:LEU:C	1:A:222:LEU:HD13	0.51	2.30	19	1
1:A:178:ALA:HB1	1:A:180:PHE:CE1	0.51	2.40	6	4
1:A:171:GLY:O	1:A:172:PRO:C	0.51	2.54	20	1
1:A:164:LEU:HD11	4:A:261:0DS:HD21	0.51	1.83	5	1
1:A:165:ALA:HB2	1:A:198:VAL:HG12	0.51	1.81	10	1
1:A:166:HIS:ND1	1:A:179:HIS:O	0.51	2.43	19	1
1:A:196:PHE:CZ	1:A:229:LEU:HB3	0.51	2.41	14	1
1:A:222:LEU:HD21	4:A:261:0DS:CB1	0.51	2.36	4	2
1:A:164:LEU:CB	1:A:186:TRP:CH2	0.51	2.93	12	2
1:A:157:PHE:CG	1:A:164:LEU:HA	0.51	2.41	10	1
1:A:204:GLY:HA3	1:A:209:LEU:HD21	0.51	1.83	2	1
1:A:97:LEU:O	1:A:132:PHE:HA	0.51	2.06	20	2
1:A:169:ALA:HB1	1:A:170:PRO:HD3	0.51	1.82	10	1
1:A:164:LEU:HD12	1:A:184:GLU:OE2	0.51	2.06	17	1
1:A:108:LEU:HB2	1:A:113:VAL:HG23	0.50	1.82	1	2
1:A:180:PHE:CE1	1:A:198:VAL:HB	0.50	2.40	1	2
1:A:148:VAL:HG22	1:A:157:PHE:H	0.50	1.66	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:LEU:CD1	1:A:245:LEU:HB3	0.50	2.37	8	4
1:A:226:LEU:H	1:A:226:LEU:CD1	0.50	2.12	11	2
1:A:162:ASN:N	1:A:193:THR:HG23	0.50	2.22	14	3
1:A:186:TRP:CE3	1:A:193:THR:OG1	0.50	2.62	20	2
1:A:164:LEU:CD1	4:A:261:0DS:HD21	0.50	2.36	5	1
1:A:223:TYR:O	1:A:223:TYR:CG	0.50	2.63	18	1
1:A:207:LEU:O	1:A:245:LEU:HD21	0.50	2.07	18	1
1:A:174:ILE:O	1:A:175:ASN:C	0.50	2.54	17	6
1:A:164:LEU:H	1:A:198:VAL:HG21	0.50	1.66	16	1
1:A:177:ASP:N	1:A:177:ASP:OD1	0.50	2.44	20	1
1:A:184:GLU:HG2	1:A:193:THR:HG21	0.50	1.81	12	5
1:A:200:ALA:HB1	1:A:218:LEU:CD2	0.50	2.37	11	3
1:A:124:TRP:CZ2	1:A:209:LEU:HD23	0.50	2.41	7	1
1:A:124:TRP:CZ3	1:A:132:PHE:CZ	0.50	3.00	14	1
1:A:161:GLY:H	1:A:193:THR:HG21	0.50	1.66	1	1
1:A:197:LEU:HB2	1:A:223:TYR:CE1	0.50	2.41	4	1
1:A:129:PRO:CD	1:A:246:TYR:CA	0.50	2.89	9	1
1:A:148:VAL:CG2	1:A:183:ASP:H	0.50	2.20	18	2
1:A:197:LEU:HD11	1:A:225:SER:HB3	0.49	1.84	1	1
1:A:164:LEU:HD11	1:A:223:TYR:CE2	0.49	2.42	4	1
1:A:157:PHE:O	1:A:157:PHE:CG	0.49	2.62	15	2
1:A:117:VAL:O	1:A:120:ALA:N	0.49	2.45	17	2
1:A:163:VAL:C	1:A:164:LEU:CG	0.49	2.82	17	4
1:A:162:ASN:O	1:A:163:VAL:HG22	0.49	2.07	20	2
1:A:142:ILE:CG2	1:A:206:SER:HB2	0.49	2.36	10	2
1:A:189:ASP:C	1:A:191:THR:N	0.49	2.69	19	1
1:A:181:ASP:C	1:A:183:ASP:H	0.49	2.13	19	6
1:A:155:TYR:HB2	1:A:156:PRO:CD	0.49	2.37	4	4
1:A:199:ALA:HB1	1:A:203:ILE:HD11	0.49	1.83	14	3
1:A:222:LEU:HD11	4:A:261:0DS:CA1	0.49	2.35	5	1
1:A:196:PHE:CZ	1:A:229:LEU:HD23	0.49	2.41	8	3
1:A:85:THR:HG23	1:A:86:PHE:N	0.49	2.21	8	1
1:A:147:ALA:O	1:A:148:VAL:CB	0.49	2.58	9	1
1:A:180:PHE:N	1:A:180:PHE:CD1	0.49	2.79	17	2
1:A:148:VAL:O	1:A:150:GLU:N	0.49	2.45	8	6
1:A:163:VAL:O	1:A:164:LEU:CB	0.49	2.60	14	6
1:A:190:THR:O	1:A:190:THR:HG22	0.49	2.06	5	2
1:A:121:LEU:CD1	1:A:203:ILE:HG21	0.49	2.37	14	2
1:A:180:PHE:CD1	1:A:180:PHE:N	0.49	2.81	14	2
1:A:116:ALA:HB1	1:A:196:PHE:HA	0.49	1.84	14	1
1:A:186:TRP:CZ3	1:A:193:THR:CB	0.49	2.95	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:ILE:N	1:A:90:PRO:CD	0.49	2.76	3	1
1:A:207:LEU:C	1:A:207:LEU:CD1	0.49	2.86	12	4
1:A:191:THR:HG21	4:A:261:ODS:CZ	0.49	2.37	13	2
1:A:191:THR:HG21	1:A:222:LEU:HD11	0.49	1.83	19	1
1:A:186:TRP:CD1	1:A:195:LEU:HD23	0.49	2.43	13	7
1:A:194:ASN:CB	1:A:223:TYR:CE2	0.49	2.96	17	3
1:A:179:HIS:CD2	1:A:179:HIS:N	0.49	2.81	19	10
1:A:162:ASN:C	1:A:163:VAL:CG2	0.49	2.84	20	3
1:A:168:TYR:O	1:A:169:ALA:HB2	0.49	2.07	18	2
1:A:164:LEU:CD2	1:A:198:VAL:CG2	0.49	2.90	12	1
1:A:143:MET:HE2	1:A:176:GLY:O	0.49	2.08	18	1
1:A:246:TYR:C	1:A:246:TYR:CD1	0.48	2.91	4	2
1:A:202:GLU:HA	1:A:205:HIS:HB2	0.48	1.85	2	1
1:A:165:ALA:H	1:A:198:VAL:HG22	0.48	1.67	16	1
1:A:223:TYR:O	1:A:223:TYR:CD2	0.48	2.66	18	1
1:A:146:PHE:CD1	1:A:146:PHE:C	0.48	2.91	1	3
1:A:123:VAL:HG23	1:A:229:LEU:CD1	0.48	2.39	8	2
1:A:197:LEU:HD12	1:A:223:TYR:CA	0.48	2.39	11	1
1:A:148:VAL:CG1	1:A:166:HIS:CE1	0.48	2.97	19	2
1:A:197:LEU:HD11	1:A:225:SER:CB	0.48	2.39	1	1
1:A:226:LEU:N	1:A:226:LEU:CD1	0.48	2.77	1	1
1:A:107:ASP:OD2	1:A:186:TRP:CG	0.48	2.67	12	1
1:A:166:HIS:ND1	1:A:179:HIS:CE1	0.48	2.80	13	1
1:A:113:VAL:HG13	1:A:195:LEU:CD1	0.48	2.39	7	6
1:A:164:LEU:N	1:A:164:LEU:CD2	0.48	2.76	17	2
1:A:243:GLN:O	1:A:246:TYR:CE1	0.48	2.66	4	2
1:A:148:VAL:HG23	1:A:149:ARG:H	0.48	1.67	6	1
1:A:163:VAL:CA	1:A:164:LEU:HD22	0.48	2.38	15	1
1:A:145:SER:C	1:A:146:PHE:CD1	0.48	2.92	18	1
1:A:153:ASP:CG	1:A:154:PHE:H	0.48	2.16	18	1
1:A:164:LEU:CG	1:A:198:VAL:CG1	0.48	2.91	2	1
1:A:209:LEU:HD12	1:A:238:ASP:HB2	0.48	1.86	6	1
1:A:222:LEU:N	4:A:261:ODS:H53	0.48	2.23	7	1
1:A:162:ASN:O	1:A:163:VAL:HG13	0.48	2.08	14	1
1:A:190:THR:C	1:A:191:THR:HG23	0.48	2.33	15	1
1:A:241:GLY:O	1:A:245:LEU:HD23	0.48	2.09	11	2
1:A:146:PHE:CG	1:A:182:ASP:OD2	0.48	2.67	14	1
1:A:166:HIS:N	1:A:179:HIS:NE2	0.48	2.61	18	1
1:A:127:VAL:CG2	1:A:242:ILE:HG21	0.47	2.39	3	2
1:A:208:GLY:C	1:A:210:PHE:H	0.47	2.17	3	3
4:A:261:ODS:H53	4:A:261:ODS:C1	0.47	2.39	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:165:ALA:CB	1:A:198:VAL:CG2	0.47	2.91	12	1
1:A:128:THR:OG1	1:A:130:LEU:HD12	0.47	2.09	14	1
1:A:186:TRP:CZ3	1:A:193:THR:OG1	0.47	2.64	20	1
1:A:234:LEU:H	1:A:234:LEU:CD1	0.47	2.21	4	3
1:A:123:VAL:HG21	1:A:232:PHE:H	0.47	1.67	13	1
1:A:121:LEU:HD12	1:A:132:PHE:HB2	0.47	1.85	5	1
1:A:164:LEU:HB2	1:A:198:VAL:HG11	0.47	1.86	8	1
1:A:165:ALA:HB2	1:A:198:VAL:HG22	0.47	1.86	12	1
1:A:163:VAL:HG22	4:A:261:ODS:HG	0.47	1.86	15	1
1:A:113:VAL:CG1	1:A:195:LEU:HG	0.47	2.39	5	5
1:A:142:ILE:CG2	1:A:206:SER:HB3	0.47	2.39	7	1
1:A:85:THR:HG22	1:A:208:GLY:HA3	0.47	1.86	8	1
1:A:207:LEU:O	1:A:207:LEU:HD13	0.47	2.09	17	1
1:A:86:PHE:CA	1:A:244:SER:HB3	0.47	2.40	13	2
1:A:187:THR:CG2	1:A:193:THR:N	0.47	2.76	3	2
1:A:164:LEU:HD13	1:A:164:LEU:N	0.47	2.24	11	2
1:A:83:PHE:CG	1:A:84:ARG:N	0.47	2.81	20	1
1:A:148:VAL:HG21	1:A:166:HIS:CD2	0.47	2.44	1	1
1:A:156:PRO:O	1:A:157:PHE:C	0.47	2.55	1	2
1:A:142:ILE:HG23	1:A:206:SER:CB	0.47	2.40	16	2
1:A:174:ILE:HD13	1:A:177:ASP:CB	0.47	2.38	13	1
1:A:151:HIS:N	1:A:151:HIS:ND1	0.47	2.62	18	1
1:A:124:TRP:CE3	1:A:234:LEU:HD11	0.47	2.44	4	1
1:A:220:TYR:O	4:A:261:ODS:H53	0.47	2.10	5	1
1:A:85:THR:HG21	1:A:208:GLY:CA	0.47	2.38	9	1
1:A:147:ALA:HA	1:A:182:ASP:HB3	0.47	1.87	10	1
1:A:167:ALA:C	1:A:168:TYR:CD2	0.47	2.93	13	2
1:A:169:ALA:CB	1:A:170:PRO:CD	0.47	2.93	14	5
1:A:194:ASN:HB3	1:A:223:TYR:CE1	0.47	2.45	10	1
1:A:235:SER:OG	1:A:238:ASP:HB2	0.46	2.09	1	1
1:A:165:ALA:H	1:A:198:VAL:HG11	0.46	1.69	7	1
1:A:129:PRO:CG	1:A:246:TYR:HA	0.46	2.40	9	1
1:A:148:VAL:CG1	1:A:166:HIS:CD2	0.46	2.98	16	1
1:A:243:GLN:C	1:A:246:TYR:CD1	0.46	2.93	19	1
1:A:162:ASN:CA	4:A:261:ODS:HB21	0.46	2.40	1	3
1:A:129:PRO:HG3	1:A:246:TYR:HA	0.46	1.86	9	1
1:A:148:VAL:HG21	1:A:181:ASP:CB	0.46	2.40	14	1
1:A:180:PHE:CD1	1:A:198:VAL:CG2	0.46	2.97	4	1
1:A:164:LEU:CD1	4:A:261:ODS:CD2	0.46	2.93	5	1
1:A:174:ILE:HD12	1:A:174:ILE:C	0.46	2.35	19	1
1:A:219:MET:SD	1:A:219:MET:N	0.46	2.88	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:209:LEU:HB2	1:A:238:ASP:CB	0.46	2.40	9	1
1:A:181:ASP:O	1:A:186:TRP:NE1	0.46	2.49	20	1
1:A:144:ILE:HD11	1:A:202:GLU:OE2	0.46	2.11	3	1
1:A:163:VAL:HG22	4:A:261:ODS:CD2	0.46	2.40	15	1
1:A:202:GLU:C	1:A:204:GLY:N	0.46	2.71	17	1
1:A:108:LEU:HB3	1:A:113:VAL:HG23	0.46	1.87	1	1
1:A:160:PRO:HA	1:A:184:GLU:HG3	0.46	1.87	1	2
1:A:234:LEU:HB2	1:A:238:ASP:CG	0.46	2.36	4	2
1:A:165:ALA:N	1:A:198:VAL:HG22	0.46	2.26	16	1
1:A:144:ILE:HD11	1:A:202:GLU:HG2	0.46	1.86	8	1
1:A:143:MET:HE3	1:A:174:ILE:HD12	0.46	1.87	10	2
1:A:108:LEU:HB2	1:A:186:TRP:CB	0.46	2.41	14	1
1:A:155:TYR:HB3	1:A:156:PRO:CD	0.46	2.41	1	1
1:A:164:LEU:HD23	1:A:198:VAL:CB	0.46	2.40	9	1
1:A:163:VAL:O	1:A:164:LEU:CG	0.46	2.64	16	1
1:A:164:LEU:HD23	1:A:198:VAL:HG21	0.46	1.88	17	1
1:A:103:ASN:O	1:A:104:TYR:CD2	0.46	2.69	20	1
1:A:235:SER:OG	1:A:238:ASP:CB	0.46	2.64	1	2
1:A:148:VAL:HG12	1:A:166:HIS:NE2	0.46	2.26	4	1
1:A:162:ASN:CB	4:A:261:ODS:HB21	0.45	2.40	1	3
1:A:124:TRP:CH2	1:A:229:LEU:CD2	0.45	2.98	4	1
1:A:98:THR:HG22	1:A:99:TYR:N	0.45	2.26	5	1
1:A:187:THR:HG23	1:A:193:THR:O	0.45	2.11	5	1
1:A:222:LEU:HD13	1:A:223:TYR:C	0.45	2.37	6	1
1:A:178:ALA:CB	1:A:202:GLU:HG3	0.45	2.42	14	2
1:A:123:VAL:C	1:A:125:GLU:N	0.45	2.73	18	1
1:A:197:LEU:HD13	1:A:198:VAL:N	0.45	2.26	3	1
1:A:181:ASP:OD2	1:A:184:GLU:OE1	0.45	2.35	17	1
1:A:242:ILE:CD1	1:A:242:ILE:N	0.45	2.79	7	2
1:A:217:ALA:HB1	1:A:235:SER:HB3	0.45	1.89	3	1
1:A:225:SER:O	1:A:227:THR:HG22	0.45	2.10	14	1
1:A:209:LEU:HD11	1:A:218:LEU:HD22	0.45	1.87	15	1
1:A:86:PHE:CB	1:A:244:SER:CB	0.45	2.95	16	6
1:A:192:GLY:C	1:A:193:THR:HG23	0.45	2.35	9	3
1:A:148:VAL:C	1:A:150:GLU:H	0.45	2.18	6	1
1:A:164:LEU:N	1:A:164:LEU:CD1	0.45	2.79	11	1
1:A:148:VAL:HG21	1:A:183:ASP:H	0.45	1.72	18	1
1:A:222:LEU:O	1:A:224:HIS:N	0.45	2.50	19	1
1:A:164:LEU:HD22	1:A:164:LEU:H	0.45	1.71	2	1
1:A:153:ASP:CB	1:A:166:HIS:CE1	0.45	2.97	3	2
1:A:229:LEU:CD2	1:A:232:PHE:CD2	0.45	3.00	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:PHE:CG	1:A:87:PRO:CD	0.45	3.00	4	1
1:A:86:PHE:CG	1:A:87:PRO:HD3	0.45	2.46	4	1
1:A:119:LYS:O	1:A:229:LEU:HD11	0.45	2.12	20	2
1:A:202:GLU:O	1:A:203:ILE:C	0.45	2.59	17	1
1:A:246:TYR:C	1:A:248:PRO:CD	0.45	2.90	18	1
1:A:222:LEU:CD2	1:A:223:TYR:N	0.45	2.70	14	3
1:A:89:ILE:HG12	1:A:245:LEU:HD13	0.45	1.89	5	1
1:A:201:HIS:O	1:A:205:HIS:HB2	0.45	2.11	5	1
1:A:184:GLU:OE1	1:A:186:TRP:CH2	0.45	2.70	11	1
1:A:180:PHE:CD2	1:A:195:LEU:HD11	0.45	2.47	12	1
1:A:188:LYS:C	1:A:190:THR:H	0.45	2.20	17	1
1:A:89:ILE:CG1	1:A:245:LEU:O	0.45	2.65	7	4
1:A:101:ILE:H	1:A:101:ILE:CD1	0.45	2.22	17	2
1:A:186:TRP:CH2	1:A:193:THR:HB	0.45	2.47	12	4
1:A:199:ALA:HB1	1:A:203:ILE:HD12	0.45	1.89	1	1
1:A:148:VAL:HG23	1:A:151:HIS:H	0.45	1.71	7	2
1:A:129:PRO:HB2	1:A:246:TYR:HA	0.44	1.89	10	1
1:A:163:VAL:O	1:A:164:LEU:HB2	0.44	2.13	20	2
1:A:244:SER:O	1:A:247:GLY:N	0.44	2.50	19	1
1:A:185:GLN:O	1:A:187:THR:HG22	0.44	2.11	8	2
1:A:129:PRO:HB2	1:A:246:TYR:CB	0.44	2.42	7	1
1:A:127:VAL:HG23	1:A:128:THR:H	0.44	1.72	9	2
1:A:164:LEU:CD2	1:A:186:TRP:CH2	0.44	2.99	10	1
1:A:164:LEU:CG	1:A:186:TRP:HH2	0.44	2.26	15	1
1:A:197:LEU:HD12	1:A:223:TYR:HB2	0.44	1.90	3	1
1:A:142:ILE:HD12	1:A:142:ILE:H	0.44	1.72	5	1
1:A:200:ALA:O	1:A:218:LEU:HD23	0.44	2.12	1	1
1:A:144:ILE:HG21	1:A:180:PHE:CD2	0.44	2.47	4	2
1:A:209:LEU:CD1	1:A:235:SER:OG	0.44	2.65	7	1
1:A:104:TYR:O	1:A:113:VAL:HG11	0.44	2.12	18	1
1:A:201:HIS:HB2	4:A:261:ODS:H53	0.44	1.88	1	1
1:A:209:LEU:CD1	1:A:238:ASP:HB2	0.44	2.43	6	1
1:A:143:MET:HE2	1:A:143:MET:N	0.44	2.27	15	2
1:A:209:LEU:C	1:A:209:LEU:HD22	0.44	2.37	16	1
1:A:209:LEU:HD13	1:A:238:ASP:CA	0.44	2.42	7	1
1:A:220:TYR:O	4:A:261:ODS:C5	0.44	2.66	9	1
1:A:107:ASP:OD2	1:A:186:TRP:CD1	0.44	2.70	19	3
1:A:130:LEU:CD1	1:A:245:LEU:HB2	0.44	2.42	12	1
1:A:238:ASP:O	1:A:242:ILE:N	0.44	2.48	18	1
1:A:113:VAL:CG2	1:A:195:LEU:HG	0.44	2.42	1	4
1:A:85:THR:CG2	1:A:245:LEU:HD21	0.44	2.43	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:196:PHE:CE1	1:A:229:LEU:HD23	0.44	2.47	10	1
1:A:105:THR:CG2	1:A:107:ASP:CG	0.44	2.91	11	2
1:A:168:TYR:O	1:A:174:ILE:HD12	0.44	2.13	13	1
1:A:113:VAL:HG22	1:A:195:LEU:CG	0.44	2.42	1	1
1:A:107:ASP:CG	1:A:108:LEU:H	0.44	2.21	12	1
1:A:130:LEU:HD13	1:A:245:LEU:HB2	0.44	1.90	13	1
1:A:143:MET:C	1:A:144:ILE:CD1	0.44	2.90	19	1
1:A:164:LEU:CD2	4:A:261:ODS:HD21	0.43	2.35	11	1
1:A:164:LEU:H	1:A:198:VAL:HG11	0.43	1.73	3	1
1:A:218:LEU:HD11	1:A:232:PHE:CE2	0.43	2.48	7	1
1:A:179:HIS:CE1	1:A:179:HIS:C	0.43	2.96	13	1
1:A:239:ILE:C	1:A:241:GLY:H	0.43	2.22	19	1
1:A:243:GLN:HA	1:A:246:TYR:CD2	0.43	2.48	6	4
1:A:85:THR:HG22	1:A:208:GLY:C	0.43	2.38	4	1
1:A:223:TYR:CD1	1:A:223:TYR:C	0.43	2.96	16	1
1:A:246:TYR:O	1:A:247:GLY:C	0.43	2.61	17	1
1:A:124:TRP:CD1	1:A:203:ILE:HG21	0.43	2.48	8	1
1:A:107:ASP:OD1	1:A:113:VAL:HG21	0.43	2.14	12	1
1:A:130:LEU:HD13	1:A:245:LEU:HD12	0.43	1.90	14	1
1:A:109:PRO:O	1:A:112:ALA:N	0.43	2.51	17	1
1:A:162:ASN:C	1:A:164:LEU:HD13	0.43	2.38	17	1
1:A:85:THR:HG23	1:A:208:GLY:HA2	0.43	1.90	18	1
1:A:153:ASP:OD2	1:A:166:HIS:CD2	0.43	2.71	18	1
1:A:199:ALA:O	1:A:203:ILE:HD12	0.43	2.13	8	1
1:A:103:ASN:CB	1:A:146:PHE:CD1	0.43	3.02	6	1
1:A:142:ILE:HG21	1:A:206:SER:HB2	0.43	1.91	8	3
1:A:124:TRP:CZ3	1:A:218:LEU:HD11	0.43	2.49	15	1
1:A:163:VAL:C	1:A:164:LEU:HD22	0.43	2.37	19	2
1:A:156:PRO:O	1:A:157:PHE:CG	0.43	2.72	1	1
1:A:164:LEU:CG	1:A:186:TRP:CH2	0.43	3.02	15	3
1:A:86:PHE:HA	1:A:244:SER:CB	0.43	2.44	3	1
1:A:164:LEU:HB3	1:A:181:ASP:CB	0.43	2.43	6	1
1:A:164:LEU:CA	1:A:181:ASP:OD1	0.43	2.67	13	1
1:A:146:PHE:CD1	1:A:182:ASP:HB2	0.43	2.48	13	2
1:A:234:LEU:HD12	1:A:234:LEU:N	0.43	2.29	4	3
1:A:99:TYR:CD1	1:A:100:ARG:N	0.43	2.87	5	1
1:A:124:TRP:CH2	1:A:204:GLY:CA	0.43	3.02	16	2
1:A:180:PHE:CE1	1:A:198:VAL:HG22	0.43	2.47	4	1
1:A:99:TYR:CD1	1:A:117:VAL:HG11	0.43	2.48	11	1
1:A:150:GLU:CG	1:A:151:HIS:H	0.43	2.26	17	1
1:A:161:GLY:CA	1:A:193:THR:CG2	0.42	2.97	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:PHE:HA	1:A:244:SER:HB3	0.42	1.91	2	3
1:A:173:GLY:HA3	1:A:177:ASP:CG	0.42	2.39	7	1
1:A:187:THR:OG1	1:A:188:LYS:N	0.42	2.52	15	1
1:A:187:THR:O	1:A:194:ASN:CG	0.42	2.62	18	1
1:A:161:GLY:C	1:A:193:THR:HG23	0.42	2.39	2	2
1:A:129:PRO:HD3	1:A:246:TYR:HA	0.42	1.89	9	1
1:A:235:SER:HB3	1:A:238:ASP:HB2	0.42	1.91	10	2
1:A:164:LEU:CB	1:A:181:ASP:CG	0.42	2.91	15	1
1:A:242:ILE:C	1:A:244:SER:H	0.42	2.19	17	1
1:A:164:LEU:HD23	1:A:193:THR:HG22	0.42	1.90	8	1
1:A:127:VAL:HG11	1:A:234:LEU:CD1	0.42	2.45	10	1
1:A:124:TRP:CH2	1:A:207:LEU:CD1	0.42	3.02	17	1
1:A:117:VAL:HA	1:A:199:ALA:CB	0.42	2.43	2	1
1:A:99:TYR:CE1	1:A:117:VAL:CG1	0.42	3.03	5	1
1:A:222:LEU:C	4:A:261:ODS:HM41	0.42	2.39	10	1
1:A:163:VAL:HG21	4:A:261:ODS:H51	0.42	1.91	16	1
1:A:161:GLY:C	1:A:162:ASN:HD22	0.42	2.23	18	1
1:A:101:ILE:N	1:A:101:ILE:CD1	0.42	2.82	20	1
1:A:185:GLN:O	1:A:186:TRP:C	0.42	2.63	20	1
1:A:103:ASN:HB3	1:A:146:PHE:CE2	0.42	2.49	1	1
1:A:155:TYR:HB2	1:A:156:PRO:HD3	0.42	1.91	7	2
1:A:105:THR:CB	1:A:146:PHE:CD2	0.42	3.02	9	1
1:A:204:GLY:CA	1:A:209:LEU:HD23	0.42	2.44	14	1
1:A:85:THR:CG2	1:A:86:PHE:N	0.42	2.83	3	1
1:A:99:TYR:CD2	1:A:142:ILE:HD13	0.42	2.50	5	1
1:A:229:LEU:HD23	1:A:232:PHE:CD2	0.42	2.50	16	1
1:A:164:LEU:HG	1:A:198:VAL:HG13	0.42	1.92	2	1
1:A:194:ASN:CG	1:A:223:TYR:CZ	0.42	2.98	20	2
1:A:226:LEU:HD23	1:A:227:THR:HG22	0.42	1.92	3	1
1:A:124:TRP:CZ3	1:A:234:LEU:HD22	0.42	2.50	6	1
1:A:104:TYR:CE1	1:A:110:LYS:HB2	0.42	2.49	19	1
1:A:148:VAL:CG2	1:A:183:ASP:CB	0.42	2.98	14	3
1:A:99:TYR:O	1:A:134:ARG:HA	0.42	2.15	5	1
1:A:123:VAL:CG2	1:A:229:LEU:HD13	0.42	2.44	8	1
1:A:209:LEU:HB2	1:A:238:ASP:CA	0.42	2.45	10	1
1:A:217:ALA:C	1:A:219:MET:N	0.42	2.77	10	2
1:A:242:ILE:HA	1:A:245:LEU:HB2	0.42	1.91	17	1
1:A:200:ALA:HB1	1:A:218:LEU:HG	0.42	1.92	9	2
1:A:99:TYR:CD1	1:A:121:LEU:HG	0.42	2.49	4	1
1:A:89:ILE:HG12	1:A:245:LEU:HD22	0.42	1.91	5	1
1:A:243:GLN:HA	1:A:246:TYR:CE2	0.42	2.50	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:ARG:H	1:A:149:ARG:CD	0.42	2.28	15	1
1:A:167:ALA:O	1:A:168:TYR:CE2	0.42	2.73	18	1
1:A:194:ASN:O	1:A:223:TYR:CE2	0.42	2.72	1	1
1:A:98:THR:CG2	1:A:99:TYR:N	0.42	2.83	5	1
1:A:98:THR:HG21	1:A:140:ALA:CB	0.42	2.45	5	1
1:A:186:TRP:C	1:A:187:THR:HG22	0.42	2.39	11	1
1:A:99:TYR:CE1	1:A:134:ARG:N	0.42	2.87	17	1
1:A:244:SER:O	1:A:245:LEU:C	0.42	2.63	18	1
1:A:163:VAL:CG2	4:A:261:ODS:H1	0.41	2.27	2	2
1:A:164:LEU:HD22	1:A:186:TRP:CZ3	0.41	2.50	10	1
1:A:194:ASN:CB	1:A:223:TYR:CE1	0.41	3.03	10	1
1:A:218:LEU:HD13	1:A:234:LEU:CD2	0.41	2.43	10	1
1:A:180:PHE:CE2	1:A:198:VAL:HG23	0.41	2.50	17	1
1:A:227:THR:HG23	1:A:228:ASP:N	0.41	2.30	17	1
1:A:197:LEU:HD13	1:A:223:TYR:HA	0.41	1.92	12	2
1:A:144:ILE:HG12	1:A:180:PHE:CZ	0.41	2.50	4	1
1:A:151:HIS:CE1	1:A:153:ASP:OD2	0.41	2.72	10	1
1:A:209:LEU:N	1:A:209:LEU:CD2	0.41	2.82	11	1
1:A:201:HIS:CE1	1:A:205:HIS:CE1	0.41	3.08	15	1
1:A:147:ALA:C	1:A:148:VAL:HG22	0.41	2.40	16	1
1:A:170:PRO:O	1:A:171:GLY:C	0.41	2.63	16	2
1:A:194:ASN:HB3	1:A:223:TYR:CE2	0.41	2.50	16	1
1:A:128:THR:C	1:A:130:LEU:H	0.41	2.23	17	1
1:A:149:ARG:CG	1:A:149:ARG:O	0.41	2.68	17	1
1:A:222:LEU:C	1:A:222:LEU:CD1	0.41	2.94	19	1
1:A:148:VAL:HB	1:A:157:PHE:N	0.41	2.30	20	1
1:A:196:PHE:CZ	1:A:229:LEU:HB2	0.41	2.51	13	1
1:A:97:LEU:HD13	1:A:130:LEU:HD21	0.41	1.90	14	1
1:A:124:TRP:CZ3	1:A:229:LEU:CD2	0.41	3.04	15	1
1:A:144:ILE:HD12	1:A:178:ALA:HB3	0.41	1.90	5	1
1:A:232:PHE:O	1:A:233:ARG:C	0.41	2.63	13	2
1:A:184:GLU:OE1	1:A:186:TRP:CZ2	0.41	2.74	11	1
1:A:198:VAL:O	1:A:199:ALA:C	0.41	2.62	17	1
1:A:207:LEU:O	1:A:207:LEU:CG	0.41	2.65	17	1
1:A:199:ALA:O	1:A:203:ILE:N	0.41	2.52	2	1
1:A:218:LEU:HD11	1:A:232:PHE:CZ	0.41	2.51	10	1
1:A:197:LEU:HB3	1:A:223:TYR:CE2	0.41	2.51	16	1
1:A:148:VAL:CG2	1:A:149:ARG:N	0.41	2.83	17	1
1:A:195:LEU:O	1:A:198:VAL:CG2	0.41	2.69	1	1
1:A:192:GLY:O	1:A:193:THR:HG23	0.41	2.16	5	1
1:A:197:LEU:HD22	4:A:261:ODS:H51	0.41	1.92	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:ASN:CB	1:A:146:PHE:CE1	0.41	3.03	8	1
1:A:124:TRP:CZ2	1:A:209:LEU:HD21	0.41	2.50	12	1
1:A:191:THR:HA	1:A:223:TYR:CE2	0.41	2.51	13	1
1:A:178:ALA:CB	1:A:202:GLU:CD	0.41	2.94	14	1
1:A:173:GLY:O	1:A:175:ASN:N	0.41	2.53	20	1
1:A:105:THR:N	1:A:146:PHE:CD2	0.41	2.89	1	1
1:A:150:GLU:HA	1:A:157:PHE:CB	0.41	2.46	1	1
4:A:261:ODS:C1	4:A:261:ODS:H52	0.41	2.46	2	1
1:A:120:ALA:O	1:A:124:TRP:CD2	0.41	2.74	4	1
1:A:190:THR:O	1:A:190:THR:CG2	0.41	2.68	7	2
1:A:229:LEU:O	1:A:229:LEU:HD23	0.41	2.15	7	1
1:A:184:GLU:HG2	1:A:193:THR:CG2	0.41	2.45	12	2
1:A:148:VAL:HG13	1:A:181:ASP:OD1	0.41	2.16	9	1
1:A:235:SER:HB3	1:A:238:ASP:CB	0.41	2.46	9	2
1:A:164:LEU:CD2	1:A:198:VAL:HG23	0.41	2.41	12	1
1:A:130:LEU:HD13	1:A:245:LEU:CB	0.41	2.46	13	1
4:A:261:ODS:H52	4:A:261:ODS:H	0.41	1.75	16	1
1:A:129:PRO:HB2	1:A:246:TYR:HB2	0.41	1.91	17	1
1:A:148:VAL:CG2	1:A:183:ASP:N	0.41	2.84	18	1
1:A:166:HIS:H	1:A:179:HIS:CE1	0.41	2.33	18	1
1:A:174:ILE:C	1:A:174:ILE:CD1	0.41	2.93	19	1
1:A:167:ALA:C	1:A:168:TYR:CD1	0.41	2.99	20	1
1:A:191:THR:HG23	1:A:192:GLY:O	0.41	2.16	20	1
1:A:209:LEU:HD22	1:A:242:ILE:CD1	0.41	2.46	5	1
1:A:184:GLU:N	1:A:184:GLU:OE1	0.41	2.54	7	1
1:A:124:TRP:O	1:A:128:THR:HG22	0.41	2.16	9	1
1:A:169:ALA:HB3	1:A:206:SER:CB	0.41	2.46	18	1
1:A:148:VAL:HG23	1:A:151:HIS:HB3	0.40	1.92	3	1
1:A:144:ILE:HG22	1:A:145:SER:H	0.40	1.76	15	2
1:A:144:ILE:CG2	1:A:180:PHE:CD1	0.40	3.04	14	1
1:A:157:PHE:C	1:A:159:GLY:H	0.40	2.25	15	1
1:A:233:ARG:O	1:A:234:LEU:O	0.40	2.39	18	1
1:A:174:ILE:O	1:A:174:ILE:CD1	0.40	2.68	19	1
1:A:222:LEU:HD11	4:A:261:ODS:CG1	0.40	2.45	4	1
1:A:117:VAL:HG22	1:A:199:ALA:CB	0.40	2.47	6	1
1:A:103:ASN:CG	1:A:104:TYR:N	0.40	2.79	7	1
1:A:86:PHE:HB2	1:A:244:SER:HB3	0.40	1.93	8	1
1:A:220:TYR:CD1	1:A:221:PRO:HD2	0.40	2.50	8	1
1:A:161:GLY:N	1:A:193:THR:HG21	0.40	2.31	9	1
1:A:195:LEU:HA	1:A:198:VAL:CG2	0.40	2.47	10	1
1:A:124:TRP:CH2	1:A:242:ILE:HD11	0.40	2.51	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:207:LEU:O	1:A:207:LEU:CD1	0.40	2.69	17	1
1:A:91:LYS:O	1:A:92:TRP:CE3	0.40	2.74	19	1
1:A:130:LEU:HD13	1:A:245:LEU:HB3	0.40	1.92	1	1
1:A:195:LEU:O	1:A:195:LEU:HD13	0.40	2.17	4	1
1:A:123:VAL:N	1:A:229:LEU:HD11	0.40	2.31	8	1
1:A:161:GLY:O	1:A:162:ASN:CB	0.40	2.69	6	1
1:A:144:ILE:HG23	1:A:178:ALA:HB3	0.40	1.94	11	1
1:A:238:ASP:O	1:A:239:ILE:C	0.40	2.64	17	1
1:A:169:ALA:C	1:A:171:GLY:N	0.40	2.75	18	1
1:A:186:TRP:C	1:A:187:THR:CG2	0.40	2.94	18	1
1:A:178:ALA:HB1	1:A:180:PHE:HE1	0.40	1.77	1	1
1:A:226:LEU:HD13	1:A:226:LEU:H	0.40	1.75	3	1
1:A:127:VAL:HB	1:A:242:ILE:HG21	0.40	1.92	10	1
1:A:147:ALA:O	1:A:148:VAL:CG1	0.40	2.63	10	1
1:A:164:LEU:CD1	1:A:186:TRP:HH2	0.40	2.30	15	1
1:A:154:PHE:CD1	1:A:168:TYR:CD1	0.40	3.09	16	1
1:A:245:LEU:C	1:A:247:GLY:H	0.40	2.25	17	1
1:A:181:ASP:HB3	1:A:184:GLU:OE1	0.40	2.16	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	164/174 (94%)	86±6 (53±3%)	43±6 (26±3%)	34±4 (21±3%)	0	2
All	All	3280/3480 (94%)	1729 (53%)	869 (26%)	682 (21%)	0	2

All 97 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	246	TYR	20
1	A	117	VAL	19
1	A	118	GLU	19
1	A	129	PRO	19

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Mol	Chain	Res	Type	Models (Total)
1	A	162	ASN	19
1	A	175	ASN	19
1	A	211	HIS	19
1	A	86	PHE	18
1	A	148	VAL	18
1	A	191	THR	18
1	A	181	ASP	17
1	A	186	TRP	16
1	A	221	PRO	16
1	A	104	TYR	16
1	A	169	ALA	15
1	A	226	LEU	15
1	A	90	PRO	14
1	A	150	GLU	14
1	A	208	GLY	14
1	A	184	GLU	14
1	A	164	LEU	13
1	A	157	PHE	13
1	A	149	ARG	11
1	A	216	GLU	11
1	A	89	ILE	10
1	A	223	TYR	10
1	A	234	LEU	10
1	A	156	PRO	10
1	A	225	SER	10
1	A	247	GLY	10
1	A	163	VAL	9
1	A	170	PRO	9
1	A	155	TYR	9
1	A	241	GLY	9
1	A	135	LEU	8
1	A	224	HIS	8
1	A	233	ARG	8
1	A	171	GLY	7
1	A	92	TRP	7
1	A	85	THR	6
1	A	138	GLY	6
1	A	231	ARG	6
1	A	235	SER	6
1	A	102	VAL	5
1	A	147	ALA	5
1	A	84	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	154	PHE	5
1	A	210	PHE	5
1	A	227	THR	5
1	A	132	PHE	5
1	A	144	ILE	5
1	A	145	SER	5
1	A	206	SER	5
1	A	190	THR	4
1	A	215	THR	4
1	A	153	ASP	4
1	A	228	ASP	4
1	A	137	GLU	3
1	A	93	ARG	3
1	A	87	PRO	3
1	A	188	LYS	3
1	A	127	VAL	3
1	A	217	ALA	3
1	A	134	ARG	3
1	A	172	PRO	3
1	A	124	TRP	3
1	A	229	LEU	3
1	A	222	LEU	2
1	A	139	GLU	2
1	A	196	PHE	2
1	A	133	SER	2
1	A	240	ASN	2
1	A	152	GLY	2
1	A	207	LEU	2
1	A	103	ASN	2
1	A	159	GLY	2
1	A	187	THR	2
1	A	105	THR	2
1	A	88	GLY	1
1	A	141	ASP	1
1	A	189	ASP	1
1	A	230	THR	1
1	A	193	THR	1
1	A	220	TYR	1
1	A	209	LEU	1
1	A	212	SER	1
1	A	108	LEU	1
1	A	120	ALA	1

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Mol	Chain	Res	Type	Models (Total)
1	A	151	HIS	1
1	A	213	ALA	1
1	A	106	PRO	1
1	A	121	LEU	1
1	A	136	TYR	1
1	A	140	ALA	1
1	A	174	ILE	1
1	A	214	ASN	1
1	A	232	PHE	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	140/148 (95%)	104±5 (75±3%)	36±5 (25±3%)	2	24
All	All	2800/2960 (95%)	2088 (75%)	712 (25%)	2	24

All 104 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	164	LEU	20
1	A	184	GLU	20
1	A	195	LEU	20
1	A	222	LEU	20
1	A	101	ILE	19
1	A	129	PRO	19
1	A	142	ILE	19
1	A	207	LEU	18
1	A	229	LEU	18
1	A	95	THR	17
1	A	143	MET	17
1	A	179	HIS	17
1	A	226	LEU	17
1	A	174	ILE	16
1	A	197	LEU	16
1	A	121	LEU	15

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Mol	Chain	Res	Type	Models (Total)
1	A	242	ILE	15
1	A	125	GLU	13
1	A	209	LEU	13
1	A	163	VAL	13
1	A	149	ARG	13
1	A	85	THR	12
1	A	187	THR	12
1	A	205	HIS	12
1	A	135	LEU	11
1	A	158	ASP	10
1	A	191	THR	10
1	A	144	ILE	10
1	A	238	ASP	10
1	A	246	TYR	10
1	A	239	ILE	9
1	A	92	TRP	9
1	A	198	VAL	9
1	A	124	TRP	8
1	A	166	HIS	8
1	A	221	PRO	8
1	A	151	HIS	8
1	A	104	TYR	7
1	A	128	THR	7
1	A	218	LEU	7
1	A	245	LEU	7
1	A	98	THR	7
1	A	113	VAL	6
1	A	227	THR	6
1	A	156	PRO	6
1	A	202	GLU	6
1	A	90	PRO	5
1	A	97	LEU	5
1	A	105	THR	5
1	A	182	ASP	5
1	A	234	LEU	5
1	A	89	ILE	5
1	A	168	TYR	5
1	A	175	ASN	5
1	A	181	ASP	5
1	A	203	ILE	5
1	A	83	PHE	5
1	A	93	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	136	TYR	4
1	A	244	SER	4
1	A	157	PHE	4
1	A	110	LYS	4
1	A	130	LEU	3
1	A	131	THR	3
1	A	194	ASN	3
1	A	232	PHE	3
1	A	86	PHE	3
1	A	190	THR	3
1	A	148	VAL	3
1	A	243	GLN	2
1	A	154	PHE	2
1	A	84	ARG	2
1	A	146	PHE	2
1	A	177	ASP	2
1	A	220	TYR	2
1	A	224	HIS	2
1	A	193	THR	2
1	A	139	GLU	2
1	A	219	MET	2
1	A	212	SER	2
1	A	216	GLU	1
1	A	127	VAL	1
1	A	206	SER	1
1	A	133	SER	1
1	A	132	PHE	1
1	A	108	LEU	1
1	A	94	LYS	1
1	A	102	VAL	1
1	A	141	ASP	1
1	A	150	GLU	1
1	A	87	PRO	1
1	A	111	ASP	1
1	A	153	ASP	1
1	A	188	LYS	1
1	A	210	PHE	1
1	A	214	ASN	1
1	A	155	TYR	1
1	A	201	HIS	1
1	A	236	GLN	1
1	A	106	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	A	91	LYS	1
1	A	180	PHE	1
1	A	189	ASP	1
1	A	228	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	0DS	A	261	2	32,32,32	1.46±0.24	2±2 (6±5%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	0DS	A	261	2	40,42,42	1.38±0.42	6±4 (14±10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	0DS	A	261	2	-	0±0,38,38,38	0±0,1,1,1

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
4	A	261	0DS	O3-N3	9.36	1.17	1.40	17	20
4	A	261	0DS	C2-C1	6.69	1.63	1.51	18	3
4	A	261	0DS	C21-N3	3.62	1.36	1.32	17	5
4	A	261	0DS	C11-C21	3.61	1.59	1.51	19	1
4	A	261	0DS	CA1-C6	3.08	1.47	1.52	20	1
4	A	261	0DS	CZ-CE2	2.59	1.43	1.38	18	1
4	A	261	0DS	C6-N2	2.41	1.38	1.32	18	1
4	A	261	0DS	CD11-CG1	2.41	1.43	1.38	19	1
4	A	261	0DS	CA-C	2.38	1.58	1.52	19	2
4	A	261	0DS	CA-N	2.36	1.50	1.45	17	1
4	A	261	0DS	CE1-CD11	2.19	1.42	1.38	18	1
4	A	261	0DS	O1-C1	2.17	1.19	1.23	20	1
4	A	261	0DS	CB1-CA1	2.12	1.49	1.54	20	1
4	A	261	0DS	O21-C21	2.11	1.27	1.23	17	1
4	A	261	0DS	C-N1	2.08	1.38	1.34	18	1
4	A	261	0DS	CD21-CG1	2.03	1.42	1.38	20	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
4	A	261	0DS	O3-N3-C21	5.77	111.26	119.79	17	6
4	A	261	0DS	CA-N-C1	5.76	134.02	121.65	11	9
4	A	261	0DS	C11-C2-C1	5.68	117.80	109.71	19	11
4	A	261	0DS	O21-C21-N3	4.86	117.31	123.27	17	1
4	A	261	0DS	CE2-CD21-CG1	4.85	113.80	120.61	18	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	261	0DS	O1-C1-C2	4.40	115.39	122.19	14	7
4	A	261	0DS	C-CA-N	4.24	122.57	111.11	11	4
4	A	261	0DS	CZ-CE1-CD11	4.12	115.16	120.24	18	2
4	A	261	0DS	CG-CB-CA	4.11	104.36	115.40	11	3
4	A	261	0DS	C5-C4-C3	3.96	125.34	111.08	20	2
4	A	261	0DS	CZ-CE2-CD21	3.94	125.10	120.24	18	2
4	A	261	0DS	O1-C1-N	3.88	116.01	122.96	17	2
4	A	261	0DS	CB1-CG1-CD11	3.85	128.07	120.90	19	3
4	A	261	0DS	CA1-N1-C	3.75	129.71	121.65	20	6
4	A	261	0DS	C2-C1-N	3.72	122.59	116.19	14	1
4	A	261	0DS	C2-C11-C21	3.67	119.53	112.33	13	12
4	A	261	0DS	C2-C3-C4	3.64	108.03	115.60	6	9
4	A	261	0DS	CB-CA-N	3.54	102.59	110.58	11	5
4	A	261	0DS	CG1-CB1-CA1	3.35	122.27	113.36	9	1
4	A	261	0DS	O2-C6-CA1	3.29	115.33	120.22	18	1
4	A	261	0DS	C11-C21-N3	3.14	119.90	115.14	3	3
4	A	261	0DS	CB1-CG1-CD21	3.09	115.15	120.90	17	2
4	A	261	0DS	CD1-CG-CB	3.06	100.07	111.08	20	1
4	A	261	0DS	CE1-CD11-CG1	2.96	116.45	120.61	19	2
4	A	261	0DS	CB-CA-C	2.80	103.96	110.59	5	2
4	A	261	0DS	CA-C-N1	2.68	122.35	116.63	19	2
4	A	261	0DS	CD2-CG-CD1	2.46	121.49	110.53	5	3
4	A	261	0DS	O21-C21-C11	2.40	118.02	121.54	18	4
4	A	261	0DS	O-C-N1	2.26	118.92	122.96	18	1
4	A	261	0DS	C6-CA1-N1	2.18	115.65	110.30	17	1
4	A	261	0DS	CD2-CG-CB	2.17	103.28	111.08	5	2
4	A	261	0DS	CE2-CZ-CE1	2.09	117.01	119.87	18	1

All unique chiral outliers are listed below.

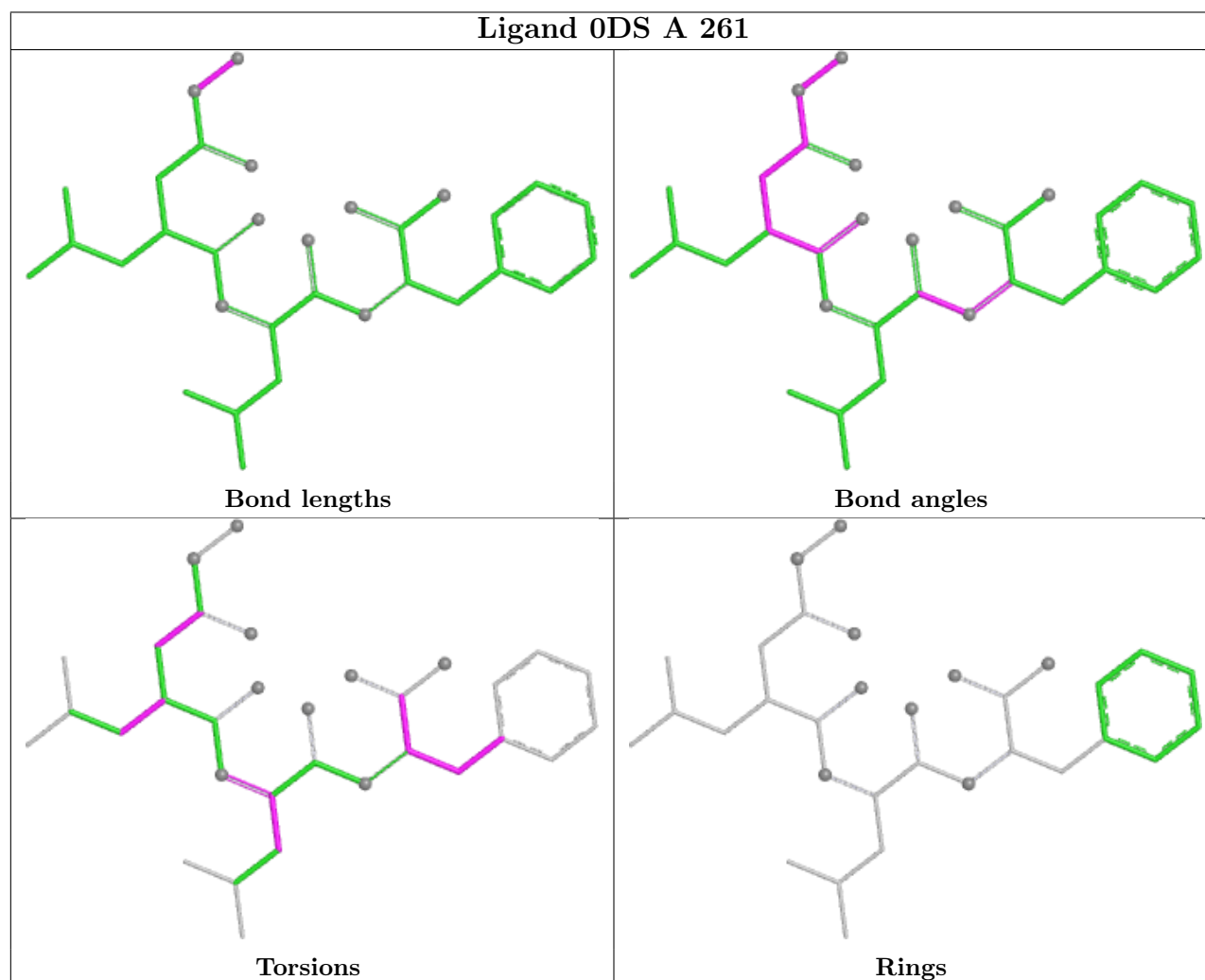
Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	261	0DS	C2	2

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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