Full wwPDB NMR Structure Validation Report (i)

Mar 15, 2026 – 01:54 PM UTC

PDB ID	:	7RSC / pdb_00007rsc
BMRB ID	:	30734
Title	:	NMR-driven structure of the KRAS4B-G12D "alpha-alpha" dimer on a lipid bilayer nanodisc
Authors	:	Lee, K.; Enomoto, M.; Gebregiworgis, T.; Gasmi-Seabrook, G.M.; Ikura, M.; Marshall, C.B.
Deposited on	:	2021-08-11

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

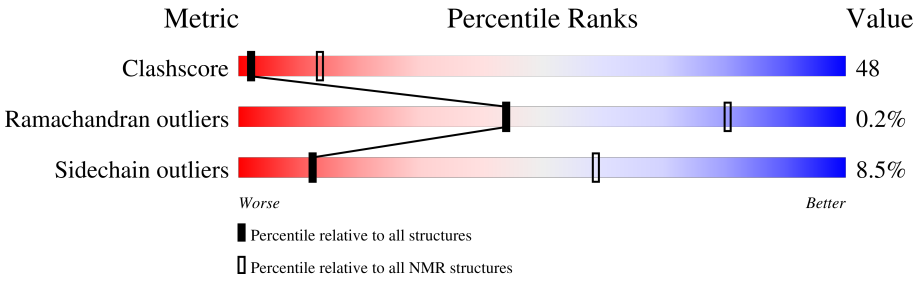
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 1%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	185	76% 14% 9% .
1	B	185	77% 12% 9% .
2	D	200	86% 7% 6%
2	E	200	82% 11% 6%

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:167, B:2-B:167 (332)	0.98	6
2	D:256-D:441, E:555-E:741 (373)	0.39	5

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14322 atoms, of which 1540 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
1	A	183	Total	C	H	N	O	S	0
			1822	917	356	255	287	7	
1	B	183	Total	C	H	N	O	S	0
			1822	917	356	255	287	7	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P01116
A	12	ASP	GLY	engineered mutation	UNP P01116
B	1	SER	-	expression tag	UNP P01116
B	12	ASP	GLY	engineered mutation	UNP P01116

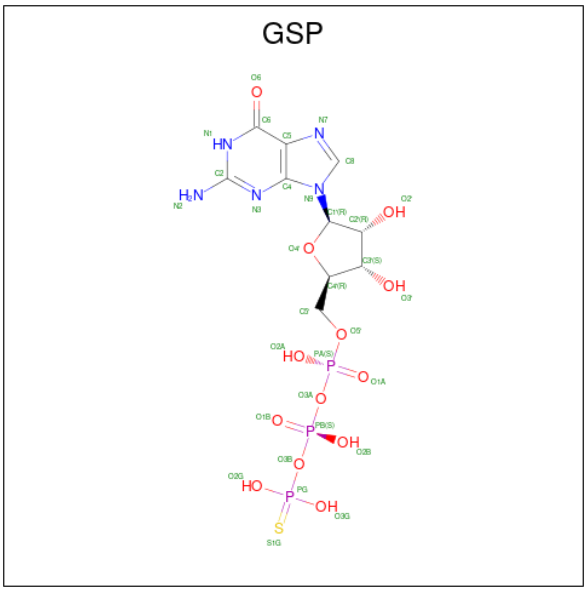
- Molecule 2 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
2	D	187	Total	C	H	N	O	S	0
			1892	960	360	273	296	3	
2	E	187	Total	C	H	N	O	S	0
			1892	960	360	273	296	3	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	242	GLY	-	expression tag	UNP P02647
D	243	PRO	-	expression tag	UNP P02647
E	542	GLY	-	expression tag	UNP P02647
E	543	PRO	-	expression tag	UNP P02647

- Molecule 3 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$) (labeled as "Ligand of Interest" by depositor).

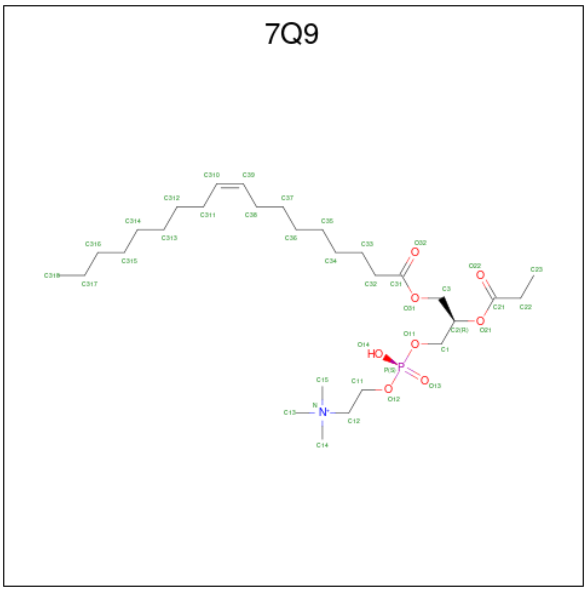


Mol	Chain	Residues	Atoms						
3	A	1	Total	C	H	N	O	P	S
			38	10	6	5	13	3	1
3	B	1	Total	C	H	N	O	P	S
			38	10	6	5	13	3	1

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	
4	A	1	Total	Mg
			1	1
4	B	1	Total	Mg
			1	1

- Molecule 5 is [(2 {R})-3-[oxidanyl-[2-(trimethyl-$l^{4}-azanyl)ethoxy]phosphoryl]oxy-2-propanoyloxy-propyl] ({Z})-octadec-9-enoate (CCD ID: 7Q9) (formula: $C_{29}H_{57}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1

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Mol	Chain	Residues	Atoms				
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1

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Mol	Chain	Residues	Atoms				
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1

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Mol	Chain	Residues	Atoms				
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1

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Mol	Chain	Residues	Atoms				
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1

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Mol	Chain	Residues	Atoms				
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1

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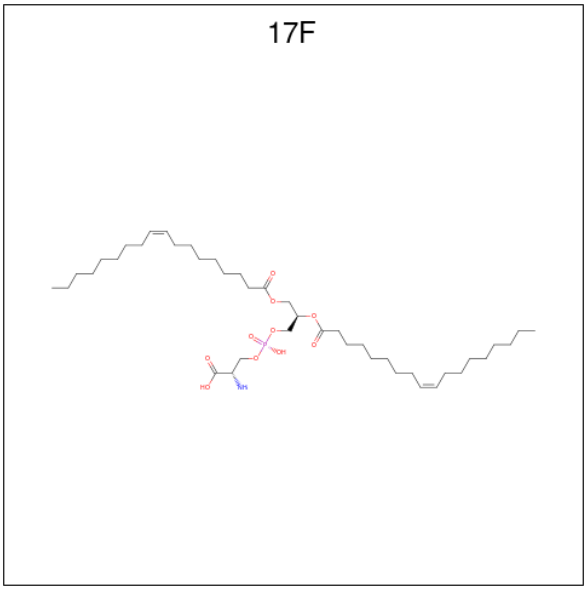
Mol	Chain	Residues	Atoms				
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1

- Molecule 6 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (CCD ID: 17F) (formula: $C_{42}H_{78}NO_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					
6	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1

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Mol	Chain	Residues	Atoms					
6	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	B	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1

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Mol	Chain	Residues	Atoms					
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1

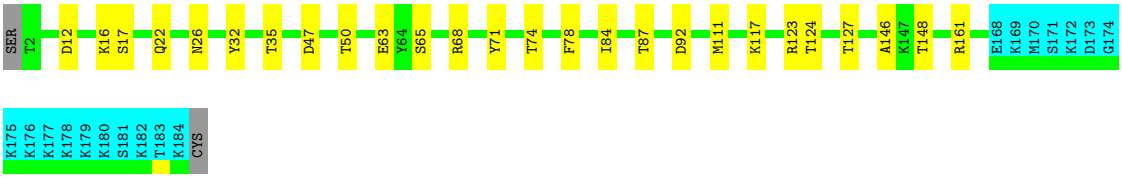
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

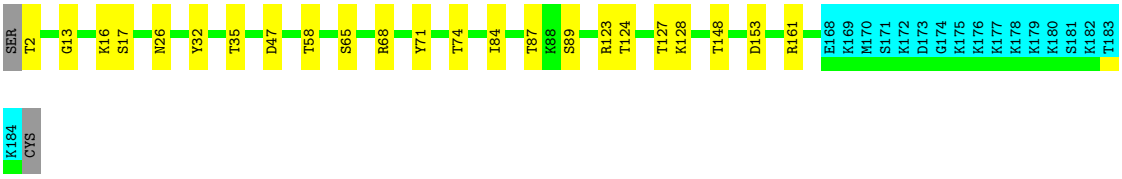
• Molecule 1: GTPase KRas

Chain A:



• Molecule 1: GTPase KRas

Chain B:

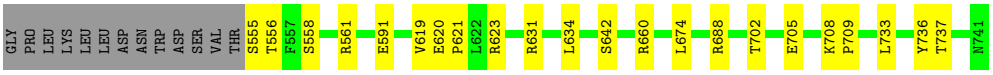


• Molecule 2: Apolipoprotein A-I

Chain D:

• Molecule 2: Apolipoprotein A-I

Chain E:



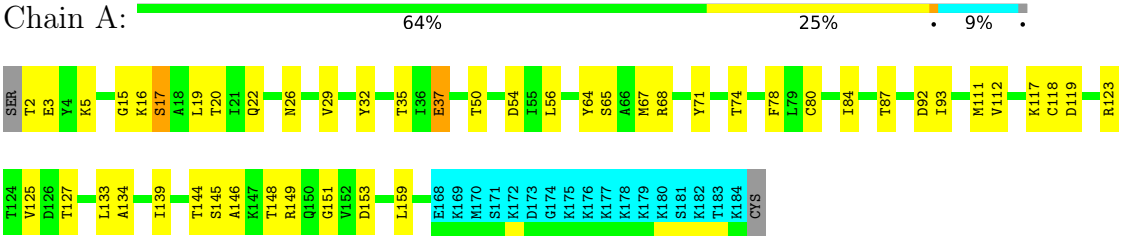
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

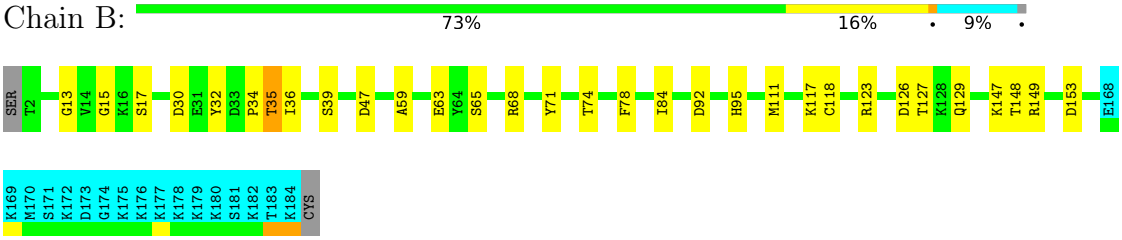
• Molecule 1: GTPase KRas

Chain A:



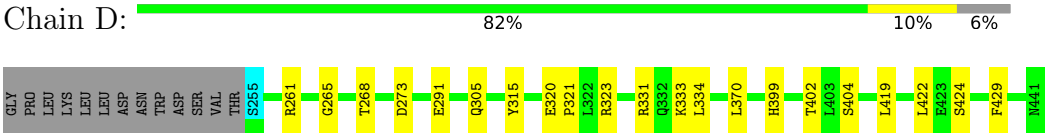
• Molecule 1: GTPase KRas

Chain B:



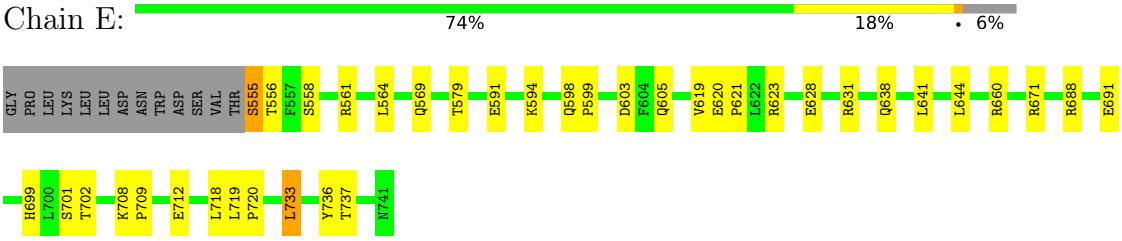
• Molecule 2: Apolipoprotein A-I

Chain D:



• Molecule 2: Apolipoprotein A-I

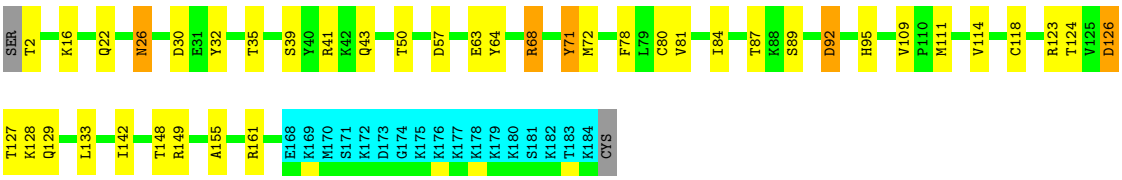
Chain E:



4.2.2 Score per residue for model 2

• Molecule 1: GTPase KRas

Chain A:

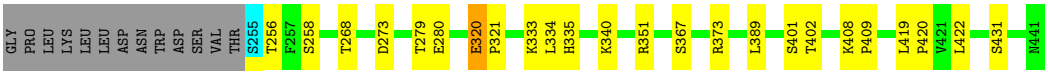


• Molecule 1: GTPase KRas

Chain B:

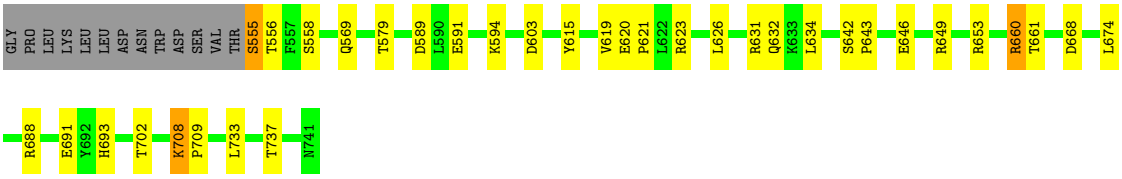
• Molecule 2: Apolipoprotein A-I

Chain D:



• Molecule 2: Apolipoprotein A-I

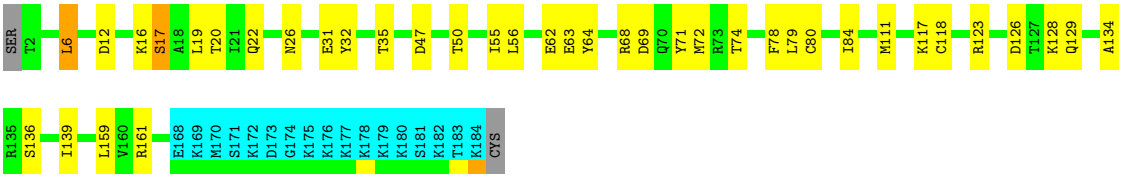
Chain E:



4.2.3 Score per residue for model 3

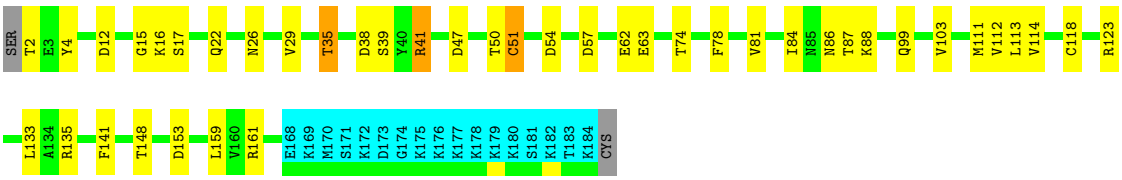
• Molecule 1: GTPase KRas

Chain A:



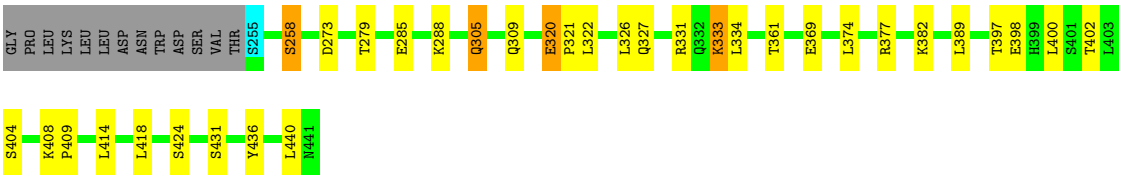
• Molecule 1: GTPase KRas

Chain B:



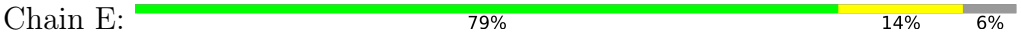
• Molecule 2: Apolipoprotein A-I

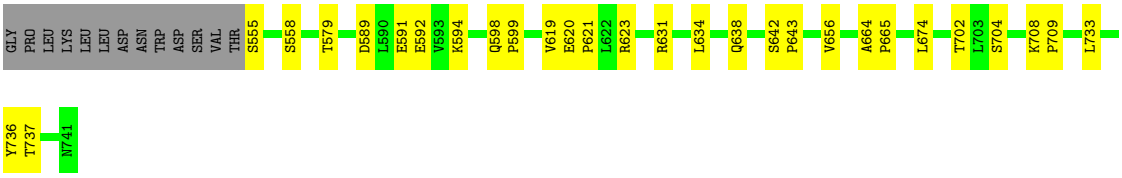
Chain D:



• Molecule 2: Apolipoprotein A-I

Chain E:

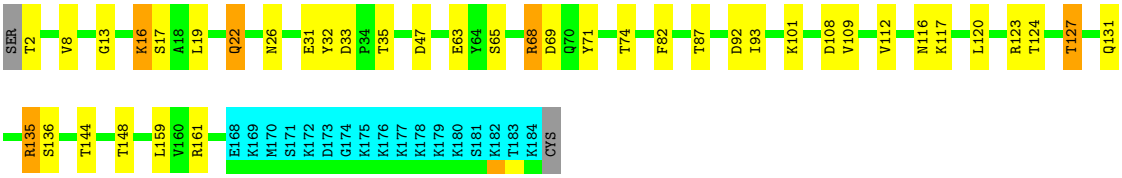




4.2.4 Score per residue for model 4

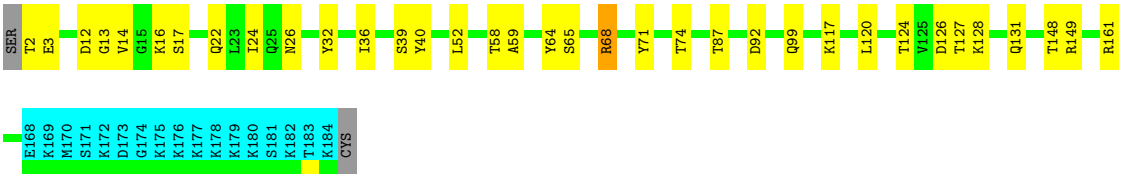
• Molecule 1: GTPase KRas

Chain A:



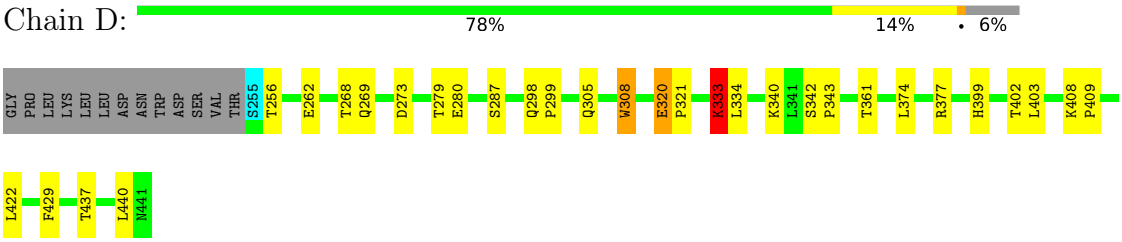
• Molecule 1: GTPase KRas

Chain B:



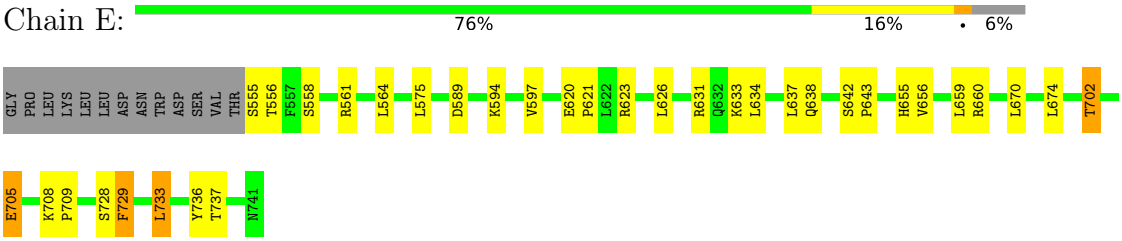
• Molecule 2: Apolipoprotein A-I

Chain D:



• Molecule 2: Apolipoprotein A-I

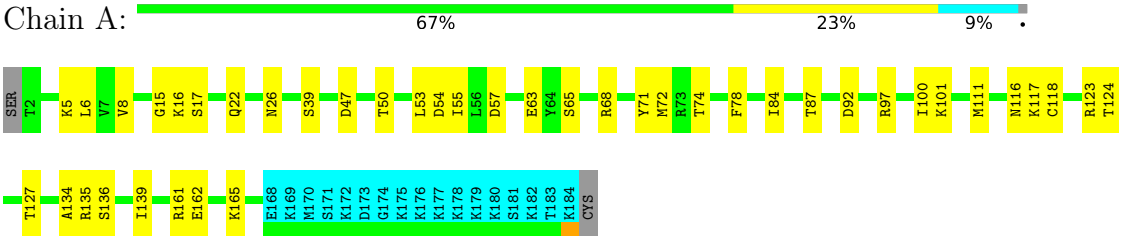
Chain E:



4.2.5 Score per residue for model 5 (medoid)

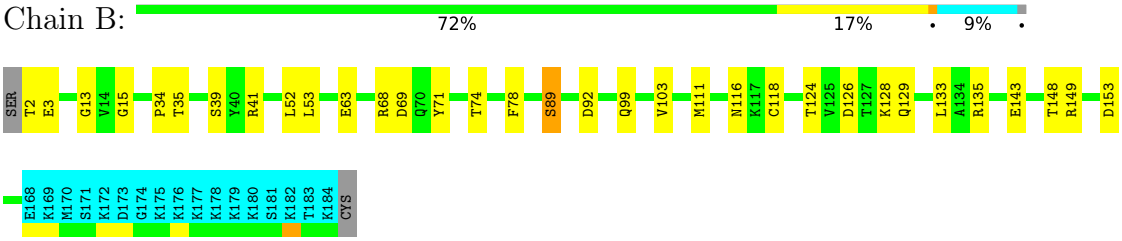
• Molecule 1: GTPase KRas

Chain A:



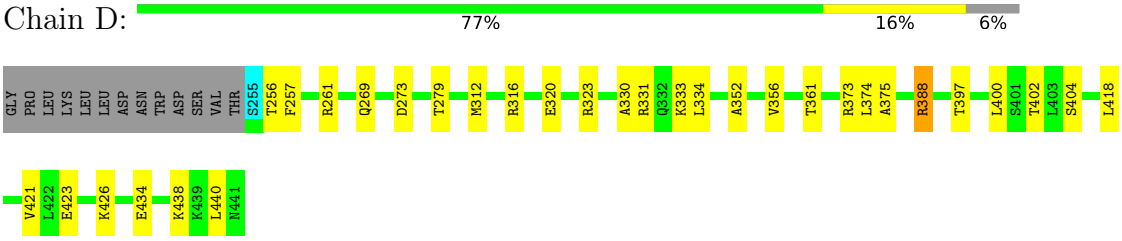
• Molecule 1: GTPase KRas

Chain B:



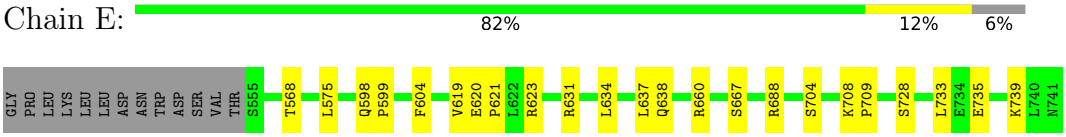
• Molecule 2: Apolipoprotein A-I

Chain D:



• Molecule 2: Apolipoprotein A-I

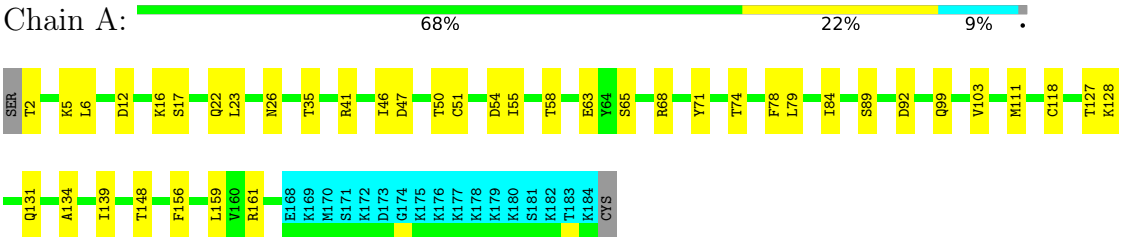
Chain E:



4.2.6 Score per residue for model 6

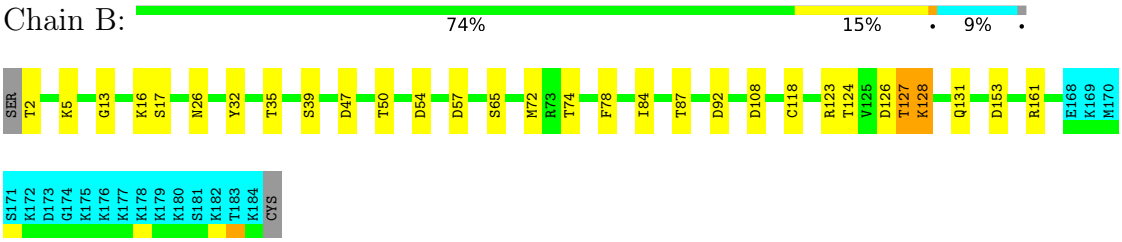
• Molecule 1: GTPase KRas

Chain A:



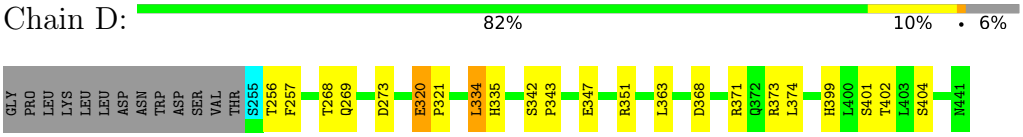
• Molecule 1: GTPase KRas

Chain B:



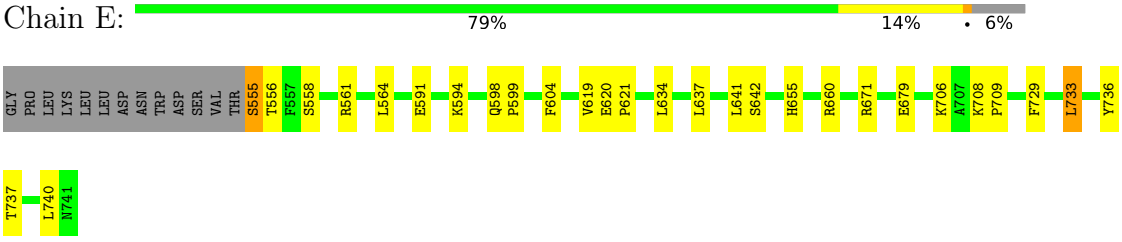
• Molecule 2: Apolipoprotein A-I

Chain D:



• Molecule 2: Apolipoprotein A-I

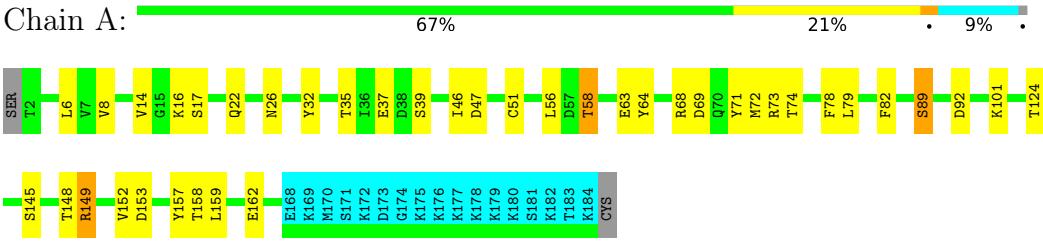
Chain E:



4.2.7 Score per residue for model 7

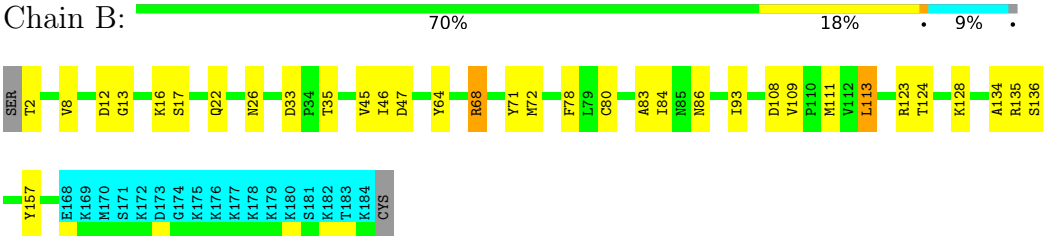
• Molecule 1: GTPase KRas

Chain A:



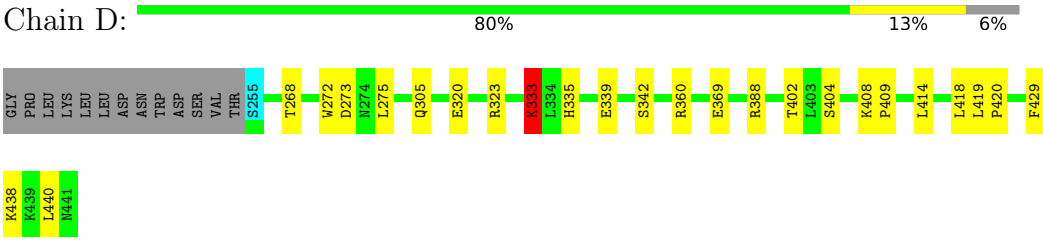
• Molecule 1: GTPase KRas

Chain B:



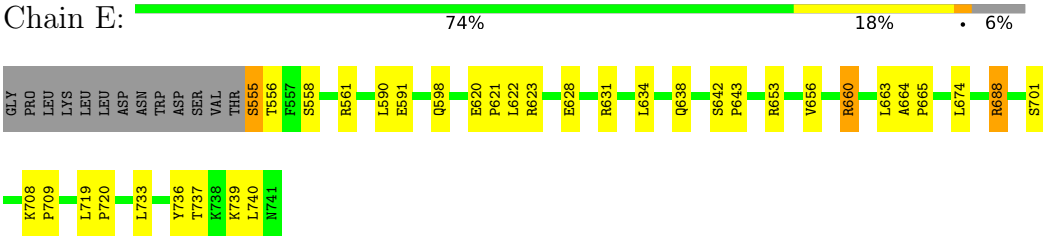
• Molecule 2: Apolipoprotein A-I

Chain D:



• Molecule 2: Apolipoprotein A-I

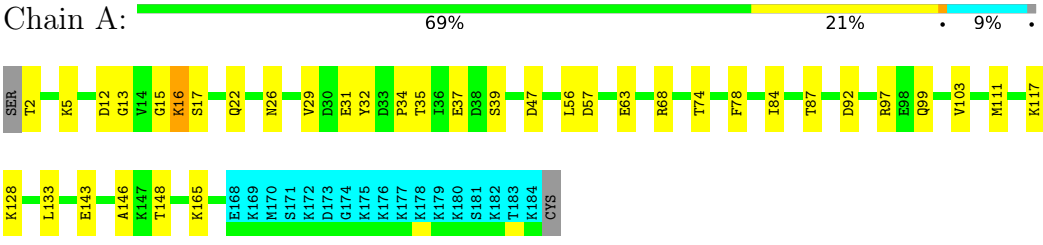
Chain E:



4.2.8 Score per residue for model 8

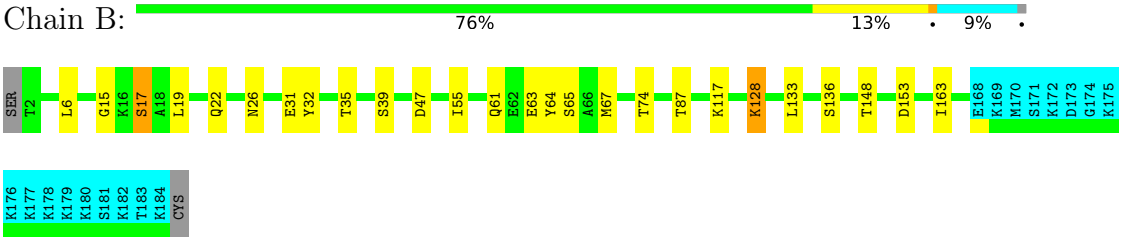
• Molecule 1: GTPase KRas

Chain A:



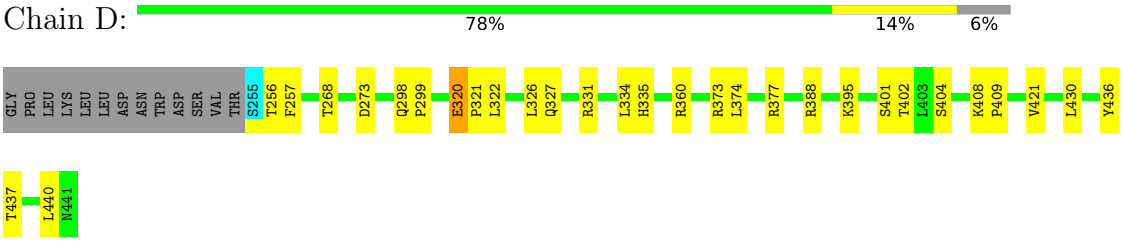
• Molecule 1: GTPase KRas

Chain B:



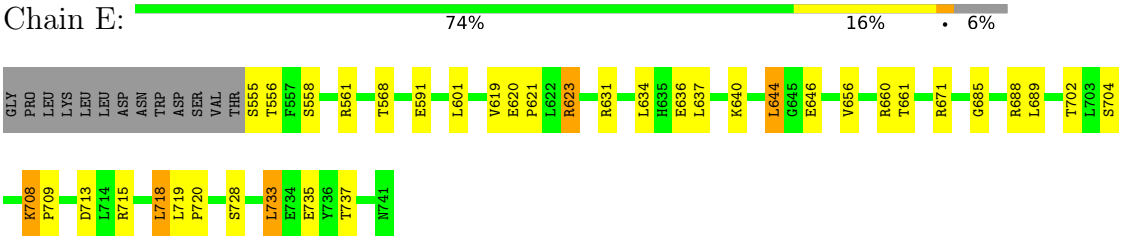
• Molecule 2: Apolipoprotein A-I

Chain D:



• Molecule 2: Apolipoprotein A-I

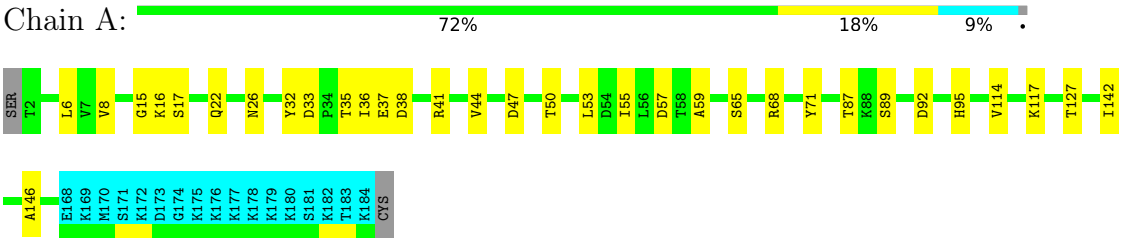
Chain E:



4.2.9 Score per residue for model 9

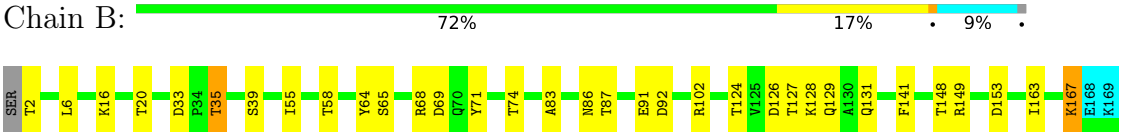
• Molecule 1: GTPase KRas

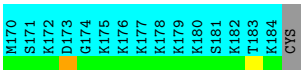
Chain A:



• Molecule 1: GTPase KRas

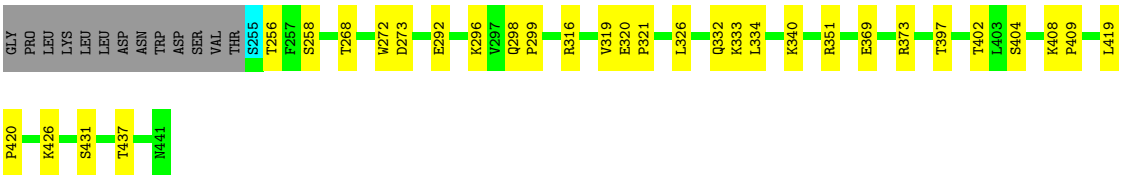
Chain B:





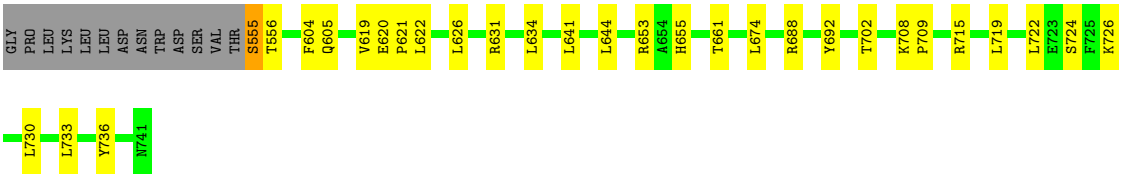
• Molecule 2: Apolipoprotein A-I

Chain D:



• Molecule 2: Apolipoprotein A-I

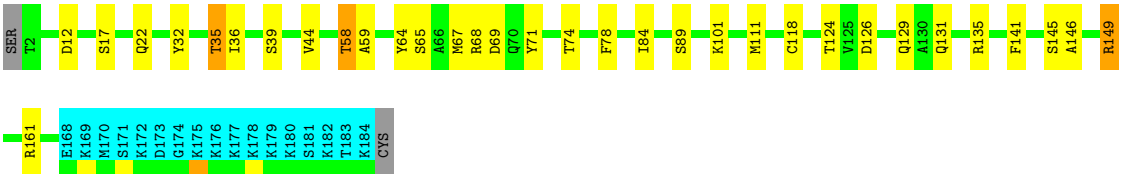
Chain E:



4.2.10 Score per residue for model 10

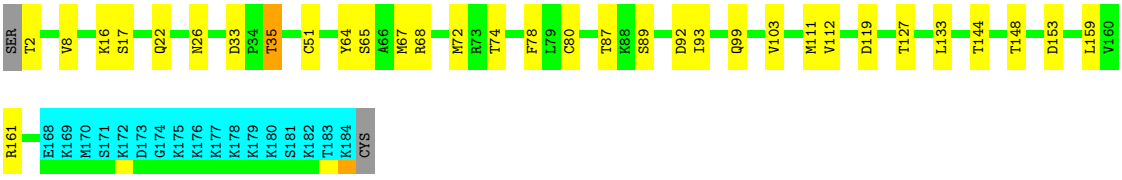
• Molecule 1: GTPase KRas

Chain A:



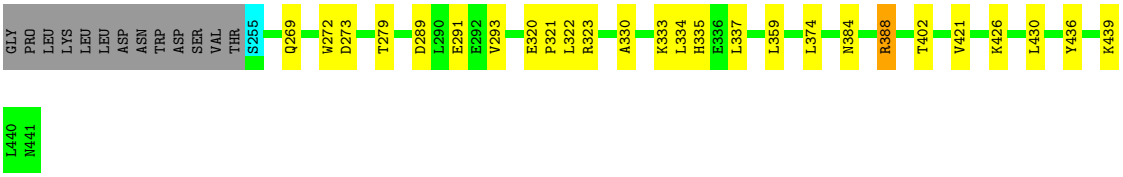
• Molecule 1: GTPase KRas

Chain B:

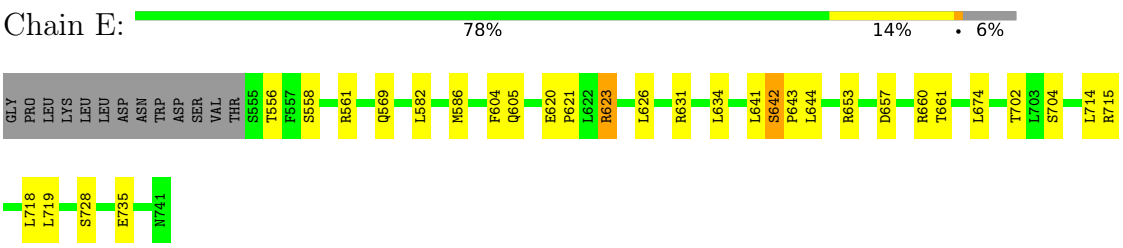


• Molecule 2: Apolipoprotein A-I

Chain D:

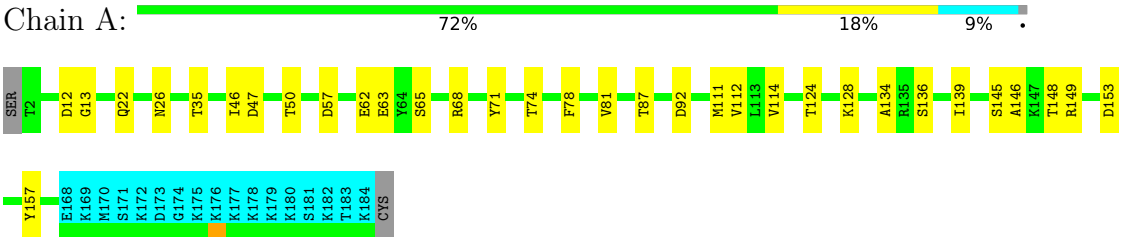


• Molecule 2: Apolipoprotein A-I

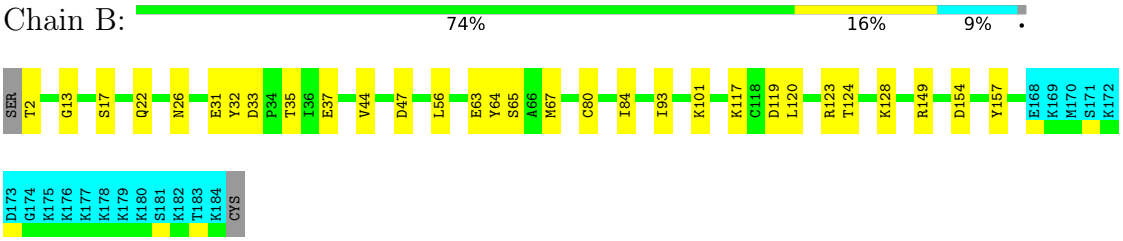


4.2.11 Score per residue for model 11

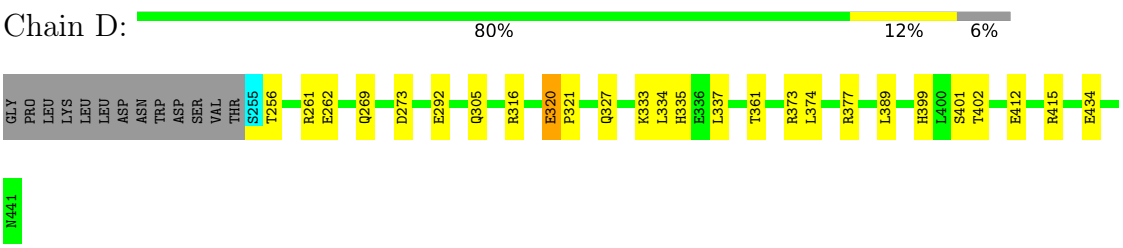
• Molecule 1: GTPase KRas



• Molecule 1: GTPase KRas

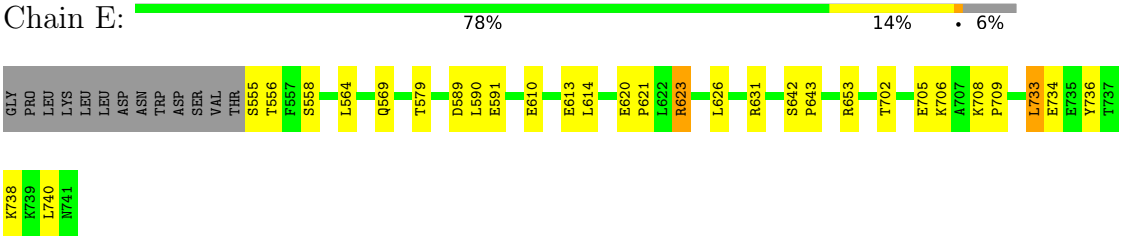


• Molecule 2: Apolipoprotein A-I



• Molecule 2: Apolipoprotein A-I

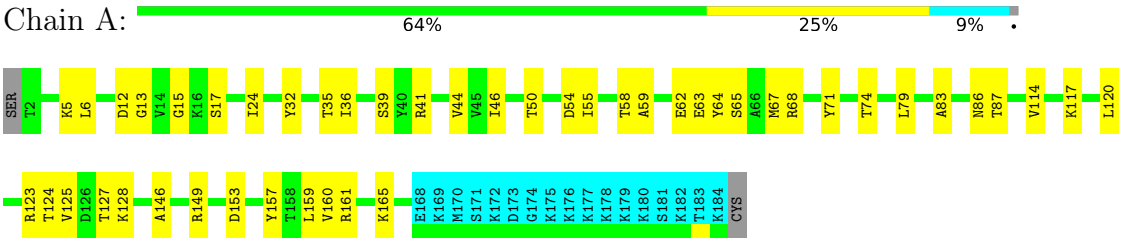
Chain E:



4.2.12 Score per residue for model 12

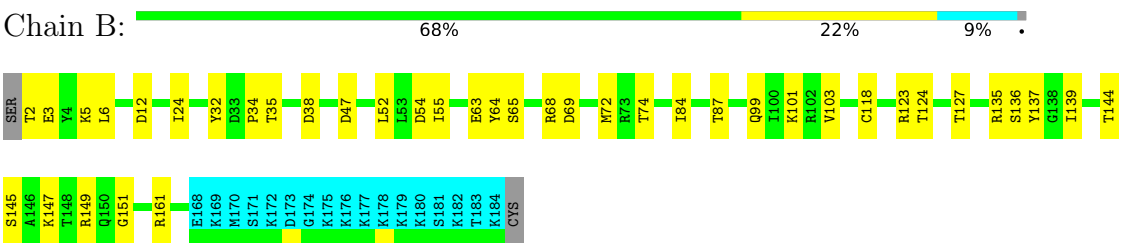
• Molecule 1: GTPase KRas

Chain A:



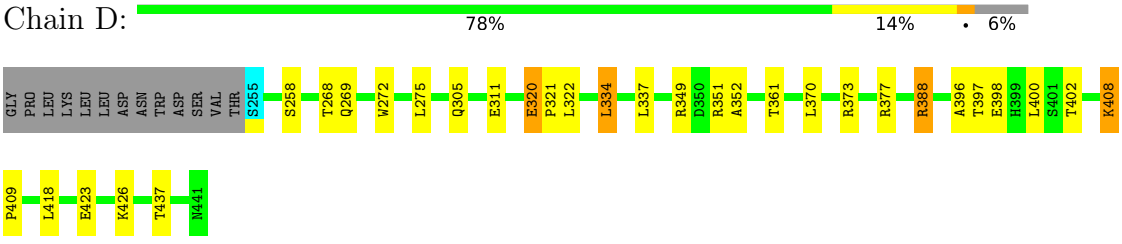
• Molecule 1: GTPase KRas

Chain B:



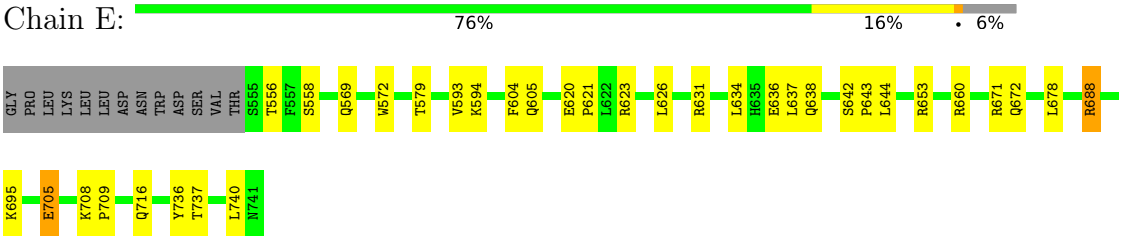
• Molecule 2: Apolipoprotein A-I

Chain D:



• Molecule 2: Apolipoprotein A-I

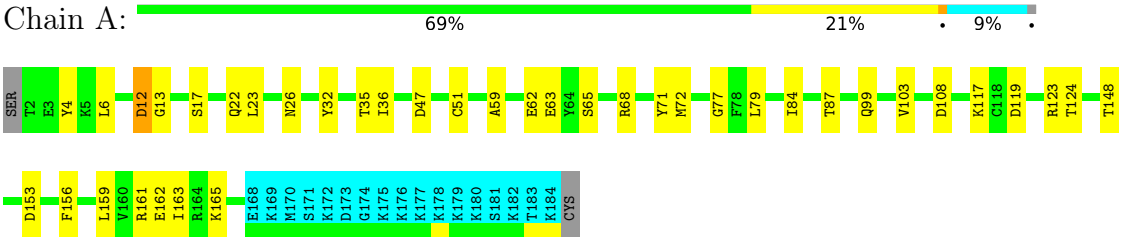
Chain E:



4.2.13 Score per residue for model 13

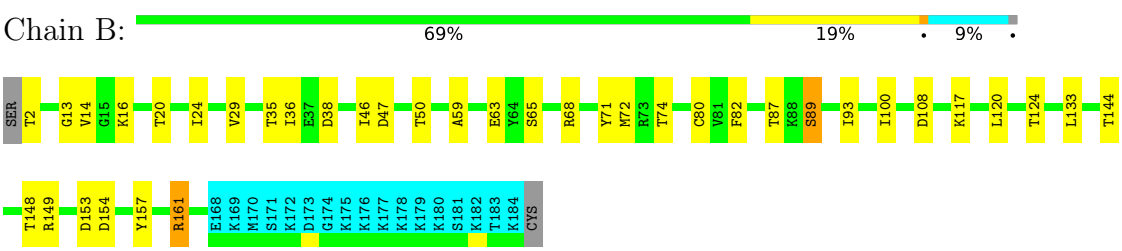
• Molecule 1: GTPase KRas

Chain A:



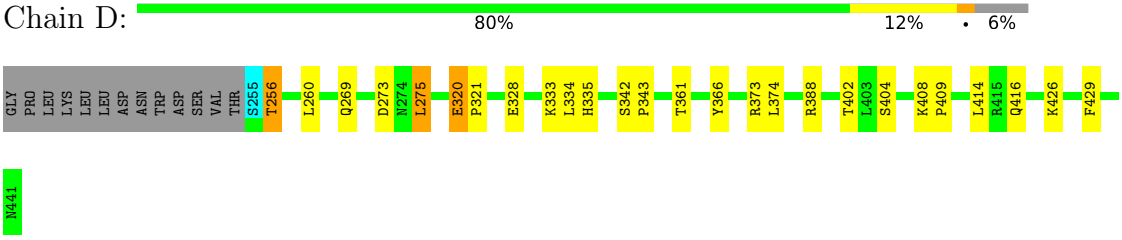
• Molecule 1: GTPase KRas

Chain B:



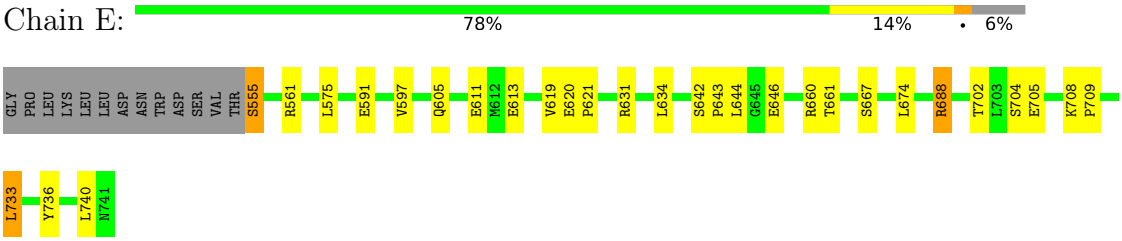
• Molecule 2: Apolipoprotein A-I

Chain D:



• Molecule 2: Apolipoprotein A-I

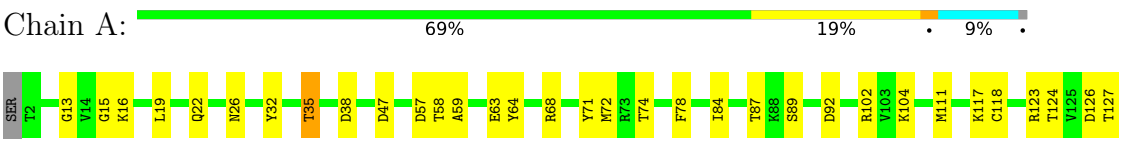
Chain E:

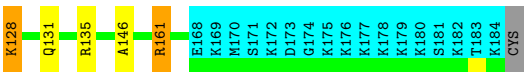


4.2.14 Score per residue for model 14

• Molecule 1: GTPase KRas

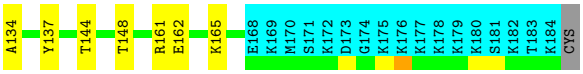
Chain A:





• Molecule 1: GTPase KRas

Chain B:

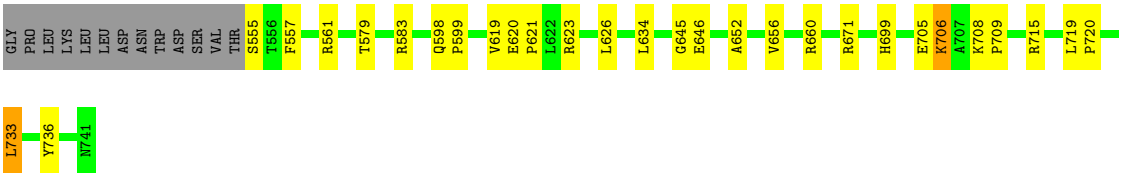


• Molecule 2: Apolipoprotein A-I

Chain D:

• Molecule 2: Apolipoprotein A-I

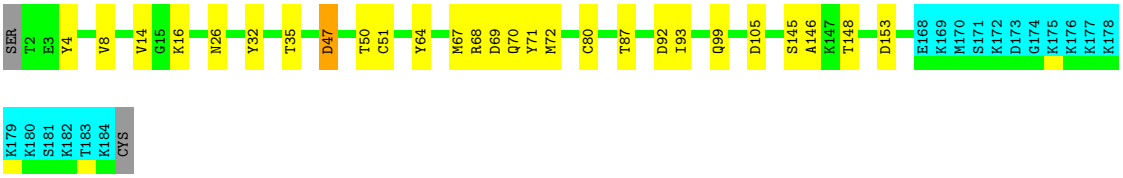
Chain E:



4.2.15 Score per residue for model 15

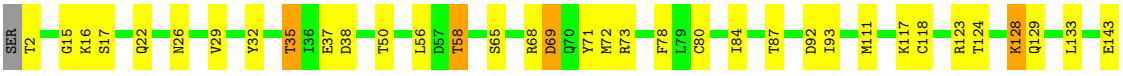
• Molecule 1: GTPase KRas

Chain A:



• Molecule 1: GTPase KRas

Chain B:



• Molecule 2: Apolipoprotein A-I

Chain D:

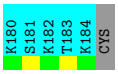
• Molecule 2: Apolipoprotein A-I

Chain E:

4.2.16 Score per residue for model 16

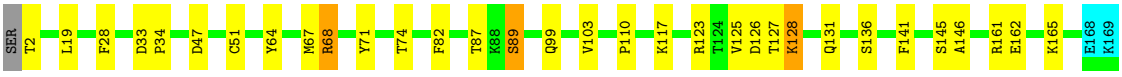
• Molecule 1: GTPase KRas

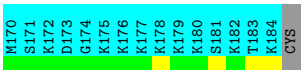
Chain A:



• Molecule 1: GTPase KRas

Chain B:



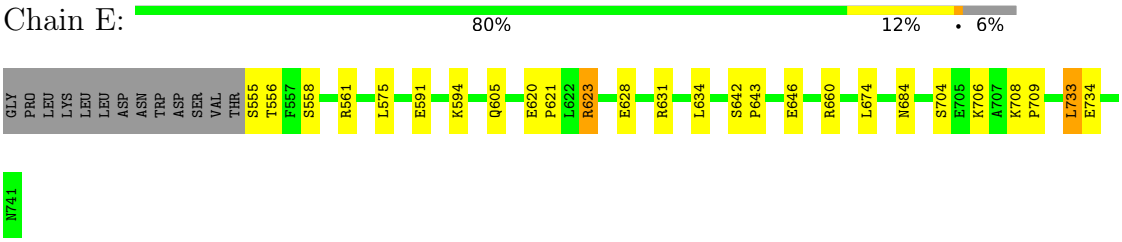


• Molecule 2: Apolipoprotein A-I

Chain D:

• Molecule 2: Apolipoprotein A-I

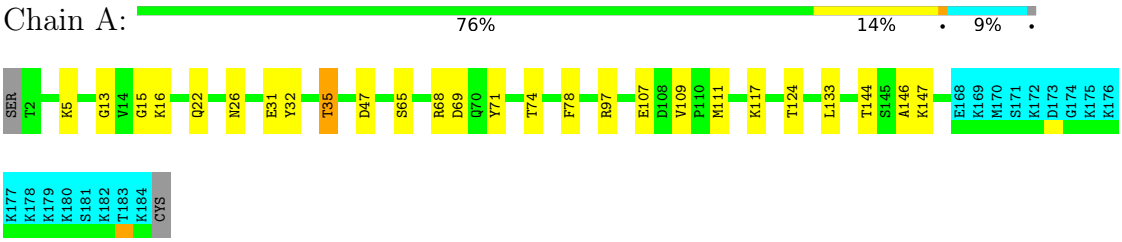
Chain E:



4.2.17 Score per residue for model 17

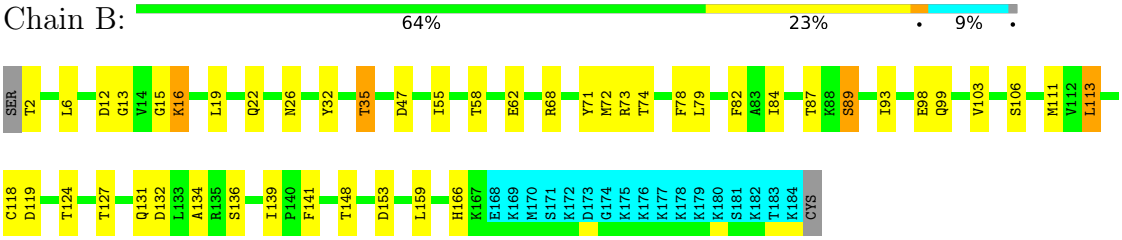
• Molecule 1: GTPase KRas

Chain A:



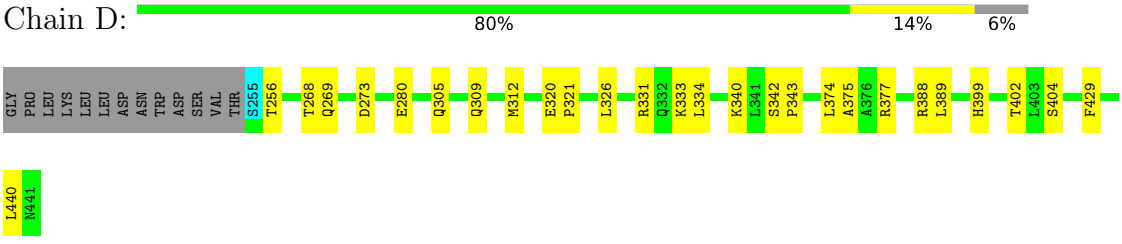
• Molecule 1: GTPase KRas

Chain B:



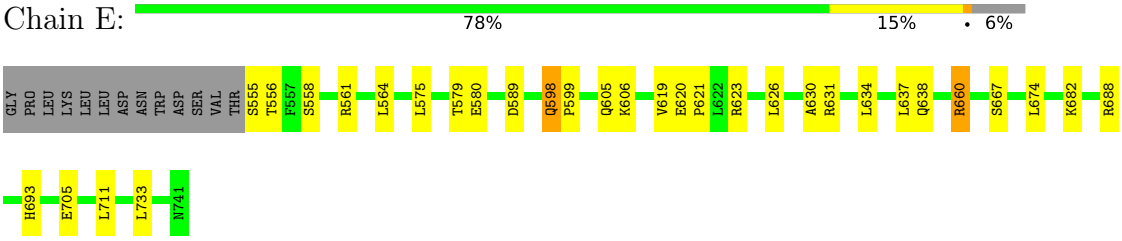
• Molecule 2: Apolipoprotein A-I

Chain D:



• Molecule 2: Apolipoprotein A-I

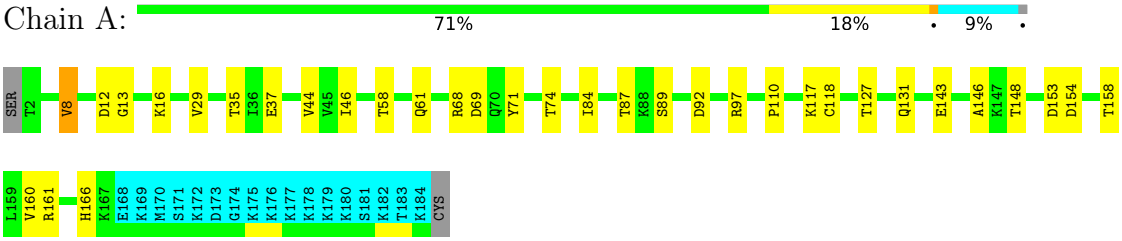
Chain E:



4.2.18 Score per residue for model 18

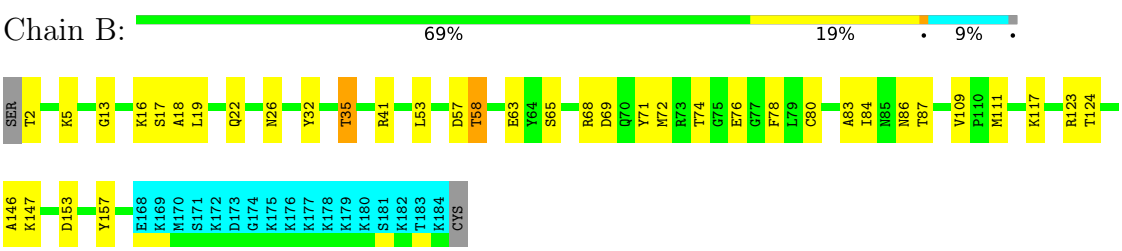
• Molecule 1: GTPase KRas

Chain A:



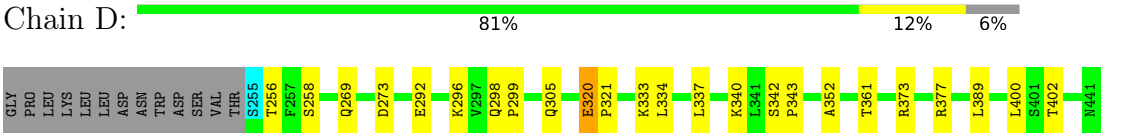
• Molecule 1: GTPase KRas

Chain B:



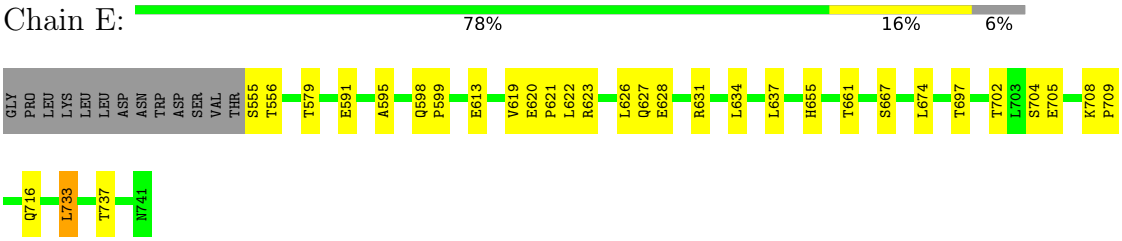
• Molecule 2: Apolipoprotein A-I

Chain D:



• Molecule 2: Apolipoprotein A-I

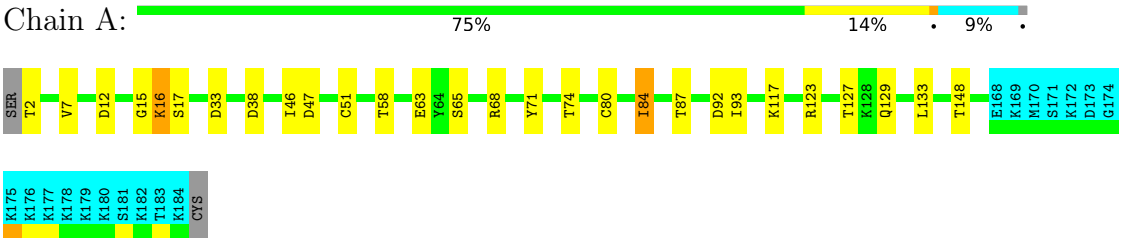
Chain E:



4.2.19 Score per residue for model 19

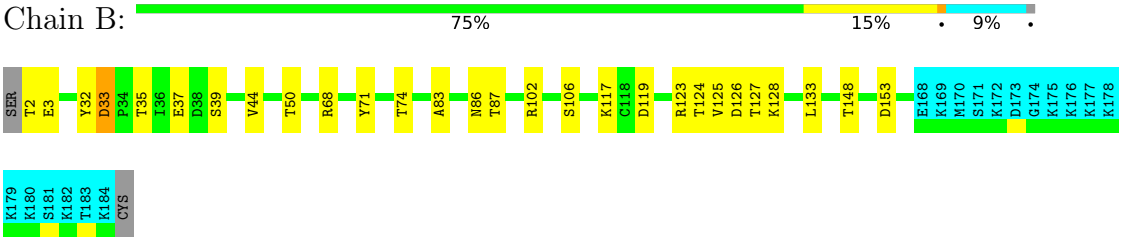
• Molecule 1: GTPase KRas

Chain A:



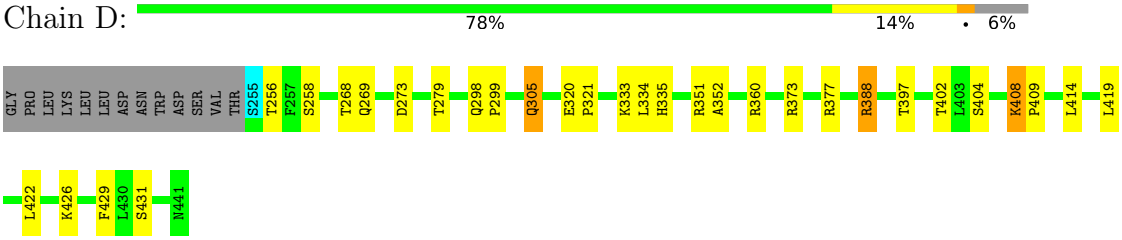
• Molecule 1: GTPase KRas

Chain B:



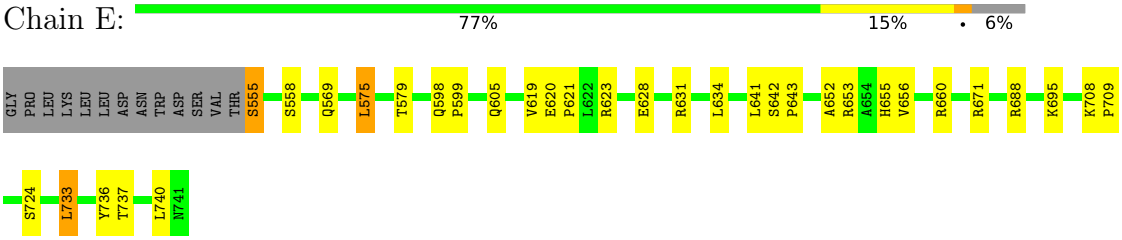
• Molecule 2: Apolipoprotein A-I

Chain D:



• Molecule 2: Apolipoprotein A-I

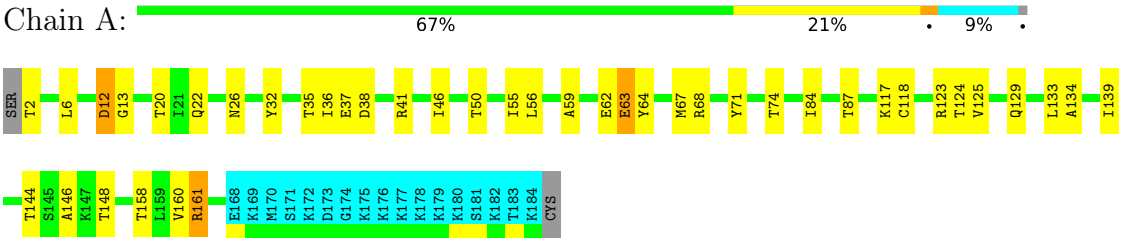
Chain E:



4.2.20 Score per residue for model 20

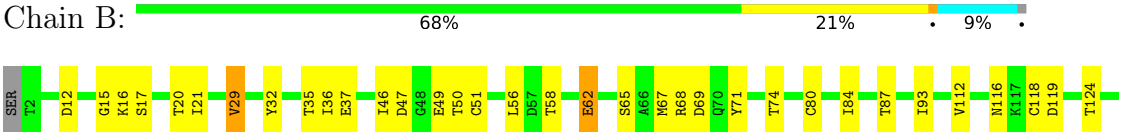
• Molecule 1: GTPase KRas

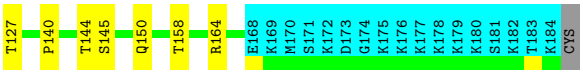
Chain A:



• Molecule 1: GTPase KRas

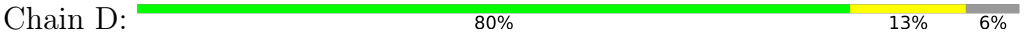
Chain B:

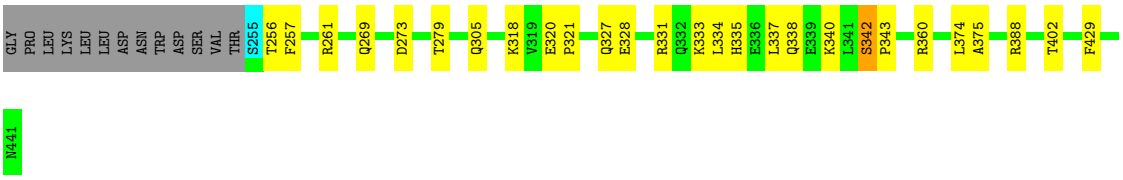




• Molecule 2: Apolipoprotein A-I

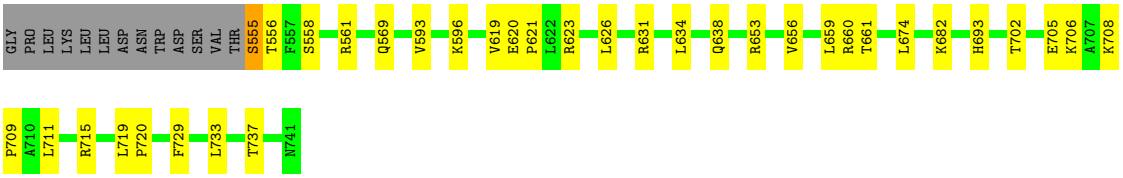
Chain D:





• Molecule 2: Apolipoprotein A-I

Chain E:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing.*

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
HADDOCK	refinement	
HADDOCK	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	154
Number of shifts mapped to atoms	61
Number of unparsed shifts	0
Number of shifts with mapping errors	93
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 17F, GSP, MG, 7Q9

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1328	306	1302	18±5
1	B	1328	306	1303	17±4
2	D	1526	358	1531	18±4
2	E	1532	360	1535	21±5
3	A	32	6	12	8±3
3	B	32	6	12	8±2
4	A	1	0	0	1±0
4	B	1	0	0	1±0
5	A	546	0	0	61±7
5	B	273	0	0	35±9
5	D	1755	0	0	187±14
5	E	2418	0	0	275±27
6	A	216	12	304	73±10
6	B	54	3	76	23±7
6	D	594	33	836	199±17
6	E	864	48	1216	213±36
All	All	250000	28760	162529	19729

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 48.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:C9	6:D:517:17F:H9	1.24	1.62	8	8
6:D:510:17F:C9	6:D:517:17F:H8A	1.23	1.64	15	12
6:D:510:17F:C12	6:D:517:17F:H8A	1.21	1.66	3	16
6:D:510:17F:C9	6:D:517:17F:H11	1.19	1.67	4	10
6:D:510:17F:H9A	6:D:517:17F:C8	1.18	1.66	18	19
6:D:510:17F:H9	6:D:517:17F:C11	1.17	1.70	2	6
6:D:510:17F:H9A	6:D:517:17F:C9	1.17	1.70	9	8
6:D:517:17F:H47	6:D:517:17F:C22	1.16	1.71	20	3
6:A:213:17F:H44	6:A:213:17F:H61	1.14	1.18	16	2
6:A:208:17F:H57	6:A:208:17F:H43	1.14	1.17	16	10
6:E:806:17F:H45	6:E:806:17F:H54	1.13	1.21	17	20
6:E:802:17F:H57	6:E:802:17F:H62	1.12	1.19	15	18
6:D:539:17F:H57	6:D:539:17F:H19A	1.12	1.21	14	19
6:D:517:17F:H39	6:D:517:17F:H47	1.12	1.19	7	16
6:D:539:17F:C18	6:D:539:17F:H57	1.12	1.73	8	1
6:A:213:17F:H8	6:A:213:17F:H12A	1.11	1.18	1	13
6:D:533:17F:O9	6:D:533:17F:H32	1.11	1.45	11	13
6:E:808:17F:H42	6:E:810:17F:H62	1.11	1.17	11	11
6:A:219:17F:H61	6:A:219:17F:H68	1.11	1.20	1	17
6:D:519:17F:H48	6:D:519:17F:H67	1.11	1.19	8	14
6:E:808:17F:H18A	6:E:810:17F:H20	1.11	1.12	12	9
6:D:534:17F:H50	6:D:534:17F:H42	1.11	1.19	20	20
6:E:819:17F:H30	6:E:819:17F:H39	1.11	1.18	17	12
6:D:510:17F:H9A	6:D:517:17F:O7	1.11	1.45	14	6
6:D:533:17F:H36	6:D:533:17F:H42	1.11	1.18	2	1
6:B:208:17F:H55	6:B:208:17F:H46	1.10	1.23	8	11
6:D:510:17F:H12	6:D:517:17F:H8A	1.10	1.14	12	13
6:D:510:17F:C8	6:D:517:17F:H19A	1.10	1.77	8	19
6:A:213:17F:H12A	6:A:213:17F:H8A	1.10	1.21	11	3
6:D:517:17F:H41	6:D:533:17F:H38	1.09	1.23	10	11
6:D:510:17F:H12	6:D:517:17F:H10A	1.09	1.19	19	8
6:D:510:17F:H60	6:D:517:17F:C12	1.09	1.77	20	1
6:D:510:17F:H12	6:D:517:17F:C8	1.09	1.75	18	18
6:D:510:17F:H5	6:D:533:17F:H19A	1.09	1.24	15	12
6:E:875:17F:H78	6:E:875:17F:H49	1.09	1.16	19	16
6:E:857:17F:H36	6:E:857:17F:H57	1.09	1.25	3	11
6:D:539:17F:C31	6:D:539:17F:H18	1.09	1.76	8	1
6:D:510:17F:O9	6:D:517:17F:H9A	1.08	1.47	3	12
6:E:808:17F:H51	6:E:808:17F:H76	1.08	1.19	6	13
6:D:510:17F:H9	6:D:517:17F:H11	1.08	1.25	5	10
6:A:219:17F:H5	6:D:518:17F:H9	1.07	1.16	6	8
6:E:857:17F:H65	6:E:875:17F:H61	1.07	1.19	20	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:213:17F:H31	6:A:213:17F:H8	1.07	1.15	11	1
6:D:519:17F:H40	6:D:519:17F:H59	1.07	1.24	11	1
6:D:517:17F:H47	6:D:517:17F:H38	1.07	1.07	13	3
6:D:539:17F:H65	6:D:539:17F:H59	1.06	1.27	8	2
6:D:510:17F:H50	6:D:517:17F:C22	1.06	1.81	1	15
6:D:539:17F:H57	6:D:539:17F:H18	1.06	1.15	8	1
6:D:510:17F:H18	6:D:517:17F:H10	1.06	1.27	6	5
6:E:839:17F:H11	6:E:839:17F:H65	1.06	1.25	14	15
6:E:819:17F:H10A	6:E:820:17F:H30	1.06	1.09	4	3
6:D:510:17F:H9	6:D:517:17F:H30	1.06	1.25	13	2
6:D:510:17F:H50	6:D:517:17F:H38	1.06	1.06	1	13
6:D:510:17F:H8A	6:D:517:17F:H19A	1.06	1.19	7	16
6:E:857:17F:H67	6:E:875:17F:H60	1.06	1.25	19	7
6:E:810:17F:H29	6:E:810:17F:H40	1.05	1.20	9	18
6:D:510:17F:H9A	6:D:517:17F:H8A	1.05	1.10	19	8
6:E:819:17F:H61	6:E:842:17F:H67	1.05	1.22	9	8
6:E:808:17F:H46	6:E:810:17F:H62	1.05	1.22	8	3
6:E:808:17F:H66	6:E:820:17F:H29	1.05	1.24	16	5
6:A:208:17F:H49	6:A:208:17F:H68	1.05	1.26	8	12
6:D:510:17F:C33	6:D:517:17F:H12A	1.05	1.79	20	1
6:B:208:17F:H57	6:B:208:17F:H63	1.05	1.28	4	18
6:D:510:17F:H1	6:D:517:17F:H6	1.05	1.28	16	8
6:D:511:17F:H76	6:E:829:17F:H54	1.05	1.24	7	2
6:D:510:17F:H46	6:D:517:17F:H68	1.05	1.29	1	17
6:D:517:17F:H38	6:D:517:17F:C27	1.04	1.82	20	3
6:E:808:17F:H20A	6:E:819:17F:H9A	1.04	1.19	7	5
6:E:808:17F:C31	6:E:820:17F:H12A	1.04	1.82	14	7
6:D:520:17F:H42	6:D:520:17F:H35	1.04	1.23	5	15
6:E:802:17F:H36	6:E:802:17F:H33	1.03	1.26	17	16
6:D:510:17F:C17	6:D:533:17F:H19A	1.03	1.82	3	7
6:E:839:17F:H33	6:E:839:17F:H40	1.03	1.22	11	4
6:D:510:17F:H9A	6:D:517:17F:H9	1.03	1.10	7	8
6:A:208:17F:H41	6:A:219:17F:H38	1.03	1.23	8	4
6:A:219:17F:H5	6:D:518:17F:H11A	1.03	1.24	1	6
6:D:510:17F:H9A	6:D:517:17F:H11	1.03	1.12	4	6
6:A:213:17F:H31	6:A:213:17F:H10A	1.03	1.09	6	5
6:E:808:17F:H55	6:E:819:17F:H76	1.03	1.31	11	8
6:D:520:17F:H64	6:D:520:17F:H56	1.03	1.14	10	5
6:D:510:17F:H9A	6:D:517:17F:C7	1.03	1.83	10	11
6:A:219:17F:H6A	6:D:518:17F:H11A	1.03	1.31	9	8
6:A:213:17F:H39	6:A:213:17F:H11A	1.03	1.23	1	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:519:17F:H20	6:D:519:17F:H12A	1.03	1.30	17	1
6:D:540:17F:H44	6:D:540:17F:H61	1.02	1.29	6	16
6:A:208:17F:H78	6:B:208:17F:H69	1.02	1.28	1	4
2:D:273:ASP:HB2	6:D:540:17F:H34	1.02	1.26	13	18
6:D:518:17F:H44	6:D:518:17F:H59	1.02	1.27	16	11
6:D:510:17F:H31	6:D:517:17F:H10	1.02	1.29	19	4
6:A:208:17F:H31	6:A:219:17F:H12A	1.02	1.28	10	6
6:A:208:17F:H72	6:B:208:17F:H69	1.01	1.22	12	6
6:A:208:17F:H45	6:A:208:17F:H64	1.01	1.32	15	2
6:E:819:17F:H41	6:E:819:17F:H71	1.01	1.30	16	1
6:D:510:17F:H5	6:D:533:17F:C19	1.01	1.84	1	10
6:E:839:17F:H19	6:E:839:17F:H56	1.01	1.33	14	20
6:D:510:17F:H8	6:D:517:17F:H19A	1.01	1.30	2	6
6:D:539:17F:H62	6:D:539:17F:H37	1.01	1.29	12	5
5:D:505:7Q9:C13	6:D:518:17F:H6A	1.01	1.85	19	2
6:D:510:17F:O3	6:D:517:17F:H4	1.01	1.54	17	19
6:D:510:17F:C6	6:D:517:17F:H4A	1.00	1.86	2	17
6:A:208:17F:H33	6:A:219:17F:H10	1.00	1.27	4	2
6:A:219:17F:O10	6:D:518:17F:H11A	1.00	1.55	5	11
5:D:512:7Q9:C13	6:D:534:17F:H4	1.00	1.87	16	12
6:E:857:17F:H68	6:E:875:17F:H61	1.00	1.32	5	4
6:D:510:17F:C5	6:D:533:17F:H19A	0.99	1.86	18	10
6:E:820:17F:H52	6:E:820:17F:H73	0.99	1.34	14	12
6:E:857:17F:H70	6:E:875:17F:H61	0.99	1.29	9	5
6:E:806:17F:H19	6:E:806:17F:H37	0.99	1.33	20	6
6:A:213:17F:H41	6:A:213:17F:H60	0.99	1.32	19	4
6:E:819:17F:H61	6:E:842:17F:H68	0.99	1.35	11	4
6:D:510:17F:C18	6:D:517:17F:H10	0.99	1.87	4	6
6:D:510:17F:H20A	6:D:517:17F:C10	0.99	1.86	15	1
2:E:555:SER:HA	6:E:873:17F:H65	0.99	1.33	3	9
5:A:216:7Q9:C318	6:D:510:17F:H42	0.99	1.87	4	7
6:D:510:17F:H12A	6:D:517:17F:H8	0.98	1.29	19	6
6:B:208:17F:H12	5:B:209:7Q9:C39	0.98	1.87	19	11
6:A:220:17F:H54	6:A:220:17F:H67	0.98	1.27	9	9
6:D:517:17F:H37	6:D:533:17F:H72	0.98	1.35	2	1
6:A:208:17F:H4	6:A:208:17F:H1	0.98	1.31	5	4
6:A:220:17F:H41	6:A:220:17F:H66	0.98	1.34	6	3
6:A:213:17F:H34	6:A:213:17F:H37	0.98	1.32	16	2
5:D:506:7Q9:C32	6:D:517:17F:H32	0.98	1.88	2	5
6:D:540:17F:H59	6:D:540:17F:H65	0.98	1.32	13	13
6:A:213:17F:C23	6:A:213:17F:H60	0.97	1.89	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:519:17F:H66	6:D:519:17F:H40	0.97	1.34	10	1
6:E:808:17F:H42	6:E:810:17F:C35	0.97	1.88	18	10
6:D:519:17F:H58	6:D:519:17F:H64	0.97	1.37	17	1
6:A:219:17F:H39	6:A:219:17F:H11	0.97	1.33	1	13
6:D:518:17F:H29	6:D:518:17F:H19	0.96	1.37	4	16
6:E:802:17F:H62	6:E:802:17F:C31	0.96	1.88	2	18
6:E:856:17F:H38	6:E:856:17F:H68	0.96	1.34	7	13
6:A:213:17F:H46	6:A:213:17F:H67	0.96	1.32	17	1
6:D:519:17F:H64	6:D:519:17F:C32	0.96	1.90	17	1
6:D:533:17F:H77	6:D:533:17F:H50	0.96	1.33	1	13
5:B:205:7Q9:C315	6:B:208:17F:H78	0.96	1.89	5	2
6:D:510:17F:H9	6:D:517:17F:H11A	0.96	1.31	2	4
6:D:510:17F:O10	6:D:533:17F:H19A	0.96	1.61	9	5
6:E:808:17F:H56	6:E:820:17F:H12A	0.96	1.29	14	3
6:D:539:17F:H75	6:D:539:17F:H50	0.96	1.36	7	3
6:D:517:17F:C24	6:D:533:17F:H38	0.96	1.91	19	7
6:E:873:17F:H36	6:E:873:17F:H20	0.96	1.35	5	7
6:D:510:17F:H12	6:D:517:17F:C10	0.96	1.90	13	6
6:A:208:17F:H30	6:B:208:17F:H19	0.96	1.37	17	2
6:A:208:17F:H31	6:A:219:17F:H10A	0.96	1.31	8	4
6:E:820:17F:H18	5:E:853:7Q9:C33	0.96	1.91	3	3
6:A:213:17F:H61	6:A:213:17F:C26	0.96	1.90	8	4
6:D:510:17F:H8A	6:D:517:17F:C19	0.96	1.91	12	6
6:A:213:17F:H36	6:A:213:17F:H45	0.95	1.35	1	5
6:E:808:17F:H60	6:E:820:17F:H29	0.95	1.38	8	1
6:D:510:17F:O7	6:D:517:17F:H4A	0.95	1.62	5	13
6:A:213:17F:H20A	6:A:213:17F:O1	0.95	1.60	9	6
6:D:520:17F:H56	6:D:520:17F:H62	0.95	1.38	11	1
6:E:857:17F:H67	6:E:875:17F:C33	0.95	1.91	13	6
6:D:517:17F:H49	6:D:517:17F:C23	0.95	1.91	3	1
6:A:213:17F:H40	6:A:213:17F:H31	0.95	1.36	1	3
6:D:510:17F:H12	6:D:517:17F:C7	0.95	1.92	2	9
6:D:510:17F:C28	6:D:517:17F:H38	0.95	1.90	9	9
6:D:510:17F:H18A	6:D:517:17F:H10	0.95	1.36	11	8
6:D:510:17F:C20	6:D:517:17F:H8	0.95	1.90	17	1
6:D:519:17F:H30	6:D:519:17F:H39	0.94	1.35	1	19
6:E:808:17F:C37	6:E:820:17F:H29	0.94	1.92	16	3
6:E:857:17F:H68	6:E:875:17F:H65	0.94	1.39	20	4
6:D:510:17F:H76	6:D:517:17F:H72	0.94	1.38	5	4
1:A:47:ASP:HA	1:B:128:LYS:HB2	0.94	1.39	9	6
6:A:213:17F:H30	5:D:509:7Q9:C22	0.94	1.93	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:871:17F:H11	5:E:872:7Q9:O14	0.94	1.62	10	3
6:D:510:17F:H20A	6:D:517:17F:H8	0.94	1.36	17	1
6:D:510:17F:H4A	6:D:517:17F:H4A	0.93	1.38	15	5
6:A:213:17F:H40	6:A:213:17F:H11A	0.93	1.35	11	1
6:D:510:17F:H20A	6:D:517:17F:C9	0.93	1.93	15	2
6:D:517:17F:H39	6:D:517:17F:C27	0.93	1.93	8	17
6:D:510:17F:H50	6:D:517:17F:H37	0.93	1.34	3	3
6:D:510:17F:H12A	6:D:517:17F:H8A	0.93	1.38	3	2
6:D:510:17F:H18A	6:D:533:17F:H20	0.93	1.38	4	1
6:E:857:17F:H69	6:E:857:17F:H58	0.93	1.36	16	15
6:E:875:17F:H49	6:E:875:17F:H72	0.92	1.37	17	4
5:B:205:7Q9:C313	6:B:208:17F:H78	0.92	1.94	8	11
6:A:208:17F:H72	6:B:208:17F:C38	0.92	1.94	12	6
6:E:808:17F:H71	6:E:819:17F:C30	0.92	1.94	5	1
6:E:810:17F:H57	6:E:810:17F:C2X	0.92	1.94	5	2
6:A:219:17F:C17	6:D:518:17F:H11A	0.92	1.94	2	2
5:E:825:7Q9:C32	6:E:842:17F:H20A	0.92	1.95	5	1
6:A:213:17F:H74	6:E:808:17F:H53	0.92	1.41	3	1
6:E:818:17F:H11	5:E:834:7Q9:C32	0.92	1.93	20	2
6:D:518:17F:H36	6:D:518:17F:H20	0.92	1.38	14	15
5:E:805:7Q9:O32	6:E:812:17F:H31	0.92	1.65	4	13
6:E:810:17F:H52	6:E:810:17F:H61	0.92	1.42	9	11
5:B:210:7Q9:C3	6:D:520:17F:H20A	0.92	1.94	2	1
6:D:540:17F:H35	6:D:540:17F:H64	0.92	1.41	10	3
6:D:539:17F:H19A	6:D:539:17F:C31	0.92	1.95	12	19
6:A:213:17F:C33	6:A:213:17F:H41	0.92	1.95	14	2
6:E:819:17F:H12	6:E:820:17F:H9A	0.92	1.40	12	1
6:E:819:17F:H1A	5:E:836:7Q9:O13	0.92	1.65	17	4
6:D:510:17F:H46	6:D:517:17F:C38	0.91	1.95	19	16
6:E:810:17F:H40	6:E:810:17F:C1X	0.91	1.95	11	17
5:E:838:7Q9:C14	6:E:842:17F:H19A	0.91	1.95	4	3
6:E:873:17F:H44	6:E:873:17F:H59	0.91	1.42	1	9
6:A:219:17F:H5	6:D:518:17F:C9	0.91	1.95	6	3
6:D:510:17F:O9	6:D:517:17F:H9	0.91	1.66	18	10
5:E:803:7Q9:O32	6:E:808:17F:H5	0.91	1.64	17	6
6:D:520:17F:H56	6:D:520:17F:C36	0.91	1.95	10	2
6:D:511:17F:H42	6:D:534:17F:H51	0.91	1.39	13	1
5:E:804:7Q9:C3	6:E:808:17F:H8A	0.91	1.95	20	3
6:D:510:17F:H8	6:D:517:17F:C19	0.91	1.94	2	6
6:E:875:17F:H78	6:E:875:17F:C28	0.91	1.94	19	13
6:E:806:17F:H73	5:E:817:7Q9:C318	0.91	1.96	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:213:17F:H41	6:A:213:17F:C34	0.91	1.96	6	5
6:D:510:17F:H9A	6:D:517:17F:C11	0.91	1.95	4	6
6:E:820:17F:H44	6:E:820:17F:H58	0.91	1.42	15	12
6:A:208:17F:H43	6:A:208:17F:C31	0.91	1.96	10	12
6:A:213:17F:H61	6:A:213:17F:H46	0.90	1.38	12	5
6:E:810:17F:H34	6:E:819:17F:H68	0.90	1.42	4	3
6:E:829:17F:H12	5:E:852:7Q9:C34	0.90	1.95	20	1
6:E:808:17F:H1	5:E:814:7Q9:C14	0.90	1.95	1	10
6:E:808:17F:C24	6:E:810:17F:H62	0.90	1.96	2	9
6:A:208:17F:H31	6:A:219:17F:C10	0.90	1.95	8	6
6:A:219:17F:C6	6:D:518:17F:H9	0.90	1.95	16	5
6:A:220:17F:H12A	6:D:519:17F:H62	0.90	1.42	17	1
6:D:518:17F:H41	5:D:551:7Q9:C39	0.90	1.97	8	6
6:E:873:17F:C20	6:E:873:17F:H36	0.90	1.96	11	8
5:D:506:7Q9:C31	6:D:517:17F:H20	0.90	1.97	8	4
6:E:842:17F:H37	5:E:877:7Q9:C31	0.90	1.97	4	3
6:D:510:17F:O8	6:D:517:17F:H19A	0.90	1.65	4	4
6:A:213:17F:H73	6:E:808:17F:H53	0.90	1.44	4	1
6:E:839:17F:H77	6:E:839:17F:H49	0.90	1.43	8	10
6:E:808:17F:H74	6:E:808:17F:H51	0.90	1.40	8	1
6:E:810:17F:H60	6:E:819:17F:H71	0.90	1.44	5	2
6:E:808:17F:H49	6:E:810:17F:H62	0.89	1.44	20	5
6:E:857:17F:C1X	6:E:875:17F:H60	0.89	1.97	8	1
6:D:520:17F:H64	6:D:520:17F:C31	0.89	1.95	12	4
6:E:839:17F:H12	6:E:857:17F:H12	0.89	1.42	17	3
6:A:219:17F:C41	6:A:219:17F:H48	0.89	1.97	14	1
6:D:510:17F:C4	6:D:517:17F:H4A	0.89	1.98	15	17
6:E:819:17F:H42	5:E:836:7Q9:C37	0.89	1.97	8	6
6:D:533:17F:H10	5:D:541:7Q9:C35	0.89	1.97	2	1
6:E:873:17F:H36	6:E:873:17F:H20A	0.89	1.44	10	14
6:E:808:17F:H33	6:E:819:17F:H9A	0.89	1.41	17	4
6:D:517:17F:H49	6:D:517:17F:H39	0.89	1.44	3	1
5:A:218:7Q9:C3	6:D:511:17F:H6	0.89	1.98	2	2
5:E:851:7Q9:C39	6:E:871:17F:H20A	0.89	1.98	4	3
6:A:213:17F:H60	6:A:213:17F:C24	0.89	1.98	20	6
6:E:810:17F:C34	6:E:819:17F:H71	0.89	1.98	3	2
6:E:819:17F:H1A	5:E:836:7Q9:O14	0.89	1.68	5	5
6:E:819:17F:H10A	6:E:820:17F:H10	0.88	1.45	16	1
6:A:213:17F:H61	6:A:213:17F:H41	0.88	1.43	17	1
6:E:820:17F:H65	5:E:837:7Q9:C36	0.88	1.98	1	5
5:A:206:7Q9:C316	6:E:802:17F:H68	0.88	1.97	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:219:17F:H61	6:A:219:17F:C38	0.88	1.99	8	17
6:E:842:17F:H9A	5:E:877:7Q9:O14	0.88	1.67	7	2
6:D:510:17F:H12A	6:D:517:17F:C8	0.88	1.99	16	5
6:D:510:17F:C1	6:D:517:17F:H6	0.88	1.97	11	7
5:A:218:7Q9:O14	6:D:511:17F:H4A	0.88	1.67	5	1
6:A:220:17F:H36	5:D:502:7Q9:C312	0.88	1.98	7	5
6:D:510:17F:H19	6:D:533:17F:H19	0.88	1.45	3	3
1:A:32:TYR:HD1	3:A:201:GSP:H5'2	0.88	1.29	4	8
6:E:857:17F:C36	6:E:875:17F:H61	0.88	1.98	4	5
6:E:808:17F:H66	6:E:820:17F:C1X	0.88	1.99	12	3
6:A:219:17F:H4A	5:D:505:7Q9:O32	0.88	1.69	18	2
6:E:808:17F:H75	6:E:819:17F:H55	0.88	1.44	1	5
6:E:873:17F:H36	6:E:873:17F:C20	0.88	1.99	7	11
6:D:510:17F:C12	6:D:517:17F:H8	0.88	1.98	13	7
6:A:219:17F:H51	5:E:828:7Q9:C317	0.88	1.99	16	2
6:D:510:17F:H46	6:D:517:17F:H64	0.87	1.41	11	13
6:D:517:17F:H39	6:D:517:17F:C28	0.87	2.00	3	1
6:D:511:17F:H11A	5:D:513:7Q9:C35	0.87	2.00	12	1
6:A:208:17F:H64	6:A:208:17F:H39	0.87	1.46	17	11
6:D:510:17F:H18A	6:D:517:17F:H9A	0.87	1.46	5	5
5:D:550:7Q9:C313	6:D:552:17F:H50	0.87	1.99	17	4
6:D:510:17F:C1	6:D:517:17F:H4	0.87	2.00	1	5
6:D:510:17F:C7	6:D:517:17F:H9	0.87	2.00	20	9
6:D:539:17F:H57	6:D:539:17F:C19	0.87	1.98	16	20
5:E:870:7Q9:C22	6:E:873:17F:H10	0.87	1.99	14	16
1:B:13:GLY:HA2	3:B:201:GSP:H5'1	0.86	1.42	18	9
1:A:32:TYR:CD1	3:A:201:GSP:H5'2	0.86	2.05	3	10
6:E:871:17F:H10A	5:E:872:7Q9:O13	0.86	1.70	16	1
6:A:213:17F:H46	6:A:213:17F:C37	0.86	2.00	17	1
5:B:205:7Q9:C311	6:B:208:17F:H78	0.86	2.00	3	1
6:A:208:17F:H68	6:A:208:17F:H46	0.86	1.47	5	1
6:A:213:17F:H45	6:A:213:17F:H35	0.86	1.45	8	3
6:D:510:17F:C26	6:D:517:17F:H68	0.86	1.99	17	11
6:E:839:17F:H40	6:E:839:17F:C1Z	0.86	2.01	11	3
6:A:219:17F:H34	5:E:801:7Q9:C32	0.86	2.00	20	1
6:A:219:17F:H66	6:D:518:17F:H37	0.86	1.45	3	1
6:D:510:17F:H63	5:D:530:7Q9:C313	0.86	1.99	3	2
6:D:539:17F:H66	6:D:539:17F:H43	0.86	1.47	8	1
6:E:839:17F:H65	6:E:839:17F:C11	0.86	2.01	18	11
6:A:213:17F:H12	6:A:213:17F:H31	0.86	1.46	10	2
6:D:510:17F:H18A	6:D:533:17F:H19A	0.86	1.48	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:219:17F:H56	6:A:219:17F:H63	0.86	1.44	12	4
6:D:511:17F:H64	6:D:511:17F:H36	0.86	1.45	20	2
6:E:808:17F:H33	6:E:819:17F:C9	0.85	2.01	17	4
6:A:220:17F:H39	6:A:220:17F:H66	0.85	1.45	12	2
6:D:510:17F:H55	6:D:533:17F:H76	0.85	1.45	16	3
5:E:804:7Q9:C31	6:E:808:17F:H8A	0.85	2.00	17	2
2:E:660:ARG:HD2	6:E:875:17F:H20A	0.85	1.46	19	6
5:E:814:7Q9:C314	6:E:819:17F:H54	0.85	2.01	17	4
6:E:802:17F:H57	6:E:802:17F:C35	0.85	2.00	17	17
6:A:219:17F:H46	5:D:505:7Q9:C311	0.85	2.01	20	9
6:D:510:17F:O7	6:D:517:17F:H9	0.85	1.71	2	9
6:A:208:17F:H34	6:A:208:17F:H46	0.85	1.48	7	1
6:D:510:17F:C42	6:D:510:17F:H53	0.85	2.01	16	2
6:E:819:17F:H78	6:E:819:17F:H45	0.85	1.47	18	9
6:D:534:17F:H50	6:D:534:17F:C24	0.85	2.02	16	20
6:A:208:17F:H43	6:A:208:17F:C1Z	0.85	2.01	2	8
5:B:205:7Q9:C37	6:B:208:17F:H72	0.85	2.01	3	1
6:D:533:17F:H50	6:D:533:17F:C42	0.85	2.02	12	9
6:A:208:17F:H31	6:A:219:17F:C12	0.85	2.01	19	7
6:E:808:17F:H18A	6:E:810:17F:C20	0.85	2.01	13	5
6:E:810:17F:C33	6:E:819:17F:H71	0.84	2.02	5	4
6:D:510:17F:H20A	6:D:517:17F:H9A	0.84	1.45	15	1
6:A:213:17F:H76	6:E:808:17F:H53	0.84	1.47	17	1
6:E:857:17F:H10A	6:E:875:17F:O10	0.84	1.71	18	2
6:E:829:17F:H9	5:E:833:7Q9:C33	0.84	2.02	1	6
6:A:208:17F:C39	6:A:208:17F:H49	0.84	2.03	16	4
6:D:517:17F:H47	6:D:517:17F:C23	0.84	2.02	14	19
6:A:213:17F:H41	6:A:213:17F:C33	0.84	2.01	6	5
6:E:820:17F:H38	6:E:820:17F:H45	0.84	1.48	19	3
5:E:838:7Q9:O32	6:E:842:17F:H12A	0.84	1.72	7	4
6:E:808:17F:H60	6:E:820:17F:H12A	0.84	1.50	19	5
5:B:205:7Q9:C312	6:B:208:17F:H78	0.84	2.02	13	1
6:D:552:17F:C7	6:D:552:17F:H57	0.84	2.02	15	16
6:A:219:17F:H6	5:D:505:7Q9:O32	0.84	1.73	7	5
6:A:208:17F:H64	6:A:208:17F:H58	0.84	1.49	3	2
6:A:213:17F:H55	6:A:213:17F:H68	0.84	1.49	10	1
6:A:220:17F:H12A	6:D:519:17F:C35	0.84	2.03	17	1
5:E:805:7Q9:C14	6:E:806:17F:H8A	0.84	2.01	10	3
6:A:219:17F:H6	5:D:505:7Q9:O21	0.84	1.73	3	1
6:E:808:17F:H55	6:E:819:17F:C42	0.84	2.02	11	7
5:E:803:7Q9:O13	6:E:808:17F:H2	0.84	1.73	16	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:C9	6:D:517:17F:C9	0.84	2.53	8	7
6:E:857:17F:H65	6:E:875:17F:C34	0.84	2.03	4	4
6:A:213:17F:H74	6:E:819:17F:H77	0.84	1.48	14	3
5:A:215:7Q9:C37	6:D:511:17F:H72	0.83	2.01	12	6
5:E:825:7Q9:C33	6:E:842:17F:H20A	0.83	2.02	17	6
6:E:812:17F:H6A	5:E:824:7Q9:C3	0.83	2.02	9	1
6:A:208:17F:H37	6:B:208:17F:H19	0.83	1.46	20	1
5:E:805:7Q9:C3	6:E:812:17F:H19	0.83	2.02	17	5
5:E:805:7Q9:C13	6:E:806:17F:H8A	0.83	2.03	6	7
5:B:205:7Q9:C312	6:B:208:17F:H12A	0.83	2.04	11	6
5:B:205:7Q9:C317	6:E:812:17F:H46	0.83	2.03	17	2
6:E:857:17F:C37	6:E:875:17F:H60	0.83	2.03	16	6
6:A:219:17F:C6	6:D:518:17F:H11A	0.83	2.04	8	4
5:E:805:7Q9:C31	6:E:812:17F:H19	0.83	2.03	7	2
6:E:839:17F:N1	6:E:875:17F:H6A	0.83	1.88	4	3
5:E:814:7Q9:C38	6:E:820:17F:H77	0.83	2.04	11	7
5:D:506:7Q9:C32	6:D:517:17F:H31	0.83	2.04	10	4
6:D:533:17F:H30	6:D:533:17F:H67	0.83	1.51	6	4
6:D:510:17F:H40	6:D:510:17F:H29	0.83	1.48	12	1
6:A:213:17F:H11A	6:A:213:17F:C23	0.83	2.03	1	6
6:A:213:17F:H8	6:A:213:17F:C12	0.83	2.04	16	13
5:B:205:7Q9:C310	6:B:208:17F:H57	0.83	2.03	10	6
6:D:510:17F:C12	6:D:517:17F:H10A	0.83	2.02	13	3
6:D:533:17F:H77	6:D:533:17F:H55	0.83	1.48	16	2
6:D:510:17F:H8	6:D:517:17F:O9	0.83	1.74	20	9
5:B:206:7Q9:C318	6:E:812:17F:H78	0.83	2.03	16	3
6:E:818:17F:H29	5:E:834:7Q9:C33	0.83	2.03	11	2
5:E:803:7Q9:O13	6:E:808:17F:H4A	0.83	1.74	14	4
6:E:819:17F:H60	6:E:842:17F:H65	0.83	1.48	11	2
6:E:842:17F:H9A	5:E:877:7Q9:C12	0.83	2.03	18	1
6:A:213:17F:H38	5:D:507:7Q9:C33	0.82	2.03	7	1
6:D:510:17F:H57	6:D:533:17F:H61	0.82	1.49	13	3
6:E:818:17F:H11	5:E:821:7Q9:C23	0.82	2.03	7	1
6:E:802:17F:H12	6:E:802:17F:H20	0.82	1.50	15	16
6:E:802:17F:H36	6:E:802:17F:C1Z	0.82	2.03	12	9
6:A:220:17F:H64	6:A:220:17F:H12	0.82	1.48	8	3
6:A:213:17F:H12A	6:A:213:17F:C8	0.82	2.02	11	16
6:D:519:17F:H67	6:D:519:17F:C27	0.82	2.02	16	14
6:E:806:17F:H45	6:E:806:17F:C30	0.82	2.05	9	20
6:E:808:17F:C33	6:E:820:17F:H12A	0.82	2.05	10	7
6:E:820:17F:H60	5:E:853:7Q9:C35	0.82	2.04	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:518:17F:H10A	6:D:518:17F:H19	0.82	1.51	11	1
6:E:875:17F:H47	6:E:875:17F:H78	0.82	1.48	2	3
6:D:552:17F:H56	6:D:552:17F:H62	0.82	1.52	6	18
5:B:205:7Q9:C314	6:B:208:17F:H71	0.82	2.04	3	1
2:E:634:LEU:HG	5:E:863:7Q9:C310	0.82	2.04	17	6
6:A:219:17F:H74	6:A:219:17F:H46	0.82	1.48	5	3
6:D:510:17F:C9	6:D:517:17F:H11A	0.82	2.04	2	2
6:D:510:17F:C26	6:D:517:17F:H64	0.82	2.03	11	12
6:E:808:17F:H38	6:E:810:17F:H20	0.82	1.50	20	3
6:E:839:17F:H35	6:E:839:17F:H33	0.82	1.51	4	4
6:A:213:17F:H40	6:A:213:17F:C11	0.82	2.04	11	2
6:A:219:17F:C5	6:D:518:17F:H9	0.82	2.04	6	6
6:E:842:17F:H39	6:E:842:17F:H29	0.82	1.51	12	8
6:E:808:17F:H71	6:E:819:17F:H55	0.82	1.51	5	2
5:D:505:7Q9:C311	5:D:505:7Q9:C37	0.82	2.58	6	16
6:E:820:17F:C22	6:E:820:17F:H45	0.82	2.05	1	17
6:A:219:17F:C37	6:D:518:17F:H37	0.82	2.04	3	1
6:E:818:17F:H61	5:E:827:7Q9:C37	0.82	2.04	3	2
6:E:808:17F:H56	6:E:820:17F:C1X	0.82	2.04	7	4
5:B:209:7Q9:C312	5:B:209:7Q9:C317	0.82	2.57	13	1
6:E:875:17F:H6	6:E:875:17F:O1	0.81	1.75	2	12
6:D:510:17F:C18	6:D:533:17F:H20	0.81	2.04	4	2
6:A:213:17F:H10A	6:A:213:17F:C1Y	0.81	2.02	6	2
6:A:213:17F:H74	6:E:819:17F:C42	0.81	2.05	20	2
6:E:808:17F:H20A	6:E:819:17F:C9	0.81	2.05	5	5
6:B:208:17F:H46	6:B:208:17F:C30	0.81	2.05	15	11
6:E:842:17F:H56	6:E:842:17F:H42	0.81	1.52	3	8
1:A:47:ASP:HA	1:B:128:LYS:HB3	0.81	1.52	4	1
5:A:218:7Q9:C1	6:D:511:17F:H6	0.81	2.06	12	3
5:E:805:7Q9:C1	6:E:812:17F:H19	0.81	2.05	9	2
6:D:510:17F:H5	6:D:533:17F:H19	0.81	1.51	1	1
6:D:510:17F:H78	6:D:510:17F:C30	0.81	2.06	8	4
6:D:511:17F:H77	6:D:511:17F:H49	0.81	1.52	9	13
6:D:510:17F:H49	6:D:517:17F:H67	0.81	1.49	12	9
6:E:808:17F:C31	6:E:820:17F:H29	0.81	2.06	4	3
6:D:510:17F:C8	6:D:517:17F:H8A	0.81	2.06	19	5
6:D:517:17F:H41	6:D:533:17F:C22	0.81	2.04	15	7
2:E:733:LEU:HG	5:E:876:7Q9:C37	0.81	2.06	19	15
6:B:208:17F:H55	6:B:208:17F:C26	0.81	2.04	3	11
6:E:857:17F:H68	6:E:875:17F:H60	0.81	1.50	9	2
6:E:819:17F:C10	6:E:820:17F:H30	0.81	2.05	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:GLY:HA2	3:A:201:GSP:H5'1	0.81	1.49	4	8
6:D:510:17F:C1X	6:D:510:17F:H43	0.81	2.06	12	1
6:E:806:17F:H54	6:E:806:17F:C26	0.81	2.06	5	20
1:B:32:TYR:HD2	3:B:201:GSP:H5'2	0.81	1.35	2	1
6:A:213:17F:H40	6:A:213:17F:H12	0.81	1.52	19	2
6:E:857:17F:H36	6:E:857:17F:C31	0.81	2.04	3	7
6:E:810:17F:H57	6:E:810:17F:H36	0.81	1.52	13	2
6:E:820:17F:H45	6:E:820:17F:C22	0.81	2.06	19	3
6:A:208:17F:H62	6:A:208:17F:H35	0.81	1.50	8	4
6:D:520:17F:H55	6:D:520:17F:H72	0.81	1.53	1	2
6:E:875:17F:O3	6:E:875:17F:H6	0.81	1.74	18	9
6:D:519:17F:H69	6:D:519:17F:H52	0.81	1.50	5	6
6:D:534:17F:H42	6:D:534:17F:C28	0.81	2.05	20	20
6:E:839:17F:H11	6:E:839:17F:C36	0.81	2.05	13	8
6:E:839:17F:H10A	6:E:857:17F:H12	0.81	1.50	7	3
6:D:518:17F:H76	6:D:518:17F:H53	0.81	1.52	7	5
6:E:802:17F:H77	6:E:802:17F:H49	0.81	1.53	2	4
5:E:870:7Q9:O12	6:E:873:17F:H9	0.81	1.75	10	8
6:A:213:17F:H53	5:D:503:7Q9:C315	0.81	2.06	8	1
6:D:539:17F:H62	6:D:539:17F:C21	0.81	2.05	12	5
6:E:839:17F:H48	6:E:839:17F:H71	0.80	1.53	20	5
6:A:208:17F:H41	6:A:219:17F:C12	0.80	2.06	13	2
6:A:219:17F:H9	5:D:505:7Q9:C34	0.80	2.04	7	4
5:A:211:7Q9:C311	6:A:213:17F:H65	0.80	2.06	17	1
6:A:219:17F:H39	6:A:219:17F:C11	0.80	2.05	6	7
6:E:839:17F:H70	6:E:875:17F:H53	0.80	1.50	14	2
5:D:523:7Q9:C32	6:D:552:17F:H36	0.80	2.05	4	5
6:A:213:17F:H30	5:D:509:7Q9:C23	0.80	2.06	11	1
6:D:518:17F:H33	5:D:528:7Q9:C37	0.80	2.07	1	7
6:E:802:17F:H10	6:E:802:17F:H18	0.80	1.54	18	8
6:E:818:17F:H18	5:E:821:7Q9:C22	0.80	2.07	5	1
6:D:510:17F:H6A	6:D:533:17F:H19A	0.80	1.53	10	1
6:D:510:17F:H47	6:D:517:17F:H37	0.80	1.52	13	2
6:A:208:17F:H49	6:A:208:17F:C38	0.80	2.05	8	10
6:E:857:17F:C38	6:E:875:17F:H61	0.80	2.06	5	4
6:E:808:17F:C31	6:E:808:17F:H30	0.80	2.06	8	1
6:E:808:17F:H30	6:E:808:17F:H57	0.80	1.53	8	1
5:A:211:7Q9:C312	6:A:213:17F:H63	0.80	2.06	9	2
6:E:839:17F:H33	6:E:839:17F:C23	0.80	2.07	11	5
6:E:875:17F:H36	6:E:875:17F:H41	0.80	1.52	3	19
6:A:219:17F:H31	5:E:801:7Q9:C34	0.80	2.06	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:512:7Q9:C33	6:D:534:17F:H6A	0.80	2.06	4	2
6:D:533:17F:H50	6:D:533:17F:H78	0.80	1.52	12	1
6:D:510:17F:H53	6:D:510:17F:H78	0.80	1.51	16	4
6:A:213:17F:H31	6:A:213:17F:C10	0.80	2.03	6	4
6:A:213:17F:H60	6:A:213:17F:H41	0.80	1.54	20	1
6:B:208:17F:H55	6:B:208:17F:H64	0.80	1.53	20	1
6:E:808:17F:H51	6:E:808:17F:C42	0.80	2.06	6	11
6:E:857:17F:H46	6:E:857:17F:H59	0.80	1.50	13	5
6:D:539:17F:H59	6:D:539:17F:C36	0.80	2.02	8	1
6:D:510:17F:C12	6:D:517:17F:C8	0.80	2.58	18	13
6:E:808:17F:H55	6:E:819:17F:H75	0.80	1.52	4	2
6:A:208:17F:H34	6:A:208:17F:H40	0.80	1.52	19	5
6:A:213:17F:H8	6:A:213:17F:C1Y	0.80	2.05	11	1
6:D:533:17F:H39	6:D:533:17F:H68	0.80	1.54	3	1
5:B:209:7Q9:C23	6:D:520:17F:H31	0.80	2.06	9	1
1:B:32:TYR:CD1	3:B:201:GSP:H5'2	0.79	2.12	17	6
6:B:208:17F:C27	6:E:812:17F:H70	0.79	2.07	3	1
6:D:518:17F:C20	6:D:518:17F:H36	0.79	2.07	8	9
6:D:519:17F:H48	6:D:519:17F:C37	0.79	2.07	18	7
6:E:802:17F:O10	6:E:808:17F:N1	0.79	2.15	12	6
6:E:808:17F:C26	6:E:810:17F:H62	0.79	2.07	8	2
6:D:510:17F:H20A	6:D:517:17F:C8	0.79	2.07	17	1
6:E:808:17F:H68	6:E:819:17F:H38	0.79	1.51	12	5
6:D:519:17F:H52	6:D:519:17F:C37	0.79	2.07	9	10
5:A:206:7Q9:C15	6:A:213:17F:H5	0.79	2.07	15	1
6:E:839:17F:C36	6:E:839:17F:H11	0.79	2.07	20	1
6:E:875:17F:H49	6:E:875:17F:C42	0.79	2.08	13	5
5:E:849:7Q9:C34	5:E:852:7Q9:C32	0.79	2.61	20	14
6:A:208:17F:H57	6:A:208:17F:C25	0.79	2.03	16	11
6:D:510:17F:C9	6:D:517:17F:C8	0.79	2.59	10	10
6:E:806:17F:H72	6:E:806:17F:C30	0.79	2.07	3	1
6:E:819:17F:C42	6:E:819:17F:H47	0.79	2.07	3	1
5:A:215:7Q9:C38	6:D:511:17F:H72	0.79	2.08	7	4
6:D:510:17F:O10	6:D:510:17F:H4	0.79	1.78	15	20
6:E:806:17F:H54	6:E:806:17F:H72	0.79	1.55	20	6
5:E:858:7Q9:C310	6:E:875:17F:H48	0.79	2.08	19	3
6:D:510:17F:H18	6:D:517:17F:C10	0.79	2.08	6	3
6:D:510:17F:O2	6:D:510:17F:N1	0.79	2.14	20	12
6:E:839:17F:H65	6:E:839:17F:H57	0.79	1.54	4	7
5:E:858:7Q9:C39	6:E:875:17F:H44	0.79	2.08	19	2
6:D:540:17F:H64	6:D:540:17F:C2X	0.79	2.06	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:539:17F:H43	6:D:539:17F:C37	0.79	2.08	8	1
6:E:842:17F:H2	6:E:842:17F:H4A	0.78	1.54	20	2
6:E:810:17F:H10A	5:E:811:7Q9:C34	0.78	2.07	3	2
6:A:208:17F:H33	6:A:219:17F:C10	0.78	2.08	4	3
6:D:519:17F:H43	6:D:519:17F:H68	0.78	1.53	10	1
6:A:208:17F:C1Y	6:A:219:17F:H10A	0.78	2.08	8	4
6:D:510:17F:H4A	6:D:517:17F:C4	0.78	2.08	15	9
5:D:512:7Q9:O13	6:D:534:17F:H4A	0.78	1.77	19	2
6:E:875:17F:O9	6:E:875:17F:H1A	0.78	1.77	19	6
6:D:552:17F:H57	6:D:552:17F:O8	0.78	1.76	15	7
6:E:819:17F:H18A	6:E:842:17F:C33	0.78	2.09	12	2
6:E:839:17F:C1Z	6:E:839:17F:H40	0.78	2.08	8	8
6:A:208:17F:H43	6:A:208:17F:H57	0.78	1.53	2	2
6:E:808:17F:H33	6:E:819:17F:C10	0.78	2.07	3	2
6:E:806:17F:C26	6:E:806:17F:H68	0.78	2.08	13	2
6:D:510:17F:O6	6:D:517:17F:H4	0.78	1.76	20	4
6:A:213:17F:H12	6:A:213:17F:H20	0.78	1.54	5	3
6:A:219:17F:H6	6:D:518:17F:H9	0.78	1.54	7	3
6:D:510:17F:H78	6:D:510:17F:H53	0.78	1.56	8	1
6:A:213:17F:H40	6:A:213:17F:C12	0.78	2.09	19	2
6:D:510:17F:H46	6:D:517:17F:C36	0.78	2.08	12	9
6:E:820:17F:H38	6:E:820:17F:C26	0.78	2.08	19	8
6:D:510:17F:C28	6:D:517:17F:H37	0.78	2.07	3	2
6:A:213:17F:H60	6:A:213:17F:H40	0.78	1.54	9	2
6:D:510:17F:H19	6:D:533:17F:C19	0.78	2.08	7	3
6:E:820:17F:O10	6:E:820:17F:H6A	0.78	1.79	1	17
6:E:873:17F:H62	6:E:873:17F:H57	0.78	1.56	5	9
2:D:305:GLN:HE22	6:D:533:17F:H10A	0.78	1.36	15	4
6:A:213:17F:H10	6:A:213:17F:C34	0.78	2.08	19	1
5:B:205:7Q9:C312	6:B:208:17F:H35	0.77	2.08	7	4
6:D:520:17F:H11	6:D:520:17F:H32	0.77	1.54	3	7
6:D:534:17F:H35	5:D:538:7Q9:C315	0.77	2.08	3	1
6:D:518:17F:O10	6:D:518:17F:H6A	0.77	1.79	20	16
6:A:208:17F:H41	6:A:219:17F:C22	0.77	2.08	8	2
6:E:802:17F:C35	6:E:802:17F:H57	0.77	2.07	11	3
2:D:269:GLN:HG2	6:D:540:17F:H33	0.77	1.56	14	4
5:B:205:7Q9:C313	6:B:208:17F:H72	0.77	2.08	5	1
6:E:839:17F:H43	5:E:858:7Q9:C312	0.77	2.09	5	2
6:E:819:17F:H39	6:E:819:17F:C1X	0.77	2.02	17	9
6:E:808:17F:H56	6:E:820:17F:H29	0.77	1.56	4	4
5:D:543:7Q9:O31	6:D:552:17F:H29	0.77	1.79	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:220:17F:H63	6:A:220:17F:H32	0.77	1.56	18	2
6:E:808:17F:H71	6:E:819:17F:H47	0.77	1.53	13	4
6:D:519:17F:H66	6:D:519:17F:C23	0.77	2.07	10	1
6:D:518:17F:H29	6:D:518:17F:C19	0.77	2.09	4	5
6:A:219:17F:H68	6:A:219:17F:C34	0.77	2.10	12	18
6:B:208:17F:O1	6:B:208:17F:H5	0.77	1.80	9	12
5:B:205:7Q9:C314	6:B:208:17F:H77	0.77	2.09	3	1
6:D:510:17F:H12	6:D:517:17F:H8	0.77	1.54	18	2
2:D:334:LEU:HB2	5:D:538:7Q9:C312	0.77	2.10	10	15
6:D:510:17F:C6	6:D:533:17F:H19A	0.77	2.10	10	4
6:D:510:17F:H58	6:D:533:17F:H71	0.77	1.54	4	2
6:D:510:17F:H56	6:D:517:17F:H11A	0.77	1.55	20	1
6:E:806:17F:C30	6:E:806:17F:H72	0.77	2.10	20	5
6:E:842:17F:H56	6:E:842:17F:C24	0.77	2.10	3	4
6:D:518:17F:O6	6:D:518:17F:H2	0.77	1.79	4	6
6:E:819:17F:H78	6:E:819:17F:C27	0.77	2.10	17	7
6:D:510:17F:H67	6:D:510:17F:H51	0.77	1.55	15	3
6:D:510:17F:H19A	5:D:530:7Q9:C3	0.76	2.09	16	5
6:D:510:17F:C21	6:D:511:17F:H56	0.76	2.09	17	2
6:E:810:17F:H34	6:E:819:17F:C38	0.76	2.08	20	2
6:D:540:17F:H8A	5:D:545:7Q9:C313	0.76	2.09	2	4
6:D:540:17F:H44	6:D:540:17F:C34	0.76	2.09	6	9
6:E:819:17F:H1	5:E:838:7Q9:C13	0.76	2.09	5	2
6:B:208:17F:H41	5:E:824:7Q9:C316	0.76	2.10	7	2
6:A:208:17F:O10	6:A:219:17F:H10	0.76	1.80	7	1
6:A:213:17F:H12	6:A:213:17F:C1Y	0.76	2.09	10	3
6:E:842:17F:H2	6:E:842:17F:C4	0.76	2.09	20	1
6:E:839:17F:H12	6:E:857:17F:C12	0.76	2.09	20	3
6:E:806:17F:H60	5:E:811:7Q9:C35	0.76	2.10	20	2
6:D:520:17F:H19A	6:D:520:17F:H10	0.76	1.58	15	12
6:E:857:17F:H68	6:E:875:17F:C34	0.76	2.10	3	6
6:A:208:17F:H64	6:A:208:17F:C23	0.76	2.10	16	5
1:A:36:ILE:HA	1:A:59:ALA:HB2	0.76	1.56	20	6
6:E:818:17F:H10A	5:E:821:7Q9:C23	0.76	2.09	20	1
6:D:552:17F:H71	6:D:552:17F:H45	0.76	1.55	3	4
6:A:219:17F:H5	6:D:518:17F:C10	0.76	2.11	2	3
6:D:510:17F:C7	6:D:517:17F:H11A	0.76	2.10	15	7
6:A:208:17F:H43	6:A:208:17F:H58	0.76	1.56	13	3
6:E:802:17F:C42	6:E:802:17F:H50	0.76	2.10	6	1
6:E:820:17F:H61	5:E:837:7Q9:C32	0.76	2.11	14	1
5:D:515:7Q9:O31	6:D:519:17F:H19	0.76	1.80	19	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:540:17F:H65	6:D:540:17F:C32	0.76	2.11	15	14
6:E:839:17F:C27	6:E:839:17F:H77	0.76	2.10	12	10
6:A:219:17F:H46	5:D:505:7Q9:C37	0.76	2.11	6	2
5:A:212:7Q9:C314	6:A:219:17F:H54	0.76	2.11	16	2
6:D:533:17F:H36	6:D:533:17F:C24	0.76	1.98	2	1
6:E:808:17F:C41	6:E:808:17F:H51	0.76	2.10	5	5
6:E:842:17F:H59	6:E:842:17F:H64	0.76	1.58	14	12
6:D:518:17F:C19	6:D:518:17F:H29	0.76	2.11	11	1
6:A:220:17F:H45	5:E:811:7Q9:C318	0.76	2.11	13	1
6:E:820:17F:C32	6:E:820:17F:H44	0.76	2.11	9	8
1:A:135:ARG:HB2	1:B:161:ARG:HD2	0.76	1.56	4	2
6:E:808:17F:C28	6:E:810:17F:H62	0.76	2.11	20	5
6:E:839:17F:C27	6:E:839:17F:H78	0.76	2.11	18	2
6:A:208:17F:C36	6:A:208:17F:H39	0.76	2.11	7	1
6:A:208:17F:H39	6:A:208:17F:C36	0.76	2.10	17	3
6:D:519:17F:H43	6:D:519:17F:C38	0.76	2.11	10	1
6:A:213:17F:H42	6:A:213:17F:H34	0.76	1.58	20	1
6:D:510:17F:O7	6:D:517:17F:C9	0.75	2.35	17	9
5:B:205:7Q9:C313	6:B:208:17F:H65	0.75	2.11	7	9
6:E:873:17F:H48	6:E:873:17F:H60	0.75	1.58	14	5
6:A:208:17F:H10	6:A:208:17F:O6	0.75	1.82	20	3
6:D:510:17F:O6	6:D:517:17F:H4A	0.75	1.81	1	12
6:E:839:17F:C33	6:E:839:17F:H9A	0.75	2.11	1	10
5:D:543:7Q9:C3	6:D:552:17F:H11A	0.75	2.10	17	4
6:E:857:17F:H78	6:E:875:17F:H65	0.75	1.59	19	4
6:A:208:17F:H39	6:A:208:17F:H68	0.75	1.55	6	2
6:D:540:17F:H10	5:D:545:7Q9:C36	0.75	2.11	7	5
5:D:541:7Q9:C318	6:E:839:17F:H51	0.75	2.11	20	2
6:D:510:17F:O7	6:D:517:17F:H11A	0.75	1.82	4	5
6:D:534:17F:H35	5:D:538:7Q9:C317	0.75	2.11	4	2
6:D:510:17F:H68	6:D:510:17F:H53	0.75	1.58	5	1
6:E:808:17F:C33	6:E:820:17F:H29	0.75	2.11	8	4
2:D:305:GLN:OE1	6:D:533:17F:H10A	0.75	1.81	1	4
5:B:205:7Q9:C314	6:B:208:17F:H44	0.75	2.10	8	4
6:E:808:17F:H47	6:E:808:17F:H74	0.75	1.58	3	1
5:D:549:7Q9:C312	5:D:549:7Q9:C38	0.75	2.62	19	3
6:A:219:17F:H48	6:A:219:17F:H74	0.75	1.57	14	1
6:A:213:17F:H53	5:D:531:7Q9:C318	0.75	2.11	18	1
5:D:505:7Q9:C15	6:D:518:17F:H6	0.75	2.11	7	2
6:D:510:17F:H74	6:D:533:17F:H76	0.75	1.57	19	1
6:A:219:17F:O10	6:A:219:17F:H6A	0.75	1.81	5	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:511:17F:H4	6:D:511:17F:O10	0.75	1.82	7	19
5:B:205:7Q9:C316	6:B:208:17F:H50	0.75	2.10	3	1
1:B:32:TYR:HD1	3:B:201:GSP:H5'2	0.75	1.42	17	6
6:D:517:17F:H55	6:D:517:17F:H70	0.75	1.56	12	1
6:E:810:17F:H10A	5:E:811:7Q9:O32	0.75	1.81	4	3
6:A:213:17F:H20A	6:A:213:17F:C22	0.75	2.12	18	2
5:D:505:7Q9:C15	6:D:518:17F:H6A	0.75	2.12	2	4
6:E:802:17F:H40	5:E:805:7Q9:C37	0.75	2.11	10	4
6:B:208:17F:H38	5:E:824:7Q9:C318	0.75	2.11	3	1
5:E:858:7Q9:C36	6:E:875:17F:H37	0.75	2.10	3	2
5:D:541:7Q9:C318	6:E:875:17F:H55	0.75	2.12	7	1
6:E:857:17F:H65	6:E:875:17F:H60	0.75	1.58	18	2
6:D:520:17F:H62	6:D:520:17F:C31	0.75	2.08	11	1
6:A:219:17F:H68	6:A:219:17F:C33	0.75	2.12	18	1
6:E:802:17F:H31	5:E:804:7Q9:C23	0.75	2.10	2	4
6:E:808:17F:C1Z	6:E:819:17F:H9A	0.75	2.10	17	3
6:A:213:17F:H42	5:D:507:7Q9:C35	0.75	2.11	7	1
6:D:520:17F:H30	5:D:550:7Q9:C318	0.75	2.11	9	1
6:D:510:17F:P1	6:D:517:17F:H6	0.74	2.22	5	6
6:D:540:17F:H59	6:D:540:17F:C36	0.74	2.08	13	13
6:E:810:17F:H10A	5:E:811:7Q9:C33	0.74	2.12	17	3
6:E:857:17F:C37	6:E:875:17F:H61	0.74	2.11	17	4
6:E:873:17F:H20	6:E:873:17F:H39	0.74	1.59	14	10
6:D:510:17F:H53	6:D:510:17F:H76	0.74	1.58	7	2
6:E:875:17F:C28	6:E:875:17F:H78	0.74	2.11	7	2
6:A:213:17F:C24	6:A:213:17F:H34	0.74	2.12	20	1
6:E:820:17F:H45	6:E:820:17F:H38	0.74	1.57	16	14
6:E:808:17F:H38	6:E:810:17F:H58	0.74	1.56	15	5
6:E:819:17F:H40	6:E:820:17F:H39	0.74	1.60	12	1
6:E:808:17F:H42	6:E:810:17F:C34	0.74	2.11	13	3
6:D:552:17F:H31	6:D:552:17F:C17	0.74	2.12	17	20
6:E:839:17F:H56	6:E:839:17F:C19	0.74	2.11	2	20
6:A:208:17F:H78	5:E:805:7Q9:C318	0.74	2.12	9	4
2:E:638:GLN:HB2	5:E:863:7Q9:C311	0.74	2.12	4	7
3:B:201:GSP:O2A	3:B:201:GSP:S1G	0.74	2.45	7	4
6:E:857:17F:H37	6:E:875:17F:H61	0.74	1.57	8	1
6:D:511:17F:H69	6:D:511:17F:C32	0.74	2.12	12	5
6:E:810:17F:H52	6:E:810:17F:C34	0.74	2.11	10	6
6:E:818:17F:H5	5:E:821:7Q9:C13	0.74	2.13	10	1
6:E:842:17F:O10	6:E:842:17F:H6A	0.74	1.82	1	18
6:E:871:17F:O10	6:E:871:17F:H6A	0.74	1.81	4	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:875:17F:H6	6:E:875:17F:P1	0.74	2.23	20	20
6:A:208:17F:C39	6:A:208:17F:H54	0.74	2.11	12	2
6:D:510:17F:H8	6:D:517:17F:C17	0.74	2.13	8	13
5:D:531:7Q9:C311	5:D:531:7Q9:C37	0.74	2.62	5	15
6:D:533:17F:H72	6:D:533:17F:H46	0.74	1.57	17	2
6:E:857:17F:C31	6:E:857:17F:H36	0.74	2.12	4	4
5:D:543:7Q9:C32	6:D:552:17F:H29	0.74	2.13	3	3
6:E:819:17F:H10A	6:E:820:17F:C10	0.74	2.13	16	1
6:D:540:17F:H1A	5:D:545:7Q9:C32	0.74	2.12	5	2
6:D:510:17F:H9	6:D:517:17F:C1X	0.74	2.10	13	1
6:D:539:17F:H19	6:D:539:17F:H2	0.74	1.59	2	1
6:D:510:17F:H50	6:D:517:17F:C21	0.74	2.13	3	4
6:A:220:17F:H41	6:A:220:17F:C37	0.74	2.11	6	1
6:A:213:17F:C23	6:A:213:17F:H11A	0.74	2.13	9	2
6:D:533:17F:H1A	5:D:541:7Q9:C13	0.74	2.12	14	2
5:E:862:7Q9:C314	5:E:862:7Q9:C310	0.74	2.66	1	20
6:D:517:17F:H38	6:D:533:17F:H38	0.74	1.58	12	1
6:A:208:17F:H78	6:B:208:17F:C38	0.73	2.09	1	2
6:E:857:17F:H56	6:E:857:17F:H63	0.73	1.58	16	15
6:D:510:17F:H76	6:D:517:17F:C40	0.73	2.10	5	2
5:A:211:7Q9:C311	6:A:213:17F:H70	0.73	2.13	17	1
5:E:834:7Q9:C32	6:E:839:17F:H31	0.73	2.13	12	3
6:A:208:17F:H58	6:A:208:17F:H40	0.73	1.56	16	7
6:E:806:17F:H37	6:E:806:17F:C19	0.73	2.13	20	3
6:E:808:17F:H49	6:E:810:17F:H64	0.73	1.58	4	3
5:E:804:7Q9:O31	6:E:808:17F:H8A	0.73	1.83	17	2
5:E:833:7Q9:C22	6:E:839:17F:H6A	0.73	2.12	11	4
6:B:208:17F:H63	6:B:208:17F:C31	0.73	2.13	20	10
6:D:510:17F:O9	6:D:517:17F:C9	0.73	2.37	5	19
6:E:873:17F:H20	6:E:873:17F:H40	0.73	1.57	13	6
6:A:208:17F:H19	5:D:505:7Q9:C32	0.73	2.13	3	1
6:E:839:17F:H52	5:E:858:7Q9:C312	0.73	2.13	17	4
6:D:519:17F:H66	6:D:519:17F:H43	0.73	1.58	12	1
6:D:510:17F:H18A	6:D:533:17F:C19	0.73	2.13	17	1
5:B:205:7Q9:C310	6:B:208:17F:H66	0.73	2.14	15	6
5:A:205:7Q9:C314	6:E:806:17F:H75	0.73	2.14	17	4
6:E:871:17F:H9A	5:E:872:7Q9:C22	0.73	2.12	6	1
6:E:802:17F:H43	5:E:807:7Q9:C316	0.73	2.13	11	1
6:A:219:17F:H63	6:A:219:17F:H40	0.73	1.58	15	2
6:E:820:17F:H44	6:E:820:17F:C32	0.73	2.13	5	7
6:D:533:17F:H42	6:D:533:17F:C2X	0.73	2.09	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:819:17F:H10	6:E:820:17F:C10	0.73	2.14	7	3
1:A:128:LYS:HG2	1:B:47:ASP:HA	0.73	1.58	7	1
6:D:510:17F:C7	6:D:517:17F:H11	0.73	2.13	19	3
6:D:520:17F:H49	5:E:840:7Q9:C317	0.73	2.13	9	3
6:A:213:17F:H74	6:E:808:17F:C30	0.73	2.13	3	1
6:E:839:17F:H12	6:E:857:17F:H9	0.73	1.57	4	1
5:E:870:7Q9:C23	6:E:873:17F:H10	0.73	2.12	5	7
6:A:208:17F:H39	6:A:208:17F:H65	0.73	1.58	7	1
6:A:219:17F:H46	5:D:505:7Q9:C312	0.73	2.14	9	3
6:E:808:17F:C42	6:E:808:17F:H51	0.73	2.13	20	1
6:E:808:17F:H75	6:E:819:17F:C30	0.73	2.13	11	3
6:D:510:17F:H46	6:D:517:17F:C37	0.73	2.14	12	6
6:D:510:17F:H6	6:D:517:17F:H4A	0.73	1.59	12	8
5:D:506:7Q9:C316	6:E:818:17F:H42	0.73	2.12	4	2
5:E:851:7Q9:C316	6:E:871:17F:H60	0.73	2.13	3	4
5:E:825:7Q9:C33	6:E:842:17F:H34	0.73	2.13	5	1
6:E:820:17F:H52	6:E:820:17F:C40	0.73	2.13	14	4
6:E:810:17F:C1Z	6:E:819:17F:H68	0.73	2.12	20	2
6:A:208:17F:H38	6:B:208:17F:C33	0.73	2.12	7	1
6:D:533:17F:H77	6:D:533:17F:C28	0.73	2.14	17	3
6:B:208:17F:O10	6:B:208:17F:H6A	0.73	1.84	6	19
6:D:518:17F:H20	6:D:518:17F:C2X	0.73	2.12	14	5
6:E:839:17F:H65	6:E:839:17F:H11	0.73	1.58	2	2
3:A:201:GSP:O2A	3:A:201:GSP:S1G	0.73	2.47	16	4
6:B:208:17F:H10	5:B:209:7Q9:C39	0.73	2.14	9	2
6:A:219:17F:H56	6:A:219:17F:C35	0.73	2.13	11	3
6:E:842:17F:H37	5:E:877:7Q9:O32	0.73	1.84	17	1
6:E:820:17F:H20	5:E:830:7Q9:O14	0.73	1.84	18	3
6:A:208:17F:H1	6:A:208:17F:H4A	0.73	1.59	20	1
2:E:733:LEU:HA	5:E:876:7Q9:C311	0.72	2.14	18	12
6:D:518:17F:H44	6:D:518:17F:C32	0.72	2.13	2	4
6:E:808:17F:C20	6:E:819:17F:H9A	0.72	2.14	17	5
6:E:818:17F:H61	5:E:827:7Q9:C36	0.72	2.13	4	2
6:E:808:17F:H51	6:E:808:17F:C41	0.72	2.14	20	8
6:D:510:17F:O7	6:D:517:17F:O7	0.72	2.07	2	20
6:A:220:17F:H61	6:A:220:17F:H50	0.72	1.60	2	1
6:D:510:17F:O9	6:D:517:17F:H11A	0.72	1.84	13	4
6:D:510:17F:H9	6:D:517:17F:H9	0.72	1.57	8	2
6:D:510:17F:H67	6:D:510:17F:C29	0.72	2.14	15	2
6:A:213:17F:H8A	6:A:213:17F:C12	0.72	2.09	11	2
6:E:819:17F:H78	6:E:819:17F:C26	0.72	2.13	20	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:515:7Q9:C313	6:D:519:17F:H78	0.72	2.13	5	4
6:E:819:17F:H47	6:E:819:17F:H78	0.72	1.60	2	2
6:A:208:17F:H20A	6:A:219:17F:H10A	0.72	1.60	3	2
6:A:208:17F:H30	6:B:208:17F:H31	0.72	1.61	4	3
6:A:208:17F:H1	6:A:208:17F:C4	0.72	2.11	5	3
6:D:510:17F:H54	6:D:517:17F:H71	0.72	1.60	15	6
6:A:213:17F:H56	6:A:213:17F:H63	0.72	1.59	5	6
5:D:506:7Q9:C32	6:D:517:17F:H20	0.72	2.13	8	5
6:A:213:17F:H31	6:A:213:17F:C8	0.72	2.07	11	1
6:D:510:17F:C20	6:D:517:17F:H9A	0.72	2.15	15	1
6:E:808:17F:H49	6:E:810:17F:C36	0.72	2.15	4	5
6:E:820:17F:H44	6:E:820:17F:H57	0.72	1.60	14	8
6:E:839:17F:HN1A	6:E:875:17F:H6A	0.72	1.43	20	2
6:D:510:17F:H49	6:D:517:17F:H69	0.72	1.61	8	1
5:E:834:7Q9:C311	6:E:839:17F:H45	0.72	2.14	11	2
6:A:220:17F:H76	5:E:825:7Q9:C315	0.72	2.14	20	1
6:D:518:17F:H34	5:D:551:7Q9:C39	0.72	2.14	17	6
6:E:839:17F:N1	6:E:839:17F:O2	0.72	2.22	2	1
6:E:873:17F:C23	6:E:873:17F:H20	0.72	2.15	15	5
6:E:802:17F:H33	6:E:802:17F:C2X	0.72	2.14	19	13
6:E:820:17F:H65	5:E:837:7Q9:C38	0.72	2.14	7	3
6:E:857:17F:H30	6:E:875:17F:H60	0.72	1.61	8	1
6:A:213:17F:C2X	6:A:213:17F:H42	0.72	2.14	16	2
6:D:520:17F:H56	6:D:520:17F:C35	0.72	2.10	11	2
6:D:510:17F:H56	6:D:517:17F:H29	0.72	1.61	11	1
6:E:857:17F:H57	6:E:857:17F:H40	0.72	1.60	13	2
6:D:520:17F:H70	6:D:520:17F:H55	0.72	1.61	18	2
5:A:215:7Q9:C38	6:D:510:17F:H39	0.72	2.14	18	1
6:D:510:17F:O2	6:D:517:17F:H6	0.72	1.85	5	6
6:E:819:17F:H59	6:E:819:17F:H65	0.72	1.61	14	5
6:E:829:17F:N1	5:E:849:7Q9:O14	0.72	2.23	4	4
6:B:208:17F:H42	6:B:208:17F:H35	0.72	1.60	17	3
6:E:842:17F:H37	5:E:877:7Q9:O31	0.72	1.85	20	4
6:E:857:17F:H29	6:E:875:17F:C33	0.72	2.14	4	1
6:A:219:17F:O10	6:D:518:17F:H11	0.72	1.84	9	2
6:D:510:17F:C8	6:D:517:17F:C19	0.72	2.65	8	11
6:D:510:17F:H70	6:D:511:17F:H74	0.72	1.61	16	2
6:E:820:17F:H75	5:E:830:7Q9:C22	0.72	2.15	10	1
6:A:213:17F:H40	6:A:213:17F:C1Y	0.72	2.14	20	1
6:D:510:17F:O10	6:D:510:17F:C4	0.72	2.38	9	13
6:D:518:17F:H18	5:D:528:7Q9:C3	0.72	2.14	17	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:856:17F:H53	5:E:868:7Q9:C315	0.72	2.15	20	2
6:E:806:17F:H45	6:E:806:17F:H72	0.72	1.60	13	2
2:D:426:LYS:HG2	6:D:539:17F:H71	0.72	1.60	13	3
6:E:819:17F:C12	6:E:820:17F:H9A	0.72	2.12	12	1
6:A:208:17F:H76	5:E:813:7Q9:C318	0.72	2.15	17	1
6:D:517:17F:H42	6:D:533:17F:H38	0.72	1.59	19	1
5:D:521:7Q9:C38	6:D:540:17F:H45	0.72	2.13	19	1
5:E:825:7Q9:C34	6:E:842:17F:H20A	0.72	2.15	7	3
6:A:213:17F:H60	6:A:213:17F:H39	0.72	1.60	7	1
3:A:201:GSP:O2A	3:A:201:GSP:H3'	0.72	1.85	11	2
6:D:510:17F:H20A	6:D:517:17F:H10	0.72	1.62	15	2
6:E:875:17F:H78	6:E:875:17F:C27	0.71	2.14	2	5
6:A:208:17F:H45	6:A:208:17F:H70	0.71	1.62	3	1
6:E:819:17F:H1A	5:E:836:7Q9:P	0.71	2.25	4	6
6:D:540:17F:H35	6:D:540:17F:C34	0.71	2.15	7	10
6:A:208:17F:N1	6:A:219:17F:O4	0.71	2.19	18	1
6:E:871:17F:H9A	5:E:872:7Q9:O14	0.71	1.86	15	3
6:A:220:17F:H67	6:A:220:17F:C30	0.71	2.12	9	5
6:E:871:17F:H58	6:E:871:17F:C21	0.71	2.15	6	8
5:E:851:7Q9:C313	6:E:871:17F:H20	0.71	2.15	7	2
6:D:511:17F:C30	6:E:829:17F:H54	0.71	2.14	18	3
6:D:518:17F:H36	6:D:518:17F:C20	0.71	2.15	12	8
6:A:220:17F:H72	5:D:515:7Q9:C318	0.71	2.15	18	1
6:E:875:17F:O9	6:E:875:17F:H1	0.71	1.84	18	1
6:E:820:17F:C7	6:E:820:17F:H4A	0.71	2.16	5	10
6:A:213:17F:H46	6:A:213:17F:H66	0.71	1.63	5	1
6:D:519:17F:O10	6:D:519:17F:H6A	0.71	1.86	6	4
1:B:32:TYR:HE1	3:B:201:GSP:H5'2	0.71	1.45	11	1
6:A:213:17F:H29	5:D:509:7Q9:O22	0.71	1.84	18	1
6:E:819:17F:H61	6:E:842:17F:C38	0.71	2.16	19	5
6:E:839:17F:H59	6:E:839:17F:H18A	0.71	1.60	2	9
5:E:849:7Q9:C312	5:E:852:7Q9:C35	0.71	2.69	3	16
6:A:213:17F:O1	6:A:213:17F:C20	0.71	2.38	5	6
6:D:517:17F:O10	6:D:517:17F:H6A	0.71	1.85	11	12
6:E:808:17F:H58	6:E:808:17F:H30	0.71	1.63	20	4
1:A:162:GLU:HA	1:A:165:LYS:HD3	0.71	1.63	13	1
1:B:92:ASP:HA	1:B:95:HIS:HD2	0.71	1.46	1	1
6:D:510:17F:O6	6:D:517:17F:C4	0.71	2.39	20	13
6:A:213:17F:H37	5:D:509:7Q9:O22	0.71	1.85	2	2
6:A:219:17F:H5	6:D:518:17F:C11	0.71	2.16	19	4
5:E:805:7Q9:C312	5:E:805:7Q9:C38	0.71	2.68	9	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:518:17F:H19	6:D:518:17F:H29	0.71	1.62	11	2
2:D:333:LYS:HE2	5:E:878:7Q9:C318	0.71	2.16	1	3
2:E:620:GLU:HA	5:E:859:7Q9:C311	0.71	2.16	19	17
6:D:520:17F:H54	5:E:841:7Q9:C318	0.71	2.16	4	3
6:D:540:17F:N1	5:D:545:7Q9:O14	0.71	2.23	6	4
2:D:327:GLN:HG3	6:D:534:17F:H78	0.71	1.62	14	3
6:D:517:17F:C37	6:D:517:17F:H49	0.71	2.15	13	1
5:D:506:7Q9:C311	6:D:517:17F:H55	0.71	2.15	20	2
5:A:217:7Q9:C39	5:A:217:7Q9:C35	0.71	2.68	10	20
6:E:857:17F:H70	6:E:875:17F:C34	0.71	2.16	16	6
5:E:865:7Q9:C39	5:E:865:7Q9:C35	0.71	2.69	11	20
6:A:220:17F:H5	6:A:220:17F:O8	0.71	1.86	8	18
1:A:128:LYS:HB2	1:B:47:ASP:HA	0.71	1.62	16	3
6:D:510:17F:C31	6:D:533:17F:H61	0.71	2.15	12	2
6:D:510:17F:H29	6:D:510:17F:H43	0.71	1.63	12	1
6:A:213:17F:H48	5:D:507:7Q9:C318	0.71	2.16	16	1
6:D:519:17F:C32	6:D:519:17F:C36	0.71	2.64	17	1
5:E:825:7Q9:O32	5:E:825:7Q9:C1	0.70	2.38	12	15
6:D:510:17F:C9	6:D:517:17F:O7	0.70	2.36	14	5
6:E:873:17F:O10	6:E:873:17F:H6A	0.70	1.86	3	10
6:A:208:17F:C1Z	6:A:219:17F:H10	0.70	2.11	4	2
6:D:519:17F:H66	6:D:519:17F:H48	0.70	1.61	6	1
6:E:810:17F:N1	6:E:819:17F:O8	0.70	2.24	14	2
6:A:213:17F:H31	6:A:213:17F:C23	0.70	2.13	1	2
2:D:334:LEU:HB3	5:D:538:7Q9:C310	0.70	2.16	20	9
6:E:829:17F:O10	6:E:829:17F:H6A	0.70	1.84	6	20
6:D:517:17F:H44	6:D:533:17F:C22	0.70	2.16	3	1
6:E:819:17F:C12	6:E:820:17F:H30	0.70	2.16	3	1
5:A:215:7Q9:C318	6:D:517:17F:H75	0.70	2.16	1	1
5:D:513:7Q9:C312	6:D:534:17F:H65	0.70	2.16	1	4
6:A:208:17F:H30	6:B:208:17F:C1Y	0.70	2.14	12	3
5:A:211:7Q9:C317	6:A:220:17F:H70	0.70	2.16	1	1
5:D:514:7Q9:C33	5:D:514:7Q9:C37	0.70	2.70	3	15
6:E:812:17F:H5	5:E:824:7Q9:C11	0.70	2.16	19	9
6:A:208:17F:H69	6:B:208:17F:C38	0.70	2.15	4	1
6:E:820:17F:H18	5:E:853:7Q9:C14	0.70	2.16	9	1
6:E:857:17F:H46	6:E:857:17F:C32	0.70	2.15	13	1
1:B:37:GLU:HG2	1:B:56:LEU:HD11	0.70	1.62	15	2
6:D:510:17F:C7	6:D:517:17F:H19A	0.70	2.16	4	9
6:D:518:17F:H59	6:D:518:17F:C25	0.70	2.14	2	2
5:B:205:7Q9:C310	6:B:208:17F:H35	0.70	2.16	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:H63	5:D:530:7Q9:C314	0.70	2.16	7	3
6:E:806:17F:H5	5:E:817:7Q9:C32	0.70	2.17	4	5
6:E:802:17F:H60	5:E:804:7Q9:C22	0.70	2.16	13	1
1:B:32:TYR:CE1	3:B:201:GSP:H5'2	0.70	2.21	11	3
5:E:805:7Q9:C31	6:E:812:17F:H31	0.70	2.16	13	4
6:A:219:17F:H47	5:D:505:7Q9:C312	0.70	2.15	2	5
6:D:511:17F:H66	6:D:511:17F:H39	0.70	1.62	14	5
6:A:208:17F:H70	6:A:208:17F:H49	0.70	1.63	13	2
6:D:518:17F:H69	5:D:528:7Q9:C311	0.70	2.17	7	1
6:A:219:17F:H34	5:E:801:7Q9:C36	0.70	2.16	12	3
5:E:803:7Q9:C314	6:E:810:17F:H66	0.70	2.16	17	1
6:E:802:17F:C17	6:E:802:17F:O8	0.70	2.39	18	19
5:E:809:7Q9:C37	5:E:809:7Q9:C33	0.70	2.70	11	20
6:E:819:17F:H61	6:E:842:17F:C37	0.70	2.16	16	6
6:D:518:17F:H36	6:D:518:17F:H20A	0.70	1.64	16	9
6:A:208:17F:H69	6:B:208:17F:H69	0.70	1.63	4	1
6:D:511:17F:C42	6:E:829:17F:H54	0.70	2.12	7	2
5:E:807:7Q9:C23	6:E:818:17F:H6A	0.70	2.17	12	1
6:E:810:17F:C1Y	6:E:819:17F:H63	0.70	2.17	17	1
6:D:533:17F:O9	6:D:533:17F:C1Y	0.70	2.35	1	13
5:E:851:7Q9:C36	6:E:871:17F:H20	0.70	2.16	1	3
6:E:810:17F:N1	6:E:819:17F:H6	0.70	2.02	10	3
6:D:511:17F:H38	5:D:513:7Q9:C315	0.70	2.17	10	2
6:D:510:17F:H29	6:D:510:17F:C23	0.70	2.16	12	1
6:D:518:17F:H58	5:D:528:7Q9:C38	0.70	2.17	7	8
6:E:808:17F:H38	6:E:810:17F:H32	0.70	1.64	12	5
6:D:517:17F:C25	6:D:533:17F:H38	0.70	2.16	3	4
5:A:211:7Q9:C318	6:E:810:17F:H54	0.70	2.17	5	1
2:D:421:VAL:HG21	2:E:735:GLU:HG2	0.70	1.62	5	3
6:D:533:17F:H77	6:D:533:17F:H46	0.70	1.63	8	1
6:D:533:17F:H55	6:D:533:17F:C42	0.70	2.16	16	1
6:B:208:17F:H4A	6:B:208:17F:O8	0.69	1.87	13	3
2:D:331:ARG:HA	5:D:538:7Q9:C310	0.69	2.17	3	5
6:E:808:17F:H4	6:E:808:17F:O10	0.69	1.85	16	15
6:A:219:17F:H4	6:A:219:17F:N1	0.69	2.01	17	1
6:B:208:17F:H12A	5:E:823:7Q9:C318	0.69	2.17	20	2
6:E:819:17F:C34	6:E:842:17F:H67	0.69	2.11	9	6
5:E:835:7Q9:C318	6:E:856:17F:H66	0.69	2.16	1	2
6:E:839:17F:H68	6:E:857:17F:H41	0.69	1.64	3	2
6:E:839:17F:C42	6:E:839:17F:H47	0.69	2.16	5	2
6:A:213:17F:H61	6:A:213:17F:H45	0.69	1.63	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:219:17F:C34	6:A:219:17F:H68	0.69	2.17	16	1
6:E:820:17F:H19A	5:E:853:7Q9:C32	0.69	2.17	2	1
6:E:839:17F:H33	6:E:839:17F:H35	0.69	1.62	17	4
2:E:555:SER:CA	6:E:873:17F:H65	0.69	2.17	8	7
6:E:802:17F:H33	6:E:802:17F:C21	0.69	2.17	15	7
6:E:808:17F:H33	6:E:819:17F:H10A	0.69	1.62	3	4
6:D:510:17F:C30	6:D:533:17F:H55	0.69	2.18	9	4
6:D:517:17F:C22	6:D:517:17F:C27	0.69	2.57	20	3
5:D:551:7Q9:C33	5:D:551:7Q9:C37	0.69	2.71	6	20
6:D:520:17F:O10	6:D:520:17F:H6A	0.69	1.87	5	2
6:D:510:17F:H9A	6:D:517:17F:C10	0.69	2.16	3	4
6:A:213:17F:H72	6:E:819:17F:H76	0.69	1.65	4	1
6:D:510:17F:O9	6:D:533:17F:H19A	0.69	1.86	5	5
6:E:839:17F:H38	5:E:858:7Q9:C312	0.69	2.17	7	2
1:A:84:ILE:HD11	1:A:118:CYS:HA	0.69	1.63	10	3
6:D:520:17F:H8A	5:D:545:7Q9:C37	0.69	2.17	7	1
5:A:209:7Q9:C313	5:A:209:7Q9:C317	0.69	2.71	9	5
5:D:512:7Q9:C13	6:D:534:17F:H1	0.69	2.17	9	1
6:A:208:17F:H49	6:A:208:17F:C39	0.69	2.18	13	3
6:E:808:17F:C18	6:E:810:17F:H18	0.69	2.18	10	2
6:A:213:17F:H47	5:D:507:7Q9:C318	0.69	2.18	11	1
6:A:213:17F:H47	5:D:507:7Q9:C316	0.69	2.16	17	1
5:E:814:7Q9:C39	6:E:820:17F:H49	0.69	2.17	14	3
5:E:841:7Q9:C32	5:E:841:7Q9:C36	0.69	2.70	11	20
6:A:208:17F:N1	6:A:219:17F:O5	0.69	2.22	10	6
6:D:517:17F:O2	6:D:517:17F:H5	0.69	1.86	13	13
2:D:327:GLN:HG3	6:D:534:17F:H56	0.69	1.64	3	2
6:E:873:17F:H29	6:E:873:17F:H19	0.69	1.63	7	3
6:D:519:17F:C38	6:D:519:17F:H52	0.69	2.17	7	1
5:B:205:7Q9:C39	6:B:208:17F:H9A	0.69	2.18	10	2
6:E:802:17F:H40	5:E:805:7Q9:C38	0.69	2.18	10	1
6:D:552:17F:H57	6:D:552:17F:O7	0.69	1.88	17	1
6:D:510:17F:H53	6:D:510:17F:C42	0.69	2.18	20	4
6:D:517:17F:H49	6:D:517:17F:C24	0.69	2.18	3	1
6:A:208:17F:H41	6:A:219:17F:H12A	0.69	1.64	13	2
6:E:808:17F:C34	6:E:820:17F:H29	0.69	2.18	14	4
6:E:856:17F:H68	6:E:856:17F:C22	0.69	2.16	19	6
6:A:213:17F:H53	5:D:503:7Q9:C314	0.69	2.17	8	1
6:E:857:17F:H29	6:E:875:17F:H60	0.69	1.63	8	1
5:A:212:7Q9:C312	5:A:212:7Q9:C38	0.69	2.66	10	2
6:D:519:17F:H52	6:D:519:17F:H77	0.69	1.63	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:220:17F:H38	5:D:502:7Q9:C317	0.69	2.18	9	3
5:D:545:7Q9:C318	5:D:545:7Q9:C314	0.69	2.70	6	20
6:B:208:17F:H1	5:B:209:7Q9:C15	0.69	2.18	5	2
6:A:213:17F:H20A	6:A:213:17F:O9	0.69	1.86	8	4
6:D:520:17F:H41	5:E:841:7Q9:C318	0.69	2.18	3	4
6:E:806:17F:H70	5:E:811:7Q9:C315	0.69	2.17	4	1
6:E:819:17F:C10	6:E:820:17F:H10A	0.69	2.18	4	2
6:E:839:17F:H12	6:E:857:17F:C9	0.69	2.17	4	2
5:B:210:7Q9:C14	6:D:520:17F:H2	0.69	2.18	6	1
6:A:213:17F:H42	6:A:213:17F:H35	0.69	1.65	16	2
6:E:808:17F:C19	6:E:810:17F:H18	0.69	2.18	10	3
6:D:518:17F:H59	6:D:518:17F:H48	0.69	1.62	15	1
6:D:510:17F:H51	6:D:510:17F:H65	0.69	1.62	18	1
6:E:857:17F:H67	6:E:875:17F:H61	0.69	1.63	18	1
6:D:510:17F:H59	6:D:533:17F:H61	0.69	1.64	20	1
6:E:802:17F:H49	6:E:802:17F:C42	0.69	2.18	2	4
6:B:208:17F:H2	6:B:208:17F:O2	0.69	1.87	4	7
6:E:810:17F:N1	6:E:819:17F:O10	0.69	2.26	17	3
6:E:857:17F:C38	6:E:875:17F:H65	0.69	2.17	20	1
5:A:215:7Q9:C318	5:A:215:7Q9:C314	0.69	2.71	2	10
5:E:837:7Q9:C317	5:E:837:7Q9:C313	0.69	2.71	2	20
6:E:873:17F:H59	6:E:873:17F:C25	0.69	2.18	1	8
6:A:213:17F:O1	6:A:213:17F:H19	0.69	1.86	2	3
5:D:545:7Q9:O32	5:D:545:7Q9:C1	0.69	2.41	17	11
6:A:208:17F:H43	6:A:208:17F:C32	0.69	2.17	4	4
1:B:68:ARG:HA	1:B:71:TYR:CZ	0.69	2.23	20	8
6:D:510:17F:H1	6:D:517:17F:C6	0.69	2.18	8	2
6:A:219:17F:C5	6:D:518:17F:H11A	0.68	2.14	1	6
2:D:273:ASP:HB2	6:D:540:17F:C1Z	0.68	2.17	18	13
6:E:802:17F:C35	6:E:802:17F:C31	0.68	2.71	1	12
6:A:219:17F:H6	5:D:505:7Q9:C31	0.68	2.17	19	2
6:B:208:17F:O8	6:B:208:17F:C4	0.68	2.42	11	16
6:E:820:17F:C22	6:E:820:17F:C26	0.68	2.71	13	20
6:E:839:17F:O2	6:E:839:17F:N1	0.68	2.24	14	7
6:E:802:17F:H60	5:E:804:7Q9:C23	0.68	2.18	20	7
6:D:510:17F:H53	6:D:510:17F:H74	0.68	1.65	11	3
6:E:873:17F:O2	6:E:873:17F:H8	0.68	1.89	6	6
6:A:220:17F:H43	5:E:811:7Q9:C318	0.68	2.18	2	1
5:A:212:7Q9:C318	6:E:806:17F:H77	0.68	2.17	4	2
6:E:839:17F:H57	6:E:839:17F:C2X	0.68	2.18	16	5
6:D:510:17F:C9	6:D:517:17F:H30	0.68	2.14	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:839:17F:N1	6:E:875:17F:O8	0.68	2.27	4	6
5:D:515:7Q9:C35	6:D:519:17F:H72	0.68	2.18	15	3
5:E:833:7Q9:C22	6:E:839:17F:H4	0.68	2.17	11	2
5:A:215:7Q9:C312	6:E:829:17F:H53	0.68	2.19	12	2
5:A:205:7Q9:C313	5:A:205:7Q9:C317	0.68	2.71	14	20
5:B:209:7Q9:C316	5:B:209:7Q9:C312	0.68	2.72	20	7
5:E:846:7Q9:C310	5:E:846:7Q9:C314	0.68	2.70	11	20
5:E:848:7Q9:O14	6:E:873:17F:H1A	0.68	1.88	19	2
6:D:520:17F:H75	5:E:823:7Q9:C39	0.68	2.18	3	1
6:D:510:17F:H53	6:D:533:17F:H77	0.68	1.65	6	2
5:E:804:7Q9:C35	5:E:804:7Q9:O22	0.68	2.42	4	3
6:A:219:17F:H75	5:D:505:7Q9:C38	0.68	2.19	6	2
6:E:820:17F:H18A	5:E:830:7Q9:O11	0.68	1.88	7	1
6:D:520:17F:H73	5:E:841:7Q9:C318	0.68	2.19	15	2
6:D:510:17F:H60	6:D:517:17F:H37	0.68	1.65	15	1
5:D:515:7Q9:C31	6:D:519:17F:H19	0.68	2.19	16	2
5:E:846:7Q9:C33	5:E:846:7Q9:C37	0.68	2.72	15	20
6:A:213:17F:H4	6:A:213:17F:O10	0.68	1.88	7	9
6:D:520:17F:H76	5:E:827:7Q9:C317	0.68	2.19	14	3
6:A:219:17F:H6A	6:D:518:17F:C11	0.68	2.16	9	3
6:E:808:17F:H58	6:E:808:17F:H12	0.68	1.66	17	7
6:E:857:17F:O4	6:E:875:17F:H4	0.68	1.89	20	2
6:E:839:17F:H37	5:E:858:7Q9:C310	0.68	2.19	8	2
1:B:17:SER:HB2	3:B:201:GSP:O1A	0.68	1.89	10	1
5:E:803:7Q9:C317	6:E:806:17F:H67	0.68	2.19	10	1
5:A:203:7Q9:C316	6:E:802:17F:H52	0.68	2.18	13	1
5:D:541:7Q9:O21	5:D:541:7Q9:O14	0.68	2.11	4	20
5:E:844:7Q9:C33	5:E:844:7Q9:C37	0.68	2.72	9	20
6:D:518:17F:H76	6:D:518:17F:C30	0.68	2.18	7	1
6:D:511:17F:C30	6:E:829:17F:H52	0.68	2.18	8	1
6:E:802:17F:H33	6:E:802:17F:H36	0.68	1.63	15	1
5:A:214:7Q9:C318	6:E:829:17F:H76	0.68	2.18	19	1
6:D:519:17F:H52	6:D:519:17F:H69	0.68	1.62	7	3
2:E:674:LEU:HD21	6:E:856:17F:H35	0.68	1.65	13	6
6:A:213:17F:H20A	6:A:213:17F:H37	0.68	1.65	4	1
6:B:208:17F:H30	6:B:208:17F:H42	0.68	1.63	9	1
6:D:519:17F:H40	6:D:519:17F:C37	0.68	2.15	10	1
6:D:517:17F:H49	6:D:517:17F:H67	0.68	1.66	13	1
6:E:802:17F:H9A	5:E:803:7Q9:C11	0.68	2.19	20	1
6:D:540:17F:H64	6:D:540:17F:C1X	0.68	2.19	20	13
5:E:841:7Q9:O32	5:E:841:7Q9:C1	0.68	2.42	17	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:845:7Q9:C314	5:E:845:7Q9:C318	0.68	2.72	1	20
6:D:510:17F:H67	6:D:510:17F:H45	0.68	1.63	4	1
5:E:816:7Q9:C31	5:E:816:7Q9:O11	0.68	2.42	8	8
5:B:205:7Q9:C316	6:B:208:17F:H75	0.68	2.19	9	1
5:E:826:7Q9:C35	5:E:826:7Q9:C31	0.67	2.72	20	20
6:A:220:17F:H52	6:A:220:17F:H70	0.67	1.66	2	2
6:D:519:17F:H50	5:D:526:7Q9:C317	0.67	2.19	9	2
6:A:208:17F:H64	6:A:208:17F:C32	0.67	2.19	3	2
6:E:829:17F:H11	5:E:833:7Q9:C38	0.67	2.18	4	3
5:E:838:7Q9:C31	6:E:842:17F:H31	0.67	2.18	4	1
6:D:540:17F:H10	5:D:545:7Q9:C33	0.67	2.19	17	1
1:A:78:PHE:HB2	1:A:111:MET:HG2	0.67	1.65	11	10
1:B:78:PHE:HB2	1:B:111:MET:HG2	0.67	1.67	18	7
6:E:818:17F:H37	6:E:839:17F:H46	0.67	1.66	1	1
6:D:533:17F:H32	6:D:533:17F:C17	0.67	2.18	2	7
6:E:839:17F:H77	6:E:839:17F:H48	0.67	1.65	4	4
6:D:511:17F:H55	6:E:829:17F:H54	0.67	1.66	9	3
6:D:539:17F:H65	6:D:539:17F:C32	0.67	2.09	8	5
3:A:201:GSP:O3G	3:A:201:GSP:O2B	0.67	2.12	7	1
6:D:510:17F:H51	6:D:510:17F:C37	0.67	2.19	17	1
2:D:331:ARG:HA	5:D:538:7Q9:C311	0.67	2.19	15	7
5:D:513:7Q9:C314	5:D:513:7Q9:C310	0.67	2.73	6	20
6:E:818:17F:H5	6:E:818:17F:O8	0.67	1.90	7	15
6:E:875:17F:O1	6:E:875:17F:C6	0.67	2.42	2	9
5:A:205:7Q9:C315	6:E:806:17F:H75	0.67	2.19	20	2
6:A:208:17F:H20A	6:A:219:17F:C10	0.67	2.20	3	1
6:D:510:17F:C17	6:D:533:17F:H20	0.67	2.20	17	2
5:E:834:7Q9:C23	6:E:839:17F:H44	0.67	2.19	15	2
5:D:521:7Q9:C317	5:D:521:7Q9:C313	0.67	2.73	12	20
6:E:819:17F:H49	5:E:836:7Q9:C311	0.67	2.19	10	6
6:E:820:17F:H31	5:E:853:7Q9:C34	0.67	2.19	2	1
6:A:213:17F:H6	5:D:503:7Q9:C14	0.67	2.18	17	1
5:A:216:7Q9:C3	6:D:517:17F:H18A	0.67	2.19	20	2
6:B:208:17F:H64	6:B:208:17F:C30	0.67	2.18	20	1
6:D:510:17F:H49	6:D:517:17F:C38	0.67	2.19	8	7
5:E:830:7Q9:O22	5:E:830:7Q9:P	0.67	2.53	2	13
6:D:511:17F:H61	6:D:511:17F:H12	0.67	1.64	17	4
6:D:518:17F:H60	6:D:518:17F:H44	0.67	1.66	3	1
6:E:808:17F:H71	6:E:819:17F:H54	0.67	1.67	5	1
6:E:819:17F:H48	6:E:819:17F:H78	0.67	1.67	5	1
6:E:857:17F:H37	6:E:875:17F:C34	0.67	2.20	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:H18A	6:D:517:17F:C10	0.67	2.18	13	4
6:A:213:17F:N1	5:D:507:7Q9:O22	0.67	2.28	14	3
5:E:865:7Q9:C315	5:E:865:7Q9:C311	0.67	2.72	8	20
5:E:830:7Q9:O22	5:E:830:7Q9:O11	0.67	2.12	5	12
6:A:220:17F:H36	5:D:502:7Q9:C311	0.67	2.19	20	4
6:A:219:17F:H46	6:A:219:17F:C41	0.67	2.19	5	2
5:B:210:7Q9:O32	6:D:520:17F:H20A	0.67	1.89	9	1
6:D:510:17F:C1Y	6:D:533:17F:H60	0.67	2.20	9	2
5:E:838:7Q9:C32	6:E:842:17F:H44	0.67	2.20	12	1
5:D:543:7Q9:C3	5:D:543:7Q9:O14	0.67	2.43	18	4
6:D:511:17F:H66	6:D:511:17F:C23	0.67	2.19	18	8
6:D:533:17F:C17	6:D:533:17F:H1	0.67	2.20	5	1
1:A:64:TYR:HB3	1:A:67:MET:HB3	0.67	1.67	1	4
6:E:810:17F:H61	6:E:810:17F:C29	0.67	2.18	10	5
6:A:213:17F:C41	6:E:808:17F:H53	0.67	2.18	3	1
6:D:510:17F:H64	6:D:533:17F:H75	0.67	1.65	5	2
5:A:203:7Q9:C36	5:A:203:7Q9:C311	0.67	2.73	7	3
6:D:511:17F:H2	6:D:511:17F:H18A	0.67	1.66	6	3
6:D:510:17F:H1	6:D:517:17F:H5	0.67	1.65	20	1
6:E:842:17F:H4A	6:E:842:17F:C2	0.67	2.20	20	1
1:A:146:ALA:HB3	3:A:201:GSP:N7	0.67	2.05	10	6
6:A:208:17F:N1	6:A:219:17F:O1	0.67	2.28	1	4
3:B:201:GSP:O3G	4:B:202:MG:MG	0.67	1.38	4	20
6:D:540:17F:H68	5:D:545:7Q9:C318	0.67	2.20	4	1
1:A:47:ASP:HA	1:B:128:LYS:HG2	0.67	1.65	5	1
6:D:540:17F:H64	6:D:540:17F:H30	0.67	1.66	20	4
5:B:205:7Q9:C311	6:B:208:17F:H72	0.67	2.20	14	3
6:A:208:17F:H19A	6:A:219:17F:H10	0.67	1.66	11	3
6:D:519:17F:H63	6:D:519:17F:H33	0.67	1.65	10	1
5:D:515:7Q9:C32	6:D:519:17F:H20A	0.67	2.20	18	1
2:E:634:LEU:HB2	5:E:878:7Q9:C315	0.67	2.19	18	1
2:E:660:ARG:HG3	6:E:875:17F:H31	0.67	1.65	7	6
5:D:523:7Q9:C32	6:D:552:17F:H12A	0.67	2.19	5	1
5:D:523:7Q9:O13	6:D:552:17F:N1	0.67	2.28	17	3
1:B:64:TYR:HB3	1:B:67:MET:HB3	0.67	1.67	11	4
6:E:857:17F:C39	6:E:875:17F:H61	0.67	2.16	9	1
6:D:519:17F:H63	6:D:519:17F:C1Z	0.67	2.20	10	1
1:A:47:ASP:HB3	1:B:128:LYS:HG3	0.67	1.67	16	2
6:E:839:17F:H8A	6:E:857:17F:H39	0.67	1.67	16	2
6:D:510:17F:H8A	6:D:517:17F:H34	0.66	1.65	13	8
6:D:510:17F:C8	6:D:517:17F:H9	0.66	2.20	9	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:539:17F:H38	6:D:539:17F:H63	0.66	1.67	14	6
6:E:839:17F:H47	6:E:839:17F:H77	0.66	1.65	1	1
6:E:839:17F:O7	6:E:839:17F:O10	0.66	2.12	12	18
5:E:844:7Q9:C310	5:E:844:7Q9:C314	0.66	2.73	4	20
5:B:210:7Q9:O32	5:B:210:7Q9:C1	0.66	2.43	7	3
5:E:864:7Q9:C22	5:E:864:7Q9:C37	0.66	2.73	17	11
5:E:849:7Q9:C313	5:E:852:7Q9:C38	0.66	2.73	3	11
6:E:820:17F:H61	5:E:837:7Q9:C34	0.66	2.19	5	2
5:E:809:7Q9:C32	6:E:812:17F:H37	0.66	2.21	6	1
5:E:807:7Q9:C14	6:E:818:17F:H4A	0.66	2.20	7	1
6:A:208:17F:H6	6:A:208:17F:O2	0.66	1.90	10	1
6:E:871:17F:H9A	5:E:872:7Q9:P	0.66	2.30	10	2
6:D:511:17F:H53	6:E:829:17F:H54	0.66	1.67	16	2
6:D:518:17F:H6A	6:D:518:17F:O10	0.66	1.89	1	2
5:E:804:7Q9:C31	5:E:804:7Q9:O22	0.66	2.44	5	10
6:D:540:17F:H1	5:D:545:7Q9:C32	0.66	2.19	18	2
6:D:518:17F:H52	5:E:847:7Q9:C317	0.66	2.19	17	4
6:D:540:17F:H8	5:D:545:7Q9:C33	0.66	2.19	4	1
6:E:808:17F:H20	6:E:810:17F:H20	0.66	1.66	11	2
6:E:819:17F:H2	6:E:819:17F:O2	0.66	1.89	19	19
5:E:874:7Q9:C21	5:E:874:7Q9:O32	0.66	2.43	20	15
5:E:858:7Q9:O32	6:E:875:17F:H10A	0.66	1.89	17	2
5:A:216:7Q9:C318	6:D:517:17F:H69	0.66	2.20	12	3
5:B:205:7Q9:O22	6:B:208:17F:N1	0.66	2.24	5	1
6:E:856:17F:H18	5:E:868:7Q9:C12	0.66	2.20	14	3
5:D:531:7Q9:C318	5:D:531:7Q9:C314	0.66	2.73	1	20
6:E:857:17F:C35	6:E:857:17F:H56	0.66	2.20	17	4
5:B:209:7Q9:C315	5:E:823:7Q9:C312	0.66	2.74	12	8
6:E:802:17F:H64	5:E:804:7Q9:C39	0.66	2.20	14	2
6:A:213:17F:C8	6:A:213:17F:C12	0.66	2.72	11	2
6:E:839:17F:H64	6:E:839:17F:C11	0.66	2.21	20	1
5:A:212:7Q9:C35	5:A:212:7Q9:C39	0.66	2.74	18	13
5:D:550:7Q9:C316	5:D:550:7Q9:C312	0.66	2.74	19	20
5:B:205:7Q9:C310	6:B:208:17F:H72	0.66	2.20	8	6
6:D:533:17F:H68	6:D:533:17F:C23	0.66	2.20	3	1
5:A:212:7Q9:C38	5:A:212:7Q9:C313	0.66	2.73	18	5
5:A:211:7Q9:C317	6:A:213:17F:H64	0.66	2.21	14	1
6:B:208:17F:H30	5:B:209:7Q9:C39	0.66	2.20	17	1
5:D:553:7Q9:C318	5:D:553:7Q9:C314	0.66	2.73	11	15
5:E:853:7Q9:O14	5:E:853:7Q9:O21	0.66	2.14	9	9
6:A:213:17F:H34	6:A:213:17F:H40	0.66	1.65	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:C17	6:D:533:17F:C19	0.66	2.74	6	6
6:E:819:17F:H39	5:E:836:7Q9:C37	0.66	2.21	3	3
6:A:208:17F:H38	6:B:208:17F:H60	0.66	1.67	7	1
6:E:818:17F:H35	6:E:818:17F:H41	0.66	1.68	13	4
6:D:533:17F:HN1	6:D:533:17F:H18A	0.66	1.49	17	2
6:A:220:17F:H46	6:A:220:17F:H30	0.66	1.67	20	1
6:D:534:17F:O7	6:D:534:17F:O10	0.66	2.14	2	8
6:A:220:17F:H12	6:A:220:17F:H65	0.66	1.67	2	1
6:E:808:17F:H49	6:E:810:17F:C35	0.66	2.19	20	4
6:E:808:17F:H47	6:E:808:17F:H78	0.66	1.68	14	5
6:E:871:17F:H53	5:E:872:7Q9:C314	0.66	2.20	16	1
5:D:506:7Q9:C32	6:D:517:17F:C1Y	0.66	2.72	2	5
5:E:843:7Q9:C31	5:E:843:7Q9:O22	0.66	2.44	15	19
6:D:510:17F:H55	6:D:517:17F:H38	0.66	1.67	15	2
6:E:873:17F:H55	6:E:873:17F:C33	0.66	2.20	17	7
6:E:808:17F:H49	6:E:810:17F:H65	0.66	1.67	3	1
1:B:118:CYS:SG	1:B:143:GLU:HG2	0.66	2.31	5	1
6:E:871:17F:H11	5:E:872:7Q9:C23	0.66	2.20	5	1
6:A:213:17F:H38	5:D:509:7Q9:C23	0.66	2.20	14	1
6:D:510:17F:O7	6:D:517:17F:H9A	0.66	1.91	1	5
6:D:518:17F:H41	5:D:551:7Q9:C310	0.66	2.20	6	8
1:B:112:VAL:HG21	1:B:159:LEU:HA	0.66	1.67	3	2
6:E:839:17F:H35	6:E:839:17F:C1Z	0.66	2.21	4	3
5:B:205:7Q9:C317	6:B:208:17F:H45	0.66	2.21	5	1
6:E:819:17F:H10	6:E:820:17F:H10A	0.66	1.66	17	4
6:D:518:17F:H19	6:D:518:17F:C10	0.66	2.20	11	1
6:E:806:17F:H6	6:E:806:17F:O1	0.66	1.90	20	1
6:D:534:17F:C24	6:D:534:17F:C28	0.65	2.74	7	17
6:E:856:17F:O10	6:E:856:17F:H6A	0.65	1.90	14	14
5:D:548:7Q9:C3	5:D:548:7Q9:O22	0.65	2.43	7	12
6:B:208:17F:H10A	5:E:823:7Q9:C318	0.65	2.20	9	1
6:A:219:17F:H45	5:D:505:7Q9:C312	0.65	2.21	12	1
6:D:510:17F:H49	6:D:517:17F:H50	0.65	1.65	12	1
5:B:210:7Q9:C315	6:D:520:17F:H76	0.65	2.21	2	1
6:B:208:17F:H47	6:E:812:17F:H70	0.65	1.68	3	1
5:E:838:7Q9:C12	6:E:842:17F:O10	0.65	2.44	7	5
6:A:208:17F:H34	6:A:208:17F:H43	0.65	1.67	6	3
6:D:518:17F:H62	6:D:518:17F:H57	0.65	1.67	8	5
5:B:205:7Q9:C312	6:B:208:17F:H63	0.65	2.21	10	1
6:E:857:17F:H67	6:E:875:17F:C32	0.65	2.22	14	1
6:A:208:17F:C1X	6:B:208:17F:H19	0.65	2.17	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:218:7Q9:C318	6:E:829:17F:H71	0.65	2.21	17	1
2:D:292:GLU:HG2	2:D:296:LYS:HD2	0.65	1.68	18	1
6:D:510:17F:C19	5:D:530:7Q9:O32	0.65	2.44	20	1
1:B:36:ILE:HA	1:B:59:ALA:HB2	0.65	1.68	4	3
5:D:554:7Q9:O32	5:D:554:7Q9:O21	0.65	2.14	17	13
6:E:857:17F:C4	6:E:857:17F:O8	0.65	2.44	15	12
6:D:519:17F:C17	6:D:519:17F:O8	0.65	2.45	17	11
5:D:543:7Q9:C31	6:D:552:17F:H29	0.65	2.21	4	6
6:E:871:17F:C17	6:E:871:17F:O8	0.65	2.44	14	7
6:E:873:17F:H60	6:E:873:17F:H44	0.65	1.68	9	4
5:E:838:7Q9:C32	6:E:842:17F:H55	0.65	2.22	13	4
6:A:213:17F:H11A	6:A:213:17F:H39	0.65	1.68	19	1
6:D:539:17F:C31	6:D:539:17F:C19	0.65	2.70	15	17
6:E:806:17F:C30	6:E:806:17F:C26	0.65	2.73	12	10
6:D:540:17F:H8	5:D:545:7Q9:C36	0.65	2.22	5	1
5:D:524:7Q9:C310	6:D:539:17F:H36	0.65	2.21	15	1
6:E:810:17F:H11A	5:E:811:7Q9:C34	0.65	2.22	19	1
6:D:510:17F:C9	6:D:517:17F:C11	0.65	2.61	2	9
6:E:820:17F:O8	6:E:820:17F:C4	0.65	2.45	20	9
1:B:16:LYS:HB2	3:B:201:GSP:O3B	0.65	1.91	3	2
6:D:510:17F:C6	6:D:517:17F:H11A	0.65	2.21	15	5
1:A:162:GLU:HA	1:A:165:LYS:HE2	0.65	1.68	5	1
5:A:211:7Q9:C312	6:A:213:17F:C35	0.65	2.75	9	1
5:D:542:7Q9:C21	5:D:542:7Q9:C31	0.65	2.75	13	1
6:A:213:17F:C11	6:A:213:17F:C23	0.65	2.74	19	2
6:E:820:17F:H6A	5:E:837:7Q9:C2	0.65	2.22	20	1
5:D:505:7Q9:C31	5:D:505:7Q9:C21	0.65	2.75	2	3
1:A:17:SER:HB2	3:A:201:GSP:O1A	0.65	1.92	6	5
6:E:819:17F:H1A	5:E:838:7Q9:C11	0.65	2.22	6	2
6:A:208:17F:O10	6:A:208:17F:H4	0.65	1.91	7	2
6:E:806:17F:H73	5:E:817:7Q9:C317	0.65	2.20	20	3
6:E:808:17F:C35	6:E:808:17F:H12A	0.65	2.22	17	1
3:A:201:GSP:O3G	4:A:202:MG:MG	0.65	1.40	3	19
2:D:320:GLU:HB3	2:D:321:PRO:HD3	0.65	1.69	18	18
6:D:519:17F:H39	6:D:519:17F:C1X	0.65	2.17	6	11
5:A:215:7Q9:C318	6:D:517:17F:H77	0.65	2.21	11	2
5:E:834:7Q9:O31	6:E:839:17F:H31	0.65	1.92	11	2
6:D:510:17F:C1X	6:D:510:17F:C25	0.65	2.75	12	1
5:D:530:7Q9:O32	5:D:530:7Q9:O21	0.65	2.15	20	16
6:D:534:17F:H38	6:D:534:17F:H69	0.65	1.68	20	5
2:E:671:ARG:HD3	5:E:858:7Q9:C22	0.65	2.22	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:857:17F:O1	6:E:857:17F:N1	0.65	2.26	9	3
5:E:870:7Q9:C14	6:E:873:17F:H8A	0.65	2.22	16	7
5:D:507:7Q9:C313	6:E:819:17F:H52	0.65	2.20	5	3
6:A:208:17F:H19A	6:A:219:17F:H10A	0.65	1.67	7	1
6:E:808:17F:H69	5:E:814:7Q9:C310	0.65	2.21	18	3
5:A:212:7Q9:C31	5:A:212:7Q9:O11	0.65	2.45	15	5
6:A:220:17F:H71	5:E:825:7Q9:C314	0.65	2.21	18	1
6:D:510:17F:H19	5:D:530:7Q9:O32	0.65	1.92	20	1
6:D:520:17F:H35	6:D:520:17F:C24	0.65	2.08	5	13
5:E:803:7Q9:C316	5:E:803:7Q9:C312	0.65	2.75	12	20
6:A:219:17F:H75	5:D:505:7Q9:C37	0.65	2.21	2	2
6:D:510:17F:H9	6:D:517:17F:H8A	0.65	1.66	5	5
5:D:514:7Q9:O13	5:D:514:7Q9:O21	0.65	2.15	8	12
6:D:510:17F:C30	6:D:517:17F:H71	0.65	2.22	12	2
5:D:505:7Q9:C13	6:D:518:17F:C6	0.65	2.72	19	1
6:D:539:17F:O10	6:D:539:17F:H6A	0.65	1.92	1	12
6:D:540:17F:C36	6:D:540:17F:H30	0.65	2.21	7	8
6:E:820:17F:C26	6:E:820:17F:H38	0.65	2.21	13	12
6:D:517:17F:H50	6:D:517:17F:H70	0.65	1.69	2	2
6:E:839:17F:C36	6:E:839:17F:C11	0.65	2.75	20	5
6:A:208:17F:H43	6:A:208:17F:C33	0.65	2.23	4	1
6:E:875:17F:H49	6:E:875:17F:C40	0.65	2.20	17	2
5:E:807:7Q9:C31	5:E:807:7Q9:C21	0.65	2.75	10	6
6:D:510:17F:P1	6:D:517:17F:H4	0.64	2.31	17	7
6:A:208:17F:H49	6:A:208:17F:H70	0.64	1.68	2	4
1:B:82:PHE:HB2	1:B:89:SER:HB2	0.64	1.67	2	4
5:D:503:7Q9:C33	6:D:519:17F:H36	0.64	2.22	3	1
6:D:510:17F:C7	6:D:517:17F:C11	0.64	2.75	15	4
6:D:510:17F:O6	6:D:517:17F:H9	0.64	1.92	4	1
6:D:519:17F:H66	6:D:519:17F:H52	0.64	1.68	4	1
6:D:540:17F:H30	6:D:540:17F:C33	0.64	2.22	4	1
6:E:857:17F:H68	6:E:875:17F:C36	0.64	2.20	20	2
6:D:510:17F:C18	6:D:517:17F:H9A	0.64	2.21	5	4
5:D:512:7Q9:C317	6:D:534:17F:H35	0.64	2.22	5	2
6:E:810:17F:H61	6:E:819:17F:H75	0.64	1.68	5	1
5:B:205:7Q9:C314	6:B:208:17F:H78	0.64	2.21	7	2
6:D:539:17F:H18	6:D:539:17F:C1Z	0.64	2.21	8	1
6:A:208:17F:C1Y	6:A:219:17F:H12A	0.64	2.22	16	3
5:A:205:7Q9:C1	5:A:205:7Q9:O32	0.64	2.44	13	1
2:E:634:LEU:HB2	5:E:878:7Q9:C316	0.64	2.22	7	10
2:E:638:GLN:HB2	5:E:863:7Q9:C312	0.64	2.22	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:539:17F:C19	6:D:539:17F:C31	0.64	2.71	5	3
5:B:205:7Q9:C316	6:B:208:17F:H44	0.64	2.23	14	1
5:D:549:7Q9:O22	5:D:549:7Q9:C3	0.64	2.44	5	17
6:E:806:17F:O9	6:E:806:17F:O8	0.64	2.14	2	19
6:D:534:17F:H37	6:D:534:17F:H66	0.64	1.67	18	6
6:E:820:17F:H58	6:E:820:17F:C25	0.64	2.20	15	4
5:E:835:7Q9:C311	5:E:835:7Q9:C37	0.64	2.75	16	17
6:D:517:17F:H44	6:D:533:17F:H38	0.64	1.68	18	4
5:E:858:7Q9:C310	6:E:875:17F:H51	0.64	2.22	8	3
6:E:808:17F:H19	6:E:810:17F:H18	0.64	1.67	18	4
6:D:510:17F:H49	6:D:517:17F:H71	0.64	1.69	1	6
5:D:542:7Q9:O14	5:D:542:7Q9:O21	0.64	2.15	8	2
5:E:864:7Q9:C35	5:E:864:7Q9:O31	0.64	2.46	11	10
2:D:273:ASP:HB2	6:D:540:17F:H56	0.64	1.69	2	2
6:D:520:17F:H47	6:D:520:17F:H71	0.64	1.69	3	3
6:E:808:17F:H51	6:E:808:17F:H74	0.64	1.69	20	3
6:E:808:17F:H58	6:E:808:17F:C1X	0.64	2.21	4	4
5:E:814:7Q9:C37	6:E:820:17F:H77	0.64	2.23	10	2
6:E:806:17F:H5	5:E:811:7Q9:C14	0.64	2.22	14	1
6:A:219:17F:C35	6:A:219:17F:H56	0.64	2.23	1	2
5:B:207:7Q9:O32	5:B:207:7Q9:C1	0.64	2.46	8	8
6:E:857:17F:H11	6:E:875:17F:H59	0.64	1.67	4	2
5:A:211:7Q9:C36	6:A:220:17F:H57	0.64	2.23	6	1
6:D:518:17F:H20	6:D:518:17F:H39	0.64	1.70	18	4
6:E:819:17F:H78	6:E:819:17F:H48	0.64	1.70	17	1
6:A:219:17F:O10	6:D:518:17F:C11	0.64	2.45	9	10
5:D:524:7Q9:O32	5:D:524:7Q9:C21	0.64	2.46	8	18
6:E:820:17F:O10	6:E:820:17F:C6	0.64	2.45	19	8
5:E:835:7Q9:C314	5:E:835:7Q9:C310	0.64	2.76	15	20
6:E:871:17F:C21	6:E:871:17F:H59	0.64	2.23	3	5
5:E:822:7Q9:C15	5:E:822:7Q9:C1	0.64	2.75	11	14
5:D:549:7Q9:C32	5:D:549:7Q9:C36	0.64	2.76	19	5
6:D:510:17F:H33	6:D:533:17F:H61	0.64	1.68	9	2
6:E:806:17F:O7	6:E:806:17F:O3	0.64	2.16	18	3
1:A:117:LYS:HE2	3:A:201:GSP:C4	0.64	2.27	1	7
6:A:208:17F:O8	6:A:208:17F:O9	0.64	2.16	16	17
6:D:510:17F:C4	6:D:517:17F:C4	0.64	2.76	10	11
6:D:540:17F:H8A	5:D:545:7Q9:C314	0.64	2.22	18	2
6:E:808:17F:H57	6:E:820:17F:H12A	0.64	1.68	7	6
6:E:808:17F:H30	6:E:808:17F:C1Z	0.64	2.22	8	1
1:B:13:GLY:HA2	3:B:201:GSP:H4'	0.64	1.68	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:72:MET:SD	1:B:100:ILE:HA	0.64	2.33	13	1
6:D:539:17F:H70	5:D:549:7Q9:O22	0.64	1.92	14	1
6:E:839:17F:H70	6:E:875:17F:C30	0.64	2.23	14	1
6:A:208:17F:H78	6:B:208:17F:C37	0.64	2.22	15	1
6:E:819:17F:C41	6:E:819:17F:H45	0.64	2.23	16	1
5:E:803:7Q9:O32	6:E:808:17F:H6A	0.64	1.92	20	1
5:D:506:7Q9:C11	5:D:506:7Q9:O21	0.64	2.45	7	2
6:D:510:17F:C42	6:D:517:17F:H72	0.64	2.19	5	3
6:D:520:17F:H42	6:D:520:17F:C2X	0.64	2.11	5	2
2:D:272:TRP:CZ3	6:D:540:17F:H71	0.64	2.28	10	3
2:E:642:SER:H	2:E:643:PRO:HD2	0.64	1.51	10	1
5:E:821:7Q9:C3	6:E:839:17F:H4A	0.64	2.22	11	1
6:A:213:17F:O10	6:A:213:17F:H6A	0.64	1.93	14	1
6:E:839:17F:H49	6:E:839:17F:C42	0.64	2.22	18	2
6:E:819:17F:H30	6:E:819:17F:C23	0.64	2.09	17	1
5:E:805:7Q9:O21	5:E:805:7Q9:O13	0.64	2.16	7	20
5:E:822:7Q9:C14	5:E:826:7Q9:O13	0.64	2.46	11	5
5:D:515:7Q9:C318	6:D:519:17F:H52	0.64	2.23	11	1
6:E:819:17F:H12A	6:E:820:17F:H9A	0.64	1.70	13	1
5:A:217:7Q9:C1	5:A:217:7Q9:C31	0.63	2.77	18	20
6:D:533:17F:O9	6:D:533:17F:O1	0.63	2.16	1	18
6:E:839:17F:O10	6:E:839:17F:C7	0.63	2.46	12	5
6:E:873:17F:H19	6:E:873:17F:C1X	0.63	2.23	3	12
5:E:840:7Q9:C311	5:E:840:7Q9:C36	0.63	2.76	7	6
6:D:510:17F:H53	6:D:533:17F:H55	0.63	1.70	10	2
2:E:631:ARG:HG3	5:E:878:7Q9:C34	0.63	2.24	8	2
5:E:835:7Q9:C318	6:E:856:17F:H70	0.63	2.24	9	4
6:E:808:17F:H38	6:E:810:17F:C20	0.63	2.22	20	2
6:E:839:17F:H8A	6:E:857:17F:H30	0.63	1.70	19	2
6:D:510:17F:H32	6:D:533:17F:H60	0.63	1.69	19	2
5:D:506:7Q9:C31	6:D:517:17F:C20	0.63	2.75	20	2
5:E:850:7Q9:C311	5:E:850:7Q9:C37	0.63	2.75	18	13
6:D:518:17F:H44	6:D:518:17F:C33	0.63	2.23	3	1
5:B:205:7Q9:C316	6:B:208:17F:H65	0.63	2.22	20	5
6:A:219:17F:C34	6:A:219:17F:C38	0.63	2.76	18	5
6:E:808:17F:H32	6:E:819:17F:H11	0.63	1.69	17	1
6:A:208:17F:H37	6:B:208:17F:C19	0.63	2.23	20	1
6:E:806:17F:C26	6:E:806:17F:C30	0.63	2.75	5	10
6:D:534:17F:C28	6:D:534:17F:C24	0.63	2.75	10	3
6:E:839:17F:H12	6:E:857:17F:C1X	0.63	2.24	20	1
5:D:522:7Q9:O21	5:D:522:7Q9:O14	0.63	2.16	2	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:523:7Q9:C34	6:D:552:17F:H40	0.63	2.22	14	3
5:B:210:7Q9:C32	6:D:520:17F:H34	0.63	2.23	2	1
6:A:219:17F:H4A	5:D:505:7Q9:C1	0.63	2.24	3	1
5:E:817:7Q9:O12	5:E:817:7Q9:C3	0.63	2.47	4	7
5:E:852:7Q9:C310	5:E:863:7Q9:C38	0.63	2.76	17	4
1:A:32:TYR:CE1	3:A:201:GSP:H5'2	0.63	2.28	13	4
5:A:214:7Q9:O32	5:A:214:7Q9:C21	0.63	2.46	1	17
6:E:806:17F:C17	6:E:806:17F:O8	0.63	2.46	1	1
6:E:873:17F:H20	6:E:873:17F:C2X	0.63	2.21	4	2
6:E:806:17F:H4	6:E:806:17F:O10	0.63	1.94	2	4
6:B:208:17F:O8	6:B:208:17F:H4A	0.63	1.92	17	12
6:E:808:17F:H55	6:E:819:17F:C41	0.63	2.22	4	1
5:D:523:7Q9:C32	6:D:552:17F:C12	0.63	2.76	5	1
1:B:6:LEU:HD21	1:B:163:ILE:HD11	0.63	1.70	8	1
6:D:539:17F:H72	5:D:549:7Q9:C31	0.63	2.23	15	1
5:A:206:7Q9:C12	5:A:211:7Q9:O22	0.63	2.47	5	3
6:E:819:17F:H46	5:E:836:7Q9:C311	0.63	2.24	10	5
6:D:510:17F:H55	6:D:533:17F:C42	0.63	2.22	16	4
6:E:857:17F:H77	6:E:875:17F:C34	0.63	2.24	14	1
5:B:210:7Q9:C32	6:D:520:17F:H57	0.63	2.23	18	3
5:D:513:7Q9:C36	5:D:532:7Q9:C39	0.63	2.77	19	9
6:E:857:17F:H78	6:E:875:17F:H61	0.63	1.71	12	3
6:E:873:17F:O9	6:E:873:17F:O1	0.63	2.17	16	11
5:B:205:7Q9:C315	6:B:208:17F:H48	0.63	2.24	19	2
6:D:534:17F:H37	6:D:534:17F:C37	0.63	2.24	18	5
6:D:533:17F:H57	6:D:533:17F:H6A	0.63	1.71	11	4
6:E:808:17F:H54	6:E:810:17F:H51	0.63	1.71	8	1
1:A:117:LYS:HG2	3:A:201:GSP:C6	0.63	2.28	9	2
2:E:605:GLN:HG3	5:E:867:7Q9:C313	0.63	2.23	19	6
6:E:819:17F:H60	6:E:842:17F:C36	0.63	2.23	11	2
6:D:510:17F:H57	6:D:533:17F:H34	0.63	1.69	20	1
1:B:13:GLY:HA2	3:B:201:GSP:C5'	0.63	2.22	6	4
5:A:206:7Q9:C317	6:E:802:17F:H69	0.63	2.24	11	1
6:E:839:17F:H73	6:E:875:17F:H53	0.63	1.69	12	1
5:A:203:7Q9:C318	6:E:802:17F:H76	0.63	2.24	15	1
2:D:388:ARG:HD2	2:E:575:LEU:HG	0.63	1.70	19	1
2:E:598:GLN:HB2	2:E:599:PRO:HD3	0.63	1.69	17	8
6:E:812:17F:O10	6:E:812:17F:H6A	0.63	1.92	15	16
5:E:844:7Q9:C21	5:E:844:7Q9:O13	0.63	2.47	3	18
6:B:208:17F:C26	6:B:208:17F:C30	0.63	2.74	3	4
2:E:634:LEU:HD13	5:E:878:7Q9:C316	0.63	2.24	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:803:7Q9:O32	5:E:803:7Q9:C2	0.63	2.45	17	7
6:E:808:17F:C41	6:E:819:17F:H76	0.63	2.23	6	1
6:A:208:17F:H40	6:A:208:17F:C32	0.63	2.24	16	2
1:B:3:GLU:HG2	1:B:52:LEU:HD23	0.63	1.70	12	1
1:B:117:LYS:HE2	3:B:201:GSP:C4	0.62	2.29	18	7
2:E:591:GLU:HG2	5:E:862:7Q9:C37	0.62	2.24	13	10
6:E:839:17F:O8	6:E:857:17F:H39	0.62	1.93	1	1
5:E:851:7Q9:O22	5:E:851:7Q9:C3	0.62	2.45	12	19
5:A:210:7Q9:C313	6:A:220:17F:H10	0.62	2.23	5	1
6:E:802:17F:C28	6:E:802:17F:H77	0.62	2.23	16	4
5:E:825:7Q9:C313	6:E:842:17F:H75	0.62	2.24	9	1
6:B:208:17F:H8A	5:B:209:7Q9:C39	0.62	2.24	13	1
6:E:857:17F:C36	6:E:875:17F:H60	0.62	2.24	18	1
6:D:517:17F:H52	6:E:839:17F:H76	0.62	1.71	20	1
6:E:875:17F:H6	6:E:875:17F:O3	0.62	1.93	20	8
6:E:819:17F:H1	5:E:838:7Q9:C11	0.62	2.23	2	1
5:B:205:7Q9:C37	6:B:208:17F:C40	0.62	2.77	3	1
6:E:839:17F:H38	5:E:858:7Q9:C39	0.62	2.24	17	4
6:E:808:17F:H20A	6:E:819:17F:C7	0.62	2.24	4	1
6:E:802:17F:H50	6:E:802:17F:H77	0.62	1.69	6	1
6:A:208:17F:H30	6:B:208:17F:H32	0.62	1.70	12	1
5:D:503:7Q9:O32	6:D:519:17F:H4	0.62	1.94	13	1
6:A:208:17F:H4	6:A:208:17F:O10	0.62	1.95	14	16
6:E:871:17F:H2	6:E:871:17F:O2	0.62	1.94	19	15
6:D:510:17F:C18	6:D:517:17F:H8	0.62	2.25	7	2
6:D:518:17F:H59	6:D:518:17F:H44	0.62	1.70	15	1
6:D:540:17F:H58	6:D:540:17F:H30	0.62	1.69	18	2
6:E:857:17F:O8	6:E:857:17F:H4	0.62	1.95	12	8
6:E:857:17F:H70	6:E:875:17F:C33	0.62	2.24	11	5
6:B:208:17F:C30	6:B:208:17F:C26	0.62	2.75	2	7
6:D:510:17F:H49	6:D:517:17F:C37	0.62	2.23	6	6
5:E:814:7Q9:C313	6:E:820:17F:H54	0.62	2.25	4	4
6:A:208:17F:HN1	6:A:219:17F:C3	0.62	2.07	10	1
6:D:518:17F:H48	6:D:518:17F:C32	0.62	2.24	15	1
5:D:531:7Q9:C21	5:D:531:7Q9:O14	0.62	2.48	4	14
5:A:215:7Q9:C314	6:E:829:17F:H52	0.62	2.25	7	1
6:E:871:17F:H9A	5:E:872:7Q9:O12	0.62	1.94	10	1
1:A:5:LYS:HA	1:A:54:ASP:HB3	0.62	1.71	12	4
5:D:514:7Q9:C21	5:D:514:7Q9:O12	0.62	2.48	6	5
6:D:519:17F:H52	6:D:519:17F:C38	0.62	2.24	1	8
5:D:536:7Q9:C14	5:D:536:7Q9:O12	0.62	2.47	4	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:849:7Q9:C315	5:E:852:7Q9:C38	0.62	2.78	5	7
5:B:210:7Q9:O31	6:D:520:17F:H20A	0.62	1.94	2	1
5:A:217:7Q9:O32	5:A:217:7Q9:C1	0.62	2.48	10	15
2:D:309:GLN:NE2	6:D:533:17F:H58	0.62	2.10	3	1
6:A:213:17F:H73	6:E:808:17F:C30	0.62	2.22	4	1
6:E:829:17F:N1	5:E:852:7Q9:O14	0.62	2.33	20	3
5:D:550:7Q9:C32	6:D:552:17F:H18	0.62	2.24	5	1
6:A:219:17F:H4	6:A:219:17F:O10	0.62	1.93	19	2
6:E:808:17F:H60	6:E:820:17F:C12	0.62	2.23	19	3
2:D:273:ASP:OD1	6:D:540:17F:H20	0.62	1.95	11	1
6:B:208:17F:H61	6:B:208:17F:C30	0.62	2.24	13	1
6:D:517:17F:H70	6:D:517:17F:H54	0.62	1.70	13	1
5:A:214:7Q9:O32	5:A:214:7Q9:O21	0.62	2.18	14	8
5:E:849:7Q9:C34	5:E:852:7Q9:O31	0.62	2.47	20	7
6:A:208:17F:H54	6:A:208:17F:H71	0.62	1.69	12	2
6:A:208:17F:C42	6:B:208:17F:H69	0.62	2.25	15	2
6:A:219:17F:C38	6:A:219:17F:C34	0.62	2.75	10	11
2:E:631:ARG:HG2	5:E:878:7Q9:C37	0.62	2.24	15	9
6:E:819:17F:H32	6:E:819:17F:O9	0.62	1.95	1	7
5:E:830:7Q9:O22	5:E:830:7Q9:C3	0.62	2.45	18	6
6:A:219:17F:H31	5:E:801:7Q9:C32	0.62	2.24	4	1
5:E:803:7Q9:O13	6:E:808:17F:N1	0.62	2.32	5	3
5:A:203:7Q9:C315	6:A:208:17F:H74	0.62	2.25	8	1
6:D:510:17F:H1A	6:D:517:17F:O1	0.62	1.95	20	1
5:A:217:7Q9:O22	5:A:217:7Q9:C3	0.62	2.46	7	17
5:E:817:7Q9:C3	5:E:817:7Q9:P	0.62	2.88	15	20
6:D:510:17F:C17	6:D:517:17F:H9A	0.62	2.24	3	6
6:D:510:17F:H66	5:D:530:7Q9:C317	0.62	2.25	5	2
5:E:849:7Q9:C22	5:E:853:7Q9:O12	0.62	2.48	7	2
6:A:219:17F:H39	6:A:219:17F:C12	0.62	2.25	6	2
6:A:208:17F:H34	6:A:208:17F:C23	0.62	2.25	19	4
6:D:518:17F:H30	6:D:518:17F:O2	0.62	1.95	11	1
6:D:539:17F:H72	5:D:549:7Q9:O32	0.62	1.95	15	1
2:D:269:GLN:HG2	6:D:540:17F:H32	0.62	1.69	17	3
6:D:539:17F:H48	5:D:549:7Q9:C23	0.62	2.24	1	2
2:E:708:LYS:HB2	2:E:709:PRO:HD3	0.62	1.72	12	17
6:D:510:17F:H9	6:D:517:17F:C8	0.62	2.23	2	4
5:B:209:7Q9:C318	5:E:824:7Q9:C310	0.62	2.78	3	1
2:D:440:LEU:HD11	5:D:543:7Q9:C313	0.62	2.25	3	3
6:D:533:17F:H1	6:D:533:17F:C18	0.62	2.24	5	1
6:A:208:17F:H40	6:A:208:17F:C1Z	0.62	2.24	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:519:17F:H40	6:D:519:17F:H62	0.62	1.72	11	1
6:E:818:17F:H11	5:E:834:7Q9:C33	0.62	2.25	20	2
6:A:208:17F:H19	5:A:212:7Q9:C34	0.62	2.24	19	1
6:D:552:17F:C17	6:D:552:17F:C1Y	0.61	2.78	17	19
6:D:511:17F:C3	5:D:532:7Q9:C12	0.61	2.78	3	2
2:D:269:GLN:CG	6:D:540:17F:H32	0.61	2.25	5	6
5:D:523:7Q9:C34	6:D:552:17F:H12A	0.61	2.24	5	1
1:A:46:ILE:HD13	1:A:157:TYR:HA	0.61	1.70	12	2
6:E:839:17F:H11	6:E:839:17F:H57	0.61	1.72	17	3
6:E:842:17F:H29	6:E:842:17F:C23	0.61	2.22	12	8
5:E:858:7Q9:C3	6:E:875:17F:C10	0.61	2.77	3	4
5:D:503:7Q9:C311	6:D:519:17F:H44	0.61	2.25	20	3
5:D:537:7Q9:O32	5:D:537:7Q9:C1	0.61	2.49	12	2
6:A:219:17F:H56	6:D:518:17F:H38	0.61	1.69	5	2
6:D:510:17F:H56	6:D:533:17F:H61	0.61	1.69	6	2
6:D:510:17F:C1X	6:D:517:17F:H8	0.61	2.25	18	2
5:E:825:7Q9:C318	6:E:842:17F:H68	0.61	2.25	7	2
5:D:523:7Q9:C21	5:D:523:7Q9:O32	0.61	2.48	17	15
6:A:220:17F:H37	5:D:502:7Q9:C312	0.61	2.25	19	3
6:E:820:17F:C7	6:E:820:17F:C4	0.61	2.78	5	5
6:E:857:17F:O10	6:E:857:17F:H6A	0.61	1.93	17	14
5:D:512:7Q9:C33	6:D:534:17F:H4	0.61	2.25	4	1
6:E:806:17F:H70	5:E:817:7Q9:C318	0.61	2.25	13	7
6:A:213:17F:H1	5:D:507:7Q9:C3	0.61	2.25	7	1
5:E:868:7Q9:C21	5:E:868:7Q9:O32	0.61	2.49	7	5
5:B:204:7Q9:C37	5:B:204:7Q9:C311	0.61	2.78	14	1
1:A:111:MET:HB3	1:A:139:ILE:HG21	0.61	1.72	16	1
5:A:218:7Q9:C13	6:D:511:17F:H4A	0.61	2.25	17	1
5:E:845:7Q9:C15	5:E:845:7Q9:O12	0.61	2.48	6	20
5:E:849:7Q9:O21	5:E:849:7Q9:O32	0.61	2.18	7	19
6:E:818:17F:H4	6:E:818:17F:O10	0.61	1.95	15	9
6:E:839:17F:C10	6:E:857:17F:H35	0.61	2.26	5	3
6:A:208:17F:N1	6:A:219:17F:C3	0.61	2.63	10	1
6:D:510:17F:H48	6:D:510:17F:H60	0.61	1.72	19	1
2:E:620:GLU:HB3	2:E:621:PRO:HD3	0.61	1.70	1	17
5:E:801:7Q9:O22	5:E:801:7Q9:O11	0.61	2.19	17	17
6:E:819:17F:H47	6:E:819:17F:C42	0.61	2.25	2	1
6:D:510:17F:H75	6:E:857:17F:H48	0.61	1.73	3	1
6:A:213:17F:H46	6:A:213:17F:C34	0.61	2.24	8	3
5:D:513:7Q9:C38	6:D:534:17F:H64	0.61	2.25	9	1
6:E:810:17F:HN1A	6:E:819:17F:H6	0.61	1.55	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:543:7Q9:C317	6:E:871:17F:H52	0.61	2.25	19	2
5:D:514:7Q9:C311	5:D:514:7Q9:C37	0.61	2.78	18	1
6:A:213:17F:H9	5:D:503:7Q9:C22	0.61	2.26	1	1
5:D:542:7Q9:C1	5:D:553:7Q9:C3	0.61	2.79	1	2
5:D:545:7Q9:C1	5:D:545:7Q9:C31	0.61	2.78	1	18
5:D:556:7Q9:C31	5:D:556:7Q9:O22	0.61	2.49	2	15
6:D:510:17F:C30	6:D:533:17F:H77	0.61	2.26	6	2
6:E:808:17F:C33	6:E:808:17F:H12	0.61	2.25	14	2
6:A:213:17F:H68	6:A:213:17F:H51	0.61	1.71	16	1
6:A:208:17F:H43	6:A:208:17F:H33	0.61	1.72	18	1
5:A:211:7Q9:C15	5:A:211:7Q9:O12	0.61	2.48	20	20
6:D:518:17F:C20	6:D:518:17F:C2X	0.61	2.79	12	10
6:E:873:17F:C20	6:E:873:17F:H39	0.61	2.26	15	6
6:A:219:17F:H71	5:D:505:7Q9:C37	0.61	2.26	4	5
6:E:871:17F:H9A	5:E:872:7Q9:C23	0.61	2.25	6	1
6:D:510:17F:C19	6:D:533:17F:H19A	0.61	2.25	7	1
6:E:842:17F:H39	6:E:842:17F:C1X	0.61	2.20	12	6
6:A:213:17F:C20	6:A:213:17F:H12	0.61	2.26	15	1
6:E:820:17F:H75	5:E:853:7Q9:C36	0.61	2.26	15	1
6:A:213:17F:H74	6:E:810:17F:H53	0.61	1.72	17	1
6:A:220:17F:H72	5:D:515:7Q9:C317	0.61	2.26	18	1
5:A:204:7Q9:O22	5:A:204:7Q9:O11	0.61	2.19	4	18
6:A:219:17F:C35	6:A:219:17F:C31	0.61	2.79	11	3
1:B:68:ARG:HA	1:B:71:TYR:CE1	0.61	2.31	1	4
5:D:526:7Q9:O14	5:D:526:7Q9:O21	0.61	2.19	4	19
6:D:540:17F:O8	6:D:540:17F:O9	0.61	2.19	2	13
5:D:556:7Q9:C15	5:D:556:7Q9:O12	0.61	2.48	3	20
5:E:849:7Q9:C34	5:E:852:7Q9:C31	0.61	2.79	8	6
6:E:829:17F:H39	6:E:829:17F:H11A	0.61	1.72	12	4
5:E:846:7Q9:C2	5:E:846:7Q9:O32	0.61	2.47	17	16
6:A:219:17F:H20	5:E:801:7Q9:C32	0.61	2.25	3	1
6:E:806:17F:H29	6:E:806:17F:H39	0.61	1.72	14	3
6:A:208:17F:H8A	6:B:208:17F:O2	0.61	1.95	6	1
1:A:149:ARG:HG2	1:A:152:VAL:HG21	0.61	1.73	7	1
5:A:210:7Q9:C316	6:A:220:17F:H49	0.61	2.25	11	1
1:A:59:ALA:HB3	1:A:64:TYR:HE2	0.61	1.55	14	1
1:B:19:LEU:HD23	1:B:146:ALA:HB2	0.61	1.71	18	1
6:D:510:17F:H59	6:D:533:17F:C34	0.61	2.25	20	1
5:A:210:7Q9:O22	5:A:210:7Q9:C3	0.61	2.46	16	17
6:D:534:17F:H60	6:D:534:17F:H10A	0.61	1.73	17	12
5:E:804:7Q9:O22	5:E:804:7Q9:O31	0.61	2.19	5	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:209:7Q9:O22	5:B:209:7Q9:O11	0.61	2.19	19	17
6:D:539:17F:H63	6:D:539:17F:C22	0.61	2.25	3	4
6:E:819:17F:H59	6:E:819:17F:C36	0.61	2.24	13	6
6:E:819:17F:H12A	6:E:820:17F:C1X	0.61	2.25	3	1
6:D:510:17F:C4	6:D:510:17F:O10	0.61	2.48	10	4
5:D:543:7Q9:C32	6:D:552:17F:H37	0.61	2.26	4	1
5:A:207:7Q9:C33	5:A:216:7Q9:C23	0.61	2.79	7	2
5:D:529:7Q9:C3	5:D:541:7Q9:O22	0.61	2.49	5	3
5:B:205:7Q9:C316	6:B:208:17F:H77	0.61	2.25	10	2
5:E:848:7Q9:O14	6:E:873:17F:N1	0.61	2.33	7	2
6:E:818:17F:O10	5:E:821:7Q9:C13	0.61	2.48	16	4
6:D:520:17F:H78	5:E:841:7Q9:C318	0.61	2.25	14	2
6:E:810:17F:H31	6:E:819:17F:H63	0.61	1.73	17	1
6:E:829:17F:H12	5:E:833:7Q9:C35	0.61	2.25	18	1
6:E:839:17F:H40	6:E:839:17F:H33	0.61	1.73	8	3
6:D:533:17F:H40	6:D:533:17F:H72	0.61	1.70	7	3
3:A:201:GSP:O1B	3:A:201:GSP:S1G	0.61	2.59	17	6
5:E:834:7Q9:C15	6:E:856:17F:H2	0.61	2.25	14	3
6:E:839:17F:H9A	6:E:839:17F:C34	0.61	2.26	14	6
6:D:540:17F:H30	6:D:540:17F:C36	0.61	2.25	20	3
5:E:805:7Q9:C3	6:E:812:17F:H31	0.61	2.26	13	2
6:E:819:17F:C33	6:E:842:17F:H65	0.61	2.25	19	2
5:D:513:7Q9:C15	5:D:513:7Q9:O12	0.60	2.48	13	20
6:E:839:17F:H77	6:E:839:17F:C27	0.60	2.26	1	3
5:E:846:7Q9:O22	5:E:846:7Q9:O11	0.60	2.19	20	16
5:B:210:7Q9:C1	5:B:210:7Q9:C31	0.60	2.79	4	4
6:E:819:17F:H65	6:E:819:17F:C32	0.60	2.26	2	6
5:D:524:7Q9:O32	5:D:524:7Q9:O21	0.60	2.18	5	9
6:D:511:17F:H8A	5:D:513:7Q9:C12	0.60	2.26	4	1
6:A:213:17F:H37	5:D:509:7Q9:C22	0.60	2.25	6	1
6:E:829:17F:H36	6:E:829:17F:H58	0.60	1.73	8	3
6:E:808:17F:H18A	6:E:810:17F:H18	0.60	1.71	10	1
5:B:205:7Q9:C311	6:B:208:17F:H10A	0.60	2.26	8	5
5:E:851:7Q9:C35	6:E:871:17F:C20	0.60	2.80	6	5
6:B:208:17F:H10	5:B:209:7Q9:C34	0.60	2.26	4	1
6:D:534:17F:H72	5:E:863:7Q9:C317	0.60	2.27	17	2
5:D:507:7Q9:O32	5:D:507:7Q9:O21	0.60	2.19	18	15
6:E:802:17F:C42	6:E:802:17F:H49	0.60	2.26	11	3
6:E:839:17F:C1Z	6:E:839:17F:C23	0.60	2.79	8	11
6:E:802:17F:H77	6:E:802:17F:C28	0.60	2.24	2	2
5:D:503:7Q9:C36	6:D:519:17F:H56	0.60	2.26	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:208:17F:H34	6:A:208:17F:C26	0.60	2.23	7	1
6:A:213:17F:C42	6:E:808:17F:H53	0.60	2.24	17	2
6:A:219:17F:H66	6:D:518:17F:H43	0.60	1.71	7	1
5:B:205:7Q9:C318	6:E:812:17F:H77	0.60	2.25	14	1
5:E:837:7Q9:O22	5:E:853:7Q9:C13	0.60	2.49	16	1
6:D:511:17F:O10	6:D:511:17F:C4	0.60	2.47	7	6
6:D:519:17F:H57	6:D:519:17F:H40	0.60	1.71	16	7
5:E:813:7Q9:C14	5:E:813:7Q9:O12	0.60	2.49	1	20
6:E:839:17F:H19	6:E:839:17F:C31	0.60	2.23	2	10
1:A:68:ARG:HA	1:A:71:TYR:CZ	0.60	2.31	11	8
5:A:215:7Q9:C12	6:D:511:17F:H5	0.60	2.26	3	1
6:A:220:17F:H37	5:D:502:7Q9:C311	0.60	2.26	15	3
6:D:520:17F:H71	5:E:841:7Q9:C318	0.60	2.25	5	3
6:E:819:17F:H47	6:E:819:17F:H77	0.60	1.73	3	1
6:A:213:17F:H39	6:A:213:17F:C33	0.60	2.26	7	1
1:B:32:TYR:CE2	3:B:201:GSP:H5'2	0.60	2.31	8	1
2:E:555:SER:N	6:E:873:17F:H68	0.60	2.11	9	4
6:D:552:17F:H41	6:D:552:17F:H66	0.60	1.73	10	2
6:A:208:17F:H72	6:B:208:17F:H68	0.60	1.73	20	1
5:B:207:7Q9:C14	5:B:207:7Q9:O12	0.60	2.50	5	20
5:B:209:7Q9:C316	5:E:823:7Q9:C312	0.60	2.79	7	3
6:D:520:17F:H4	6:D:520:17F:O10	0.60	1.97	6	6
5:E:821:7Q9:C2	6:E:839:17F:H18	0.60	2.26	6	1
5:E:822:7Q9:C22	5:E:826:7Q9:C35	0.60	2.80	9	6
5:A:205:7Q9:C316	6:E:806:17F:H75	0.60	2.26	7	1
1:B:15:GLY:O	1:B:19:LEU:HG	0.60	1.95	17	2
6:E:808:17F:H20	6:E:810:17F:C20	0.60	2.27	11	2
6:D:540:17F:H65	6:D:540:17F:C1X	0.60	2.26	18	1
5:D:516:7Q9:O11	5:D:516:7Q9:C31	0.60	2.50	11	10
5:D:528:7Q9:O12	5:D:528:7Q9:C13	0.60	2.49	19	20
5:E:844:7Q9:C22	5:E:845:7Q9:C14	0.60	2.80	6	5
5:D:525:7Q9:C21	5:D:525:7Q9:O32	0.60	2.49	7	12
5:A:210:7Q9:O13	6:A:220:17F:N1	0.60	2.34	16	2
5:D:521:7Q9:C31	5:D:521:7Q9:O11	0.60	2.50	17	4
6:E:842:17F:H4A	6:E:842:17F:O4	0.60	1.96	16	1
6:D:519:17F:H58	6:D:519:17F:C36	0.60	2.10	17	1
5:E:870:7Q9:C11	6:E:873:17F:H8A	0.60	2.25	19	1
5:D:524:7Q9:C15	6:D:539:17F:O5	0.60	2.50	2	4
5:E:817:7Q9:C3	5:E:817:7Q9:O12	0.60	2.50	20	12
5:E:868:7Q9:C3	5:E:868:7Q9:O22	0.60	2.48	8	10
5:A:212:7Q9:O22	5:A:212:7Q9:C3	0.60	2.47	8	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:220:17F:H12	6:A:220:17F:C36	0.60	2.25	2	2
2:E:736:TYR:HD1	5:E:876:7Q9:C310	0.60	2.09	4	7
6:E:808:17F:H30	6:E:808:17F:C32	0.60	2.25	7	6
5:E:845:7Q9:C311	5:E:845:7Q9:C37	0.60	2.79	11	11
6:D:533:17F:H42	5:D:541:7Q9:C313	0.60	2.26	7	2
1:A:68:ARG:HA	1:A:71:TYR:CE1	0.60	2.32	6	3
6:D:511:17F:H2	6:D:511:17F:C18	0.60	2.26	6	2
5:A:203:7Q9:O32	6:A:208:17F:H12A	0.60	1.97	7	1
6:A:219:17F:H76	5:D:505:7Q9:C316	0.60	2.27	9	4
5:B:205:7Q9:C310	6:B:208:17F:H11	0.60	2.27	14	2
6:A:208:17F:H64	6:A:208:17F:H45	0.60	1.72	17	1
1:A:37:GLU:HG2	1:A:56:LEU:HD11	0.60	1.72	20	4
5:D:505:7Q9:O32	5:D:505:7Q9:O21	0.60	2.20	6	11
1:A:81:VAL:HG12	1:A:114:VAL:HB	0.60	1.72	2	1
5:B:205:7Q9:C316	6:B:208:17F:H71	0.60	2.27	10	3
6:B:208:17F:H48	6:E:812:17F:H70	0.60	1.73	3	1
2:D:400:LEU:HG	5:D:548:7Q9:C312	0.60	2.26	3	2
6:D:552:17F:H41	6:D:552:17F:C37	0.60	2.26	10	1
6:E:810:17F:H31	6:E:819:17F:C35	0.60	2.26	17	1
5:A:204:7Q9:C31	5:A:204:7Q9:C21	0.60	2.78	18	1
5:B:203:7Q9:O12	5:B:203:7Q9:C15	0.60	2.50	13	20
6:D:540:17F:H30	6:D:540:17F:H65	0.60	1.74	7	4
5:E:832:7Q9:C3	5:E:832:7Q9:O22	0.60	2.47	20	12
6:E:871:17F:H58	6:E:871:17F:C2X	0.60	2.26	6	10
6:E:871:17F:O10	6:E:871:17F:C6	0.60	2.46	15	6
5:B:205:7Q9:C316	6:E:812:17F:H75	0.60	2.26	12	1
5:D:549:7Q9:C14	5:D:549:7Q9:O12	0.60	2.50	1	20
6:E:812:17F:O10	6:E:812:17F:C6	0.60	2.47	8	15
5:E:841:7Q9:O22	5:E:841:7Q9:C3	0.60	2.45	11	18
5:B:206:7Q9:C310	6:B:208:17F:H74	0.60	2.27	15	3
6:E:818:17F:H20	5:E:834:7Q9:O32	0.60	1.97	4	1
6:E:819:17F:H10A	6:E:820:17F:C1X	0.60	2.05	4	3
5:E:851:7Q9:C316	6:E:871:17F:H61	0.60	2.26	5	1
6:A:208:17F:H78	6:B:208:17F:H67	0.60	1.73	15	1
5:D:549:7Q9:C11	5:D:551:7Q9:C23	0.60	2.79	18	1
5:A:211:7Q9:C313	5:A:211:7Q9:C38	0.59	2.80	11	6
5:A:215:7Q9:O22	5:A:215:7Q9:C3	0.59	2.47	11	6
6:E:871:17F:H35	6:E:871:17F:H58	0.59	1.74	2	8
5:A:203:7Q9:C3	5:A:203:7Q9:O22	0.59	2.48	2	13
5:E:853:7Q9:C3	5:E:853:7Q9:C12	0.59	2.80	6	5
6:E:856:17F:H29	6:E:856:17F:C33	0.59	2.27	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:220:17F:H52	6:A:220:17F:C33	0.59	2.27	6	1
5:E:825:7Q9:C35	6:E:842:17F:H34	0.59	2.27	7	2
5:E:849:7Q9:C34	5:E:852:7Q9:C33	0.59	2.80	7	2
6:E:806:17F:H46	6:E:806:17F:H72	0.59	1.71	11	1
6:E:873:17F:H20	6:E:873:17F:C23	0.59	2.27	11	7
5:E:803:7Q9:C31	6:E:810:17F:H18A	0.59	2.26	12	2
5:E:860:7Q9:O32	5:E:860:7Q9:C21	0.59	2.50	4	17
6:D:510:17F:H5	6:D:533:17F:C20	0.59	2.27	2	2
6:D:510:17F:H10A	6:D:517:17F:H34	0.59	1.73	2	3
6:D:510:17F:H49	6:D:517:17F:H68	0.59	1.74	7	4
6:E:829:17F:H37	5:E:830:7Q9:C318	0.59	2.27	5	1
6:D:519:17F:H51	5:D:526:7Q9:C318	0.59	2.27	8	1
6:D:510:17F:H43	6:D:510:17F:H30	0.59	1.72	12	1
5:E:817:7Q9:O32	5:E:817:7Q9:O12	0.59	2.20	12	1
5:A:211:7Q9:C22	6:A:213:17F:H33	0.59	2.27	20	1
5:D:508:7Q9:O12	5:D:508:7Q9:C14	0.59	2.50	4	20
6:A:208:17F:H77	6:A:208:17F:H54	0.59	1.74	11	2
6:E:820:17F:H31	5:E:853:7Q9:C35	0.59	2.27	2	1
6:E:839:17F:H18A	6:E:839:17F:C32	0.59	2.26	2	2
6:A:213:17F:H12	6:A:213:17F:C20	0.59	2.28	16	3
6:A:220:17F:H50	5:E:811:7Q9:C318	0.59	2.27	5	3
6:D:510:17F:H5	6:D:533:17F:C18	0.59	2.28	14	3
6:D:511:17F:H43	5:D:513:7Q9:C316	0.59	2.27	17	1
6:A:213:17F:H20A	6:A:213:17F:H38	0.59	1.75	20	2
5:D:532:7Q9:C39	5:D:532:7Q9:C22	0.59	2.80	18	19
5:E:813:7Q9:C13	5:E:817:7Q9:C22	0.59	2.80	10	9
5:A:206:7Q9:C318	6:E:802:17F:H68	0.59	2.27	2	1
5:D:538:7Q9:C21	5:D:538:7Q9:O32	0.59	2.50	19	10
6:A:208:17F:H68	6:A:208:17F:C23	0.59	2.26	3	1
6:D:510:17F:C27	6:D:517:17F:H37	0.59	2.27	19	3
6:D:511:17F:H76	6:E:829:17F:H50	0.59	1.74	3	1
5:E:834:7Q9:O13	6:E:839:17F:H20A	0.59	1.97	3	1
5:A:216:7Q9:C34	6:D:517:17F:H31	0.59	2.28	12	1
6:E:812:17F:H45	6:E:812:17F:H77	0.59	1.74	12	1
5:A:212:7Q9:C313	6:A:219:17F:H54	0.59	2.27	16	1
6:D:517:17F:C27	6:D:517:17F:C23	0.59	2.78	10	14
6:D:540:17F:H4	6:D:540:17F:O10	0.59	1.95	9	12
6:D:552:17F:H2	6:D:552:17F:O1	0.59	1.98	7	11
5:E:811:7Q9:C15	5:E:811:7Q9:O12	0.59	2.51	20	20
6:A:208:17F:H43	6:A:208:17F:H34	0.59	1.75	2	2
5:A:215:7Q9:C21	5:A:215:7Q9:O32	0.59	2.51	2	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:E:555:SER:OG	6:E:873:17F:H65	0.59	1.98	14	2
6:E:802:17F:C31	6:E:802:17F:C35	0.59	2.66	3	6
2:E:656:VAL:HG13	6:E:857:17F:H64	0.59	1.74	20	5
5:D:523:7Q9:C313	6:D:552:17F:H38	0.59	2.28	5	1
5:E:831:7Q9:C315	6:E:871:17F:H46	0.59	2.28	5	1
6:E:839:17F:C31	6:E:839:17F:H35	0.59	2.28	16	6
6:D:539:17F:H73	5:D:549:7Q9:O32	0.59	1.97	9	1
6:A:220:17F:H66	6:A:220:17F:C23	0.59	2.26	12	1
5:B:205:7Q9:C315	6:E:812:17F:H70	0.59	2.27	15	2
5:D:512:7Q9:C34	6:D:534:17F:H6A	0.59	2.27	20	1
5:A:216:7Q9:O32	5:A:216:7Q9:O21	0.59	2.21	5	15
5:D:509:7Q9:O22	5:D:509:7Q9:C3	0.59	2.44	16	19
5:D:512:7Q9:C13	5:D:512:7Q9:O12	0.59	2.51	19	20
5:D:531:7Q9:O12	5:D:531:7Q9:C14	0.59	2.50	18	20
5:E:821:7Q9:O32	5:E:821:7Q9:O21	0.59	2.21	10	10
5:A:205:7Q9:C3	5:A:205:7Q9:O22	0.59	2.47	2	11
5:D:543:7Q9:C2	5:D:543:7Q9:O32	0.59	2.48	13	9
2:E:634:LEU:HB2	5:E:878:7Q9:C317	0.59	2.27	13	7
5:E:860:7Q9:O32	5:E:860:7Q9:O21	0.59	2.19	2	7
5:E:814:7Q9:C37	6:E:820:17F:H36	0.59	2.28	3	3
5:E:848:7Q9:O31	6:E:873:17F:N1	0.59	2.35	3	3
6:A:208:17F:C38	6:B:208:17F:H69	0.59	2.27	4	1
5:D:515:7Q9:C318	6:D:519:17F:H68	0.59	2.28	4	2
6:E:839:17F:H5	6:E:839:17F:O2	0.59	1.98	18	5
6:A:208:17F:H68	6:A:208:17F:C26	0.59	2.23	5	1
6:E:839:17F:C42	6:E:839:17F:C27	0.59	2.80	5	1
5:E:807:7Q9:C13	6:E:818:17F:H4A	0.59	2.27	6	1
1:B:46:ILE:HG23	1:B:157:TYR:HD1	0.59	1.57	7	1
6:E:819:17F:H40	6:E:820:17F:C23	0.59	2.26	12	1
6:A:208:17F:C25	6:A:219:17F:H12A	0.59	2.28	20	1
6:A:213:17F:H45	6:A:213:17F:C2X	0.59	2.26	8	5
5:D:509:7Q9:O12	5:D:509:7Q9:C13	0.59	2.51	15	20
5:D:542:7Q9:O21	5:D:542:7Q9:O12	0.59	2.21	15	8
6:E:808:17F:H58	6:E:808:17F:C12	0.59	2.28	4	6
6:A:208:17F:H40	6:A:208:17F:H58	0.59	1.74	9	2
6:E:873:17F:H56	6:E:873:17F:H39	0.59	1.74	19	4
6:E:839:17F:C1Z	6:E:839:17F:H39	0.59	2.28	19	2
5:A:204:7Q9:C14	5:A:204:7Q9:O12	0.59	2.51	11	20
6:B:208:17F:H4A	6:B:208:17F:C7	0.59	2.27	7	16
6:E:857:17F:H5	6:E:857:17F:O1	0.59	1.97	4	7
1:B:68:ARG:HG2	1:B:72:MET:HE3	0.59	1.75	18	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:540:17F:H30	6:D:540:17F:C32	0.59	2.27	4	2
6:D:520:17F:H76	5:E:827:7Q9:C318	0.59	2.28	6	1
6:D:510:17F:C19	6:D:533:17F:C19	0.59	2.80	7	1
5:E:803:7Q9:C32	6:E:810:17F:H18A	0.59	2.28	14	4
6:A:219:17F:H6A	6:D:518:17F:H9	0.59	1.74	16	3
6:D:510:17F:H48	6:D:510:17F:C33	0.59	2.28	19	1
5:A:205:7Q9:O12	5:A:205:7Q9:C14	0.59	2.51	6	20
2:E:623:ARG:HB2	5:E:859:7Q9:C313	0.59	2.27	12	10
5:E:847:7Q9:C3	5:E:847:7Q9:O22	0.59	2.47	9	13
5:E:850:7Q9:C21	5:E:850:7Q9:O32	0.59	2.51	1	10
6:D:510:17F:O6	6:D:517:17F:H6	0.59	1.98	14	4
6:E:819:17F:H65	6:E:819:17F:H59	0.59	1.73	2	1
6:D:533:17F:H42	5:D:541:7Q9:C310	0.59	2.27	4	2
5:D:541:7Q9:C1	5:D:541:7Q9:C14	0.59	2.81	10	6
6:E:810:17F:C1Z	6:E:819:17F:H63	0.59	2.27	4	1
6:E:802:17F:H42	6:E:802:17F:H35	0.59	1.75	5	5
6:D:511:17F:H77	6:D:511:17F:C28	0.59	2.27	9	3
5:E:817:7Q9:C311	5:E:826:7Q9:C313	0.59	2.81	7	2
6:E:839:17F:H57	6:E:839:17F:H35	0.59	1.73	10	3
6:A:213:17F:H40	6:A:213:17F:H61	0.59	1.73	15	1
5:D:537:7Q9:C13	5:D:537:7Q9:O12	0.59	2.51	8	20
6:D:510:17F:C11	6:D:517:17F:H8A	0.59	2.28	10	5
6:A:219:17F:C1Y	5:E:801:7Q9:C32	0.59	2.81	4	1
6:E:839:17F:H37	5:E:858:7Q9:C39	0.59	2.28	8	2
2:D:275:LEU:HG	2:E:688:ARG:HD2	0.59	1.75	13	2
2:E:630:ALA:HB1	5:E:878:7Q9:C314	0.59	2.28	17	1
5:E:858:7Q9:C3	6:E:875:17F:H10	0.59	2.27	17	1
6:E:802:17F:H39	5:E:805:7Q9:C38	0.59	2.28	18	1
5:A:205:7Q9:C21	5:A:205:7Q9:O32	0.59	2.51	19	1
6:A:220:17F:H4	6:A:220:17F:O10	0.58	1.97	20	4
5:D:521:7Q9:C14	5:D:521:7Q9:O12	0.58	2.51	14	20
5:D:551:7Q9:C22	5:D:551:7Q9:C13	0.58	2.81	1	13
5:A:206:7Q9:C2	5:A:206:7Q9:O32	0.58	2.49	11	12
6:E:808:17F:C12	6:E:808:17F:H58	0.58	2.27	3	1
6:D:517:17F:C2X	6:D:533:17F:H38	0.58	2.27	17	3
6:B:208:17F:O2	6:B:208:17F:H2	0.58	1.98	6	1
1:A:47:ASP:HA	1:B:128:LYS:HG3	0.58	1.73	7	1
6:D:540:17F:H76	2:E:692:TYR:HE2	0.58	1.58	9	1
2:E:634:LEU:HD11	5:E:863:7Q9:C312	0.58	2.27	10	1
6:D:510:17F:C30	6:D:533:17F:H76	0.58	2.24	16	4
5:D:543:7Q9:C15	5:D:543:7Q9:O12	0.58	2.51	7	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:550:7Q9:O12	5:D:550:7Q9:C13	0.58	2.52	3	20
5:E:816:7Q9:O12	5:E:816:7Q9:C13	0.58	2.51	10	20
5:E:836:7Q9:C15	5:E:836:7Q9:O12	0.58	2.51	18	20
5:E:868:7Q9:C14	5:E:868:7Q9:O12	0.58	2.50	16	20
6:E:806:17F:O1	6:E:806:17F:N1	0.58	2.25	9	5
6:D:540:17F:H35	6:D:540:17F:C33	0.58	2.28	18	8
2:E:641:LEU:HG	5:E:852:7Q9:C313	0.58	2.28	10	3
6:E:819:17F:H78	6:E:819:17F:H47	0.58	1.76	17	3
1:A:68:ARG:HG2	1:A:72:MET:HE3	0.58	1.73	16	3
6:A:208:17F:H65	6:A:208:17F:C23	0.58	2.26	7	1
6:E:808:17F:H46	6:E:810:17F:C35	0.58	2.14	8	2
2:D:292:GLU:HG2	2:D:296:LYS:HE3	0.58	1.74	9	1
6:D:519:17F:C38	6:D:519:17F:H48	0.58	2.28	12	1
6:E:839:17F:H51	5:E:858:7Q9:C313	0.58	2.28	16	2
6:D:540:17F:H1	5:D:545:7Q9:C33	0.58	2.27	13	1
6:A:208:17F:H44	6:A:219:17F:H12A	0.58	1.73	20	1
1:B:47:ASP:HB2	1:B:164:ARG:HH12	0.58	1.57	20	1
5:A:217:7Q9:C1	5:A:217:7Q9:O32	0.58	2.51	18	5
6:E:812:17F:O6	6:E:812:17F:O8	0.58	2.21	7	13
5:E:827:7Q9:C13	5:E:827:7Q9:O12	0.58	2.51	19	20
5:E:877:7Q9:O32	5:E:877:7Q9:C21	0.58	2.51	20	11
5:D:542:7Q9:C1	5:D:553:7Q9:O22	0.58	2.52	12	5
6:E:819:17F:H4	6:E:819:17F:O10	0.58	1.98	16	11
6:D:517:17F:H50	6:D:517:17F:H66	0.58	1.75	10	2
6:D:510:17F:H19	6:D:533:17F:C20	0.58	2.29	7	1
6:D:519:17F:H43	6:D:519:17F:H59	0.58	1.75	7	2
5:B:205:7Q9:C39	6:B:208:17F:H66	0.58	2.29	15	3
6:D:518:17F:O2	6:D:518:17F:H2	0.58	1.99	11	1
5:D:523:7Q9:O22	6:D:552:17F:H19A	0.58	1.98	11	1
6:E:839:17F:H8A	6:E:857:17F:C23	0.58	2.27	16	2
6:A:213:17F:H49	6:A:213:17F:H68	0.58	1.73	17	1
6:D:552:17F:H9A	6:D:552:17F:C31	0.58	2.28	20	1
5:A:203:7Q9:O12	5:A:203:7Q9:C13	0.58	2.51	7	20
5:A:217:7Q9:C13	5:A:217:7Q9:O12	0.58	2.52	6	20
5:D:544:7Q9:C14	5:D:544:7Q9:O12	0.58	2.51	17	20
2:E:733:LEU:HA	5:E:876:7Q9:C310	0.58	2.29	16	7
5:E:825:7Q9:O12	5:E:825:7Q9:C14	0.58	2.51	5	20
5:E:846:7Q9:C15	5:E:846:7Q9:O12	0.58	2.51	10	20
5:E:876:7Q9:C14	5:E:876:7Q9:O12	0.58	2.52	1	20
6:E:871:17F:O1	6:E:871:17F:H5	0.58	1.99	3	12
6:E:875:17F:C6	6:E:875:17F:O1	0.58	2.51	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:811:7Q9:O21	5:E:826:7Q9:C37	0.58	2.51	5	1
6:A:208:17F:H68	6:A:208:17F:C28	0.58	2.16	8	2
6:A:219:17F:H58	5:D:508:7Q9:C317	0.58	2.28	8	1
5:E:843:7Q9:C2	5:E:843:7Q9:O32	0.58	2.49	18	1
6:E:818:17F:H51	5:E:821:7Q9:C318	0.58	2.28	20	1
5:D:501:7Q9:C14	5:D:501:7Q9:O12	0.58	2.51	3	20
5:D:554:7Q9:O22	5:D:554:7Q9:O12	0.58	2.22	1	4
5:E:849:7Q9:C14	5:E:849:7Q9:O12	0.58	2.51	14	20
6:D:511:17F:C28	6:D:511:17F:H77	0.58	2.28	2	2
6:D:540:17F:H65	6:D:540:17F:H30	0.58	1.76	12	5
5:D:544:7Q9:C12	5:D:544:7Q9:O32	0.58	2.51	3	2
5:E:864:7Q9:C32	5:E:874:7Q9:C32	0.58	2.81	3	8
6:D:510:17F:H48	6:D:510:17F:H61	0.58	1.75	4	3
6:D:518:17F:C2X	6:D:518:17F:H20A	0.58	2.29	20	2
5:B:206:7Q9:O22	5:B:206:7Q9:C3	0.58	2.47	9	4
6:D:518:17F:H29	6:D:518:17F:C18	0.58	2.29	11	1
6:A:208:17F:C1Z	6:A:219:17F:H12A	0.58	2.29	16	2
5:D:529:7Q9:C1	5:D:529:7Q9:O22	0.58	2.49	12	1
6:E:857:17F:O8	6:E:857:17F:C4	0.58	2.51	12	1
6:E:806:17F:H68	6:E:806:17F:H46	0.58	1.73	13	1
1:A:147:LYS:HB2	3:A:201:GSP:HN1	0.58	1.59	17	1
6:D:540:17F:C10	5:D:545:7Q9:C33	0.58	2.81	17	1
6:A:213:17F:H19A	6:A:213:17F:O1	0.58	1.98	20	3
1:B:15:GLY:HA2	3:B:201:GSP:H8	0.58	1.59	3	4
5:D:515:7Q9:O12	5:D:515:7Q9:C13	0.58	2.52	17	20
6:E:808:17F:O10	6:E:810:17F:H18	0.58	1.98	1	2
5:E:869:7Q9:C14	5:E:869:7Q9:O12	0.58	2.51	10	20
6:E:839:17F:C23	6:E:839:17F:H33	0.58	2.28	14	5
5:E:835:7Q9:C318	6:E:856:17F:H67	0.58	2.28	4	2
6:D:533:17F:H49	6:E:857:17F:H76	0.58	1.75	7	2
5:D:524:7Q9:O13	5:D:543:7Q9:C14	0.58	2.51	6	1
6:E:820:17F:H44	6:E:820:17F:C31	0.58	2.28	19	6
6:D:519:17F:H52	6:D:519:17F:H67	0.58	1.75	9	2
6:A:213:17F:H54	5:D:503:7Q9:C315	0.58	2.28	10	1
2:E:623:ARG:HB3	5:E:859:7Q9:C310	0.58	2.29	10	1
5:D:501:7Q9:C317	5:E:809:7Q9:C39	0.58	2.82	19	2
5:A:218:7Q9:C14	5:A:218:7Q9:O12	0.58	2.52	10	20
6:D:534:17F:O10	6:D:534:17F:C7	0.58	2.51	2	17
5:E:814:7Q9:C310	6:E:820:17F:H49	0.58	2.28	1	4
1:B:80:CYS:HB3	1:B:93:ILE:HD12	0.58	1.75	20	7
5:B:206:7Q9:O22	5:D:501:7Q9:C12	0.58	2.51	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:273:ASP:HB2	6:D:540:17F:C31	0.58	2.29	14	5
5:D:554:7Q9:O11	5:D:554:7Q9:O22	0.58	2.20	14	12
6:E:820:17F:H61	5:E:837:7Q9:C36	0.58	2.28	7	3
5:E:821:7Q9:C31	5:E:821:7Q9:C21	0.58	2.82	15	3
5:D:513:7Q9:O31	5:D:513:7Q9:O22	0.58	2.22	17	13
6:E:808:17F:C1Y	6:E:819:17F:H9A	0.58	2.28	17	2
5:E:821:7Q9:O22	5:E:821:7Q9:O31	0.58	2.22	20	3
6:D:518:17F:H57	6:D:518:17F:C35	0.58	2.29	11	1
5:E:804:7Q9:C22	6:E:808:17F:H8A	0.58	2.29	16	1
2:E:623:ARG:HD3	5:E:859:7Q9:C310	0.58	2.28	20	1
5:D:505:7Q9:C14	5:D:505:7Q9:O12	0.58	2.51	19	20
5:D:521:7Q9:O22	5:D:521:7Q9:C3	0.58	2.49	15	11
5:D:546:7Q9:C15	5:D:546:7Q9:O12	0.58	2.52	4	20
5:E:814:7Q9:C314	6:E:819:17F:H52	0.58	2.28	18	3
5:E:830:7Q9:C14	5:E:830:7Q9:O12	0.58	2.52	8	20
5:E:833:7Q9:C14	5:E:833:7Q9:O12	0.58	2.52	17	20
5:E:837:7Q9:C13	5:E:837:7Q9:O12	0.58	2.51	15	20
5:E:850:7Q9:O12	5:E:850:7Q9:C14	0.58	2.52	14	20
5:E:878:7Q9:C15	5:E:878:7Q9:O12	0.58	2.52	14	20
5:B:209:7Q9:O12	5:B:209:7Q9:C13	0.58	2.52	6	19
6:E:819:17F:H46	5:E:836:7Q9:C310	0.58	2.29	2	1
2:D:333:LYS:HD3	5:E:878:7Q9:C318	0.58	2.29	10	3
6:E:819:17F:O6	6:E:819:17F:C7	0.58	2.51	17	4
5:E:877:7Q9:O22	5:E:877:7Q9:C3	0.58	2.49	3	5
5:A:218:7Q9:C31	5:A:218:7Q9:O22	0.58	2.51	5	5
5:E:803:7Q9:O13	6:E:808:17F:C2	0.58	2.51	19	3
6:E:819:17F:H42	5:E:836:7Q9:C311	0.58	2.29	5	2
5:B:210:7Q9:C14	5:B:210:7Q9:O12	0.58	2.51	6	1
5:D:502:7Q9:O14	5:D:502:7Q9:O21	0.58	2.21	10	5
1:A:77:GLY:HA3	1:A:163:ILE:HD11	0.58	1.74	13	1
6:A:213:17F:H52	5:D:503:7Q9:C314	0.58	2.29	19	1
5:A:212:7Q9:O13	5:A:212:7Q9:O21	0.58	2.22	1	10
5:D:522:7Q9:O22	5:D:522:7Q9:C3	0.58	2.50	4	18
5:D:536:7Q9:O32	5:D:536:7Q9:C21	0.58	2.52	17	14
6:E:857:17F:C7	6:E:857:17F:H4A	0.58	2.29	4	13
5:E:860:7Q9:C14	5:E:860:7Q9:O12	0.58	2.52	12	20
6:D:540:17F:H30	6:D:540:17F:H64	0.58	1.74	2	1
5:D:542:7Q9:P	5:D:542:7Q9:O21	0.58	2.62	9	16
5:E:853:7Q9:C3	5:E:853:7Q9:O22	0.58	2.50	6	13
5:D:537:7Q9:C311	5:D:537:7Q9:C37	0.58	2.81	12	3
6:E:818:17F:H29	5:E:834:7Q9:C32	0.58	2.29	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:819:17F:H42	5:E:836:7Q9:C310	0.58	2.28	4	5
5:E:833:7Q9:C22	5:E:833:7Q9:C13	0.58	2.81	18	3
5:A:218:7Q9:O22	5:A:218:7Q9:O31	0.58	2.22	17	5
6:D:517:17F:H76	6:E:839:17F:H73	0.58	1.74	5	1
5:E:825:7Q9:C37	6:E:842:17F:H58	0.58	2.29	17	2
5:A:218:7Q9:C35	6:D:511:17F:H64	0.58	2.29	9	1
6:D:511:17F:H55	6:E:829:17F:C30	0.58	2.28	9	1
6:E:857:17F:H63	6:E:857:17F:C31	0.58	2.24	16	8
6:A:219:17F:H56	5:E:801:7Q9:C36	0.58	2.29	10	1
6:E:829:17F:H12	5:E:833:7Q9:C33	0.58	2.29	10	2
3:B:201:GSP:S1G	3:B:201:GSP:O3A	0.58	2.62	16	3
6:A:219:17F:H19	6:A:219:17F:O8	0.58	1.99	13	1
5:A:216:7Q9:O32	5:B:207:7Q9:C35	0.58	2.52	17	1
6:D:510:17F:H60	6:D:517:17F:H12A	0.58	0.83	20	1
5:A:203:7Q9:C38	5:A:203:7Q9:C313	0.58	2.82	1	2
5:A:206:7Q9:C13	5:A:206:7Q9:P	0.58	2.92	16	9
5:A:215:7Q9:C13	5:A:215:7Q9:O12	0.58	2.51	8	20
6:D:518:17F:C2X	6:D:518:17F:C20	0.58	2.82	1	3
5:E:858:7Q9:C14	5:E:858:7Q9:O12	0.58	2.51	16	20
6:D:510:17F:H12	6:D:517:17F:C9	0.58	2.29	13	4
5:D:535:7Q9:O22	5:D:535:7Q9:C3	0.58	2.49	16	13
6:D:510:17F:O9	6:D:517:17F:C10	0.58	2.51	4	4
5:E:840:7Q9:C21	5:E:840:7Q9:O32	0.58	2.52	4	3
2:D:272:TRP:HZ3	6:D:540:17F:H71	0.58	1.59	10	1
1:A:13:GLY:HA2	3:A:201:GSP:C5'	0.58	2.29	20	5
5:A:210:7Q9:O14	5:D:502:7Q9:C12	0.58	2.51	19	1
1:A:22:GLN:O	1:A:26:ASN:HA	0.57	1.99	4	14
5:E:867:7Q9:O31	5:E:867:7Q9:O22	0.57	2.22	8	20
6:E:875:17F:H36	6:E:875:17F:C24	0.57	2.26	17	13
5:D:547:7Q9:O32	5:D:547:7Q9:C2	0.57	2.50	15	13
5:B:210:7Q9:C311	5:E:823:7Q9:C317	0.57	2.82	19	11
5:E:851:7Q9:C35	6:E:871:17F:H20	0.57	2.29	6	4
6:E:856:17F:H53	5:E:868:7Q9:C317	0.57	2.28	6	2
5:E:864:7Q9:C1	5:E:874:7Q9:C32	0.57	2.82	19	4
6:A:213:17F:H52	5:D:503:7Q9:C315	0.57	2.29	13	2
5:D:555:7Q9:O31	6:E:857:17F:H32	0.57	1.99	17	1
6:E:839:17F:C11	6:E:857:17F:H35	0.57	2.29	20	1
1:A:84:ILE:HD12	1:A:123:ARG:HB3	0.57	1.76	2	8
5:A:209:7Q9:O31	5:A:209:7Q9:C13	0.57	2.52	1	1
5:B:205:7Q9:O12	5:B:205:7Q9:C13	0.57	2.52	10	20
5:B:210:7Q9:O12	5:B:210:7Q9:C14	0.57	2.52	14	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:507:7Q9:C14	5:D:507:7Q9:O12	0.57	2.52	6	20
6:D:510:17F:C28	6:D:517:17F:C22	0.57	2.72	4	10
5:D:548:7Q9:O12	5:D:548:7Q9:C13	0.57	2.51	6	20
5:E:862:7Q9:C14	5:E:862:7Q9:O12	0.57	2.52	8	20
6:A:208:17F:C20	6:A:219:17F:H10A	0.57	2.29	3	2
2:D:305:GLN:NE2	6:D:533:17F:H10A	0.57	2.14	11	4
1:B:83:ALA:HB3	1:B:86:ASN:HB3	0.57	1.76	19	4
6:A:220:17F:H41	6:A:220:17F:H73	0.57	1.75	8	2
6:D:520:17F:C39	6:D:520:17F:H55	0.57	2.29	9	1
6:E:808:17F:H76	6:E:808:17F:C29	0.57	2.21	14	4
6:A:213:17F:H51	5:D:503:7Q9:C314	0.57	2.29	12	1
6:D:519:17F:H55	5:E:843:7Q9:C318	0.57	2.29	20	1
5:E:822:7Q9:C15	5:E:822:7Q9:O12	0.57	2.53	1	19
5:E:838:7Q9:C15	5:E:838:7Q9:O12	0.57	2.53	7	20
5:E:840:7Q9:O12	5:E:840:7Q9:C13	0.57	2.51	2	20
5:E:861:7Q9:C15	5:E:861:7Q9:O12	0.57	2.53	12	20
5:E:867:7Q9:C15	5:E:867:7Q9:O12	0.57	2.52	11	20
6:D:519:17F:C37	6:D:519:17F:H52	0.57	2.29	8	3
6:E:857:17F:C31	6:E:857:17F:H63	0.57	2.28	8	3
5:B:210:7Q9:C1	5:B:210:7Q9:O32	0.57	2.52	4	1
5:E:817:7Q9:C1	5:E:817:7Q9:O22	0.57	2.51	5	3
5:D:555:7Q9:C3	5:E:833:7Q9:C3	0.57	2.82	7	2
5:D:543:7Q9:C34	6:D:552:17F:H73	0.57	2.29	6	1
6:E:839:17F:H73	6:E:875:17F:C30	0.57	2.29	12	1
6:E:808:17F:H69	5:E:814:7Q9:C311	0.57	2.29	15	1
6:A:219:17F:H68	6:A:219:17F:H61	0.57	1.76	16	1
5:A:214:7Q9:C15	5:A:214:7Q9:C1	0.57	2.83	1	10
6:B:208:17F:O10	6:B:208:17F:C6	0.57	2.46	6	6
5:E:805:7Q9:C14	5:E:805:7Q9:O12	0.57	2.51	14	20
5:E:815:7Q9:C15	5:E:815:7Q9:O12	0.57	2.53	19	20
6:E:818:17F:O10	6:E:818:17F:H4	0.57	1.98	16	5
6:D:510:17F:H9	6:D:517:17F:C9	0.57	2.29	2	3
6:A:219:17F:H66	6:D:518:17F:C21	0.57	2.27	3	1
1:B:120:LEU:HD11	3:B:201:GSP:N2	0.57	2.14	4	3
6:D:517:17F:H76	6:E:839:17F:H74	0.57	1.74	7	3
6:D:540:17F:H30	6:D:540:17F:H58	0.57	1.74	4	1
6:E:818:17F:H49	5:E:821:7Q9:C316	0.57	2.29	5	1
6:A:213:17F:O10	6:A:213:17F:C4	0.57	2.48	7	3
6:D:519:17F:H43	6:D:519:17F:C32	0.57	2.29	7	1
6:E:839:17F:C28	6:E:875:17F:H53	0.57	2.29	7	1
5:D:513:7Q9:C311	6:D:534:17F:H65	0.57	2.29	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:808:17F:C18	6:E:810:17F:H20	0.57	2.29	11	3
6:A:219:17F:H48	6:A:219:17F:H75	0.57	1.73	14	1
2:D:340:LYS:HE2	2:E:622:LEU:HD22	0.57	1.76	18	1
5:A:211:7Q9:C23	6:A:213:17F:H33	0.57	2.30	20	1
5:D:530:7Q9:C14	5:D:530:7Q9:O12	0.57	2.53	6	19
5:D:545:7Q9:C1	5:D:545:7Q9:O32	0.57	2.52	16	7
5:D:545:7Q9:C14	5:D:545:7Q9:O12	0.57	2.51	14	20
5:E:828:7Q9:C15	5:E:828:7Q9:O12	0.57	2.53	4	20
5:E:834:7Q9:C14	5:E:834:7Q9:O12	0.57	2.52	10	20
5:E:835:7Q9:C1	5:E:835:7Q9:O22	0.57	2.50	15	7
5:E:843:7Q9:C14	5:E:843:7Q9:O12	0.57	2.53	3	20
5:E:844:7Q9:C15	5:E:844:7Q9:O12	0.57	2.52	20	20
5:E:862:7Q9:O22	5:E:862:7Q9:C1	0.57	2.49	1	13
5:E:878:7Q9:O11	5:E:878:7Q9:O22	0.57	2.23	6	14
5:B:203:7Q9:O32	5:B:203:7Q9:O21	0.57	2.23	13	16
6:D:518:17F:H53	6:D:518:17F:C41	0.57	2.29	4	2
6:E:808:17F:C31	6:E:820:17F:C1X	0.57	2.81	4	3
5:A:215:7Q9:C37	6:D:511:17F:H74	0.57	2.29	5	1
6:D:511:17F:H76	6:E:829:17F:C30	0.57	2.15	7	2
5:E:833:7Q9:C23	6:E:857:17F:H39	0.57	2.29	12	1
6:E:808:17F:H70	6:E:819:17F:C42	0.57	2.29	13	1
6:E:810:17F:H29	6:E:810:17F:C23	0.57	2.17	17	1
5:A:206:7Q9:O22	5:A:206:7Q9:C1	0.57	2.49	1	9
5:D:505:7Q9:C14	6:D:518:17F:O8	0.57	2.52	11	3
6:D:518:17F:O10	6:D:518:17F:C6	0.57	2.50	9	16
5:D:538:7Q9:O32	5:D:538:7Q9:O21	0.57	2.21	17	14
5:D:555:7Q9:O12	5:D:555:7Q9:C13	0.57	2.51	12	19
5:A:203:7Q9:O13	5:A:204:7Q9:C13	0.57	2.52	15	5
5:D:514:7Q9:C15	5:D:514:7Q9:O12	0.57	2.52	9	14
5:E:878:7Q9:C37	5:E:878:7Q9:C311	0.57	2.82	19	9
6:D:517:17F:C17	6:D:517:17F:H1A	0.57	2.29	3	1
5:D:555:7Q9:C2	5:D:555:7Q9:O32	0.57	2.48	5	11
5:E:870:7Q9:O22	5:E:870:7Q9:C1	0.57	2.49	11	5
5:E:813:7Q9:C13	5:E:817:7Q9:O22	0.57	2.53	13	4
1:A:82:PHE:HB2	1:A:89:SER:HB2	0.57	1.77	7	1
6:D:518:17F:H35	6:D:518:17F:H20	0.57	1.74	11	1
5:A:206:7Q9:C13	5:A:206:7Q9:O12	0.57	2.53	3	20
5:B:210:7Q9:C3	5:B:210:7Q9:O22	0.57	2.51	16	13
6:D:510:17F:C7	6:D:517:17F:C9	0.57	2.83	9	4
6:D:511:17F:H8A	5:D:513:7Q9:C14	0.57	2.30	16	4
5:D:530:7Q9:C33	5:D:530:7Q9:C37	0.57	2.83	5	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:541:7Q9:O12	5:D:541:7Q9:C14	0.57	2.52	1	14
5:E:815:7Q9:O11	5:E:815:7Q9:O22	0.57	2.21	19	14
5:E:840:7Q9:C3	5:E:840:7Q9:O22	0.57	2.50	12	8
5:B:210:7Q9:O13	5:B:210:7Q9:C2	0.57	2.52	5	9
6:D:517:17F:C23	6:D:517:17F:C28	0.57	2.71	3	1
5:E:834:7Q9:C12	5:E:858:7Q9:O14	0.57	2.53	17	4
6:E:829:17F:H71	5:E:830:7Q9:C36	0.57	2.30	5	1
6:A:208:17F:O2	6:A:208:17F:C6	0.57	2.53	10	1
6:E:806:17F:O7	6:E:806:17F:P1	0.57	2.62	12	3
6:D:511:17F:H10A	5:D:513:7Q9:C23	0.57	2.29	19	2
1:B:93:ILE:HG21	1:B:113:LEU:HD11	0.57	1.75	17	1
6:D:510:17F:H65	6:D:510:17F:C29	0.57	2.30	18	1
5:A:209:7Q9:C13	5:A:209:7Q9:O12	0.57	2.52	6	20
1:B:84:ILE:HD12	1:B:123:ARG:HB3	0.57	1.76	14	9
5:D:524:7Q9:O12	5:D:524:7Q9:C15	0.57	2.51	5	18
6:E:812:17F:H75	5:E:823:7Q9:C316	0.57	2.30	14	5
5:E:832:7Q9:C14	5:E:832:7Q9:O12	0.57	2.52	20	20
5:B:204:7Q9:C317	6:E:812:17F:H54	0.57	2.30	3	1
6:E:839:17F:H9A	6:E:839:17F:H60	0.57	1.75	5	3
6:E:839:17F:H47	6:E:839:17F:H78	0.57	1.76	5	1
5:A:209:7Q9:C15	5:A:209:7Q9:C32	0.57	2.83	9	2
5:D:514:7Q9:C2	5:D:514:7Q9:O32	0.57	2.51	11	8
5:D:525:7Q9:C14	5:D:525:7Q9:O12	0.57	2.52	16	19
5:D:530:7Q9:C1	5:D:530:7Q9:O22	0.57	2.51	1	7
5:D:532:7Q9:O22	5:D:532:7Q9:C3	0.57	2.49	1	16
5:E:833:7Q9:C1	5:E:833:7Q9:O22	0.57	2.47	13	10
5:E:834:7Q9:C31	5:E:834:7Q9:C35	0.57	2.82	1	19
5:B:203:7Q9:C311	5:B:203:7Q9:C37	0.57	2.80	3	1
6:A:220:17F:H12A	5:D:502:7Q9:C311	0.57	2.30	4	1
5:B:204:7Q9:C36	5:B:204:7Q9:C311	0.57	2.83	18	2
5:A:203:7Q9:C39	6:A:208:17F:H72	0.57	2.29	5	1
6:A:208:17F:H46	6:A:208:17F:C38	0.57	2.27	5	1
2:D:404:SER:HB2	5:D:548:7Q9:C311	0.57	2.30	5	2
6:E:839:17F:H57	6:E:839:17F:H36	0.57	1.76	16	2
1:B:8:VAL:HG12	1:B:16:LYS:HD2	0.57	1.76	7	2
6:B:208:17F:C7	6:B:208:17F:C4	0.57	2.83	7	1
6:D:510:17F:H10A	6:D:517:17F:H59	0.57	1.77	8	2
6:A:219:17F:H64	6:D:518:17F:H47	0.57	1.77	11	1
5:D:502:7Q9:O22	5:D:502:7Q9:O31	0.57	2.23	17	16
5:E:869:7Q9:O22	5:E:869:7Q9:C3	0.57	2.49	8	15
6:A:208:17F:C4	6:A:208:17F:H1	0.57	2.29	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:518:17F:O10	5:D:528:7Q9:C1	0.57	2.53	4	2
6:E:802:17F:H20A	5:E:804:7Q9:C22	0.57	2.30	5	1
5:E:826:7Q9:C39	5:E:845:7Q9:C39	0.57	2.83	10	5
5:E:811:7Q9:C12	5:E:817:7Q9:O32	0.57	2.53	8	2
6:A:208:17F:H33	6:A:219:17F:H41	0.57	1.76	20	2
6:A:219:17F:C17	6:A:219:17F:O8	0.57	2.53	16	1
6:A:213:17F:C12	6:A:213:17F:C23	0.57	2.83	19	1
5:D:504:7Q9:C3	5:D:504:7Q9:O22	0.56	2.50	6	11
5:D:513:7Q9:O21	5:D:513:7Q9:C31	0.56	2.53	1	5
5:D:526:7Q9:O12	5:D:526:7Q9:C15	0.56	2.53	20	20
5:D:532:7Q9:O12	5:D:532:7Q9:C15	0.56	2.53	10	20
5:D:549:7Q9:O31	5:D:549:7Q9:C34	0.56	2.53	7	13
5:E:803:7Q9:O12	5:E:803:7Q9:C13	0.56	2.52	7	20
5:E:824:7Q9:C14	5:E:824:7Q9:O12	0.56	2.53	8	20
6:E:857:17F:C4	6:E:857:17F:C7	0.56	2.83	12	11
6:E:875:17F:O7	6:E:875:17F:O10	0.56	2.23	4	18
5:A:212:7Q9:C35	5:A:212:7Q9:C31	0.56	2.83	5	4
5:D:555:7Q9:C15	6:E:857:17F:H5	0.56	2.30	5	3
6:E:842:17F:H64	6:E:842:17F:C32	0.56	2.28	4	1
6:E:857:17F:O5	6:E:875:17F:H4	0.56	2.00	4	1
2:D:400:LEU:HG	5:D:548:7Q9:C310	0.56	2.29	5	1
2:E:631:ARG:HG2	5:E:878:7Q9:C34	0.56	2.30	7	3
5:E:863:7Q9:C13	5:E:863:7Q9:P	0.56	2.93	18	2
6:A:213:17F:C2X	6:A:213:17F:C24	0.56	2.83	16	2
2:D:400:LEU:HG	5:D:548:7Q9:C313	0.56	2.30	12	1
5:A:211:7Q9:C22	6:A:213:17F:H57	0.56	2.30	17	1
6:A:213:17F:H62	6:A:213:17F:H10	0.56	1.75	17	1
6:A:219:17F:H42	5:D:505:7Q9:C37	0.56	2.28	20	1
5:A:212:7Q9:C15	5:A:212:7Q9:O12	0.56	2.53	4	20
6:D:510:17F:P1	6:D:510:17F:HN1	0.56	2.23	5	8
5:E:807:7Q9:C15	5:E:807:7Q9:O12	0.56	2.54	8	20
5:E:868:7Q9:C34	5:E:868:7Q9:O31	0.56	2.53	11	14
6:E:857:17F:H56	6:E:857:17F:C35	0.56	2.30	18	11
6:E:875:17F:H4	6:E:875:17F:O10	0.56	2.00	2	1
5:E:837:7Q9:O22	5:E:837:7Q9:C1	0.56	2.47	20	13
5:D:513:7Q9:C11	5:D:513:7Q9:O21	0.56	2.53	18	12
1:B:33:ASP:O	3:B:201:GSP:S1G	0.56	2.63	7	5
6:D:517:17F:C42	6:E:839:17F:H74	0.56	2.30	20	3
6:A:219:17F:H52	5:E:816:7Q9:C318	0.56	2.30	10	1
5:E:833:7Q9:O22	6:E:839:17F:H4	0.56	2.00	18	1
5:B:204:7Q9:C3	5:B:204:7Q9:O22	0.56	2.49	2	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:204:7Q9:O12	5:B:204:7Q9:C14	0.56	2.53	19	20
5:D:535:7Q9:C13	5:D:535:7Q9:O12	0.56	2.54	17	20
6:D:539:17F:H72	5:D:549:7Q9:C22	0.56	2.30	14	2
5:E:805:7Q9:C3	5:E:805:7Q9:O22	0.56	2.49	4	15
5:E:834:7Q9:O22	5:E:834:7Q9:O31	0.56	2.22	4	16
5:E:870:7Q9:O12	5:E:870:7Q9:C15	0.56	2.53	10	20
5:E:874:7Q9:C14	5:E:874:7Q9:O12	0.56	2.53	7	20
1:A:92:ASP:HA	1:A:95:HIS:HD2	0.56	1.61	9	2
5:A:211:7Q9:C15	5:A:211:7Q9:C1	0.56	2.83	18	3
2:D:389:LEU:HD21	5:D:546:7Q9:C313	0.56	2.29	15	4
5:D:503:7Q9:O31	5:D:503:7Q9:O22	0.56	2.23	13	6
6:D:510:17F:HN1	6:D:510:17F:P1	0.56	2.23	7	8
6:E:806:17F:H78	5:E:817:7Q9:C317	0.56	2.30	3	1
5:E:854:7Q9:O14	5:E:854:7Q9:O21	0.56	2.23	15	5
6:A:213:17F:H38	5:D:507:7Q9:C35	0.56	2.30	5	1
5:D:515:7Q9:C2	5:D:515:7Q9:O32	0.56	2.51	12	7
6:D:520:17F:C30	6:D:520:17F:H72	0.56	2.30	7	4
6:E:857:17F:H65	6:E:875:17F:C33	0.56	2.30	7	2
6:E:810:17F:H48	6:E:810:17F:H60	0.56	1.78	8	2
5:D:554:7Q9:O14	5:E:848:7Q9:C12	0.56	2.52	10	3
5:E:805:7Q9:C38	5:E:805:7Q9:C312	0.56	2.83	18	2
6:A:213:17F:H51	5:D:503:7Q9:C313	0.56	2.31	12	1
1:B:144:THR:HG22	1:B:151:GLY:HA3	0.56	1.78	15	2
1:B:117:LYS:HE2	3:B:201:GSP:N7	0.56	2.14	14	1
1:A:147:LYS:HB2	3:A:201:GSP:N1	0.56	2.15	17	1
6:E:806:17F:C7	6:E:806:17F:O9	0.56	2.53	17	1
5:E:863:7Q9:C13	5:E:863:7Q9:O12	0.56	2.54	18	1
6:A:213:17F:H39	6:A:213:17F:C11	0.56	2.30	17	2
5:D:506:7Q9:C2	5:D:506:7Q9:O32	0.56	2.53	19	10
5:D:542:7Q9:O21	5:D:542:7Q9:P	0.56	2.63	15	3
5:D:550:7Q9:O22	5:D:550:7Q9:O11	0.56	2.23	15	17
5:E:854:7Q9:O32	5:E:854:7Q9:O21	0.56	2.23	10	11
5:B:205:7Q9:C313	6:B:208:17F:C42	0.56	2.83	10	7
5:D:516:7Q9:O12	5:D:516:7Q9:C14	0.56	2.53	15	19
5:B:205:7Q9:C314	6:B:208:17F:C42	0.56	2.83	7	2
5:D:555:7Q9:C12	6:E:857:17F:O10	0.56	2.54	3	1
6:D:520:17F:H54	5:E:841:7Q9:C317	0.56	2.30	4	3
5:D:524:7Q9:C12	5:D:524:7Q9:O22	0.56	2.53	20	3
5:D:528:7Q9:O22	5:D:528:7Q9:C3	0.56	2.52	6	8
6:E:871:17F:H1	6:E:871:17F:H4	0.56	1.77	5	1
5:D:523:7Q9:C32	6:D:552:17F:H40	0.56	2.31	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:839:17F:H71	6:E:839:17F:C27	0.56	2.28	20	2
5:E:845:7Q9:C14	5:E:865:7Q9:O22	0.56	2.53	19	4
6:D:519:17F:H12A	6:D:519:17F:C20	0.56	2.20	17	1
6:D:533:17F:O2	5:D:541:7Q9:C13	0.56	2.54	17	1
5:D:554:7Q9:O12	5:D:554:7Q9:C13	0.56	2.54	10	20
5:E:809:7Q9:O12	5:E:809:7Q9:C14	0.56	2.53	19	20
5:D:554:7Q9:O22	5:D:554:7Q9:P	0.56	2.64	5	6
5:E:816:7Q9:O32	5:E:828:7Q9:C2	0.56	2.53	12	6
5:E:817:7Q9:C12	5:E:832:7Q9:O13	0.56	2.54	5	5
5:A:218:7Q9:O21	5:A:218:7Q9:O13	0.56	2.22	3	1
5:B:205:7Q9:C310	6:B:208:17F:H63	0.56	2.30	13	4
5:D:524:7Q9:C33	5:D:543:7Q9:C34	0.56	2.83	3	3
5:E:814:7Q9:C33	5:E:830:7Q9:O13	0.56	2.53	3	3
2:D:340:LYS:HD3	2:E:626:LEU:HD21	0.56	1.77	17	4
2:D:375:ALA:HB2	5:D:535:7Q9:C35	0.56	2.31	20	3
6:E:839:17F:H77	6:E:839:17F:C28	0.56	2.29	13	7
6:D:510:17F:H54	6:D:517:17F:H72	0.56	1.77	11	2
6:D:511:17F:H53	6:E:829:17F:C30	0.56	2.29	16	1
6:D:511:17F:O9	6:D:511:17F:O8	0.56	2.24	9	17
5:D:553:7Q9:C14	5:D:553:7Q9:O12	0.56	2.54	18	20
6:E:829:17F:O10	6:E:829:17F:C6	0.56	2.52	11	11
5:E:872:7Q9:O12	5:E:872:7Q9:C13	0.56	2.54	11	20
5:A:207:7Q9:C36	5:B:207:7Q9:C314	0.56	2.84	2	2
5:A:216:7Q9:C1	5:A:216:7Q9:O22	0.56	2.48	4	9
6:D:517:17F:C23	6:D:517:17F:C27	0.56	2.74	14	3
6:E:842:17F:H42	6:E:842:17F:C31	0.56	2.29	3	1
5:E:849:7Q9:C37	5:E:852:7Q9:C32	0.56	2.83	4	4
6:D:534:17F:H40	5:D:538:7Q9:C317	0.56	2.30	20	2
6:E:839:17F:H71	6:E:875:17F:H53	0.56	1.78	5	1
6:E:808:17F:H75	6:E:819:17F:H76	0.56	1.76	6	1
6:D:518:17F:H45	5:D:549:7Q9:C311	0.56	2.30	7	1
6:D:520:17F:C27	6:D:520:17F:C39	0.56	2.84	8	1
5:E:822:7Q9:C12	5:E:826:7Q9:O13	0.56	2.54	10	2
6:A:213:17F:H37	6:A:213:17F:C1Z	0.56	2.26	10	2
6:A:213:17F:H66	6:A:213:17F:H43	0.56	1.77	11	1
6:E:842:17F:H59	6:E:842:17F:C36	0.56	2.26	14	1
6:E:806:17F:O3	6:E:806:17F:H8	0.56	2.01	17	1
6:E:812:17F:H61	5:E:824:7Q9:C32	0.56	2.31	17	2
5:E:809:7Q9:C315	6:E:818:17F:H52	0.56	2.31	19	1
5:A:210:7Q9:C13	5:A:210:7Q9:O12	0.56	2.53	16	20
5:D:502:7Q9:C32	5:D:525:7Q9:C22	0.56	2.84	9	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:506:7Q9:C21	5:D:506:7Q9:O14	0.56	2.54	1	3
5:D:527:7Q9:C1	5:D:527:7Q9:O22	0.56	2.53	16	9
5:B:207:7Q9:C1	5:B:207:7Q9:C31	0.56	2.83	16	9
6:D:517:17F:O2	6:D:517:17F:C5	0.56	2.54	13	8
5:D:504:7Q9:C38	5:D:508:7Q9:C313	0.56	2.83	20	3
2:D:429:PHE:CE1	6:D:539:17F:H66	0.56	2.35	4	4
5:A:205:7Q9:C315	6:E:806:17F:H71	0.56	2.31	5	1
5:E:844:7Q9:C2	5:E:844:7Q9:O32	0.56	2.52	5	6
5:A:218:7Q9:C310	6:D:511:17F:H52	0.56	2.30	17	1
5:A:214:7Q9:C15	5:A:214:7Q9:O12	0.56	2.53	20	20
5:E:866:7Q9:C15	5:E:866:7Q9:O12	0.56	2.53	12	20
5:D:525:7Q9:C3	5:D:525:7Q9:O22	0.56	2.51	9	4
6:A:208:17F:C33	6:A:208:17F:H43	0.56	2.31	3	1
5:D:526:7Q9:C313	5:D:544:7Q9:C314	0.56	2.84	7	4
6:A:208:17F:C39	6:B:208:17F:H69	0.56	2.30	4	1
6:D:510:17F:H45	6:D:510:17F:C37	0.56	2.30	4	1
5:E:840:7Q9:O21	5:E:840:7Q9:O32	0.56	2.23	5	1
6:A:208:17F:H19A	6:A:219:17F:C10	0.56	2.31	7	1
6:E:806:17F:H45	6:E:806:17F:H68	0.56	1.74	13	2
6:D:510:17F:H18A	6:D:517:17F:C9	0.56	2.30	18	2
6:E:802:17F:H20	6:E:802:17F:H36	0.56	1.77	20	1
1:B:15:GLY:HA2	3:B:201:GSP:C8	0.56	2.36	3	2
5:D:514:7Q9:C14	5:D:525:7Q9:O22	0.56	2.54	19	3
5:E:824:7Q9:O32	5:E:824:7Q9:O21	0.56	2.24	14	15
5:E:831:7Q9:O12	5:E:831:7Q9:C14	0.56	2.54	5	20
5:E:833:7Q9:O32	5:E:833:7Q9:O21	0.56	2.23	20	13
5:E:849:7Q9:C310	5:E:852:7Q9:C311	0.56	2.84	14	13
6:E:875:17F:H11A	6:E:875:17F:HN1A	0.56	1.60	17	5
5:E:801:7Q9:O32	5:E:801:7Q9:O21	0.56	2.23	17	12
6:E:812:17F:H34	6:E:812:17F:H8	0.56	1.77	3	2
5:A:207:7Q9:O32	5:A:209:7Q9:C13	0.56	2.53	4	1
5:A:211:7Q9:C1	6:A:213:17F:H18	0.56	2.31	7	1
2:D:322:LEU:HD22	2:E:644:LEU:HD12	0.56	1.78	10	1
6:E:812:17F:H77	6:E:812:17F:C26	0.56	2.31	12	1
2:E:645:GLY:HA2	5:E:852:7Q9:C318	0.56	2.31	14	1
6:E:819:17F:H68	5:E:825:7Q9:C318	0.56	2.31	18	1
5:D:526:7Q9:O22	5:D:526:7Q9:C3	0.56	2.52	8	17
5:E:847:7Q9:C14	5:E:847:7Q9:O12	0.56	2.54	5	20
6:D:510:17F:C12	6:D:517:17F:C7	0.56	2.80	14	3
6:E:806:17F:H5	5:E:817:7Q9:C31	0.56	2.31	3	3
2:D:333:LYS:HE2	2:E:633:LYS:HG2	0.56	1.78	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:518:17F:H19	6:D:518:17F:C1X	0.56	2.23	4	9
6:E:808:17F:H20A	6:E:819:17F:C10	0.56	2.30	5	1
6:A:213:17F:C33	6:A:213:17F:C24	0.56	2.83	9	2
6:A:219:17F:C6	5:D:505:7Q9:O32	0.56	2.53	6	2
6:E:857:17F:P1	6:E:857:17F:HN1	0.56	2.23	11	6
5:D:531:7Q9:O32	5:D:531:7Q9:C11	0.56	2.54	9	3
6:A:219:17F:H63	6:A:219:17F:C31	0.56	2.23	11	2
2:D:262:GLU:HG3	5:D:545:7Q9:C316	0.56	2.31	11	1
6:D:510:17F:H29	6:D:510:17F:C25	0.56	2.29	12	1
6:A:219:17F:H68	5:D:505:7Q9:C37	0.56	2.30	15	1
5:A:204:7Q9:O13	5:A:211:7Q9:C15	0.56	2.54	18	1
2:E:620:GLU:HB2	2:E:621:PRO:HD3	0.56	1.78	18	2
6:E:839:17F:H12	6:E:857:17F:C21	0.56	2.31	18	1
6:A:208:17F:H34	6:A:208:17F:C25	0.56	2.31	20	1
6:A:208:17F:C21	6:B:208:17F:H19	0.56	2.27	20	1
5:A:216:7Q9:C14	5:A:216:7Q9:O12	0.55	2.53	19	20
5:D:502:7Q9:C14	5:D:502:7Q9:O12	0.55	2.54	11	20
5:E:826:7Q9:C14	5:E:826:7Q9:O12	0.55	2.54	18	20
5:E:848:7Q9:C14	5:E:848:7Q9:O12	0.55	2.54	3	20
6:E:871:17F:H30	6:E:871:17F:H56	0.55	1.79	10	8
6:E:857:17F:C38	6:E:875:17F:H60	0.55	2.31	2	3
6:A:208:17F:C40	6:B:208:17F:H69	0.55	2.31	4	1
5:A:215:7Q9:C313	6:D:517:17F:H73	0.55	2.31	5	1
6:D:511:17F:H29	6:D:534:17F:H53	0.55	1.77	6	1
6:A:208:17F:N1	6:A:219:17F:H1	0.55	2.17	15	3
6:A:208:17F:H31	6:A:219:17F:H12	0.55	1.77	14	3
5:A:215:7Q9:C14	6:D:511:17F:H6	0.55	2.31	10	1
5:E:811:7Q9:C3	5:E:822:7Q9:C23	0.55	2.84	10	1
5:E:803:7Q9:C22	6:E:806:17F:H33	0.55	2.31	12	1
5:E:833:7Q9:C312	5:E:852:7Q9:C34	0.55	2.84	19	1
5:E:858:7Q9:O31	6:E:875:17F:H9	0.55	2.01	20	1
5:D:512:7Q9:O11	5:D:512:7Q9:O22	0.55	2.23	7	13
5:D:542:7Q9:O12	5:D:542:7Q9:C13	0.55	2.54	14	19
5:E:852:7Q9:C13	5:E:852:7Q9:O12	0.55	2.53	16	20
5:A:212:7Q9:P	5:A:212:7Q9:O21	0.55	2.65	10	9
6:D:510:17F:O9	6:D:517:17F:C11	0.55	2.54	4	2
5:D:506:7Q9:C32	6:D:517:17F:C20	0.55	2.84	8	2
5:A:211:7Q9:O12	5:A:211:7Q9:C3	0.55	2.54	7	1
6:D:520:17F:C17	6:D:520:17F:O8	0.55	2.54	14	6
6:E:819:17F:H10	6:E:820:17F:H10	0.55	1.77	7	1
5:D:507:7Q9:C12	5:D:527:7Q9:O22	0.55	2.54	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:814:7Q9:C35	6:E:820:17F:H12	0.55	2.30	17	2
6:E:806:17F:H4	5:E:811:7Q9:C14	0.55	2.31	13	1
6:E:839:17F:H8A	6:E:857:17F:C24	0.55	2.31	15	1
5:D:526:7Q9:C315	5:D:544:7Q9:C314	0.55	2.85	1	4
5:E:803:7Q9:C32	6:E:810:17F:H9A	0.55	2.31	12	3
5:E:804:7Q9:C13	5:E:804:7Q9:O12	0.55	2.54	3	20
5:E:827:7Q9:C2	5:E:827:7Q9:O32	0.55	2.53	20	14
5:E:853:7Q9:C15	5:E:853:7Q9:O12	0.55	2.54	14	19
5:E:863:7Q9:O12	5:E:863:7Q9:C13	0.55	2.54	14	19
5:E:864:7Q9:C15	5:E:864:7Q9:O12	0.55	2.55	17	19
5:A:215:7Q9:C36	6:D:511:17F:H72	0.55	2.32	9	2
6:D:510:17F:C8	6:D:517:17F:H11A	0.55	2.31	2	1
1:A:13:GLY:CA	3:A:201:GSP:H5'1	0.55	2.29	4	3
5:D:502:7Q9:C34	5:D:525:7Q9:C23	0.55	2.84	4	1
1:A:58:THR:HG21	1:A:71:TYR:CE1	0.55	2.36	10	3
6:A:213:17F:H29	5:D:503:7Q9:C37	0.55	2.32	12	1
5:D:523:7Q9:C314	6:D:552:17F:H55	0.55	2.32	12	1
5:D:523:7Q9:O32	6:D:552:17F:H39	0.55	2.02	19	1
5:D:503:7Q9:C13	5:D:503:7Q9:O12	0.55	2.55	18	19
6:D:510:17F:N1	6:D:510:17F:P1	0.55	2.80	18	9
5:D:542:7Q9:O31	5:D:542:7Q9:O22	0.55	2.24	3	19
5:D:547:7Q9:C13	5:D:547:7Q9:O12	0.55	2.55	5	20
5:E:811:7Q9:C12	5:E:817:7Q9:C32	0.55	2.85	10	4
5:D:524:7Q9:O22	5:D:524:7Q9:C3	0.55	2.52	6	3
6:D:552:17F:O10	6:D:552:17F:H6A	0.55	2.01	2	9
6:E:802:17F:H32	5:E:807:7Q9:C38	0.55	2.30	2	1
6:D:540:17F:C33	6:D:540:17F:C2X	0.55	2.84	17	6
1:B:117:LYS:HG2	3:B:201:GSP:C6	0.55	2.36	19	2
6:E:842:17F:H38	5:E:877:7Q9:C34	0.55	2.31	7	3
6:A:219:17F:H74	6:A:219:17F:H48	0.55	1.75	6	1
1:B:17:SER:HB2	3:B:201:GSP:O2A	0.55	2.01	7	1
1:A:13:GLY:C	3:A:201:GSP:H5'1	0.55	2.26	20	2
5:D:506:7Q9:C31	6:D:517:17F:H18A	0.55	2.31	11	1
6:E:810:17F:H48	6:E:810:17F:C34	0.55	2.32	16	1
6:D:533:17F:H53	6:E:839:17F:H75	0.55	1.79	17	1
1:A:68:ARG:HA	1:A:71:TYR:CE2	0.55	2.37	4	5
5:D:506:7Q9:C13	5:D:506:7Q9:O12	0.55	2.55	1	20
5:D:522:7Q9:C15	5:D:522:7Q9:O12	0.55	2.55	4	20
5:E:877:7Q9:C14	5:E:877:7Q9:O12	0.55	2.54	14	20
2:D:419:LEU:HB3	2:D:420:PRO:HD3	0.55	1.79	7	4
6:A:208:17F:H4	6:A:208:17F:C1	0.55	2.21	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:513:7Q9:C37	5:D:532:7Q9:C39	0.55	2.85	10	3
5:E:803:7Q9:C314	6:E:810:17F:H72	0.55	2.31	13	3
6:A:219:17F:H75	6:A:219:17F:H42	0.55	1.79	12	1
5:E:821:7Q9:O31	6:E:839:17F:H6	0.55	2.02	13	1
5:A:209:7Q9:C13	5:A:209:7Q9:C32	0.55	2.84	14	1
5:E:804:7Q9:O21	6:E:808:17F:H8A	0.55	2.02	14	1
1:B:146:ALA:HB3	3:B:201:GSP:N7	0.55	2.16	16	1
6:D:534:17F:H69	6:D:534:17F:C22	0.55	2.30	20	2
6:A:213:17F:H61	6:A:213:17F:C24	0.55	2.26	17	1
5:D:523:7Q9:C14	5:D:523:7Q9:O12	0.55	2.54	14	20
5:D:541:7Q9:O22	5:D:541:7Q9:C3	0.55	2.50	16	10
5:E:826:7Q9:O32	5:E:826:7Q9:O21	0.55	2.25	18	14
6:E:856:17F:H37	5:E:858:7Q9:C317	0.55	2.32	1	2
5:E:859:7Q9:C15	5:E:859:7Q9:O12	0.55	2.54	13	20
5:E:872:7Q9:O32	5:E:872:7Q9:O21	0.55	2.25	5	19
5:E:803:7Q9:O22	5:E:803:7Q9:O11	0.55	2.24	17	14
5:E:814:7Q9:O22	5:E:814:7Q9:C1	0.55	2.49	5	9
5:E:850:7Q9:O32	5:E:850:7Q9:O21	0.55	2.23	11	12
6:A:220:17F:H54	6:A:220:17F:H61	0.55	1.78	5	2
5:E:825:7Q9:C32	6:E:842:17F:H18A	0.55	2.31	20	2
5:D:527:7Q9:O31	5:D:531:7Q9:O31	0.55	2.25	7	8
6:E:873:17F:C20	6:E:873:17F:C2X	0.55	2.82	7	2
5:E:804:7Q9:O31	5:E:804:7Q9:O22	0.55	2.24	17	7
2:E:734:GLU:HG2	2:E:738:LYS:HE3	0.55	1.78	11	1
6:E:808:17F:H56	6:E:820:17F:C12	0.55	2.18	14	1
6:A:213:17F:H60	6:A:213:17F:H42	0.55	1.74	20	1
6:A:213:17F:H47	5:D:507:7Q9:C35	0.55	2.32	20	1
5:D:551:7Q9:O12	5:D:551:7Q9:C15	0.55	2.55	2	20
5:E:823:7Q9:O22	5:E:823:7Q9:O31	0.55	2.24	9	18
5:B:209:7Q9:C2	5:B:209:7Q9:O32	0.55	2.53	8	8
6:A:220:17F:H12A	5:D:502:7Q9:C38	0.55	2.32	5	1
5:E:803:7Q9:C315	6:E:810:17F:H70	0.55	2.32	7	3
6:D:520:17F:H10	6:D:520:17F:O8	0.55	2.01	17	5
5:D:523:7Q9:C32	6:D:552:17F:C2X	0.55	2.84	7	1
6:A:208:17F:H35	6:A:208:17F:C35	0.55	2.32	18	3
6:E:839:17F:H40	6:E:839:17F:H34	0.55	1.79	8	1
6:E:839:17F:H35	6:E:839:17F:H57	0.55	1.79	8	2
6:A:208:17F:H41	6:A:219:17F:H37	0.55	1.77	12	1
6:B:208:17F:H12	5:B:209:7Q9:C318	0.55	2.32	13	1
6:D:539:17F:H52	5:E:801:7Q9:C315	0.55	2.32	15	1
5:D:501:7Q9:O22	5:D:501:7Q9:O11	0.55	2.24	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:538:7Q9:C15	5:D:538:7Q9:O12	0.55	2.55	17	19
6:E:806:17F:H73	5:E:817:7Q9:C316	0.55	2.31	1	2
5:E:849:7Q9:C313	5:E:852:7Q9:C311	0.55	2.85	14	9
5:E:851:7Q9:C15	5:E:851:7Q9:O12	0.55	2.54	3	20
5:A:204:7Q9:C32	5:A:211:7Q9:C37	0.55	2.85	11	4
6:D:511:17F:H69	6:D:511:17F:H58	0.55	1.78	12	4
6:E:819:17F:H12A	6:E:820:17F:H30	0.55	1.75	3	3
5:D:549:7Q9:O14	5:D:549:7Q9:O21	0.55	2.24	6	5
6:E:839:17F:H35	6:E:839:17F:C31	0.55	2.31	10	3
1:A:15:GLY:CA	3:A:201:GSP:H8	0.55	2.15	17	2
6:E:839:17F:H10	6:E:857:17F:H35	0.55	1.77	5	1
6:E:856:17F:H18	5:E:868:7Q9:C11	0.55	2.32	5	2
6:E:818:17F:C1X	5:E:834:7Q9:C33	0.55	2.84	7	2
6:D:519:17F:C1Z	6:D:519:17F:C35	0.55	2.85	10	1
6:E:857:17F:H77	6:E:875:17F:H61	0.55	1.78	14	2
6:A:213:17F:H76	6:E:819:17F:H77	0.55	1.79	12	1
6:A:219:17F:H57	5:D:508:7Q9:C317	0.55	2.32	12	1
5:A:209:7Q9:O32	5:A:209:7Q9:O21	0.55	2.24	15	10
5:B:206:7Q9:C15	5:B:206:7Q9:O12	0.55	2.55	11	20
5:E:814:7Q9:O32	5:E:814:7Q9:O21	0.55	2.25	1	10
5:E:817:7Q9:C3	5:E:817:7Q9:O13	0.55	2.55	8	11
5:E:823:7Q9:O12	5:E:823:7Q9:C14	0.55	2.54	1	20
5:E:854:7Q9:C13	5:E:854:7Q9:O12	0.55	2.55	7	20
5:E:855:7Q9:C21	5:E:855:7Q9:O32	0.55	2.55	5	17
6:A:208:17F:C32	6:A:208:17F:C36	0.55	2.84	3	1
5:D:553:7Q9:O22	5:D:553:7Q9:O11	0.55	2.24	20	3
5:A:209:7Q9:C1	5:A:209:7Q9:O22	0.55	2.53	13	11
6:A:208:17F:N1	6:A:219:17F:O2	0.55	2.40	6	2
3:B:201:GSP:S1G	3:B:201:GSP:O1B	0.55	2.65	5	5
2:D:388:ARG:HB3	2:E:575:LEU:HD21	0.55	1.79	5	1
6:A:220:17F:H66	6:A:220:17F:C24	0.55	2.24	6	1
5:D:506:7Q9:C11	5:D:506:7Q9:C3	0.55	2.85	7	1
5:A:215:7Q9:C37	6:D:511:17F:H54	0.55	2.32	8	1
5:D:512:7Q9:C15	6:D:534:17F:H1	0.55	2.31	19	3
1:B:131:GLN:HG2	1:B:141:PHE:CD2	0.55	2.36	9	1
6:E:820:17F:H41	5:E:836:7Q9:C38	0.55	2.32	12	1
5:D:507:7Q9:O31	5:D:509:7Q9:C23	0.55	2.55	14	1
6:E:802:17F:H12	6:E:802:17F:C20	0.55	2.31	18	1
6:E:839:17F:H10A	6:E:857:17F:C22	0.55	2.32	18	1
2:D:340:LYS:HD2	2:E:626:LEU:HD21	0.55	1.78	20	1
2:D:370:LEU:HD21	5:E:877:7Q9:C316	0.55	2.31	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:504:7Q9:O12	5:D:504:7Q9:C13	0.55	2.55	6	20
5:E:831:7Q9:O32	5:E:831:7Q9:O21	0.55	2.25	18	14
5:E:841:7Q9:C1	5:E:841:7Q9:C31	0.55	2.85	18	20
6:A:219:17F:C7	6:A:219:17F:O9	0.55	2.55	2	2
6:D:510:17F:H76	6:D:517:17F:C41	0.55	2.32	2	1
5:B:210:7Q9:C317	6:D:520:17F:H76	0.55	2.31	3	1
5:E:865:7Q9:C21	5:E:865:7Q9:O13	0.55	2.55	10	11
5:E:804:7Q9:O22	5:E:804:7Q9:C35	0.55	2.55	5	7
5:E:804:7Q9:C1	5:E:814:7Q9:C14	0.55	2.85	10	3
6:A:208:17F:H40	6:A:208:17F:H34	0.55	1.78	12	1
6:D:540:17F:HN1	5:D:545:7Q9:C32	0.55	2.15	19	2
2:D:408:LYS:HB3	2:D:409:PRO:HD3	0.55	1.79	13	2
5:A:206:7Q9:C311	6:E:802:17F:H70	0.55	2.32	18	1
5:B:207:7Q9:O22	5:B:207:7Q9:C3	0.54	2.50	1	11
5:E:801:7Q9:O12	5:E:801:7Q9:C13	0.54	2.55	1	20
5:E:863:7Q9:O22	5:E:863:7Q9:C1	0.54	2.54	16	4
5:A:207:7Q9:O22	5:B:203:7Q9:C12	0.54	2.55	11	4
6:D:552:17F:H62	6:D:552:17F:C31	0.54	2.26	15	12
6:E:808:17F:O4	5:E:814:7Q9:C14	0.54	2.56	19	7
5:E:821:7Q9:O12	5:E:821:7Q9:C14	0.54	2.54	11	18
6:E:871:17F:H10A	5:E:872:7Q9:O14	0.54	2.02	2	1
6:D:540:17F:C32	6:D:540:17F:C36	0.54	2.78	20	9
6:E:819:17F:O5	5:E:825:7Q9:C15	0.54	2.55	6	3
6:A:219:17F:H52	5:E:828:7Q9:C317	0.54	2.31	6	1
6:A:213:17F:C11	6:A:213:17F:C34	0.54	2.86	7	1
6:E:829:17F:H36	6:E:829:17F:C32	0.54	2.32	8	2
6:E:806:17F:C30	6:E:806:17F:H68	0.54	2.31	19	3
2:E:740:LEU:HD21	5:E:870:7Q9:C318	0.54	2.32	12	1
5:E:854:7Q9:O14	5:E:854:7Q9:C13	0.54	2.55	15	2
5:E:803:7Q9:C312	6:E:806:17F:H64	0.54	2.32	13	2
5:B:209:7Q9:C36	6:D:520:17F:H61	0.54	2.31	16	1
5:E:869:7Q9:O32	5:E:869:7Q9:C21	0.54	2.54	18	1
5:E:803:7Q9:C2	5:E:803:7Q9:O32	0.54	2.53	11	10
5:E:841:7Q9:C11	5:E:850:7Q9:C22	0.54	2.86	18	4
6:E:873:17F:H44	6:E:873:17F:C32	0.54	2.33	12	5
5:A:212:7Q9:C311	5:A:212:7Q9:C37	0.54	2.83	7	2
6:D:534:17F:O2	6:D:534:17F:O9	0.54	2.24	2	8
5:E:853:7Q9:C23	5:E:878:7Q9:C22	0.54	2.85	3	4
5:D:504:7Q9:C37	5:D:508:7Q9:C313	0.54	2.85	5	2
5:E:845:7Q9:O22	5:E:845:7Q9:C3	0.54	2.52	19	11
5:E:840:7Q9:O32	5:E:840:7Q9:C21	0.54	2.55	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:208:17F:O10	6:B:208:17F:H20A	0.54	2.02	6	1
2:D:322:LEU:HD22	2:E:644:LEU:HD22	0.54	1.79	8	1
5:D:524:7Q9:C13	6:D:539:17F:O5	0.54	2.55	18	2
6:E:819:17F:H20	5:E:838:7Q9:C12	0.54	2.32	12	2
1:A:12:ASP:HA	3:A:201:GSP:O1B	0.54	2.03	13	2
6:E:857:17F:H37	6:E:857:17F:H68	0.54	1.80	14	1
6:B:208:17F:H12	5:B:209:7Q9:C310	0.54	2.32	18	1
6:E:842:17F:H4A	6:E:842:17F:C3	0.54	2.32	20	1
6:A:208:17F:O9	6:A:208:17F:C7	0.54	2.55	19	15
6:A:213:17F:O1	6:A:213:17F:O9	0.54	2.26	20	8
5:B:205:7Q9:O32	6:B:208:17F:H1	0.54	2.02	1	1
5:D:527:7Q9:C314	5:D:531:7Q9:C316	0.54	2.86	18	3
5:D:546:7Q9:O22	5:D:546:7Q9:O31	0.54	2.25	16	17
5:E:816:7Q9:O22	5:E:816:7Q9:C1	0.54	2.49	5	16
5:E:853:7Q9:C312	5:E:853:7Q9:C38	0.54	2.81	1	7
6:D:510:17F:C25	6:D:517:17F:H64	0.54	2.33	2	6
5:E:834:7Q9:O13	5:E:834:7Q9:C2	0.54	2.55	20	8
2:D:374:LEU:HD23	5:D:535:7Q9:C39	0.54	2.32	4	5
5:D:515:7Q9:C311	5:D:515:7Q9:C37	0.54	2.85	8	2
5:E:835:7Q9:C317	6:E:856:17F:H67	0.54	2.32	3	2
5:E:835:7Q9:O32	5:E:835:7Q9:O21	0.54	2.26	19	11
6:D:533:17F:H49	6:E:857:17F:C42	0.54	2.33	7	2
6:D:539:17F:C35	6:D:539:17F:H38	0.54	2.33	6	3
6:A:208:17F:O7	6:A:208:17F:P1	0.54	2.65	10	1
6:A:219:17F:O8	6:A:219:17F:C17	0.54	2.56	13	1
5:A:203:7Q9:C15	5:B:203:7Q9:O32	0.54	2.55	16	1
6:A:219:17F:H57	5:E:801:7Q9:C36	0.54	2.32	17	1
5:A:205:7Q9:C33	5:A:212:7Q9:C32	0.54	2.85	20	1
5:E:854:7Q9:C311	5:E:854:7Q9:C37	0.54	2.82	9	16
6:E:857:17F:C7	6:E:857:17F:C4	0.54	2.84	4	2
5:B:206:7Q9:O21	5:B:206:7Q9:C11	0.54	2.55	15	2
5:E:826:7Q9:C33	5:E:845:7Q9:C38	0.54	2.85	4	2
6:A:219:17F:O9	6:D:518:17F:H11A	0.54	2.01	6	1
5:E:849:7Q9:C317	5:E:852:7Q9:C316	0.54	2.85	14	4
5:D:512:7Q9:O13	6:D:534:17F:C4	0.54	2.56	8	2
5:D:507:7Q9:C32	5:D:509:7Q9:C23	0.54	2.85	9	1
6:E:819:17F:H58	6:E:842:17F:H53	0.54	1.80	12	1
5:D:524:7Q9:C15	6:D:539:17F:H1A	0.54	2.32	15	1
6:E:802:17F:O8	6:E:802:17F:H10	0.54	2.02	14	6
5:E:852:7Q9:O22	5:E:852:7Q9:C3	0.54	2.51	12	6
2:E:674:LEU:HD21	6:E:856:17F:H12	0.54	1.78	4	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:806:17F:H20	5:E:811:7Q9:C22	0.54	2.33	3	1
6:B:208:17F:H12A	5:B:209:7Q9:C39	0.54	2.32	4	1
5:E:814:7Q9:C33	5:E:830:7Q9:C22	0.54	2.85	5	2
6:D:540:17F:C2X	6:D:540:17F:C33	0.54	2.86	7	6
6:D:533:17F:H77	6:D:533:17F:C26	0.54	2.33	8	1
6:A:219:17F:C26	5:D:505:7Q9:C37	0.54	2.85	10	1
5:E:822:7Q9:O21	5:E:822:7Q9:O12	0.54	2.26	10	1
5:A:215:7Q9:C15	5:A:216:7Q9:O13	0.54	2.56	18	1
6:D:520:17F:C27	6:D:520:17F:H70	0.54	2.33	19	1
1:A:126:ASP:O	1:A:129:GLN:HG2	0.54	2.03	3	3
6:A:213:17F:O1	6:A:213:17F:C19	0.54	2.55	18	4
6:A:219:17F:O10	6:D:518:17F:H9	0.54	2.03	2	1
5:D:523:7Q9:C3	5:D:523:7Q9:O22	0.54	2.50	19	4
6:E:808:17F:C28	6:E:808:17F:H74	0.54	2.33	7	2
5:E:809:7Q9:C38	6:E:812:17F:H37	0.54	2.32	2	2
5:E:822:7Q9:O31	5:E:822:7Q9:O22	0.54	2.26	10	6
5:A:215:7Q9:C313	5:A:216:7Q9:C316	0.54	2.86	7	2
5:D:555:7Q9:C35	6:E:857:17F:H54	0.54	2.33	4	1
6:E:810:17F:C31	6:E:810:17F:H29	0.54	2.32	5	1
2:D:430:LEU:CD2	6:D:539:17F:H33	0.54	2.32	7	2
5:B:205:7Q9:C315	6:B:208:17F:H44	0.54	2.32	8	2
6:D:540:17F:C36	6:D:540:17F:C32	0.54	2.80	13	2
6:A:220:17F:H67	6:A:220:17F:H48	0.54	1.79	19	2
5:A:206:7Q9:C15	5:A:211:7Q9:C22	0.54	2.85	11	4
2:D:437:THR:HG23	5:D:543:7Q9:O31	0.54	2.02	12	1
5:E:821:7Q9:C21	5:E:821:7Q9:O14	0.54	2.55	13	1
6:A:213:17F:H74	6:E:810:17F:C30	0.54	2.32	17	1
6:D:539:17F:H47	5:D:549:7Q9:C23	0.54	2.33	18	1
6:D:511:17F:H1A	5:D:513:7Q9:C15	0.54	2.33	20	1
6:E:806:17F:O1	6:E:806:17F:C6	0.54	2.55	20	1
5:A:204:7Q9:O32	5:A:204:7Q9:O21	0.54	2.26	19	16
1:B:147:LYS:HB2	3:B:201:GSP:N1	0.54	2.18	12	2
5:B:210:7Q9:C316	5:D:501:7Q9:C312	0.54	2.85	15	6
5:E:835:7Q9:O12	5:E:835:7Q9:C15	0.54	2.56	9	20
6:D:520:17F:H64	6:D:520:17F:H59	0.54	1.80	5	2
1:A:79:LEU:HD13	1:A:159:LEU:HD22	0.54	1.80	13	3
6:D:540:17F:C34	6:D:540:17F:H35	0.54	2.32	6	3
2:D:273:ASP:CB	6:D:540:17F:H34	0.54	2.20	10	1
6:D:539:17F:H62	6:D:539:17F:C22	0.54	2.33	16	1
1:B:84:ILE:HD13	1:B:118:CYS:HA	0.54	1.78	6	6
5:D:503:7Q9:C31	5:D:503:7Q9:O22	0.54	2.56	18	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:818:17F:O10	5:E:821:7Q9:C14	0.54	2.56	1	2
5:E:841:7Q9:C13	5:E:841:7Q9:O12	0.54	2.56	9	20
5:E:847:7Q9:P	5:E:847:7Q9:C14	0.54	2.96	10	3
5:B:206:7Q9:C21	5:B:206:7Q9:O32	0.54	2.56	6	13
6:E:808:17F:C42	6:E:808:17F:H47	0.54	2.32	10	9
6:E:820:17F:C4	6:E:820:17F:C7	0.54	2.85	14	5
6:A:213:17F:H51	5:D:507:7Q9:C318	0.54	2.33	3	2
6:E:839:17F:H43	5:E:858:7Q9:C310	0.54	2.32	18	3
5:E:849:7Q9:C13	5:E:853:7Q9:O14	0.54	2.54	3	2
6:A:219:17F:O10	6:A:219:17F:C6	0.54	2.49	4	2
6:E:808:17F:H57	6:E:820:17F:H29	0.54	1.80	4	1
5:D:502:7Q9:O32	5:D:525:7Q9:C15	0.54	2.55	15	3
6:D:517:17F:H19	6:D:517:17F:H1A	0.54	1.80	10	1
6:D:520:17F:H76	5:E:823:7Q9:C39	0.54	2.33	13	1
6:D:510:17F:C5	6:D:517:17F:H9	0.54	2.32	15	1
6:A:219:17F:O8	6:A:219:17F:H19	0.54	2.03	16	1
2:D:333:LYS:HE3	5:D:538:7Q9:C313	0.54	2.33	17	1
5:E:825:7Q9:O22	5:E:825:7Q9:C3	0.54	2.52	17	15
5:E:825:7Q9:C2	5:E:825:7Q9:O13	0.54	2.56	13	17
2:E:733:LEU:HD12	5:E:876:7Q9:C311	0.54	2.33	7	4
5:D:528:7Q9:C3	5:D:528:7Q9:O22	0.54	2.54	15	6
5:E:811:7Q9:O31	5:E:826:7Q9:C37	0.54	2.56	4	1
1:A:15:GLY:HA3	3:A:201:GSP:C8	0.54	2.38	9	4
6:D:518:17F:O10	5:D:528:7Q9:C2	0.54	2.56	20	6
5:E:821:7Q9:C1	5:E:821:7Q9:O22	0.54	2.50	11	3
6:E:808:17F:O2	5:E:814:7Q9:C14	0.54	2.56	16	5
5:D:516:7Q9:O22	5:D:537:7Q9:C15	0.54	2.55	8	2
6:D:540:17F:H35	6:D:540:17F:C36	0.54	2.26	10	1
5:E:838:7Q9:C32	6:E:842:17F:H50	0.54	2.33	12	1
6:E:873:17F:H39	6:E:873:17F:C20	0.54	2.33	17	2
5:D:515:7Q9:C32	6:D:519:17F:H19	0.54	2.33	20	1
5:A:207:7Q9:C13	5:A:207:7Q9:O12	0.54	2.55	12	20
5:D:544:7Q9:O21	5:D:544:7Q9:O32	0.54	2.26	10	13
5:E:828:7Q9:C1	5:E:828:7Q9:O22	0.54	2.52	14	10
6:E:839:17F:C19	6:E:839:17F:C31	0.54	2.84	2	8
5:D:542:7Q9:C21	5:D:542:7Q9:O31	0.54	2.56	16	4
6:A:213:17F:O8	5:D:503:7Q9:C15	0.54	2.56	3	1
1:B:64:TYR:O	1:B:68:ARG:HB2	0.54	2.02	4	1
5:D:516:7Q9:C34	5:D:516:7Q9:O31	0.54	2.55	14	8
1:A:6:LEU:HD22	1:A:159:LEU:HG	0.54	1.78	13	2
6:D:511:17F:H55	6:E:829:17F:H52	0.54	1.79	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:839:17F:H51	5:E:858:7Q9:C315	0.54	2.33	9	1
3:B:201:GSP:H5'1	3:B:201:GSP:O1B	0.54	2.03	11	1
5:A:210:7Q9:C12	5:A:210:7Q9:C34	0.54	2.86	12	1
5:A:216:7Q9:C34	6:D:517:17F:C1Y	0.54	2.86	12	1
6:E:839:17F:O8	6:E:857:17F:H35	0.54	2.03	12	1
5:D:506:7Q9:C3	5:D:506:7Q9:O13	0.54	2.56	17	1
6:D:533:17F:H20A	6:D:533:17F:O1	0.54	2.02	17	1
5:D:538:7Q9:C31	5:D:538:7Q9:O11	0.54	2.56	17	1
5:D:531:7Q9:C312	5:D:531:7Q9:C38	0.54	2.86	18	1
5:D:506:7Q9:C316	6:E:818:17F:H45	0.54	2.32	20	1
5:D:505:7Q9:O22	5:D:505:7Q9:O11	0.53	2.26	6	8
5:D:515:7Q9:O32	5:D:515:7Q9:C2	0.53	2.53	7	8
5:D:529:7Q9:O12	5:D:529:7Q9:C14	0.53	2.56	2	20
5:E:815:7Q9:O32	5:E:815:7Q9:O21	0.53	2.26	10	17
1:A:8:VAL:HG12	1:A:16:LYS:HD2	0.53	1.80	5	4
5:D:525:7Q9:C37	5:D:547:7Q9:C37	0.53	2.86	4	1
5:E:804:7Q9:C13	5:E:815:7Q9:O22	0.53	2.56	6	1
6:D:539:17F:C40	5:D:549:7Q9:O32	0.53	2.56	9	1
2:D:337:LEU:HG	2:E:626:LEU:HB3	0.53	1.80	12	1
6:D:510:17F:C1X	6:D:510:17F:C23	0.53	2.82	12	1
6:D:534:17F:H9A	5:D:538:7Q9:C37	0.53	2.32	17	1
5:E:804:7Q9:C31	6:E:808:17F:C8	0.53	2.83	17	1
6:E:819:17F:H12A	6:E:820:17F:C21	0.53	2.33	17	2
5:A:203:7Q9:C37	6:A:208:17F:H61	0.53	2.33	19	1
5:B:209:7Q9:C14	5:B:209:7Q9:O12	0.53	2.56	1	1
5:B:210:7Q9:C317	5:E:823:7Q9:C38	0.53	2.87	15	10
5:E:807:7Q9:C15	5:E:807:7Q9:C21	0.53	2.86	8	6
5:E:861:7Q9:O21	5:E:861:7Q9:O32	0.53	2.25	19	20
6:E:875:17F:P1	6:E:875:17F:C6	0.53	2.96	20	16
5:A:211:7Q9:C1	5:A:211:7Q9:O22	0.53	2.50	3	8
6:B:208:17F:C4	6:B:208:17F:C7	0.53	2.87	8	15
5:D:512:7Q9:O32	5:D:512:7Q9:O21	0.53	2.26	4	14
5:A:209:7Q9:C13	5:A:209:7Q9:O31	0.53	2.56	6	6
6:D:518:17F:O6	6:D:518:17F:C2	0.53	2.55	4	2
2:D:440:LEU:HD22	6:D:552:17F:H78	0.53	1.81	7	1
6:E:808:17F:H30	6:E:808:17F:H33	0.53	1.80	8	1
6:B:208:17F:H42	6:B:208:17F:C1X	0.53	2.33	9	1
5:E:814:7Q9:C313	6:E:820:17F:H49	0.53	2.33	9	1
6:E:829:17F:H34	5:E:830:7Q9:O32	0.53	2.03	18	2
5:D:502:7Q9:C312	5:D:502:7Q9:C38	0.53	2.85	12	3
6:E:839:17F:O8	6:E:839:17F:H5	0.53	2.03	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:502:7Q9:O22	5:D:514:7Q9:C13	0.53	2.56	18	1
6:E:871:17F:C21	6:E:871:17F:C32	0.53	2.86	12	9
6:A:208:17F:H57	6:A:208:17F:C26	0.53	2.33	2	2
1:B:79:LEU:HD13	1:B:159:LEU:HD22	0.53	1.79	2	2
6:D:518:17F:H60	6:D:518:17F:H39	0.53	1.80	3	1
5:E:858:7Q9:C31	6:E:875:17F:H10A	0.53	2.33	17	2
5:E:855:7Q9:O11	5:E:855:7Q9:C14	0.53	2.56	20	4
5:E:809:7Q9:C33	6:E:812:17F:H37	0.53	2.32	6	1
5:E:804:7Q9:O22	5:E:804:7Q9:C31	0.53	2.56	19	4
6:A:220:17F:H64	6:A:220:17F:C12	0.53	2.30	8	1
6:D:539:17F:C18	6:D:539:17F:C31	0.53	2.56	8	1
6:E:808:17F:H72	6:E:819:17F:H54	0.53	1.80	8	1
5:D:529:7Q9:C13	5:D:553:7Q9:O13	0.53	2.56	9	1
5:E:853:7Q9:C15	5:E:853:7Q9:O11	0.53	2.56	13	1
6:E:820:17F:H76	5:E:830:7Q9:C23	0.53	2.33	14	1
6:E:871:17F:H75	6:E:871:17F:H48	0.53	1.81	17	1
6:E:806:17F:C40	5:E:817:7Q9:C318	0.53	2.85	20	2
2:D:429:PHE:CD1	6:D:539:17F:H69	0.53	2.38	19	3
5:E:825:7Q9:C1	5:E:825:7Q9:C31	0.53	2.86	7	15
5:E:876:7Q9:C3	5:E:876:7Q9:O22	0.53	2.52	8	4
6:E:820:17F:H19A	5:E:853:7Q9:C33	0.53	2.33	8	2
6:A:213:17F:C12	6:A:213:17F:C8	0.53	2.86	19	2
1:A:15:GLY:HA2	3:A:201:GSP:H8	0.53	1.62	14	5
6:D:510:17F:H5	6:D:533:17F:H18	0.53	1.80	6	2
5:E:840:7Q9:O32	5:E:841:7Q9:C22	0.53	2.56	7	2
5:A:207:7Q9:C36	5:B:207:7Q9:C34	0.53	2.87	10	1
6:E:808:17F:C22	6:E:810:17F:H32	0.53	2.34	13	3
5:E:843:7Q9:O22	5:E:843:7Q9:O31	0.53	2.27	17	4
6:D:518:17F:H20A	6:D:518:17F:C2X	0.53	2.33	17	5
5:E:853:7Q9:C3	5:E:853:7Q9:C11	0.53	2.87	20	3
6:D:533:17F:O2	5:D:541:7Q9:C15	0.53	2.56	3	1
5:A:205:7Q9:C13	5:A:210:7Q9:O32	0.53	2.56	4	3
5:D:543:7Q9:C1	5:D:543:7Q9:O22	0.53	2.54	17	6
6:A:219:17F:H71	5:D:505:7Q9:C38	0.53	2.33	20	3
5:E:840:7Q9:C34	5:E:841:7Q9:C22	0.53	2.86	11	2
6:A:213:17F:H51	6:A:213:17F:C38	0.53	2.33	16	1
5:D:515:7Q9:O13	5:D:525:7Q9:C13	0.53	2.57	1	1
2:E:605:GLN:HB2	5:E:867:7Q9:C313	0.53	2.34	1	1
5:E:836:7Q9:O32	5:E:836:7Q9:O21	0.53	2.27	20	13
6:E:839:17F:O2	6:E:839:17F:H5	0.53	2.04	11	4
1:A:161:ARG:NH1	1:B:131:GLN:HB3	0.53	2.18	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:534:17F:H6	5:D:538:7Q9:C14	0.53	2.33	2	1
6:E:856:17F:O9	6:E:856:17F:O8	0.53	2.27	3	1
6:A:208:17F:C24	6:A:219:17F:H12A	0.53	2.34	4	2
6:B:208:17F:H35	6:B:208:17F:C24	0.53	2.29	17	3
5:D:514:7Q9:C35	5:D:516:7Q9:C39	0.53	2.86	20	3
5:D:526:7Q9:C313	5:D:544:7Q9:C313	0.53	2.86	4	2
6:E:871:17F:H32	6:E:871:17F:H12	0.53	1.81	7	3
5:B:203:7Q9:C314	5:E:803:7Q9:C318	0.53	2.86	7	1
5:E:833:7Q9:O22	6:E:839:17F:H4A	0.53	2.02	8	1
5:A:217:7Q9:O11	5:A:217:7Q9:C13	0.53	2.56	10	1
6:D:517:17F:H70	6:D:517:17F:C30	0.53	2.33	12	1
6:E:819:17F:C33	6:E:842:17F:H53	0.53	2.33	12	2
5:E:832:7Q9:C21	5:E:832:7Q9:O32	0.53	2.57	16	4
5:E:803:7Q9:C313	6:E:806:17F:H64	0.53	2.33	13	1
5:A:216:7Q9:O22	5:A:216:7Q9:C1	0.53	2.55	9	7
1:B:84:ILE:CD1	1:B:118:CYS:HA	0.53	2.33	17	6
5:E:809:7Q9:C14	6:E:818:17F:O1	0.53	2.55	1	2
5:E:817:7Q9:C15	5:E:817:7Q9:O12	0.53	2.57	2	4
6:A:219:17F:O4	5:D:504:7Q9:C15	0.53	2.57	19	3
5:D:508:7Q9:O22	5:D:508:7Q9:C3	0.53	2.52	17	9
6:D:510:17F:P1	6:D:510:17F:N1	0.53	2.82	14	10
5:D:554:7Q9:O12	5:D:554:7Q9:O22	0.53	2.27	13	7
6:E:820:17F:H4A	6:E:820:17F:O8	0.53	2.02	3	4
2:D:342:SER:HB3	2:D:343:PRO:HD3	0.53	1.78	4	1
6:D:510:17F:C17	6:D:517:17F:H10	0.53	2.33	4	2
6:D:533:17F:O10	6:D:533:17F:H4	0.53	2.03	17	4
5:D:516:7Q9:O22	5:D:548:7Q9:C15	0.53	2.57	5	3
6:D:517:17F:H74	6:D:533:17F:C30	0.53	2.34	5	2
5:E:838:7Q9:O21	5:E:838:7Q9:C15	0.53	2.57	5	2
1:B:46:ILE:HG23	1:B:157:TYR:CD1	0.53	2.38	7	1
6:D:511:17F:H42	6:D:534:17F:C29	0.53	2.26	13	1
6:A:213:17F:HN1A	5:D:507:7Q9:C23	0.53	2.17	1	1
6:D:510:17F:H6	6:D:517:17F:C4	0.53	2.34	6	4
5:E:853:7Q9:O31	5:E:853:7Q9:C11	0.53	2.56	5	1
5:D:509:7Q9:C312	5:D:531:7Q9:C316	0.53	2.87	20	2
5:E:834:7Q9:C23	5:E:858:7Q9:C35	0.53	2.87	7	1
6:A:219:17F:C26	5:D:505:7Q9:C312	0.53	2.86	9	2
6:B:208:17F:O4	5:B:209:7Q9:C15	0.53	2.57	9	3
6:D:518:17F:O9	6:D:518:17F:O1	0.53	2.26	12	4
5:D:503:7Q9:C312	5:D:503:7Q9:C38	0.53	2.83	13	2
1:B:117:LYS:HE2	3:B:201:GSP:C5	0.53	2.38	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:126:ASP:OD2	1:B:128:LYS:HB3	0.53	2.04	16	1
5:B:204:7Q9:O13	5:B:205:7Q9:O12	0.53	2.26	16	1
5:D:531:7Q9:O21	5:D:531:7Q9:O32	0.53	2.27	19	15
6:E:810:17F:O7	6:E:810:17F:O10	0.53	2.27	20	17
5:D:524:7Q9:C15	5:D:524:7Q9:O12	0.53	2.57	15	2
6:D:534:17F:O10	6:D:534:17F:H9	0.53	2.04	7	9
1:A:72:MET:HA	1:A:78:PHE:HZ	0.53	1.63	7	2
6:A:220:17F:H54	6:A:220:17F:C34	0.53	2.33	3	1
5:B:205:7Q9:C310	6:B:208:17F:H74	0.53	2.34	4	1
2:D:269:GLN:HG3	6:D:540:17F:H32	0.53	1.81	5	1
6:D:533:17F:H54	6:E:857:17F:H74	0.53	1.79	5	2
6:D:517:17F:H39	6:D:517:17F:H64	0.53	1.81	8	1
5:A:218:7Q9:C2	5:A:218:7Q9:O32	0.53	2.54	9	1
5:E:822:7Q9:O21	5:E:822:7Q9:P	0.53	2.67	10	1
6:A:213:17F:H10	5:D:503:7Q9:C22	0.53	2.34	11	1
5:D:503:7Q9:O22	5:D:503:7Q9:C31	0.53	2.56	13	1
6:A:208:17F:C1Z	6:A:208:17F:H40	0.53	2.33	18	2
6:D:520:17F:H55	6:D:520:17F:C39	0.53	2.34	15	2
6:A:208:17F:HN1A	6:A:219:17F:H1	0.53	1.63	1	2
5:D:528:7Q9:C318	6:E:873:17F:H50	0.53	2.33	1	1
5:E:855:7Q9:C14	5:E:855:7Q9:O12	0.53	2.57	12	20
5:D:513:7Q9:O32	5:D:513:7Q9:O21	0.53	2.27	2	1
6:E:808:17F:H69	5:E:814:7Q9:C312	0.53	2.34	3	3
6:E:856:17F:O8	6:E:856:17F:C17	0.53	2.57	3	1
5:E:851:7Q9:C38	6:E:871:17F:H20A	0.53	2.34	5	2
2:D:423:GLU:HA	2:D:426:LYS:HE2	0.53	1.80	12	2
5:D:509:7Q9:O14	5:D:526:7Q9:C14	0.53	2.57	5	3
5:A:203:7Q9:O32	6:A:208:17F:H9	0.53	2.03	7	1
6:B:208:17F:O1	6:B:208:17F:H2	0.53	2.02	7	1
6:E:802:17F:H1A	6:E:802:17F:H4	0.53	1.80	14	2
5:E:834:7Q9:C316	6:E:839:17F:H53	0.53	2.34	14	1
5:A:215:7Q9:C317	5:E:821:7Q9:C314	0.53	2.86	17	1
2:E:711:LEU:HB2	5:E:866:7Q9:C311	0.53	2.34	17	1
6:E:806:17F:H74	5:E:811:7Q9:C315	0.53	2.34	17	1
5:D:555:7Q9:O22	5:D:555:7Q9:C1	0.52	2.53	20	8
5:D:501:7Q9:O22	5:D:501:7Q9:C3	0.52	2.52	3	13
5:E:876:7Q9:O22	5:E:876:7Q9:C3	0.52	2.54	6	8
5:D:541:7Q9:C14	5:D:541:7Q9:O12	0.52	2.57	17	6
6:A:213:17F:H63	6:A:213:17F:C31	0.52	2.28	5	4
6:A:220:17F:H11	5:D:515:7Q9:C23	0.52	2.33	5	2
6:D:517:17F:C42	6:E:839:17F:H73	0.52	2.34	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:833:7Q9:C316	6:E:857:17F:H55	0.52	2.34	10	1
5:E:864:7Q9:C13	5:E:874:7Q9:O13	0.52	2.57	10	1
6:D:519:17F:H46	5:D:526:7Q9:C312	0.52	2.34	16	1
6:E:808:17F:H69	6:E:820:17F:H37	0.52	1.81	16	1
6:A:213:17F:H44	5:D:507:7Q9:C36	0.52	2.34	17	1
6:A:213:17F:H50	5:D:507:7Q9:C318	0.52	2.34	1	1
1:B:17:SER:OG	3:B:201:GSP:O3G	0.52	2.26	20	8
1:B:131:GLN:HE21	1:B:141:PHE:HD2	0.52	1.45	2	1
5:E:809:7Q9:O22	5:E:809:7Q9:O31	0.52	2.27	20	3
5:E:851:7Q9:C313	6:E:871:17F:H20A	0.52	2.35	3	1
6:B:208:17F:O1	6:B:208:17F:C5	0.52	2.56	9	3
5:A:218:7Q9:O14	6:D:511:17F:C4	0.52	2.50	5	1
6:E:810:17F:C2X	6:E:810:17F:C31	0.52	2.82	5	2
5:E:870:7Q9:C12	6:E:873:17F:O4	0.52	2.57	13	1
6:E:839:17F:C28	6:E:875:17F:H51	0.52	2.34	17	1
5:B:204:7Q9:C318	6:E:818:17F:H53	0.52	2.34	19	1
6:E:806:17F:H69	5:E:817:7Q9:C318	0.52	2.34	19	1
5:D:512:7Q9:C13	6:D:534:17F:C4	0.52	2.88	15	5
5:E:849:7Q9:O21	5:E:849:7Q9:C31	0.52	2.57	7	10
5:E:826:7Q9:C1	5:E:826:7Q9:O22	0.52	2.56	3	10
5:E:863:7Q9:O32	5:E:863:7Q9:O21	0.52	2.27	16	14
6:D:540:17F:C10	5:D:545:7Q9:C36	0.52	2.86	7	3
6:D:510:17F:O10	6:D:533:17F:C20	0.52	2.58	4	2
5:E:858:7Q9:C3	6:E:875:17F:H9	0.52	2.34	4	3
6:E:839:17F:H49	6:E:875:17F:H55	0.52	1.82	5	1
6:D:520:17F:H72	6:D:520:17F:H55	0.52	1.80	7	1
5:D:524:7Q9:O13	5:D:543:7Q9:C12	0.52	2.58	8	4
6:E:829:17F:O8	5:E:833:7Q9:C12	0.52	2.58	8	1
5:E:803:7Q9:C315	6:E:810:17F:H72	0.52	2.35	9	2
6:A:220:17F:H30	6:A:220:17F:C23	0.52	2.34	10	1
6:D:510:17F:H40	6:D:510:17F:C1X	0.52	2.19	12	1
6:A:213:17F:C24	6:A:213:17F:H56	0.52	2.35	13	1
5:D:502:7Q9:O21	5:D:502:7Q9:P	0.52	2.67	14	17
6:D:511:17F:H38	5:D:513:7Q9:C314	0.52	2.33	1	1
5:D:513:7Q9:O21	5:D:513:7Q9:O32	0.52	2.28	1	3
5:D:527:7Q9:C15	5:D:527:7Q9:O12	0.52	2.57	13	20
5:E:814:7Q9:O12	5:E:814:7Q9:C15	0.52	2.58	14	15
5:D:553:7Q9:C21	5:D:553:7Q9:C12	0.52	2.87	17	3
5:E:855:7Q9:C32	5:E:859:7Q9:C35	0.52	2.88	7	4
6:A:213:17F:H38	6:A:213:17F:H34	0.52	1.81	4	1
1:B:68:ARG:HB3	1:B:99:GLN:HE22	0.52	1.64	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:819:17F:C10	6:E:820:17F:C10	0.52	2.87	17	3
6:E:839:17F:C10	6:E:857:17F:H12	0.52	2.34	4	1
6:E:802:17F:H20	6:E:802:17F:C12	0.52	2.33	18	4
6:A:213:17F:H9	5:D:503:7Q9:C23	0.52	2.35	12	3
5:D:556:7Q9:C12	5:E:865:7Q9:O22	0.52	2.57	9	1
5:E:807:7Q9:C14	5:E:807:7Q9:O32	0.52	2.57	9	2
5:E:853:7Q9:O22	5:E:859:7Q9:C14	0.52	2.57	13	1
6:E:857:17F:H59	6:E:857:17F:C26	0.52	2.30	13	1
6:E:857:17F:C42	6:E:875:17F:H65	0.52	2.34	16	2
5:E:807:7Q9:C22	6:E:818:17F:H4A	0.52	2.34	19	1
5:E:865:7Q9:O12	5:E:865:7Q9:C14	0.52	2.57	13	15
6:A:220:17F:O8	6:A:220:17F:C5	0.52	2.53	2	5
5:D:509:7Q9:C312	5:D:527:7Q9:C314	0.52	2.87	2	2
6:D:517:17F:H37	6:D:533:17F:C40	0.52	2.24	2	1
5:E:874:7Q9:O32	5:E:874:7Q9:O21	0.52	2.27	2	10
5:D:544:7Q9:O32	5:D:544:7Q9:O21	0.52	2.28	17	2
5:D:503:7Q9:O32	5:D:503:7Q9:C2	0.52	2.54	20	8
6:E:802:17F:H57	6:E:802:17F:H63	0.52	1.80	12	3
6:E:808:17F:C20	6:E:810:17F:H20	0.52	2.33	11	1
6:E:819:17F:H40	5:E:836:7Q9:C37	0.52	2.34	15	1
5:E:811:7Q9:C2	5:E:811:7Q9:O32	0.52	2.54	20	9
5:E:814:7Q9:C15	5:E:814:7Q9:O13	0.52	2.58	15	15
1:A:57:ASP:OD2	3:A:201:GSP:O3G	0.52	2.27	2	5
5:D:555:7Q9:C13	5:D:555:7Q9:O14	0.52	2.57	3	10
6:E:819:17F:H42	5:E:836:7Q9:C39	0.52	2.35	17	2
5:E:859:7Q9:C1	5:E:859:7Q9:O22	0.52	2.54	3	5
5:B:205:7Q9:O22	5:B:205:7Q9:C1	0.52	2.56	5	8
5:D:548:7Q9:O22	5:D:548:7Q9:C3	0.52	2.56	14	3
5:A:207:7Q9:C13	5:A:207:7Q9:O11	0.52	2.57	7	2
6:B:208:17F:C4	6:B:208:17F:O8	0.52	2.57	7	1
6:E:808:17F:H12	6:E:808:17F:H58	0.52	1.80	14	1
5:A:203:7Q9:C14	5:B:203:7Q9:O32	0.52	2.58	16	1
5:E:862:7Q9:C2	5:E:877:7Q9:C11	0.52	2.88	17	1
6:E:839:17F:H39	6:E:839:17F:H34	0.52	1.80	19	1
5:A:215:7Q9:C12	5:A:216:7Q9:O14	0.52	2.58	20	1
5:D:529:7Q9:O32	5:D:529:7Q9:O21	0.52	2.28	16	14
5:D:532:7Q9:C13	5:D:532:7Q9:C32	0.52	2.88	13	2
1:B:126:ASP:OD2	1:B:128:LYS:HB2	0.52	2.04	4	1
6:D:517:17F:O10	6:D:517:17F:C6	0.52	2.52	13	8
5:E:824:7Q9:O22	5:E:846:7Q9:C13	0.52	2.57	5	1
5:D:516:7Q9:C1	5:D:548:7Q9:C15	0.52	2.88	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:860:7Q9:C3	5:E:865:7Q9:C15	0.52	2.88	15	4
6:A:208:17F:H58	6:A:208:17F:H45	0.52	1.82	7	1
5:B:205:7Q9:C318	6:E:812:17F:H46	0.52	2.35	7	1
5:D:516:7Q9:O13	5:D:548:7Q9:C15	0.52	2.57	15	4
5:E:825:7Q9:C35	6:E:842:17F:H20A	0.52	2.35	7	2
5:E:833:7Q9:C312	5:E:852:7Q9:C36	0.52	2.88	9	1
5:D:526:7Q9:O14	5:D:526:7Q9:C2	0.52	2.57	13	3
5:E:833:7Q9:C23	6:E:857:17F:H12	0.52	2.35	13	1
1:B:6:LEU:HB2	1:B:55:ILE:HG12	0.52	1.81	14	1
6:D:539:17F:O7	6:D:539:17F:O6	0.52	2.28	12	6
5:A:205:7Q9:C14	5:A:205:7Q9:C22	0.52	2.88	6	6
6:D:510:17F:C28	6:D:517:17F:H67	0.52	2.33	2	3
5:D:512:7Q9:C21	5:D:512:7Q9:O32	0.52	2.58	12	2
6:E:820:17F:O2	5:E:830:7Q9:C12	0.52	2.58	17	3
5:D:528:7Q9:O22	5:D:528:7Q9:O11	0.52	2.28	11	3
6:D:533:17F:H30	6:D:533:17F:C37	0.52	2.35	12	4
6:A:208:17F:H56	5:D:505:7Q9:C36	0.52	2.35	5	1
5:E:863:7Q9:C1	5:E:863:7Q9:O22	0.52	2.55	9	5
5:A:218:7Q9:C15	6:D:511:17F:O2	0.52	2.58	6	1
6:A:220:17F:H52	6:A:220:17F:C34	0.52	2.35	6	1
5:A:211:7Q9:C15	5:A:211:7Q9:O32	0.52	2.57	7	1
6:E:810:17F:C1X	6:E:810:17F:C23	0.52	2.76	9	3
2:E:641:LEU:HG	5:E:852:7Q9:C312	0.52	2.35	9	1
5:B:205:7Q9:C310	6:B:208:17F:C31	0.52	2.85	10	1
5:D:526:7Q9:C22	5:D:544:7Q9:O31	0.52	2.58	11	1
5:E:805:7Q9:C14	5:E:816:7Q9:O22	0.52	2.58	12	1
5:A:214:7Q9:C318	6:E:820:17F:H76	0.52	2.35	13	1
6:E:810:17F:H48	6:E:810:17F:H61	0.52	1.81	16	1
6:E:875:17F:O9	6:E:875:17F:C1	0.52	2.57	18	1
5:D:507:7Q9:O32	5:D:507:7Q9:C21	0.52	2.57	17	15
5:E:865:7Q9:C2	5:E:865:7Q9:O32	0.52	2.54	12	6
1:B:57:ASP:OD2	3:B:201:GSP:O3G	0.52	2.28	14	4
5:B:204:7Q9:C316	6:E:802:17F:H53	0.52	2.35	4	1
6:B:208:17F:O2	6:B:208:17F:C2	0.52	2.58	17	3
5:D:514:7Q9:O32	5:D:514:7Q9:C2	0.52	2.56	19	6
5:A:203:7Q9:C13	5:B:205:7Q9:O14	0.52	2.58	7	1
5:D:556:7Q9:O32	5:D:556:7Q9:C2	0.52	2.56	10	1
6:D:518:17F:O2	6:D:518:17F:C2	0.52	2.58	11	1
1:B:117:LYS:HE2	3:B:201:GSP:N3	0.52	2.20	13	1
6:D:511:17F:C10	5:D:513:7Q9:C23	0.52	2.87	13	1
6:D:510:17F:H50	6:D:517:17F:C23	0.52	2.35	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:511:17F:H43	5:D:513:7Q9:C315	0.52	2.34	17	1
6:E:839:17F:C8	6:E:857:17F:H30	0.52	2.34	19	1
6:E:839:17F:H8	6:E:857:17F:H41	0.52	1.82	1	2
6:E:819:17F:C42	6:E:819:17F:C27	0.52	2.85	3	1
5:E:838:7Q9:C11	6:E:842:17F:O10	0.52	2.58	3	1
6:A:219:17F:H56	6:D:518:17F:C22	0.52	2.35	5	1
5:A:211:7Q9:C316	6:A:220:17F:H34	0.52	2.35	7	1
1:A:34:PRO:HA	3:A:201:GSP:S1G	0.52	2.45	8	1
5:E:870:7Q9:O22	6:E:873:17F:H9A	0.52	2.05	10	1
6:D:510:17F:H56	6:D:517:17F:C1X	0.52	2.34	11	1
2:D:396:ALA:HA	5:D:537:7Q9:C316	0.52	2.34	15	2
6:D:510:17F:H6A	6:D:517:17F:H11A	0.52	1.82	15	1
6:A:219:17F:H31	5:E:801:7Q9:C36	0.52	2.34	17	1
6:D:510:17F:H74	6:E:857:17F:H48	0.52	1.81	17	1
6:A:219:17F:O8	5:D:505:7Q9:C35	0.52	2.58	18	1
6:D:510:17F:C1X	6:D:517:17F:H8A	0.52	2.35	20	1
5:D:516:7Q9:C22	5:D:537:7Q9:C14	0.51	2.87	1	3
2:E:628:GLU:OE2	2:E:631:ARG:HD3	0.51	2.05	18	2
5:A:211:7Q9:C312	6:A:213:17F:C36	0.51	2.88	3	1
6:E:808:17F:O10	6:E:808:17F:C4	0.51	2.54	14	6
5:E:838:7Q9:C314	5:E:867:7Q9:C318	0.51	2.88	3	3
5:B:206:7Q9:O32	5:B:206:7Q9:O21	0.51	2.28	5	4
6:E:839:17F:H49	6:E:875:17F:H53	0.51	1.82	7	1
5:D:537:7Q9:C22	5:D:548:7Q9:C39	0.51	2.87	8	1
6:B:208:17F:O4	5:B:209:7Q9:C12	0.51	2.59	9	1
6:D:519:17F:H48	6:D:519:17F:H69	0.51	1.82	12	1
6:D:510:17F:H8	6:D:517:17F:H19	0.51	1.82	14	1
5:A:214:7Q9:C313	5:A:218:7Q9:C315	0.51	2.87	19	1
5:E:813:7Q9:O22	5:E:813:7Q9:O31	0.51	2.28	19	15
5:E:855:7Q9:O21	5:E:855:7Q9:O32	0.51	2.28	9	3
5:D:555:7Q9:C15	6:E:857:17F:O1	0.51	2.58	3	6
5:E:825:7Q9:C39	5:E:843:7Q9:C34	0.51	2.88	4	2
5:A:205:7Q9:C13	5:A:205:7Q9:C22	0.51	2.88	4	1
6:E:806:17F:H36	6:E:806:17F:H41	0.51	1.81	4	2
6:E:810:17F:H57	6:E:810:17F:H35	0.51	1.78	13	2
5:A:218:7Q9:C39	6:D:511:17F:H42	0.51	2.35	10	1
6:E:829:17F:H43	6:E:829:17F:C34	0.51	2.35	10	2
5:D:513:7Q9:C37	6:D:534:17F:H62	0.51	2.34	11	1
6:A:213:17F:C42	6:E:819:17F:H77	0.51	2.35	12	1
6:E:802:17F:H50	6:E:802:17F:H65	0.51	1.82	12	1
5:A:215:7Q9:C13	5:A:216:7Q9:O22	0.51	2.58	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:867:7Q9:C33	5:E:877:7Q9:C35	0.51	2.88	14	1
5:D:514:7Q9:C312	5:D:525:7Q9:C318	0.51	2.89	15	1
5:A:203:7Q9:C12	5:B:203:7Q9:O31	0.51	2.58	17	1
5:A:203:7Q9:C318	6:A:208:17F:H76	0.51	2.35	19	1
5:E:854:7Q9:O11	5:E:854:7Q9:C13	0.51	2.58	1	1
5:E:858:7Q9:O32	5:E:858:7Q9:O21	0.51	2.27	2	14
2:D:408:LYS:HB2	2:D:409:PRO:HD3	0.51	1.81	12	8
5:B:205:7Q9:C310	6:B:208:17F:C35	0.51	2.89	3	1
5:A:205:7Q9:C3	6:A:208:17F:H5	0.51	2.35	4	1
6:E:873:17F:O2	6:E:873:17F:C8	0.51	2.58	9	4
5:A:212:7Q9:C33	5:D:505:7Q9:C32	0.51	2.88	7	1
2:D:404:SER:HB2	5:D:548:7Q9:C312	0.51	2.35	19	4
2:D:430:LEU:HD21	6:D:539:17F:H33	0.51	1.81	8	1
5:A:218:7Q9:O22	5:A:218:7Q9:O11	0.51	2.29	18	3
5:E:825:7Q9:C38	6:E:842:17F:H69	0.51	2.35	9	2
5:D:549:7Q9:C22	5:E:801:7Q9:C35	0.51	2.88	10	1
1:A:17:SER:OG	3:A:201:GSP:O3G	0.51	2.29	12	2
3:B:201:GSP:O3G	3:B:201:GSP:O2B	0.51	2.29	13	1
6:E:802:17F:H39	5:E:805:7Q9:C312	0.51	2.36	13	1
6:A:213:17F:C22	5:D:509:7Q9:C23	0.51	2.89	14	1
6:E:802:17F:H61	5:E:804:7Q9:C22	0.51	2.36	14	1
5:D:521:7Q9:C39	5:D:542:7Q9:C37	0.51	2.89	16	1
6:E:808:17F:H12A	6:E:808:17F:H63	0.51	1.81	17	1
5:A:204:7Q9:C318	6:E:802:17F:H75	0.51	2.35	18	1
6:E:819:17F:C34	6:E:842:17F:H65	0.51	2.35	19	1
5:A:204:7Q9:C13	5:A:205:7Q9:C23	0.51	2.89	20	1
6:D:510:17F:O7	6:D:517:17F:C4	0.51	2.50	5	2
6:D:510:17F:H43	6:D:510:17F:H36	0.51	1.83	13	5
6:D:511:17F:O4	5:D:532:7Q9:C12	0.51	2.59	20	2
5:D:526:7Q9:C318	5:E:838:7Q9:C310	0.51	2.89	4	2
5:E:817:7Q9:C36	5:E:817:7Q9:C311	0.51	2.88	4	2
5:D:556:7Q9:O22	5:D:556:7Q9:O31	0.51	2.28	11	3
5:E:850:7Q9:O32	5:E:850:7Q9:C21	0.51	2.58	16	7
1:A:46:ILE:HB	1:A:51:CYS:SG	0.51	2.46	6	3
5:B:209:7Q9:C311	6:D:520:17F:H61	0.51	2.35	7	2
6:D:517:17F:H67	6:D:517:17F:H50	0.51	1.82	12	2
5:D:532:7Q9:C35	5:D:532:7Q9:O31	0.51	2.58	8	2
6:D:539:17F:H57	6:D:539:17F:C17	0.51	2.35	8	1
6:E:842:17F:C4	6:E:842:17F:H2	0.51	2.35	15	2
6:D:510:17F:H54	6:D:533:17F:H55	0.51	1.83	9	1
5:D:506:7Q9:C34	6:D:517:17F:C31	0.51	2.88	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:802:17F:H59	5:E:804:7Q9:C39	0.51	2.35	11	2
6:D:510:17F:C25	6:D:510:17F:H30	0.51	2.34	12	1
5:A:212:7Q9:C36	5:D:505:7Q9:C34	0.51	2.89	14	1
5:E:847:7Q9:C13	5:E:848:7Q9:O13	0.51	2.58	15	1
2:D:440:LEU:HD13	6:D:552:17F:H78	0.51	1.82	16	1
6:A:208:17F:H30	6:B:208:17F:C19	0.51	2.26	17	1
6:D:534:17F:H29	5:D:538:7Q9:C315	0.51	2.35	17	1
6:E:812:17F:H6A	5:E:824:7Q9:C11	0.51	2.35	17	1
6:A:220:17F:H65	6:A:220:17F:H10A	0.51	1.83	18	1
5:D:508:7Q9:O22	5:D:508:7Q9:O11	0.51	2.29	18	1
1:A:84:ILE:CD1	1:A:118:CYS:HA	0.51	2.35	6	4
5:A:205:7Q9:O22	5:A:205:7Q9:C3	0.51	2.56	17	5
6:D:510:17F:C5	6:D:533:17F:C19	0.51	2.73	1	2
2:E:623:ARG:HD2	5:E:859:7Q9:C310	0.51	2.36	1	1
6:E:842:17F:O10	6:E:842:17F:C6	0.51	2.47	1	9
5:E:825:7Q9:C33	5:E:825:7Q9:C37	0.51	2.89	5	5
6:E:839:17F:H2	6:E:875:17F:O8	0.51	2.05	11	3
6:E:856:17F:O8	6:E:856:17F:C20	0.51	2.59	3	1
5:E:838:7Q9:C32	6:E:842:17F:H31	0.51	2.35	7	3
6:E:857:17F:H36	6:E:857:17F:H56	0.51	1.82	4	1
2:E:733:LEU:HG	5:E:876:7Q9:C38	0.51	2.36	5	2
6:D:519:17F:H33	6:D:519:17F:C35	0.51	2.35	10	1
5:E:864:7Q9:C13	5:E:874:7Q9:C1	0.51	2.88	10	1
6:D:519:17F:H62	6:D:519:17F:C23	0.51	2.36	11	1
5:E:834:7Q9:O31	5:E:834:7Q9:O22	0.51	2.29	16	2
6:A:213:17F:H76	6:E:819:17F:C42	0.51	2.35	12	1
6:E:829:17F:H30	5:E:833:7Q9:C35	0.51	2.35	12	3
5:E:834:7Q9:C15	6:E:856:17F:C2	0.51	2.88	12	1
5:D:505:7Q9:C14	5:D:505:7Q9:C1	0.51	2.89	16	1
5:E:825:7Q9:C316	6:E:842:17F:H71	0.51	2.36	18	1
6:A:208:17F:C4	6:A:208:17F:C1	0.51	2.87	5	3
5:E:878:7Q9:C2	5:E:878:7Q9:O32	0.51	2.53	1	9
5:D:505:7Q9:C15	6:D:518:17F:O10	0.51	2.59	2	3
5:B:204:7Q9:C14	5:B:204:7Q9:O13	0.51	2.58	10	4
5:E:817:7Q9:O12	5:E:817:7Q9:C15	0.51	2.58	15	16
6:E:819:17F:H77	6:E:819:17F:C27	0.51	2.35	3	1
5:E:844:7Q9:O13	5:E:844:7Q9:O21	0.51	2.29	3	3
5:D:503:7Q9:O22	5:D:503:7Q9:O11	0.51	2.29	20	7
5:E:809:7Q9:C13	6:E:818:17F:O2	0.51	2.59	11	2
5:E:815:7Q9:O22	5:E:815:7Q9:O11	0.51	2.28	6	2
5:E:854:7Q9:C1	5:E:854:7Q9:O22	0.51	2.55	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:834:7Q9:C11	5:E:858:7Q9:O13	0.51	2.58	7	1
5:A:211:7Q9:C311	6:A:213:17F:H57	0.51	2.35	8	1
5:E:847:7Q9:C22	5:E:848:7Q9:C34	0.51	2.88	15	2
2:D:436:TYR:HD1	2:E:718:LEU:HD11	0.51	1.64	10	1
5:D:515:7Q9:C3	6:D:519:17F:H19	0.51	2.34	10	1
2:D:333:LYS:HD2	5:E:878:7Q9:C318	0.51	2.36	11	3
6:E:839:17F:H77	6:E:839:17F:H47	0.51	1.81	11	2
5:E:874:7Q9:C3	5:E:874:7Q9:O22	0.51	2.56	14	1
6:E:819:17F:H45	6:E:819:17F:H75	0.51	1.81	16	1
6:D:552:17F:C7	6:D:552:17F:O6	0.51	2.58	17	1
5:E:803:7Q9:P	6:E:808:17F:H2	0.51	2.46	15	2
5:E:848:7Q9:C1	5:E:848:7Q9:O22	0.51	2.53	15	10
5:D:516:7Q9:C1	5:D:516:7Q9:O22	0.51	2.52	13	6
6:D:519:17F:H30	6:D:519:17F:C23	0.51	2.24	2	2
6:D:533:17F:C17	6:D:533:17F:C1Y	0.51	2.89	8	6
1:A:117:LYS:HE2	3:A:201:GSP:N7	0.51	2.20	3	1
6:A:208:17F:C1X	6:B:208:17F:H31	0.51	2.36	3	2
5:E:804:7Q9:C311	5:E:815:7Q9:C315	0.51	2.89	6	1
5:A:207:7Q9:O22	5:B:203:7Q9:C14	0.51	2.59	8	1
6:E:820:17F:O8	6:E:820:17F:H4A	0.51	2.04	20	3
6:D:518:17F:H34	5:D:551:7Q9:C38	0.51	2.36	9	1
5:A:211:7Q9:C1	5:A:211:7Q9:C15	0.51	2.89	12	1
6:E:857:17F:H67	6:E:875:17F:C34	0.51	2.36	18	2
2:E:682:LYS:HG3	5:E:868:7Q9:O32	0.51	2.06	17	2
6:A:208:17F:H18A	5:A:212:7Q9:C36	0.51	2.35	20	1
6:A:213:17F:H12A	6:A:213:17F:O2	0.51	2.06	20	1
5:A:216:7Q9:C33	5:B:207:7Q9:C35	0.51	2.88	7	4
6:D:534:17F:H10A	6:D:534:17F:C33	0.51	2.35	17	5
5:D:542:7Q9:O31	5:D:542:7Q9:C21	0.51	2.58	5	15
2:E:641:LEU:HD23	5:E:852:7Q9:C313	0.51	2.36	1	2
5:E:867:7Q9:C1	5:E:877:7Q9:O13	0.51	2.58	9	5
5:A:216:7Q9:C34	5:D:506:7Q9:O32	0.51	2.58	15	3
6:D:533:17F:O10	6:D:533:17F:H6A	0.51	2.06	12	4
6:D:539:17F:H37	6:D:539:17F:C35	0.51	2.36	2	3
6:D:540:17F:C36	6:D:540:17F:C1X	0.51	2.89	9	5
6:A:213:17F:C40	6:E:819:17F:H76	0.51	2.35	4	1
6:E:802:17F:H1	6:E:802:17F:H4	0.51	1.81	5	1
5:A:206:7Q9:O13	5:A:206:7Q9:C12	0.51	2.58	16	7
5:B:206:7Q9:C316	6:E:812:17F:H50	0.51	2.35	7	1
6:A:220:17F:H39	6:A:220:17F:C37	0.51	2.27	12	1
6:E:820:17F:H18	5:E:853:7Q9:C11	0.51	2.36	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:808:17F:H50	6:E:808:17F:H74	0.51	1.83	1	1
6:E:857:17F:H10A	6:E:875:17F:H5	0.51	1.83	6	2
5:B:205:7Q9:C314	6:B:208:17F:H39	0.51	2.36	10	2
5:B:209:7Q9:O32	5:B:209:7Q9:C2	0.51	2.56	9	8
6:D:511:17F:H69	6:D:511:17F:H59	0.51	1.82	12	2
6:A:219:17F:C37	6:D:518:17F:H60	0.51	2.36	5	1
5:E:824:7Q9:O22	5:E:846:7Q9:C12	0.51	2.59	5	1
5:A:211:7Q9:C313	6:A:220:17F:H34	0.51	2.36	6	2
5:E:822:7Q9:C13	5:E:826:7Q9:O13	0.51	2.59	6	1
5:A:211:7Q9:C3	5:A:211:7Q9:C15	0.51	2.89	8	1
5:B:206:7Q9:C37	5:B:210:7Q9:C39	0.51	2.89	20	2
6:D:510:17F:H53	6:D:510:17F:H68	0.51	1.82	11	1
6:E:829:17F:H70	5:E:830:7Q9:C35	0.51	2.36	12	2
6:E:810:17F:HN1	6:E:819:17F:H6	0.51	1.66	14	1
6:A:219:17F:H68	5:D:505:7Q9:C38	0.51	2.36	15	1
6:A:213:17F:H20A	6:A:213:17F:C21	0.51	2.36	18	1
6:A:213:17F:H12	6:A:213:17F:C23	0.51	2.31	19	1
6:A:213:17F:H78	6:E:819:17F:H51	0.51	1.82	20	1
2:E:711:LEU:HD22	5:E:866:7Q9:C311	0.51	2.36	20	1
6:D:510:17F:H49	6:D:517:17F:C39	0.51	2.35	1	3
5:D:554:7Q9:C13	5:D:554:7Q9:O14	0.51	2.59	3	6
5:E:848:7Q9:O32	5:E:848:7Q9:O21	0.51	2.29	16	18
5:E:831:7Q9:O22	5:E:831:7Q9:C1	0.51	2.57	4	6
5:E:865:7Q9:C14	5:E:865:7Q9:O11	0.51	2.59	10	14
5:A:207:7Q9:C22	5:B:204:7Q9:C32	0.51	2.89	4	1
5:D:555:7Q9:C11	5:E:833:7Q9:C2	0.51	2.89	4	3
5:A:217:7Q9:C38	5:D:514:7Q9:C39	0.51	2.89	5	2
5:E:845:7Q9:C14	5:E:865:7Q9:O13	0.51	2.59	5	2
6:D:510:17F:C28	6:D:517:17F:H68	0.51	2.35	7	1
6:D:539:17F:H66	6:D:539:17F:H38	0.51	1.81	8	1
6:E:873:17F:O2	6:E:873:17F:H2	0.51	2.06	12	4
5:B:205:7Q9:C314	6:B:208:17F:H35	0.51	2.35	10	1
5:D:505:7Q9:C14	5:D:505:7Q9:O13	0.51	2.59	11	1
2:D:374:LEU:HD23	5:D:535:7Q9:C310	0.51	2.35	13	1
1:B:10:GLY:O	1:B:60:GLY:HA3	0.51	2.06	14	1
5:A:216:7Q9:C2	6:D:517:17F:H18A	0.51	2.36	20	1
6:D:540:17F:H65	6:D:540:17F:H59	0.50	1.81	12	2
6:D:539:17F:H63	6:D:539:17F:H38	0.50	1.82	3	2
5:E:838:7Q9:O31	5:E:838:7Q9:O22	0.50	2.29	4	9
5:E:864:7Q9:C37	5:E:864:7Q9:C23	0.50	2.90	16	2
6:A:220:17F:H48	6:A:220:17F:H65	0.50	1.83	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:99:GLN:O	1:B:103:VAL:HG23	0.50	2.07	17	6
5:D:508:7Q9:O13	5:D:524:7Q9:C11	0.50	2.59	4	1
6:E:808:17F:O5	5:E:814:7Q9:C13	0.50	2.59	4	1
6:D:520:17F:O8	6:D:520:17F:O9	0.50	2.29	6	4
5:E:861:7Q9:C1	5:E:861:7Q9:O22	0.50	2.57	7	3
5:A:215:7Q9:C22	5:A:216:7Q9:C23	0.50	2.89	12	1
6:E:818:17F:H35	6:E:818:17F:C24	0.50	2.35	19	2
5:D:506:7Q9:O12	5:D:506:7Q9:O21	0.50	2.29	15	1
2:D:257:PHE:HE2	2:E:706:LYS:HD3	0.50	1.66	16	1
5:D:505:7Q9:O32	6:D:518:17F:H9A	0.50	2.05	16	1
6:A:213:17F:C23	6:A:213:17F:C12	0.50	2.88	17	1
5:A:206:7Q9:C312	6:E:802:17F:H70	0.50	2.36	18	1
6:A:219:17F:H57	5:E:801:7Q9:C34	0.50	2.36	18	1
6:E:810:17F:H30	5:E:811:7Q9:C33	0.50	2.36	19	1
6:A:208:17F:O4	5:A:212:7Q9:C14	0.50	2.58	19	3
6:A:213:17F:O1	6:A:213:17F:C17	0.50	2.59	2	5
6:B:208:17F:H57	6:B:208:17F:C35	0.50	2.23	13	3
5:D:554:7Q9:O22	5:D:554:7Q9:O11	0.50	2.28	10	3
5:D:514:7Q9:O13	5:D:514:7Q9:C21	0.50	2.59	9	2
5:D:555:7Q9:C15	6:E:857:17F:O6	0.50	2.59	15	3
1:A:6:LEU:O	1:A:55:ILE:HA	0.50	2.06	3	3
6:D:534:17F:H6	5:D:538:7Q9:C35	0.50	2.36	3	1
5:E:827:7Q9:O32	5:E:827:7Q9:C2	0.50	2.56	16	5
6:A:220:17F:O2	5:D:503:7Q9:C15	0.50	2.59	7	1
5:E:838:7Q9:C34	6:E:842:17F:H44	0.50	2.36	20	2
6:E:839:17F:H10A	6:E:857:17F:C12	0.50	2.30	7	1
5:D:523:7Q9:C312	5:D:523:7Q9:C38	0.50	2.89	8	1
2:D:439:LYS:HG3	2:E:714:LEU:HD12	0.50	1.82	10	1
5:D:550:7Q9:O21	6:D:552:17F:N1	0.50	2.44	13	1
6:A:219:17F:C32	6:A:219:17F:H35	0.50	2.36	14	1
5:E:840:7Q9:C11	5:E:866:7Q9:C36	0.50	2.89	14	1
6:D:510:17F:H8	6:D:517:17F:O7	0.50	2.05	16	1
6:B:208:17F:H51	5:D:504:7Q9:C318	0.50	2.36	17	1
6:E:802:17F:O9	6:E:802:17F:O8	0.50	2.29	20	1
5:A:211:7Q9:C317	6:A:220:17F:H78	0.50	2.36	1	1
5:D:516:7Q9:O13	5:D:516:7Q9:C14	0.50	2.59	1	1
6:E:802:17F:C28	6:E:802:17F:C42	0.50	2.89	9	5
6:E:818:17F:O10	6:E:818:17F:C4	0.50	2.57	15	3
6:E:818:17F:O8	5:E:821:7Q9:C13	0.50	2.59	2	2
5:A:216:7Q9:C15	5:B:207:7Q9:C33	0.50	2.89	16	4
1:B:22:GLN:O	1:B:26:ASN:HA	0.50	2.06	7	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:520:17F:C24	6:D:520:17F:C2X	0.50	2.80	5	2
6:E:808:17F:H47	6:E:808:17F:C41	0.50	2.32	3	1
5:E:863:7Q9:O32	5:E:878:7Q9:C14	0.50	2.59	4	1
5:D:546:7Q9:C15	5:D:546:7Q9:O22	0.50	2.59	14	2
1:B:109:VAL:HB	1:B:111:MET:HE3	0.50	1.82	7	1
5:B:205:7Q9:C312	6:B:208:17F:C35	0.50	2.89	10	2
5:D:556:7Q9:O13	5:E:845:7Q9:C13	0.50	2.59	13	3
5:E:830:7Q9:O11	5:E:830:7Q9:O22	0.50	2.29	7	1
5:E:833:7Q9:O22	5:E:833:7Q9:C1	0.50	2.55	18	3
2:E:619:VAL:HA	2:E:622:LEU:HD12	0.50	1.82	9	2
5:D:531:7Q9:O32	5:D:531:7Q9:O21	0.50	2.28	10	1
5:A:206:7Q9:C318	6:E:802:17F:H64	0.50	2.37	11	1
5:E:870:7Q9:O22	6:E:873:17F:H9	0.50	2.06	11	1
6:E:812:17F:H42	6:E:812:17F:H71	0.50	1.83	12	1
5:D:514:7Q9:C1	5:D:514:7Q9:C15	0.50	2.89	20	3
5:D:501:7Q9:C315	5:E:809:7Q9:C310	0.50	2.90	18	1
5:D:513:7Q9:C14	5:D:532:7Q9:O13	0.50	2.60	19	1
5:D:546:7Q9:O22	5:D:546:7Q9:C12	0.50	2.60	2	8
5:E:837:7Q9:O32	5:E:837:7Q9:O21	0.50	2.28	12	8
5:B:204:7Q9:C22	5:B:207:7Q9:C311	0.50	2.90	2	2
6:E:839:17F:H33	6:E:839:17F:H39	0.50	1.83	2	2
5:E:864:7Q9:C35	5:E:864:7Q9:O32	0.50	2.59	7	4
6:D:518:17F:H60	6:D:518:17F:C25	0.50	2.37	3	1
6:E:810:17F:H34	6:E:819:17F:H63	0.50	1.84	4	1
5:E:835:7Q9:C317	6:E:856:17F:C37	0.50	2.89	4	1
5:B:203:7Q9:C1	5:B:203:7Q9:O22	0.50	2.55	8	3
6:D:517:17F:C21	6:D:533:17F:H38	0.50	2.37	5	1
6:E:819:17F:C1	5:E:838:7Q9:C13	0.50	2.88	5	2
1:B:72:MET:HA	1:B:78:PHE:HZ	0.50	1.66	7	3
6:E:808:17F:C31	6:E:820:17F:C12	0.50	2.89	7	1
6:D:510:17F:H19	5:D:530:7Q9:C3	0.50	2.36	8	1
5:E:803:7Q9:C313	6:E:806:17F:H61	0.50	2.36	12	2
5:E:864:7Q9:C32	5:E:874:7Q9:C34	0.50	2.90	8	1
5:E:835:7Q9:C34	6:E:856:17F:H19A	0.50	2.36	9	1
6:A:220:17F:H11A	5:D:515:7Q9:C23	0.50	2.36	12	1
5:D:507:7Q9:O22	5:D:507:7Q9:C3	0.50	2.51	12	1
1:A:127:THR:O	1:A:131:GLN:HG3	0.50	2.05	14	1
2:D:269:GLN:CG	6:D:540:17F:H33	0.50	2.35	14	1
6:A:213:17F:C1X	5:D:509:7Q9:O22	0.50	2.58	18	1
6:E:818:17F:C10	5:E:821:7Q9:C23	0.50	2.89	20	1
5:A:217:7Q9:C38	5:D:514:7Q9:C310	0.50	2.89	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:527:7Q9:O32	5:D:527:7Q9:O21	0.50	2.29	14	8
5:D:554:7Q9:O14	5:E:848:7Q9:C13	0.50	2.59	7	6
5:E:831:7Q9:C1	5:E:831:7Q9:O22	0.50	2.55	9	7
5:E:844:7Q9:O32	5:E:844:7Q9:C2	0.50	2.57	6	6
5:B:206:7Q9:C21	5:D:501:7Q9:C15	0.50	2.90	5	1
5:D:513:7Q9:O31	6:D:534:17F:H9	0.50	2.05	9	1
6:D:519:17F:H59	6:D:519:17F:C23	0.50	2.18	11	1
5:E:805:7Q9:C12	5:E:816:7Q9:O22	0.50	2.59	12	1
6:E:806:17F:P1	6:E:806:17F:HN1	0.50	2.30	20	2
6:D:534:17F:H61	6:D:534:17F:H10A	0.50	1.82	14	1
5:D:542:7Q9:C15	5:D:553:7Q9:O22	0.50	2.60	14	1
6:A:219:17F:H40	6:A:219:17F:C35	0.50	2.33	15	1
5:B:206:7Q9:C318	6:E:812:17F:H45	0.50	2.35	16	1
6:D:539:17F:H62	6:D:539:17F:H38	0.50	1.84	16	1
6:E:802:17F:H46	5:E:807:7Q9:C318	0.50	2.37	16	1
2:D:269:GLN:HG2	6:D:540:17F:C1Y	0.50	2.35	17	1
6:E:875:17F:H41	6:E:875:17F:C2X	0.50	2.36	17	1
5:E:811:7Q9:O13	5:E:822:7Q9:O11	0.50	2.29	18	1
6:E:808:17F:C33	6:E:820:17F:C12	0.50	2.87	10	3
5:D:503:7Q9:C21	5:D:503:7Q9:C11	0.50	2.90	2	1
6:D:511:17F:O9	6:D:511:17F:C7	0.50	2.59	8	8
5:D:547:7Q9:O22	5:D:547:7Q9:C1	0.50	2.58	10	9
5:E:813:7Q9:C34	5:E:828:7Q9:C313	0.50	2.89	14	3
5:E:859:7Q9:O32	5:E:859:7Q9:O21	0.50	2.30	20	13
1:A:16:LYS:HG2	3:A:201:GSP:O2B	0.50	2.07	17	2
6:A:219:17F:C26	5:D:505:7Q9:C311	0.50	2.87	15	3
5:B:205:7Q9:C39	6:B:208:17F:H63	0.50	2.37	3	1
6:A:213:17F:O9	6:A:213:17F:O8	0.50	2.29	20	3
5:B:206:7Q9:P	5:B:206:7Q9:C15	0.50	2.99	4	1
5:D:521:7Q9:C15	5:D:522:7Q9:O14	0.50	2.60	4	1
5:E:838:7Q9:O32	6:E:842:17F:H19	0.50	2.07	4	1
6:E:839:17F:H73	6:E:857:17F:H41	0.50	1.84	7	3
1:B:129:GLN:O	1:B:133:LEU:HB2	0.50	2.05	15	2
5:B:206:7Q9:C318	6:E:812:17F:H74	0.50	2.37	5	1
2:D:342:SER:HB2	2:D:343:PRO:HD3	0.50	1.83	6	5
5:E:865:7Q9:C14	5:E:865:7Q9:O12	0.50	2.59	10	5
6:A:208:17F:H10A	6:A:208:17F:O2	0.50	2.06	7	1
1:B:93:ILE:HG21	1:B:113:LEU:HD21	0.50	1.83	7	1
5:E:870:7Q9:C11	6:E:873:17F:H9	0.50	2.37	9	2
5:D:506:7Q9:C34	6:D:517:17F:H56	0.50	2.37	10	1
5:E:809:7Q9:C1	5:E:809:7Q9:O22	0.50	2.58	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:352:ALA:HB1	5:D:527:7Q9:C317	0.50	2.37	12	2
5:B:204:7Q9:C14	5:B:204:7Q9:O11	0.50	2.60	18	1
5:E:843:7Q9:C22	5:E:843:7Q9:C13	0.50	2.90	18	1
6:E:812:17F:C6	6:E:812:17F:O10	0.50	2.53	19	1
5:E:807:7Q9:O21	5:E:807:7Q9:C31	0.50	2.60	1	13
1:A:16:LYS:HB2	3:A:201:GSP:O3B	0.50	2.06	2	2
6:D:519:17F:O8	6:D:519:17F:H10A	0.50	2.06	15	11
5:D:555:7Q9:C23	2:E:653:ARG:HA	0.50	2.37	2	1
5:E:847:7Q9:C14	5:E:847:7Q9:P	0.50	2.99	16	11
5:B:205:7Q9:C316	6:B:208:17F:C28	0.50	2.89	3	1
6:E:808:17F:H56	6:E:820:17F:H30	0.50	1.83	5	1
6:E:839:17F:H49	6:E:875:17F:C30	0.50	2.37	5	2
5:D:555:7Q9:O14	5:D:555:7Q9:C13	0.50	2.60	6	1
5:E:863:7Q9:O13	5:E:863:7Q9:C12	0.50	2.58	18	2
5:E:870:7Q9:C22	6:E:873:17F:H12A	0.50	2.37	7	1
6:A:213:17F:O9	6:A:213:17F:C20	0.50	2.60	8	2
6:A:220:17F:H30	6:A:220:17F:H39	0.50	1.84	10	1
6:E:819:17F:O4	5:E:825:7Q9:C15	0.50	2.60	14	2
6:D:511:17F:O1	5:D:513:7Q9:C14	0.50	2.60	11	2
6:D:520:17F:H9	5:D:550:7Q9:C39	0.50	2.36	12	1
6:D:510:17F:C17	6:D:517:17F:H9	0.50	2.36	13	2
2:D:399:HIS:CE1	2:E:561:ARG:HA	0.50	2.41	16	2
5:A:216:7Q9:O32	5:B:207:7Q9:C34	0.50	2.60	17	1
5:D:507:7Q9:C313	5:E:814:7Q9:C315	0.50	2.89	18	1
6:E:802:17F:H19	5:E:804:7Q9:C22	0.50	2.36	18	1
6:D:517:17F:H78	6:E:839:17F:H74	0.50	1.82	20	1
1:A:80:CYS:HB3	1:A:93:ILE:HD12	0.50	1.84	1	4
2:D:399:HIS:HE1	2:E:564:LEU:HB2	0.50	1.65	1	1
6:D:510:17F:C8	6:D:517:17F:C17	0.50	2.89	9	3
5:D:541:7Q9:C317	6:E:875:17F:H50	0.50	2.37	4	3
5:B:204:7Q9:O22	5:B:204:7Q9:C3	0.50	2.57	11	5
6:E:857:17F:C11	6:E:875:17F:H59	0.50	2.36	4	2
6:A:220:17F:H12A	5:D:502:7Q9:C37	0.50	2.37	5	2
6:E:829:17F:H71	5:E:830:7Q9:C316	0.50	2.37	7	1
5:D:506:7Q9:O32	6:D:517:17F:H20	0.50	2.05	8	1
5:A:218:7Q9:C33	6:D:511:17F:H9	0.50	2.36	10	1
6:D:510:17F:C9	6:D:517:17F:C7	0.50	2.88	14	1
5:D:553:7Q9:C22	5:D:553:7Q9:C13	0.50	2.90	17	2
5:B:206:7Q9:C317	6:E:812:17F:H75	0.50	2.36	15	1
6:D:519:17F:H29	5:D:526:7Q9:C310	0.50	2.37	18	1
1:B:35:THR:OG1	3:B:201:GSP:O3G	0.50	2.29	2	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:811:7Q9:C14	5:E:817:7Q9:O32	0.50	2.59	8	5
5:E:826:7Q9:O22	5:E:826:7Q9:C1	0.50	2.58	5	6
5:E:866:7Q9:O22	5:E:866:7Q9:C3	0.50	2.58	11	9
5:B:205:7Q9:C317	6:B:208:17F:C26	0.50	2.90	5	1
2:D:275:LEU:HG	2:E:688:ARG:HG3	0.50	1.84	7	1
6:A:219:17F:H34	5:E:801:7Q9:C34	0.50	2.37	9	1
5:E:809:7Q9:C23	6:E:818:17F:H65	0.50	2.36	9	2
6:D:519:17F:H40	6:D:519:17F:C32	0.50	2.17	11	1
5:D:546:7Q9:C313	5:D:546:7Q9:C38	0.50	2.89	12	1
6:A:208:17F:C42	6:B:208:17F:C38	0.50	2.90	15	1
5:A:210:7Q9:C36	5:A:217:7Q9:C22	0.50	2.90	16	1
5:E:872:7Q9:C1	5:E:872:7Q9:O22	0.49	2.56	6	4
5:E:825:7Q9:C316	6:E:842:17F:H75	0.49	2.37	2	4
6:A:208:17F:H76	5:B:205:7Q9:C318	0.49	2.36	3	1
6:D:510:17F:H37	6:D:511:17F:H56	0.49	1.83	3	2
6:E:856:17F:H29	6:E:856:17F:C34	0.49	2.37	4	1
5:E:851:7Q9:C315	6:E:871:17F:H60	0.49	2.37	5	2
6:D:552:17F:C31	6:D:552:17F:C9	0.49	2.90	20	4
5:D:544:7Q9:O14	5:D:544:7Q9:C21	0.49	2.60	11	5
6:E:819:17F:O10	5:E:825:7Q9:C13	0.49	2.60	19	2
6:A:208:17F:C24	6:A:219:17F:H38	0.49	2.17	8	1
6:A:213:17F:H31	6:A:213:17F:C12	0.49	2.29	10	1
5:B:210:7Q9:C32	6:D:520:17F:H60	0.49	2.37	16	1
5:B:209:7Q9:C314	5:E:840:7Q9:C314	0.49	2.90	17	1
5:D:543:7Q9:C3	6:D:552:17F:H29	0.49	2.37	17	1
2:D:422:LEU:HG	2:D:426:LYS:HE2	0.49	1.82	19	1
5:D:513:7Q9:C311	5:D:513:7Q9:C37	0.49	2.87	20	1
6:A:220:17F:H18A	5:D:503:7Q9:C15	0.49	2.37	1	1
5:E:864:7Q9:C33	5:E:868:7Q9:C22	0.49	2.90	1	2
1:A:64:TYR:O	1:A:68:ARG:HD2	0.49	2.06	2	1
6:A:220:17F:H65	6:A:220:17F:C12	0.49	2.35	2	1
5:E:874:7Q9:O32	5:E:874:7Q9:C21	0.49	2.59	2	3
2:D:333:LYS:HG3	5:E:878:7Q9:C318	0.49	2.37	5	1
5:D:509:7Q9:O14	5:D:526:7Q9:C13	0.49	2.61	5	1
6:D:511:17F:H1A	5:D:532:7Q9:C12	0.49	2.37	5	1
5:A:210:7Q9:C313	6:A:220:17F:H9	0.49	2.38	6	2
5:D:508:7Q9:C22	5:D:508:7Q9:C12	0.49	2.90	16	4
5:D:523:7Q9:C3	6:D:552:17F:H19A	0.49	2.37	10	2
2:E:715:ARG:O	2:E:719:LEU:HG	0.49	2.07	8	5
6:D:520:17F:C31	6:D:520:17F:C35	0.49	2.80	11	1
6:D:533:17F:H50	6:D:533:17F:H77	0.49	1.81	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:847:7Q9:C13	6:E:873:17F:O5	0.49	2.60	12	1
6:E:808:17F:H70	6:E:819:17F:H76	0.49	1.83	13	1
1:A:47:ASP:CG	1:B:132:ASP:HB2	0.49	2.32	14	1
5:A:211:7Q9:C318	6:A:220:17F:H53	0.49	2.36	17	1
5:D:516:7Q9:C14	5:D:516:7Q9:O13	0.49	2.60	5	3
5:E:868:7Q9:C312	5:E:868:7Q9:C38	0.49	2.87	6	3
6:D:518:17F:H57	6:D:518:17F:H63	0.49	1.84	11	1
1:A:46:ILE:HD12	1:A:160:VAL:HG21	0.49	1.84	18	2
1:B:24:ILE:HD11	1:B:55:ILE:HD12	0.49	1.84	12	1
2:E:660:ARG:HD2	6:E:875:17F:C20	0.49	2.30	19	3
5:D:527:7Q9:C314	5:D:531:7Q9:C315	0.49	2.89	20	2
6:A:213:17F:H35	6:A:213:17F:C24	0.49	2.29	16	1
5:D:542:7Q9:O21	5:D:542:7Q9:C13	0.49	2.60	17	1
6:D:511:17F:C7	6:D:511:17F:O9	0.49	2.60	18	5
6:D:518:17F:H54	6:D:518:17F:C41	0.49	2.37	3	1
5:D:527:7Q9:O22	5:D:527:7Q9:C1	0.49	2.54	10	7
5:E:835:7Q9:C22	5:E:835:7Q9:C13	0.49	2.91	18	5
6:E:810:17F:H29	6:E:810:17F:H56	0.49	1.83	5	1
5:D:555:7Q9:C13	5:D:555:7Q9:O12	0.49	2.60	6	1
6:E:839:17F:C23	6:E:839:17F:H34	0.49	2.37	16	4
5:E:807:7Q9:C311	6:E:818:17F:H8	0.49	2.37	7	1
6:E:839:17F:C1Z	6:E:839:17F:H35	0.49	2.37	8	1
6:A:220:17F:H52	6:A:220:17F:H59	0.49	1.84	10	1
5:E:822:7Q9:P	5:E:822:7Q9:O21	0.49	2.71	13	1
6:A:213:17F:H66	6:A:213:17F:H46	0.49	1.84	15	1
6:A:208:17F:H40	6:A:208:17F:C31	0.49	2.37	16	2
6:A:213:17F:O10	6:A:213:17F:N1	0.49	2.43	17	1
1:A:110:PRO:HG3	1:A:166:HIS:HB2	0.49	1.82	18	1
6:D:511:17F:H53	6:E:829:17F:H50	0.49	1.84	18	1
6:A:208:17F:H31	6:A:219:17F:H10	0.49	1.81	20	1
5:E:803:7Q9:O32	6:E:808:17F:C6	0.49	2.60	20	1
5:E:807:7Q9:C13	6:E:818:17F:O2	0.49	2.60	20	1
5:D:549:7Q9:C314	5:E:870:7Q9:C313	0.49	2.90	15	2
2:D:367:SER:HB3	5:D:544:7Q9:C38	0.49	2.37	2	2
5:D:503:7Q9:O13	5:D:503:7Q9:C13	0.49	2.60	16	2
5:D:526:7Q9:O11	5:D:531:7Q9:C15	0.49	2.61	16	2
6:E:806:17F:O9	6:E:806:17F:C7	0.49	2.60	20	11
6:A:208:17F:H45	6:A:208:17F:C39	0.49	2.36	3	1
2:D:389:LEU:HD11	5:D:546:7Q9:C38	0.49	2.38	3	2
6:E:806:17F:H78	5:E:817:7Q9:C318	0.49	2.37	7	2
2:E:660:ARG:HH11	6:E:875:17F:H20A	0.49	1.68	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:519:17F:O10	6:D:519:17F:C6	0.49	2.49	6	2
6:E:839:17F:H34	6:E:839:17F:H39	0.49	1.84	16	3
6:D:510:17F:H73	5:E:833:7Q9:C315	0.49	2.37	7	1
6:E:810:17F:H48	6:E:810:17F:C33	0.49	2.37	8	1
6:E:820:17F:H19A	5:E:853:7Q9:C35	0.49	2.38	8	1
6:E:829:17F:H30	5:E:849:7Q9:C22	0.49	2.38	8	1
5:E:836:7Q9:C1	5:E:836:7Q9:O22	0.49	2.52	12	3
5:A:215:7Q9:C33	6:D:511:17F:H65	0.49	2.38	11	1
5:D:526:7Q9:O32	5:D:526:7Q9:C1	0.49	2.60	13	1
5:E:834:7Q9:C22	6:E:839:17F:H20	0.49	2.37	13	1
5:E:803:7Q9:O32	6:E:808:17F:C5	0.49	2.51	17	1
6:A:219:17F:O10	6:D:518:17F:H12	0.49	2.08	1	1
5:D:521:7Q9:O31	5:D:521:7Q9:P	0.49	2.71	7	2
5:E:865:7Q9:O13	5:E:865:7Q9:C21	0.49	2.60	5	2
5:D:541:7Q9:C318	6:E:875:17F:H50	0.49	2.38	3	1
5:E:858:7Q9:C3	6:E:875:17F:H10A	0.49	2.38	3	1
5:A:217:7Q9:C13	5:A:217:7Q9:O11	0.49	2.60	8	4
1:A:68:ARG:HG3	1:A:71:TYR:CE2	0.49	2.43	5	2
6:E:871:17F:C32	6:E:871:17F:C21	0.49	2.90	5	2
6:D:510:17F:N1	6:D:510:17F:O2	0.49	2.35	7	2
5:E:836:7Q9:C13	5:E:836:7Q9:O22	0.49	2.59	7	2
6:E:873:17F:C33	6:E:873:17F:H48	0.49	2.37	7	1
2:E:685:GLY:O	2:E:689:LEU:HG	0.49	2.07	8	1
6:D:520:17F:H8A	5:D:550:7Q9:C39	0.49	2.38	9	1
6:B:208:17F:H76	6:E:812:17F:H76	0.49	1.85	10	1
1:B:16:LYS:HG2	3:B:201:GSP:O2B	0.49	2.08	20	2
5:A:217:7Q9:C36	5:D:516:7Q9:C37	0.49	2.90	13	2
5:D:516:7Q9:O22	5:D:516:7Q9:C1	0.49	2.59	6	8
5:D:543:7Q9:C32	6:D:552:17F:H73	0.49	2.37	1	2
5:E:849:7Q9:C310	5:E:852:7Q9:C38	0.49	2.90	16	8
5:A:203:7Q9:C12	5:B:203:7Q9:C31	0.49	2.91	2	3
5:D:537:7Q9:O13	5:D:546:7Q9:C12	0.49	2.60	18	3
5:E:837:7Q9:O14	5:E:855:7Q9:C12	0.49	2.61	2	3
5:D:528:7Q9:O32	5:D:551:7Q9:C38	0.49	2.61	3	1
6:A:208:17F:O5	5:A:212:7Q9:C14	0.49	2.61	5	1
6:B:208:17F:H42	5:E:824:7Q9:C318	0.49	2.37	5	1
5:E:833:7Q9:C315	6:E:857:17F:H51	0.49	2.38	18	2
6:E:875:17F:H11A	6:E:875:17F:N1	0.49	2.23	5	2
6:E:857:17F:P1	6:E:857:17F:N1	0.49	2.86	11	4
6:E:856:17F:H56	6:E:856:17F:H36	0.49	1.85	7	1
6:E:820:17F:H67	5:E:853:7Q9:C311	0.49	2.38	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:816:7Q9:O32	5:E:816:7Q9:C14	0.49	2.61	10	1
6:A:220:17F:C42	6:A:220:17F:H47	0.49	2.38	12	1
6:B:208:17F:O4	5:D:508:7Q9:C15	0.49	2.61	12	1
5:D:513:7Q9:C314	6:D:534:17F:H45	0.49	2.38	14	1
6:E:857:17F:H37	6:E:857:17F:C38	0.49	2.37	14	1
5:B:205:7Q9:C312	6:B:208:17F:C12	0.49	2.90	15	1
6:E:810:17F:H11A	5:E:811:7Q9:C33	0.49	2.37	16	1
6:A:213:17F:C23	6:A:213:17F:H12	0.49	2.37	17	1
6:E:839:17F:H65	6:E:839:17F:H11A	0.49	1.83	18	1
6:E:875:17F:O3	6:E:875:17F:C6	0.49	2.58	18	1
2:D:257:PHE:HB3	2:D:261:ARG:NH1	0.49	2.23	20	1
5:D:505:7Q9:O21	5:D:505:7Q9:C31	0.49	2.61	6	9
6:E:873:17F:H20	6:E:873:17F:C1X	0.49	2.38	4	2
5:B:205:7Q9:C38	6:B:208:17F:H10A	0.49	2.38	3	1
6:D:518:17F:H54	6:D:518:17F:H74	0.49	1.84	3	1
5:D:551:7Q9:C1	5:D:551:7Q9:O22	0.49	2.54	12	4
5:A:215:7Q9:C14	5:A:218:7Q9:O14	0.49	2.60	4	2
6:E:812:17F:O10	5:E:824:7Q9:C11	0.49	2.61	17	2
5:D:556:7Q9:O31	5:E:854:7Q9:C39	0.49	2.61	6	1
6:E:839:17F:P1	6:E:839:17F:N1	0.49	2.86	19	4
5:D:528:7Q9:C36	5:D:551:7Q9:C314	0.49	2.90	7	1
6:E:802:17F:H69	5:E:804:7Q9:C312	0.49	2.38	7	1
5:D:549:7Q9:C38	5:D:551:7Q9:C312	0.49	2.90	9	1
2:D:337:LEU:HG	2:E:626:LEU:HD13	0.49	1.84	10	3
5:D:554:7Q9:C13	5:E:813:7Q9:C15	0.49	2.91	11	1
5:B:205:7Q9:C39	6:B:208:17F:H33	0.49	2.38	13	1
1:A:72:MET:SD	1:A:99:GLN:HG2	0.49	2.48	15	1
5:D:525:7Q9:O31	5:D:546:7Q9:O11	0.49	2.31	17	1
5:D:528:7Q9:C313	5:D:551:7Q9:C318	0.49	2.91	20	1
5:D:541:7Q9:O11	5:D:541:7Q9:C12	0.49	2.61	1	1
5:E:847:7Q9:O13	5:E:847:7Q9:C12	0.49	2.61	3	16
5:E:834:7Q9:C23	5:E:858:7Q9:C34	0.49	2.91	3	2
5:E:848:7Q9:O21	5:E:848:7Q9:C31	0.49	2.61	12	4
6:A:213:17F:H54	6:A:213:17F:H78	0.49	1.85	5	1
6:D:517:17F:C41	6:D:533:17F:H53	0.49	2.37	5	1
5:E:868:7Q9:O22	5:E:868:7Q9:C3	0.49	2.59	16	4
5:A:212:7Q9:C12	6:A:219:17F:O2	0.49	2.60	8	1
5:D:545:7Q9:O32	5:D:545:7Q9:C15	0.49	2.61	20	2
6:E:806:17F:H54	6:E:806:17F:H68	0.49	1.83	10	1
6:E:819:17F:H12A	6:E:820:17F:C10	0.49	2.38	10	1
6:E:819:17F:O2	6:E:819:17F:C2	0.49	2.60	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:322:LEU:HD23	2:E:644:LEU:HD22	0.49	1.84	12	1
6:D:534:17F:H76	5:D:538:7Q9:C313	0.49	2.37	12	1
6:D:511:17F:C30	6:E:829:17F:H78	0.49	2.38	20	1
2:D:422:LEU:HD13	5:E:876:7Q9:C318	0.49	2.38	2	3
6:E:802:17F:H4A	5:E:804:7Q9:C15	0.49	2.38	1	1
6:A:219:17F:O9	6:A:219:17F:O8	0.49	2.31	2	2
5:E:869:7Q9:C34	5:E:874:7Q9:C37	0.49	2.91	13	5
5:E:869:7Q9:C31	5:E:874:7Q9:C13	0.49	2.91	8	7
5:A:216:7Q9:C13	5:D:506:7Q9:O13	0.49	2.61	8	1
6:E:873:17F:H20	6:E:873:17F:H36	0.49	1.84	8	2
1:B:6:LEU:O	1:B:55:ILE:HA	0.49	2.08	14	3
5:E:864:7Q9:O12	5:E:874:7Q9:C32	0.49	2.61	15	3
6:E:856:17F:H2	5:E:858:7Q9:C15	0.49	2.38	10	1
6:E:873:17F:H54	6:E:873:17F:C42	0.49	2.38	10	1
5:B:209:7Q9:C313	6:D:520:17F:H64	0.49	2.38	11	1
5:E:834:7Q9:C31	6:E:839:17F:H31	0.49	2.38	16	2
3:B:201:GSP:S1G	3:B:201:GSP:PA	0.49	3.11	12	2
5:D:537:7Q9:O22	5:D:548:7Q9:C39	0.49	2.61	13	1
5:A:205:7Q9:C13	5:A:210:7Q9:O22	0.49	2.61	15	1
5:D:505:7Q9:C13	5:D:528:7Q9:O14	0.49	2.61	15	1
5:E:865:7Q9:C34	5:E:865:7Q9:O32	0.49	2.60	15	1
5:A:206:7Q9:O12	6:A:213:17F:H18A	0.49	2.07	17	1
6:D:510:17F:H49	6:D:517:17F:H38	0.49	1.82	17	1
2:E:693:HIS:HB2	5:E:864:7Q9:C39	0.49	2.38	20	2
5:E:807:7Q9:O22	5:E:815:7Q9:C13	0.49	2.61	17	1
6:D:519:17F:H69	6:D:519:17F:C29	0.49	2.38	18	2
6:A:213:17F:C34	6:A:213:17F:C10	0.49	2.88	19	1
5:E:853:7Q9:O22	5:E:853:7Q9:C3	0.48	2.59	13	6
5:D:514:7Q9:O22	5:D:514:7Q9:C1	0.48	2.60	7	3
5:D:543:7Q9:O32	6:D:552:17F:H29	0.48	2.08	2	1
2:E:642:SER:N	2:E:643:PRO:HD2	0.48	2.23	13	9
6:D:518:17F:H29	6:D:518:17F:C20	0.48	2.37	4	2
6:D:533:17F:H1	6:D:533:17F:H18A	0.48	1.85	5	1
6:A:213:17F:H41	6:A:213:17F:H61	0.48	1.82	6	1
5:E:826:7Q9:C33	5:E:845:7Q9:C36	0.48	2.91	9	4
6:A:208:17F:H65	6:A:208:17F:C22	0.48	2.37	7	1
6:A:208:17F:H58	6:A:208:17F:H64	0.48	1.85	7	1
5:E:853:7Q9:O12	5:E:853:7Q9:C15	0.48	2.61	7	1
5:E:840:7Q9:C12	5:E:866:7Q9:C34	0.48	2.91	8	1
5:E:822:7Q9:O21	5:E:822:7Q9:C15	0.48	2.61	10	1
6:D:533:17F:HN1	6:D:533:17F:C18	0.48	2.20	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:520:17F:H70	5:E:841:7Q9:C318	0.48	2.38	17	1
5:D:542:7Q9:C13	5:D:542:7Q9:O12	0.48	2.61	17	1
6:D:517:17F:H38	6:D:517:17F:C26	0.48	2.38	19	1
5:D:504:7Q9:O14	5:D:508:7Q9:C13	0.48	2.61	20	1
5:D:537:7Q9:O22	5:D:537:7Q9:C3	0.48	2.55	19	9
6:D:510:17F:O6	6:D:517:17F:C6	0.48	2.61	2	3
5:E:811:7Q9:O32	5:E:811:7Q9:C2	0.48	2.59	14	7
5:D:516:7Q9:C13	6:D:518:17F:O10	0.48	2.61	3	1
5:D:550:7Q9:C32	6:D:552:17F:H19	0.48	2.38	4	2
2:E:558:SER:OG	6:E:873:17F:H63	0.48	2.08	8	2
6:E:820:17F:C18	5:E:853:7Q9:C33	0.48	2.91	4	3
6:E:873:17F:H2	6:E:873:17F:O2	0.48	2.08	3	1
5:D:502:7Q9:C31	5:D:525:7Q9:C12	0.48	2.91	4	1
5:A:207:7Q9:C315	5:E:821:7Q9:C314	0.48	2.91	5	1
5:E:853:7Q9:C15	5:E:853:7Q9:O13	0.48	2.61	8	4
6:E:808:17F:H12	6:E:808:17F:C32	0.48	2.38	14	2
6:E:802:17F:C33	5:E:804:7Q9:C39	0.48	2.90	7	1
5:A:206:7Q9:C22	5:B:203:7Q9:C13	0.48	2.91	8	1
5:E:807:7Q9:C312	5:E:815:7Q9:C38	0.48	2.91	8	1
5:E:815:7Q9:O13	6:E:829:17F:H4	0.48	2.08	8	1
5:A:207:7Q9:C32	5:A:215:7Q9:C1	0.48	2.92	12	1
5:E:803:7Q9:C311	6:E:810:17F:H69	0.48	2.38	12	1
6:A:208:17F:H58	6:A:208:17F:C25	0.48	2.36	13	1
6:A:213:17F:H72	5:D:503:7Q9:C313	0.48	2.38	15	1
6:D:510:17F:C33	6:D:517:17F:H37	0.48	2.36	15	1
6:D:510:17F:C18	6:D:533:17F:C20	0.48	2.90	17	1
5:E:814:7Q9:C3	5:E:830:7Q9:O13	0.48	2.60	17	1
6:D:552:17F:C9	6:D:552:17F:C31	0.48	2.91	19	1
6:A:220:17F:H46	6:A:220:17F:C1X	0.48	2.35	20	1
6:E:802:17F:H18	6:E:802:17F:H12	0.48	1.83	20	1
6:A:213:17F:H36	6:A:213:17F:C26	0.48	2.25	1	1
2:D:389:LEU:HD11	5:D:546:7Q9:C313	0.48	2.39	2	1
6:D:518:17F:C17	6:D:518:17F:O8	0.48	2.61	3	1
5:A:216:7Q9:C318	6:D:510:17F:C24	0.48	2.90	13	3
6:D:510:17F:O7	6:D:517:17F:C11	0.48	2.61	11	3
6:D:540:17F:C8	5:D:545:7Q9:C33	0.48	2.90	4	1
6:E:808:17F:H43	6:E:810:17F:H62	0.48	1.84	4	2
6:E:820:17F:C6	5:E:837:7Q9:O22	0.48	2.62	7	3
5:A:211:7Q9:C23	6:A:213:17F:H63	0.48	2.39	7	1
6:E:871:17F:H53	5:E:872:7Q9:C315	0.48	2.38	7	1
6:A:219:17F:C31	5:E:801:7Q9:C36	0.48	2.90	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:217:7Q9:C14	5:D:502:7Q9:O14	0.48	2.61	11	1
5:E:821:7Q9:O21	5:E:821:7Q9:C31	0.48	2.61	19	4
2:D:272:TRP:CE3	6:D:540:17F:H78	0.48	2.43	14	1
5:D:543:7Q9:C35	6:D:552:17F:H73	0.48	2.38	14	2
5:E:837:7Q9:C13	5:E:855:7Q9:O14	0.48	2.62	15	1
1:B:127:THR:HG22	1:B:131:GLN:HG3	0.48	1.86	17	1
1:B:147:LYS:HE3	3:B:201:GSP:N1	0.48	2.24	18	1
5:A:217:7Q9:C36	5:D:516:7Q9:C39	0.48	2.91	6	4
5:D:516:7Q9:C14	5:D:516:7Q9:O12	0.48	2.61	1	1
6:D:520:17F:O9	6:D:520:17F:O8	0.48	2.31	1	6
5:D:532:7Q9:C2	6:D:534:17F:H34	0.48	2.39	2	1
6:D:520:17F:O10	6:D:520:17F:C6	0.48	2.51	5	1
5:A:218:7Q9:C12	6:D:511:17F:O2	0.48	2.61	19	2
6:A:213:17F:C23	6:A:213:17F:C33	0.48	2.78	7	1
6:D:517:17F:H35	6:D:533:17F:H38	0.48	1.84	7	2
6:D:518:17F:H53	6:D:518:17F:C42	0.48	2.37	10	2
5:D:516:7Q9:O11	5:D:516:7Q9:O32	0.48	2.32	8	3
6:D:510:17F:C20	6:D:533:17F:H60	0.48	2.38	9	1
5:A:211:7Q9:C15	5:A:211:7Q9:C3	0.48	2.92	10	2
6:E:842:17F:C23	6:E:842:17F:C1X	0.48	2.90	13	2
6:D:518:17F:H31	5:D:528:7Q9:O22	0.48	2.08	15	1
6:D:518:17F:H32	5:D:551:7Q9:C38	0.48	2.38	16	1
5:E:848:7Q9:O32	6:E:873:17F:H12	0.48	2.09	16	1
5:D:515:7Q9:C318	6:D:519:17F:H73	0.48	2.38	17	1
5:E:809:7Q9:C13	6:E:818:17F:O1	0.48	2.62	16	2
5:D:555:7Q9:O32	5:D:555:7Q9:C2	0.48	2.60	4	3
6:A:213:17F:C20	6:A:213:17F:O9	0.48	2.62	3	1
5:E:828:7Q9:O21	5:E:828:7Q9:O32	0.48	2.30	19	9
1:B:14:VAL:HG23	1:B:16:LYS:HG3	0.48	1.85	4	1
6:A:219:17F:O5	5:D:504:7Q9:C13	0.48	2.61	6	4
6:D:539:17F:H61	5:D:549:7Q9:O22	0.48	2.08	7	1
5:E:851:7Q9:C315	6:E:871:17F:H34	0.48	2.39	7	1
6:E:808:17F:H68	6:E:819:17F:H44	0.48	1.85	8	1
5:E:864:7Q9:O22	5:E:864:7Q9:C1	0.48	2.56	20	3
5:E:835:7Q9:C15	5:E:835:7Q9:O11	0.48	2.61	11	1
5:A:216:7Q9:O32	5:B:207:7Q9:C33	0.48	2.61	13	1
5:E:833:7Q9:C22	6:E:839:17F:C4	0.48	2.92	15	1
1:B:68:ARG:HA	1:B:71:TYR:CE2	0.48	2.43	16	1
5:D:549:7Q9:O13	5:E:801:7Q9:C3	0.48	2.61	16	1
5:D:556:7Q9:C2	5:D:556:7Q9:O32	0.48	2.56	16	1
6:E:819:17F:H30	5:E:836:7Q9:C37	0.48	2.39	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:220:17F:H53	6:E:810:17F:C39	0.48	2.38	18	1
5:A:206:7Q9:C11	5:A:211:7Q9:O22	0.48	2.61	2	1
6:D:510:17F:C6	6:D:517:17F:C4	0.48	2.77	2	2
6:A:208:17F:H58	6:A:208:17F:C36	0.48	2.32	3	1
5:B:205:7Q9:C314	6:B:208:17F:H65	0.48	2.38	3	1
5:E:811:7Q9:C3	5:E:826:7Q9:C35	0.48	2.91	3	1
5:D:538:7Q9:O32	5:D:538:7Q9:C21	0.48	2.61	17	5
6:D:540:17F:C33	6:D:540:17F:C1X	0.48	2.92	4	1
1:A:16:LYS:HB2	3:A:201:GSP:O2G	0.48	2.08	5	1
5:E:864:7Q9:C23	5:E:868:7Q9:C22	0.48	2.91	20	2
5:E:828:7Q9:O13	5:E:831:7Q9:C32	0.48	2.61	7	1
5:A:204:7Q9:C311	5:A:204:7Q9:C37	0.48	2.91	11	3
5:A:211:7Q9:C22	6:A:213:17F:H6A	0.48	2.38	9	1
5:E:835:7Q9:C35	6:E:856:17F:H32	0.48	2.38	9	1
5:E:870:7Q9:C14	6:E:873:17F:O4	0.48	2.62	13	2
5:A:203:7Q9:C22	5:B:203:7Q9:O32	0.48	2.62	13	2
5:D:509:7Q9:C31	5:D:509:7Q9:C1	0.48	2.91	14	1
5:E:837:7Q9:O14	5:E:855:7Q9:C15	0.48	2.62	14	1
5:A:207:7Q9:C33	5:A:215:7Q9:C2	0.48	2.91	16	1
1:A:158:THR:HA	1:A:161:ARG:HE	0.48	1.68	20	1
2:E:719:LEU:HB2	2:E:720:PRO:HD3	0.48	1.84	8	5
1:B:32:TYR:CD2	3:B:201:GSP:H5'2	0.48	2.28	2	1
6:D:510:17F:C4	6:D:517:17F:H4	0.48	2.38	2	2
5:D:543:7Q9:O22	5:D:543:7Q9:C1	0.48	2.58	14	6
6:E:873:17F:O10	6:E:873:17F:C6	0.48	2.54	5	4
6:D:539:17F:H50	6:D:539:17F:C41	0.48	2.37	13	3
5:A:218:7Q9:C11	6:D:511:17F:H4A	0.48	2.39	6	1
5:A:211:7Q9:O11	6:A:213:17F:C18	0.48	2.62	7	1
6:E:839:17F:P1	6:E:839:17F:HN1	0.48	2.32	19	3
5:E:865:7Q9:O32	5:E:865:7Q9:C2	0.48	2.54	15	4
6:E:856:17F:O10	6:E:856:17F:C6	0.48	2.59	9	2
6:E:819:17F:H5	5:E:825:7Q9:C13	0.48	2.39	10	1
5:E:870:7Q9:C22	6:E:873:17F:C10	0.48	2.86	16	3
1:A:62:GLU:HG3	1:A:63:GLU:H	0.48	1.68	12	2
5:E:823:7Q9:C14	5:E:840:7Q9:O14	0.48	2.61	15	3
6:E:806:17F:C39	5:E:817:7Q9:C317	0.48	2.92	13	1
5:D:506:7Q9:C3	5:D:506:7Q9:C11	0.48	2.91	17	1
5:E:825:7Q9:C33	6:E:842:17F:H18A	0.48	2.38	20	1
5:E:827:7Q9:C318	5:E:841:7Q9:C313	0.48	2.92	1	1
5:B:206:7Q9:C316	5:E:809:7Q9:C312	0.48	2.92	15	4
5:B:210:7Q9:C31	6:D:520:17F:H34	0.48	2.38	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:518:17F:C18	5:D:551:7Q9:C33	0.48	2.91	18	4
6:E:842:17F:C8	5:E:867:7Q9:O14	0.48	2.61	2	1
5:E:852:7Q9:O32	5:E:852:7Q9:O21	0.48	2.31	2	6
1:A:17:SER:HB2	3:A:201:GSP:PA	0.48	2.49	3	1
1:A:117:LYS:HB3	1:A:120:LEU:HD12	0.48	1.85	4	2
6:D:534:17F:O10	6:D:534:17F:O7	0.48	2.31	8	5
6:E:839:17F:C11	6:E:857:17F:H12	0.48	2.38	4	1
2:D:257:PHE:HE2	2:E:706:LYS:HD2	0.48	1.67	6	1
6:A:208:17F:H38	6:B:208:17F:C34	0.48	2.39	7	1
5:A:211:7Q9:O11	6:A:213:17F:H18	0.48	2.09	7	1
1:A:114:VAL:HG12	1:A:142:ILE:HB	0.48	1.86	9	1
5:B:205:7Q9:C317	6:E:812:17F:H71	0.48	2.39	10	1
5:E:833:7Q9:C2	6:E:857:17F:H6A	0.48	2.39	13	1
6:E:818:17F:H9	5:E:821:7Q9:C22	0.48	2.39	16	1
6:A:213:17F:C12	6:A:213:17F:H40	0.48	2.37	17	1
5:E:850:7Q9:O22	5:E:850:7Q9:C3	0.48	2.53	18	1
1:B:116:ASN:OD1	1:B:145:SER:HA	0.48	2.09	20	1
5:D:506:7Q9:C31	6:D:517:17F:H20A	0.48	2.38	20	1
6:D:510:17F:H58	6:D:533:17F:H66	0.48	1.85	20	1
6:D:540:17F:C33	6:D:540:17F:H36	0.48	2.38	2	3
5:D:553:7Q9:C3	5:D:553:7Q9:O22	0.48	2.54	1	1
5:E:870:7Q9:C21	6:E:873:17F:H10	0.48	2.39	2	1
6:E:802:17F:C34	5:E:804:7Q9:C39	0.48	2.92	6	3
6:E:829:17F:N1	5:E:852:7Q9:O13	0.48	2.47	3	1
6:E:875:17F:H49	6:E:875:17F:H78	0.48	1.86	3	1
5:B:204:7Q9:C22	5:B:207:7Q9:C310	0.48	2.91	11	3
6:E:819:17F:H48	6:E:819:17F:C42	0.48	2.37	5	1
6:E:842:17F:O5	5:E:877:7Q9:C13	0.48	2.62	5	1
6:A:219:17F:H6A	6:A:219:17F:O10	0.48	2.08	8	4
1:A:97:ARG:HG3	1:A:111:MET:HE1	0.48	1.86	17	2
6:A:213:17F:C34	6:A:213:17F:H39	0.48	2.39	8	1
6:A:213:17F:HN1	6:A:213:17F:H19A	0.48	1.67	9	1
5:B:209:7Q9:C315	5:E:823:7Q9:C314	0.48	2.91	12	3
5:E:849:7Q9:O22	5:E:849:7Q9:C1	0.48	2.57	20	6
5:D:544:7Q9:C14	5:D:544:7Q9:O32	0.48	2.62	12	2
6:A:219:17F:O8	6:A:219:17F:C19	0.48	2.62	13	2
6:E:802:17F:O2	5:E:807:7Q9:C12	0.48	2.61	18	1
6:A:213:17F:H37	5:D:509:7Q9:C3	0.48	2.39	19	1
5:E:846:7Q9:O32	5:E:846:7Q9:C2	0.48	2.56	1	4
5:E:867:7Q9:O31	5:E:867:7Q9:C21	0.48	2.61	2	19
5:D:506:7Q9:O32	5:D:506:7Q9:C2	0.48	2.60	16	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:856:17F:H38	6:E:856:17F:C38	0.48	2.39	2	3
5:B:207:7Q9:C1	5:B:207:7Q9:O32	0.48	2.61	3	1
6:E:839:17F:H68	6:E:857:17F:C24	0.48	2.37	3	1
5:E:854:7Q9:O14	5:E:854:7Q9:C12	0.48	2.62	3	2
5:E:838:7Q9:C14	6:E:842:17F:H18	0.48	2.38	5	1
5:D:553:7Q9:O22	5:D:553:7Q9:C3	0.48	2.55	6	4
6:A:213:17F:C34	6:A:213:17F:H11	0.48	2.38	7	1
2:E:656:VAL:CG1	6:E:857:17F:H64	0.48	2.38	7	2
6:A:213:17F:O9	6:A:213:17F:O1	0.48	2.32	8	2
6:E:808:17F:H68	6:E:819:17F:C25	0.48	2.39	8	1
5:E:849:7Q9:C312	5:E:852:7Q9:C34	0.48	2.92	8	1
6:D:520:17F:H19A	6:D:520:17F:C10	0.48	2.39	9	2
5:E:864:7Q9:O12	5:E:864:7Q9:C15	0.48	2.61	15	1
5:D:550:7Q9:C12	6:D:552:17F:O5	0.48	2.62	18	1
1:B:112:VAL:HG22	1:B:140:PRO:HG2	0.48	1.84	20	1
5:D:514:7Q9:O12	5:D:514:7Q9:C15	0.47	2.62	13	3
5:A:215:7Q9:O32	5:A:215:7Q9:O21	0.47	2.32	14	4
6:A:220:17F:H10A	6:A:220:17F:H63	0.47	1.84	11	2
5:E:821:7Q9:O13	5:E:821:7Q9:C12	0.47	2.62	2	7
6:D:517:17F:H2	6:D:517:17F:H19	0.47	1.85	3	1
6:D:510:17F:O8	6:D:517:17F:C19	0.47	2.50	4	1
6:D:510:17F:C10	6:D:517:17F:H8A	0.47	2.35	16	3
5:D:555:7Q9:C12	5:E:833:7Q9:O22	0.47	2.62	4	2
6:D:510:17F:H29	6:D:517:17F:H8	0.47	1.86	5	1
6:E:808:17F:H74	6:E:808:17F:C29	0.47	2.39	20	2
6:D:518:17F:C17	5:D:551:7Q9:C33	0.47	2.91	19	3
2:D:327:GLN:HG3	6:D:534:17F:C42	0.47	2.39	8	1
5:A:217:7Q9:C35	5:D:516:7Q9:C39	0.47	2.91	10	1
6:E:819:17F:O1	5:E:838:7Q9:C11	0.47	2.62	11	1
5:B:203:7Q9:C23	5:B:204:7Q9:O31	0.47	2.62	12	1
5:D:543:7Q9:O32	5:D:543:7Q9:C2	0.47	2.58	20	2
6:A:213:17F:H11	5:D:503:7Q9:C23	0.47	2.38	16	1
5:B:210:7Q9:C318	5:E:823:7Q9:C38	0.47	2.92	16	1
6:A:219:17F:H4	6:A:219:17F:C2	0.47	2.39	17	1
6:E:818:17F:H40	6:E:818:17F:H30	0.47	1.86	20	1
6:A:213:17F:H38	6:A:213:17F:C20	0.47	2.38	1	1
5:D:543:7Q9:C318	5:E:872:7Q9:C315	0.47	2.93	3	1
2:E:664:ALA:HB3	2:E:665:PRO:HD3	0.47	1.85	3	1
5:D:530:7Q9:O22	5:D:530:7Q9:C1	0.47	2.58	19	7
5:A:205:7Q9:C316	6:E:806:17F:H53	0.47	2.39	5	1
5:E:803:7Q9:C3	6:E:810:17F:O1	0.47	2.62	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:804:7Q9:C311	5:E:815:7Q9:C38	0.47	2.92	5	2
6:E:829:17F:H11	5:E:833:7Q9:C37	0.47	2.39	5	1
5:A:218:7Q9:C31	5:A:218:7Q9:C21	0.47	2.92	7	1
6:D:510:17F:O3	6:D:517:17F:H6	0.47	2.09	19	3
5:D:514:7Q9:C32	5:D:516:7Q9:C37	0.47	2.92	8	1
2:E:634:LEU:HG	5:E:863:7Q9:C312	0.47	2.40	12	1
1:A:4:TYR:CD2	1:A:51:CYS:HB3	0.47	2.45	15	2
6:E:820:17F:H20	5:E:830:7Q9:C11	0.47	2.39	13	1
6:E:808:17F:C30	6:E:819:17F:H76	0.47	2.38	15	1
5:D:543:7Q9:C316	6:E:871:17F:H52	0.47	2.38	16	1
6:E:808:17F:H68	6:E:819:17F:C22	0.47	2.39	17	1
6:E:875:17F:H18A	6:E:875:17F:N1	0.47	2.23	20	1
5:E:833:7Q9:C14	6:E:857:17F:O8	0.47	2.62	2	1
1:B:113:LEU:O	1:B:141:PHE:HA	0.47	2.08	3	1
5:E:837:7Q9:O21	5:E:837:7Q9:C31	0.47	2.62	9	13
5:A:217:7Q9:O14	5:A:217:7Q9:C2	0.47	2.62	8	3
5:D:502:7Q9:O21	5:D:502:7Q9:O14	0.47	2.33	20	7
6:D:510:17F:H11A	6:D:517:17F:H8A	0.47	1.85	14	2
1:B:127:THR:O	1:B:131:GLN:HG3	0.47	2.10	16	2
5:B:209:7Q9:C318	5:E:824:7Q9:C314	0.47	2.92	9	2
6:E:873:17F:H44	6:E:873:17F:C33	0.47	2.39	9	3
1:A:83:ALA:HB3	1:A:86:ASN:HB3	0.47	1.84	12	1
5:E:803:7Q9:C22	6:E:806:17F:C1Z	0.47	2.92	12	1
6:E:808:17F:O5	5:E:814:7Q9:C14	0.47	2.62	12	1
5:A:210:7Q9:C38	5:A:210:7Q9:C22	0.47	2.93	19	2
6:A:220:17F:O10	6:A:220:17F:C4	0.47	2.59	13	2
5:E:822:7Q9:C15	5:E:822:7Q9:C3	0.47	2.92	13	1
5:D:509:7Q9:C1	5:D:509:7Q9:O32	0.47	2.62	14	1
5:E:826:7Q9:C318	5:E:845:7Q9:C313	0.47	2.93	14	1
5:A:203:7Q9:C317	6:E:802:17F:H76	0.47	2.40	15	1
6:D:517:17F:H41	6:D:533:17F:C23	0.47	2.40	15	1
5:D:556:7Q9:O14	5:E:854:7Q9:C15	0.47	2.62	15	1
6:E:820:17F:H65	5:E:837:7Q9:C37	0.47	2.39	15	1
6:D:510:17F:H48	6:D:510:17F:C34	0.47	2.39	17	1
6:E:839:17F:H33	6:E:839:17F:C2X	0.47	2.35	17	1
6:E:875:17F:H66	6:E:875:17F:H46	0.47	1.86	17	1
6:A:208:17F:H71	6:A:208:17F:H54	0.47	1.84	18	1
1:A:7:VAL:HG11	1:A:71:TYR:CD2	0.47	2.44	19	1
5:B:203:7Q9:C3	5:B:204:7Q9:C15	0.47	2.92	19	1
5:D:554:7Q9:C32	5:E:832:7Q9:C22	0.47	2.92	19	1
6:B:208:17F:H46	5:E:824:7Q9:C316	0.47	2.39	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:804:7Q9:O32	6:E:808:17F:H9	0.47	2.09	20	1
5:E:834:7Q9:C11	6:E:839:17F:H2	0.47	2.38	20	1
5:A:204:7Q9:C34	5:A:211:7Q9:C37	0.47	2.93	1	4
6:A:208:17F:O4	5:A:212:7Q9:C12	0.47	2.63	1	1
5:A:211:7Q9:O22	5:A:211:7Q9:C1	0.47	2.60	8	8
6:D:520:17F:H59	6:D:520:17F:C36	0.47	2.39	5	2
5:A:211:7Q9:C13	5:A:211:7Q9:O32	0.47	2.63	10	4
1:B:16:LYS:HB2	3:B:201:GSP:PG	0.47	2.49	3	1
2:D:322:LEU:O	2:D:326:LEU:HG	0.47	2.09	3	2
6:D:540:17F:O10	6:D:540:17F:H4	0.47	2.09	17	3
6:E:808:17F:H66	5:E:814:7Q9:C310	0.47	2.40	4	1
1:A:47:ASP:OD2	1:A:161:ARG:HD2	0.47	2.10	5	2
6:D:518:17F:C20	6:D:518:17F:C1X	0.47	2.93	20	2
5:E:828:7Q9:O22	5:E:828:7Q9:C1	0.47	2.55	16	5
6:A:219:17F:H52	5:E:828:7Q9:C318	0.47	2.39	6	1
5:E:821:7Q9:C3	6:E:839:17F:O9	0.47	2.62	6	1
1:A:118:CYS:SG	1:A:143:GLU:HB3	0.47	2.49	8	2
5:D:506:7Q9:C1	5:D:506:7Q9:O22	0.47	2.56	8	5
5:E:822:7Q9:O12	5:E:822:7Q9:C15	0.47	2.62	10	1
6:A:208:17F:C36	6:A:208:17F:H35	0.47	2.39	16	2
6:B:208:17F:O8	6:B:208:17F:H4	0.47	2.08	11	1
6:E:871:17F:C11	5:E:872:7Q9:O14	0.47	2.62	11	1
6:A:208:17F:H54	6:A:208:17F:H70	0.47	1.84	12	1
2:D:349:ARG:HD3	5:D:527:7Q9:C39	0.47	2.39	12	1
5:D:527:7Q9:C37	5:D:527:7Q9:C311	0.47	2.89	13	2
5:E:813:7Q9:C14	5:E:817:7Q9:O22	0.47	2.62	15	1
6:E:839:17F:H52	5:E:858:7Q9:C311	0.47	2.40	15	1
5:D:512:7Q9:O22	5:D:536:7Q9:C15	0.47	2.62	17	1
5:A:205:7Q9:O32	5:A:205:7Q9:O21	0.47	2.32	19	1
2:D:268:THR:HG23	2:E:695:LYS:HD2	0.47	1.86	19	1
6:D:511:17F:H10	5:D:513:7Q9:C12	0.47	2.39	20	1
5:E:835:7Q9:C15	6:E:856:17F:O5	0.47	2.62	1	1
5:E:855:7Q9:C14	5:E:855:7Q9:O11	0.47	2.63	2	7
5:E:858:7Q9:O22	5:E:858:7Q9:C1	0.47	2.60	6	7
6:E:802:17F:C42	6:E:802:17F:C28	0.47	2.92	2	3
5:D:549:7Q9:C318	5:E:876:7Q9:C311	0.47	2.92	3	1
6:E:873:17F:H19	6:E:873:17F:H30	0.47	1.85	10	2
6:A:208:17F:C26	6:A:208:17F:H64	0.47	2.39	5	1
5:D:502:7Q9:C21	5:D:502:7Q9:O31	0.47	2.63	5	2
6:E:839:17F:C39	6:E:875:17F:H53	0.47	2.39	5	1
6:D:510:17F:H8	6:D:517:17F:C18	0.47	2.39	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:134:ALA:HB1	1:B:139:ILE:O	0.47	2.09	17	2
1:A:146:ALA:N	3:A:201:GSP:O6	0.47	2.48	14	7
5:D:555:7Q9:C1	5:E:852:7Q9:C22	0.47	2.93	8	1
6:D:510:17F:H58	6:D:517:17F:H37	0.47	1.84	11	1
6:E:857:17F:H11A	6:E:875:17F:O10	0.47	2.09	12	1
2:D:326:LEU:HD22	2:E:637:LEU:HG	0.47	1.87	17	1
6:E:839:17F:H8	6:E:857:17F:C21	0.47	2.39	19	1
6:E:839:17F:O8	6:E:857:17F:H12	0.47	2.10	19	1
6:D:534:17F:C23	5:D:538:7Q9:C316	0.47	2.93	20	1
5:D:523:7Q9:O14	5:D:523:7Q9:C12	0.47	2.62	8	3
5:E:824:7Q9:C1	5:E:824:7Q9:O22	0.47	2.58	15	4
5:E:803:7Q9:C315	6:E:810:17F:H66	0.47	2.40	3	3
1:A:127:THR:HG22	1:A:131:GLN:HG3	0.47	1.86	4	2
6:B:208:17F:C10	5:B:209:7Q9:C37	0.47	2.93	4	1
6:A:213:17F:H66	6:A:213:17F:C26	0.47	2.37	5	1
5:E:807:7Q9:C1	5:E:807:7Q9:O22	0.47	2.60	5	1
6:E:871:17F:C21	6:E:871:17F:H58	0.47	2.40	5	2
5:E:877:7Q9:O32	5:E:877:7Q9:O21	0.47	2.33	5	1
5:E:859:7Q9:O22	5:E:859:7Q9:C1	0.47	2.60	15	6
2:D:414:LEU:HD21	2:E:740:LEU:HD23	0.47	1.86	7	3
2:E:722:LEU:HG	2:E:726:LYS:HE3	0.47	1.86	9	1
6:A:213:17F:H68	6:A:213:17F:C30	0.47	2.33	10	1
5:D:506:7Q9:O31	6:D:517:17F:H18A	0.47	2.10	10	1
6:D:540:17F:C8	5:D:545:7Q9:C313	0.47	2.93	10	1
6:E:873:17F:H54	6:E:873:17F:H76	0.47	1.85	10	1
5:A:214:7Q9:C35	5:A:218:7Q9:C34	0.47	2.92	13	1
6:E:839:17F:C23	6:E:839:17F:C1Z	0.47	2.92	14	3
6:A:220:17F:O4	5:D:515:7Q9:C13	0.47	2.63	17	1
5:D:503:7Q9:C317	6:E:842:17F:H74	0.47	2.39	17	1
6:D:510:17F:H57	5:D:530:7Q9:C310	0.47	2.39	17	1
6:D:510:17F:H50	6:D:517:17F:H39	0.47	1.85	18	1
6:D:534:17F:C37	6:D:534:17F:C21	0.47	2.93	18	1
6:E:875:17F:H18A	6:E:875:17F:O4	0.47	2.10	19	1
6:A:219:17F:O10	6:D:518:17F:C8	0.47	2.63	20	1
5:D:549:7Q9:C23	5:D:549:7Q9:C35	0.47	2.93	20	1
2:D:399:HIS:CE1	2:E:564:LEU:HB2	0.47	2.45	17	5
5:D:509:7Q9:O32	5:D:509:7Q9:C1	0.47	2.63	1	1
6:D:510:17F:C5	6:D:517:17F:H9A	0.47	2.38	17	5
5:D:513:7Q9:C312	6:D:534:17F:H71	0.47	2.40	1	1
5:D:515:7Q9:O13	5:D:525:7Q9:C12	0.47	2.62	17	2
6:E:812:17F:O6	6:E:812:17F:C7	0.47	2.63	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:821:7Q9:C14	5:E:821:7Q9:O12	0.47	2.63	1	2
5:E:864:7Q9:C35	5:E:864:7Q9:C31	0.47	2.92	12	13
5:D:506:7Q9:C318	6:E:839:17F:H76	0.47	2.39	2	1
5:E:814:7Q9:C15	5:E:814:7Q9:O12	0.47	2.63	3	5
5:E:823:7Q9:C14	5:E:823:7Q9:P	0.47	3.03	2	1
6:A:213:17F:O1	6:A:213:17F:O7	0.47	2.32	3	1
6:D:510:17F:O10	6:D:533:17F:C19	0.47	2.63	12	3
5:E:827:7Q9:C14	5:E:850:7Q9:C13	0.47	2.92	16	2
5:E:854:7Q9:C13	5:E:854:7Q9:P	0.47	3.03	3	5
5:E:860:7Q9:C311	5:E:860:7Q9:C37	0.47	2.89	3	1
6:E:873:17F:H19	6:E:873:17F:H29	0.47	1.85	3	2
6:E:820:17F:H20	5:E:830:7Q9:O11	0.47	2.09	4	1
6:D:517:17F:H36	6:D:533:17F:H38	0.47	1.86	5	2
6:E:806:17F:H4A	5:E:811:7Q9:C14	0.47	2.39	5	1
5:E:830:7Q9:C38	5:E:853:7Q9:C311	0.47	2.93	5	1
5:A:207:7Q9:O14	5:B:203:7Q9:C14	0.47	2.63	15	2
5:D:545:7Q9:O22	5:D:545:7Q9:C3	0.47	2.60	17	10
5:A:210:7Q9:C315	6:A:220:17F:H45	0.47	2.40	7	2
1:B:72:MET:HA	1:B:78:PHE:CZ	0.47	2.45	7	3
6:D:517:17F:H74	6:D:533:17F:H53	0.47	1.85	11	2
6:A:220:17F:H1A	5:D:503:7Q9:C14	0.47	2.40	10	1
6:D:517:17F:C28	6:D:517:17F:H70	0.47	2.40	10	1
5:D:525:7Q9:C14	5:D:525:7Q9:O11	0.47	2.63	10	1
6:E:806:17F:H69	5:E:817:7Q9:C317	0.47	2.39	19	2
5:A:217:7Q9:C14	5:D:502:7Q9:C22	0.47	2.92	11	1
6:B:208:17F:H61	6:B:208:17F:H53	0.47	1.86	13	1
6:B:208:17F:H61	6:B:208:17F:H55	0.47	1.85	13	1
2:D:366:TYR:HD1	2:E:597:VAL:HG13	0.47	1.70	13	1
5:E:822:7Q9:O12	5:E:822:7Q9:O21	0.47	2.33	15	2
6:D:534:17F:O2	5:D:538:7Q9:C14	0.47	2.62	15	1
5:A:211:7Q9:C314	6:A:220:17F:H33	0.47	2.40	16	1
6:D:511:17F:H66	6:D:511:17F:H40	0.47	1.86	16	1
6:E:808:17F:H69	6:E:820:17F:C21	0.47	2.39	16	1
6:D:510:17F:C41	6:E:857:17F:H48	0.47	2.39	17	1
6:D:552:17F:C31	6:D:552:17F:H9A	0.47	2.39	19	1
5:E:809:7Q9:C312	5:E:827:7Q9:C316	0.47	2.93	20	1
2:D:265:GLY:HA2	2:E:699:HIS:HE1	0.47	1.69	14	3
5:D:502:7Q9:O31	5:D:502:7Q9:C21	0.47	2.63	10	12
5:E:830:7Q9:O13	5:E:830:7Q9:C2	0.47	2.62	17	5
5:E:838:7Q9:C15	5:E:838:7Q9:O11	0.47	2.62	20	8
2:D:440:LEU:HD11	5:D:543:7Q9:C314	0.47	2.40	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:501:7Q9:O13	5:D:521:7Q9:C13	0.47	2.63	3	1
6:D:534:17F:C2X	5:D:538:7Q9:C315	0.47	2.88	3	1
1:A:33:ASP:O	3:A:201:GSP:S1G	0.47	2.73	16	2
1:A:47:ASP:CA	1:B:128:LYS:HB3	0.47	2.35	4	1
5:E:855:7Q9:O32	5:E:855:7Q9:O21	0.47	2.33	17	5
6:D:539:17F:H43	6:D:539:17F:H67	0.47	1.85	13	2
5:E:825:7Q9:C33	6:E:842:17F:C20	0.47	2.89	20	2
1:B:126:ASP:OD2	1:B:128:LYS:HG2	0.47	2.09	19	2
5:A:209:7Q9:C15	5:A:218:7Q9:O13	0.47	2.62	11	2
5:A:206:7Q9:C316	6:E:802:17F:H69	0.47	2.40	13	1
2:E:633:LYS:HB3	5:E:878:7Q9:C317	0.47	2.40	15	1
6:E:820:17F:H48	6:E:820:17F:C38	0.47	2.38	15	1
6:A:213:17F:H68	6:A:213:17F:C29	0.47	2.38	16	1
6:D:533:17F:H77	6:D:533:17F:C30	0.47	2.31	16	1
5:D:537:7Q9:C13	5:D:546:7Q9:C11	0.47	2.93	16	1
2:D:333:LYS:HE3	5:D:538:7Q9:C314	0.47	2.39	17	1
5:E:849:7Q9:O22	5:E:849:7Q9:C13	0.47	2.63	20	2
6:D:510:17F:C6	6:D:517:17F:H9A	0.47	2.39	17	4
6:E:802:17F:O7	6:E:802:17F:O6	0.47	2.32	20	5
5:A:206:7Q9:C15	5:A:211:7Q9:O22	0.47	2.63	3	2
6:D:519:17F:O8	6:D:519:17F:O9	0.47	2.33	11	4
5:D:554:7Q9:O32	5:E:832:7Q9:C22	0.47	2.63	7	3
5:E:844:7Q9:C1	5:E:845:7Q9:C34	0.47	2.92	4	2
2:D:418:LEU:HD23	2:E:739:LYS:HD2	0.47	1.87	7	2
5:B:210:7Q9:C14	6:D:520:17F:O4	0.47	2.62	6	1
6:D:540:17F:H76	2:E:692:TYR:CE2	0.47	2.42	9	1
5:A:218:7Q9:C39	6:D:511:17F:H35	0.47	2.40	10	1
6:A:213:17F:H43	6:A:213:17F:C37	0.47	2.39	11	1
5:A:218:7Q9:C316	5:E:814:7Q9:C318	0.47	2.93	12	1
6:A:220:17F:H47	6:A:220:17F:H77	0.47	1.85	12	1
2:D:373:ARG:O	2:D:377:ARG:HG3	0.47	2.10	12	1
6:D:510:17F:C7	6:D:517:17F:H4A	0.47	2.40	20	2
6:E:802:17F:C36	5:E:804:7Q9:C39	0.47	2.93	14	1
5:E:836:7Q9:O31	5:E:838:7Q9:C23	0.47	2.63	14	1
6:E:839:17F:H52	5:E:858:7Q9:C310	0.47	2.40	15	1
1:A:46:ILE:HG21	1:A:160:VAL:HG21	0.47	1.85	16	1
6:D:510:17F:C18	6:D:517:17F:C10	0.47	2.82	16	1
1:B:84:ILE:HD11	1:B:118:CYS:HA	0.47	1.87	17	1
5:D:503:7Q9:C3	6:D:519:17F:O2	0.47	2.63	17	1
6:D:511:17F:H43	5:D:513:7Q9:C317	0.47	2.40	17	1
6:D:539:17F:O10	5:D:549:7Q9:O11	0.47	2.32	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:538:7Q9:C15	5:D:538:7Q9:P	0.47	3.03	17	2
1:A:142:ILE:HD13	1:A:155:ALA:HA	0.47	1.86	2	1
6:D:518:17F:H18	5:D:551:7Q9:C33	0.47	2.40	2	1
5:E:815:7Q9:O21	5:E:815:7Q9:C31	0.47	2.63	3	14
5:D:554:7Q9:C21	5:E:817:7Q9:C22	0.47	2.93	3	1
5:E:803:7Q9:C317	6:E:810:17F:H69	0.47	2.40	7	3
5:E:851:7Q9:C315	6:E:871:17F:H20	0.47	2.40	7	2
1:B:14:VAL:CG2	1:B:16:LYS:HG3	0.47	2.40	4	2
1:A:72:MET:SD	1:A:100:ILE:HA	0.47	2.50	5	1
5:D:516:7Q9:O22	5:D:537:7Q9:C14	0.47	2.63	6	1
5:A:217:7Q9:C35	5:D:516:7Q9:C38	0.47	2.93	7	1
5:A:207:7Q9:O14	5:B:203:7Q9:C13	0.47	2.63	13	1
5:D:554:7Q9:O21	5:D:554:7Q9:C31	0.47	2.63	14	1
1:A:46:ILE:HD13	1:A:160:VAL:HG21	0.47	1.86	20	1
6:A:220:17F:H52	6:A:220:17F:C39	0.46	2.40	2	1
6:E:842:17F:H9A	5:E:867:7Q9:O14	0.46	2.09	2	1
6:E:839:17F:N1	6:E:839:17F:P1	0.46	2.88	11	2
5:E:853:7Q9:O22	5:E:859:7Q9:C13	0.46	2.63	11	3
1:B:24:ILE:HG13	1:B:40:TYR:CD2	0.46	2.46	4	1
2:D:305:GLN:HA	2:D:308:TRP:HE3	0.46	1.70	4	1
5:D:502:7Q9:C34	5:D:525:7Q9:C22	0.46	2.93	20	3
6:E:802:17F:H35	6:E:802:17F:C24	0.46	2.36	5	5
6:D:533:17F:H11	5:D:541:7Q9:C35	0.46	2.40	6	1
5:A:215:7Q9:C34	6:D:511:17F:H68	0.46	2.40	9	1
6:E:812:17F:H6A	6:E:812:17F:O10	0.46	2.10	9	1
2:D:388:ARG:HB3	2:E:572:TRP:HZ3	0.46	1.70	12	1
5:A:217:7Q9:O14	5:A:217:7Q9:C12	0.46	2.63	16	1
5:B:205:7Q9:C315	6:E:812:17F:H75	0.46	2.40	18	1
1:A:84:ILE:HB	1:A:123:ARG:HB2	0.46	1.87	19	1
1:A:84:ILE:HD13	1:A:118:CYS:HA	0.46	1.87	2	5
6:A:220:17F:C35	6:A:220:17F:H32	0.46	2.41	2	1
5:D:530:7Q9:C12	5:D:532:7Q9:C33	0.46	2.93	2	1
5:E:809:7Q9:C22	5:E:809:7Q9:C35	0.46	2.93	11	2
1:A:16:LYS:HA	1:A:19:LEU:HD12	0.46	1.88	3	1
5:A:204:7Q9:C11	5:A:205:7Q9:C22	0.46	2.94	3	2
5:E:841:7Q9:O22	5:E:874:7Q9:C37	0.46	2.63	4	2
5:A:212:7Q9:C34	5:D:505:7Q9:C34	0.46	2.93	7	2
5:D:513:7Q9:C312	6:D:534:17F:H64	0.46	2.39	5	1
5:D:543:7Q9:C32	6:D:552:17F:C1X	0.46	2.93	5	1
6:D:511:17F:H37	5:D:513:7Q9:C315	0.46	2.39	8	1
5:A:207:7Q9:C22	5:B:203:7Q9:C22	0.46	2.94	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:H43	6:D:517:17F:H64	0.46	1.88	18	3
5:D:509:7Q9:C33	5:D:509:7Q9:O13	0.46	2.62	13	1
5:D:524:7Q9:C13	6:D:539:17F:O1	0.46	2.63	13	1
5:E:821:7Q9:C3	6:E:839:17F:H6	0.46	2.41	13	1
5:D:554:7Q9:O21	5:D:554:7Q9:O32	0.46	2.32	14	1
2:E:652:ALA:O	2:E:656:VAL:HG23	0.46	2.09	14	2
5:E:804:7Q9:C15	5:E:807:7Q9:C3	0.46	2.93	14	1
5:E:869:7Q9:C36	5:E:874:7Q9:C38	0.46	2.93	14	1
6:D:510:17F:C20	6:D:517:17F:C10	0.46	2.78	15	1
5:E:834:7Q9:C312	6:E:839:17F:H54	0.46	2.39	16	1
6:A:213:17F:C11	6:A:213:17F:H40	0.46	2.40	17	1
5:D:523:7Q9:C3	6:D:552:17F:H20A	0.46	2.40	20	1
1:B:15:GLY:CA	3:B:201:GSP:C8	0.46	2.98	3	2
6:D:520:17F:H6A	5:D:545:7Q9:C38	0.46	2.40	1	1
5:D:541:7Q9:C14	5:D:541:7Q9:C1	0.46	2.93	5	4
6:E:839:17F:H8A	6:E:857:17F:C21	0.46	2.40	2	1
5:A:203:7Q9:C37	6:A:208:17F:H8A	0.46	2.40	3	1
6:A:208:17F:H41	6:A:208:17F:H57	0.46	1.88	3	1
5:B:207:7Q9:C14	5:D:506:7Q9:O14	0.46	2.64	5	2
6:D:520:17F:H47	6:D:520:17F:C39	0.46	2.38	3	2
6:E:819:17F:C23	5:E:836:7Q9:C37	0.46	2.93	3	1
5:E:849:7Q9:C36	5:E:852:7Q9:O31	0.46	2.63	3	1
6:D:534:17F:H18A	5:D:538:7Q9:C35	0.46	2.41	5	1
6:E:808:17F:H57	6:E:820:17F:C12	0.46	2.40	7	2
5:A:211:7Q9:O22	6:A:213:17F:C31	0.46	2.64	7	1
5:E:859:7Q9:C23	5:E:878:7Q9:C38	0.46	2.93	20	3
1:A:128:LYS:HB3	1:B:47:ASP:HA	0.46	1.87	8	2
6:D:510:17F:H77	6:D:517:17F:H75	0.46	1.87	8	2
5:E:834:7Q9:C314	6:E:839:17F:H53	0.46	2.41	8	1
6:A:208:17F:C42	5:E:805:7Q9:C318	0.46	2.93	19	2
1:B:163:ILE:HG22	1:B:167:LYS:HE2	0.46	1.88	9	1
5:D:514:7Q9:C13	5:D:525:7Q9:O22	0.46	2.63	9	2
5:E:833:7Q9:C23	6:E:839:17F:H6A	0.46	2.40	10	2
5:D:514:7Q9:O12	5:D:514:7Q9:C21	0.46	2.63	14	1
6:E:839:17F:H8A	6:E:857:17F:H41	0.46	1.87	15	1
5:D:524:7Q9:C14	6:D:539:17F:O5	0.46	2.63	16	1
6:D:540:17F:C1X	6:D:540:17F:C36	0.46	2.93	16	1
6:E:802:17F:O4	5:E:807:7Q9:C14	0.46	2.63	16	1
6:A:220:17F:H77	6:A:220:17F:H42	0.46	1.86	18	1
1:B:5:LYS:HB2	1:B:76:GLU:HG3	0.46	1.87	18	1
2:E:593:VAL:HA	2:E:596:LYS:HE2	0.46	1.86	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:540:17F:C34	6:D:540:17F:C2X	0.46	2.94	2	2
6:E:839:17F:H57	6:E:839:17F:C36	0.46	2.37	2	2
6:D:510:17F:H56	6:D:517:17F:H12A	0.46	1.86	3	1
6:D:518:17F:O8	6:D:518:17F:O9	0.46	2.33	3	1
1:A:82:PHE:HB3	1:A:93:ILE:HD11	0.46	1.88	4	1
5:E:870:7Q9:C15	5:E:870:7Q9:O14	0.46	2.63	10	11
5:D:506:7Q9:C316	5:E:834:7Q9:C314	0.46	2.94	5	1
5:E:831:7Q9:C317	6:E:871:17F:H50	0.46	2.41	5	1
2:D:363:LEU:HD21	5:E:877:7Q9:C314	0.46	2.41	6	1
6:E:829:17F:C8	5:E:833:7Q9:C33	0.46	2.93	6	1
1:A:158:THR:O	1:A:162:GLU:HG2	0.46	2.09	7	1
5:D:550:7Q9:C14	6:D:552:17F:H1	0.46	2.41	8	1
5:D:542:7Q9:C21	5:D:542:7Q9:O14	0.46	2.64	9	2
1:A:131:GLN:HG2	1:A:141:PHE:CD2	0.46	2.45	10	1
5:E:816:7Q9:O32	5:E:816:7Q9:C11	0.46	2.64	10	1
6:D:519:17F:H66	6:D:519:17F:C25	0.46	2.35	12	1
6:A:213:17F:C12	6:A:213:17F:O2	0.46	2.63	13	1
2:D:256:THR:O	2:D:260:LEU:HG	0.46	2.10	13	2
6:A:219:17F:O8	5:D:505:7Q9:C34	0.46	2.64	14	1
5:A:206:7Q9:C15	5:A:211:7Q9:O13	0.46	2.64	15	1
5:A:212:7Q9:O13	5:A:217:7Q9:C22	0.46	2.63	15	1
6:A:213:17F:H34	6:A:213:17F:C21	0.46	2.22	16	2
5:E:840:7Q9:C37	5:E:841:7Q9:C23	0.46	2.94	15	1
2:D:404:SER:HB3	5:D:548:7Q9:C315	0.46	2.40	16	1
6:D:552:17F:C37	6:D:552:17F:H41	0.46	2.41	17	1
2:E:605:GLN:HG3	2:E:606:LYS:N	0.46	2.26	17	1
6:A:220:17F:H47	6:A:220:17F:C33	0.46	2.40	19	1
6:D:511:17F:O4	5:D:513:7Q9:C14	0.46	2.63	20	1
5:B:203:7Q9:O22	5:B:203:7Q9:C1	0.46	2.60	1	4
6:D:510:17F:H1	6:D:517:17F:H4	0.46	1.86	1	1
5:D:530:7Q9:O21	5:D:530:7Q9:C31	0.46	2.64	12	5
5:E:803:7Q9:C316	6:E:810:17F:H72	0.46	2.41	8	3
5:B:206:7Q9:C318	6:E:812:17F:C42	0.46	2.91	3	1
6:E:810:17F:O7	6:E:810:17F:C17	0.46	2.63	10	9
6:A:213:17F:H29	5:D:509:7Q9:C22	0.46	2.41	5	1
5:E:807:7Q9:C35	5:E:807:7Q9:C311	0.46	2.93	13	3
5:E:828:7Q9:O13	5:E:831:7Q9:C33	0.46	2.64	9	2
5:B:205:7Q9:C22	5:B:209:7Q9:C3	0.46	2.93	6	1
2:D:333:LYS:HB2	2:D:333:LYS:NZ	0.46	2.25	7	1
6:D:533:17F:H46	6:D:533:17F:C42	0.46	2.37	8	1
5:D:544:7Q9:O32	5:D:544:7Q9:C12	0.46	2.63	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:546:7Q9:C318	5:D:556:7Q9:C316	0.46	2.94	9	1
6:E:871:17F:H58	6:E:871:17F:H35	0.46	1.86	9	2
1:B:78:PHE:HB2	1:B:111:MET:HG3	0.46	1.87	10	1
5:A:206:7Q9:C15	6:A:213:17F:O10	0.46	2.64	11	1
5:E:860:7Q9:O32	5:E:860:7Q9:C23	0.46	2.64	15	2
1:B:15:GLY:HA3	3:B:201:GSP:C8	0.46	2.45	15	2
6:E:839:17F:C8	6:E:857:17F:H41	0.46	2.41	15	1
5:E:834:7Q9:C15	6:E:856:17F:O5	0.46	2.63	16	1
6:D:510:17F:C17	6:D:533:17F:C20	0.46	2.93	17	1
6:A:208:17F:O2	6:A:208:17F:C10	0.46	2.63	20	1
1:A:17:SER:N	3:A:201:GSP:O1A	0.46	2.49	1	2
5:E:801:7Q9:C13	5:E:801:7Q9:P	0.46	3.04	11	6
5:E:821:7Q9:C14	5:E:821:7Q9:P	0.46	3.03	12	7
5:E:823:7Q9:O31	5:E:823:7Q9:C21	0.46	2.64	10	7
6:E:873:17F:C20	6:E:873:17F:C1X	0.46	2.94	4	2
6:A:220:17F:O2	5:D:503:7Q9:C14	0.46	2.63	2	1
5:D:514:7Q9:C14	5:D:514:7Q9:O22	0.46	2.63	2	1
5:E:836:7Q9:C22	5:E:837:7Q9:C22	0.46	2.93	2	1
5:B:204:7Q9:C14	5:B:205:7Q9:O13	0.46	2.64	3	1
5:D:505:7Q9:C21	5:D:505:7Q9:O31	0.46	2.62	7	2
2:D:440:LEU:HD11	5:D:543:7Q9:C315	0.46	2.40	4	1
6:E:873:17F:C2X	6:E:873:17F:C20	0.46	2.94	4	1
5:B:205:7Q9:C317	6:B:208:17F:H48	0.46	2.40	10	2
5:E:852:7Q9:C39	5:E:863:7Q9:C317	0.46	2.94	8	1
6:A:213:17F:C21	5:D:509:7Q9:O22	0.46	2.64	9	1
5:D:521:7Q9:O32	5:D:542:7Q9:C36	0.46	2.63	9	1
5:D:537:7Q9:C310	5:D:556:7Q9:C316	0.46	2.94	9	1
5:E:872:7Q9:O22	5:E:872:7Q9:C1	0.46	2.57	10	4
6:D:519:17F:H66	6:D:519:17F:C22	0.46	2.41	10	1
6:D:540:17F:C2X	6:D:540:17F:C36	0.46	2.90	10	1
6:D:510:17F:C29	6:D:517:17F:H71	0.46	2.40	12	1
6:A:219:17F:H74	6:A:219:17F:C26	0.46	2.41	13	1
6:B:208:17F:H10	5:B:209:7Q9:C310	0.46	2.40	13	1
5:E:844:7Q9:C15	5:E:845:7Q9:O13	0.46	2.64	13	1
2:D:257:PHE:CE2	2:E:706:LYS:HG2	0.46	2.45	14	1
5:D:508:7Q9:O12	5:D:508:7Q9:O21	0.46	2.32	16	3
6:A:208:17F:C21	6:B:208:17F:H31	0.46	2.40	17	1
5:E:826:7Q9:C11	5:E:845:7Q9:O32	0.46	2.63	17	1
6:E:839:17F:C12	6:E:857:17F:H12	0.46	2.31	17	1
5:D:504:7Q9:C311	5:D:508:7Q9:C3	0.46	2.94	18	1
6:A:208:17F:O2	6:A:208:17F:H10A	0.46	2.10	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:875:17F:HN1	6:E:875:17F:C18	0.46	2.24	20	1
5:A:217:7Q9:C35	5:D:516:7Q9:C37	0.46	2.93	19	4
6:D:519:17F:N1	5:D:535:7Q9:O13	0.46	2.47	2	1
5:D:527:7Q9:O32	5:D:531:7Q9:C32	0.46	2.64	16	3
2:E:623:ARG:HD2	5:E:859:7Q9:C316	0.46	2.41	2	1
5:E:850:7Q9:C314	5:E:868:7Q9:C314	0.46	2.93	2	2
5:E:803:7Q9:C39	6:E:808:17F:H41	0.46	2.41	3	1
6:E:802:17F:C23	5:E:805:7Q9:C37	0.46	2.94	5	2
6:E:820:17F:H57	6:E:820:17F:H40	0.46	1.86	5	2
5:D:514:7Q9:P	5:D:514:7Q9:O21	0.46	2.74	6	2
5:E:827:7Q9:C1	5:E:827:7Q9:O22	0.46	2.57	6	1
5:E:841:7Q9:C1	5:E:841:7Q9:O32	0.46	2.64	6	1
1:B:113:LEU:HD12	1:B:139:ILE:HD11	0.46	1.87	7	1
5:A:211:7Q9:C23	6:A:213:17F:C6	0.46	2.94	10	1
5:D:554:7Q9:O14	5:D:554:7Q9:C13	0.46	2.64	10	1
6:D:540:17F:N1	5:D:545:7Q9:O32	0.46	2.44	11	1
5:A:203:7Q9:C14	5:B:203:7Q9:C31	0.46	2.94	12	2
6:A:208:17F:H58	6:A:208:17F:C23	0.46	2.40	12	1
2:D:370:LEU:HD13	2:E:593:VAL:HG11	0.46	1.88	12	1
6:E:806:17F:H45	6:E:806:17F:C40	0.46	2.37	13	1
5:E:847:7Q9:C33	5:E:851:7Q9:C23	0.46	2.94	14	1
5:D:512:7Q9:O22	5:D:512:7Q9:O11	0.46	2.33	17	1
5:E:803:7Q9:C311	6:E:808:17F:H42	0.46	2.41	17	1
6:E:857:17F:C35	6:E:857:17F:C31	0.46	2.85	17	2
6:E:875:17F:H46	6:E:875:17F:C37	0.46	2.41	17	1
5:D:550:7Q9:C22	6:D:552:17F:HN1	0.46	2.24	18	1
5:D:514:7Q9:C311	5:D:525:7Q9:C318	0.46	2.93	19	1
6:E:808:17F:H61	6:E:820:17F:H29	0.46	1.87	19	1
6:D:510:17F:H56	6:D:517:17F:C11	0.46	2.34	20	1
5:E:807:7Q9:O21	5:E:807:7Q9:O32	0.46	2.33	1	7
5:E:826:7Q9:C31	5:E:826:7Q9:O21	0.46	2.62	12	3
5:E:844:7Q9:O22	5:E:845:7Q9:C15	0.46	2.64	1	1
6:D:517:17F:C28	6:D:517:17F:C24	0.46	2.90	3	1
1:B:68:ARG:HB3	1:B:99:GLN:NE2	0.46	2.26	4	1
5:B:209:7Q9:C318	5:E:840:7Q9:C312	0.46	2.93	7	2
5:E:863:7Q9:O21	5:E:863:7Q9:C31	0.46	2.64	17	6
5:E:822:7Q9:O32	5:E:843:7Q9:C14	0.46	2.64	5	1
5:E:847:7Q9:O22	5:E:847:7Q9:C3	0.46	2.58	15	4
5:D:513:7Q9:C3	6:D:534:17F:H5	0.46	2.41	7	1
5:D:522:7Q9:C14	5:D:553:7Q9:C1	0.46	2.93	7	1
6:E:808:17F:C37	5:E:814:7Q9:C310	0.46	2.94	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:840:7Q9:O22	5:E:840:7Q9:C3	0.46	2.61	20	4
6:A:219:17F:H46	6:A:219:17F:H75	0.46	1.86	8	1
6:D:518:17F:H20	6:D:518:17F:C23	0.46	2.40	8	2
5:D:556:7Q9:O13	5:E:845:7Q9:C14	0.46	2.64	18	3
6:D:520:17F:H55	6:D:520:17F:C40	0.46	2.40	9	1
2:E:610:GLU:O	2:E:614:LEU:HG	0.46	2.11	11	1
6:E:839:17F:C2	6:E:875:17F:O8	0.46	2.63	11	1
1:B:32:TYR:HE1	3:B:201:GSP:O1B	0.46	1.94	15	1
5:D:555:7Q9:C12	6:E:857:17F:H18	0.46	2.41	15	1
1:B:123:ARG:HD3	1:B:125:VAL:O	0.46	2.11	19	2
5:E:877:7Q9:O32	5:E:877:7Q9:C34	0.46	2.63	17	3
2:E:628:GLU:HA	2:E:631:ARG:HD3	0.46	1.86	19	1
5:E:844:7Q9:C22	5:E:865:7Q9:C1	0.46	2.94	19	1
6:E:839:17F:H10A	6:E:857:17F:H35	0.46	1.87	20	1
6:D:510:17F:H54	6:D:517:17F:H74	0.46	1.86	1	2
5:E:822:7Q9:C21	5:E:822:7Q9:O31	0.46	2.64	17	7
5:D:523:7Q9:C316	5:E:846:7Q9:C318	0.46	2.94	3	1
5:E:878:7Q9:O32	5:E:878:7Q9:C2	0.46	2.59	20	4
5:E:809:7Q9:O22	5:E:809:7Q9:C1	0.46	2.60	4	1
1:A:15:GLY:CA	3:A:201:GSP:C8	0.46	2.99	5	2
5:B:209:7Q9:C316	5:E:840:7Q9:C312	0.46	2.93	5	1
5:E:863:7Q9:O32	5:E:878:7Q9:C13	0.46	2.64	5	2
1:A:99:GLN:O	1:A:103:VAL:HG23	0.46	2.11	13	3
6:A:220:17F:H32	6:A:220:17F:C35	0.46	2.41	6	1
1:A:69:ASP:O	1:A:73:ARG:HG3	0.46	2.11	7	1
5:A:217:7Q9:C37	5:D:514:7Q9:C310	0.46	2.93	7	2
6:D:517:17F:H76	6:E:839:17F:C41	0.46	2.41	7	1
5:D:544:7Q9:C1	5:D:544:7Q9:O22	0.46	2.60	7	2
5:E:821:7Q9:C1	6:E:839:17F:O9	0.46	2.64	7	1
5:D:523:7Q9:C14	5:D:523:7Q9:P	0.46	3.04	8	2
1:B:20:THR:HG23	1:B:55:ILE:HD12	0.46	1.87	9	1
2:D:359:LEU:HD13	2:E:604:PHE:HD1	0.46	1.71	10	1
6:E:873:17F:C20	6:E:873:17F:C23	0.46	2.94	13	3
5:E:811:7Q9:C22	5:E:817:7Q9:C36	0.46	2.94	11	1
5:E:870:7Q9:O22	6:E:873:17F:C9	0.46	2.64	11	1
5:D:550:7Q9:C14	6:D:552:17F:C3	0.46	2.94	12	2
6:E:806:17F:P1	6:E:806:17F:N1	0.46	2.89	12	2
6:A:219:17F:H49	5:E:828:7Q9:C318	0.46	2.40	13	1
6:E:802:17F:H31	5:E:804:7Q9:C22	0.46	2.41	13	1
5:E:807:7Q9:C15	5:E:807:7Q9:O21	0.46	2.64	18	2
2:D:378:LEU:HD21	5:D:535:7Q9:C318	0.46	2.41	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:871:17F:C32	6:E:871:17F:H30	0.46	2.41	16	1
5:A:206:7Q9:C13	6:A:213:17F:HN1A	0.46	2.24	17	1
6:E:839:17F:C11	6:E:839:17F:C36	0.46	2.87	17	1
5:E:855:7Q9:P	5:E:855:7Q9:C14	0.46	3.04	19	1
1:A:123:ARG:HD3	1:A:125:VAL:O	0.46	2.11	1	3
1:A:134:ALA:HB1	1:A:139:ILE:O	0.46	2.11	3	6
6:D:534:17F:O10	6:D:534:17F:C9	0.46	2.64	1	2
6:D:520:17F:H52	5:E:841:7Q9:C311	0.46	2.41	2	2
5:B:205:7Q9:C310	6:B:208:17F:H65	0.46	2.41	3	1
6:D:510:17F:H9A	6:D:517:17F:H10A	0.46	1.86	3	1
6:D:533:17F:H32	6:D:533:17F:C6	0.46	2.40	3	1
5:D:550:7Q9:O11	5:D:550:7Q9:C21	0.46	2.64	9	6
5:A:217:7Q9:C12	5:A:217:7Q9:O21	0.46	2.63	4	4
6:D:510:17F:C32	6:D:533:17F:H71	0.46	2.35	4	1
6:A:219:17F:O10	6:A:219:17F:C4	0.46	2.58	6	1
5:E:838:7Q9:C313	5:E:867:7Q9:C312	0.46	2.94	7	1
6:D:533:17F:H68	6:D:533:17F:H30	0.46	1.88	8	1
5:E:807:7Q9:O32	5:E:807:7Q9:O21	0.46	2.34	9	1
1:A:22:GLN:HB3	1:A:149:ARG:HG3	0.46	1.88	10	1
5:A:207:7Q9:C1	5:A:207:7Q9:O22	0.46	2.57	10	2
6:E:829:17F:H43	6:E:829:17F:H61	0.46	1.88	10	1
6:A:219:17F:H39	6:A:219:17F:H12A	0.46	1.88	14	1
6:A:213:17F:H31	6:A:213:17F:H12	0.46	1.88	15	1
5:D:504:7Q9:O14	5:D:504:7Q9:C2	0.46	2.63	16	1
1:B:113:LEU:HB3	1:B:141:PHE:HD1	0.46	1.71	17	1
5:A:205:7Q9:O11	5:A:212:7Q9:C1	0.46	2.63	19	1
5:D:523:7Q9:C22	5:D:550:7Q9:C312	0.46	2.94	19	1
5:E:838:7Q9:C31	6:E:842:17F:H12A	0.46	2.41	20	1
5:E:845:7Q9:C318	5:E:865:7Q9:C312	0.46	2.94	20	1
6:A:213:17F:C1X	5:D:509:7Q9:C22	0.45	2.94	1	2
5:D:546:7Q9:O31	5:D:546:7Q9:C21	0.45	2.63	16	6
5:E:836:7Q9:O22	5:E:836:7Q9:C1	0.45	2.60	14	7
1:A:35:THR:OG1	3:A:201:GSP:O3G	0.45	2.33	4	8
6:A:208:17F:H30	6:B:208:17F:H34	0.45	1.88	3	1
5:D:501:7Q9:C318	5:E:809:7Q9:C312	0.45	2.94	3	2
5:D:514:7Q9:O21	5:D:514:7Q9:O13	0.45	2.35	6	2
6:D:510:17F:H18A	6:D:517:17F:H8	0.45	1.86	7	1
2:E:636:GLU:HG2	2:E:640:LYS:HE2	0.45	1.88	8	1
6:D:510:17F:H33	6:D:533:17F:C34	0.45	2.41	9	1
5:D:529:7Q9:C12	5:D:541:7Q9:O22	0.45	2.64	9	1
6:B:208:17F:C3	5:B:209:7Q9:C12	0.45	2.94	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:514:7Q9:C15	5:D:514:7Q9:C1	0.45	2.94	11	1
2:E:705:GLU:HG3	2:E:706:LYS:H	0.45	1.70	14	2
6:E:810:17F:H38	5:E:825:7Q9:C314	0.45	2.41	11	1
6:E:806:17F:C26	6:E:806:17F:H72	0.45	2.36	13	1
5:E:858:7Q9:C33	6:E:875:17F:H37	0.45	2.41	13	1
5:E:824:7Q9:C22	5:E:846:7Q9:C34	0.45	2.94	18	2
5:E:826:7Q9:C12	5:E:845:7Q9:O32	0.45	2.64	17	1
5:E:854:7Q9:C3	5:E:854:7Q9:C12	0.45	2.94	18	1
1:A:129:GLN:O	1:A:133:LEU:HB2	0.45	2.12	20	2
5:E:862:7Q9:C3	5:E:877:7Q9:C15	0.45	2.94	19	1
5:D:549:7Q9:C22	5:E:801:7Q9:C22	0.45	2.94	20	1
1:B:34:PRO:HA	3:B:201:GSP:S1G	0.45	2.50	5	3
5:D:508:7Q9:C312	5:D:508:7Q9:C38	0.45	2.94	1	4
5:E:864:7Q9:O14	5:E:864:7Q9:C12	0.45	2.64	8	5
5:A:218:7Q9:C39	6:D:511:17F:H48	0.45	2.41	4	1
6:B:208:17F:H12A	5:B:209:7Q9:C310	0.45	2.41	4	1
6:E:820:17F:H31	5:E:830:7Q9:C22	0.45	2.42	4	1
6:A:208:17F:C1Z	6:A:219:17F:C10	0.45	2.91	5	2
6:A:219:17F:H67	6:D:518:17F:H60	0.45	1.88	5	1
5:D:516:7Q9:C33	5:D:516:7Q9:O14	0.45	2.64	20	2
5:D:524:7Q9:O11	5:D:543:7Q9:C11	0.45	2.64	5	1
5:E:850:7Q9:O32	5:E:864:7Q9:C22	0.45	2.65	15	2
5:D:503:7Q9:C13	5:D:503:7Q9:O13	0.45	2.64	15	7
5:E:844:7Q9:O22	5:E:845:7Q9:C34	0.45	2.63	8	1
6:D:510:17F:C1Z	6:D:533:17F:H61	0.45	2.41	9	1
6:E:819:17F:O3	5:E:838:7Q9:C11	0.45	2.64	10	1
1:A:112:VAL:HG12	1:A:114:VAL:HG23	0.45	1.87	11	1
5:A:207:7Q9:C39	5:A:215:7Q9:C23	0.45	2.94	12	1
5:D:509:7Q9:C31	5:D:509:7Q9:O11	0.45	2.64	13	1
6:E:875:17F:H54	6:E:875:17F:H72	0.45	1.88	13	1
6:E:873:17F:H62	6:E:873:17F:C31	0.45	2.30	14	3
5:A:217:7Q9:C2	5:A:217:7Q9:O13	0.45	2.64	15	1
6:B:208:17F:H48	6:E:812:17F:C38	0.45	2.42	15	1
5:A:203:7Q9:O13	5:A:204:7Q9:C12	0.45	2.65	16	1
2:D:396:ALA:HB1	5:D:537:7Q9:C314	0.45	2.40	16	1
5:A:203:7Q9:O32	5:B:205:7Q9:C12	0.45	2.63	17	1
5:A:218:7Q9:C39	6:E:829:17F:H78	0.45	2.41	17	1
5:D:513:7Q9:O31	5:D:513:7Q9:C21	0.45	2.64	17	2
6:E:819:17F:C1X	6:E:819:17F:C23	0.45	2.79	17	1
1:B:18:ALA:O	1:B:22:GLN:HG3	0.45	2.11	18	1
5:E:853:7Q9:C15	5:E:853:7Q9:P	0.45	3.04	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:208:17F:C20	6:A:219:17F:C10	0.45	2.92	3	1
5:D:504:7Q9:C32	5:D:508:7Q9:C36	0.45	2.95	5	3
5:D:521:7Q9:C13	5:D:522:7Q9:C22	0.45	2.95	17	2
6:D:552:17F:H56	6:D:552:17F:C35	0.45	2.39	15	4
6:D:510:17F:H19	6:D:533:17F:H20	0.45	1.86	7	1
5:E:838:7Q9:C15	5:E:838:7Q9:O21	0.45	2.64	7	3
5:E:816:7Q9:O14	5:E:824:7Q9:C13	0.45	2.65	14	2
5:D:513:7Q9:C313	6:D:534:17F:H55	0.45	2.41	9	1
5:D:556:7Q9:C12	5:E:865:7Q9:C22	0.45	2.94	12	1
5:E:814:7Q9:C313	6:E:820:17F:H50	0.45	2.41	15	1
6:A:213:17F:H62	6:A:213:17F:C10	0.45	2.41	17	1
5:E:838:7Q9:C38	5:E:861:7Q9:C39	0.45	2.94	17	1
5:A:212:7Q9:C313	5:D:505:7Q9:C312	0.45	2.94	19	1
6:D:510:17F:H5	6:D:533:17F:H20	0.45	1.87	20	1
6:D:520:17F:H52	5:E:841:7Q9:C312	0.45	2.41	20	1
6:E:802:17F:O8	6:E:802:17F:O9	0.45	2.34	14	8
5:E:843:7Q9:C37	5:E:843:7Q9:C314	0.45	2.95	13	7
5:D:543:7Q9:C15	5:D:543:7Q9:P	0.45	3.04	14	9
5:E:809:7Q9:C14	5:E:809:7Q9:P	0.45	3.04	8	3
5:D:527:7Q9:C3	5:D:531:7Q9:O31	0.45	2.65	11	3
6:D:534:17F:C6	5:D:538:7Q9:C35	0.45	2.95	3	1
5:E:825:7Q9:C35	6:E:842:17F:H30	0.45	2.42	3	1
6:E:873:17F:O2	6:E:873:17F:C2	0.45	2.65	13	5
5:D:524:7Q9:C33	5:D:543:7Q9:O32	0.45	2.65	4	1
6:D:540:17F:H8	5:D:545:7Q9:C35	0.45	2.41	11	2
5:E:868:7Q9:O13	5:E:868:7Q9:C2	0.45	2.64	12	3
6:E:871:17F:H1	6:E:871:17F:C4	0.45	2.41	5	1
6:E:857:17F:H37	6:E:875:17F:C33	0.45	2.41	8	1
5:D:507:7Q9:C313	5:E:814:7Q9:C316	0.45	2.94	9	1
5:D:549:7Q9:C22	5:E:801:7Q9:C33	0.45	2.93	10	1
5:E:826:7Q9:C39	5:E:845:7Q9:C38	0.45	2.94	18	2
2:E:557:PHE:CZ	6:E:873:17F:H71	0.45	2.47	14	1
5:B:210:7Q9:C318	6:E:812:17F:H77	0.45	2.41	15	1
5:D:515:7Q9:O32	6:D:519:17F:H19	0.45	2.11	18	1
5:E:830:7Q9:C316	5:E:849:7Q9:C23	0.45	2.95	19	1
5:A:214:7Q9:C32	5:A:218:7Q9:O13	0.45	2.64	20	1
5:D:554:7Q9:O32	5:E:832:7Q9:C23	0.45	2.64	20	1
1:A:112:VAL:HG21	1:A:159:LEU:HA	0.45	1.88	1	2
5:D:503:7Q9:C13	5:D:503:7Q9:P	0.45	3.05	1	2
5:D:532:7Q9:C22	5:D:532:7Q9:C38	0.45	2.95	12	3
6:E:808:17F:O10	6:E:808:17F:H4	0.45	2.12	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:817:7Q9:P	5:E:817:7Q9:C15	0.45	3.04	1	4
5:E:840:7Q9:C22	5:E:866:7Q9:C36	0.45	2.94	1	2
6:E:873:17F:H39	6:E:873:17F:H34	0.45	1.87	1	1
5:D:551:7Q9:O22	5:D:551:7Q9:C1	0.45	2.62	13	6
5:E:823:7Q9:O14	5:E:840:7Q9:C3	0.45	2.65	2	1
5:E:861:7Q9:O21	5:E:861:7Q9:C31	0.45	2.64	14	10
6:D:519:17F:H54	6:E:842:17F:H77	0.45	1.88	3	1
5:E:838:7Q9:C14	6:E:842:17F:C19	0.45	2.94	5	1
5:E:824:7Q9:O22	5:E:824:7Q9:C1	0.45	2.62	20	2
6:D:540:17F:H10A	5:D:545:7Q9:C311	0.45	2.42	7	1
5:E:833:7Q9:O21	5:E:833:7Q9:C31	0.45	2.65	14	3
6:A:208:17F:C31	6:A:208:17F:H40	0.45	2.42	9	1
6:D:520:17F:H55	6:D:520:17F:H70	0.45	1.88	9	1
5:E:803:7Q9:C313	6:E:806:17F:H66	0.45	2.42	12	2
5:D:503:7Q9:O13	5:D:503:7Q9:C12	0.45	2.65	13	2
6:E:857:17F:O7	6:E:857:17F:H10	0.45	2.11	18	2
5:D:514:7Q9:C22	5:D:546:7Q9:O11	0.45	2.64	13	1
5:E:840:7Q9:C37	5:E:841:7Q9:C22	0.45	2.94	15	1
1:B:28:PHE:CZ	3:B:201:GSP:H2'	0.45	2.46	16	1
6:D:510:17F:C18	6:D:517:17F:C9	0.45	2.93	18	1
6:E:819:17F:C38	5:E:825:7Q9:C318	0.45	2.94	18	1
6:A:208:17F:H30	6:B:208:17F:H19A	0.45	1.88	19	1
6:D:510:17F:H31	6:D:517:17F:C10	0.45	2.22	19	1
1:A:16:LYS:HB2	3:A:201:GSP:O2B	0.45	2.11	1	1
1:B:5:LYS:HA	1:B:54:ASP:HB3	0.45	1.88	6	3
6:D:517:17F:H70	6:D:517:17F:C28	0.45	2.40	2	1
5:E:826:7Q9:O13	5:E:826:7Q9:C12	0.45	2.64	3	6
2:D:308:TRP:HH2	2:E:659:LEU:HD13	0.45	1.72	4	1
2:E:702:THR:HA	2:E:705:GLU:HG2	0.45	1.89	4	1
6:A:208:17F:O5	5:A:212:7Q9:C13	0.45	2.65	5	1
5:D:513:7Q9:O21	5:D:513:7Q9:O14	0.45	2.34	12	2
6:E:802:17F:H59	5:E:807:7Q9:C38	0.45	2.41	8	1
5:B:210:7Q9:O22	5:B:210:7Q9:C3	0.45	2.61	9	2
6:A:208:17F:H8A	5:B:205:7Q9:C32	0.45	2.42	10	1
6:E:802:17F:C18	6:E:802:17F:H10	0.45	2.41	10	1
5:A:216:7Q9:C3	6:D:517:17F:O10	0.45	2.65	13	1
1:A:39:SER:HB2	1:A:41:ARG:NH1	0.45	2.27	16	1
6:A:208:17F:H58	6:A:208:17F:C2X	0.45	2.42	16	1
6:D:519:17F:H40	6:D:519:17F:C31	0.45	2.40	16	1
6:E:857:17F:H78	6:E:875:17F:C36	0.45	2.41	16	1
5:A:214:7Q9:C23	5:A:214:7Q9:C13	0.45	2.95	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:518:17F:H5	5:D:528:7Q9:O13	0.45	2.12	17	1
5:A:203:7Q9:C313	6:B:208:17F:H68	0.45	2.42	18	1
6:A:213:17F:H10	6:A:213:17F:H61	0.45	1.88	19	1
5:D:506:7Q9:C32	6:D:517:17F:H20A	0.45	2.42	20	1
6:E:875:17F:N1	6:E:875:17F:C18	0.45	2.79	20	1
5:A:210:7Q9:O31	5:A:210:7Q9:C34	0.45	2.64	16	9
5:A:218:7Q9:C11	6:D:511:17F:O2	0.45	2.65	1	1
5:E:838:7Q9:O31	5:E:838:7Q9:C21	0.45	2.65	11	11
5:E:849:7Q9:C316	5:E:852:7Q9:C316	0.45	2.94	16	4
5:D:515:7Q9:C32	6:D:519:17F:H20	0.45	2.42	2	1
5:A:215:7Q9:C310	5:A:216:7Q9:C316	0.45	2.95	3	1
5:D:514:7Q9:C3	5:D:516:7Q9:C32	0.45	2.95	4	1
5:A:210:7Q9:C317	6:A:220:17F:H44	0.45	2.41	5	1
5:B:206:7Q9:C15	5:B:206:7Q9:C1	0.45	2.94	12	3
6:B:208:17F:C24	5:E:824:7Q9:C318	0.45	2.95	5	1
6:D:510:17F:H19A	5:D:530:7Q9:O21	0.45	2.12	5	1
6:D:540:17F:O10	6:D:540:17F:C4	0.45	2.62	11	3
6:E:802:17F:C20	5:E:804:7Q9:C22	0.45	2.94	5	1
5:E:824:7Q9:C312	5:E:840:7Q9:C311	0.45	2.95	8	1
5:D:505:7Q9:C318	5:D:554:7Q9:C314	0.45	2.95	9	2
5:D:554:7Q9:C310	5:E:826:7Q9:C316	0.45	2.94	11	1
5:B:209:7Q9:C318	5:E:824:7Q9:C312	0.45	2.95	12	1
5:D:508:7Q9:C38	5:D:524:7Q9:C34	0.45	2.95	12	1
5:E:836:7Q9:O13	5:E:838:7Q9:C13	0.45	2.64	12	1
1:A:23:LEU:HD22	1:A:156:PHE:CD2	0.45	2.47	13	1
1:B:15:GLY:CA	3:B:201:GSP:H8	0.45	2.25	15	1
6:E:812:17F:H39	6:E:812:17F:H30	0.45	1.88	15	1
6:D:552:17F:H57	6:D:552:17F:C9	0.45	2.42	19	2
5:D:546:7Q9:C318	5:D:556:7Q9:C317	0.45	2.95	2	2
6:A:220:17F:O4	5:D:502:7Q9:C12	0.45	2.65	2	1
6:D:510:17F:C10	6:D:517:17F:H34	0.45	2.40	2	2
6:D:533:17F:H6A	6:D:533:17F:H57	0.45	1.87	2	1
6:E:808:17F:H49	6:E:810:17F:H51	0.45	1.88	2	1
5:E:864:7Q9:C15	5:E:864:7Q9:P	0.45	3.05	16	9
1:A:72:MET:HA	1:A:78:PHE:CZ	0.45	2.45	7	3
6:E:806:17F:H39	6:E:806:17F:C1X	0.45	2.39	14	2
5:A:203:7Q9:O22	5:A:203:7Q9:C3	0.45	2.58	5	4
1:B:116:ASN:ND2	3:B:201:GSP:N7	0.45	2.65	5	1
1:A:47:ASP:HA	1:B:128:LYS:CB	0.45	2.30	6	1
5:B:210:7Q9:O32	6:D:520:17F:H57	0.45	2.11	6	1
5:A:207:7Q9:C14	5:B:207:7Q9:C3	0.45	2.94	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:507:7Q9:C314	6:E:819:17F:H52	0.45	2.42	7	1
6:E:829:17F:H9A	5:E:833:7Q9:C35	0.45	2.41	7	1
5:D:555:7Q9:C312	5:E:849:7Q9:C316	0.45	2.95	8	1
6:E:808:17F:H72	6:E:819:17F:C30	0.45	2.42	8	1
5:A:215:7Q9:C14	6:D:511:17F:H4A	0.45	2.41	10	1
6:E:808:17F:C19	6:E:810:17F:H20	0.45	2.42	11	1
1:B:137:TYR:HB2	1:B:139:ILE:HG12	0.45	1.88	12	1
5:D:537:7Q9:O13	5:D:546:7Q9:C1	0.45	2.65	12	1
6:E:819:17F:C10	6:E:820:17F:H9A	0.45	2.42	16	1
5:A:203:7Q9:O32	5:B:205:7Q9:C13	0.45	2.65	17	1
6:D:552:17F:C7	6:D:552:17F:C4	0.45	2.95	17	1
5:D:544:7Q9:C23	5:D:544:7Q9:O14	0.45	2.65	1	1
5:E:814:7Q9:C312	6:E:819:17F:H54	0.45	2.42	1	1
5:E:826:7Q9:C14	5:E:826:7Q9:P	0.45	3.05	3	5
6:D:510:17F:C6	6:D:517:17F:H9	0.45	2.42	15	2
5:E:836:7Q9:O14	5:E:838:7Q9:C13	0.45	2.65	2	1
6:E:871:17F:H35	6:E:871:17F:C32	0.45	2.42	3	2
5:A:218:7Q9:C13	5:D:513:7Q9:O13	0.45	2.64	4	1
6:E:806:17F:H44	5:E:817:7Q9:C317	0.45	2.42	4	1
1:B:13:GLY:CA	3:B:201:GSP:H5'1	0.45	2.37	6	1
5:D:505:7Q9:O31	5:D:505:7Q9:O22	0.45	2.34	7	1
5:A:205:7Q9:O14	5:A:205:7Q9:C2	0.45	2.65	10	4
5:A:203:7Q9:C12	5:B:203:7Q9:O32	0.45	2.65	10	1
6:D:540:17F:H61	6:D:540:17F:C25	0.45	2.37	10	1
5:D:507:7Q9:C313	6:E:820:17F:H55	0.45	2.42	11	1
5:E:851:7Q9:C15	5:E:851:7Q9:O13	0.45	2.65	11	1
5:A:218:7Q9:P	5:A:218:7Q9:O21	0.45	2.74	20	2
2:D:269:GLN:HG2	6:D:540:17F:C1Z	0.45	2.41	12	3
6:E:808:17F:C34	6:E:820:17F:H12A	0.45	2.41	12	1
6:D:539:17F:H38	6:D:539:17F:C35	0.45	2.40	14	2
1:A:126:ASP:OD2	1:A:128:LYS:HB3	0.45	2.11	14	1
5:D:524:7Q9:C11	5:D:524:7Q9:C2	0.45	2.95	15	1
6:D:533:17F:C1Y	6:D:533:17F:O1	0.45	2.65	17	1
5:A:212:7Q9:O14	5:A:212:7Q9:O31	0.45	2.35	19	1
5:D:505:7Q9:C13	6:D:518:17F:O10	0.45	2.65	19	1
5:E:814:7Q9:C39	6:E:820:17F:H37	0.45	2.42	19	1
6:D:510:17F:H9	6:D:517:17F:C10	0.45	2.42	20	1
5:D:530:7Q9:O12	5:D:530:7Q9:C14	0.45	2.64	20	1
5:D:531:7Q9:C1	5:D:531:7Q9:O22	0.45	2.61	3	3
5:B:203:7Q9:O31	5:B:203:7Q9:O11	0.45	2.35	2	4
5:E:834:7Q9:C13	6:E:839:17F:O4	0.45	2.65	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:842:17F:C32	6:E:842:17F:C36	0.45	2.92	4	1
5:D:509:7Q9:O13	5:D:527:7Q9:C3	0.45	2.65	6	1
5:D:516:7Q9:C21	5:D:537:7Q9:C14	0.45	2.95	6	1
5:D:538:7Q9:C15	5:D:538:7Q9:O13	0.45	2.65	6	3
5:A:203:7Q9:O13	5:A:204:7Q9:C15	0.45	2.65	19	2
5:E:831:7Q9:C34	5:E:851:7Q9:C1	0.45	2.95	8	1
5:D:513:7Q9:C13	5:D:513:7Q9:C31	0.45	2.95	10	2
5:D:550:7Q9:C2	5:D:550:7Q9:O32	0.45	2.62	11	4
5:D:550:7Q9:C13	6:D:552:17F:O5	0.45	2.65	13	1
1:B:17:SER:HB2	3:B:201:GSP:O3B	0.45	2.11	14	1
6:D:539:17F:C35	6:D:539:17F:C22	0.45	2.95	14	1
5:A:212:7Q9:C317	6:A:219:17F:H54	0.45	2.42	18	2
6:E:819:17F:H63	6:E:842:17F:H67	0.45	1.89	15	1
5:E:866:7Q9:C15	5:E:866:7Q9:O13	0.45	2.65	18	1
5:A:210:7Q9:C314	6:A:220:17F:H10	0.45	2.42	19	1
6:E:806:17F:H68	6:E:806:17F:H55	0.45	1.89	19	1
1:A:6:LEU:HB2	1:A:55:ILE:HG12	0.45	1.87	20	1
2:E:660:ARG:NH1	6:E:875:17F:H20A	0.44	2.26	1	1
5:A:207:7Q9:C15	5:B:203:7Q9:O22	0.44	2.65	2	1
5:E:811:7Q9:C3	5:E:822:7Q9:C22	0.44	2.95	2	1
5:E:853:7Q9:C12	5:E:853:7Q9:O11	0.44	2.65	2	1
6:D:517:17F:H49	6:D:517:17F:C22	0.44	2.39	3	1
5:E:854:7Q9:C13	5:E:854:7Q9:O14	0.44	2.65	7	2
6:D:511:17F:O1	5:D:513:7Q9:C15	0.44	2.65	4	1
6:E:829:17F:H8A	5:E:833:7Q9:C33	0.44	2.42	6	1
5:D:512:7Q9:C33	6:D:534:17F:C6	0.44	2.95	7	1
6:D:518:17F:H50	5:D:549:7Q9:C312	0.44	2.42	8	1
2:D:330:ALA:HA	2:D:333:LYS:HE3	0.44	1.88	10	1
6:B:208:17F:C7	6:B:208:17F:H4A	0.44	2.42	11	1
1:A:6:LEU:HD13	1:A:159:LEU:HD23	0.44	1.89	13	1
6:D:510:17F:C9	6:D:517:17F:C1X	0.44	2.86	13	1
5:D:503:7Q9:C34	6:D:519:17F:H56	0.44	2.41	14	1
5:D:526:7Q9:P	5:D:526:7Q9:O21	0.44	2.75	15	1
5:E:852:7Q9:C36	5:E:852:7Q9:C311	0.44	2.96	18	2
5:D:521:7Q9:C34	5:D:521:7Q9:O31	0.44	2.64	17	1
5:D:502:7Q9:C32	5:D:525:7Q9:C23	0.44	2.95	18	1
5:D:515:7Q9:O22	5:D:515:7Q9:C1	0.44	2.60	1	1
5:A:205:7Q9:C36	5:A:210:7Q9:C23	0.44	2.95	2	1
6:A:213:17F:H37	5:D:509:7Q9:C21	0.44	2.42	2	1
5:D:542:7Q9:O21	5:D:542:7Q9:O14	0.44	2.34	18	9
1:B:41:ARG:HD2	1:B:54:ASP:OD1	0.44	2.12	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:530:7Q9:C312	5:D:530:7Q9:C38	0.44	2.95	7	2
6:E:808:17F:H74	6:E:808:17F:C27	0.44	2.36	3	1
6:E:808:17F:H51	6:E:808:17F:H75	0.44	1.89	3	1
5:E:822:7Q9:O31	5:E:822:7Q9:C21	0.44	2.64	10	3
5:A:211:7Q9:C318	6:A:220:17F:H52	0.44	2.42	4	1
6:A:213:17F:H30	5:D:509:7Q9:O22	0.44	2.12	4	1
5:D:536:7Q9:C22	5:D:536:7Q9:C311	0.44	2.94	14	2
6:D:510:17F:H54	6:D:517:17F:C40	0.44	2.41	5	1
6:E:875:17F:N1	6:E:875:17F:H18A	0.44	2.26	5	1
5:A:210:7Q9:C13	5:A:210:7Q9:P	0.44	3.05	8	2
1:B:39:SER:HA	1:B:55:ILE:O	0.44	2.12	8	1
6:D:539:17F:H8	6:D:539:17F:O5	0.44	2.12	9	1
6:A:213:17F:C7	6:A:213:17F:O9	0.44	2.65	11	1
6:A:219:17F:C1Y	5:E:801:7Q9:C34	0.44	2.95	11	1
6:E:808:17F:H75	6:E:819:17F:H54	0.44	1.88	11	1
6:D:519:17F:H50	5:D:526:7Q9:C318	0.44	2.42	12	1
6:E:819:17F:C32	6:E:842:17F:H53	0.44	2.41	12	1
6:A:213:17F:H56	6:A:213:17F:H41	0.44	1.89	13	1
5:E:841:7Q9:C3	5:E:874:7Q9:C39	0.44	2.95	13	1
6:A:213:17F:O10	6:A:213:17F:C6	0.44	2.54	14	1
6:E:857:17F:C38	6:E:857:17F:C21	0.44	2.96	14	1
5:B:206:7Q9:C39	6:B:208:17F:H74	0.44	2.42	15	1
6:E:842:17F:O6	6:E:842:17F:H2	0.44	2.12	18	1
6:A:220:17F:H30	6:A:220:17F:C26	0.44	2.39	20	1
5:D:504:7Q9:C1	5:D:508:7Q9:C34	0.44	2.95	20	1
6:E:802:17F:O9	6:E:802:17F:C7	0.44	2.65	20	1
5:E:838:7Q9:C32	6:E:842:17F:H41	0.44	2.42	20	1
6:E:856:17F:O4	5:E:858:7Q9:C15	0.44	2.65	20	1
5:D:529:7Q9:C13	5:D:553:7Q9:C11	0.44	2.95	15	3
5:E:855:7Q9:O32	5:E:855:7Q9:C21	0.44	2.65	11	3
5:D:524:7Q9:O12	5:D:524:7Q9:C2	0.44	2.65	3	1
6:E:839:17F:HN1	6:E:839:17F:P1	0.44	2.35	6	4
1:A:47:ASP:HA	1:B:128:LYS:CG	0.44	2.38	5	1
1:B:41:ARG:HA	1:B:53:LEU:O	0.44	2.13	18	2
5:B:206:7Q9:C315	5:E:809:7Q9:C314	0.44	2.95	5	2
2:E:736:TYR:O	2:E:740:LEU:HG	0.44	2.12	11	2
6:A:220:17F:H67	6:A:220:17F:H50	0.44	1.89	8	1
6:E:806:17F:O7	6:E:806:17F:O6	0.44	2.34	14	3
5:D:503:7Q9:O31	5:D:503:7Q9:C21	0.44	2.65	12	1
5:A:205:7Q9:C1	5:A:205:7Q9:C31	0.44	2.95	13	1
6:A:220:17F:H47	6:A:220:17F:H65	0.44	1.90	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:526:7Q9:C1	5:D:526:7Q9:C31	0.44	2.95	13	1
6:E:842:17F:H8	5:E:867:7Q9:O14	0.44	2.12	13	1
5:B:205:7Q9:C317	6:E:812:17F:H77	0.44	2.42	14	2
5:A:207:7Q9:O14	5:B:203:7Q9:C12	0.44	2.66	15	1
6:A:219:17F:H63	6:A:219:17F:C23	0.44	2.37	15	1
6:E:871:17F:H29	5:E:872:7Q9:C23	0.44	2.43	16	1
5:D:506:7Q9:C312	5:E:821:7Q9:C318	0.44	2.95	17	1
5:E:834:7Q9:O12	6:E:839:17F:H2	0.44	2.12	17	1
5:E:838:7Q9:O32	6:E:842:17F:C12	0.44	2.62	20	1
5:D:501:7Q9:O11	5:D:501:7Q9:C21	0.44	2.66	13	2
5:D:531:7Q9:C11	5:D:531:7Q9:O21	0.44	2.66	3	3
5:D:515:7Q9:C14	6:D:519:17F:H4A	0.44	2.43	3	1
6:D:518:17F:H4A	6:D:518:17F:H2	0.44	1.90	3	1
5:E:804:7Q9:C12	6:E:808:17F:O4	0.44	2.65	4	1
5:E:841:7Q9:O13	5:E:841:7Q9:C2	0.44	2.65	20	4
1:B:89:SER:HA	1:B:92:ASP:HB2	0.44	1.89	5	1
5:D:523:7Q9:O13	5:D:550:7Q9:C14	0.44	2.65	5	1
6:E:808:17F:H65	6:E:819:17F:H38	0.44	1.89	8	1
6:A:213:17F:H51	6:A:213:17F:H71	0.44	1.89	10	1
5:D:507:7Q9:C39	5:D:512:7Q9:C315	0.44	2.95	10	1
6:A:220:17F:C23	6:A:220:17F:H73	0.44	2.42	12	1
6:E:857:17F:O10	6:E:857:17F:H20A	0.44	2.13	14	2
6:D:539:17F:H43	5:D:549:7Q9:O32	0.44	2.11	15	1
6:E:819:17F:H10	6:E:820:17F:H9A	0.44	1.88	16	1
6:E:829:17F:H72	5:E:830:7Q9:C316	0.44	2.42	16	1
5:E:851:7Q9:C311	5:E:851:7Q9:C37	0.44	2.93	16	1
6:D:510:17F:H18A	6:D:533:17F:C20	0.44	2.40	17	1
6:B:208:17F:H54	6:E:812:17F:H68	0.44	1.89	1	1
5:D:537:7Q9:C37	5:D:546:7Q9:C318	0.44	2.95	1	1
5:E:804:7Q9:C34	5:E:807:7Q9:C34	0.44	2.95	1	1
6:D:539:17F:O10	6:D:539:17F:C6	0.44	2.53	9	4
1:A:79:LEU:HB2	1:A:159:LEU:HD22	0.44	1.89	3	1
6:D:510:17F:C9	6:D:517:17F:C10	0.44	2.92	3	2
5:E:804:7Q9:O32	6:E:808:17F:C8	0.44	2.66	3	1
5:E:835:7Q9:C37	5:E:835:7Q9:C311	0.44	2.93	4	1
5:D:514:7Q9:O13	5:D:537:7Q9:C15	0.44	2.65	5	1
5:E:844:7Q9:C312	5:E:860:7Q9:C313	0.44	2.96	5	1
5:E:861:7Q9:O22	5:E:861:7Q9:C1	0.44	2.59	13	5
5:D:508:7Q9:C14	5:D:508:7Q9:C1	0.44	2.95	11	2
5:D:513:7Q9:C21	5:D:513:7Q9:O31	0.44	2.64	13	2
6:E:820:17F:H60	5:E:853:7Q9:C36	0.44	2.41	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:820:17F:H64	5:E:837:7Q9:C38	0.44	2.42	12	1
5:B:206:7Q9:C15	5:B:206:7Q9:O11	0.44	2.65	13	1
5:E:830:7Q9:C1	5:E:853:7Q9:C35	0.44	2.95	20	2
6:A:208:17F:H72	6:B:208:17F:H61	0.44	1.89	18	1
6:E:810:17F:N1	6:E:819:17F:H5	0.44	2.28	20	1
6:A:213:17F:H31	6:A:213:17F:C22	0.44	2.43	1	1
5:E:854:7Q9:O22	5:E:854:7Q9:C1	0.44	2.61	1	3
1:B:4:TYR:HE2	1:B:51:CYS:HG	0.44	1.56	2	1
5:D:515:7Q9:C316	5:E:822:7Q9:C318	0.44	2.96	2	1
6:B:208:17F:O2	5:B:209:7Q9:C12	0.44	2.66	3	1
5:E:835:7Q9:C318	6:E:856:17F:H71	0.44	2.43	20	2
5:E:843:7Q9:C311	5:E:843:7Q9:C37	0.44	2.96	3	2
5:E:848:7Q9:C14	5:E:848:7Q9:P	0.44	3.05	3	1
6:E:857:17F:O10	6:E:857:17F:C6	0.44	2.63	13	5
1:A:116:ASN:ND2	3:A:201:GSP:N7	0.44	2.64	4	2
6:A:219:17F:O5	5:D:504:7Q9:C15	0.44	2.66	12	2
5:D:555:7Q9:C14	5:E:833:7Q9:O22	0.44	2.65	5	3
6:E:839:17F:C27	6:E:839:17F:C42	0.44	2.93	12	5
5:A:207:7Q9:O22	5:A:207:7Q9:C3	0.44	2.59	5	1
6:A:208:17F:H56	5:A:212:7Q9:C32	0.44	2.43	6	1
2:D:305:GLN:CD	6:D:533:17F:H10A	0.44	2.38	7	1
5:E:863:7Q9:C11	5:E:878:7Q9:C14	0.44	2.96	7	1
6:E:875:17F:N1	6:E:875:17F:H10	0.44	2.28	7	3
6:D:520:17F:H71	6:D:520:17F:C27	0.44	2.41	8	1
5:D:556:7Q9:O14	5:E:854:7Q9:C14	0.44	2.65	13	2
6:E:808:17F:H38	6:E:810:17F:C1Y	0.44	2.42	8	1
5:E:826:7Q9:C36	5:E:826:7Q9:O32	0.44	2.66	9	2
5:A:218:7Q9:C15	6:D:511:17F:O1	0.44	2.66	16	2
2:D:320:GLU:O	2:D:323:ARG:HG2	0.44	2.12	10	1
5:D:536:7Q9:O22	5:D:536:7Q9:C3	0.44	2.62	11	1
6:E:819:17F:C19	6:E:842:17F:H57	0.44	2.43	12	1
5:E:834:7Q9:C312	6:E:839:17F:H52	0.44	2.43	12	1
1:B:16:LYS:HB2	3:B:201:GSP:O2G	0.44	2.13	15	1
2:E:591:GLU:CD	2:E:594:LYS:HZ2	0.44	2.21	16	1
5:A:216:7Q9:C3	6:D:517:17F:C18	0.44	2.95	17	1
5:A:216:7Q9:O31	6:D:517:17F:H18A	0.44	2.11	20	2
5:E:805:7Q9:O32	6:E:812:17F:C1Y	0.44	2.64	17	1
6:E:806:17F:H43	5:E:817:7Q9:C317	0.44	2.42	17	1
5:A:217:7Q9:O13	5:D:516:7Q9:C32	0.44	2.66	18	1
5:D:502:7Q9:C38	5:D:515:7Q9:C22	0.44	2.96	18	1
6:D:520:17F:C39	6:D:520:17F:H47	0.44	2.43	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:E:659:LEU:HD21	6:E:875:17F:H68	0.44	1.90	20	1
6:E:820:17F:H69	6:E:820:17F:H52	0.44	1.89	20	1
2:D:315:TYR:CE2	2:E:644:LEU:HG	0.44	2.48	1	1
6:D:510:17F:C7	6:D:517:17F:O9	0.44	2.66	1	1
5:D:529:7Q9:C11	5:D:541:7Q9:O22	0.44	2.66	1	1
5:E:851:7Q9:C15	5:E:851:7Q9:P	0.44	3.06	11	6
6:D:533:17F:O9	6:D:533:17F:P1	0.44	2.75	3	3
5:E:838:7Q9:O32	6:E:842:17F:H31	0.44	2.11	3	1
5:B:206:7Q9:O14	5:B:206:7Q9:C12	0.44	2.66	4	2
6:D:510:17F:H62	5:D:530:7Q9:C313	0.44	2.42	4	1
5:E:840:7Q9:O32	5:E:840:7Q9:O21	0.44	2.36	4	1
5:E:841:7Q9:C13	5:E:841:7Q9:P	0.44	3.06	4	2
5:D:530:7Q9:O21	5:D:530:7Q9:O32	0.44	2.36	5	1
6:E:842:17F:C8	5:E:877:7Q9:O14	0.44	2.66	5	1
1:A:153:ASP:O	1:A:157:TYR:HB2	0.44	2.13	7	1
5:D:556:7Q9:O13	5:E:845:7Q9:C12	0.44	2.66	7	1
5:A:207:7Q9:C35	5:A:216:7Q9:C23	0.44	2.95	13	2
1:B:89:SER:O	1:B:93:ILE:HG12	0.44	2.12	10	1
5:D:521:7Q9:C31	5:D:521:7Q9:C1	0.44	2.96	10	1
6:D:533:17F:P1	6:D:533:17F:O9	0.44	2.76	10	1
5:D:514:7Q9:C23	5:D:537:7Q9:C13	0.44	2.96	20	2
5:E:870:7Q9:O22	6:E:873:17F:C10	0.44	2.65	11	1
6:D:517:17F:H38	6:D:533:17F:C22	0.44	2.40	12	1
6:D:519:17F:H69	6:D:519:17F:C27	0.44	2.43	12	1
5:A:204:7Q9:C12	5:A:205:7Q9:O22	0.44	2.66	13	1
2:D:334:LEU:HB3	5:D:538:7Q9:C312	0.44	2.42	13	1
6:E:802:17F:H56	5:E:807:7Q9:C316	0.44	2.43	13	1
5:E:849:7Q9:C315	5:E:852:7Q9:C311	0.44	2.96	15	1
6:E:806:17F:HN1	6:E:806:17F:P1	0.44	2.35	17	1
5:E:833:7Q9:C14	5:E:833:7Q9:C21	0.44	2.96	19	1
5:D:502:7Q9:C36	5:D:515:7Q9:C22	0.44	2.96	20	1
5:D:543:7Q9:O31	6:D:552:17F:H11A	0.44	2.13	20	1
6:E:820:17F:H6A	6:E:820:17F:O10	0.44	2.12	20	1
5:D:532:7Q9:C1	6:D:534:17F:H31	0.44	2.43	2	1
6:E:818:17F:O8	6:E:818:17F:C5	0.44	2.53	7	3
2:D:414:LEU:O	2:D:418:LEU:HG	0.44	2.12	3	1
6:D:540:17F:H76	5:E:864:7Q9:C316	0.44	2.43	3	1
5:E:849:7Q9:C315	5:E:852:7Q9:C314	0.44	2.96	8	3
6:A:213:17F:H73	6:E:810:17F:H55	0.44	1.89	5	1
5:D:503:7Q9:C318	5:D:526:7Q9:C316	0.44	2.96	6	1
6:E:829:17F:H30	5:E:833:7Q9:C36	0.44	2.43	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:207:7Q9:O22	5:A:207:7Q9:C1	0.44	2.64	7	3
5:D:504:7Q9:O22	5:D:504:7Q9:C3	0.44	2.63	8	2
6:D:518:17F:H62	6:D:518:17F:C31	0.44	2.40	8	1
6:E:802:17F:H77	6:E:802:17F:H50	0.44	1.87	9	2
1:A:64:TYR:HB3	1:A:67:MET:HB2	0.44	1.88	12	1
5:A:210:7Q9:C34	5:A:210:7Q9:O31	0.44	2.66	12	1
6:D:539:17F:C21	6:D:539:17F:C35	0.44	2.89	12	1
6:D:517:17F:H49	6:D:517:17F:H66	0.44	1.86	13	1
5:A:215:7Q9:C1	5:A:216:7Q9:C22	0.44	2.95	14	1
5:D:514:7Q9:O21	5:D:514:7Q9:P	0.44	2.76	19	2
6:D:510:17F:C30	6:D:517:17F:H38	0.44	2.39	15	1
5:E:827:7Q9:O13	5:E:841:7Q9:C15	0.44	2.66	15	1
5:D:549:7Q9:C22	5:E:801:7Q9:O32	0.44	2.66	17	1
6:E:839:17F:H78	6:E:839:17F:H48	0.44	1.89	18	1
5:E:849:7Q9:C15	5:E:853:7Q9:O14	0.44	2.65	18	1
5:D:529:7Q9:C35	5:D:541:7Q9:C312	0.44	2.95	19	1
1:A:15:GLY:O	1:A:19:LEU:HG	0.44	2.13	1	1
5:A:216:7Q9:O21	5:A:216:7Q9:C31	0.44	2.66	3	3
5:D:550:7Q9:O32	5:D:550:7Q9:C2	0.44	2.61	2	3
1:B:4:TYR:CE2	1:B:51:CYS:HB3	0.44	2.48	3	1
2:D:436:TYR:O	2:D:440:LEU:HG	0.44	2.12	8	2
5:E:854:7Q9:O21	5:E:854:7Q9:O32	0.44	2.36	7	3
5:D:506:7Q9:C311	6:D:517:17F:H53	0.44	2.43	5	1
5:D:526:7Q9:C314	5:E:838:7Q9:C315	0.44	2.95	20	2
6:E:829:17F:C12	5:E:833:7Q9:C38	0.44	2.96	5	1
5:E:833:7Q9:O31	5:E:852:7Q9:O13	0.44	2.36	5	1
5:A:218:7Q9:O32	5:A:218:7Q9:C2	0.44	2.63	16	2
5:D:521:7Q9:C36	5:D:542:7Q9:C310	0.44	2.96	6	1
6:D:533:17F:O5	5:D:541:7Q9:C15	0.44	2.66	6	1
5:E:855:7Q9:C14	5:E:855:7Q9:P	0.44	3.06	6	2
5:E:832:7Q9:O32	5:E:832:7Q9:C34	0.44	2.65	7	3
5:D:503:7Q9:C35	6:D:519:17F:H56	0.44	2.43	8	1
5:D:543:7Q9:C12	5:D:543:7Q9:O13	0.44	2.65	10	2
3:A:201:GSP:O1A	3:A:201:GSP:O2B	0.44	2.36	10	1
6:E:810:17F:C22	5:E:825:7Q9:C314	0.44	2.95	11	1
5:E:826:7Q9:O21	5:E:826:7Q9:O32	0.44	2.36	12	1
6:E:819:17F:C1	5:E:838:7Q9:C11	0.44	2.96	13	1
6:D:534:17F:H10A	6:D:534:17F:C34	0.44	2.43	14	1
5:E:854:7Q9:C13	5:E:854:7Q9:O11	0.44	2.66	19	2
6:D:520:17F:O4	5:D:545:7Q9:C13	0.44	2.65	16	1
6:E:819:17F:H75	6:E:819:17F:C26	0.44	2.43	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:208:17F:H10	5:B:209:7Q9:C33	0.44	2.43	17	1
6:D:510:17F:H58	5:D:530:7Q9:C313	0.44	2.43	17	1
6:E:808:17F:C12	6:E:808:17F:H63	0.44	2.43	17	1
5:E:805:7Q9:C316	6:E:812:17F:H48	0.44	2.43	19	1
6:A:213:17F:O1	6:A:213:17F:H12	0.44	2.13	20	1
5:A:206:7Q9:C318	6:E:802:17F:C38	0.43	2.96	2	1
5:B:204:7Q9:C14	5:B:204:7Q9:P	0.43	3.06	4	4
2:D:280:GLU:HG3	5:D:542:7Q9:C315	0.43	2.43	2	1
5:D:513:7Q9:C36	5:D:532:7Q9:O21	0.43	2.66	2	1
5:E:868:7Q9:O31	5:E:868:7Q9:C34	0.43	2.64	2	1
6:D:511:17F:H11A	5:D:532:7Q9:C37	0.43	2.43	3	1
5:D:538:7Q9:O31	5:D:538:7Q9:O11	0.43	2.36	3	5
6:E:857:17F:H11	6:E:875:17F:C32	0.43	2.42	4	1
2:D:330:ALA:HB1	6:D:534:17F:H78	0.43	1.89	5	1
2:E:555:SER:N	6:E:873:17F:H65	0.43	2.28	7	2
6:D:520:17F:C39	6:D:520:17F:H48	0.43	2.43	8	1
5:D:555:7Q9:C310	5:E:849:7Q9:C316	0.43	2.96	8	1
6:E:820:17F:O1	5:E:830:7Q9:C14	0.43	2.66	8	1
5:E:849:7Q9:C13	5:E:849:7Q9:O22	0.43	2.66	11	2
5:D:523:7Q9:C1	5:D:550:7Q9:C23	0.43	2.96	9	1
2:D:439:LYS:HE3	2:E:714:LEU:HA	0.43	1.90	10	1
6:D:533:17F:O1	6:D:533:17F:O7	0.43	2.35	14	2
5:D:542:7Q9:C33	5:D:553:7Q9:C38	0.43	2.95	10	1
5:A:214:7Q9:C315	5:A:218:7Q9:C316	0.43	2.96	11	1
6:A:220:17F:H42	5:E:811:7Q9:C316	0.43	2.43	11	1
1:B:37:GLU:HG3	1:B:56:LEU:HD11	0.43	1.90	11	1
5:D:522:7Q9:C36	5:D:529:7Q9:O13	0.43	2.66	11	1
6:A:219:17F:H48	5:E:828:7Q9:C318	0.43	2.43	12	1
5:A:216:7Q9:C318	6:D:510:17F:C23	0.43	2.96	13	1
5:A:218:7Q9:O31	5:A:218:7Q9:C21	0.43	2.65	19	3
5:B:205:7Q9:C312	6:B:208:17F:C42	0.43	2.89	13	1
5:A:206:7Q9:C34	5:B:203:7Q9:C311	0.43	2.96	15	1
6:D:518:17F:H59	6:D:518:17F:C27	0.43	2.39	15	1
5:B:206:7Q9:O32	5:B:206:7Q9:C21	0.43	2.66	16	1
5:D:537:7Q9:C312	5:D:546:7Q9:C318	0.43	2.96	19	1
6:E:875:17F:O4	6:E:875:17F:C18	0.43	2.66	19	1
1:B:21:ILE:HD12	1:B:29:VAL:HG21	0.43	1.90	20	1
6:E:818:17F:C11	5:E:834:7Q9:C33	0.43	2.96	20	1
5:A:206:7Q9:O32	5:A:206:7Q9:C2	0.43	2.64	1	3
5:A:206:7Q9:C12	5:A:206:7Q9:O13	0.43	2.66	2	1
6:E:839:17F:H5	6:E:839:17F:O8	0.43	2.12	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:216:7Q9:C15	5:D:506:7Q9:O13	0.43	2.66	3	1
5:E:852:7Q9:C39	5:E:863:7Q9:C38	0.43	2.95	3	2
6:E:819:17F:C1	5:E:836:7Q9:O14	0.43	2.67	7	2
6:E:839:17F:H11A	6:E:857:17F:H35	0.43	1.89	4	1
6:A:213:17F:H71	6:A:213:17F:H49	0.43	1.89	5	1
6:A:213:17F:C22	5:D:507:7Q9:C33	0.43	2.96	5	2
6:D:510:17F:H68	6:D:510:17F:C30	0.43	2.44	11	2
5:D:531:7Q9:O21	5:D:531:7Q9:C11	0.43	2.66	15	2
6:E:819:17F:O10	6:E:819:17F:C4	0.43	2.63	6	1
5:A:214:7Q9:O32	5:A:218:7Q9:C22	0.43	2.67	7	1
6:E:808:17F:C41	6:E:808:17F:C29	0.43	2.96	7	1
5:D:512:7Q9:C3	5:D:536:7Q9:C13	0.43	2.96	8	1
5:E:864:7Q9:C11	5:E:874:7Q9:C33	0.43	2.96	8	1
5:E:843:7Q9:C12	5:E:860:7Q9:O13	0.43	2.66	11	1
5:A:205:7Q9:C1	5:A:212:7Q9:C1	0.43	2.95	12	1
5:E:859:7Q9:C22	5:E:878:7Q9:C38	0.43	2.97	12	1
5:D:542:7Q9:C13	5:D:542:7Q9:C1	0.43	2.96	13	1
2:E:579:THR:O	2:E:583:ARG:HG3	0.43	2.13	14	1
2:D:349:ARG:HG3	5:D:527:7Q9:C39	0.43	2.44	15	1
1:B:64:TYR:HB3	1:B:67:MET:HB2	0.43	1.90	16	1
5:D:503:7Q9:O11	5:D:503:7Q9:C21	0.43	2.66	17	1
5:A:217:7Q9:C314	5:D:554:7Q9:C316	0.43	2.96	20	1
5:D:529:7Q9:O22	5:D:529:7Q9:C1	0.43	2.63	20	1
6:E:829:17F:C12	5:E:852:7Q9:C34	0.43	2.85	20	1
5:E:852:7Q9:O32	5:E:852:7Q9:C21	0.43	2.66	11	6
6:E:875:17F:C6	6:E:875:17F:P1	0.43	3.06	2	1
5:B:205:7Q9:C315	6:B:208:17F:H71	0.43	2.42	3	1
6:B:208:17F:O2	5:B:209:7Q9:C15	0.43	2.66	3	1
5:D:513:7Q9:C22	5:D:513:7Q9:C13	0.43	2.96	3	1
6:E:857:17F:C31	6:E:857:17F:C35	0.43	2.95	3	2
5:A:210:7Q9:C35	5:A:210:7Q9:O14	0.43	2.66	4	2
2:D:312:MET:HE1	6:D:533:17F:H64	0.43	1.89	17	2
6:D:510:17F:C17	6:D:533:17F:H19	0.43	2.42	6	1
5:E:835:7Q9:O22	5:E:835:7Q9:C1	0.43	2.62	6	3
5:D:512:7Q9:O11	5:D:512:7Q9:C21	0.43	2.66	7	2
6:A:220:17F:P1	5:D:503:7Q9:C14	0.43	3.06	12	1
6:E:806:17F:H54	6:E:806:17F:C39	0.43	2.43	13	1
1:A:47:ASP:HB3	1:B:132:ASP:HB2	0.43	1.89	17	1
6:D:510:17F:C21	6:D:511:17F:C31	0.43	2.92	17	1
5:E:813:7Q9:O13	5:E:813:7Q9:C2	0.43	2.66	18	1
6:A:208:17F:C10	6:A:208:17F:P1	0.43	3.06	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:511:17F:O4	5:D:532:7Q9:C13	0.43	2.67	20	1
5:B:210:7Q9:C311	5:E:823:7Q9:C318	0.43	2.95	1	2
6:E:808:17F:H49	6:E:810:17F:C29	0.43	2.43	12	2
5:E:831:7Q9:C34	5:E:851:7Q9:O13	0.43	2.67	2	1
6:D:511:17F:H61	6:D:511:17F:H36	0.43	1.90	3	1
5:D:513:7Q9:O22	5:D:513:7Q9:C1	0.43	2.62	3	1
5:D:530:7Q9:C35	5:D:532:7Q9:C34	0.43	2.96	3	1
5:A:218:7Q9:C15	5:D:513:7Q9:O13	0.43	2.67	4	1
6:D:520:17F:C30	5:E:841:7Q9:C318	0.43	2.94	4	2
5:E:825:7Q9:C32	6:E:842:17F:C20	0.43	2.84	5	1
5:E:838:7Q9:O13	6:E:842:17F:H5	0.43	2.13	5	1
6:E:857:17F:C39	6:E:875:17F:H65	0.43	2.42	5	1
6:A:208:17F:C4	6:A:208:17F:O10	0.43	2.64	8	1
2:D:326:LEU:HD22	2:E:637:LEU:HD12	0.43	1.90	8	1
6:D:511:17F:H55	6:E:829:17F:C29	0.43	2.44	8	1
6:D:520:17F:H48	6:D:520:17F:H70	0.43	1.89	8	1
6:A:208:17F:H35	6:A:208:17F:H65	0.43	1.89	11	1
6:D:510:17F:H10	6:D:517:17F:H19A	0.43	1.90	14	1
6:A:213:17F:H35	5:D:509:7Q9:O22	0.43	2.13	16	1
5:E:821:7Q9:O22	5:E:821:7Q9:C1	0.43	2.64	16	2
5:D:538:7Q9:O13	5:D:538:7Q9:C12	0.43	2.65	17	1
5:E:867:7Q9:C33	5:E:877:7Q9:C33	0.43	2.96	17	1
5:D:502:7Q9:C38	5:D:502:7Q9:C312	0.43	2.94	18	1
1:A:117:LYS:HE2	3:A:201:GSP:N3	0.43	2.27	19	1
6:A:220:17F:C21	5:D:502:7Q9:C312	0.43	2.96	19	1
1:B:25:GLN:HB3	1:B:27:HIS:CD2	0.43	2.48	2	1
6:B:208:17F:C1X	5:B:209:7Q9:C39	0.43	2.97	3	1
5:B:204:7Q9:O14	5:B:204:7Q9:C12	0.43	2.66	4	2
2:D:298:GLN:N	2:D:299:PRO:HD2	0.43	2.29	8	6
6:A:208:17F:C22	6:B:208:17F:H60	0.43	2.42	7	1
6:A:208:17F:H55	5:E:816:7Q9:C315	0.43	2.43	7	1
6:E:873:17F:O7	6:E:873:17F:O6	0.43	2.36	7	2
5:D:503:7Q9:C313	6:D:519:17F:H45	0.43	2.43	8	1
6:A:219:17F:C42	5:D:505:7Q9:C316	0.43	2.97	9	1
5:E:821:7Q9:P	5:E:821:7Q9:C14	0.43	3.06	10	1
1:A:81:VAL:HA	1:A:114:VAL:O	0.43	2.13	11	1
5:D:546:7Q9:C21	5:D:546:7Q9:O31	0.43	2.67	11	1
6:E:839:17F:O10	6:E:839:17F:H9A	0.43	2.13	12	1
5:D:526:7Q9:C313	5:D:544:7Q9:C310	0.43	2.96	13	1
5:E:849:7Q9:C313	5:E:852:7Q9:C35	0.43	2.96	13	1
5:D:538:7Q9:O12	5:D:538:7Q9:C15	0.43	2.66	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:538:7Q9:O22	5:D:538:7Q9:C3	0.43	2.62	18	1
6:E:839:17F:C42	6:E:839:17F:C28	0.43	2.97	18	1
6:D:511:17F:H58	6:D:511:17F:H63	0.43	1.50	2	6
6:D:539:17F:H63	6:D:539:17F:C21	0.43	2.43	2	2
6:E:818:17F:H58	6:E:818:17F:H63	0.43	1.54	5	8
2:D:418:LEU:HD22	2:E:736:TYR:HD2	0.43	1.74	3	3
1:B:58:THR:HG21	1:B:71:TYR:CE1	0.43	2.48	18	4
6:E:806:17F:H74	5:E:811:7Q9:C313	0.43	2.43	4	1
6:E:839:17F:H52	5:E:858:7Q9:C313	0.43	2.44	5	1
6:D:510:17F:C17	6:D:517:17F:C9	0.43	2.97	18	2
2:D:430:LEU:HD22	6:D:539:17F:H33	0.43	1.89	7	1
5:D:504:7Q9:C311	5:D:508:7Q9:C310	0.43	2.95	7	1
6:E:818:17F:C11	5:E:821:7Q9:C23	0.43	2.88	7	1
5:E:862:7Q9:C3	5:E:877:7Q9:C11	0.43	2.97	7	1
5:E:816:7Q9:O31	5:E:816:7Q9:C34	0.43	2.66	8	4
6:E:857:17F:H71	6:E:875:17F:H61	0.43	1.89	8	1
6:E:808:17F:H18A	6:E:810:17F:C18	0.43	2.42	10	1
6:E:875:17F:H78	6:E:875:17F:C30	0.43	2.43	13	1
5:D:514:7Q9:C15	5:D:525:7Q9:O22	0.43	2.67	15	1
6:A:208:17F:H49	6:A:208:17F:H71	0.43	1.88	16	1
6:A:208:17F:H58	6:A:208:17F:H36	0.43	1.89	16	1
6:E:812:17F:H70	5:E:823:7Q9:C316	0.43	2.44	16	1
5:D:537:7Q9:C38	5:D:546:7Q9:C37	0.43	2.96	17	1
6:E:819:17F:O9	6:E:819:17F:O8	0.43	2.35	18	1
5:A:207:7Q9:C33	5:A:215:7Q9:C3	0.43	2.96	19	1
5:E:849:7Q9:O14	5:E:878:7Q9:C15	0.43	2.66	19	1
6:A:213:17F:C24	6:A:213:17F:C1Z	0.43	2.94	20	1
6:D:510:17F:H18	6:D:517:17F:H8	0.43	1.91	1	1
5:E:813:7Q9:C32	5:E:816:7Q9:C312	0.43	2.96	1	1
5:A:211:7Q9:O31	5:A:211:7Q9:C34	0.43	2.66	2	1
5:E:877:7Q9:C34	5:E:877:7Q9:O32	0.43	2.65	3	1
6:E:820:17F:H6A	5:E:837:7Q9:O22	0.43	2.14	7	1
5:A:206:7Q9:C318	6:E:802:17F:H67	0.43	2.44	9	1
2:D:319:VAL:HG23	2:E:644:LEU:HD21	0.43	1.90	9	1
5:D:509:7Q9:C36	5:D:531:7Q9:C312	0.43	2.96	9	1
5:E:828:7Q9:O13	5:E:851:7Q9:C2	0.43	2.67	9	1
5:D:512:7Q9:C2	5:D:536:7Q9:C13	0.43	2.96	10	1
6:E:808:17F:H72	5:E:814:7Q9:C312	0.43	2.44	11	1
5:A:209:7Q9:C13	5:A:209:7Q9:P	0.43	3.06	13	1
6:B:208:17F:H40	5:D:508:7Q9:C318	0.43	2.43	17	1
5:D:537:7Q9:P	5:D:546:7Q9:C12	0.43	3.07	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:520:17F:H70	6:D:520:17F:H48	0.43	1.91	19	1
6:A:220:17F:H10A	6:A:220:17F:C35	0.43	2.44	2	1
5:E:809:7Q9:C313	6:E:812:17F:H55	0.43	2.43	2	1
5:E:803:7Q9:O11	5:E:803:7Q9:C21	0.43	2.67	9	5
5:A:205:7Q9:C35	5:A:212:7Q9:O32	0.43	2.66	4	1
5:E:831:7Q9:C22	5:E:831:7Q9:C39	0.43	2.96	19	3
6:E:839:17F:H8A	6:E:857:17F:H12	0.43	1.91	5	1
5:E:833:7Q9:O11	5:E:833:7Q9:O31	0.43	2.37	6	2
5:E:847:7Q9:C13	6:E:873:17F:O4	0.43	2.67	6	2
5:D:512:7Q9:C317	6:D:534:17F:H40	0.43	2.43	7	1
6:D:518:17F:C26	5:D:549:7Q9:C311	0.43	2.97	7	1
6:E:802:17F:O8	5:E:803:7Q9:C12	0.43	2.67	8	1
2:D:272:TRP:HZ2	2:E:695:LYS:HB2	0.43	1.74	12	1
5:E:865:7Q9:P	5:E:865:7Q9:O21	0.43	2.77	12	2
6:A:213:17F:H8	6:A:213:17F:O2	0.43	2.13	20	2
5:A:215:7Q9:O22	5:A:216:7Q9:C22	0.43	2.66	14	1
6:E:808:17F:C33	6:E:808:17F:C12	0.43	2.96	14	1
5:D:515:7Q9:C15	6:D:519:17F:O10	0.43	2.67	15	1
1:B:19:LEU:HG	1:B:146:ALA:HB2	0.43	1.91	16	1
1:B:131:GLN:HG2	1:B:141:PHE:CE2	0.43	2.49	16	1
5:E:835:7Q9:C15	6:E:856:17F:O4	0.43	2.67	16	1
6:D:540:17F:C32	6:D:540:17F:H30	0.43	2.44	17	1
5:E:830:7Q9:C15	5:E:853:7Q9:C13	0.43	2.97	17	1
5:E:864:7Q9:C23	5:E:868:7Q9:C23	0.43	2.97	17	1
2:E:628:GLU:HA	2:E:631:ARG:CD	0.43	2.44	19	2
5:D:543:7Q9:C15	5:D:543:7Q9:O13	0.43	2.67	19	1
5:E:838:7Q9:C36	6:E:842:17F:H50	0.43	2.44	20	1
6:E:857:17F:H8	6:E:875:17F:O10	0.43	2.13	20	1
6:A:213:17F:H62	6:A:213:17F:H41	0.43	1.91	1	1
5:E:817:7Q9:C311	5:E:826:7Q9:C311	0.43	2.97	6	2
5:E:834:7Q9:O22	6:E:839:17F:H20	0.43	2.13	5	2
2:E:591:GLU:HA	2:E:594:LYS:HE2	0.43	1.90	2	1
5:E:809:7Q9:O14	5:E:809:7Q9:C12	0.43	2.67	8	4
5:D:521:7Q9:C14	5:D:522:7Q9:O14	0.43	2.67	3	1
6:E:820:17F:H58	6:E:820:17F:H62	0.43	1.63	13	4
5:E:835:7Q9:O14	5:E:850:7Q9:C12	0.43	2.66	3	1
6:E:839:17F:H29	5:E:858:7Q9:C310	0.43	2.44	9	1
2:D:434:GLU:OE1	2:D:434:GLU:HA	0.43	2.14	11	1
5:D:537:7Q9:C1	5:D:537:7Q9:C31	0.43	2.96	12	1
6:D:517:17F:H66	6:D:517:17F:C28	0.43	2.43	13	1
5:D:550:7Q9:C23	6:D:552:17F:HN1A	0.43	2.27	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:839:17F:H50	6:E:875:17F:H51	0.43	1.91	17	1
2:E:631:ARG:HB2	5:E:878:7Q9:C35	0.43	2.42	18	1
6:A:213:17F:H40	6:A:213:17F:C10	0.43	2.43	19	1
5:E:817:7Q9:O22	5:E:817:7Q9:C1	0.43	2.62	1	2
2:E:615:TYR:O	2:E:619:VAL:HG23	0.43	2.13	2	1
5:E:815:7Q9:O11	5:E:815:7Q9:C21	0.43	2.67	2	4
5:E:827:7Q9:O22	5:E:827:7Q9:C1	0.43	2.62	2	4
1:A:64:TYR:O	1:A:68:ARG:HB2	0.43	2.14	3	1
6:A:208:17F:H33	6:A:219:17F:H10A	0.43	1.90	3	1
2:D:327:GLN:OE1	6:D:534:17F:H32	0.43	2.14	3	1
6:D:510:17F:H36	6:D:510:17F:C25	0.43	2.44	13	2
6:E:806:17F:H5	5:E:817:7Q9:O32	0.43	2.14	3	1
5:E:838:7Q9:C37	5:E:861:7Q9:C39	0.43	2.97	3	1
5:E:848:7Q9:C12	5:E:848:7Q9:O13	0.43	2.67	3	1
2:D:320:GLU:HA	2:D:323:ARG:HD3	0.43	1.89	5	1
5:D:555:7Q9:O32	5:E:852:7Q9:C22	0.43	2.66	5	1
1:A:131:GLN:HB3	1:B:161:ARG:CZ	0.43	2.43	6	1
5:D:553:7Q9:C14	5:D:553:7Q9:O14	0.43	2.67	7	1
6:E:871:17F:H59	6:E:871:17F:H62	0.43	1.60	7	2
5:E:869:7Q9:O32	5:E:874:7Q9:C23	0.43	2.67	8	1
1:B:126:ASP:HB3	1:B:129:GLN:HG2	0.43	1.90	9	1
5:A:214:7Q9:C22	5:D:507:7Q9:C23	0.43	2.96	10	1
5:A:212:7Q9:C23	5:A:217:7Q9:C2	0.43	2.97	11	1
5:D:505:7Q9:O21	5:D:505:7Q9:O32	0.43	2.37	12	2
6:D:510:17F:H57	6:D:533:17F:C34	0.43	2.33	13	1
6:A:213:17F:O1	6:A:213:17F:H20A	0.43	2.13	14	1
5:E:811:7Q9:C23	5:E:817:7Q9:C38	0.43	2.97	14	1
6:E:857:17F:C11	6:E:875:17F:H5	0.43	2.44	14	1
5:B:206:7Q9:O32	5:B:206:7Q9:C34	0.43	2.67	15	1
6:E:819:17F:H45	6:E:819:17F:H74	0.43	1.90	16	1
6:E:808:17F:C30	6:E:819:17F:H75	0.43	2.36	17	1
5:E:814:7Q9:C314	6:E:819:17F:C30	0.43	2.88	17	1
5:E:862:7Q9:O21	5:E:877:7Q9:C1	0.43	2.67	17	1
5:E:807:7Q9:C15	5:E:807:7Q9:O11	0.43	2.67	18	1
6:E:819:17F:O10	6:E:819:17F:H4	0.43	2.14	18	1
5:E:853:7Q9:O13	5:E:853:7Q9:C12	0.42	2.67	20	3
1:B:49:GLU:HB3	1:B:164:ARG:NH2	0.42	2.29	20	2
5:D:532:7Q9:C13	5:D:532:7Q9:C31	0.42	2.97	3	1
6:E:856:17F:O8	6:E:856:17F:H20A	0.42	2.14	3	1
5:E:870:7Q9:C22	6:E:873:17F:C12	0.42	2.97	3	1
5:D:502:7Q9:C21	5:D:502:7Q9:O14	0.42	2.67	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:507:7Q9:C317	5:E:836:7Q9:C316	0.42	2.97	5	1
2:D:347:GLU:O	2:D:351:ARG:HG3	0.42	2.13	6	1
1:A:14:VAL:CG2	1:A:16:LYS:HG3	0.42	2.44	7	2
5:A:216:7Q9:C32	6:D:517:17F:H31	0.42	2.44	7	1
6:E:808:17F:H74	6:E:808:17F:H50	0.42	1.90	7	1
6:D:519:17F:C1X	6:D:519:17F:C23	0.42	2.92	9	3
5:D:525:7Q9:C14	5:D:525:7Q9:C1	0.42	2.97	9	2
5:A:212:7Q9:C34	5:A:212:7Q9:O32	0.42	2.67	10	1
6:E:808:17F:H59	6:E:808:17F:H63	0.42	1.62	10	1
6:D:518:17F:H29	6:D:518:17F:H18A	0.42	1.90	11	1
5:E:827:7Q9:C13	5:E:850:7Q9:C13	0.42	2.97	11	1
2:D:272:TRP:CZ2	2:E:695:LYS:HB2	0.42	2.49	12	1
5:D:553:7Q9:C12	5:D:553:7Q9:O11	0.42	2.67	12	2
5:B:205:7Q9:C312	6:B:208:17F:H65	0.42	2.44	13	1
2:D:421:VAL:HB	2:E:736:TYR:HE2	0.42	1.73	14	1
5:A:204:7Q9:C32	5:A:211:7Q9:C39	0.42	2.96	16	1
2:E:716:GLN:OE1	2:E:716:GLN:HA	0.42	2.14	18	1
6:A:219:17F:H42	5:D:505:7Q9:C36	0.42	2.44	20	1
5:D:506:7Q9:C314	6:D:517:17F:H53	0.42	2.44	20	1
5:A:206:7Q9:C311	5:A:206:7Q9:C37	0.42	2.96	1	1
6:E:839:17F:H8A	6:E:857:17F:C22	0.42	2.45	1	1
6:E:875:17F:O10	6:E:875:17F:C4	0.42	2.58	2	1
6:D:518:17F:H18A	5:D:551:7Q9:C33	0.42	2.45	4	1
6:E:842:17F:C22	5:E:877:7Q9:C34	0.42	2.98	4	1
5:B:206:7Q9:O22	5:D:501:7Q9:C15	0.42	2.67	5	1
5:E:837:7Q9:O21	5:E:837:7Q9:O32	0.42	2.38	6	2
5:A:212:7Q9:C34	5:D:505:7Q9:C32	0.42	2.97	7	1
6:D:519:17F:H67	6:D:519:17F:H52	0.42	1.88	7	1
5:A:210:7Q9:O14	5:A:210:7Q9:C12	0.42	2.66	8	2
6:E:873:17F:C17	6:E:873:17F:O8	0.42	2.67	9	2
5:E:823:7Q9:C13	5:E:824:7Q9:C1	0.42	2.97	10	1
5:E:824:7Q9:C311	5:E:840:7Q9:C310	0.42	2.97	11	1
2:E:634:LEU:HD22	5:E:878:7Q9:C315	0.42	2.44	12	1
6:E:802:17F:H5	5:E:804:7Q9:O14	0.42	2.14	12	1
6:E:857:17F:N1	6:E:857:17F:P1	0.42	2.92	13	1
5:D:525:7Q9:C312	5:D:546:7Q9:C310	0.42	2.97	14	1
5:A:212:7Q9:C314	6:A:219:17F:C30	0.42	2.94	16	1
5:A:217:7Q9:C13	5:A:217:7Q9:P	0.42	3.07	16	1
2:D:257:PHE:CE2	2:E:706:LYS:HD3	0.42	2.49	16	1
6:E:808:17F:H55	6:E:819:17F:H78	0.42	1.90	16	1
5:E:811:7Q9:C23	5:E:817:7Q9:C311	0.42	2.97	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:802:17F:O8	5:E:803:7Q9:C11	0.42	2.66	20	1
5:E:841:7Q9:C39	5:E:850:7Q9:C317	0.42	2.97	20	1
2:D:419:LEU:HD12	2:D:422:LEU:HD23	0.42	1.91	1	1
5:E:811:7Q9:O22	5:E:811:7Q9:C1	0.42	2.63	1	1
6:E:812:17F:O8	6:E:812:17F:C4	0.42	2.67	1	3
5:E:844:7Q9:C23	5:E:865:7Q9:C1	0.42	2.97	1	2
5:B:206:7Q9:C317	6:E:812:17F:H76	0.42	2.45	2	1
5:D:504:7Q9:C1	5:D:508:7Q9:C14	0.42	2.97	3	1
5:E:807:7Q9:O22	5:E:807:7Q9:C1	0.42	2.63	3	1
6:E:873:17F:H36	6:E:873:17F:H39	0.42	1.60	17	6
5:B:207:7Q9:C13	5:D:506:7Q9:O14	0.42	2.67	4	1
6:D:552:17F:C1Y	6:D:552:17F:O10	0.42	2.67	4	1
6:D:533:17F:H18A	6:D:533:17F:C1	0.42	2.43	5	1
6:E:810:17F:C31	6:E:810:17F:C1X	0.42	2.97	5	1
6:E:818:17F:O10	5:E:821:7Q9:C11	0.42	2.68	5	2
5:E:835:7Q9:C35	6:E:856:17F:C33	0.42	2.97	5	1
6:E:808:17F:C33	6:E:820:17F:C1X	0.42	2.96	6	2
1:A:126:ASP:OD1	1:A:128:LYS:HD3	0.42	2.15	7	1
5:D:513:7Q9:O31	6:D:534:17F:H5	0.42	2.14	7	1
5:E:817:7Q9:C13	5:E:826:7Q9:O22	0.42	2.68	7	1
5:A:210:7Q9:C312	5:A:210:7Q9:C38	0.42	2.97	8	1
5:E:805:7Q9:O22	5:E:805:7Q9:C3	0.42	2.64	10	1
5:D:524:7Q9:C13	6:D:539:17F:H1A	0.42	2.43	11	1
5:A:203:7Q9:C15	5:B:203:7Q9:O31	0.42	2.66	13	1
1:A:15:GLY:HA2	3:A:201:GSP:C8	0.42	2.49	14	1
2:E:627:GLN:O	2:E:631:ARG:HG3	0.42	2.14	15	1
5:E:833:7Q9:C22	6:E:839:17F:C6	0.42	2.96	15	1
5:A:211:7Q9:C311	6:A:213:17F:C36	0.42	2.90	17	1
5:B:209:7Q9:C317	5:E:823:7Q9:C313	0.42	2.98	17	1
6:E:839:17F:H12	6:E:857:17F:H37	0.42	1.90	18	1
5:A:209:7Q9:C23	5:A:214:7Q9:C34	0.42	2.97	19	1
6:E:842:17F:C21	5:E:877:7Q9:O31	0.42	2.64	20	1
6:A:219:17F:H75	6:A:219:17F:H46	0.42	1.90	12	2
6:D:517:17F:C5	6:D:517:17F:O2	0.42	2.68	1	1
6:E:806:17F:O8	6:E:806:17F:O9	0.42	2.37	1	1
5:E:813:7Q9:O31	5:E:813:7Q9:C21	0.42	2.67	14	4
5:A:204:7Q9:O31	5:A:211:7Q9:O22	0.42	2.36	3	1
2:D:258:SER:HB3	5:D:550:7Q9:C38	0.42	2.44	3	1
6:D:533:17F:H46	6:D:533:17F:C40	0.42	2.44	3	1
5:A:205:7Q9:C22	5:A:205:7Q9:C14	0.42	2.98	4	1
5:D:512:7Q9:O21	5:D:512:7Q9:C31	0.42	2.67	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:843:7Q9:C310	5:E:862:7Q9:C313	0.42	2.96	4	1
5:D:502:7Q9:O31	5:D:502:7Q9:O22	0.42	2.37	5	2
5:D:524:7Q9:C310	6:D:539:17F:H11	0.42	2.44	8	1
5:E:807:7Q9:C315	6:E:818:17F:H53	0.42	2.45	8	1
5:E:865:7Q9:O32	5:E:865:7Q9:C34	0.42	2.68	10	2
5:D:526:7Q9:O21	5:D:526:7Q9:P	0.42	2.78	9	2
5:D:526:7Q9:C32	5:D:531:7Q9:C36	0.42	2.97	11	1
5:E:824:7Q9:C14	5:E:824:7Q9:P	0.42	3.07	12	1
2:D:334:LEU:CB	5:D:538:7Q9:C312	0.42	2.98	13	1
6:E:842:17F:H29	6:E:842:17F:C24	0.42	2.44	13	1
5:A:209:7Q9:C32	5:A:209:7Q9:C15	0.42	2.98	14	1
5:E:815:7Q9:C310	6:E:818:17F:H55	0.42	2.45	14	1
1:B:118:CYS:SG	1:B:143:GLU:HB3	0.42	2.55	15	1
5:A:205:7Q9:C1	5:A:212:7Q9:O32	0.42	2.67	17	1
1:B:49:GLU:HG2	1:B:50:THR:N	0.42	2.29	20	1
5:A:215:7Q9:C37	6:D:511:17F:H78	0.42	2.44	18	2
6:D:510:17F:C8	6:D:517:17F:O9	0.42	2.65	8	2
5:E:845:7Q9:C37	5:E:845:7Q9:C311	0.42	2.98	2	1
5:D:550:7Q9:C315	6:D:552:17F:H50	0.42	2.44	3	1
6:B:208:17F:H18A	5:D:504:7Q9:O32	0.42	2.14	4	1
5:D:525:7Q9:C23	5:D:525:7Q9:O32	0.42	2.67	4	1
6:E:808:17F:C25	6:E:810:17F:H62	0.42	2.44	4	1
6:E:839:17F:O10	6:E:839:17F:H9	0.42	2.13	4	1
6:E:873:17F:O8	6:E:873:17F:H10A	0.42	2.14	4	1
5:E:803:7Q9:C314	6:E:810:17F:H70	0.42	2.44	6	1
5:E:811:7Q9:C12	5:E:817:7Q9:C31	0.42	2.98	6	1
5:A:215:7Q9:C21	5:A:216:7Q9:C22	0.42	2.97	7	1
5:D:504:7Q9:C317	5:E:831:7Q9:C318	0.42	2.97	7	1
1:B:32:TYR:CZ	3:B:201:GSP:H5'2	0.42	2.49	8	1
5:D:551:7Q9:C15	5:D:551:7Q9:O11	0.42	2.68	9	1
6:E:857:17F:C39	6:E:875:17F:C34	0.42	2.92	9	1
5:E:801:7Q9:O11	5:E:801:7Q9:C21	0.42	2.68	19	3
5:A:209:7Q9:C12	5:A:209:7Q9:O14	0.42	2.67	16	2
5:E:849:7Q9:C314	5:E:852:7Q9:C35	0.42	2.96	13	1
5:D:544:7Q9:O12	5:D:544:7Q9:O21	0.42	2.37	14	1
5:E:834:7Q9:C23	6:E:839:17F:H20	0.42	2.44	14	1
5:B:206:7Q9:C15	5:B:206:7Q9:P	0.42	3.08	15	1
6:E:806:17F:O10	6:E:806:17F:H4	0.42	2.14	15	1
5:E:836:7Q9:O22	5:E:836:7Q9:C13	0.42	2.67	15	1
6:B:208:17F:C12	5:E:823:7Q9:C318	0.42	2.98	17	1
2:D:352:ALA:HB1	5:D:527:7Q9:C316	0.42	2.44	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:208:17F:C25	6:A:219:17F:C12	0.42	2.97	20	1
6:D:520:17F:H52	5:E:841:7Q9:C313	0.42	2.44	20	1
5:D:524:7Q9:C13	6:D:539:17F:H8	0.42	2.44	1	1
6:E:871:17F:C9	5:E:872:7Q9:O14	0.42	2.65	1	1
5:A:204:7Q9:O11	5:A:204:7Q9:C21	0.42	2.68	2	3
6:D:517:17F:C21	6:D:533:17F:H72	0.42	2.25	2	1
6:E:820:17F:O1	5:E:830:7Q9:C12	0.42	2.67	3	1
5:A:216:7Q9:C311	5:A:216:7Q9:C37	0.42	2.94	4	1
2:E:659:LEU:HD21	6:E:875:17F:H69	0.42	1.90	4	1
6:E:819:17F:C3	5:E:825:7Q9:C13	0.42	2.97	5	1
5:E:838:7Q9:C14	6:E:842:17F:C18	0.42	2.98	5	1
5:D:506:7Q9:C15	6:D:517:17F:O5	0.42	2.67	6	1
6:E:802:17F:H50	6:E:802:17F:H78	0.42	1.90	6	1
6:A:208:17F:C21	6:B:208:17F:H34	0.42	2.44	7	1
5:A:215:7Q9:C316	5:E:821:7Q9:C310	0.42	2.98	8	1
5:D:530:7Q9:C14	5:D:530:7Q9:P	0.42	3.08	8	1
6:D:510:17F:H40	6:D:510:17F:H36	0.42	1.52	9	1
6:E:871:17F:H64	6:E:871:17F:H38	0.42	1.90	9	1
2:D:289:ASP:O	2:D:293:VAL:HG23	0.42	2.15	10	1
6:A:208:17F:C19	6:A:219:17F:H10	0.42	2.41	11	1
2:D:412:GLU:OE2	2:D:415:ARG:HD3	0.42	2.15	11	1
6:E:875:17F:H78	6:E:875:17F:H54	0.42	1.91	13	1
5:A:203:7Q9:C39	6:A:208:17F:H61	0.42	2.45	14	1
6:D:533:17F:H39	6:D:533:17F:H36	0.42	1.57	14	2
6:A:220:17F:H53	6:E:810:17F:H73	0.42	1.91	18	1
6:E:839:17F:H49	6:E:839:17F:H77	0.42	1.89	18	1
6:D:518:17F:O7	6:D:518:17F:O2	0.42	2.37	20	1
5:E:874:7Q9:C14	5:E:874:7Q9:C22	0.42	2.98	20	1
5:A:211:7Q9:C22	6:A:220:17F:H19A	0.42	2.44	1	1
5:A:212:7Q9:C37	5:D:505:7Q9:C36	0.42	2.97	1	2
6:A:219:17F:H5	6:D:518:17F:H10	0.42	1.88	2	1
6:D:510:17F:C5	6:D:533:17F:C20	0.42	2.97	2	1
5:A:204:7Q9:C3	5:A:206:7Q9:C11	0.42	2.98	3	1
6:E:812:17F:H34	6:E:812:17F:C8	0.42	2.44	3	1
6:E:808:17F:H74	6:E:808:17F:H47	0.42	1.91	4	1
5:E:801:7Q9:C318	6:E:871:17F:H67	0.42	2.45	5	1
6:E:808:17F:C12	6:E:808:17F:C32	0.42	2.98	6	1
5:E:821:7Q9:O22	6:E:839:17F:H18	0.42	2.15	6	1
6:A:213:17F:C30	5:D:503:7Q9:C315	0.42	2.91	8	1
5:A:218:7Q9:O22	5:D:513:7Q9:C14	0.42	2.67	8	1
6:E:875:17F:H58	6:E:875:17F:H63	0.42	1.62	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:214:7Q9:C3	5:D:513:7Q9:C1	0.42	2.98	11	1
6:E:810:17F:C37	6:E:810:17F:H52	0.42	2.45	11	1
5:A:217:7Q9:C3	5:A:217:7Q9:O22	0.42	2.61	12	1
5:E:803:7Q9:C314	6:E:810:17F:C40	0.42	2.97	12	1
5:A:206:7Q9:C11	5:A:211:7Q9:C22	0.42	2.98	13	1
6:E:808:17F:H63	6:E:808:17F:H59	0.42	1.65	14	2
1:A:19:LEU:HD23	1:A:146:ALA:HB2	0.42	1.91	14	1
6:E:820:17F:H73	6:E:820:17F:C29	0.42	2.24	14	1
5:D:506:7Q9:O21	5:D:506:7Q9:P	0.42	2.78	15	1
6:D:540:17F:H49	5:D:542:7Q9:C313	0.42	2.44	15	1
6:E:806:17F:H18A	6:E:806:17F:H10	0.42	1.92	17	1
5:E:826:7Q9:C12	5:E:826:7Q9:O13	0.42	2.68	17	1
6:A:219:17F:H6	6:D:518:17F:H11A	0.42	1.88	18	1
5:B:204:7Q9:C21	5:B:204:7Q9:O32	0.42	2.68	18	1
6:E:842:17F:C36	6:E:842:17F:H59	0.42	2.43	19	1
5:D:536:7Q9:O32	5:D:536:7Q9:O21	0.42	2.38	12	2
5:E:870:7Q9:C1	5:E:870:7Q9:O22	0.42	2.63	1	1
5:A:218:7Q9:C21	5:A:218:7Q9:O31	0.42	2.67	2	1
6:A:219:17F:C4	6:D:518:17F:H9	0.42	2.45	2	1
5:B:206:7Q9:O22	5:D:501:7Q9:C13	0.42	2.68	2	1
6:D:510:17F:H55	6:D:533:17F:H77	0.42	1.91	2	1
6:A:208:17F:H46	6:A:208:17F:H64	0.42	1.90	5	1
2:D:335:HIS:O	2:D:339:GLU:HB2	0.42	2.15	7	1
5:D:549:7Q9:C314	5:E:870:7Q9:C315	0.42	2.97	7	1
1:A:41:ARG:HA	1:A:53:LEU:O	0.42	2.15	9	1
5:A:211:7Q9:C23	6:A:213:17F:H6A	0.42	2.45	10	1
5:B:210:7Q9:C315	5:D:501:7Q9:C33	0.42	2.98	10	1
6:E:873:17F:H39	6:E:873:17F:H56	0.42	1.91	10	1
6:D:518:17F:H63	6:D:518:17F:C31	0.42	2.41	11	1
6:E:839:17F:O10	6:E:839:17F:C9	0.42	2.67	12	1
5:A:212:7Q9:O32	5:A:212:7Q9:C34	0.42	2.68	13	1
6:E:857:17F:H69	6:E:857:17F:C21	0.42	2.45	14	1
5:D:527:7Q9:O21	5:D:527:7Q9:C31	0.42	2.67	15	2
5:D:550:7Q9:C14	6:D:552:17F:O4	0.42	2.68	16	1
5:D:524:7Q9:C318	5:D:543:7Q9:C39	0.42	2.97	17	1
6:E:808:17F:H65	6:E:819:17F:H37	0.42	1.91	17	1
5:E:855:7Q9:O14	5:E:855:7Q9:C12	0.42	2.67	19	1
1:B:36:ILE:HG22	1:B:67:MET:HE1	0.42	1.90	20	1
6:D:510:17F:H31	6:D:510:17F:C17	0.42	2.45	20	1
6:D:552:17F:H56	6:D:552:17F:H9A	0.42	1.92	20	1
6:E:820:17F:H18A	5:E:853:7Q9:C33	0.42	2.44	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:835:7Q9:C318	6:E:856:17F:C39	0.42	2.97	20	1
1:B:92:ASP:HA	1:B:95:HIS:CD2	0.42	2.37	1	1
6:A:220:17F:H58	6:A:220:17F:H63	0.42	1.65	3	2
2:D:434:GLU:O	2:D:438:LYS:HG3	0.42	2.14	7	2
6:D:510:17F:H29	6:D:517:17F:C8	0.42	2.44	5	1
5:E:814:7Q9:C39	6:E:820:17F:C21	0.42	2.98	6	1
6:A:208:17F:H19	5:A:212:7Q9:C37	0.42	2.45	7	1
5:E:807:7Q9:C311	5:E:807:7Q9:C35	0.42	2.98	7	1
6:E:829:17F:H64	5:E:830:7Q9:C318	0.42	2.45	7	1
5:E:837:7Q9:C310	5:E:853:7Q9:C318	0.42	2.98	7	1
1:A:37:GLU:HA	1:A:57:ASP:O	0.42	2.15	9	1
6:D:552:17F:H56	6:D:552:17F:H9	0.42	1.90	9	1
6:D:518:17F:H36	6:D:518:17F:H39	0.42	1.64	16	6
5:D:531:7Q9:O22	5:D:531:7Q9:C1	0.42	2.64	19	3
6:A:208:17F:H60	5:A:212:7Q9:C36	0.42	2.45	13	1
5:E:826:7Q9:C310	5:E:845:7Q9:C39	0.42	2.97	13	1
5:A:211:7Q9:C22	6:A:213:17F:C31	0.42	2.98	17	1
5:A:206:7Q9:C34	5:B:203:7Q9:C313	0.42	2.98	18	1
6:E:806:17F:O2	6:E:806:17F:N1	0.42	2.41	18	1
5:E:847:7Q9:C22	5:E:848:7Q9:C32	0.42	2.98	18	1
6:A:219:17F:O4	5:D:504:7Q9:C13	0.42	2.67	19	1
2:D:257:PHE:CZ	2:E:706:LYS:HG2	0.42	2.49	20	1
5:D:506:7Q9:C314	6:D:517:17F:C30	0.42	2.98	20	1
6:D:510:17F:C42	6:D:533:17F:H76	0.42	2.45	20	1
6:D:517:17F:C22	6:D:517:17F:C26	0.42	2.98	20	1
5:D:524:7Q9:C13	6:D:539:17F:H10	0.42	2.45	1	1
1:B:146:ALA:N	3:B:201:GSP:O6	0.42	2.52	2	1
5:D:526:7Q9:O22	5:D:544:7Q9:C3	0.42	2.68	2	1
5:D:529:7Q9:O14	5:D:529:7Q9:C12	0.42	2.68	3	1
6:D:552:17F:H39	6:D:552:17F:H35	0.42	1.58	18	3
6:D:517:17F:C41	6:D:533:17F:C30	0.42	2.98	5	1
5:D:538:7Q9:O11	5:D:538:7Q9:O31	0.42	2.38	5	1
6:D:518:17F:C18	5:D:551:7Q9:C37	0.42	2.98	6	1
6:E:819:17F:H40	6:E:820:17F:H38	0.42	1.92	7	1
6:A:208:17F:C1Y	6:A:219:17F:C10	0.42	2.82	8	1
6:D:539:17F:H63	5:D:549:7Q9:C22	0.42	2.44	8	1
5:E:835:7Q9:C33	6:E:856:17F:H19A	0.42	2.44	9	1
5:D:503:7Q9:O14	6:D:519:17F:H31	0.42	2.15	10	1
5:E:850:7Q9:C316	5:E:868:7Q9:C314	0.42	2.98	11	1
5:D:537:7Q9:O22	5:D:548:7Q9:C310	0.42	2.67	12	1
5:E:817:7Q9:O21	5:E:817:7Q9:C31	0.42	2.68	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:205:7Q9:C22	5:B:206:7Q9:C33	0.42	2.97	14	1
5:D:544:7Q9:O22	5:D:544:7Q9:C1	0.42	2.62	17	2
5:E:813:7Q9:C1	5:E:816:7Q9:C2	0.42	2.98	14	1
6:D:518:17F:H48	6:D:518:17F:C33	0.42	2.44	15	1
6:A:213:17F:C12	6:A:213:17F:H31	0.42	2.38	16	1
5:D:508:7Q9:O14	5:D:523:7Q9:C15	0.42	2.67	17	1
5:D:505:7Q9:C31	5:D:505:7Q9:O21	0.42	2.67	19	1
6:D:533:17F:H53	6:E:839:17F:C41	0.42	2.45	20	1
1:A:145:SER:HB3	1:A:148:THR:OG1	0.41	2.15	1	1
5:D:509:7Q9:C1	5:D:509:7Q9:C31	0.41	2.98	1	1
5:D:505:7Q9:C15	6:D:518:17F:O8	0.41	2.68	2	2
6:D:517:17F:H49	6:D:517:17F:H42	0.41	1.87	3	1
5:D:546:7Q9:O12	5:D:546:7Q9:C2	0.41	2.67	3	2
6:E:810:17F:H62	6:E:819:17F:H75	0.41	1.90	3	1
6:A:208:17F:H41	6:A:219:17F:H10A	0.41	1.90	6	2
6:E:856:17F:H39	6:E:856:17F:H36	0.41	1.54	8	2
6:E:819:17F:C10	6:E:820:17F:H10	0.41	2.45	7	1
6:D:510:17F:H20	6:D:533:17F:H60	0.41	1.92	9	1
6:D:552:17F:O1	6:D:552:17F:C2	0.41	2.68	9	1
2:D:384:ASN:O	2:D:388:ARG:HD3	0.41	2.15	10	1
2:D:374:LEU:HD13	2:E:590:LEU:HD22	0.41	1.92	11	1
1:B:109:VAL:HB	1:B:111:MET:HE2	0.41	1.91	18	2
5:E:827:7Q9:C318	5:E:841:7Q9:C310	0.41	2.98	15	1
6:E:819:17F:H10A	6:E:820:17F:C9	0.41	2.45	16	1
2:E:711:LEU:O	2:E:715:ARG:HG2	0.41	2.15	20	1
5:E:817:7Q9:C39	5:E:832:7Q9:C23	0.41	2.98	20	1
5:E:816:7Q9:C34	5:E:828:7Q9:O22	0.41	2.69	16	2
2:D:333:LYS:HD2	5:D:538:7Q9:C314	0.41	2.45	2	1
5:B:203:7Q9:C22	5:B:203:7Q9:C11	0.41	2.98	3	1
5:E:822:7Q9:O32	5:E:843:7Q9:C13	0.41	2.68	3	1
5:E:828:7Q9:O21	5:E:828:7Q9:C31	0.41	2.68	3	2
5:D:530:7Q9:O13	5:D:530:7Q9:C12	0.41	2.68	7	2
6:E:808:17F:H35	6:E:808:17F:H40	0.41	1.65	6	2
6:A:219:17F:H56	6:A:219:17F:H62	0.41	1.90	8	1
2:D:395:LYS:HD3	2:E:568:THR:HG23	0.41	1.91	8	1
2:D:326:LEU:HD11	2:E:641:LEU:HD13	0.41	1.92	9	1
5:D:535:7Q9:O14	5:D:535:7Q9:C12	0.41	2.67	14	2
5:D:524:7Q9:O13	5:D:543:7Q9:C13	0.41	2.68	14	2
6:E:842:17F:H29	6:E:842:17F:H39	0.41	1.92	11	1
5:A:210:7Q9:C22	5:A:211:7Q9:C34	0.41	2.98	12	1
5:E:862:7Q9:C21	5:E:877:7Q9:C11	0.41	2.98	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:208:17F:C12	5:B:209:7Q9:C39	0.41	2.87	16	1
5:B:209:7Q9:C318	5:E:824:7Q9:C315	0.41	2.98	16	1
6:E:802:17F:H62	6:E:802:17F:C1Z	0.41	2.45	18	1
5:E:814:7Q9:C15	5:E:814:7Q9:P	0.41	3.09	1	1
1:A:126:ASP:HB3	1:A:128:LYS:HG2	0.41	1.92	3	2
6:D:539:17F:H52	5:E:801:7Q9:C313	0.41	2.45	2	1
5:D:528:7Q9:O32	5:D:528:7Q9:C34	0.41	2.68	4	1
6:D:540:17F:C33	6:D:540:17F:H35	0.41	2.46	4	1
6:D:552:17F:H35	6:D:552:17F:H39	0.41	1.58	9	3
2:E:729:PHE:CE2	6:E:871:17F:H66	0.41	2.50	4	1
6:A:219:17F:C34	6:A:219:17F:H40	0.41	2.46	6	1
2:D:374:LEU:HD11	5:D:535:7Q9:C318	0.41	2.44	6	1
2:E:664:ALA:N	2:E:665:PRO:HD2	0.41	2.30	7	1
6:A:208:17F:H44	6:A:219:17F:H50	0.41	1.92	8	1
2:D:426:LYS:O	2:D:430:LEU:HG	0.41	2.16	10	1
2:E:582:LEU:HG	2:E:586:MET:HE3	0.41	1.92	10	1
6:E:802:17F:O6	6:E:802:17F:O7	0.41	2.38	11	2
5:E:811:7Q9:C23	5:E:826:7Q9:C37	0.41	2.98	12	1
6:A:219:17F:O8	6:A:219:17F:O9	0.41	2.39	13	1
6:D:517:17F:C37	6:D:517:17F:C28	0.41	2.94	13	1
6:E:806:17F:C4	5:E:811:7Q9:C14	0.41	2.99	13	1
5:B:204:7Q9:O13	5:B:204:7Q9:C2	0.41	2.69	14	1
5:B:204:7Q9:C12	5:B:204:7Q9:C1	0.41	2.98	18	1
6:A:213:17F:C33	6:A:213:17F:C10	0.41	2.99	19	1
2:E:671:ARG:HD2	5:E:858:7Q9:C22	0.41	2.45	19	1
5:D:501:7Q9:C2	5:D:522:7Q9:O22	0.41	2.69	20	1
2:E:729:PHE:CE2	6:E:871:17F:H63	0.41	2.51	20	1
6:E:857:17F:HN1	6:E:857:17F:P1	0.41	2.39	20	1
6:A:208:17F:H11A	6:A:208:17F:O1	0.41	2.15	1	1
5:D:505:7Q9:O11	5:D:505:7Q9:C21	0.41	2.69	1	2
6:E:875:17F:H49	6:E:875:17F:C41	0.41	2.45	11	2
5:B:204:7Q9:C317	6:E:812:17F:H49	0.41	2.45	3	1
5:D:535:7Q9:O13	5:D:535:7Q9:C2	0.41	2.69	11	2
2:E:674:LEU:CD2	6:E:856:17F:H12	0.41	2.45	4	1
6:A:213:17F:H66	6:A:213:17F:H49	0.41	1.93	5	1
6:D:540:17F:C8	5:D:545:7Q9:C36	0.41	2.98	5	1
5:E:803:7Q9:C312	6:E:806:17F:C37	0.41	2.98	6	1
6:E:808:17F:H40	6:E:808:17F:H35	0.41	1.70	7	2
5:D:549:7Q9:C37	5:D:551:7Q9:C312	0.41	2.97	10	1
5:E:835:7Q9:C38	5:E:850:7Q9:C310	0.41	2.98	11	1
5:E:851:7Q9:C39	6:E:871:17F:H20	0.41	2.45	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:213:17F:H48	6:A:213:17F:H66	0.41	1.91	12	1
6:E:802:17F:HN1	5:E:807:7Q9:C37	0.41	2.28	13	1
5:E:823:7Q9:O13	5:E:823:7Q9:C12	0.41	2.68	13	1
6:A:220:17F:H63	6:A:220:17F:H58	0.41	1.67	14	2
5:D:521:7Q9:O31	5:D:521:7Q9:C34	0.41	2.69	14	1
6:E:829:17F:H72	5:E:830:7Q9:C315	0.41	2.45	14	1
6:E:875:17F:H63	6:E:875:17F:H58	0.41	1.64	15	1
6:D:540:17F:C36	6:D:540:17F:H35	0.41	2.45	19	1
5:E:854:7Q9:O21	5:E:854:7Q9:C31	0.41	2.68	19	1
6:D:540:17F:H51	5:D:542:7Q9:C318	0.41	2.45	1	1
5:E:851:7Q9:C35	6:E:871:17F:H20A	0.41	2.46	2	1
2:D:334:LEU:CB	5:D:538:7Q9:C310	0.41	2.98	3	1
5:E:849:7Q9:C22	5:E:853:7Q9:C11	0.41	2.98	4	2
5:E:851:7Q9:O13	5:E:851:7Q9:C12	0.41	2.69	3	1
5:A:214:7Q9:C15	5:A:214:7Q9:O11	0.41	2.69	4	1
5:D:502:7Q9:O32	5:D:515:7Q9:P	0.41	2.78	4	1
2:E:558:SER:OG	6:E:873:17F:H69	0.41	2.16	4	1
6:D:539:17F:C36	6:D:539:17F:H59	0.41	2.45	6	1
5:A:212:7Q9:C35	5:A:212:7Q9:O32	0.41	2.68	7	1
5:A:212:7Q9:C23	5:A:217:7Q9:O22	0.41	2.68	7	1
5:A:214:7Q9:O22	5:A:214:7Q9:C3	0.41	2.65	7	1
5:D:521:7Q9:C3	5:D:521:7Q9:O14	0.41	2.68	7	1
6:D:517:17F:H47	6:D:517:17F:H64	0.41	1.92	8	1
6:D:539:17F:C36	6:D:539:17F:C32	0.41	2.79	8	1
6:E:812:17F:H41	6:E:812:17F:H36	0.41	1.91	8	1
5:A:204:7Q9:C12	5:A:205:7Q9:C23	0.41	2.98	10	1
6:B:208:17F:H39	6:B:208:17F:H35	0.41	1.62	11	1
2:D:269:GLN:HG3	6:D:540:17F:H33	0.41	1.93	11	1
6:D:519:17F:H55	5:D:544:7Q9:C316	0.41	2.45	13	1
2:E:623:ARG:HA	2:E:626:LEU:HD12	0.41	1.91	14	1
5:D:516:7Q9:C14	5:D:516:7Q9:P	0.41	3.09	15	1
5:E:825:7Q9:C33	6:E:842:17F:C34	0.41	2.99	15	1
6:A:219:17F:O10	6:D:518:17F:H8	0.41	2.16	17	1
6:A:220:17F:C22	5:E:822:7Q9:C315	0.41	2.98	17	1
1:B:73:ARG:HG3	1:B:103:VAL:CG1	0.41	2.46	17	1
5:E:851:7Q9:C38	6:E:871:17F:H19A	0.41	2.46	20	2
6:A:208:17F:H35	6:A:208:17F:C36	0.41	2.46	18	1
6:D:510:17F:C25	6:D:510:17F:H36	0.41	2.46	18	1
5:D:522:7Q9:C14	5:D:553:7Q9:C31	0.41	2.99	18	1
6:A:220:17F:H48	6:A:220:17F:C37	0.41	2.44	19	1
5:E:868:7Q9:C38	5:E:868:7Q9:C312	0.41	2.97	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:215:7Q9:C39	6:D:510:17F:H41	0.41	2.45	1	1
5:B:209:7Q9:O13	5:B:209:7Q9:C2	0.41	2.68	1	1
5:E:853:7Q9:P	5:E:853:7Q9:O21	0.41	2.79	1	1
5:B:210:7Q9:C312	5:E:823:7Q9:C317	0.41	2.99	2	1
6:E:806:17F:O10	6:E:806:17F:C4	0.41	2.59	2	1
1:B:86:ASN:OD1	1:B:88:LYS:HB3	0.41	2.15	3	1
5:E:851:7Q9:C315	6:E:871:17F:C20	0.41	2.98	3	1
1:A:17:SER:N	3:A:201:GSP:O2B	0.41	2.52	4	1
6:E:839:17F:H42	6:E:839:17F:H71	0.41	1.92	4	1
2:D:352:ALA:O	2:D:356:VAL:HG23	0.41	2.16	5	2
6:E:829:17F:H72	5:E:830:7Q9:C310	0.41	2.44	5	1
2:E:663:LEU:HD21	6:E:875:17F:H42	0.41	1.92	7	1
2:E:601:LEU:HB3	5:E:867:7Q9:C37	0.41	2.46	8	1
6:D:511:17F:H40	6:D:511:17F:H66	0.41	1.93	11	1
1:A:79:LEU:HG	1:A:114:VAL:HG21	0.41	1.93	12	1
5:D:523:7Q9:C1	5:D:550:7Q9:C35	0.41	2.99	12	1
6:A:213:17F:H39	6:A:213:17F:H36	0.41	1.63	13	2
1:A:110:PRO:HB3	1:A:162:GLU:HB3	0.41	1.93	16	1
5:D:502:7Q9:O14	5:D:502:7Q9:C21	0.41	2.69	16	1
5:E:846:7Q9:O11	5:E:846:7Q9:C21	0.41	2.69	16	1
6:A:213:17F:O8	5:D:503:7Q9:C14	0.41	2.68	17	2
5:B:205:7Q9:C39	6:B:208:17F:C9	0.41	2.98	17	1
2:D:333:LYS:CD	5:E:878:7Q9:C318	0.41	2.98	17	1
5:D:508:7Q9:O32	5:D:524:7Q9:C32	0.41	2.69	18	1
1:A:16:LYS:HG3	3:A:201:GSP:O2G	0.41	2.15	19	1
6:D:510:17F:C32	6:D:533:17F:H66	0.41	2.46	20	1
5:E:858:7Q9:O21	5:E:858:7Q9:C31	0.41	2.69	1	1
1:A:68:ARG:HB3	1:A:72:MET:HE3	0.41	1.93	2	1
1:A:109:VAL:HB	1:A:111:MET:HE2	0.41	1.92	2	1
5:D:505:7Q9:C13	5:D:528:7Q9:P	0.41	3.09	2	1
1:A:117:LYS:HE2	3:A:201:GSP:C5	0.41	2.50	3	1
1:B:81:VAL:HA	1:B:114:VAL:O	0.41	2.16	3	1
6:D:518:17F:H62	5:D:528:7Q9:C39	0.41	2.46	3	1
5:E:838:7Q9:P	5:E:838:7Q9:O21	0.41	2.79	3	1
5:E:861:7Q9:C3	5:E:867:7Q9:C14	0.41	2.99	3	1
5:A:207:7Q9:C34	5:A:215:7Q9:C3	0.41	2.99	4	1
1:B:3:GLU:HG3	1:B:52:LEU:HD23	0.41	1.92	5	2
6:E:819:17F:H12A	6:E:820:17F:C22	0.41	2.46	4	1
1:A:97:ARG:HD3	1:A:101:LYS:HE2	0.41	1.93	5	1
5:A:218:7Q9:O11	6:D:511:17F:H6	0.41	2.16	5	1
6:E:802:17F:H1	6:E:802:17F:C4	0.41	2.45	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:511:17F:H18A	6:D:511:17F:C2	0.41	2.43	6	2
5:E:869:7Q9:O32	5:E:874:7Q9:C15	0.41	2.69	7	1
1:B:15:GLY:HA2	3:B:201:GSP:O5'	0.41	2.15	8	1
5:E:835:7Q9:O21	5:E:835:7Q9:C31	0.41	2.69	8	2
5:A:212:7Q9:C31	5:A:212:7Q9:C1	0.41	2.98	9	1
5:A:218:7Q9:O11	5:A:218:7Q9:C21	0.41	2.69	9	2
6:E:819:17F:H49	5:E:836:7Q9:C312	0.41	2.45	10	1
5:E:848:7Q9:O22	5:E:848:7Q9:C1	0.41	2.66	10	1
5:D:506:7Q9:C34	6:D:517:17F:H32	0.41	2.45	11	1
5:D:512:7Q9:C23	5:D:536:7Q9:C33	0.41	2.98	11	1
5:D:506:7Q9:C15	6:D:517:17F:C3	0.41	2.99	12	1
5:A:218:7Q9:C2	6:D:511:17F:H6	0.41	2.46	13	1
6:E:842:17F:H2	6:E:842:17F:O2	0.41	2.16	13	1
5:D:513:7Q9:C313	5:D:532:7Q9:C315	0.41	2.99	14	1
5:D:513:7Q9:C315	6:D:534:17F:H45	0.41	2.46	14	1
5:E:835:7Q9:C318	6:E:856:17F:H75	0.41	2.45	14	1
5:A:207:7Q9:C22	5:A:207:7Q9:C15	0.41	2.99	16	1
1:B:110:PRO:HB3	1:B:162:GLU:HB3	0.41	1.92	16	1
5:D:550:7Q9:C23	6:D:552:17F:N1	0.41	2.83	18	1
5:E:833:7Q9:C13	6:E:839:17F:H4A	0.41	2.45	19	1
6:A:219:17F:H69	6:D:518:17F:H35	0.41	1.93	20	1
6:D:552:17F:O10	6:D:552:17F:C6	0.41	2.65	20	1
6:E:842:17F:H2	6:E:842:17F:O6	0.41	2.14	20	1
1:A:144:THR:HG22	1:A:151:GLY:HA3	0.41	1.91	1	1
5:B:209:7Q9:C12	5:B:209:7Q9:O14	0.41	2.69	1	1
1:B:158:THR:HA	1:B:161:ARG:HE	0.41	1.76	2	1
6:A:213:17F:H37	5:D:509:7Q9:C23	0.41	2.45	3	1
6:D:534:17F:H37	6:D:534:17F:H69	0.41	1.92	3	1
5:E:851:7Q9:C313	6:E:871:17F:C20	0.41	2.99	3	2
5:E:877:7Q9:C14	5:E:877:7Q9:P	0.41	3.09	3	1
6:E:812:17F:H2	6:E:812:17F:O6	0.41	2.16	4	1
6:E:842:17F:H29	6:E:842:17F:H41	0.41	1.92	4	1
5:A:204:7Q9:C38	5:A:211:7Q9:C37	0.41	2.98	5	1
6:E:829:17F:H30	5:E:849:7Q9:C23	0.41	2.46	8	1
5:E:833:7Q9:O21	5:E:833:7Q9:O32	0.41	2.39	9	1
5:D:535:7Q9:C3	5:D:535:7Q9:O22	0.41	2.64	10	1
6:A:213:17F:H66	6:A:213:17F:C27	0.41	2.46	12	1
5:A:212:7Q9:O21	5:A:212:7Q9:P	0.41	2.79	13	1
5:B:205:7Q9:O13	5:B:206:7Q9:C13	0.41	2.69	13	1
6:E:802:17F:H32	5:E:807:7Q9:C37	0.41	2.46	14	1
5:A:212:7Q9:O21	5:A:212:7Q9:O13	0.41	2.39	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:117:LYS:HG2	3:B:201:GSP:C2	0.41	2.50	16	1
6:E:819:17F:H67	5:E:825:7Q9:C318	0.41	2.46	16	1
6:E:875:17F:HN1A	6:E:875:17F:C11	0.41	2.29	16	1
5:E:816:7Q9:C1	5:E:816:7Q9:O32	0.41	2.69	20	2
5:B:210:7Q9:O32	6:D:520:17F:H31	0.41	2.16	18	1
5:D:509:7Q9:C34	5:D:527:7Q9:O32	0.41	2.69	18	1
6:D:519:17F:H63	6:D:519:17F:H59	0.41	1.61	18	1
5:D:544:7Q9:C315	5:E:877:7Q9:C315	0.41	2.98	18	1
1:A:15:GLY:HA2	3:A:201:GSP:PA	0.41	2.55	19	1
3:A:201:GSP:O5'	3:A:201:GSP:H2'	0.41	2.16	19	1
6:E:818:17F:C34	5:E:827:7Q9:C37	0.41	2.98	20	1
5:A:215:7Q9:C35	6:D:511:17F:H68	0.41	2.46	1	1
5:B:204:7Q9:C14	5:B:204:7Q9:C1	0.41	2.99	1	1
2:E:736:TYR:CE1	5:E:876:7Q9:C318	0.41	3.04	1	1
5:E:855:7Q9:O32	5:E:855:7Q9:C23	0.41	2.69	1	1
5:A:218:7Q9:O31	5:A:218:7Q9:O22	0.41	2.38	2	1
2:D:340:LYS:HG2	2:E:626:LEU:HD21	0.41	1.93	2	1
5:D:527:7Q9:C34	5:D:527:7Q9:O31	0.41	2.69	3	1
5:E:811:7Q9:C310	5:E:826:7Q9:C312	0.41	2.99	3	1
5:E:823:7Q9:C23	5:E:827:7Q9:C22	0.41	2.98	4	1
5:E:828:7Q9:C310	5:E:847:7Q9:C37	0.41	2.99	4	1
6:E:829:17F:H11A	6:E:829:17F:H39	0.41	1.93	4	1
6:E:810:17F:C3	5:E:825:7Q9:C12	0.41	2.98	5	1
5:E:824:7Q9:O21	5:E:824:7Q9:C31	0.41	2.69	5	1
5:E:866:7Q9:C315	5:E:869:7Q9:C316	0.41	2.99	5	1
6:E:875:17F:N1	6:E:875:17F:C11	0.41	2.84	5	1
6:A:208:17F:H37	6:B:208:17F:H34	0.41	1.93	7	1
5:A:211:7Q9:C23	6:A:213:17F:H56	0.41	2.46	7	1
5:A:216:7Q9:C31	6:D:517:17F:H31	0.41	2.45	7	1
6:E:808:17F:H57	6:E:808:17F:C1X	0.41	2.38	8	1
6:E:819:17F:H45	6:E:819:17F:C42	0.41	2.41	8	1
5:D:549:7Q9:C314	5:E:870:7Q9:C314	0.41	2.99	9	1
6:A:208:17F:N1	5:D:504:7Q9:O14	0.41	2.54	10	1
5:A:214:7Q9:C310	5:A:218:7Q9:C315	0.41	2.99	10	1
6:A:220:17F:C23	6:A:220:17F:C1X	0.41	2.97	10	1
6:D:540:17F:H39	6:D:540:17F:C33	0.41	2.46	10	1
5:E:821:7Q9:C12	5:E:821:7Q9:O13	0.41	2.69	10	1
1:A:24:ILE:HD11	1:A:55:ILE:HD12	0.41	1.91	12	1
5:A:204:7Q9:C22	5:A:210:7Q9:C21	0.41	2.98	12	1
6:A:220:17F:H77	6:A:220:17F:C27	0.41	2.46	12	1
6:D:517:17F:C37	6:D:517:17F:H50	0.41	2.46	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:534:17F:H35	6:D:534:17F:H40	0.41	1.70	12	1
5:E:805:7Q9:C15	5:E:816:7Q9:O22	0.41	2.69	12	1
6:E:839:17F:O8	6:E:839:17F:C5	0.41	2.64	12	1
6:A:208:17F:H45	6:A:208:17F:C36	0.41	2.43	13	1
6:D:510:17F:H53	6:D:533:17F:H76	0.41	1.92	13	1
6:A:219:17F:C6	6:A:219:17F:O10	0.41	2.65	14	1
1:B:162:GLU:O	1:B:165:LYS:HG2	0.41	2.16	14	1
5:E:832:7Q9:O22	5:E:832:7Q9:C3	0.41	2.61	14	1
5:A:210:7Q9:C34	5:A:210:7Q9:O14	0.41	2.68	15	1
6:D:510:17F:C20	6:D:517:17F:H10	0.41	2.42	15	1
6:E:873:17F:O1	6:E:873:17F:O9	0.41	2.39	15	1
5:D:556:7Q9:C23	5:E:854:7Q9:C38	0.41	2.98	16	1
2:E:628:GLU:HG3	2:E:631:ARG:NH2	0.41	2.30	16	1
6:E:857:17F:C42	6:E:875:17F:H61	0.41	2.46	16	1
2:D:309:GLN:OE1	6:D:533:17F:H62	0.41	2.15	17	1
5:E:860:7Q9:O22	5:E:865:7Q9:C15	0.41	2.69	17	1
6:D:510:17F:H45	6:D:510:17F:H64	0.41	1.91	18	1
5:D:514:7Q9:O14	5:D:514:7Q9:C12	0.41	2.68	18	1
6:E:819:17F:H4A	5:E:825:7Q9:C13	0.41	2.45	18	1
6:E:875:17F:O10	6:E:875:17F:O7	0.41	2.39	18	1
1:B:46:ILE:HB	1:B:51:CYS:SG	0.41	2.56	20	1
1:B:62:GLU:OE1	1:B:62:GLU:HA	0.41	2.15	20	1
2:D:318:LYS:O	2:D:321:PRO:HD2	0.41	2.16	20	1
3:B:201:GSP:O1B	3:B:201:GSP:S1G	0.41	2.79	2	1
5:E:823:7Q9:C12	5:E:823:7Q9:O13	0.41	2.69	2	1
2:D:382:LYS:HD2	5:D:547:7Q9:O32	0.41	2.16	3	1
6:D:540:17F:C1X	6:D:540:17F:H64	0.41	2.46	3	1
6:E:802:17F:H10	6:E:802:17F:O8	0.41	2.15	3	1
6:A:208:17F:H45	6:A:208:17F:C37	0.41	2.46	4	1
6:D:552:17F:H31	6:D:552:17F:O10	0.41	2.16	6	2
6:E:857:17F:O1	6:E:857:17F:C5	0.41	2.67	4	1
1:A:6:LEU:HD11	1:A:53:LEU:HD22	0.41	1.92	5	1
6:A:219:17F:H61	6:A:219:17F:C39	0.41	2.44	5	1
5:D:516:7Q9:O13	5:D:548:7Q9:C14	0.41	2.69	6	1
6:D:517:17F:H5	6:D:517:17F:O2	0.41	2.16	7	1
6:D:533:17F:H36	6:D:533:17F:H39	0.41	1.62	7	1
5:E:813:7Q9:O31	5:E:813:7Q9:O22	0.41	2.38	7	2
2:E:671:ARG:HD2	5:E:858:7Q9:C23	0.41	2.45	8	1
6:D:511:17F:H63	6:D:511:17F:H58	0.41	1.58	9	1
5:E:878:7Q9:O11	5:E:878:7Q9:C21	0.41	2.69	14	2
6:A:213:17F:C41	6:E:819:17F:H77	0.41	2.45	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:543:7Q9:C318	5:E:872:7Q9:C316	0.41	2.99	12	1
6:A:208:17F:H45	6:A:208:17F:H68	0.41	1.92	13	1
6:E:820:17F:H52	6:E:820:17F:H69	0.41	1.92	13	1
6:A:208:17F:H34	6:A:208:17F:C24	0.41	2.46	14	1
5:A:209:7Q9:C1	5:A:209:7Q9:C12	0.41	2.99	15	1
6:E:806:17F:H70	5:E:817:7Q9:C317	0.41	2.46	15	1
5:E:814:7Q9:C315	6:E:819:17F:H52	0.41	2.45	15	1
5:A:206:7Q9:C23	5:A:209:7Q9:C314	0.41	2.99	16	1
1:B:113:LEU:HB3	1:B:141:PHE:CD1	0.41	2.51	17	1
6:D:510:17F:H37	6:D:511:17F:C31	0.41	2.44	17	1
6:D:519:17F:H64	6:D:519:17F:H59	0.41	1.83	17	1
5:D:523:7Q9:O32	5:D:523:7Q9:O21	0.41	2.39	17	1
5:E:851:7Q9:C3	5:E:851:7Q9:O22	0.41	2.64	17	1
6:E:802:17F:H6A	6:E:808:17F:HN1A	0.41	1.76	18	1
6:E:839:17F:H78	6:E:839:17F:C28	0.41	2.45	18	1
2:D:333:LYS:HE3	2:D:337:LEU:HD22	0.41	1.91	20	1
1:B:16:LYS:N	3:B:201:GSP:O2B	0.40	2.52	2	1
6:D:511:17F:H77	6:D:511:17F:H50	0.40	1.90	2	1
6:D:517:17F:H40	6:D:517:17F:H35	0.40	1.64	2	1
5:E:833:7Q9:C14	5:E:833:7Q9:C1	0.40	2.99	2	1
6:A:208:17F:H20A	6:A:219:17F:C9	0.40	2.46	3	1
5:E:833:7Q9:O14	5:E:852:7Q9:C14	0.40	2.69	3	1
5:E:850:7Q9:C37	5:E:850:7Q9:C311	0.40	2.99	3	2
5:A:209:7Q9:C37	5:A:209:7Q9:C311	0.40	2.99	4	1
5:D:513:7Q9:O21	5:D:513:7Q9:P	0.40	2.79	5	1
5:E:841:7Q9:C3	5:E:841:7Q9:O22	0.40	2.63	5	1
5:E:844:7Q9:O14	5:E:860:7Q9:C34	0.40	2.69	5	1
5:B:203:7Q9:O11	5:B:203:7Q9:O31	0.40	2.39	6	1
5:E:846:7Q9:O13	5:E:872:7Q9:C14	0.40	2.69	6	1
5:A:211:7Q9:C317	6:A:213:17F:H70	0.40	2.45	8	1
6:A:213:17F:O1	6:A:213:17F:H19A	0.40	2.15	8	1
6:A:219:17F:H5	6:D:518:17F:C8	0.40	2.46	8	1
5:A:212:7Q9:C1	5:A:212:7Q9:O32	0.40	2.69	9	1
6:A:213:17F:H38	5:D:509:7Q9:C22	0.40	2.46	12	1
5:D:555:7Q9:C13	5:D:555:7Q9:P	0.40	3.09	12	1
5:E:847:7Q9:C13	6:E:873:17F:C3	0.40	2.98	12	1
1:B:47:ASP:OD2	1:B:161:ARG:HD2	0.40	2.16	13	1
1:B:59:ALA:HA	3:B:201:GSP:O2G	0.40	2.14	13	1
5:D:502:7Q9:C31	5:D:525:7Q9:C22	0.40	2.99	13	1
5:D:556:7Q9:C32	5:E:854:7Q9:C310	0.40	2.99	14	1
5:E:803:7Q9:O11	5:E:803:7Q9:O22	0.40	2.39	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:528:7Q9:C1	5:D:551:7Q9:C32	0.40	2.99	15	1
5:E:807:7Q9:C13	5:E:809:7Q9:O13	0.40	2.69	15	1
6:D:510:17F:C8	6:D:517:17F:O7	0.40	2.68	16	1
6:A:213:17F:H49	6:A:213:17F:C38	0.40	2.44	17	1
5:D:528:7Q9:C35	5:D:551:7Q9:C311	0.40	2.99	19	1
5:D:509:7Q9:C32	5:D:531:7Q9:C34	0.40	2.99	20	1
1:B:126:ASP:O	1:B:129:GLN:HG2	0.40	2.16	1	1
6:E:871:17F:C10	5:E:872:7Q9:O14	0.40	2.69	1	1
5:A:214:7Q9:C34	5:A:218:7Q9:C31	0.40	2.99	4	1
6:D:518:17F:C1X	6:D:518:17F:C20	0.40	2.99	4	1
1:B:126:ASP:OD1	1:B:128:LYS:HD3	0.40	2.15	5	1
5:E:851:7Q9:C38	6:E:871:17F:C20	0.40	2.99	5	1
1:B:47:ASP:OD2	1:B:161:ARG:HD3	0.40	2.17	6	1
2:D:368:ASP:O	2:D:371:ARG:HG2	0.40	2.16	6	1
5:D:555:7Q9:C1	5:D:555:7Q9:O22	0.40	2.65	8	1
5:E:807:7Q9:C15	5:E:807:7Q9:C22	0.40	2.99	8	1
5:E:815:7Q9:C33	5:E:821:7Q9:C35	0.40	2.99	9	1
6:E:806:17F:H53	5:E:813:7Q9:C314	0.40	2.47	11	1
6:E:810:17F:H52	6:E:810:17F:H67	0.40	1.92	11	1
5:D:507:7Q9:O13	5:D:509:7Q9:C11	0.40	2.69	12	1
6:D:534:17F:C42	5:D:538:7Q9:C313	0.40	2.99	12	1
5:E:837:7Q9:C32	5:E:853:7Q9:C35	0.40	2.99	12	1
1:B:69:ASP:O	1:B:73:ARG:HG3	0.40	2.15	15	1
6:D:510:17F:H59	6:D:510:17F:H62	0.40	1.64	15	1
5:D:505:7Q9:C13	6:D:518:17F:H6	0.40	2.45	16	1
5:A:209:7Q9:C3	5:A:218:7Q9:O14	0.40	2.69	17	1
5:E:827:7Q9:O22	5:E:841:7Q9:C12	0.40	2.69	18	1
5:D:513:7Q9:C14	5:D:532:7Q9:O14	0.40	2.69	20	1
5:E:816:7Q9:O11	5:E:816:7Q9:O32	0.40	2.39	20	1
6:E:819:17F:H10	6:E:820:17F:H30	0.40	1.88	20	1
5:E:872:7Q9:O21	5:E:872:7Q9:C31	0.40	2.69	14	3
6:A:219:17F:O10	6:A:219:17F:H4	0.40	2.15	2	1
6:D:519:17F:C23	6:D:519:17F:C1X	0.40	2.90	2	1
6:E:806:17F:O6	6:E:806:17F:O7	0.40	2.38	2	1
6:D:518:17F:H62	5:D:528:7Q9:C38	0.40	2.46	3	1
5:D:505:7Q9:C33	5:D:505:7Q9:C22	0.40	2.99	4	1
1:B:13:GLY:HA2	3:B:201:GSP:C4'	0.40	2.46	6	1
5:E:843:7Q9:C314	5:E:843:7Q9:C37	0.40	2.99	6	1
6:A:213:17F:H78	6:E:808:17F:H53	0.40	1.93	7	1
2:E:590:LEU:HD21	5:E:862:7Q9:C318	0.40	2.47	7	1
5:E:805:7Q9:O32	6:E:812:17F:H19	0.40	2.13	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:809:7Q9:C12	6:E:818:17F:O1	0.40	2.70	7	1
2:D:374:LEU:HD21	5:D:535:7Q9:C317	0.40	2.46	10	2
5:D:537:7Q9:C37	5:D:537:7Q9:C311	0.40	2.98	15	2
2:E:623:ARG:HD2	2:E:623:ARG:O	0.40	2.15	8	1
5:D:553:7Q9:O11	5:D:553:7Q9:C12	0.40	2.70	11	1
5:D:556:7Q9:C35	5:E:854:7Q9:C310	0.40	2.99	13	1
5:E:801:7Q9:O14	5:E:801:7Q9:C12	0.40	2.68	14	1
5:E:853:7Q9:O32	5:E:853:7Q9:C34	0.40	2.70	14	1
1:A:5:LYS:HD2	1:A:74:THR:HG22	0.40	1.93	17	1
5:A:218:7Q9:C39	6:E:829:17F:C42	0.40	2.98	17	1
6:E:812:17F:C6	5:E:824:7Q9:C11	0.40	3.00	17	1
5:E:817:7Q9:O14	5:E:817:7Q9:C12	0.40	2.69	17	1
6:E:818:17F:H50	5:E:821:7Q9:C318	0.40	2.46	17	1
1:B:58:THR:HG21	1:B:71:TYR:CZ	0.40	2.51	18	1
5:D:553:7Q9:C12	5:D:553:7Q9:O21	0.40	2.69	18	1
6:E:829:17F:H9A	5:E:833:7Q9:C33	0.40	2.46	19	1
6:D:520:17F:H50	5:E:841:7Q9:C317	0.40	2.47	20	1
6:E:808:17F:O4	5:E:814:7Q9:C13	0.40	2.70	20	1
6:D:510:17F:C8	6:D:517:17F:C18	0.40	2.99	1	1
6:E:802:17F:H51	5:E:807:7Q9:C316	0.40	2.46	1	1
5:D:527:7Q9:C15	5:D:527:7Q9:P	0.40	3.09	2	1
6:B:208:17F:H41	5:E:824:7Q9:C317	0.40	2.47	3	1
6:E:829:17F:C11	5:E:833:7Q9:C38	0.40	2.97	4	1
6:E:808:17F:C39	6:E:819:17F:H54	0.40	2.42	5	1
5:D:505:7Q9:C13	6:D:518:17F:O8	0.40	2.69	6	1
6:A:220:17F:C22	5:D:502:7Q9:C317	0.40	3.00	7	1
5:E:833:7Q9:C37	5:E:849:7Q9:O32	0.40	2.69	8	1
5:E:860:7Q9:O32	5:E:865:7Q9:C12	0.40	2.70	8	1
6:D:520:17F:H46	5:E:840:7Q9:C317	0.40	2.46	9	1
6:E:857:17F:H68	6:E:875:17F:C33	0.40	2.35	9	1
5:D:515:7Q9:C36	6:D:519:17F:H75	0.40	2.47	10	1
6:E:820:17F:C41	5:E:830:7Q9:C22	0.40	2.97	10	1
5:E:834:7Q9:C37	6:E:839:17F:H44	0.40	2.47	11	1
5:E:834:7Q9:O14	5:E:858:7Q9:C34	0.40	2.69	11	1
6:A:220:17F:H41	6:A:220:17F:H77	0.40	1.94	12	1
6:D:520:17F:O10	6:D:520:17F:H4	0.40	2.15	12	1
6:A:208:17F:O9	6:A:208:17F:O8	0.40	2.39	13	1
5:A:211:7Q9:C312	6:A:213:17F:H5	0.40	2.46	13	1
1:B:20:THR:O	1:B:24:ILE:HG12	0.40	2.15	13	1
5:D:516:7Q9:O11	5:D:516:7Q9:C34	0.40	2.70	13	1
5:D:555:7Q9:C310	5:E:849:7Q9:C318	0.40	2.99	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:134:ALA:HA	1:B:137:TYR:CD2	0.40	2.51	14	1
6:A:213:17F:H61	6:A:213:17F:C23	0.40	2.46	15	1
5:D:547:7Q9:C1	5:D:547:7Q9:O22	0.40	2.65	15	1
5:E:801:7Q9:C12	5:E:801:7Q9:O14	0.40	2.69	15	1
3:B:201:GSP:O1A	3:B:201:GSP:O2B	0.40	2.39	16	1
6:E:839:17F:H78	6:E:839:17F:H47	0.40	1.89	18	1
6:D:520:17F:H70	6:D:520:17F:H47	0.40	1.92	19	1
6:D:510:17F:O9	6:D:510:17F:H31	0.40	2.16	20	1
5:E:874:7Q9:O32	5:E:874:7Q9:C34	0.40	2.70	20	1
5:B:209:7Q9:C14	5:B:209:7Q9:P	0.40	3.10	1	1
1:B:139:ILE:HB	1:B:140:PRO:HD2	0.40	1.93	2	1
6:E:820:17F:H65	5:E:837:7Q9:C39	0.40	2.46	2	1
5:E:865:7Q9:O22	5:E:865:7Q9:C1	0.40	2.65	2	1
6:D:518:17F:H60	6:D:518:17F:C23	0.40	2.46	3	1
5:D:524:7Q9:C2	5:D:524:7Q9:C11	0.40	2.99	3	1
2:E:736:TYR:HB2	5:E:876:7Q9:C310	0.40	2.46	3	1
5:D:549:7Q9:C22	5:E:801:7Q9:C23	0.40	3.00	4	1
5:A:206:7Q9:C1	5:A:206:7Q9:O22	0.40	2.61	6	1
5:E:847:7Q9:C12	5:E:847:7Q9:O13	0.40	2.69	6	1
6:B:208:17F:O1	6:B:208:17F:C2	0.40	2.70	7	1
5:D:555:7Q9:C15	6:E:857:17F:O10	0.40	2.70	7	1
2:E:598:GLN:HG2	5:E:877:7Q9:C313	0.40	2.47	7	1
6:D:511:17F:C21	5:D:513:7Q9:C315	0.40	3.00	8	1
5:E:828:7Q9:O32	5:E:828:7Q9:O21	0.40	2.39	8	1
5:D:515:7Q9:C12	6:D:519:17F:H6	0.40	2.47	9	1
2:E:730:LEU:HD12	2:E:733:LEU:HD22	0.40	1.93	9	1
5:E:821:7Q9:O21	5:E:821:7Q9:O14	0.40	2.39	9	1
5:A:214:7Q9:C313	5:E:814:7Q9:C318	0.40	2.99	10	1
1:B:46:ILE:HG21	1:B:157:TYR:CG	0.40	2.52	13	1
5:B:209:7Q9:C312	5:B:209:7Q9:C316	0.40	2.99	13	1
5:E:844:7Q9:O13	5:E:845:7Q9:C15	0.40	2.69	13	1
5:E:854:7Q9:C37	5:E:854:7Q9:C311	0.40	2.96	13	1
6:D:517:17F:H37	6:D:533:17F:H71	0.40	1.92	14	1
6:E:871:17F:H30	6:E:871:17F:C32	0.40	2.47	14	1
5:E:869:7Q9:C34	5:E:874:7Q9:C38	0.40	3.00	15	1
6:D:540:17F:C1	5:D:545:7Q9:C32	0.40	2.99	16	1
1:A:32:TYR:CE1	3:A:201:GSP:S1G	0.40	3.15	17	1
5:A:216:7Q9:O31	6:D:517:17F:C18	0.40	2.70	17	1
2:E:595:ALA:HA	2:E:598:GLN:NE2	0.40	2.31	18	1
5:E:814:7Q9:O21	5:E:814:7Q9:C31	0.40	2.70	18	1
5:E:816:7Q9:C1	5:E:816:7Q9:O22	0.40	2.65	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:513:7Q9:C13	5:D:532:7Q9:O13	0.40	2.70	19	1
5:D:524:7Q9:O32	5:D:524:7Q9:C23	0.40	2.69	19	1
5:E:838:7Q9:C310	5:E:877:7Q9:C35	0.40	2.99	19	1
6:E:829:17F:H12	5:E:852:7Q9:C33	0.40	2.44	20	1
5:E:859:7Q9:O21	5:E:859:7Q9:C31	0.40	2.69	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	165/185 (89%)	156±2 (95±1%)	8±2 (5±1%)	0±1 (0±0%)	49	83
1	B	165/185 (89%)	156±2 (94±1%)	9±2 (5±1%)	0±1 (0±0%)	44	80
2	D	185/200 (92%)	182±2 (98±1%)	3±2 (2±1%)	0±1 (0±0%)	44	80
2	E	185/200 (92%)	180±2 (97±1%)	4±2 (2±1%)	0±1 (0±0%)	44	80
All	All	14000/15400 (91%)	13482 (96%)	493 (4%)	25 (0%)	44	80

All 18 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	47	ASP	3
1	B	64	TYR	3
2	E	718	LEU	2
2	E	708	LYS	2
2	D	333	LYS	2
1	B	47	ASP	1
2	D	403	LEU	1
2	E	642	SER	1
1	B	34	PRO	1
2	D	408	LYS	1
2	E	705	GLU	1
1	A	153	ASP	1
1	B	154	ASP	1

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Mol	Chain	Res	Type	Models (Total)
2	D	265	GLY	1
2	D	400	LEU	1
2	E	598	GLN	1
1	B	37	GLU	1
2	D	419	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	147/165 (89%)	132±4 (90±2%)	15±4 (10±2%)	9 54
1	B	147/165 (89%)	133±3 (90±2%)	14±3 (10±2%)	10 55
2	D	162/175 (93%)	152±3 (94±2%)	10±3 (6±2%)	18 67
2	E	163/175 (93%)	150±3 (92±2%)	13±3 (8±2%)	13 61
All	All	12380/13600 (91%)	11332 (92%)	1048 (8%)	12 59

All 247 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)
2	D	402	THR	19
1	B	74	THR	17
1	B	2	THR	17
2	E	556	THR	15
1	A	35	THR	14
1	A	74	THR	14
1	A	87	THR	14
1	B	35	THR	14
1	B	65	SER	14
1	B	124	THR	14
2	D	256	THR	14
1	B	87	THR	14
1	A	92	ASP	13
2	E	702	THR	13
1	A	65	SER	12
1	B	148	THR	12

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Mol	Chain	Res	Type	Models (Total)
1	B	153	ASP	12
2	D	268	THR	12
2	E	619	VAL	12
2	E	737	THR	12
1	A	63	GLU	12
1	A	124	THR	12
2	D	320	GLU	12
1	A	50	THR	11
2	E	558	SER	11
2	E	733	LEU	11
1	A	148	THR	11
1	A	12	ASP	11
2	E	555	SER	10
2	E	688	ARG	10
2	D	335	HIS	10
2	D	373	ARG	10
2	D	388	ARG	10
1	B	63	GLU	9
1	B	127	THR	9
2	E	561	ARG	9
2	E	579	THR	9
2	D	279	THR	9
1	A	161	ARG	9
1	A	2	THR	8
1	A	127	THR	8
1	B	39	SER	8
2	D	258	SER	8
2	E	623	ARG	8
2	E	704	SER	8
1	B	149	ARG	7
2	E	569	GLN	7
1	A	89	SER	7
1	B	12	ASP	7
1	B	69	ASP	7
2	E	661	THR	7
1	A	69	ASP	7
2	D	361	THR	7
2	D	377	ARG	7
2	E	705	GLU	7
2	E	653	ARG	7
1	A	149	ARG	6
1	A	39	SER	6

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Mol	Chain	Res	Type	Models (Total)
1	A	68	ARG	6
1	B	92	ASP	6
1	B	161	ARG	6
2	D	431	SER	6
2	E	660	ARG	6
1	B	50	THR	6
2	E	637	LEU	6
1	A	58	THR	6
1	B	58	THR	6
1	A	17	SER	5
1	A	153	ASP	5
1	B	17	SER	5
2	D	404	SER	5
2	E	594	LYS	5
1	B	89	SER	5
2	D	351	ARG	5
2	E	589	ASP	5
2	E	646	GLU	5
1	B	133	LEU	5
2	D	333	LYS	5
2	D	397	THR	5
1	A	16	LYS	5
2	E	575	LEU	5
2	E	655	HIS	5
2	E	604	PHE	5
1	B	136	SER	5
1	B	119	ASP	5
1	A	29	VAL	4
1	A	133	LEU	4
2	D	261	ARG	4
1	A	41	ARG	4
2	D	401	SER	4
1	A	31	GLU	4
1	A	136	SER	4
1	B	29	VAL	4
1	B	38	ASP	4
1	B	135	ARG	4
2	E	728	SER	4
2	E	667	SER	4
1	B	16	LYS	4
1	B	128	LYS	4
1	A	145	SER	4

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Mol	Chain	Res	Type	Models (Total)
2	D	360	ARG	4
1	A	38	ASP	4
1	A	44	VAL	4
1	B	144	THR	4
1	A	20	THR	3
1	A	6	LEU	3
1	A	62	GLU	3
1	B	51	CYS	3
1	B	62	GLU	3
2	D	305	GLN	3
2	D	369	GLU	3
1	A	101	LYS	3
1	A	135	ARG	3
1	A	144	THR	3
1	B	68	ARG	3
2	D	280	GLU	3
2	D	437	THR	3
2	D	257	PHE	3
2	D	316	ARG	3
1	B	108	ASP	3
1	A	8	VAL	3
2	E	631	ARG	3
2	E	613	GLU	3
1	A	37	GLU	2
1	A	119	ASP	2
2	D	291	GLU	2
2	D	323	ARG	2
2	D	424	SER	2
2	E	603	ASP	2
2	E	691	GLU	2
2	E	701	SER	2
1	A	26	ASN	2
1	A	80	CYS	2
2	D	398	GLU	2
1	A	108	ASP	2
1	A	109	VAL	2
2	D	308	TRP	2
2	E	729	PHE	2
1	A	128	LYS	2
2	D	334	LEU	2
1	B	113	LEU	2
1	B	150	GLN	2

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Mol	Chain	Res	Type	Models (Total)
2	D	342	SER	2
1	A	165	LYS	2
1	B	31	GLU	2
2	E	644	LEU	2
1	A	33	ASP	2
2	E	724	SER	2
1	B	33	ASP	2
1	B	80	CYS	2
1	B	44	VAL	2
1	B	101	LYS	2
1	B	157	TYR	2
1	B	145	SER	2
2	D	311	GLU	2
2	D	328	GLU	2
1	B	165	LYS	2
2	E	627	GLN	2
2	E	674	LEU	2
1	B	106	SER	2
1	A	3	GLU	1
1	B	30	ASP	1
2	E	638	GLN	1
2	E	712	GLU	1
1	A	30	ASP	1
1	A	43	GLN	1
1	A	71	TYR	1
1	A	126	ASP	1
2	E	632	GLN	1
2	E	649	ARG	1
2	E	668	ASP	1
2	E	693	HIS	1
1	A	56	LEU	1
1	B	41	ARG	1
2	D	285	GLU	1
2	D	288	LYS	1
2	E	592	GLU	1
1	A	19	LEU	1
1	A	22	GLN	1
1	A	123	ARG	1
1	B	131	GLN	1
2	D	262	GLU	1
2	D	287	SER	1
2	E	597	VAL	1

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Mol	Chain	Res	Type	Models (Total)
2	E	670	LEU	1
2	E	568	THR	1
1	A	23	LEU	1
1	A	55	ILE	1
1	A	156	PHE	1
1	B	26	ASN	1
1	B	126	ASP	1
2	E	642	SER	1
2	E	671	ARG	1
2	E	679	GLU	1
1	A	64	TYR	1
1	B	45	VAL	1
2	E	622	LEU	1
2	E	628	GLU	1
1	A	5	LYS	1
1	B	61	GLN	1
2	E	713	ASP	1
2	E	718	LEU	1
1	B	91	GLU	1
1	B	167	LYS	1
2	D	332	GLN	1
2	D	426	LYS	1
2	E	657	ASP	1
1	B	154	ASP	1
2	D	292	GLU	1
1	A	159	LEU	1
1	B	6	LEU	1
2	E	636	GLU	1
2	E	672	GLN	1
2	E	678	LEU	1
2	E	716	GLN	1
2	D	275	LEU	1
2	D	416	GLN	1
2	E	611	GLU	1
1	A	102	ARG	1
1	A	104	LYS	1
2	E	706	LYS	1
1	A	70	GLN	1
1	A	105	ASP	1
2	D	278	GLU	1
2	D	415	ARG	1
2	E	616	ARG	1

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Mol	Chain	Res	Type	Models (Total)
2	E	639	GLU	1
2	D	276	GLU	1
2	E	684	ASN	1
2	E	734	GLU	1
1	A	107	GLU	1
1	B	47	ASP	1
1	B	166	HIS	1
2	E	580	GLU	1
1	A	61	GLN	1
1	A	97	ARG	1
1	A	154	ASP	1
1	A	158	THR	1
2	D	389	LEU	1
2	E	697	THR	1
1	A	84	ILE	1
1	B	3	GLU	1
1	B	102	ARG	1
2	D	408	LYS	1
1	B	20	THR	1
1	B	158	THR	1
2	D	338	GLN	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

Of 164 ligands modelled in this entry, 2 are monoatomic - leaving 162 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
5	7Q9	E	823	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	525	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	542	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	847	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	830	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	D	533	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	E	852	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	837	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	543	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	216	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	549	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	841	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	524	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	859	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	528	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	815	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	A	219	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	D	520	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	A	204	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	544	-	38,38,38	0.80±0.00	0±0 (0±0%)
3	GSP	A	201	-	33,34,34	1.17±0.01	1±0 (3±0%)
5	7Q9	D	541	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	550	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	B	204	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	527	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	554	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	856	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	D	519	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	A	220	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	521	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	870	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	866	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	808	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	D	506	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	555	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	871	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	512	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	860	-	38,38,38	0.80±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
5	7Q9	E	822	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	813	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	515	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	207	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	834	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	877	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	840	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	817	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	B	209	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	211	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	838	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	802	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	553	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	513	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	A	217	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	540	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	538	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	811	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	210	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	873	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	B	208	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	547	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	218	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	209	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	872	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	548	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	D	511	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	A	213	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	804	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	861	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	818	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	D	508	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	833	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	212	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	857	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	556	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	531	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	874	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	507	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	805	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	510	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	865	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	832	-	38,38,38	0.81±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
5	7Q9	D	545	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	518	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	853	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	530	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	801	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	825	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	850	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	812	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	B	205	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	516	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	537	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	A	208	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	D	523	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	848	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	505	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	878	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	819	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	863	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	820	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	A	206	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	803	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	862	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	529	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	210	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	D	552	-	52,53,53	0.82±0.00	0±0 (0±0%)
6	17F	E	806	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	522	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	814	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	846	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	867	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	842	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	E	826	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	836	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	810	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	D	517	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	532	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	839	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	A	205	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	828	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	551	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	864	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	851	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	504	-	38,38,38	0.81±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
5	7Q9	D	509	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	534	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	845	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	809	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	514	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	A	203	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	849	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	829	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	B	206	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	526	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	503	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	876	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	807	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	539	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	824	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	835	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	546	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	502	-	38,38,38	0.81±0.00	0±0 (0±0%)
3	GSP	B	201	-	33,34,34	1.18±0.01	1±0 (3±1%)
5	7Q9	D	501	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	827	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	821	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	858	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	536	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	855	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	869	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	207	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	214	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	843	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	535	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	854	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	816	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	875	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	A	215	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	203	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	831	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	844	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	868	-	38,38,38	0.80±0.00	0±0 (0±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
5	7Q9	E	823	-	44,46,46	0.99±0.02	3±0 (7±1%)
5	7Q9	D	525	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	D	542	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	E	847	-	44,46,46	1.02±0.02	4±0 (8±1%)
5	7Q9	E	830	-	44,46,46	0.99±0.02	3±0 (7±0%)
6	17F	D	533	-	54,60,60	1.14±0.05	5±0 (8±0%)
5	7Q9	E	852	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	E	837	-	44,46,46	0.99±0.02	4±0 (8±1%)
5	7Q9	D	543	-	44,46,46	1.01±0.01	3±0 (7±0%)
5	7Q9	A	216	-	44,46,46	1.01±0.04	3±0 (7±1%)
5	7Q9	D	549	-	44,46,46	1.02±0.03	4±0 (8±1%)
5	7Q9	E	841	-	44,46,46	0.96±0.02	3±0 (6±0%)
5	7Q9	D	524	-	44,46,46	0.99±0.02	3±0 (7±0%)
5	7Q9	E	859	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	D	528	-	44,46,46	1.02±0.02	4±0 (9±0%)
5	7Q9	E	815	-	44,46,46	1.02±0.02	4±0 (7±1%)
6	17F	A	219	-	54,60,60	1.15±0.03	4±0 (8±0%)
6	17F	D	520	-	54,60,60	1.12±0.03	4±0 (7±0%)
5	7Q9	A	204	-	44,46,46	0.98±0.02	3±0 (6±0%)
5	7Q9	D	544	-	44,46,46	0.99±0.02	3±0 (6±0%)
3	GSP	A	201	-	47,54,54	1.73±0.03	12±1 (25±1%)
5	7Q9	D	541	-	44,46,46	1.01±0.02	3±0 (6±0%)
5	7Q9	D	550	-	44,46,46	1.02±0.01	3±0 (7±0%)
5	7Q9	B	204	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	D	527	-	44,46,46	1.00±0.01	3±0 (7±0%)
5	7Q9	D	554	-	44,46,46	1.00±0.03	3±0 (7±0%)
6	17F	E	856	-	54,60,60	1.10±0.02	4±0 (7±0%)
6	17F	D	519	-	54,60,60	1.11±0.03	4±0 (7±0%)
6	17F	A	220	-	54,60,60	1.12±0.02	4±0 (8±0%)
5	7Q9	D	521	-	44,46,46	0.99±0.02	3±0 (7±0%)
5	7Q9	E	870	-	44,46,46	1.01±0.02	4±0 (8±0%)
5	7Q9	E	866	-	44,46,46	1.00±0.02	3±0 (7±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
6	17F	E	808	-	54,60,60	1.09±0.02	4±0 (8±0%)
5	7Q9	D	506	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	D	555	-	44,46,46	1.01±0.01	3±0 (6±0%)
6	17F	E	871	-	54,60,60	1.13±0.03	4±0 (7±0%)
5	7Q9	D	512	-	44,46,46	1.01±0.01	3±0 (6±0%)
5	7Q9	E	860	-	44,46,46	1.01±0.02	3±0 (6±0%)
5	7Q9	E	822	-	44,46,46	1.05±0.02	4±0 (8±0%)
5	7Q9	E	813	-	44,46,46	1.06±0.02	4±0 (9±0%)
5	7Q9	D	515	-	44,46,46	1.02±0.02	3±0 (7±0%)
5	7Q9	A	207	-	44,46,46	1.02±0.02	3±0 (7±1%)
5	7Q9	E	834	-	44,46,46	1.00±0.02	4±1 (8±1%)
5	7Q9	E	877	-	44,46,46	1.00±0.02	3±0 (7±1%)
5	7Q9	E	840	-	44,46,46	0.99±0.01	3±0 (7±0%)
5	7Q9	E	817	-	44,46,46	0.96±0.03	3±0 (6±0%)
5	7Q9	B	209	-	44,46,46	1.00±0.02	3±0 (7±1%)
5	7Q9	A	211	-	44,46,46	1.00±0.02	3±0 (7±1%)
5	7Q9	E	838	-	44,46,46	1.02±0.03	4±0 (8±0%)
6	17F	E	802	-	54,60,60	1.13±0.03	4±0 (7±0%)
5	7Q9	D	553	-	44,46,46	1.02±0.01	4±0 (7±1%)
5	7Q9	D	513	-	44,46,46	1.00±0.02	3±0 (7±1%)
5	7Q9	A	217	-	44,46,46	1.00±0.02	3±0 (7±0%)
6	17F	D	540	-	54,60,60	1.13±0.03	4±0 (7±0%)
5	7Q9	D	538	-	44,46,46	0.99±0.01	3±0 (6±0%)
5	7Q9	E	811	-	44,46,46	1.02±0.02	3±0 (7±0%)
5	7Q9	A	210	-	44,46,46	1.02±0.02	4±0 (8±0%)
6	17F	E	873	-	54,60,60	1.17±0.03	4±0 (8±0%)
6	17F	B	208	-	54,60,60	1.08±0.03	4±0 (7±0%)
5	7Q9	D	547	-	44,46,46	0.99±0.01	3±0 (6±0%)
5	7Q9	A	218	-	44,46,46	1.00±0.03	3±0 (7±0%)
5	7Q9	A	209	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	E	872	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	D	548	-	44,46,46	1.02±0.01	4±0 (8±0%)
6	17F	D	511	-	54,60,60	1.10±0.03	4±0 (8±0%)
6	17F	A	213	-	54,60,60	1.13±0.06	4±1 (8±1%)
5	7Q9	E	804	-	44,46,46	0.99±0.02	3±0 (7±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
5	7Q9	E	861	-	44,46,46	1.02±0.02	3±0 (7±0%)
6	17F	E	818	-	54,60,60	1.10±0.03	4±0 (7±0%)
5	7Q9	D	508	-	44,46,46	1.01±0.01	3±0 (7±0%)
5	7Q9	E	833	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	A	212	-	44,46,46	1.00±0.03	3±0 (7±1%)
6	17F	E	857	-	54,60,60	1.16±0.04	4±0 (7±0%)
5	7Q9	D	556	-	44,46,46	1.00±0.02	4±0 (8±0%)
5	7Q9	D	531	-	44,46,46	0.98±0.02	3±0 (6±0%)
5	7Q9	E	874	-	44,46,46	0.99±0.03	3±0 (6±0%)
5	7Q9	D	507	-	44,46,46	0.99±0.01	3±0 (6±0%)
5	7Q9	E	805	-	44,46,46	1.02±0.01	4±0 (8±1%)
6	17F	D	510	-	54,60,60	1.07±0.07	4±1 (6±1%)
5	7Q9	E	865	-	44,46,46	1.00±0.01	3±0 (7±0%)
5	7Q9	E	832	-	44,46,46	1.00±0.01	4±0 (8±1%)
5	7Q9	D	545	-	44,46,46	0.98±0.02	3±0 (7±0%)
6	17F	D	518	-	54,60,60	1.16±0.03	5±0 (8±0%)
5	7Q9	E	853	-	44,46,46	1.03±0.02	4±0 (8±0%)
5	7Q9	D	530	-	44,46,46	0.98±0.01	3±0 (6±0%)
5	7Q9	E	801	-	44,46,46	1.01±0.01	3±0 (6±0%)
5	7Q9	E	825	-	44,46,46	0.97±0.02	3±0 (6±0%)
5	7Q9	E	850	-	44,46,46	1.00±0.01	3±0 (6±0%)
6	17F	E	812	-	54,60,60	1.08±0.04	4±0 (7±0%)
5	7Q9	B	205	-	44,46,46	1.00±0.02	3±0 (7±1%)
5	7Q9	D	516	-	44,46,46	0.96±0.04	3±0 (7±0%)
5	7Q9	D	537	-	44,46,46	1.01±0.03	4±0 (8±0%)
6	17F	A	208	-	54,60,60	1.09±0.03	4±0 (7±0%)
5	7Q9	D	523	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	E	848	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	D	505	-	44,46,46	1.01±0.03	3±0 (7±1%)
5	7Q9	E	878	-	44,46,46	1.02±0.01	3±0 (7±0%)
6	17F	E	819	-	54,60,60	1.06±0.02	4±0 (7±0%)
5	7Q9	E	863	-	44,46,46	0.99±0.02	3±0 (7±0%)
6	17F	E	820	-	54,60,60	1.07±0.03	4±0 (7±0%)
5	7Q9	A	206	-	44,46,46	1.00±0.01	3±0 (7±0%)
5	7Q9	E	803	-	44,46,46	1.02±0.01	3±1 (7±1%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
5	7Q9	E	862	-	44,46,46	1.00±0.02	4±0 (7±1%)
5	7Q9	D	529	-	44,46,46	1.02±0.01	3±0 (6±0%)
5	7Q9	B	210	-	44,46,46	0.99±0.02	3±0 (7±1%)
6	17F	D	552	-	54,60,60	1.13±0.02	5±0 (9±0%)
6	17F	E	806	-	54,60,60	1.12±0.03	4±0 (7±0%)
5	7Q9	D	522	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	814	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	E	846	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	867	-	44,46,46	0.99±0.03	3±0 (6±0%)
6	17F	E	842	-	54,60,60	1.10±0.03	4±0 (7±0%)
5	7Q9	E	826	-	44,46,46	1.00±0.01	3±0 (6±0%)
5	7Q9	E	836	-	44,46,46	0.97±0.02	3±0 (6±0%)
6	17F	E	810	-	54,60,60	1.18±0.03	5±0 (9±0%)
6	17F	D	517	-	54,60,60	1.07±0.03	4±0 (7±0%)
5	7Q9	D	532	-	44,46,46	1.10±0.02	4±0 (9±0%)
6	17F	E	839	-	54,60,60	1.13±0.04	5±0 (9±0%)
5	7Q9	A	205	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	E	828	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	D	551	-	44,46,46	1.01±0.02	4±0 (8±0%)
5	7Q9	E	864	-	44,46,46	1.03±0.02	4±0 (7±1%)
5	7Q9	E	851	-	44,46,46	1.01±0.01	4±0 (8±1%)
5	7Q9	D	504	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	D	509	-	44,46,46	1.02±0.04	4±0 (8±0%)
6	17F	D	534	-	54,60,60	1.12±0.03	5±0 (9±0%)
5	7Q9	E	845	-	44,46,46	1.01±0.01	3±0 (7±1%)
5	7Q9	E	809	-	44,46,46	0.97±0.02	3±0 (6±0%)
5	7Q9	D	514	-	44,46,46	0.99±0.03	3±0 (7±0%)
5	7Q9	A	203	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	E	849	-	44,46,46	1.00±0.01	3±0 (6±0%)
6	17F	E	829	-	54,60,60	1.10±0.02	4±0 (7±0%)
5	7Q9	B	206	-	44,46,46	1.00±0.01	3±0 (7±0%)
5	7Q9	D	526	-	44,46,46	1.04±0.02	4±0 (8±0%)
5	7Q9	D	503	-	44,46,46	1.02±0.03	3±1 (7±1%)
5	7Q9	E	876	-	44,46,46	0.99±0.01	3±0 (6±0%)
5	7Q9	E	807	-	44,46,46	1.05±0.02	4±0 (8±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
6	17F	D	539	-	54,60,60	1.10±0.03	4±0 (7±0%)
5	7Q9	E	824	-	44,46,46	1.02±0.02	3±0 (6±0%)
5	7Q9	E	835	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	D	546	-	44,46,46	1.01±0.02	4±0 (8±0%)
5	7Q9	D	502	-	44,46,46	1.00±0.02	4±0 (7±1%)
3	GSP	B	201	-	47,54,54	1.71±0.03	12±1 (24±1%)
5	7Q9	D	501	-	44,46,46	0.99±0.02	3±0 (7±0%)
5	7Q9	E	827	-	44,46,46	0.99±0.01	3±0 (6±0%)
5	7Q9	E	821	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	858	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	D	536	-	44,46,46	1.00±0.01	3±0 (6±0%)
5	7Q9	E	855	-	44,46,46	1.00±0.01	3±0 (6±0%)
5	7Q9	E	869	-	44,46,46	1.01±0.02	4±0 (7±1%)
5	7Q9	B	207	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	A	214	-	44,46,46	1.01±0.01	3±0 (6±0%)
5	7Q9	E	843	-	44,46,46	0.97±0.02	3±0 (7±1%)
5	7Q9	D	535	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	854	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	E	816	-	44,46,46	1.00±0.02	3±0 (7±0%)
6	17F	E	875	-	54,60,60	1.11±0.03	4±0 (8±0%)
5	7Q9	A	215	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	B	203	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	E	831	-	44,46,46	1.02±0.01	3±0 (6±0%)
5	7Q9	E	844	-	44,46,46	1.00±0.02	3±0 (7±1%)
5	7Q9	E	868	-	44,46,46	0.99±0.01	3±0 (6±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
5	7Q9	D	543	-	-	0±0,42,42,42	-
6	17F	E	856	-	-	0±0,59,59,59	-
5	7Q9	E	813	-	-	0±0,42,42,42	-
5	7Q9	E	837	-	-	0±0,42,42,42	-
6	17F	D	511	-	-	0±0,59,59,59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	17F	E	818	-	-	0±0,59,59,59	-
6	17F	D	520	-	-	0±0,59,59,59	-
5	7Q9	D	554	-	-	0±0,42,42,42	-
6	17F	E	812	-	-	0±0,59,59,59	-
5	7Q9	D	542	-	-	0±0,42,42,42	-
5	7Q9	D	525	-	-	0±0,42,42,42	-
5	7Q9	D	503	-	-	0±0,42,42,42	-
5	7Q9	D	502	-	-	0±0,42,42,42	-
5	7Q9	D	538	-	-	0±0,42,42,42	-
5	7Q9	D	546	-	-	0±0,42,42,42	-
5	7Q9	E	855	-	-	0±0,42,42,42	-
5	7Q9	A	214	-	-	0±0,42,42,42	-
3	GSP	B	201	-	-	0±0,21,38,38	0±0,3,3,3
6	17F	E	875	-	-	0±0,59,59,59	-
5	7Q9	D	515	-	-	0±0,42,42,42	-
6	17F	E	857	-	-	0±0,59,59,59	-
6	17F	B	208	-	-	0±0,59,59,59	-
5	7Q9	D	547	-	-	0±0,42,42,42	-
5	7Q9	D	529	-	-	0±0,42,42,42	-
5	7Q9	E	841	-	-	0±0,42,42,42	-
5	7Q9	E	809	-	-	0±0,42,42,42	-
5	7Q9	E	867	-	-	0±0,42,42,42	-
5	7Q9	E	849	-	-	0±0,42,42,42	-
5	7Q9	D	513	-	-	0±0,42,42,42	-
6	17F	D	552	-	-	0±0,59,59,59	-
5	7Q9	E	840	-	-	0±0,42,42,42	-
6	17F	A	213	-	-	0±0,59,59,59	-
5	7Q9	B	209	-	-	0±0,42,42,42	-
5	7Q9	E	801	-	-	0±0,42,42,42	-
6	17F	A	220	-	-	0±0,59,59,59	-
5	7Q9	E	858	-	-	0±0,42,42,42	-
5	7Q9	D	544	-	-	0±0,42,42,42	-
5	7Q9	D	553	-	-	0±0,42,42,42	-
5	7Q9	E	803	-	-	0±0,42,42,42	-
5	7Q9	D	509	-	-	0±0,42,42,42	-
5	7Q9	E	805	-	-	0±0,42,42,42	-
5	7Q9	E	807	-	-	0±0,42,42,42	-
5	7Q9	D	521	-	-	0±0,42,42,42	-
5	7Q9	E	865	-	-	0±0,42,42,42	-
5	7Q9	D	555	-	-	0±0,42,42,42	-
5	7Q9	E	821	-	-	0±0,42,42,42	-
5	7Q9	E	811	-	-	0±0,42,42,42	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	7Q9	A	216	-	-	0±0,42,42,42	-
5	7Q9	B	207	-	-	0±0,42,42,42	-
5	7Q9	D	541	-	-	0±0,42,42,42	-
6	17F	D	539	-	-	0±0,59,59,59	-
5	7Q9	D	505	-	-	0±0,42,42,42	-
5	7Q9	A	204	-	-	0±0,42,42,42	-
5	7Q9	E	825	-	-	0±0,42,42,42	-
5	7Q9	D	550	-	-	0±0,42,42,42	-
5	7Q9	E	872	-	-	0±0,42,42,42	-
5	7Q9	B	204	-	-	0±0,42,42,42	-
5	7Q9	E	843	-	-	0±0,42,42,42	-
5	7Q9	D	523	-	-	0±0,42,42,42	-
5	7Q9	D	522	-	-	0±0,42,42,42	-
5	7Q9	E	861	-	-	0±0,42,42,42	-
6	17F	E	829	-	-	0±0,59,59,59	-
5	7Q9	E	838	-	-	0±0,42,42,42	-
5	7Q9	B	206	-	-	0±0,42,42,42	-
5	7Q9	D	524	-	-	0±0,42,42,42	-
5	7Q9	E	844	-	-	0±0,42,42,42	-
6	17F	D	518	-	-	0±0,59,59,59	-
5	7Q9	E	833	-	-	0±0,42,42,42	-
5	7Q9	D	506	-	-	0±0,42,42,42	-
5	7Q9	A	217	-	-	0±0,42,42,42	-
5	7Q9	E	859	-	-	0±0,42,42,42	-
6	17F	E	871	-	-	0±0,59,59,59	-
3	GSP	A	201	-	-	0±0,21,38,38	0±0,3,3,3
5	7Q9	A	218	-	-	0±0,42,42,42	-
5	7Q9	D	528	-	-	0±0,42,42,42	-
6	17F	E	873	-	-	0±0,59,59,59	-
5	7Q9	E	832	-	-	0±0,42,42,42	-
5	7Q9	E	877	-	-	0±0,42,42,42	-
5	7Q9	D	527	-	-	0±0,42,42,42	-
5	7Q9	D	536	-	-	0±0,42,42,42	-
5	7Q9	E	827	-	-	0±0,42,42,42	-
5	7Q9	E	868	-	-	0±0,42,42,42	-
6	17F	E	808	-	-	0±0,59,59,59	-
5	7Q9	E	846	-	-	0±0,42,42,42	-
5	7Q9	E	870	-	-	0±0,42,42,42	-
5	7Q9	A	215	-	-	0±0,42,42,42	-
5	7Q9	D	526	-	-	0±0,42,42,42	-
5	7Q9	E	845	-	-	0±0,42,42,42	-
5	7Q9	E	866	-	-	0±0,42,42,42	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	7Q9	D	532	-	-	0±0,42,42,42	-
5	7Q9	E	822	-	-	0±0,42,42,42	-
5	7Q9	E	828	-	-	0±0,42,42,42	-
5	7Q9	A	211	-	-	0±0,42,42,42	-
6	17F	D	519	-	-	0±0,59,59,59	-
5	7Q9	E	830	-	-	0±0,42,42,42	-
5	7Q9	D	507	-	-	0±0,42,42,42	-
5	7Q9	A	212	-	-	0±0,42,42,42	-
5	7Q9	D	548	-	-	0±0,42,42,42	-
6	17F	D	534	-	-	0±0,59,59,59	-
5	7Q9	E	831	-	-	0±0,42,42,42	-
5	7Q9	E	854	-	-	0±0,42,42,42	-
6	17F	E	810	-	-	0±0,59,59,59	-
5	7Q9	A	209	-	-	0±0,42,42,42	-
5	7Q9	E	835	-	-	0±0,42,42,42	-
5	7Q9	E	804	-	-	0±0,42,42,42	-
5	7Q9	B	205	-	-	0±0,42,42,42	-
6	17F	E	819	-	-	0±0,59,59,59	-
5	7Q9	E	851	-	-	0±0,42,42,42	-
5	7Q9	D	556	-	-	0±0,42,42,42	-
5	7Q9	E	823	-	-	0±0,42,42,42	-
5	7Q9	E	852	-	-	0±0,42,42,42	-
5	7Q9	D	535	-	-	0±0,42,42,42	-
5	7Q9	D	514	-	-	0±0,42,42,42	-
6	17F	A	219	-	-	0±0,59,59,59	-
5	7Q9	E	853	-	-	0±0,42,42,42	-
5	7Q9	D	501	-	-	0±0,42,42,42	-
5	7Q9	A	206	-	-	0±0,42,42,42	-
5	7Q9	B	210	-	-	0±0,42,42,42	-
5	7Q9	E	864	-	-	0±0,42,42,42	-
5	7Q9	E	815	-	-	0±0,42,42,42	-
5	7Q9	D	530	-	-	0±0,42,42,42	-
5	7Q9	E	834	-	-	0±0,42,42,42	-
6	17F	E	820	-	-	0±0,59,59,59	-
5	7Q9	E	862	-	-	0±0,42,42,42	-
5	7Q9	E	817	-	-	0±0,42,42,42	-
5	7Q9	D	512	-	-	0±0,42,42,42	-
5	7Q9	D	504	-	-	0±0,42,42,42	-
5	7Q9	E	847	-	-	0±0,42,42,42	-
5	7Q9	E	850	-	-	0±0,42,42,42	-
5	7Q9	A	205	-	-	0±0,42,42,42	-
6	17F	D	533	-	-	0±0,59,59,59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	17F	D	540	-	-	0±0,59,59,59	-
5	7Q9	D	508	-	-	0±0,42,42,42	-
6	17F	D	517	-	-	0±0,59,59,59	-
6	17F	E	802	-	-	0±0,59,59,59	-
5	7Q9	D	549	-	-	0±0,42,42,42	-
5	7Q9	A	207	-	-	0±0,42,42,42	-
5	7Q9	E	863	-	-	0±0,42,42,42	-
5	7Q9	E	814	-	-	0±0,42,42,42	-
5	7Q9	E	860	-	-	0±0,42,42,42	-
5	7Q9	D	545	-	-	0±0,42,42,42	-
5	7Q9	E	876	-	-	0±0,42,42,42	-
5	7Q9	D	551	-	-	0±0,42,42,42	-
5	7Q9	E	878	-	-	0±0,42,42,42	-
5	7Q9	D	516	-	-	0±0,42,42,42	-
5	7Q9	E	874	-	-	0±0,42,42,42	-
6	17F	E	842	-	-	0±0,59,59,59	-
5	7Q9	A	210	-	-	0±0,42,42,42	-
6	17F	A	208	-	-	0±0,59,59,59	-
5	7Q9	E	824	-	-	0±0,42,42,42	-
5	7Q9	E	848	-	-	0±0,42,42,42	-
6	17F	E	839	-	-	0±0,59,59,59	-
5	7Q9	E	826	-	-	0±0,42,42,42	-
5	7Q9	D	531	-	-	0±0,42,42,42	-
5	7Q9	E	869	-	-	0±0,42,42,42	-
5	7Q9	D	537	-	-	0±0,42,42,42	-
5	7Q9	B	203	-	-	0±0,42,42,42	-
6	17F	E	806	-	-	0±0,59,59,59	-
6	17F	D	510	-	-	0±0,59,59,59	-
5	7Q9	E	836	-	-	0±0,42,42,42	-
5	7Q9	E	816	-	-	0±0,42,42,42	-
5	7Q9	A	203	-	-	0±0,42,42,42	-

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
3	A	201	GSP	C5-N7	3.00	1.33	1.39	15	20
3	B	201	GSP	C5-N7	3.00	1.33	1.39	14	20
3	B	201	GSP	PA-O3A	2.04	1.61	1.59	16	2
3	B	201	GSP	PB-O3B	2.01	1.61	1.59	20	1
3	A	201	GSP	C4-N9	2.01	1.32	1.38	11	1
3	A	201	GSP	PA-O3A	2.01	1.61	1.59	15	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
3	A	201	GSP	C2-N3-C4	5.31	121.44	112.30	14	20
3	B	201	GSP	C2-N3-C4	5.28	121.40	112.30	9	20
6	E	839	17F	O3-C1-C2	5.25	112.64	108.06	2	20
6	E	806	17F	O3-C1-C2	5.19	112.58	108.06	10	20
3	A	201	GSP	C5-C4-N3	4.96	120.49	128.39	11	20
3	B	201	GSP	C5-C4-N3	4.93	120.55	128.39	7	20
6	E	857	17F	O3-C1-C2	4.74	112.19	108.06	9	20
6	E	810	17F	O3-C1-C2	4.63	112.10	108.06	19	20
6	D	510	17F	O3-C1-C2	4.52	112.00	108.06	9	20
6	D	552	17F	O3-C1-C2	4.51	111.99	108.06	19	20
6	D	533	17F	O3-C1-C2	4.50	111.98	108.06	1	20
6	E	812	17F	O3-C1-C2	4.45	111.94	108.06	8	20
6	B	208	17F	O3-C1-C2	4.45	111.94	108.06	7	20
6	E	871	17F	O3-C1-C2	4.43	111.92	108.06	15	20
6	D	510	17F	O9-C17-C18	4.43	121.06	111.48	15	20
6	E	818	17F	O3-C1-C2	4.42	111.92	108.06	10	20
6	E	875	17F	O3-C1-C2	4.42	111.91	108.06	18	20
6	E	873	17F	O3-C1-C2	4.35	111.85	108.06	16	20
6	D	539	17F	O3-C1-C2	4.28	111.79	108.06	16	20
6	D	534	17F	O3-C1-C2	4.26	111.77	108.06	18	20
6	D	533	17F	O9-C17-C18	4.26	120.69	111.48	19	20
6	A	208	17F	O3-C1-C2	4.26	111.77	108.06	16	20
6	D	518	17F	O3-C1-C2	4.25	111.76	108.06	13	20
3	B	201	GSP	C4'-O4'-C1'	4.24	100.11	109.47	10	2
6	E	842	17F	O3-C1-C2	4.23	111.75	108.06	13	20
6	D	511	17F	O3-C1-C2	4.22	111.74	108.06	7	20
6	A	213	17F	O9-C17-C18	4.21	120.59	111.48	19	20
6	D	517	17F	O3-C1-C2	4.21	111.73	108.06	11	20
6	E	819	17F	O3-C1-C2	4.19	111.71	108.06	20	20
6	E	802	17F	O9-C17-C18	4.16	120.49	111.48	4	20
6	A	219	17F	O3-C1-C2	4.16	111.68	108.06	5	20
6	D	540	17F	O9-C17-C18	4.13	120.41	111.48	12	20
6	A	219	17F	O9-C17-C18	4.12	120.39	111.48	11	20
6	D	520	17F	O3-C1-C2	4.09	111.63	108.06	14	20
5	D	532	7Q9	C2-O21-C21	4.06	108.07	117.80	15	20
6	A	220	17F	O3-C1-C2	4.06	111.59	108.06	6	20
6	E	873	17F	O9-C17-C18	4.05	120.25	111.48	20	20
3	A	201	GSP	C4'-O4'-C1'	4.03	100.57	109.47	6	3
6	E	802	17F	C5-O9-C17	4.03	108.15	117.80	4	20
6	E	829	17F	O3-C1-C2	4.03	111.57	108.06	19	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
6	D	520	17F	O9-C17-C18	4.02	120.17	111.48	18	20
6	E	873	17F	C5-O9-C17	4.01	108.19	117.80	10	20
5	E	864	7Q9	C2-O21-C21	4.01	108.21	117.80	19	20
6	D	520	17F	C5-O9-C17	4.01	108.20	117.80	18	20
6	A	213	17F	O3-C1-C2	4.00	111.54	108.06	2	20
6	E	820	17F	O3-C1-C2	3.99	111.54	108.06	12	20
6	E	857	17F	O9-C17-C18	3.99	120.11	111.48	13	20
6	E	806	17F	O9-C17-C18	3.99	120.11	111.48	1	20
6	D	518	17F	O9-C17-C18	3.97	120.06	111.48	16	20
6	D	540	17F	C5-O9-C17	3.96	108.32	117.80	11	20
6	E	810	17F	O9-C17-C18	3.95	120.03	111.48	4	20
6	D	539	17F	O9-C17-C18	3.94	120.00	111.48	17	20
3	A	201	GSP	PB-O3B-PG	3.93	118.78	133.17	7	20
6	E	802	17F	O3-C1-C2	3.93	111.49	108.06	6	20
6	D	519	17F	O9-C17-C18	3.93	119.98	111.48	5	20
6	D	517	17F	O9-C17-C18	3.91	119.94	111.48	12	20
6	E	857	17F	C5-O9-C17	3.90	108.47	117.80	13	20
6	E	871	17F	O9-C17-C18	3.87	119.84	111.48	9	20
6	D	534	17F	O9-C17-C18	3.86	119.82	111.48	11	20
6	D	539	17F	C5-O9-C17	3.83	108.62	117.80	17	20
6	D	519	17F	C5-O9-C17	3.82	108.65	117.80	4	20
6	A	220	17F	O9-C17-C18	3.82	119.75	111.48	17	20
5	E	852	7Q9	C2-O21-C21	3.81	108.67	117.80	3	20
5	A	210	7Q9	C2-O21-C21	3.80	108.71	117.80	14	20
6	E	806	17F	C5-O9-C17	3.80	108.71	117.80	1	20
6	E	808	17F	O3-C1-C2	3.79	111.37	108.06	10	20
6	E	808	17F	O9-C17-C18	3.80	119.69	111.48	8	20
5	E	801	7Q9	C2-O21-C21	3.79	108.73	117.80	5	20
6	A	208	17F	O9-C17-C18	3.79	119.67	111.48	15	20
6	E	842	17F	O9-C17-C18	3.78	119.67	111.48	1	20
6	D	519	17F	O3-C1-C2	3.78	111.36	108.06	19	20
5	D	523	7Q9	C2-O21-C21	3.78	108.75	117.80	15	20
5	A	218	7Q9	C2-O21-C21	3.77	108.76	117.80	16	20
6	D	510	17F	C5-O9-C17	3.77	108.77	117.80	17	11
5	E	811	7Q9	C2-O21-C21	3.77	108.78	117.80	7	20
6	E	875	17F	O9-C17-C18	3.76	119.62	111.48	13	20
6	E	839	17F	O9-C17-C18	3.76	119.61	111.48	20	20
6	A	219	17F	C5-O9-C17	3.76	108.80	117.80	12	20
6	E	856	17F	O3-C1-C2	3.75	111.33	108.06	3	20
5	B	204	7Q9	C2-O21-C21	3.75	108.81	117.80	11	20
6	E	856	17F	O9-C17-C18	3.75	119.60	111.48	8	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
5	A	207	7Q9	C2-O21-C21	3.75	108.82	117.80	15	20
5	D	506	7Q9	C2-O21-C21	3.75	108.83	117.80	19	20
6	D	552	17F	O9-C17-C18	3.74	119.56	111.48	17	20
6	E	829	17F	O9-C17-C18	3.73	119.56	111.48	16	20
6	B	208	17F	O9-C17-C18	3.73	119.55	111.48	9	20
5	E	822	7Q9	C2-O21-C21	3.72	108.90	117.80	11	20
6	A	213	17F	C5-O9-C17	3.71	108.91	117.80	14	19
5	A	214	7Q9	C2-O21-C21	3.71	108.92	117.80	17	20
5	E	855	7Q9	C2-O21-C21	3.71	108.93	117.80	9	20
6	D	511	17F	O9-C17-C18	3.71	119.50	111.48	20	20
5	E	807	7Q9	C2-O21-C21	3.70	108.93	117.80	20	20
6	E	818	17F	O9-C17-C18	3.70	119.48	111.48	5	20
5	E	874	7Q9	C2-O21-C21	3.69	108.97	117.80	3	20
6	D	518	17F	C5-O9-C17	3.69	108.97	117.80	2	20
6	D	533	17F	C5-O9-C17	3.68	108.98	117.80	20	20
5	D	550	7Q9	C2-O21-C21	3.67	109.00	117.80	2	20
5	E	877	7Q9	C2-O21-C21	3.67	109.00	117.80	6	20
6	E	820	17F	O9-C17-C18	3.67	119.43	111.48	5	20
5	B	206	7Q9	C2-O21-C21	3.66	109.03	117.80	16	20
5	E	865	7Q9	C2-O21-C21	3.66	109.03	117.80	4	20
5	D	529	7Q9	C2-O21-C21	3.66	109.04	117.80	15	20
5	E	859	7Q9	C2-O21-C21	3.66	109.04	117.80	14	20
5	A	205	7Q9	C2-O21-C21	3.66	109.04	117.80	8	20
5	B	203	7Q9	C2-O21-C21	3.66	109.05	117.80	3	20
6	E	812	17F	O9-C17-C18	3.65	119.38	111.48	6	20
6	E	810	17F	C5-O9-C17	3.65	109.06	117.80	4	20
5	E	866	7Q9	C2-O21-C21	3.64	109.08	117.80	10	20
5	E	869	7Q9	C2-O21-C21	3.64	109.09	117.80	4	20
6	D	540	17F	O3-C1-C2	3.64	111.23	108.06	3	20
5	D	507	7Q9	C2-O21-C21	3.63	109.10	117.80	18	20
5	A	209	7Q9	C2-O21-C21	3.63	109.11	117.80	18	20
5	D	508	7Q9	C2-O21-C21	3.63	109.11	117.80	14	20
5	D	514	7Q9	C2-O21-C21	3.63	109.11	117.80	11	20
5	D	525	7Q9	C2-O21-C21	3.63	109.11	117.80	6	20
5	A	216	7Q9	C2-O21-C21	3.63	109.12	117.80	18	20
5	E	831	7Q9	C2-O21-C21	3.62	109.12	117.80	16	20
5	A	215	7Q9	C2-O21-C21	3.62	109.13	117.80	12	20
5	D	536	7Q9	C2-O21-C21	3.62	109.13	117.80	6	20
5	E	844	7Q9	C2-O21-C21	3.62	109.13	117.80	16	20
5	E	835	7Q9	C2-O21-C21	3.61	109.15	117.80	20	20
5	E	805	7Q9	C2-O21-C21	3.60	109.18	117.80	12	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
6	A	220	17F	C5-O9-C17	3.60	109.18	117.80	8	20
5	E	848	7Q9	C2-O21-C21	3.60	109.19	117.80	5	20
5	D	543	7Q9	C2-O21-C21	3.60	109.19	117.80	12	20
5	E	861	7Q9	C2-O21-C21	3.59	109.19	117.80	11	20
5	D	512	7Q9	C2-O21-C21	3.59	109.20	117.80	17	20
5	D	501	7Q9	C2-O21-C21	3.59	109.21	117.80	6	20
5	D	524	7Q9	C2-O21-C21	3.59	109.21	117.80	20	20
5	E	828	7Q9	C2-O21-C21	3.59	109.21	117.80	19	20
5	D	551	7Q9	C2-O21-C21	3.59	109.22	117.80	5	20
6	E	871	17F	C5-O9-C17	3.58	109.22	117.80	9	20
6	A	208	17F	C5-O9-C17	3.58	109.23	117.80	1	20
5	E	860	7Q9	C2-O21-C21	3.58	109.23	117.80	5	20
5	D	555	7Q9	C2-O21-C21	3.58	109.24	117.80	8	20
5	D	553	7Q9	C2-O21-C21	3.57	109.24	117.80	19	20
5	E	833	7Q9	C2-O21-C21	3.57	109.25	117.80	9	20
5	D	515	7Q9	C2-O21-C21	3.57	109.25	117.80	8	20
5	E	821	7Q9	C2-O21-C21	3.57	109.26	117.80	1	20
5	D	538	7Q9	C2-O21-C21	3.56	109.27	117.80	19	20
5	E	845	7Q9	C2-O21-C21	3.55	109.29	117.80	5	20
5	A	206	7Q9	C2-O21-C21	3.55	109.29	117.80	4	20
5	E	850	7Q9	C2-O21-C21	3.55	109.30	117.80	20	20
5	E	824	7Q9	C2-O21-C21	3.54	109.31	117.80	12	20
5	E	862	7Q9	C2-O21-C21	3.54	109.32	117.80	13	20
5	D	513	7Q9	C2-O21-C21	3.54	109.32	117.80	13	20
5	E	827	7Q9	C2-O21-C21	3.54	109.32	117.80	20	20
5	D	541	7Q9	C2-O21-C21	3.54	109.33	117.80	1	20
5	D	556	7Q9	C2-O21-C21	3.54	109.33	117.80	16	20
5	E	870	7Q9	C2-O21-C21	3.53	109.34	117.80	15	20
5	D	549	7Q9	C2-O21-C21	3.53	109.34	117.80	4	20
5	E	854	7Q9	C2-O21-C21	3.53	109.35	117.80	6	20
6	D	552	17F	C5-O9-C17	3.53	109.35	117.80	15	20
5	B	207	7Q9	C2-O21-C21	3.53	109.36	117.80	11	20
5	E	878	7Q9	C2-O21-C21	3.52	109.36	117.80	20	20
5	A	211	7Q9	C2-O21-C21	3.52	109.37	117.80	5	20
5	B	209	7Q9	C2-O21-C21	3.52	109.37	117.80	10	20
5	E	838	7Q9	C2-O21-C21	3.52	109.38	117.80	1	20
5	D	554	7Q9	C2-O21-C21	3.51	109.40	117.80	6	20
5	D	504	7Q9	C2-O21-C21	3.51	109.40	117.80	3	20
5	E	814	7Q9	C2-O21-C21	3.51	109.40	117.80	10	20
5	E	840	7Q9	C2-O21-C21	3.51	109.40	117.80	5	20
5	D	505	7Q9	C2-O21-C21	3.50	109.42	117.80	5	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
5	D	509	7Q9	C2-O21-C21	3.50	109.42	117.80	10	20
5	E	803	7Q9	C2-O21-C21	3.50	109.42	117.80	19	20
5	D	544	7Q9	C2-O21-C21	3.50	109.43	117.80	18	20
5	E	809	7Q9	C2-O21-C21	3.50	109.43	117.80	16	20
5	D	503	7Q9	C2-O21-C21	3.49	109.43	117.80	12	20
5	D	542	7Q9	C2-O21-C21	3.49	109.44	117.80	5	20
5	E	853	7Q9	C2-O21-C21	3.49	109.44	117.80	1	20
5	A	217	7Q9	C2-O21-C21	3.49	109.45	117.80	12	20
5	D	522	7Q9	C2-O21-C21	3.49	109.45	117.80	6	20
5	D	537	7Q9	C2-O21-C21	3.49	109.45	117.80	1	20
5	E	832	7Q9	C2-O21-C21	3.49	109.45	117.80	18	20
5	E	851	7Q9	C2-O21-C21	3.48	109.46	117.80	2	20
5	E	858	7Q9	C2-O21-C21	3.48	109.47	117.80	3	20
3	B	201	GSP	PB-O3B-PG	3.47	120.45	133.17	16	20
5	E	847	7Q9	C2-O21-C21	3.47	109.49	117.80	12	20
5	E	825	7Q9	C2-O21-C21	3.46	109.50	117.80	3	20
5	D	535	7Q9	C2-O21-C21	3.46	109.52	117.80	18	20
5	E	815	7Q9	C2-O21-C21	3.46	109.53	117.80	14	20
5	E	876	7Q9	C2-O21-C21	3.45	109.53	117.80	2	20
5	D	527	7Q9	C2-O21-C21	3.45	109.54	117.80	11	20
5	E	816	7Q9	C2-O21-C21	3.45	109.54	117.80	1	20
5	E	846	7Q9	C2-O21-C21	3.45	109.54	117.80	2	20
5	D	530	7Q9	C2-O21-C21	3.43	109.59	117.80	9	20
5	E	863	7Q9	C2-O21-C21	3.43	109.59	117.80	3	20
5	E	836	7Q9	C2-O21-C21	3.42	109.60	117.80	11	20
5	E	867	7Q9	C2-O21-C21	3.42	109.60	117.80	6	20
5	E	813	7Q9	C2-O21-C21	3.42	109.61	117.80	8	20
5	D	502	7Q9	C2-O21-C21	3.41	109.62	117.80	6	20
6	E	819	17F	O9-C17-C18	3.42	118.87	111.48	18	20
5	D	531	7Q9	C2-O21-C21	3.41	109.63	117.80	8	20
5	E	826	7Q9	C2-O21-C21	3.40	109.65	117.80	16	20
5	D	516	7Q9	C2-O21-C21	3.40	109.66	117.80	4	20
6	E	842	17F	C5-O9-C17	3.39	109.67	117.80	2	20
5	E	872	7Q9	C2-O21-C21	3.39	109.69	117.80	11	20
6	E	808	17F	C5-O9-C17	3.38	109.70	117.80	11	20
5	A	203	7Q9	C2-O21-C21	3.38	109.70	117.80	2	20
5	D	528	7Q9	C2-O21-C21	3.37	109.72	117.80	12	20
5	D	547	7Q9	C2-O21-C21	3.37	109.72	117.80	8	20
5	B	205	7Q9	C2-O21-C21	3.37	109.73	117.80	7	20
5	E	868	7Q9	C2-O21-C21	3.37	109.73	117.80	17	20
5	E	837	7Q9	C2-O21-C21	3.37	109.73	117.80	2	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
5	E	841	7Q9	C2-O21-C21	3.37	109.73	117.80	5	20
6	E	856	17F	C5-O9-C17	3.37	109.73	117.80	7	20
5	E	849	7Q9	C2-O21-C21	3.36	109.75	117.80	12	20
6	E	818	17F	C5-O9-C17	3.36	109.76	117.80	4	20
3	A	201	GSP	C2-N1-C6	3.35	119.03	125.11	16	20
5	D	545	7Q9	C2-O21-C21	3.35	109.77	117.80	4	20
5	D	548	7Q9	C2-O21-C21	3.35	109.77	117.80	9	20
5	E	834	7Q9	C2-O21-C21	3.35	109.78	117.80	20	20
5	A	204	7Q9	C2-O21-C21	3.35	109.78	117.80	6	20
5	A	212	7Q9	C2-O21-C21	3.35	109.78	117.80	5	20
6	B	208	17F	C5-O9-C17	3.35	109.79	117.80	10	20
6	D	517	17F	C5-O9-C17	3.35	109.78	117.80	7	20
5	B	210	7Q9	C2-O21-C21	3.34	109.80	117.80	19	20
5	E	804	7Q9	C2-O21-C21	3.34	109.80	117.80	3	20
3	B	201	GSP	C2-N1-C6	3.34	119.05	125.11	9	20
5	E	817	7Q9	C2-O21-C21	3.34	109.81	117.80	15	20
6	D	534	17F	C5-O9-C17	3.34	109.81	117.80	11	20
5	D	526	7Q9	C2-O21-C21	3.31	109.88	117.80	5	20
5	D	521	7Q9	C2-O21-C21	3.31	109.88	117.80	12	20
5	D	546	7Q9	C2-O21-C21	3.31	109.89	117.80	11	20
6	D	511	17F	C5-O9-C17	3.30	109.90	117.80	17	20
5	E	823	7Q9	C2-O21-C21	3.29	109.92	117.80	10	20
5	E	843	7Q9	C2-O21-C21	3.27	109.97	117.80	18	20
3	A	201	GSP	N9-C4-N3	3.26	132.47	125.95	14	20
3	B	201	GSP	N9-C4-N3	3.24	132.44	125.95	9	20
6	E	812	17F	C5-O9-C17	3.23	110.06	117.80	3	20
6	E	820	17F	C5-O9-C17	3.21	110.10	117.80	5	20
6	E	829	17F	C5-O9-C17	3.20	110.13	117.80	6	20
5	E	830	7Q9	C2-O21-C21	3.18	110.19	117.80	20	20
6	E	875	17F	C5-O9-C17	3.17	110.20	117.80	14	20
5	D	532	7Q9	O31-C31-C32	3.06	121.17	111.83	10	20
6	E	839	17F	C5-O9-C17	3.05	110.50	117.80	20	20
3	B	201	GSP	O4'-C1'-N9	3.00	115.16	108.36	16	17
6	E	810	17F	O7-C7-C8	3.00	120.97	111.83	1	20
6	E	819	17F	C5-O9-C17	2.96	110.70	117.80	18	20
6	A	213	17F	O7-C7-C8	2.96	120.86	111.83	14	20
6	D	510	17F	O7-C7-C8	2.92	120.75	111.83	10	20
5	E	813	7Q9	O31-C31-C32	2.89	120.65	111.83	19	20
6	E	839	17F	O7-C7-C8	2.89	120.65	111.83	10	20
6	D	518	17F	O7-C7-C8	2.87	120.57	111.83	9	20
5	E	817	7Q9	O31-C31-C32	2.86	120.54	111.83	12	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
5	D	503	7Q9	O31-C31-C32	2.85	120.53	111.83	10	20
5	D	509	7Q9	O31-C31-C32	2.84	120.48	111.83	10	20
5	D	526	7Q9	O31-C31-C32	2.82	120.42	111.83	4	20
5	E	822	7Q9	O31-C31-C32	2.81	120.41	111.83	10	20
5	E	860	7Q9	O31-C31-C32	2.81	120.40	111.83	3	20
5	A	212	7Q9	O31-C31-C32	2.81	120.39	111.83	20	20
5	A	216	7Q9	O31-C31-C32	2.80	120.38	111.83	7	20
5	E	838	7Q9	O31-C31-C32	2.80	120.36	111.83	6	20
5	D	537	7Q9	O31-C31-C32	2.79	120.35	111.83	16	20
5	D	549	7Q9	O31-C31-C32	2.78	120.30	111.83	12	20
5	E	821	7Q9	O31-C31-C32	2.77	120.28	111.83	18	20
5	E	807	7Q9	O31-C31-C32	2.77	120.27	111.83	7	20
5	D	548	7Q9	O31-C31-C32	2.76	120.26	111.83	20	20
5	E	864	7Q9	O31-C31-C32	2.76	120.26	111.83	6	20
3	A	201	GSP	O4'-C1'-N9	2.76	114.62	108.36	6	19
6	E	812	17F	O7-C7-C8	2.76	120.25	111.83	3	20
5	D	528	7Q9	O31-C31-C32	2.75	120.22	111.83	17	20
5	A	210	7Q9	O31-C31-C32	2.74	120.19	111.83	2	20
5	A	218	7Q9	O31-C31-C32	2.74	120.19	111.83	7	20
6	A	219	17F	O7-C7-C8	2.73	120.17	111.83	2	20
5	E	851	7Q9	O31-C31-C32	2.72	120.13	111.83	15	20
5	E	847	7Q9	O31-C31-C32	2.72	120.12	111.83	15	20
5	D	505	7Q9	O31-C31-C32	2.71	120.11	111.83	18	20
5	E	816	7Q9	O31-C31-C32	2.71	120.10	111.83	12	20
5	E	844	7Q9	O31-C31-C32	2.71	120.09	111.83	17	20
5	E	837	7Q9	O31-C31-C32	2.71	120.09	111.83	6	20
5	E	870	7Q9	O31-C31-C32	2.71	120.08	111.83	5	20
6	D	534	17F	O7-C7-C8	2.71	120.09	111.83	5	20
5	D	501	7Q9	O31-C31-C32	2.70	120.07	111.83	5	20
6	E	873	17F	O7-C7-C8	2.70	120.07	111.83	5	20
5	D	546	7Q9	O31-C31-C32	2.70	120.07	111.83	17	20
6	E	857	17F	O7-C7-C8	2.70	120.06	111.83	1	20
5	D	525	7Q9	O31-C31-C32	2.70	120.06	111.83	20	20
5	A	217	7Q9	O31-C31-C32	2.69	120.05	111.83	19	20
5	E	846	7Q9	O31-C31-C32	2.69	120.04	111.83	3	20
6	D	552	17F	O7-C7-C8	2.69	120.04	111.83	1	20
5	E	811	7Q9	O31-C31-C32	2.68	120.01	111.83	4	20
5	E	801	7Q9	O31-C31-C32	2.68	120.01	111.83	2	20
5	E	815	7Q9	O31-C31-C32	2.68	119.99	111.83	6	20
5	E	853	7Q9	O31-C31-C32	2.67	119.98	111.83	1	20
6	D	511	17F	O7-C7-C8	2.67	119.99	111.83	18	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
5	D	553	7Q9	O31-C31-C32	2.67	119.98	111.83	10	20
6	A	213	17F	C6-O7-C7	2.67	107.37	117.12	9	10
6	A	220	17F	O7-C7-C8	2.67	119.97	111.83	16	20
5	D	524	7Q9	O31-C31-C32	2.66	119.96	111.83	6	20
5	E	845	7Q9	O31-C31-C32	2.66	119.95	111.83	6	20
5	D	527	7Q9	O31-C31-C32	2.66	119.93	111.83	10	20
5	A	214	7Q9	O31-C31-C32	2.65	119.92	111.83	1	20
5	E	834	7Q9	O31-C31-C32	2.65	119.92	111.83	5	20
6	E	808	17F	O7-C7-C8	2.65	119.92	111.83	2	20
5	A	206	7Q9	O31-C31-C32	2.65	119.91	111.83	11	20
6	E	802	17F	O7-C7-C8	2.65	119.91	111.83	14	20
5	B	205	7Q9	O31-C31-C32	2.65	119.91	111.83	1	20
5	D	544	7Q9	O31-C31-C32	2.65	119.90	111.83	4	20
5	D	554	7Q9	O31-C31-C32	2.64	119.90	111.83	14	20
5	E	828	7Q9	O31-C31-C32	2.64	119.90	111.83	2	20
5	D	551	7Q9	O31-C31-C32	2.64	119.89	111.83	14	20
5	A	211	7Q9	O31-C31-C32	2.64	119.88	111.83	15	20
5	B	209	7Q9	O31-C31-C32	2.64	119.87	111.83	15	20
5	D	513	7Q9	O31-C31-C32	2.64	119.88	111.83	9	20
6	A	208	17F	O7-C7-C8	2.63	119.87	111.83	9	20
5	D	532	7Q9	C3-O31-C31	2.63	107.50	117.12	10	20
5	E	843	7Q9	O31-C31-C32	2.63	119.86	111.83	1	20
5	E	878	7Q9	O31-C31-C32	2.63	119.86	111.83	11	20
6	E	875	17F	O7-C7-C8	2.63	119.85	111.83	6	20
6	D	540	17F	O7-C7-C8	2.62	119.84	111.83	4	20
5	E	854	7Q9	O31-C31-C32	2.62	119.83	111.83	3	20
5	E	863	7Q9	O31-C31-C32	2.62	119.83	111.83	17	20
5	E	840	7Q9	O31-C31-C32	2.62	119.82	111.83	4	20
5	D	514	7Q9	O31-C31-C32	2.62	119.82	111.83	20	20
5	D	530	7Q9	O31-C31-C32	2.61	119.80	111.83	19	20
5	A	205	7Q9	O31-C31-C32	2.61	119.80	111.83	19	20
5	D	535	7Q9	O31-C31-C32	2.61	119.80	111.83	9	20
5	D	545	7Q9	O31-C31-C32	2.61	119.80	111.83	20	20
5	E	824	7Q9	O31-C31-C32	2.61	119.80	111.83	2	20
5	E	835	7Q9	O31-C31-C32	2.61	119.79	111.83	8	20
5	E	869	7Q9	O31-C31-C32	2.61	119.79	111.83	17	20
5	E	823	7Q9	O31-C31-C32	2.61	119.78	111.83	15	20
5	E	848	7Q9	O31-C31-C32	2.61	119.79	111.83	7	20
5	D	522	7Q9	O31-C31-C32	2.61	119.78	111.83	3	20
5	E	862	7Q9	O31-C31-C32	2.61	119.78	111.83	12	20
5	D	543	7Q9	O31-C31-C32	2.61	119.78	111.83	16	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
6	D	519	17F	O7-C7-C8	2.60	119.77	111.83	14	20
5	D	506	7Q9	O31-C31-C32	2.60	119.76	111.83	6	20
5	E	805	7Q9	O31-C31-C32	2.60	119.76	111.83	13	20
5	E	832	7Q9	O31-C31-C32	2.60	119.76	111.83	7	20
5	D	536	7Q9	O31-C31-C32	2.60	119.75	111.83	11	20
5	E	849	7Q9	O31-C31-C32	2.60	119.75	111.83	20	20
5	E	868	7Q9	O31-C31-C32	2.60	119.75	111.83	9	20
5	B	204	7Q9	O31-C31-C32	2.59	119.74	111.83	1	20
5	D	515	7Q9	O31-C31-C32	2.59	119.74	111.83	18	20
5	D	556	7Q9	O31-C31-C32	2.59	119.74	111.83	12	20
5	D	516	7Q9	O31-C31-C32	2.59	119.74	111.83	10	20
5	E	826	7Q9	O31-C31-C32	2.59	119.74	111.83	10	20
5	E	861	7Q9	O31-C31-C32	2.59	119.74	111.83	14	20
5	A	203	7Q9	O31-C31-C32	2.59	119.72	111.83	20	20
5	D	504	7Q9	O31-C31-C32	2.59	119.73	111.83	2	20
5	B	207	7Q9	O31-C31-C32	2.59	119.72	111.83	16	20
5	E	833	7Q9	O31-C31-C32	2.58	119.71	111.83	14	20
5	E	865	7Q9	O31-C31-C32	2.58	119.71	111.83	9	20
6	B	208	17F	O7-C7-C8	2.58	119.71	111.83	2	20
5	E	874	7Q9	O31-C31-C32	2.58	119.70	111.83	20	20
6	D	533	17F	O7-C7-C8	2.58	119.71	111.83	14	20
5	A	215	7Q9	O31-C31-C32	2.58	119.70	111.83	16	20
5	D	523	7Q9	O31-C31-C32	2.58	119.70	111.83	3	20
5	D	555	7Q9	O31-C31-C32	2.58	119.70	111.83	9	20
6	D	520	17F	O7-C7-C8	2.57	119.68	111.83	2	20
5	B	206	7Q9	O31-C31-C32	2.57	119.67	111.83	11	20
5	A	216	7Q9	C3-O31-C31	2.57	107.74	117.12	6	6
6	E	819	17F	O7-C7-C8	2.57	119.66	111.83	15	20
5	E	877	7Q9	O31-C31-C32	2.56	119.65	111.83	13	20
6	E	818	17F	O7-C7-C8	2.56	119.65	111.83	15	20
6	E	829	17F	O7-C7-C8	2.56	119.65	111.83	1	20
5	A	207	7Q9	O31-C31-C32	2.56	119.64	111.83	3	20
5	D	502	7Q9	O31-C31-C32	2.56	119.64	111.83	11	20
5	E	872	7Q9	O31-C31-C32	2.56	119.64	111.83	14	20
5	E	841	7Q9	O31-C31-C32	2.56	119.63	111.83	13	20
5	D	550	7Q9	O31-C31-C32	2.55	119.62	111.83	6	20
5	E	830	7Q9	O31-C31-C32	2.55	119.62	111.83	8	20
5	E	814	7Q9	O31-C31-C32	2.55	119.61	111.83	13	20
5	D	508	7Q9	O31-C31-C32	2.55	119.60	111.83	13	20
5	B	210	7Q9	O31-C31-C32	2.54	119.58	111.83	11	20
5	E	803	7Q9	O31-C31-C32	2.54	119.58	111.83	11	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
5	E	831	7Q9	O31-C31-C32	2.54	119.57	111.83	7	20
6	D	517	17F	O7-C7-C8	2.54	119.57	111.83	12	20
6	E	871	17F	O7-C7-C8	2.54	119.57	111.83	3	20
5	D	507	7Q9	O31-C31-C32	2.53	119.56	111.83	12	20
5	D	521	7Q9	O31-C31-C32	2.54	119.57	111.83	13	20
5	E	850	7Q9	O31-C31-C32	2.53	119.55	111.83	18	20
5	D	529	7Q9	O31-C31-C32	2.53	119.53	111.83	17	20
5	E	859	7Q9	O31-C31-C32	2.52	119.53	111.83	3	20
5	E	867	7Q9	O31-C31-C32	2.52	119.53	111.83	15	20
6	E	820	17F	O7-C7-C8	2.52	119.52	111.83	2	20
6	E	856	17F	O7-C7-C8	2.52	119.52	111.83	6	20
5	D	541	7Q9	O31-C31-C32	2.52	119.50	111.83	10	20
5	B	203	7Q9	O31-C31-C32	2.51	119.49	111.83	18	20
5	D	509	7Q9	C3-O31-C31	2.51	107.94	117.12	11	16
5	E	852	7Q9	O21-C21-C22	2.51	120.15	110.93	3	20
5	E	866	7Q9	O31-C31-C32	2.51	119.49	111.83	19	20
5	E	804	7Q9	O31-C31-C32	2.51	119.48	111.83	11	20
6	E	810	17F	C6-O7-C7	2.51	107.96	117.12	1	19
5	A	209	7Q9	O31-C31-C32	2.50	119.47	111.83	5	20
5	E	859	7Q9	O21-C21-C22	2.50	120.12	110.93	13	20
5	E	813	7Q9	C3-O31-C31	2.50	107.97	117.12	19	20
5	E	876	7Q9	O31-C31-C32	2.50	119.46	111.83	20	20
5	D	531	7Q9	O31-C31-C32	2.49	119.43	111.83	8	20
5	D	542	7Q9	O31-C31-C32	2.49	119.43	111.83	13	20
5	E	858	7Q9	O31-C31-C32	2.49	119.42	111.83	1	20
5	E	864	7Q9	O21-C21-C22	2.49	120.08	110.93	5	20
5	D	512	7Q9	O31-C31-C32	2.49	119.42	111.83	15	20
5	E	825	7Q9	O31-C31-C32	2.48	119.40	111.83	11	20
5	D	538	7Q9	O31-C31-C32	2.48	119.40	111.83	20	20
5	D	547	7Q9	O31-C31-C32	2.48	119.39	111.83	10	20
6	E	842	17F	O7-C7-C8	2.48	119.40	111.83	9	20
5	D	523	7Q9	O21-C21-C22	2.48	120.03	110.93	15	20
5	D	532	7Q9	O21-C21-C22	2.48	120.03	110.93	15	20
5	E	807	7Q9	C3-O31-C31	2.47	108.08	117.12	7	19
6	D	539	17F	O7-C7-C8	2.47	119.37	111.83	9	20
5	A	204	7Q9	O31-C31-C32	2.47	119.36	111.83	10	20
5	D	514	7Q9	O21-C21-C22	2.46	119.97	110.93	1	20
5	D	549	7Q9	C3-O31-C31	2.46	108.13	117.12	12	14
5	E	836	7Q9	O21-C21-C22	2.46	119.97	110.93	14	20
5	E	861	7Q9	O21-C21-C22	2.46	119.97	110.93	11	20
5	D	508	7Q9	O21-C21-C22	2.46	119.95	110.93	14	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
5	E	809	7Q9	O31-C31-C32	2.45	119.32	111.83	20	20
3	A	201	GSP	C4-C5-N7	2.45	106.78	110.67	7	19
5	A	214	7Q9	O21-C21-C22	2.45	119.94	110.93	17	20
6	D	518	17F	C6-O7-C7	2.45	108.15	117.12	6	17
5	D	529	7Q9	O21-C21-C22	2.45	119.94	110.93	5	20
5	E	803	7Q9	O21-C21-C22	2.45	119.93	110.93	6	20
5	D	555	7Q9	O21-C21-C22	2.45	119.92	110.93	3	20
5	E	850	7Q9	O21-C21-C22	2.45	119.92	110.93	16	20
6	E	806	17F	O7-C7-C8	2.45	119.29	111.83	17	20
5	E	836	7Q9	O31-C31-C32	2.44	119.29	111.83	17	20
5	A	215	7Q9	O21-C21-C22	2.44	119.90	110.93	20	20
5	D	503	7Q9	C3-O31-C31	2.44	108.19	117.12	10	7
5	E	860	7Q9	O21-C21-C22	2.44	119.90	110.93	5	20
5	D	531	7Q9	O21-C21-C22	2.44	119.89	110.93	13	20
5	E	862	7Q9	O21-C21-C22	2.44	119.90	110.93	13	20
6	E	839	17F	C6-O7-C7	2.44	108.20	117.12	15	20
5	E	835	7Q9	O21-C21-C22	2.44	119.89	110.93	5	20
5	E	874	7Q9	O21-C21-C22	2.44	119.89	110.93	4	20
5	A	216	7Q9	O21-C21-C22	2.43	119.87	110.93	9	20
5	E	845	7Q9	O21-C21-C22	2.44	119.88	110.93	3	20
5	E	822	7Q9	O21-C21-C22	2.43	119.87	110.93	14	20
5	E	827	7Q9	O31-C31-C32	2.43	119.26	111.83	4	20
5	E	821	7Q9	O21-C21-C22	2.43	119.86	110.93	1	20
5	D	526	7Q9	O21-C21-C22	2.43	119.86	110.93	5	20
5	A	212	7Q9	C3-O31-C31	2.43	108.24	117.12	2	8
5	D	505	7Q9	C3-O31-C31	2.43	108.24	117.12	18	7
5	D	524	7Q9	O21-C21-C22	2.43	119.85	110.93	19	20
5	D	543	7Q9	O21-C21-C22	2.43	119.85	110.93	13	20
5	B	207	7Q9	O21-C21-C22	2.43	119.84	110.93	12	20
5	B	210	7Q9	O21-C21-C22	2.43	119.84	110.93	19	20
5	E	834	7Q9	O21-C21-C22	2.43	119.85	110.93	6	20
5	E	804	7Q9	O21-C21-C22	2.43	119.84	110.93	18	20
5	E	855	7Q9	O21-C21-C22	2.43	119.84	110.93	14	20
5	B	203	7Q9	O21-C21-C22	2.42	119.83	110.93	1	20
5	D	513	7Q9	O21-C21-C22	2.43	119.84	110.93	11	20
5	E	877	7Q9	O21-C21-C22	2.43	119.84	110.93	7	20
5	D	501	7Q9	O21-C21-C22	2.42	119.83	110.93	11	20
5	A	205	7Q9	O21-C21-C22	2.42	119.83	110.93	8	20
5	A	207	7Q9	O21-C21-C22	2.42	119.82	110.93	15	20
5	D	512	7Q9	O21-C21-C22	2.42	119.82	110.93	17	20
5	E	828	7Q9	O21-C21-C22	2.42	119.82	110.93	8	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
5	E	847	7Q9	O21-C21-C22	2.42	119.82	110.93	9	20
5	E	870	7Q9	O21-C21-C22	2.42	119.82	110.93	11	20
5	D	526	7Q9	C3-O31-C31	2.42	108.27	117.12	17	19
5	E	805	7Q9	O21-C21-C22	2.42	119.82	110.93	12	20
5	A	210	7Q9	O21-C21-C22	2.42	119.81	110.93	14	20
5	D	550	7Q9	O21-C21-C22	2.42	119.81	110.93	3	20
5	E	855	7Q9	O31-C31-C32	2.42	119.21	111.83	10	20
5	E	840	7Q9	O21-C21-C22	2.42	119.81	110.93	12	20
5	D	522	7Q9	O21-C21-C22	2.42	119.81	110.93	16	20
5	A	211	7Q9	O21-C21-C22	2.42	119.80	110.93	5	20
5	D	528	7Q9	C3-O31-C31	2.42	108.29	117.12	6	20
5	D	547	7Q9	O21-C21-C22	2.42	119.81	110.93	13	20
5	E	825	7Q9	O21-C21-C22	2.42	119.81	110.93	13	20
5	E	851	7Q9	O21-C21-C22	2.42	119.81	110.93	10	20
5	E	852	7Q9	O31-C31-C32	2.42	119.20	111.83	17	20
5	E	867	7Q9	O21-C21-C22	2.42	119.81	110.93	6	20
5	A	209	7Q9	O21-C21-C22	2.41	119.79	110.93	3	20
5	B	204	7Q9	O21-C21-C22	2.41	119.79	110.93	11	20
5	B	206	7Q9	O21-C21-C22	2.41	119.80	110.93	12	20
5	B	209	7Q9	O21-C21-C22	2.41	119.80	110.93	14	20
5	D	553	7Q9	O21-C21-C22	2.41	119.80	110.93	19	20
5	D	554	7Q9	O21-C21-C22	2.41	119.80	110.93	1	20
5	E	849	7Q9	O21-C21-C22	2.41	119.79	110.93	12	20
5	E	833	7Q9	O21-C21-C22	2.41	119.79	110.93	7	20
5	E	866	7Q9	O21-C21-C22	2.41	119.79	110.93	18	20
5	A	218	7Q9	O21-C21-C22	2.41	119.78	110.93	7	20
5	D	506	7Q9	O21-C21-C22	2.41	119.78	110.93	10	20
5	E	838	7Q9	O21-C21-C22	2.41	119.78	110.93	15	20
5	D	546	7Q9	O21-C21-C22	2.41	119.78	110.93	14	20
5	E	809	7Q9	O21-C21-C22	2.41	119.78	110.93	18	20
5	D	544	7Q9	O21-C21-C22	2.41	119.77	110.93	8	20
5	D	541	7Q9	O21-C21-C22	2.41	119.77	110.93	5	20
5	D	549	7Q9	O21-C21-C22	2.41	119.77	110.93	4	20
5	E	824	7Q9	O21-C21-C22	2.41	119.77	110.93	2	20
5	E	831	7Q9	O21-C21-C22	2.41	119.77	110.93	1	20
5	E	853	7Q9	C3-O31-C31	2.41	108.33	117.12	16	17
5	E	844	7Q9	O21-C21-C22	2.40	119.76	110.93	5	20
5	E	846	7Q9	O21-C21-C22	2.40	119.76	110.93	6	20
5	D	525	7Q9	O21-C21-C22	2.40	119.75	110.93	19	20
5	D	537	7Q9	O21-C21-C22	2.40	119.76	110.93	17	20
5	D	551	7Q9	O21-C21-C22	2.40	119.76	110.93	2	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
5	E	813	7Q9	O21-C21-C22	2.40	119.76	110.93	13	20
5	E	801	7Q9	O21-C21-C22	2.40	119.75	110.93	5	20
5	E	876	7Q9	O21-C21-C22	2.40	119.76	110.93	9	20
5	D	502	7Q9	O21-C21-C22	2.40	119.75	110.93	16	20
5	D	515	7Q9	O21-C21-C22	2.40	119.75	110.93	7	20
5	D	542	7Q9	O21-C21-C22	2.40	119.75	110.93	17	20
5	E	815	7Q9	O21-C21-C22	2.40	119.75	110.93	14	20
5	E	832	7Q9	O21-C21-C22	2.40	119.75	110.93	12	20
5	E	869	7Q9	O21-C21-C22	2.40	119.74	110.93	2	20
5	D	505	7Q9	O21-C21-C22	2.40	119.73	110.93	3	20
5	D	521	7Q9	O21-C21-C22	2.40	119.73	110.93	8	20
5	D	536	7Q9	O21-C21-C22	2.40	119.73	110.93	11	20
5	E	816	7Q9	O21-C21-C22	2.40	119.74	110.93	8	20
5	E	837	7Q9	O21-C21-C22	2.40	119.73	110.93	10	20
5	E	848	7Q9	O21-C21-C22	2.40	119.73	110.93	13	20
5	E	865	7Q9	O21-C21-C22	2.40	119.73	110.93	3	20
5	E	854	7Q9	O21-C21-C22	2.39	119.71	110.93	15	20
5	E	863	7Q9	O21-C21-C22	2.39	119.72	110.93	3	20
5	E	878	7Q9	O21-C21-C22	2.39	119.71	110.93	12	20
6	E	812	17F	C6-O7-C7	2.39	108.38	117.12	16	4
5	D	527	7Q9	O21-C21-C22	2.39	119.71	110.93	12	20
5	D	538	7Q9	O21-C21-C22	2.39	119.71	110.93	15	20
5	A	217	7Q9	O21-C21-C22	2.39	119.70	110.93	9	20
5	D	503	7Q9	O21-C21-C22	2.39	119.71	110.93	16	20
5	D	507	7Q9	O21-C21-C22	2.39	119.71	110.93	16	20
5	D	535	7Q9	O21-C21-C22	2.39	119.70	110.93	7	20
5	D	545	7Q9	O21-C21-C22	2.39	119.70	110.93	2	20
5	E	807	7Q9	O21-C21-C22	2.39	119.70	110.93	4	20
5	A	204	7Q9	O21-C21-C22	2.39	119.70	110.93	5	20
5	A	212	7Q9	O21-C21-C22	2.39	119.70	110.93	4	20
5	E	841	7Q9	O21-C21-C22	2.39	119.69	110.93	7	20
5	E	843	7Q9	O21-C21-C22	2.39	119.70	110.93	10	20
5	E	853	7Q9	O21-C21-C22	2.38	119.69	110.93	1	20
5	E	868	7Q9	O21-C21-C22	2.38	119.69	110.93	12	20
5	D	504	7Q9	O21-C21-C22	2.38	119.68	110.93	11	20
5	D	509	7Q9	O21-C21-C22	2.38	119.68	110.93	19	20
5	E	827	7Q9	O21-C21-C22	2.38	119.68	110.93	3	20
5	D	530	7Q9	O21-C21-C22	2.38	119.68	110.93	6	20
5	E	811	7Q9	O21-C21-C22	2.38	119.68	110.93	6	20
5	E	826	7Q9	O21-C21-C22	2.38	119.67	110.93	15	20
5	E	858	7Q9	O21-C21-C22	2.38	119.67	110.93	15	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
5	B	205	7Q9	O21-C21-C22	2.38	119.66	110.93	16	20
5	E	823	7Q9	O21-C21-C22	2.38	119.66	110.93	12	20
5	D	556	7Q9	O21-C21-C22	2.37	119.65	110.93	10	20
5	A	203	7Q9	O21-C21-C22	2.37	119.64	110.93	3	20
5	A	206	7Q9	O21-C21-C22	2.37	119.64	110.93	5	20
5	A	210	7Q9	C3-O31-C31	2.37	108.45	117.12	6	17
5	E	822	7Q9	C3-O31-C31	2.37	108.45	117.12	10	19
5	E	830	7Q9	O21-C21-C22	2.37	119.63	110.93	20	20
5	E	816	7Q9	C3-O31-C31	2.37	108.47	117.12	12	4
5	E	814	7Q9	O21-C21-C22	2.37	119.62	110.93	16	20
5	D	528	7Q9	O21-C21-C22	2.36	119.61	110.93	19	20
5	D	548	7Q9	O21-C21-C22	2.36	119.61	110.93	17	20
5	E	817	7Q9	O21-C21-C22	2.36	119.59	110.93	15	20
5	E	872	7Q9	O21-C21-C22	2.36	119.60	110.93	11	20
3	A	201	GSP	C3'-C2'-C1'	2.36	97.00	101.46	19	13
5	D	516	7Q9	O21-C21-C22	2.36	119.58	110.93	15	20
5	D	548	7Q9	C3-O31-C31	2.35	108.54	117.12	20	17
5	E	838	7Q9	C3-O31-C31	2.35	108.54	117.12	13	15
6	A	220	17F	C6-O7-C7	2.34	108.58	117.12	16	10
5	D	550	7Q9	C3-C2-C1	2.33	106.35	111.78	19	3
5	D	537	7Q9	C3-O31-C31	2.32	108.63	117.12	3	16
5	D	551	7Q9	C3-O31-C31	2.32	108.65	117.12	14	18
5	E	870	7Q9	C3-O31-C31	2.31	108.67	117.12	6	18
6	A	219	17F	C6-O7-C7	2.31	108.68	117.12	6	9
5	E	864	7Q9	C3-O31-C31	2.30	108.70	117.12	8	10
5	E	830	7Q9	C3-C2-C1	2.30	106.42	111.78	12	2
5	B	205	7Q9	C3-O31-C31	2.29	108.74	117.12	1	6
5	D	513	7Q9	C3-O31-C31	2.29	108.75	117.12	9	8
6	D	510	17F	C6-O7-C7	2.29	108.75	117.12	6	3
6	D	534	17F	C6-O7-C7	2.29	108.75	117.12	9	19
5	E	832	7Q9	C3-O31-C31	2.28	108.77	117.12	7	14
5	E	834	7Q9	C3-O31-C31	2.28	108.78	117.12	5	11
5	E	843	7Q9	C3-O31-C31	2.28	108.78	117.12	1	6
3	A	201	GSP	C8-N7-C5	2.28	108.32	104.26	7	20
5	D	546	7Q9	C3-O31-C31	2.26	108.84	117.12	14	15
5	A	218	7Q9	C3-O31-C31	2.26	108.85	117.12	7	5
5	E	817	7Q9	C3-O31-C31	2.25	108.88	117.12	12	1
3	A	201	GSP	O6-C6-C5	2.25	120.59	126.53	16	20
5	E	847	7Q9	C3-O31-C31	2.25	108.90	117.12	14	11
3	B	201	GSP	C4-C5-N7	2.24	107.12	110.67	19	18
5	B	206	7Q9	C3-O31-C31	2.24	108.93	117.12	9	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
5	D	524	7Q9	C3-O31-C31	2.24	108.94	117.12	2	2
3	B	201	GSP	O6-C6-C5	2.23	120.63	126.53	9	20
6	D	533	17F	C6-O7-C7	2.23	108.95	117.12	19	13
3	B	201	GSP	C3'-C2'-C1'	2.23	97.25	101.46	1	15
3	A	201	GSP	N9-C8-N7	2.22	109.28	113.40	11	20
5	D	535	7Q9	C3-O31-C31	2.22	109.01	117.12	19	8
5	E	860	7Q9	C3-O31-C31	2.22	109.01	117.12	3	1
3	B	201	GSP	N9-C8-N7	2.22	109.29	113.40	4	19
6	D	552	17F	C6-O7-C7	2.21	109.03	117.12	5	18
5	D	544	7Q9	C3-O31-C31	2.20	109.06	117.12	4	1
5	E	851	7Q9	C3-O31-C31	2.20	109.06	117.12	15	13
3	B	201	GSP	C8-N7-C5	2.20	108.18	104.26	3	20
6	D	519	17F	C6-O7-C7	2.20	109.08	117.12	7	2
5	E	862	7Q9	C3-O31-C31	2.20	109.08	117.12	10	10
5	E	804	7Q9	C3-C2-C1	2.20	106.66	111.78	5	2
5	D	501	7Q9	C3-O31-C31	2.20	109.09	117.12	5	4
5	E	837	7Q9	C3-O31-C31	2.20	109.09	117.12	13	13
6	E	875	17F	C6-O7-C7	2.20	109.09	117.12	20	10
5	E	821	7Q9	C3-O31-C31	2.20	109.09	117.12	18	8
6	D	511	17F	C6-O7-C7	2.19	109.13	117.12	17	9
6	E	873	17F	C6-O7-C7	2.19	109.12	117.12	5	7
5	D	516	7Q9	C3-O31-C31	2.19	109.13	117.12	12	4
5	B	204	7Q9	C3-O31-C31	2.18	109.14	117.12	1	7
5	D	536	7Q9	C3-O31-C31	2.18	109.14	117.12	11	1
3	A	201	GSP	C5-C6-N1	2.18	118.80	113.25	7	20
5	E	823	7Q9	C3-O31-C31	2.18	109.15	117.12	15	6
5	D	502	7Q9	C3-O31-C31	2.18	109.16	117.12	5	10
5	A	215	7Q9	C3-O31-C31	2.18	109.16	117.12	16	4
5	D	545	7Q9	C3-O31-C31	2.18	109.16	117.12	3	4
6	E	808	17F	C6-O7-C7	2.17	109.17	117.12	8	9
5	D	507	7Q9	C3-O31-C31	2.17	109.17	117.12	12	1
5	D	554	7Q9	C3-O31-C31	2.17	109.19	117.12	14	2
5	D	514	7Q9	C3-O31-C31	2.17	109.20	117.12	14	5
5	E	878	7Q9	C3-O31-C31	2.17	109.20	117.12	11	5
5	E	825	7Q9	C3-O31-C31	2.16	109.22	117.12	13	1
5	E	877	7Q9	C3-O31-C31	2.16	109.23	117.12	17	6
6	E	857	17F	C6-O7-C7	2.16	109.23	117.12	9	5
5	E	814	7Q9	C3-O31-C31	2.16	109.24	117.12	13	2
5	E	866	7Q9	C3-O31-C31	2.15	109.25	117.12	19	2
5	A	211	7Q9	C3-O31-C31	2.15	109.27	117.12	2	7
5	D	506	7Q9	C3-C2-C1	2.15	106.78	111.78	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	201	GSP	C5-C6-N1	2.15	118.71	113.25	12	19
5	A	207	7Q9	C3-O31-C31	2.14	109.28	117.12	20	8
5	D	553	7Q9	C3-C2-C1	2.14	106.79	111.78	17	1
5	E	805	7Q9	C3-O31-C31	2.14	109.29	117.12	6	14
5	E	846	7Q9	C3-O31-C31	2.14	109.29	117.12	5	9
5	A	204	7Q9	C3-C2-C1	2.14	106.80	111.78	1	1
5	D	522	7Q9	C3-O31-C31	2.14	109.31	117.12	3	7
5	A	205	7Q9	C3-O31-C31	2.14	109.31	117.12	11	2
5	D	504	7Q9	C3-O31-C31	2.13	109.32	117.12	5	5
5	E	811	7Q9	C3-O31-C31	2.13	109.32	117.12	18	4
6	E	829	17F	C6-O7-C7	2.13	109.32	117.12	16	5
5	B	210	7Q9	C3-O31-C31	2.13	109.35	117.12	18	9
5	D	553	7Q9	C3-O31-C31	2.12	109.36	117.12	7	9
5	E	863	7Q9	C3-O31-C31	2.12	109.36	117.12	17	3
3	A	201	GSP	O4'-C1'-C2'	2.12	102.09	106.62	1	1
6	E	842	17F	C6-C5-C4	2.11	106.86	111.78	5	1
5	E	844	7Q9	C3-O31-C31	2.11	109.41	117.12	20	9
5	D	556	7Q9	C3-O31-C31	2.11	109.42	117.12	5	16
5	E	869	7Q9	C3-O31-C31	2.11	109.42	117.12	14	10
5	D	525	7Q9	C3-O31-C31	2.10	109.44	117.12	19	5
5	E	840	7Q9	C3-O31-C31	2.10	109.43	117.12	3	2
5	B	209	7Q9	C3-O31-C31	2.10	109.45	117.12	11	6
5	E	861	7Q9	C3-O31-C31	2.10	109.46	117.12	13	2
5	A	217	7Q9	C3-O31-C31	2.09	109.47	117.12	19	2
5	A	214	7Q9	C3-O31-C31	2.09	109.47	117.12	10	1
5	E	845	7Q9	C3-O31-C31	2.09	109.48	117.12	20	9
5	E	850	7Q9	C3-O31-C31	2.09	109.48	117.12	18	1
6	E	871	17F	C6-O7-C7	2.08	109.50	117.12	20	2
5	E	876	7Q9	C3-O31-C31	2.08	109.51	117.12	12	1
5	D	521	7Q9	C3-C2-C1	2.08	106.93	111.78	4	1
5	A	203	7Q9	C3-O31-C31	2.08	109.52	117.12	8	5
5	E	828	7Q9	C3-O31-C31	2.08	109.53	117.12	16	5
5	D	527	7Q9	C3-O31-C31	2.08	109.53	117.12	2	3
6	B	208	17F	C6-O7-C7	2.08	109.53	117.12	16	2
5	E	835	7Q9	C3-O31-C31	2.07	109.54	117.12	4	2
5	A	216	7Q9	C3-C2-C1	2.07	106.95	111.78	14	1
5	D	521	7Q9	C3-O31-C31	2.07	109.55	117.12	13	3
5	D	543	7Q9	C3-O31-C31	2.07	109.55	117.12	8	5
5	E	815	7Q9	C3-O31-C31	2.07	109.55	117.12	5	10
5	E	830	7Q9	C3-O31-C31	2.07	109.55	117.12	8	2
5	D	503	7Q9	C3-C2-C1	2.07	106.97	111.78	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
5	E	824	7Q9	C3-O31-C31	2.06	109.59	117.12	8	1
6	D	539	17F	C6-O7-C7	2.06	109.58	117.12	9	1
5	E	803	7Q9	C3-C2-C1	2.06	106.99	111.78	8	2
5	E	833	7Q9	C3-O31-C31	2.06	109.60	117.12	16	1
6	A	208	17F	C6-O7-C7	2.06	109.60	117.12	12	1
6	E	819	17F	C6-O7-C7	2.06	109.60	117.12	16	2
5	A	206	7Q9	C3-O31-C31	2.05	109.64	117.12	18	3
6	E	842	17F	C6-O7-C7	2.04	109.65	117.12	15	2
5	D	508	7Q9	C3-O31-C31	2.04	109.65	117.12	13	3
5	E	865	7Q9	C3-O31-C31	2.04	109.66	117.12	9	4
5	E	854	7Q9	C3-O31-C31	2.04	109.67	117.12	2	2
6	E	820	17F	C6-O7-C7	2.04	109.66	117.12	6	1
5	D	515	7Q9	C3-O31-C31	2.04	109.68	117.12	8	2
5	D	541	7Q9	C3-O31-C31	2.04	109.68	117.12	10	1
5	E	859	7Q9	C11-C12-N	2.03	109.30	115.82	18	1
5	B	207	7Q9	C3-O31-C31	2.03	109.69	117.12	11	1
5	E	848	7Q9	C3-O31-C31	2.03	109.70	117.12	20	3
5	D	530	7Q9	C3-O31-C31	2.03	109.70	117.12	19	1
5	D	555	7Q9	C3-O31-C31	2.02	109.72	117.12	7	1
6	D	540	17F	C6-O7-C7	2.02	109.72	117.12	19	2
5	E	804	7Q9	C3-O31-C31	2.02	109.73	117.12	11	1
5	E	849	7Q9	C3-O31-C31	2.02	109.73	117.12	9	1
5	D	515	7Q9	C3-C2-C1	2.02	107.08	111.78	13	1
6	D	520	17F	C6-O7-C7	2.02	109.75	117.12	2	1
6	E	818	17F	C6-O7-C7	2.02	109.75	117.12	2	3
5	D	550	7Q9	C3-O31-C31	2.01	109.75	117.12	18	1
5	E	803	7Q9	C3-O31-C31	2.01	109.75	117.12	7	2
5	E	867	7Q9	C3-O31-C31	2.01	109.76	117.12	15	1
5	E	834	7Q9	C11-C12-N	2.01	109.37	115.82	2	1
5	D	548	7Q9	C11-C12-N	2.00	109.40	115.82	7	1

There are no chirality outliers.

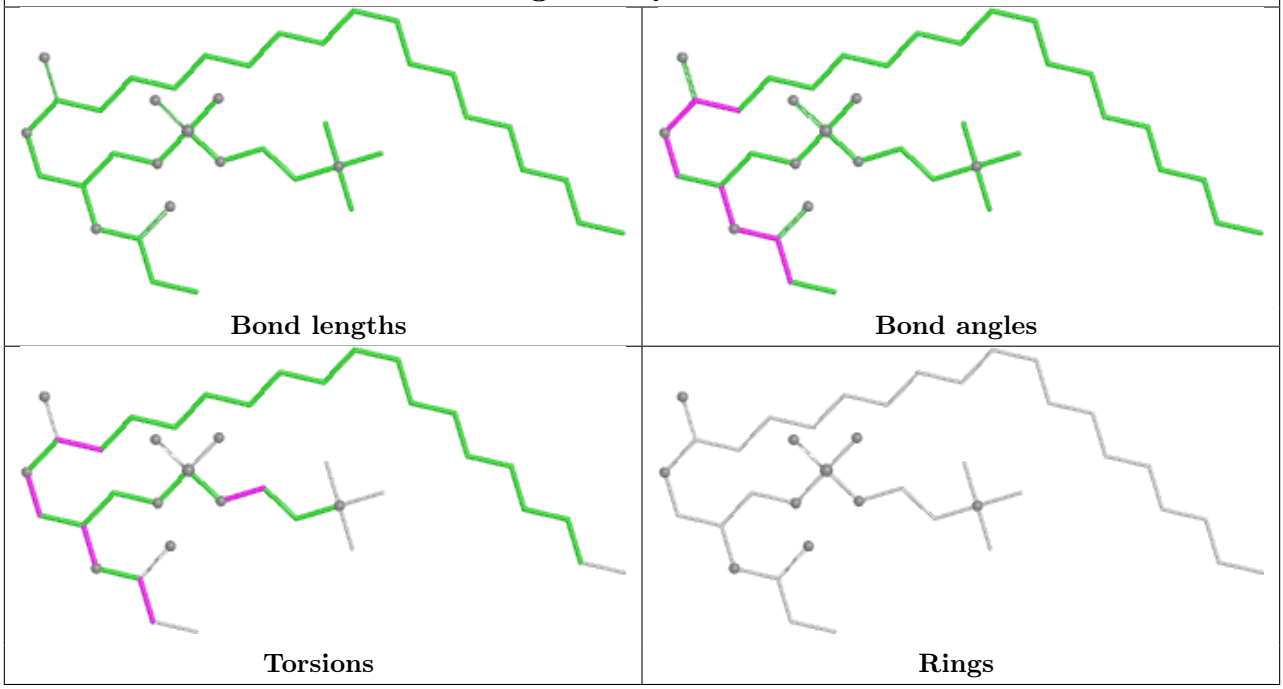
There are no torsion outliers.

There are no ring outliers.

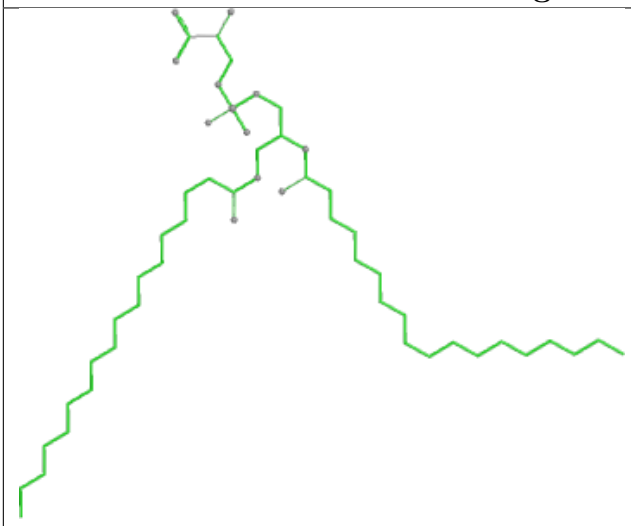
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

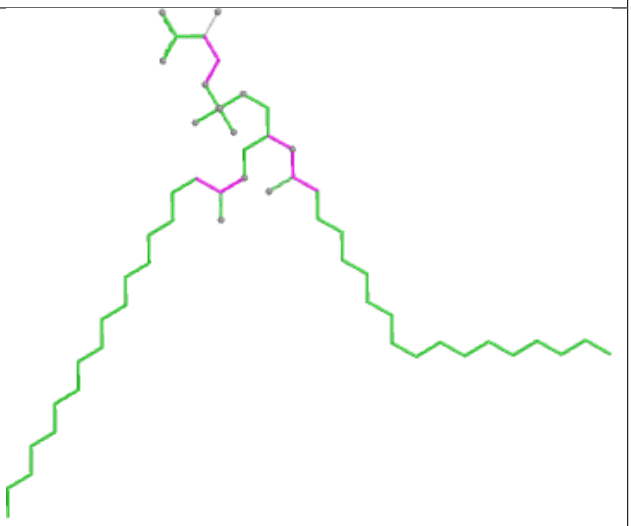
Ligand 7Q9 D 543



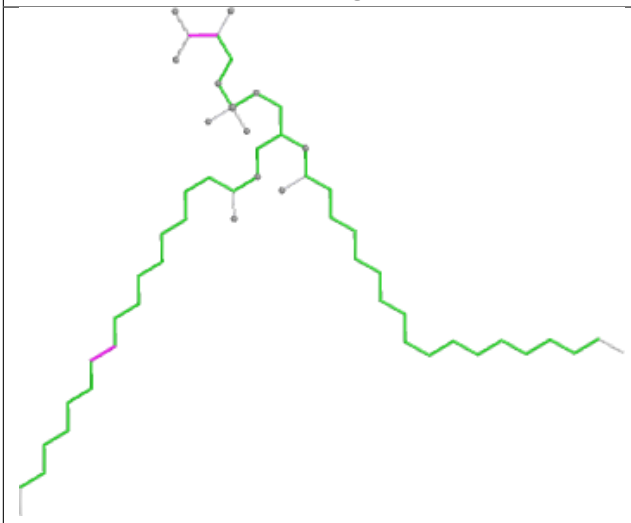
Ligand 17F E 856



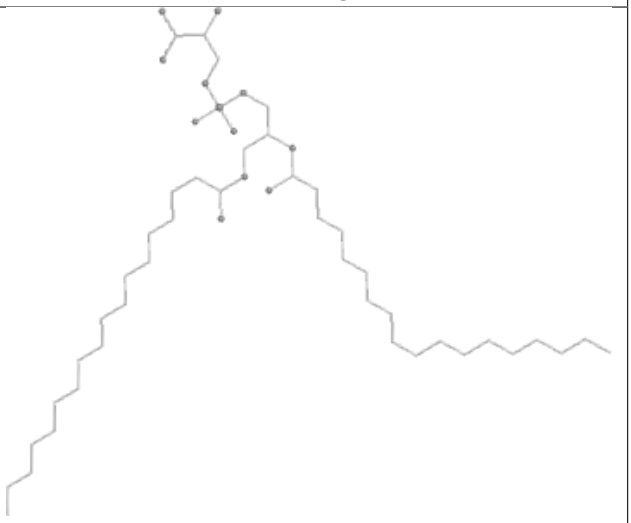
Bond lengths



Bond angles

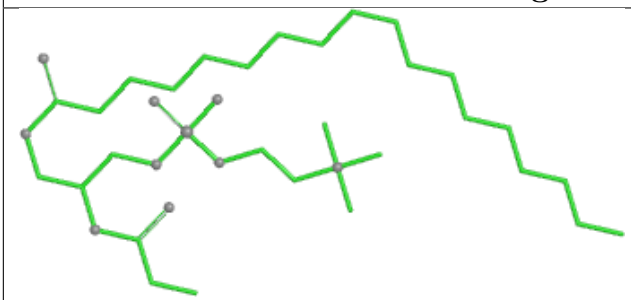


Torsions

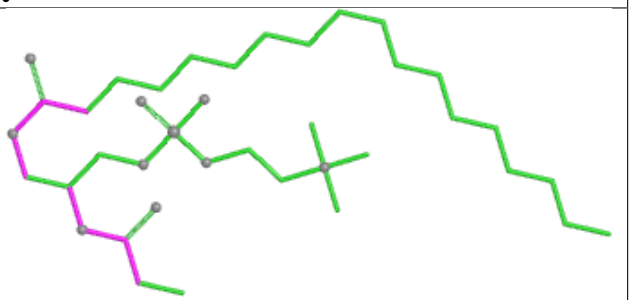


Rings

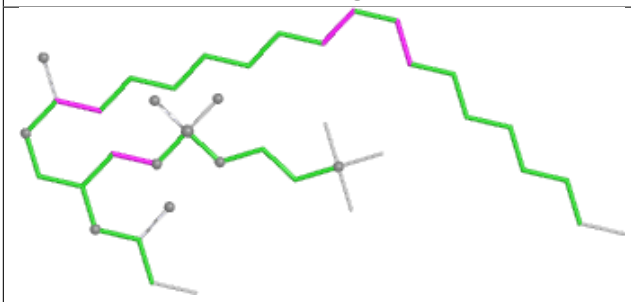
Ligand 7Q9 E 813



Bond lengths



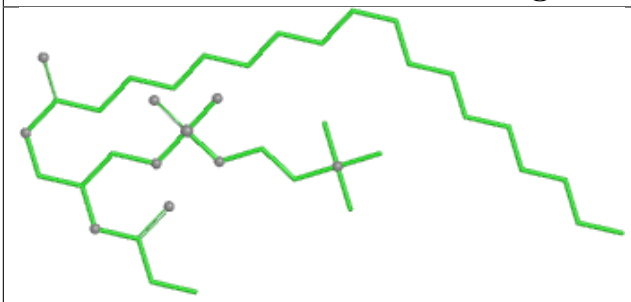
Bond angles



Torsions

Rings

Ligand 7Q9 E 837



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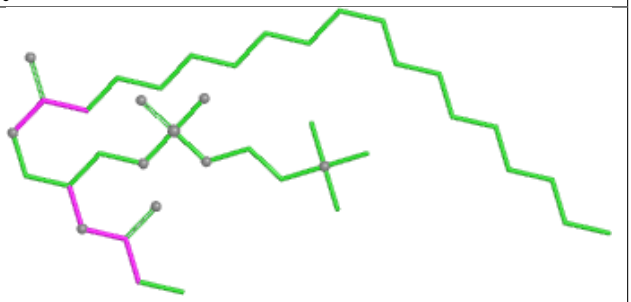
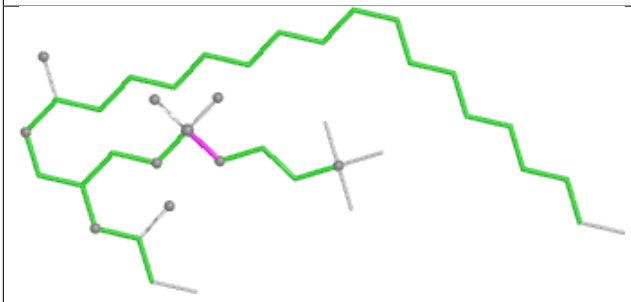


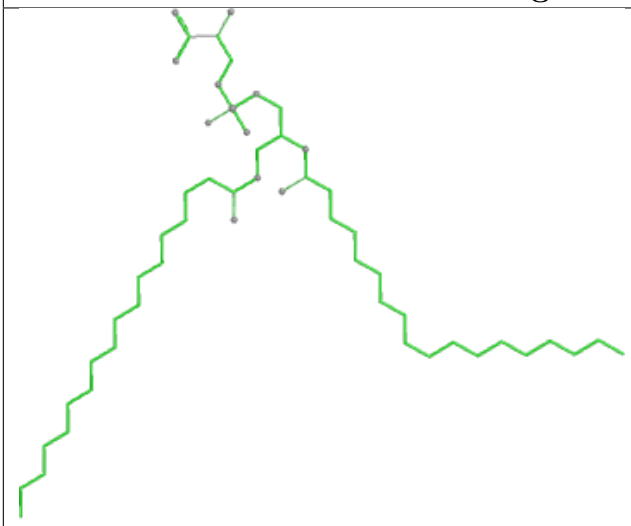
Bond angles



Torsions

Rings

Ligand 17F D 511



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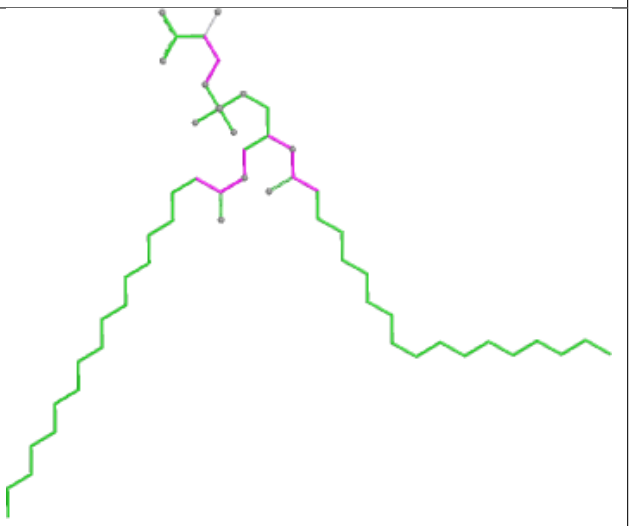
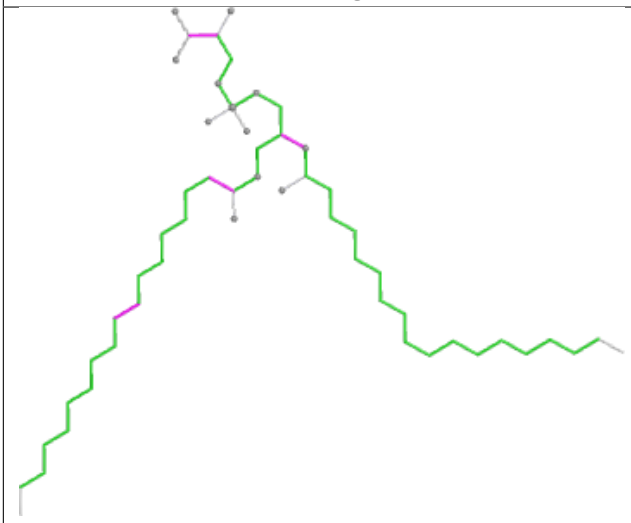
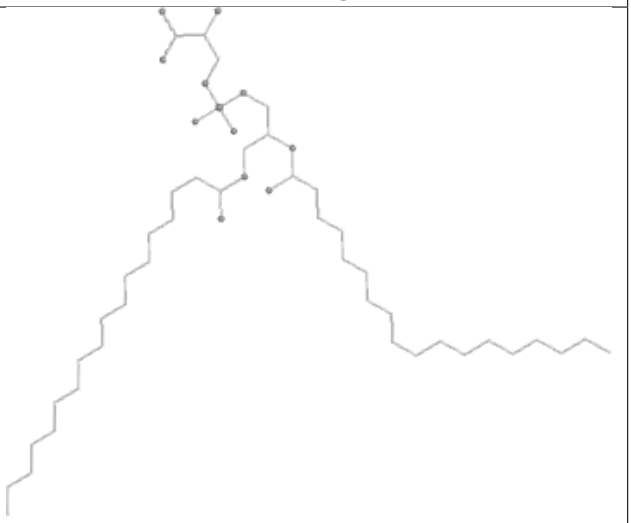


Bond angles

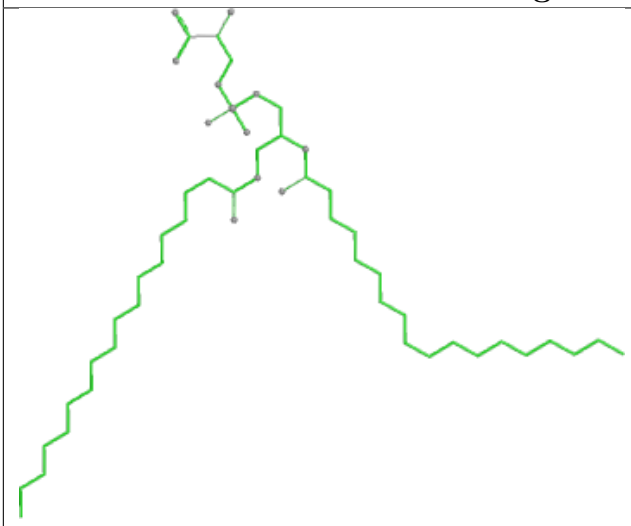


Torsions

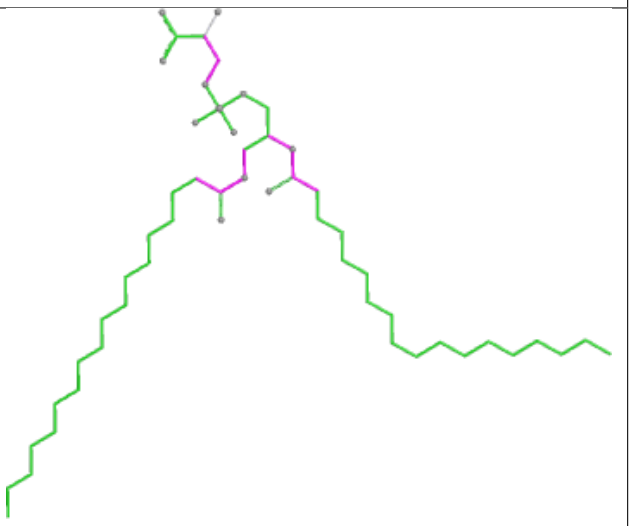


Rings

Ligand 17F E 818



Bond lengths



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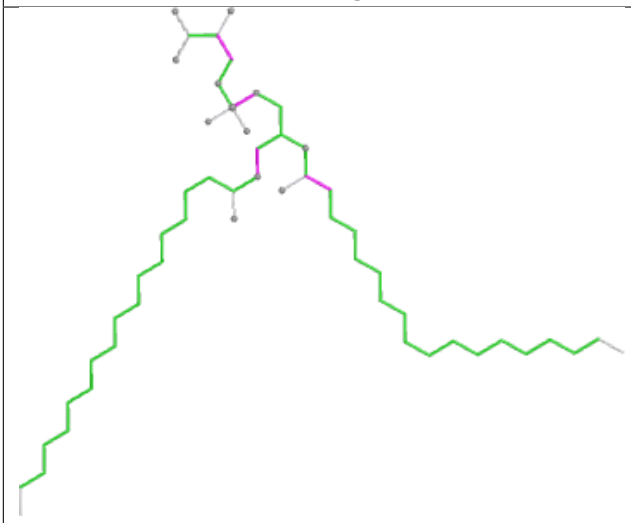

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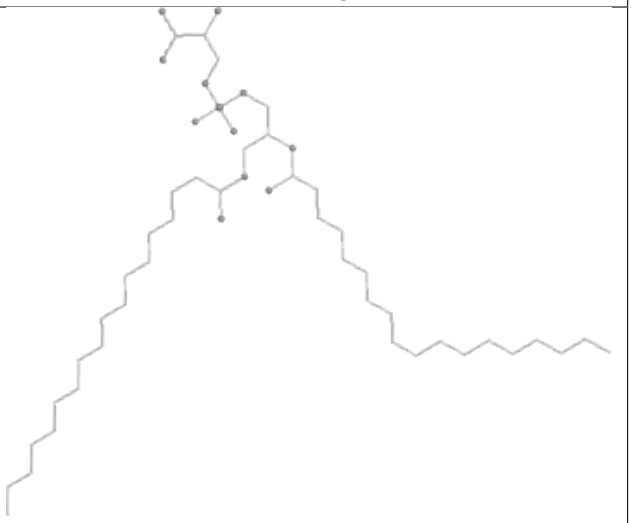
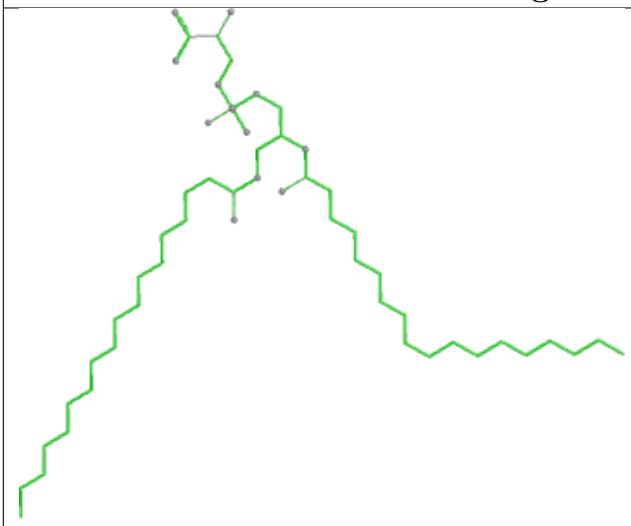


Rings

Ligand 17F D 520



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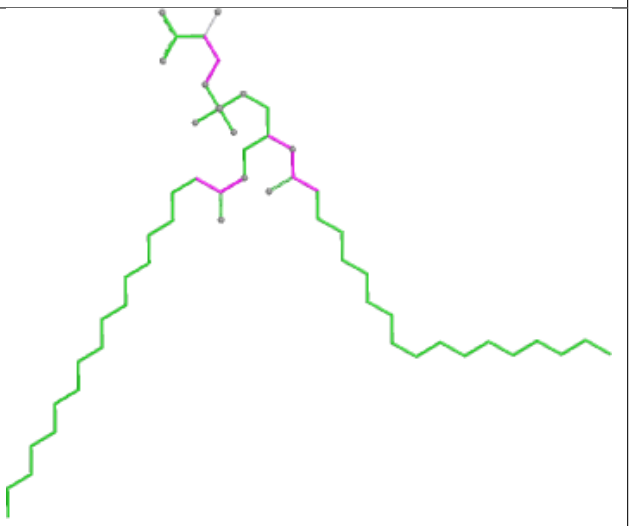

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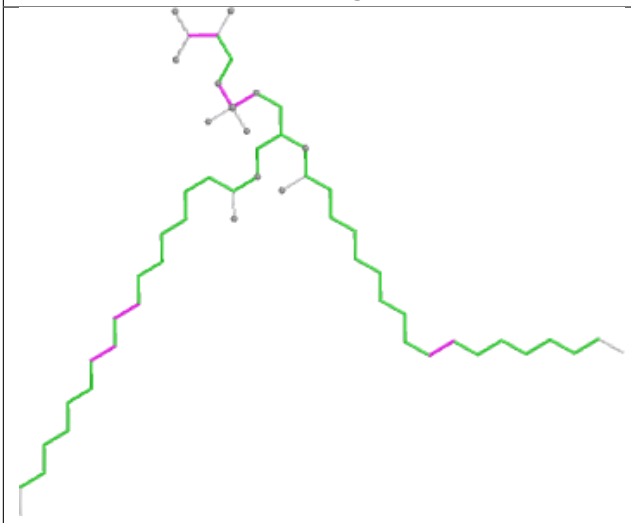

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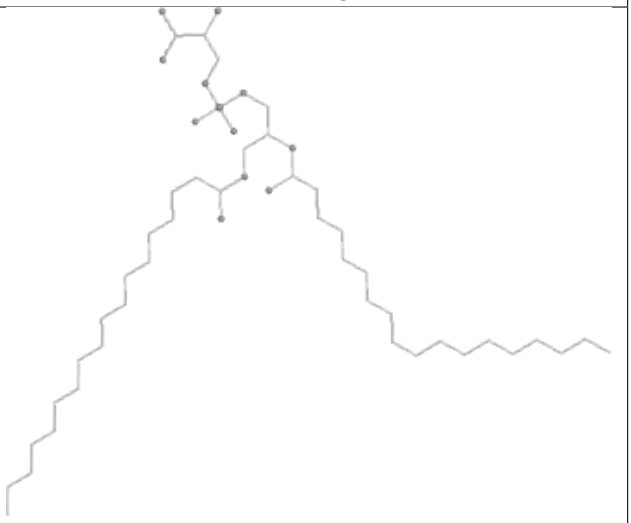
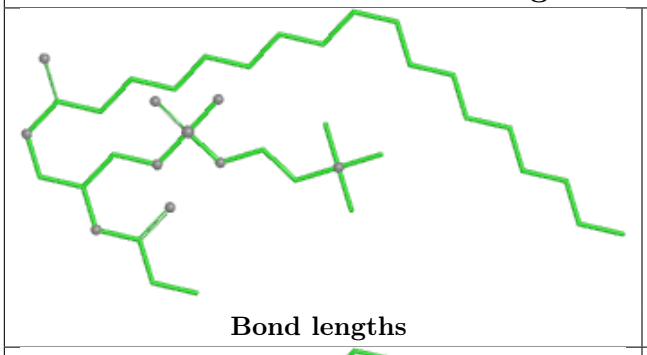


Rings

Ligand 7Q9 D 554



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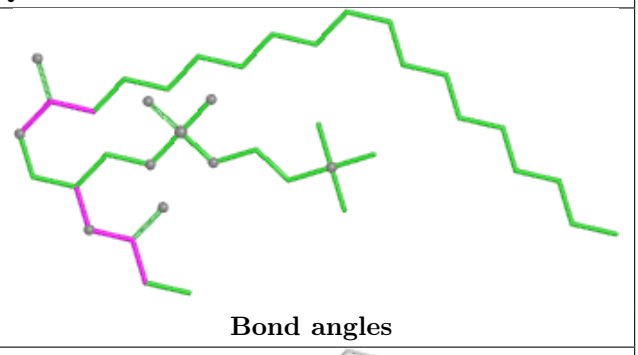

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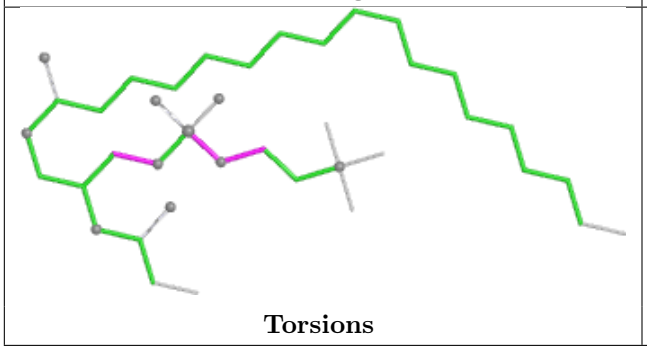

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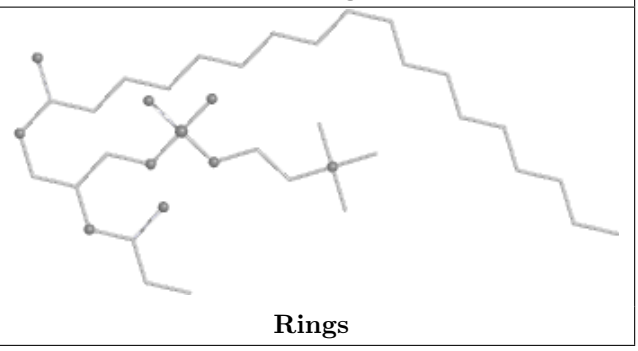
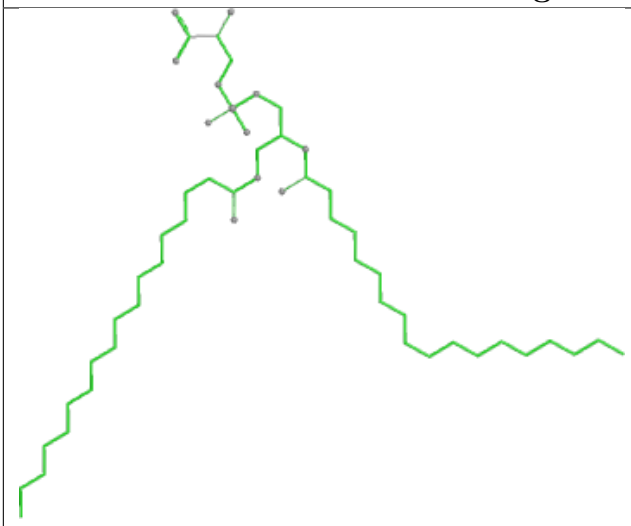


Rings

Ligand 17F E 812



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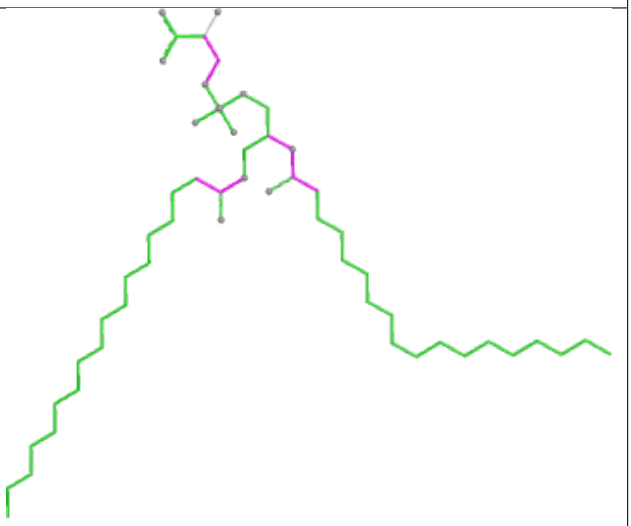
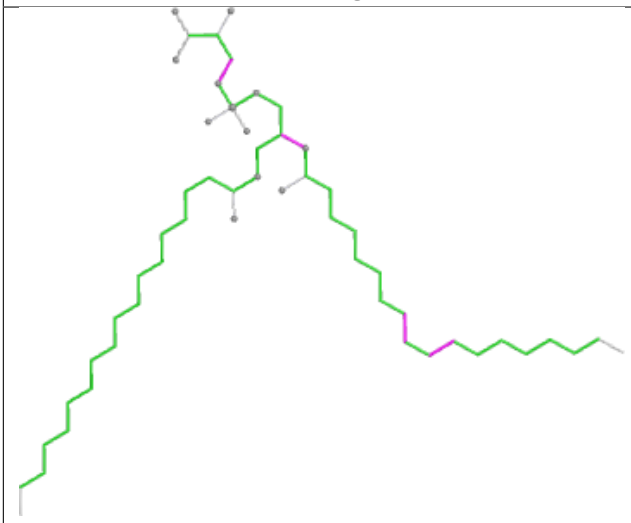


Bond angles



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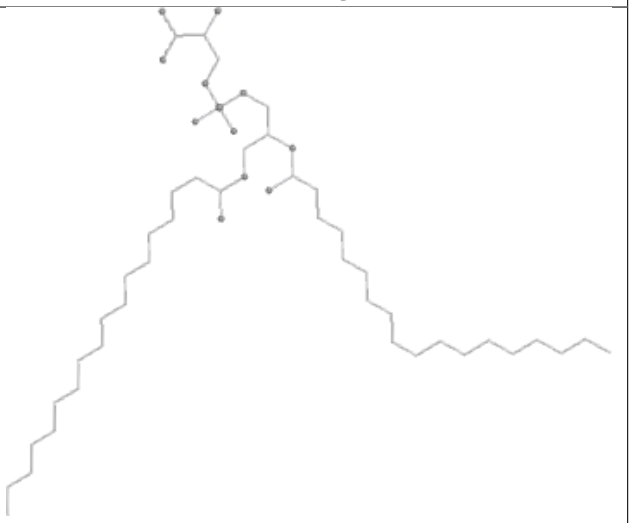
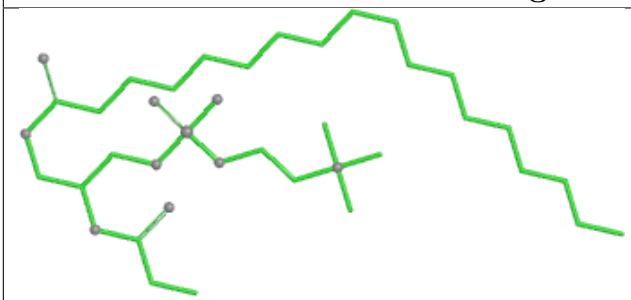


Rings

Ligand 7Q9 D 542



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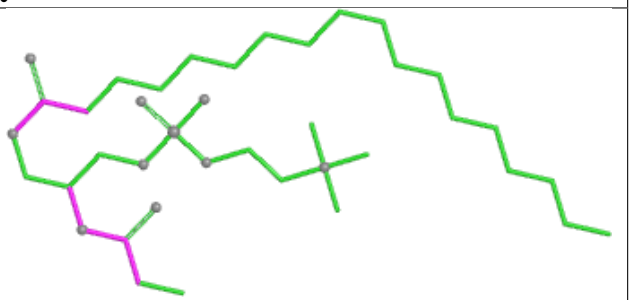
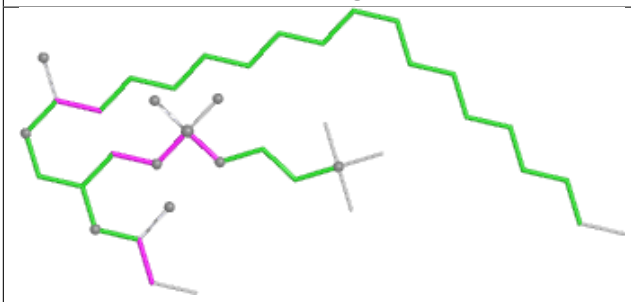


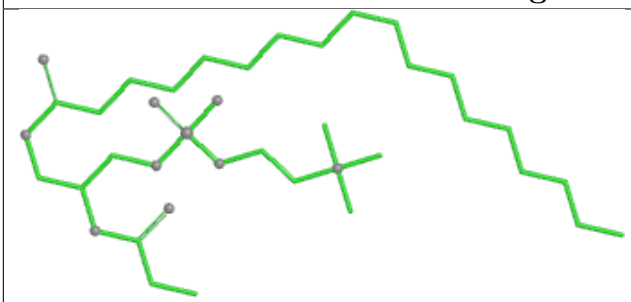
Bond angles



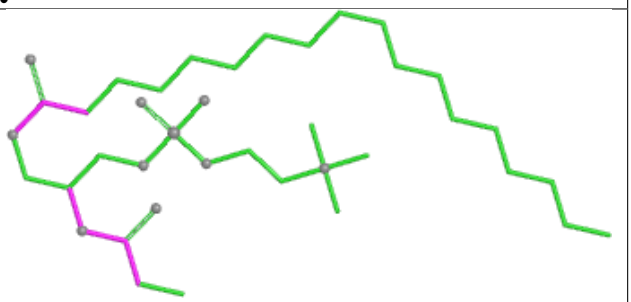
Torsions

Rings

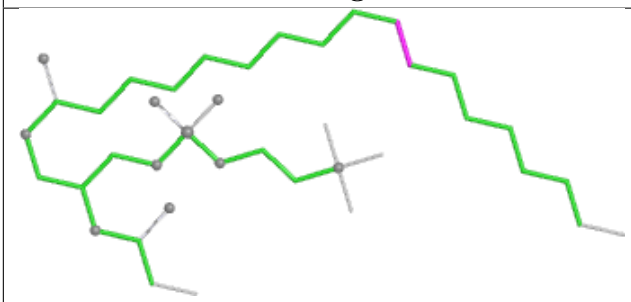
Ligand 7Q9 D 525



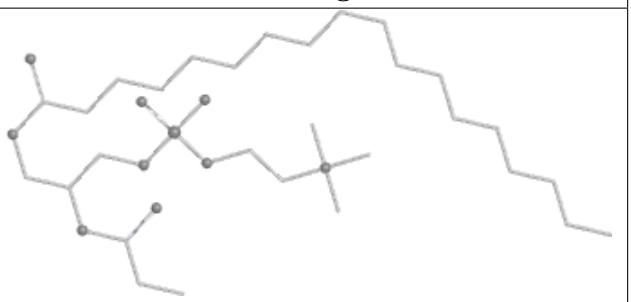
Bond lengths



Bond angles

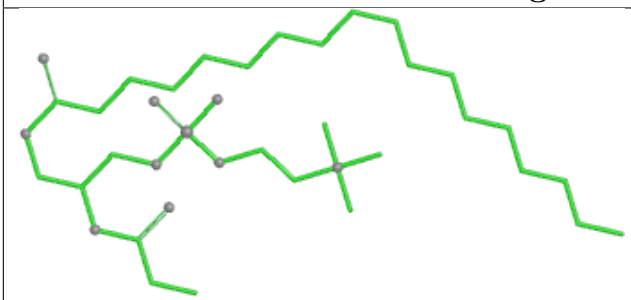


Torsions

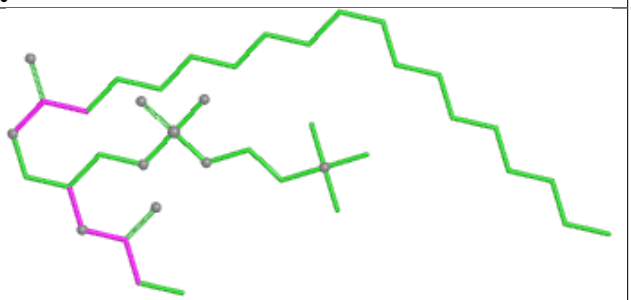


Rings

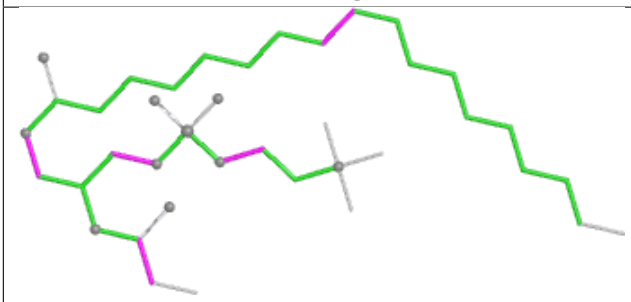
Ligand 7Q9 D 503



Bond lengths



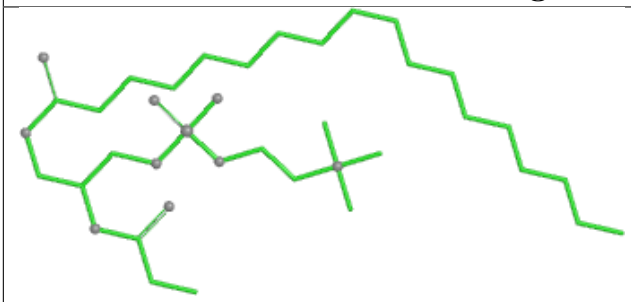
Bond angles



Torsions

Rings

Ligand 7Q9 D 502



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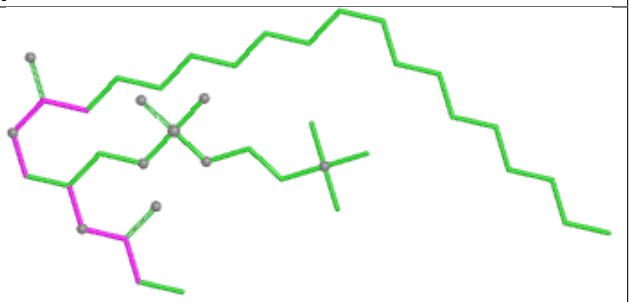
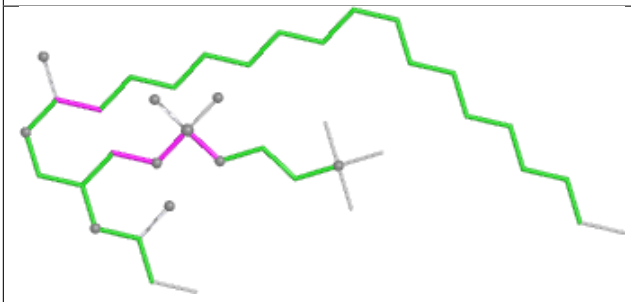


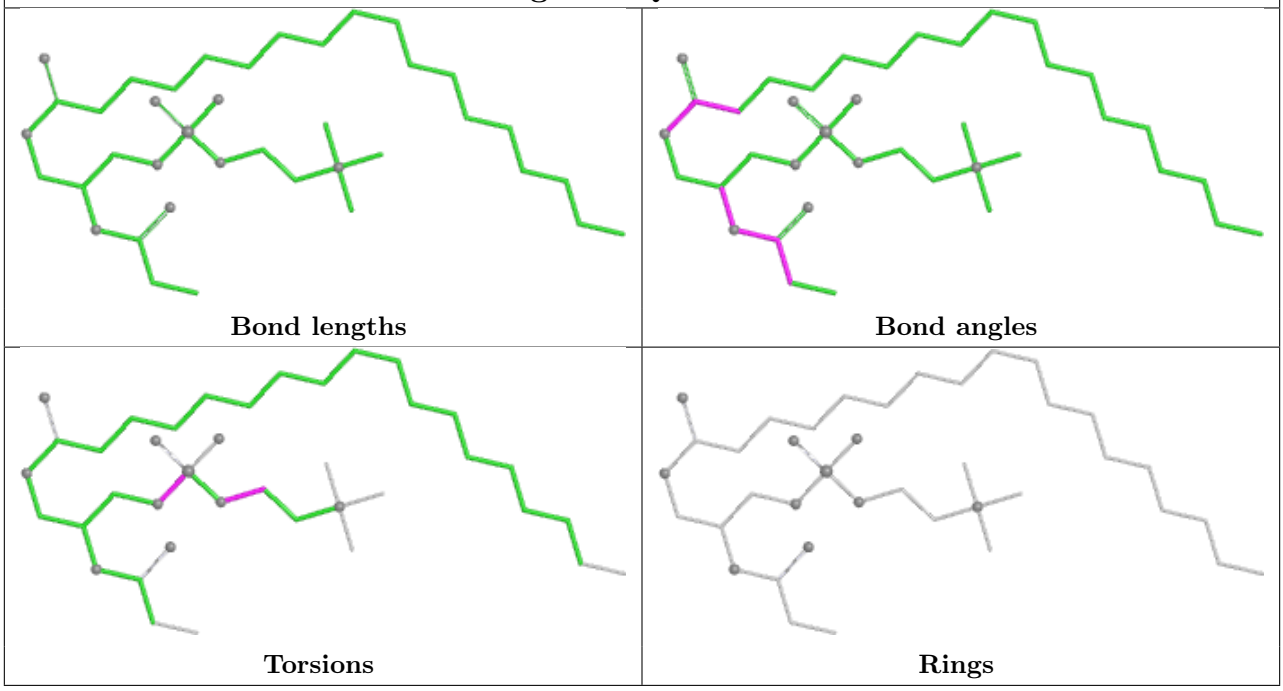
Bond angles



Torsions

Rings

Ligand 7Q9 D 538



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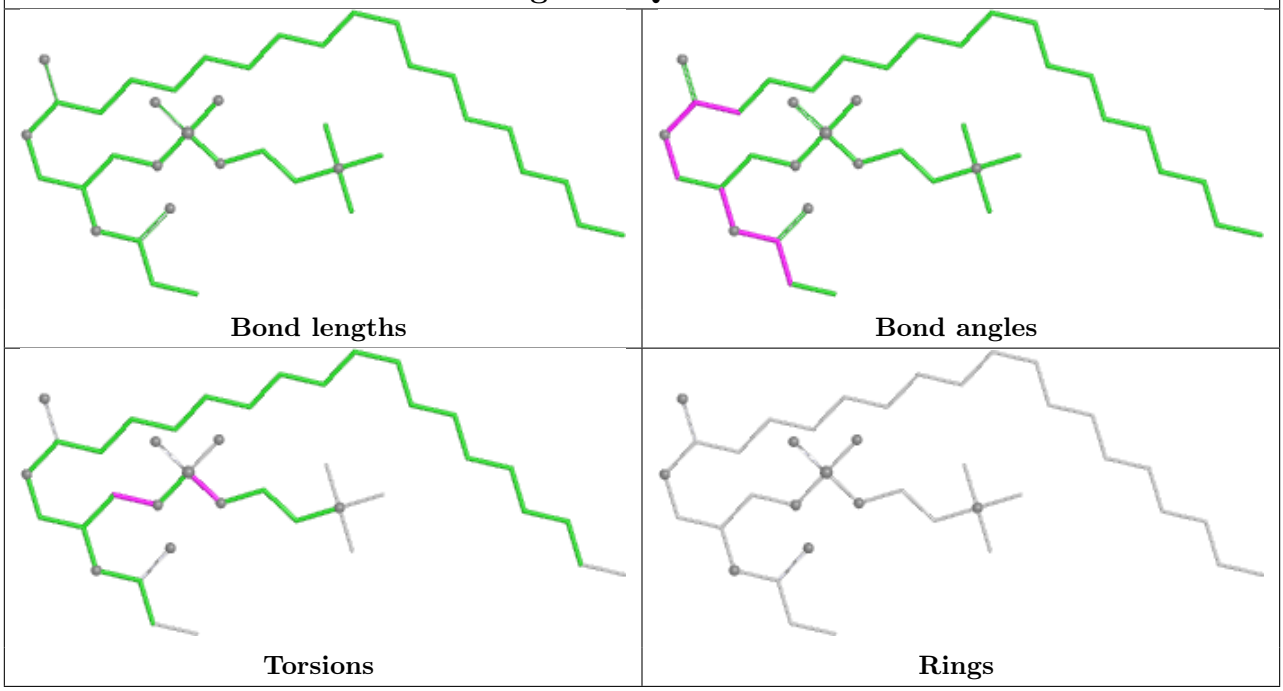
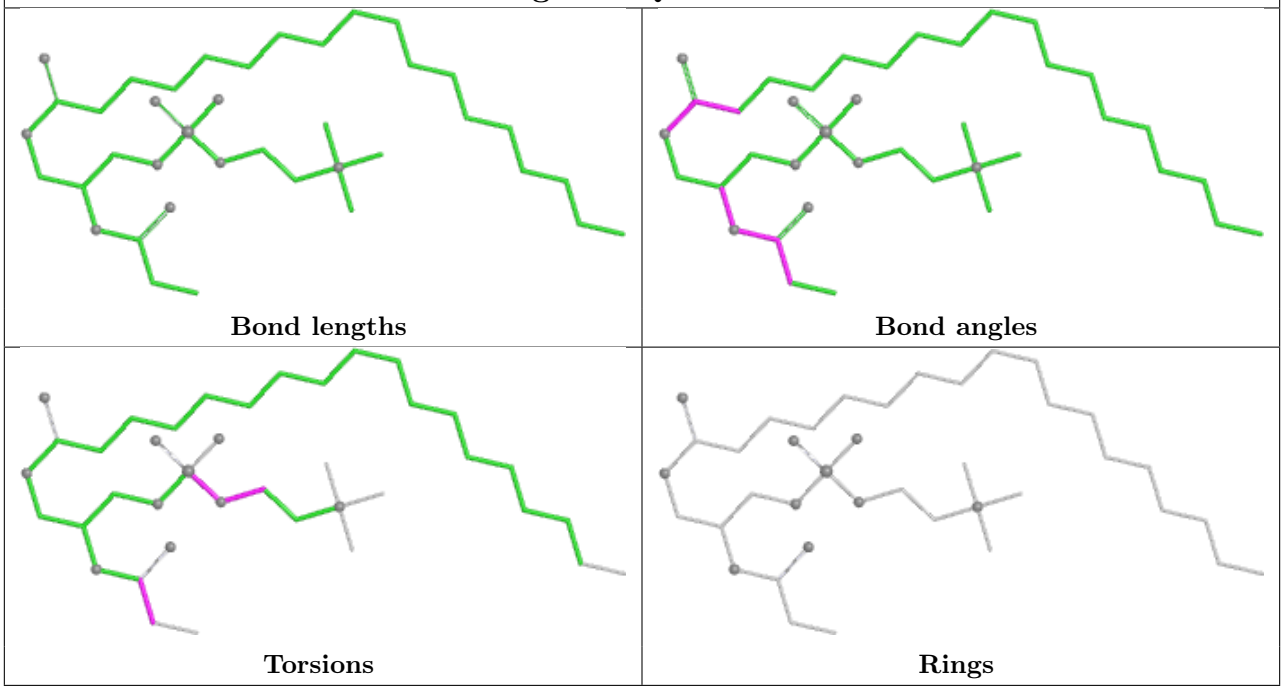
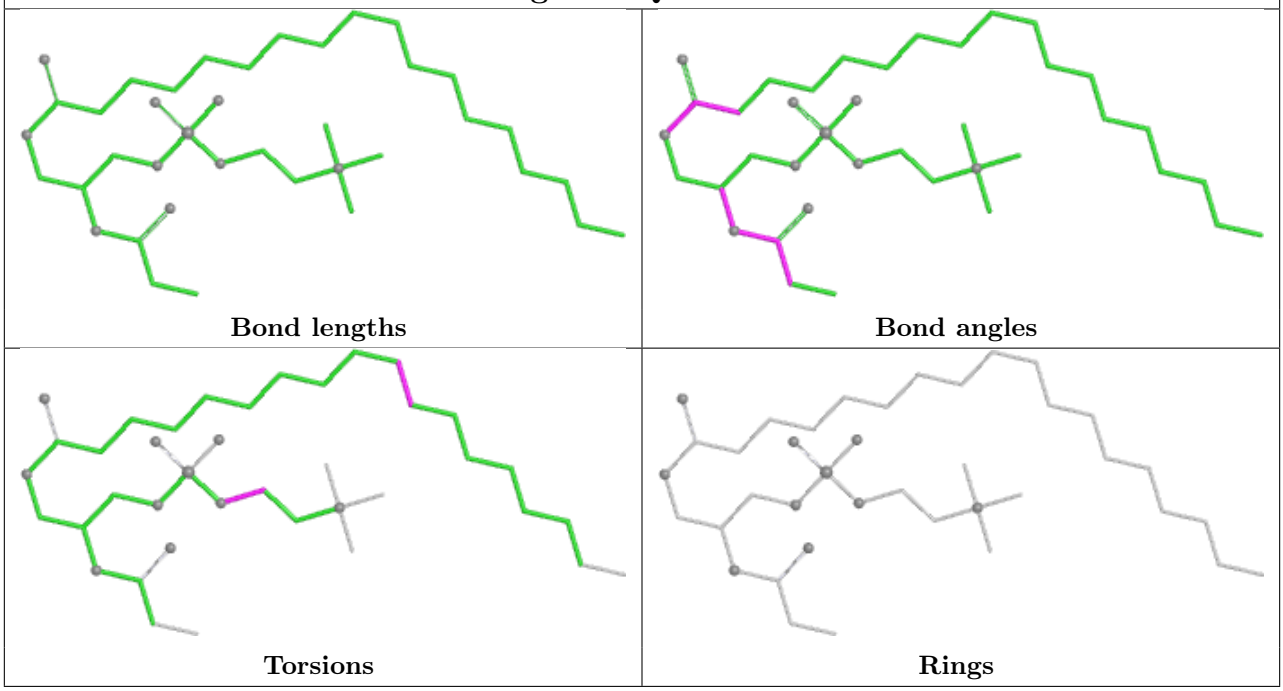


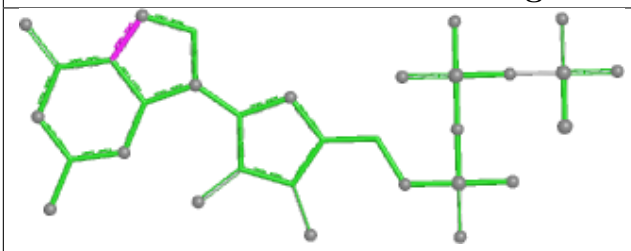
Ligand 7Q9 E 855



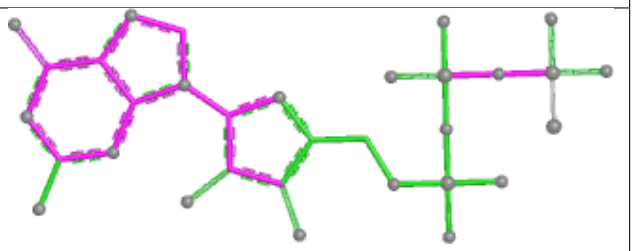
Ligand 7Q9 A 214



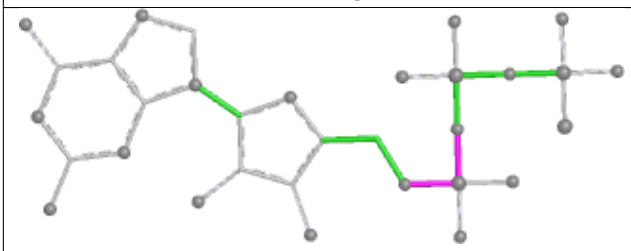
Ligand GSP B 201



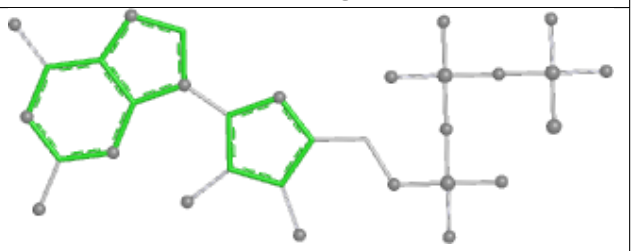
Bond lengths



Bond angles

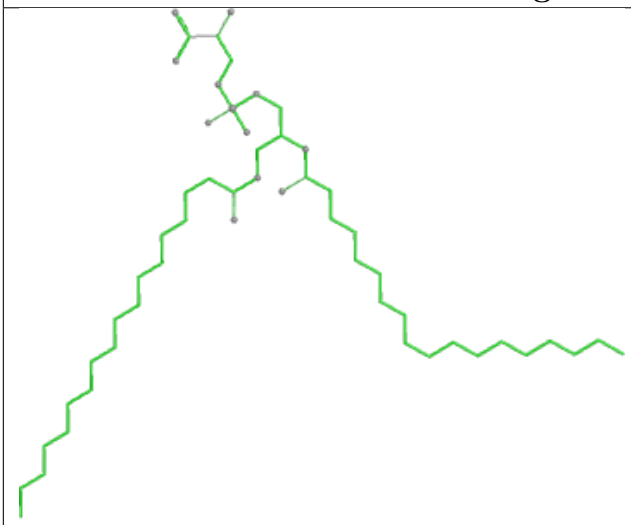


Torsions



Rings

Ligand 17F E 875



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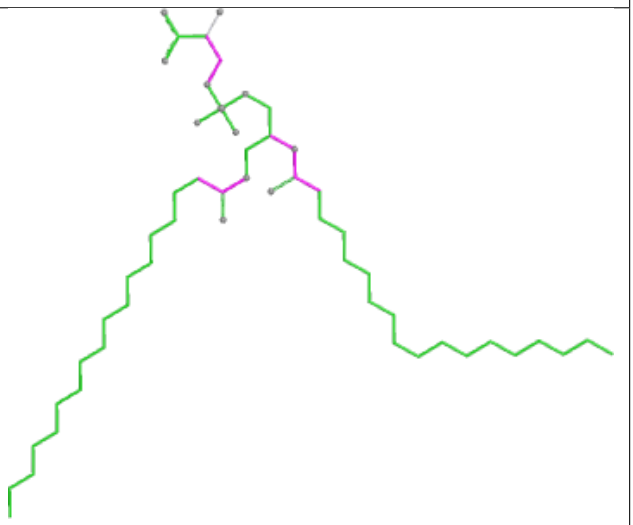
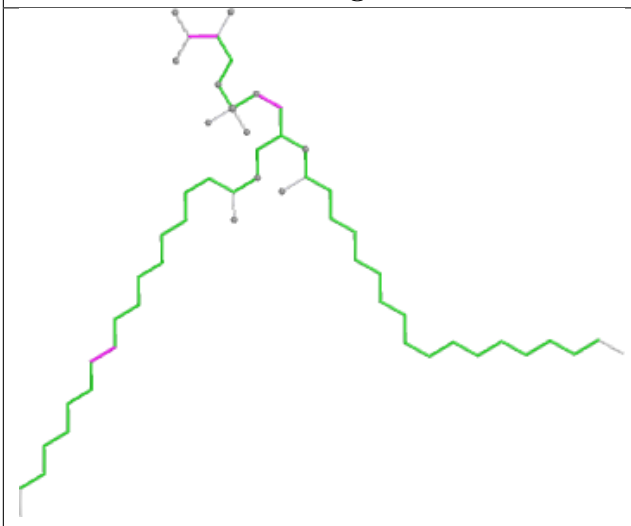


Bond angles



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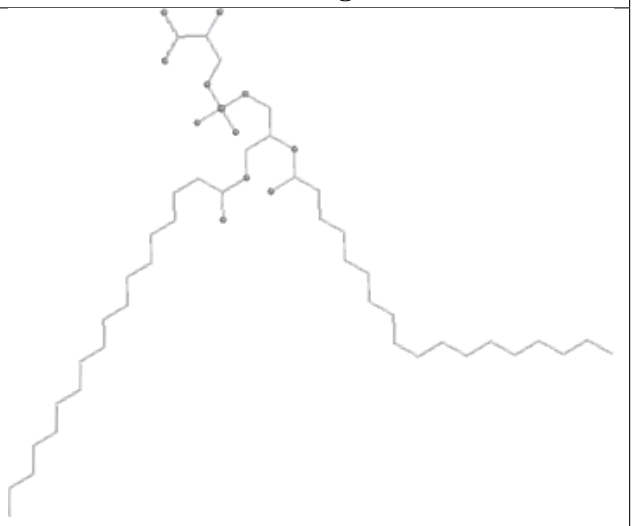
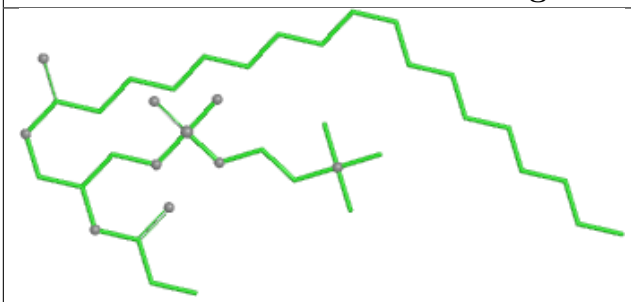


Rings

Ligand 7Q9 D 515



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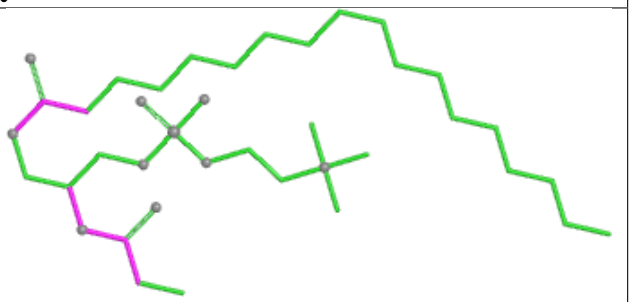
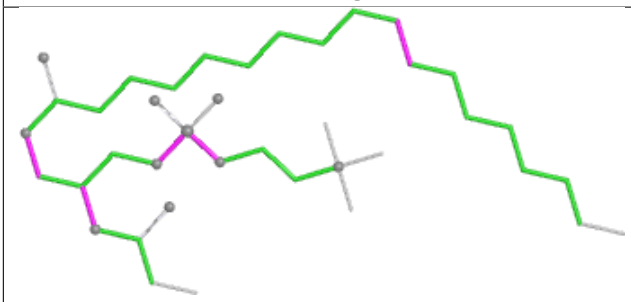


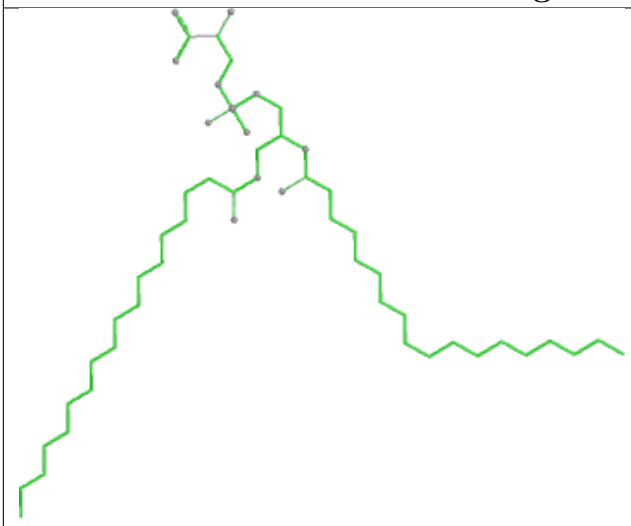
Bond angles



Torsions

Rings

Ligand 17F E 857



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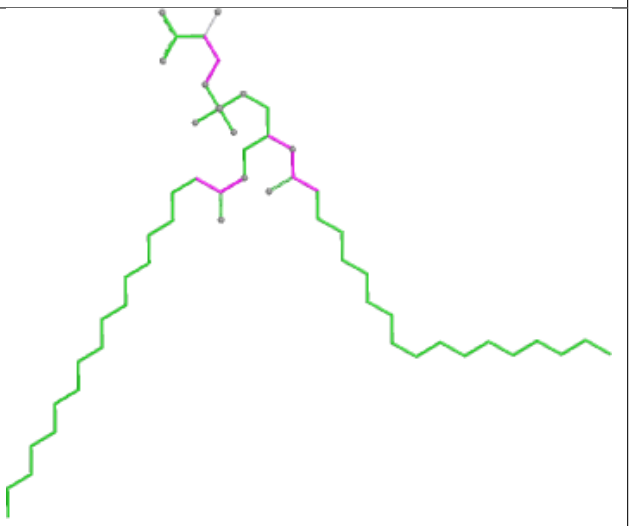
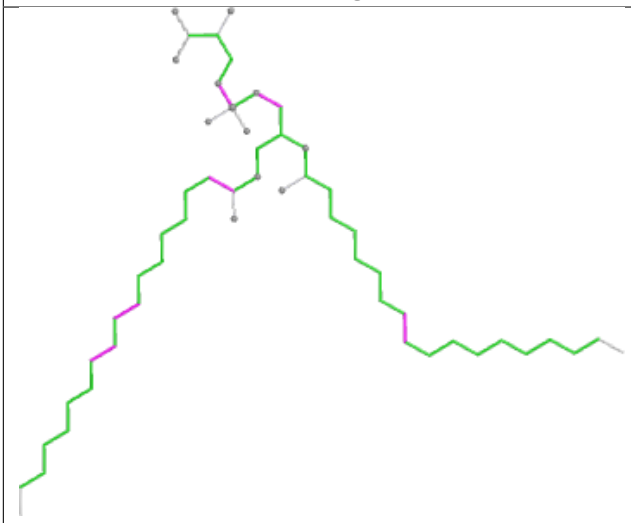


Bond angles



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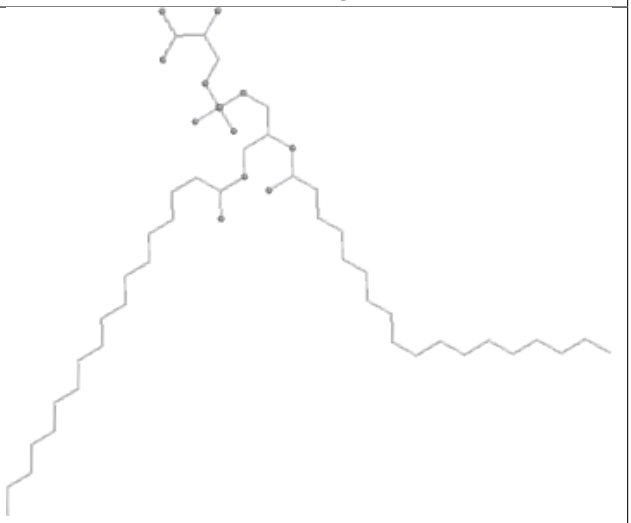
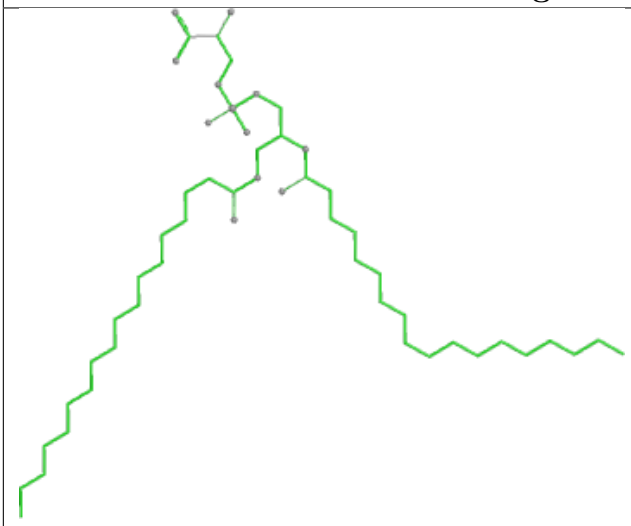


Rings

Ligand 17F B 208



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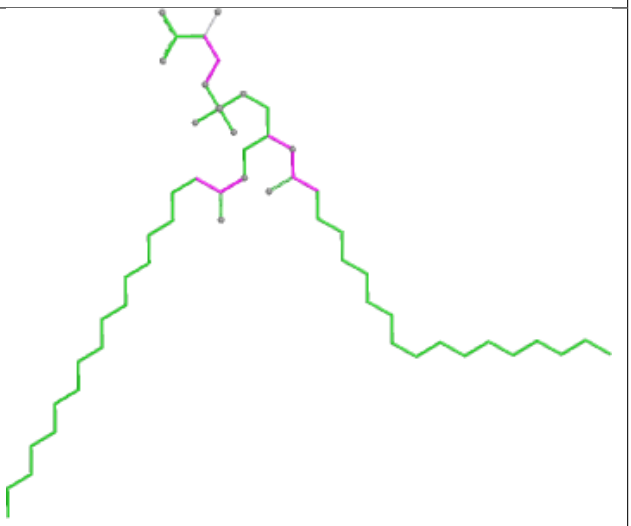
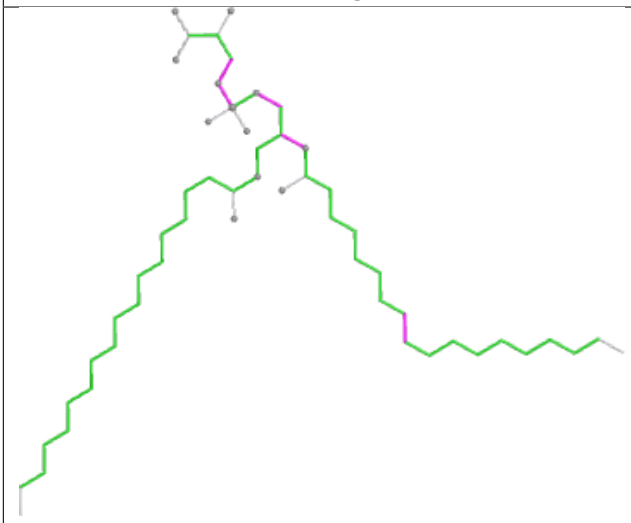
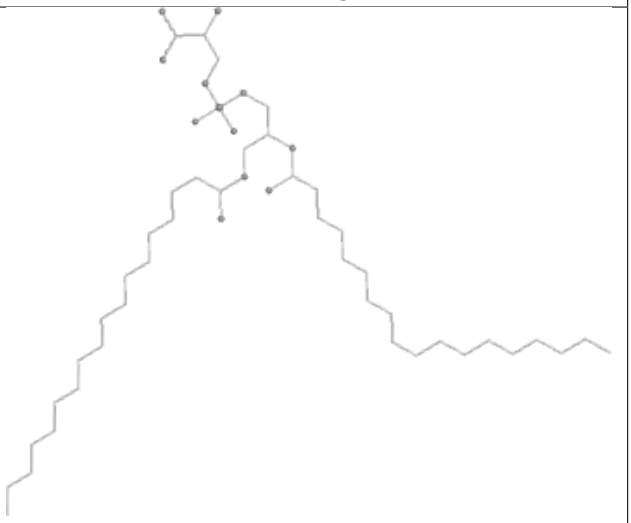


Bond angles

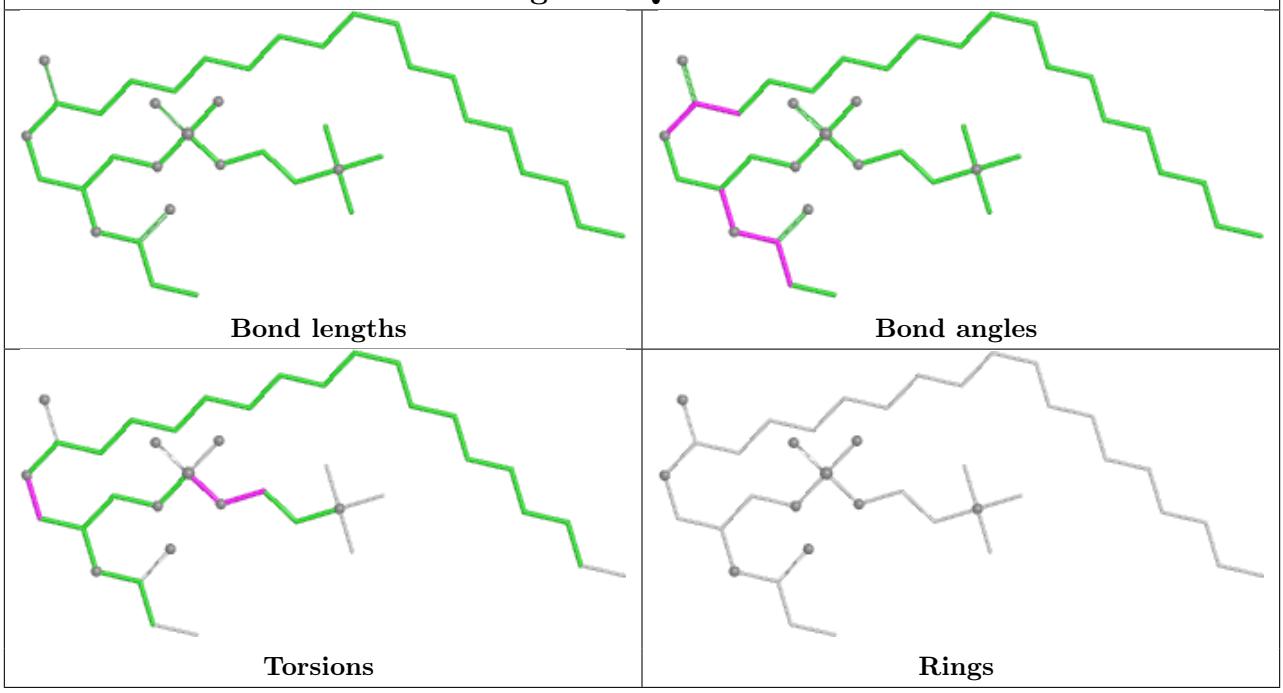


Torsions

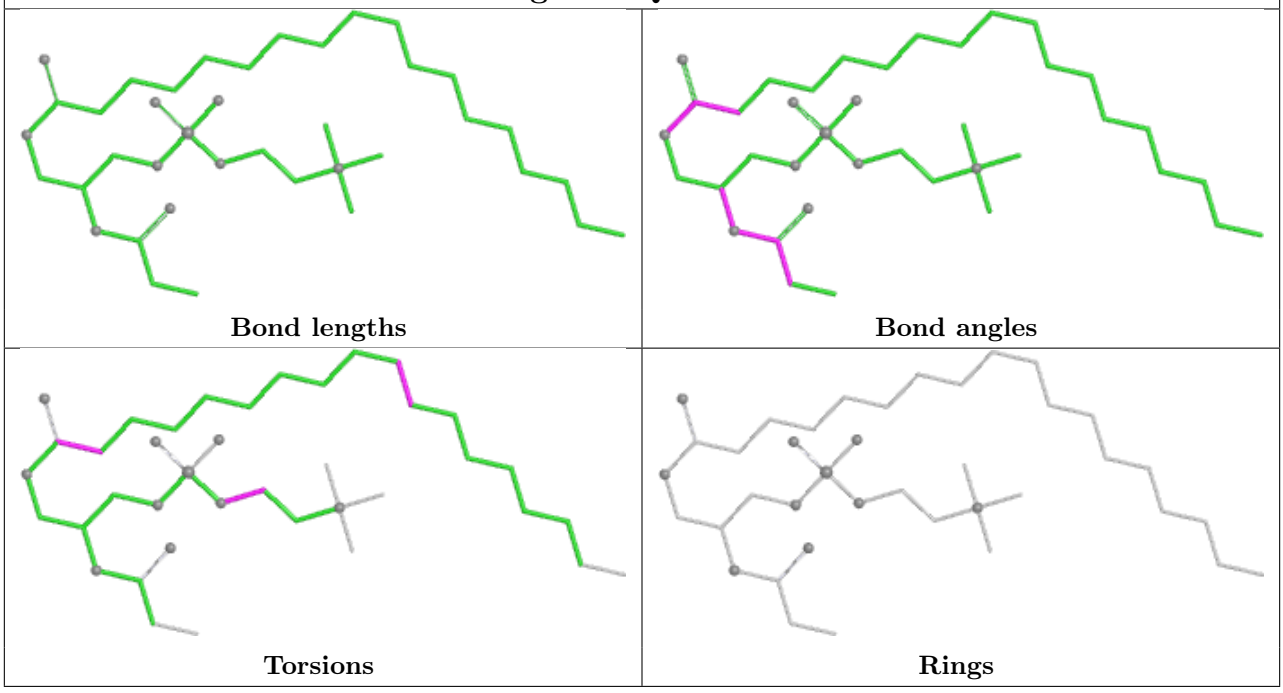


Rings

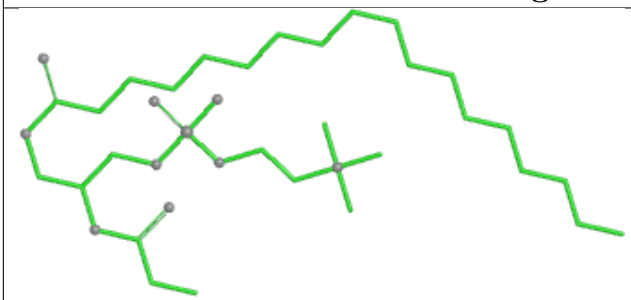
Ligand 7Q9 D 547



Ligand 7Q9 D 529



Ligand 7Q9 E 841



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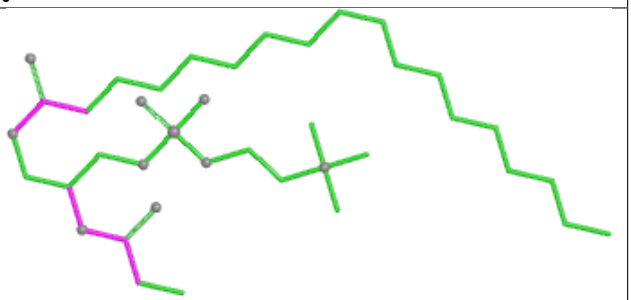
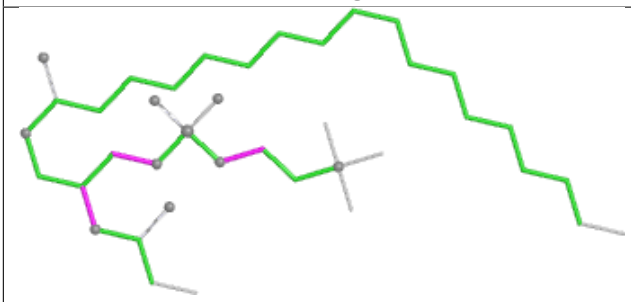


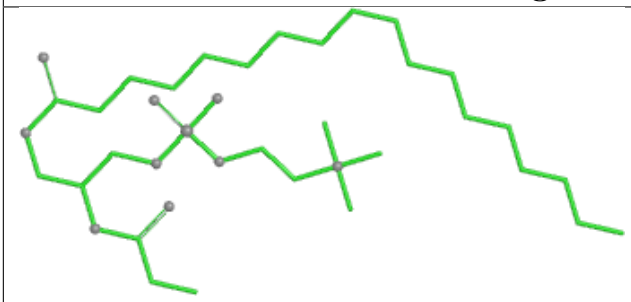
Bond angles



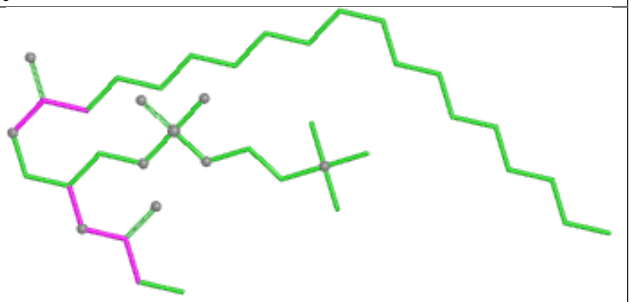
Torsions

Rings

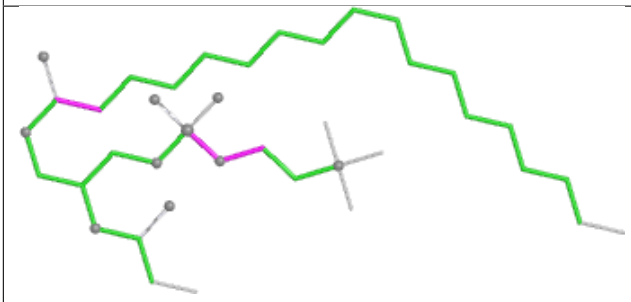
Ligand 7Q9 E 809



Bond lengths



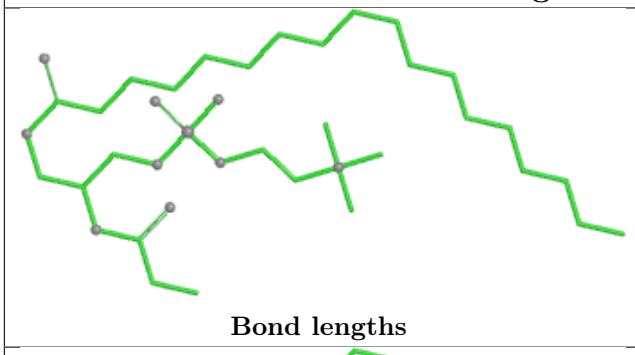
Bond angles



Torsions

Rings

Ligand 7Q9 E 867



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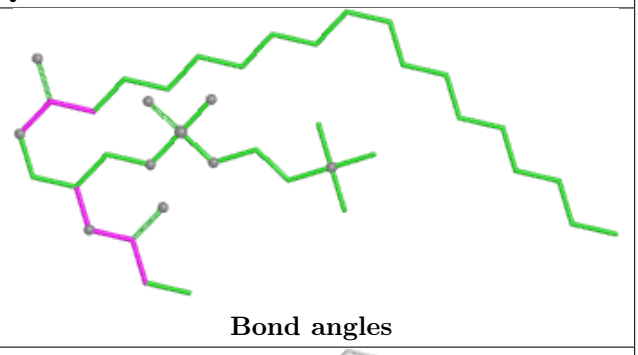
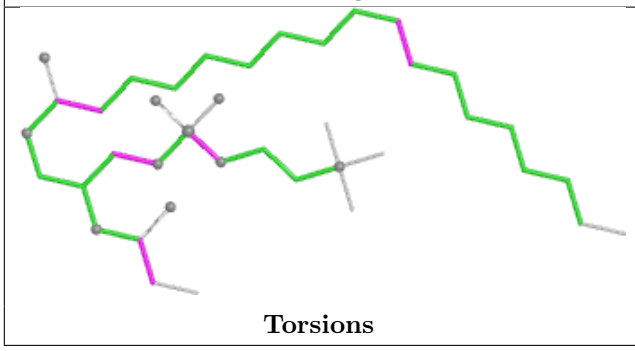


Bond angles



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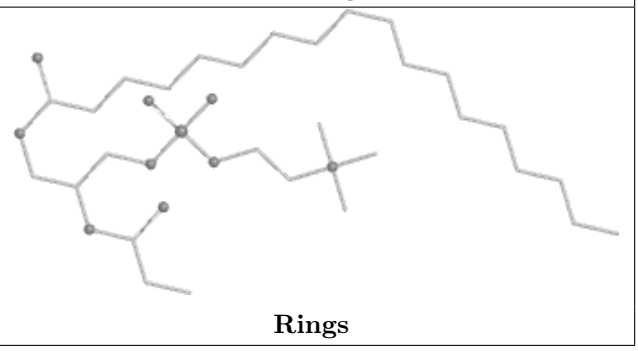
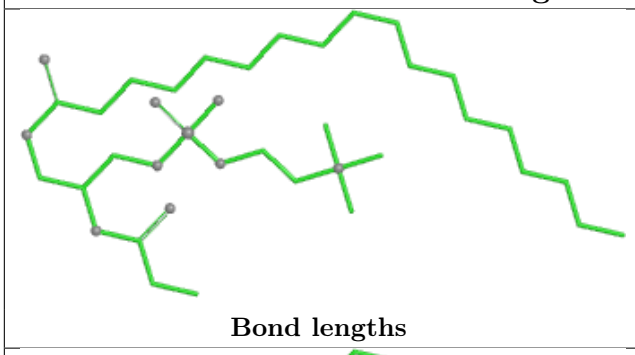
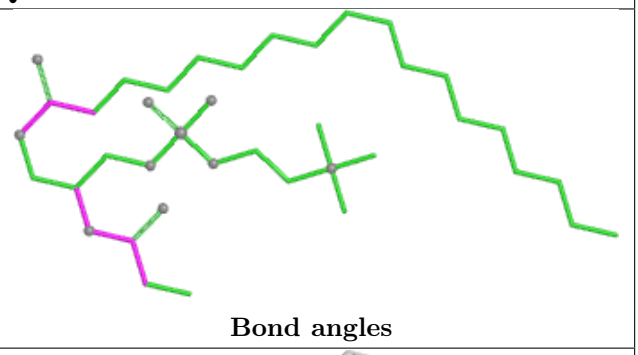


Rings

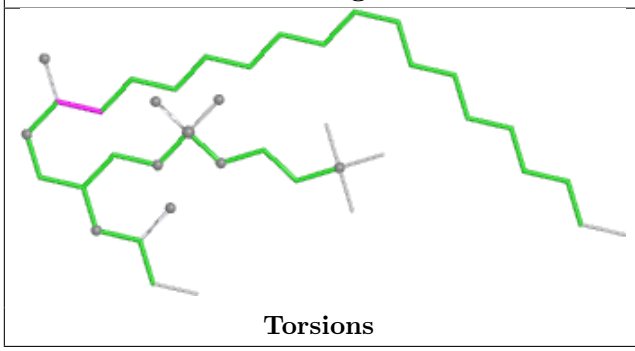
Ligand 7Q9 E 849



Bond lengths



Bond angles



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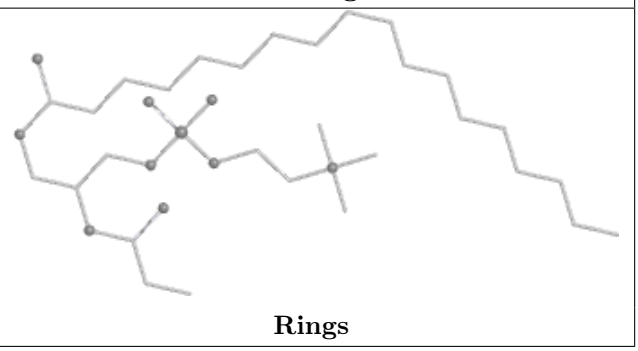
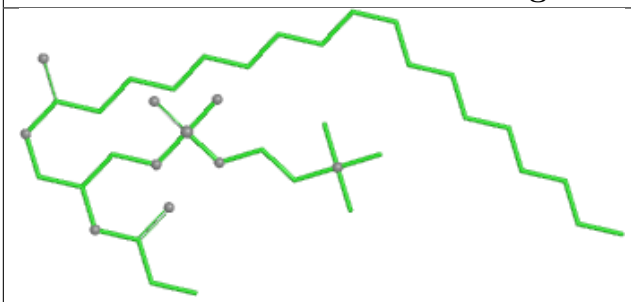


Rings

Ligand 7Q9 D 513



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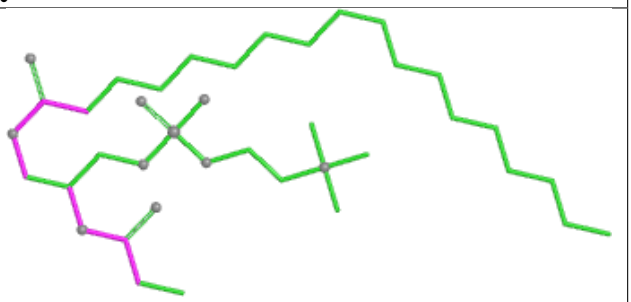
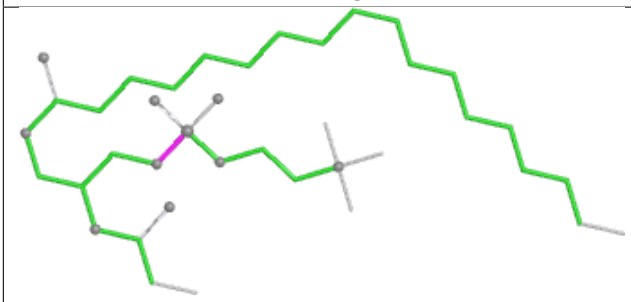


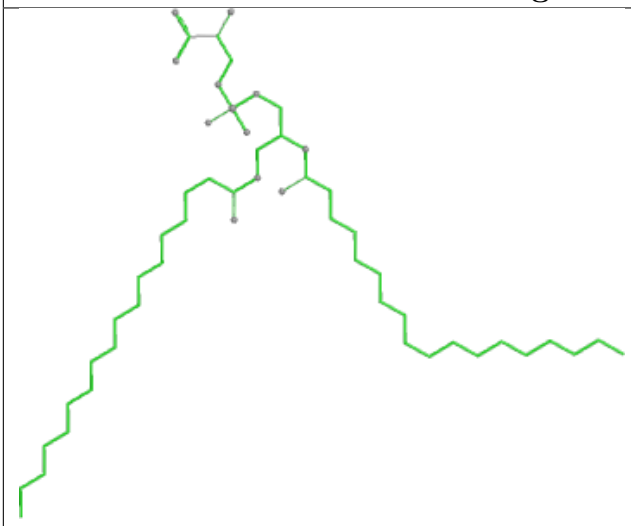
Bond angles



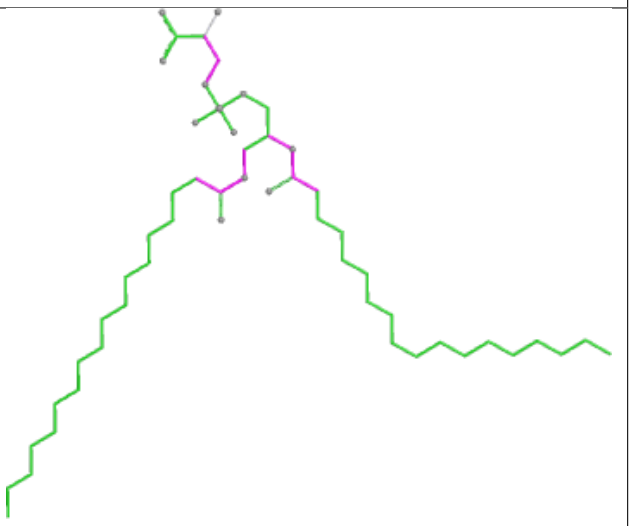
Torsions

Rings

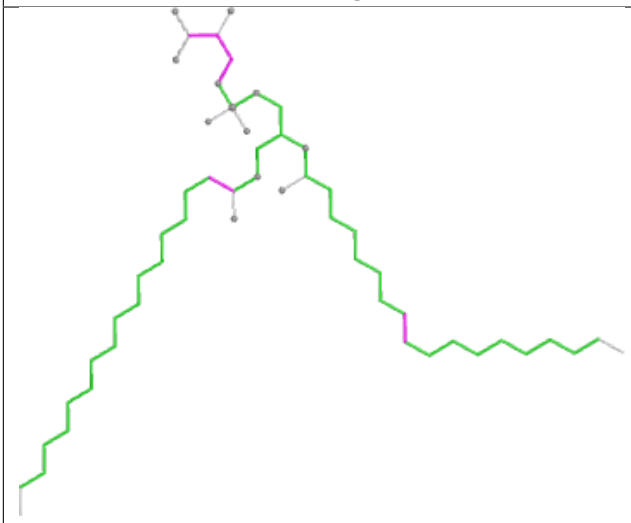
Ligand 17F D 552



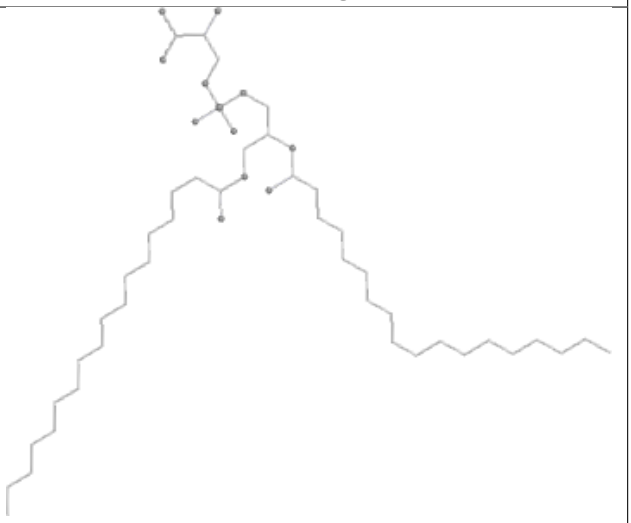
Bond lengths



Bond angles

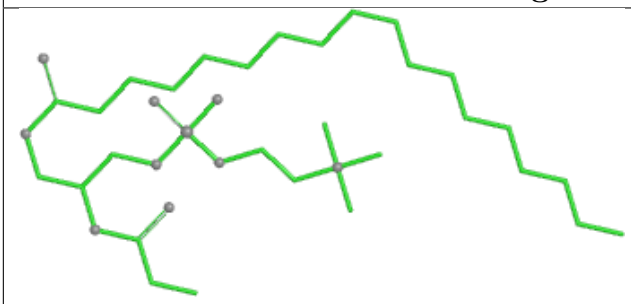


Torsions

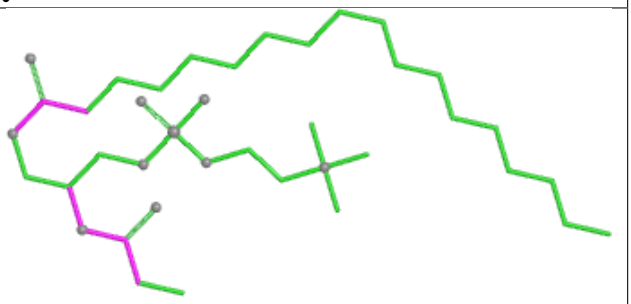


Rings

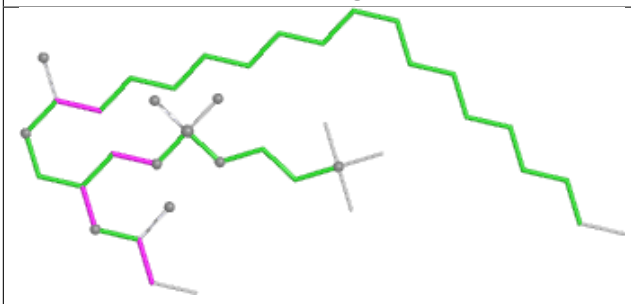
Ligand 7Q9 E 840



Bond lengths



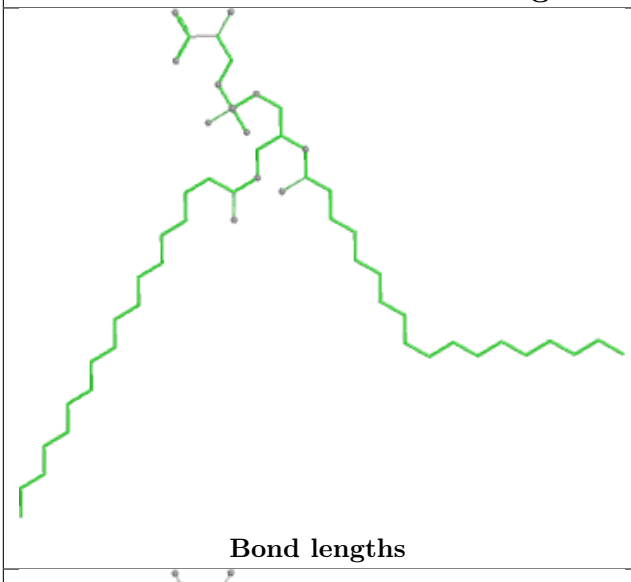
Bond angles



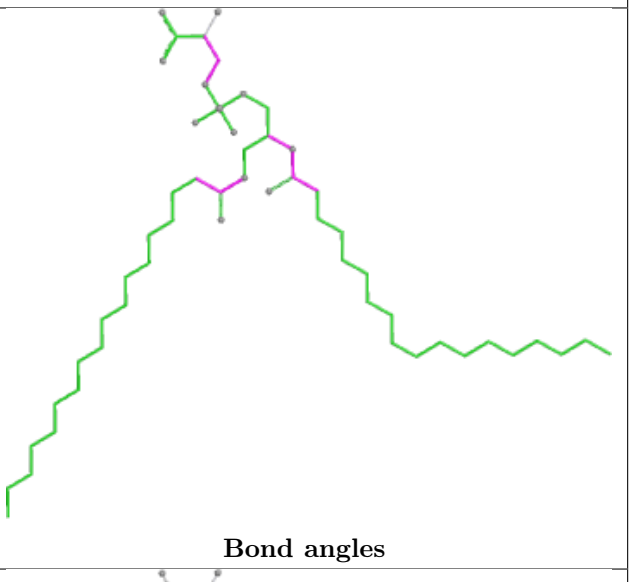
Torsions

Rings

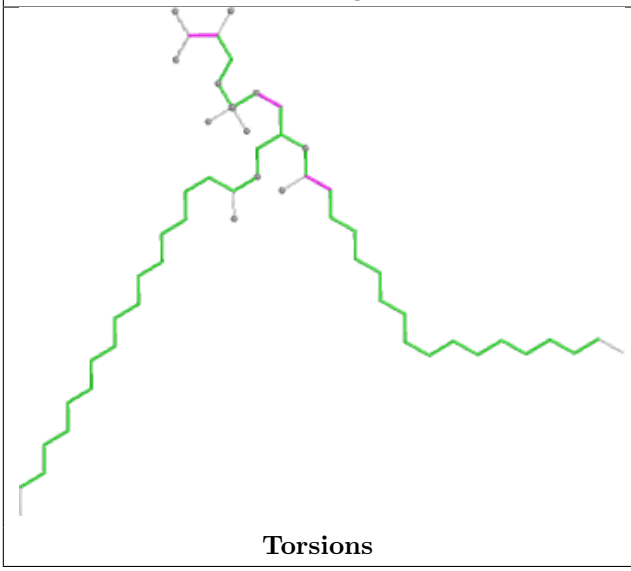
Ligand 17F A 213



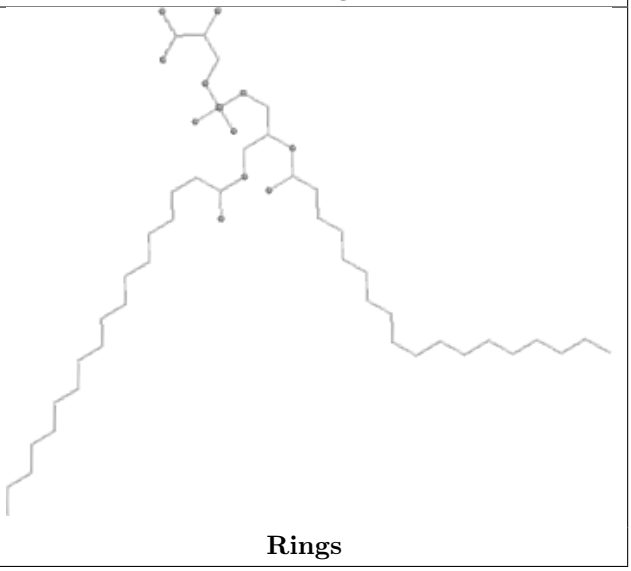
Bond lengths



Bond angles

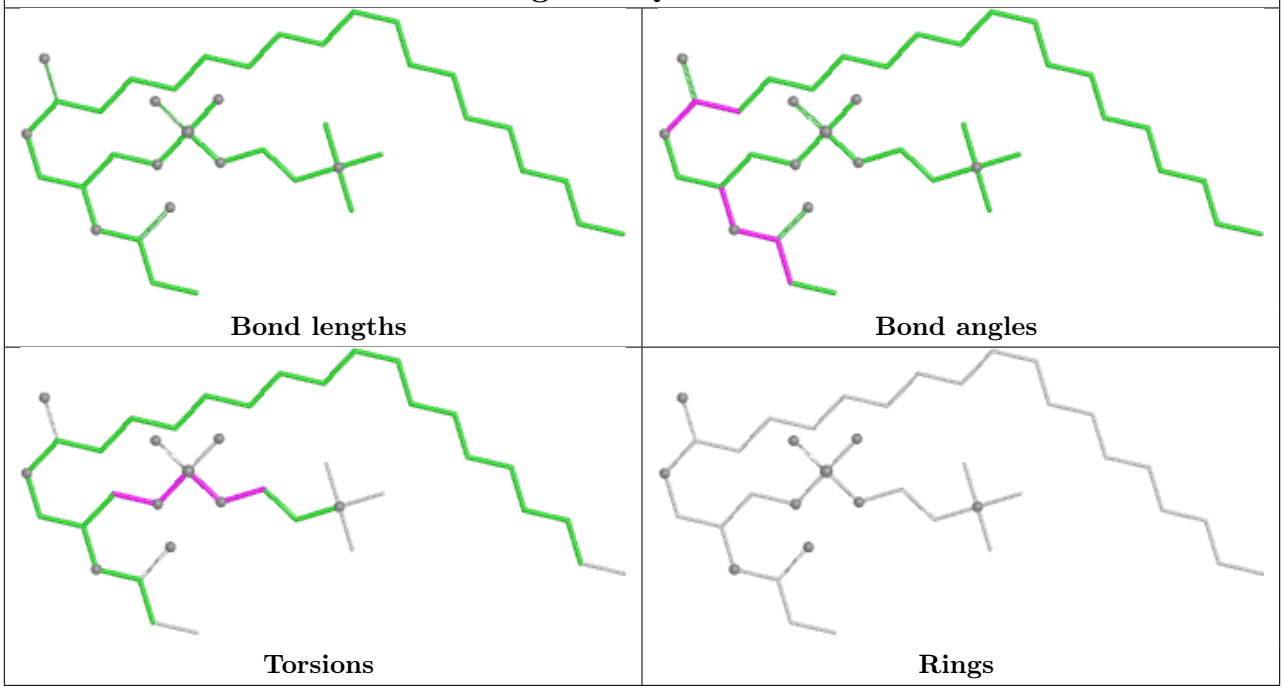


Torsions

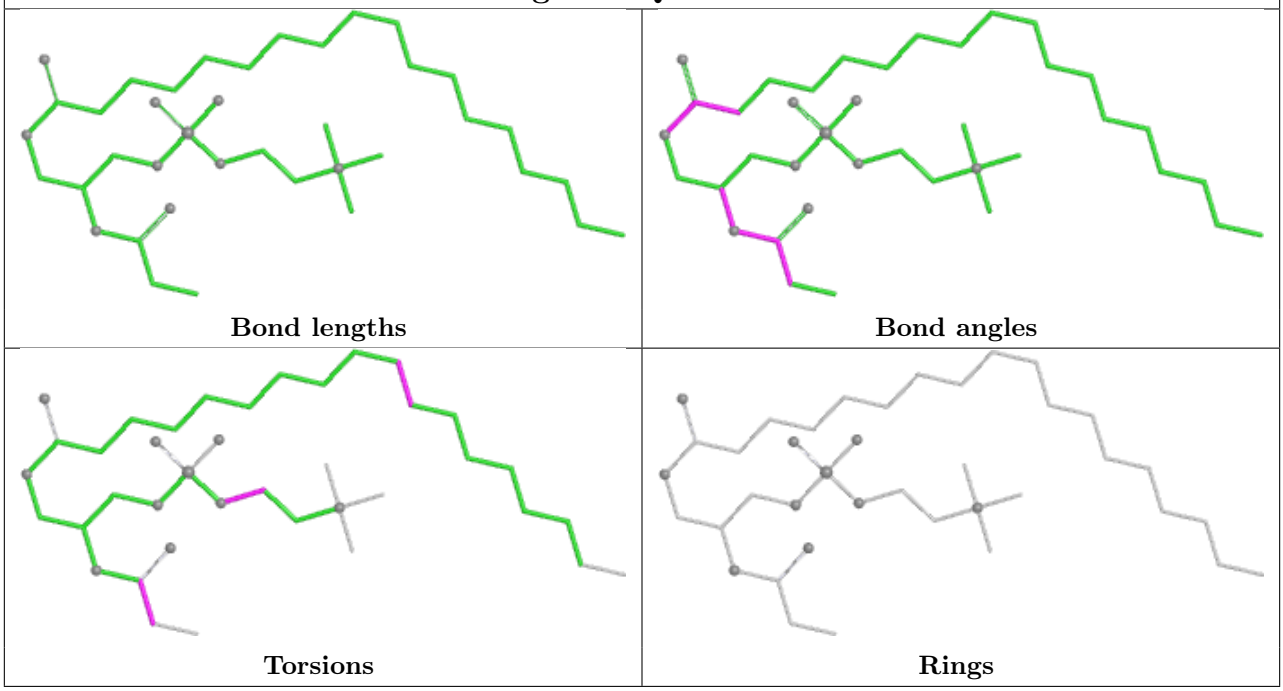


Rings

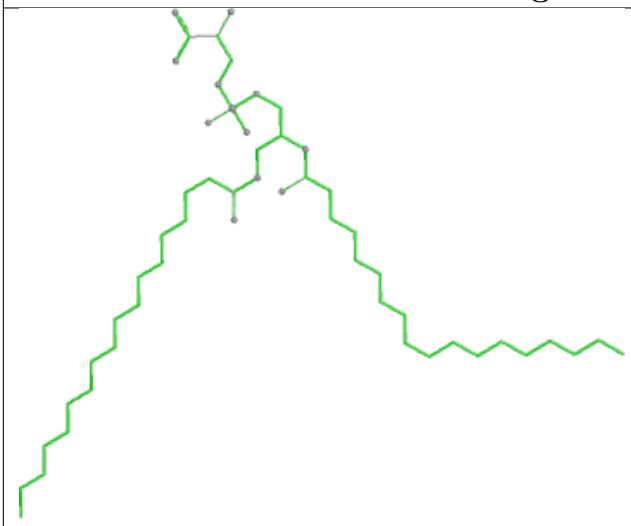
Ligand 7Q9 B 209



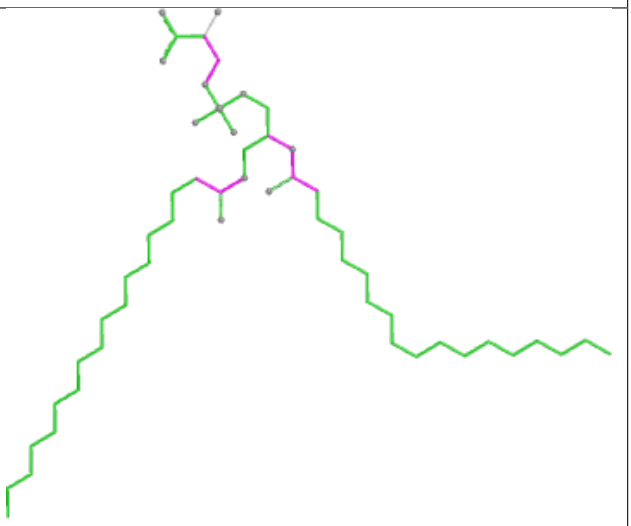
Ligand 7Q9 E 801



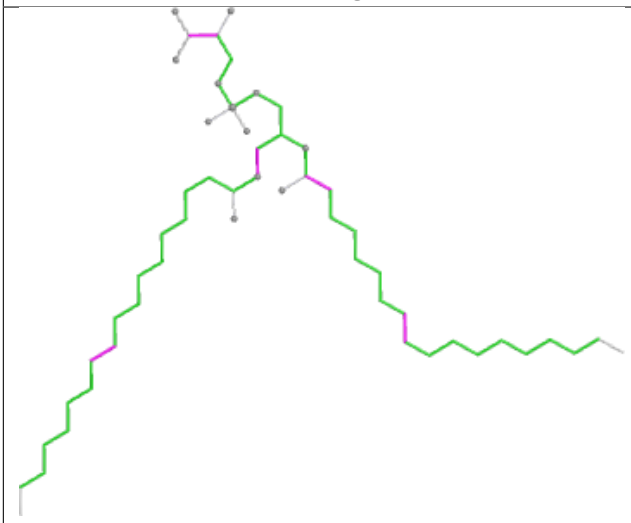
Ligand 17F A 220



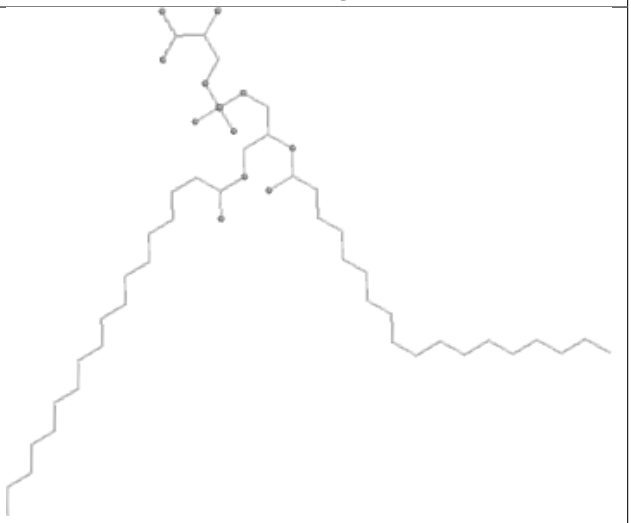
Bond lengths



Bond angles

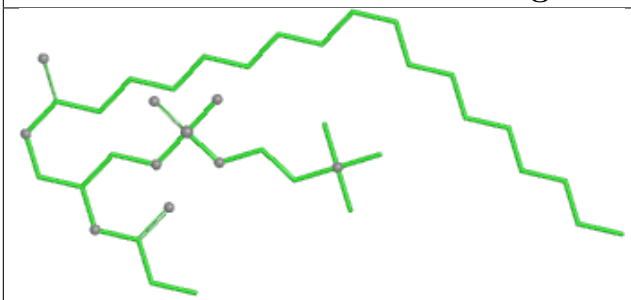


Torsions

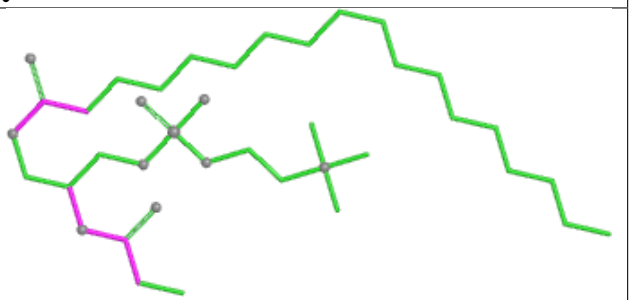


Rings

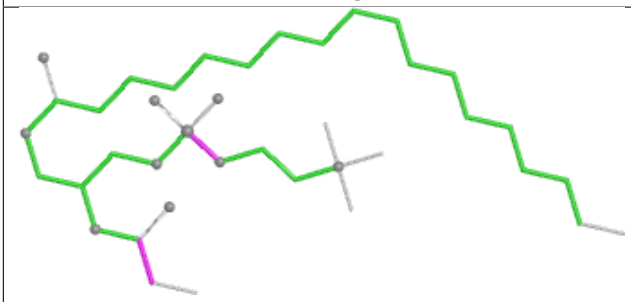
Ligand 7Q9 E 858



Bond lengths



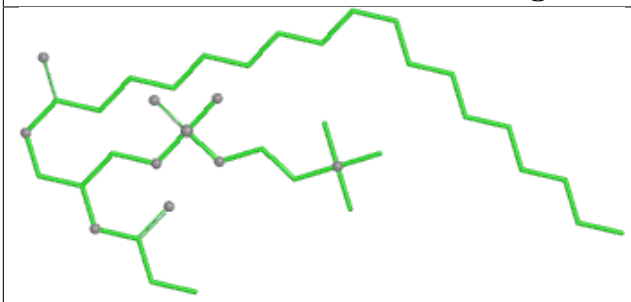
Bond angles



Torsions

Rings

Ligand 7Q9 D 544



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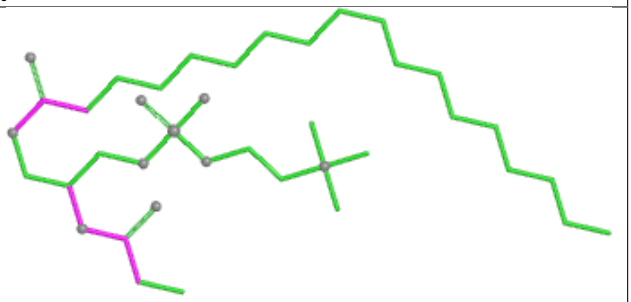
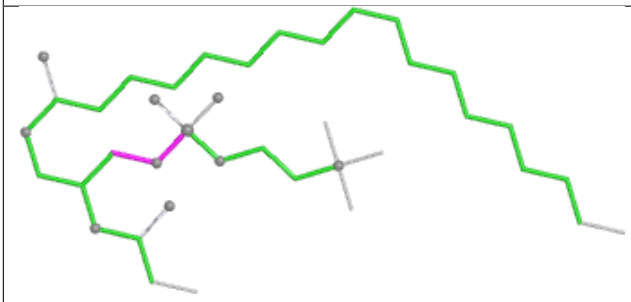


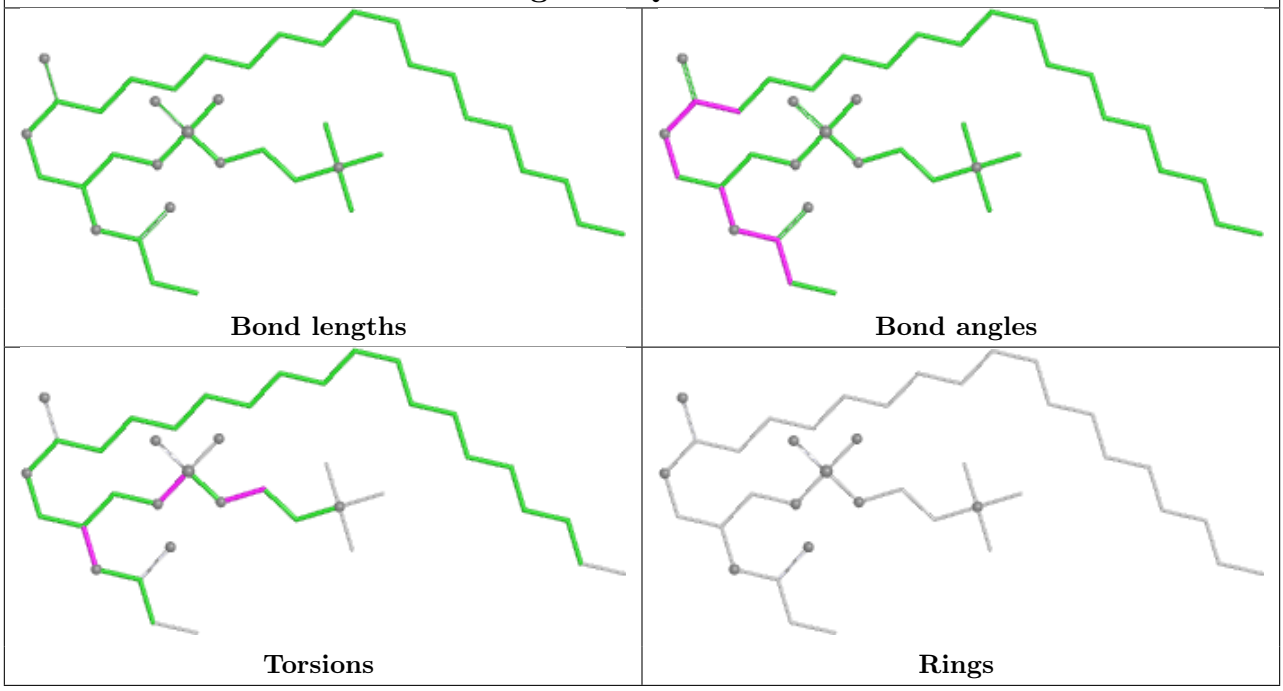
Bond angles



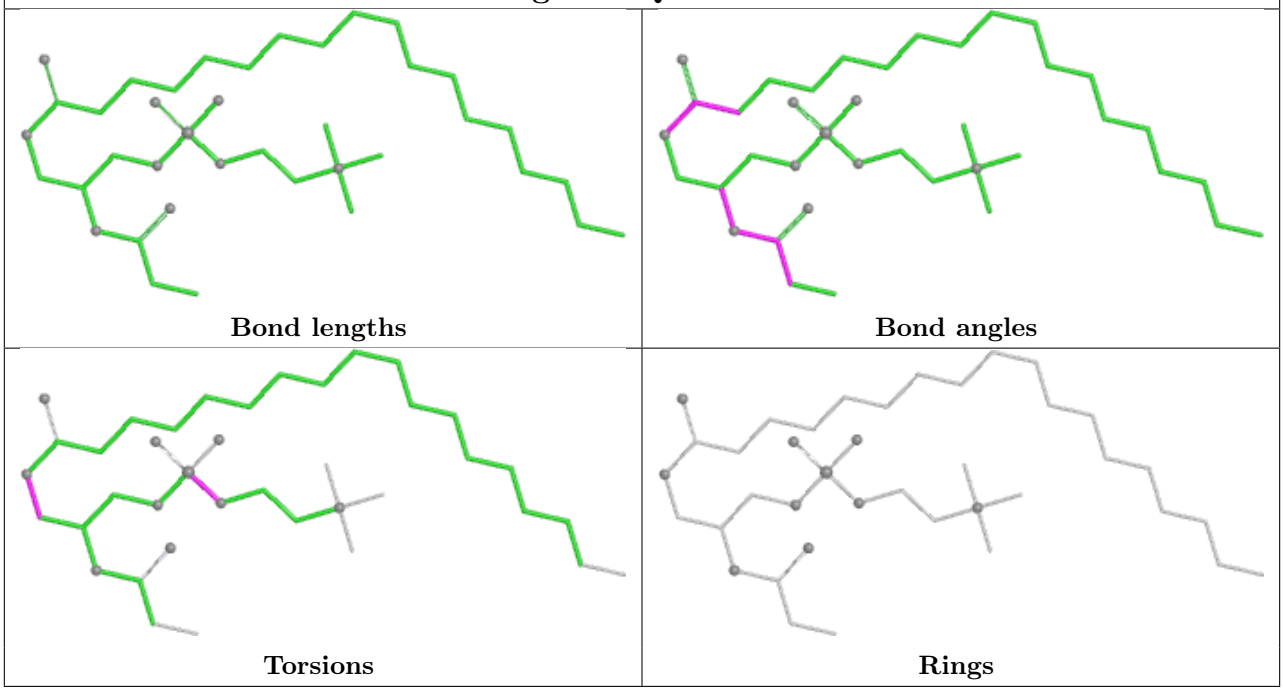
Torsions

Rings

Ligand 7Q9 D 553



Ligand 7Q9 E 803



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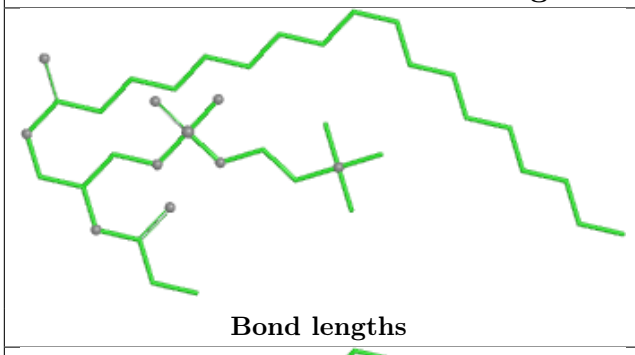

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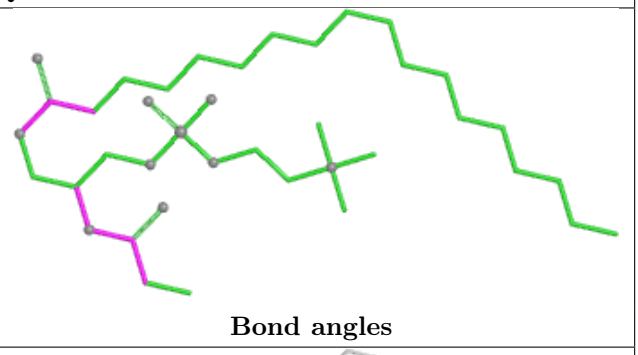
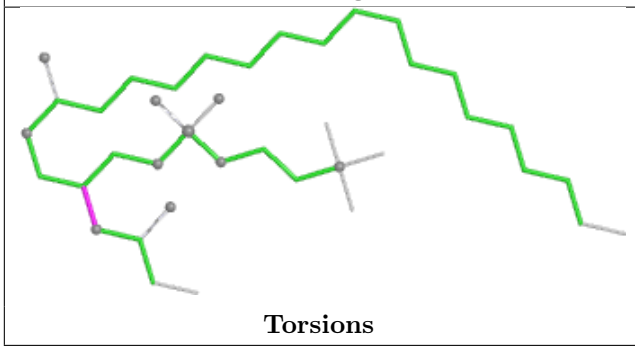


Bond angles



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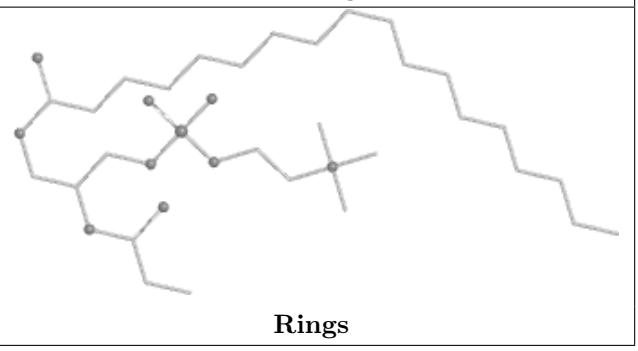
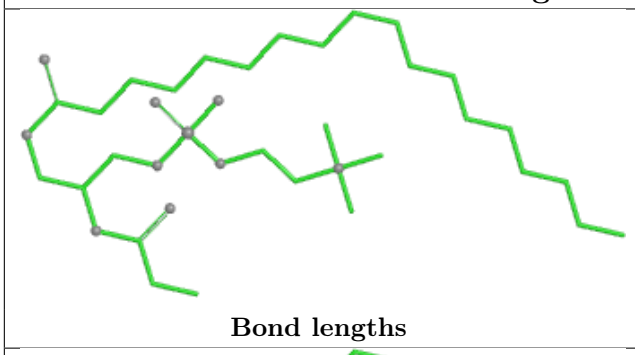


Rings

Ligand 7Q9 E 805



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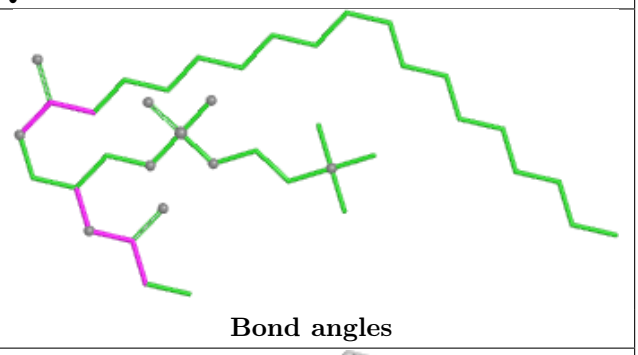
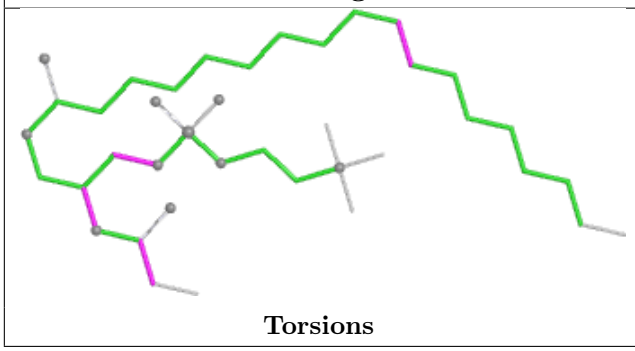


Bond angles



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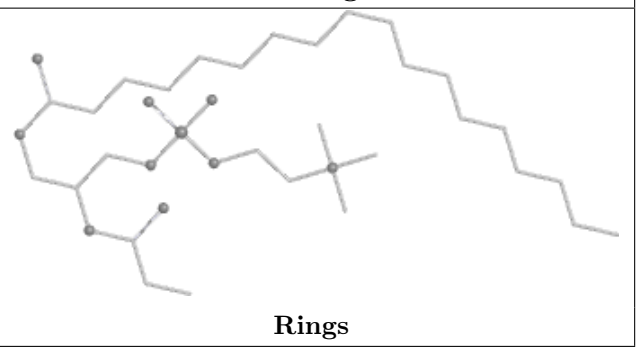
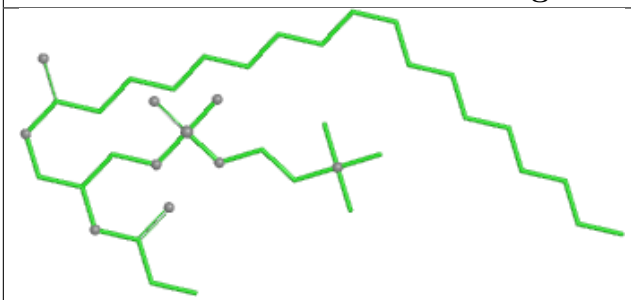


Rings

Ligand 7Q9 E 807



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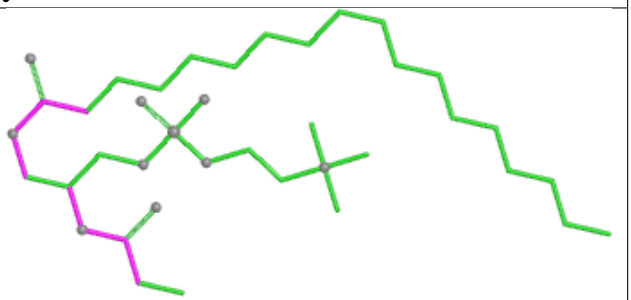
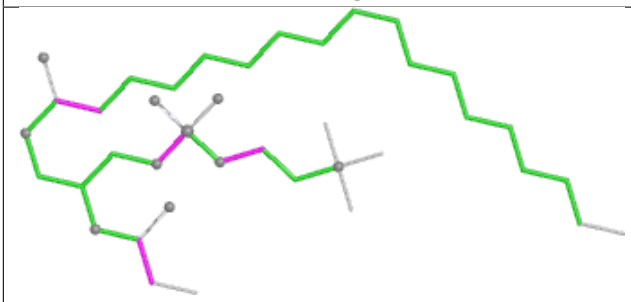


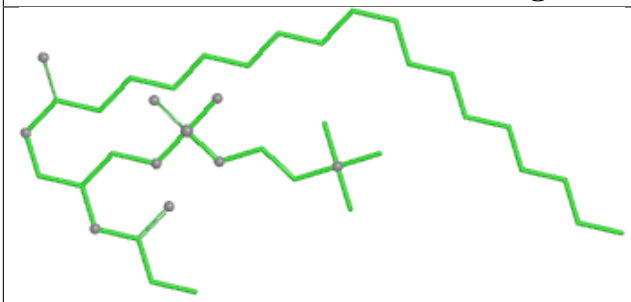
Bond angles



Torsions

Rings

Ligand 7Q9 D 521



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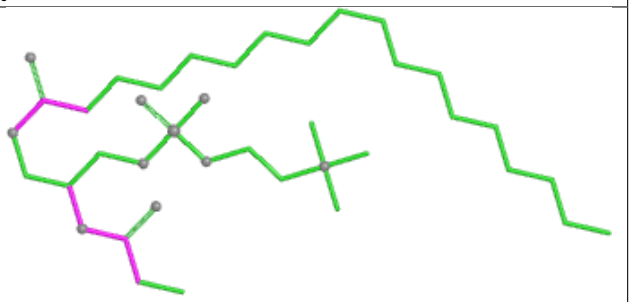
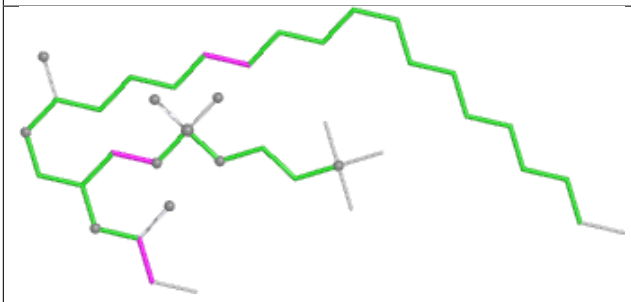


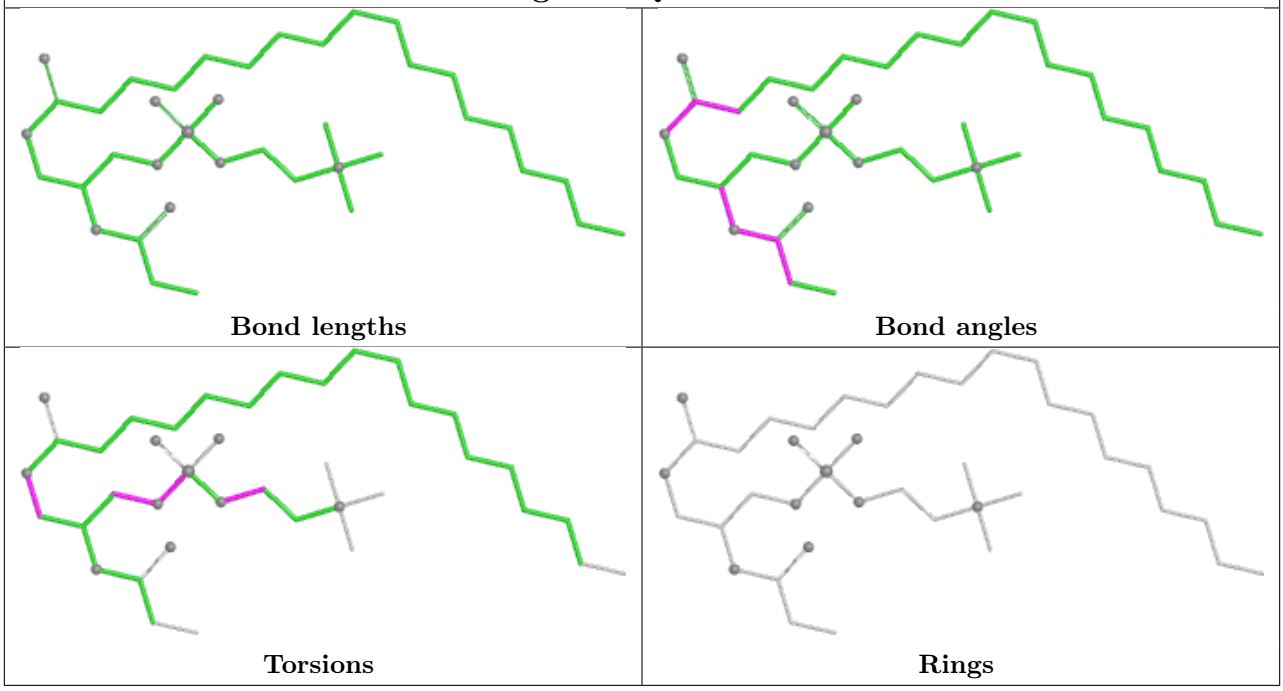
Bond angles



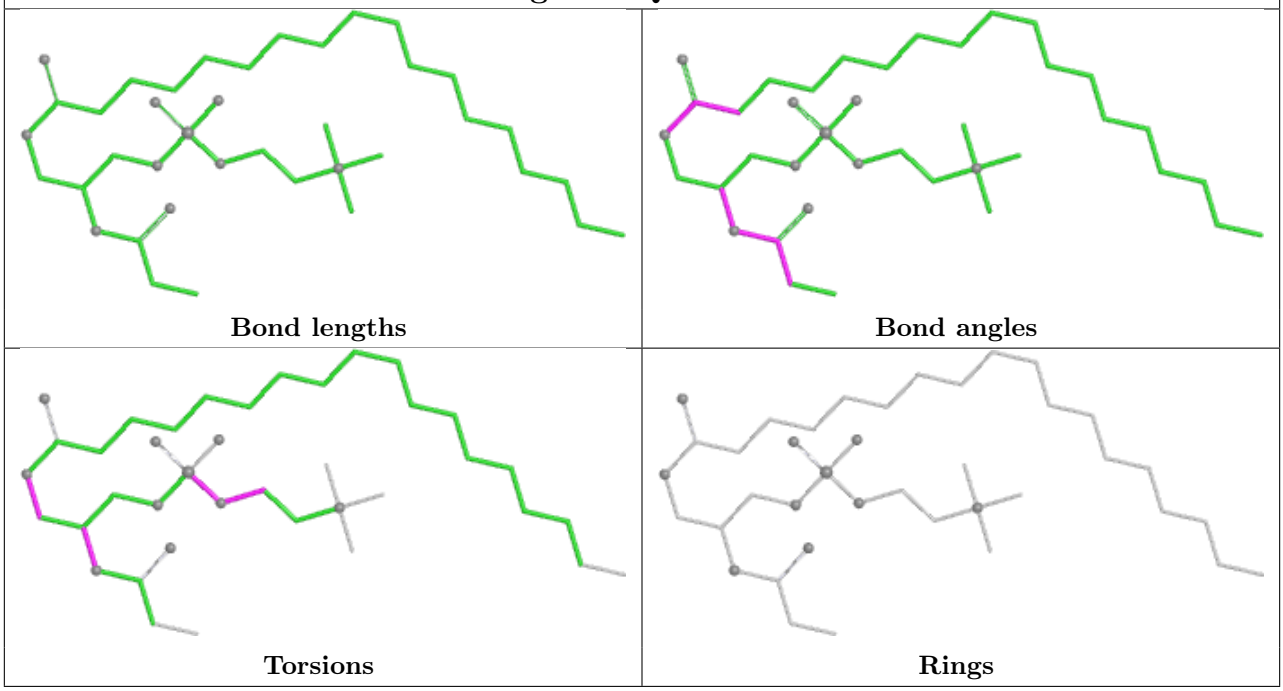
Torsions

Rings

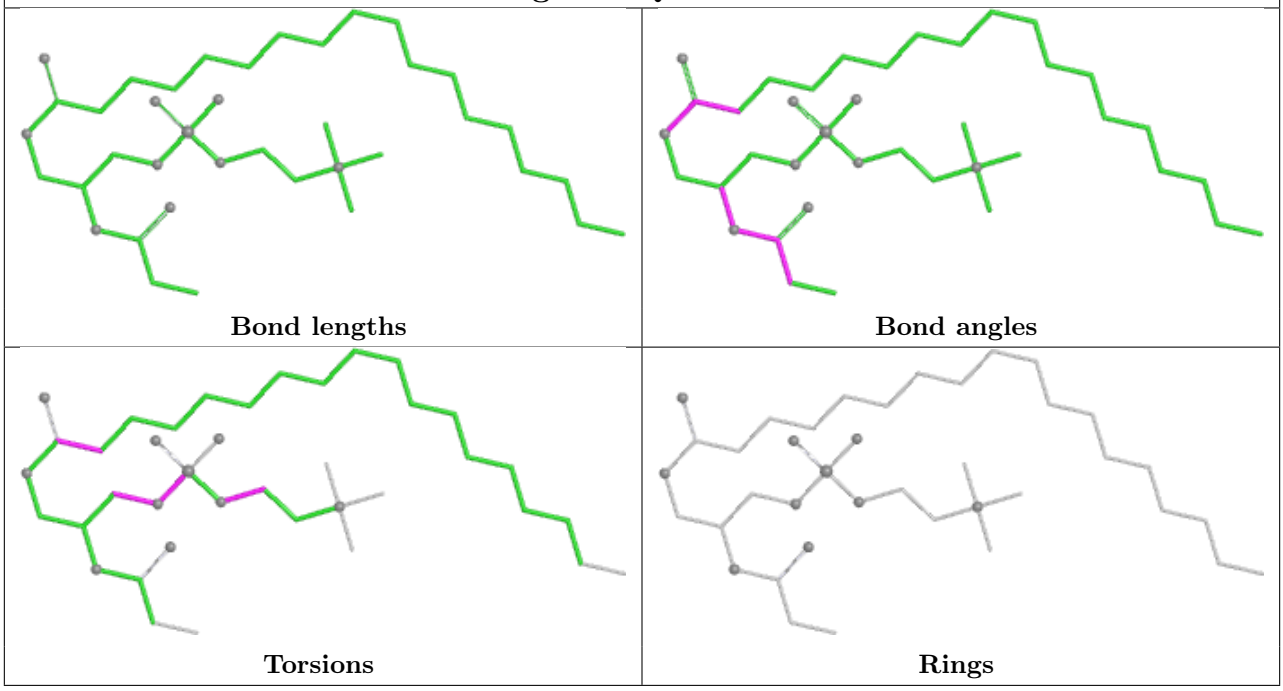
Ligand 7Q9 E 865



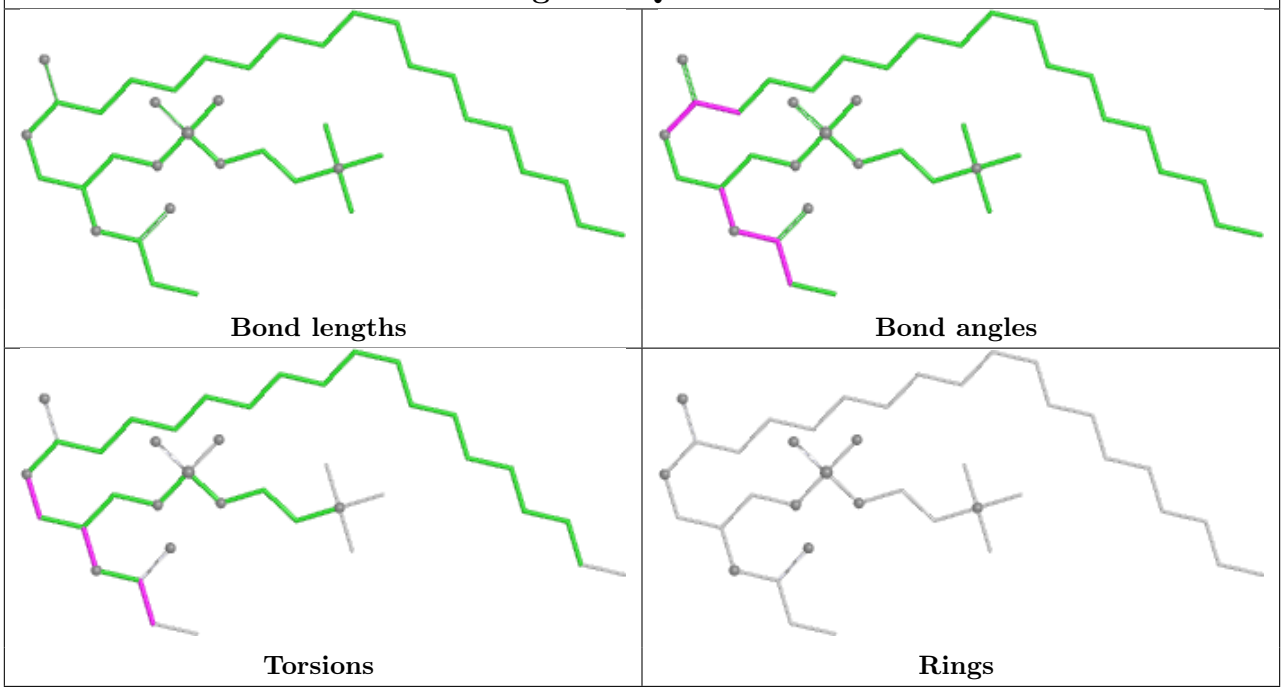
Ligand 7Q9 D 555



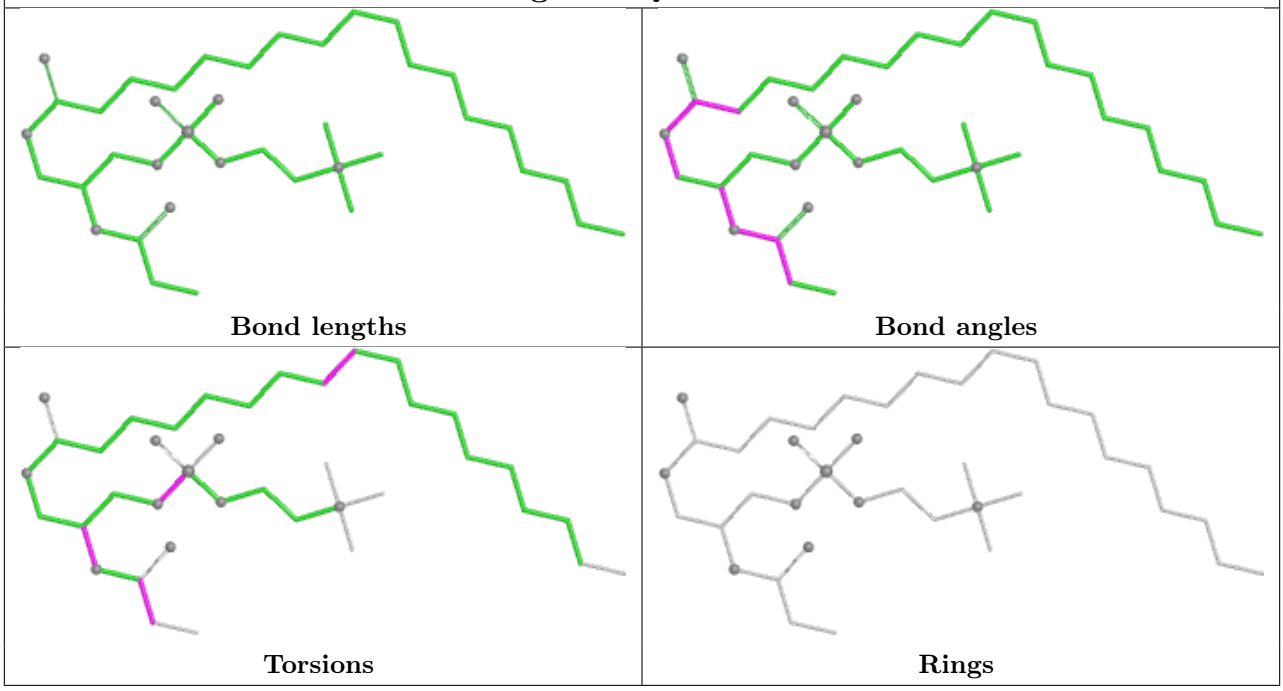
Ligand 7Q9 E 821



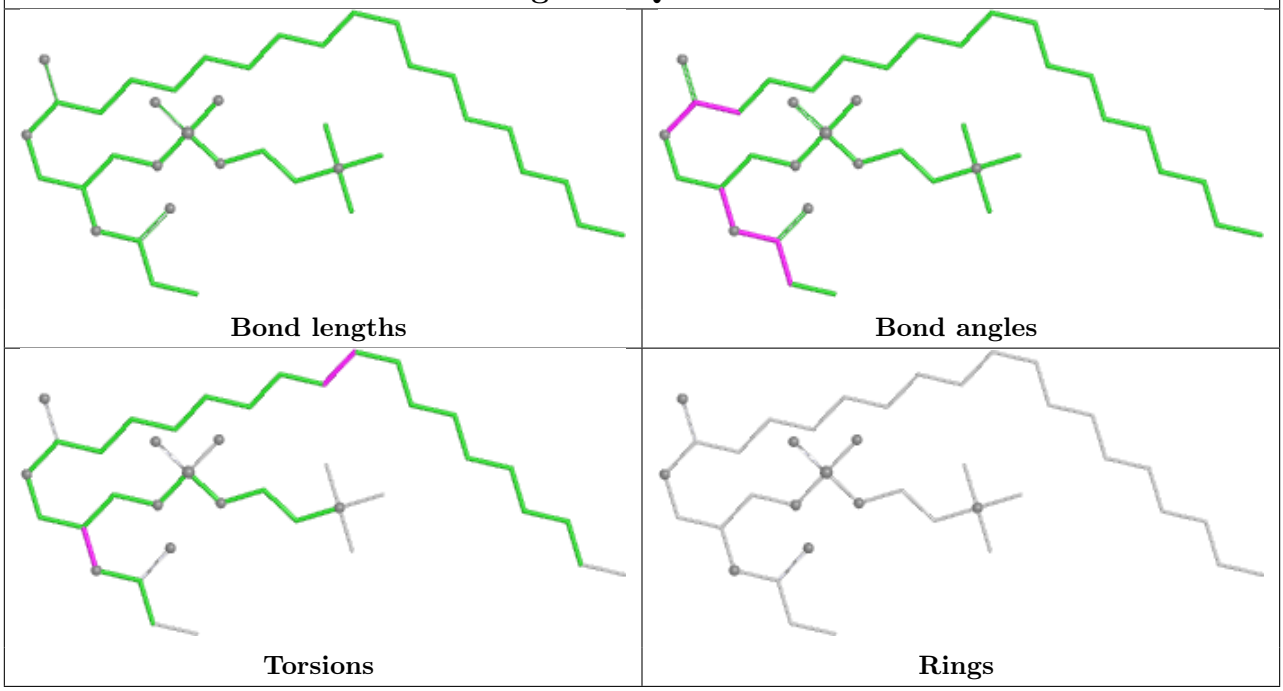
Ligand 7Q9 E 811



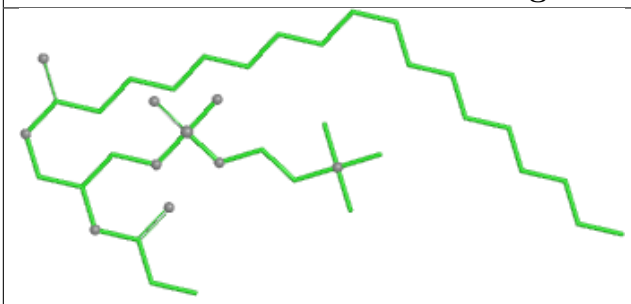
Ligand 7Q9 A 216



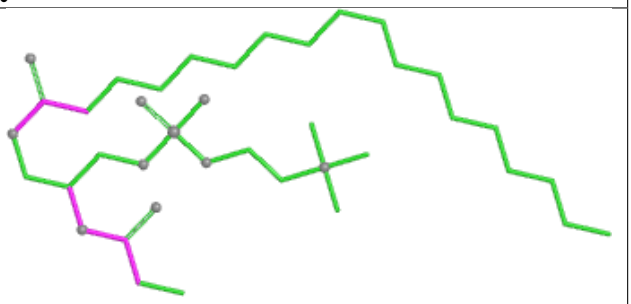
Ligand 7Q9 B 207



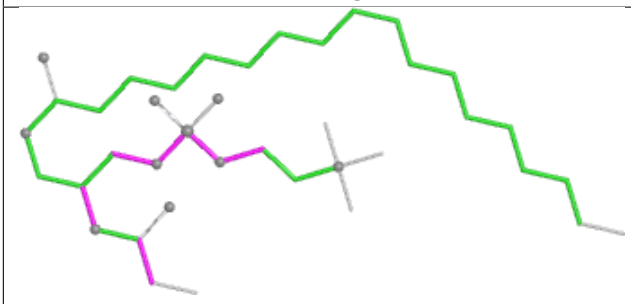
Ligand 7Q9 D 541



Bond lengths



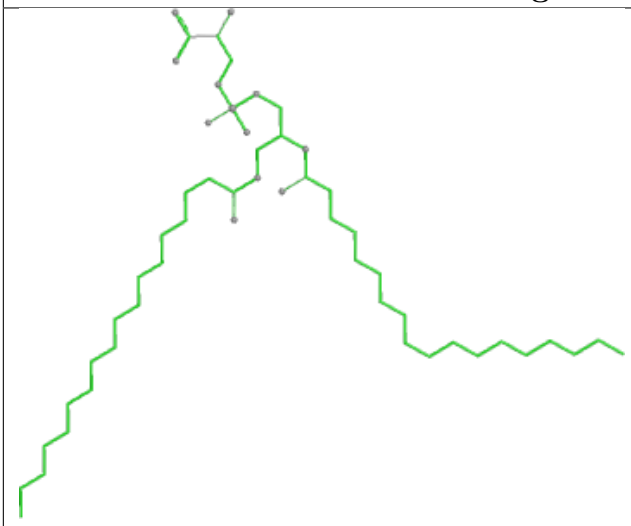
Bond angles



Torsions

Rings

Ligand 17F D 539



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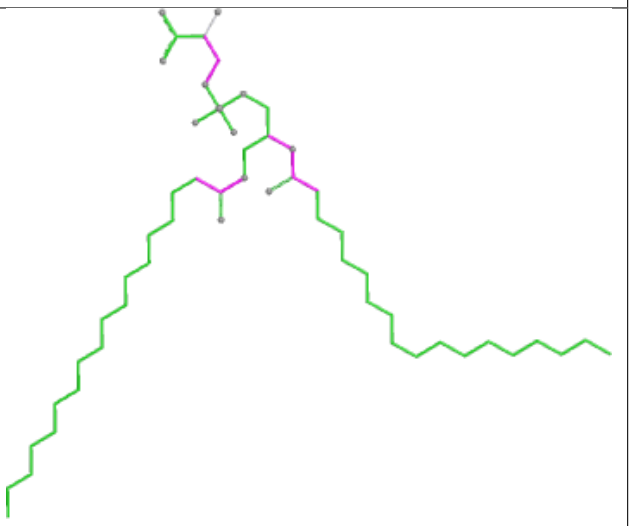
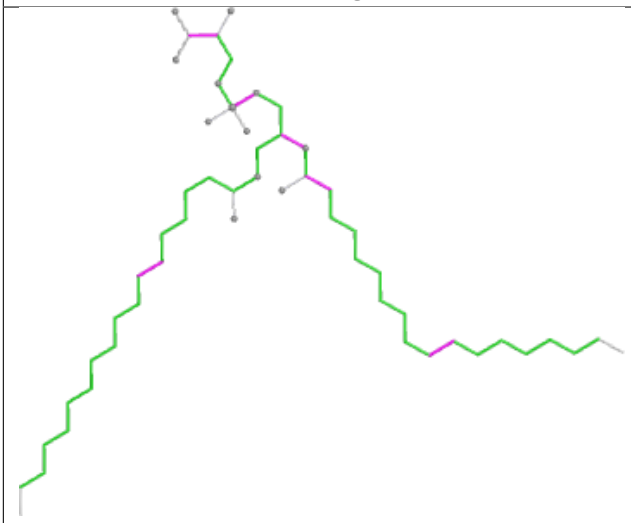
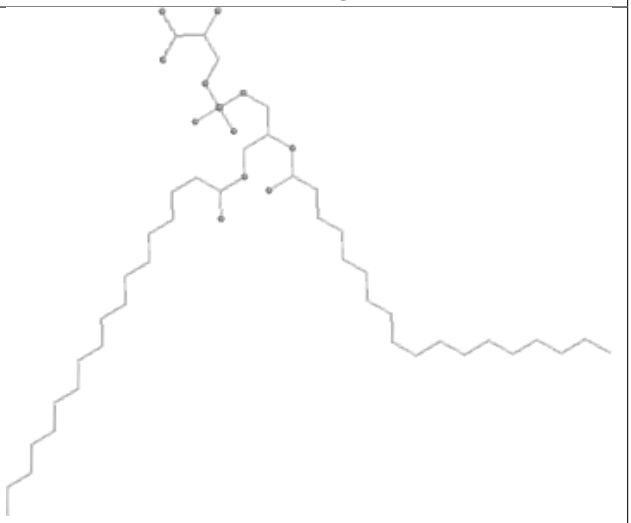


Bond angles

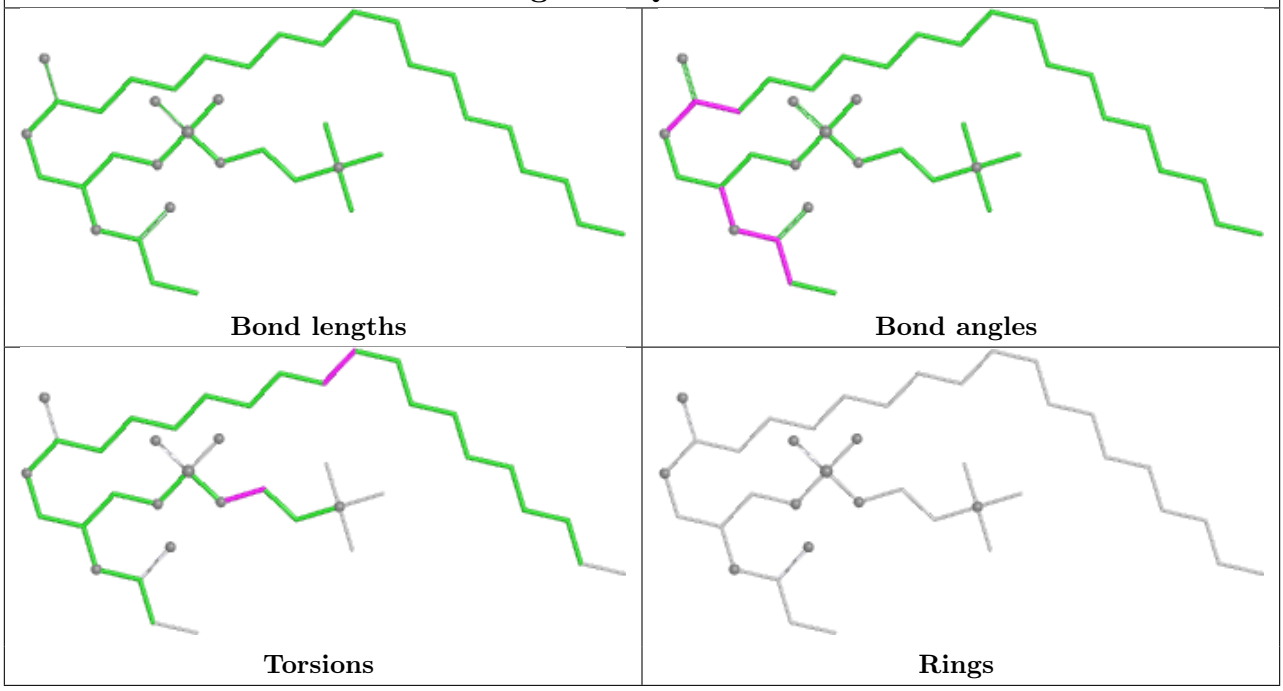


Torsions

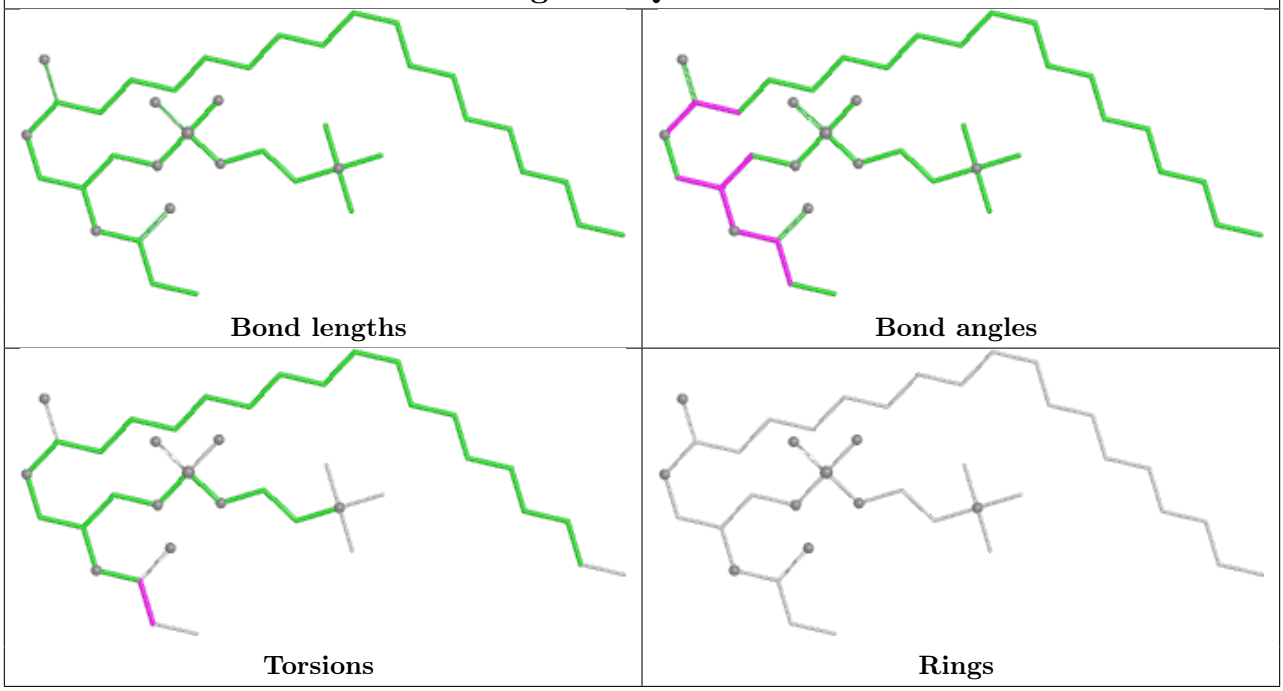


Rings

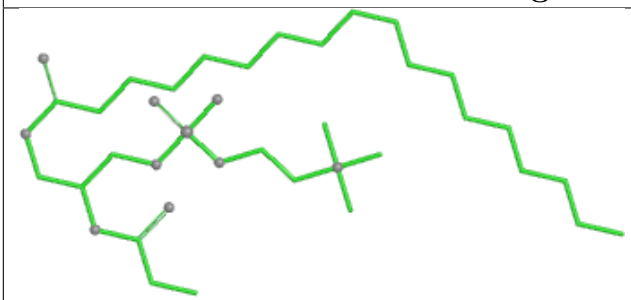
Ligand 7Q9 D 505



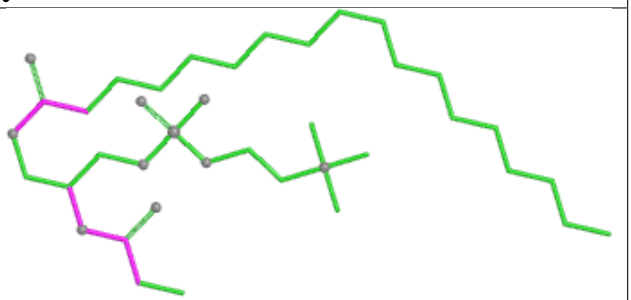
Ligand 7Q9 A 204



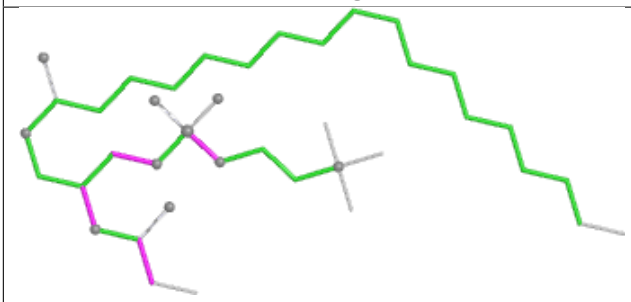
Ligand 7Q9 E 825



Bond lengths



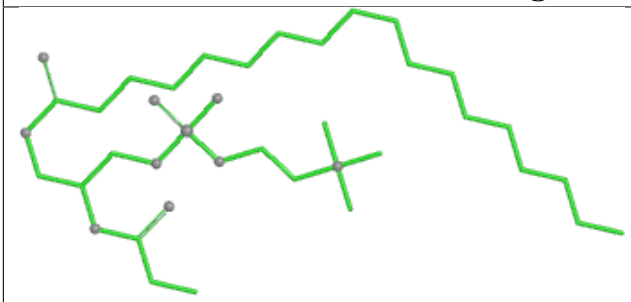
Bond angles



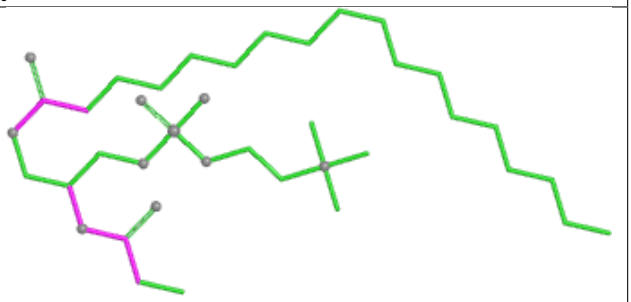
Torsions

Rings

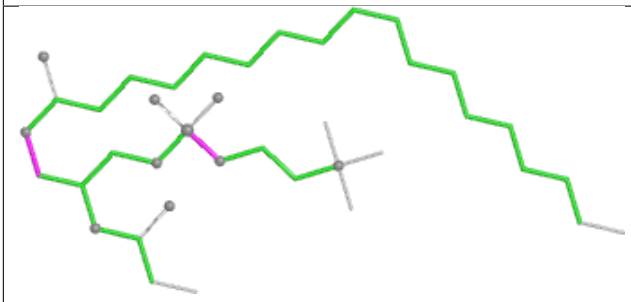
Ligand 7Q9 D 550



Bond lengths



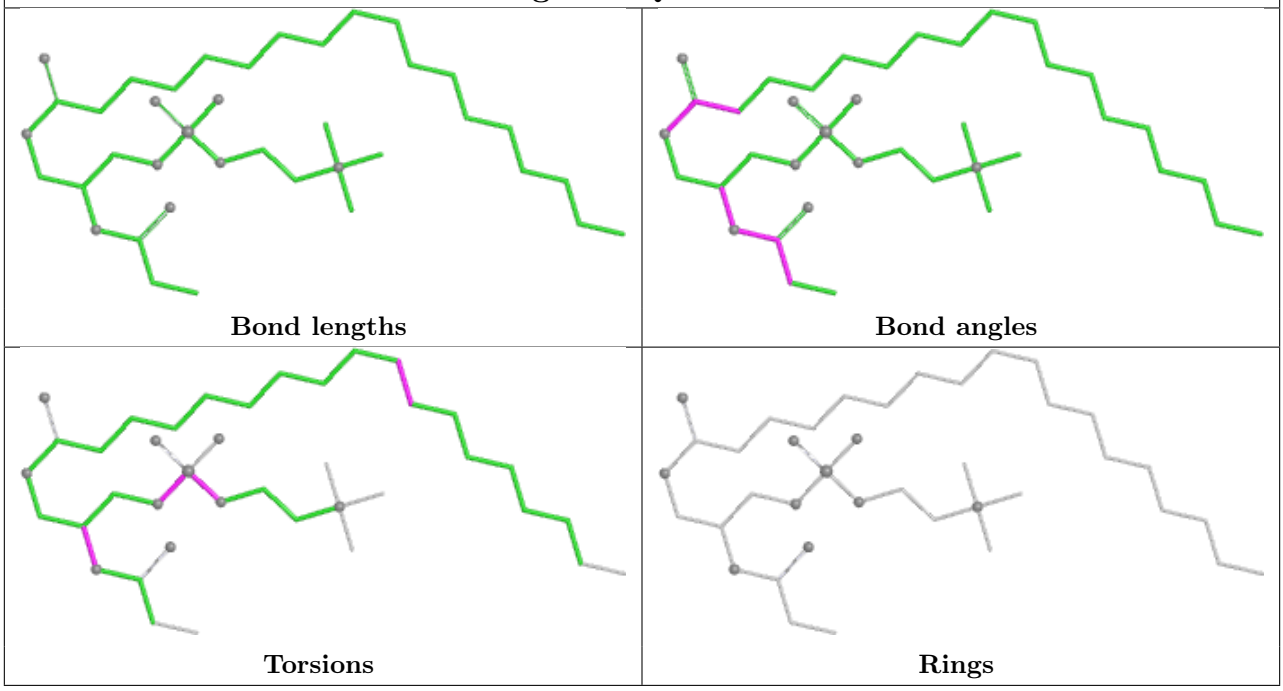
Bond angles



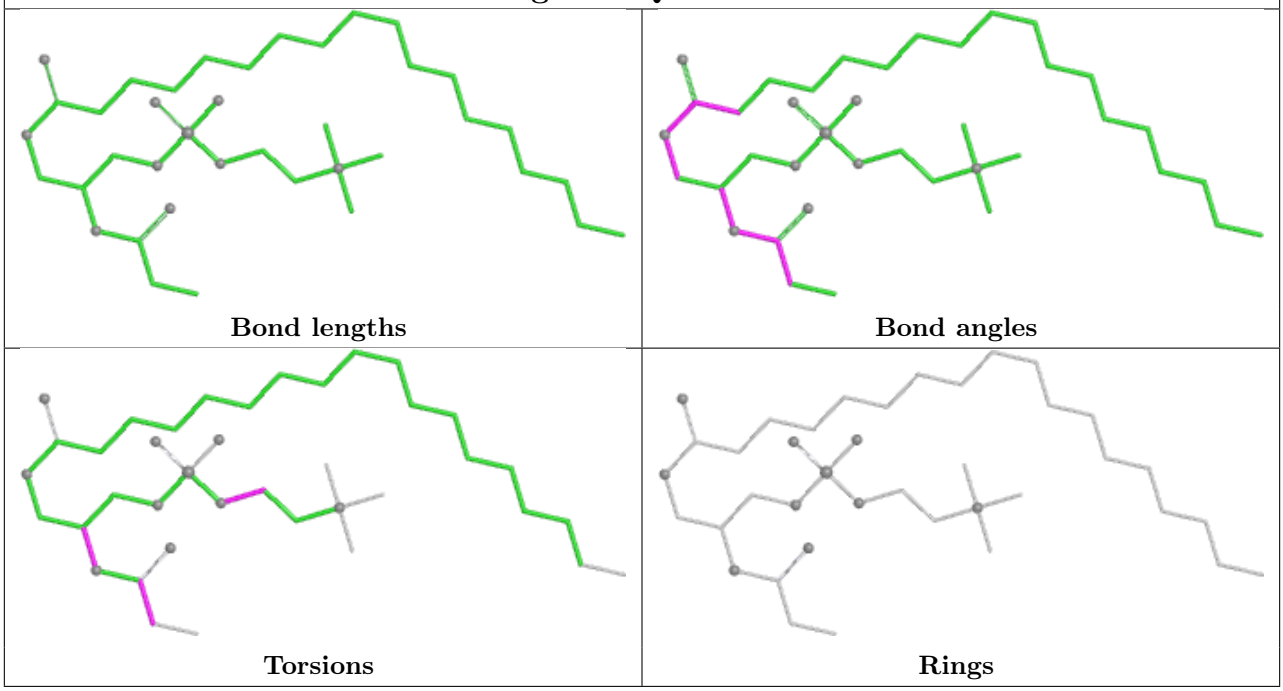
Torsions

Rings

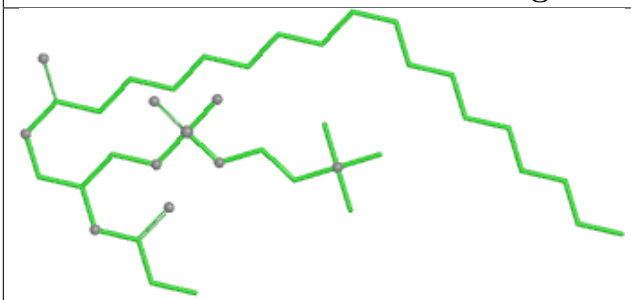
Ligand 7Q9 E 872



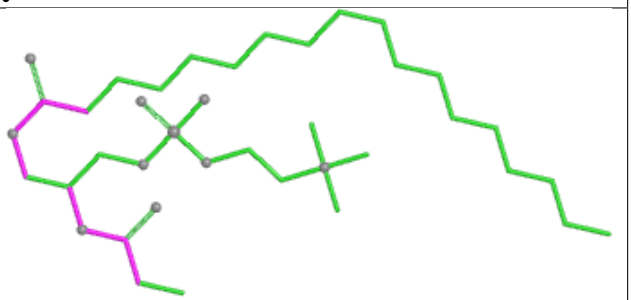
Ligand 7Q9 B 204



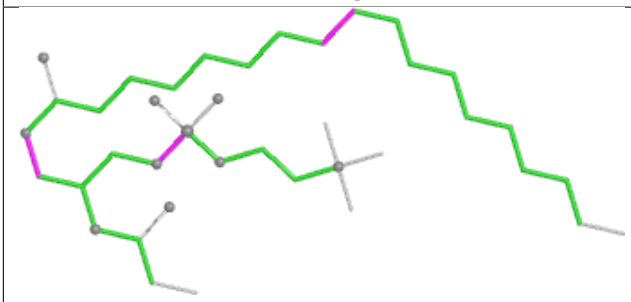
Ligand 7Q9 E 843



Bond lengths



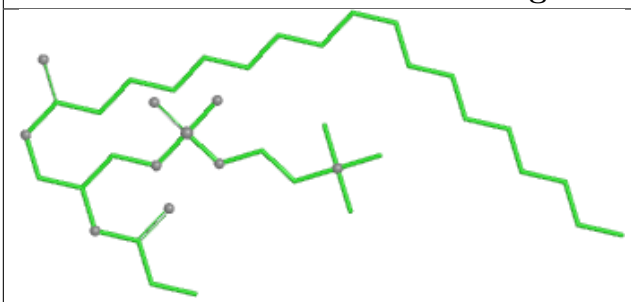
Bond angles



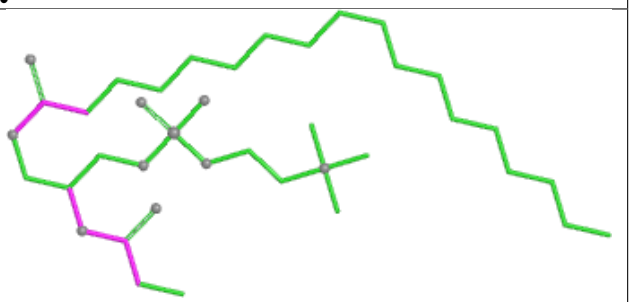
Torsions

Rings

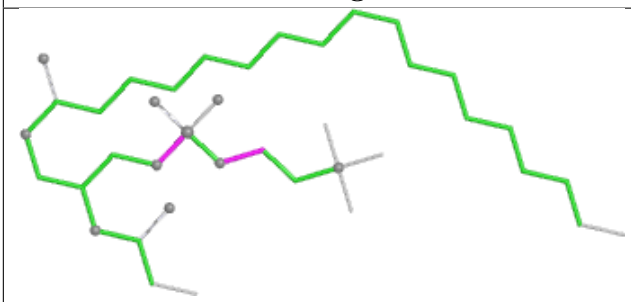
Ligand 7Q9 D 523



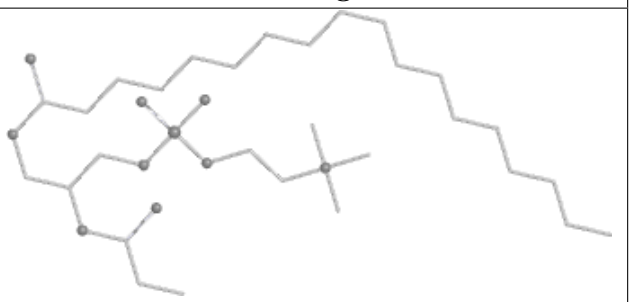
Bond lengths



Bond angles

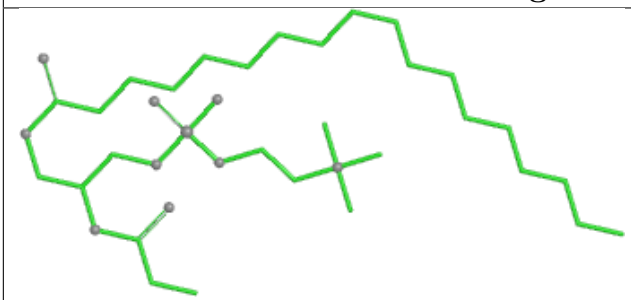


Torsions

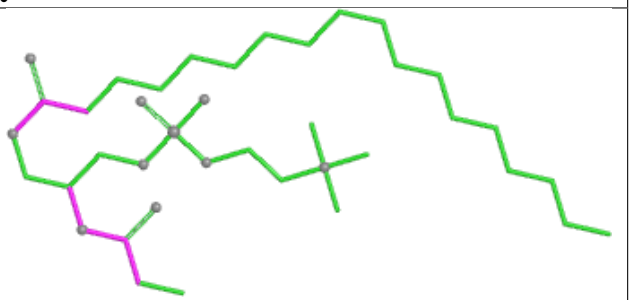


Rings

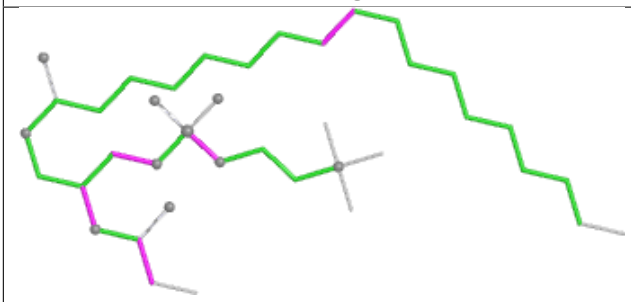
Ligand 7Q9 D 522



Bond lengths



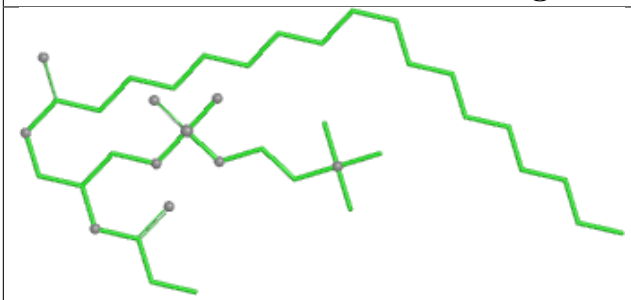
Bond angles



Torsions

Rings

Ligand 7Q9 E 861



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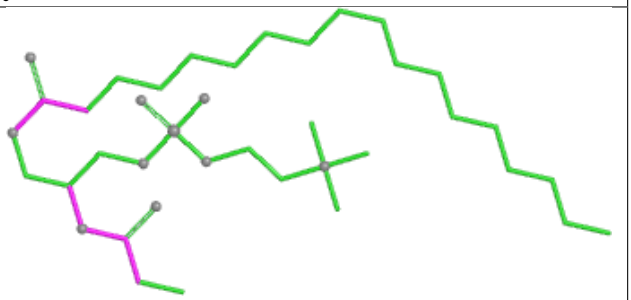
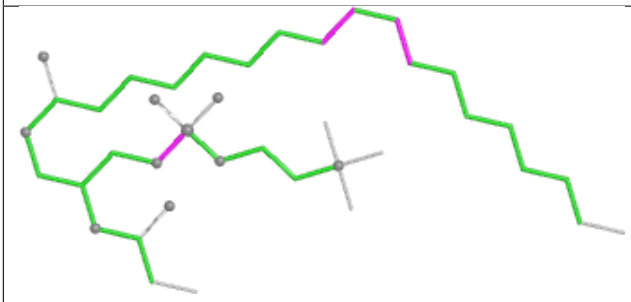


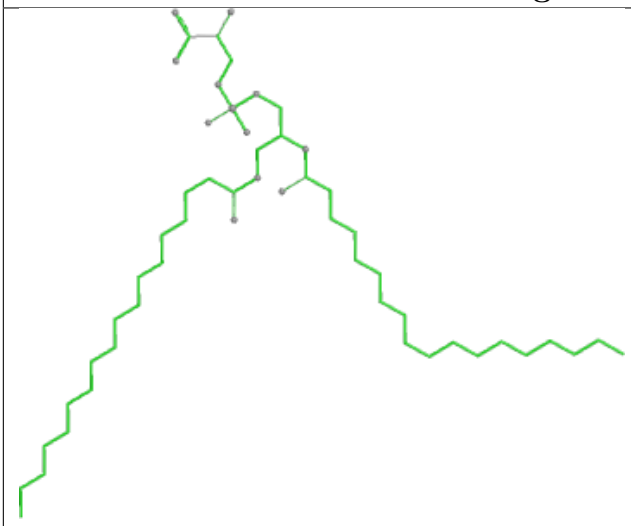
Bond angles



Torsions

Rings

Ligand 17F E 829



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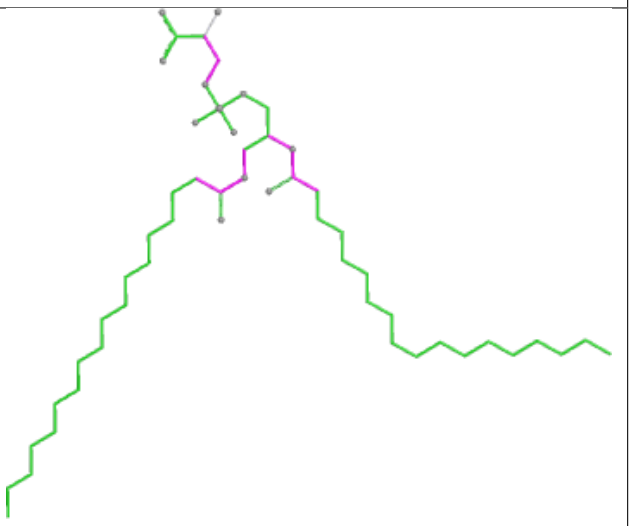
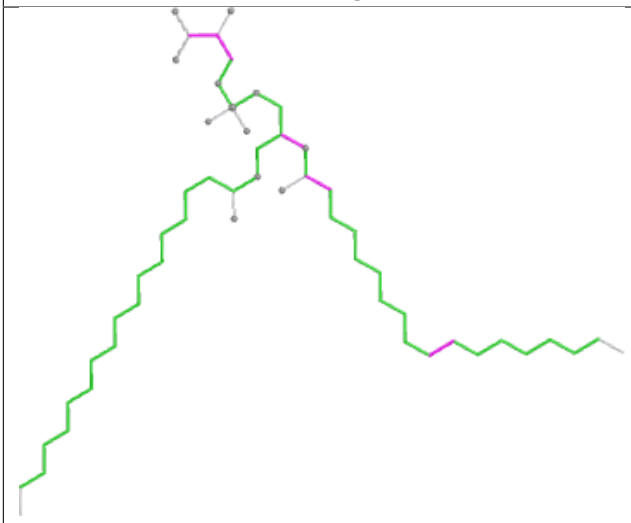
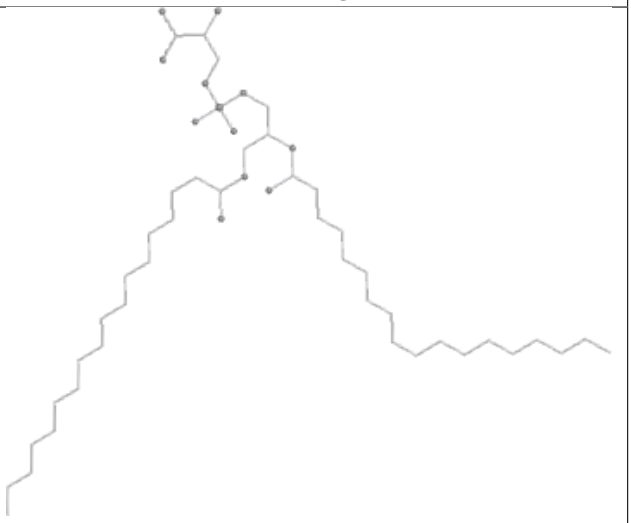


Bond angles

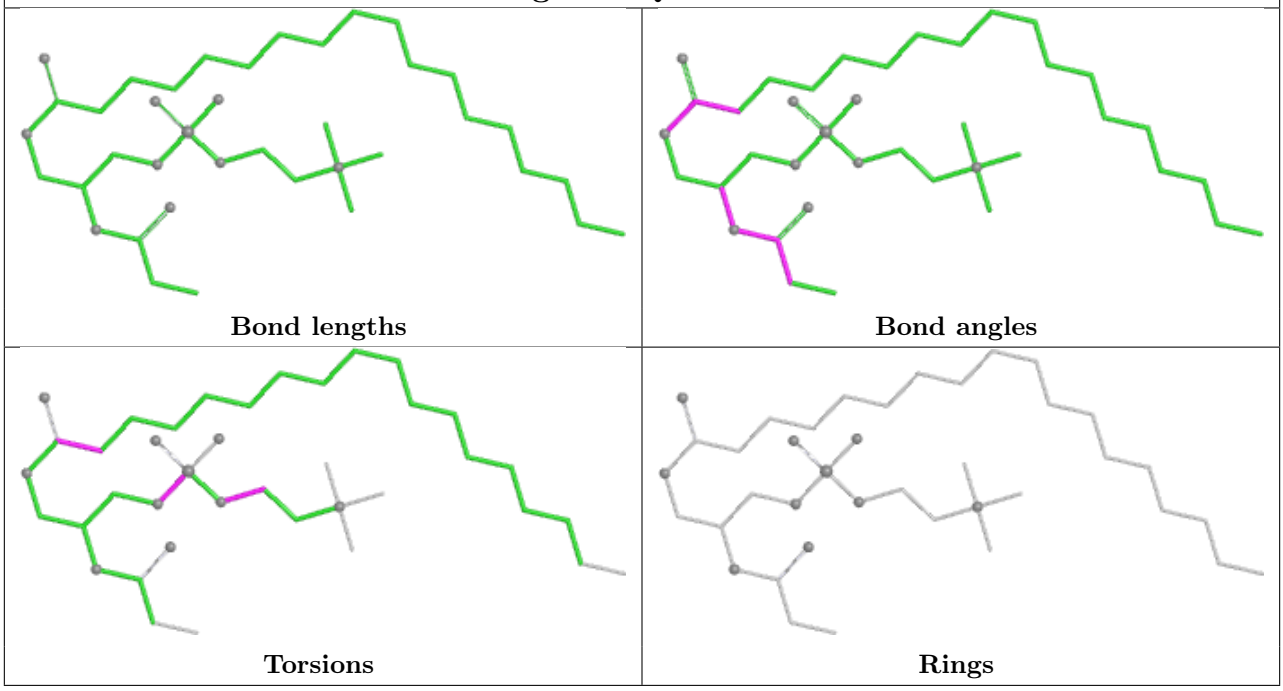


Torsions

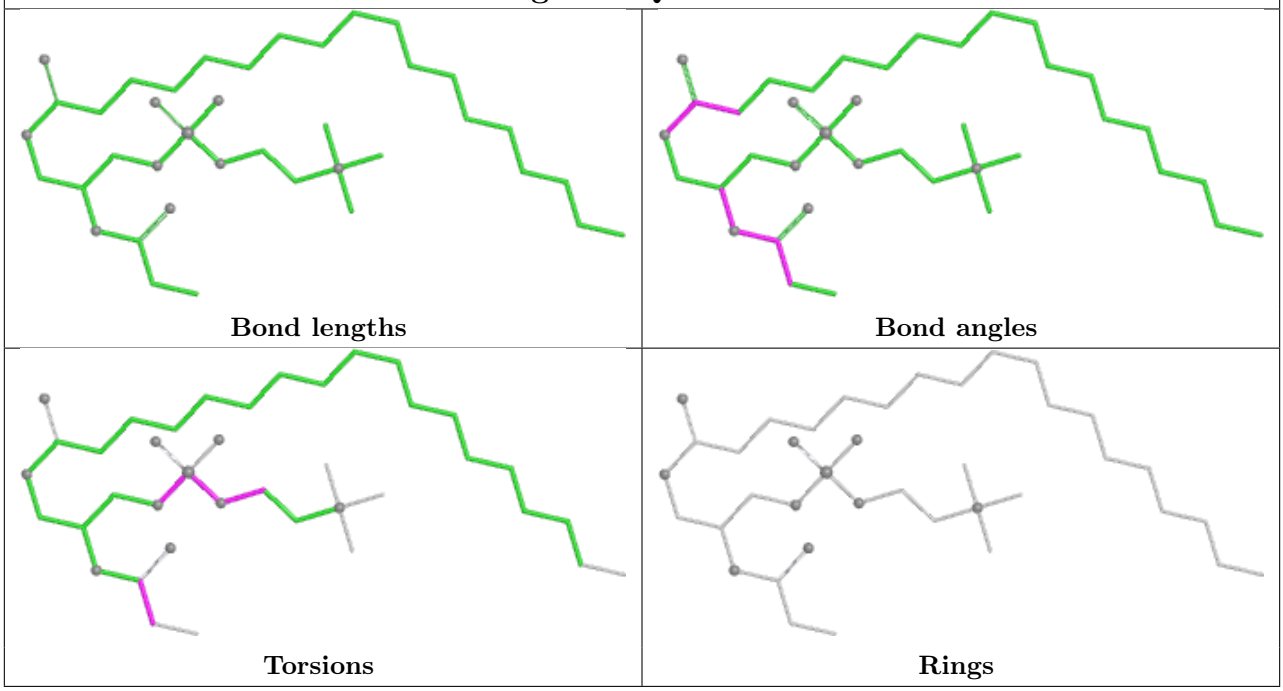


Rings

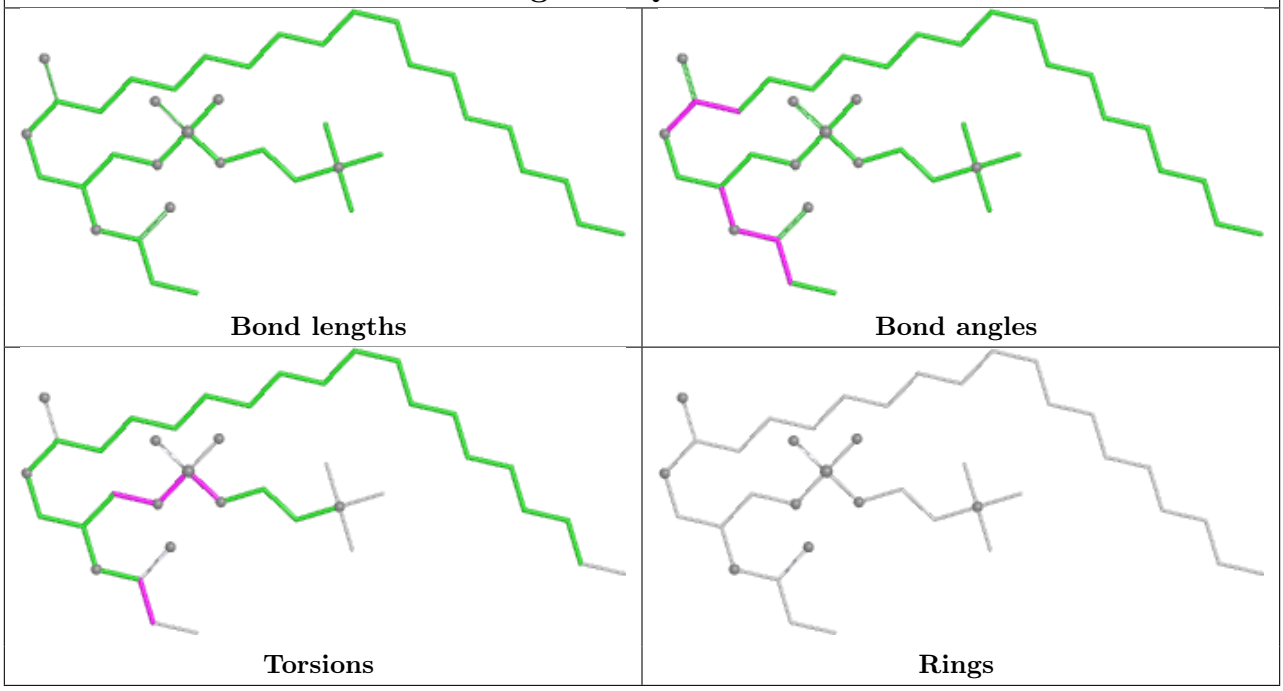
Ligand 7Q9 E 838



Ligand 7Q9 B 206



Ligand 7Q9 D 524



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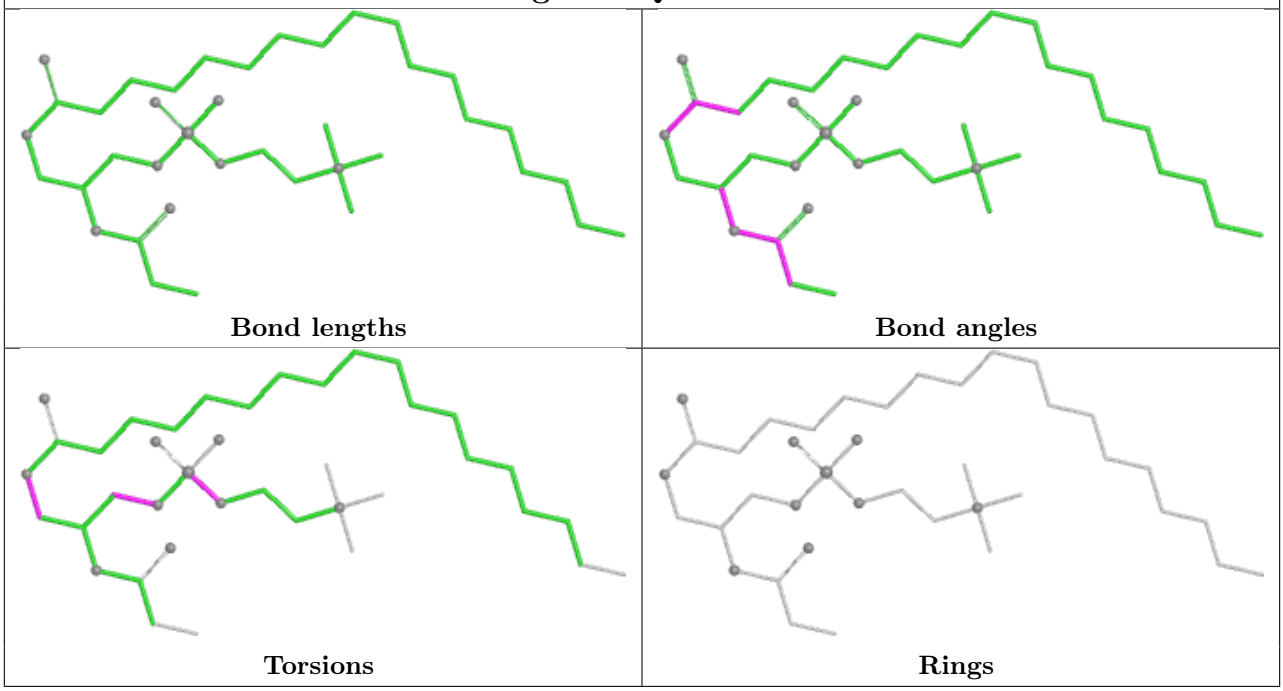
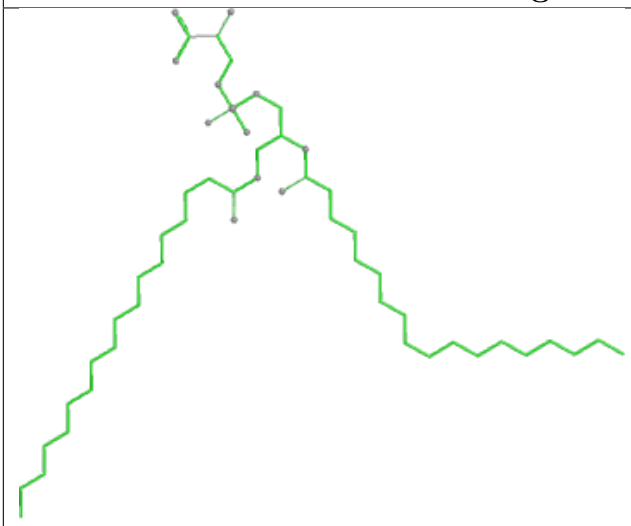
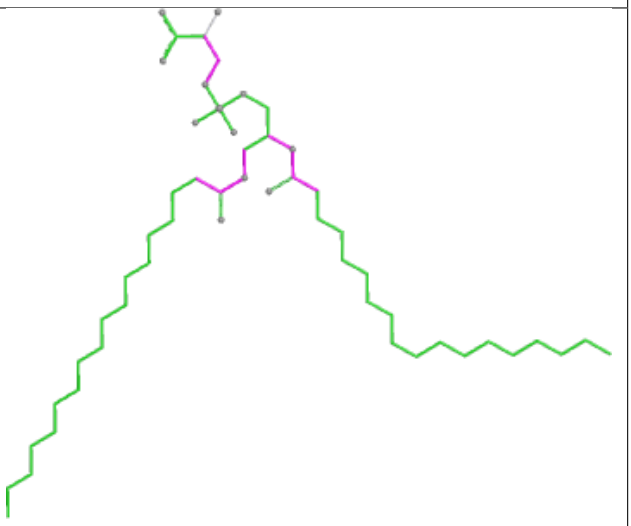


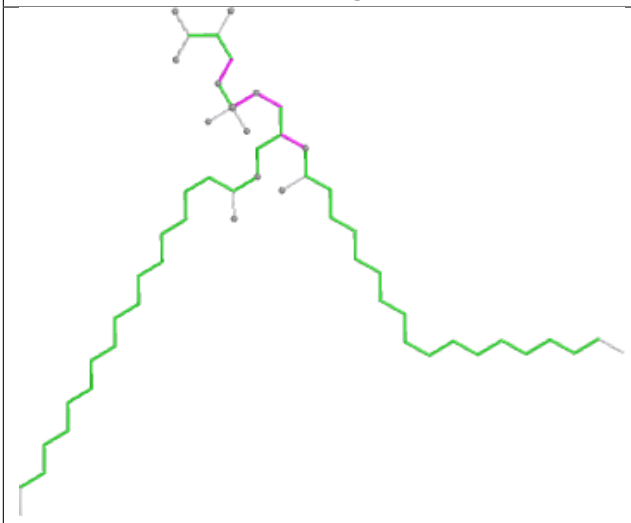
Ligand 17F D 518



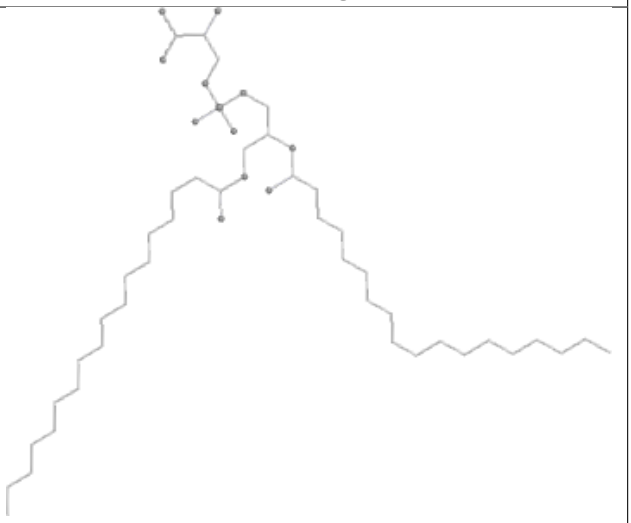
Bond lengths



Bond angles

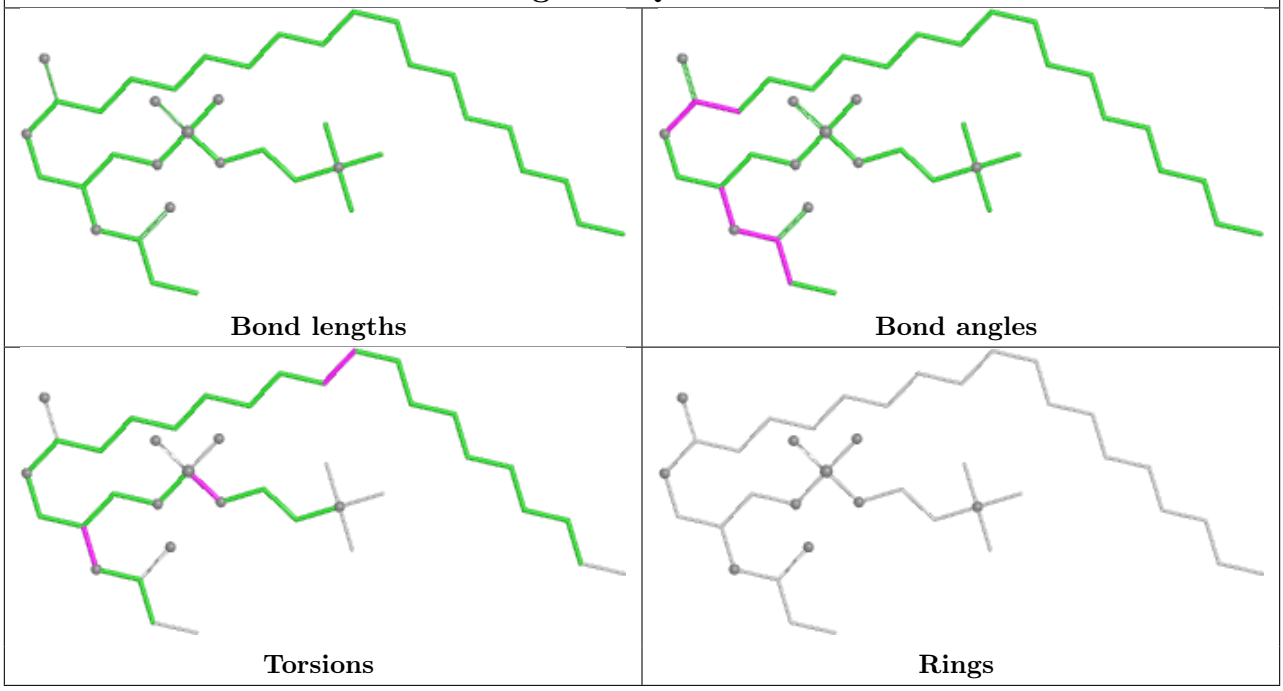


Torsions

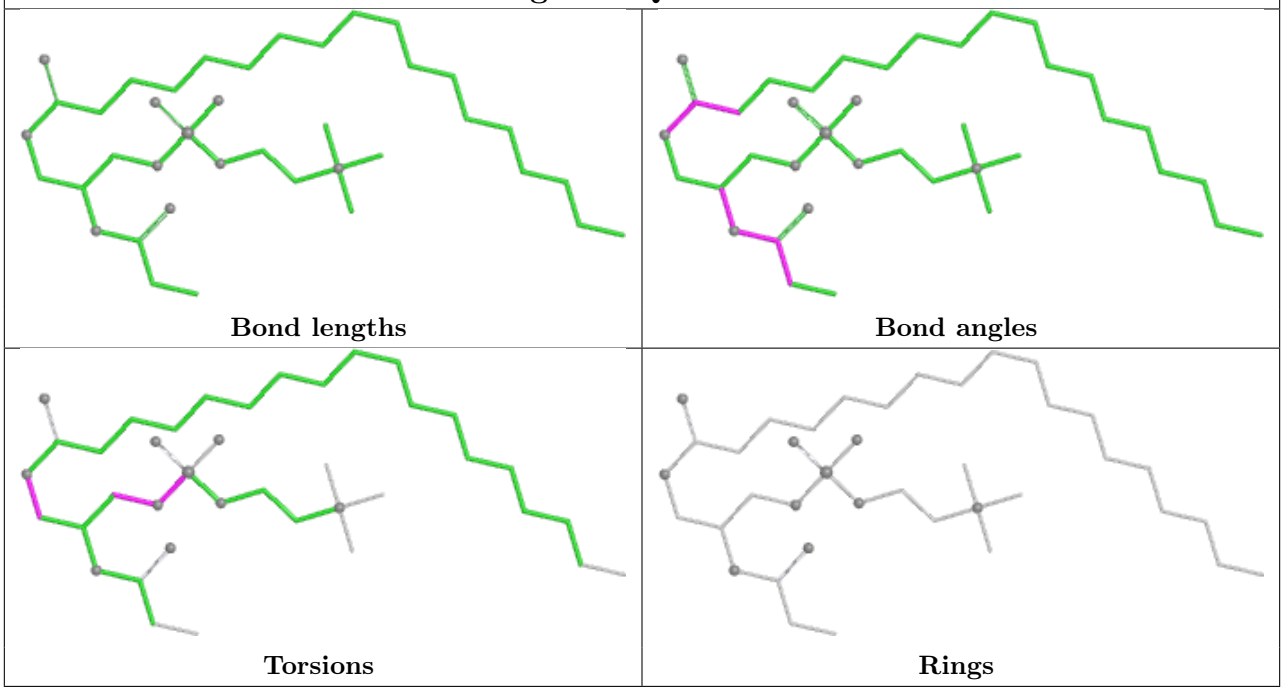


Rings

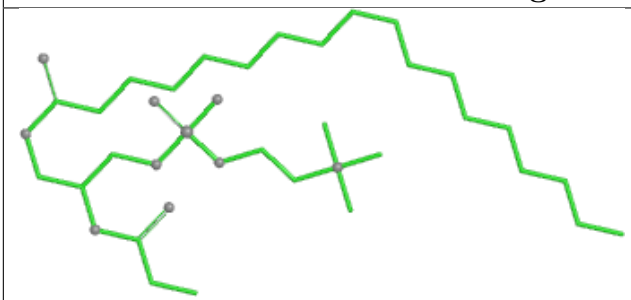
Ligand 7Q9 E 833



Ligand 7Q9 D 506



Ligand 7Q9 A 217



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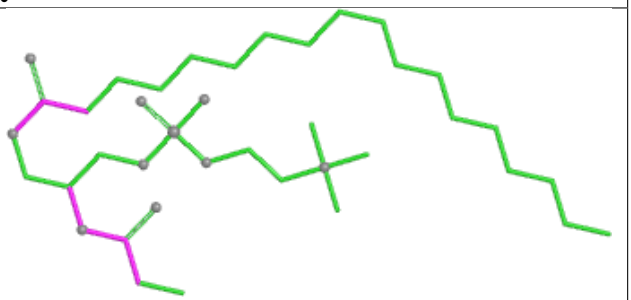
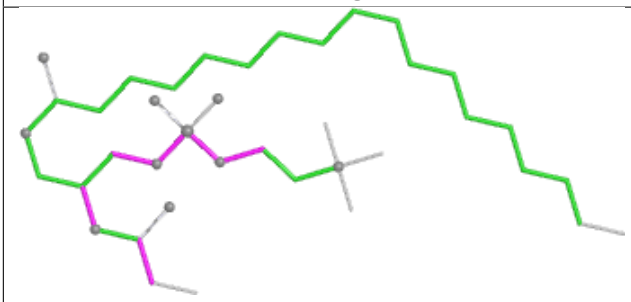


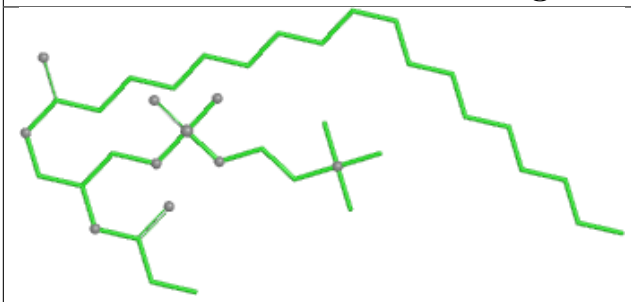
Bond angles



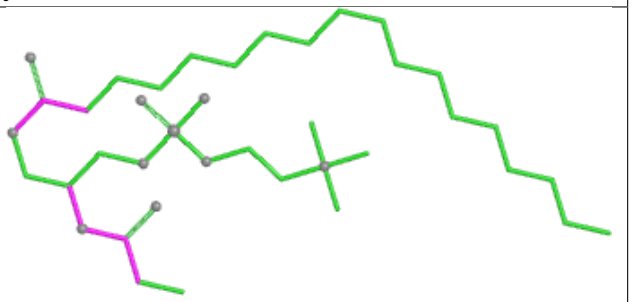
Torsions

Rings

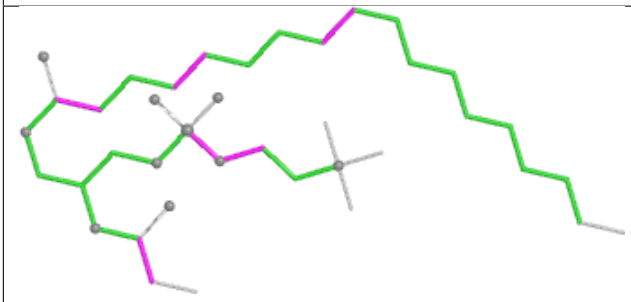
Ligand 7Q9 E 859



Bond lengths



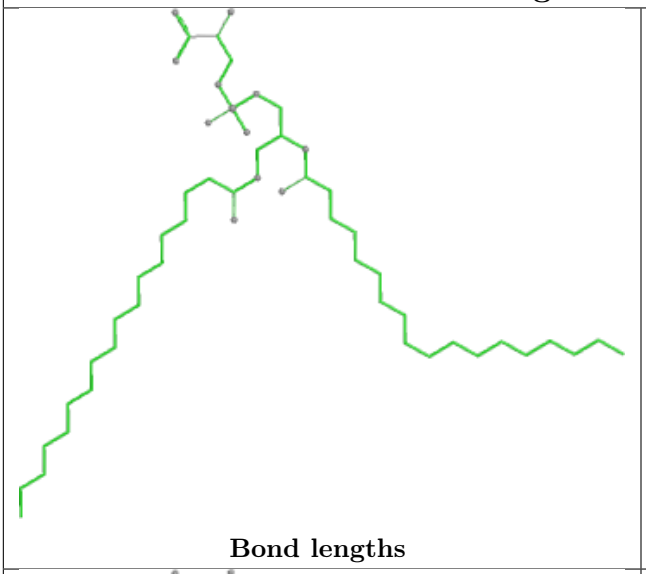
Bond angles



Torsions

Rings

Ligand 17F E 871



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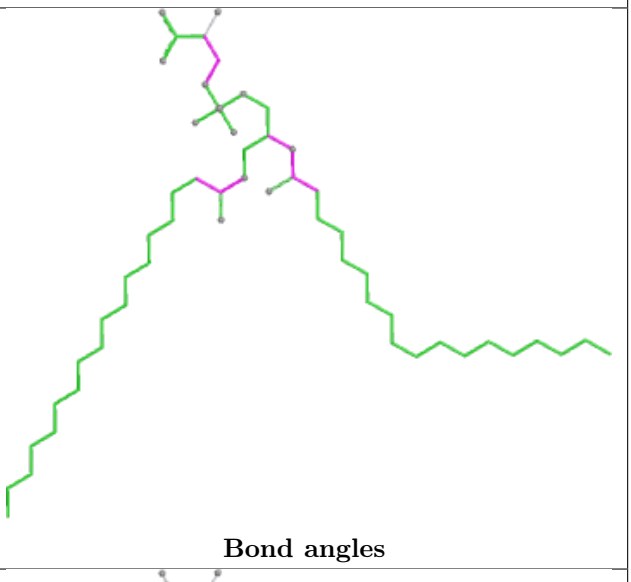
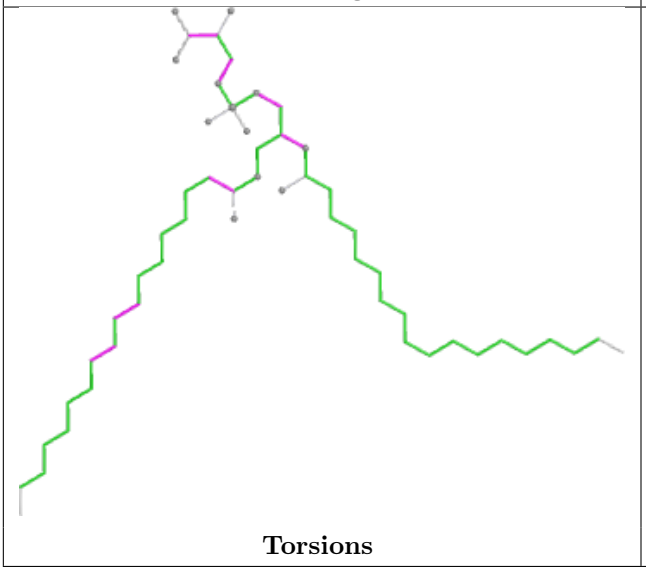
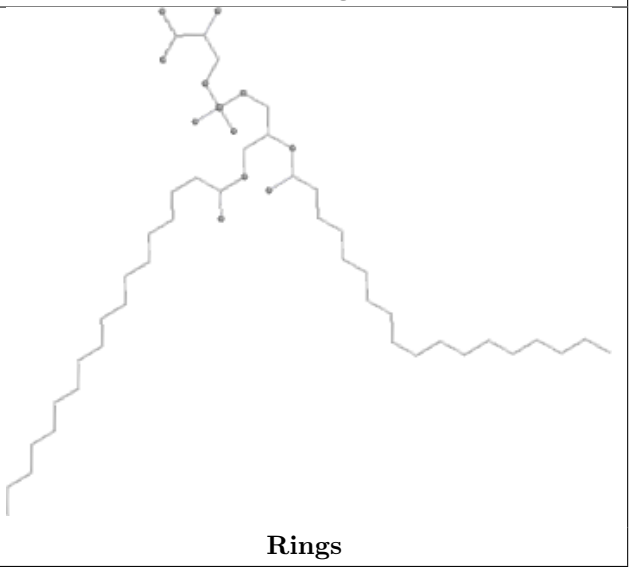


Bond angles

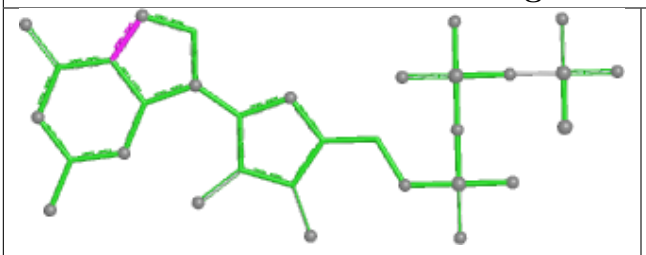


Torsions

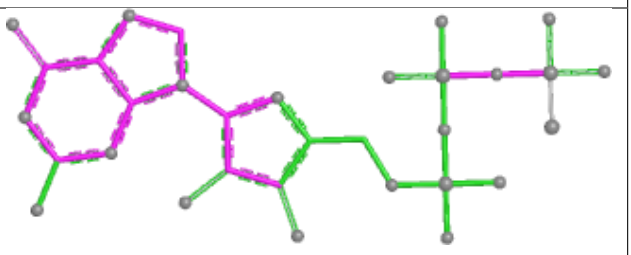


Rings

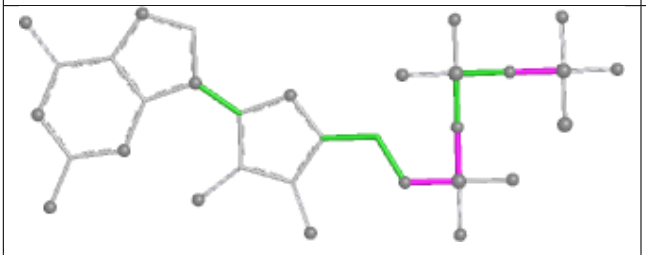
Ligand GSP A 201



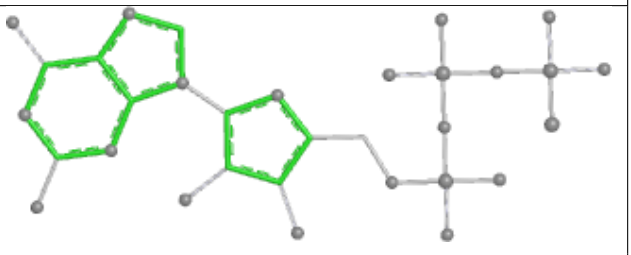
Bond lengths



Bond angles

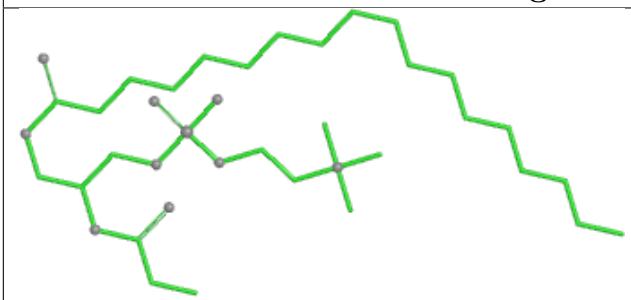


Torsions



Rings

Ligand 7Q9 A 218



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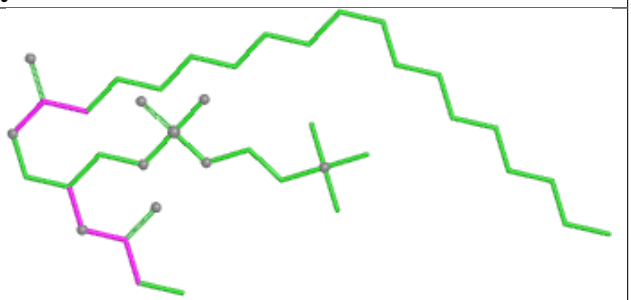
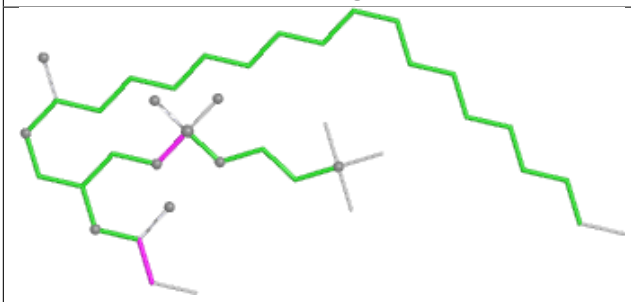


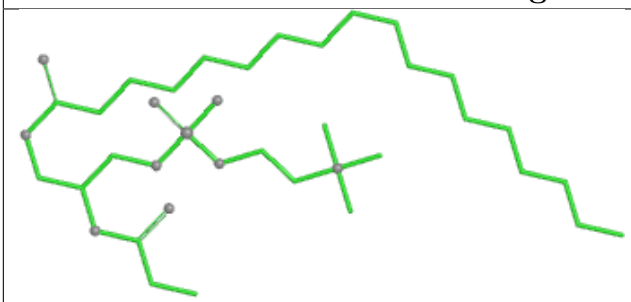
Bond angles



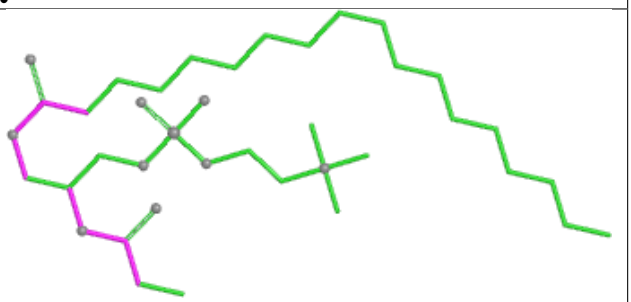
Torsions

Rings

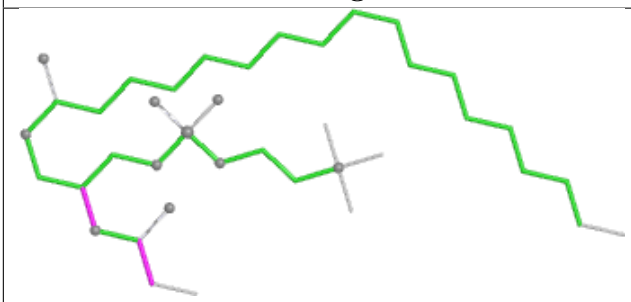
Ligand 7Q9 D 528



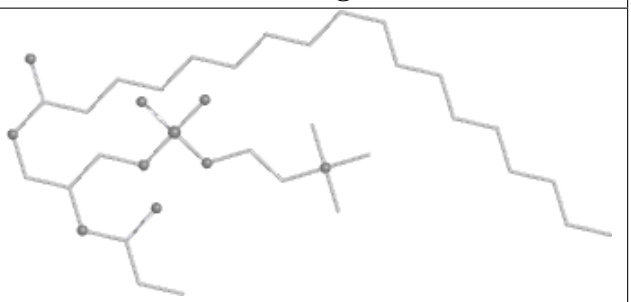
Bond lengths



Bond angles

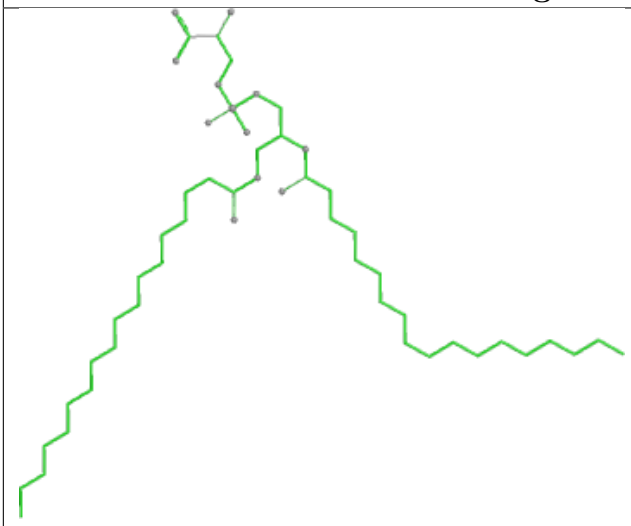


Torsions

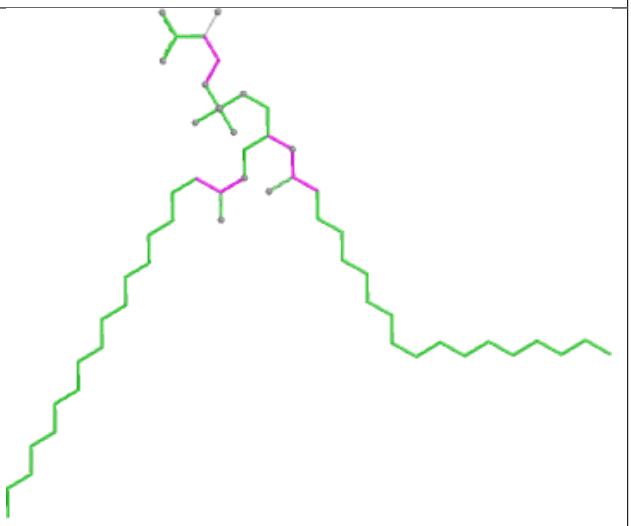


Rings

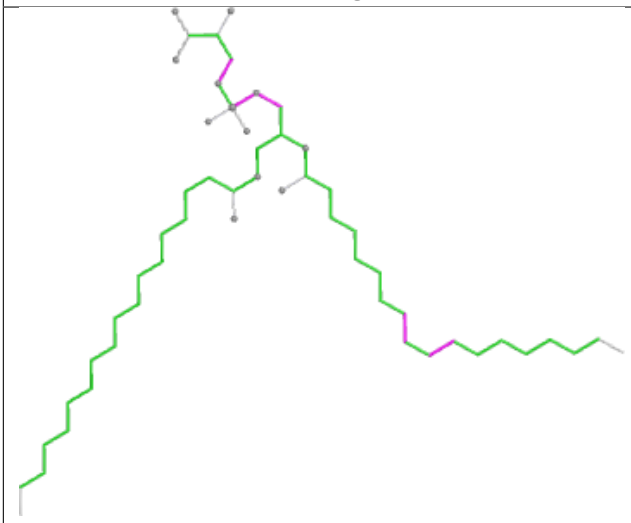
Ligand 17F E 873



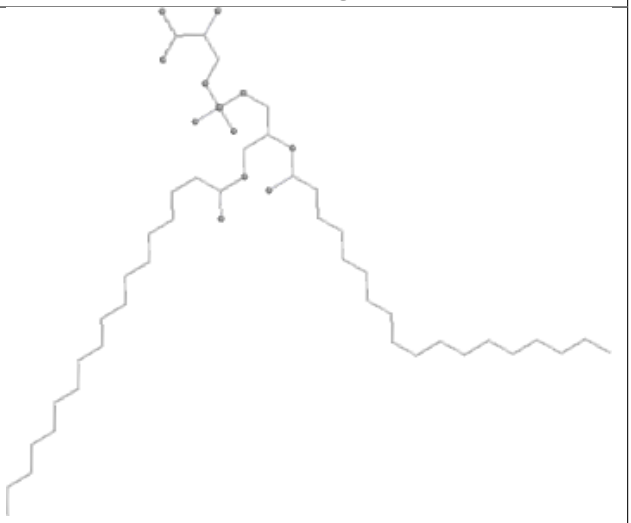
Bond lengths



Bond angles

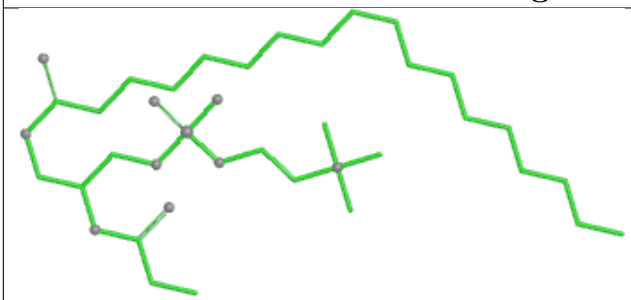


Torsions

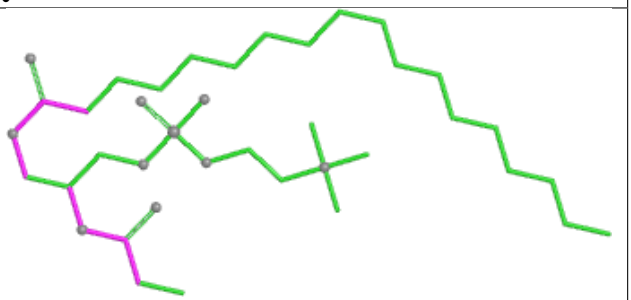


Rings

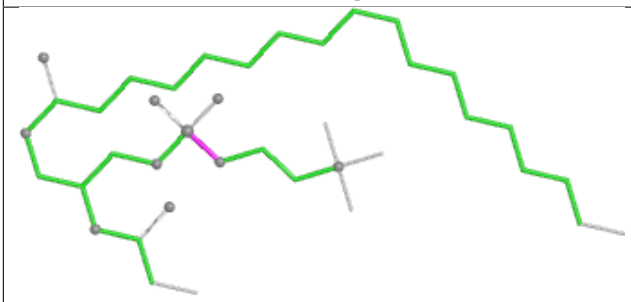
Ligand 7Q9 E 832



Bond lengths



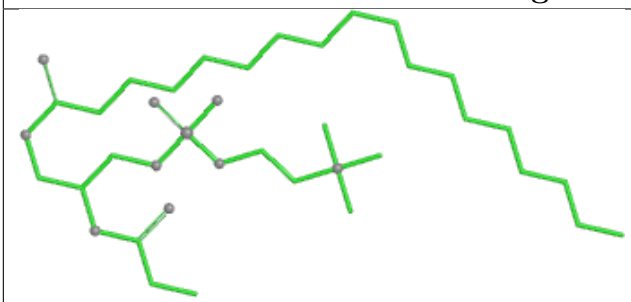
Bond angles



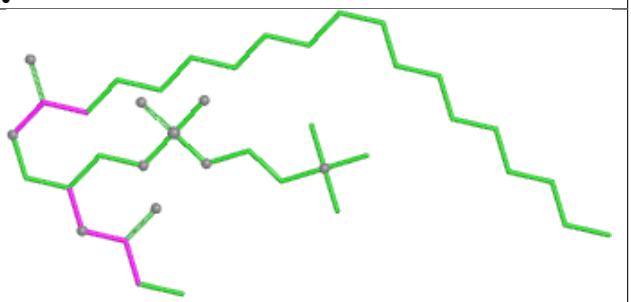
Torsions

Rings

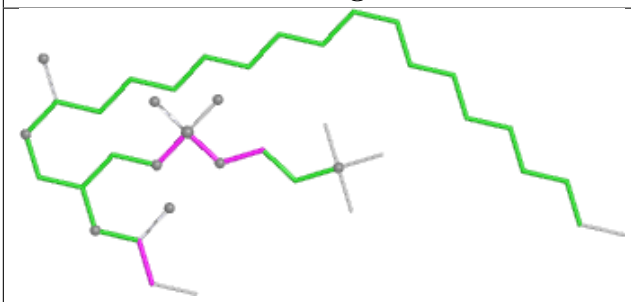
Ligand 7Q9 E 877



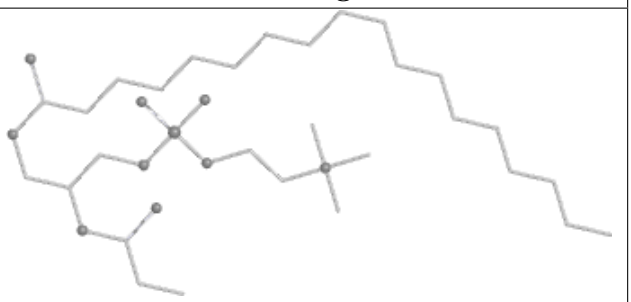
Bond lengths



Bond angles

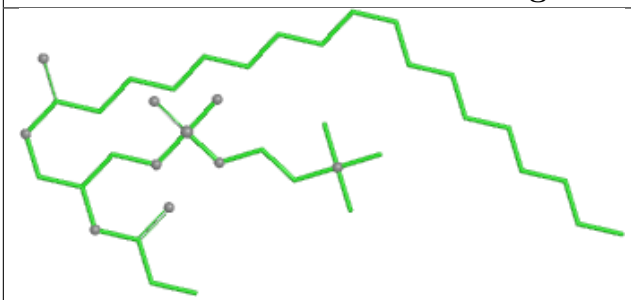


Torsions



Rings

Ligand 7Q9 D 527



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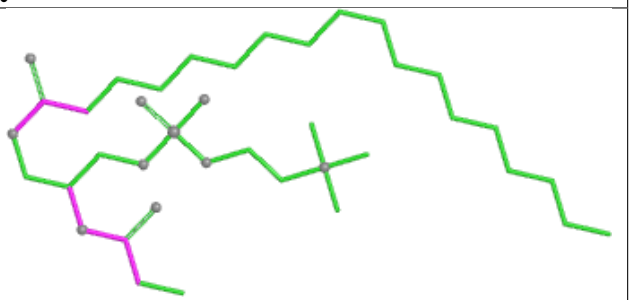
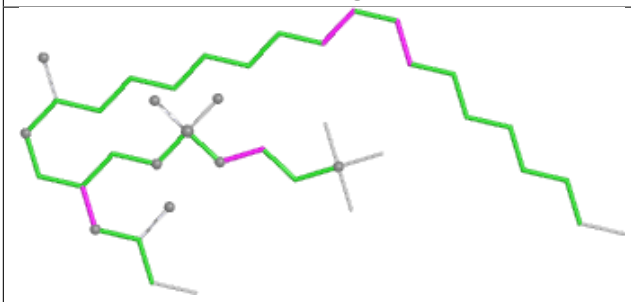


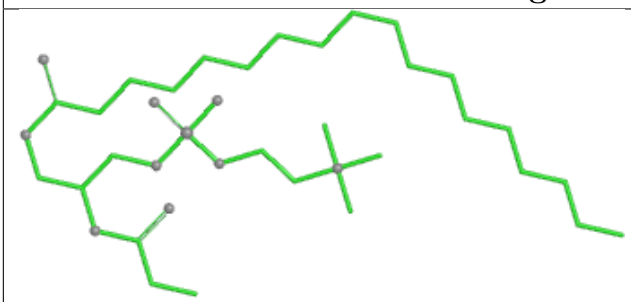
Bond angles



Torsions

Rings

Ligand 7Q9 D 536



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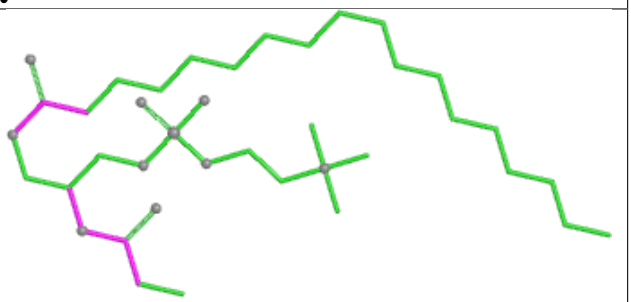
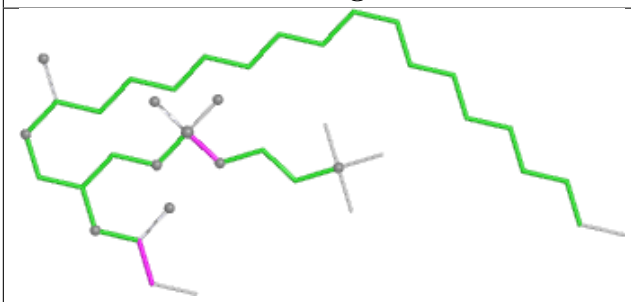
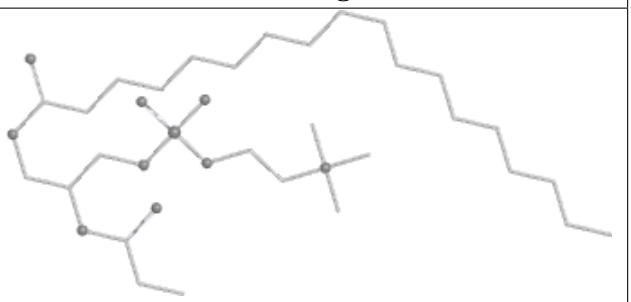


Bond angles

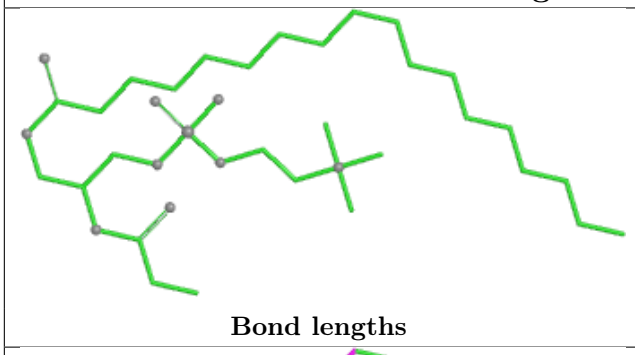


Torsions

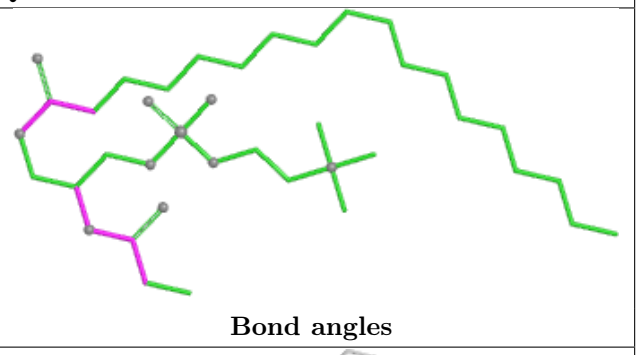


Rings

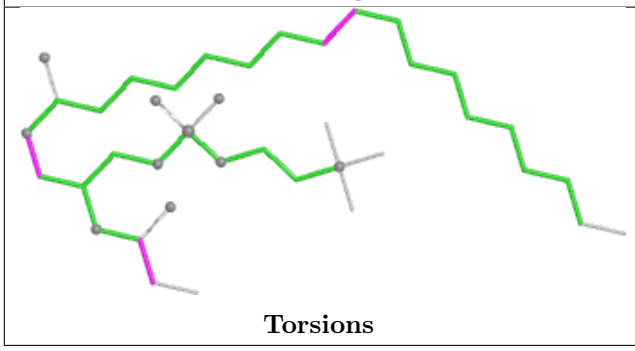
Ligand 7Q9 E 827



Bond lengths



Bond angles



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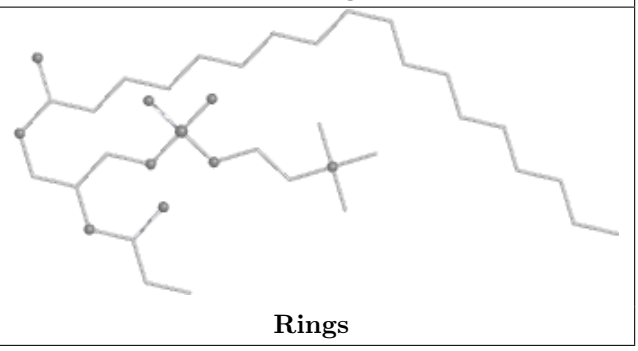
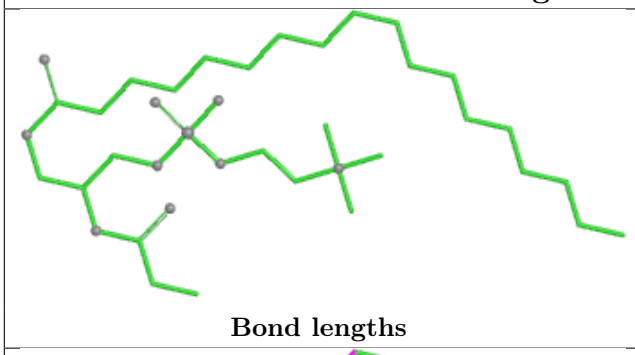


Rings

Ligand 7Q9 E 868



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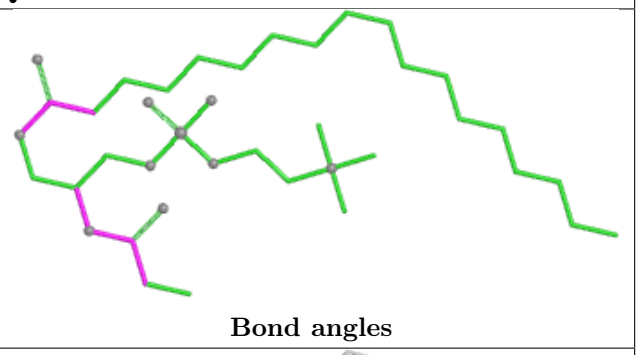
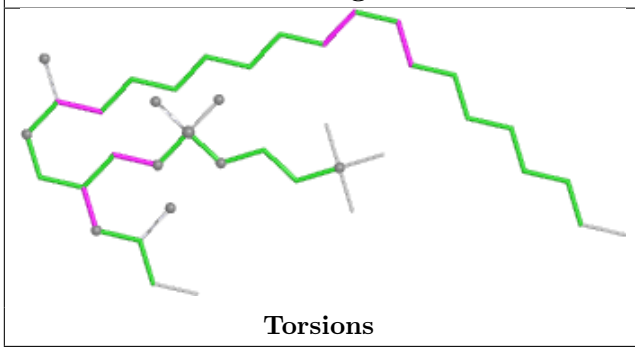


Bond angles



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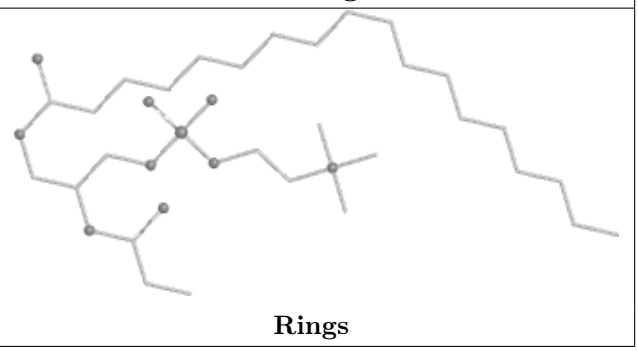
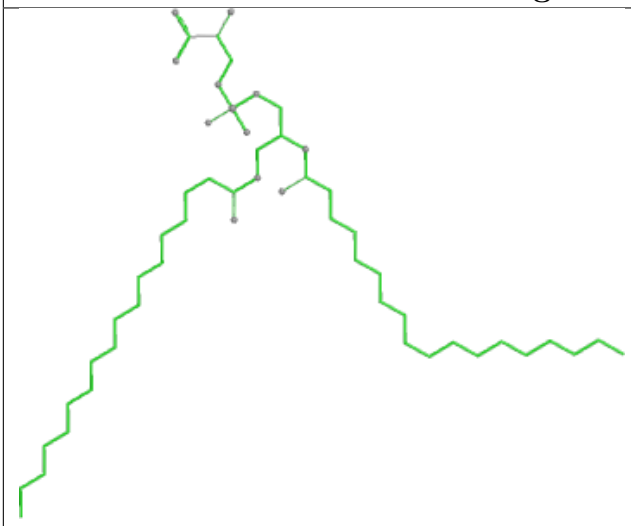


Rings

Ligand 17F E 808



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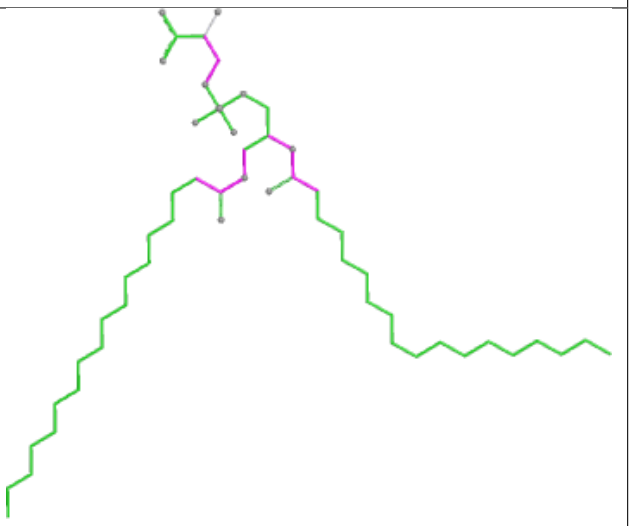
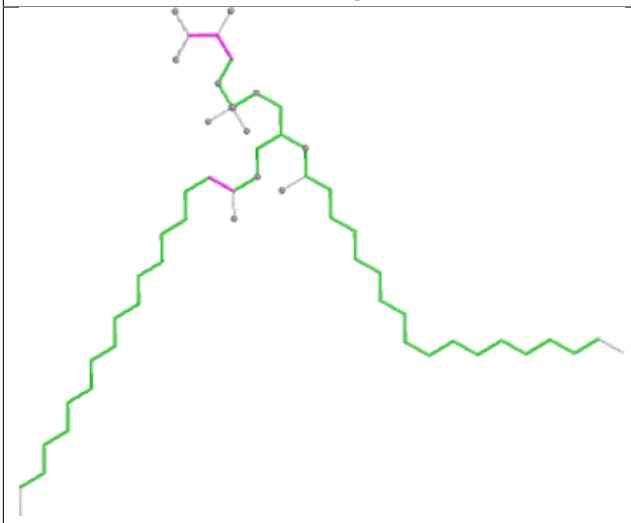


Bond angles



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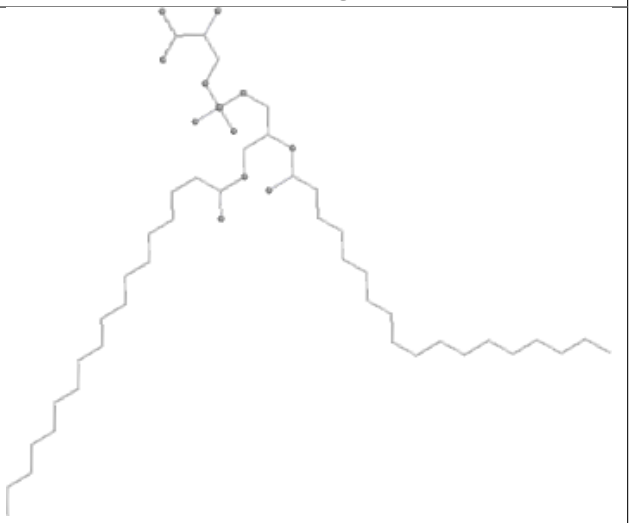
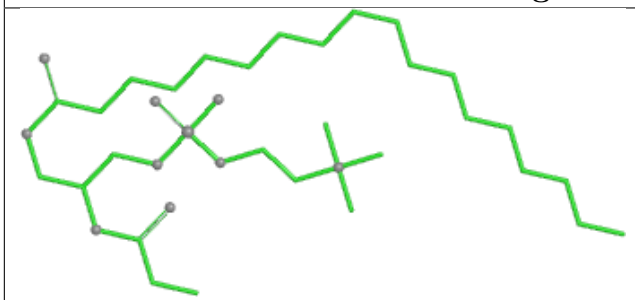


Rings

Ligand 7Q9 E 846



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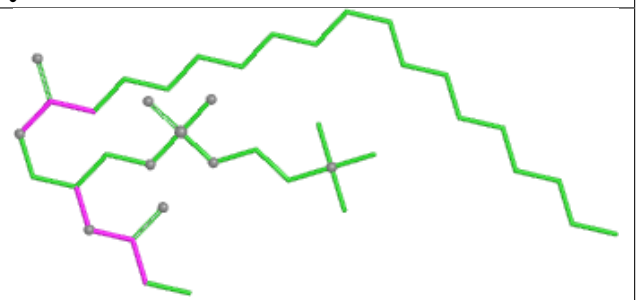
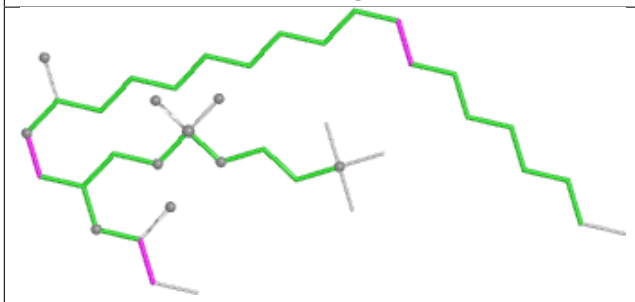


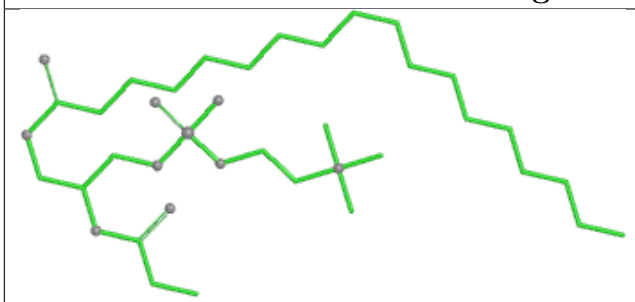
Bond angles



Torsions

Rings

Ligand 7Q9 E 870



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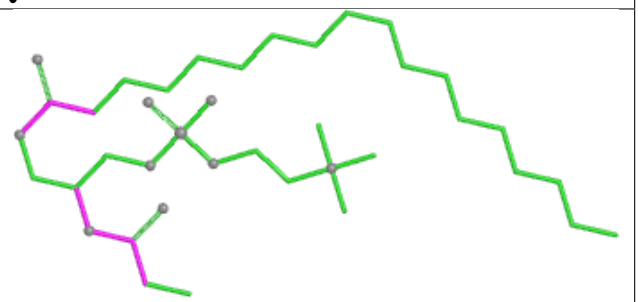
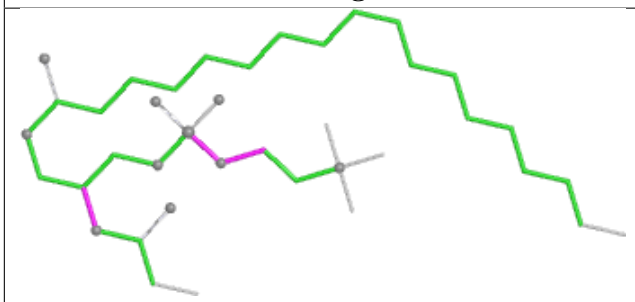
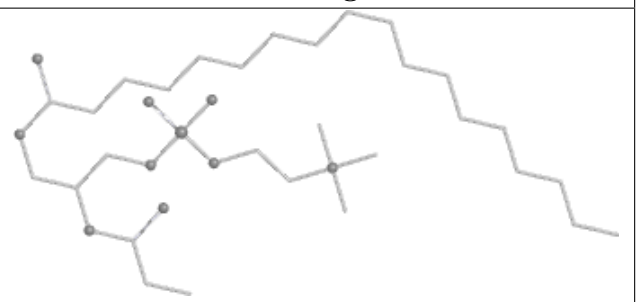


Bond angles

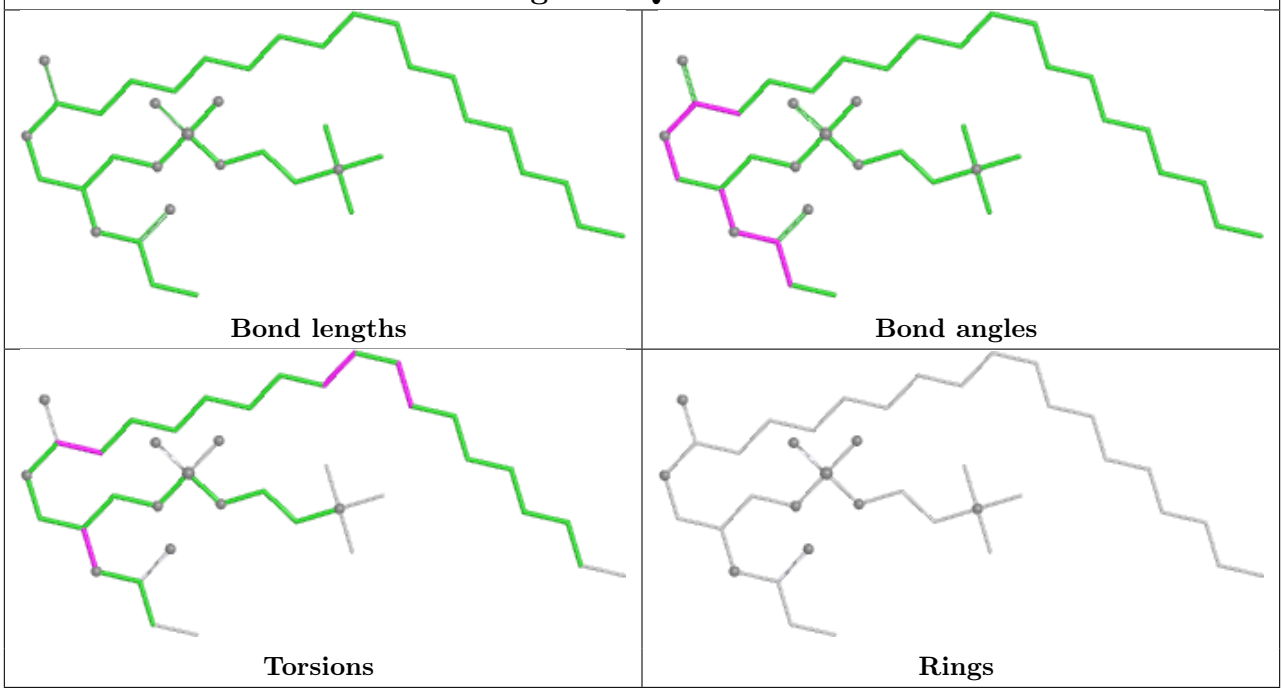


Torsions

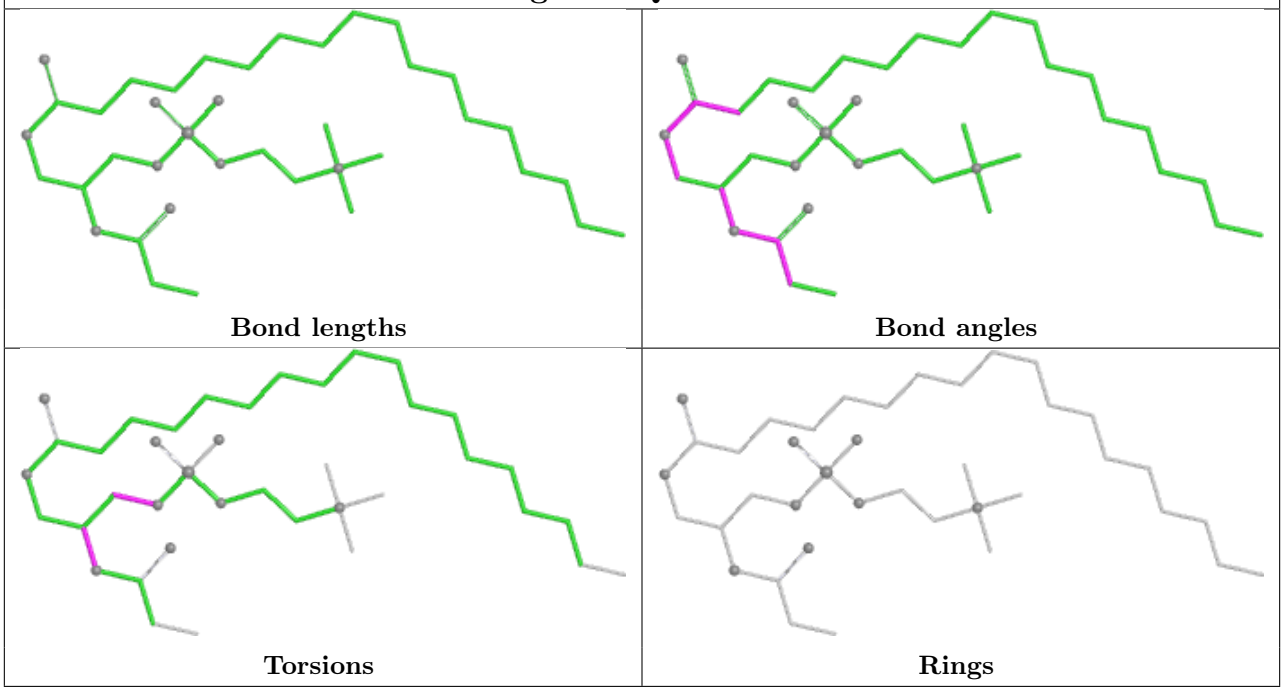


Rings

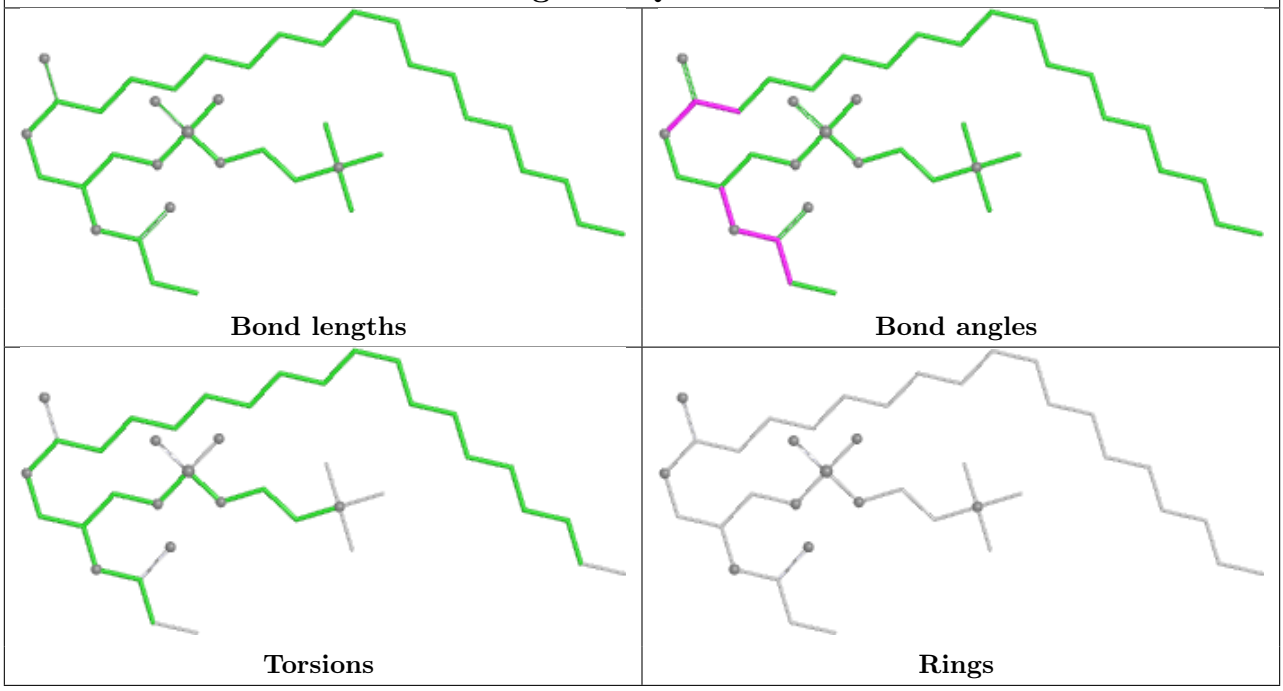
Ligand 7Q9 A 215



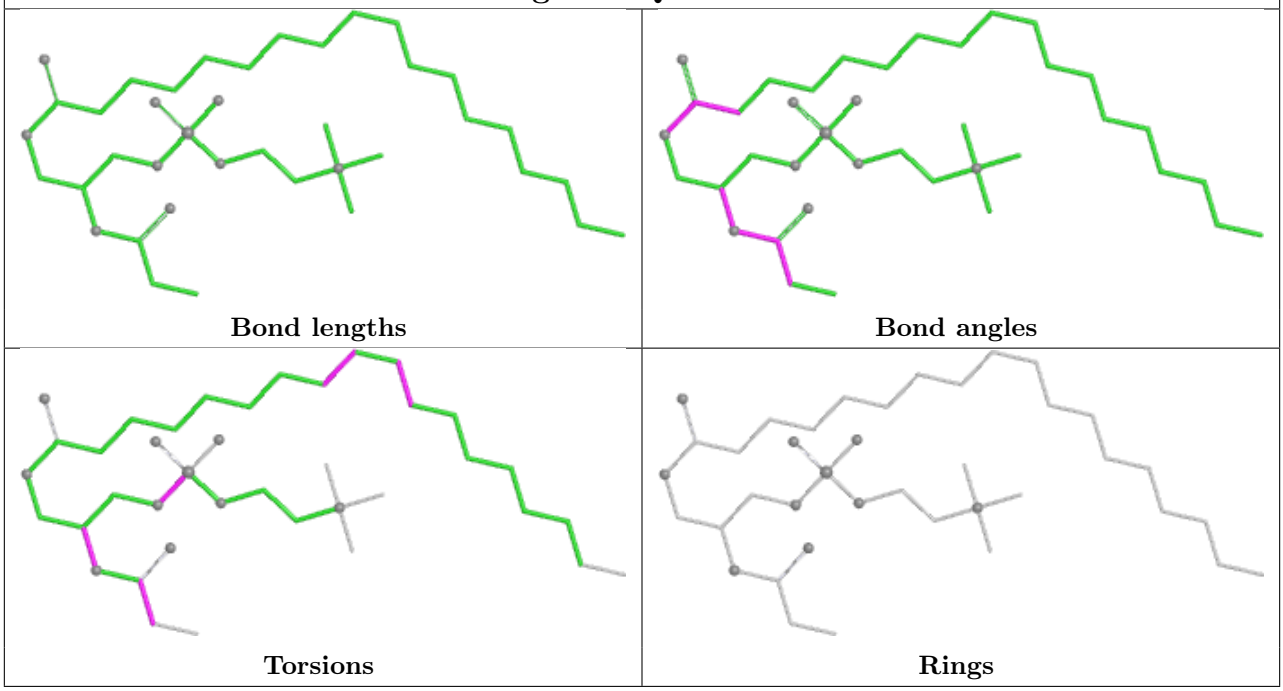
Ligand 7Q9 D 526



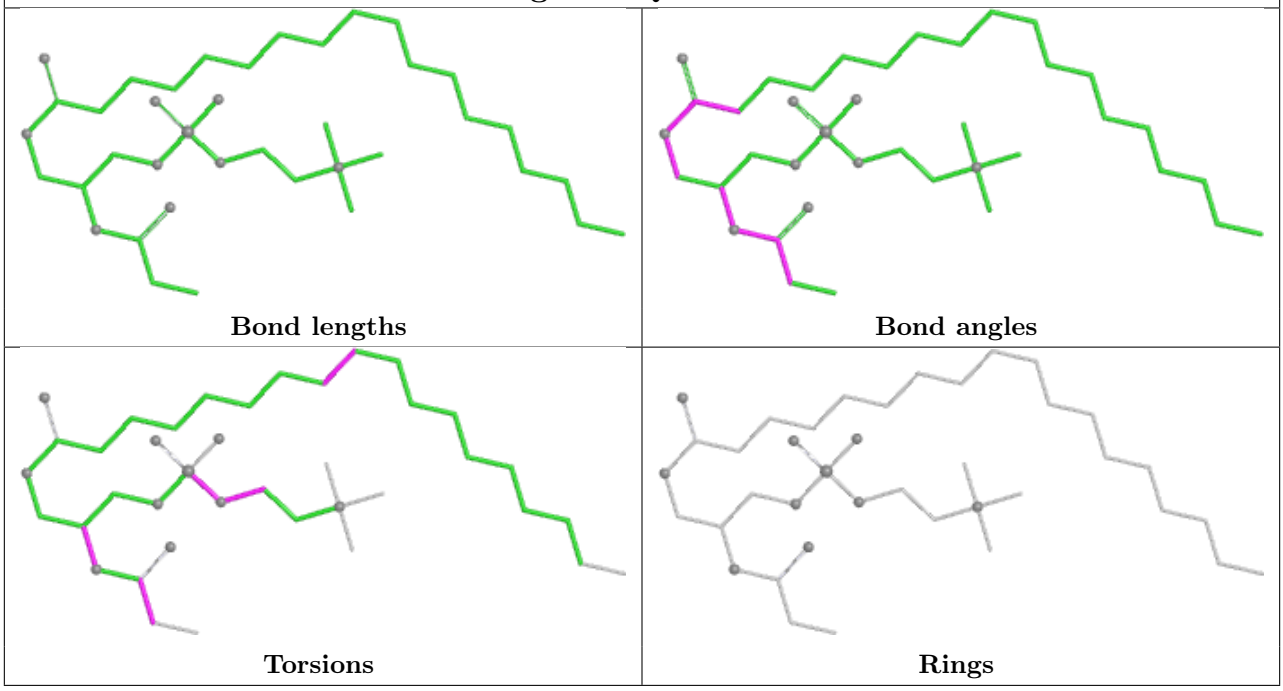
Ligand 7Q9 E 845



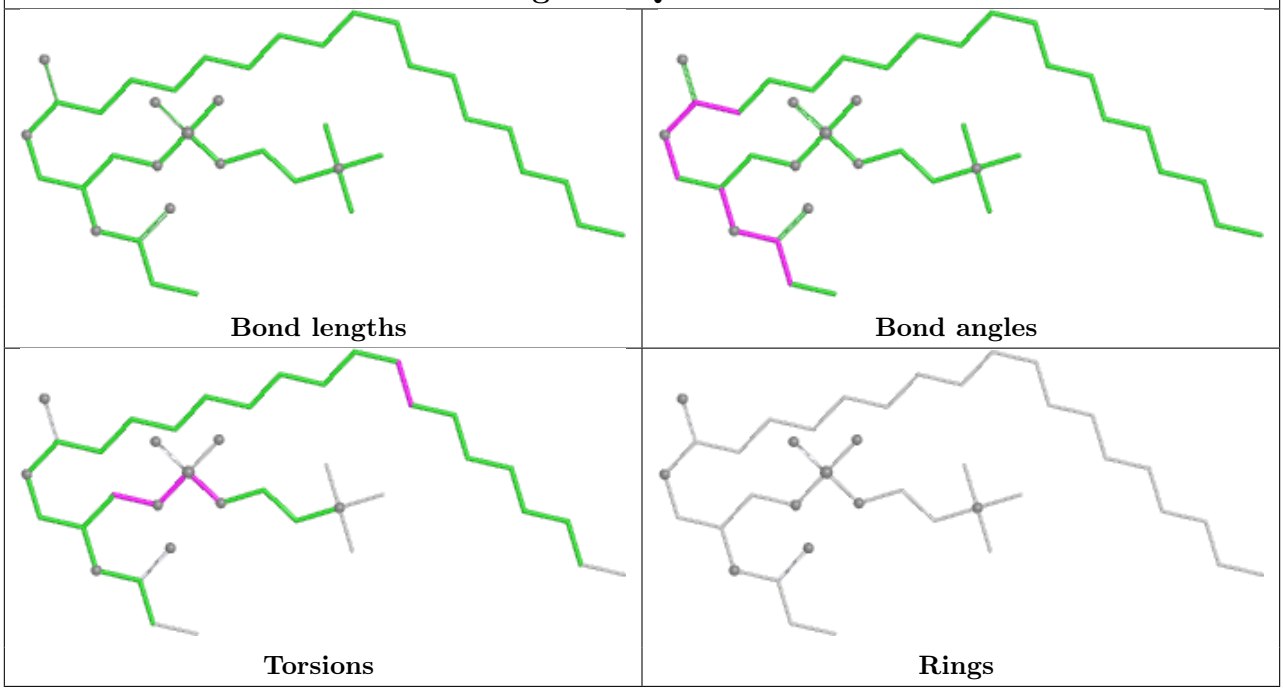
Ligand 7Q9 E 866



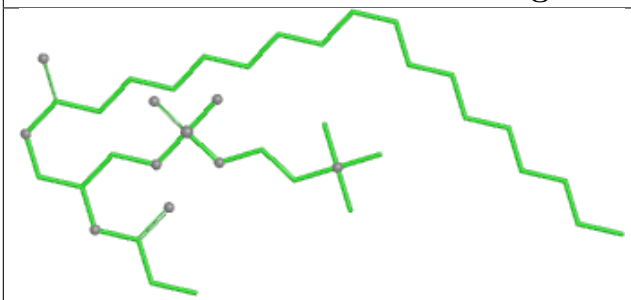
Ligand 7Q9 D 532



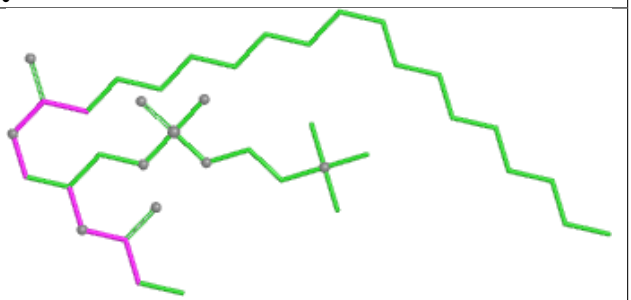
Ligand 7Q9 E 822



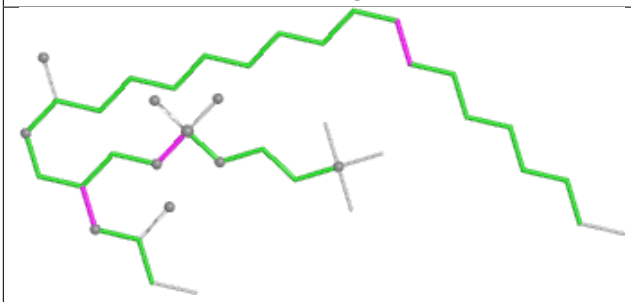
Ligand 7Q9 E 828



Bond lengths



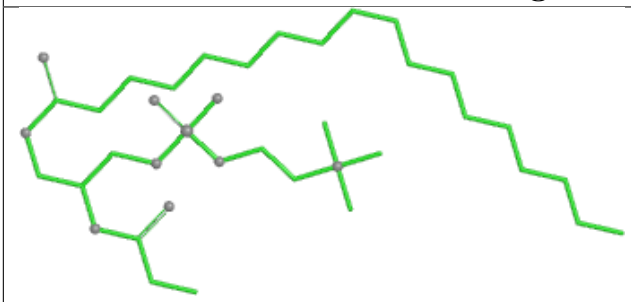
Bond angles



Torsions

Rings

Ligand 7Q9 A 211



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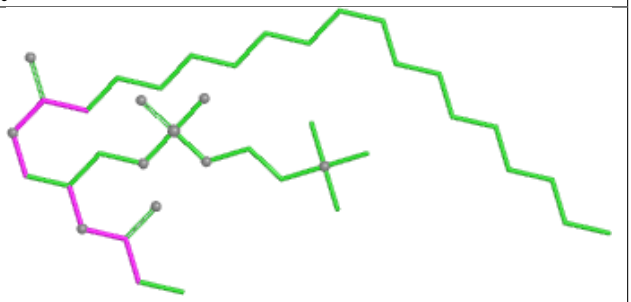
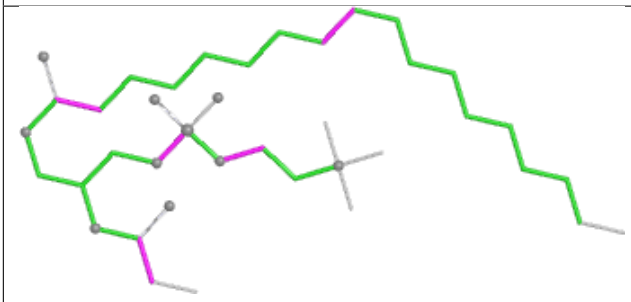


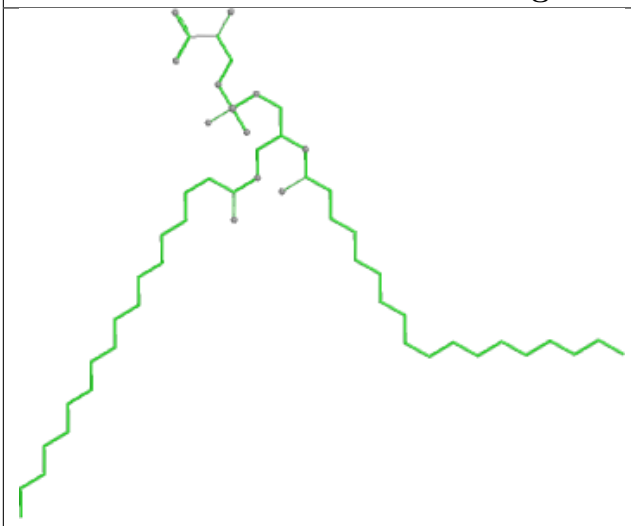
Bond angles



Torsions

Rings

Ligand 17F D 519



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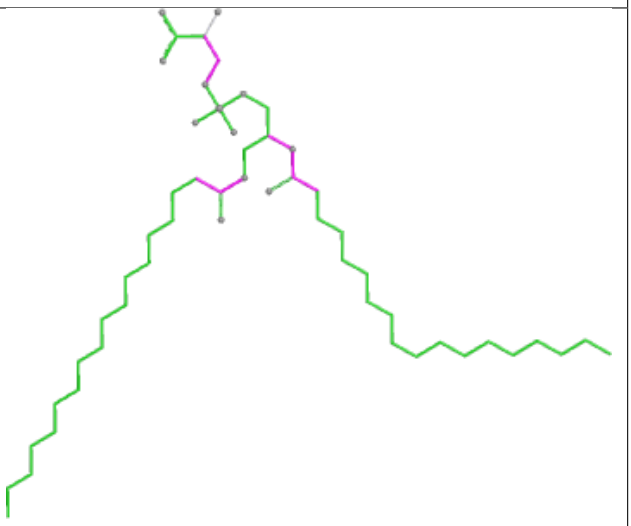
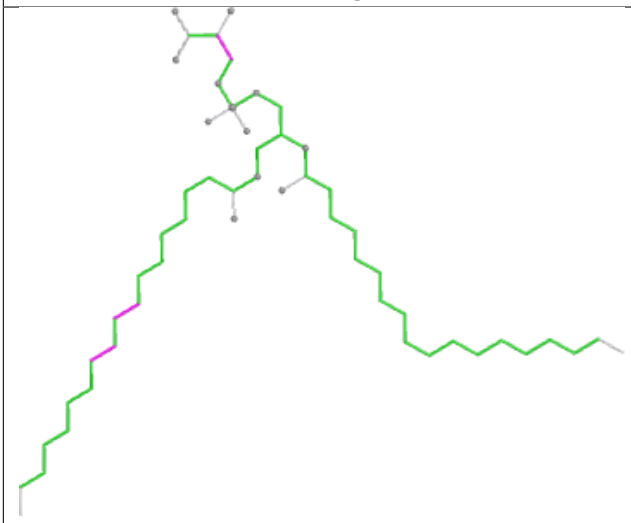
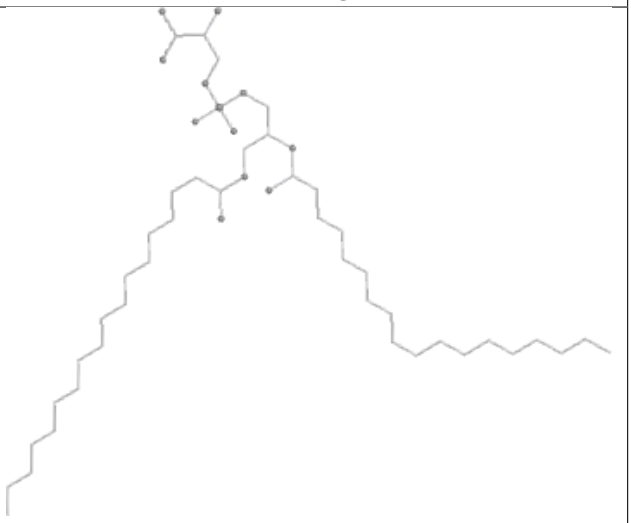


Bond angles

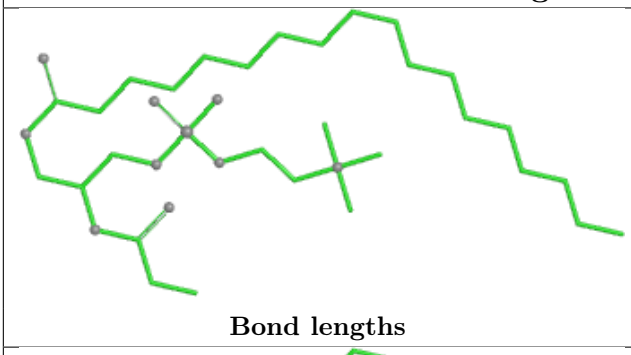


Torsions

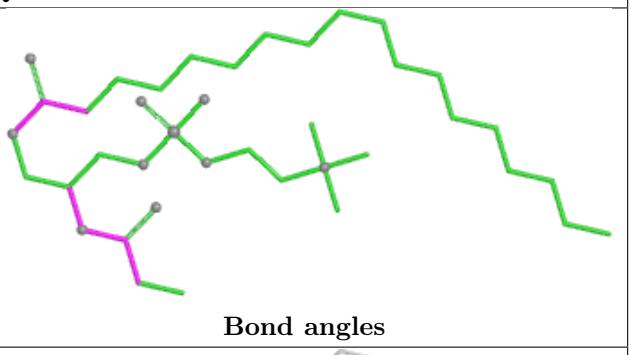


Rings

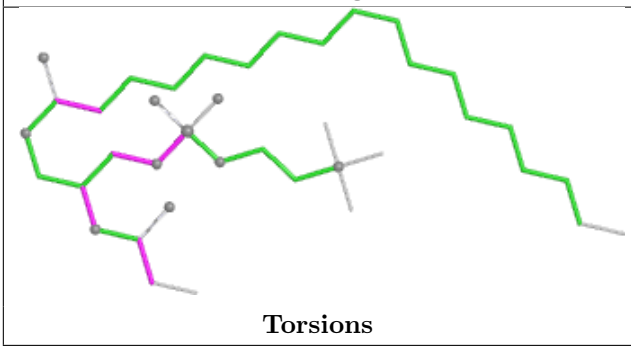
Ligand 7Q9 E 830



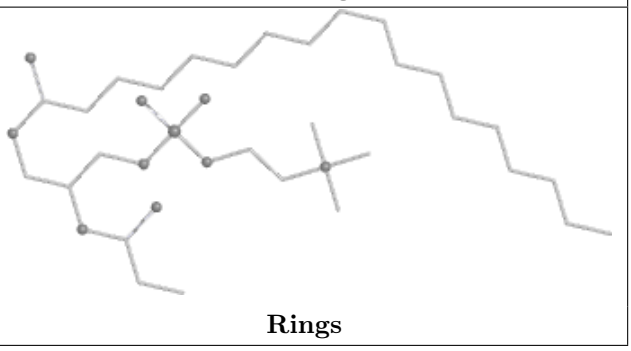
Bond lengths



Bond angles

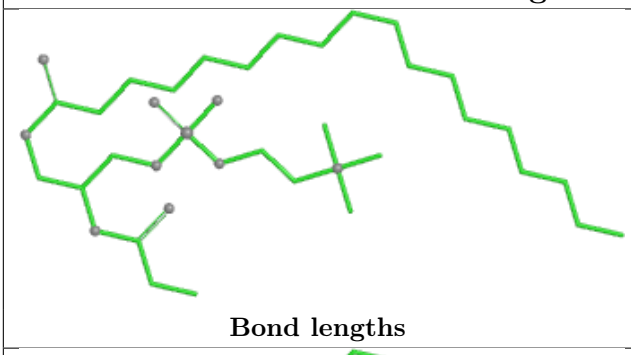


Torsions

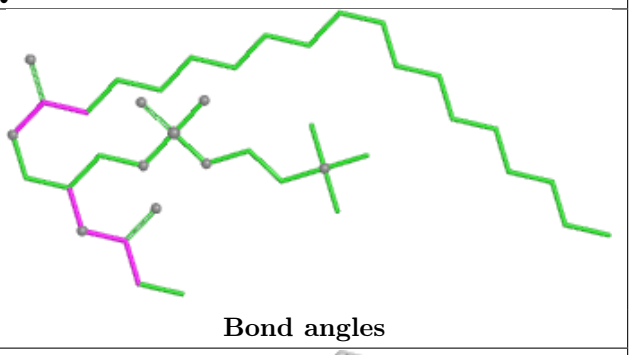


Rings

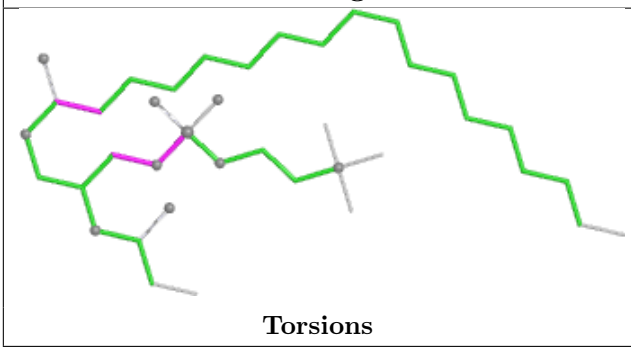
Ligand 7Q9 D 507



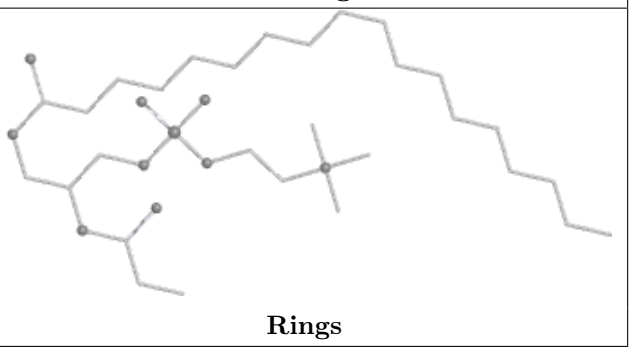
Bond lengths



Bond angles

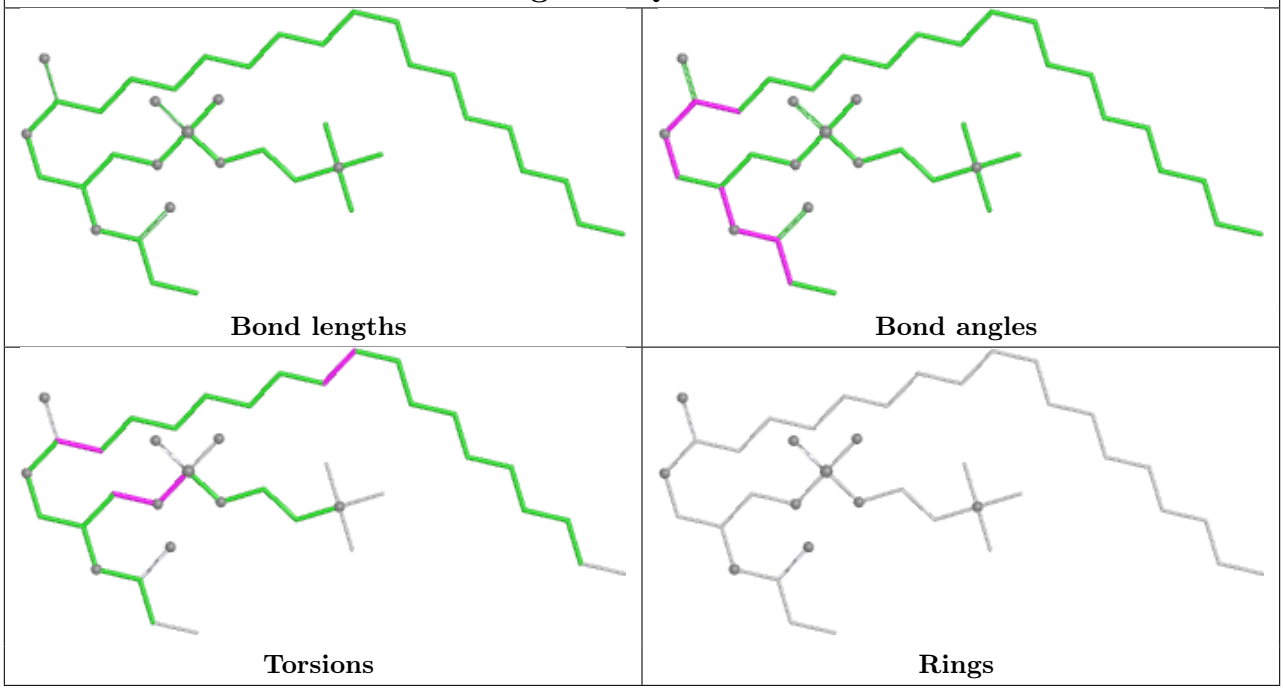


Torsions

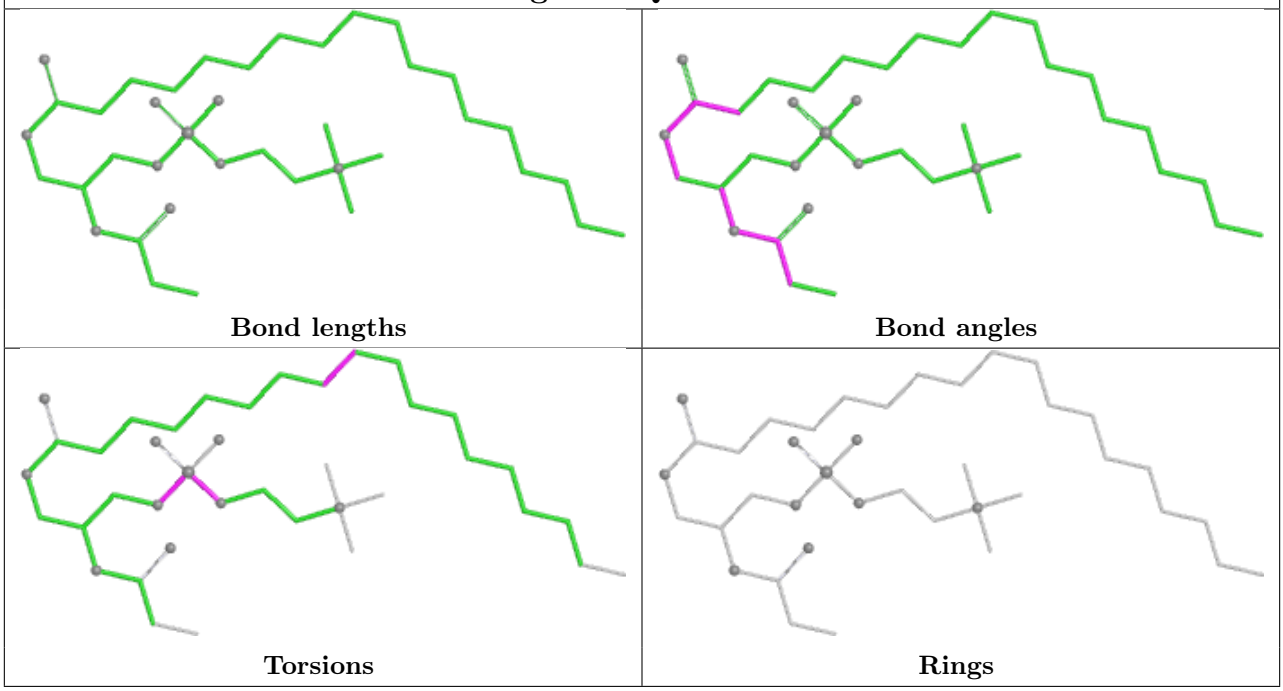


Rings

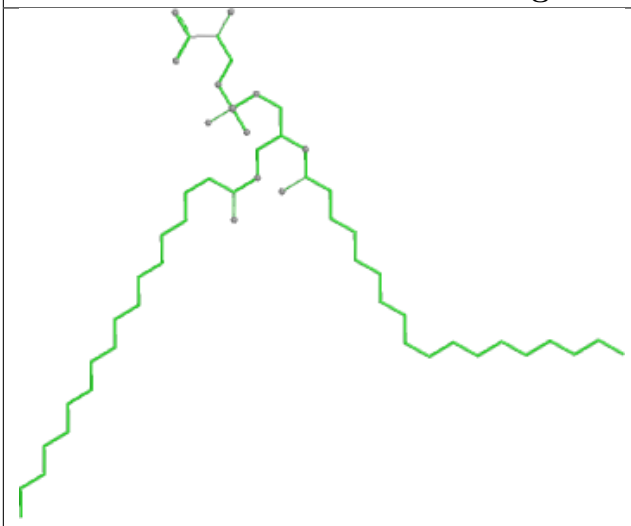
Ligand 7Q9 A 212



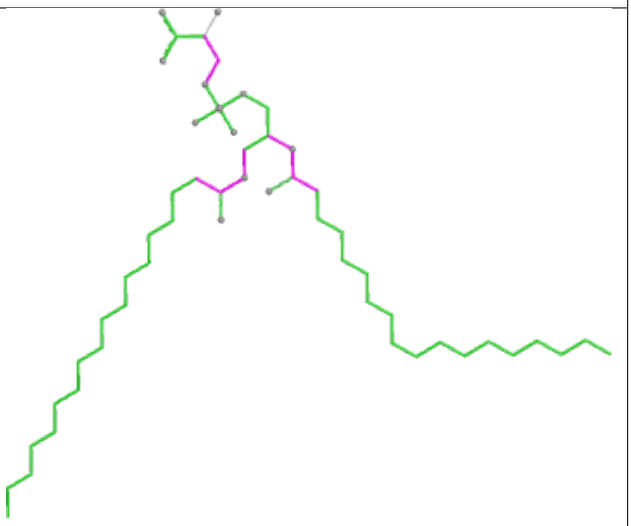
Ligand 7Q9 D 548



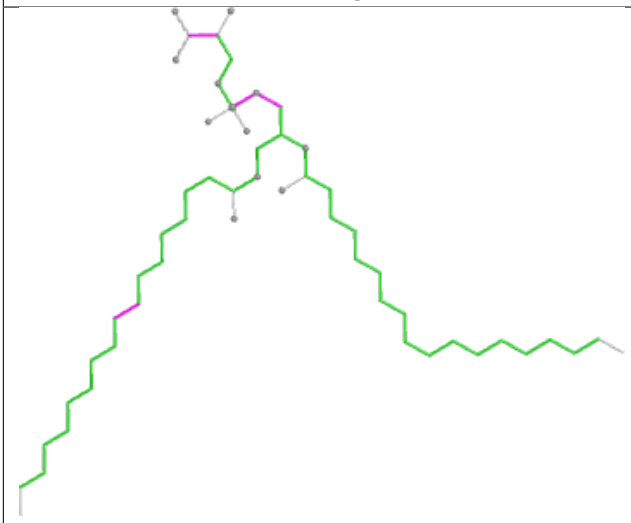
Ligand 17F D 534



Bond lengths



Bond angles



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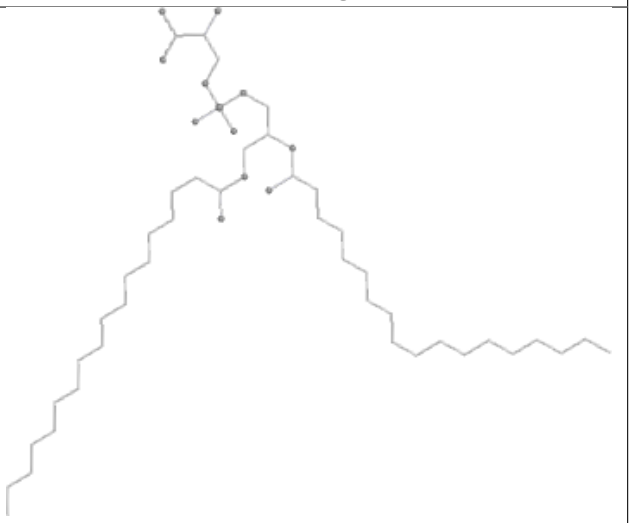
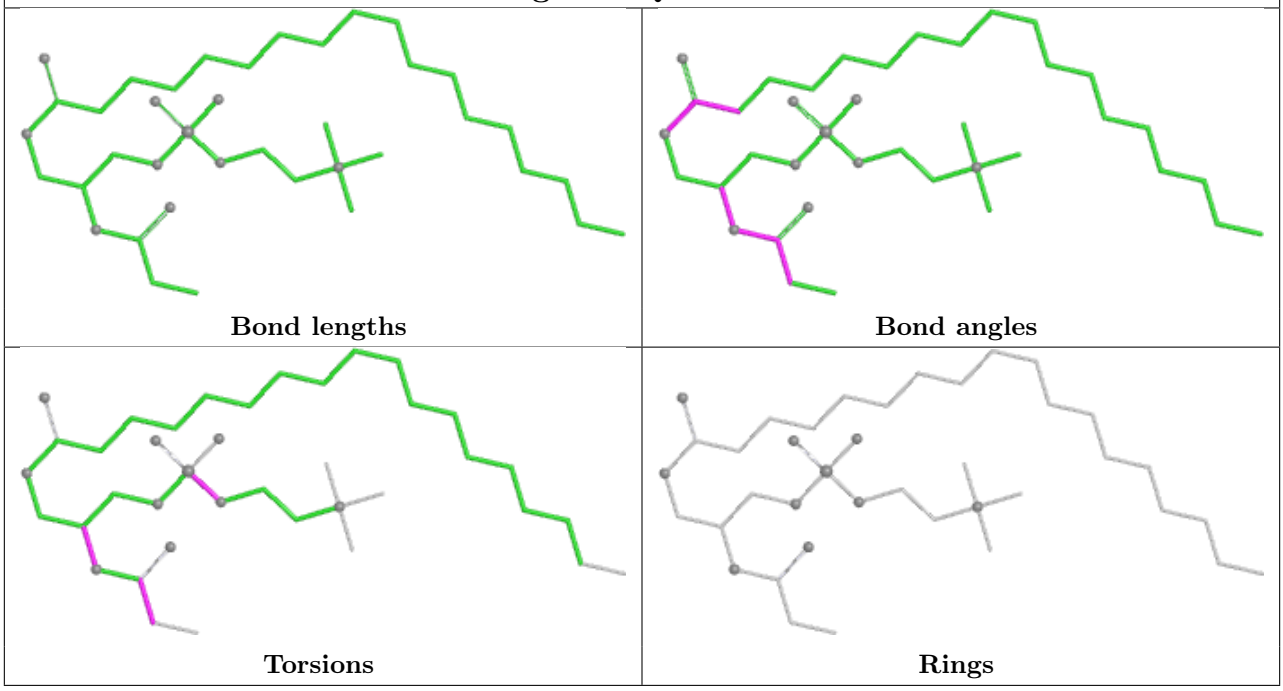
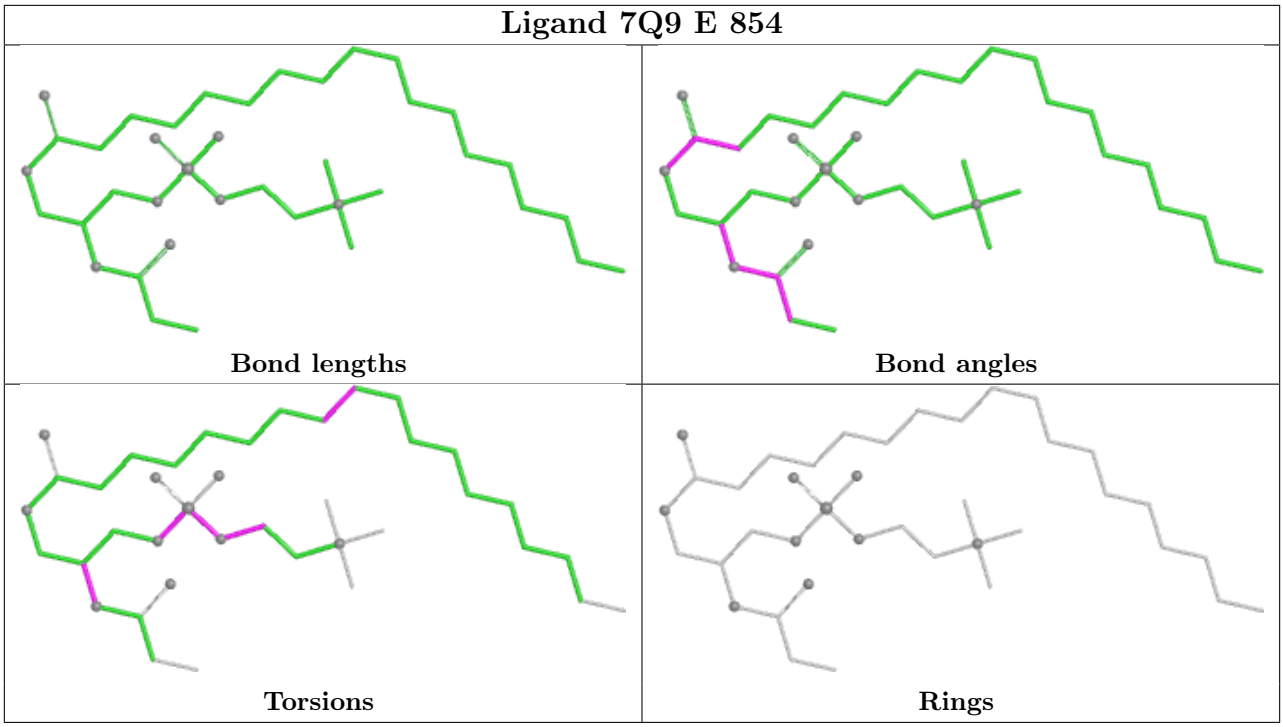


Rings

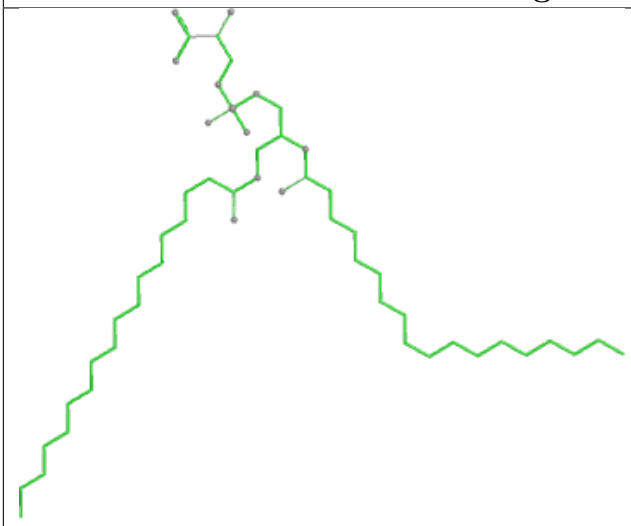
Ligand 7Q9 E 831



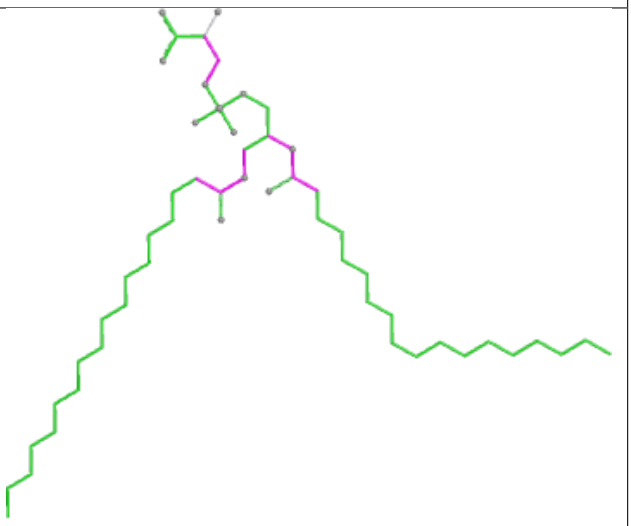
Ligand 7Q9 E 854



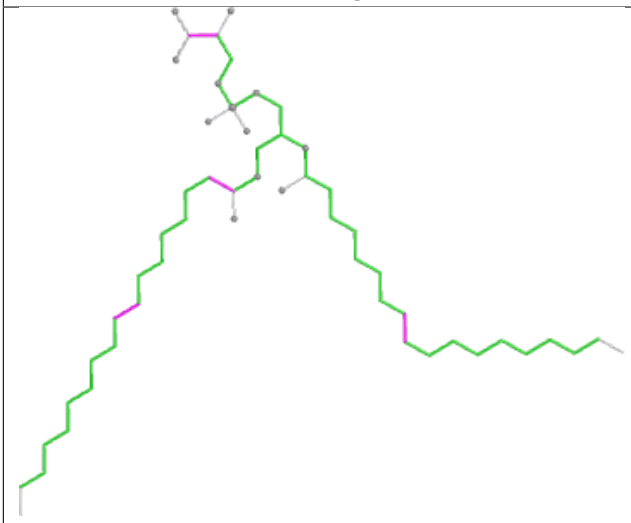
Ligand 17F E 810



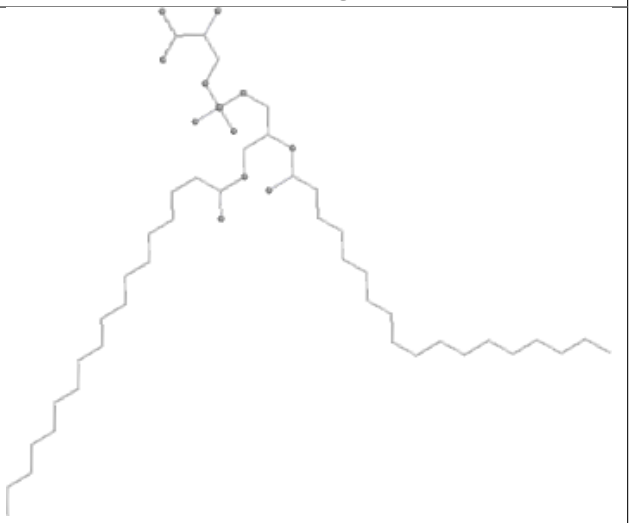
Bond lengths



Bond angles

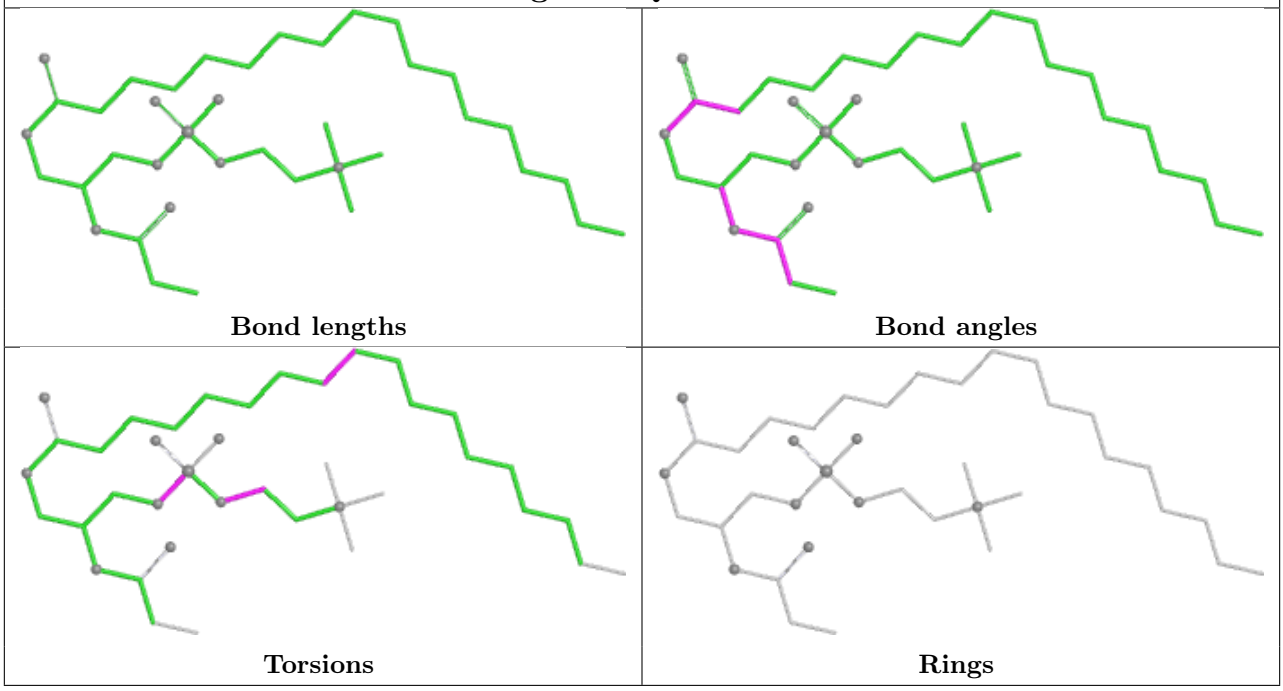


Torsions

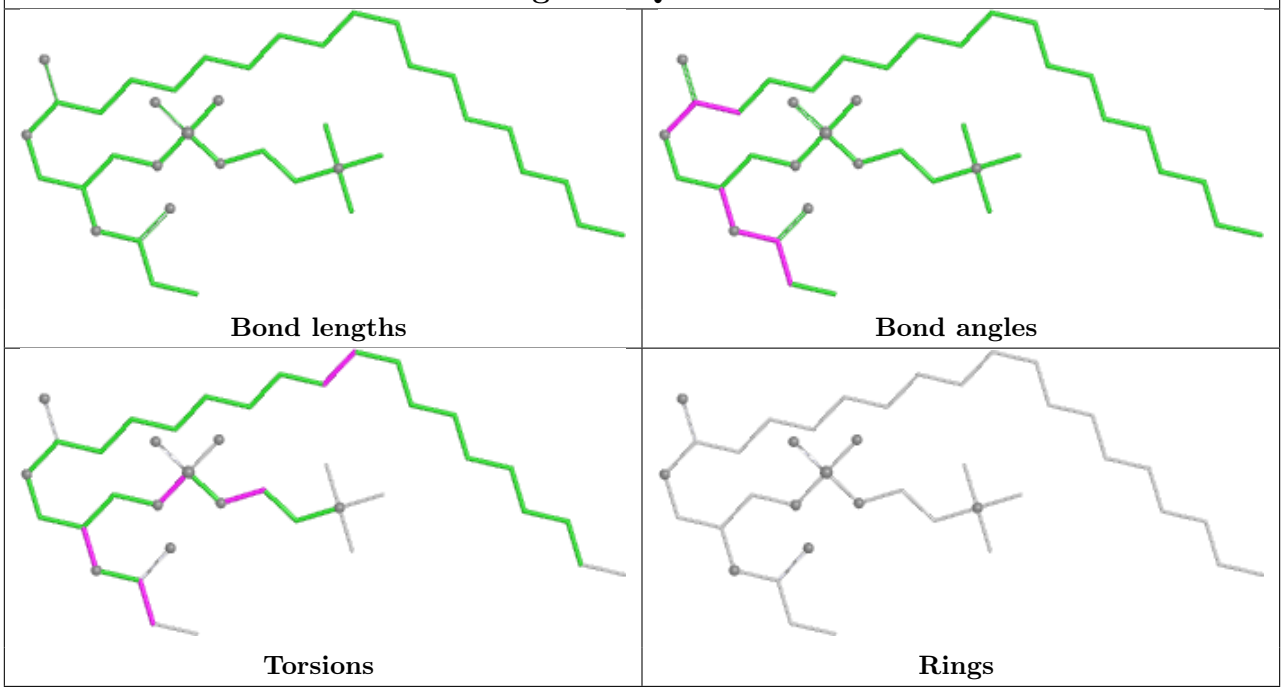


Rings

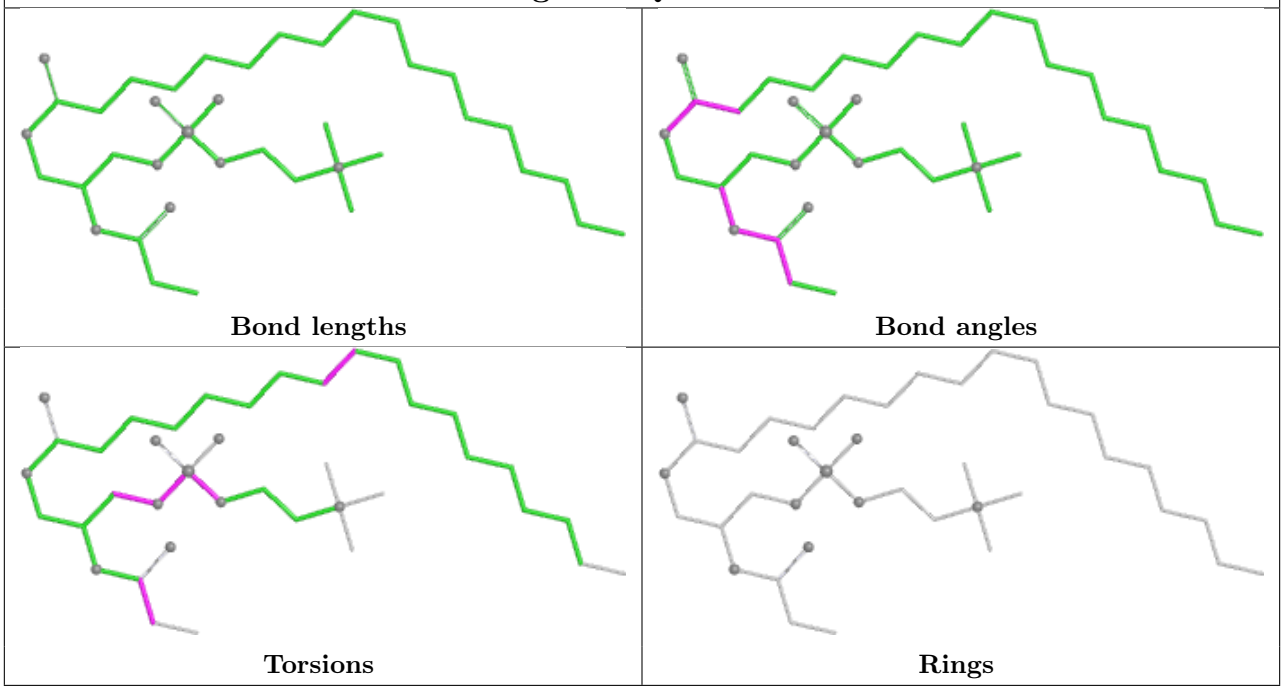
Ligand 7Q9 A 209



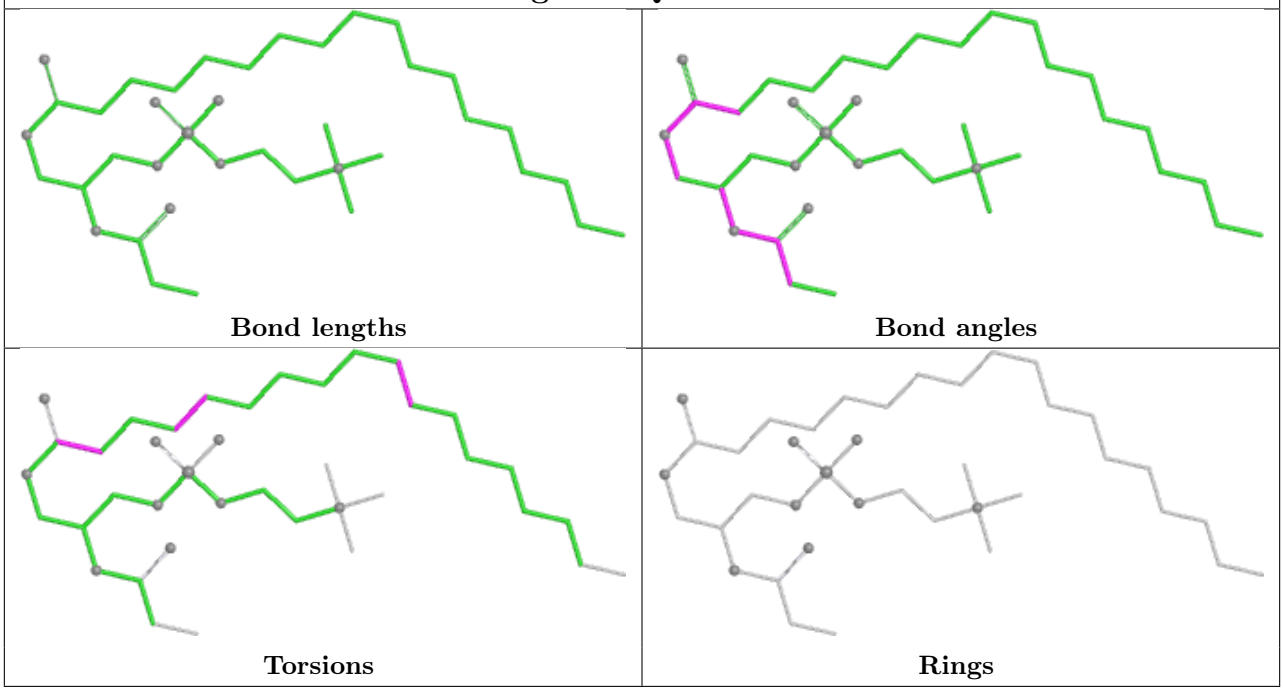
Ligand 7Q9 E 835



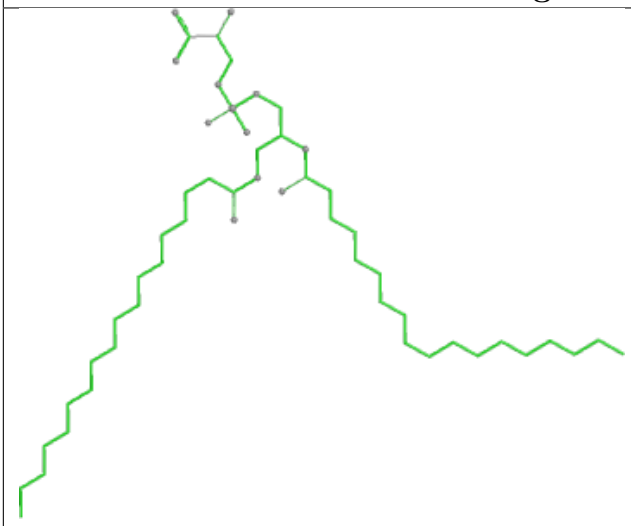
Ligand 7Q9 E 804



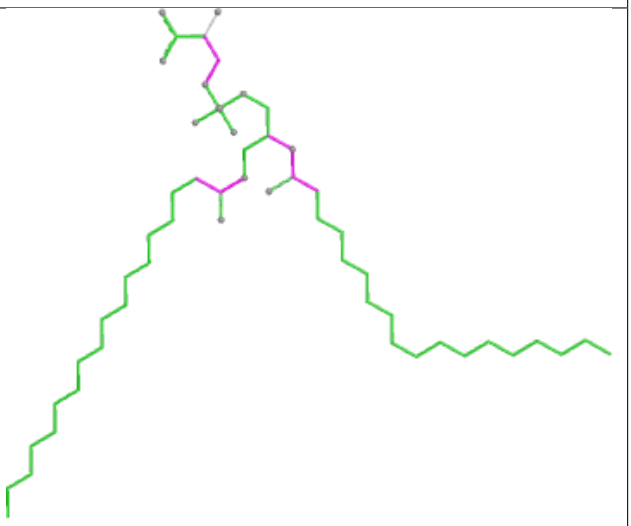
Ligand 7Q9 B 205



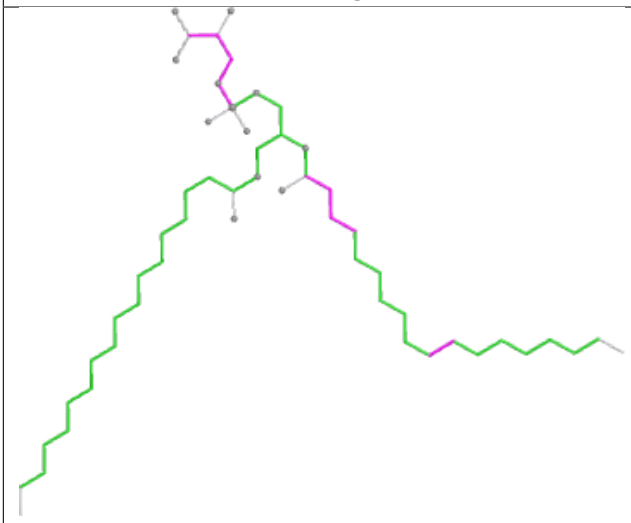
Ligand 17F E 819



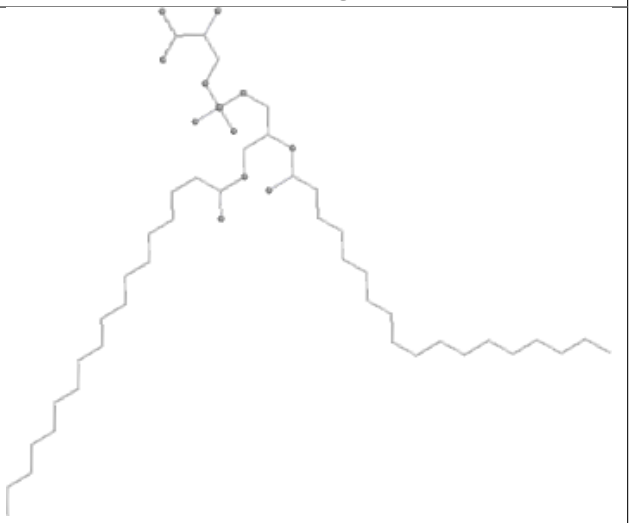
Bond lengths



Bond angles

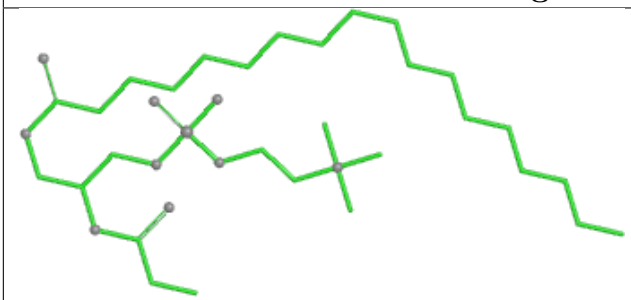


Torsions



Rings

Ligand 7Q9 E 851



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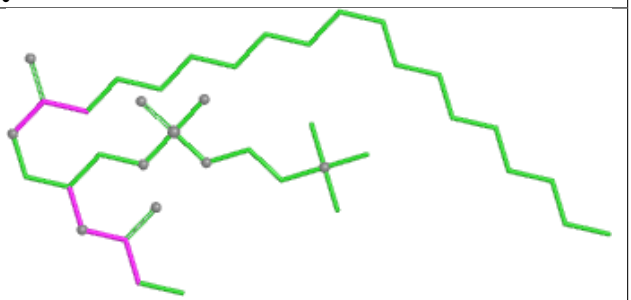
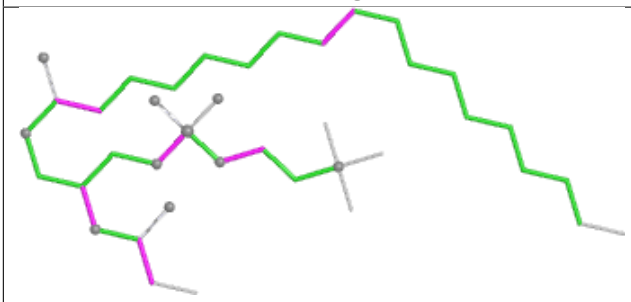


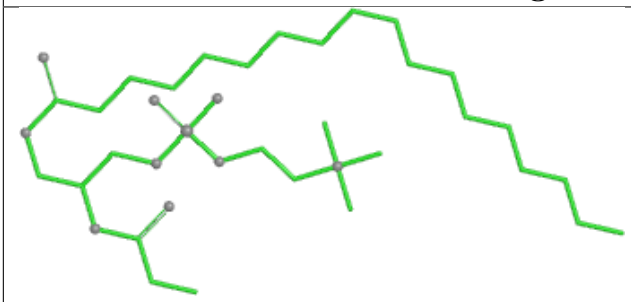
Bond angles



Torsions

Rings

Ligand 7Q9 D 556



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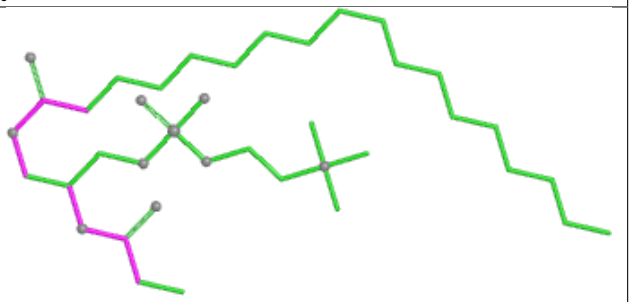
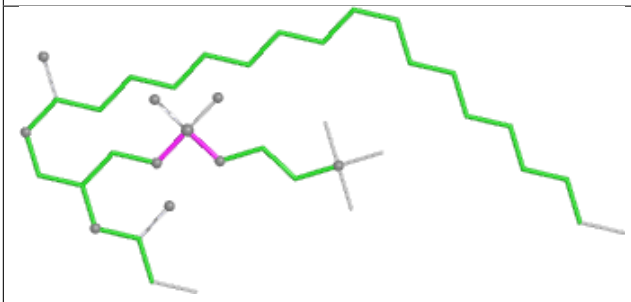


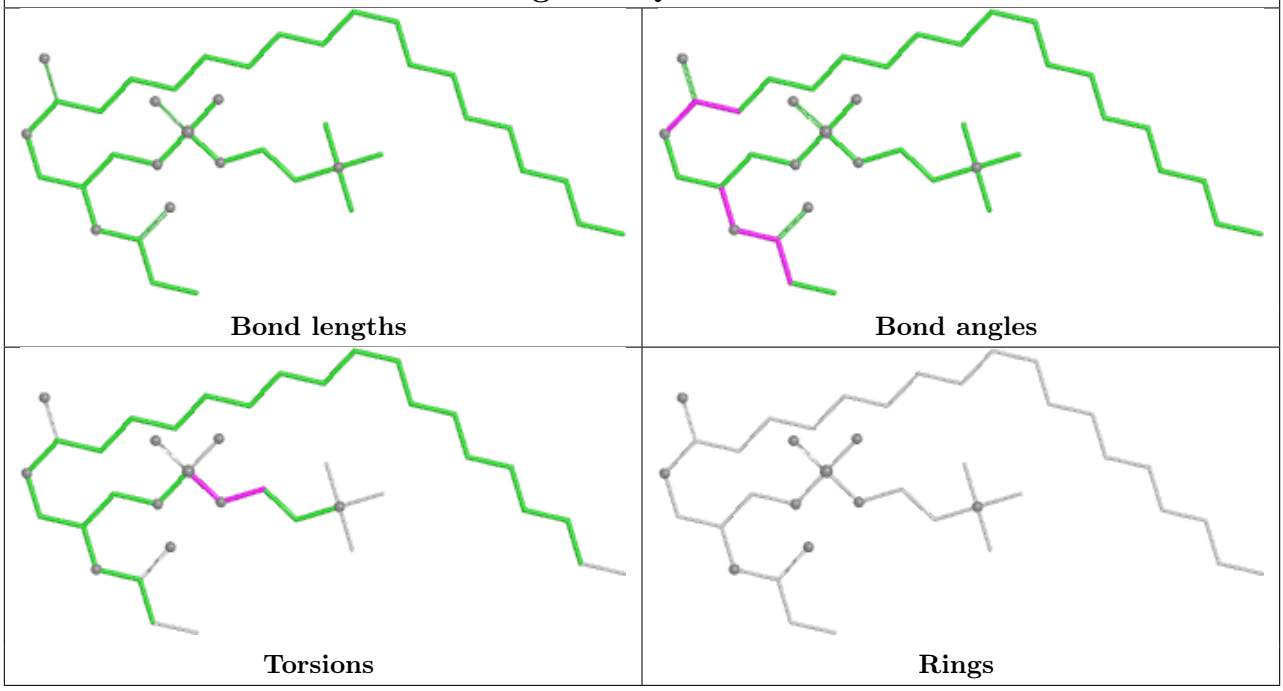
Bond angles



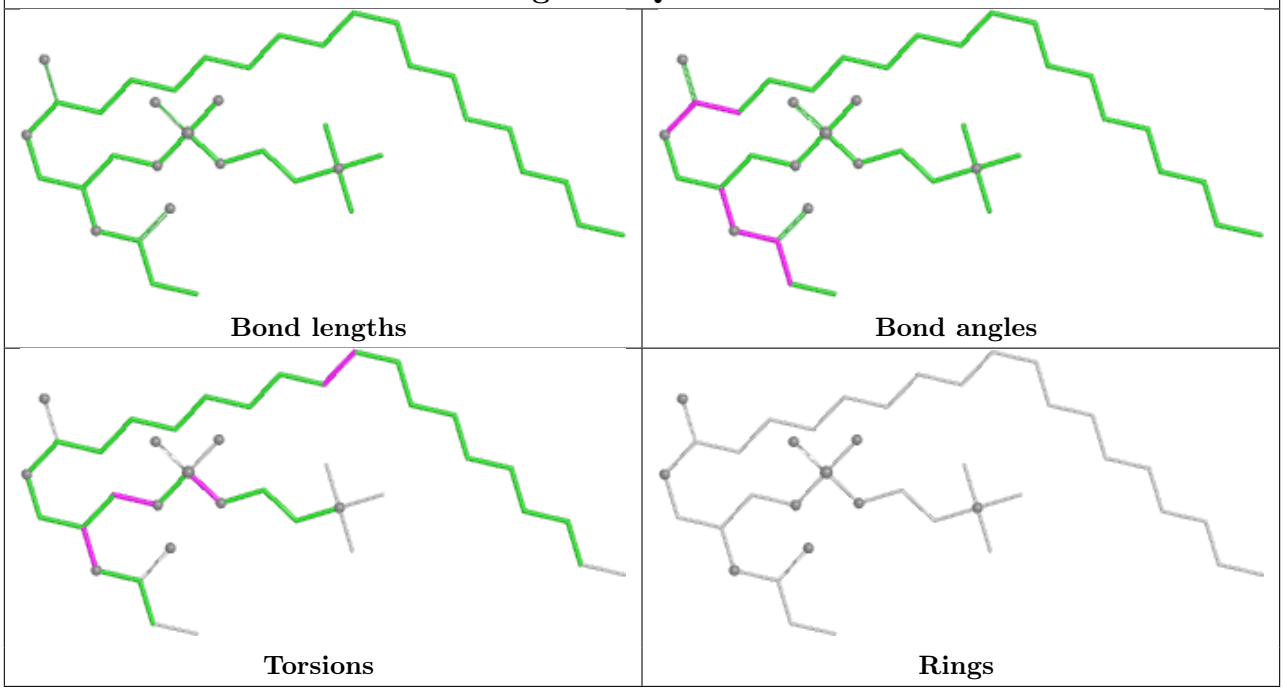
Torsions

Rings

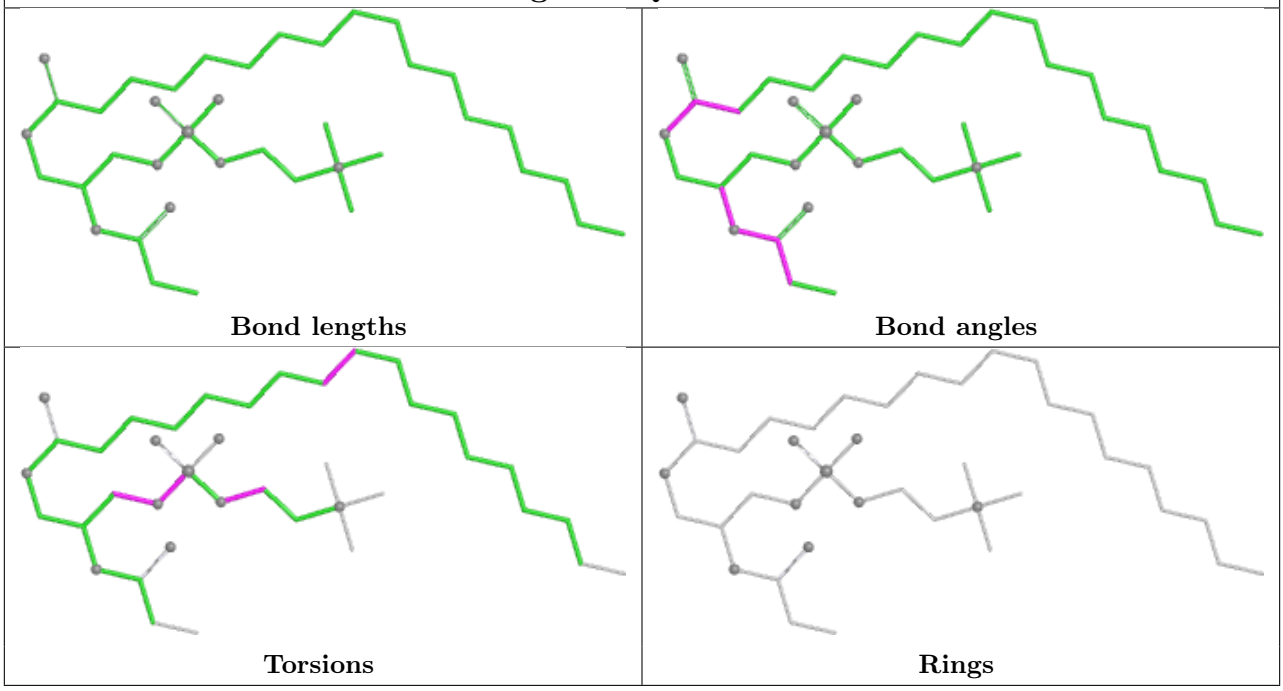
Ligand 7Q9 E 823



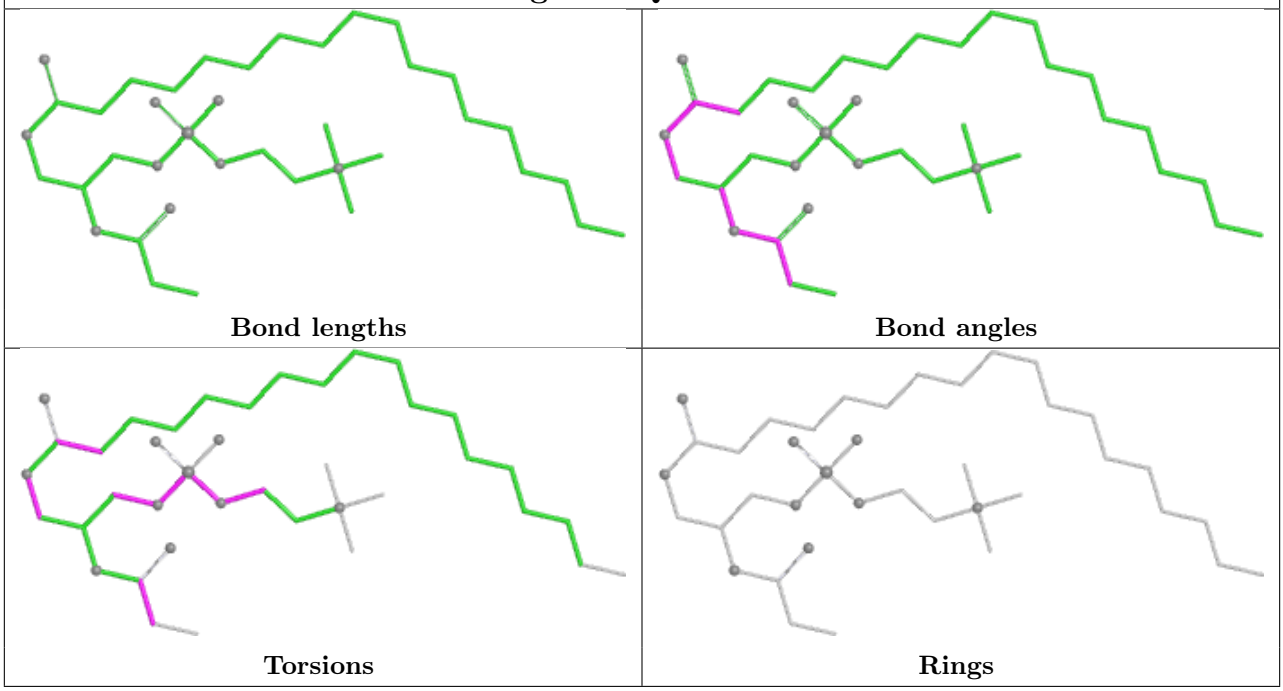
Ligand 7Q9 E 852



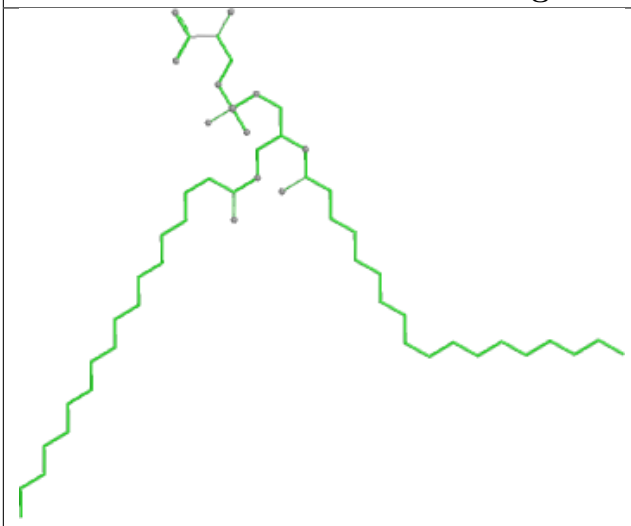
Ligand 7Q9 D 535



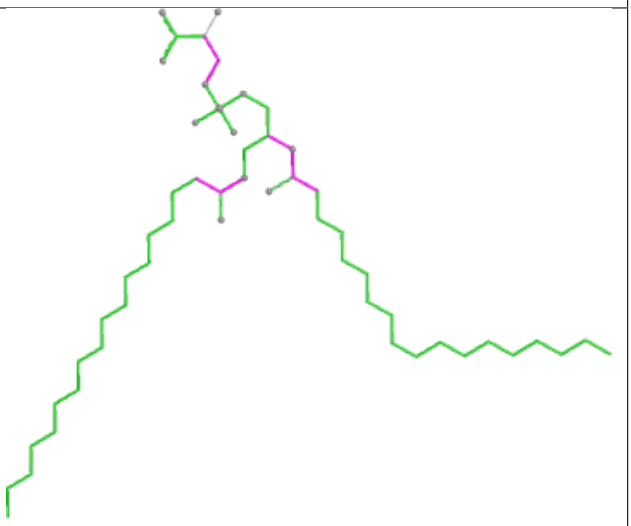
Ligand 7Q9 D 514



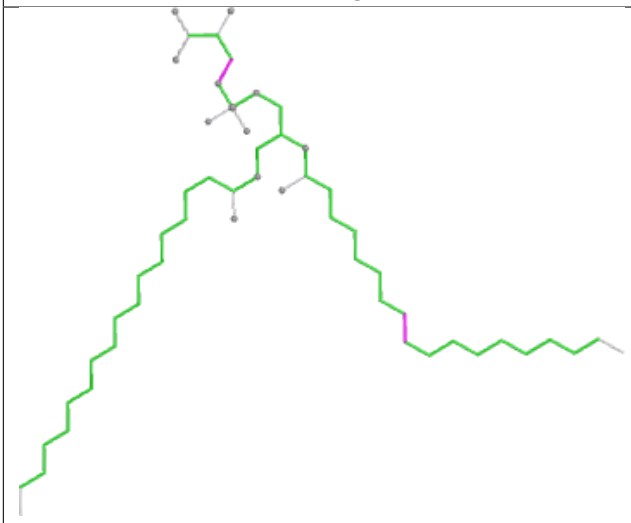
Ligand 17F A 219



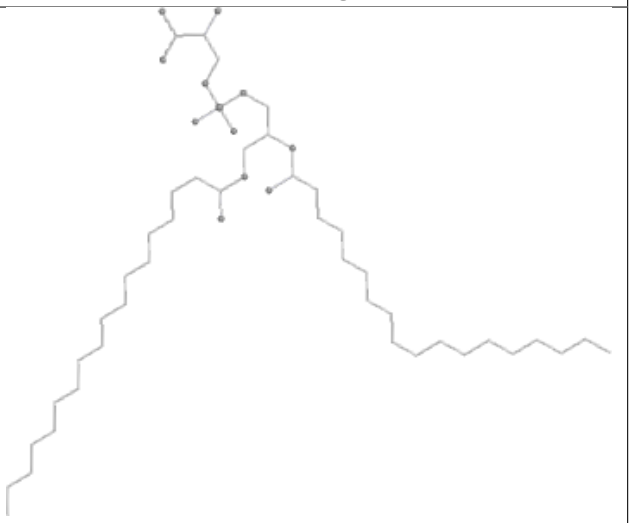
Bond lengths



Bond angles

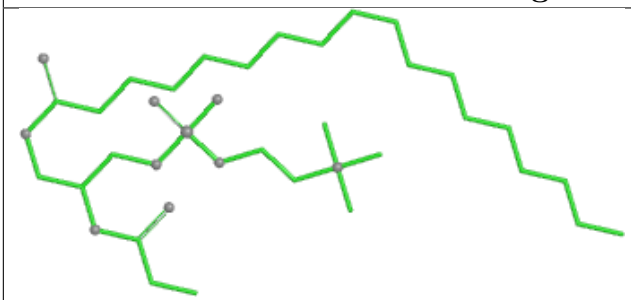


Torsions



Rings

Ligand 7Q9 E 853



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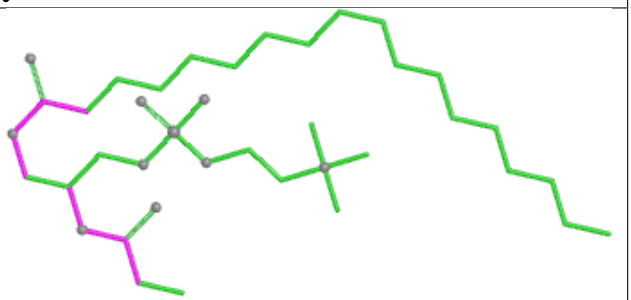
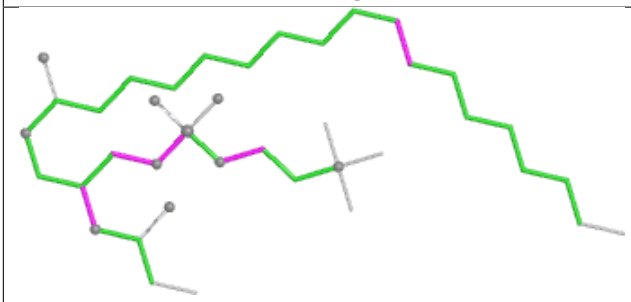


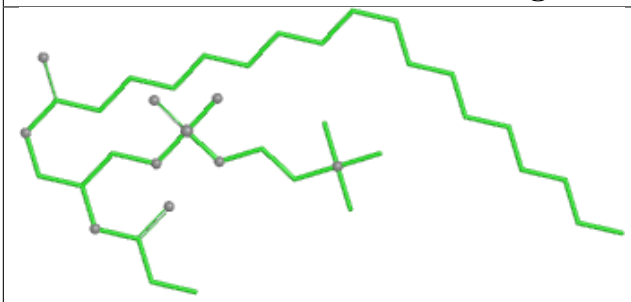
Bond angles



Torsions

Rings

Ligand 7Q9 D 501



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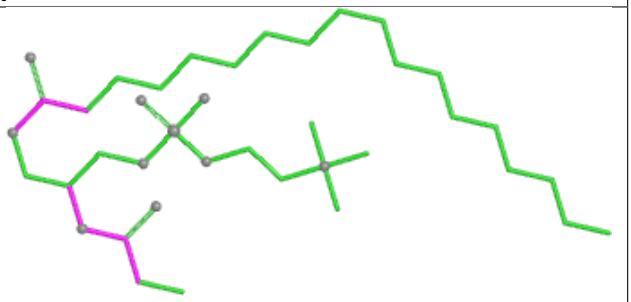
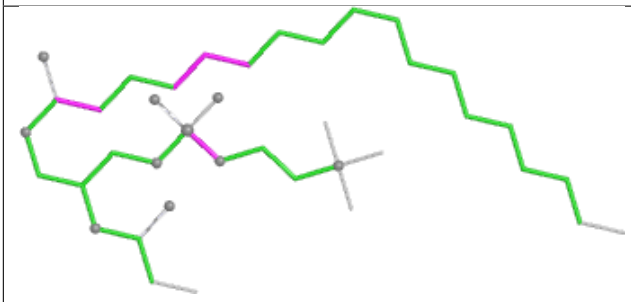


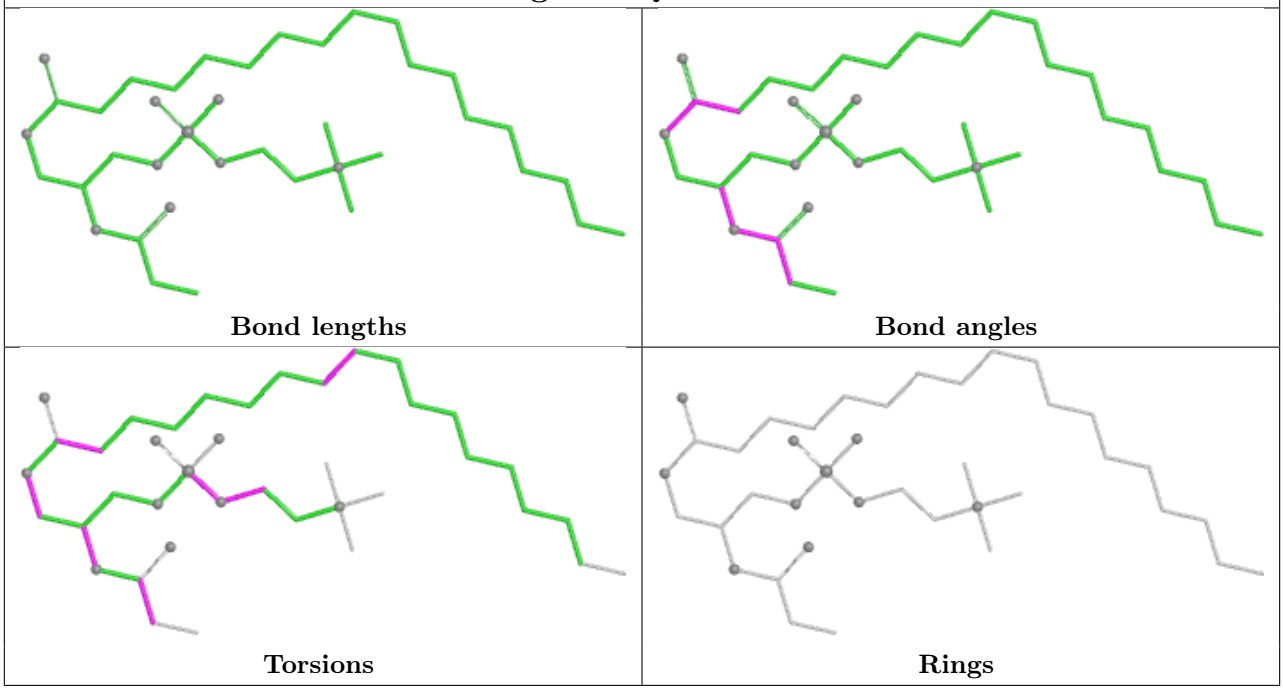
Bond angles



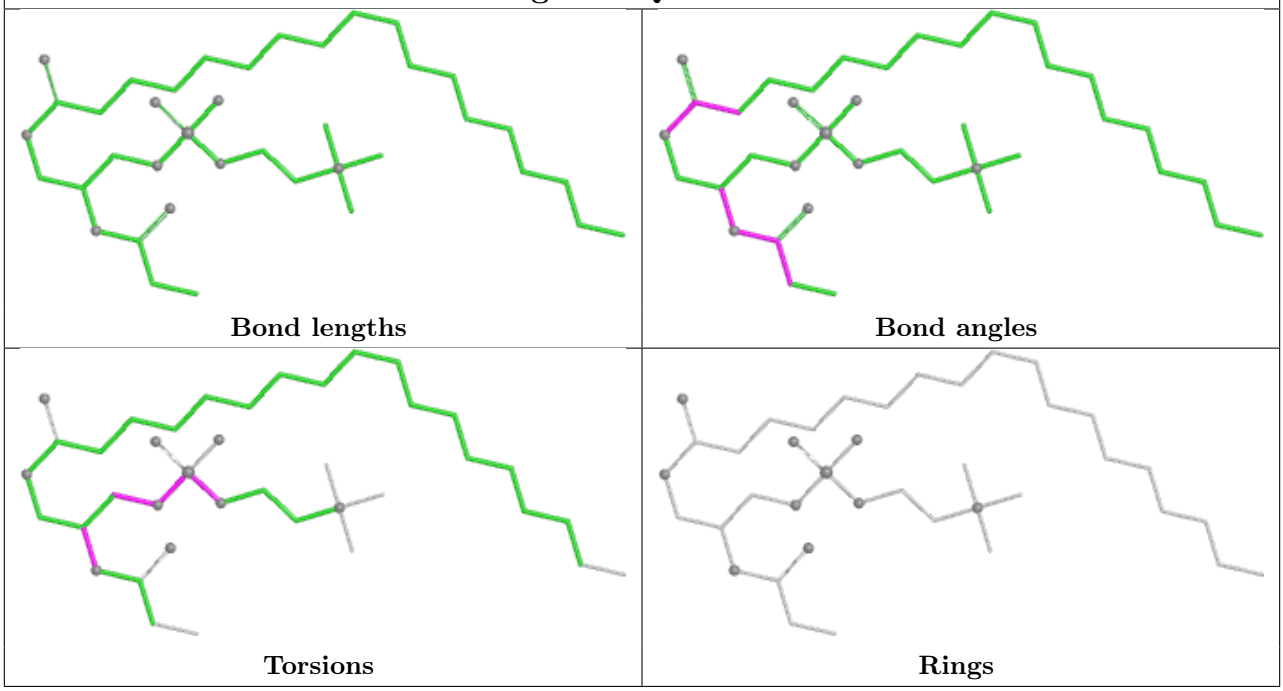
Torsions

Rings

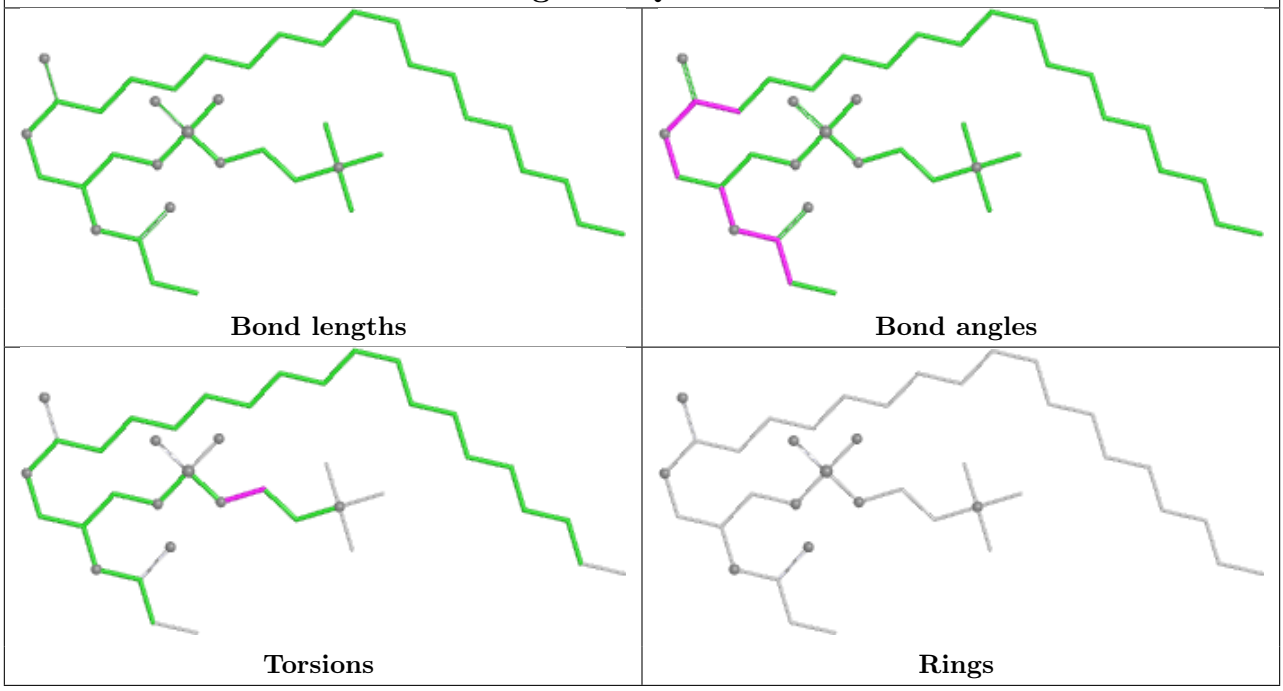
Ligand 7Q9 A 206



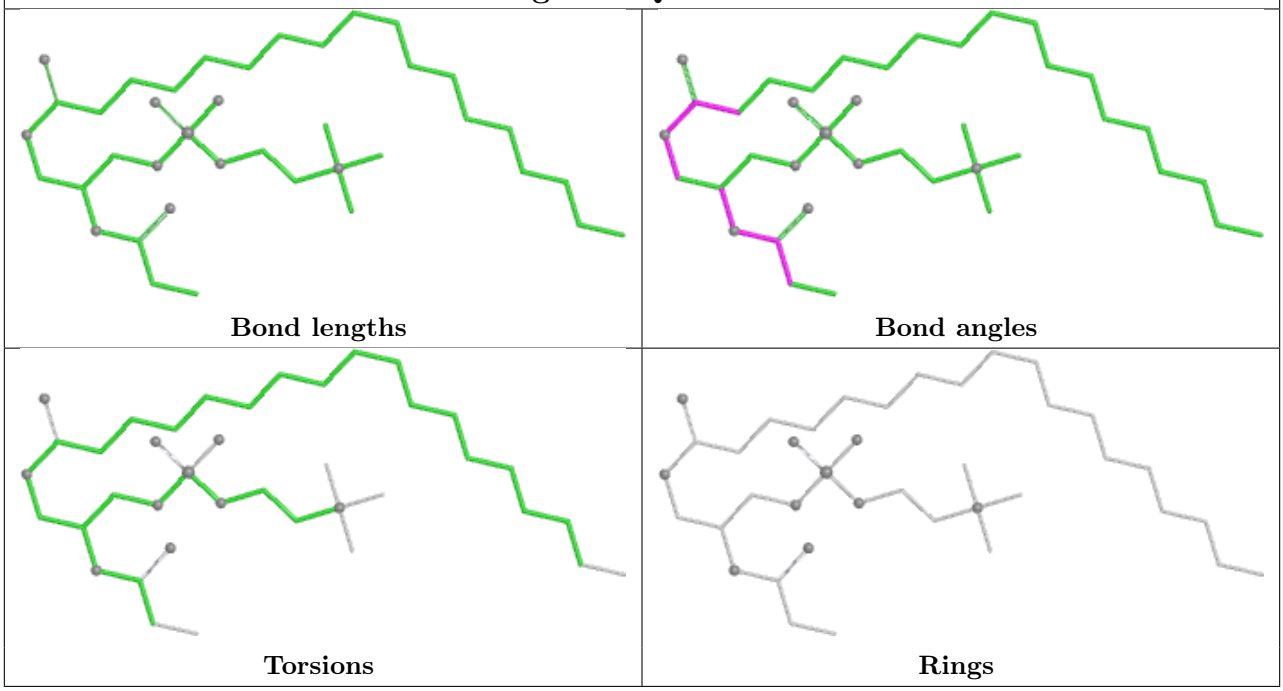
Ligand 7Q9 B 210



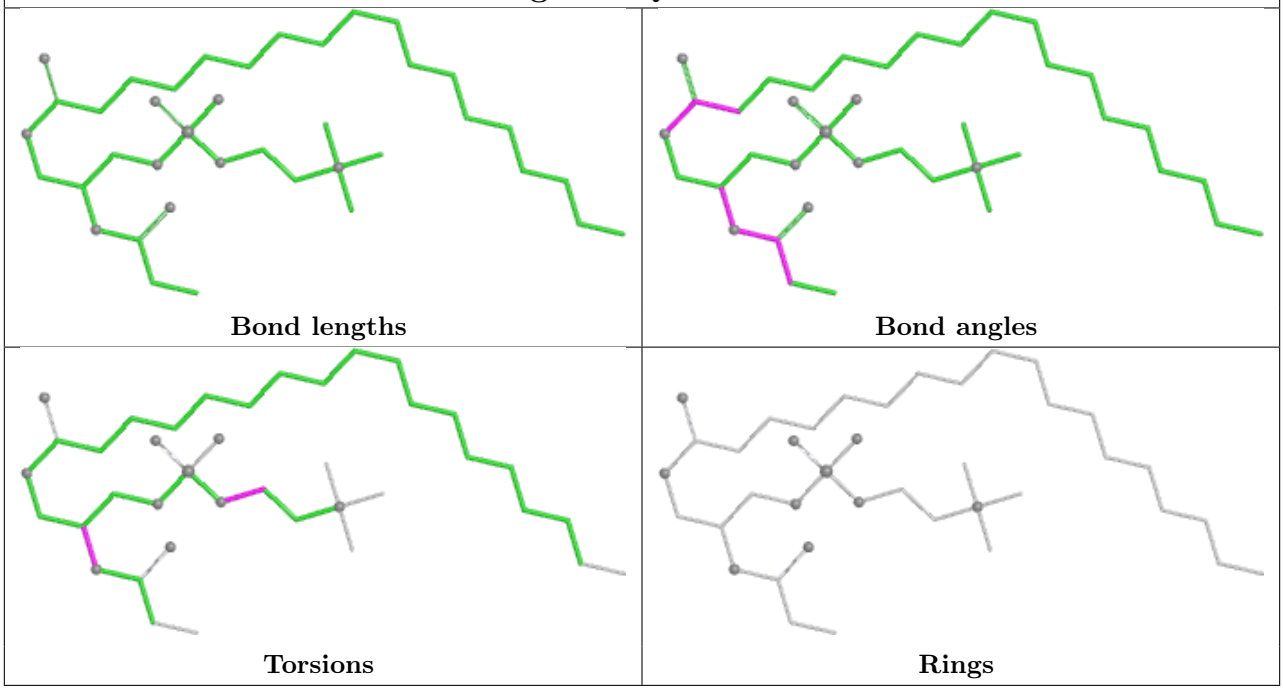
Ligand 7Q9 E 864



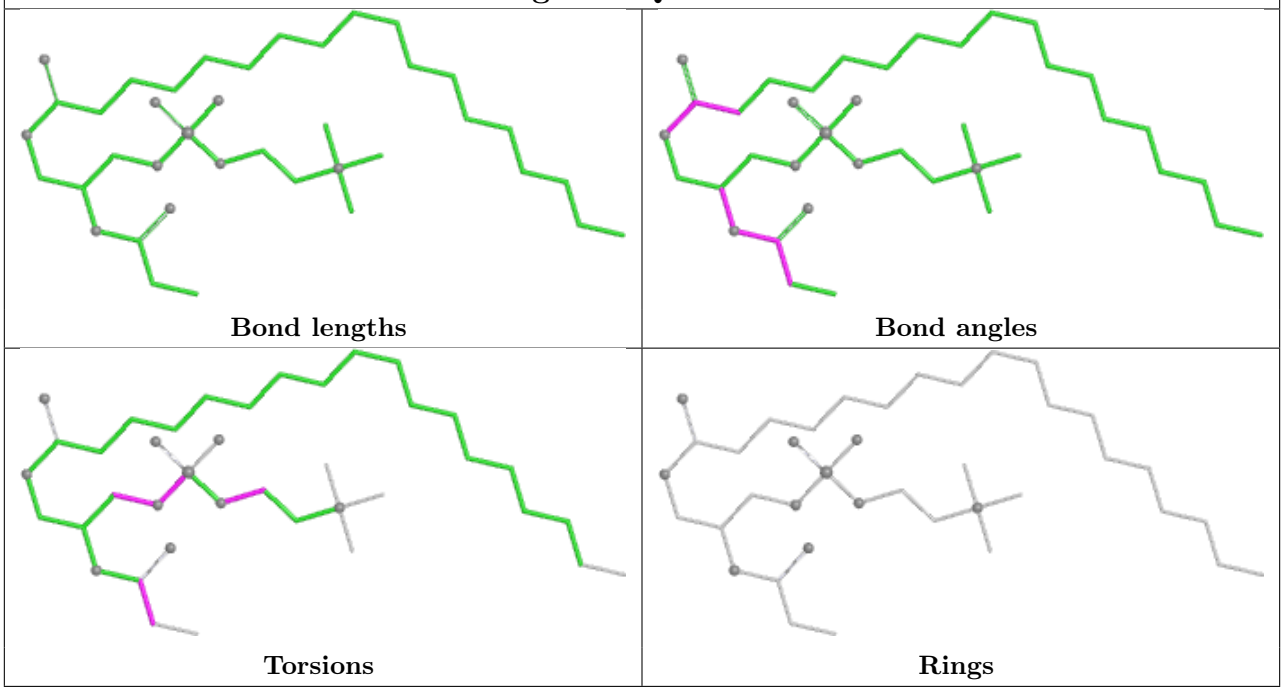
Ligand 7Q9 E 815



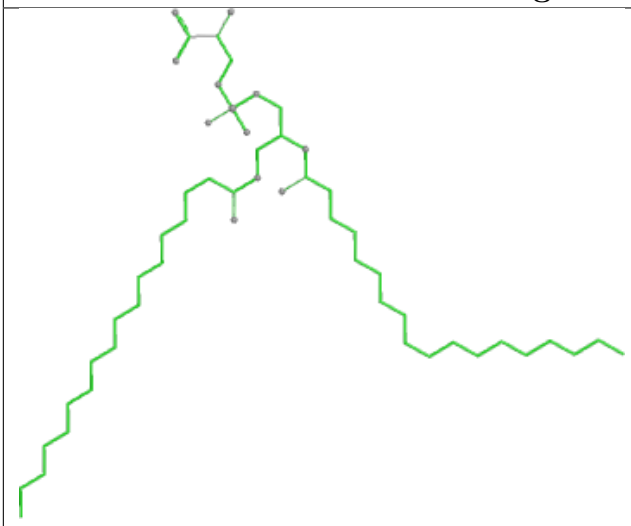
Ligand 7Q9 D 530



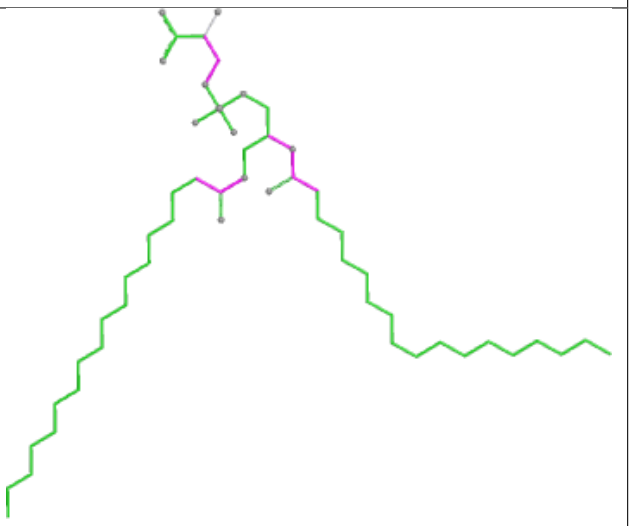
Ligand 7Q9 E 834



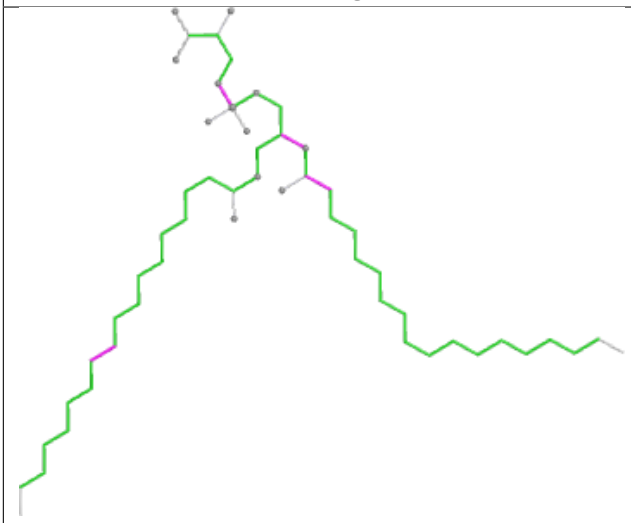
Ligand 17F E 820



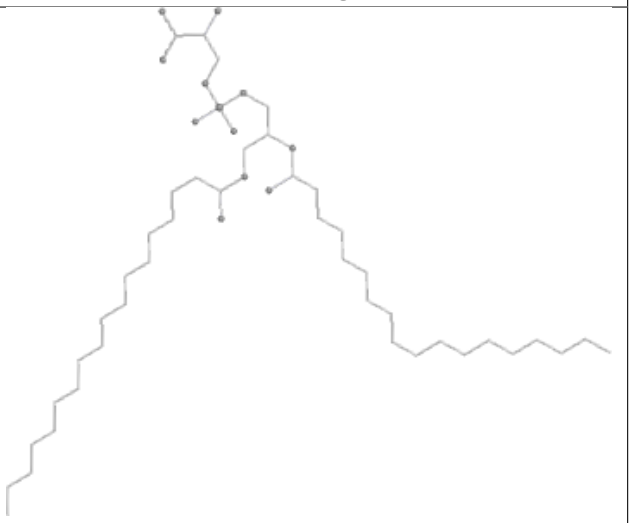
Bond lengths



Bond angles

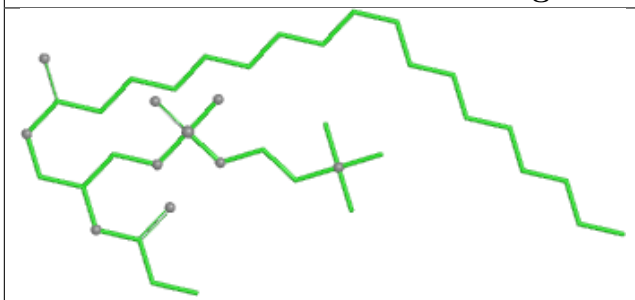


Torsions

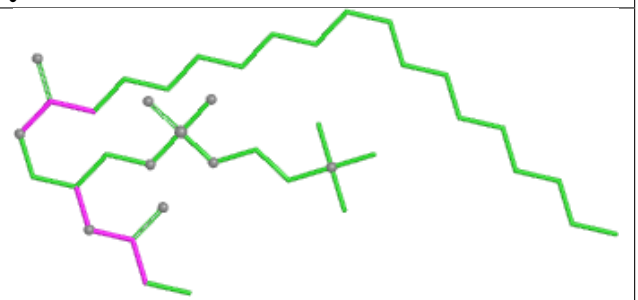


Rings

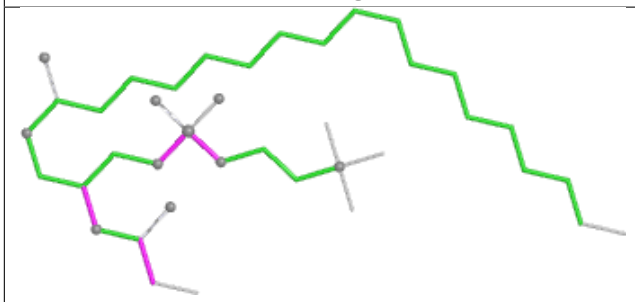
Ligand 7Q9 E 862



Bond lengths



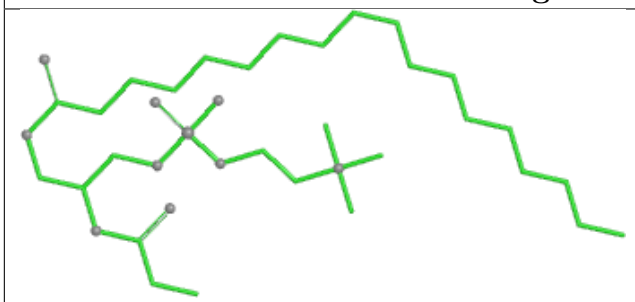
Bond angles



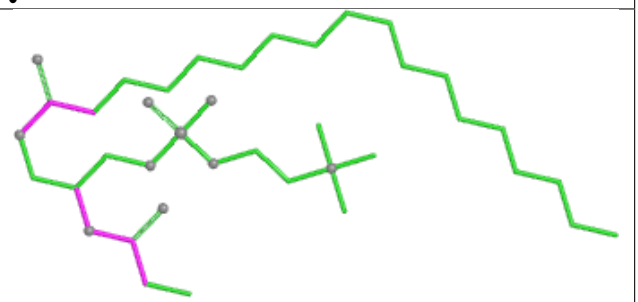
Torsions

Rings

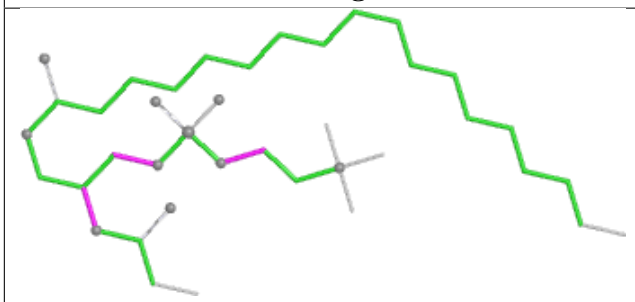
Ligand 7Q9 E 817



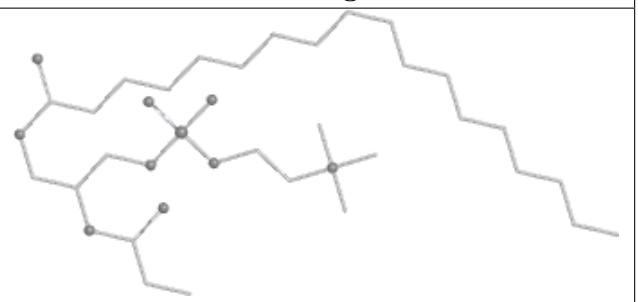
Bond lengths



Bond angles

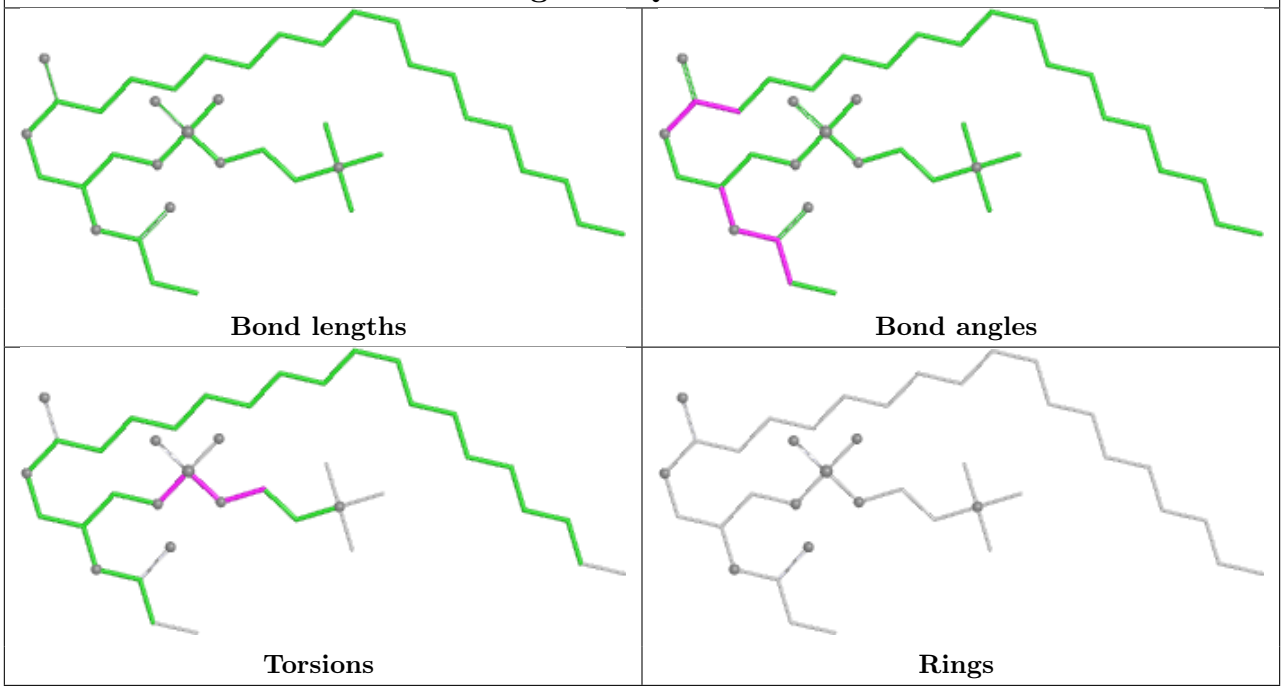


Torsions

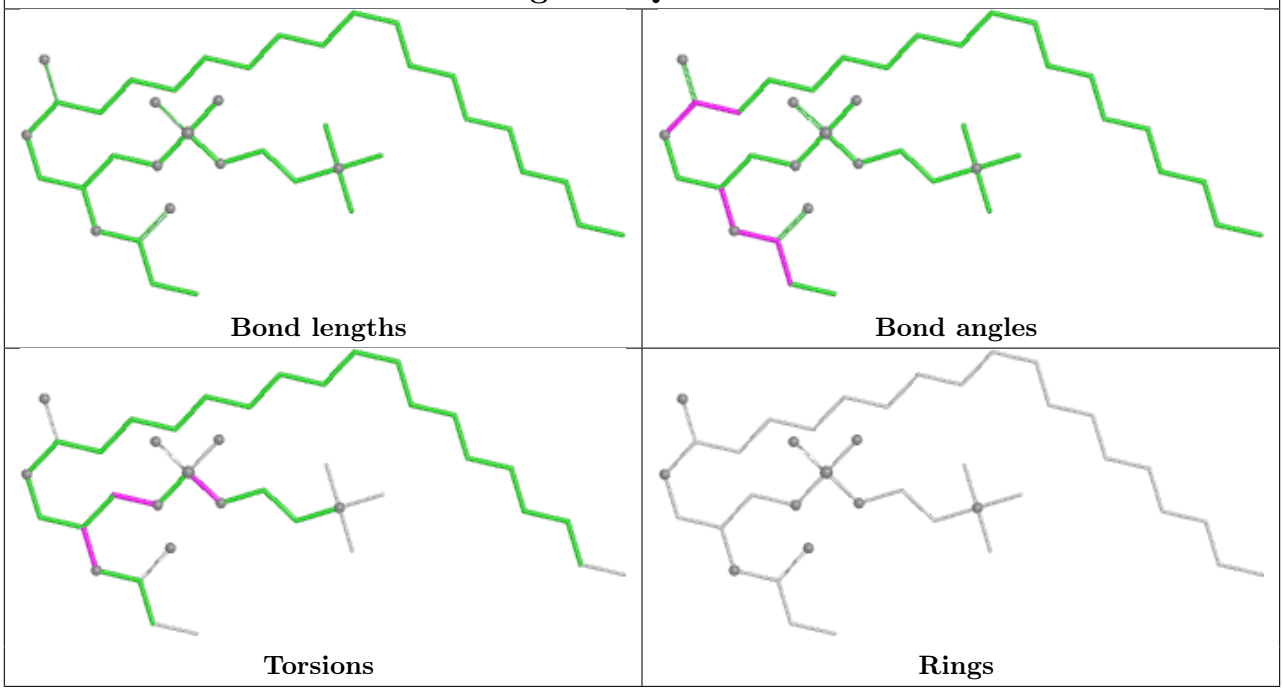


Rings

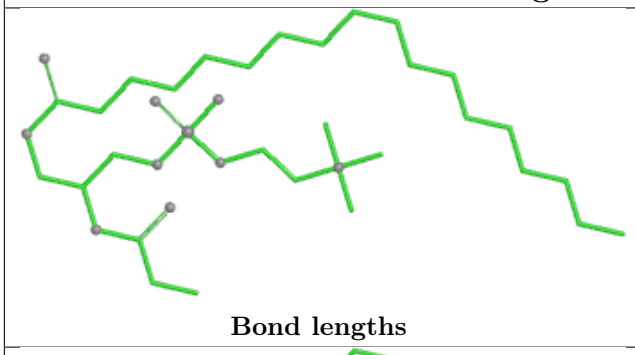
Ligand 7Q9 D 512



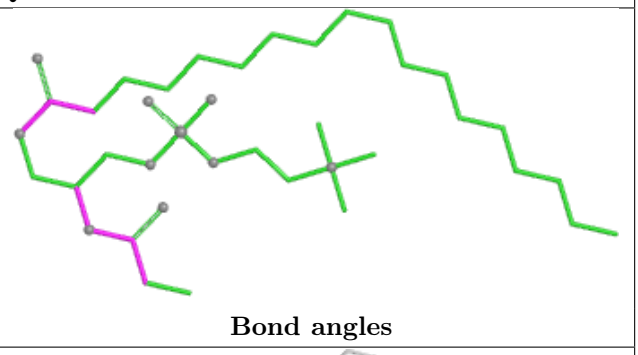
Ligand 7Q9 D 504



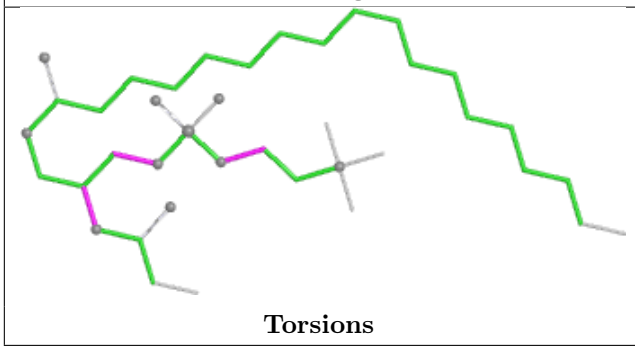
Ligand 7Q9 E 847



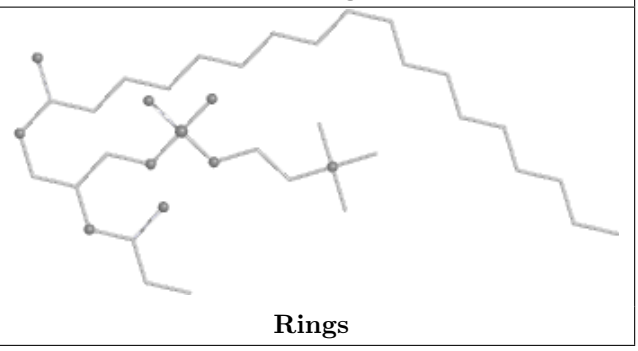
Bond lengths



Bond angles

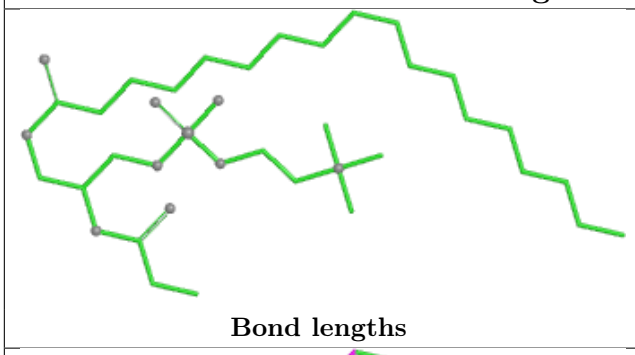


Torsions

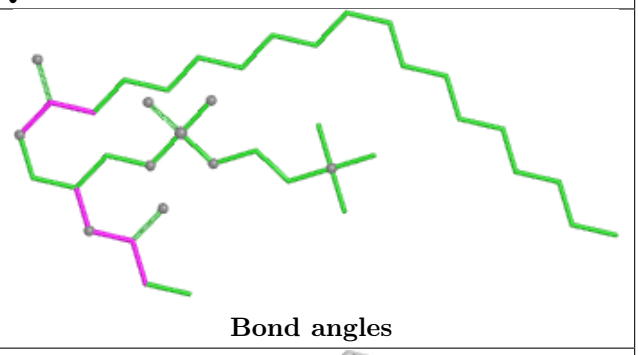


Rings

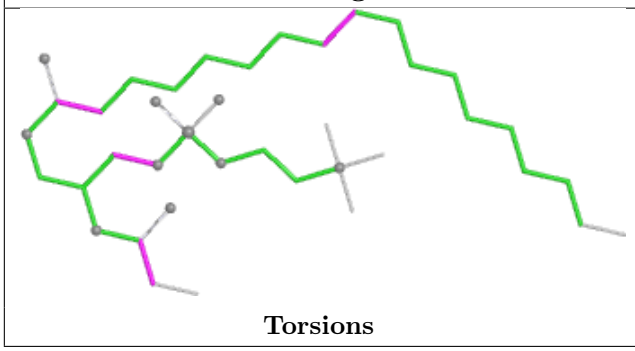
Ligand 7Q9 E 850



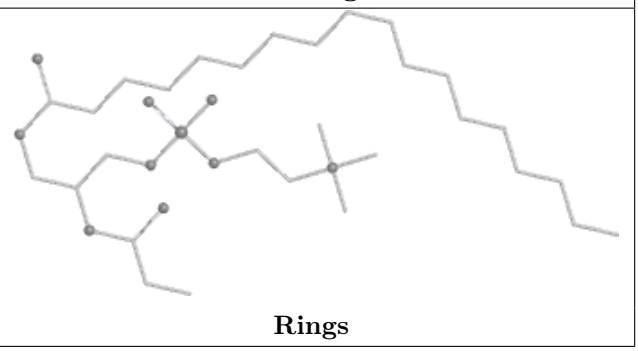
Bond lengths



Bond angles

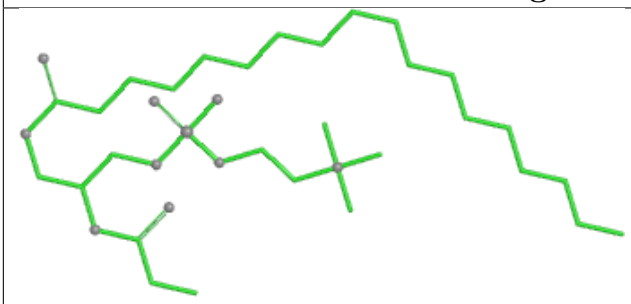


Torsions



Rings

Ligand 7Q9 A 205



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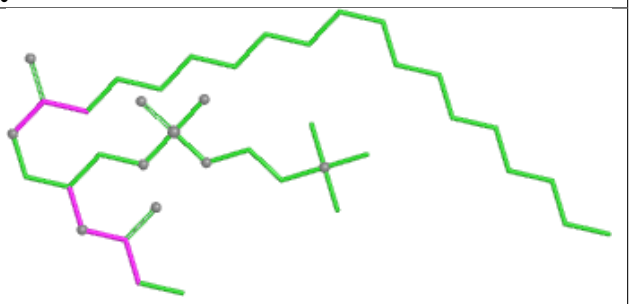
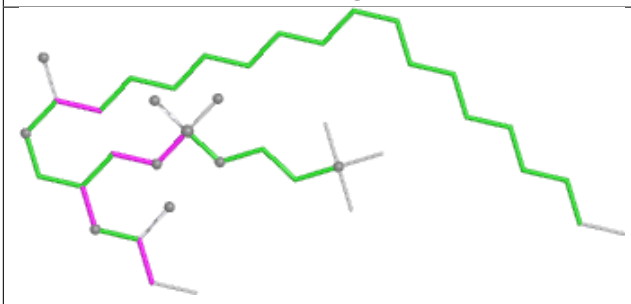


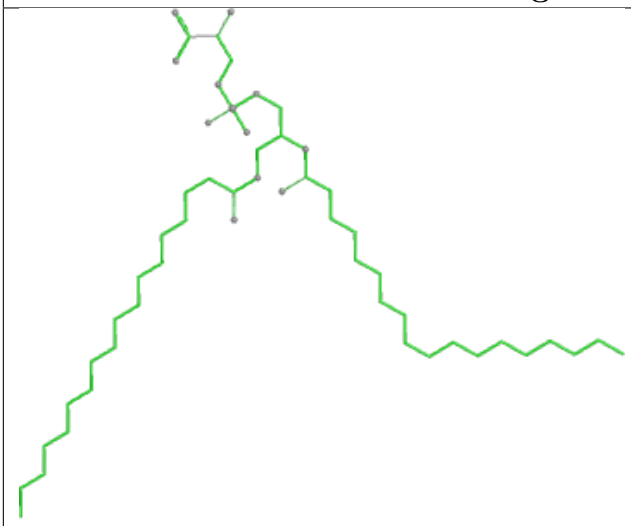
Bond angles



Torsions

Rings

Ligand 17F D 533



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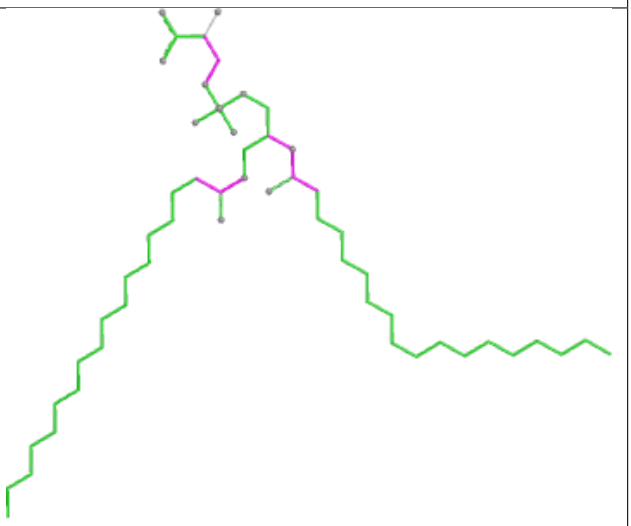
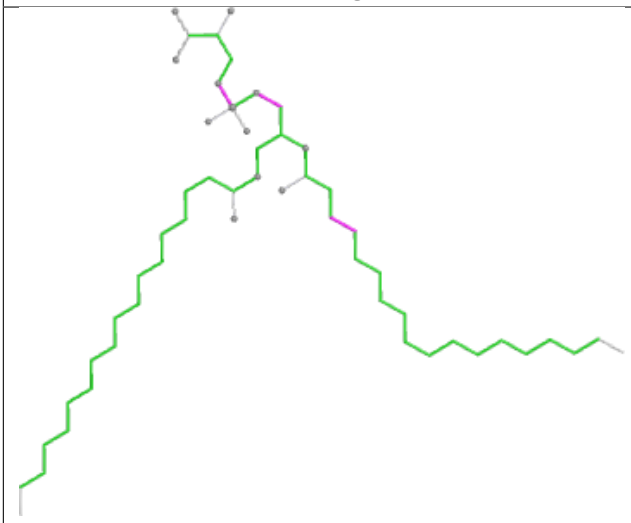
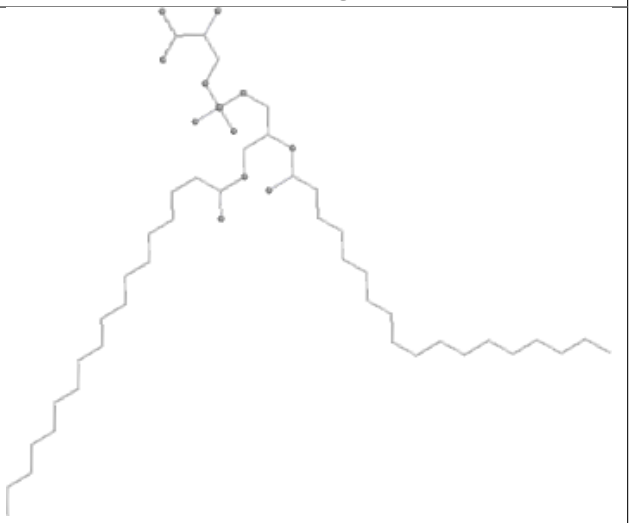


Bond angles

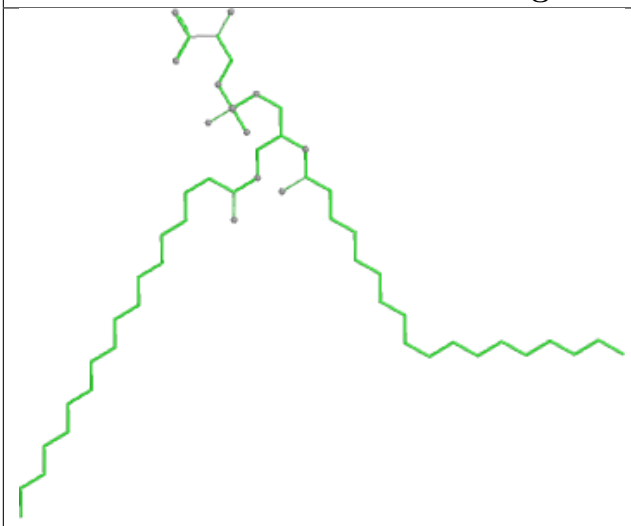


Torsions



Rings

Ligand 17F D 540



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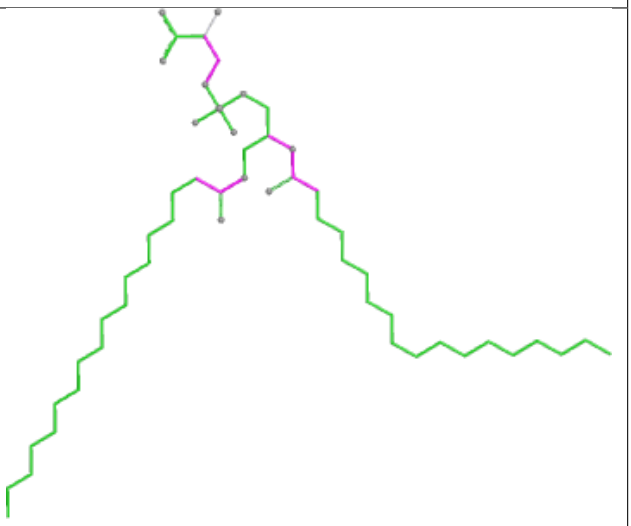
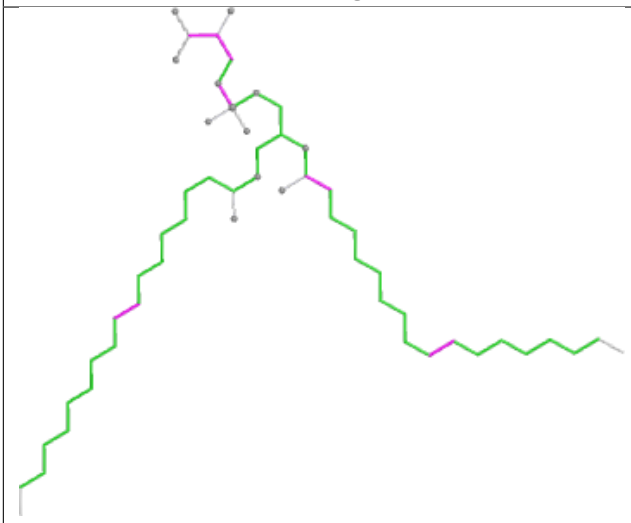


Bond angles



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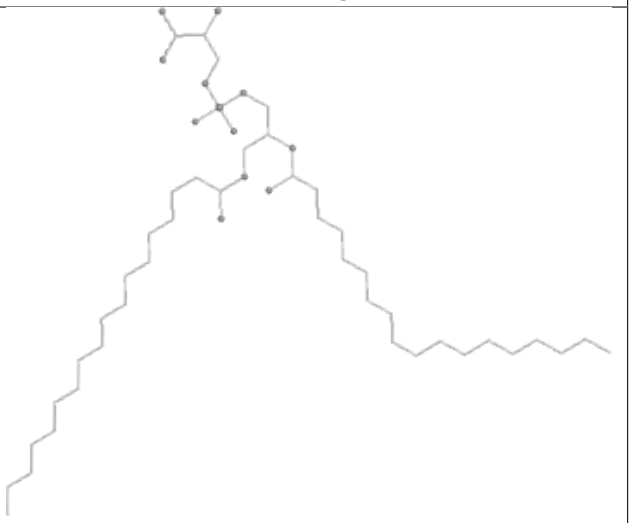
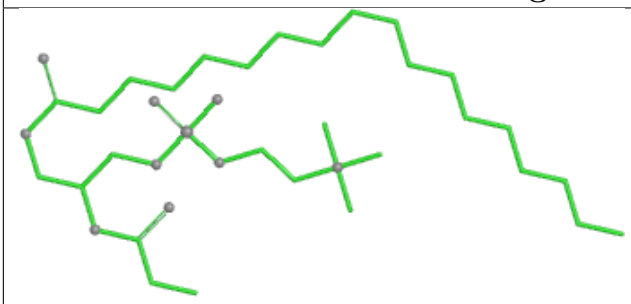


Rings

Ligand 7Q9 D 508



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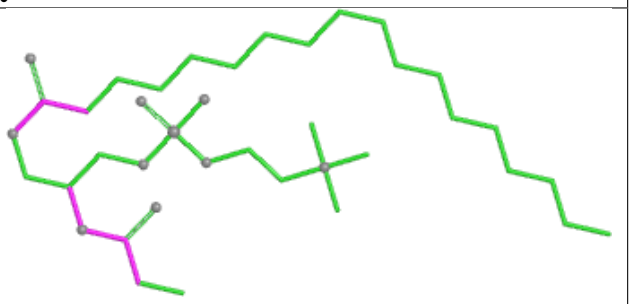
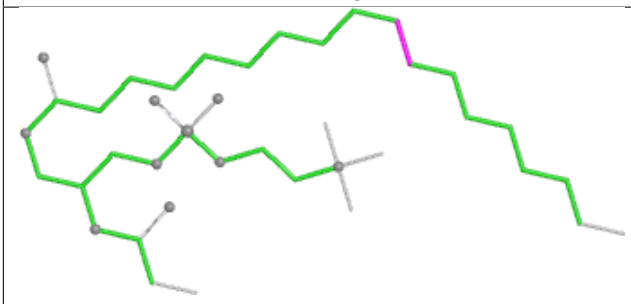


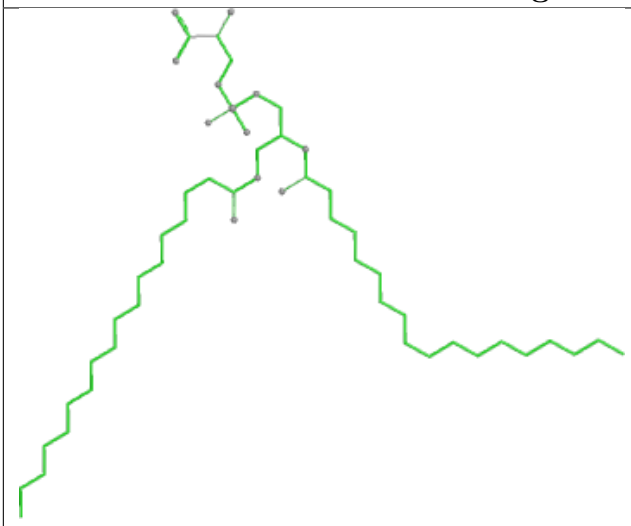
Bond angles



Torsions

Rings

Ligand 17F D 517



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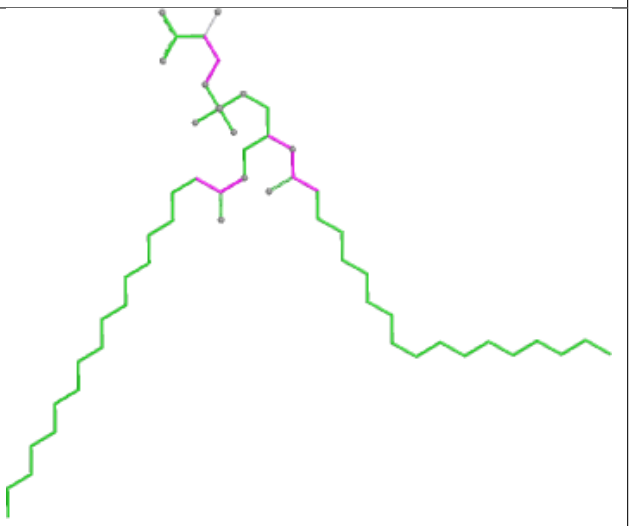
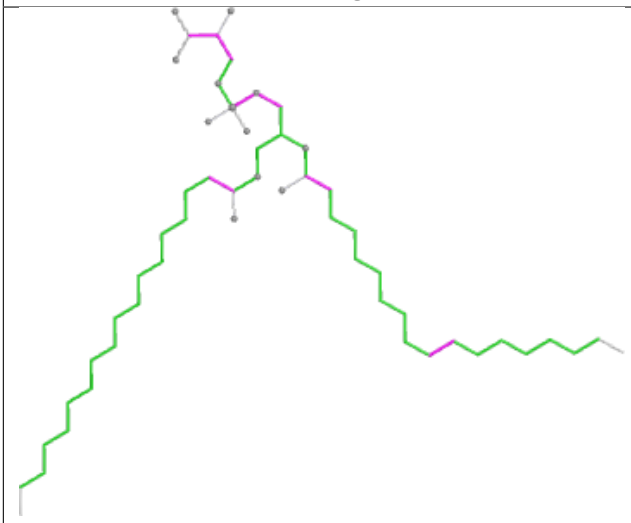
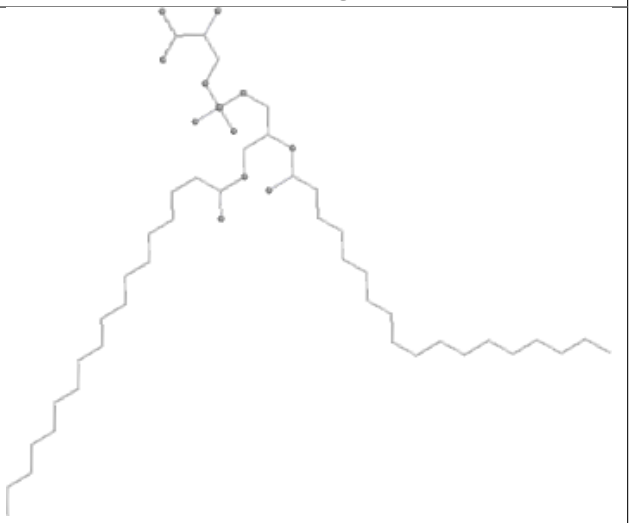


Bond angles

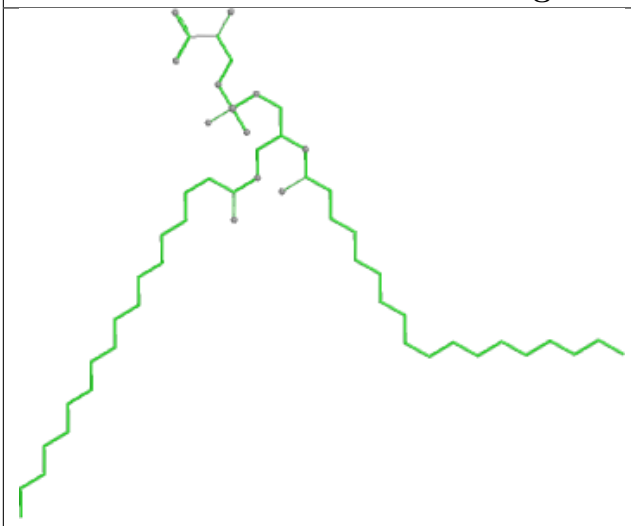


Torsions



Rings

Ligand 17F E 802



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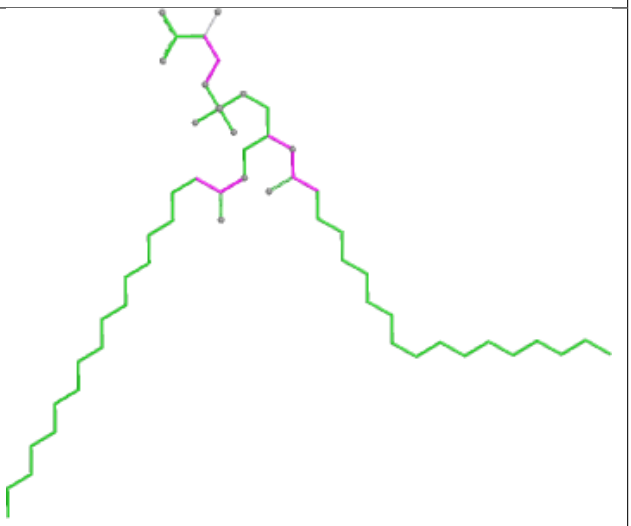
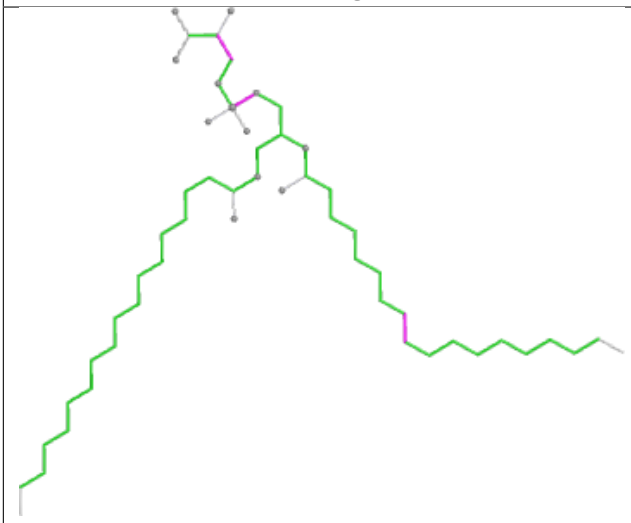
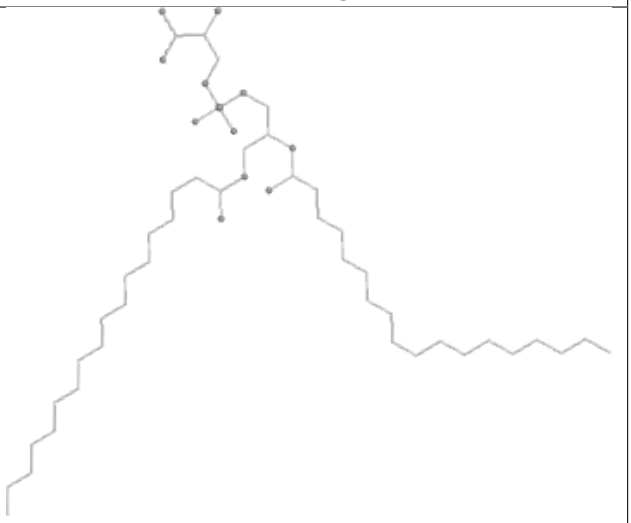


Bond angles

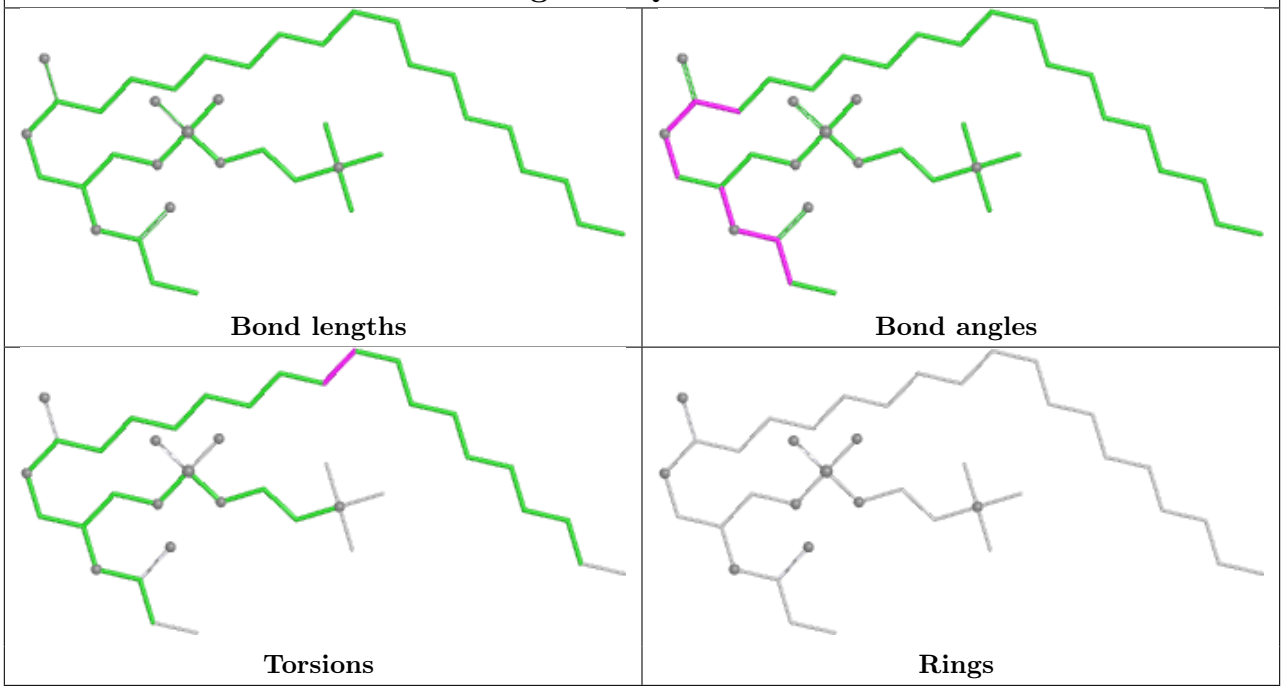


Torsions

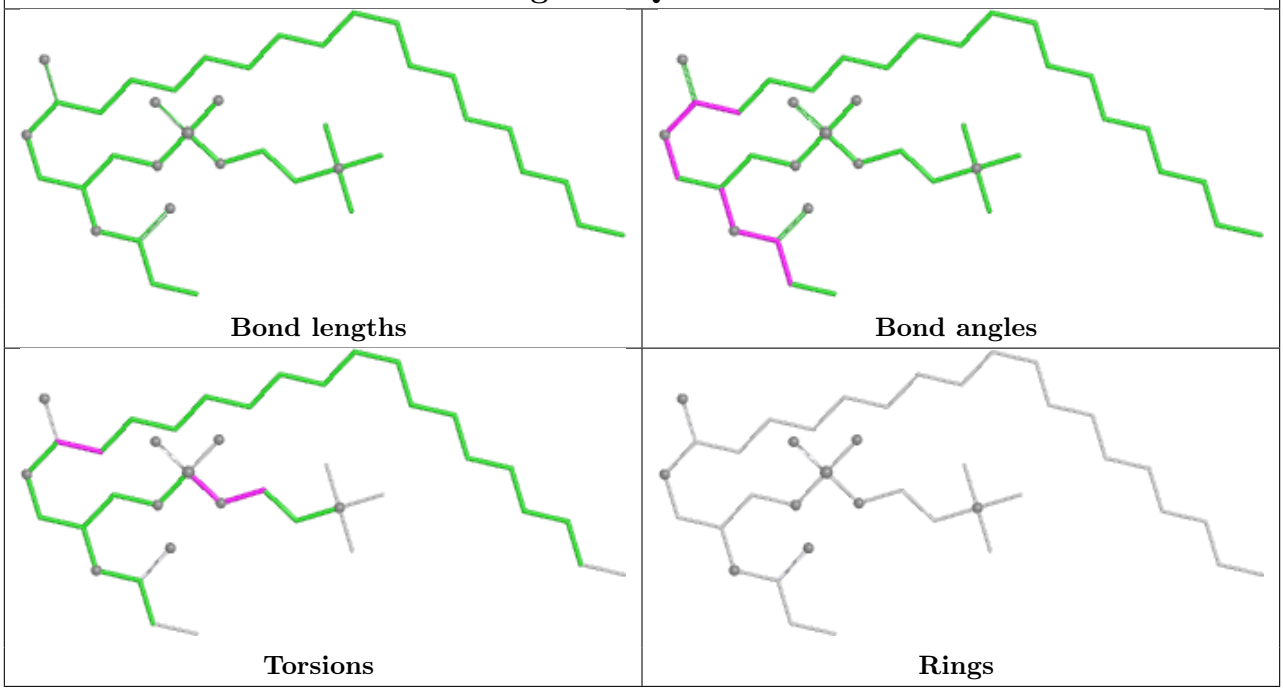


Rings

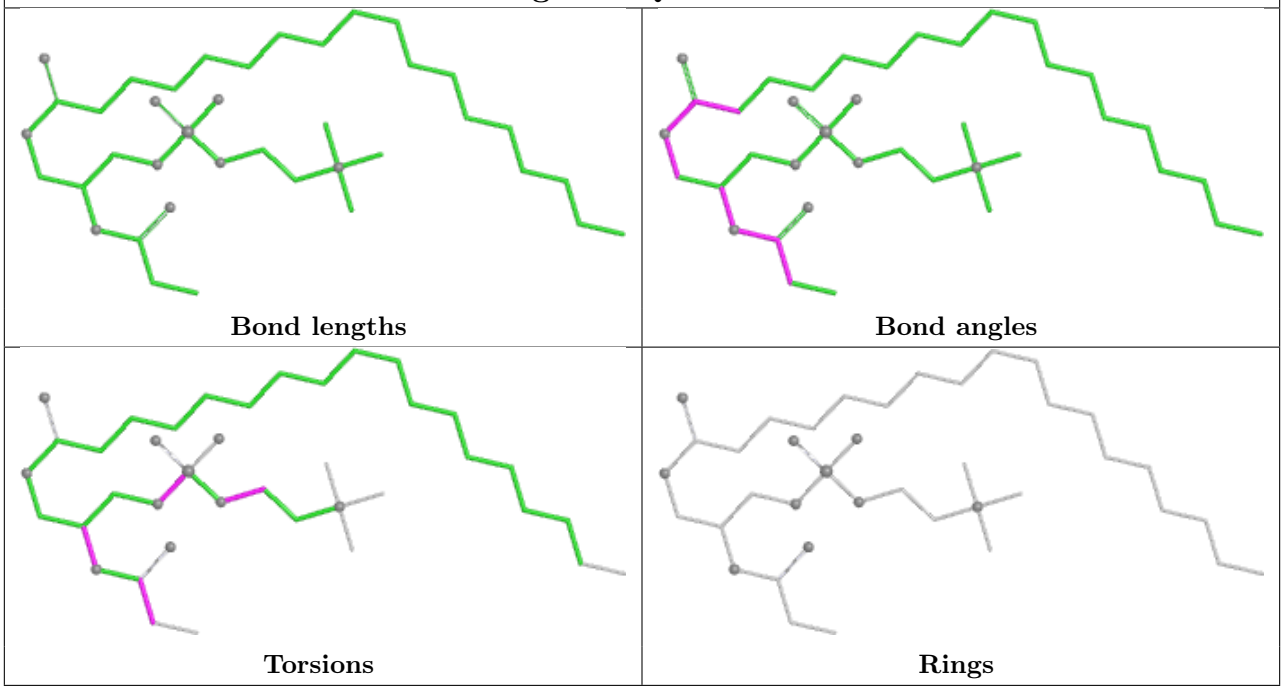
Ligand 7Q9 D 549



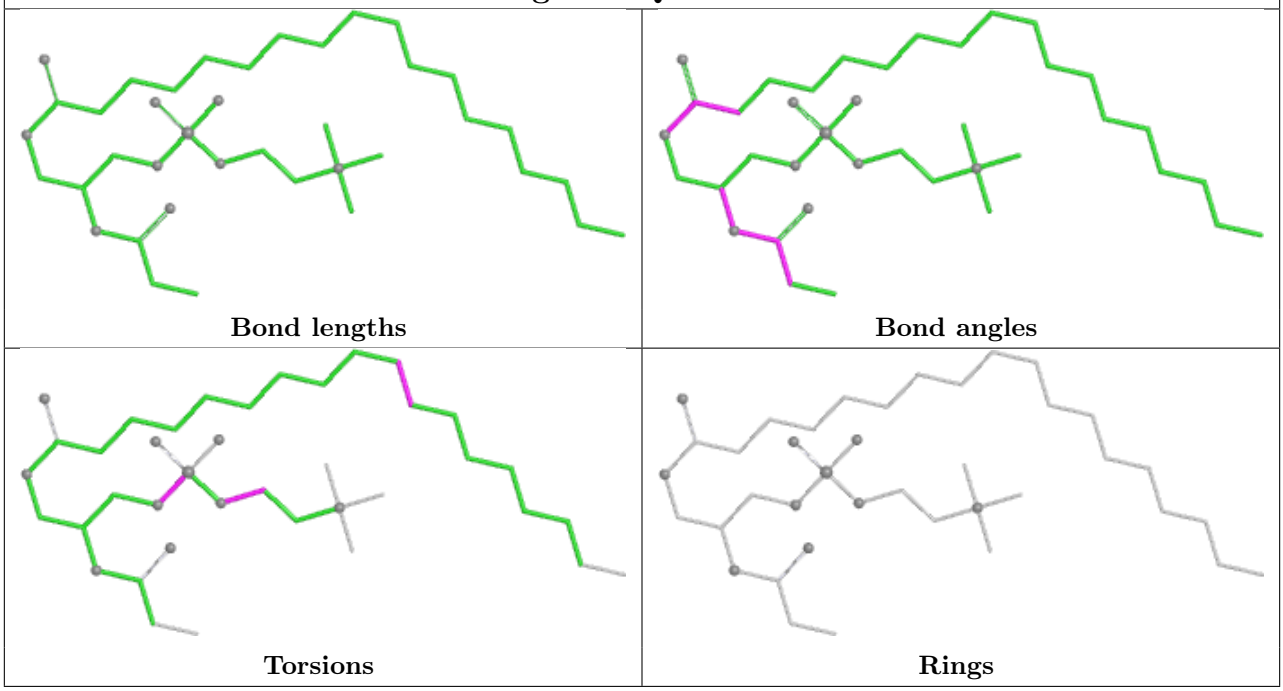
Ligand 7Q9 A 207



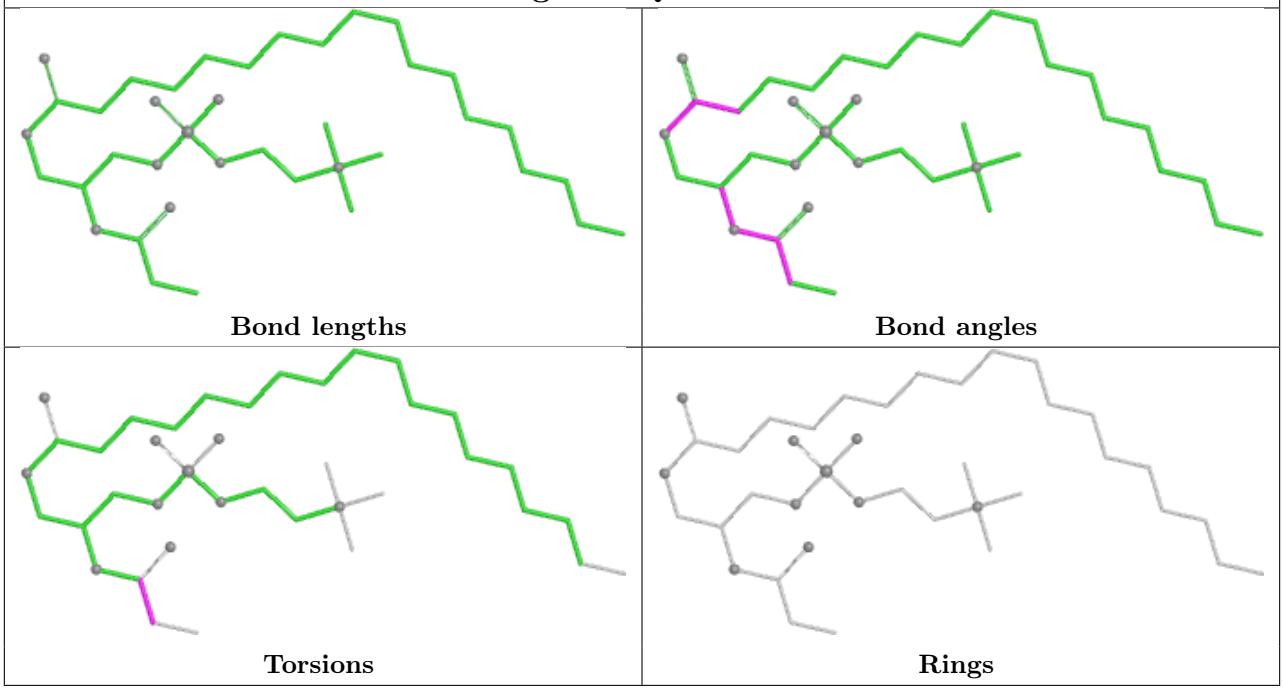
Ligand 7Q9 E 863



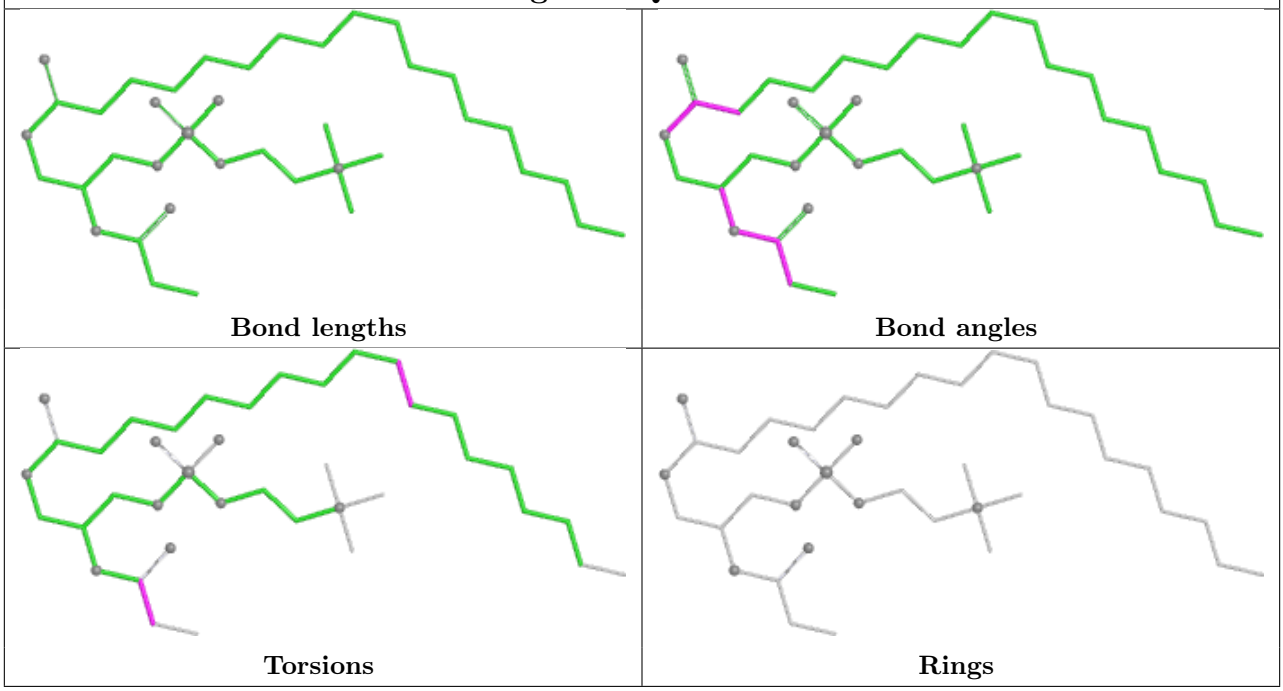
Ligand 7Q9 E 814



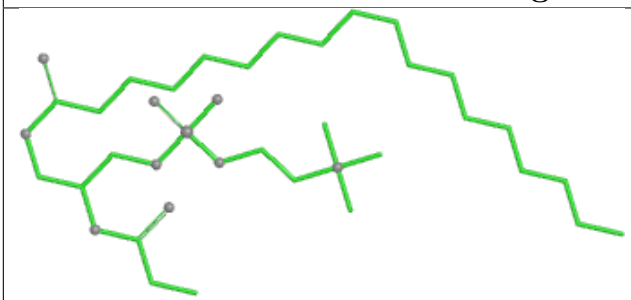
Ligand 7Q9 E 860



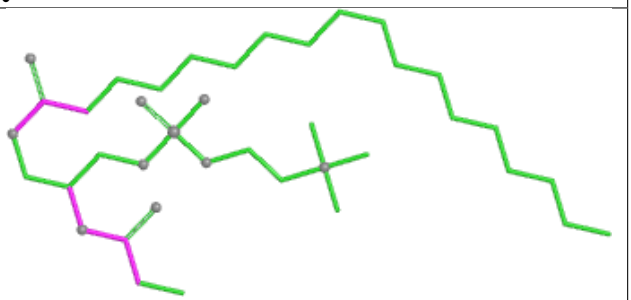
Ligand 7Q9 D 545



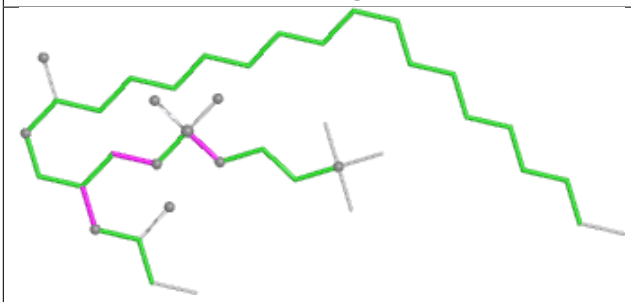
Ligand 7Q9 E 876



Bond lengths



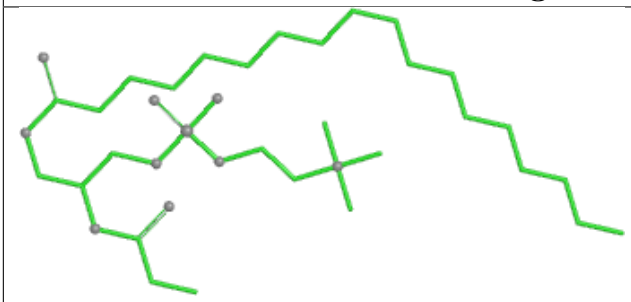
Bond angles



Torsions

Rings

Ligand 7Q9 D 551



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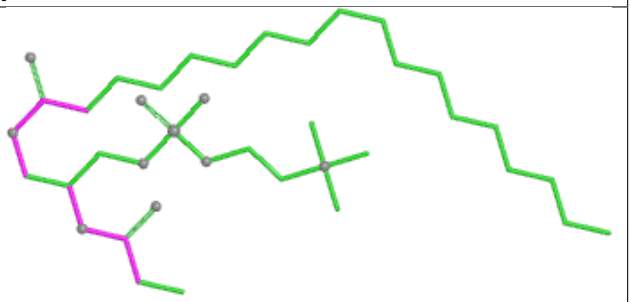
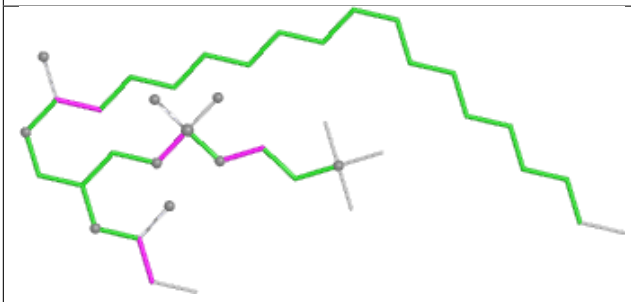


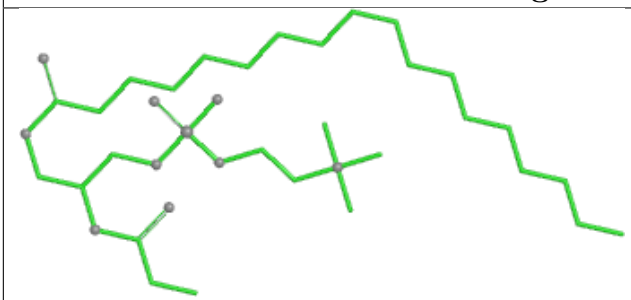
Bond angles



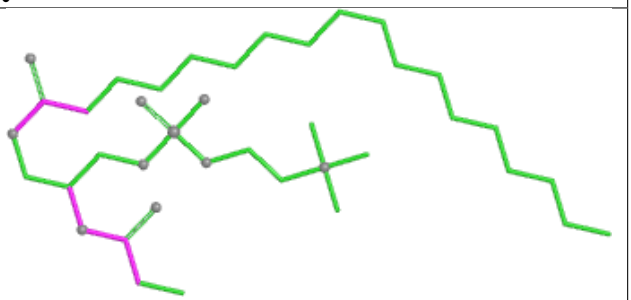
Torsions

Rings

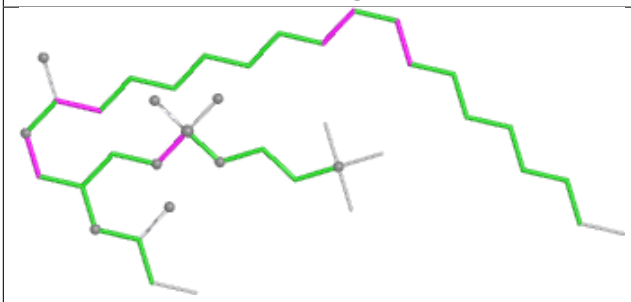
Ligand 7Q9 E 878



Bond lengths



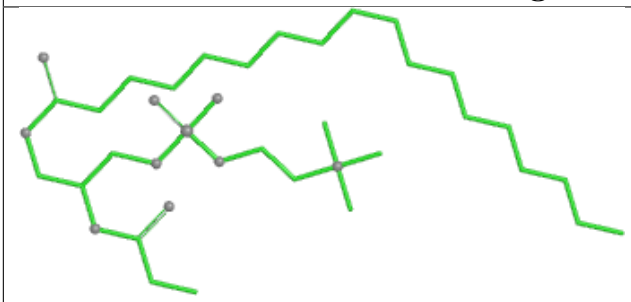
Bond angles



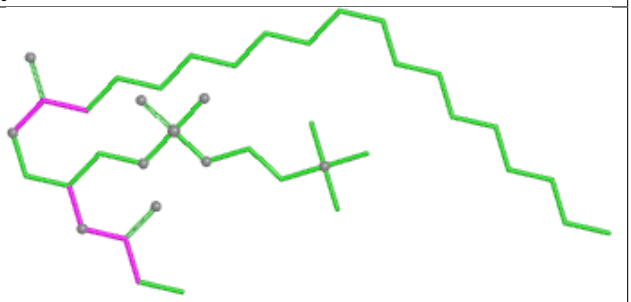
Torsions

Rings

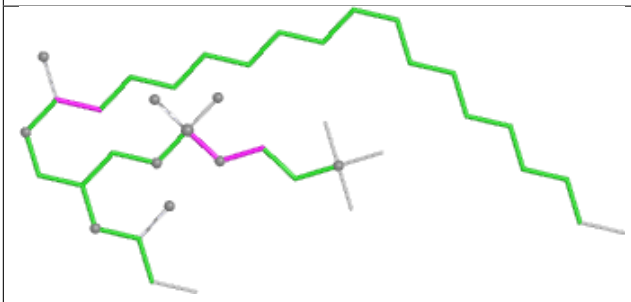
Ligand 7Q9 D 516



Bond lengths



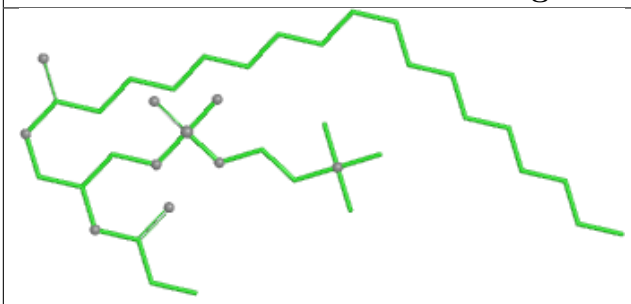
Bond angles



Torsions

Rings

Ligand 7Q9 E 874



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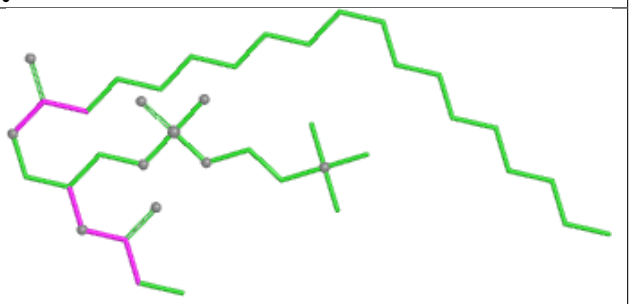
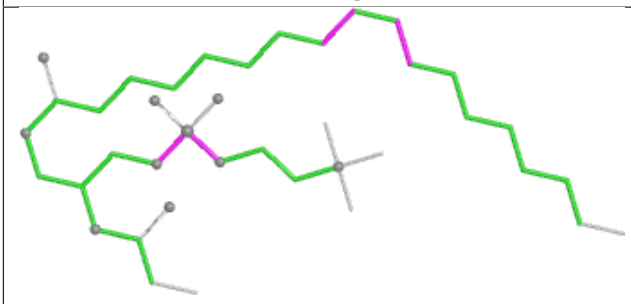


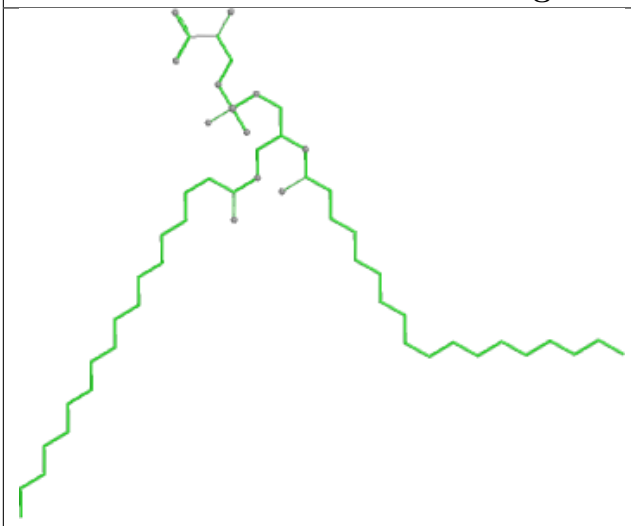
Bond angles



Torsions

Rings

Ligand 17F E 842



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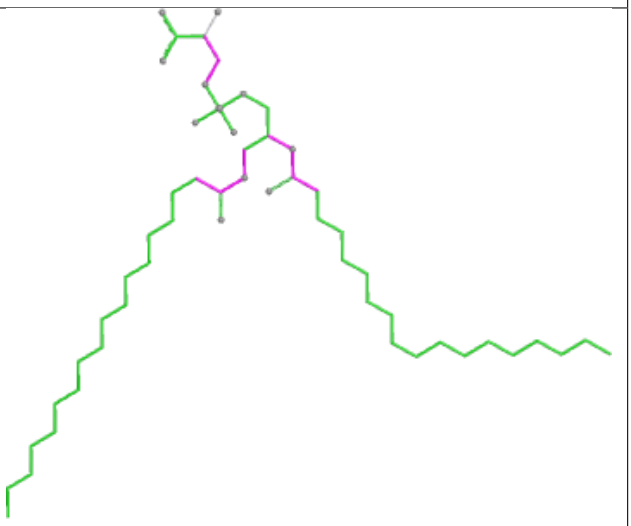

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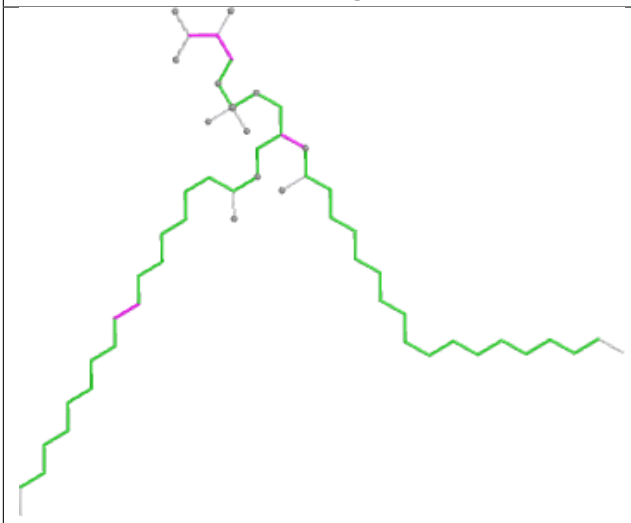
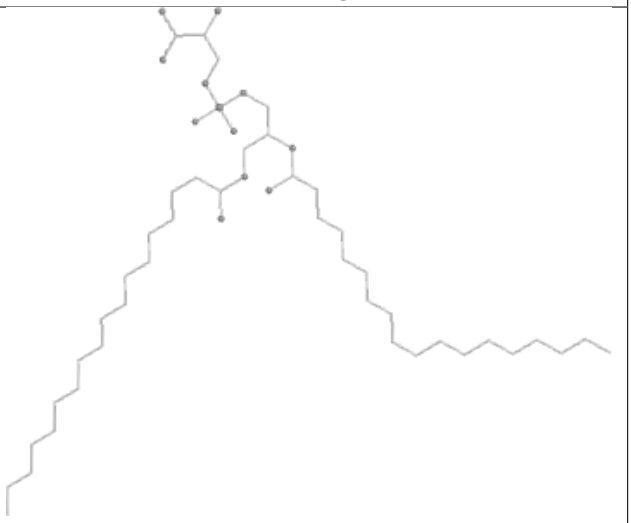
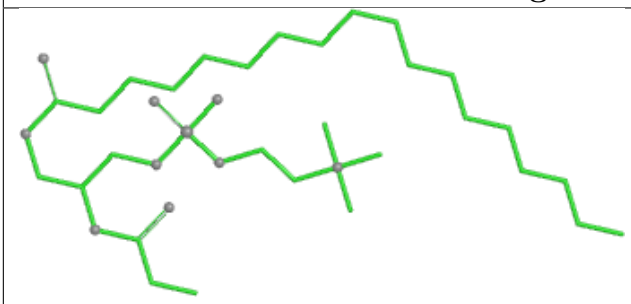


Torsions



Rings

Ligand 7Q9 A 210



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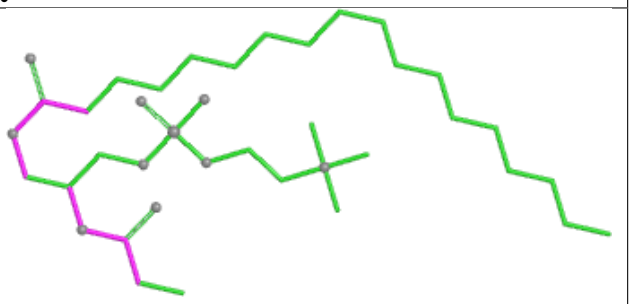
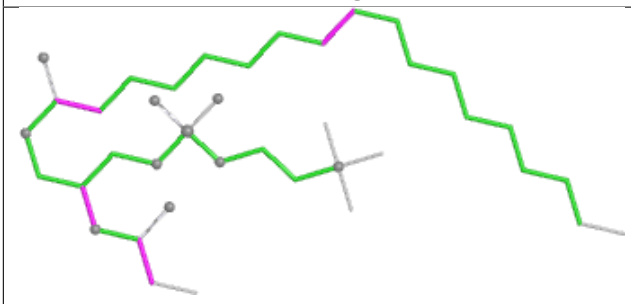


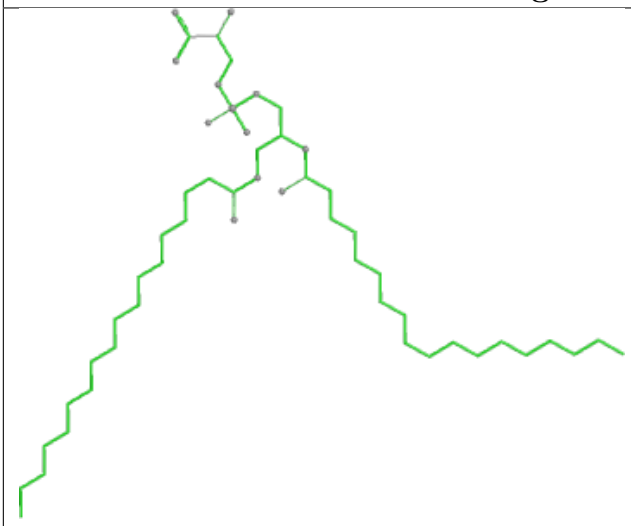
Bond angles



Torsions

Rings

Ligand 17F A 208



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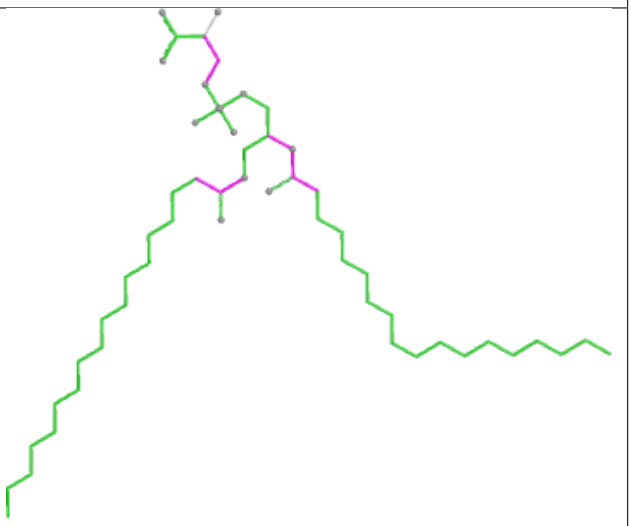

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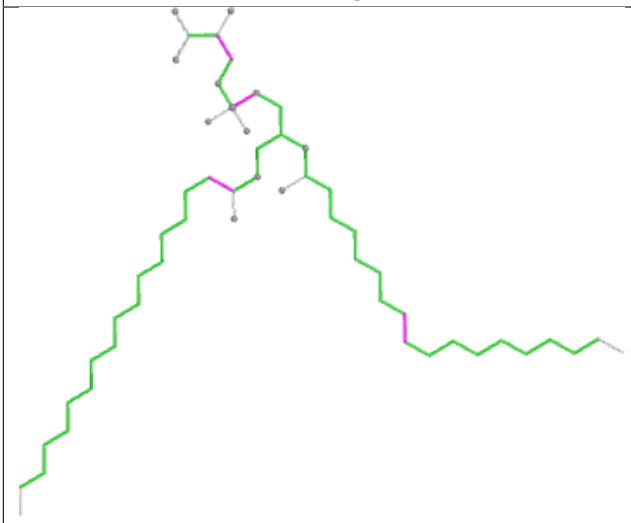
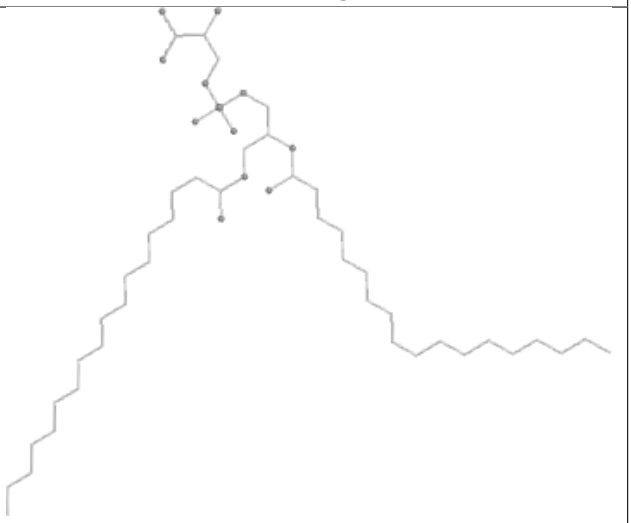
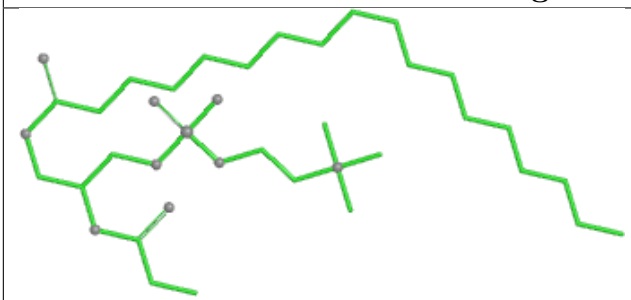


Torsions

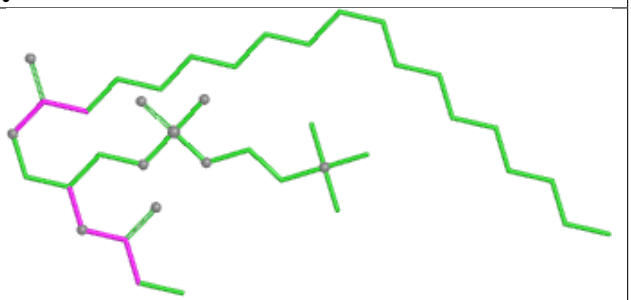


Rings

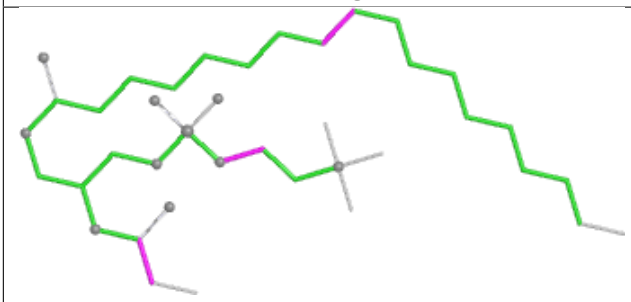
Ligand 7Q9 E 824



Bond lengths



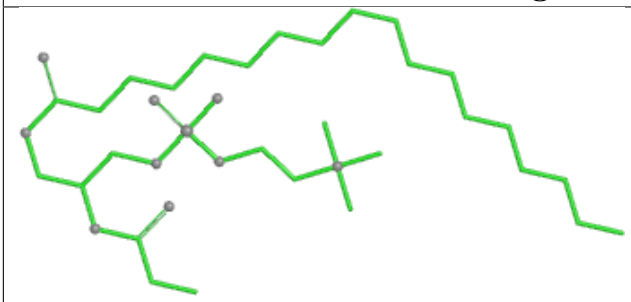
Bond angles



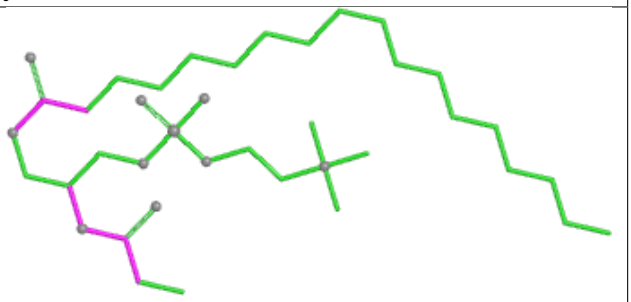
Torsions

Rings

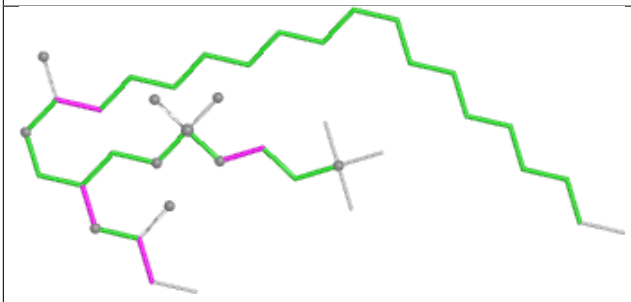
Ligand 7Q9 E 848



Bond lengths



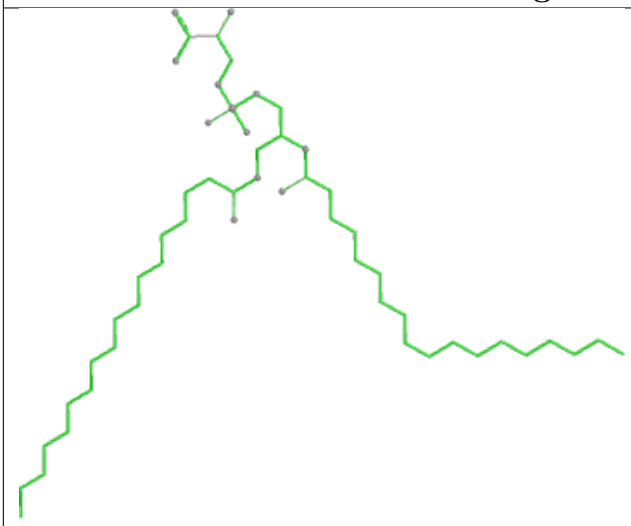
Bond angles



Torsions

Rings

Ligand 17F E 839



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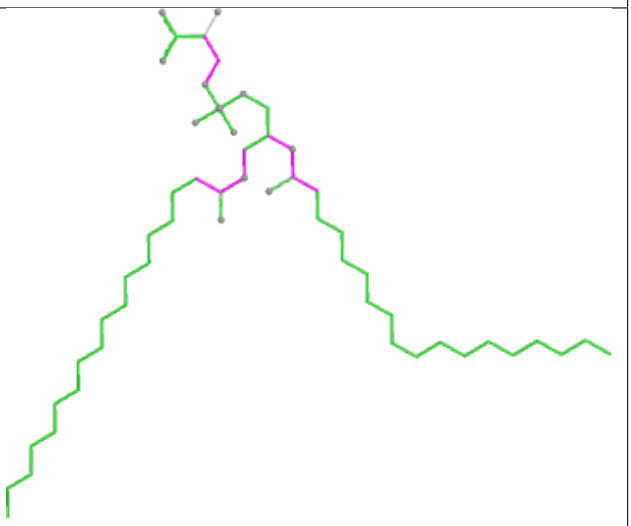
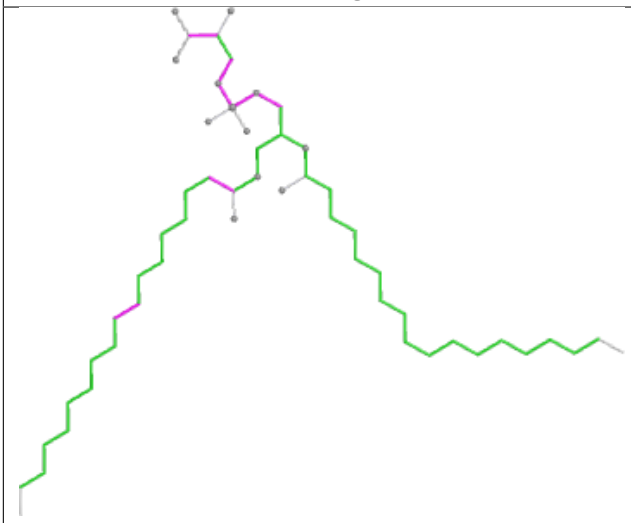


Bond angles



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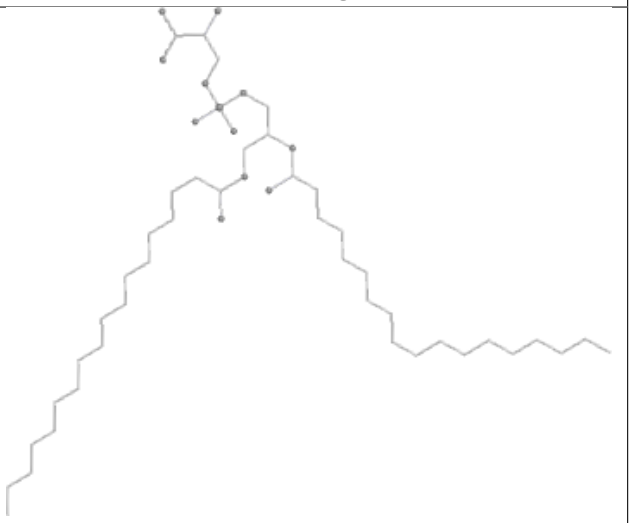
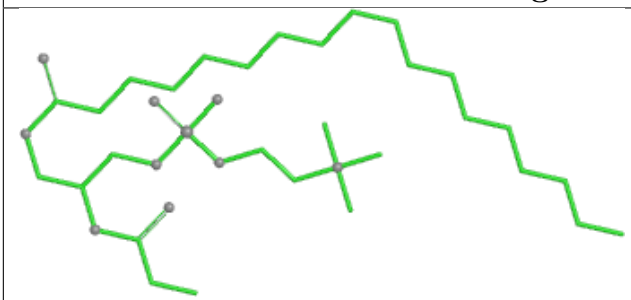


Rings

Ligand 7Q9 E 826



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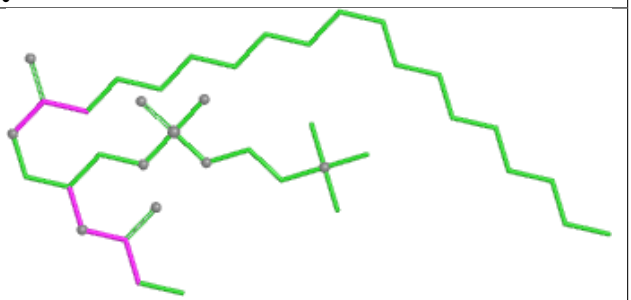
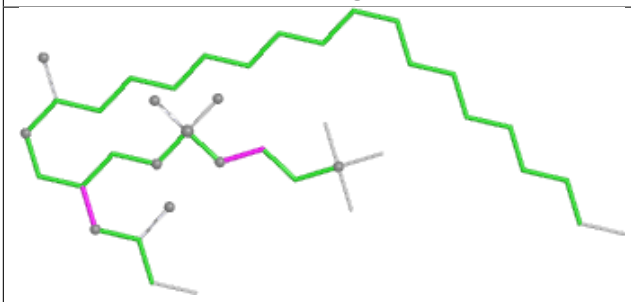


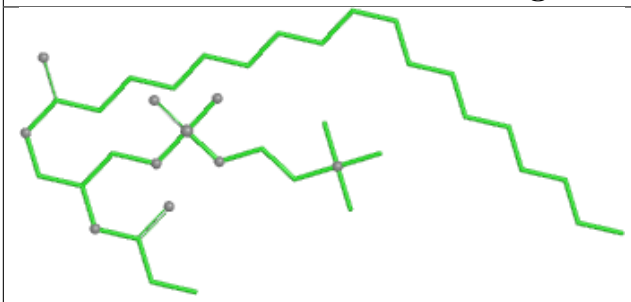
Bond angles



Torsions

Rings

Ligand 7Q9 D 531



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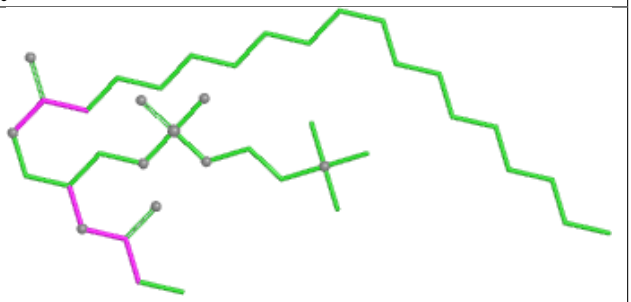
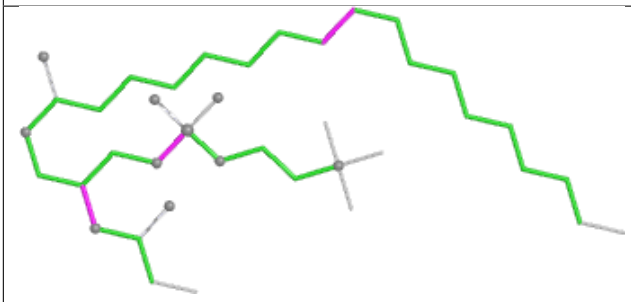


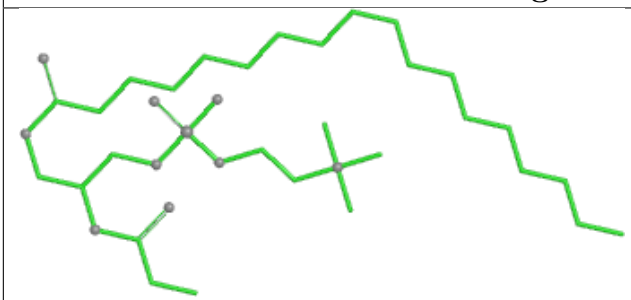
Bond angles



Torsions

Rings

Ligand 7Q9 E 869



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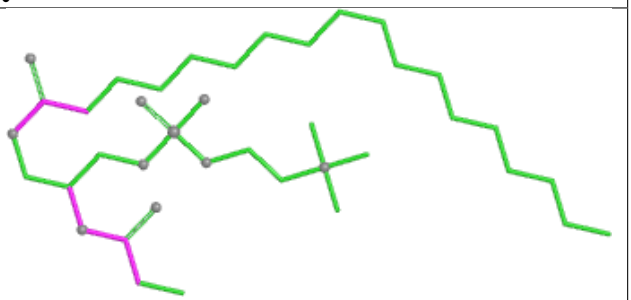

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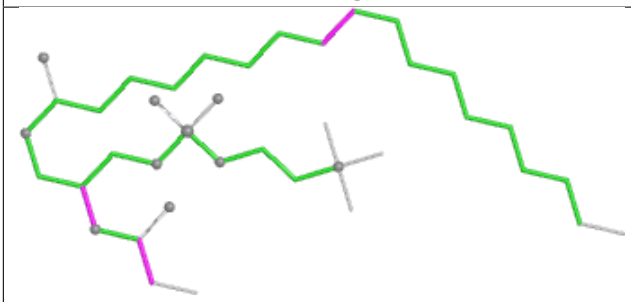
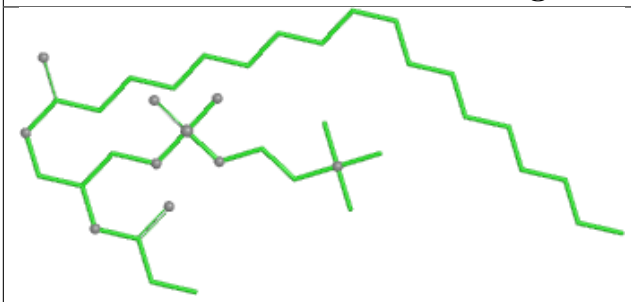


Torsions

Rings

Ligand 7Q9 D 537



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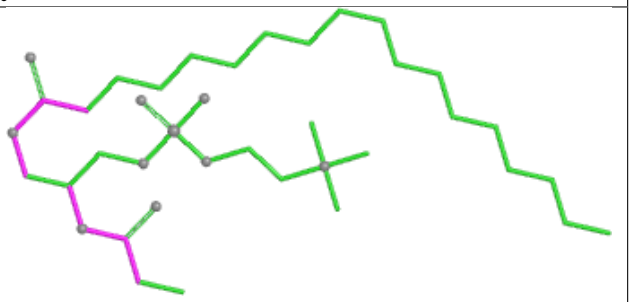

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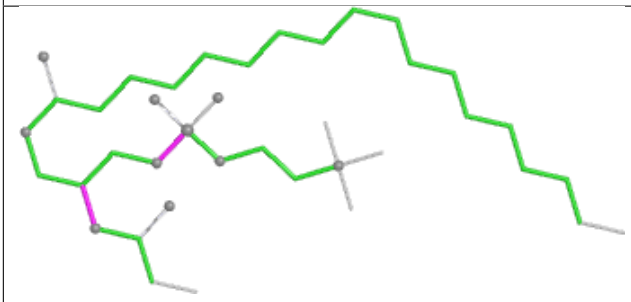
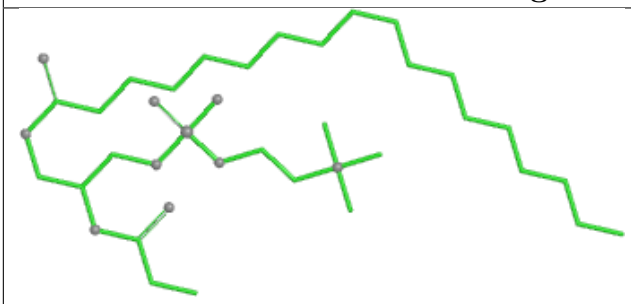


Torsions

Rings

Ligand 7Q9 B 203



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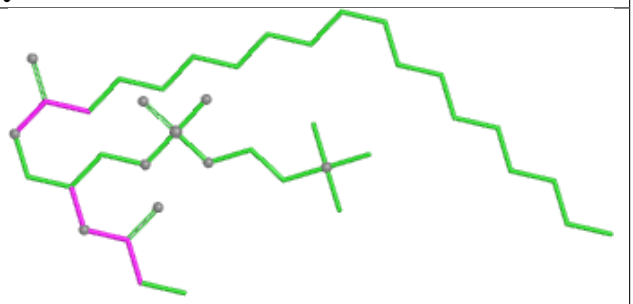
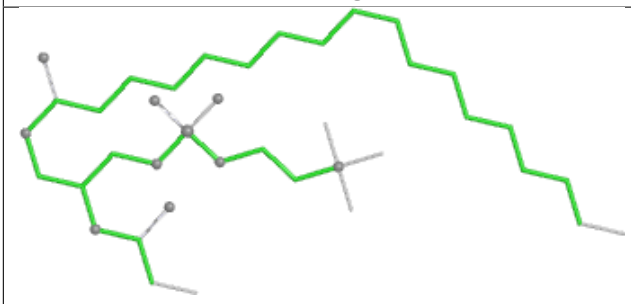


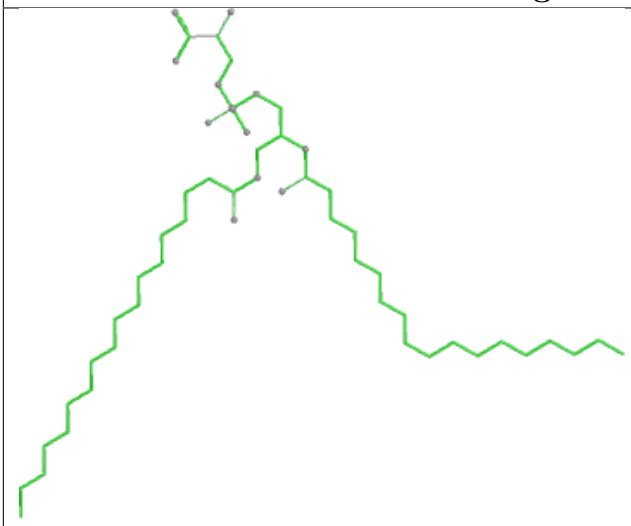
Bond angles



Torsions

Rings

Ligand 17F E 806



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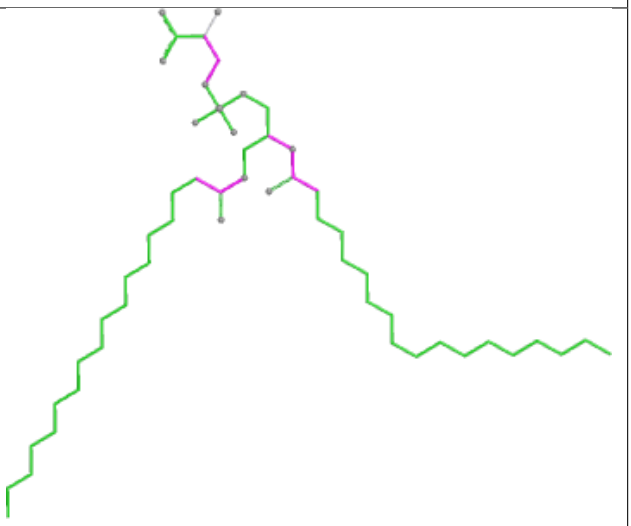
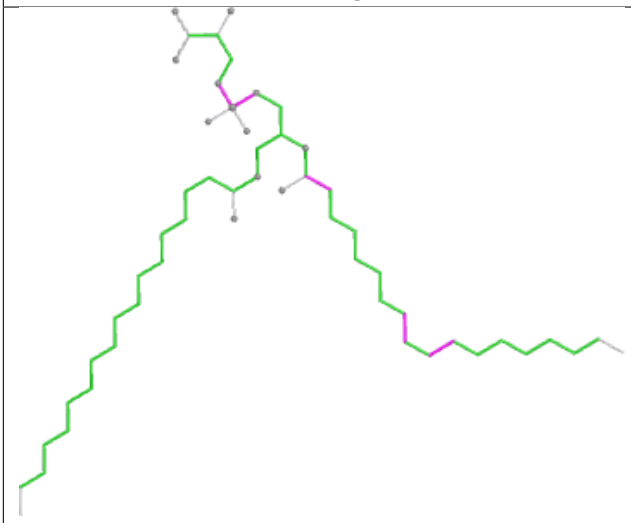
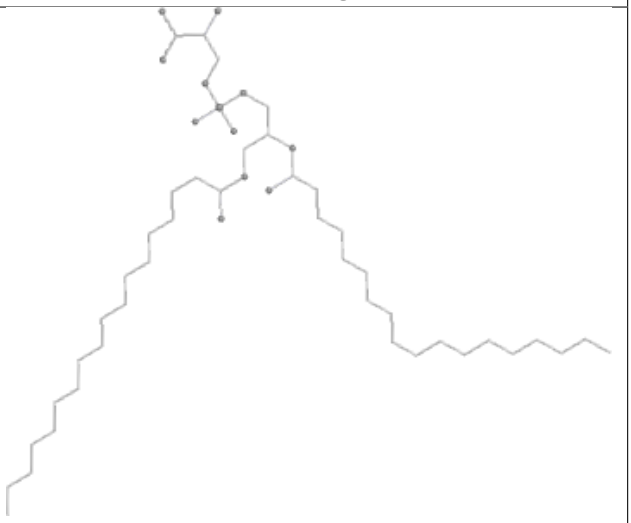


Bond angles

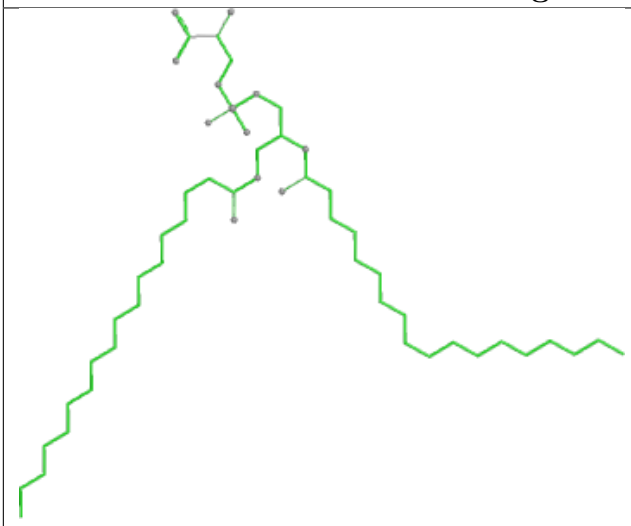


Torsions



Rings

Ligand 17F D 510



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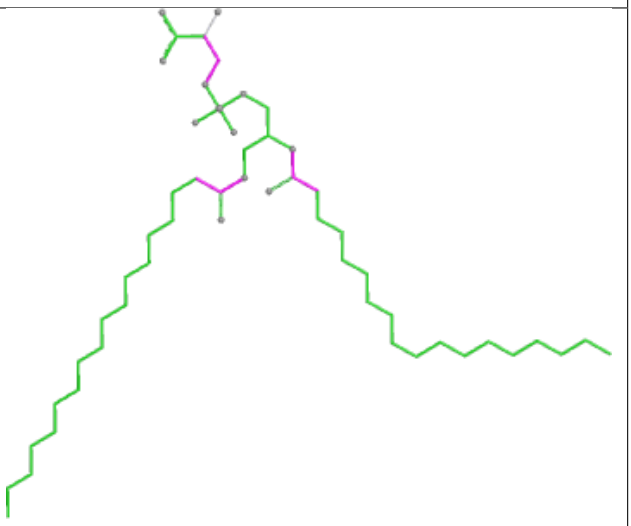
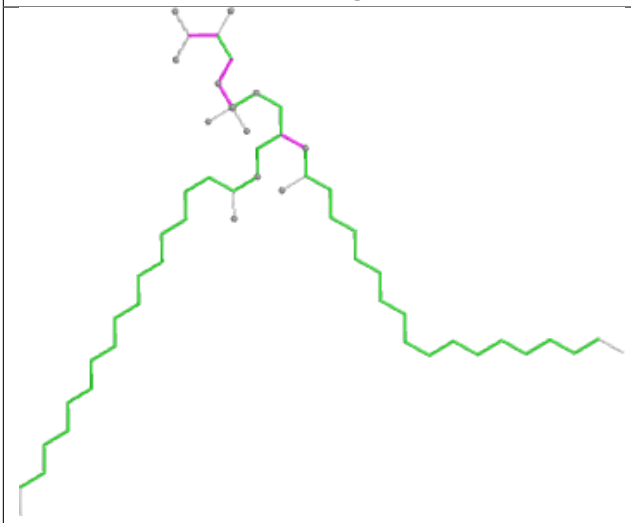


Bond angles



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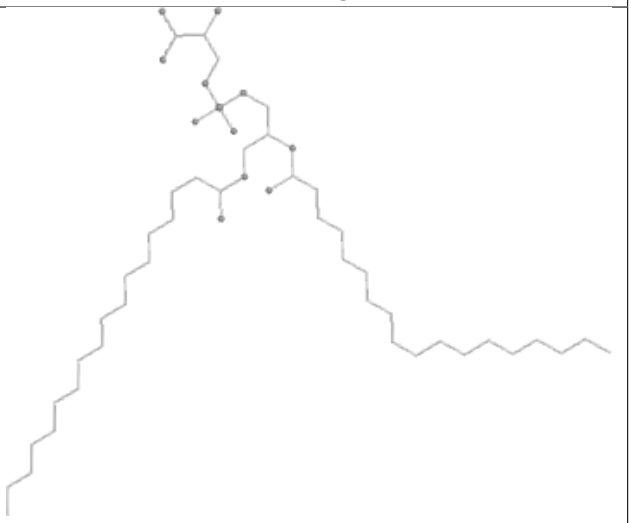
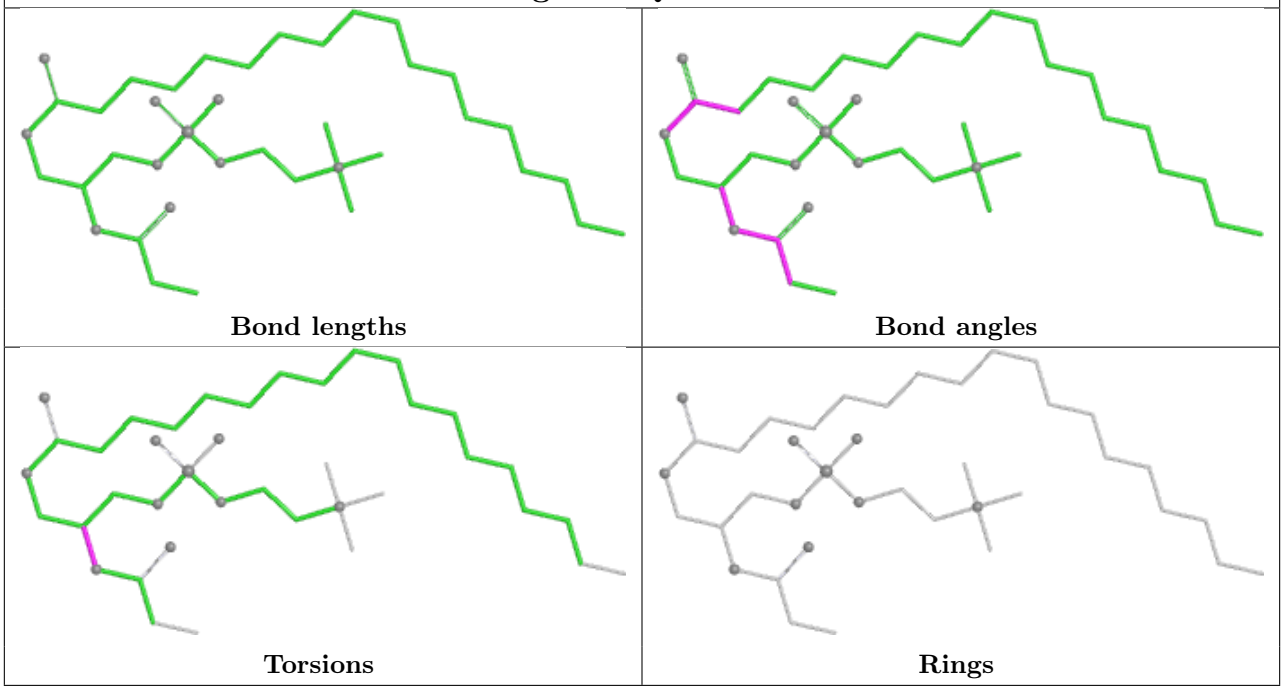
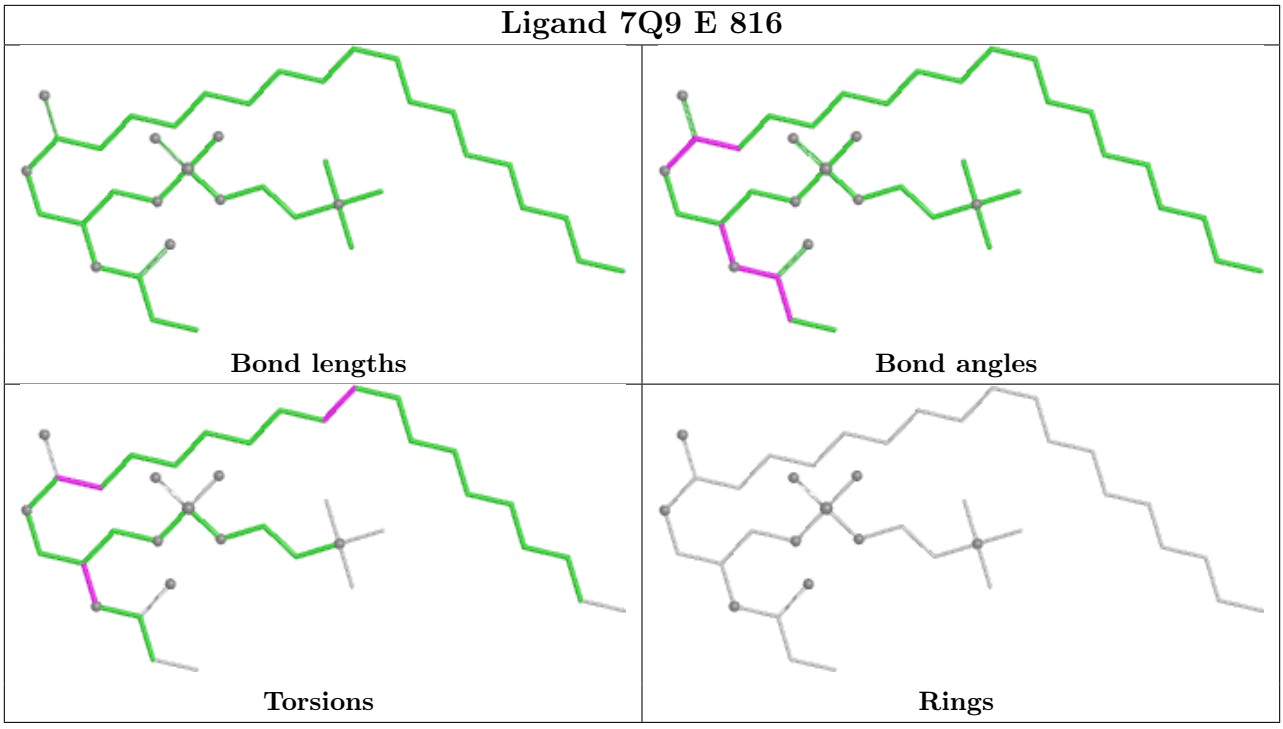


Rings

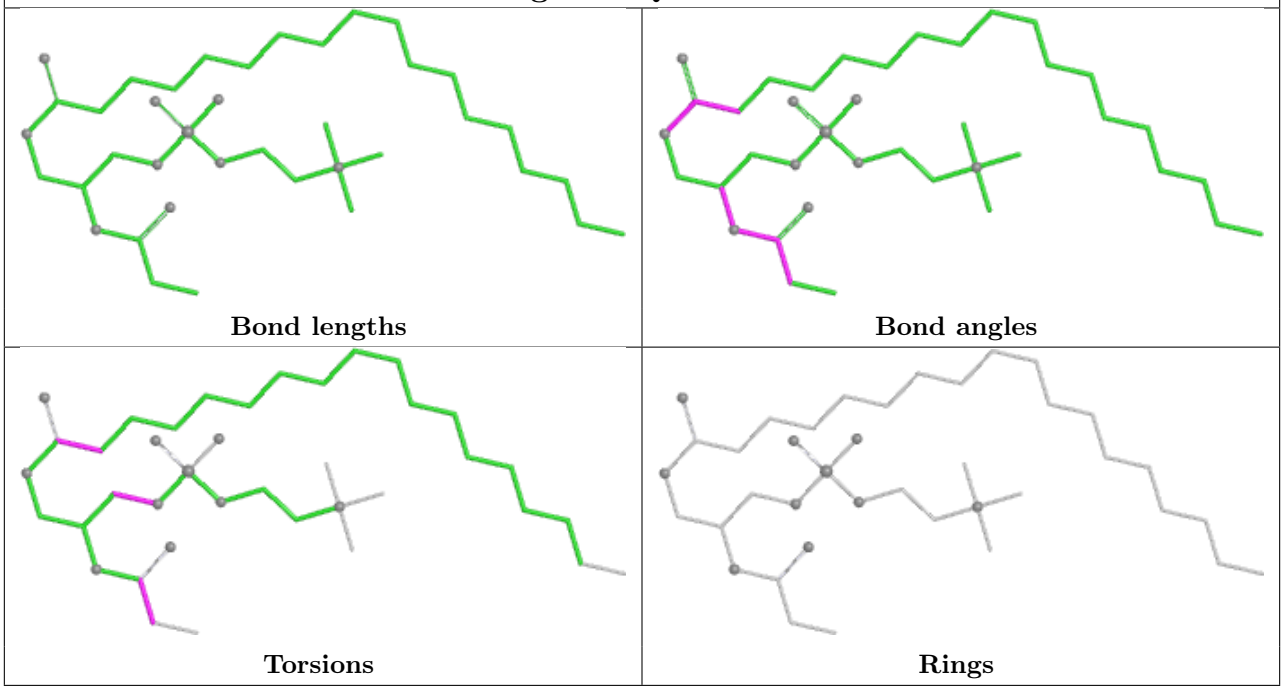
Ligand 7Q9 E 836



Ligand 7Q9 E 816



Ligand 7Q9 A 203



6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 1% for the well-defined parts and 1% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	154
Number of shifts mapped to atoms	61
Number of unparsed shifts	0
Number of shifts with mapping errors	93
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 93 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	LEU	HD11	0.763	.	2
1	A	6	LEU	HD12	0.763	.	2
1	A	6	LEU	HD13	0.763	.	2
1	A	8	VAL	HG21	0.7528	.	2
1	A	8	VAL	HG22	0.7528	.	2
1	A	8	VAL	HG23	0.7528	.	2
1	A	14	VAL	HG21	0.9725	.	2
1	A	14	VAL	HG22	0.9725	.	2
1	A	14	VAL	HG23	0.9725	.	2
1	A	19	LEU	HD11	0.4104	.	2
1	A	19	LEU	HD12	0.4104	.	2
1	A	19	LEU	HD13	0.4104	.	2
1	A	19	LEU	HD21	0.5804	.	2
1	A	19	LEU	HD22	0.5804	.	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	19	LEU	HD23	0.5804	.	2
1	A	21	ILE	HD11	0.4182	.	1
1	A	21	ILE	HD12	0.4182	.	1
1	A	21	ILE	HD13	0.4182	.	1
1	A	23	LEU	HD11	-0.477	.	2
1	A	23	LEU	HD12	-0.477	.	2
1	A	23	LEU	HD13	-0.477	.	2
1	A	24	ILE	HD11	0.2691	.	1
1	A	24	ILE	HD12	0.2691	.	1
1	A	24	ILE	HD13	0.2691	.	1
1	A	36	ILE	HD11	0.5397	.	1
1	A	36	ILE	HD12	0.5397	.	1
1	A	36	ILE	HD13	0.5397	.	1
1	A	44	VAL	HG11	0.5353	.	2
1	A	44	VAL	HG12	0.5353	.	2
1	A	44	VAL	HG13	0.5353	.	2
1	A	45	VAL	HG11	0.4379	.	2
1	A	45	VAL	HG12	0.4379	.	2
1	A	45	VAL	HG13	0.4379	.	2
1	A	46	ILE	HD11	0.2525	.	1
1	A	46	ILE	HD12	0.2525	.	1
1	A	46	ILE	HD13	0.2525	.	1
1	A	55	ILE	HD11	0.3369	.	1
1	A	55	ILE	HD12	0.3369	.	1
1	A	55	ILE	HD13	0.3369	.	1
1	A	56	LEU	HD11	0.5372	.	2
1	A	56	LEU	HD12	0.5372	.	2
1	A	56	LEU	HD13	0.5372	.	2
1	A	79	LEU	HD11	-0.1312	.	2
1	A	79	LEU	HD12	-0.1312	.	2
1	A	79	LEU	HD13	-0.1312	.	2
1	A	79	LEU	HD21	-0.015	.	2
1	A	79	LEU	HD22	-0.015	.	2
1	A	79	LEU	HD23	-0.015	.	2
1	A	81	VAL	HG21	0.4663	.	2
1	A	81	VAL	HG22	0.4663	.	2
1	A	81	VAL	HG23	0.4663	.	2
1	A	84	ILE	HD11	0.5865	.	1
1	A	84	ILE	HD12	0.5865	.	1
1	A	84	ILE	HD13	0.5865	.	1
1	A	93	ILE	HD11	0.6063	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	ILE	HD12	0.6063	.	1
1	A	93	ILE	HD13	0.6063	.	1
1	A	100	ILE	HD11	0.0964	.	1
1	A	100	ILE	HD12	0.0964	.	1
1	A	100	ILE	HD13	0.0964	.	1
1	A	103	VAL	HG11	0.8243	.	2
1	A	103	VAL	HG12	0.8243	.	2
1	A	103	VAL	HG13	0.8243	.	2
1	A	112	VAL	HG11	0.5953	.	2
1	A	112	VAL	HG12	0.5953	.	2
1	A	112	VAL	HG13	0.5953	.	2
1	A	113	LEU	HD11	0.8748	.	2
1	A	113	LEU	HD12	0.8748	.	2
1	A	113	LEU	HD13	0.8748	.	2
1	A	120	LEU	HD11	0.6958	.	2
1	A	120	LEU	HD12	0.6958	.	2
1	A	120	LEU	HD13	0.6958	.	2
1	A	125	VAL	HG11	-0.3248	.	2
1	A	125	VAL	HG12	-0.3248	.	2
1	A	125	VAL	HG13	-0.3248	.	2
1	A	133	LEU	HD11	0.2014	.	2
1	A	133	LEU	HD12	0.2014	.	2
1	A	133	LEU	HD13	0.2014	.	2
1	A	139	ILE	HD11	0.7118	.	1
1	A	139	ILE	HD12	0.7118	.	1
1	A	139	ILE	HD13	0.7118	.	1
1	A	142	ILE	HD11	0.5035	.	1
1	A	142	ILE	HD12	0.5035	.	1
1	A	142	ILE	HD13	0.5035	.	1
1	A	159	LEU	HD11	0.51	.	2
1	A	159	LEU	HD12	0.51	.	2
1	A	159	LEU	HD13	0.51	.	2
1	A	160	VAL	HG11	-0.2062	.	2
1	A	160	VAL	HG12	-0.2062	.	2
1	A	160	VAL	HG13	-0.2062	.	2
1	A	163	ILE	HD11	0.5261	.	1
1	A	163	ILE	HD12	0.5261	.	1
1	A	163	ILE	HD13	0.5261	.	1

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 140 atoms were assigned a chemical shift out of a possible 9884. 0 out of 126 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	16/3515 (0%)	8/1422 (1%)	0/1410 (0%)	8/683 (1%)
Sidechain	124/5741 (2%)	93/3690 (3%)	31/1795 (2%)	0/256 (0%)
Aromatic	0/628 (0%)	0/310 (0%)	0/296 (0%)	0/22 (0%)
Overall	140/9884 (1%)	101/5422 (2%)	31/3501 (1%)	8/961 (1%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 1%, i.e. 154 atoms were assigned a chemical shift out of a possible 10390. 0 out of 126 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	30/3692 (1%)	15/1494 (1%)	0/1480 (0%)	15/718 (2%)
Sidechain	124/6070 (2%)	93/3894 (2%)	31/1900 (2%)	0/276 (0%)
Aromatic	0/628 (0%)	0/310 (0%)	0/296 (0%)	0/22 (0%)
Overall	154/10390 (1%)	108/5698 (2%)	31/3676 (1%)	15/1016 (1%)

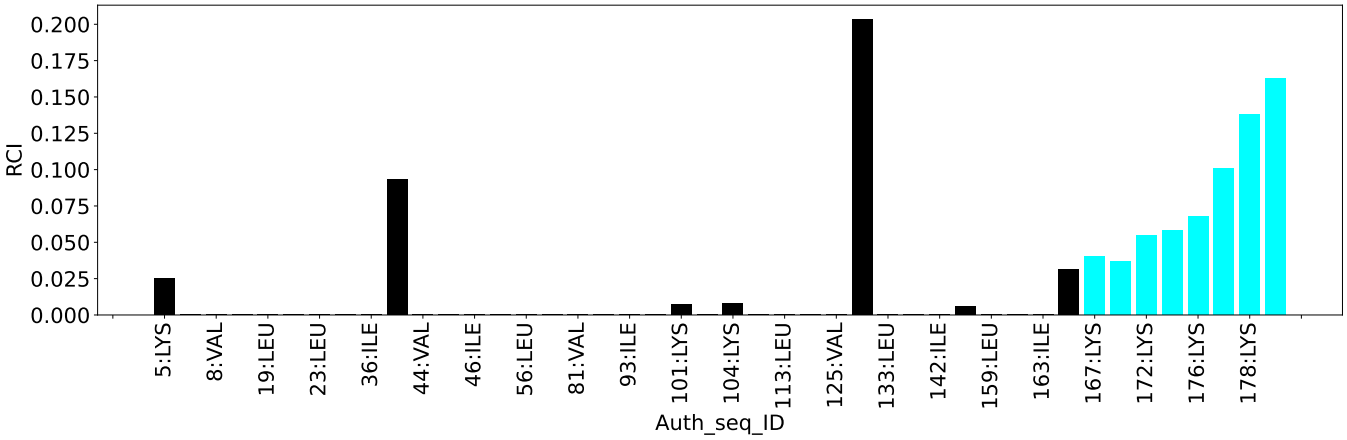
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
5:LYS
8:VAL
19:LEU
23:LEU
36:ILE
44:VAL
46:ILE
56:LEU
81:VAL
93:ILE
101:LYS
104:LYS
113:LEU
125:VAL
133:LEU
142:ILE
159:LEU
163:ILE
167:LYS
172:LYS
176:LYS
178:LYS
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	75
Intra-residue (|i-j|=0)	1
Sequential (|i-j|=1)	0
Medium range (|i-j|>1 and |i-j|<5)	0
Long range (|i-j|≥5)	21
Inter-chain	53
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue[1]	0.0

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å
are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	None	None
0.2-0.5 (Medium)	None	None
>0.5 (Large)	36.0	25.61

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

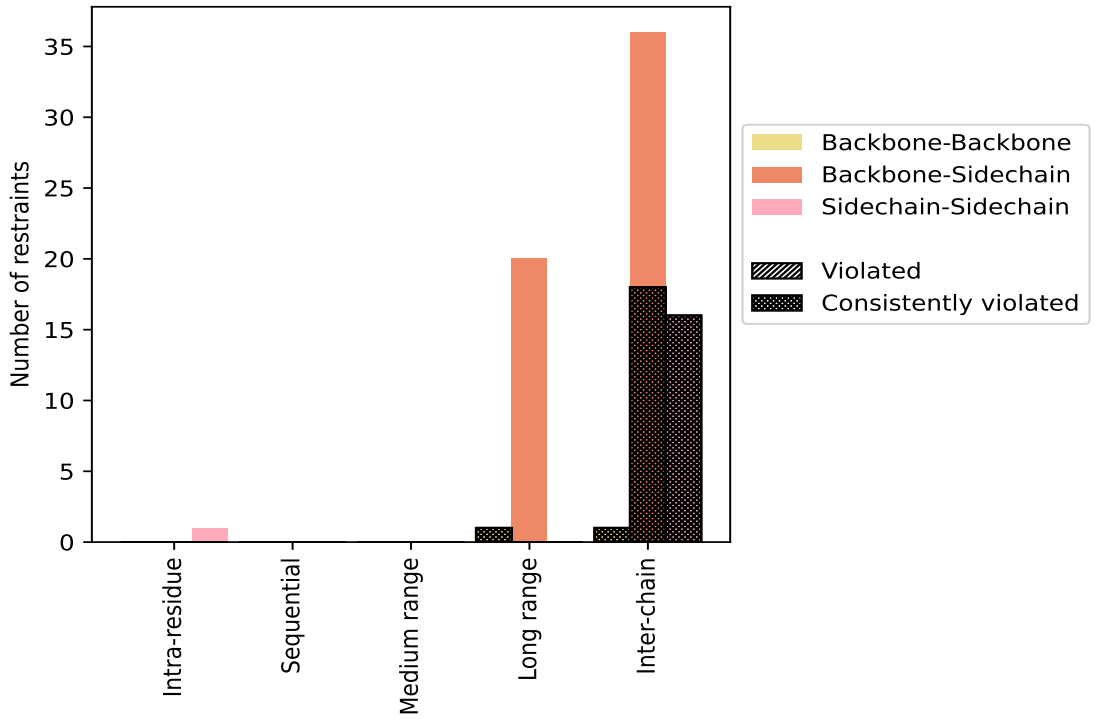
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	1	1.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1	1.3	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	21	28.0	1	4.8	1.3	1	4.8	1.3
Backbone-Backbone	1	1.3	1	100.0	1.3	1	100.0	1.3
Backbone-Sidechain	20	26.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	53	70.7	35	66.0	46.7	35	66.0	46.7
Backbone-Backbone	1	1.3	1	100.0	1.3	1	100.0	1.3
Backbone-Sidechain	36	48.0	18	50.0	24.0	18	50.0	24.0
Sidechain-Sidechain	16	21.3	16	100.0	21.3	16	100.0	21.3
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	75	100.0	36	48.0	48.0	36	48.0	48.0
Backbone-Backbone	2	2.7	2	100.0	2.7	2	100.0	2.7
Backbone-Sidechain	56	74.7	18	32.1	24.0	18	32.1	24.0
Sidechain-Sidechain	17	22.7	16	94.1	21.3	16	94.1	21.3

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å
are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	36	36	12.55	17.19	2.97	13.4
2	0	0	0	0	36	36	12.49	17.3	2.23	12.42
3	0	0	0	0	36	36	12.72	18.59	2.96	12.9
4	0	0	0	0	36	36	13.13	18.82	2.74	13.16
5	0	0	0	0	36	36	12.46	16.89	2.88	12.7
6	0	0	0	0	36	36	13.07	18.3	2.37	12.95
7	0	0	0	0	36	36	12.74	17.25	3.28	13.02
8	0	0	0	0	36	36	12.84	20.35	2.35	12.52
9	0	0	0	0	36	36	13.07	18.38	2.09	12.81
10	0	0	0	0	36	36	12.54	19.49	2.93	12.48

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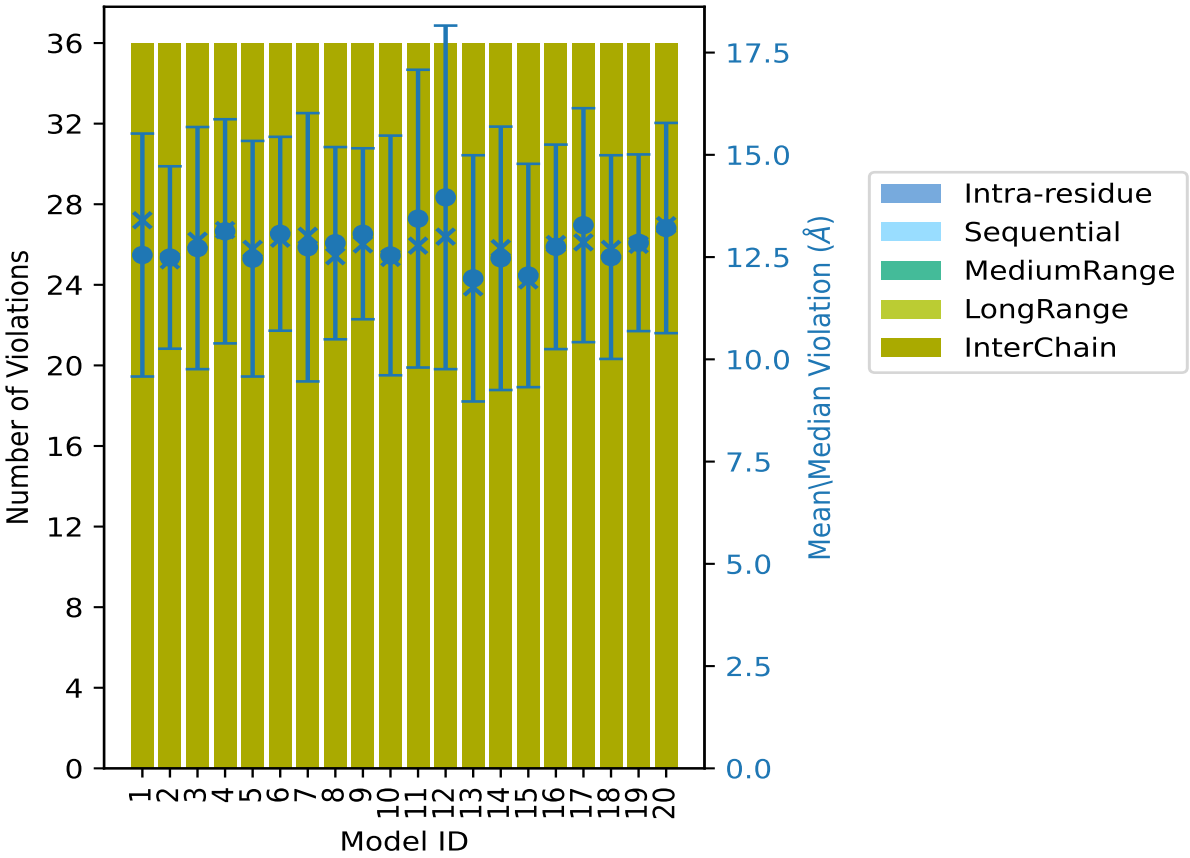
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	0	0	0	36	36	13.44	22.7	3.64	12.78
12	0	0	0	0	36	36	13.96	25.61	4.2	13.0
13	0	0	0	0	36	36	11.98	19.54	3.01	11.76
14	0	0	0	0	36	36	12.47	17.85	3.22	12.72
15	0	0	0	0	36	36	12.05	16.86	2.73	11.93
16	0	0	0	0	36	36	12.75	16.27	2.5	12.82
17	0	0	0	0	36	36	13.28	22.56	2.86	12.86
18	0	0	0	0	36	36	12.5	19.04	2.49	12.7
19	0	0	0	0	36	36	12.85	17.46	2.16	12.8
20	0	0	0	0	36	36	13.21	17.48	2.57	13.28

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

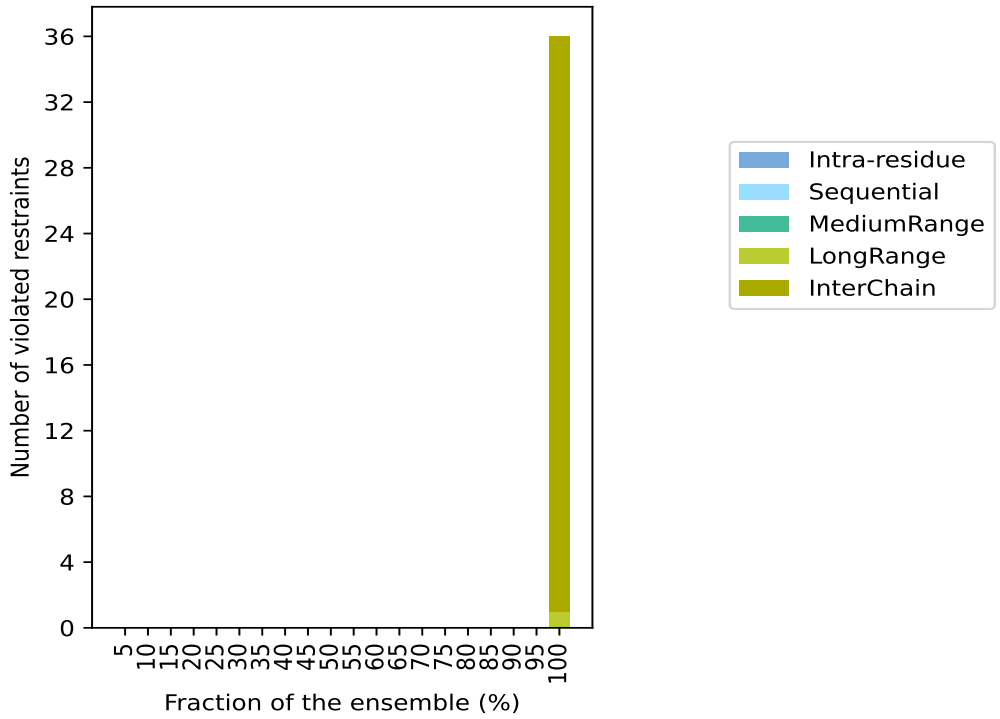
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 39(IR:1, SQ:0, MR:0, LR:20, IC:18) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	1	35	36	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

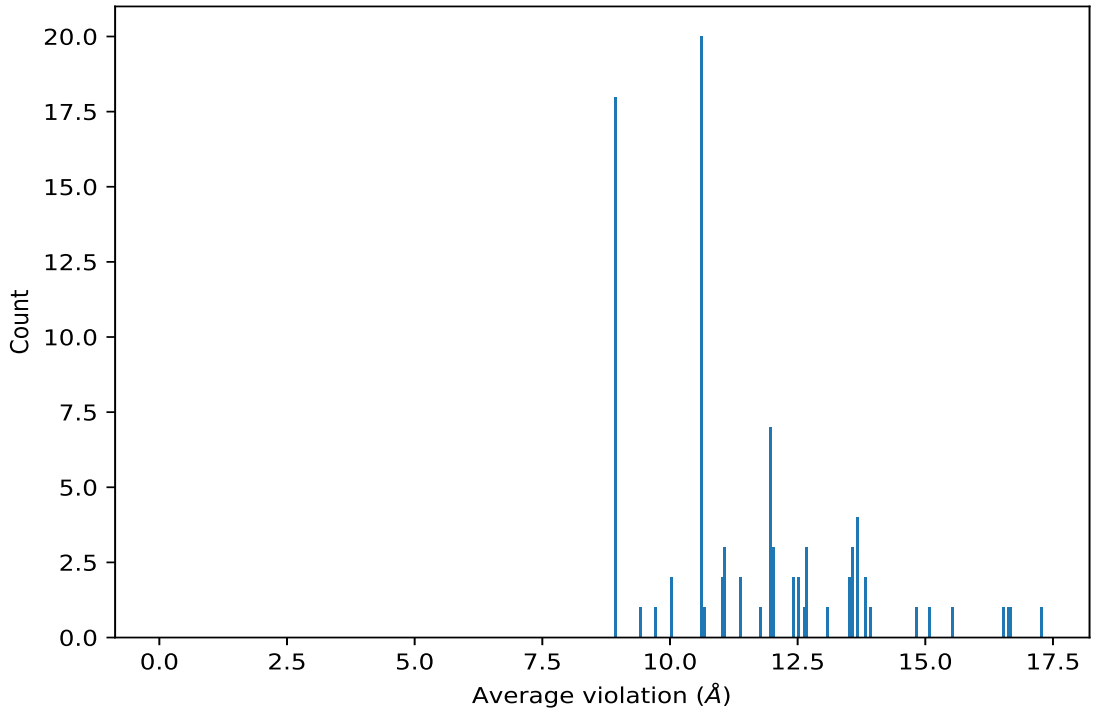
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of theviolation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	20	17.26	2.48	17.1
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	20	16.67	0.99	16.31
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	20	16.65	0.81	16.32
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	20	16.54	2.4	17.23
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	20	15.53	2.09	15.84
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	20	15.1	1.57	15.08
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	20	14.85	1.82	15.0
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	20	13.95	1.66	13.64
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	20	13.85	0.17	13.92
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	20	13.81	1.68	13.73
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	20	13.66	0.48	13.57
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	20	13.66	0.48	13.57
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	20	13.65	0.47	13.69
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	20	13.65	0.47	13.69
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	20	13.6	0.56	13.7
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	20	13.6	0.56	13.7

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	20	13.6	0.83	13.94
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	20	13.52	0.36	13.59
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	20	13.52	0.36	13.59
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	20	13.06	1.56	12.76
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	20	12.69	1.22	12.54
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	20	12.67	0.12	12.74
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	20	12.67	0.12	12.74
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	20	12.64	1.42	12.41
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	20	12.54	0.29	12.71
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	20	12.54	0.29	12.71
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	20	12.45	0.82	12.24
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	20	12.45	0.82	12.24
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	20	12.03	1.86	11.84
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	20	12.02	0.91	12.07
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	20	12.02	0.91	12.07
(3,4)	1:103:B:VAL:CG1	6:219:A:17F:N1	20	11.96	2.07	12.1
(3,4)	1:103:B:VAL:CG1	5:218:A:7Q9:N	20	11.96	2.07	12.1
(3,4)	1:103:B:VAL:CG1	5:210:A:7Q9:N	20	11.96	2.07	12.1
(3,4)	1:103:B:VAL:CG1	5:216:A:7Q9:N	20	11.96	2.07	12.1
(3,4)	1:103:B:VAL:CG1	5:209:A:7Q9:N	20	11.96	2.07	12.1
(3,4)	1:103:B:VAL:CG2	5:216:A:7Q9:N	20	11.96	2.07	12.1
(3,4)	1:103:B:VAL:CG1	5:212:A:7Q9:N	20	11.96	2.07	12.1
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	20	11.78	1.72	12.08
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	20	11.38	0.66	11.58
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	20	11.38	0.66	11.58
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	20	11.1	0.68	11.04
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	20	11.1	0.68	11.04
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	20	11.08	1.13	10.93
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	20	11.02	0.88	11.02
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	20	11.0	1.18	10.94
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	20	10.67	1.01	10.66
(1,35)	1:184:B:LYS:HZ3	6:213:A:17F:N1	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:HZ2	6:219:A:17F:N1	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:O	5:207:A:7Q9:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:HZ3	5:203:A:7Q9:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:CA	5:207:A:7Q9:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:HZ2	5:203:A:7Q9:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:HZ2	6:208:A:17F:N1	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:HZ1	5:217:A:7Q9:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:O	6:208:A:17F:N1	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:H	5:203:A:7Q9:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:O	6:220:A:17F:N1	20	10.61	7.33	10.32

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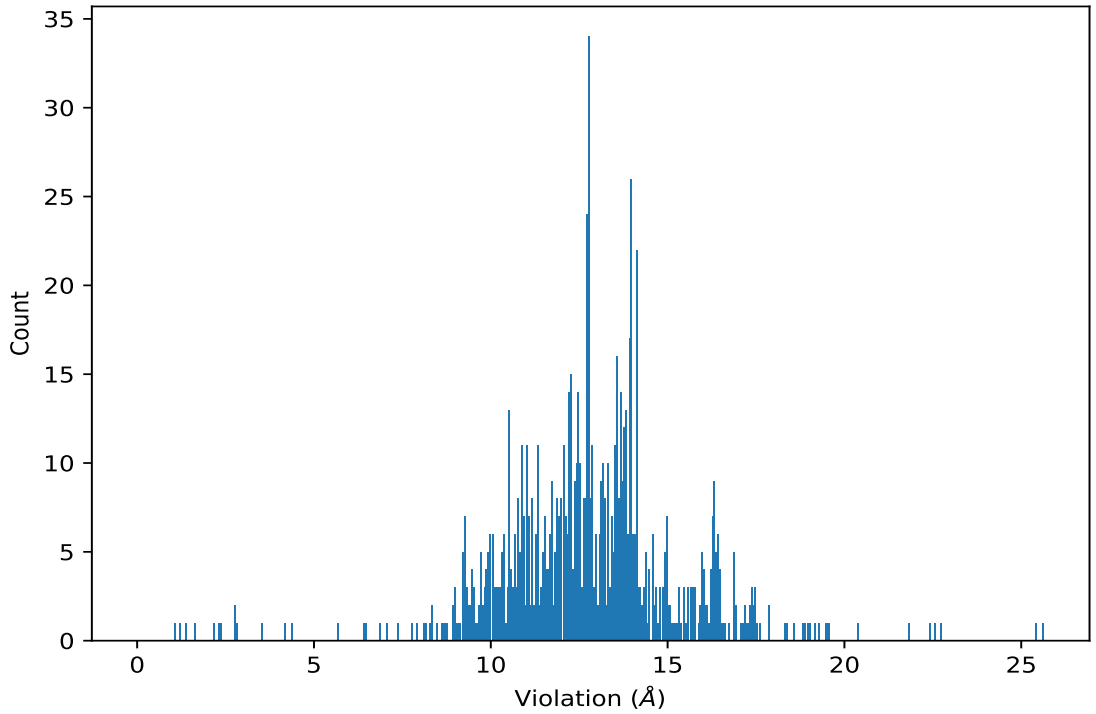
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,35)	1:184:B:LYS:N	5:216:A:7Q9:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:O	5:206:A:7Q9:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:HZ3	5:207:A:7Q9:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:HZ3	5:217:A:7Q9:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:C	5:217:A:7Q9:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:HZ3	5:216:A:7Q9:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:O	5:212:A:7Q9:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:HZ1	1:63:A:GLU:N	20	10.61	7.33	10.32
(1,35)	1:184:B:LYS:H	6:208:A:17F:N1	20	10.61	7.33	10.32
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	20	10.03	0.92	10.21
(3,3)	1:100:B:ILE:CD1	1:48:A:GLY:N	20	10.03	0.92	10.21
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	20	9.71	0.92	9.97
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	20	9.43	0.81	9.35
(1,34)	1:184:A:LYS:O	6:208:A:17F:N1	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:O	5:218:A:7Q9:N	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:N	6:219:A:17F:N1	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:HZ2	6:213:A:17F:N1	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:CB	6:208:A:17F:N1	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:HZ3	5:216:A:7Q9:N	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:HZ1	5:205:A:7Q9:N	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:C	6:219:A:17F:N1	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:CD	5:216:A:7Q9:N	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:N	5:217:A:7Q9:N	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:HZ1	6:208:A:17F:N1	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:C	5:217:A:7Q9:N	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:H	5:216:A:7Q9:N	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:O	5:217:A:7Q9:N	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:O	5:209:A:7Q9:N	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:H	6:220:A:17F:N1	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:H	6:208:A:17F:N1	20	8.94	5.7	6.97
(1,34)	1:184:A:LYS:CB	5:218:A:7Q9:N	20	8.94	5.7	6.97

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:184:B:LYS:N	5:216:A:7Q9:N	12	25.61
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	12	25.4
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	11	22.7
(1,35)	1:184:B:LYS:HZ3	5:216:A:7Q9:N	17	22.56
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	12	22.4
(1,34)	1:184:A:LYS:HZ1	6:208:A:17F:N1	11	21.81
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	8	20.35
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	12	19.58
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	13	19.54
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	10	19.49
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	11	19.27
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	11	19.17
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	18	19.04
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	12	18.95
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	17	18.87
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	4	18.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	3	18.59
(1,35)	1:184:B:LYS:O	6:208:A:17F:N1	9	18.38
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	6	18.3
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	11	17.87
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	14	17.85
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	10	17.64
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	6	17.52
(1,35)	1:184:B:LYS:H	6:208:A:17F:N1	20	17.48
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	12	17.48
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	19	17.46
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	3	17.41
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	3	17.4
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	4	17.38
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	17	17.38
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	12	17.37
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	8	17.34
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	2	17.3
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	7	17.25
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	20	17.21
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	1	17.19
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	20	17.18
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	17	17.13
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	9	17.07
(1,35)	1:184:B:LYS:HZ2	5:203:A:7Q9:N	6	16.93
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	11	16.93
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	5	16.89
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	14	16.87
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	15	16.86
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	17	16.86
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	12	16.86
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	7	16.73
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	13	16.63
(1,35)	1:184:B:LYS:H	5:203:A:7Q9:N	10	16.58
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	10	16.5
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	11	16.49
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	18	16.47
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	1	16.46
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	10	16.46
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	6	16.44
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	10	16.44
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	8	16.44
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	5	16.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	18	16.4
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	19	16.4
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	14	16.38
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	13	16.37
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	2	16.36
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	11	16.36
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	8	16.35
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	12	16.34
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	7	16.33
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	18	16.33
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	14	16.32
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	20	16.32
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	1	16.3
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	6	16.3
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	1	16.3
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	7	16.3
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	3	16.29
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	7	16.28
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	5	16.28
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	15	16.28
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	16	16.27
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	2	16.26
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	20	16.26
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	15	16.24
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	5	16.23
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	9	16.23
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	19	16.21
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	5	16.15
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	14	16.12
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	16	16.11
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	7	16.07
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	4	16.06
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	17	16.04
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	4	16.03
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	7	16.03
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	1	16.0
(1,25)	1:169:B:LYS:CG	1:128:A:LYS:N	9	15.99
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	20	15.98
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	8	15.95
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	14	15.95
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	19	15.95
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	17	15.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	16	15.92
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	16	15.89
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	5	15.78
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	14	15.77
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	5	15.75
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	15	15.74
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	6	15.72
(1,34)	1:184:A:LYS:C	6:219:A:17F:N1	8	15.71
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	4	15.69
(1,34)	1:184:A:LYS:O	5:218:A:7Q9:N	16	15.68
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	10	15.65
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	8	15.59
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	18	15.57
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	1	15.55
(1,34)	1:184:A:LYS:H	6:208:A:17F:N1	19	15.54
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	4	15.49
(1,35)	1:184:B:LYS:HZ1	1:63:A:GLU:N	19	15.48
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	16	15.47
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	3	15.37
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	9	15.33
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	16	15.33
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	14	15.32
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	12	15.26
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	7	15.2
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	4	15.16
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	10	15.14
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	17	15.06
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	19	15.05
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	2	15.02
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	9	15.01
(3,4)	1:103:B:VAL:CG1	5:210:A:7Q9:N	3	14.99
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	1	14.99
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	13	14.98
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	20	14.97
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	3	14.96
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	19	14.96
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	11	14.95
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	11	14.93
(3,4)	1:103:B:VAL:CG1	5:218:A:7Q9:N	20	14.92
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	18	14.92
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	1	14.9
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	15	14.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	6	14.87
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	5	14.87
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	9	14.87
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	14	14.79
(1,9)	1:169:A:LYS:CG	1:128:B:LYS:N	13	14.79
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	20	14.75
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	16	14.72
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	4	14.68
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	20	14.67
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	15	14.65
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	3	14.64
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	9	14.62
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	20	14.58
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	4	14.58
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	20	14.57
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	16	14.56
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	1	14.56
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	9	14.55
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	5	14.49
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	5	14.49
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	20	14.47
(3,4)	1:103:B:VAL:CG1	5:218:A:7Q9:N	4	14.46
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	17	14.41
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	10	14.39
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	10	14.39
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	20	14.35
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	2	14.35
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	2	14.35
(1,34)	1:184:A:LYS:H	5:216:A:7Q9:N	13	14.34
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	13	14.3
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	13	14.3
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	7	14.28
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	19	14.27
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	3	14.23
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	18	14.22
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	18	14.22
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	6	14.16
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	7	14.16
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	7	14.16
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	13	14.14
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	13	14.14
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	4	14.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	4	14.14
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	17	14.14
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	17	14.14
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	6	14.13
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	15	14.13
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	15	14.13
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	15	14.13
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	15	14.13
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	12	14.12
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	12	14.11
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	12	14.11
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	12	14.1
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	12	14.1
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	19	14.1
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	19	14.1
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	14	14.1
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	14	14.1
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	19	14.1
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	19	14.1
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	5	14.09
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	5	14.09
(1,32)	1:169:B:LYS:CG	1:179:A:LYS:N	2	14.08
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	6	14.08
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	9	14.08
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	9	14.08
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	17	14.03
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	17	14.03
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	18	14.03
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	11	14.02
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	11	14.02
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	19	14.0
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	8	13.99
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	8	13.99
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	5	13.99
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	10	13.98
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	16	13.97
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	18	13.97
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	18	13.97
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	12	13.97
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	13	13.97
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	3	13.97
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	3	13.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	6	13.97
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	17	13.97
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	20	13.96
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	16	13.96
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	16	13.96
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	2	13.96
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	1	13.96
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	8	13.96
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	2	13.95
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	3	13.95
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	15	13.95
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	4	13.95
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	10	13.95
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	2	13.95
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	2	13.95
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	13	13.94
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	1	13.94
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	14	13.94
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	2	13.94
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	9	13.94
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	14	13.94
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	20	13.94
(3,4)	1:103:B:VAL:CG1	6:219:A:17F:N1	11	13.93
(1,34)	1:184:A:LYS:CD	5:216:A:7Q9:N	9	13.93
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	7	13.93
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	5	13.93
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	6	13.93
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	6	13.93
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	11	13.93
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	5	13.92
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	17	13.9
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	9	13.9
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	9	13.88
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	18	13.87
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	3	13.85
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	3	13.85
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	10	13.85
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	10	13.85
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	19	13.84
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	10	13.83
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	11	13.83
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	11	13.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	16	13.83
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	10	13.82
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	10	13.82
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	18	13.82
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	4	13.82
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	17	13.82
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	17	13.82
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	15	13.8
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	15	13.8
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	5	13.79
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	5	13.79
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	14	13.79
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	14	13.79
(3,4)	1:103:B:VAL:CG1	6:219:A:17F:N1	1	13.78
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	2	13.77
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	15	13.77
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	15	13.77
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	17	13.77
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	16	13.77
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	16	13.77
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	2	13.76
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	9	13.73
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	9	13.73
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	3	13.73
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	3	13.73
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	6	13.72
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	8	13.72
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	4	13.71
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	12	13.7
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	12	13.7
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	3	13.69
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	3	13.69
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	6	13.69
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	6	13.68
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	6	13.68
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	1	13.67
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	18	13.67
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	18	13.67
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	6	13.67
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	6	13.67
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	12	13.66
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	1	13.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	1	13.65
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	7	13.65
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	4	13.64
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	4	13.64
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	4	13.64
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	4	13.64
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	3	13.64
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	11	13.63
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	2	13.62
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	2	13.62
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	1	13.59
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	1	13.59
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	2	13.59
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	2	13.59
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	12	13.59
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	12	13.59
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	16	13.59
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	1	13.59
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	1	13.59
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	7	13.56
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	7	13.56
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	3	13.55
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	1	13.55
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	1	13.55
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	20	13.55
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	20	13.55
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	5	13.53
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	5	13.53
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	19	13.52
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	19	13.52
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	17	13.52
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	17	13.52
(3,4)	1:103:B:VAL:CG1	6:219:A:17F:N1	5	13.51
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	4	13.51
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	1	13.51
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	9	13.5
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	9	13.5
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	2	13.47
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	9	13.45
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	15	13.45
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	11	13.45
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	11	13.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	17	13.44
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	17	13.44
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	11	13.41
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	11	13.41
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	8	13.41
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	8	13.41
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	7	13.41
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	20	13.38
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	20	13.38
(3,4)	1:103:B:VAL:CG1	6:219:A:17F:N1	13	13.35
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	7	13.34
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	7	13.34
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	7	13.34
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	7	13.34
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	18	13.34
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	18	13.34
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	14	13.33
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	13	13.33
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	13	13.33
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	1	13.3
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	7	13.26
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	13	13.25
(1,19)	1:118:B:CYS:SG	1:46:A:ILE:CD1	16	13.24
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	8	13.23
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	8	13.23
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	7	13.22
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	4	13.2
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	4	13.2
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	10	13.2
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	10	13.2
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	20	13.19
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	20	13.19
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	14	13.17
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	14	13.17
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	5	13.16
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	10	13.16
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	3	13.16
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	3	13.16
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	6	13.15
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	6	13.15
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	14	13.12
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	14	13.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	6	13.12
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	6	13.12
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	12	13.12
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	4	13.11
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	4	13.11
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	16	13.1
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	16	13.1
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	20	13.08
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	20	13.08
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	16	13.08
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	13	13.07
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	13	13.07
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	3	13.05
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	8	13.0
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	15	13.0
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	18	12.98
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	14	12.98
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	14	12.98
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	18	12.96
(3,4)	1:103:B:VAL:CG1	5:212:A:7Q9:N	19	12.95
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	18	12.95
(1,34)	1:184:A:LYS:HZ2	6:213:A:17F:N1	17	12.94
(1,35)	1:184:B:LYS:HZ3	5:203:A:7Q9:N	4	12.93
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	19	12.9
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	16	12.89
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	19	12.89
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	19	12.89
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	12	12.89
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	4	12.89
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	4	12.89
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	4	12.87
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	19	12.86
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	2	12.85
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	10	12.85
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	10	12.85
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	4	12.84
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG1	9	12.83
(1,17)	1:118:B:CYS:SG	1:44:A:VAL:CG2	9	12.83
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	7	12.83
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	7	12.81
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	8	12.81
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	11	12.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	11	12.81
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	9	12.79
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	9	12.79
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	15	12.79
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	15	12.79
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	17	12.79
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	17	12.79
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	9	12.78
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	9	12.78
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	6	12.78
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	6	12.78
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	6	12.78
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	8	12.77
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	8	12.77
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	1	12.77
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	1	12.77
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	7	12.77
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	7	12.77
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	18	12.77
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	18	12.77
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	3	12.76
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	3	12.76
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	15	12.76
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	15	12.76
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	8	12.75
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	4	12.75
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	4	12.75
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	5	12.75
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	5	12.75
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	11	12.75
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	11	12.75
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	9	12.75
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	9	12.75
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	16	12.75
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	16	12.75
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	12	12.74
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	12	12.74
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	7	12.74
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	9	12.74
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	2	12.74
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	2	12.74
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	19	12.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	19	12.74
(3,4)	1:103:B:VAL:CG1	6:219:A:17F:N1	8	12.73
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG1	7	12.73
(1,5)	1:118:A:CYS:SG	1:160:B:VAL:CG2	7	12.73
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	14	12.73
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	14	12.73
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	6	12.72
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	18	12.72
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	18	12.72
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	1	12.71
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	1	12.71
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	14	12.71
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	14	12.71
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	13	12.71
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	13	12.71
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	11	12.7
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	20	12.7
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	15	12.69
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	13	12.68
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	13	12.68
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	18	12.68
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	20	12.67
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	5	12.66
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	20	12.65
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	20	12.65
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	14	12.64
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	6	12.63
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	5	12.63
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	5	12.63
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	11	12.61
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	11	12.61
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	10	12.6
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	10	12.6
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	2	12.58
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	2	12.58
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	14	12.57
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	8	12.54
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	8	12.54
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	3	12.53
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	3	12.53
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	7	12.52
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	4	12.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	15	12.5
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	8	12.5
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	20	12.5
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	20	12.5
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	16	12.49
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	16	12.49
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	12	12.49
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	12	12.49
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	20	12.49
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	20	12.49
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	19	12.48
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	3	12.48
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	3	12.48
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	18	12.47
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	6	12.46
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	6	12.46
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	8	12.46
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	8	12.46
(3,3)	1:100:B:ILE:CD1	1:48:A:GLY:N	16	12.44
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	4	12.44
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	17	12.44
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	7	12.43
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	4	12.41
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	7	12.41
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	7	12.41
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG1	4	12.41
(1,2)	1:118:A:CYS:SG	1:45:B:VAL:CG2	4	12.41
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	6	12.4
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	12	12.39
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	12	12.39
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	17	12.37
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	11	12.37
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	17	12.36
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	17	12.36
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	13	12.36
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	10	12.35
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	10	12.35
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	11	12.34
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	14	12.31
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG1	16	12.31
(1,21)	1:118:B:CYS:SG	1:160:A:VAL:CG2	16	12.31
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	6	12.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	6	12.28
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	3	12.27
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	3	12.27
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	7	12.27
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	7	12.27
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	19	12.27
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	19	12.27
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	16	12.26
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	11	12.25
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	11	12.25
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	2	12.25
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	2	12.25
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	4	12.25
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	4	12.25
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	9	12.24
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	9	12.24
(3,4)	1:103:B:VAL:CG1	5:216:A:7Q9:N	16	12.23
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	12	12.22
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	12	12.22
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	17	12.22
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	17	12.22
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG1	12	12.22
(1,1)	1:118:A:CYS:SG	1:44:B:VAL:CG2	12	12.22
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	2	12.21
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	2	12.21
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	17	12.2
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	18	12.2
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	18	12.2
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	16	12.18
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	16	12.18
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	13	12.17
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	19	12.16
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	8	12.15
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	8	12.15
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	2	12.14
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	6	12.14
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	6	12.14
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	15	12.13
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	12	12.12
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	19	12.12
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	2	12.1
(1,31)	1:169:B:LYS:CG	1:178:A:LYS:N	19	12.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	1	12.09
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	1	12.09
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	2	12.07
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	3	12.07
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	20	12.07
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	4	12.07
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	4	12.07
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	14	12.05
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	19	12.05
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	19	12.05
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	10	11.97
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	8	11.97
(3,4)	1:103:B:VAL:CG2	5:216:A:7Q9:N	9	11.96
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	5	11.96
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	20	11.96
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	11	11.96
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	11	11.96
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	1	11.95
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	8	11.92
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	8	11.92
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	20	11.92
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	20	11.92
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	11	11.91
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	9	11.91
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	9	11.91
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	18	11.89
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	18	11.89
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	3	11.89
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	3	11.89
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	19	11.88
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	19	11.88
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	6	11.85
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	12	11.85
(3,4)	1:103:B:VAL:CG1	5:209:A:7Q9:N	17	11.84
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	3	11.83
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG1	19	11.83
(1,18)	1:118:B:CYS:SG	1:45:A:VAL:CG2	19	11.83
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	3	11.8
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	2	11.78
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	2	11.78
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	15	11.73
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	2	11.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	2	11.72
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	18	11.71
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	6	11.71
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	7	11.7
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	7	11.7
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	20	11.7
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	20	11.7
(1,35)	1:184:B:LYS:HZ2	6:219:A:17F:N1	2	11.69
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	11	11.69
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	11	11.69
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	16	11.68
(1,15)	1:169:A:LYS:CG	1:178:B:LYS:N	16	11.66
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	1	11.65
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	4	11.64
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	6	11.62
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	6	11.62
(1,34)	1:184:A:LYS:N	6:219:A:17F:N1	3	11.6
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	16	11.59
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	15	11.58
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	15	11.58
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	16	11.55
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	9	11.54
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	7	11.53
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	7	11.53
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	20	11.53
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	1	11.52
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	1	11.52
(3,4)	1:103:B:VAL:CG1	5:209:A:7Q9:N	7	11.5
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	10	11.47
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	10	11.47
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	17	11.46
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	17	11.46
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	17	11.46
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	20	11.44
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	20	11.44
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	15	11.44
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	17	11.38
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	13	11.36
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	10	11.34
(1,16)	1:169:A:LYS:CG	1:179:B:LYS:N	4	11.34
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	5	11.34
(1,29)	1:169:B:LYS:CG	1:176:A:LYS:N	8	11.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	16	11.32
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	16	11.32
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	14	11.31
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	14	11.31
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	13	11.31
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	13	11.31
(1,35)	1:184:B:LYS:O	5:212:A:7Q9:N	18	11.3
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	1	11.28
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	7	11.27
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	14	11.26
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	14	11.26
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	5	11.26
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	17	11.25
(1,30)	1:169:B:LYS:CG	1:177:A:LYS:N	8	11.22
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	13	11.2
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	6	11.16
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	19	11.16
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	18	11.16
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	18	11.16
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	8	11.15
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	8	11.15
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	9	11.15
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	9	11.15
(3,4)	1:103:B:VAL:CG1	5:210:A:7Q9:N	14	11.14
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	15	11.13
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	11	11.08
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	8	11.08
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	12	11.08
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	12	11.08
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	9	11.07
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	2	11.07
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	8	11.05
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	8	11.03
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	15	11.02
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	13	11.01
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	9	11.0
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	10	11.0
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	10	11.0
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	10	11.0
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	10	11.0
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	3	11.0
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD1	5	11.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:169:A:LYS:CG	1:113:B:LEU:CD2	5	11.0
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	2	10.99
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	10	10.97
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	2	10.94
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	1	10.92
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	1	10.92
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	18	10.92
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	19	10.92
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	17	10.91
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	17	10.91
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	8	10.89
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	8	10.89
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	14	10.88
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	18	10.88
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	18	10.88
(1,13)	1:169:A:LYS:CG	1:176:B:LYS:N	9	10.88
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	9	10.87
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	9	10.87
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	16	10.86
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	16	10.86
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	12	10.85
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	5	10.84
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	5	10.84
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	3	10.82
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	16	10.8
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	16	10.8
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	1	10.79
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	10	10.79
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	4	10.77
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	10	10.75
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	2	10.75
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	19	10.75
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	19	10.75
(1,14)	1:169:A:LYS:CG	1:177:B:LYS:N	13	10.75
(3,4)	1:103:B:VAL:CG1	5:216:A:7Q9:N	6	10.71
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	8	10.71
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	17	10.7
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	3	10.68
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	15	10.68
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	5	10.66
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	5	10.66
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	13	10.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	13	10.65
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	15	10.64
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	11	10.64
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	14	10.62
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	12	10.56
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	7	10.55
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	18	10.55
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	12	10.55
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD1	15	10.54
(1,22)	1:169:B:LYS:CG	1:113:A:LEU:CD2	15	10.54
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	6	10.54
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	1	10.53
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	1	10.53
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	13	10.52
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	15	10.51
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	15	10.51
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	1	10.5
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	18	10.5
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	15	10.5
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	13	10.5
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	8	10.5
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	16	10.48
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	15	10.47
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	18	10.47
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	20	10.44
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	5	10.39
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	14	10.39
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	14	10.39
(3,3)	1:100:B:ILE:CD1	1:48:A:GLY:N	13	10.37
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	7	10.37
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	9	10.35
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	19	10.34
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	5	10.33
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	17	10.33
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	8	10.31
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	2	10.31
(1,11)	1:169:A:LYS:CG	1:172:B:LYS:N	3	10.28
(3,4)	1:103:B:VAL:CG1	5:216:A:7Q9:N	15	10.26
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	1	10.25
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	14	10.24
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	14	10.24
(1,3)	1:118:A:CYS:SG	1:46:B:ILE:CD1	13	10.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	8	10.19
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	2	10.16
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	19	10.15
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	15	10.12
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	15	10.12
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	19	10.1
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	6	10.09
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	10	10.07
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	5	10.06
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	5	10.06
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	18	10.05
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	11	10.05
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	8	9.98
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	13	9.98
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	5	9.98
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	3	9.98
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	5	9.97
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	9	9.96
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD1	13	9.92
(1,23)	1:169:B:LYS:CG	1:133:A:LEU:CD2	13	9.92
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD1	13	9.9
(1,7)	1:169:A:LYS:CG	1:133:B:LEU:CD2	13	9.9
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	11	9.9
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	10	9.89
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	19	9.87
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	5	9.87
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	17	9.86
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	14	9.84
(1,27)	1:169:B:LYS:CG	1:172:A:LYS:N	11	9.84
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	13	9.83
(1,8)	1:169:A:LYS:CG	1:139:B:ILE:CD1	15	9.77
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	14	9.76
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	20	9.74
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	20	9.73
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	2	9.7
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	10	9.7
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	5	9.7
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	4	9.66
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	18	9.65
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	12	9.61
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	19	9.58
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	17	9.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	11	9.53
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	3	9.52
(1,26)	1:169:B:LYS:CG	1:169:A:LYS:N	12	9.49
(1,10)	1:169:A:LYS:CG	1:169:B:LYS:N	11	9.49
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	12	9.47
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	3	9.45
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	15	9.43
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	6	9.43
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	5	9.38
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	15	9.36
(1,35)	1:184:B:LYS:HZ3	5:217:A:7Q9:N	15	9.34
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	16	9.34
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	2	9.32
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	18	9.29
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	9	9.27
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	1	9.27
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	12	9.26
(1,35)	1:184:B:LYS:HZ1	5:217:A:7Q9:N	8	9.26
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	3	9.26
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	18	9.25
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	11	9.24
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	10	9.24
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	9	9.24
(1,12)	1:169:A:LYS:CG	1:175:B:LYS:N	10	9.23
(1,28)	1:169:B:LYS:CG	1:175:A:LYS:N	13	9.21
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	1	9.13
(3,4)	1:103:B:VAL:CG1	5:218:A:7Q9:N	2	9.06
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	17	9.04
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	1	8.99
(3,4)	1:103:B:VAL:CG1	5:218:A:7Q9:N	10	8.98
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	20	8.97
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	16	8.93
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	13	8.91
(1,24)	1:169:B:LYS:CG	1:139:A:ILE:CD1	13	8.75
(1,34)	1:184:A:LYS:C	5:217:A:7Q9:N	12	8.7
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	10	8.65
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	6	8.6
(3,4)	1:103:B:VAL:CG1	5:218:A:7Q9:N	12	8.49
(3,3)	1:100:B:ILE:CD1	1:47:A:ASP:N	17	8.32
(3,4)	1:103:B:VAL:CG1	5:218:A:7Q9:N	18	8.31
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	10	8.26
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	7	8.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:184:B:LYS:CA	5:207:A:7Q9:N	5	8.14
(1,4)	1:118:A:CYS:SG	1:142:B:ILE:CD1	14	7.91
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	19	7.75
(1,20)	1:118:B:CYS:SG	1:142:A:ILE:CD1	4	7.35
(1,34)	1:184:A:LYS:HZ3	5:216:A:7Q9:N	6	7.08
(1,34)	1:184:A:LYS:H	6:220:A:17F:N1	18	6.86
(1,34)	1:184:A:LYS:O	6:208:A:17F:N1	1	6.45
(1,34)	1:184:A:LYS:N	5:217:A:7Q9:N	10	6.42
(1,34)	1:184:A:LYS:O	5:218:A:7Q9:N	2	5.68
(1,34)	1:184:A:LYS:CB	5:218:A:7Q9:N	20	4.38
(1,35)	1:184:B:LYS:O	6:220:A:17F:N1	11	4.15
(1,34)	1:184:A:LYS:O	5:217:A:7Q9:N	14	3.52
(1,35)	1:184:B:LYS:C	5:217:A:7Q9:N	16	2.81
(1,35)	1:184:B:LYS:HZ3	5:207:A:7Q9:N	14	2.78
(1,34)	1:184:A:LYS:CB	6:208:A:17F:N1	5	2.78
(1,35)	1:184:B:LYS:HZ2	6:208:A:17F:N1	7	2.35
(1,34)	1:184:A:LYS:HZ2	6:213:A:17F:N1	4	2.34
(1,35)	1:184:B:LYS:HZ3	6:213:A:17F:N1	1	2.16
(1,34)	1:184:A:LYS:O	5:209:A:7Q9:N	15	1.64
(1,34)	1:184:A:LYS:HZ1	5:205:A:7Q9:N	7	1.37
(1,35)	1:184:B:LYS:O	5:207:A:7Q9:N	3	1.22
(1,35)	1:184:B:LYS:O	5:206:A:7Q9:N	13	1.08

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found