



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:50 PM UTC

PDB ID : 1MT5 / pdb_00001mt5
Title : CRYSTAL STRUCTURE OF FATTY ACID AMIDE HYDROLASE
Authors : Bracey, M.H.; Hanson, M.A.; Masuda, K.R.; Stevens, R.C.; Cravatt, B.F.
Deposited on : 2002-09-20
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

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)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

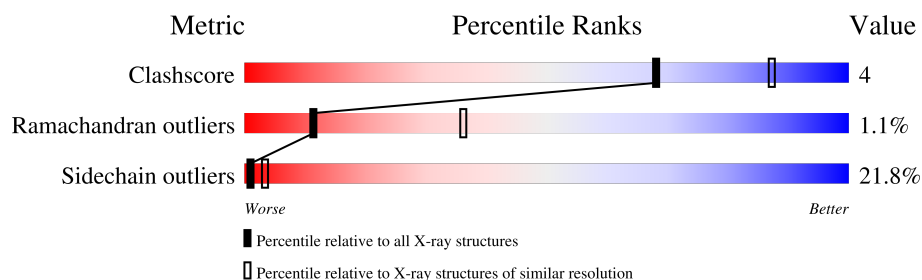
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	537	74% 23% .
1	B	537	75% 20% . .
1	C	537	75% 20% 5%
1	D	537	75% 20% . .
1	E	537	74% 21% . .
1	F	537	73% 21% 6%
1	G	537	74% 22% . .
1	H	537	73% 22% .

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Mol	Chain	Length	Quality of chain
1	I	537	 74%21%.
1	J	537	 74%21%5%.
1	K	537	 74%22%. .
1	L	537	 74%22%. .
1	M	537	 64%30%. .
1	N	537	 70%23%6%. .
1	O	537	 72%24%. .
1	P	537	 73%22%. .

2 Entry composition

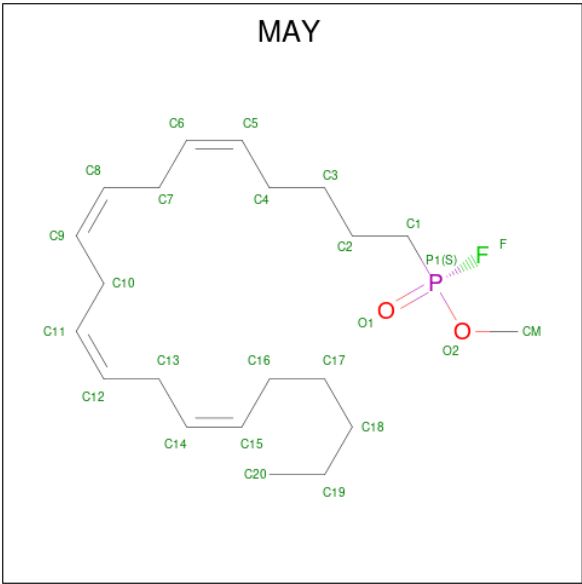
There are 2 unique types of molecules in this entry. The entry contains 64524 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fatty-acid amide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	B	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	C	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	D	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	E	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	F	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	G	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	H	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	I	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	J	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	K	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	L	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	M	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	N	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	O	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	P	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			

- Molecule 2 is METHYL ARACHIDONYL FLUOROPHOSPHONATE (CCD ID: MAY) (formula: C₂₁H₃₆FO₂P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			24	21	2	1		
2	B	1	Total	C	O	P	0	0
			24	21	2	1		
2	C	1	Total	C	O	P	0	0
			24	21	2	1		
2	D	1	Total	C	O	P	0	0
			24	21	2	1		
2	E	1	Total	C	O	P	0	0
			24	21	2	1		
2	F	1	Total	C	O	P	0	0
			24	21	2	1		
2	G	1	Total	C	O	P	0	0
			24	21	2	1		
2	H	1	Total	C	O	P	0	0
			24	21	2	1		
2	I	1	Total	C	O	P	0	0
			24	21	2	1		
2	J	1	Total	C	O	P	0	0
			24	21	2	1		
2	K	1	Total	C	O	P	0	0
			24	21	2	1		
2	L	1	Total	C	O	P	0	0
			24	21	2	1		

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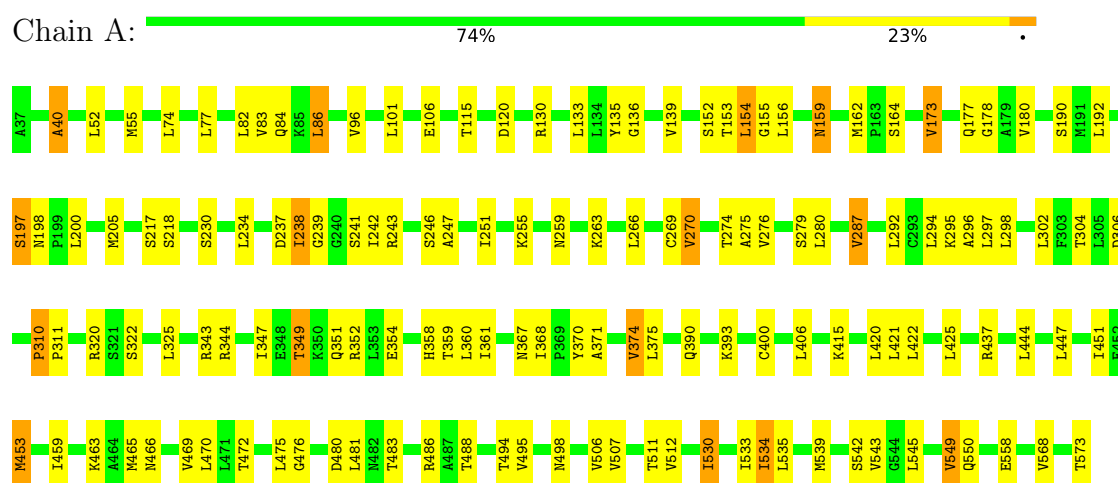
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	M	1	Total	C	O	P	0	0
			24	21	2	1		
2	N	1	Total	C	O	P	0	0
			24	21	2	1		
2	O	1	Total	C	O	P	0	0
			24	21	2	1		
2	P	1	Total	C	O	P	0	0
			24	21	2	1		

3 Residue-property plots

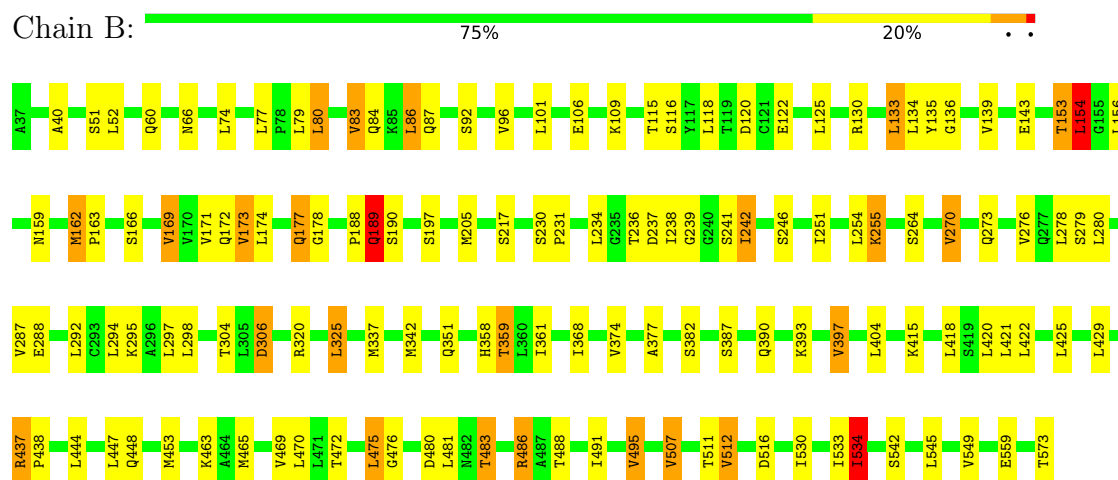
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: Fatty-acid amide hydrolase

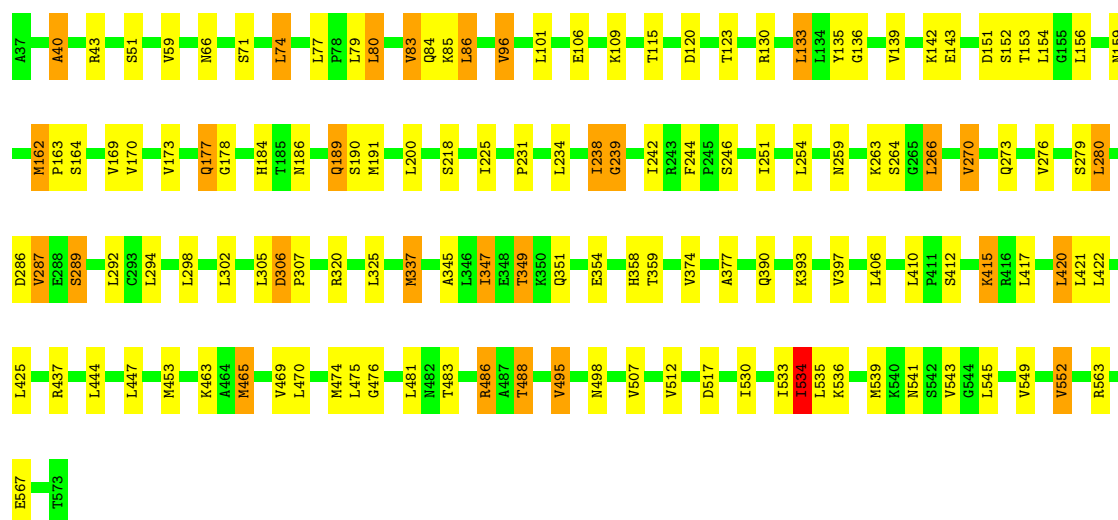


• Molecule 1: Fatty-acid amide hydrolase



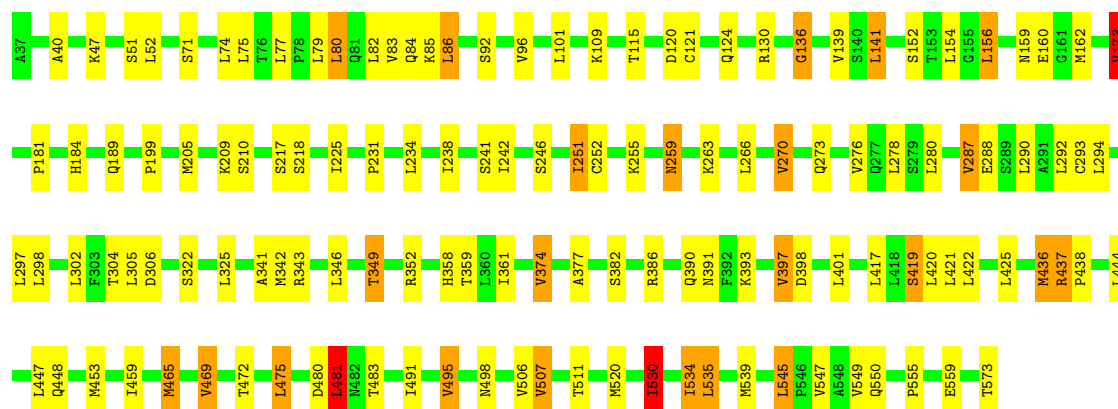
• Molecule 1: Fatty-acid amide hydrolase





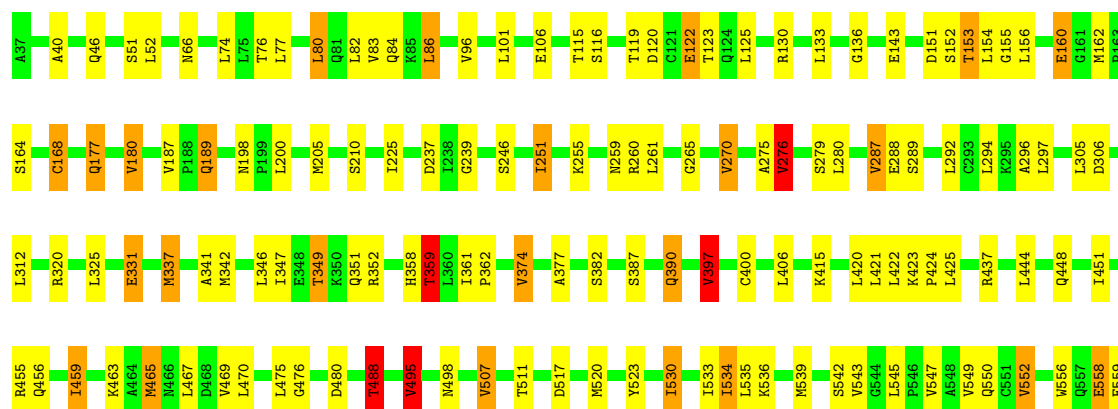
• Molecule 1: Fatty-acid amide hydrolase

Chain D: 75% 20%



• Molecule 1: Fatty-acid amide hydrolase

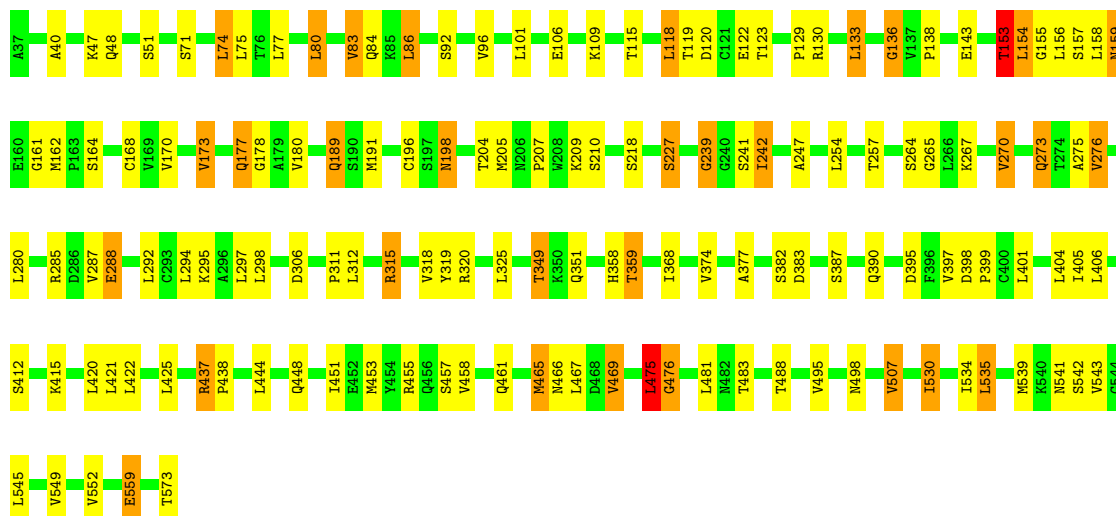
Chain E: 74% 21%





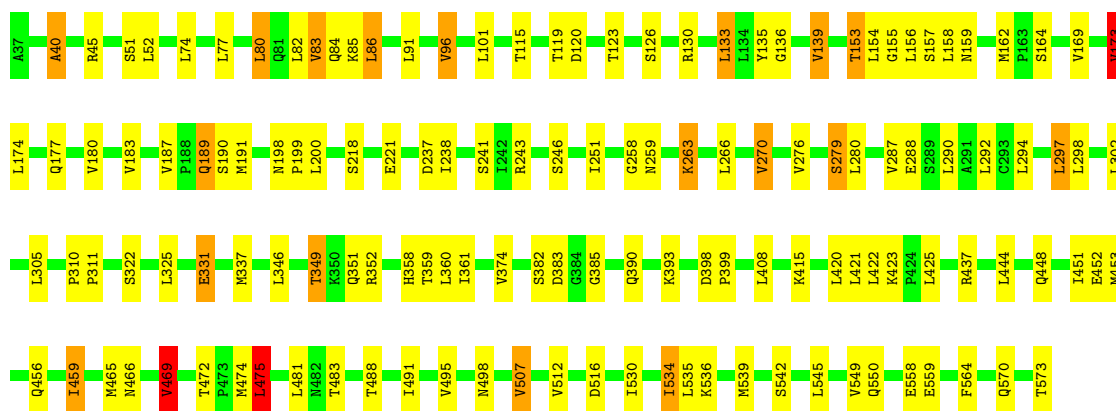
• Molecule 1: Fatty-acid amide hydrolase

Chain F:  73% 21% 6%



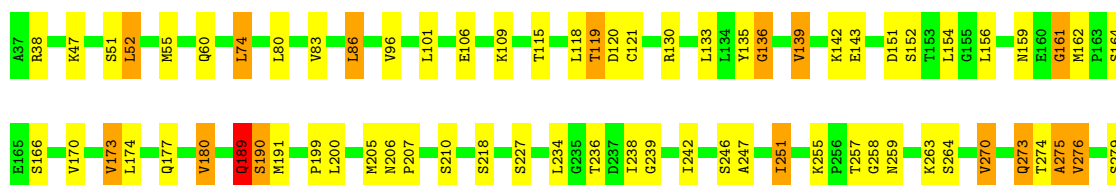
• Molecule 1: Fatty-acid amide hydrolase

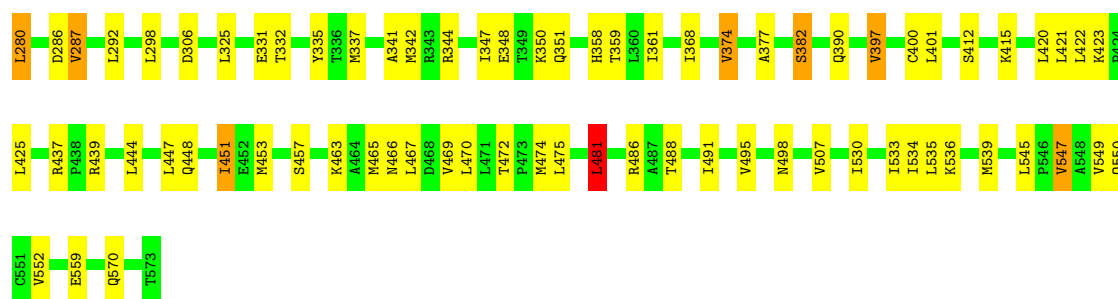
Chain G:  74% 22% 4%



• Molecule 1: Fatty-acid amide hydrolase

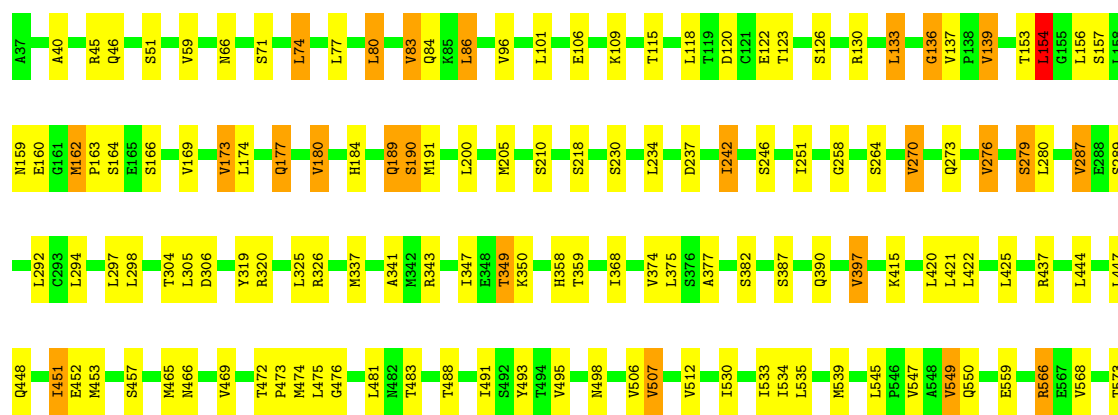
Chain H:  73% 22% 5%





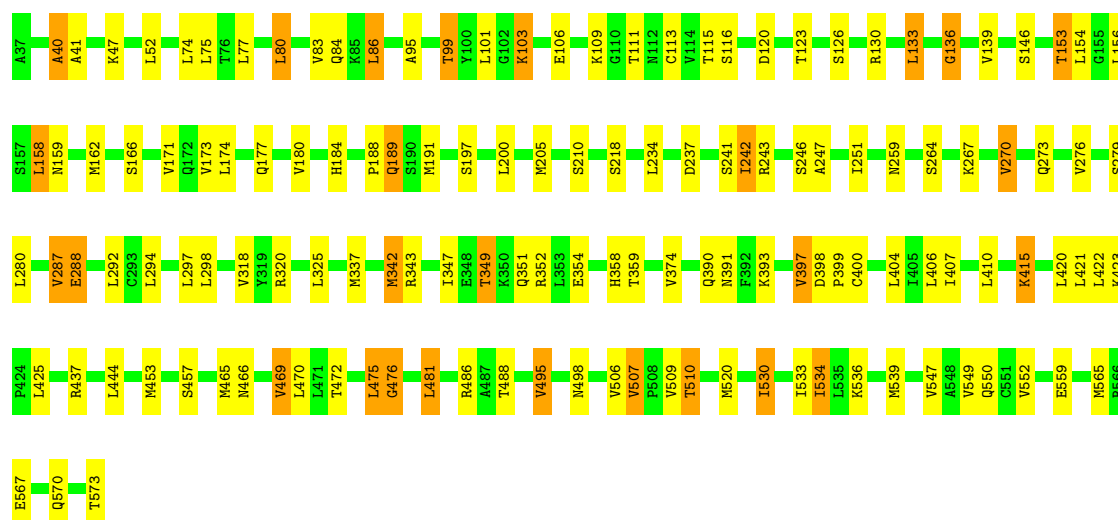
- Molecule 1: Fatty-acid amide hydrolase

Chain I: 74% 21%



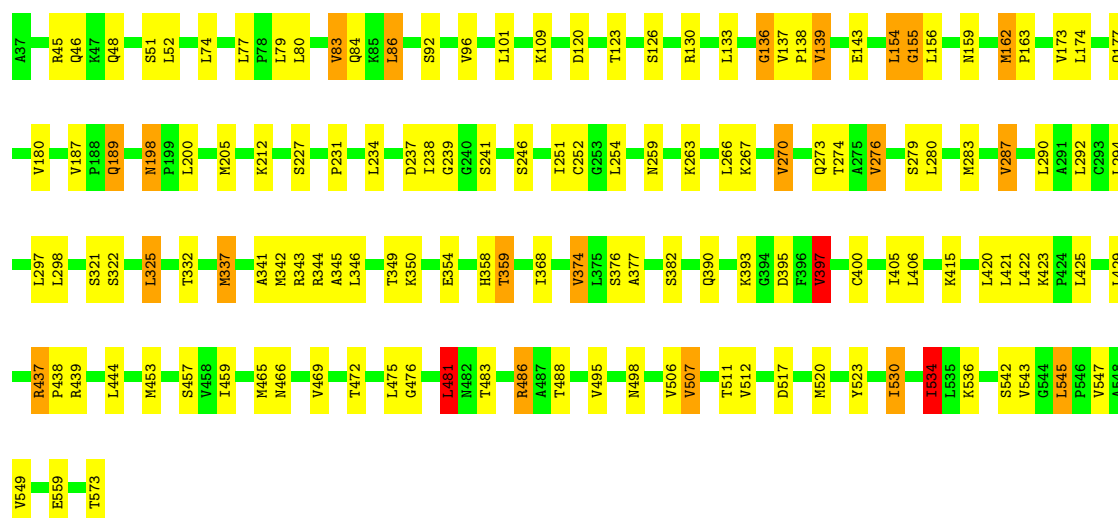
- Molecule 1: Fatty-acid amide hydrolase

Chain J: 74% 21% 5%



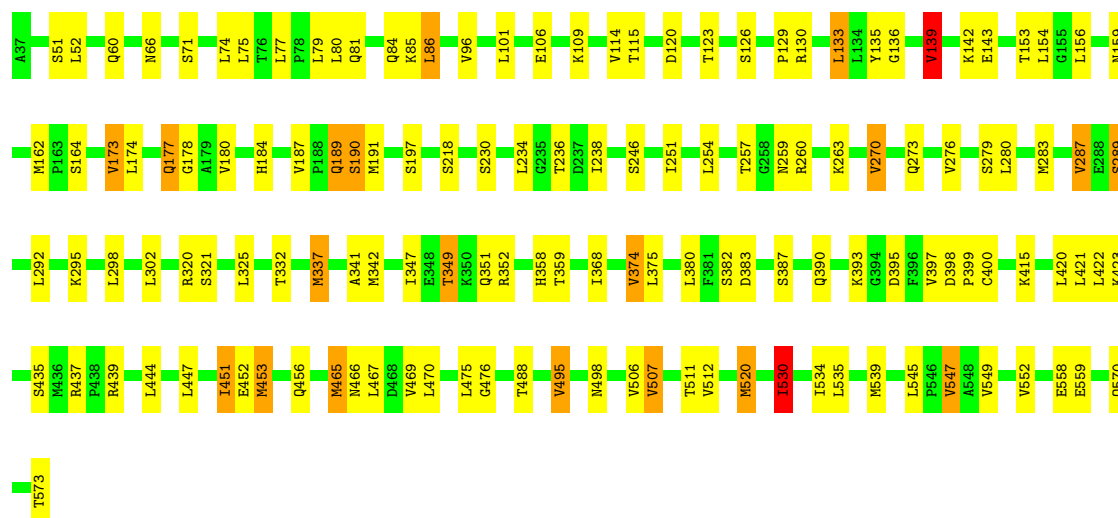
- Molecule 1: Fatty-acid amide hydrolase

Chain K: 74% 22%



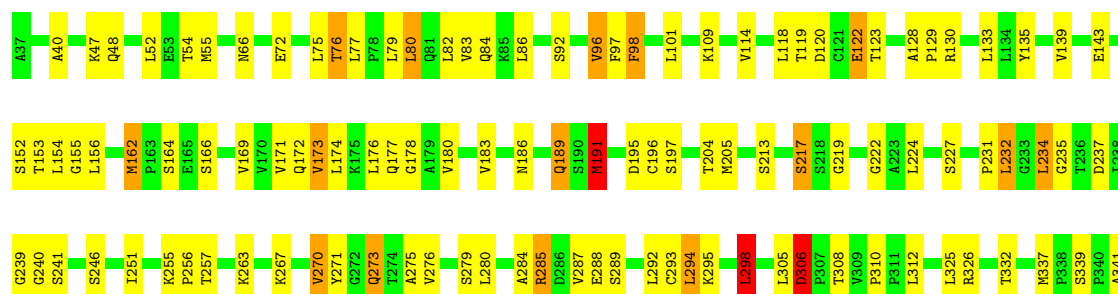
• Molecule 1: Fatty-acid amide hydrolase

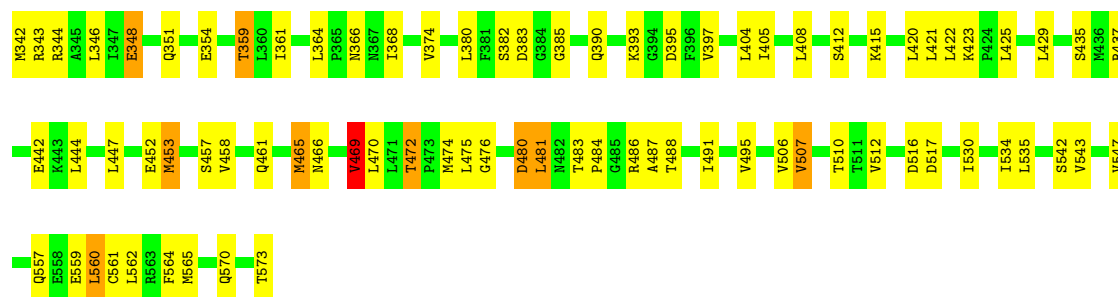
Chain L: 74% 22%



• Molecule 1: Fatty-acid amide hydrolase

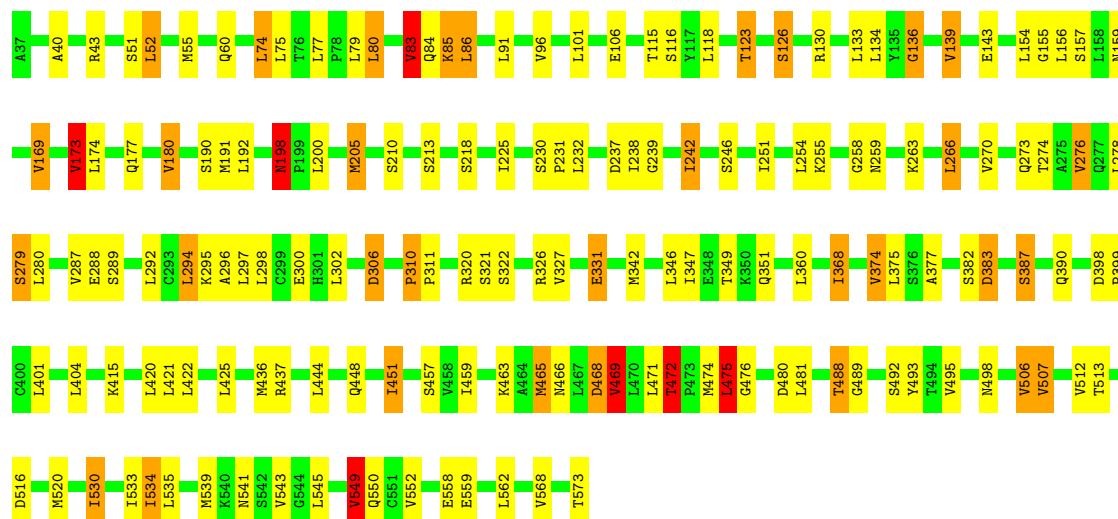
Chain M: 64% 30%





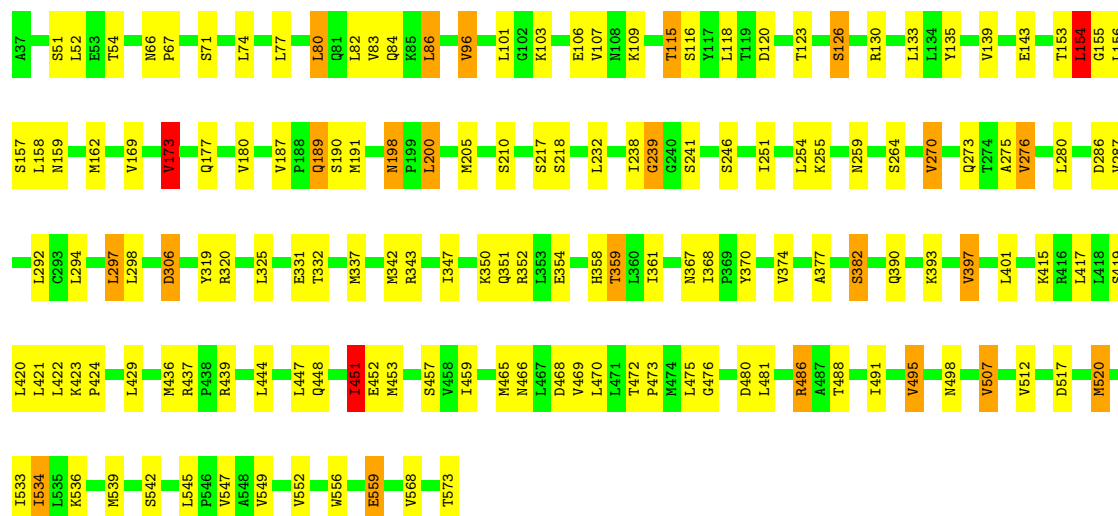
- Molecule 1: Fatty-acid amide hydrolase

Chain N: 70% 23% 6% •



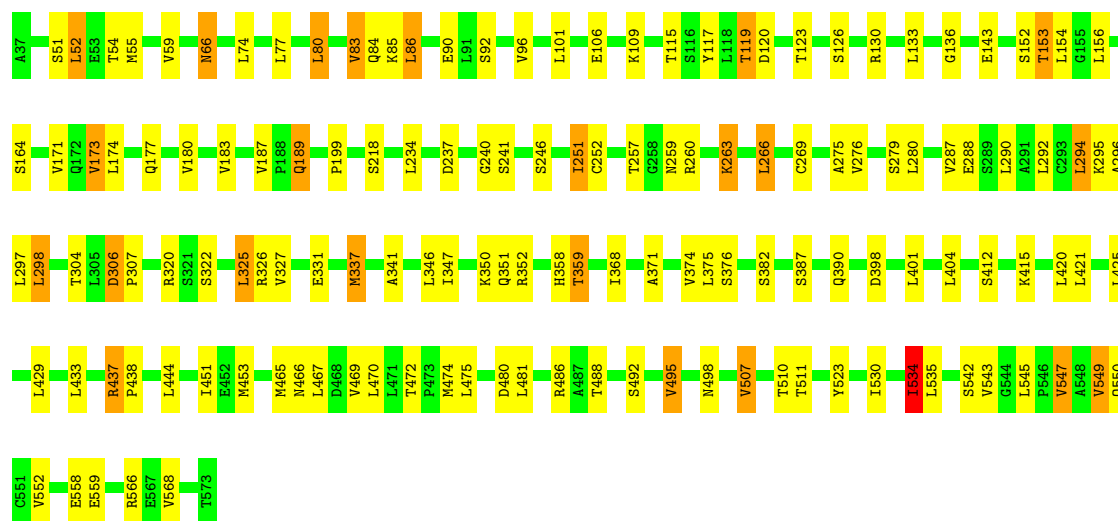
- Molecule 1: Fatty-acid amide hydrolase

Chain O: 72% 24% • •



- Molecule 1: Fatty-acid amide hydrolase

Chain P:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	147.11Å 272.02Å 147.22Å 90.00° 115.21° 90.00°	Depositor
Resolution (Å)	141.42 – 2.80	Depositor
% Data completeness (in resolution range)	71.4 (141.42-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.218 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	64524	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAY

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 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	1.25	23/4102 (0.6%)	1.15	0/5589
1	B	1.28	21/4100 (0.5%)	1.14	0/5586
1	C	1.25	21/4100 (0.5%)	1.15	5/5586 (0.1%)
1	D	1.25	19/4100 (0.5%)	1.15	3/5586 (0.1%)
1	E	1.30	27/4100 (0.7%)	1.12	1/5586 (0.0%)
1	F	1.29	22/4100 (0.5%)	1.16	5/5586 (0.1%)
1	G	1.26	20/4102 (0.5%)	1.14	6/5589 (0.1%)
1	H	1.22	17/4100 (0.4%)	1.14	5/5586 (0.1%)
1	I	1.27	24/4102 (0.6%)	1.13	4/5589 (0.1%)
1	J	1.27	21/4100 (0.5%)	1.14	2/5586 (0.0%)
1	K	1.29	23/4100 (0.6%)	1.15	2/5586 (0.0%)
1	L	1.31	20/4102 (0.5%)	1.16	4/5589 (0.1%)
1	M	1.47	34/4102 (0.8%)	1.18	7/5589 (0.1%)
1	N	1.40	34/4100 (0.8%)	1.16	1/5586 (0.0%)
1	O	1.26	23/4102 (0.6%)	1.15	4/5589 (0.1%)
1	P	1.32	20/4100 (0.5%)	1.15	2/5586 (0.0%)
All	All	1.29	369/65612 (0.6%)	1.15	51/89394 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	4
1	E	0	4
1	F	0	6
1	G	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	6
1	I	0	5
1	J	0	4
1	K	0	3
1	L	0	1
1	M	0	4
1	N	0	4
1	O	0	4
1	P	0	2
All	All	0	57

All (369) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	368	ILE	CA-CB	12.93	1.60	1.54
1	P	507	VAL	CA-CB	11.90	1.63	1.54
1	F	368	ILE	CA-CB	11.68	1.59	1.54
1	B	368	ILE	CA-CB	11.51	1.59	1.54
1	L	287	VAL	CA-CB	10.26	1.66	1.54
1	L	368	ILE	CA-CB	10.02	1.59	1.54
1	D	507	VAL	CA-CB	9.84	1.66	1.54
1	P	368	ILE	CA-CB	9.79	1.59	1.54
1	F	83	VAL	CA-CB	9.58	1.66	1.54
1	O	436	MET	SD-CE	-9.43	1.55	1.79
1	L	453	MET	SD-CE	9.28	2.02	1.79
1	P	507	VAL	CA-C	9.23	1.59	1.52
1	B	270	VAL	CA-CB	9.21	1.65	1.54
1	A	549	VAL	CA-CB	9.15	1.67	1.54
1	B	83	VAL	CA-CB	9.09	1.66	1.54
1	I	287	VAL	CA-CB	9.04	1.65	1.54
1	J	347	ILE	CA-CB	8.98	1.65	1.54
1	G	173	VAL	CA-CB	8.83	1.66	1.54
1	N	83	VAL	CA-CB	8.77	1.65	1.54
1	D	453	MET	SD-CE	8.74	2.01	1.79
1	M	507	VAL	CA-CB	8.64	1.65	1.54
1	I	349	THR	CA-CB	8.63	1.67	1.53
1	A	287	VAL	CA-CB	8.61	1.67	1.54
1	F	349	THR	CA-CB	8.53	1.67	1.53
1	I	568	VAL	CA-CB	8.30	1.64	1.54
1	P	173	VAL	CA-CB	8.29	1.66	1.54
1	F	270	VAL	CA-CB	8.18	1.65	1.54
1	C	552	VAL	CA-CB	8.16	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	507	VAL	CA-CB	8.16	1.60	1.54
1	D	270	VAL	CA-CB	8.14	1.65	1.54
1	N	191	MET	SD-CE	8.07	1.99	1.79
1	E	349	THR	CA-CB	8.03	1.67	1.53
1	D	374	VAL	CA-CB	7.98	1.64	1.54
1	N	533	ILE	CA-CB	7.96	1.63	1.54
1	K	287	VAL	CA-CB	7.92	1.65	1.54
1	B	453	MET	SD-CE	7.92	1.99	1.79
1	P	83	VAL	CA-CB	7.83	1.65	1.54
1	J	533	ILE	CA-CB	7.80	1.63	1.54
1	L	270	VAL	CA-CB	7.79	1.66	1.54
1	I	507	VAL	CA-CB	7.78	1.64	1.54
1	O	276	VAL	CA-CB	7.75	1.65	1.54
1	F	453	MET	SD-CE	7.74	1.99	1.79
1	D	397	VAL	CA-CB	7.71	1.63	1.54
1	H	474	MET	SD-CE	-7.71	1.60	1.79
1	E	153	THR	CA-CB	7.68	1.62	1.53
1	J	397	VAL	CA-CB	7.68	1.63	1.54
1	G	83	VAL	CA-CB	7.67	1.65	1.54
1	P	453	MET	SD-CE	7.67	1.98	1.79
1	N	242	ILE	CA-CB	7.59	1.64	1.54
1	H	368	ILE	CA-CB	7.56	1.57	1.54
1	E	495	VAL	CA-CB	7.53	1.65	1.54
1	N	507	VAL	CA-CB	7.51	1.63	1.54
1	K	332	THR	CA-CB	7.46	1.66	1.53
1	C	238	ILE	CA-CB	7.45	1.63	1.54
1	L	512	VAL	CA-CB	7.45	1.62	1.53
1	F	469	VAL	CA-C	7.42	1.60	1.52
1	M	83	VAL	CA-CB	7.40	1.63	1.54
1	C	191	MET	SD-CE	7.37	1.98	1.79
1	E	534	ILE	CA-CB	7.35	1.64	1.54
1	G	187	VAL	CA-CB	7.35	1.61	1.55
1	D	495	VAL	CA-CB	7.34	1.64	1.54
1	M	284	ALA	N-CA	7.31	1.55	1.46
1	A	173	VAL	CA-CB	7.31	1.64	1.54
1	G	349	THR	CA-CB	7.30	1.66	1.53
1	J	507	VAL	CA-CB	7.28	1.63	1.54
1	B	507	VAL	CA-CB	7.25	1.63	1.54
1	L	530	ILE	CA-CB	7.21	1.64	1.54
1	F	465	MET	SD-CE	7.20	1.97	1.79
1	M	306	ASP	N-CA	7.18	1.56	1.46
1	M	96	VAL	CA-CB	7.14	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	495	VAL	CA-CB	7.10	1.64	1.54
1	D	139	VAL	CA-CB	7.08	1.64	1.54
1	E	180	VAL	CA-CB	7.07	1.63	1.54
1	C	533	ILE	CA-CB	7.04	1.62	1.54
1	F	153	THR	CA-CB	7.04	1.64	1.53
1	C	453	MET	SD-CE	7.03	1.97	1.79
1	I	270	VAL	CA-CB	7.01	1.64	1.54
1	M	173	VAL	CA-CB	6.99	1.63	1.54
1	G	139	VAL	CA-CB	6.99	1.63	1.54
1	A	368	ILE	CA-CB	6.97	1.57	1.54
1	O	368	ILE	CA-CB	6.97	1.63	1.54
1	C	337	MET	SD-CE	6.95	1.97	1.79
1	E	397	VAL	CA-CB	6.93	1.62	1.54
1	B	512	VAL	CA-CB	6.92	1.62	1.53
1	C	474	MET	SD-CE	-6.91	1.62	1.79
1	F	173	VAL	CA-CB	6.91	1.63	1.54
1	N	534	ILE	CA-CB	6.90	1.62	1.54
1	O	306	ASP	N-CA	6.88	1.55	1.46
1	E	530	ILE	CA-CB	6.88	1.64	1.54
1	I	180	VAL	CA-CB	6.88	1.63	1.54
1	J	247	ALA	CA-CB	-6.87	1.41	1.53
1	O	397	VAL	CA-CB	6.85	1.62	1.54
1	K	359	THR	CA-CB	6.80	1.63	1.53
1	I	276	VAL	N-CA	6.79	1.54	1.46
1	P	347	ILE	CA-CB	6.79	1.64	1.54
1	K	374	VAL	CA-CB	6.76	1.62	1.54
1	N	465	MET	SD-CE	6.76	1.96	1.79
1	O	451	ILE	CA-CB	6.75	1.62	1.54
1	L	507	VAL	CA-CB	6.75	1.62	1.54
1	N	310	PRO	CA-C	6.74	1.58	1.52
1	K	83	VAL	CA-CB	6.74	1.63	1.54
1	E	533	ILE	CA-CB	6.72	1.62	1.54
1	I	491	ILE	CA-CB	6.72	1.62	1.54
1	I	83	VAL	CA-CB	6.71	1.64	1.54
1	J	565	MET	SD-CE	6.71	1.96	1.79
1	D	162	MET	SD-CE	6.68	1.96	1.79
1	M	270	VAL	CA-CB	6.66	1.63	1.54
1	E	507	VAL	CA-CB	6.65	1.62	1.54
1	G	453	MET	SD-CE	6.65	1.96	1.79
1	N	374	VAL	CA-CB	6.65	1.64	1.54
1	C	270	VAL	CA-CB	6.64	1.62	1.54
1	D	173	VAL	CA-CB	6.64	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	512	VAL	CA-CB	6.63	1.61	1.53
1	G	40	ALA	CA-C	6.63	1.61	1.52
1	B	359	THR	CA-CB	6.62	1.62	1.53
1	J	270	VAL	CA-CB	6.62	1.62	1.54
1	C	83	VAL	CA-CB	6.60	1.64	1.54
1	C	244	PHE	N-CA	6.59	1.51	1.46
1	F	318	VAL	CA-CB	6.59	1.63	1.54
1	K	507	VAL	CA-CB	6.56	1.62	1.54
1	A	530	ILE	CA-CB	6.55	1.64	1.54
1	N	568	VAL	CA-CB	6.54	1.62	1.54
1	A	270	VAL	CA-CB	6.54	1.64	1.55
1	I	59	VAL	CA-CB	6.54	1.63	1.54
1	K	397	VAL	CA-CB	6.53	1.62	1.54
1	K	453	MET	SD-CE	6.52	1.95	1.79
1	B	469	VAL	CA-CB	6.52	1.64	1.55
1	N	139	VAL	CA-CB	6.50	1.62	1.54
1	O	359	THR	CA-CB	6.50	1.63	1.53
1	G	162	MET	SD-CE	6.48	1.95	1.79
1	H	180	VAL	CA-CB	6.47	1.62	1.54
1	M	139	VAL	CA-CB	6.46	1.63	1.54
1	J	349	THR	CA-CB	6.46	1.64	1.53
1	E	337	MET	SD-CE	6.44	1.95	1.79
1	I	173	VAL	CA-CB	6.44	1.62	1.54
1	C	139	VAL	CA-CB	6.42	1.62	1.54
1	E	552	VAL	CA-CB	6.42	1.63	1.54
1	L	187	VAL	CA-CB	6.41	1.60	1.55
1	G	96	VAL	CA-CB	6.41	1.62	1.54
1	L	465	MET	SD-CE	6.41	1.95	1.79
1	O	512	VAL	CA-CB	6.40	1.61	1.53
1	E	287	VAL	CA-CB	6.39	1.62	1.54
1	L	173	VAL	CA-CB	6.39	1.63	1.54
1	O	533	ILE	CA-CB	6.38	1.61	1.54
1	B	306	ASP	CA-C	6.38	1.60	1.52
1	O	83	VAL	CA-CB	6.38	1.62	1.54
1	A	180	VAL	CA-CB	6.38	1.62	1.54
1	C	347	ILE	CA-CB	6.37	1.62	1.54
1	H	533	ILE	CA-CB	6.34	1.61	1.54
1	J	534	ILE	CA-CB	6.33	1.61	1.54
1	J	453	MET	SD-CE	6.33	1.95	1.79
1	N	472	THR	CA-C	6.32	1.59	1.52
1	M	191	MET	SD-CE	6.30	1.95	1.79
1	N	173	VAL	CA-CB	6.30	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	318	VAL	CA-CB	6.30	1.63	1.54
1	M	491	ILE	CA-CB	6.29	1.61	1.54
1	G	270	VAL	CA-CB	6.29	1.64	1.55
1	N	475	LEU	N-CA	6.28	1.54	1.46
1	K	270	VAL	CA-CB	6.27	1.62	1.54
1	N	530	ILE	CA-CB	6.23	1.65	1.54
1	G	451	ILE	CA-CB	6.21	1.62	1.54
1	I	451	ILE	CA-CB	6.21	1.62	1.54
1	N	552	VAL	CA-C	6.20	1.60	1.52
1	O	173	VAL	CA-CB	6.19	1.63	1.54
1	P	59	VAL	CA-CB	6.19	1.62	1.54
1	L	191	MET	SD-CE	6.18	1.95	1.79
1	M	483	THR	CA-C	6.16	1.60	1.52
1	M	469	VAL	CA-C	6.16	1.60	1.52
1	M	423	LYS	CA-C	6.15	1.58	1.52
1	B	361	ILE	CA-CB	6.14	1.59	1.54
1	O	453	MET	SD-CE	6.14	1.94	1.79
1	B	533	ILE	CA-CB	6.13	1.61	1.54
1	L	337	MET	SD-CE	6.12	1.94	1.79
1	N	368	ILE	CA-CB	6.12	1.62	1.54
1	I	154	LEU	C-O	-6.09	1.15	1.24
1	P	153	THR	CA-CB	6.08	1.61	1.53
1	N	451	ILE	CA-CB	6.06	1.62	1.54
1	B	491	ILE	CA-CB	6.05	1.61	1.54
1	L	114	VAL	CA-CB	6.04	1.61	1.53
1	A	453	MET	SD-CE	6.04	1.94	1.79
1	M	114	VAL	CA-CB	6.04	1.62	1.54
1	F	451	ILE	CA-CB	6.03	1.61	1.54
1	A	533	ILE	CA-CB	6.02	1.62	1.54
1	F	247	ALA	CA-CB	-6.02	1.43	1.53
1	K	238	ILE	CA-C	6.01	1.61	1.52
1	L	180	VAL	CA-CB	6.00	1.61	1.54
1	C	512	VAL	CA-CB	6.00	1.61	1.53
1	D	287	VAL	CA-CB	5.99	1.61	1.54
1	B	189	GLN	C-O	-5.97	1.16	1.24
1	K	276	VAL	CA-CB	5.97	1.62	1.54
1	N	506	VAL	CA-CB	5.96	1.62	1.54
1	N	276	VAL	CA-CB	5.95	1.62	1.54
1	N	230	SER	CA-C	5.93	1.58	1.52
1	K	459	ILE	CA-CB	5.92	1.61	1.54
1	E	83	VAL	CA-CB	5.91	1.61	1.54
1	K	534	ILE	CA-CB	5.90	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	347	ILE	CA-CB	5.89	1.61	1.54
1	G	474	MET	SD-CE	-5.87	1.64	1.79
1	H	397	VAL	CA-CB	5.86	1.61	1.54
1	A	247	ALA	CA-CB	-5.86	1.43	1.53
1	E	187	VAL	CA-C	5.85	1.59	1.52
1	O	191	MET	SD-CE	5.85	1.94	1.79
1	I	397	VAL	CA-CB	5.83	1.61	1.54
1	J	407	ILE	CA-CB	5.83	1.62	1.54
1	F	552	VAL	CA-C	5.82	1.59	1.52
1	D	349	THR	CA-CB	5.81	1.63	1.53
1	K	483	THR	CA-C	5.80	1.60	1.52
1	I	347	ILE	CA-CB	5.79	1.61	1.54
1	K	337	MET	SD-CE	5.78	1.94	1.79
1	A	238	ILE	N-CA	5.78	1.51	1.46
1	H	270	VAL	CA-CB	5.78	1.64	1.55
1	L	349	THR	CA-CB	5.77	1.62	1.53
1	M	98	PHE	CA-C	5.77	1.60	1.52
1	M	560	LEU	CA-C	5.77	1.60	1.52
1	B	173	VAL	CA-CB	5.76	1.62	1.54
1	E	423	LYS	CA-CB	5.75	1.59	1.54
1	H	173	VAL	CA-CB	5.75	1.62	1.54
1	C	242	ILE	CA-CB	5.74	1.63	1.54
1	C	465	MET	SD-CE	5.73	1.93	1.79
1	N	474	MET	CA-C	5.73	1.59	1.52
1	E	359	THR	CA-CB	5.73	1.62	1.53
1	E	276	VAL	CA-CB	5.72	1.62	1.54
1	J	153	THR	CA-CB	5.71	1.62	1.53
1	N	513	THR	CA-CB	5.71	1.62	1.53
1	O	187	VAL	CA-CB	5.70	1.61	1.54
1	A	349	THR	CA-CB	5.70	1.63	1.53
1	D	534	ILE	CA-CB	5.69	1.61	1.54
1	O	423	LYS	N-CA	5.69	1.52	1.46
1	E	270	VAL	CA-CB	5.68	1.62	1.54
1	K	342	MET	SD-CE	-5.67	1.65	1.79
1	N	205	MET	SD-CE	5.66	1.93	1.79
1	A	274	THR	CA-CB	5.66	1.60	1.53
1	F	242	ILE	CA-CB	5.66	1.62	1.54
1	M	472	THR	CA-C	5.66	1.57	1.52
1	N	327	VAL	CA-CB	5.66	1.60	1.53
1	D	251	ILE	CA-CB	5.66	1.62	1.54
1	I	368	ILE	CA-C	5.64	1.59	1.52
1	M	368	ILE	CA-CB	5.64	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	530	ILE	N-CA	5.64	1.53	1.46
1	I	453	MET	SD-CE	5.64	1.93	1.79
1	I	368	ILE	CA-CB	5.63	1.56	1.54
1	N	306	ASP	N-CA	5.63	1.54	1.46
1	H	547	VAL	CA-CB	5.62	1.62	1.54
1	M	122	GLU	N-CA	5.61	1.53	1.46
1	N	274	THR	CA-CB	5.61	1.62	1.54
1	J	423	LYS	CA-CB	5.60	1.60	1.53
1	I	549	VAL	CA-CB	5.59	1.64	1.54
1	A	374	VAL	CA-CB	5.59	1.60	1.55
1	D	469	VAL	CA-CB	5.58	1.62	1.54
1	N	469	VAL	CA-CB	5.57	1.62	1.54
1	P	66	ASN	CA-C	5.57	1.59	1.52
1	C	287	VAL	CA-CB	5.56	1.62	1.54
1	B	171	VAL	CA-CB	5.54	1.60	1.54
1	M	119	THR	CA-CB	5.54	1.61	1.53
1	M	162	MET	SD-CE	5.54	1.93	1.79
1	K	189	GLN	C-O	-5.54	1.17	1.24
1	A	40	ALA	CA-C	5.54	1.60	1.52
1	A	310	PRO	CA-C	5.53	1.57	1.52
1	F	276	VAL	CA-CB	5.53	1.61	1.54
1	K	187	VAL	CA-CB	5.53	1.59	1.55
1	C	488	THR	CA-CB	5.52	1.63	1.53
1	P	119	THR	CA-CB	5.52	1.62	1.53
1	E	565	MET	SD-CE	-5.52	1.65	1.79
1	J	530	ILE	CA-CB	5.51	1.62	1.54
1	O	507	VAL	CA-CB	5.51	1.61	1.54
1	C	59	VAL	CA-CB	5.49	1.61	1.54
1	M	359	THR	CA-CB	5.49	1.61	1.53
1	G	491	ILE	CA-CB	5.49	1.61	1.54
1	J	469	VAL	CA-C	5.49	1.58	1.52
1	M	337	MET	SD-CE	5.49	1.93	1.79
1	D	306	ASP	CA-C	5.48	1.59	1.52
1	P	549	VAL	CA-CB	5.48	1.62	1.54
1	B	368	ILE	CA-C	5.47	1.58	1.52
1	B	154	LEU	C-O	-5.47	1.15	1.23
1	D	436	MET	SD-CE	-5.46	1.65	1.79
1	F	530	ILE	CA-CB	5.45	1.62	1.54
1	E	347	ILE	CA-CB	5.44	1.61	1.54
1	I	533	ILE	CA-CB	5.44	1.60	1.54
1	N	347	ILE	CA-CB	5.44	1.60	1.54
1	F	359	THR	CA-CB	5.44	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	469	VAL	CA-CB	5.43	1.61	1.54
1	N	300	GLU	CA-C	5.43	1.60	1.52
1	I	512	VAL	CA-CB	5.43	1.60	1.53
1	D	530	ILE	CA-CB	5.42	1.62	1.54
1	K	530	ILE	CA-CB	5.42	1.63	1.54
1	F	138	PRO	CA-C	5.42	1.58	1.52
1	E	459	ILE	CA-CB	5.40	1.61	1.54
1	M	235	GLY	N-CA	5.39	1.49	1.44
1	M	510	THR	CA-CB	5.38	1.62	1.53
1	D	459	ILE	CA-CB	5.38	1.61	1.54
1	J	40	ALA	CA-CB	-5.38	1.45	1.52
1	P	510	THR	CA-CB	5.37	1.62	1.53
1	N	180	VAL	CA-CB	5.37	1.61	1.54
1	M	458	VAL	CA-CB	5.37	1.61	1.54
1	G	534	ILE	CA-CB	5.36	1.61	1.54
1	B	534	ILE	CA-CB	5.36	1.61	1.54
1	I	474	MET	SD-CE	-5.36	1.66	1.79
1	N	270	VAL	CA-CB	5.35	1.62	1.54
1	H	83	VAL	CA-CB	5.35	1.62	1.54
1	H	287	VAL	CA-CB	5.35	1.62	1.54
1	M	139	VAL	N-CA	5.35	1.52	1.46
1	B	153	THR	CA-CB	5.34	1.61	1.53
1	M	453	MET	SD-CE	5.33	1.92	1.79
1	O	347	ILE	CA-CB	5.33	1.61	1.54
1	P	187	VAL	CA-CB	5.33	1.59	1.55
1	A	568	VAL	CA-CB	5.32	1.61	1.54
1	M	512	VAL	CA-CB	5.31	1.60	1.54
1	E	361	ILE	CA-C	5.29	1.57	1.52
1	F	122	GLU	N-CA	5.29	1.53	1.46
1	P	327	VAL	CA-CB	5.28	1.60	1.54
1	B	242	ILE	CA-CB	5.28	1.61	1.54
1	G	507	VAL	CA-CB	5.28	1.60	1.54
1	H	247	ALA	CA-CB	-5.27	1.45	1.53
1	L	139	VAL	CA-CB	5.27	1.60	1.54
1	I	191	MET	SD-CE	5.26	1.92	1.79
1	A	230	SER	CA-C	5.25	1.58	1.52
1	A	368	ILE	CA-C	5.25	1.58	1.52
1	G	423	LYS	CA-CB	5.25	1.60	1.53
1	J	83	VAL	CA-CB	5.25	1.62	1.54
1	G	187	VAL	CA-C	5.25	1.56	1.52
1	O	568	VAL	CA-CB	5.25	1.61	1.54
1	A	512	VAL	CA-CB	5.23	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	459	ILE	CA-CB	5.23	1.61	1.54
1	P	566	ARG	NE-CZ	5.23	1.38	1.33
1	M	366	ASN	N-CA	5.22	1.52	1.45
1	J	287	VAL	CA-CB	5.22	1.60	1.54
1	G	361	ILE	CA-CB	5.21	1.58	1.54
1	C	96	VAL	CA-CB	5.21	1.61	1.54
1	H	119	THR	CA-CB	5.21	1.61	1.53
1	A	242	ILE	CA-CB	5.21	1.61	1.54
1	E	374	VAL	CA-CB	5.20	1.61	1.54
1	K	274	THR	N-CA	5.18	1.52	1.46
1	P	359	THR	CA-CB	5.17	1.61	1.53
1	L	190	SER	CA-CB	-5.17	1.45	1.53
1	H	491	ILE	CA-CB	5.17	1.60	1.54
1	P	534	ILE	CA-CB	5.16	1.61	1.54
1	E	465	MET	SD-CE	5.15	1.92	1.79
1	E	260	ARG	NE-CZ	5.15	1.38	1.33
1	M	310	PRO	CA-C	5.15	1.56	1.52
1	A	83	VAL	CA-CB	5.14	1.61	1.54
1	L	374	VAL	CA-CB	5.14	1.61	1.54
1	J	495	VAL	CA-CB	5.13	1.61	1.54
1	K	423	LYS	N-CA	5.12	1.51	1.46
1	O	67	PRO	CA-C	5.12	1.57	1.52
1	F	458	VAL	CA-CB	5.12	1.61	1.54
1	H	275	ALA	C-O	-5.12	1.17	1.23
1	H	374	VAL	CA-CB	5.11	1.61	1.54
1	A	55	MET	SD-CE	-5.11	1.66	1.79
1	I	306	ASP	N-CA	5.10	1.53	1.46
1	O	270	VAL	CA-CB	5.09	1.62	1.54
1	O	115	THR	CA-CB	5.09	1.61	1.53
1	E	276	VAL	N-CA	5.08	1.52	1.46
1	F	191	MET	SD-CE	5.08	1.92	1.79
1	M	237	ASP	CA-C	5.08	1.58	1.52
1	H	276	VAL	N-CA	5.08	1.52	1.46
1	E	488	THR	N-CA	5.08	1.52	1.46
1	H	274	THR	N-CA	5.06	1.52	1.45
1	B	495	VAL	CA-CB	5.04	1.61	1.54
1	D	83	VAL	CA-CB	5.03	1.61	1.54
1	O	107	VAL	CA-CB	5.03	1.61	1.54
1	C	534	ILE	CA-CB	5.02	1.60	1.54
1	N	198	ASN	CA-C	5.02	1.58	1.52
1	N	549	VAL	CA-CB	5.02	1.62	1.55
1	J	510	THR	CA-CB	5.01	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	54	THR	CA-CB	5.01	1.62	1.53
1	P	568	VAL	CA-CB	5.01	1.60	1.54
1	C	225	ILE	CA-CB	5.01	1.59	1.54
1	M	481	LEU	CA-C	-5.01	1.49	1.52
1	P	306	ASP	N-CA	5.00	1.53	1.46

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	GLN	N-CA-C	7.94	120.64	111.11
1	M	139	VAL	N-CA-C	6.86	118.35	108.48
1	L	374	VAL	N-CA-C	6.55	118.14	111.00
1	C	169	VAL	N-CA-C	6.47	116.63	110.42
1	I	137	VAL	N-CA-C	6.19	113.95	108.63
1	G	135	TYR	N-CA-C	6.07	118.39	111.11
1	O	139	VAL	N-CA-C	5.93	116.41	108.11
1	M	480	ASP	CA-C-N	-5.80	115.53	122.44
1	M	480	ASP	C-N-CA	-5.80	115.53	122.44
1	J	264	SER	N-CA-C	5.76	119.13	111.75
1	L	423	LYS	N-CA-C	5.76	121.46	113.45
1	J	481	LEU	N-CA-C	5.72	117.60	111.36
1	G	139	VAL	N-CA-C	5.71	116.11	108.11
1	K	139	VAL	N-CA-C	5.67	116.11	108.17
1	N	374	VAL	N-CA-C	5.66	116.72	111.45
1	F	241	SER	N-CA-C	5.58	119.34	112.54
1	K	423	LYS	N-CA-C	5.57	121.19	113.45
1	M	285	ARG	N-CA-C	5.56	118.27	111.82
1	G	189	GLN	N-CA-C	5.55	118.04	111.33
1	L	259	ASN	N-CA-C	5.50	119.09	112.93
1	M	169	VAL	N-CA-C	5.43	115.87	110.23
1	D	374	VAL	N-CA-C	5.35	116.41	111.81
1	O	135	TYR	N-CA-C	5.32	116.77	110.97
1	P	189	GLN	N-CA-C	5.32	117.77	111.33
1	G	221	GLU	N-CA-C	5.30	117.06	111.28
1	M	284	ALA	N-CA-C	5.27	115.32	107.88
1	G	169	VAL	N-CA-C	5.25	115.46	110.42
1	O	169	VAL	N-CA-C	5.20	115.42	110.42
1	P	492	SER	N-CA-C	5.20	117.35	111.11
1	L	189	GLN	N-CA-C	5.19	116.93	111.28
1	O	189	GLN	N-CA-C	5.19	116.93	111.28
1	C	189	GLN	N-CA-C	5.18	117.32	111.11
1	C	162	MET	N-CA-C	5.17	118.42	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	461	GLN	CA-C-N	5.15	127.18	120.28
1	F	461	GLN	C-N-CA	5.15	127.18	120.28
1	H	374	VAL	CB-CA-C	5.13	118.64	111.92
1	C	186	ASN	N-CA-C	5.13	117.67	110.23
1	M	470	LEU	N-CA-C	5.12	116.87	108.52
1	E	119	THR	N-CA-C	5.11	118.29	111.75
1	G	483	THR	N-CA-C	5.09	121.06	109.81
1	H	423	LYS	N-CA-C	5.09	119.87	113.25
1	I	189	GLN	CA-C-N	-5.07	114.54	122.65
1	I	189	GLN	C-N-CA	-5.07	114.54	122.65
1	I	483	THR	N-CA-C	5.06	121.00	109.81
1	F	189	GLN	N-CA-C	5.05	119.70	111.37
1	H	348	GLU	N-CA-C	5.04	116.85	111.36
1	F	119	THR	N-CA-C	5.04	118.20	111.75
1	C	420	LEU	CA-CB-CG	5.04	133.93	116.30
1	H	135	TYR	N-CA-C	5.03	116.84	111.36
1	D	386	ARG	N-CA-C	5.01	116.44	111.07
1	H	189	GLN	N-CA-C	5.01	117.39	111.33

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ASP	Peptide
1	A	197	SER	Peptide
1	B	120	ASP	Peptide
1	B	40	ALA	Peptide
1	B	475	LEU	Peptide
1	C	120	ASP	Peptide
1	C	40	ALA	Peptide
1	D	120	ASP	Peptide
1	D	136	GLY	Peptide
1	D	40	ALA	Peptide
1	D	475	LEU	Peptide
1	E	120	ASP	Peptide
1	E	276	VAL	Peptide
1	E	359	THR	Peptide
1	E	40	ALA	Peptide
1	F	118	LEU	Peptide
1	F	120	ASP	Peptide
1	F	136	GLY	Peptide
1	F	161	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	F	40	ALA	Peptide
1	F	475	LEU	Peptide
1	G	120	ASP	Peptide
1	G	40	ALA	Peptide
1	G	475	LEU	Peptide
1	H	118	LEU	Peptide
1	H	120	ASP	Peptide
1	H	136	GLY	Peptide
1	H	161	GLY	Peptide
1	H	190	SER	Peptide
1	H	38	ARG	Peptide
1	I	118	LEU	Peptide
1	I	120	ASP	Peptide
1	I	136	GLY	Peptide
1	I	190	SER	Peptide
1	I	40	ALA	Peptide
1	J	120	ASP	Peptide
1	J	136	GLY	Peptide
1	J	40	ALA	Peptide
1	J	475	LEU	Peptide
1	K	120	ASP	Peptide
1	K	136	GLY	Peptide
1	K	155	GLY	Peptide
1	L	120	ASP	Peptide
1	M	120	ASP	Peptide
1	M	155	GLY	Peptide
1	M	40	ALA	Peptide
1	M	476	GLY	Peptide
1	N	136	GLY	Peptide
1	N	40	ALA	Peptide
1	N	468	ASP	Peptide
1	N	475	LEU	Peptide
1	O	118	LEU	Peptide
1	O	120	ASP	Peptide
1	O	154	LEU	Peptide
1	O	468	ASP	Peptide
1	P	120	ASP	Peptide
1	P	136	GLY	Peptide

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4010	0	3953	31	0
1	B	4008	0	3953	28	0
1	C	4008	0	3953	28	0
1	D	4008	0	3953	32	0
1	E	4008	0	3953	30	0
1	F	4008	0	3953	30	0
1	G	4010	0	3953	30	0
1	H	4008	0	3953	27	0
1	I	4010	0	3953	22	0
1	J	4008	0	3953	28	0
1	K	4008	0	3953	28	0
1	L	4010	0	3953	25	0
1	M	4010	0	3953	30	0
1	N	4008	0	3953	39	0
1	O	4010	0	3953	27	0
1	P	4008	0	3953	30	0
2	A	24	0	36	5	0
2	B	24	0	36	3	0
2	C	24	0	36	3	0
2	D	24	0	36	4	0
2	E	24	0	36	3	0
2	F	24	0	36	4	0
2	G	24	0	36	1	0
2	H	24	0	36	4	0
2	I	24	0	36	2	0
2	J	24	0	36	2	0
2	K	24	0	36	3	0
2	L	24	0	36	1	0
2	M	24	0	36	2	0
2	N	24	0	36	4	0
2	O	24	0	36	3	0
2	P	24	0	36	2	0
All	All	64524	0	63824	463	0

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 4.

All (463) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:453:MET:SD	1:L:453:MET:CE	2.02	1.48
1:D:325:LEU:H	1:D:358:HIS:HD2	1.18	0.90
1:A:155:GLY:HA3	1:A:198:ASN:HD21	1.38	0.87
1:C:325:LEU:H	1:C:358:HIS:HD2	1.27	0.81
1:D:86:LEU:HG	1:D:136:GLY:HA3	1.64	0.80
1:K:397:VAL:HG11	1:K:405:ILE:HG21	1.64	0.80
1:A:155:GLY:CA	1:A:198:ASN:HD21	1.98	0.77
1:J:95:ALA:O	1:J:99:THR:OG1	2.05	0.74
1:I:86:LEU:HG	1:I:136:GLY:HA3	1.72	0.72
1:E:155:GLY:HA2	1:E:198:ASN:HD22	1.55	0.71
1:P:325:LEU:H	1:P:358:HIS:HD2	1.36	0.71
1:E:86:LEU:HG	1:E:136:GLY:HA3	1.72	0.71
1:K:325:LEU:H	1:K:358:HIS:HD2	1.37	0.70
1:O:325:LEU:H	1:O:358:HIS:HD2	1.40	0.69
1:J:325:LEU:H	1:J:358:HIS:HD2	1.40	0.69
1:A:325:LEU:H	1:A:358:HIS:HD2	1.39	0.69
1:K:86:LEU:HG	1:K:136:GLY:HA3	1.75	0.69
1:B:86:LEU:HG	1:B:136:GLY:HA3	1.73	0.69
1:G:325:LEU:H	1:G:358:HIS:HD2	1.41	0.68
1:C:495:VAL:HA	1:C:498:ASN:HD22	1.61	0.66
1:G:155:GLY:HA2	1:G:198:ASN:HD22	1.60	0.66
1:P:86:LEU:HD21	1:P:96:VAL:HG21	1.78	0.65
1:H:325:LEU:H	1:H:358:HIS:HD2	1.43	0.64
1:L:495:VAL:HG11	2:L:600:MAY:H15	1.79	0.64
1:A:86:LEU:HD21	1:A:96:VAL:HG21	1.79	0.64
1:B:325:LEU:H	1:B:358:HIS:HD2	1.45	0.64
1:L:142:LYS:NZ	1:L:236:THR:OG1	2.27	0.64
1:N:375:LEU:HD22	1:N:451:ILE:HG13	1.79	0.64
1:M:80:LEU:HD11	1:M:288:GLU:HB3	1.79	0.64
1:D:495:VAL:HG11	2:D:600:MAY:H15	1.79	0.64
1:G:246:SER:HA	1:G:251:ILE:HG13	1.79	0.63
1:C:495:VAL:HG11	2:C:600:MAY:H15	1.81	0.63
1:N:80:LEU:HD11	1:N:288:GLU:HB3	1.80	0.62
1:M:495:VAL:HG11	2:M:600:MAY:H15	1.82	0.62
1:B:80:LEU:HD11	1:B:288:GLU:HB3	1.81	0.62
1:E:495:VAL:HA	1:E:498:ASN:HD22	1.64	0.62
1:A:86:LEU:HG	1:A:136:GLY:HA3	1.82	0.62
1:N:331:GLU:HG3	1:N:346:LEU:HD12	1.81	0.62
1:E:495:VAL:HG11	2:E:600:MAY:H15	1.81	0.62
1:A:246:SER:HA	1:A:251:ILE:HG13	1.80	0.62
1:F:325:LEU:H	1:F:358:HIS:HD2	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:375:LEU:HD13	1:L:451:ILE:HG12	1.82	0.61
1:C:246:SER:HA	1:C:251:ILE:HG13	1.82	0.61
1:J:80:LEU:HD11	1:J:288:GLU:HB3	1.83	0.61
1:H:495:VAL:HA	1:H:498:ASN:HD22	1.65	0.61
1:A:495:VAL:HG11	2:A:600:MAY:H15	1.83	0.60
1:G:495:VAL:HA	1:G:498:ASN:HD22	1.67	0.60
1:B:154:LEU:O	1:B:189:GLN:O	2.20	0.60
1:G:243:ARG:HH22	1:G:498:ASN:HD21	1.50	0.59
1:F:86:LEU:HD21	1:F:96:VAL:HG21	1.84	0.59
1:H:86:LEU:HG	1:H:136:GLY:HA3	1.83	0.59
1:A:486:ARG:HB2	1:A:534:ILE:HG21	1.85	0.59
1:O:495:VAL:HG11	2:O:600:MAY:H15	1.85	0.59
1:N:155:GLY:HA3	1:N:198:ASN:ND2	2.17	0.58
1:H:246:SER:HA	1:H:251:ILE:HG13	1.86	0.58
1:K:495:VAL:HA	1:K:498:ASN:HD22	1.68	0.58
1:J:246:SER:HA	1:J:251:ILE:HG13	1.86	0.58
1:A:162:MET:SD	1:A:162:MET:N	2.76	0.57
1:K:495:VAL:HG11	2:K:600:MAY:H15	1.85	0.57
1:D:173:VAL:HG22	1:D:297:LEU:HD23	1.86	0.57
1:K:154:LEU:HD21	1:K:267:LYS:HG2	1.86	0.57
1:I:495:VAL:HA	1:I:498:ASN:HD22	1.69	0.57
1:H:275:ALA:HB1	1:H:451:ILE:HD12	1.87	0.57
1:B:153:THR:HA	1:B:159:ASN:HB2	1.85	0.57
1:M:562:LEU:HA	1:M:565:MET:HB2	1.87	0.56
1:B:86:LEU:HD21	1:B:96:VAL:HG21	1.87	0.56
1:N:173:VAL:HG11	1:N:302:LEU:HD12	1.88	0.56
1:P:472:THR:HG21	1:P:550:GLN:HE21	1.71	0.56
1:G:258:GLY:HA2	1:G:279:SER:HB3	1.88	0.56
1:L:189:GLN:HE22	1:L:397:VAL:HA	1.71	0.56
1:P:495:VAL:HG11	2:P:600:MAY:H15	1.87	0.56
1:I:237:ASP:HB2	1:I:242:ILE:HD12	1.88	0.56
1:N:495:VAL:HA	1:N:498:ASN:HD22	1.71	0.56
1:F:495:VAL:HG11	2:F:600:MAY:H15	1.87	0.55
1:N:74:LEU:HD11	1:N:96:VAL:HG12	1.89	0.55
1:C:133:LEU:H	1:C:177:GLN:HG3	1.71	0.55
1:G:243:ARG:NH2	1:G:498:ASN:HD21	2.04	0.55
1:C:189:GLN:HE22	1:C:397:VAL:HA	1.72	0.55
1:O:495:VAL:HA	1:O:498:ASN:HD22	1.71	0.55
1:C:486:ARG:HB2	1:C:534:ILE:HG21	1.89	0.55
1:F:153:THR:HA	1:F:159:ASN:HB2	1.88	0.55
1:G:139:VAL:HG21	1:G:174:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:325:LEU:H	1:J:358:HIS:CD2	2.24	0.55
1:N:86:LEU:HG	1:N:136:GLY:HA3	1.87	0.55
1:A:155:GLY:HA3	1:A:198:ASN:ND2	2.16	0.55
1:O:155:GLY:HA2	1:O:198:ASN:HD22	1.72	0.55
1:P:294:LEU:HD22	1:P:298:LEU:HD22	1.87	0.55
1:K:325:LEU:H	1:K:358:HIS:CD2	2.23	0.55
1:P:371:ALA:HA	1:P:375:LEU:HD12	1.89	0.55
1:J:133:LEU:HB2	1:J:177:GLN:HE21	1.70	0.55
1:E:377:ALA:HA	2:E:600:MAY:H12	1.89	0.54
1:G:153:THR:HA	1:G:159:ASN:HB2	1.89	0.54
1:H:238:ILE:HG22	2:H:600:MAY:HMB	1.88	0.54
1:F:189:GLN:NE2	1:F:398:ASP:H	2.05	0.54
1:J:86:LEU:HG	1:J:136:GLY:HA3	1.89	0.54
1:B:495:VAL:HG11	2:B:600:MAY:H15	1.90	0.54
1:D:199:PRO:HD3	1:D:398:ASP:HB2	1.88	0.54
1:B:189:GLN:HE22	1:B:397:VAL:HA	1.72	0.54
1:E:86:LEU:HD21	1:E:96:VAL:HG21	1.89	0.54
1:H:133:LEU:HB2	1:H:177:GLN:HE21	1.73	0.54
1:M:488:THR:HG23	2:M:600:MAY:H7A	1.90	0.54
1:N:86:LEU:HD21	1:N:96:VAL:HG21	1.89	0.54
1:A:263:LYS:HG2	1:A:266:LEU:HD22	1.90	0.53
1:E:325:LEU:H	1:E:358:HIS:HD2	1.56	0.53
1:G:80:LEU:HD21	1:G:288:GLU:HB3	1.89	0.53
1:G:243:ARG:HH22	1:G:498:ASN:ND2	2.05	0.53
1:J:111:THR:HG1	1:J:113:CYS:HG	1.57	0.53
1:G:86:LEU:HD21	1:G:96:VAL:HG21	1.89	0.53
1:G:472:THR:HB	1:G:550:GLN:HB3	1.89	0.53
1:I:495:VAL:HG11	2:I:600:MAY:H15	1.90	0.53
1:A:177:GLN:HG2	1:A:296:ALA:HB1	1.90	0.53
1:P:252:CYS:HB3	1:P:290:LEU:HD11	1.90	0.53
1:D:495:VAL:HA	1:D:498:ASN:HD22	1.74	0.53
1:C:86:LEU:HG	1:C:136:GLY:HA3	1.91	0.53
1:F:86:LEU:HG	1:F:136:GLY:HA3	1.89	0.53
1:N:472:THR:HG21	1:N:550:GLN:HE21	1.72	0.53
1:M:246:SER:HA	1:M:251:ILE:HG13	1.91	0.53
1:N:139:VAL:HG21	1:N:174:LEU:HD13	1.90	0.53
1:N:512:VAL:HG13	1:N:516:ASP:HB2	1.91	0.52
1:B:188:PRO:HA	1:B:197:SER:O	2.10	0.52
1:H:52:LEU:HA	1:H:55:MET:HE2	1.91	0.52
1:L:162:MET:SD	1:L:162:MET:N	2.79	0.52
1:A:237:ASP:HB3	1:A:255:LYS:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:ALA:HB1	1:D:547:VAL:HG21	1.90	0.52
1:E:470:LEU:HB3	1:E:552:VAL:HB	1.89	0.52
1:J:509:VAL:HG23	1:J:510:THR:HG22	1.92	0.52
1:G:263:LYS:HB3	1:G:266:LEU:HD22	1.92	0.52
1:K:341:ALA:HB1	1:K:547:VAL:HG21	1.92	0.52
1:K:377:ALA:HA	2:K:600:MAY:H12	1.92	0.52
1:B:133:LEU:H	1:B:177:GLN:HG3	1.75	0.52
1:H:273:GLN:OE1	1:H:275:ALA:O	2.28	0.52
1:K:246:SER:HA	1:K:251:ILE:HG13	1.91	0.52
1:O:367:ASN:HB3	1:O:370:TYR:HB3	1.92	0.52
1:F:475:LEU:HD22	1:F:476:GLY:H	1.74	0.51
1:L:246:SER:HA	1:L:251:ILE:HG13	1.93	0.51
1:N:258:GLY:HA2	1:N:279:SER:HB3	1.92	0.51
1:O:198:ASN:HD21	1:O:200:LEU:HB2	1.74	0.51
1:F:488:THR:HG23	2:F:600:MAY:H7A	1.92	0.51
1:K:86:LEU:HD21	1:K:96:VAL:HG21	1.91	0.51
1:L:86:LEU:HD21	1:L:96:VAL:HG21	1.92	0.51
1:H:139:VAL:HG21	1:H:174:LEU:HD13	1.92	0.51
1:O:470:LEU:HB3	1:O:552:VAL:HB	1.93	0.51
1:K:239:GLY:HA2	1:K:495:VAL:HG23	1.93	0.51
1:H:470:LEU:HB3	1:H:552:VAL:HB	1.92	0.51
1:N:198:ASN:HD21	1:N:200:LEU:HB2	1.76	0.51
1:F:495:VAL:HA	1:F:498:ASN:HD22	1.76	0.51
1:L:79:LEU:HD23	1:L:289:SER:HB3	1.93	0.51
1:P:260:ARG:NH2	1:P:558:GLU:OE1	2.44	0.50
1:F:535:LEU:HG	1:F:539:MET:HE2	1.92	0.50
1:G:535:LEU:HG	1:G:539:MET:HE2	1.93	0.50
1:A:488:THR:HG23	2:A:600:MAY:H7A	1.93	0.50
1:H:495:VAL:HG11	2:H:600:MAY:H15	1.93	0.50
1:J:472:THR:HG21	1:J:550:GLN:HE21	1.77	0.50
1:L:133:LEU:H	1:L:177:GLN:HG3	1.77	0.50
1:O:275:ALA:HB1	1:O:451:ILE:HD12	1.93	0.50
1:P:325:LEU:H	1:P:358:HIS:CD2	2.24	0.50
1:B:169:VAL:HA	1:B:172:GLN:HE21	1.77	0.50
1:I:325:LEU:H	1:I:358:HIS:HD2	1.59	0.50
1:J:139:VAL:HG21	1:J:174:LEU:HD13	1.94	0.50
1:I:319:TYR:O	1:I:566:ARG:NH1	2.45	0.49
1:I:154:LEU:O	1:I:189:GLN:O	2.30	0.49
1:N:535:LEU:HG	1:N:539:MET:HE2	1.94	0.49
1:I:246:SER:HA	1:I:251:ILE:HG13	1.93	0.49
1:M:232:LEU:HD11	1:M:293:CYS:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:486:ARG:HB2	1:O:534:ILE:HG21	1.94	0.49
1:E:535:LEU:HG	1:E:539:MET:HE2	1.94	0.49
1:F:325:LEU:H	1:F:358:HIS:CD2	2.28	0.49
1:I:375:LEU:HD22	1:I:451:ILE:HG13	1.95	0.49
1:J:495:VAL:HA	1:J:498:ASN:HD22	1.77	0.49
1:N:169:VAL:O	1:N:173:VAL:HG12	2.12	0.49
1:O:86:LEU:HD21	1:O:96:VAL:HG21	1.94	0.49
1:P:486:ARG:HB2	1:P:534:ILE:HG21	1.94	0.49
1:D:246:SER:HA	1:D:251:ILE:HG13	1.94	0.49
1:L:470:LEU:HB3	1:L:552:VAL:HB	1.94	0.49
1:C:162:MET:SD	1:C:162:MET:N	2.85	0.49
1:M:239:GLY:HA2	1:M:495:VAL:HG23	1.94	0.49
1:B:162:MET:SD	1:B:162:MET:N	2.85	0.49
1:C:286:ASP:OD2	1:C:289:SER:OG	2.31	0.49
1:M:135:TYR:HA	1:M:178:GLY:HA3	1.95	0.49
1:M:469:VAL:HG11	1:M:564:PHE:CG	2.47	0.49
1:J:470:LEU:HB3	1:J:552:VAL:HB	1.95	0.49
1:G:331:GLU:HG3	1:G:346:LEU:HD12	1.94	0.49
1:B:486:ARG:HG3	1:B:534:ILE:HG12	1.94	0.48
1:D:325:LEU:H	1:D:358:HIS:CD2	2.11	0.48
1:D:377:ALA:HA	2:D:600:MAY:H12	1.94	0.48
1:P:294:LEU:O	1:P:298:LEU:HB2	2.13	0.48
1:P:488:THR:HG23	2:P:600:MAY:H7A	1.94	0.48
1:A:495:VAL:HA	1:A:498:ASN:HD22	1.79	0.48
1:B:377:ALA:HA	2:B:600:MAY:H12	1.95	0.48
1:C:74:LEU:HD11	1:C:96:VAL:HG12	1.95	0.48
1:H:382:SER:HA	1:H:439:ARG:HH11	1.78	0.48
1:E:80:LEU:HD11	1:E:288:GLU:HB3	1.95	0.48
1:P:80:LEU:HD11	1:P:288:GLU:HB3	1.95	0.48
1:A:154:LEU:HD23	1:A:269:CYS:HB3	1.95	0.48
1:A:472:THR:HB	1:A:550:GLN:HB3	1.95	0.48
1:E:122:GLU:HA	1:E:125:LEU:HB2	1.94	0.48
1:C:86:LEU:HD21	1:C:96:VAL:HG21	1.96	0.48
1:A:243:ARG:HH22	1:A:498:ASN:HD21	1.61	0.48
1:J:495:VAL:HG11	2:J:600:MAY:H15	1.94	0.48
1:N:239:GLY:HA2	1:N:495:VAL:HG23	1.96	0.48
1:G:199:PRO:HD3	1:G:398:ASP:HB2	1.96	0.47
1:J:488:THR:HG23	2:J:600:MAY:H7A	1.96	0.47
1:P:495:VAL:HA	1:P:498:ASN:HD22	1.79	0.47
1:P:199:PRO:HD3	1:P:398:ASP:HB2	1.96	0.47
1:C:307:PRO:HB2	1:D:555:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:GLY:HA2	1:E:495:VAL:HG23	1.95	0.47
1:O:520:MET:HE2	1:O:539:MET:HB2	1.96	0.47
1:K:139:VAL:HG21	1:K:174:LEU:HD13	1.96	0.47
1:A:325:LEU:N	1:A:358:HIS:HD2	2.09	0.47
1:G:80:LEU:HD22	1:G:80:LEU:H	1.79	0.47
1:O:259:ASN:HB3	1:O:556:TRP:HH2	1.80	0.47
1:A:238:ILE:HG22	2:A:600:MAY:HMB	1.95	0.47
1:E:488:THR:HG23	2:E:600:MAY:H7A	1.97	0.47
1:G:86:LEU:HG	1:G:136:GLY:HA3	1.95	0.47
1:N:237:ASP:HB3	1:N:255:LYS:HG3	1.97	0.47
1:P:51:SER:HB3	1:P:117:TYR:H	1.79	0.47
1:D:86:LEU:HD21	1:D:96:VAL:HG21	1.96	0.47
1:E:168:CYS:HB2	1:E:265:GLY:HA3	1.96	0.47
1:D:520:MET:HE2	1:D:539:MET:HB2	1.96	0.47
1:E:80:LEU:H	1:E:80:LEU:HD22	1.80	0.47
1:P:133:LEU:H	1:P:177:GLN:HG3	1.79	0.47
1:F:397:VAL:HG11	1:F:405:ILE:HG21	1.97	0.46
1:G:189:GLN:NE2	1:G:398:ASP:H	2.12	0.46
1:H:341:ALA:HB1	1:H:547:VAL:HG21	1.98	0.46
1:O:488:THR:HG23	2:O:600:MAY:H7A	1.97	0.46
1:C:80:LEU:H	1:C:80:LEU:HD22	1.81	0.46
1:I:258:GLY:HA2	1:I:279:SER:HB3	1.96	0.46
1:P:171:VAL:HA	1:P:174:LEU:HD12	1.97	0.46
1:P:275:ALA:HB1	1:P:451:ILE:HD12	1.97	0.46
1:E:523:TYR:HB3	1:E:536:LYS:HG3	1.98	0.46
1:E:312:LEU:HD11	1:F:311:PRO:HD2	1.96	0.46
1:D:238:ILE:HD12	1:D:278:LEU:HB2	1.98	0.46
1:C:79:LEU:HD13	1:C:231:PRO:HB2	1.97	0.46
1:I:377:ALA:HA	2:I:600:MAY:H12	1.97	0.46
1:P:177:GLN:HG2	1:P:296:ALA:HB1	1.98	0.46
1:A:153:THR:HA	1:A:159:ASN:HB2	1.97	0.46
1:A:535:LEU:HG	1:A:539:MET:HE2	1.98	0.46
1:B:512:VAL:HG13	1:B:516:ASP:HB2	1.97	0.46
1:F:319:TYR:HB2	1:F:559:GLU:HB2	1.96	0.46
1:M:273:GLN:NE2	1:M:275:ALA:O	2.49	0.46
1:J:75:LEU:HD13	1:J:103:LYS:HE3	1.97	0.46
1:H:236:THR:HG22	1:H:280:LEU:HB3	1.98	0.46
1:I:535:LEU:HG	1:I:539:MET:HE2	1.98	0.46
1:M:195:ASP:HB2	1:M:484:PRO:HG2	1.98	0.46
1:A:275:ALA:HB1	1:A:451:ILE:HD12	1.97	0.46
1:D:141:LEU:HD11	1:D:181:PRO:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:CYS:HB3	1:D:290:LEU:HD11	1.98	0.46
1:E:331:GLU:HG3	1:E:346:LEU:HD12	1.98	0.46
1:F:168:CYS:HB2	1:F:265:GLY:HA3	1.98	0.46
1:H:142:LYS:NZ	1:H:236:THR:OG1	2.49	0.46
1:D:535:LEU:HG	1:D:539:MET:HE2	1.97	0.45
1:L:139:VAL:HG21	1:L:174:LEU:HD13	1.98	0.45
1:D:217:SER:H	1:D:241:SER:CB	2.29	0.45
1:H:535:LEU:HG	1:H:539:MET:HE2	1.99	0.45
1:I:86:LEU:HD21	1:I:96:VAL:HG21	1.97	0.45
1:J:243:ARG:HH22	1:J:498:ASN:HD21	1.63	0.45
1:O:123:THR:HA	1:O:126:SER:HB2	1.98	0.45
1:H:74:LEU:HD13	1:H:96:VAL:HG12	1.99	0.45
1:P:326:ARG:HE	1:P:326:ARG:HB3	1.53	0.45
1:L:520:MET:HE2	1:L:539:MET:HB2	1.99	0.45
1:F:196:CYS:HB3	1:F:204:THR:HB	1.98	0.45
1:N:79:LEU:O	1:N:83:VAL:HG12	2.17	0.45
1:C:239:GLY:HA2	1:C:495:VAL:HG23	1.99	0.45
1:K:79:LEU:HD13	1:K:231:PRO:HB2	1.97	0.45
1:N:495:VAL:HG11	2:N:600:MAY:H15	1.99	0.45
1:D:437:ARG:HA	1:D:438:PRO:HD3	1.83	0.45
1:B:255:LYS:HB3	1:B:255:LYS:HE3	1.64	0.45
1:D:491:ILE:HD11	2:D:600:MAY:C14	2.47	0.45
1:G:133:LEU:H	1:G:177:GLN:HG3	1.82	0.45
1:I:139:VAL:HG21	1:I:174:LEU:HD13	1.97	0.45
1:P:263:LYS:HA	1:P:266:LEU:HD13	1.98	0.45
1:B:162:MET:HA	1:B:163:PRO:HD2	1.89	0.44
1:C:377:ALA:HA	2:C:600:MAY:H12	1.99	0.44
1:D:472:THR:HG21	1:D:550:GLN:HE21	1.82	0.44
1:H:206:ASN:HA	1:H:207:PRO:HD2	1.85	0.44
1:I:472:THR:HB	1:I:550:GLN:HB3	1.98	0.44
1:L:435:SER:HA	1:L:439:ARG:HH22	1.82	0.44
1:A:371:ALA:HA	1:A:375:LEU:HD12	2.00	0.44
1:F:80:LEU:HD11	1:F:288:GLU:HB3	1.99	0.44
1:D:481:LEU:HD13	1:D:481:LEU:HA	1.91	0.44
1:L:495:VAL:HA	1:L:498:ASN:HD22	1.83	0.44
1:M:72:GLU:O	1:M:76:THR:OG1	2.34	0.44
1:N:133:LEU:H	1:N:177:GLN:HG3	1.82	0.44
1:D:156:LEU:HG	1:D:391:ASN:HB3	1.98	0.44
1:M:361:ILE:HG21	1:M:465:MET:HG2	1.99	0.44
1:P:52:LEU:HA	1:P:55:MET:HE2	1.99	0.44
1:C:345:ALA:O	1:C:349:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:GLN:NE2	1:L:398:ASP:H	2.14	0.44
1:M:385:GLY:HA3	1:M:408:LEU:HD22	1.99	0.44
1:N:198:ASN:ND2	1:N:200:LEU:H	2.15	0.44
1:A:239:GLY:O	1:A:494:THR:OG1	2.34	0.44
1:E:225:ILE:HG22	1:E:251:ILE:HG21	1.98	0.44
1:I:74:LEU:HD11	1:I:96:VAL:HG12	2.00	0.44
1:N:123:THR:HA	1:N:126:SER:HB2	2.00	0.44
1:O:246:SER:HA	1:O:251:ILE:HG13	1.98	0.44
1:O:377:ALA:HA	2:O:600:MAY:H12	1.99	0.44
1:C:470:LEU:HB3	1:C:552:VAL:HB	2.00	0.44
1:D:209:LYS:HD2	1:D:545:LEU:HD21	1.99	0.44
1:M:128:ALA:HA	1:M:129:PRO:HD3	1.84	0.44
1:N:85:LYS:HB3	1:N:91:LEU:HD12	1.99	0.44
1:A:243:ARG:HH22	1:A:498:ASN:ND2	2.16	0.44
1:B:139:VAL:HG21	1:B:174:LEU:HD13	2.00	0.44
1:C:170:VAL:HG11	1:C:280:LEU:HD11	2.00	0.44
1:D:246:SER:HB2	1:D:506:VAL:HG11	1.98	0.44
1:D:259:ASN:HD22	1:D:259:ASN:HA	1.68	0.44
1:G:325:LEU:H	1:G:358:HIS:CD2	2.27	0.44
1:M:217:SER:H	1:M:241:SER:CB	2.30	0.44
1:N:294:LEU:HD12	1:N:562:LEU:HD11	1.99	0.44
1:B:246:SER:HA	1:B:251:ILE:HG13	1.99	0.44
1:E:151:ASP:HB3	1:E:153:THR:HG23	2.00	0.44
1:I:133:LEU:H	1:I:177:GLN:HG3	1.83	0.44
1:F:239:GLY:HA2	1:F:495:VAL:HG23	1.99	0.43
1:H:377:ALA:HA	2:H:600:MAY:H12	2.00	0.43
1:M:474:MET:HG2	1:M:506:VAL:HG21	2.00	0.43
1:C:40:ALA:HB1	1:C:43:ARG:HB2	2.00	0.43
1:C:563:ARG:HH12	1:C:567:GLU:HB2	1.83	0.43
1:K:523:TYR:HB3	1:K:536:LYS:HG3	2.00	0.43
1:I:80:LEU:HD22	1:I:80:LEU:H	1.83	0.43
1:K:162:MET:HA	1:K:163:PRO:HD2	1.95	0.43
1:F:189:GLN:HE21	1:F:398:ASP:H	1.65	0.43
1:F:377:ALA:HA	2:F:600:MAY:H12	2.00	0.43
1:E:246:SER:HA	1:E:251:ILE:HG13	1.99	0.43
1:J:188:PRO:HA	1:J:197:SER:O	2.19	0.43
1:C:263:LYS:HA	1:C:266:LEU:HD13	2.00	0.43
1:L:129:PRO:HD2	1:L:178:GLY:HA2	2.01	0.43
1:E:275:ALA:HB2	1:E:448:GLN:HG3	2.01	0.43
1:L:535:LEU:HG	1:L:539:MET:HE2	2.00	0.43
1:M:306:ASP:OD2	1:M:308:THR:OG1	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:469:VAL:HG11	1:M:564:PHE:CD2	2.53	0.43
1:O:80:LEU:H	1:O:80:LEU:HD22	1.83	0.43
1:C:238:ILE:HG22	2:C:600:MAY:HMB	1.99	0.43
1:D:238:ILE:HG22	2:D:600:MAY:HMB	2.01	0.43
1:G:495:VAL:HG11	2:G:600:MAY:H15	2.01	0.43
1:O:239:GLY:HA2	1:O:495:VAL:HG23	1.99	0.43
1:O:472:THR:HG22	1:O:473:PRO:O	2.19	0.43
1:C:410:LEU:HB2	1:C:415:LYS:HD2	1.99	0.43
1:E:237:ASP:HB3	1:E:255:LYS:HG3	2.01	0.43
1:K:198:ASN:HD21	1:K:200:LEU:HB2	1.84	0.43
1:J:398:ASP:HA	1:J:399:PRO:HD2	1.88	0.43
1:K:437:ARG:HD3	1:K:439:ARG:HG3	2.00	0.43
1:M:294:LEU:HD22	1:M:298:LEU:HD22	2.00	0.43
1:N:79:LEU:HD13	1:N:231:PRO:HB2	2.00	0.43
1:N:310:PRO:HA	1:N:311:PRO:HD3	1.82	0.43
1:E:189:GLN:HE22	1:E:397:VAL:HA	1.84	0.42
1:H:335:TYR:OH	2:H:600:MAY:H19A	2.19	0.42
1:K:345:ALA:O	1:K:349:THR:HG23	2.19	0.42
1:N:192:LEU:HG	2:N:600:MAY:H8	2.01	0.42
1:O:217:SER:H	1:O:241:SER:CB	2.31	0.42
1:C:535:LEU:HG	1:C:539:MET:HE2	2.00	0.42
1:D:79:LEU:HD13	1:D:231:PRO:HB2	2.01	0.42
1:K:237:ASP:HA	1:K:241:SER:HB2	2.01	0.42
1:L:86:LEU:HG	1:L:136:GLY:HA3	2.00	0.42
1:N:225:ILE:HB	1:N:251:ILE:HD13	2.01	0.42
1:N:349:THR:HG21	1:N:549:VAL:HG21	2.01	0.42
1:N:383:ASP:OD2	1:N:387:SER:OG	2.34	0.42
1:O:74:LEU:HD11	1:O:96:VAL:HA	2.01	0.42
1:E:556:TRP:HA	1:E:558:GLU:OE1	2.19	0.42
1:G:398:ASP:HA	1:G:399:PRO:HD2	1.88	0.42
1:J:41:ALA:HB1	1:J:200:LEU:HA	2.01	0.42
1:P:341:ALA:HB1	1:P:547:VAL:HG21	2.01	0.42
1:G:512:VAL:HG13	1:G:516:ASP:HB2	2.01	0.42
1:J:189:GLN:HE21	1:J:398:ASP:H	1.66	0.42
1:G:237:ASP:HA	1:G:241:SER:HB2	2.01	0.42
1:L:135:TYR:HA	1:L:178:GLY:HA3	2.00	0.42
1:N:246:SER:HA	1:N:251:ILE:HG13	2.02	0.42
1:O:325:LEU:H	1:O:358:HIS:CD2	2.28	0.42
1:B:237:ASP:HB3	1:B:255:LYS:HG3	2.01	0.42
1:C:162:MET:HA	1:C:163:PRO:HD2	1.93	0.42
1:F:398:ASP:HA	1:F:399:PRO:HD2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:196:CYS:SG	1:M:219:GLY:HA3	2.60	0.42
1:P:470:LEU:HB3	1:P:552:VAL:HB	2.02	0.42
1:F:207:PRO:HB3	1:F:227:SER:HB3	2.01	0.42
1:G:385:GLY:HA3	1:G:408:LEU:HD22	2.02	0.42
1:K:486:ARG:HB2	1:K:534:ILE:HD13	2.01	0.42
1:M:183:VAL:HG21	1:M:224:LEU:HD21	2.02	0.42
1:P:246:SER:HA	1:P:251:ILE:HG13	2.00	0.42
1:P:237:ASP:HA	1:P:241:SER:HB2	2.01	0.42
1:P:337:MET:HB3	1:P:523:TYR:CE2	2.54	0.42
1:A:310:PRO:HA	1:A:311:PRO:HD2	1.92	0.42
1:B:238:ILE:HG22	2:B:600:MAY:HMB	2.02	0.42
1:M:341:ALA:HB2	1:M:516:ASP:HB3	2.02	0.42
1:A:217:SER:H	1:A:241:SER:CB	2.33	0.42
1:B:236:THR:HB	1:B:278:LEU:HD11	2.02	0.42
1:K:137:VAL:HA	1:K:138:PRO:HD3	1.90	0.42
1:H:189:GLN:HB2	1:H:199:PRO:HD3	2.02	0.41
1:J:237:ASP:HB2	1:J:242:ILE:HD12	2.02	0.41
1:N:489:GLY:HA2	2:N:600:MAY:H18	2.01	0.41
1:B:135:TYR:HA	1:B:178:GLY:HA3	2.02	0.41
1:J:237:ASP:HA	1:J:241:SER:HB2	2.02	0.41
1:E:341:ALA:HB1	1:E:547:VAL:HG21	2.01	0.41
1:I:341:ALA:HB1	1:I:547:VAL:HG21	2.01	0.41
1:K:252:CYS:HB3	1:K:290:LEU:HD11	2.01	0.41
1:L:453:MET:CE	1:L:453:MET:CG	2.96	0.41
1:N:238:ILE:HD12	1:N:278:LEU:HB2	2.02	0.41
1:A:135:TYR:HA	1:A:178:GLY:HA3	2.02	0.41
1:G:469:VAL:HG11	1:G:564:PHE:CG	2.56	0.41
1:K:155:GLY:HA2	1:K:198:ASN:ND2	2.34	0.41
1:K:212:LYS:HG3	1:K:545:LEU:HD11	2.03	0.41
1:B:238:ILE:HD12	1:B:278:LEU:HB2	2.03	0.41
1:F:437:ARG:HA	1:F:438:PRO:HD3	1.94	0.41
1:K:481:LEU:HD13	1:K:481:LEU:HA	1.96	0.41
1:O:154:LEU:HD12	1:O:154:LEU:HA	1.91	0.41
1:C:135:TYR:HA	1:C:178:GLY:HA3	2.03	0.41
1:E:160:GLU:HG2	1:E:200:LEU:HD21	2.02	0.41
1:L:398:ASP:HA	1:L:399:PRO:HD2	1.78	0.41
1:M:174:LEU:HD11	1:M:234:LEU:HD22	2.02	0.41
2:A:600:MAY:H4	2:A:600:MAY:H7	1.94	0.41
1:L:325:LEU:H	1:L:358:HIS:CD2	2.38	0.41
1:L:341:ALA:HB1	1:L:547:VAL:HG21	2.02	0.41
1:N:177:GLN:HG2	1:N:296:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:162:MET:HA	1:I:163:PRO:HD2	1.90	0.41
1:J:520:MET:HE2	1:J:539:MET:HB2	2.02	0.41
1:M:255:LYS:HA	1:M:256:PRO:HD2	1.95	0.41
1:M:557:GLN:HB3	1:M:560:LEU:HB3	2.03	0.41
1:N:263:LYS:HA	1:N:266:LEU:HD13	2.01	0.41
1:O:173:VAL:HG22	1:O:297:LEU:HD12	2.03	0.41
1:P:437:ARG:HA	1:P:438:PRO:HD3	1.90	0.41
1:A:367:ASN:HB3	1:A:370:TYR:HB3	2.02	0.41
1:B:122:GLU:HA	1:B:125:LEU:HB2	2.03	0.41
1:B:217:SER:H	1:B:241:SER:CB	2.34	0.41
1:B:437:ARG:HA	1:B:438:PRO:HD3	1.87	0.41
1:D:80:LEU:HD11	1:D:288:GLU:HB3	2.03	0.41
1:F:155:GLY:CA	1:F:198:ASN:ND2	2.84	0.41
1:H:472:THR:HG21	1:H:550:GLN:HE21	1.85	0.41
1:H:472:THR:HB	1:H:550:GLN:HB3	2.02	0.41
1:H:481:LEU:HD13	1:H:481:LEU:HA	2.00	0.41
1:I:473:PRO:HG2	1:I:493:TYR:CE1	2.56	0.41
1:J:158:LEU:HD22	1:J:391:ASN:HD22	1.85	0.41
1:J:410:LEU:HB2	1:J:415:LYS:HD2	2.02	0.41
1:O:382:SER:HA	1:O:439:ARG:HH11	1.85	0.41
1:F:74:LEU:HD11	1:F:96:VAL:HG12	2.02	0.41
1:F:133:LEU:H	1:F:177:GLN:HG3	1.86	0.41
1:M:186:ASN:ND2	1:M:204:THR:OG1	2.54	0.41
1:O:319:TYR:HB2	1:O:559:GLU:HB2	2.03	0.41
1:O:459:ILE:HD13	1:P:307:PRO:HD2	2.03	0.41
1:D:361:ILE:HG21	1:D:465:MET:HG2	2.03	0.40
1:E:177:GLN:HG2	1:E:296:ALA:HB1	2.03	0.40
1:J:171:VAL:HA	1:J:174:LEU:HD12	2.03	0.40
1:K:437:ARG:HA	1:K:438:PRO:HD3	1.96	0.40
1:M:79:LEU:HD13	1:M:231:PRO:HB2	2.03	0.40
1:N:52:LEU:HA	1:N:55:MET:HE2	2.03	0.40
1:D:79:LEU:HD12	1:D:82:LEU:HD23	2.03	0.40
1:H:207:PRO:HB3	1:H:227:SER:HB3	2.02	0.40
1:K:488:THR:HG23	2:K:600:MAY:H7A	2.02	0.40
1:F:129:PRO:HD2	1:F:178:GLY:HA2	2.04	0.40
1:H:239:GLY:HA2	1:H:495:VAL:HG23	2.03	0.40
1:I:162:MET:SD	1:I:162:MET:N	2.94	0.40
1:L:260:ARG:NH2	1:L:558:GLU:OE2	2.48	0.40
1:M:222:GLY:HA2	1:M:251:ILE:HD11	2.02	0.40
1:N:377:ALA:HA	2:N:600:MAY:H12	2.02	0.40
1:A:192:LEU:HG	2:A:600:MAY:H8	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LEU:HD13	1:B:231:PRO:HB2	2.04	0.40
1:F:273:GLN:OE1	1:F:275:ALA:O	2.39	0.40
1:F:312:LEU:HD22	1:F:315:ARG:HH12	1.86	0.40
1:G:173:VAL:HG22	1:G:297:LEU:HD12	2.03	0.40
1:G:310:PRO:HA	1:G:311:PRO:HD3	1.90	0.40
1:M:344:ARG:O	1:M:348:GLU:HB2	2.21	0.40
1:D:530:ILE:HG21	1:E:424:PRO:O	2.21	0.40
1:E:390:GLN:HE21	1:E:390:GLN:HB2	1.72	0.40
1:F:154:LEU:O	1:F:189:GLN:O	2.38	0.40
2:F:600:MAY:H4	2:F:600:MAY:H7	1.88	0.40
1:J:342:MET:HG3	1:J:476:GLY:HA2	2.03	0.40
1:N:398:ASP:HA	1:N:399:PRO:HD2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	535/537 (100%)	498 (93%)	31 (6%)	6 (1%)	11	36
1	B	535/537 (100%)	503 (94%)	24 (4%)	8 (2%)	8	28
1	C	535/537 (100%)	507 (95%)	23 (4%)	5 (1%)	14	41
1	D	535/537 (100%)	499 (93%)	31 (6%)	5 (1%)	14	41
1	E	535/537 (100%)	491 (92%)	36 (7%)	8 (2%)	8	28
1	F	535/537 (100%)	502 (94%)	27 (5%)	6 (1%)	11	36
1	G	535/537 (100%)	506 (95%)	26 (5%)	3 (1%)	21	51
1	H	535/537 (100%)	498 (93%)	31 (6%)	6 (1%)	11	36
1	I	535/537 (100%)	496 (93%)	37 (7%)	2 (0%)	30	60
1	J	535/537 (100%)	506 (95%)	26 (5%)	3 (1%)	21	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	535/537 (100%)	497 (93%)	32 (6%)	6 (1%)	11	36
1	L	535/537 (100%)	494 (92%)	36 (7%)	5 (1%)	14	41
1	M	535/537 (100%)	466 (87%)	57 (11%)	12 (2%)	5	19
1	N	535/537 (100%)	494 (92%)	33 (6%)	8 (2%)	8	28
1	O	535/537 (100%)	499 (93%)	30 (6%)	6 (1%)	11	36
1	P	535/537 (100%)	497 (93%)	34 (6%)	4 (1%)	18	47
All	All	8560/8592 (100%)	7953 (93%)	514 (6%)	93 (1%)	11	36

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	ASP
1	A	480	ASP
1	E	189	GLN
1	E	480	ASP
1	E	488	THR
1	F	306	ASP
1	L	530	ILE
1	M	189	GLN
1	M	480	ASP
1	N	306	ASP
1	N	480	ASP
1	N	488	THR
1	A	40	ALA
1	B	189	GLN
1	B	476	GLY
1	E	276	VAL
1	G	475	LEU
1	H	258	GLY
1	I	276	VAL
1	J	476	GLY
1	K	481	LEU
1	M	98	PHE
1	M	197	SER
1	M	298	LEU
1	M	487	ALA
1	N	476	GLY
1	N	493	TYR
1	O	476	GLY
1	O	480	ASP

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Mol	Chain	Res	Type
1	B	480	ASP
1	C	476	GLY
1	D	480	ASP
1	E	306	ASP
1	H	191	MET
1	J	191	MET
1	K	189	GLN
1	M	227	SER
1	N	276	VAL
1	A	197	SER
1	B	143	GLU
1	B	483	THR
1	C	276	VAL
1	C	306	ASP
1	D	276	VAL
1	D	481	LEU
1	F	227	SER
1	H	276	VAL
1	H	481	LEU
1	I	476	GLY
1	J	276	VAL
1	K	227	SER
1	L	197	SER
1	L	276	VAL
1	M	97	PHE
1	M	276	VAL
1	O	239	GLY
1	O	276	VAL
1	O	306	ASP
1	P	276	VAL
1	A	276	VAL
1	B	276	VAL
1	B	306	ASP
1	F	276	VAL
1	F	483	THR
1	K	376	SER
1	L	321	SER
1	M	191	MET
1	N	492	SER
1	P	306	ASP
1	P	480	ASP
1	D	419	SER

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Mol	Chain	Res	Type
1	E	455	ARG
1	F	476	GLY
1	G	191	MET
1	G	276	VAL
1	H	306	ASP
1	K	276	VAL
1	K	476	GLY
1	M	240	GLY
1	A	476	GLY
1	C	239	GLY
1	H	161	GLY
1	E	476	GLY
1	M	306	ASP
1	B	239	GLY
1	F	239	GLY
1	L	476	GLY
1	O	424	PRO
1	D	483	THR
1	N	469	VAL
1	P	240	GLY
1	C	483	THR
1	E	362	PRO

5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	426/455 (94%)	345 (81%)	81 (19%)	1	5
1	B	425/455 (93%)	336 (79%)	89 (21%)	1	4
1	C	425/455 (93%)	338 (80%)	87 (20%)	1	4
1	D	425/455 (93%)	341 (80%)	84 (20%)	1	5
1	E	425/455 (93%)	337 (79%)	88 (21%)	1	4
1	F	425/455 (93%)	329 (77%)	96 (23%)	1	3
1	G	426/455 (94%)	340 (80%)	86 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	425/455 (93%)	330 (78%)	95 (22%)	1	3
1	I	426/455 (94%)	332 (78%)	94 (22%)	1	3
1	J	425/455 (93%)	337 (79%)	88 (21%)	1	4
1	K	425/455 (93%)	335 (79%)	90 (21%)	1	4
1	L	426/455 (94%)	330 (78%)	96 (22%)	1	3
1	M	426/455 (94%)	310 (73%)	116 (27%)	0	1
1	N	425/455 (93%)	326 (77%)	99 (23%)	1	3
1	O	426/455 (94%)	324 (76%)	102 (24%)	1	3
1	P	425/455 (93%)	333 (78%)	92 (22%)	1	3
All	All	6806/7280 (94%)	5323 (78%)	1483 (22%)	1	3

All (1483) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	74	LEU
1	A	77	LEU
1	A	82	LEU
1	A	84	GLN
1	A	86	LEU
1	A	101	LEU
1	A	106	GLU
1	A	115	THR
1	A	130	ARG
1	A	133	LEU
1	A	139	VAL
1	A	152	SER
1	A	154	LEU
1	A	156	LEU
1	A	159	ASN
1	A	164	SER
1	A	173	VAL
1	A	190	SER
1	A	200	LEU
1	A	205	MET
1	A	218	SER
1	A	234	LEU
1	A	259	ASN
1	A	270	VAL

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Mol	Chain	Res	Type
1	A	279	SER
1	A	280	LEU
1	A	287	VAL
1	A	292	LEU
1	A	294	LEU
1	A	295	LYS
1	A	297	LEU
1	A	298	LEU
1	A	302	LEU
1	A	304	THR
1	A	320	ARG
1	A	322	SER
1	A	343	ARG
1	A	344	ARG
1	A	347	ILE
1	A	349	THR
1	A	351	GLN
1	A	352	ARG
1	A	354	GLU
1	A	359	THR
1	A	360	LEU
1	A	361	ILE
1	A	374	VAL
1	A	390	GLN
1	A	393	LYS
1	A	400	CYS
1	A	406	LEU
1	A	415	LYS
1	A	420	LEU
1	A	421	LEU
1	A	422	LEU
1	A	425	LEU
1	A	437	ARG
1	A	444	LEU
1	A	447	LEU
1	A	453	MET
1	A	459	ILE
1	A	463	LYS
1	A	465	MET
1	A	466	ASN
1	A	469	VAL
1	A	470	LEU

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Mol	Chain	Res	Type
1	A	475	LEU
1	A	481	LEU
1	A	483	THR
1	A	506	VAL
1	A	507	VAL
1	A	511	THR
1	A	530	ILE
1	A	534	ILE
1	A	542	SER
1	A	543	VAL
1	A	545	LEU
1	A	549	VAL
1	A	558	GLU
1	A	573	THR
1	B	51	SER
1	B	52	LEU
1	B	60	GLN
1	B	66	ASN
1	B	74	LEU
1	B	77	LEU
1	B	80	LEU
1	B	83	VAL
1	B	84	GLN
1	B	86	LEU
1	B	87	GLN
1	B	92	SER
1	B	101	LEU
1	B	106	GLU
1	B	109	LYS
1	B	115	THR
1	B	116	SER
1	B	118	LEU
1	B	130	ARG
1	B	133	LEU
1	B	134	LEU
1	B	154	LEU
1	B	156	LEU
1	B	162	MET
1	B	166	SER
1	B	169	VAL
1	B	173	VAL
1	B	177	GLN

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Mol	Chain	Res	Type
1	B	190	SER
1	B	205	MET
1	B	230	SER
1	B	234	LEU
1	B	242	ILE
1	B	254	LEU
1	B	255	LYS
1	B	264	SER
1	B	270	VAL
1	B	273	GLN
1	B	279	SER
1	B	280	LEU
1	B	287	VAL
1	B	292	LEU
1	B	294	LEU
1	B	295	LYS
1	B	297	LEU
1	B	298	LEU
1	B	304	THR
1	B	320	ARG
1	B	325	LEU
1	B	337	MET
1	B	342	MET
1	B	351	GLN
1	B	359	THR
1	B	374	VAL
1	B	382	SER
1	B	387	SER
1	B	390	GLN
1	B	393	LYS
1	B	397	VAL
1	B	404	LEU
1	B	415	LYS
1	B	418	LEU
1	B	420	LEU
1	B	421	LEU
1	B	422	LEU
1	B	425	LEU
1	B	429	LEU
1	B	437	ARG
1	B	444	LEU
1	B	447	LEU

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Mol	Chain	Res	Type
1	B	448	GLN
1	B	463	LYS
1	B	465	MET
1	B	470	LEU
1	B	472	THR
1	B	475	LEU
1	B	481	LEU
1	B	483	THR
1	B	486	ARG
1	B	488	THR
1	B	507	VAL
1	B	511	THR
1	B	530	ILE
1	B	534	ILE
1	B	542	SER
1	B	545	LEU
1	B	549	VAL
1	B	559	GLU
1	B	573	THR
1	C	51	SER
1	C	66	ASN
1	C	71	SER
1	C	74	LEU
1	C	77	LEU
1	C	80	LEU
1	C	83	VAL
1	C	84	GLN
1	C	85	LYS
1	C	86	LEU
1	C	101	LEU
1	C	106	GLU
1	C	109	LYS
1	C	115	THR
1	C	123	THR
1	C	130	ARG
1	C	133	LEU
1	C	142	LYS
1	C	143	GLU
1	C	151	ASP
1	C	152	SER
1	C	153	THR
1	C	154	LEU

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Mol	Chain	Res	Type
1	C	156	LEU
1	C	159	ASN
1	C	164	SER
1	C	173	VAL
1	C	177	GLN
1	C	184	HIS
1	C	190	SER
1	C	200	LEU
1	C	218	SER
1	C	234	LEU
1	C	254	LEU
1	C	259	ASN
1	C	264	SER
1	C	266	LEU
1	C	270	VAL
1	C	273	GLN
1	C	279	SER
1	C	280	LEU
1	C	287	VAL
1	C	289	SER
1	C	292	LEU
1	C	294	LEU
1	C	298	LEU
1	C	302	LEU
1	C	305	LEU
1	C	306	ASP
1	C	320	ARG
1	C	337	MET
1	C	347	ILE
1	C	349	THR
1	C	351	GLN
1	C	354	GLU
1	C	359	THR
1	C	374	VAL
1	C	390	GLN
1	C	393	LYS
1	C	406	LEU
1	C	412	SER
1	C	415	LYS
1	C	417	LEU
1	C	420	LEU
1	C	421	LEU

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Mol	Chain	Res	Type
1	C	422	LEU
1	C	425	LEU
1	C	437	ARG
1	C	444	LEU
1	C	447	LEU
1	C	463	LYS
1	C	465	MET
1	C	469	VAL
1	C	475	LEU
1	C	481	LEU
1	C	486	ARG
1	C	488	THR
1	C	495	VAL
1	C	507	VAL
1	C	517	ASP
1	C	530	ILE
1	C	534	ILE
1	C	536	LYS
1	C	541	ASN
1	C	543	VAL
1	C	545	LEU
1	C	549	VAL
1	D	47	LYS
1	D	51	SER
1	D	52	LEU
1	D	71	SER
1	D	74	LEU
1	D	75	LEU
1	D	77	LEU
1	D	80	LEU
1	D	84	GLN
1	D	85	LYS
1	D	86	LEU
1	D	92	SER
1	D	101	LEU
1	D	109	LYS
1	D	115	THR
1	D	121	CYS
1	D	124	GLN
1	D	130	ARG
1	D	141	LEU
1	D	152	SER

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Mol	Chain	Res	Type
1	D	154	LEU
1	D	156	LEU
1	D	159	ASN
1	D	160	GLU
1	D	173	VAL
1	D	184	HIS
1	D	205	MET
1	D	210	SER
1	D	218	SER
1	D	225	ILE
1	D	234	LEU
1	D	242	ILE
1	D	255	LYS
1	D	259	ASN
1	D	263	LYS
1	D	266	LEU
1	D	270	VAL
1	D	273	GLN
1	D	280	LEU
1	D	287	VAL
1	D	292	LEU
1	D	293	CYS
1	D	294	LEU
1	D	298	LEU
1	D	302	LEU
1	D	304	THR
1	D	305	LEU
1	D	322	SER
1	D	342	MET
1	D	343	ARG
1	D	346	LEU
1	D	349	THR
1	D	352	ARG
1	D	359	THR
1	D	374	VAL
1	D	382	SER
1	D	390	GLN
1	D	393	LYS
1	D	397	VAL
1	D	401	LEU
1	D	417	LEU
1	D	419	SER

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Mol	Chain	Res	Type
1	D	420	LEU
1	D	421	LEU
1	D	422	LEU
1	D	425	LEU
1	D	436	MET
1	D	437	ARG
1	D	444	LEU
1	D	447	LEU
1	D	448	GLN
1	D	465	MET
1	D	469	VAL
1	D	475	LEU
1	D	481	LEU
1	D	507	VAL
1	D	511	THR
1	D	530	ILE
1	D	534	ILE
1	D	535	LEU
1	D	545	LEU
1	D	549	VAL
1	D	559	GLU
1	D	573	THR
1	E	46	GLN
1	E	51	SER
1	E	52	LEU
1	E	66	ASN
1	E	74	LEU
1	E	76	THR
1	E	77	LEU
1	E	80	LEU
1	E	82	LEU
1	E	84	GLN
1	E	86	LEU
1	E	101	LEU
1	E	106	GLU
1	E	115	THR
1	E	116	SER
1	E	122	GLU
1	E	123	THR
1	E	130	ARG
1	E	133	LEU
1	E	143	GLU

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Mol	Chain	Res	Type
1	E	152	SER
1	E	154	LEU
1	E	156	LEU
1	E	160	GLU
1	E	162	MET
1	E	164	SER
1	E	168	CYS
1	E	177	GLN
1	E	180	VAL
1	E	205	MET
1	E	210	SER
1	E	251	ILE
1	E	259	ASN
1	E	261	LEU
1	E	270	VAL
1	E	279	SER
1	E	280	LEU
1	E	287	VAL
1	E	289	SER
1	E	292	LEU
1	E	294	LEU
1	E	297	LEU
1	E	305	LEU
1	E	320	ARG
1	E	331	GLU
1	E	337	MET
1	E	342	MET
1	E	349	THR
1	E	351	GLN
1	E	352	ARG
1	E	359	THR
1	E	374	VAL
1	E	382	SER
1	E	387	SER
1	E	390	GLN
1	E	397	VAL
1	E	400	CYS
1	E	406	LEU
1	E	415	LYS
1	E	420	LEU
1	E	421	LEU
1	E	422	LEU

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Mol	Chain	Res	Type
1	E	425	LEU
1	E	437	ARG
1	E	444	LEU
1	E	451	ILE
1	E	456	GLN
1	E	459	ILE
1	E	463	LYS
1	E	465	MET
1	E	467	LEU
1	E	469	VAL
1	E	475	LEU
1	E	495	VAL
1	E	507	VAL
1	E	511	THR
1	E	517	ASP
1	E	520	MET
1	E	530	ILE
1	E	534	ILE
1	E	542	SER
1	E	543	VAL
1	E	545	LEU
1	E	549	VAL
1	E	550	GLN
1	E	558	GLU
1	E	559	GLU
1	E	573	THR
1	F	47	LYS
1	F	48	GLN
1	F	51	SER
1	F	71	SER
1	F	74	LEU
1	F	75	LEU
1	F	77	LEU
1	F	80	LEU
1	F	83	VAL
1	F	84	GLN
1	F	86	LEU
1	F	92	SER
1	F	101	LEU
1	F	106	GLU
1	F	109	LYS
1	F	115	THR

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Mol	Chain	Res	Type
1	F	118	LEU
1	F	123	THR
1	F	130	ARG
1	F	133	LEU
1	F	143	GLU
1	F	153	THR
1	F	154	LEU
1	F	156	LEU
1	F	157	SER
1	F	158	LEU
1	F	159	ASN
1	F	162	MET
1	F	164	SER
1	F	170	VAL
1	F	173	VAL
1	F	177	GLN
1	F	180	VAL
1	F	198	ASN
1	F	205	MET
1	F	209	LYS
1	F	210	SER
1	F	218	SER
1	F	242	ILE
1	F	254	LEU
1	F	257	THR
1	F	264	SER
1	F	267	LYS
1	F	270	VAL
1	F	273	GLN
1	F	280	LEU
1	F	285	ARG
1	F	287	VAL
1	F	288	GLU
1	F	292	LEU
1	F	294	LEU
1	F	295	LYS
1	F	297	LEU
1	F	298	LEU
1	F	315	ARG
1	F	320	ARG
1	F	349	THR
1	F	351	GLN

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Mol	Chain	Res	Type
1	F	359	THR
1	F	374	VAL
1	F	382	SER
1	F	383	ASP
1	F	387	SER
1	F	390	GLN
1	F	395	ASP
1	F	401	LEU
1	F	404	LEU
1	F	406	LEU
1	F	412	SER
1	F	415	LYS
1	F	420	LEU
1	F	421	LEU
1	F	422	LEU
1	F	425	LEU
1	F	437	ARG
1	F	444	LEU
1	F	448	GLN
1	F	455	ARG
1	F	457	SER
1	F	465	MET
1	F	466	ASN
1	F	467	LEU
1	F	469	VAL
1	F	475	LEU
1	F	481	LEU
1	F	507	VAL
1	F	530	ILE
1	F	534	ILE
1	F	535	LEU
1	F	541	ASN
1	F	542	SER
1	F	543	VAL
1	F	545	LEU
1	F	549	VAL
1	F	559	GLU
1	F	573	THR
1	G	45	ARG
1	G	51	SER
1	G	52	LEU
1	G	74	LEU

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Mol	Chain	Res	Type
1	G	77	LEU
1	G	80	LEU
1	G	82	LEU
1	G	83	VAL
1	G	84	GLN
1	G	85	LYS
1	G	86	LEU
1	G	91	LEU
1	G	101	LEU
1	G	115	THR
1	G	119	THR
1	G	123	THR
1	G	126	SER
1	G	130	ARG
1	G	133	LEU
1	G	153	THR
1	G	154	LEU
1	G	156	LEU
1	G	157	SER
1	G	158	LEU
1	G	164	SER
1	G	173	VAL
1	G	180	VAL
1	G	183	VAL
1	G	190	SER
1	G	200	LEU
1	G	218	SER
1	G	238	ILE
1	G	259	ASN
1	G	263	LYS
1	G	270	VAL
1	G	279	SER
1	G	280	LEU
1	G	287	VAL
1	G	290	LEU
1	G	292	LEU
1	G	294	LEU
1	G	297	LEU
1	G	298	LEU
1	G	302	LEU
1	G	305	LEU
1	G	322	SER

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Mol	Chain	Res	Type
1	G	331	GLU
1	G	337	MET
1	G	349	THR
1	G	351	GLN
1	G	352	ARG
1	G	359	THR
1	G	360	LEU
1	G	374	VAL
1	G	382	SER
1	G	383	ASP
1	G	390	GLN
1	G	393	LYS
1	G	415	LYS
1	G	420	LEU
1	G	421	LEU
1	G	422	LEU
1	G	425	LEU
1	G	437	ARG
1	G	444	LEU
1	G	448	GLN
1	G	452	GLU
1	G	456	GLN
1	G	459	ILE
1	G	465	MET
1	G	466	ASN
1	G	469	VAL
1	G	475	LEU
1	G	481	LEU
1	G	488	THR
1	G	507	VAL
1	G	530	ILE
1	G	534	ILE
1	G	536	LYS
1	G	542	SER
1	G	545	LEU
1	G	549	VAL
1	G	558	GLU
1	G	559	GLU
1	G	570	GLN
1	G	573	THR
1	H	47	LYS
1	H	51	SER

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Mol	Chain	Res	Type
1	H	52	LEU
1	H	60	GLN
1	H	74	LEU
1	H	80	LEU
1	H	86	LEU
1	H	101	LEU
1	H	106	GLU
1	H	109	LYS
1	H	115	THR
1	H	119	THR
1	H	121	CYS
1	H	130	ARG
1	H	139	VAL
1	H	143	GLU
1	H	151	ASP
1	H	152	SER
1	H	154	LEU
1	H	156	LEU
1	H	159	ASN
1	H	162	MET
1	H	164	SER
1	H	166	SER
1	H	170	VAL
1	H	173	VAL
1	H	180	VAL
1	H	189	GLN
1	H	190	SER
1	H	200	LEU
1	H	205	MET
1	H	210	SER
1	H	218	SER
1	H	234	LEU
1	H	242	ILE
1	H	251	ILE
1	H	255	LYS
1	H	257	THR
1	H	259	ASN
1	H	263	LYS
1	H	264	SER
1	H	270	VAL
1	H	273	GLN
1	H	279	SER

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Mol	Chain	Res	Type
1	H	280	LEU
1	H	286	ASP
1	H	287	VAL
1	H	292	LEU
1	H	298	LEU
1	H	331	GLU
1	H	332	THR
1	H	337	MET
1	H	342	MET
1	H	344	ARG
1	H	347	ILE
1	H	350	LYS
1	H	351	GLN
1	H	359	THR
1	H	361	ILE
1	H	374	VAL
1	H	382	SER
1	H	390	GLN
1	H	397	VAL
1	H	400	CYS
1	H	401	LEU
1	H	412	SER
1	H	415	LYS
1	H	420	LEU
1	H	421	LEU
1	H	422	LEU
1	H	425	LEU
1	H	437	ARG
1	H	444	LEU
1	H	447	LEU
1	H	448	GLN
1	H	451	ILE
1	H	453	MET
1	H	457	SER
1	H	463	LYS
1	H	465	MET
1	H	466	ASN
1	H	467	LEU
1	H	469	VAL
1	H	475	LEU
1	H	481	LEU
1	H	486	ARG

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Mol	Chain	Res	Type
1	H	488	THR
1	H	507	VAL
1	H	530	ILE
1	H	534	ILE
1	H	536	LYS
1	H	545	LEU
1	H	549	VAL
1	H	559	GLU
1	H	570	GLN
1	I	45	ARG
1	I	46	GLN
1	I	51	SER
1	I	66	ASN
1	I	71	SER
1	I	74	LEU
1	I	77	LEU
1	I	80	LEU
1	I	83	VAL
1	I	84	GLN
1	I	86	LEU
1	I	101	LEU
1	I	106	GLU
1	I	109	LYS
1	I	115	THR
1	I	122	GLU
1	I	123	THR
1	I	126	SER
1	I	130	ARG
1	I	133	LEU
1	I	139	VAL
1	I	153	THR
1	I	154	LEU
1	I	156	LEU
1	I	157	SER
1	I	159	ASN
1	I	160	GLU
1	I	162	MET
1	I	164	SER
1	I	166	SER
1	I	169	VAL
1	I	173	VAL
1	I	177	GLN

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Mol	Chain	Res	Type
1	I	180	VAL
1	I	184	HIS
1	I	190	SER
1	I	200	LEU
1	I	205	MET
1	I	210	SER
1	I	218	SER
1	I	230	SER
1	I	234	LEU
1	I	242	ILE
1	I	264	SER
1	I	270	VAL
1	I	273	GLN
1	I	279	SER
1	I	280	LEU
1	I	287	VAL
1	I	289	SER
1	I	292	LEU
1	I	294	LEU
1	I	297	LEU
1	I	298	LEU
1	I	304	THR
1	I	305	LEU
1	I	320	ARG
1	I	326	ARG
1	I	337	MET
1	I	343	ARG
1	I	349	THR
1	I	350	LYS
1	I	359	THR
1	I	374	VAL
1	I	382	SER
1	I	387	SER
1	I	390	GLN
1	I	397	VAL
1	I	415	LYS
1	I	420	LEU
1	I	421	LEU
1	I	422	LEU
1	I	425	LEU
1	I	437	ARG
1	I	444	LEU

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Mol	Chain	Res	Type
1	I	447	LEU
1	I	448	GLN
1	I	452	GLU
1	I	457	SER
1	I	465	MET
1	I	466	ASN
1	I	469	VAL
1	I	475	LEU
1	I	481	LEU
1	I	488	THR
1	I	506	VAL
1	I	507	VAL
1	I	530	ILE
1	I	534	ILE
1	I	545	LEU
1	I	549	VAL
1	I	559	GLU
1	I	566	ARG
1	I	573	THR
1	J	47	LYS
1	J	52	LEU
1	J	74	LEU
1	J	77	LEU
1	J	80	LEU
1	J	84	GLN
1	J	86	LEU
1	J	99	THR
1	J	101	LEU
1	J	103	LYS
1	J	106	GLU
1	J	109	LYS
1	J	115	THR
1	J	116	SER
1	J	123	THR
1	J	126	SER
1	J	130	ARG
1	J	133	LEU
1	J	146	SER
1	J	153	THR
1	J	154	LEU
1	J	156	LEU
1	J	158	LEU

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Mol	Chain	Res	Type
1	J	159	ASN
1	J	162	MET
1	J	166	SER
1	J	173	VAL
1	J	180	VAL
1	J	184	HIS
1	J	189	GLN
1	J	205	MET
1	J	210	SER
1	J	218	SER
1	J	234	LEU
1	J	242	ILE
1	J	259	ASN
1	J	267	LYS
1	J	270	VAL
1	J	273	GLN
1	J	279	SER
1	J	280	LEU
1	J	287	VAL
1	J	288	GLU
1	J	292	LEU
1	J	294	LEU
1	J	297	LEU
1	J	298	LEU
1	J	320	ARG
1	J	337	MET
1	J	342	MET
1	J	343	ARG
1	J	349	THR
1	J	351	GLN
1	J	352	ARG
1	J	354	GLU
1	J	359	THR
1	J	374	VAL
1	J	390	GLN
1	J	393	LYS
1	J	397	VAL
1	J	400	CYS
1	J	404	LEU
1	J	406	LEU
1	J	415	LYS
1	J	420	LEU

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Mol	Chain	Res	Type
1	J	421	LEU
1	J	422	LEU
1	J	425	LEU
1	J	437	ARG
1	J	444	LEU
1	J	457	SER
1	J	465	MET
1	J	466	ASN
1	J	469	VAL
1	J	475	LEU
1	J	481	LEU
1	J	486	ARG
1	J	506	VAL
1	J	507	VAL
1	J	530	ILE
1	J	534	ILE
1	J	536	LYS
1	J	547	VAL
1	J	549	VAL
1	J	559	GLU
1	J	567	GLU
1	J	570	GLN
1	J	573	THR
1	K	45	ARG
1	K	46	GLN
1	K	48	GLN
1	K	51	SER
1	K	52	LEU
1	K	74	LEU
1	K	77	LEU
1	K	80	LEU
1	K	83	VAL
1	K	84	GLN
1	K	86	LEU
1	K	92	SER
1	K	101	LEU
1	K	109	LYS
1	K	123	THR
1	K	126	SER
1	K	130	ARG
1	K	133	LEU
1	K	143	GLU

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Mol	Chain	Res	Type
1	K	154	LEU
1	K	156	LEU
1	K	159	ASN
1	K	162	MET
1	K	173	VAL
1	K	177	GLN
1	K	180	VAL
1	K	198	ASN
1	K	205	MET
1	K	234	LEU
1	K	254	LEU
1	K	259	ASN
1	K	263	LYS
1	K	266	LEU
1	K	270	VAL
1	K	273	GLN
1	K	279	SER
1	K	280	LEU
1	K	283	MET
1	K	287	VAL
1	K	292	LEU
1	K	294	LEU
1	K	297	LEU
1	K	298	LEU
1	K	321	SER
1	K	322	SER
1	K	325	LEU
1	K	337	MET
1	K	343	ARG
1	K	344	ARG
1	K	346	LEU
1	K	350	LYS
1	K	354	GLU
1	K	359	THR
1	K	374	VAL
1	K	382	SER
1	K	390	GLN
1	K	393	LYS
1	K	395	ASP
1	K	397	VAL
1	K	400	CYS
1	K	406	LEU

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Mol	Chain	Res	Type
1	K	415	LYS
1	K	420	LEU
1	K	421	LEU
1	K	422	LEU
1	K	425	LEU
1	K	429	LEU
1	K	437	ARG
1	K	444	LEU
1	K	457	SER
1	K	465	MET
1	K	466	ASN
1	K	469	VAL
1	K	472	THR
1	K	475	LEU
1	K	481	LEU
1	K	486	ARG
1	K	506	VAL
1	K	507	VAL
1	K	511	THR
1	K	517	ASP
1	K	520	MET
1	K	530	ILE
1	K	534	ILE
1	K	542	SER
1	K	543	VAL
1	K	545	LEU
1	K	549	VAL
1	K	559	GLU
1	K	573	THR
1	L	51	SER
1	L	52	LEU
1	L	60	GLN
1	L	66	ASN
1	L	71	SER
1	L	74	LEU
1	L	75	LEU
1	L	77	LEU
1	L	80	LEU
1	L	81	GLN
1	L	84	GLN
1	L	85	LYS
1	L	86	LEU

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Mol	Chain	Res	Type
1	L	101	LEU
1	L	106	GLU
1	L	109	LYS
1	L	115	THR
1	L	123	THR
1	L	126	SER
1	L	130	ARG
1	L	133	LEU
1	L	139	VAL
1	L	143	GLU
1	L	153	THR
1	L	154	LEU
1	L	156	LEU
1	L	159	ASN
1	L	164	SER
1	L	173	VAL
1	L	177	GLN
1	L	184	HIS
1	L	190	SER
1	L	218	SER
1	L	230	SER
1	L	234	LEU
1	L	238	ILE
1	L	254	LEU
1	L	257	THR
1	L	263	LYS
1	L	270	VAL
1	L	273	GLN
1	L	279	SER
1	L	280	LEU
1	L	283	MET
1	L	287	VAL
1	L	289	SER
1	L	292	LEU
1	L	295	LYS
1	L	298	LEU
1	L	302	LEU
1	L	320	ARG
1	L	332	THR
1	L	337	MET
1	L	342	MET
1	L	349	THR

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Mol	Chain	Res	Type
1	L	351	GLN
1	L	352	ARG
1	L	359	THR
1	L	374	VAL
1	L	380	LEU
1	L	382	SER
1	L	383	ASP
1	L	387	SER
1	L	390	GLN
1	L	393	LYS
1	L	395	ASP
1	L	400	CYS
1	L	415	LYS
1	L	420	LEU
1	L	421	LEU
1	L	422	LEU
1	L	437	ARG
1	L	444	LEU
1	L	447	LEU
1	L	451	ILE
1	L	452	GLU
1	L	456	GLN
1	L	465	MET
1	L	466	ASN
1	L	467	LEU
1	L	469	VAL
1	L	475	LEU
1	L	488	THR
1	L	495	VAL
1	L	506	VAL
1	L	507	VAL
1	L	511	THR
1	L	520	MET
1	L	530	ILE
1	L	534	ILE
1	L	545	LEU
1	L	547	VAL
1	L	549	VAL
1	L	559	GLU
1	L	570	GLN
1	L	573	THR
1	M	47	LYS

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Mol	Chain	Res	Type
1	M	48	GLN
1	M	52	LEU
1	M	55	MET
1	M	66	ASN
1	M	75	LEU
1	M	76	THR
1	M	77	LEU
1	M	80	LEU
1	M	82	LEU
1	M	84	GLN
1	M	86	LEU
1	M	92	SER
1	M	96	VAL
1	M	101	LEU
1	M	109	LYS
1	M	118	LEU
1	M	122	GLU
1	M	123	THR
1	M	130	ARG
1	M	133	LEU
1	M	143	GLU
1	M	152	SER
1	M	153	THR
1	M	154	LEU
1	M	156	LEU
1	M	162	MET
1	M	164	SER
1	M	166	SER
1	M	171	VAL
1	M	172	GLN
1	M	173	VAL
1	M	176	LEU
1	M	177	GLN
1	M	180	VAL
1	M	189	GLN
1	M	191	MET
1	M	205	MET
1	M	213	SER
1	M	217	SER
1	M	232	LEU
1	M	234	LEU
1	M	257	THR

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Mol	Chain	Res	Type
1	M	263	LYS
1	M	267	LYS
1	M	270	VAL
1	M	271	TYR
1	M	273	GLN
1	M	279	SER
1	M	280	LEU
1	M	285	ARG
1	M	287	VAL
1	M	289	SER
1	M	292	LEU
1	M	294	LEU
1	M	295	LYS
1	M	298	LEU
1	M	305	LEU
1	M	312	LEU
1	M	325	LEU
1	M	326	ARG
1	M	332	THR
1	M	339	SER
1	M	342	MET
1	M	343	ARG
1	M	346	LEU
1	M	348	GLU
1	M	351	GLN
1	M	354	GLU
1	M	359	THR
1	M	364	LEU
1	M	374	VAL
1	M	380	LEU
1	M	382	SER
1	M	383	ASP
1	M	390	GLN
1	M	393	LYS
1	M	395	ASP
1	M	397	VAL
1	M	404	LEU
1	M	405	ILE
1	M	412	SER
1	M	415	LYS
1	M	420	LEU
1	M	421	LEU

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Mol	Chain	Res	Type
1	M	422	LEU
1	M	425	LEU
1	M	429	LEU
1	M	435	SER
1	M	437	ARG
1	M	442	GLU
1	M	444	LEU
1	M	447	LEU
1	M	452	GLU
1	M	453	MET
1	M	457	SER
1	M	461	GLN
1	M	465	MET
1	M	466	ASN
1	M	469	VAL
1	M	472	THR
1	M	475	LEU
1	M	481	LEU
1	M	486	ARG
1	M	507	VAL
1	M	517	ASP
1	M	530	ILE
1	M	534	ILE
1	M	535	LEU
1	M	542	SER
1	M	543	VAL
1	M	547	VAL
1	M	559	GLU
1	M	561	CYS
1	M	570	GLN
1	M	573	THR
1	N	43	ARG
1	N	51	SER
1	N	52	LEU
1	N	60	GLN
1	N	74	LEU
1	N	75	LEU
1	N	77	LEU
1	N	80	LEU
1	N	83	VAL
1	N	84	GLN
1	N	85	LYS

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Mol	Chain	Res	Type
1	N	86	LEU
1	N	101	LEU
1	N	106	GLU
1	N	115	THR
1	N	116	SER
1	N	118	LEU
1	N	123	THR
1	N	126	SER
1	N	130	ARG
1	N	134	LEU
1	N	143	GLU
1	N	154	LEU
1	N	156	LEU
1	N	157	SER
1	N	159	ASN
1	N	169	VAL
1	N	173	VAL
1	N	180	VAL
1	N	190	SER
1	N	198	ASN
1	N	205	MET
1	N	210	SER
1	N	213	SER
1	N	218	SER
1	N	232	LEU
1	N	242	ILE
1	N	254	LEU
1	N	259	ASN
1	N	266	LEU
1	N	273	GLN
1	N	279	SER
1	N	280	LEU
1	N	287	VAL
1	N	289	SER
1	N	292	LEU
1	N	294	LEU
1	N	295	LYS
1	N	297	LEU
1	N	298	LEU
1	N	320	ARG
1	N	321	SER
1	N	322	SER

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Mol	Chain	Res	Type
1	N	326	ARG
1	N	331	GLU
1	N	342	MET
1	N	351	GLN
1	N	360	LEU
1	N	368	ILE
1	N	374	VAL
1	N	382	SER
1	N	383	ASP
1	N	387	SER
1	N	390	GLN
1	N	401	LEU
1	N	404	LEU
1	N	415	LYS
1	N	420	LEU
1	N	421	LEU
1	N	422	LEU
1	N	425	LEU
1	N	436	MET
1	N	437	ARG
1	N	444	LEU
1	N	448	GLN
1	N	457	SER
1	N	459	ILE
1	N	463	LYS
1	N	465	MET
1	N	466	ASN
1	N	468	ASP
1	N	469	VAL
1	N	471	LEU
1	N	472	THR
1	N	475	LEU
1	N	481	LEU
1	N	488	THR
1	N	506	VAL
1	N	507	VAL
1	N	520	MET
1	N	530	ILE
1	N	534	ILE
1	N	541	ASN
1	N	543	VAL
1	N	545	LEU

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Mol	Chain	Res	Type
1	N	549	VAL
1	N	558	GLU
1	N	559	GLU
1	N	573	THR
1	O	51	SER
1	O	52	LEU
1	O	54	THR
1	O	66	ASN
1	O	71	SER
1	O	77	LEU
1	O	80	LEU
1	O	82	LEU
1	O	84	GLN
1	O	86	LEU
1	O	96	VAL
1	O	101	LEU
1	O	103	LYS
1	O	106	GLU
1	O	109	LYS
1	O	115	THR
1	O	116	SER
1	O	126	SER
1	O	130	ARG
1	O	133	LEU
1	O	143	GLU
1	O	153	THR
1	O	154	LEU
1	O	156	LEU
1	O	157	SER
1	O	158	LEU
1	O	159	ASN
1	O	162	MET
1	O	173	VAL
1	O	177	GLN
1	O	180	VAL
1	O	189	GLN
1	O	190	SER
1	O	198	ASN
1	O	200	LEU
1	O	205	MET
1	O	210	SER
1	O	218	SER

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Mol	Chain	Res	Type
1	O	232	LEU
1	O	238	ILE
1	O	254	LEU
1	O	255	LYS
1	O	264	SER
1	O	270	VAL
1	O	273	GLN
1	O	280	LEU
1	O	286	ASP
1	O	287	VAL
1	O	292	LEU
1	O	294	LEU
1	O	297	LEU
1	O	298	LEU
1	O	320	ARG
1	O	331	GLU
1	O	332	THR
1	O	337	MET
1	O	342	MET
1	O	343	ARG
1	O	350	LYS
1	O	351	GLN
1	O	352	ARG
1	O	354	GLU
1	O	359	THR
1	O	361	ILE
1	O	374	VAL
1	O	382	SER
1	O	390	GLN
1	O	393	LYS
1	O	397	VAL
1	O	401	LEU
1	O	415	LYS
1	O	417	LEU
1	O	419	SER
1	O	420	LEU
1	O	421	LEU
1	O	422	LEU
1	O	429	LEU
1	O	437	ARG
1	O	444	LEU
1	O	447	LEU

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Mol	Chain	Res	Type
1	O	448	GLN
1	O	451	ILE
1	O	452	GLU
1	O	457	SER
1	O	465	MET
1	O	466	ASN
1	O	469	VAL
1	O	475	LEU
1	O	481	LEU
1	O	486	ARG
1	O	491	ILE
1	O	507	VAL
1	O	517	ASP
1	O	520	MET
1	O	534	ILE
1	O	536	LYS
1	O	542	SER
1	O	545	LEU
1	O	547	VAL
1	O	549	VAL
1	O	559	GLU
1	O	573	THR
1	P	52	LEU
1	P	54	THR
1	P	66	ASN
1	P	74	LEU
1	P	77	LEU
1	P	80	LEU
1	P	83	VAL
1	P	84	GLN
1	P	85	LYS
1	P	86	LEU
1	P	90	GLU
1	P	92	SER
1	P	101	LEU
1	P	106	GLU
1	P	109	LYS
1	P	115	THR
1	P	119	THR
1	P	123	THR
1	P	126	SER
1	P	130	ARG

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Mol	Chain	Res	Type
1	P	143	GLU
1	P	152	SER
1	P	153	THR
1	P	154	LEU
1	P	156	LEU
1	P	164	SER
1	P	173	VAL
1	P	180	VAL
1	P	183	VAL
1	P	189	GLN
1	P	218	SER
1	P	234	LEU
1	P	251	ILE
1	P	257	THR
1	P	259	ASN
1	P	263	LYS
1	P	266	LEU
1	P	269	CYS
1	P	279	SER
1	P	280	LEU
1	P	287	VAL
1	P	292	LEU
1	P	294	LEU
1	P	295	LYS
1	P	297	LEU
1	P	298	LEU
1	P	304	THR
1	P	320	ARG
1	P	322	SER
1	P	325	LEU
1	P	331	GLU
1	P	337	MET
1	P	346	LEU
1	P	350	LYS
1	P	351	GLN
1	P	352	ARG
1	P	359	THR
1	P	374	VAL
1	P	376	SER
1	P	382	SER
1	P	387	SER
1	P	390	GLN

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Mol	Chain	Res	Type
1	P	401	LEU
1	P	404	LEU
1	P	412	SER
1	P	415	LYS
1	P	420	LEU
1	P	421	LEU
1	P	425	LEU
1	P	429	LEU
1	P	433	LEU
1	P	437	ARG
1	P	444	LEU
1	P	465	MET
1	P	466	ASN
1	P	467	LEU
1	P	469	VAL
1	P	474	MET
1	P	475	LEU
1	P	481	LEU
1	P	495	VAL
1	P	507	VAL
1	P	511	THR
1	P	530	ILE
1	P	534	ILE
1	P	535	LEU
1	P	542	SER
1	P	543	VAL
1	P	545	LEU
1	P	547	VAL
1	P	549	VAL
1	P	559	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (181) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	60	GLN
1	A	159	ASN
1	A	189	GLN
1	A	198	ASN
1	A	259	ASN
1	A	358	HIS
1	A	366	ASN

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Mol	Chain	Res	Type
1	A	448	GLN
1	A	498	ASN
1	B	48	GLN
1	B	84	GLN
1	B	159	ASN
1	B	172	GLN
1	B	189	GLN
1	B	198	ASN
1	B	259	ASN
1	B	273	GLN
1	B	334	ASN
1	B	358	HIS
1	B	448	GLN
1	B	498	ASN
1	C	81	GLN
1	C	189	GLN
1	C	198	ASN
1	C	259	ASN
1	C	273	GLN
1	C	358	HIS
1	C	391	ASN
1	C	482	ASN
1	C	498	ASN
1	D	48	GLN
1	D	84	GLN
1	D	87	GLN
1	D	150	HIS
1	D	189	GLN
1	D	198	ASN
1	D	259	ASN
1	D	273	GLN
1	D	351	GLN
1	D	358	HIS
1	D	434	ASN
1	D	482	ASN
1	D	498	ASN
1	E	48	GLN
1	E	66	ASN
1	E	189	GLN
1	E	259	ASN
1	E	358	HIS
1	E	498	ASN

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Mol	Chain	Res	Type
1	F	48	GLN
1	F	84	GLN
1	F	108	ASN
1	F	159	ASN
1	F	189	GLN
1	F	198	ASN
1	F	259	ASN
1	F	273	GLN
1	F	358	HIS
1	F	434	ASN
1	F	498	ASN
1	G	48	GLN
1	G	66	ASN
1	G	87	GLN
1	G	177	GLN
1	G	189	GLN
1	G	198	ASN
1	G	259	ASN
1	G	358	HIS
1	G	366	ASN
1	G	434	ASN
1	G	482	ASN
1	G	498	ASN
1	G	557	GLN
1	H	48	GLN
1	H	66	ASN
1	H	87	GLN
1	H	159	ASN
1	H	177	GLN
1	H	189	GLN
1	H	259	ASN
1	H	273	GLN
1	H	351	GLN
1	H	358	HIS
1	H	366	ASN
1	H	391	ASN
1	H	448	GLN
1	H	456	GLN
1	H	498	ASN
1	I	46	GLN
1	I	48	GLN
1	I	66	ASN

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Mol	Chain	Res	Type
1	I	84	GLN
1	I	186	ASN
1	I	189	GLN
1	I	259	ASN
1	I	358	HIS
1	I	391	ASN
1	I	434	ASN
1	I	498	ASN
1	I	541	ASN
1	J	48	GLN
1	J	87	GLN
1	J	177	GLN
1	J	189	GLN
1	J	203	GLN
1	J	259	ASN
1	J	301	HIS
1	J	358	HIS
1	J	391	ASN
1	J	434	ASN
1	J	482	ASN
1	J	498	ASN
1	K	46	GLN
1	K	66	ASN
1	K	81	GLN
1	K	84	GLN
1	K	189	GLN
1	K	198	ASN
1	K	259	ASN
1	K	358	HIS
1	K	391	ASN
1	K	498	ASN
1	L	48	GLN
1	L	66	ASN
1	L	87	GLN
1	L	189	GLN
1	L	273	GLN
1	L	334	ASN
1	L	358	HIS
1	L	366	ASN
1	L	482	ASN
1	L	498	ASN
1	M	124	GLN

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Mol	Chain	Res	Type
1	M	159	ASN
1	M	172	GLN
1	M	198	ASN
1	M	273	GLN
1	M	351	GLN
1	M	391	ASN
1	M	456	GLN
1	M	482	ASN
1	M	498	ASN
1	N	48	GLN
1	N	81	GLN
1	N	84	GLN
1	N	159	ASN
1	N	189	GLN
1	N	198	ASN
1	N	259	ASN
1	N	334	ASN
1	N	358	HIS
1	N	434	ASN
1	N	448	GLN
1	N	482	ASN
1	N	498	ASN
1	N	541	ASN
1	O	87	GLN
1	O	124	GLN
1	O	177	GLN
1	O	189	GLN
1	O	198	ASN
1	O	259	ASN
1	O	273	GLN
1	O	351	GLN
1	O	358	HIS
1	O	366	ASN
1	O	456	GLN
1	O	498	ASN
1	P	48	GLN
1	P	66	ASN
1	P	159	ASN
1	P	189	GLN
1	P	259	ASN
1	P	358	HIS
1	P	367	ASN

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Mol	Chain	Res	Type
1	P	390	GLN
1	P	391	ASN
1	P	434	ASN
1	P	456	GLN
1	P	498	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MAY	G	600	1	20,23,24	0.34	0	18,23,26	0.65	0
2	MAY	N	600	1	20,23,24	0.45	0	18,23,26	0.57	0
2	MAY	B	600	1	20,23,24	0.46	0	18,23,26	0.57	0
2	MAY	K	600	1	20,23,24	0.44	0	18,23,26	0.53	0
2	MAY	C	600	1	20,23,24	0.33	0	18,23,26	0.57	0
2	MAY	E	600	1	20,23,24	0.44	0	18,23,26	0.58	0
2	MAY	A	600	1	20,23,24	0.38	0	18,23,26	0.63	0
2	MAY	M	600	1	20,23,24	0.34	0	18,23,26	0.60	0
2	MAY	L	600	1	20,23,24	0.44	0	18,23,26	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAY	P	600	1	20,23,24	0.40	0	18,23,26	0.52	0
2	MAY	O	600	1	20,23,24	0.46	0	18,23,26	0.50	0
2	MAY	H	600	1	20,23,24	0.44	0	18,23,26	0.61	0
2	MAY	F	600	1	20,23,24	0.44	0	18,23,26	0.46	0
2	MAY	J	600	1	20,23,24	0.46	0	18,23,26	0.55	0
2	MAY	I	600	1	20,23,24	0.34	0	18,23,26	0.60	0
2	MAY	D	600	1	20,23,24	0.37	0	18,23,26	0.64	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
2	MAY	G	600	1	-	8/18/22/24	-
2	MAY	N	600	1	-	8/18/22/24	-
2	MAY	B	600	1	-	9/18/22/24	-
2	MAY	K	600	1	-	8/18/22/24	-
2	MAY	C	600	1	-	8/18/22/24	-
2	MAY	E	600	1	-	7/18/22/24	-
2	MAY	A	600	1	-	7/18/22/24	-
2	MAY	M	600	1	-	7/18/22/24	-
2	MAY	L	600	1	-	9/18/22/24	-
2	MAY	P	600	1	-	7/18/22/24	-
2	MAY	O	600	1	-	8/18/22/24	-
2	MAY	H	600	1	-	9/18/22/24	-
2	MAY	F	600	1	-	8/18/22/24	-
2	MAY	J	600	1	-	8/18/22/24	-
2	MAY	I	600	1	-	7/18/22/24	-
2	MAY	D	600	1	-	9/18/22/24	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	600	MAY	P1-C1-C2-C3
2	K	600	MAY	P1-C1-C2-C3
2	M	600	MAY	P1-C1-C2-C3
2	O	600	MAY	C1-C2-C3-C4
2	D	600	MAY	C1-C2-C3-C4
2	G	600	MAY	C1-C2-C3-C4
2	J	600	MAY	C1-C2-C3-C4
2	C	600	MAY	C1-C2-C3-C4
2	L	600	MAY	C1-C2-C3-C4
2	I	600	MAY	C2-C3-C4-C5
2	N	600	MAY	C2-C3-C4-C5
2	D	600	MAY	C2-C3-C4-C5
2	A	600	MAY	C2-C3-C4-C5
2	G	600	MAY	C2-C3-C4-C5
2	O	600	MAY	C2-C3-C4-C5
2	P	600	MAY	C2-C3-C4-C5
2	I	600	MAY	C1-C2-C3-C4
2	C	600	MAY	C2-C3-C4-C5
2	F	600	MAY	C2-C3-C4-C5
2	H	600	MAY	C2-C3-C4-C5
2	J	600	MAY	C2-C3-C4-C5
2	M	600	MAY	C2-C3-C4-C5
2	A	600	MAY	C1-C2-C3-C4
2	E	600	MAY	C1-C2-C3-C4
2	H	600	MAY	C1-C2-C3-C4
2	M	600	MAY	C1-C2-C3-C4
2	N	600	MAY	C1-C2-C3-C4
2	P	600	MAY	C1-C2-C3-C4
2	B	600	MAY	C1-C2-C3-C4
2	F	600	MAY	C1-C2-C3-C4
2	K	600	MAY	C1-C2-C3-C4
2	B	600	MAY	P1-C1-C2-C3
2	C	600	MAY	P1-C1-C2-C3
2	E	600	MAY	P1-C1-C2-C3
2	I	600	MAY	P1-C1-C2-C3
2	L	600	MAY	P1-C1-C2-C3
2	N	600	MAY	P1-C1-C2-C3
2	P	600	MAY	P1-C1-C2-C3
2	B	600	MAY	C2-C3-C4-C5
2	K	600	MAY	C2-C3-C4-C5
2	L	600	MAY	C2-C3-C4-C5
2	P	600	MAY	C15-C16-C17-C18
2	A	600	MAY	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
2	C	600	MAY	C15-C16-C17-C18
2	E	600	MAY	C2-C3-C4-C5
2	E	600	MAY	C15-C16-C17-C18
2	G	600	MAY	C15-C16-C17-C18
2	H	600	MAY	C15-C16-C17-C18
2	I	600	MAY	C15-C16-C17-C18
2	J	600	MAY	C15-C16-C17-C18
2	K	600	MAY	C15-C16-C17-C18
2	M	600	MAY	C15-C16-C17-C18
2	O	600	MAY	C15-C16-C17-C18
2	B	600	MAY	C15-C16-C17-C18
2	D	600	MAY	C15-C16-C17-C18
2	F	600	MAY	C15-C16-C17-C18
2	L	600	MAY	C15-C16-C17-C18
2	N	600	MAY	C15-C16-C17-C18
2	A	600	MAY	C6-C7-C8-C9
2	B	600	MAY	C6-C7-C8-C9
2	B	600	MAY	C12-C13-C14-C15
2	C	600	MAY	C6-C7-C8-C9
2	D	600	MAY	C6-C7-C8-C9
2	E	600	MAY	C6-C7-C8-C9
2	F	600	MAY	C6-C7-C8-C9
2	G	600	MAY	C6-C7-C8-C9
2	H	600	MAY	C6-C7-C8-C9
2	H	600	MAY	C9-C10-C11-C12
2	I	600	MAY	C6-C7-C8-C9
2	J	600	MAY	C6-C7-C8-C9
2	K	600	MAY	C6-C7-C8-C9
2	L	600	MAY	C6-C7-C8-C9
2	M	600	MAY	C6-C7-C8-C9
2	N	600	MAY	C6-C7-C8-C9
2	O	600	MAY	C6-C7-C8-C9
2	P	600	MAY	C6-C7-C8-C9
2	N	600	MAY	C17-C18-C19-C20
2	O	600	MAY	C17-C18-C19-C20
2	M	600	MAY	C17-C18-C19-C20
2	B	600	MAY	C17-C18-C19-C20
2	F	600	MAY	C17-C18-C19-C20
2	A	600	MAY	C17-C18-C19-C20
2	I	600	MAY	C17-C18-C19-C20
2	J	600	MAY	C17-C18-C19-C20
2	C	600	MAY	C17-C18-C19-C20

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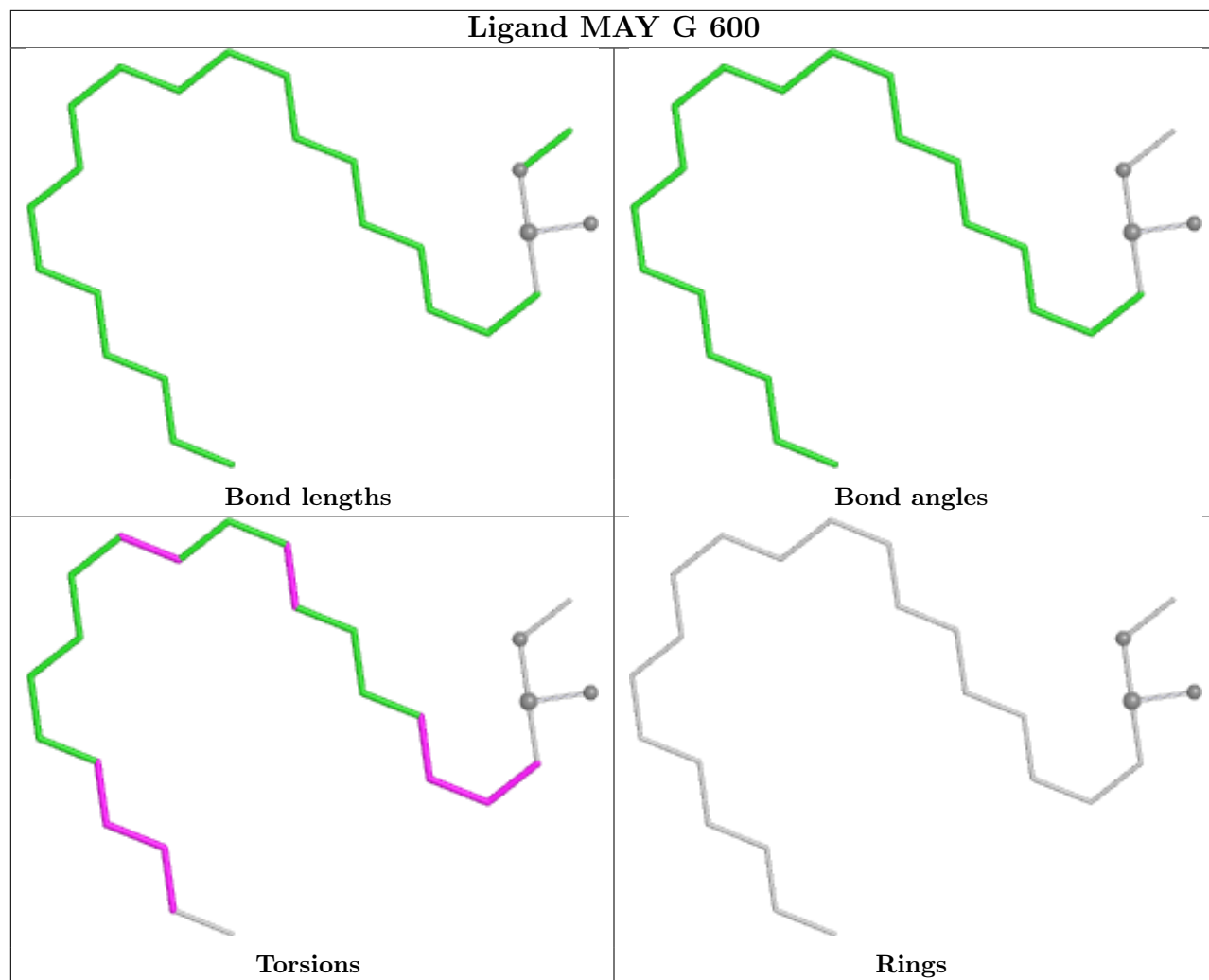
Mol	Chain	Res	Type	Atoms
2	L	600	MAY	C17-C18-C19-C20
2	K	600	MAY	C17-C18-C19-C20
2	A	600	MAY	P1-C1-C2-C3
2	D	600	MAY	P1-C1-C2-C3
2	E	600	MAY	C17-C18-C19-C20
2	P	600	MAY	C17-C18-C19-C20
2	G	600	MAY	C17-C18-C19-C20
2	H	600	MAY	C17-C18-C19-C20
2	D	600	MAY	C17-C18-C19-C20
2	D	600	MAY	C16-C17-C18-C19
2	G	600	MAY	P1-C1-C2-C3
2	H	600	MAY	P1-C1-C2-C3
2	J	600	MAY	P1-C1-C2-C3
2	O	600	MAY	P1-C1-C2-C3
2	A	600	MAY	C9-C10-C11-C12
2	B	600	MAY	C9-C10-C11-C12
2	C	600	MAY	C9-C10-C11-C12
2	D	600	MAY	C9-C10-C11-C12
2	D	600	MAY	C12-C13-C14-C15
2	E	600	MAY	C9-C10-C11-C12
2	F	600	MAY	C9-C10-C11-C12
2	G	600	MAY	C9-C10-C11-C12
2	H	600	MAY	C12-C13-C14-C15
2	I	600	MAY	C9-C10-C11-C12
2	J	600	MAY	C9-C10-C11-C12
2	J	600	MAY	C12-C13-C14-C15
2	K	600	MAY	C9-C10-C11-C12
2	L	600	MAY	C9-C10-C11-C12
2	L	600	MAY	C12-C13-C14-C15
2	M	600	MAY	C9-C10-C11-C12
2	N	600	MAY	C9-C10-C11-C12
2	N	600	MAY	C12-C13-C14-C15
2	O	600	MAY	C9-C10-C11-C12
2	P	600	MAY	C9-C10-C11-C12
2	G	600	MAY	C16-C17-C18-C19
2	H	600	MAY	C16-C17-C18-C19
2	K	600	MAY	C16-C17-C18-C19
2	O	600	MAY	C16-C17-C18-C19
2	L	600	MAY	C16-C17-C18-C19
2	B	600	MAY	C16-C17-C18-C19
2	C	600	MAY	C16-C17-C18-C19
2	F	600	MAY	C16-C17-C18-C19

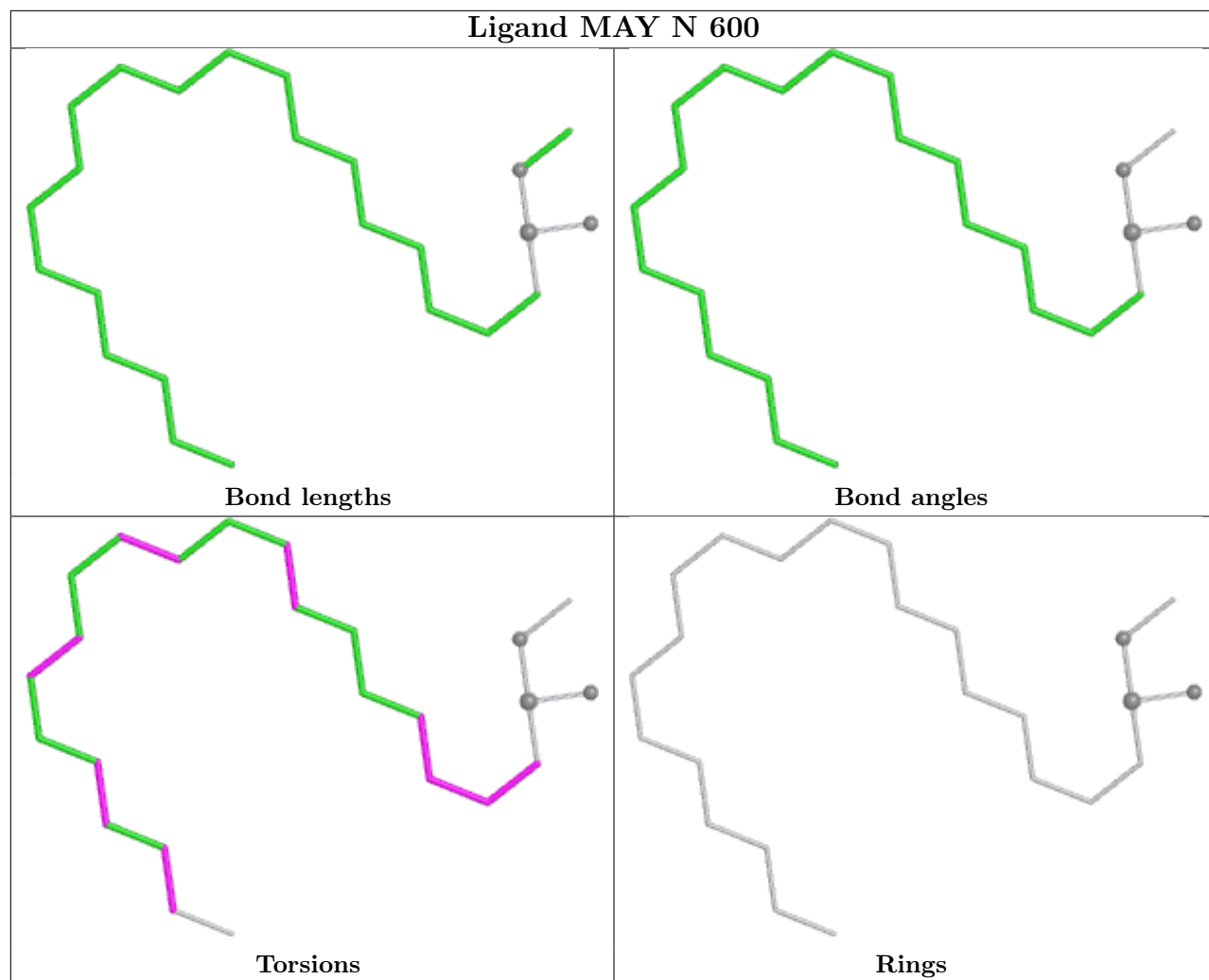
There are no ring outliers.

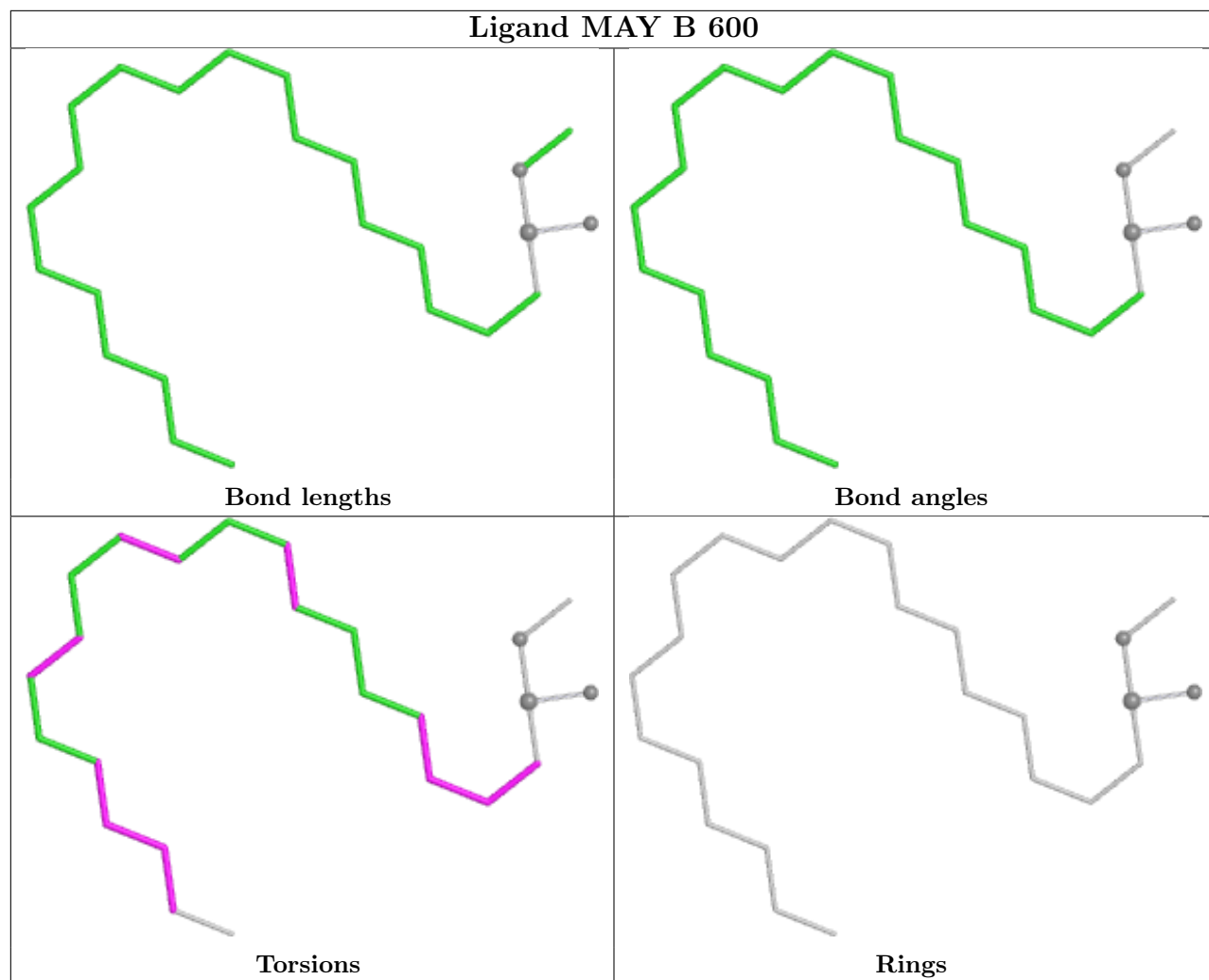
16 monomers are involved in 46 short contacts:

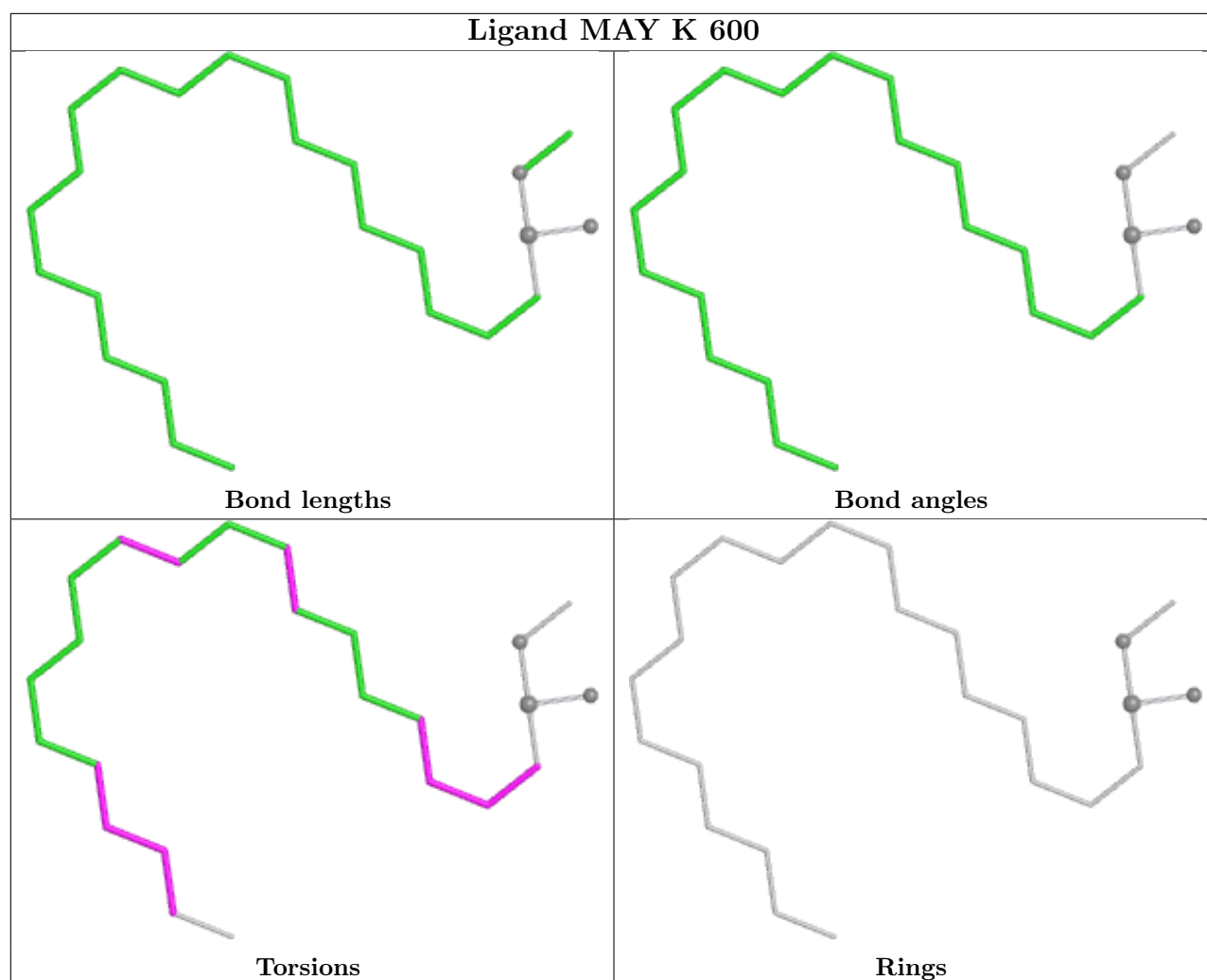
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	600	MAY	1	0
2	N	600	MAY	4	0
2	B	600	MAY	3	0
2	K	600	MAY	3	0
2	C	600	MAY	3	0
2	E	600	MAY	3	0
2	A	600	MAY	5	0
2	M	600	MAY	2	0
2	L	600	MAY	1	0
2	P	600	MAY	2	0
2	O	600	MAY	3	0
2	H	600	MAY	4	0
2	F	600	MAY	4	0
2	J	600	MAY	2	0
2	I	600	MAY	2	0
2	D	600	MAY	4	0

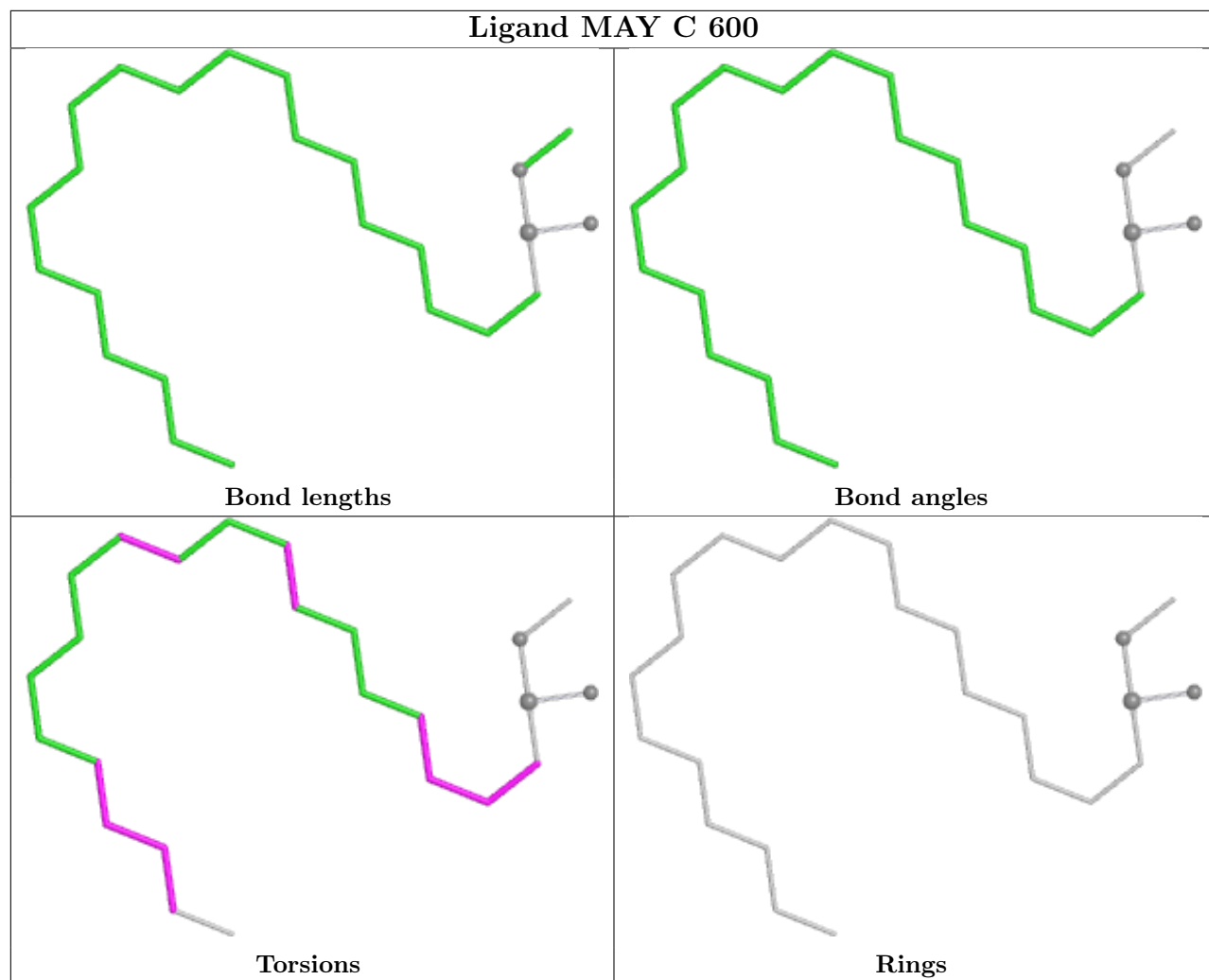
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

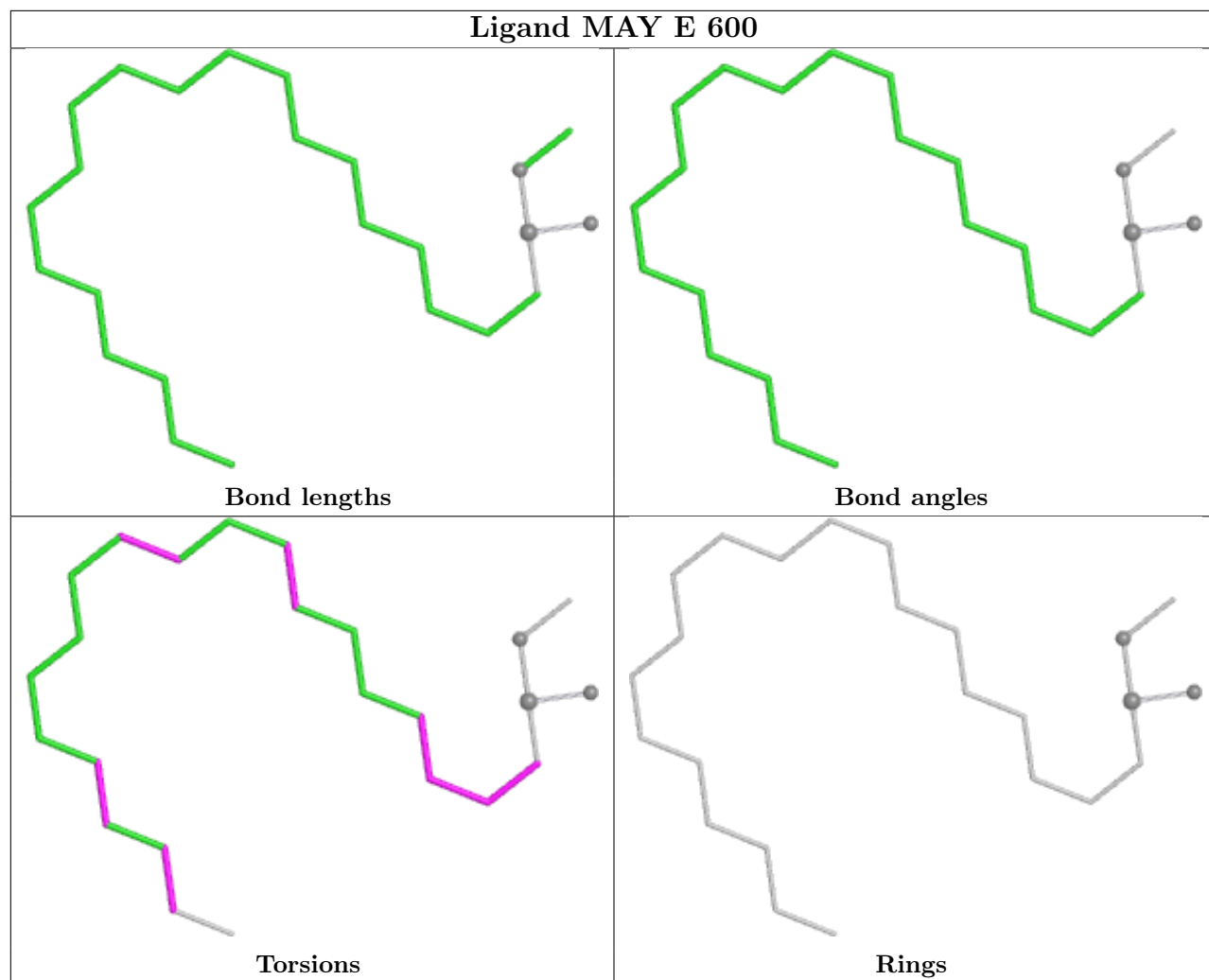


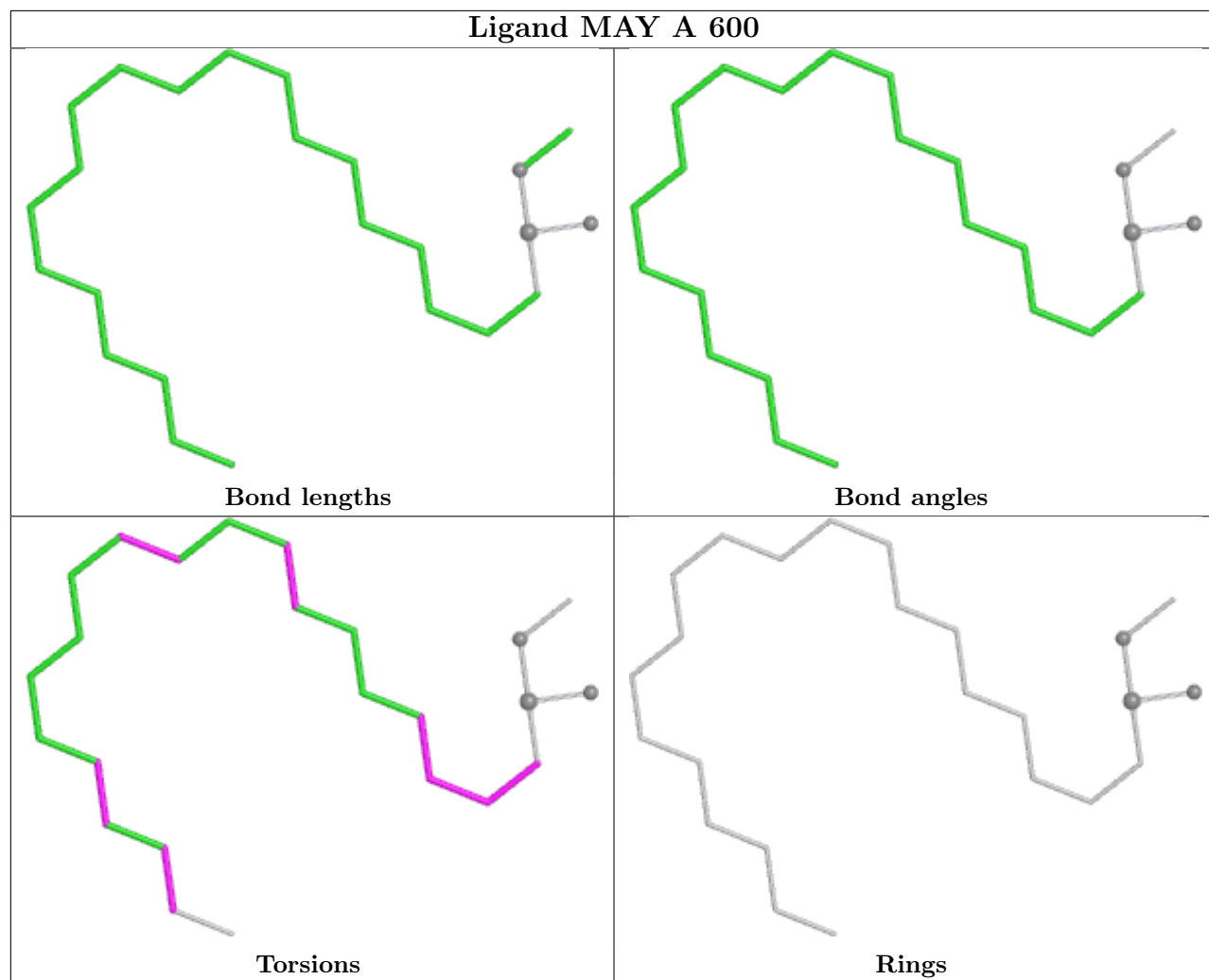


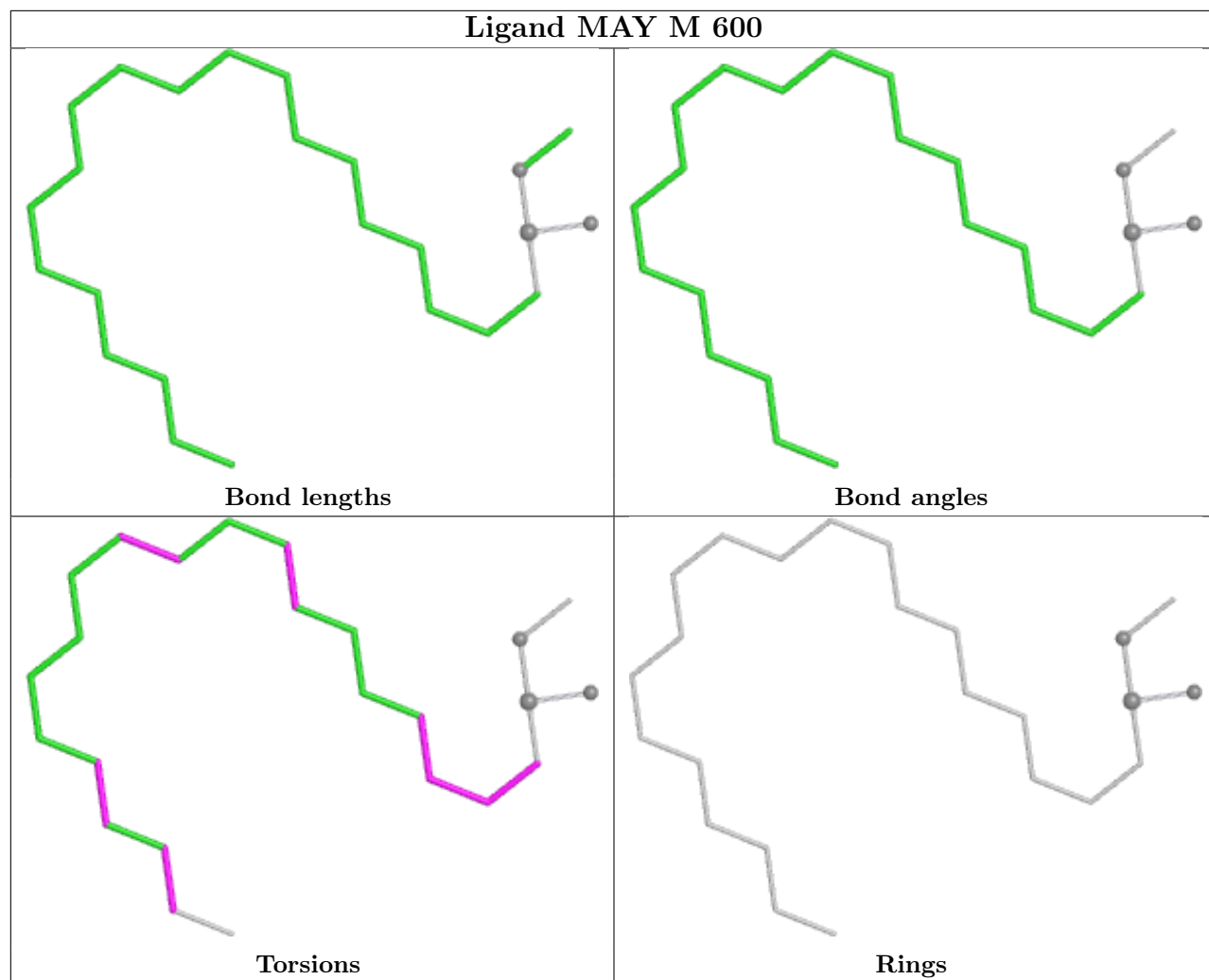


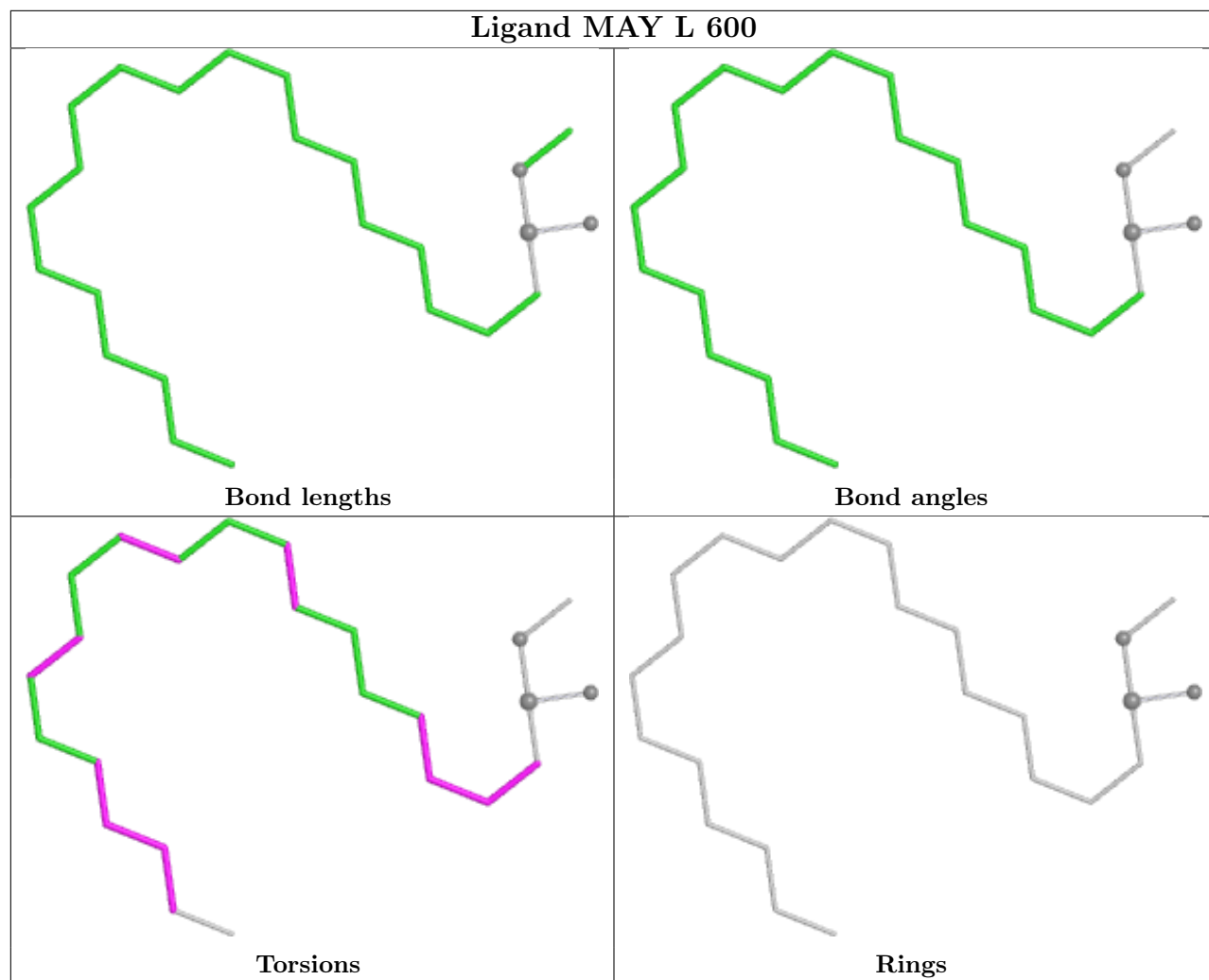


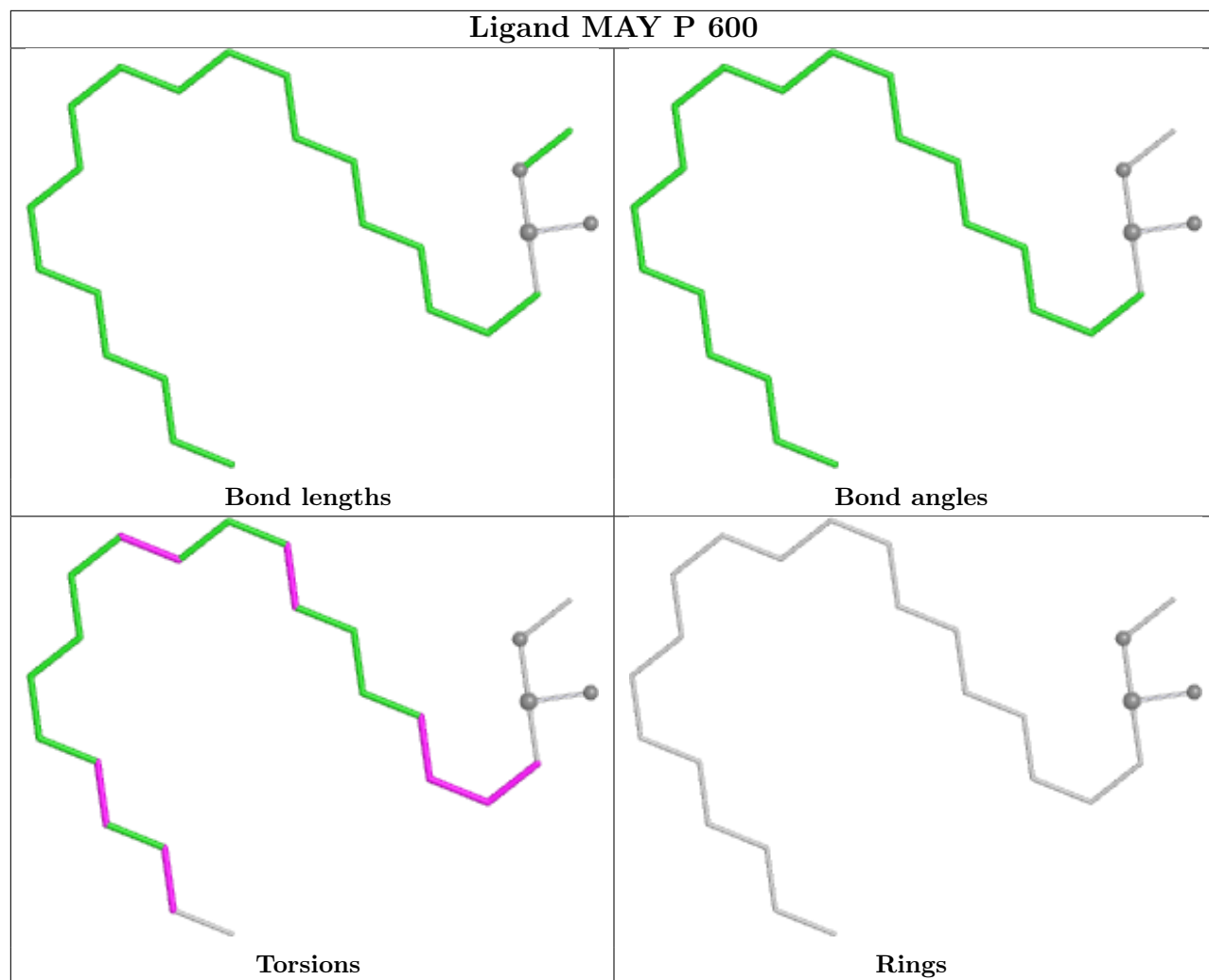


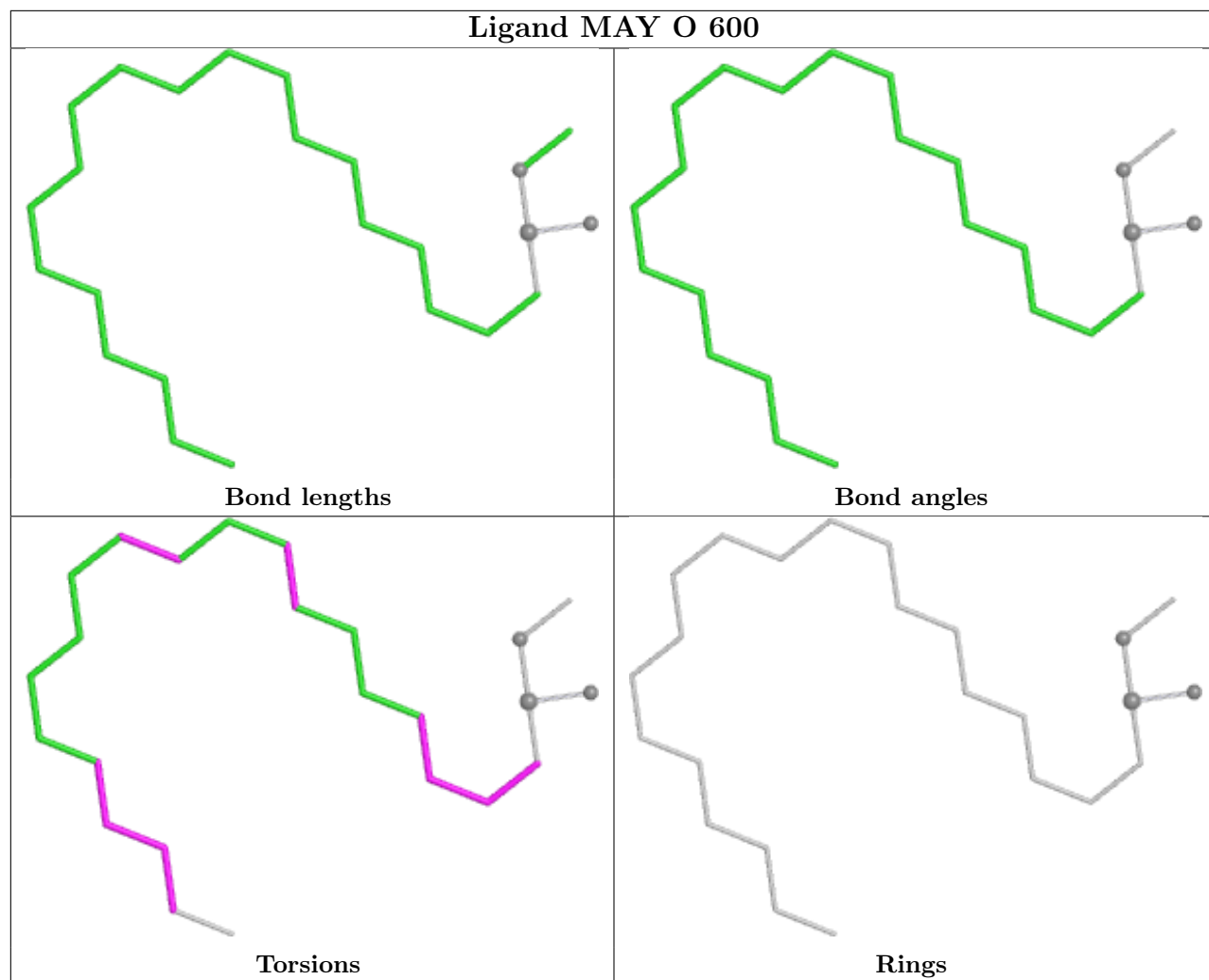


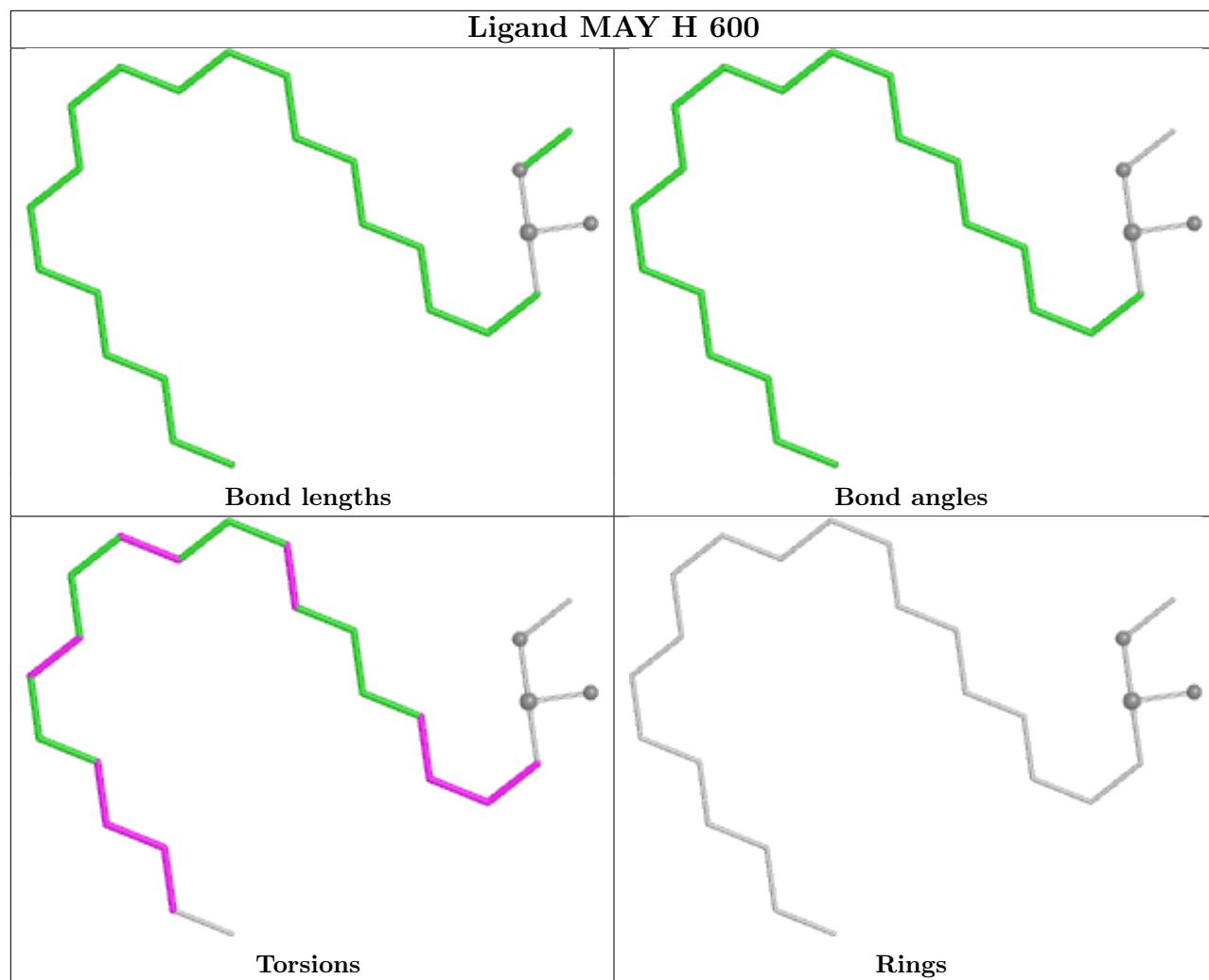


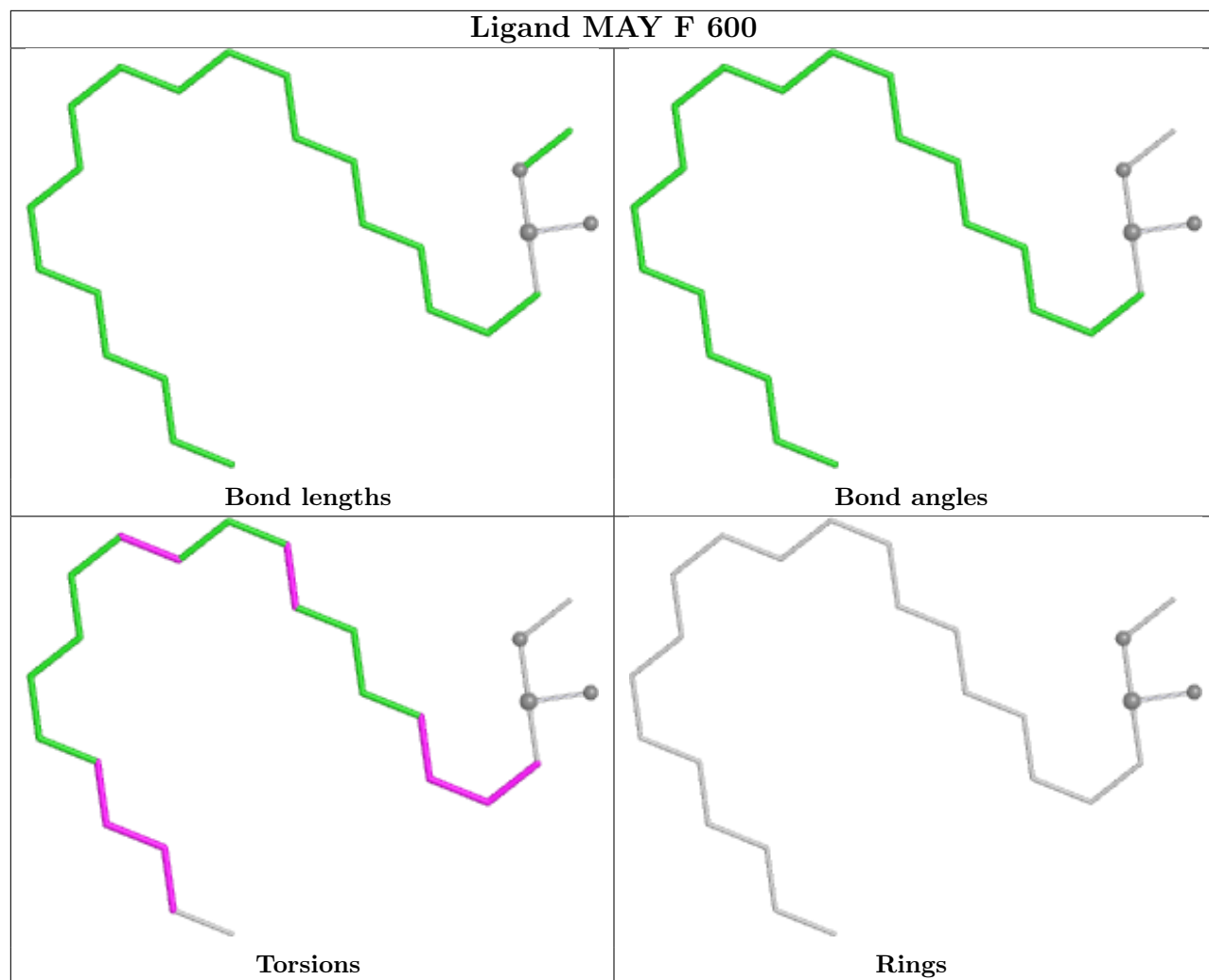


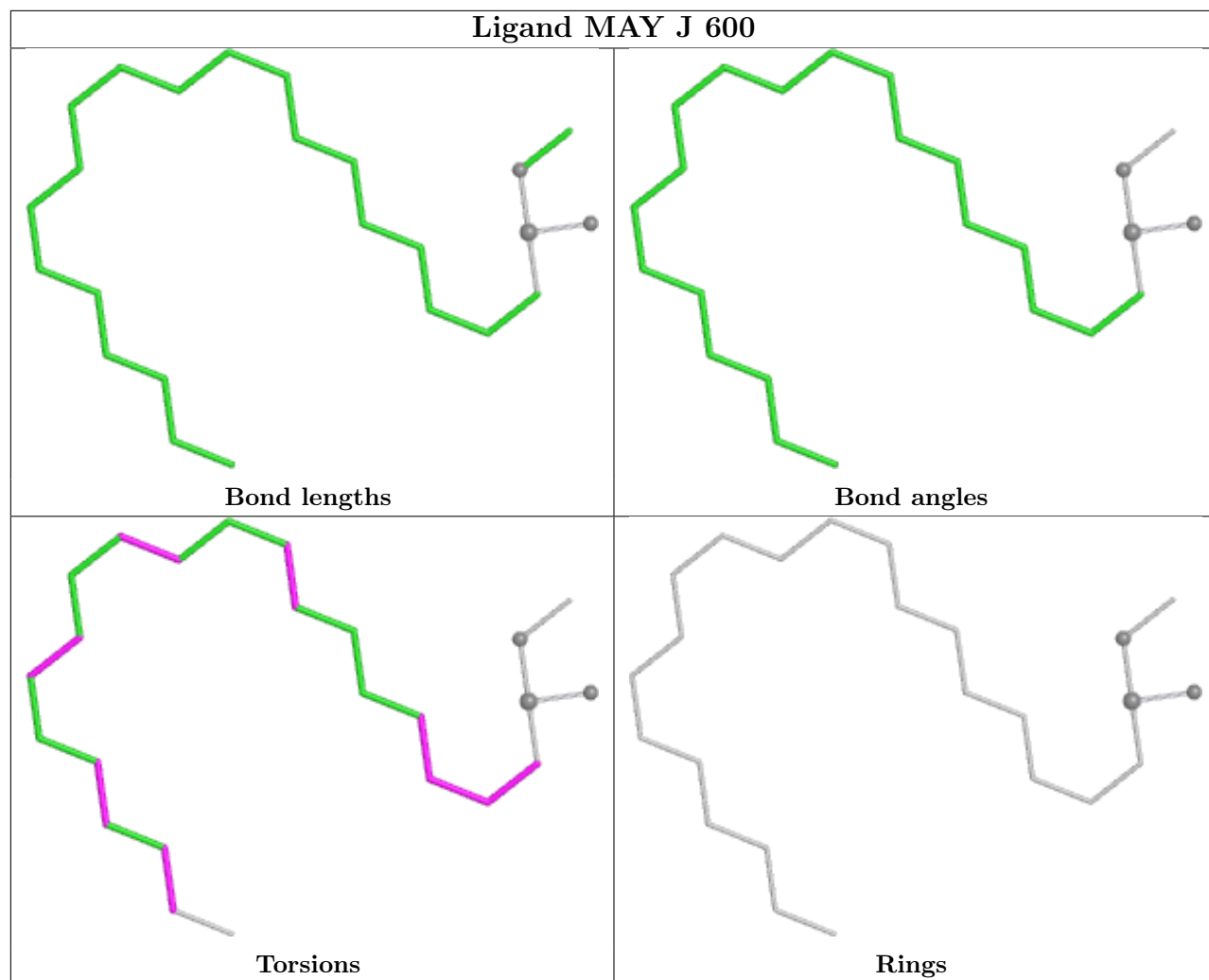


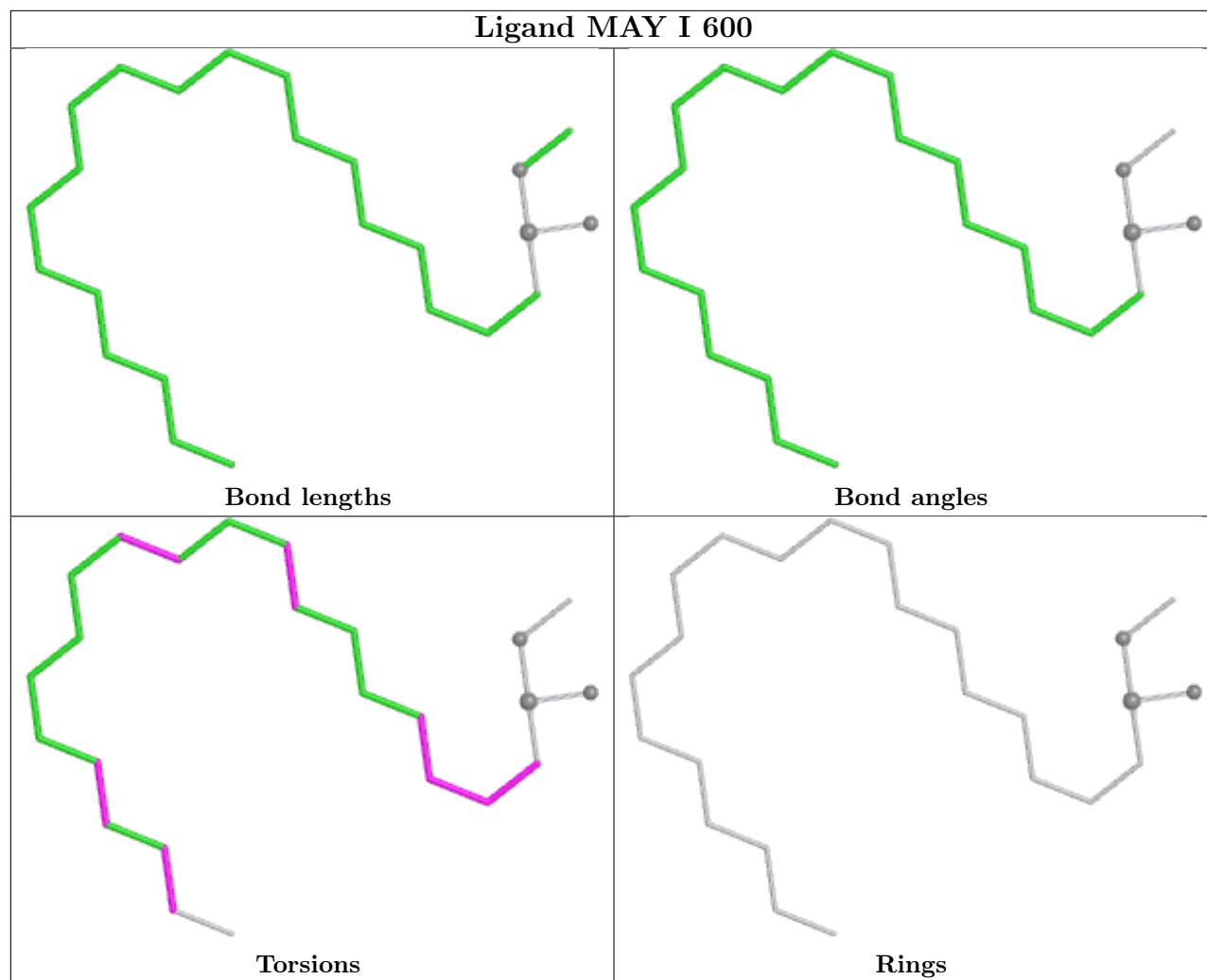


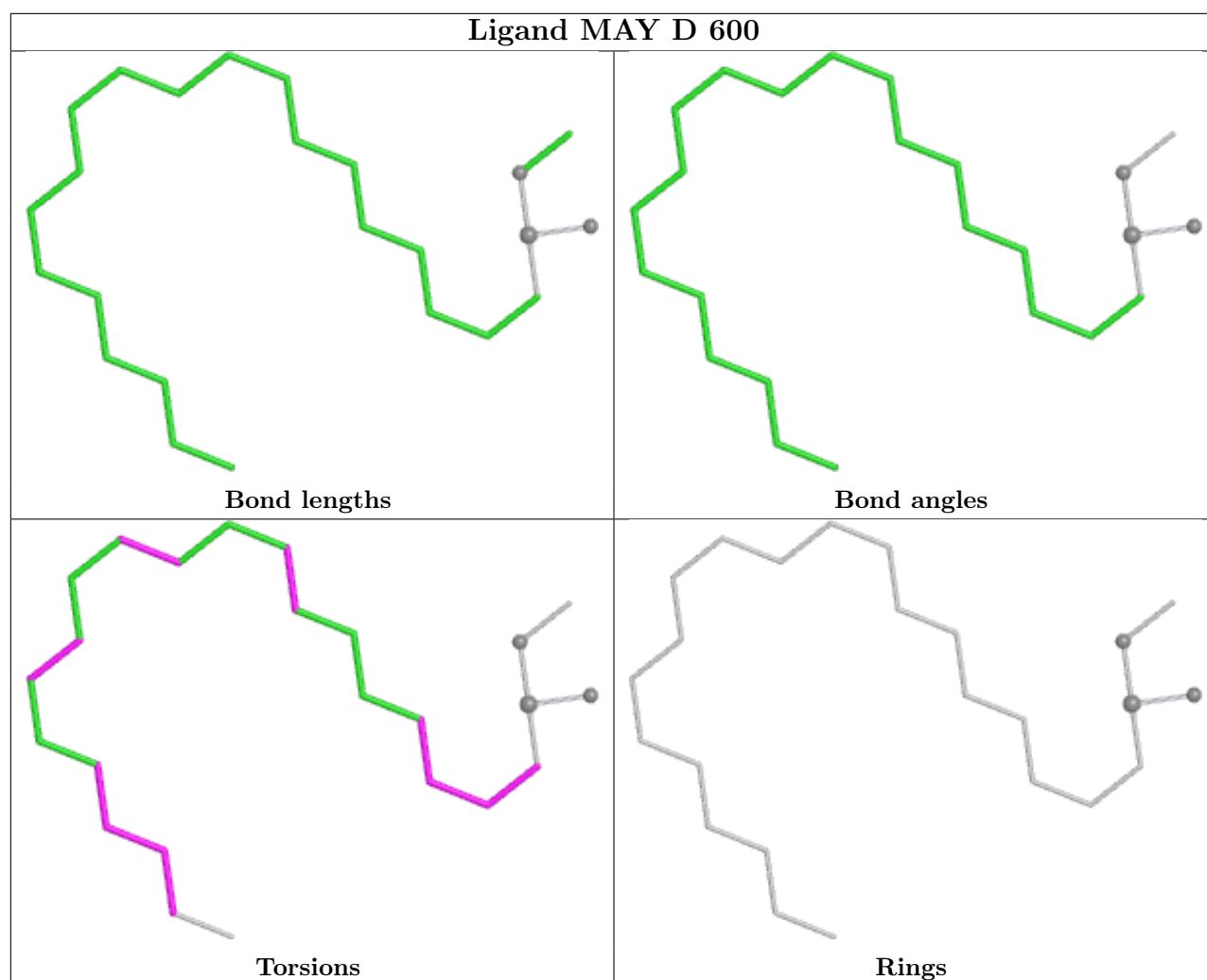












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.