Full wwPDB NMR Structure Validation Report (i)

Sep 17, 2020 – 07:02 PM EDT

PDB ID	:	1UMS
Title	:	STROMELYSIN-1 CATALYTIC DOMAIN WITH HYDROPHOBIC INHIBITOR BOUND, PH 7.0, 32OC, 20 MM CACL2, 15% ACETONITRILE; NMR ENSEMBLE OF 20 STRUCTURES
Authors	:	Van Doren, S.R.; Kurochkin, A.V.; Hu, W.; Zuiderweg, E.R.P.
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 (i) symbol.

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

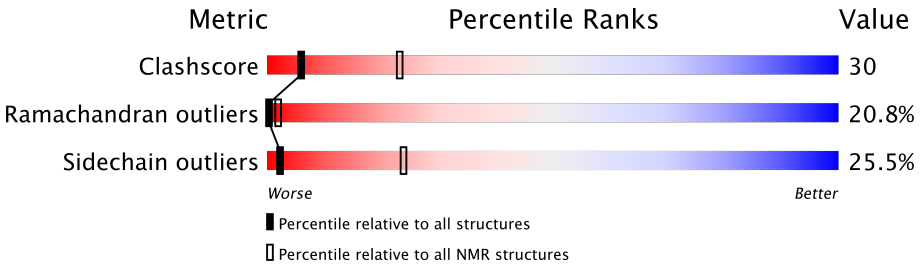
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.14.4
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	174	32% 39% 19% 6% 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)	0.63	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

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
			Total	C	H	N	O	S	
1	A	166	2572	851	1248	221	250	2	0

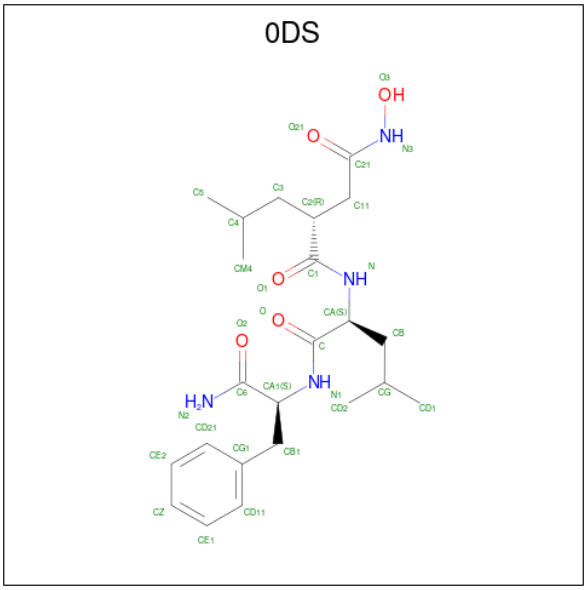
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
3	A	1	1	1

- Molecule 4 is N-{(2R)-2-[2-(hydroxyamino)-2-oxoethyl]-4-methylpentanoyl}-L-leucyl-L-phenylalaninamide (three-letter code: 0DS) (formula: $C_{23}H_{36}N_4O_5$).



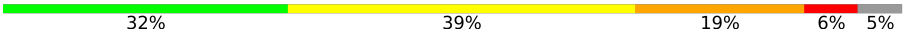
Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
4	A	1	68	23	36	4	5

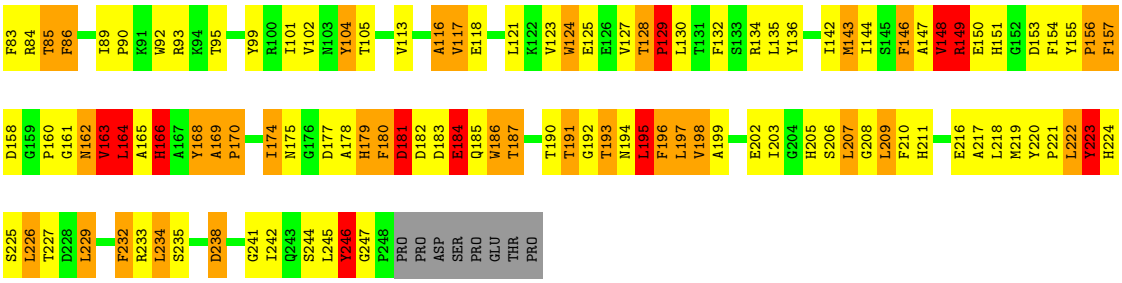
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: STROMELYSIN-1

Chain A: 

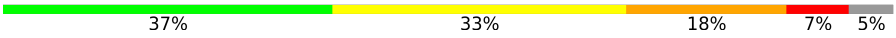


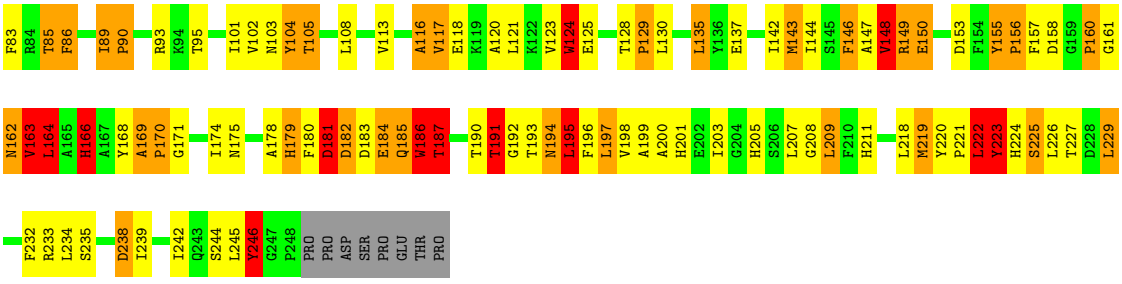
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: STROMELYSIN-1

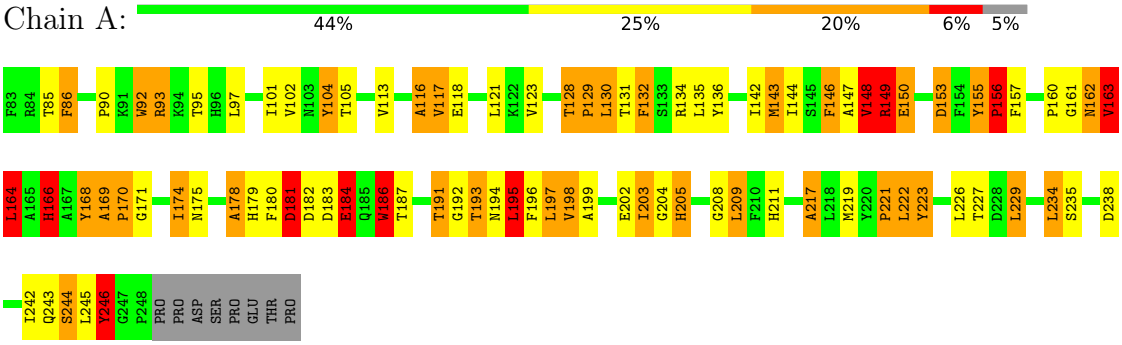
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: STROMELYSIN-1

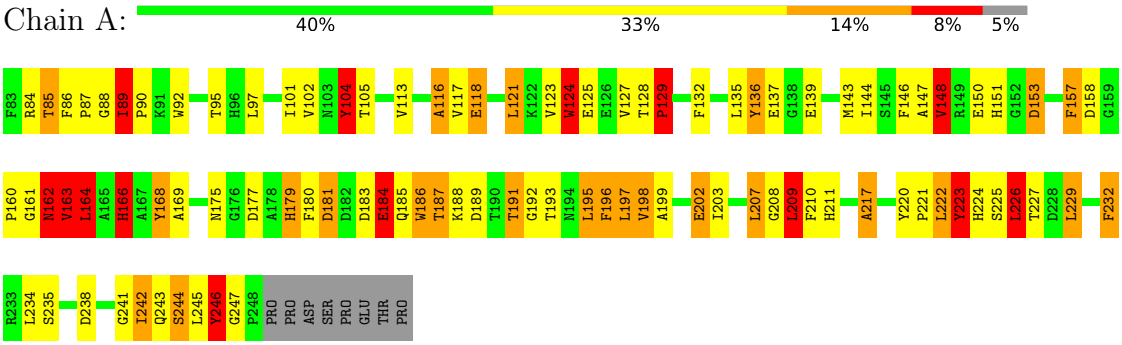
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: STROMELYSIN-1

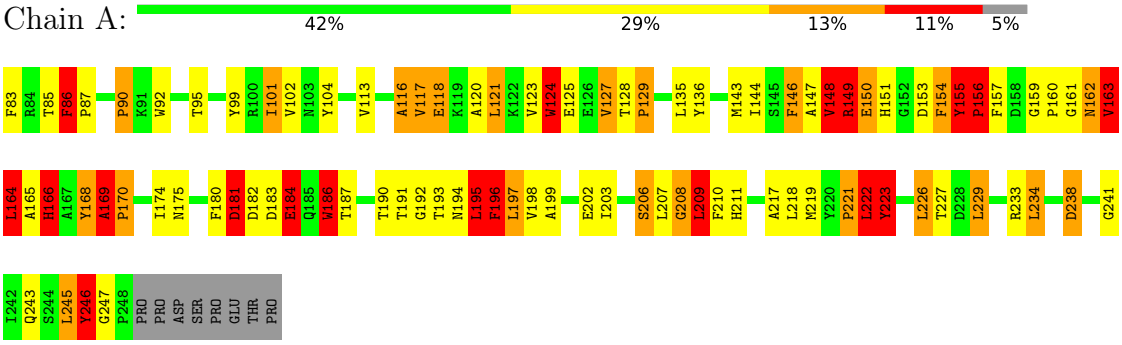
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: STROMELYSIN-1

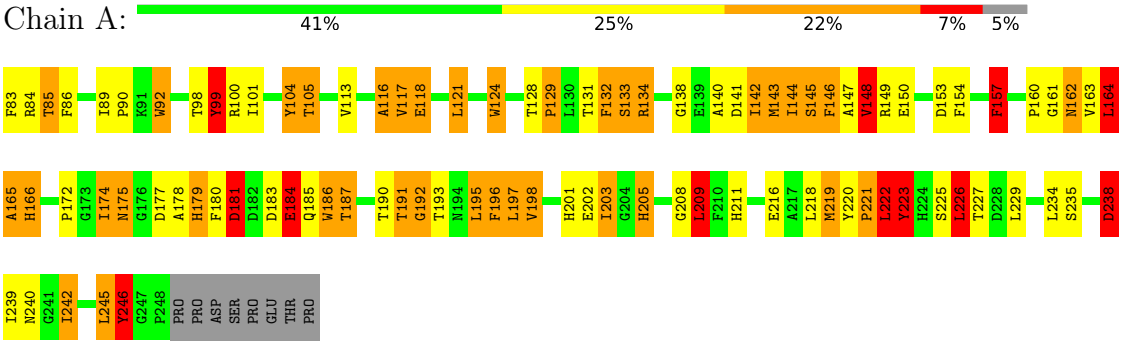
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: STROMELYSIN-1

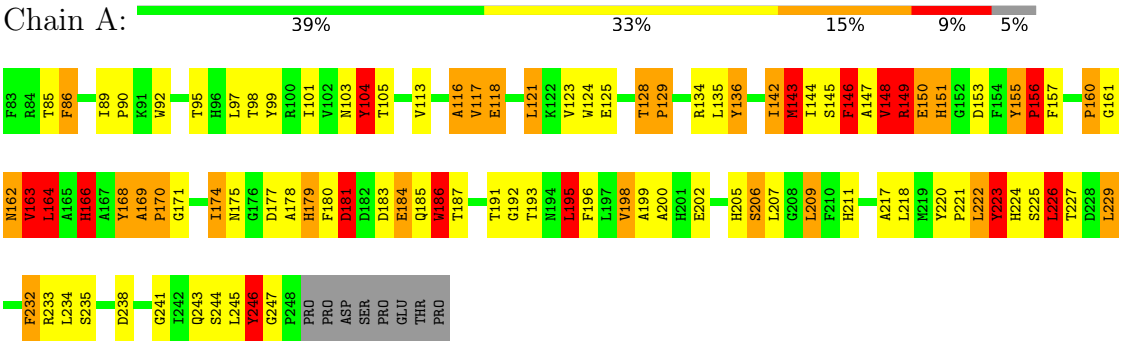
Chain A:



4.2.6 Score per residue for model 6 (medoid)

• Molecule 1: STROMELYSIN-1

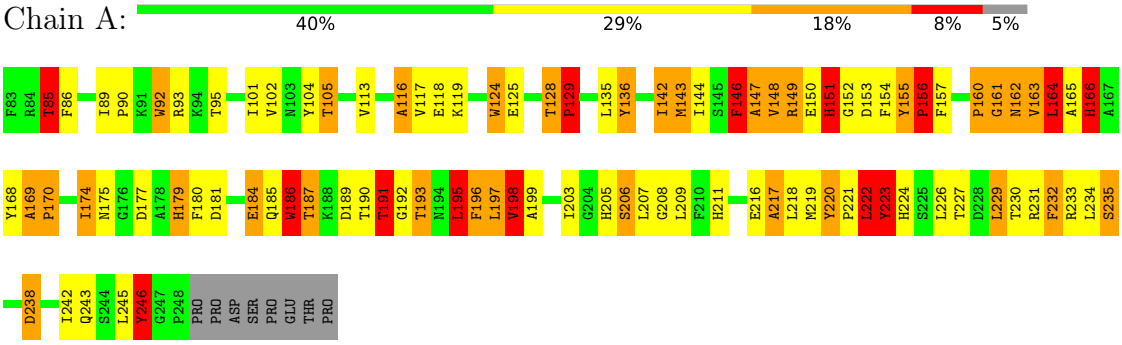
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: STROMELYSIN-1

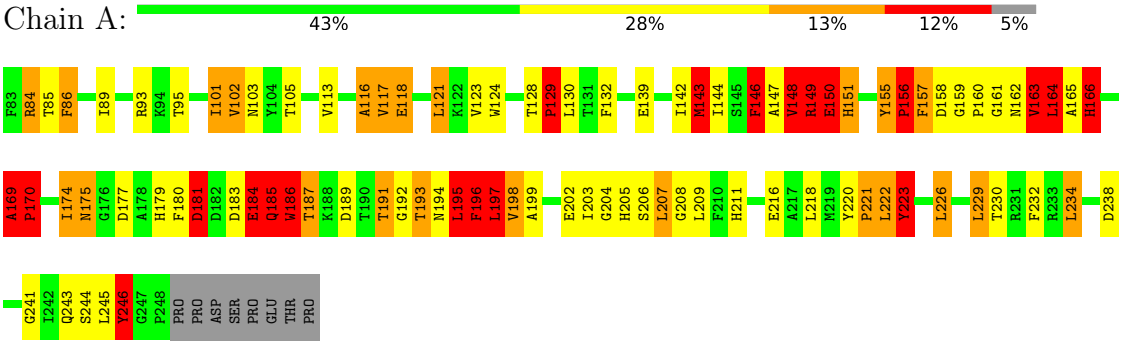
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: STROMELYSIN-1

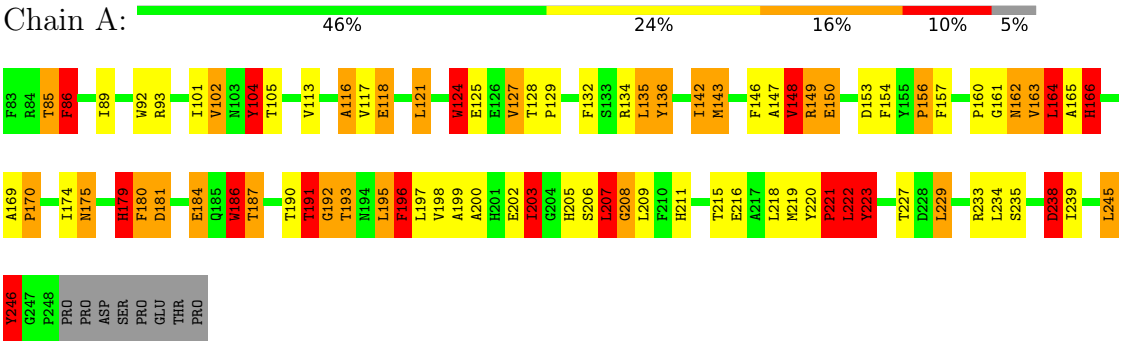
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: STROMELYSIN-1

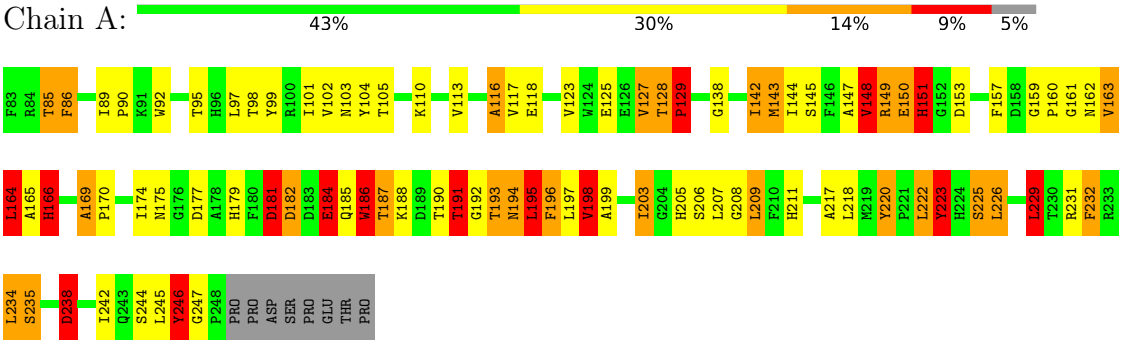
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: STROMELYSIN-1

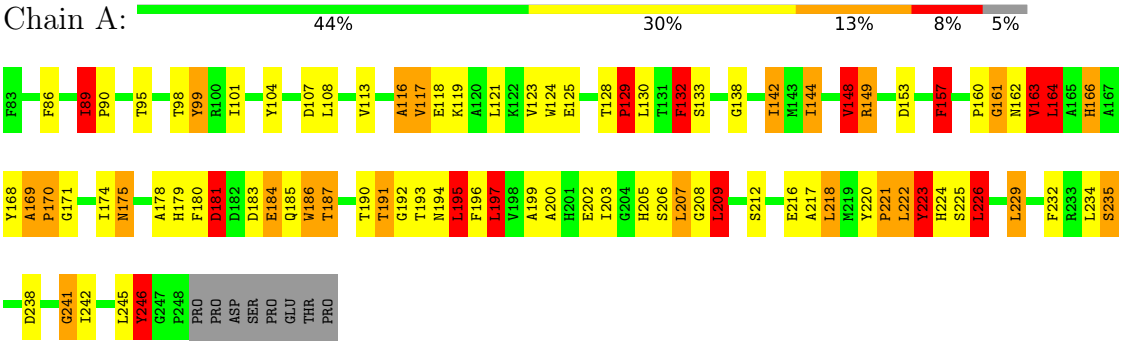
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: STROMELYSIN-1

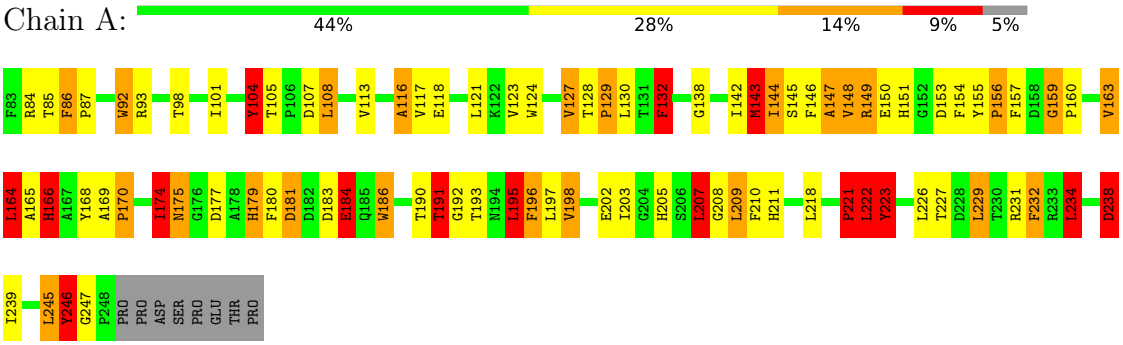
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: STROMELYSIN-1

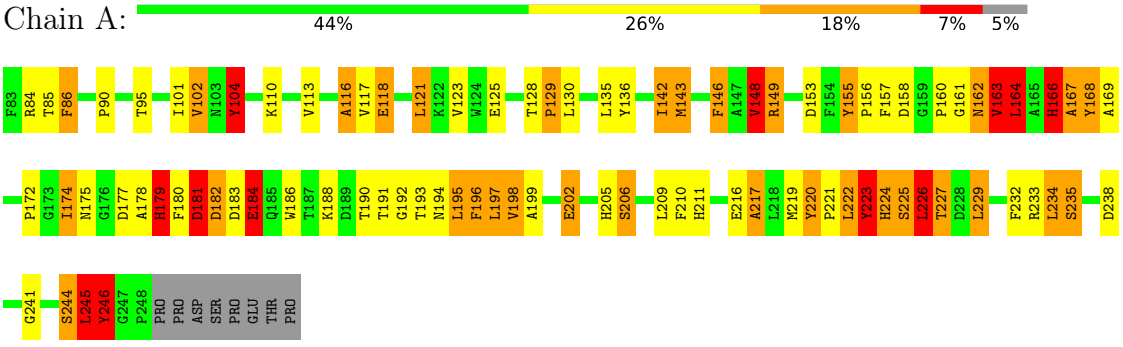
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: STROMELYSIN-1

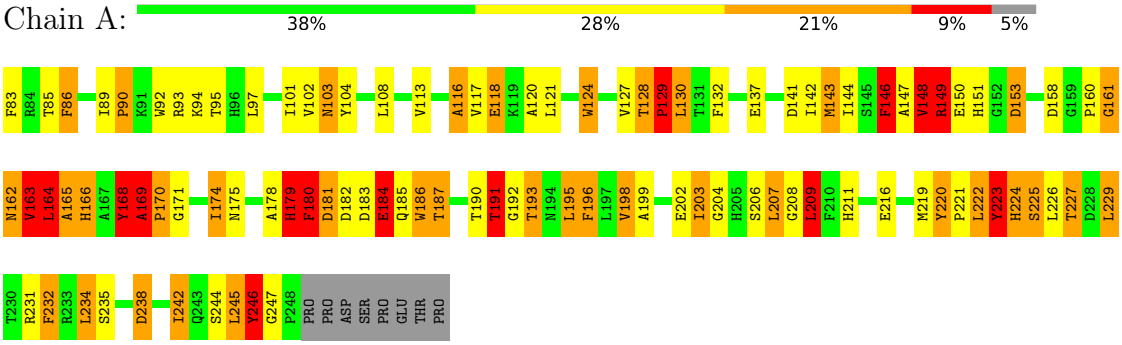
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: STROMELYSIN-1

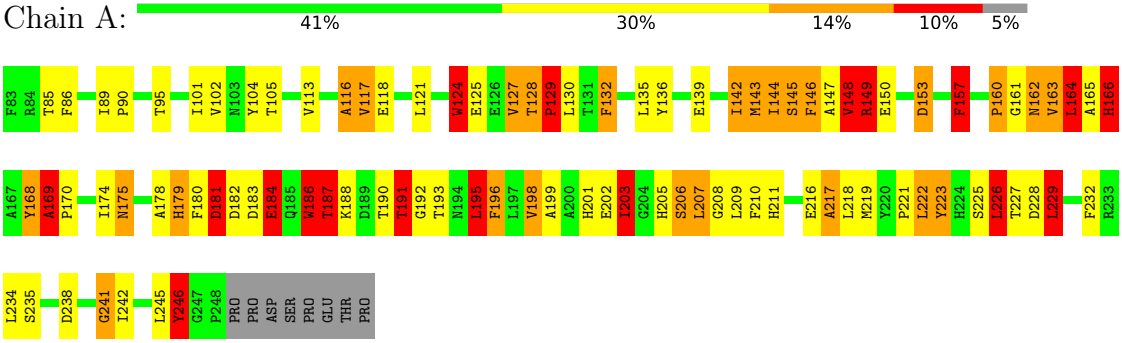
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: STROMELYSIN-1

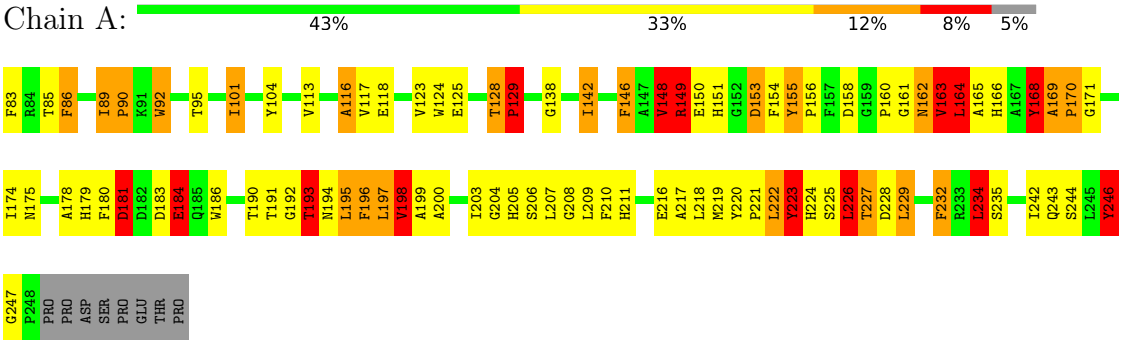
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: STROMELYSIN-1

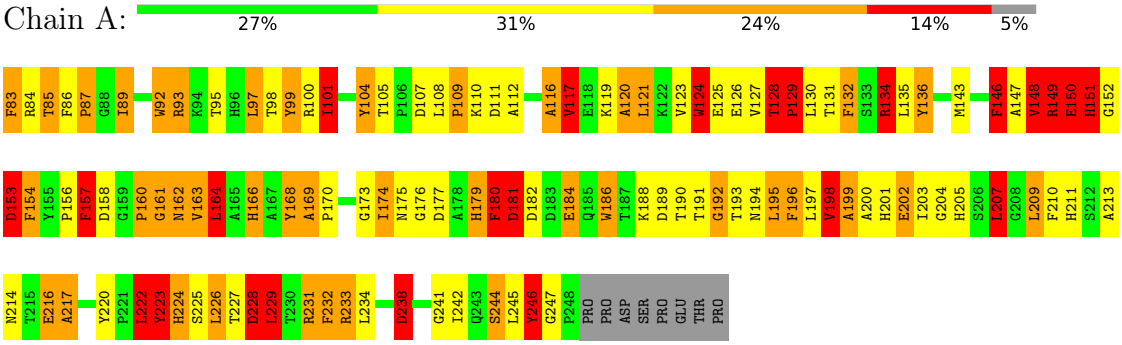
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: STROMELYSIN-1

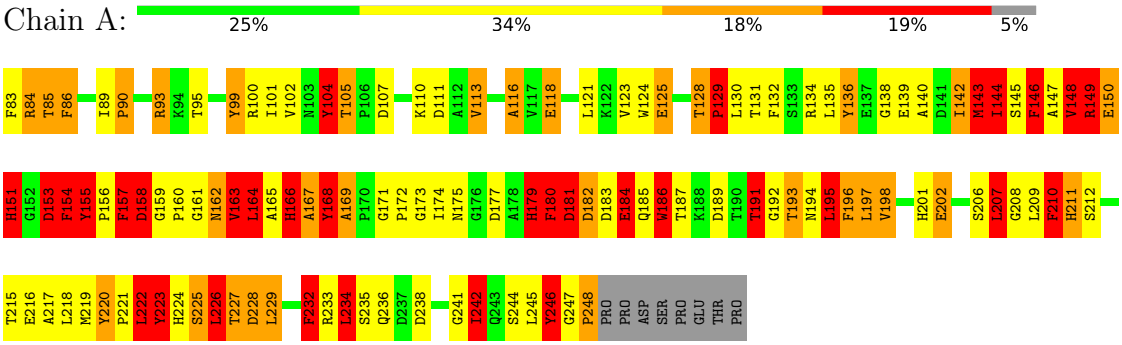
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: STROMELYSIN-1

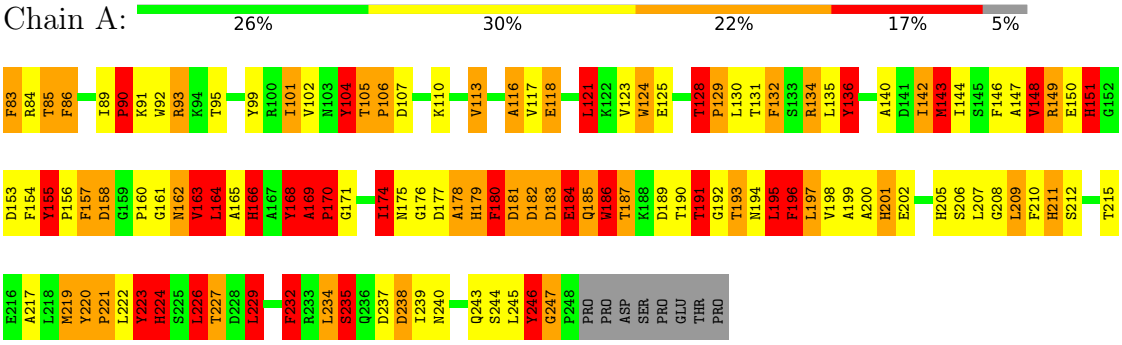
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: STROMELYSIN-1

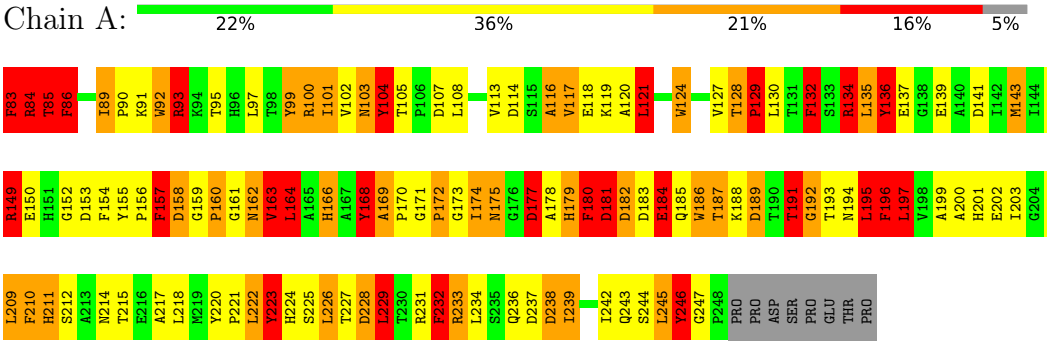
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: STROMELYSIN-1

Chain A:



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. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 0DS, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.93±0.31	2±3/1366 (0.1± 0.2%)	1.95±0.32	49±28/1864 (2.6± 1.5%)
All	All	0.98	30/27320 (0.1%)	1.98	971/37280 (2.6%)

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	244	SER	CA-CB	-7.29	1.42	1.52	18	1
1	A	159	GLY	CA-C	6.71	1.62	1.51	18	1
1	A	155	TYR	CE1-CZ	6.54	1.47	1.38	19	1
1	A	212	SER	CB-OG	-6.42	1.33	1.42	19	1
1	A	156	PRO	N-CD	-6.31	1.39	1.47	18	1
1	A	235	SER	CA-CB	-6.28	1.43	1.52	19	1
1	A	161	GLY	N-CA	-5.76	1.37	1.46	20	3
1	A	186	TRP	CD2-CE3	-5.74	1.31	1.40	20	1
1	A	99	TYR	CZ-OH	-5.73	1.28	1.37	18	1
1	A	144	ILE	N-CA	-5.64	1.35	1.46	18	1
1	A	206	SER	CA-CB	-5.64	1.44	1.52	19	1
1	A	176	GLY	N-CA	-5.63	1.37	1.46	17	1
1	A	201	HIS	CB-CG	5.49	1.59	1.50	19	1
1	A	220	TYR	CE2-CZ	5.43	1.45	1.38	17	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	211	HIS	CB-CG	5.41	1.59	1.50	18	1
1	A	223	TYR	CG-CD1	5.39	1.46	1.39	18	1
1	A	128	THR	N-CA	-5.33	1.35	1.46	17	1
1	A	198	VAL	CA-CB	-5.32	1.43	1.54	17	1
1	A	162	ASN	N-CA	-5.30	1.35	1.46	19	1
1	A	206	SER	CB-OG	-5.24	1.35	1.42	19	1
1	A	238	ASP	N-CA	-5.22	1.35	1.46	20	1
1	A	145	SER	CB-OG	5.22	1.49	1.42	20	1
1	A	134	ARG	CZ-NH2	5.21	1.39	1.33	19	1
1	A	149	ARG	CZ-NH2	-5.21	1.26	1.33	19	1
1	A	137	GLU	CD-OE2	5.13	1.31	1.25	20	1
1	A	196	PHE	CB-CG	5.05	1.59	1.51	20	1
1	A	180	PHE	CG-CD2	5.04	1.46	1.38	20	1
1	A	199	ALA	N-CA	-5.01	1.36	1.46	17	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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	231	ARG	NE-CZ-NH2	-18.37	111.11	120.30	17	1
1	A	246	TYR	CB-CG-CD2	-16.84	110.89	121.00	20	19
1	A	149	ARG	NE-CZ-NH1	16.30	128.45	120.30	20	3
1	A	196	PHE	CB-CG-CD1	-15.70	109.81	120.80	20	1
1	A	160	PRO	N-CA-CB	15.61	122.03	103.30	20	20
1	A	146	PHE	CB-CG-CD2	-15.35	110.05	120.80	15	5
1	A	146	PHE	CB-CG-CD1	-14.46	110.68	120.80	2	4
1	A	148	VAL	CA-CB-CG1	13.83	131.65	110.90	5	7
1	A	164	LEU	CB-CG-CD2	13.36	133.71	111.00	15	11
1	A	84	ARG	NE-CZ-NH2	-13.28	113.66	120.30	19	2
1	A	192	GLY	N-CA-C	-13.20	80.11	113.10	20	20
1	A	191	THR	C-N-CA	12.85	149.29	122.30	3	10
1	A	223	TYR	CB-CG-CD2	-12.79	113.33	121.00	18	8
1	A	105	THR	CA-CB-CG2	12.40	129.76	112.40	18	2
1	A	168	TYR	CB-CG-CD2	-12.19	113.69	121.00	19	3
1	A	180	PHE	CB-CG-CD1	-11.83	112.52	120.80	18	4
1	A	238	ASP	CB-CA-C	11.82	134.03	110.40	19	8
1	A	149	ARG	NE-CZ-NH2	-11.77	114.41	120.30	18	3
1	A	166	HIS	CB-CA-C	11.46	133.33	110.40	13	18
1	A	104	TYR	CB-CG-CD2	-11.30	114.22	121.00	19	8
1	A	191	THR	CA-CB-CG2	10.95	127.72	112.40	20	9
1	A	246	TYR	CB-CG-CD1	10.77	127.47	121.00	17	12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	148	VAL	CG1-CB-CG2	10.62	127.88	110.90	17	10
1	A	150	GLU	OE1-CD-OE2	10.32	135.69	123.30	18	1
1	A	116	ALA	CB-CA-C	10.18	125.37	110.10	17	20
1	A	143	MET	CA-CB-CG	10.14	130.53	113.30	6	6
1	A	148	VAL	C-N-CA	10.12	147.01	121.70	7	3
1	A	223	TYR	CB-CG-CD1	9.86	126.92	121.00	19	4
1	A	179	HIS	CG-ND1-CE1	-9.65	93.16	105.70	13	1
1	A	246	TYR	CA-CB-CG	9.59	131.63	113.40	17	20
1	A	207	LEU	CB-CG-CD1	9.57	127.28	111.00	17	6
1	A	166	HIS	CA-CB-CG	9.51	129.77	113.60	8	17
1	A	163	VAL	N-CA-CB	9.51	132.41	111.50	17	2
1	A	181	ASP	CA-CB-CG	9.50	134.31	113.40	2	9
1	A	183	ASP	CB-CG-OD2	-9.49	109.75	118.30	19	2
1	A	186	TRP	CE2-CD2-CG	9.35	114.78	107.30	20	3
1	A	102	VAL	CG1-CB-CG2	-9.25	96.09	110.90	8	5
1	A	163	VAL	CG1-CB-CG2	9.21	125.64	110.90	7	7
1	A	166	HIS	N-CA-C	-9.15	86.29	111.00	18	8
1	A	210	PHE	CB-CG-CD1	-9.07	114.45	120.80	18	1
1	A	127	VAL	CB-CA-C	9.07	128.63	111.40	20	1
1	A	164	LEU	CB-CG-CD1	9.01	126.32	111.00	20	10
1	A	154	PHE	CB-CG-CD1	-8.95	114.53	120.80	17	2
1	A	100	ARG	NE-CZ-NH2	8.82	124.71	120.30	18	2
1	A	93	ARG	NE-CZ-NH1	-8.78	115.91	120.30	18	2
1	A	223	TYR	CA-CB-CG	-8.77	96.73	113.40	20	1
1	A	189	ASP	CB-CG-OD2	-8.73	110.45	118.30	20	1
1	A	163	VAL	CA-CB-CG1	-8.69	97.86	110.90	8	8
1	A	148	VAL	CB-CA-C	-8.61	95.04	111.40	18	3
1	A	158	ASP	CB-CG-OD2	-8.59	110.57	118.30	18	1
1	A	177	ASP	CB-CA-C	-8.53	93.34	110.40	20	8
1	A	186	TRP	CZ3-CH2-CZ2	-8.50	111.40	121.60	20	4
1	A	163	VAL	N-CA-C	-8.41	88.30	111.00	20	4
1	A	136	TYR	CB-CG-CD2	-8.39	115.97	121.00	18	3
1	A	181	ASP	CB-CG-OD1	-8.35	110.79	118.30	19	6
1	A	105	THR	CA-CB-OG1	-8.33	91.51	109.00	18	1
1	A	217	ALA	N-CA-CB	-8.32	98.45	110.10	17	10
1	A	182	ASP	CB-CG-OD1	-8.30	110.83	118.30	19	2
1	A	223	TYR	C-N-CA	8.27	142.36	121.70	14	7
1	A	228	ASP	CB-CG-OD1	-8.25	110.87	118.30	18	2
1	A	232	PHE	CB-CG-CD2	-8.11	115.12	120.80	17	3
1	A	180	PHE	CB-CG-CD2	8.07	126.45	120.80	17	3
1	A	238	ASP	N-CA-CB	-8.04	96.12	110.60	20	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	216	GLU	C-N-CA	8.03	141.78	121.70	17	1
1	A	163	VAL	O-C-N	8.03	135.55	122.70	18	3
1	A	232	PHE	CB-CG-CD1	8.02	126.41	120.80	19	2
1	A	149	ARG	C-N-CA	7.97	141.63	121.70	18	13
1	A	223	TYR	CG-CD1-CE1	-7.92	114.96	121.30	18	2
1	A	186	TRP	CD1-CG-CD2	-7.91	99.97	106.30	18	2
1	A	168	TYR	CB-CG-CD1	-7.89	116.27	121.00	20	2
1	A	231	ARG	NE-CZ-NH1	7.89	124.24	120.30	17	1
1	A	195	LEU	N-CA-CB	-7.88	94.64	110.40	18	3
1	A	229	LEU	CB-CG-CD1	7.85	124.35	111.00	20	3
1	A	107	ASP	CB-CG-OD2	-7.83	111.25	118.30	18	2
1	A	166	HIS	C-N-CA	7.74	141.05	121.70	19	1
1	A	207	LEU	C-N-CA	7.70	138.46	122.30	8	1
1	A	173	GLY	C-N-CA	7.61	140.73	121.70	18	1
1	A	165	ALA	N-CA-CB	7.59	120.72	110.10	14	3
1	A	102	VAL	CA-CB-CG1	7.57	122.25	110.90	13	10
1	A	129	PRO	N-CA-CB	-7.50	94.30	103.30	18	2
1	A	198	VAL	CA-CB-CG2	7.48	122.12	110.90	19	6
1	A	220	TYR	CB-CG-CD2	7.42	125.45	121.00	18	1
1	A	102	VAL	CB-CA-C	7.36	125.39	111.40	8	3
1	A	166	HIS	O-C-N	7.36	134.48	122.70	19	1
1	A	206	SER	CB-CA-C	7.34	124.06	110.10	4	1
1	A	161	GLY	C-N-CA	7.33	140.03	121.70	5	5
1	A	108	LEU	N-CA-C	-7.33	91.21	111.00	17	2
1	A	143	MET	CB-CA-C	7.22	124.85	110.40	20	6
1	A	153	ASP	CB-CG-OD2	-7.20	111.82	118.30	18	3
1	A	195	LEU	CB-CG-CD1	-7.17	98.81	111.00	18	3
1	A	134	ARG	CB-CA-C	-7.14	96.12	110.40	17	2
1	A	211	HIS	CA-CB-CG	-7.12	101.50	113.60	20	1
1	A	195	LEU	CB-CA-C	7.11	123.70	110.20	19	12
1	A	221	PRO	CA-N-CD	-7.11	101.55	111.50	12	1
1	A	174	ILE	CB-CG1-CD1	7.10	133.77	113.90	18	1
1	A	166	HIS	CG-ND1-CE1	-7.03	96.56	105.70	19	4
1	A	157	PHE	CA-CB-CG	7.01	130.72	113.90	19	3
1	A	226	LEU	CB-CG-CD1	6.99	122.88	111.00	5	2
1	A	177	ASP	CB-CG-OD2	-6.99	112.01	118.30	19	1
1	A	209	LEU	C-N-CA	6.99	139.16	121.70	3	7
1	A	148	VAL	N-CA-CB	-6.97	96.17	111.50	7	7
1	A	163	VAL	CA-CB-CG2	6.94	121.31	110.90	17	1
1	A	109	PRO	N-CA-CB	6.94	111.63	103.30	17	1
1	A	124	TRP	N-CA-CB	-6.94	98.11	110.60	17	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	151	HIS	CA-CB-CG	6.92	125.37	113.60	6	5
1	A	124	TRP	CA-CB-CG	6.92	126.84	113.70	17	4
1	A	246	TYR	N-CA-CB	-6.88	98.21	110.60	14	11
1	A	197	LEU	CB-CG-CD2	-6.88	99.31	111.00	19	3
1	A	130	LEU	N-CA-CB	6.88	124.16	110.40	20	1
1	A	164	LEU	N-CA-C	6.87	129.56	111.00	12	5
1	A	124	TRP	CB-CA-C	-6.87	96.65	110.40	19	1
1	A	168	TYR	C-N-CA	6.86	138.84	121.70	15	8
1	A	154	PHE	N-CA-CB	-6.83	98.30	110.60	18	1
1	A	86	PHE	CB-CG-CD1	6.83	125.58	120.80	20	1
1	A	186	TRP	CB-CA-C	6.83	124.06	110.40	4	11
1	A	136	TYR	CB-CG-CD1	6.82	125.09	121.00	18	1
1	A	100	ARG	NE-CZ-NH1	-6.80	116.90	120.30	20	1
1	A	121	LEU	CB-CA-C	-6.78	97.31	110.20	17	4
1	A	151	HIS	N-CA-CB	-6.77	98.41	110.60	6	2
1	A	154	PHE	CB-CG-CD2	6.77	125.54	120.80	17	1
1	A	124	TRP	NE1-CE2-CZ2	6.77	137.84	130.40	17	1
1	A	143	MET	N-CA-CB	6.73	122.72	110.60	18	6
1	A	210	PHE	CG-CD1-CE1	-6.73	113.40	120.80	20	1
1	A	164	LEU	N-CA-CB	-6.73	96.95	110.40	10	8
1	A	186	TRP	NE1-CE2-CD2	-6.73	100.57	107.30	19	2
1	A	127	VAL	CA-CB-CG2	6.72	120.97	110.90	20	4
1	A	136	TYR	CA-CB-CG	6.71	126.14	113.40	18	1
1	A	117	VAL	CA-CB-CG1	6.70	120.96	110.90	17	1
1	A	160	PRO	CA-N-CD	-6.70	102.12	111.50	20	1
1	A	156	PRO	CA-N-CD	-6.70	102.12	111.50	4	4
1	A	83	PHE	CB-CG-CD1	-6.68	116.12	120.80	17	3
1	A	150	GLU	N-CA-CB	-6.66	98.61	110.60	17	2
1	A	165	ALA	N-CA-C	-6.66	93.03	111.00	19	3
1	A	163	VAL	CB-CA-C	6.66	124.05	111.40	10	6
1	A	205	HIS	CG-ND1-CE1	-6.65	97.05	105.70	20	1
1	A	163	VAL	CA-C-N	-6.64	102.60	117.20	12	3
1	A	99	TYR	CG-CD2-CE2	-6.63	116.00	121.30	20	1
1	A	135	LEU	CB-CG-CD2	6.62	122.26	111.00	18	1
1	A	170	PRO	CA-N-CD	-6.60	102.26	111.50	19	2
1	A	233	ARG	NE-CZ-NH1	6.59	123.60	120.30	17	1
1	A	136	TYR	CG-CD2-CE2	-6.58	116.04	121.30	17	1
1	A	108	LEU	CB-CG-CD2	6.57	122.17	111.00	20	1
1	A	245	LEU	CB-CG-CD2	6.57	122.16	111.00	20	1
1	A	174	ILE	N-CA-C	-6.57	93.28	111.00	19	15
1	A	238	ASP	N-CA-C	-6.57	93.27	111.00	19	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	128	THR	CA-CB-CG2	6.51	121.52	112.40	20	1
1	A	84	ARG	NE-CZ-NH1	6.51	123.56	120.30	20	3
1	A	203	ILE	CA-CB-CG1	6.50	123.35	111.00	7	13
1	A	107	ASP	CB-CG-OD1	-6.50	112.45	118.30	17	1
1	A	192	GLY	C-N-CA	6.48	137.90	121.70	5	2
1	A	161	GLY	O-C-N	6.48	133.07	122.70	19	2
1	A	179	HIS	CA-CB-CG	6.48	124.61	113.60	7	3
1	A	99	TYR	CG-CD1-CE1	-6.47	116.13	121.30	20	2
1	A	134	ARG	NE-CZ-NH2	-6.45	117.07	120.30	17	1
1	A	151	HIS	ND1-CE1-NE2	6.45	124.10	109.90	18	1
1	A	131	THR	O-C-N	6.44	133.01	122.70	19	1
1	A	246	TYR	CZ-CE2-CD2	-6.43	114.01	119.80	18	1
1	A	111	ASP	CB-CG-OD2	-6.41	112.53	118.30	18	1
1	A	187	THR	CA-CB-CG2	6.41	121.37	112.40	19	1
1	A	166	HIS	CA-C-N	-6.40	103.13	117.20	19	2
1	A	155	TYR	CZ-CE2-CD2	6.39	125.55	119.80	18	1
1	A	139	GLU	OE1-CD-OE2	6.38	130.96	123.30	18	1
1	A	223	TYR	O-C-N	6.38	132.90	122.70	20	1
1	A	199	ALA	N-CA-CB	6.38	119.03	110.10	9	2
1	A	149	ARG	O-C-N	6.37	132.89	122.70	18	1
1	A	211	HIS	CG-ND1-CE1	-6.34	97.46	105.70	19	3
1	A	146	PHE	CG-CD2-CE2	-6.33	113.83	120.80	15	1
1	A	186	TRP	NE1-CE2-CZ2	6.32	137.36	130.40	19	1
1	A	189	ASP	C-N-CA	6.30	137.46	121.70	17	1
1	A	114	ASP	CB-CG-OD1	-6.30	112.63	118.30	20	1
1	A	234	LEU	CB-CA-C	6.29	122.14	110.20	7	1
1	A	164	LEU	CB-CA-C	6.28	122.13	110.20	19	2
1	A	85	THR	C-N-CA	6.27	137.37	121.70	9	3
1	A	166	HIS	ND1-CE1-NE2	6.25	123.66	109.90	19	1
1	A	177	ASP	CB-CG-OD1	-6.24	112.68	118.30	18	1
1	A	224	HIS	N-CA-C	-6.24	94.16	111.00	17	4
1	A	207	LEU	N-CA-C	-6.21	94.24	111.00	4	1
1	A	99	TYR	CB-CG-CD2	-6.21	117.28	121.00	5	1
1	A	143	MET	N-CA-C	-6.20	94.25	111.00	19	2
1	A	173	GLY	N-CA-C	-6.19	97.61	113.10	17	1
1	A	102	VAL	C-N-CA	6.19	137.16	121.70	10	4
1	A	170	PRO	N-CD-CG	6.18	112.48	103.20	19	1
1	A	198	VAL	CA-CB-CG1	-6.18	101.63	110.90	6	7
1	A	143	MET	CG-SD-CE	-6.17	90.33	100.20	6	3
1	A	132	PHE	CB-CG-CD2	-6.16	116.49	120.80	11	2
1	A	170	PRO	CA-C-N	-6.15	103.89	116.20	20	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	124	TRP	CE3-CZ3-CH2	-6.15	114.44	121.20	18	1
1	A	180	PHE	CG-CD1-CE1	-6.15	114.04	120.80	18	1
1	A	222	LEU	CB-CG-CD1	-6.14	100.56	111.00	5	3
1	A	160	PRO	O-C-N	6.12	133.60	123.20	19	1
1	A	186	TRP	CD2-CE3-CZ3	6.12	126.75	118.80	20	1
1	A	134	ARG	CD-NE-CZ	6.11	132.15	123.60	18	1
1	A	190	THR	CA-CB-CG2	-6.10	103.86	112.40	14	2
1	A	116	ALA	N-CA-CB	-6.10	101.56	110.10	19	1
1	A	167	ALA	CB-CA-C	-6.09	100.96	110.10	13	2
1	A	197	LEU	CA-CB-CG	6.09	129.30	115.30	18	2
1	A	90	PRO	N-CA-CB	6.08	110.59	103.30	20	1
1	A	151	HIS	CG-ND1-CE1	-6.06	97.82	105.70	19	5
1	A	193	THR	N-CA-CB	-6.05	98.80	110.30	9	5
1	A	191	THR	CA-C-N	-6.04	104.13	116.20	10	5
1	A	187	THR	C-N-CA	6.03	136.78	121.70	15	1
1	A	143	MET	O-C-N	6.03	132.34	122.70	20	1
1	A	149	ARG	N-CA-C	-6.02	94.76	111.00	19	1
1	A	161	GLY	CA-C-N	-6.01	103.97	117.20	19	3
1	A	101	ILE	N-CA-C	-5.99	94.82	111.00	19	3
1	A	150	GLU	C-N-CA	5.98	136.66	121.70	17	1
1	A	210	PHE	C-N-CA	5.98	136.65	121.70	19	1
1	A	222	LEU	CB-CG-CD2	5.98	121.17	111.00	1	3
1	A	185	GLN	N-CA-C	-5.97	94.87	111.00	20	12
1	A	224	HIS	CA-CB-CG	-5.96	103.46	113.60	17	1
1	A	193	THR	CA-CB-CG2	-5.96	104.06	112.40	16	1
1	A	210	PHE	CB-CG-CD2	5.95	124.97	120.80	18	1
1	A	170	PRO	N-CA-CB	5.95	110.44	103.30	17	4
1	A	169	ALA	N-CA-CB	-5.94	101.78	110.10	17	6
1	A	104	TYR	CG-CD2-CE2	-5.93	116.56	121.30	19	1
1	A	85	THR	CA-CB-CG2	5.92	120.69	112.40	3	2
1	A	232	PHE	CA-CB-CG	5.89	128.04	113.90	18	2
1	A	223	TYR	CZ-CE2-CD2	-5.88	114.51	119.80	19	1
1	A	103	ASN	C-N-CA	5.87	136.36	121.70	14	2
1	A	179	HIS	N-CA-C	-5.86	95.19	111.00	18	1
1	A	225	SER	C-N-CA	5.84	136.30	121.70	20	5
1	A	248	PRO	CA-N-CD	-5.83	103.34	111.50	18	1
1	A	245	LEU	N-CA-C	-5.82	95.29	111.00	20	2
1	A	124	TRP	CG-CD1-NE1	-5.79	104.31	110.10	17	1
1	A	104	TYR	CB-CG-CD1	5.78	124.47	121.00	19	2
1	A	113	VAL	CB-CA-C	5.78	122.38	111.40	18	1
1	A	237	ASP	CB-CG-OD2	-5.77	113.11	118.30	20	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	238	ASP	CB-CG-OD2	-5.76	113.12	118.30	17	1
1	A	234	LEU	CB-CG-CD2	-5.75	101.22	111.00	19	2
1	A	234	LEU	CB-CG-CD1	5.75	120.77	111.00	11	4
1	A	105	THR	N-CA-CB	5.75	121.22	110.30	17	1
1	A	246	TYR	CG-CD2-CE2	5.74	125.89	121.30	18	1
1	A	118	GLU	OE1-CD-OE2	5.73	130.18	123.30	19	1
1	A	136	TYR	CA-C-N	-5.73	104.59	117.20	20	1
1	A	186	TRP	CH2-CZ2-CE2	-5.70	111.70	117.40	17	1
1	A	203	ILE	CB-CG1-CD1	5.70	129.84	113.90	20	1
1	A	90	PRO	O-C-N	5.69	131.80	122.70	18	1
1	A	156	PRO	O-C-N	5.68	131.80	122.70	17	1
1	A	156	PRO	CB-CA-C	-5.66	97.84	112.00	20	1
1	A	150	GLU	CB-CA-C	5.66	121.71	110.40	8	1
1	A	131	THR	CA-C-N	-5.65	104.76	117.20	19	1
1	A	148	VAL	N-CA-C	5.63	126.19	111.00	3	1
1	A	103	ASN	O-C-N	5.62	131.69	122.70	20	1
1	A	100	ARG	CA-CB-CG	5.61	125.74	113.40	17	1
1	A	147	ALA	C-N-CA	5.61	135.72	121.70	7	1
1	A	233	ARG	CD-NE-CZ	-5.59	115.77	123.60	20	1
1	A	148	VAL	CA-CB-CG2	-5.59	102.52	110.90	8	2
1	A	196	PHE	O-C-N	-5.58	113.76	122.70	19	1
1	A	230	THR	C-N-CA	5.57	135.63	121.70	7	1
1	A	155	TYR	CB-CG-CD1	-5.57	117.66	121.00	19	1
1	A	171	GLY	CA-C-O	-5.55	110.60	120.60	18	1
1	A	193	THR	O-C-N	-5.55	113.82	122.70	18	1
1	A	179	HIS	CG-CD2-NE2	-5.55	98.66	109.20	13	1
1	A	222	LEU	C-N-CA	5.54	135.56	121.70	12	2
1	A	129	PRO	CA-N-CD	-5.54	103.74	111.50	18	8
1	A	152	GLY	N-CA-C	-5.52	99.30	113.10	17	1
1	A	233	ARG	NE-CZ-NH2	-5.52	117.54	120.30	17	1
1	A	105	THR	OG1-CB-CG2	-5.51	97.33	110.00	20	1
1	A	124	TRP	CB-CG-CD2	5.50	133.76	126.60	1	4
1	A	189	ASP	CB-CG-OD1	-5.50	113.35	118.30	18	1
1	A	148	VAL	CA-C-N	-5.49	105.12	117.20	19	1
1	A	195	LEU	CB-CG-CD2	5.49	120.33	111.00	8	3
1	A	179	HIS	CB-CA-C	5.49	121.37	110.40	13	1
1	A	174	ILE	C-N-CA	5.48	135.41	121.70	18	1
1	A	244	SER	O-C-N	5.47	131.46	122.70	17	2
1	A	132	PHE	CB-CG-CD1	-5.45	116.98	120.80	20	1
1	A	90	PRO	CA-N-CD	-5.44	103.88	111.50	19	1
1	A	245	LEU	C-N-CA	5.43	135.28	121.70	5	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	97	LEU	CA-CB-CG	-5.42	102.83	115.30	17	1
1	A	140	ALA	C-N-CA	5.42	135.25	121.70	18	1
1	A	187	THR	N-CA-C	5.42	125.62	111.00	1	1
1	A	242	ILE	CB-CA-C	5.39	122.38	111.60	18	1
1	A	183	ASP	CB-CA-C	-5.39	99.62	110.40	19	1
1	A	237	ASP	O-C-N	5.39	131.32	122.70	19	1
1	A	149	ARG	CA-C-N	-5.38	105.36	117.20	8	2
1	A	144	ILE	N-CA-CB	-5.38	98.42	110.80	18	1
1	A	135	LEU	CB-CA-C	-5.38	99.99	110.20	18	1
1	A	89	ILE	CA-CB-CG2	5.37	121.63	110.90	20	2
1	A	220	TYR	CB-CG-CD1	-5.36	117.78	121.00	19	1
1	A	104	TYR	CA-CB-CG	5.36	123.58	113.40	1	3
1	A	158	ASP	CB-CG-OD1	-5.36	113.48	118.30	19	1
1	A	197	LEU	CA-C-N	5.35	128.98	117.20	20	1
1	A	178	ALA	CB-CA-C	5.35	118.13	110.10	2	2
1	A	156	PRO	N-CA-C	5.34	125.99	112.10	1	1
1	A	224	HIS	C-N-CA	5.34	135.04	121.70	7	2
1	A	229	LEU	CB-CG-CD2	5.33	120.07	111.00	19	2
1	A	221	PRO	C-N-CA	5.33	135.04	121.70	19	1
1	A	209	LEU	CB-CG-CD2	-5.32	101.96	111.00	20	2
1	A	232	PHE	N-CA-CB	-5.31	101.04	110.60	17	2
1	A	229	LEU	C-N-CA	5.31	134.96	121.70	9	1
1	A	242	ILE	CG1-CB-CG2	5.29	123.04	111.40	18	1
1	A	190	THR	C-N-CA	5.29	134.92	121.70	4	1
1	A	124	TRP	CD2-CE2-CZ2	-5.27	115.97	122.30	17	1
1	A	246	TYR	CG-CD1-CE1	-5.26	117.09	121.30	20	2
1	A	173	GLY	CA-C-N	-5.26	105.62	117.20	18	1
1	A	181	ASP	N-CA-CB	5.26	120.06	110.60	19	1
1	A	149	ARG	CD-NE-CZ	5.25	130.96	123.60	19	1
1	A	168	TYR	CG-CD2-CE2	-5.25	117.10	121.30	19	1
1	A	150	GLU	CA-CB-CG	5.25	124.96	113.40	18	1
1	A	206	SER	C-N-CA	-5.25	108.57	121.70	19	1
1	A	163	VAL	CA-C-O	-5.24	109.10	120.10	18	1
1	A	236	GLN	N-CA-CB	-5.24	101.17	110.60	20	1
1	A	134	ARG	NE-CZ-NH1	5.23	122.92	120.30	20	1
1	A	180	PHE	CD1-CG-CD2	-5.23	111.50	118.30	17	1
1	A	232	PHE	O-C-N	5.22	131.05	122.70	20	1
1	A	209	LEU	N-CA-CB	5.22	120.84	110.40	17	1
1	A	186	TRP	CB-CG-CD2	5.22	133.38	126.60	20	1
1	A	126	GLU	OE1-CD-OE2	5.21	129.55	123.30	17	1
1	A	194	ASN	CB-CA-C	5.20	120.80	110.40	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	146	PHE	CG-CD1-CE1	-5.20	115.08	120.80	2	2
1	A	141	ASP	CB-CG-OD2	-5.19	113.63	118.30	20	1
1	A	247	GLY	CA-C-O	-5.18	111.28	120.60	19	1
1	A	164	LEU	CA-CB-CG	-5.17	103.40	115.30	11	3
1	A	235	SER	CB-CA-C	-5.17	100.27	110.10	10	1
1	A	202	GLU	CA-CB-CG	-5.16	102.04	113.40	19	1
1	A	129	PRO	CA-CB-CG	-5.16	94.20	104.00	20	1
1	A	234	LEU	C-N-CA	5.15	134.58	121.70	16	1
1	A	125	GLU	N-CA-CB	-5.12	101.38	110.60	17	1
1	A	147	ALA	CA-C-N	-5.11	105.95	117.20	12	1
1	A	228	ASP	CB-CG-OD2	-5.11	113.70	118.30	20	1
1	A	239	ILE	N-CA-C	-5.10	97.23	111.00	20	1
1	A	93	ARG	NE-CZ-NH2	-5.09	117.76	120.30	20	1
1	A	146	PHE	CB-CA-C	5.08	120.57	110.40	17	1
1	A	186	TRP	CG-CD1-NE1	5.08	115.18	110.10	18	1
1	A	184	GLU	C-N-CA	5.08	134.39	121.70	20	1
1	A	172	PRO	C-N-CA	-5.07	111.66	122.30	18	1
1	A	187	THR	OG1-CB-CG2	-5.07	98.35	110.00	18	1
1	A	225	SER	CA-C-N	-5.06	106.06	117.20	1	1
1	A	123	VAL	CA-C-O	-5.06	109.47	120.10	19	1
1	A	124	TRP	CZ3-CH2-CZ2	-5.05	115.53	121.60	19	1
1	A	186	TRP	CE2-CD2-CE3	-5.05	112.64	118.70	20	1
1	A	99	TYR	CB-CG-CD1	-5.05	117.97	121.00	20	1
1	A	121	LEU	N-CA-CB	-5.04	100.31	110.40	20	1
1	A	86	PHE	CB-CA-C	5.04	120.48	110.40	9	1
1	A	221	PRO	N-CA-C	5.04	125.20	112.10	9	1
1	A	207	LEU	CB-CG-CD2	-5.04	102.44	111.00	8	1
1	A	170	PRO	C-N-CA	5.04	132.87	122.30	17	1
1	A	225	SER	N-CA-CB	-5.03	102.96	110.50	20	1
1	A	142	ILE	CA-C-N	-5.02	106.15	117.20	18	1
1	A	131	THR	C-N-CA	5.02	134.25	121.70	5	1
1	A	143	MET	CA-C-N	-5.01	106.18	117.20	20	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	223	TYR	Sidechain	19
1	A	128	THR	Peptide	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	132	PHE	Sidechain	7
1	A	180	PHE	Sidechain	7
1	A	155	TYR	Peptide,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	154	PHE	Sidechain	3
1	A	89	ILE	Peptide	3
1	A	159	GLY	Peptide	3
1	A	169	ALA	Peptide	3
1	A	86	PHE	Sidechain	2
1	A	105	THR	Peptide	1
1	A	149	ARG	Sidechain	1
1	A	210	PHE	Sidechain	1
1	A	93	ARG	Sidechain	1
1	A	100	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	1324	1248	1252	70±11
4	A	32	36	35	14±3
All	All	27180	25680	25736	1566

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 30.

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	9
4:A:261:0DS:CG1	4:A:261:0DS:CE2	1.11	2.29	18	6
4:A:261:0DS:CD11	4:A:261:0DS:HD1	1.11	0.97	6	11
4:A:261:0DS:HD2	4:A:261:0DS:CD21	1.10	0.97	7	10
4:A:261:0DS:CD21	4:A:261:0DS:HD2	1.08	0.97	17	10
1:A:164:LEU:HD23	1:A:198:VAL:HG13	1.05	1.13	15	4
4:A:261:0DS:CE2	4:A:261:0DS:CG1	1.00	2.37	20	14
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	20	9
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: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:HD2	4:A:261:0DS:CG1	0.83	2.04	19	11
1:A:148:VAL:HG12	1:A:166:HIS:CE1	0.83	2.08	13	1
4:A:261:0DS:CE2	4:A:261:0DS:HD2	0.82	2.04	19	13
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
1:A:163:VAL:C	1:A:164:LEU:HD13	0.81	1.95	16	14
4:A:261:0DS:HD2	4:A:261:0DS:CE2	0.81	2.05	17	7
4:A:261:0DS:CE1	4:A:261:0DS:HD1	0.80	2.06	3	11
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:CG1	4:A:261:0DS:HD2	0.80	2.07	3	9
4:A:261:0DS:HD1	4:A:261:0DS:CG1	0.80	2.06	20	13
4:A:261:0DS:HD1	4:A:261:0DS:CE1	0.80	2.07	8	9
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	2.07	4	7
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:184:GLU:CD	1:A:193:THR:HG21	0.74	2.02	11	5
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
1:A:166:HIS:CE1	1:A:179:HIS:CE1	0.72	2.77	13	1
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:261:0DS:HB31	0.71	1.62	4	6
1:A:164:LEU:HD22	1:A:164:LEU:H	0.71	1.45	12	2
1:A:222:LEU:HD11	4:A:261:0DS: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:HD12	1:A:226:LEU:H	0.70	1.46	11	1
1:A:163:VAL:HG21	4:A:261:0DS: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:O	1:A:174:ILE:HD12	0.68	1.88	8	2
1:A:169:ALA:HB1	1:A:170:PRO:HD2	0.68	1.65	1	11
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:261:0DS:CD1	0.67	2.19	5	4
1:A:163:VAL:HG11	4:A:261:0DS:HA	0.67	1.64	12	2
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:261:0DS:C5	0.66	2.20	17	1
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:HD12	1:A:226:LEU:N	0.65	2.07	1	1
1:A:164:LEU:HD11	4:A:261:0DS:CD2	0.65	2.22	13	7
1:A:197:LEU:HD11	4:A:261:0DS: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:143:MET:O	1:A:144:ILE:HD12	0.64	1.90	18	1
1:A:162:ASN:HA	4:A:261:0DS: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:223:TYR:C	1:A:223:TYR:CD2	0.63	2.72	20	1
1:A:197:LEU:HD13	1:A:197:LEU:C	0.63	2.13	3	3
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:202:GLU:CD	1:A:202:GLU:C	0.63	2.57	18	2
1:A:164:LEU:HB3	1:A:186:TRP:CH2	0.62	2.29	12	1
1:A:162:ASN:HA	4:A:261:0DS: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:178:ALA:HB2	1:A:202:GLU:CD	0.62	2.15	11	4
1:A:164:LEU:HD12	1:A:186:TRP:CH2	0.62	2.30	12	3
1:A:108:LEU:CB	1:A:113:VAL:HG23	0.62	2.25	1	1
1:A:105:THR:CG2	1:A:186:TRP:CD1	0.62	2.82	6	10
1:A:85:THR:HG22	1:A:86:PHE:N	0.62	2.09	9	3
1:A:163:VAL:C	1:A:164:LEU:HG	0.62	2.13	10	1
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:162:ASN:C	1:A:163:VAL:HG22	0.61	2.15	20	4
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:146:PHE:CD1	1:A:146:PHE:N	0.60	2.68	18	1
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
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	1
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:200:ALA:O	1:A:201:HIS:C	0.59	2.39	19	3
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: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:N	1:A:164:LEU:HD22	0.57	2.14	2	3
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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
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:HD22	4:A:261:0DS:H1	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:163:VAL:HG21	4:A:261:0DS:CD1	0.56	2.30	8	6
1:A:148:VAL:HG23	1:A:183:ASP:HB2	0.56	1.78	11	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:119:LYS:O	1:A:120:ALA:C	0.56	2.43	17	1
1:A:101:ILE:N	1:A:101:ILE:HD13	0.56	2.16	20	1
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:O	1:A:190:THR:HG22	0.56	2.00	7	2
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:H	1:A:226:LEU:HD12	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: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:N	1:A:164:LEU:CD2	0.54	2.69	1	5
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:LEU:HD13	1:A:223:TYR:CD1	0.54	2.37	10	3
1:A:180:PHE:O	1:A:182:ASP:N	0.54	2.40	18	6
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
1:A:186:TRP:CD2	1:A:195:LEU:HD23	0.54	2.38	9	4
1:A:146:PHE:N	1:A:146:PHE:CD1	0.54	2.75	8	1
1:A:222:LEU:CG	1:A:223:TYR:H	0.54	2.15	17	7
1:A:144:ILE:HG13	1:A:178:ALA:HB3	0.54	1.80	19	2
1:A:163:VAL:O	1:A:164:LEU:CD2	0.54	2.55	5	8
1:A:121:LEU:HD22	1:A:121:LEU:H	0.54	1.61	14	3
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:196:PHE:CD1	1:A:196:PHE:C	0.54	2.79	17	2
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:OD1	1:A:182:ASP:O	0.54	2.26	17	1
1:A:162:ASN:O	1:A:164:LEU:HD13	0.54	2.03	1	1
1:A:163:VAL:C	1:A:164:LEU:CD1	0.53	2.74	3	3
1:A:166:HIS:ND1	1:A:179:HIS:HB2	0.53	2.18	11	1
1:A:186:TRP:O	1:A:187:THR:HB	0.53	2.02	20	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:148:VAL:HG11	1:A:166:HIS:CE1	0.53	2.39	19	1
1:A:164:LEU:HD11	4:A:261:0DS:HD12	0.53	1.80	16	2
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:164:LEU:HB3	1:A:181:ASP:CG	0.53	2.24	15	1
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:191:THR:HG21	1:A:223:TYR:O	0.52	2.03	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:VAL:HG11	1:A:232:PHE:H	0.52	1.63	3	1
1:A:234:LEU:HD12	1:A:234:LEU:H	0.52	1.63	4	5
1:A:163:VAL:HG22	4:A:261:0DS:CD1	0.52	2.27	7	1
1:A:164:LEU:N	1:A:164:LEU:CD1	0.52	2.71	10	2
1:A:124:TRP:CZ3	1:A:242:ILE:HD11	0.52	2.39	11	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:186:TRP:CE2	1:A:195:LEU:HD23	0.52	2.39	4	4
1:A:165:ALA:HB2	1:A:198:VAL:CG2	0.52	2.34	12	2
1:A:218:LEU:HD22	1:A:234:LEU:HD23	0.52	1.80	8	1
1:A:159:GLY:HA2	1:A:183:ASP:CG	0.52	2.25	12	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:165:ALA:HB1	1:A:202:GLU:HG3	0.52	1.82	4	1
1:A:85:THR:H	1:A:208:GLY:HA3	0.52	1.65	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:99:TYR:CZ	1:A:144:ILE:HD11	0.51	2.40	5	1
1:A:178:ALA:HB1	1:A:180:PHE:CE1	0.51	2.40	6	4
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:VAL:HG22	1:A:157:PHE:H	0.50	1.66	5	1
1:A:190:THR:HG22	1:A:190:THR:O	0.50	2.06	5	3
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: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:164:LEU:H	1:A:198:VAL:HG21	0.50	1.66	16	1
1:A:177:ASP:OD1	1:A:177:ASP:N	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:143:MET:C	1:A:144:ILE:HD12	0.49	2.26	19	2
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:162:ASN:O	1:A:163:VAL:HG22	0.49	2.07	20	2
1:A:168:TYR:O	1:A:169:ALA:HB2	0.49	2.07	18	2
1:A:160:PRO:HA	1:A:184:GLU:CD	0.49	2.27	15	4
1:A:142:ILE:CG2	1:A:206:SER:HB2	0.49	2.36	10	2
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:180:PHE:N	1:A:180:PHE:CD1	0.49	2.79	17	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:197:LEU:C	1:A:197:LEU:HD13	0.49	2.28	20	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:121:LEU:CD1	1:A:203:ILE:HG21	0.49	2.37	14	2
1:A:116:ALA:HB1	1:A:196:PHE:HA	0.49	1.84	14	1
1:A:180:PHE:CD1	1:A:180:PHE:N	0.49	2.81	14	1
1:A:186:TRP:CZ3	1:A:193:THR:CB	0.49	2.95	20	1

Continued on next page...

Continued from previous page...

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:191:THR:HG21	4:A:261:0DS: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	7
1:A:164:LEU:CD2	1:A:198:VAL:CG2	0.49	2.90	12	1
1:A:101:ILE:HD13	1:A:101:ILE:N	0.48	2.21	17	1
1:A:181:ASP:C	1:A:183:ASP:N	0.48	2.65	19	5
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:CD2	1:A:223:TYR:O	0.48	2.66	18	1
1:A:164:LEU:H	1:A:164:LEU:HD22	0.48	1.67	4	1
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:CD1	1:A:226:LEU:N	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:189:ASP:C	1:A:191:THR:H	0.48	2.12	19	1
1:A:113:VAL:HG13	1:A:195:LEU:CD1	0.48	2.39	7	6
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: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:261:0DS:H53	0.48	2.23	7	1
1:A:148:VAL:HG21	1:A:181:ASP:CG	0.48	2.29	10	1
1:A:162:ASN:O	1:A:163:VAL:HG13	0.48	2.08	14	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:134:ARG:O	1:A:135:LEU:C	0.48	2.53	20	1
1:A:127:VAL:CG2	1:A:242:ILE:HG21	0.47	2.39	3	2
4:A:261:0DS:H53	4:A:261:0DS:C1	0.47	2.39	8	1
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	2
1:A:123:VAL:HG21	1:A:232:PHE:H	0.47	1.67	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:261:0DS: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:N	1:A:164:LEU:HD13	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: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:ND1	1:A:151:HIS:N	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:261:0DS: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: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:158:ASP:O	1:A:158:ASP:CG	0.47	2.53	20	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:162:ASN:CA	4:A:261:0DS: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:186:TRP:CE3	1:A:193:THR:OG1	0.46	2.62	20	3
1:A:222:LEU:HD13	1:A:222:LEU:C	0.46	2.30	19	1
1:A:171:GLY:O	1:A:172:PRO:C	0.46	2.54	20	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:261:0DS:CD2	0.46	2.93	5	1
1:A:219:MET:N	1:A:219:MET:SD	0.46	2.88	19	3
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:261:0DS:CD2	0.46	2.40	15	1
1:A:187:THR:OG1	1:A:188:LYS:N	0.46	2.47	20	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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:261:0DS: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:187:THR:HG23	1:A:193:THR:O	0.45	2.11	5	1
1:A:98:THR:HG22	1:A:99:TYR:N	0.45	2.26	5	1
1:A:178:ALA:CB	1:A:202:GLU:HG3	0.45	2.42	14	2
1:A:179:HIS:N	1:A:179:HIS:CD2	0.45	2.84	1	3
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:217:ALA:HB1	1:A:235:SER:HB3	0.45	1.89	3	1
1:A:181:ASP:C	1:A:183:ASP:H	0.45	2.13	19	2
1:A:162:ASN:C	1:A:163:VAL:CG2	0.45	2.84	20	2
1:A:242:ILE:N	1:A:242:ILE:CD1	0.45	2.79	7	1
1:A:174:ILE:O	1:A:175:ASN:C	0.45	2.54	17	1
1:A:226:LEU:N	1:A:226:LEU:HD12	0.45	2.27	18	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:164:LEU:CD1	1:A:164:LEU:N	0.45	2.80	8	3
1:A:148:VAL:HG21	1:A:183:ASP:H	0.45	1.72	18	1
1:A:163:VAL:C	1:A:164:LEU:CG	0.45	2.82	17	2
1:A:222:LEU:O	1:A:224:HIS:N	0.45	2.50	19	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
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:222:LEU:CD2	1:A:223:TYR:N	0.45	2.70	14	3
1:A:201:HIS:O	1:A:205:HIS:HB2	0.45	2.11	5	1
1:A:89:ILE:HG12	1:A:245:LEU:HD13	0.45	1.89	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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	1
1:A:189:ASP:C	1:A:191:THR:N	0.45	2.69	19	1
1:A:199:ALA:HB1	1:A:203:ILE:HD12	0.45	1.89	1	1
1:A:186:TRP:CH2	1:A:193:THR:HB	0.45	2.47	12	4
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:207:LEU:C	1:A:207:LEU:CD1	0.44	2.86	12	1
1:A:164:LEU:CG	1:A:186:TRP:HH2	0.44	2.26	15	1
1:A:156:PRO:O	1:A:157:PHE:C	0.44	2.55	1	1
1:A:197:LEU:HD12	1:A:223:TYR:HB2	0.44	1.90	3	1
1:A:142:ILE:H	1:A:142:ILE:HD12	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:190:THR:C	1:A:191:THR:HG23	0.44	2.33	15	1
1:A:104:TYR:O	1:A:113:VAL:HG11	0.44	2.12	18	1
1:A:201:HIS:HB2	4:A:261:0DS: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:209:LEU:HD13	1:A:238:ASP:CA	0.44	2.42	7	1
1:A:220:TYR:O	4:A:261:0DS: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:246:TYR:C	1:A:246:TYR:CD1	0.44	2.91	4	1
1:A:85:THR:CG2	1:A:245:LEU:HD21	0.44	2.43	4	2
1:A:196:PHE:CE1	1:A:229:LEU:HD23	0.44	2.47	10	1
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:130:LEU:HD13	1:A:245:LEU:HB2	0.44	1.90	13	1
1:A:164:LEU:CD2	4:A:261:0DS:HD21	0.43	2.35	11	1
1:A:146:PHE:CD1	1:A:146:PHE:C	0.43	2.91	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:243:GLN:HA	1:A:246:TYR:CD2	0.43	2.48	6	4
1:A:242:ILE:CD1	1:A:242:ILE:N	0.43	2.81	2	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:145:SER:C	1:A:146:PHE:CD1	0.43	2.92	18	1
1:A:153:ASP:OD2	1:A:166:HIS:CD2	0.43	2.71	18	1
1:A:85:THR:HG23	1:A:208:GLY:HA2	0.43	1.90	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:158:ASP:CG	1:A:158:ASP:O	0.43	2.56	18	1
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:208:GLY:C	1:A:210:PHE:H	0.43	2.17	3	1
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
1:A:86:PHE:HA	1:A:244:SER:HB3	0.42	1.91	2	3
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:167:ALA:C	1:A:168:TYR:CD2	0.42	2.93	13	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:153:ASP:CG	1:A:154:PHE:H	0.42	2.16	18	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:163:VAL:HG21	4:A:261:0DS:H51	0.42	1.91	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:ILE:CD1	1:A:101:ILE:N	0.42	2.82	20	1
1:A:103:ASN:HB3	1:A:146:PHE:CE2	0.42	2.49	1	1
1:A:146:PHE:C	1:A:146:PHE:CD1	0.42	2.92	7	2
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: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:197:LEU:CD1	1:A:197:LEU:C	0.42	2.87	3	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:227:THR:HG23	1:A:228:ASP:N	0.42	2.30	17	1
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
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:243:GLN:C	1:A:246:TYR:CD1	0.42	2.93	19	1
1:A:194:ASN:O	1:A:223:TYR:CE2	0.42	2.72	1	1
1:A:98:THR:HG21	1:A:140:ALA:CB	0.42	2.45	5	1
1:A:98:THR:CG2	1:A:99:TYR:N	0.42	2.83	5	1
1:A:99:TYR:CE1	1:A:134:ARG:N	0.42	2.87	17	1
1:A:163:VAL:CG2	4:A:261:0DS: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:197:LEU:HD13	1:A:223:TYR:HA	0.41	1.92	12	2
1:A:174:ILE:C	1:A:174:ILE:HD12	0.41	2.35	19	1
1:A:101:ILE:CD1	1:A:101:ILE:H	0.41	2.24	20	1
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:194:ASN:HB3	1:A:223:TYR:CE2	0.41	2.50	16	1
1:A:149:ARG:CG	1:A:149:ARG:O	0.41	2.68	17	1
1:A:202:GLU:C	1:A:204:GLY:N	0.41	2.71	17	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:184:GLU:OE1	1:A:186:TRP:CZ2	0.41	2.74	11	1
1:A:234:LEU:CD1	1:A:234:LEU:H	0.41	2.28	16	1
1:A:207:LEU:CG	1:A:207:LEU:O	0.41	2.65	17	1
1:A:199:ALA:O	1:A:203:ILE:N	0.41	2.52	2	1
1:A:157:PHE:CG	1:A:157:PHE:O	0.41	2.74	3	1
1:A:234:LEU:HB2	1:A:238:ASP:CG	0.41	2.36	4	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:261:0DS:H51	0.41	1.92	7	1
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:123:VAL:C	1:A:125:GLU:N	0.41	2.73	18	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:261:0DS:C1	4:A:261:0DS: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	1
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:261:0DS:H52	4:A:261:0DS: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:166:HIS:H	1:A:179:HIS:CE1	0.41	2.33	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:VAL:CG2	1:A:183:ASP:N	0.41	2.84	18	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:148:VAL:C	1:A:150:GLU:H	0.41	2.18	6	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:190:THR:CG2	1:A:190:THR:O	0.40	2.68	5	1
1:A:144:ILE:HG22	1:A:145:SER:H	0.40	1.76	15	2
1:A:222:LEU:HD13	1:A:223:TYR:C	0.40	2.37	6	1
1:A:192:GLY:C	1:A:193:THR:HG23	0.40	2.35	9	1
1:A:144:ILE:CG2	1:A:180:PHE:CD1	0.40	3.04	14	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:261:0DS: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:220:TYR:CD1	1:A:221:PRO:HD2	0.40	2.50	8	1
1:A:86:PHE:HB2	1:A:244:SER:HB3	0.40	1.93	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
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:HD13	1:A:195:LEU:O	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:202:GLU:O	1:A:203:ILE:C	0.40	2.59	17	1
1:A:246:TYR:C	1:A:248:PRO:CD	0.40	2.90	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:181:ASP:HB3	1:A:184:GLU:OE1	0.40	2.16	20	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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	118	GLU	19
1	A	117	VAL	19
1	A	211	HIS	19
1	A	175	ASN	19
1	A	129	PRO	19
1	A	162	ASN	19
1	A	191	THR	18
1	A	148	VAL	18
1	A	86	PHE	18
1	A	181	ASP	17
1	A	104	TYR	16
1	A	221	PRO	16
1	A	186	TRP	16
1	A	169	ALA	15
1	A	226	LEU	15
1	A	184	GLU	14
1	A	90	PRO	14
1	A	208	GLY	14
1	A	150	GLU	14
1	A	157	PHE	13
1	A	164	LEU	13
1	A	149	ARG	11
1	A	216	GLU	11
1	A	223	TYR	10
1	A	247	GLY	10
1	A	225	SER	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	89	ILE	10
1	A	156	PRO	10
1	A	234	LEU	10
1	A	155	TYR	9
1	A	170	PRO	9
1	A	163	VAL	9
1	A	241	GLY	9
1	A	224	HIS	8
1	A	233	ARG	8
1	A	135	LEU	8
1	A	171	GLY	7
1	A	92	TRP	7
1	A	138	GLY	6
1	A	235	SER	6
1	A	85	THR	6
1	A	231	ARG	6
1	A	227	THR	5
1	A	206	SER	5
1	A	84	ARG	5
1	A	144	ILE	5
1	A	145	SER	5
1	A	132	PHE	5
1	A	147	ALA	5
1	A	210	PHE	5
1	A	102	VAL	5
1	A	154	PHE	5
1	A	153	ASP	4
1	A	190	THR	4
1	A	228	ASP	4
1	A	215	THR	4
1	A	93	ARG	3
1	A	87	PRO	3
1	A	217	ALA	3
1	A	134	ARG	3
1	A	127	VAL	3
1	A	124	TRP	3
1	A	137	GLU	3
1	A	188	LYS	3
1	A	229	LEU	3
1	A	172	PRO	3
1	A	207	LEU	2
1	A	133	SER	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	139	GLU	2
1	A	196	PHE	2
1	A	159	GLY	2
1	A	187	THR	2
1	A	103	ASN	2
1	A	222	LEU	2
1	A	105	THR	2
1	A	240	ASN	2
1	A	152	GLY	2
1	A	140	ALA	1
1	A	193	THR	1
1	A	213	ALA	1
1	A	88	GLY	1
1	A	174	ILE	1
1	A	141	ASP	1
1	A	136	TYR	1
1	A	232	PHE	1
1	A	121	LEU	1
1	A	151	HIS	1
1	A	214	ASN	1
1	A	189	ASP	1
1	A	212	SER	1
1	A	230	THR	1
1	A	120	ALA	1
1	A	106	PRO	1
1	A	220	TYR	1
1	A	108	LEU	1
1	A	209	LEU	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	140/148 (95%)	104±4 (74±3%)	36±4 (26±3%)	2 24
All	All	2800/2960 (95%)	2085 (74%)	715 (26%)	2 24

All 108 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	195	LEU	20
1	A	184	GLU	20
1	A	164	LEU	20
1	A	222	LEU	19
1	A	101	ILE	19
1	A	129	PRO	19
1	A	149	ARG	18
1	A	143	MET	18
1	A	229	LEU	18
1	A	95	THR	17
1	A	226	LEU	17
1	A	207	LEU	16
1	A	179	HIS	15
1	A	142	ILE	14
1	A	205	HIS	14
1	A	209	LEU	14
1	A	125	GLU	13
1	A	197	LEU	13
1	A	187	THR	12
1	A	166	HIS	12
1	A	219	MET	12
1	A	85	THR	12
1	A	163	VAL	12
1	A	238	ASP	12
1	A	93	ARG	10
1	A	158	ASP	10
1	A	246	TYR	10
1	A	92	TRP	10
1	A	191	THR	9
1	A	198	VAL	9
1	A	174	ILE	9
1	A	124	TRP	9
1	A	242	ILE	8
1	A	221	PRO	8
1	A	121	LEU	8
1	A	104	TYR	7
1	A	232	PHE	7
1	A	128	THR	7
1	A	245	LEU	7
1	A	157	PHE	6
1	A	227	THR	6
1	A	175	ASN	6
1	A	168	TYR	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	239	ILE	6
1	A	136	TYR	6
1	A	182	ASP	6
1	A	194	ASN	6
1	A	181	ASP	6
1	A	156	PRO	6
1	A	202	GLU	6
1	A	151	HIS	6
1	A	135	LEU	6
1	A	223	TYR	5
1	A	90	PRO	5
1	A	98	THR	5
1	A	234	LEU	5
1	A	83	PHE	5
1	A	220	TYR	5
1	A	244	SER	4
1	A	153	ASP	4
1	A	110	LYS	4
1	A	134	ARG	4
1	A	218	LEU	4
1	A	105	THR	4
1	A	146	PHE	4
1	A	131	THR	3
1	A	84	ARG	3
1	A	130	LEU	3
1	A	196	PHE	3
1	A	148	VAL	3
1	A	89	ILE	3
1	A	203	ILE	3
1	A	86	PHE	3
1	A	150	GLU	3
1	A	189	ASP	3
1	A	210	PHE	3
1	A	193	THR	2
1	A	224	HIS	2
1	A	139	GLU	2
1	A	144	ILE	2
1	A	185	GLN	2
1	A	177	ASP	2
1	A	212	SER	2
1	A	154	PHE	2
1	A	162	ASN	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	243	GLN	2
1	A	155	TYR	1
1	A	133	SER	1
1	A	228	ASP	1
1	A	206	SER	1
1	A	87	PRO	1
1	A	113	VAL	1
1	A	99	TYR	1
1	A	141	ASP	1
1	A	170	PRO	1
1	A	97	LEU	1
1	A	201	HIS	1
1	A	111	ASP	1
1	A	132	PHE	1
1	A	214	ASN	1
1	A	127	VAL	1
1	A	180	PHE	1
1	A	91	LYS	1
1	A	188	LYS	1
1	A	94	LYS	1
1	A	236	GLN	1
1	A	106	PRO	1
1	A	108	LEU	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

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	1.28±0.00	1±0 (3±0%)

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	41,42,42	1.18±0.00	0±0 (0±0%)

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.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
4	A	261	0DS	O3-N3	6.16	1.24	1.40	9	20

There are no bond-angle outliers.

All unique chiral outliers are listed below.

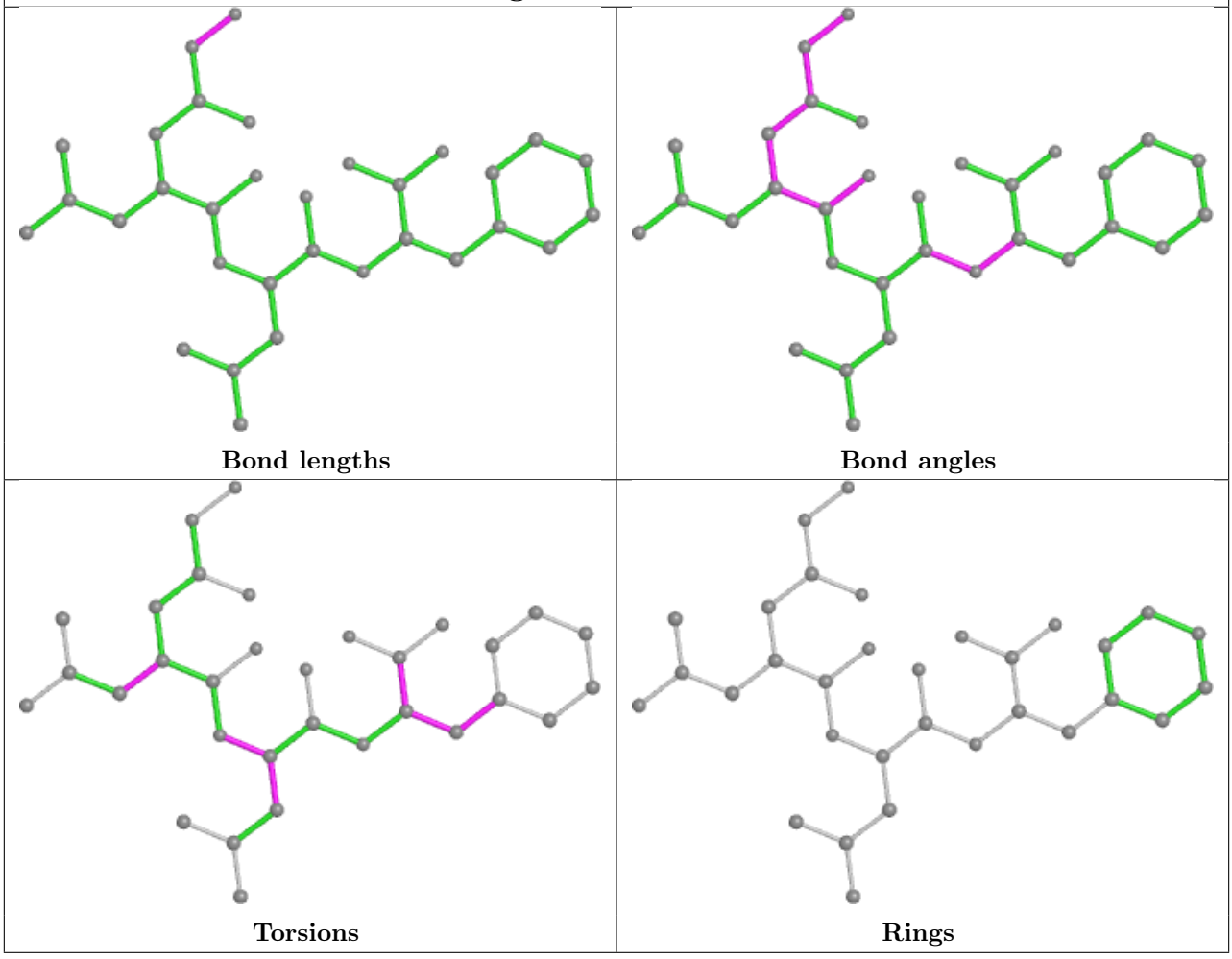
Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	261	0DS	C2	2

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 then 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.

Ligand 0DS A 261



6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided