



## Full wwPDB EM Model Validation Report ⓘ

Mar 12, 2020 – 02:25 PM EDT

PDB ID : 6QL5  
EMDB ID : EMD-4577  
Title : Structure of fatty acid synthase complex with bound gamma subunit from *Saccharomyces cerevisiae* at 2.8 angstrom  
Authors : Singh, K.; Graf, B.; Linden, A.; Sautner, V.; Urlaub, H.; Tittmann, K.; Stark, H.; Chari, A.  
Deposited on : 2019-01-31  
Resolution : 2.80 Å(reported)

This is a Full wwPDB EM Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

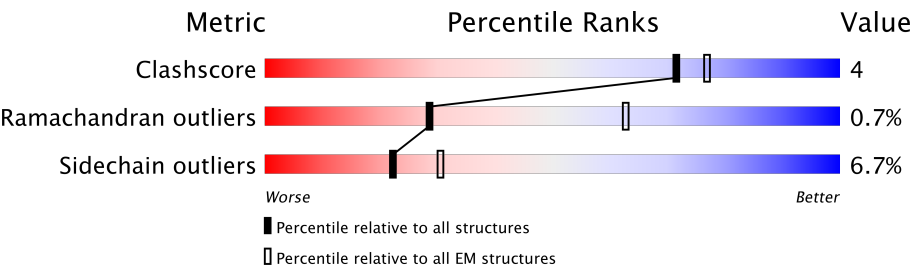
MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.8

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 Å.

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












Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1887	
1	B	1887	
1	C	1887	
1	D	1887	
1	E	1887	
1	F	1887	
2	G	2040	
2	H	2040	
2	I	2040	

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Mol	Chain	Length	Quality of chain
2	J	2040	 86% 12% .
2	K	2040	 86% 12% .
2	L	2040	 86% 12% .
3	M	148	 60% 12% . 24%
3	N	148	 60% 11% . 24%
3	O	148	 60% 12% . 24%
3	P	148	 60% 11% . 24%
3	Q	148	 60% 12% . 24%
3	R	148	 60% 11% . 24%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 183444 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	B	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	C	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	D	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	E	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	F	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	H	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	I	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	J	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	K	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	L	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		

- Molecule 3 is a protein called Translation machinery-associated protein 17.

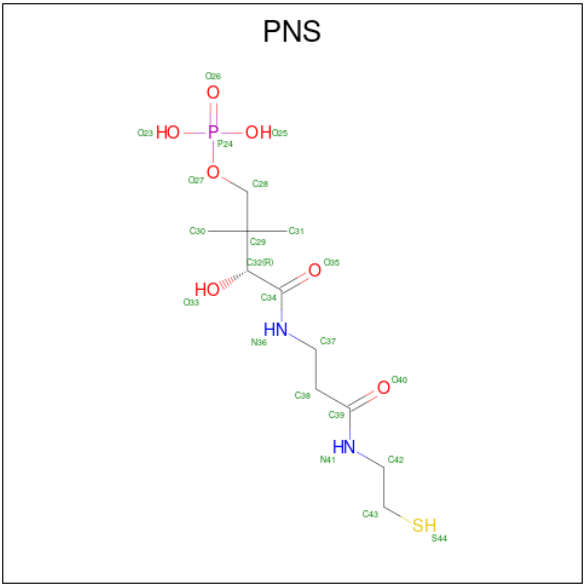
Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	112	Total	C	N	O	S	0	0
			879	542	155	179	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	O	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	P	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	Q	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	R	112	Total	C	N	O	S	0	0
			879	542	155	179	3		

- Molecule 4 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>PS).



Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total 21	C 11	N 2	O 6	P 1	S 1	0
4	B	1	Total 21	C 11	N 2	O 6	P 1	S 1	0
4	C	1	Total 21	C 11	N 2	O 6	P 1	S 1	0
4	D	1	Total 21	C 11	N 2	O 6	P 1	S 1	0
4	E	1	Total 21	C 11	N 2	O 6	P 1	S 1	0
4	F	1	Total 21	C 11	N 2	O 6	P 1	S 1	0

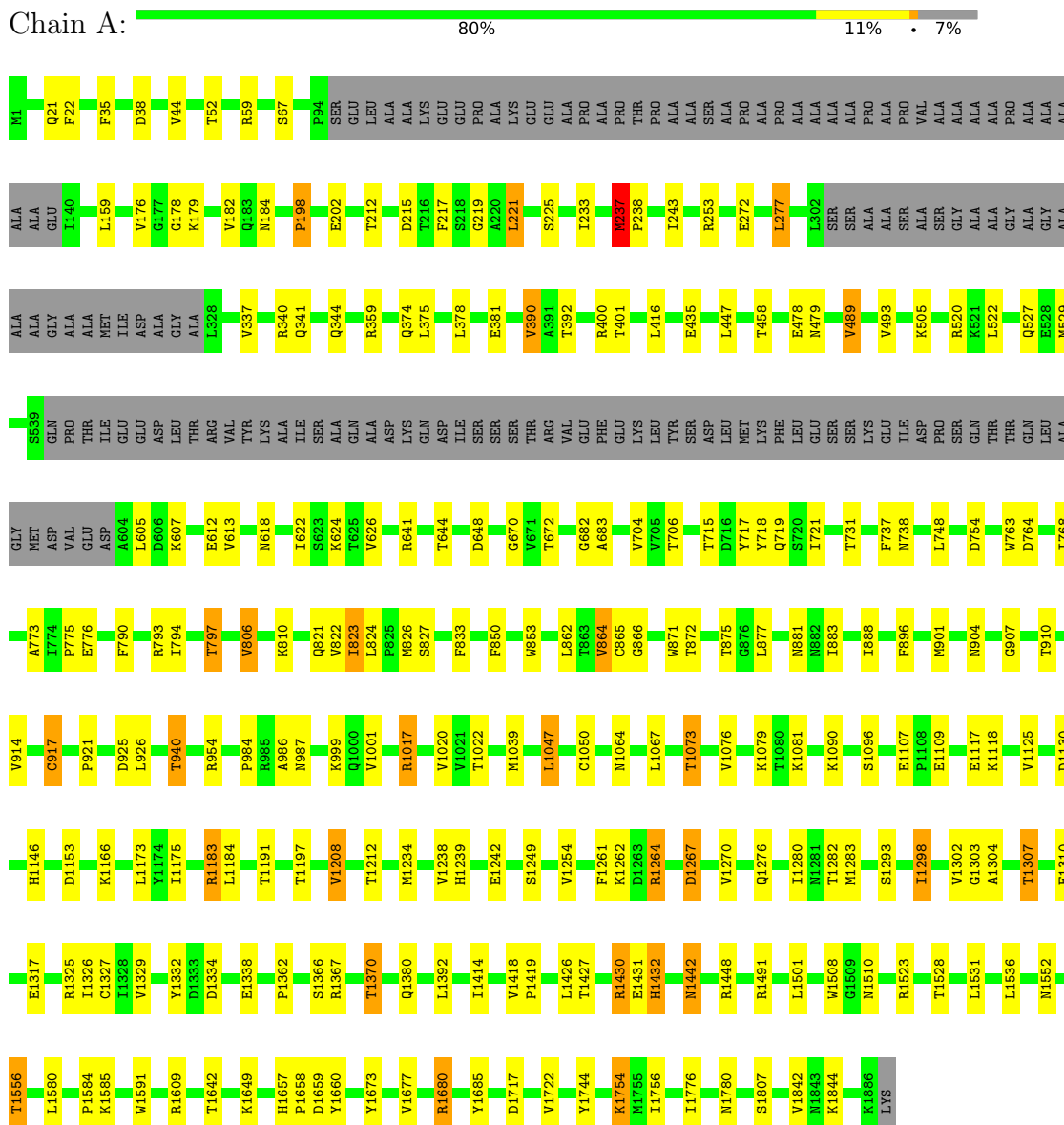
- 
- The image displays the chemical structure of Flavin Mononucleotide (FMN). It features an isoalloxazine ring system, which is a tricyclic aromatic heterocycle consisting of a benzene ring fused to two pyrimidine rings. The atoms in the ring are labeled: N1, N5, N10 for nitrogen; C2, C4, C6, C7, C8, C9 for carbon. Substituents include a carbonyl group at C2 (O2), a carbonyl group at C4 (O4), and a dimethylaminomethyl group at C10 (C10A, C10B, N10B, N10C). Attached to the C10 position is a ribityl chain (C1, C2, C3, C4) with hydroxyl groups at C2 (O2), C3 (O3), and C4 (O4). The C4 carbon is also attached to a phosphate group (P, O1P, O2P, O3P).

Mol	Chain	Residues	Atoms					AltConf
5	G	1	Total 31	C 17	N 4	O 9	P 1	0
5	H	1	Total 31	C 17	N 4	O 9	P 1	0
5	I	1	Total 31	C 17	N 4	O 9	P 1	0
5	J	1	Total 31	C 17	N 4	O 9	P 1	0
5	K	1	Total 31	C 17	N 4	O 9	P 1	0
5	L	1	Total 31	C 17	N 4	O 9	P 1	0

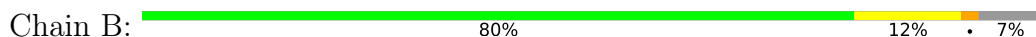
### 3 Residue-property plots

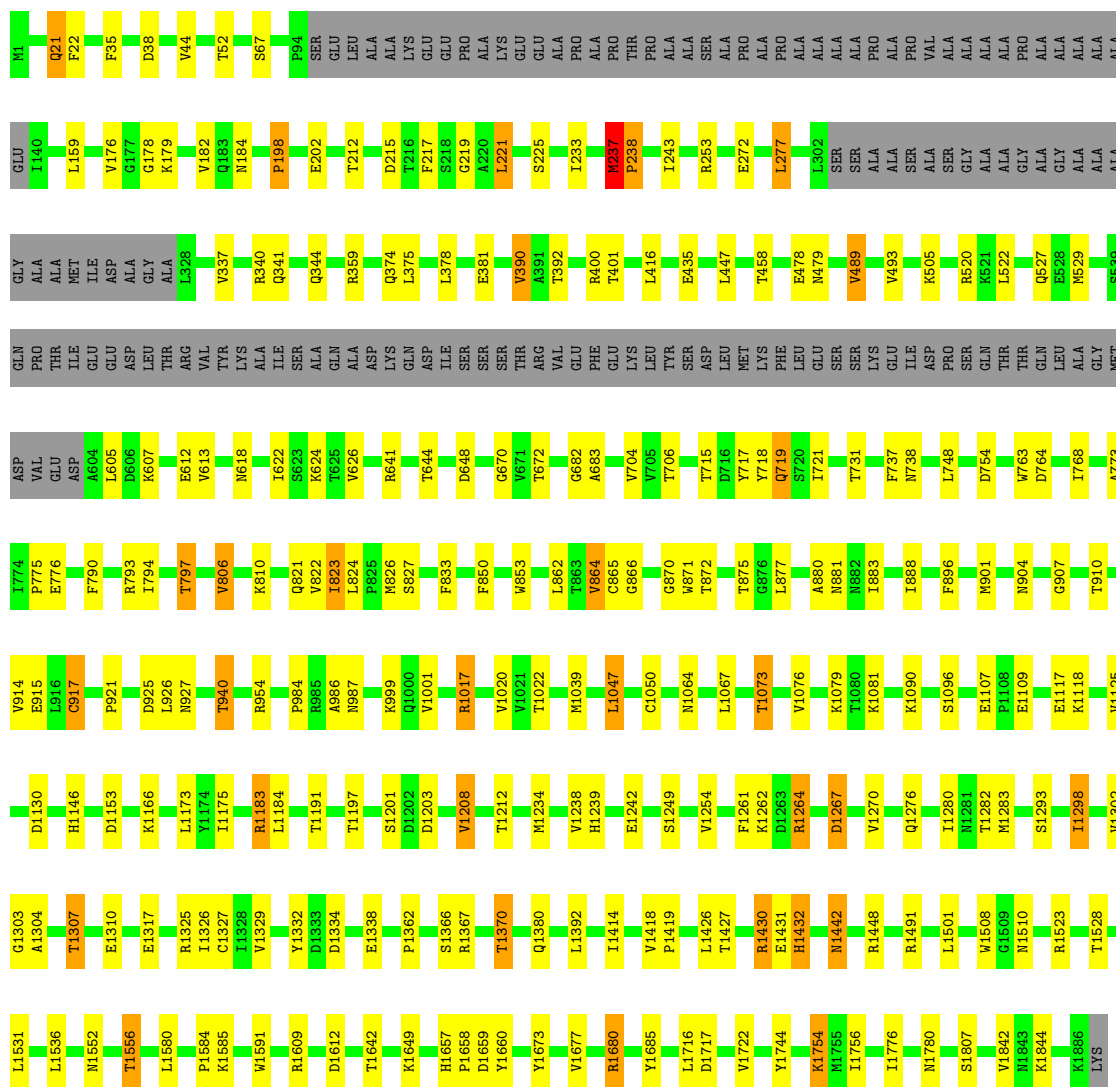
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fatty acid synthase subunit alpha



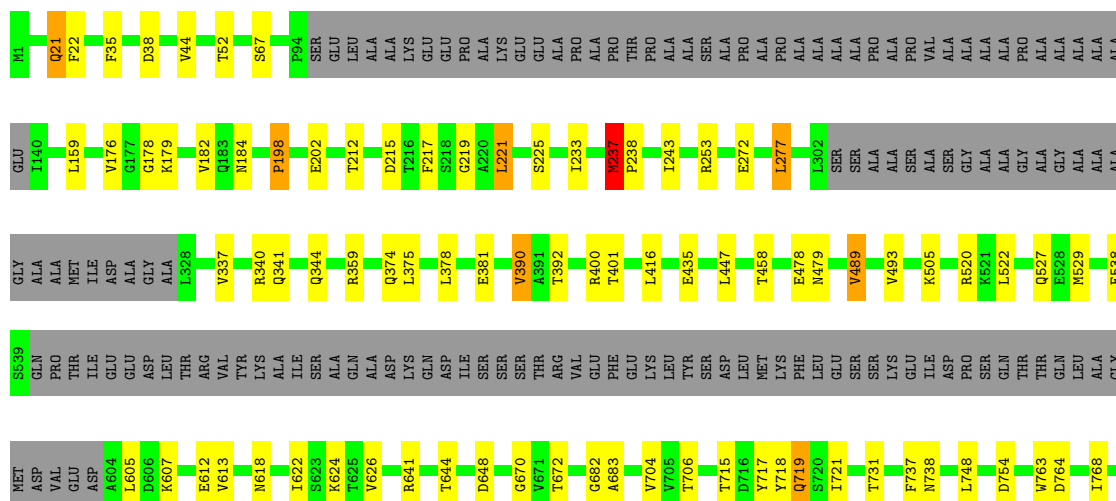
- Molecule 1: Fatty acid synthase subunit alpha



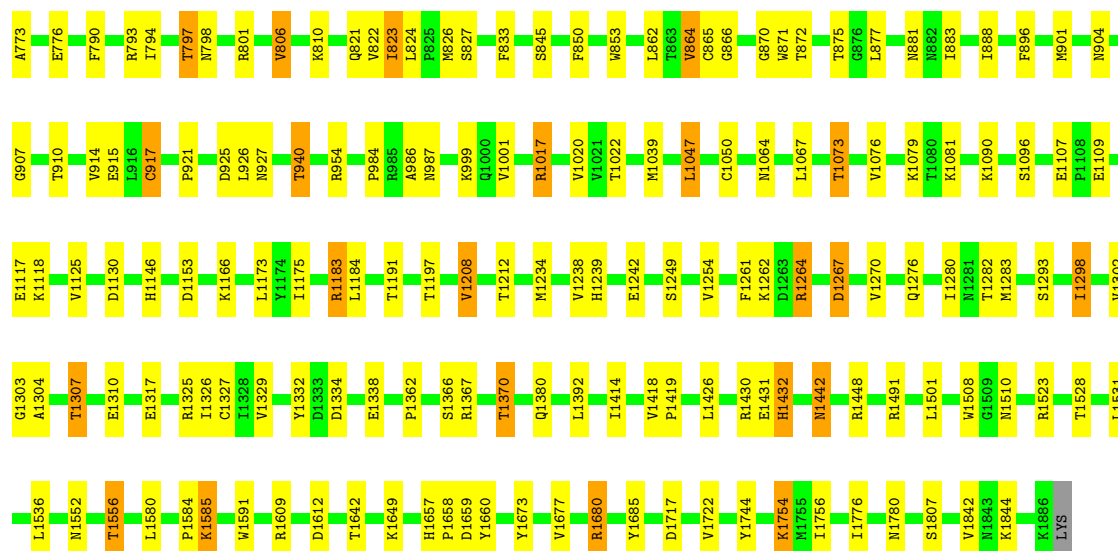


### • Molecule 1: Fatty acid synthase subunit alpha


Chain C: 80% 12% 7%

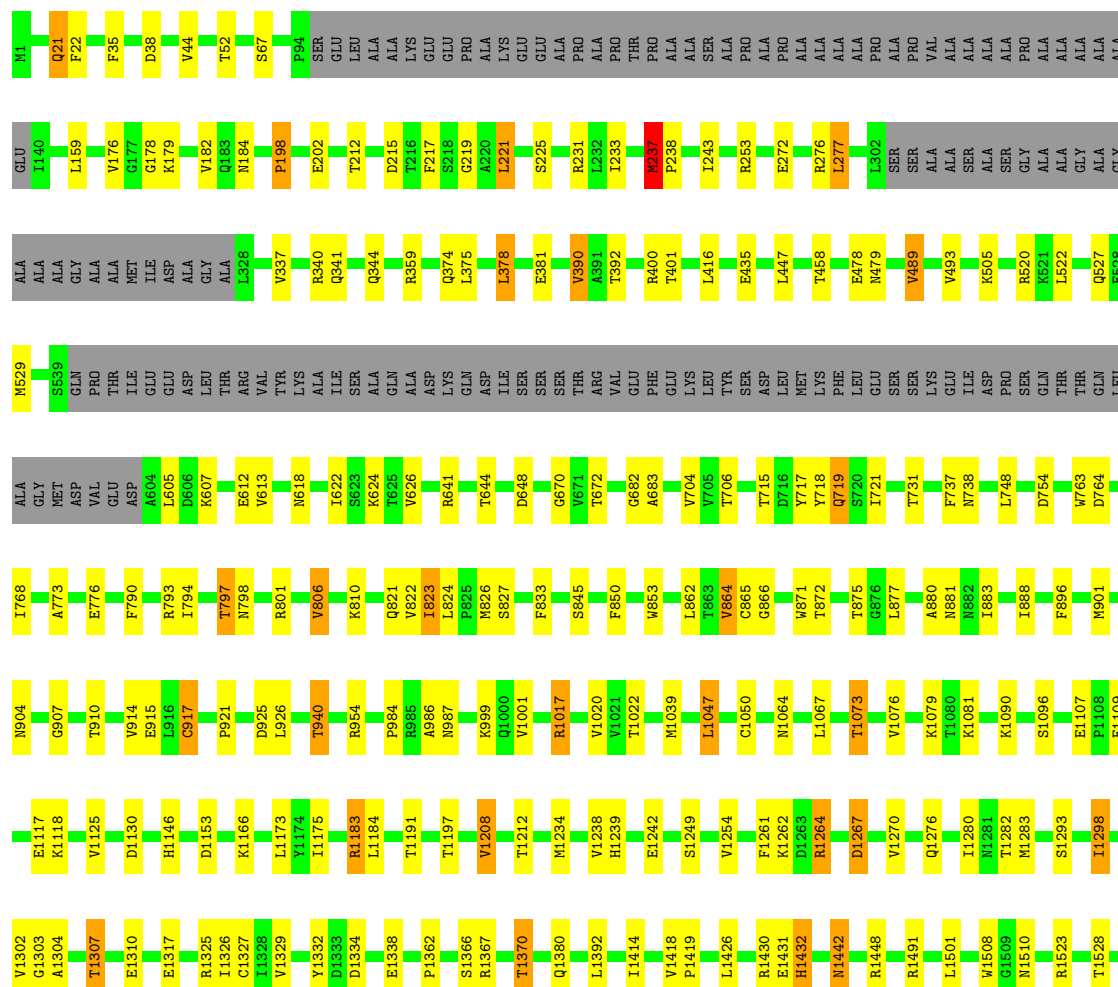






- Molecule 1: Fatty acid synthase subunit alpha

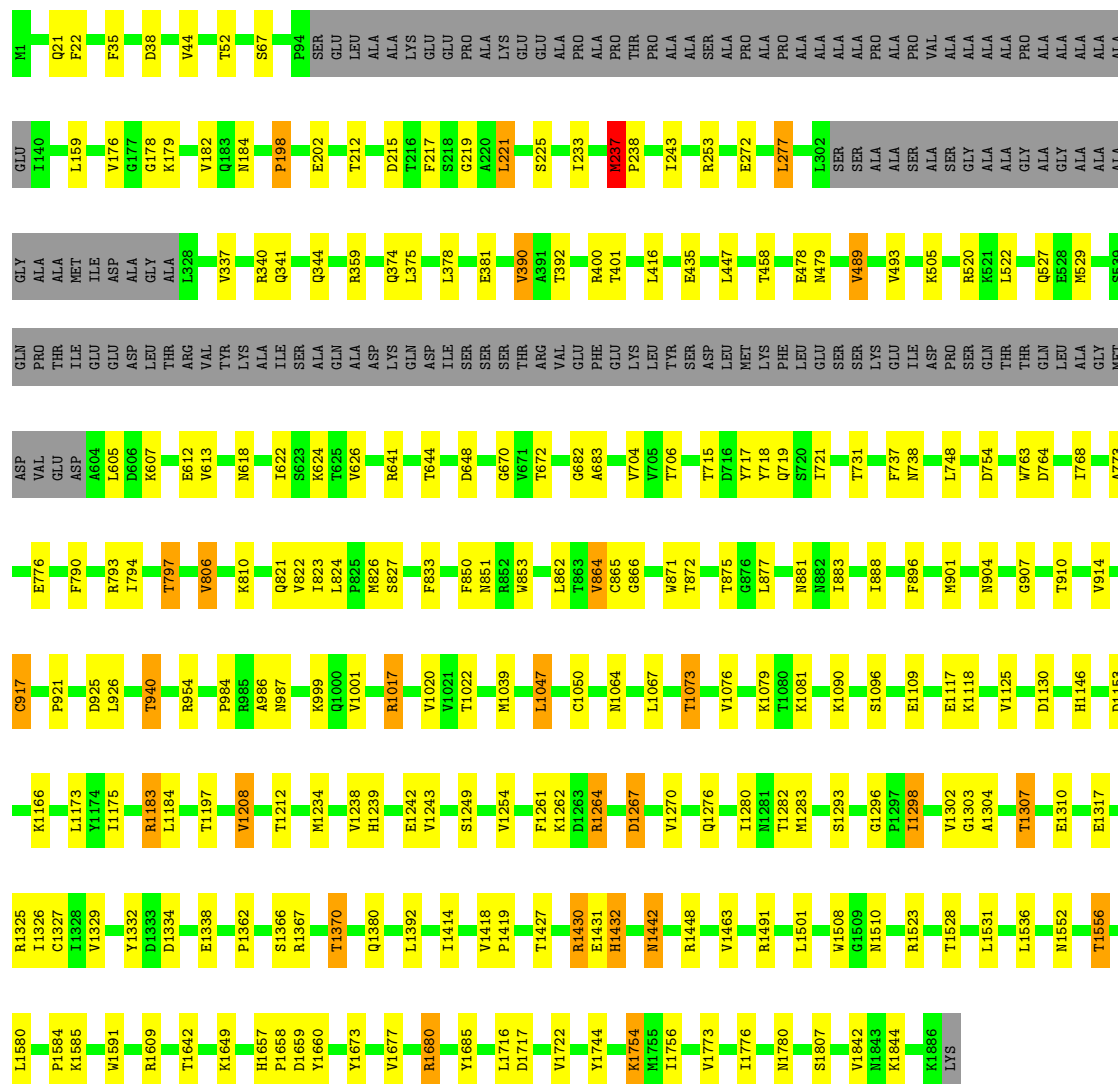
Chain D:  80% 11% 7%





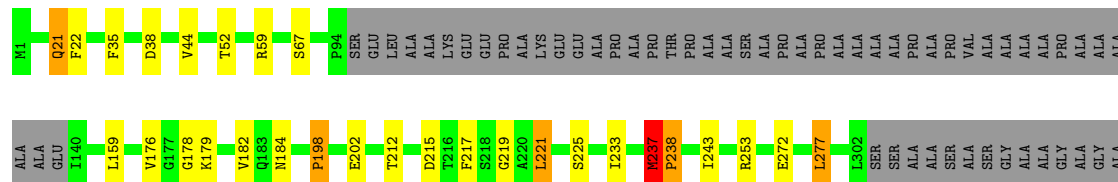
• Molecule 1: Fatty acid synthase subunit alpha

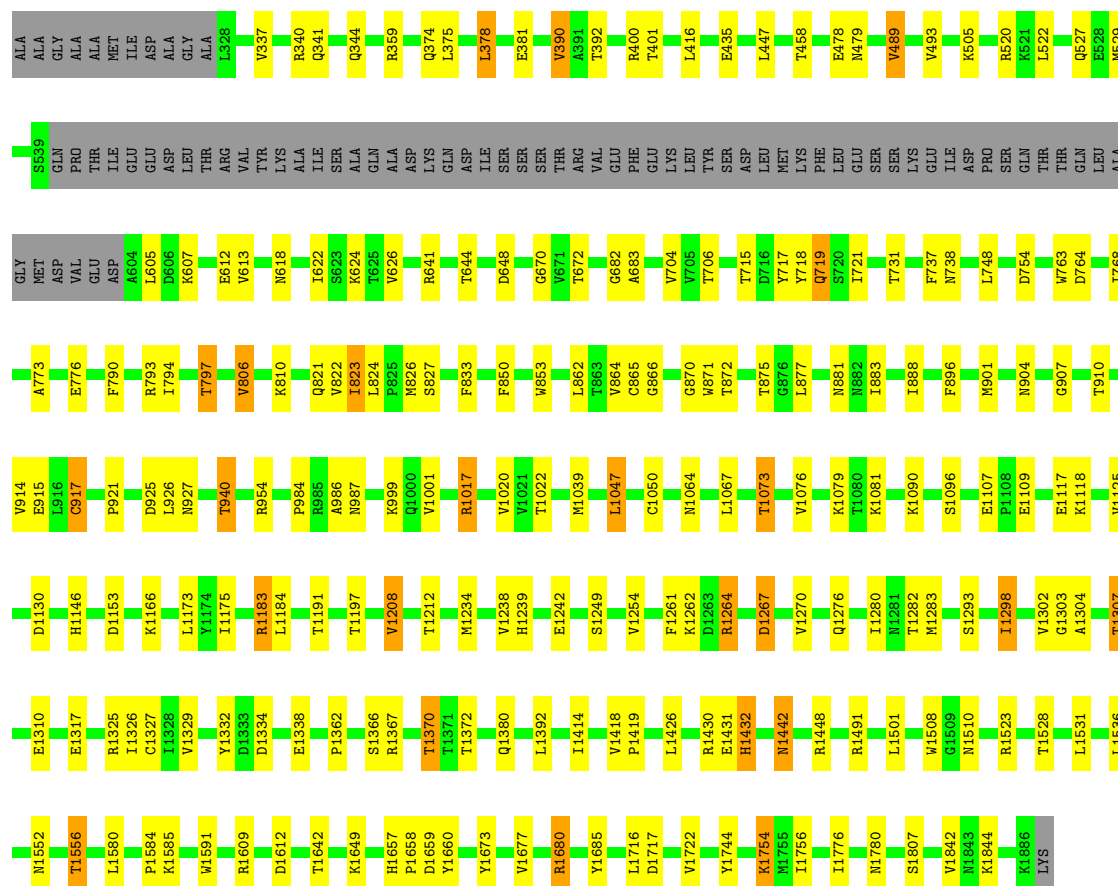
Chain E: 80% 11% 7%



• Molecule 1: Fatty acid synthase subunit alpha

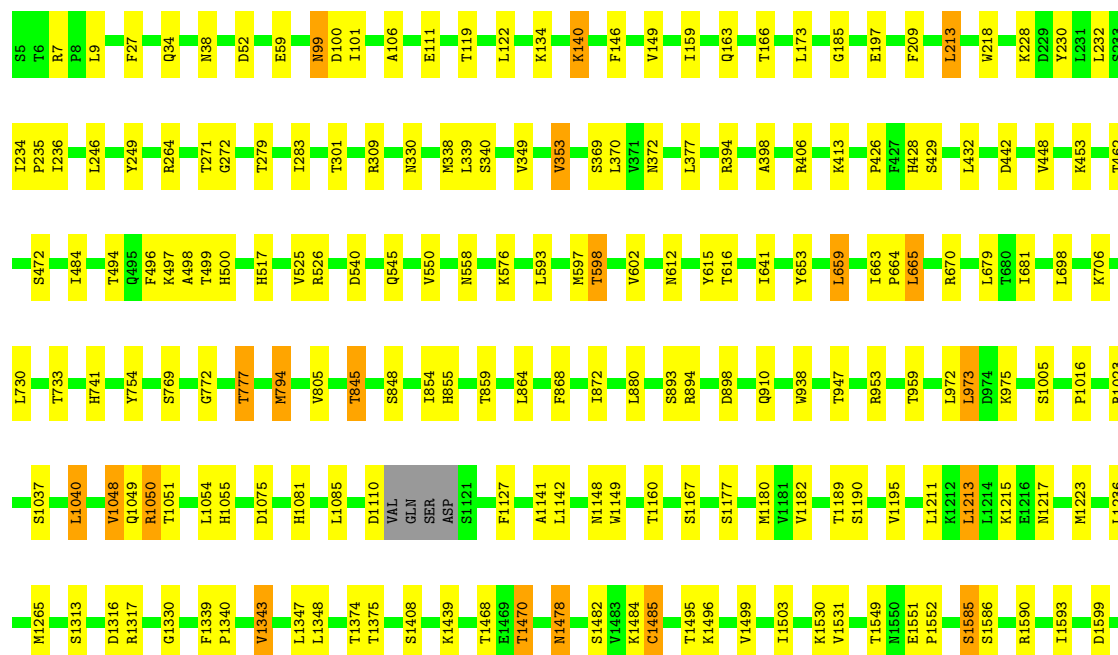
Chain F: 80% 11% 7%

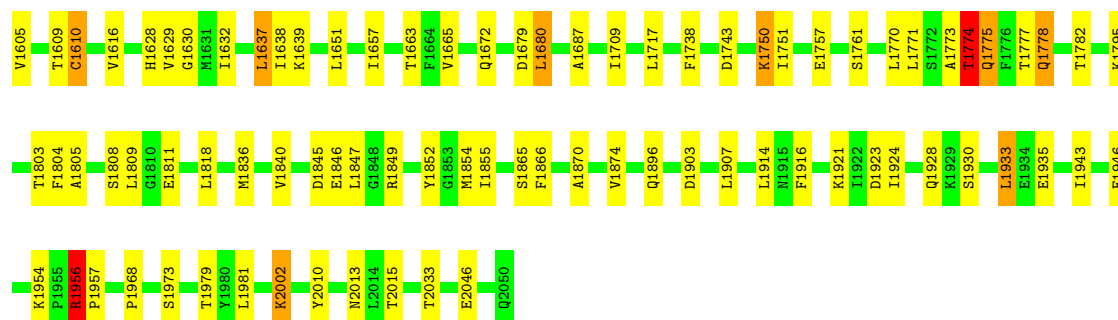




• Molecule 2: Fatty acid synthase subunit beta

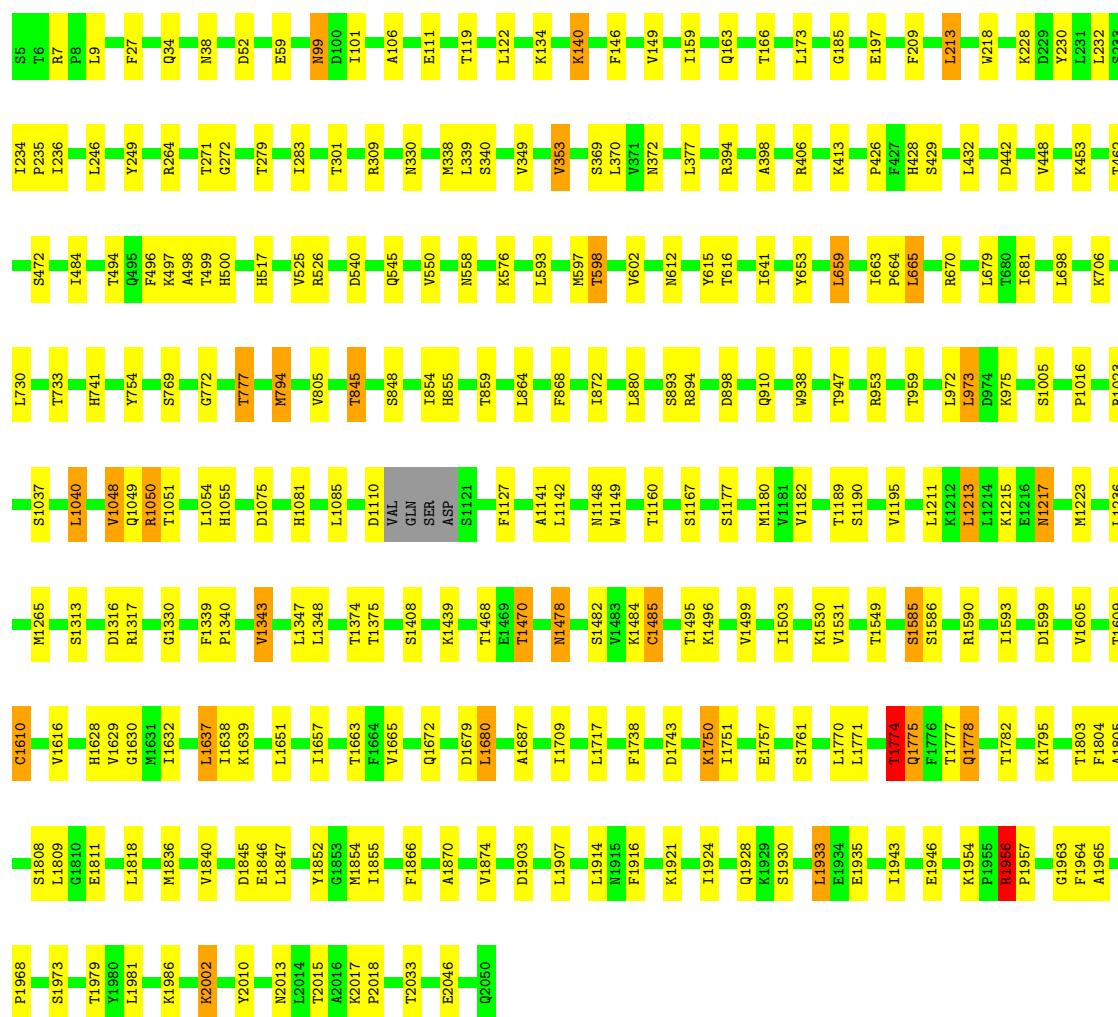
Chain G: 86% 12%

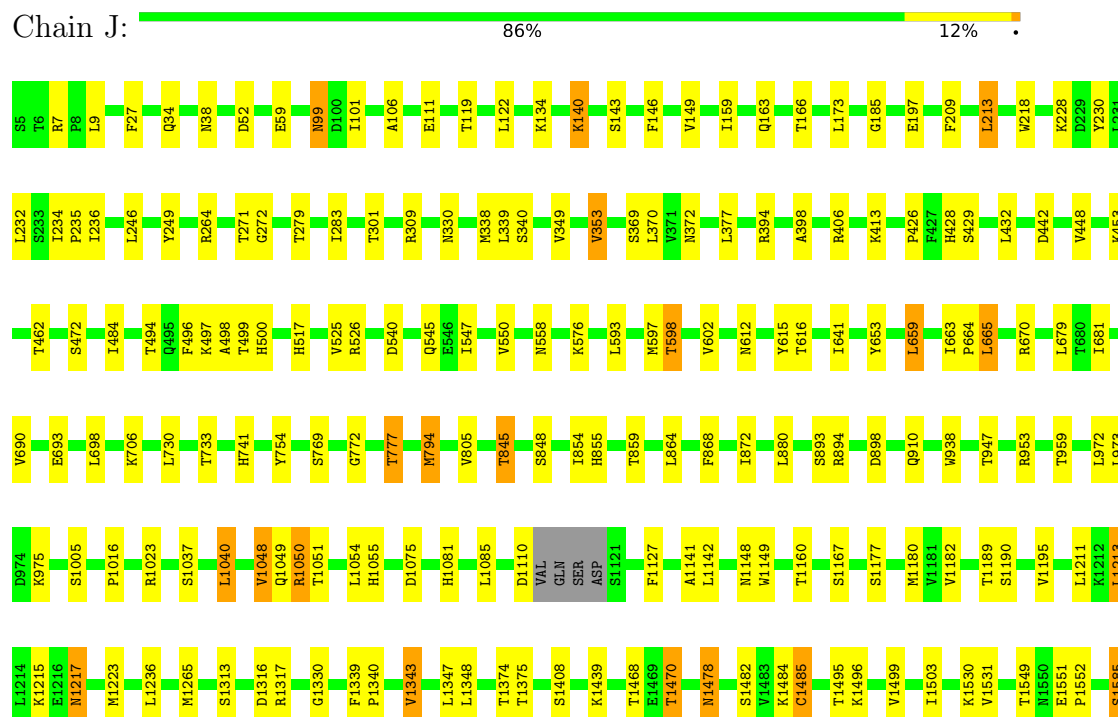


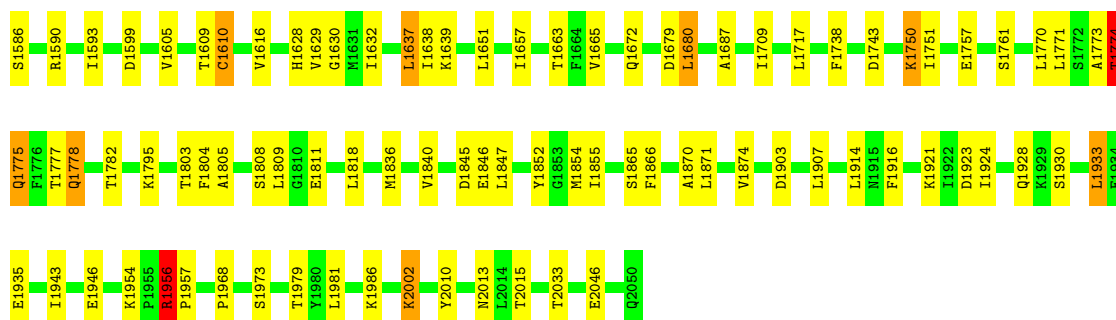


• Molecule 2: Fatty acid synthase subunit beta

Chain H: 86% 12% .

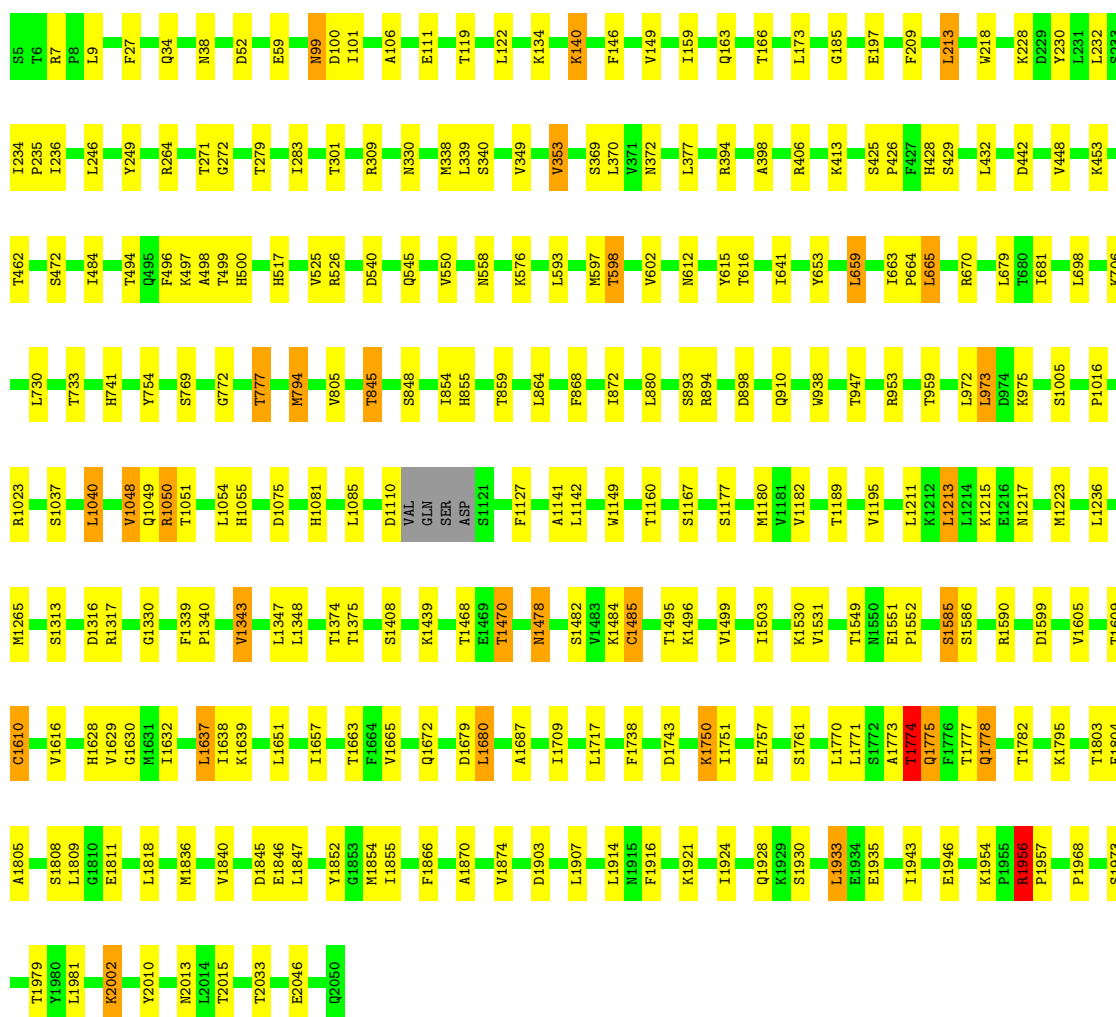






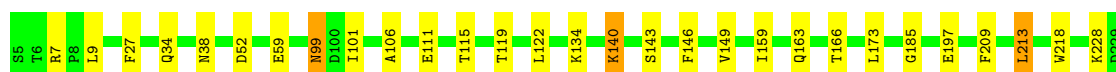
• Molecule 2: Fatty acid synthase subunit beta

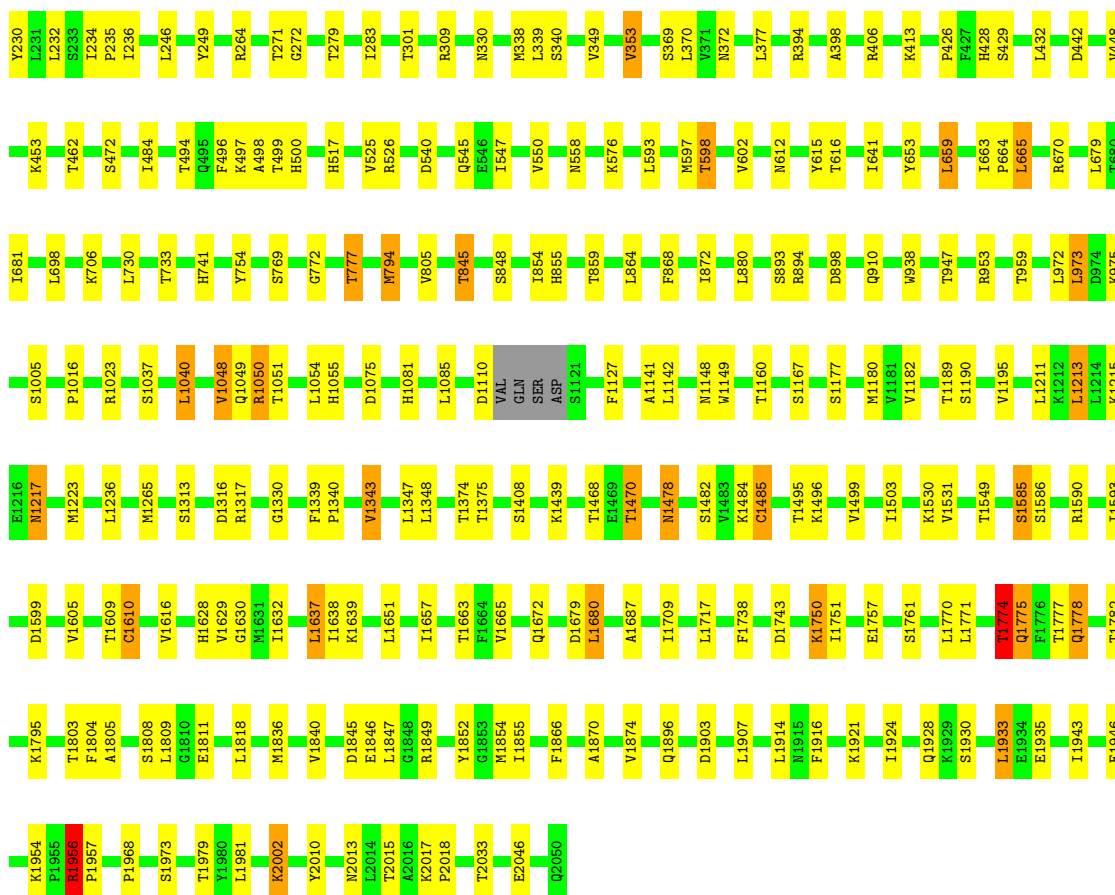
Chain K: 86% 12% .



• Molecule 2: Fatty acid synthase subunit beta

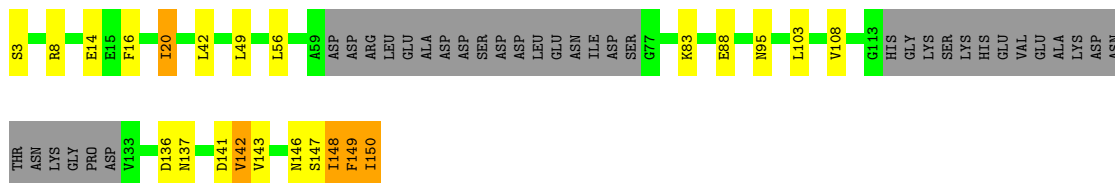
Chain L: 86% 12% .





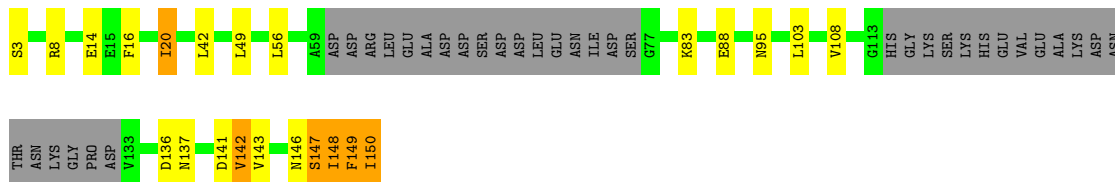
• Molecule 3: Translation machinery-associated protein 17

Chain M: 60% 12% 24%



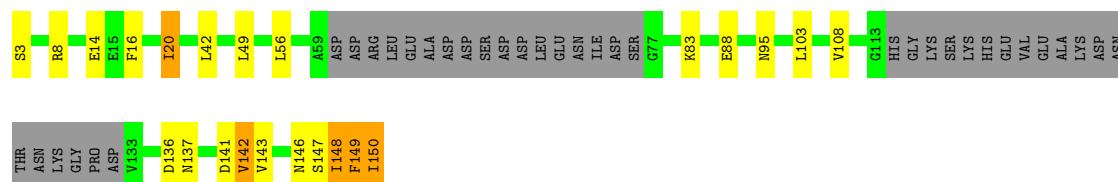
• Molecule 3: Translation machinery-associated protein 17

Chain N: 60% 11% 24%

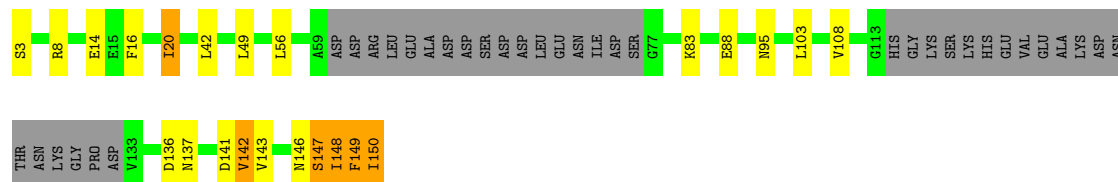


• Molecule 3: Translation machinery-associated protein 17

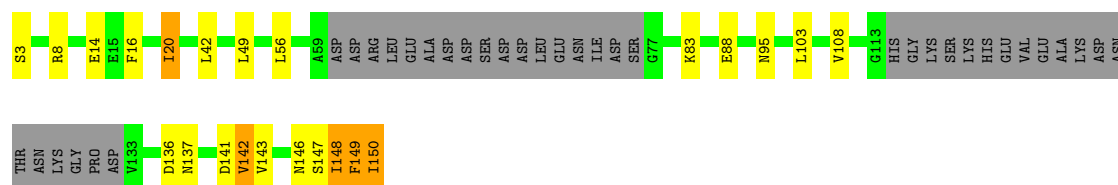
Chain O: 60% 12% 24%



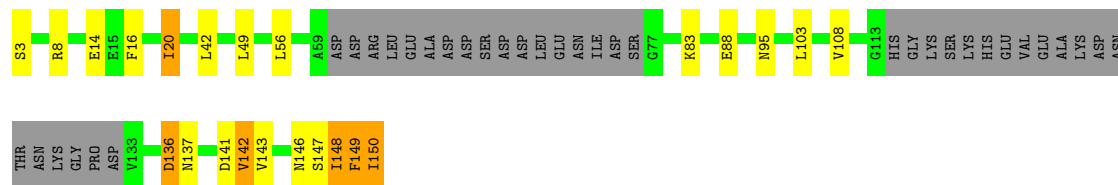
• Molecule 3: Translation machinery-associated protein 17



• Molecule 3: Translation machinery-associated protein 17



• Molecule 3: Translation machinery-associated protein 17





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	110597	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	132000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.75	0/13878	0.93	4/18755 (0.0%)
1	B	0.75	0/13878	0.93	4/18755 (0.0%)
1	C	0.75	0/13878	0.93	4/18755 (0.0%)
1	D	0.75	0/13878	0.93	4/18755 (0.0%)
1	E	0.75	0/13878	0.93	4/18755 (0.0%)
1	F	0.75	0/13878	0.93	4/18755 (0.0%)
2	G	0.67	0/16383	0.86	1/22229 (0.0%)
2	H	0.67	0/16383	0.86	1/22229 (0.0%)
2	I	0.67	0/16383	0.87	1/22229 (0.0%)
2	J	0.67	0/16383	0.86	1/22229 (0.0%)
2	K	0.67	0/16383	0.86	1/22229 (0.0%)
2	L	0.67	0/16383	0.86	1/22229 (0.0%)
3	M	0.76	0/885	0.91	0/1189
3	N	0.76	0/885	0.91	0/1189
3	O	0.76	0/885	0.91	0/1189
3	P	0.76	0/885	0.91	0/1189
3	Q	0.76	0/885	0.91	0/1189
3	R	0.76	0/885	0.91	0/1189
All	All	0.71	0/186876	0.90	30/253038 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
2	G	0	6
2	H	0	6
2	I	0	6
2	J	0	6
2	K	0	6
2	L	0	6
All	All	0	42

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1264	ARG	CG-CD-NE	-6.20	98.78	111.80
1	E	1264	ARG	CG-CD-NE	-6.20	98.79	111.80
1	D	1264	ARG	CG-CD-NE	-6.20	98.79	111.80
1	F	1264	ARG	CG-CD-NE	-6.19	98.79	111.80
1	C	1264	ARG	CG-CD-NE	-6.18	98.81	111.80
1	B	1264	ARG	CG-CD-NE	-6.16	98.86	111.80
2	K	1956	ARG	NE-CZ-NH2	-5.71	117.45	120.30
2	I	1956	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	1680	ARG	CG-CD-NE	-5.64	99.95	111.80
1	D	1680	ARG	CG-CD-NE	-5.64	99.96	111.80
1	C	1680	ARG	CG-CD-NE	-5.62	100.00	111.80
1	E	1680	ARG	CG-CD-NE	-5.61	100.03	111.80
1	F	1680	ARG	CG-CD-NE	-5.59	100.06	111.80
2	J	1956	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	1680	ARG	CG-CD-NE	-5.55	100.15	111.80
2	G	1956	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	L	1956	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	1017	ARG	CB-CA-C	5.50	121.41	110.40
1	F	1017	ARG	CB-CA-C	5.49	121.37	110.40
1	A	1017	ARG	CB-CA-C	5.48	121.36	110.40
1	C	1017	ARG	CB-CA-C	5.48	121.36	110.40
1	E	1017	ARG	CB-CA-C	5.48	121.36	110.40
2	H	1956	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	D	1017	ARG	CB-CA-C	5.46	121.32	110.40
1	E	1183	ARG	CG-CD-NE	5.08	122.48	111.80
1	B	1183	ARG	CG-CD-NE	5.07	122.45	111.80
1	C	1183	ARG	CG-CD-NE	5.07	122.44	111.80
1	A	1183	ARG	CG-CD-NE	5.06	122.43	111.80
1	D	1183	ARG	CG-CD-NE	5.04	122.39	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1183	ARG	CG-CD-NE	5.04	122.38	111.80

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	MET	Peptide
1	B	237	MET	Peptide
1	C	237	MET	Peptide
1	D	237	MET	Peptide
1	E	237	MET	Peptide
1	F	237	MET	Peptide
2	G	1050	ARG	Peptide
2	G	1223	MET	Peptide
2	G	1605	VAL	Peptide
2	G	1750	LYS	Peptide
2	G	2046	GLU	Peptide
2	G	975	LYS	Peptide
2	H	1050	ARG	Peptide
2	H	1223	MET	Peptide
2	H	1605	VAL	Peptide
2	H	1750	LYS	Peptide
2	H	2046	GLU	Peptide
2	H	975	LYS	Peptide
2	I	1050	ARG	Peptide
2	I	1223	MET	Peptide
2	I	1605	VAL	Peptide
2	I	1750	LYS	Peptide
2	I	2046	GLU	Peptide
2	I	975	LYS	Peptide
2	J	1050	ARG	Peptide
2	J	1223	MET	Peptide
2	J	1605	VAL	Peptide
2	J	1750	LYS	Peptide
2	J	2046	GLU	Peptide
2	J	975	LYS	Peptide
2	K	1050	ARG	Peptide
2	K	1223	MET	Peptide
2	K	1605	VAL	Peptide
2	K	1750	LYS	Peptide
2	K	2046	GLU	Peptide
2	K	975	LYS	Peptide

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Mol	Chain	Res	Type	Group
2	L	1050	ARG	Peptide
2	L	1223	MET	Peptide
2	L	1605	VAL	Peptide
2	L	1750	LYS	Peptide
2	L	2046	GLU	Peptide
2	L	975	LYS	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13625	0	13615	117	0
1	B	13625	0	13615	123	0
1	C	13625	0	13615	123	0
1	D	13625	0	13615	124	0
1	E	13625	0	13615	117	0
1	F	13625	0	13615	120	0
2	G	16018	0	15993	117	0
2	H	16018	0	15993	113	0
2	I	16018	0	15993	114	0
2	J	16018	0	15993	114	0
2	K	16018	0	15993	112	0
2	L	16018	0	15993	114	0
3	M	879	0	871	19	0
3	N	879	0	871	20	0
3	O	879	0	871	19	0
3	P	879	0	871	19	0
3	Q	879	0	871	18	0
3	R	879	0	871	20	0
4	A	21	0	21	3	0
4	B	21	0	21	4	0
4	C	21	0	21	3	0
4	D	21	0	21	3	0
4	E	21	0	21	3	0
4	F	21	0	21	3	0
5	G	31	0	19	3	0
5	H	31	0	19	3	0
5	I	31	0	19	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	31	0	19	3	0
5	K	31	0	19	3	0
5	L	31	0	19	3	0
All	All	183444	0	183114	1374	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1374) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1811:GLU:OE2	2:L:2010:TYR:OH	1.80	1.00
2:H:1811:GLU:OE2	2:H:2010:TYR:OH	1.80	1.00
2:K:1811:GLU:OE2	2:K:2010:TYR:OH	1.80	0.99
2:G:1811:GLU:OE2	2:G:2010:TYR:OH	1.80	0.99
2:I:1811:GLU:OE2	2:I:2010:TYR:OH	1.80	0.99
2:J:1811:GLU:OE2	2:J:2010:TYR:OH	1.80	0.98
2:H:894:ARG:NH1	2:H:898:ASP:OD2	2.15	0.80
2:L:894:ARG:NH1	2:L:898:ASP:OD2	2.15	0.80
2:I:894:ARG:NH1	2:I:898:ASP:OD2	2.15	0.80
2:J:894:ARG:NH1	2:J:898:ASP:OD2	2.15	0.80
2:G:894:ARG:NH1	2:G:898:ASP:OD2	2.15	0.79
2:K:894:ARG:NH1	2:K:898:ASP:OD2	2.15	0.79
1:C:871:TRP:HA	3:O:146:ASN:ND2	2.04	0.73
1:D:871:TRP:HA	3:P:146:ASN:ND2	2.05	0.72
1:E:871:TRP:HA	3:Q:146:ASN:ND2	2.06	0.71
1:F:871:TRP:HA	3:R:146:ASN:ND2	2.05	0.70
1:C:1552:ASN:O	1:C:1556:THR:HG22	1.91	0.70
1:D:1552:ASN:O	1:D:1556:THR:HG22	1.91	0.70
1:B:1552:ASN:O	1:B:1556:THR:HG22	1.91	0.70
1:F:1552:ASN:O	1:F:1556:THR:HG22	1.91	0.70
1:A:871:TRP:HA	3:M:146:ASN:ND2	2.07	0.70
1:C:872:THR:H	3:O:146:ASN:HD21	1.40	0.69
1:A:1552:ASN:O	1:A:1556:THR:HG22	1.91	0.69
1:B:871:TRP:HA	3:N:146:ASN:ND2	2.07	0.69
1:E:1552:ASN:O	1:E:1556:THR:HG22	1.91	0.69
1:B:793:ARG:HA	1:B:797:THR:HG23	1.76	0.68
1:F:793:ARG:HA	1:F:797:THR:HG23	1.76	0.68
1:A:793:ARG:HA	1:A:797:THR:HG23	1.76	0.68
1:E:793:ARG:HA	1:E:797:THR:HG23	1.76	0.68
1:C:793:ARG:HA	1:C:797:THR:HG23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:793:ARG:HA	1:D:797:THR:HG23	1.76	0.68
2:I:406:ARG:HG2	3:O:88:GLU:HG2	1.76	0.67
2:L:406:ARG:HG2	3:R:88:GLU:HG2	1.76	0.67
2:J:406:ARG:HG2	3:P:88:GLU:HG2	1.77	0.67
2:L:612:ASN:HD21	2:L:641:ILE:HA	1.60	0.67
2:H:612:ASN:HD21	2:H:641:ILE:HA	1.61	0.66
1:C:400:ARG:NH1	1:C:715:THR:HG21	2.11	0.66
1:D:400:ARG:NH1	1:D:715:THR:HG21	2.11	0.66
2:G:612:ASN:HD21	2:G:641:ILE:HA	1.60	0.66
2:K:612:ASN:HD21	2:K:641:ILE:HA	1.60	0.66
1:A:717:TYR:CZ	1:A:721:ILE:HD11	2.31	0.66
1:E:400:ARG:NH1	1:E:715:THR:HG21	2.11	0.66
1:E:717:TYR:CZ	1:E:721:ILE:HD11	2.31	0.66
1:A:400:ARG:NH1	1:A:715:THR:HG21	2.11	0.66
1:E:872:THR:H	3:Q:146:ASN:HD21	1.42	0.66
1:F:872:THR:H	3:R:146:ASN:HD21	1.41	0.66
1:B:400:ARG:NH1	1:B:715:THR:HG21	2.11	0.66
1:C:717:TYR:CZ	1:C:721:ILE:HD11	2.31	0.65
1:D:717:TYR:CZ	1:D:721:ILE:HD11	2.31	0.65
1:F:400:ARG:NH1	1:F:715:THR:HG21	2.11	0.65
2:J:612:ASN:HD21	2:J:641:ILE:HA	1.60	0.65
1:B:717:TYR:CZ	1:B:721:ILE:HD11	2.31	0.65
2:G:1924:ILE:O	2:G:1928:GLN:HB2	1.97	0.65
2:H:406:ARG:HG2	3:N:88:GLU:HG2	1.76	0.65
1:F:717:TYR:CZ	1:F:721:ILE:HD11	2.31	0.65
2:K:1924:ILE:O	2:K:1928:GLN:HB2	1.97	0.65
2:G:406:ARG:HG2	3:M:88:GLU:HG2	1.77	0.65
2:I:1924:ILE:O	2:I:1928:GLN:HB2	1.97	0.65
2:I:612:ASN:HD21	2:I:641:ILE:HA	1.60	0.65
2:J:1924:ILE:O	2:J:1928:GLN:HB2	1.97	0.65
2:K:406:ARG:HG2	3:Q:88:GLU:HG2	1.78	0.65
2:G:848:SER:HB3	2:G:854:ILE:HD11	1.79	0.65
1:D:872:THR:H	3:P:146:ASN:HD21	1.45	0.65
2:K:848:SER:HB3	2:K:854:ILE:HD11	1.79	0.64
1:B:1491:ARG:NH1	1:B:1744:TYR:O	2.31	0.64
2:L:848:SER:HB3	2:L:854:ILE:HD11	1.79	0.64
1:C:1491:ARG:NH1	1:C:1744:TYR:O	2.31	0.64
1:D:1491:ARG:NH1	1:D:1744:TYR:O	2.31	0.64
1:F:1491:ARG:NH1	1:F:1744:TYR:O	2.31	0.64
2:H:848:SER:HB3	2:H:854:ILE:HD11	1.79	0.64
2:J:848:SER:HB3	2:J:854:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:848:SER:HB3	2:I:854:ILE:HD11	1.79	0.64
1:B:872:THR:H	3:N:146:ASN:HD21	1.44	0.64
4:D:1901:PNS:H382	2:L:372:ASN:HD21	1.63	0.64
1:E:1491:ARG:NH1	1:E:1744:TYR:O	2.30	0.64
1:F:1448:ARG:HD2	1:F:1508:TRP:O	1.98	0.63
2:L:1924:ILE:O	2:L:1928:GLN:HB2	1.97	0.63
1:A:1448:ARG:HD2	1:A:1508:TRP:O	1.98	0.63
1:B:1448:ARG:HD2	1:B:1508:TRP:O	1.98	0.63
2:H:1924:ILE:O	2:H:1928:GLN:HB2	1.97	0.63
1:A:1491:ARG:NH1	1:A:1744:TYR:O	2.31	0.63
1:D:1448:ARG:HD2	1:D:1508:TRP:O	1.98	0.63
1:C:1448:ARG:HD2	1:C:1508:TRP:O	1.98	0.63
1:E:1448:ARG:HD2	1:E:1508:TRP:O	1.98	0.63
1:A:872:THR:H	3:M:146:ASN:HD21	1.45	0.62
4:C:1901:PNS:H421	2:H:163:GLN:O	1.99	0.62
1:B:1125:VAL:HG11	1:B:1175:ILE:HD12	1.81	0.62
1:F:1125:VAL:HG11	1:F:1175:ILE:HD12	1.81	0.62
4:B:1901:PNS:H382	2:G:372:ASN:HD21	1.64	0.62
1:D:1064:ASN:ND2	1:D:1073:THR:OG1	2.33	0.62
1:B:1064:ASN:ND2	1:B:1073:THR:OG1	2.33	0.61
1:C:1064:ASN:ND2	1:C:1073:THR:OG1	2.33	0.61
1:F:1064:ASN:ND2	1:F:1073:THR:OG1	2.33	0.61
4:A:1901:PNS:H382	2:I:372:ASN:HD21	1.65	0.61
1:A:1064:ASN:ND2	1:A:1073:THR:OG1	2.33	0.61
1:E:1064:ASN:ND2	1:E:1073:THR:OG1	2.33	0.61
1:C:1414:ILE:HG12	1:F:1293:SER:HB2	1.83	0.61
1:E:1125:VAL:HG11	1:E:1175:ILE:HD12	1.81	0.61
2:I:1771:LEU:O	2:I:1777:THR:OG1	2.19	0.61
1:B:1017:ARG:HG2	1:B:1510:ASN:HD22	1.66	0.61
2:J:1771:LEU:O	2:J:1777:THR:OG1	2.19	0.61
1:A:1125:VAL:HG11	1:A:1175:ILE:HD12	1.81	0.61
4:A:1901:PNS:O23	4:A:1901:PNS:H312	2.00	0.61
1:C:1125:VAL:HG11	1:C:1175:ILE:HD12	1.81	0.61
1:F:1017:ARG:HG2	1:F:1510:ASN:HD22	1.66	0.61
1:D:1125:VAL:HG11	1:D:1175:ILE:HD12	1.81	0.61
1:F:237:MET:HB2	1:F:277:LEU:HD12	1.82	0.61
2:L:1632:ILE:HG22	2:L:1637:LEU:HD23	1.83	0.61
4:B:1901:PNS:O23	4:B:1901:PNS:H312	2.01	0.60
1:B:237:MET:HB2	1:B:277:LEU:HD12	1.82	0.60
4:F:1901:PNS:H312	4:F:1901:PNS:O26	2.00	0.60
4:D:1901:PNS:O26	4:D:1901:PNS:H312	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1632:ILE:HG22	2:H:1637:LEU:HD23	1.83	0.60
2:G:1771:LEU:O	2:G:1777:THR:OG1	2.19	0.60
2:K:1771:LEU:O	2:K:1777:THR:OG1	2.19	0.60
1:A:1017:ARG:HG2	1:A:1510:ASN:HD22	1.66	0.60
1:C:1017:ARG:HG2	1:C:1510:ASN:HD22	1.66	0.60
1:D:1017:ARG:HG2	1:D:1510:ASN:HD22	1.66	0.60
2:K:101:ILE:HD11	2:K:122:LEU:CD2	2.32	0.60
4:E:1901:PNS:O26	4:E:1901:PNS:H312	2.00	0.60
4:A:1901:PNS:H421	2:I:163:GLN:O	2.01	0.60
4:C:1901:PNS:H312	4:C:1901:PNS:O23	2.00	0.60
1:C:237:MET:HB2	1:C:277:LEU:HD12	1.82	0.60
1:E:1017:ARG:HG2	1:E:1510:ASN:HD22	1.66	0.60
1:B:1293:SER:HB2	1:D:1414:ILE:HG12	1.84	0.60
1:C:1208:VAL:HG13	1:C:1212:THR:HB	1.84	0.60
1:A:1293:SER:HB2	1:E:1414:ILE:HG12	1.83	0.60
1:D:1208:VAL:HG13	1:D:1212:THR:HB	1.84	0.60
2:G:101:ILE:HD11	2:G:122:LEU:CD2	2.32	0.60
2:H:1771:LEU:O	2:H:1777:THR:OG1	2.19	0.59
2:I:1632:ILE:HG22	2:I:1637:LEU:HD23	1.83	0.59
2:J:1632:ILE:HG22	2:J:1637:LEU:HD23	1.83	0.59
1:A:1208:VAL:HG13	1:A:1212:THR:HB	1.84	0.59
1:E:1208:VAL:HG13	1:E:1212:THR:HB	1.84	0.59
4:F:1901:PNS:H382	2:K:372:ASN:HD21	1.67	0.59
2:L:1771:LEU:O	2:L:1777:THR:OG1	2.19	0.59
2:K:1632:ILE:HG22	2:K:1637:LEU:HD23	1.83	0.59
1:B:1039:MET:O	1:B:1609:ARG:NH2	2.36	0.59
1:F:1039:MET:O	1:F:1609:ARG:NH2	2.36	0.59
2:G:1632:ILE:HG22	2:G:1637:LEU:HD23	1.83	0.59
2:L:101:ILE:HD11	2:L:122:LEU:CD2	2.32	0.59
1:A:237:MET:HB2	1:A:277:LEU:HD12	1.82	0.59
1:D:237:MET:HB2	1:D:277:LEU:HD12	1.82	0.59
1:F:1208:VAL:HG13	1:F:1212:THR:HB	1.84	0.59
2:I:101:ILE:HD11	2:I:122:LEU:CD2	2.32	0.59
1:B:1208:VAL:HG13	1:B:1212:THR:HB	1.84	0.59
2:H:101:ILE:HD11	2:H:122:LEU:CD2	2.32	0.59
1:C:1293:SER:HB2	1:F:1414:ILE:HG12	1.83	0.59
1:C:1234:MET:HE3	1:C:1326:ILE:HG21	1.84	0.59
1:C:1039:MET:O	1:C:1609:ARG:NH2	2.35	0.59
1:D:1234:MET:HE3	1:D:1326:ILE:HG21	1.84	0.59
4:E:1901:PNS:H421	2:J:163:GLN:O	2.02	0.59
4:D:1901:PNS:H421	2:L:163:GLN:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:MET:O	1:A:1609:ARG:NH2	2.36	0.59
1:B:1276:GLN:O	1:B:1282:THR:HG21	2.03	0.59
1:D:1039:MET:O	1:D:1609:ARG:NH2	2.36	0.59
1:E:237:MET:HB2	1:E:277:LEU:HD12	1.82	0.59
1:F:1276:GLN:O	1:F:1282:THR:HG21	2.03	0.59
2:J:101:ILE:HD11	2:J:122:LEU:CD2	2.32	0.59
4:E:1901:PNS:H382	2:J:372:ASN:HD21	1.68	0.59
1:A:1234:MET:HE3	1:A:1326:ILE:HG21	1.84	0.59
1:B:1414:ILE:HG12	1:D:1293:SER:HB2	1.84	0.59
4:F:1901:PNS:H421	2:K:163:GLN:O	2.02	0.59
1:D:1276:GLN:O	1:D:1282:THR:HG21	2.03	0.58
1:E:1039:MET:O	1:E:1609:ARG:NH2	2.36	0.58
1:C:1276:GLN:O	1:C:1282:THR:HG21	2.03	0.58
1:A:1276:GLN:O	1:A:1282:THR:HG21	2.03	0.58
1:A:1414:ILE:HG12	1:E:1293:SER:HB2	1.84	0.58
1:E:1276:GLN:O	1:E:1282:THR:HG21	2.03	0.58
1:B:1234:MET:HE3	1:B:1326:ILE:HG21	1.86	0.58
3:M:16:PHE:CE2	3:M:20:ILE:HD12	2.40	0.57
1:F:1238:VAL:HG22	1:F:1325:ARG:HD3	1.86	0.57
2:K:1775:GLN:HG2	2:K:1836:MET:HE2	1.87	0.57
3:Q:16:PHE:CE2	3:Q:20:ILE:HD12	2.40	0.57
1:E:1234:MET:HE3	1:E:1326:ILE:HG21	1.85	0.57
3:P:16:PHE:CE2	3:P:20:ILE:HD12	2.40	0.57
1:B:1238:VAL:HG22	1:B:1325:ARG:HD3	1.87	0.57
4:B:1901:PNS:H421	2:G:163:GLN:O	2.03	0.57
2:L:1680:LEU:HD13	2:L:1687:ALA:HB2	1.86	0.57
1:A:833:PHE:CZ	3:M:150:ILE:HG13	2.40	0.57
2:H:1680:LEU:HD13	2:H:1687:ALA:HB2	1.86	0.57
3:O:16:PHE:CE2	3:O:20:ILE:HD12	2.40	0.57
2:G:1680:LEU:HD13	2:G:1687:ALA:HB2	1.86	0.56
3:N:16:PHE:CE2	3:N:20:ILE:HD12	2.40	0.56
3:R:16:PHE:CE2	3:R:20:ILE:HD12	2.40	0.56
1:D:833:PHE:CZ	3:P:150:ILE:HG13	2.40	0.56
4:C:1901:PNS:H382	2:H:372:ASN:HD21	1.69	0.56
2:K:1680:LEU:HD13	2:K:1687:ALA:HB2	1.86	0.56
1:B:221:LEU:O	1:B:225:SER:OG	2.23	0.56
2:H:218:TRP:HH2	2:H:236:ILE:HD11	1.71	0.56
2:L:845:THR:HG22	2:L:855:HIS:CD2	2.40	0.56
1:F:221:LEU:O	1:F:225:SER:OG	2.22	0.56
2:I:1680:LEU:HD13	2:I:1687:ALA:HB2	1.86	0.56
2:G:615:TYR:OH	2:G:1075:ASP:OD1	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:845:THR:HG22	2:H:855:HIS:CD2	2.41	0.56
2:J:845:THR:HG22	2:J:855:HIS:CD2	2.41	0.56
2:G:845:THR:HG22	2:G:855:HIS:CD2	2.40	0.56
2:I:845:THR:HG22	2:I:855:HIS:CD2	2.41	0.56
2:J:1680:LEU:HD13	2:J:1687:ALA:HB2	1.86	0.56
2:L:1343:VAL:O	2:L:1343:VAL:HG22	2.06	0.56
1:A:1238:VAL:HG22	1:A:1325:ARG:HD3	1.87	0.56
2:K:845:THR:HG22	2:K:855:HIS:CD2	2.41	0.56
2:G:1775:GLN:HG2	2:G:1836:MET:HE2	1.88	0.56
2:H:1343:VAL:HG22	2:H:1343:VAL:O	2.06	0.56
2:I:1343:VAL:O	2:I:1343:VAL:HG22	2.06	0.56
2:I:1775:GLN:HG2	2:I:1836:MET:CE	2.36	0.56
2:H:1610:CYS:SG	2:H:1651:LEU:HD22	2.46	0.56
2:J:1775:GLN:HG2	2:J:1836:MET:CE	2.36	0.56
1:E:1238:VAL:HG22	1:E:1325:ARG:HD3	1.87	0.55
2:I:1610:CYS:SG	2:I:1651:LEU:HD22	2.46	0.55
2:J:1343:VAL:O	2:J:1343:VAL:HG22	2.06	0.55
2:J:1610:CYS:SG	2:J:1651:LEU:HD22	2.46	0.55
2:K:1343:VAL:O	2:K:1343:VAL:HG22	2.06	0.55
1:A:768:ILE:HD11	1:A:806:VAL:HG11	1.88	0.55
1:E:768:ILE:HD11	1:E:806:VAL:HG11	1.88	0.55
2:G:1775:GLN:HG2	2:G:1836:MET:CE	2.36	0.55
2:H:1866:PHE:CE1	2:H:1870:ALA:HB1	2.42	0.55
2:L:1610:CYS:SG	2:L:1651:LEU:HD22	2.46	0.55
1:B:833:PHE:CZ	3:N:150:ILE:HG13	2.42	0.55
1:C:940:THR:HG21	3:O:150:ILE:C	2.26	0.55
2:G:1343:VAL:HG22	2:G:1343:VAL:O	2.06	0.55
2:K:218:TRP:HH2	2:K:236:ILE:HD11	1.71	0.55
1:F:768:ILE:HD11	1:F:806:VAL:HG11	1.88	0.55
2:K:1775:GLN:HG2	2:K:1836:MET:CE	2.36	0.55
2:L:1866:PHE:CE1	2:L:1870:ALA:HB1	2.42	0.55
1:E:833:PHE:CZ	3:Q:150:ILE:HG13	2.42	0.55
1:C:1238:VAL:HG22	1:C:1325:ARG:HD3	1.87	0.55
1:D:877:LEU:HD12	1:D:883:ILE:CG2	2.37	0.55
2:H:597:MET:HA	5:H:2101:FMN:N5	2.22	0.55
2:H:106:ALA:HB2	2:H:545:GLN:HG2	1.89	0.55
2:L:1775:GLN:HG2	2:L:1836:MET:CE	2.36	0.55
2:L:218:TRP:HH2	2:L:236:ILE:HD11	1.72	0.55
1:B:768:ILE:HD11	1:B:806:VAL:HG11	1.88	0.55
1:D:1238:VAL:HG22	1:D:1325:ARG:HD3	1.87	0.55
2:H:1775:GLN:HG2	2:H:1836:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:877:LEU:HD12	1:C:883:ILE:CG2	2.37	0.55
2:J:615:TYR:OH	2:J:1075:ASP:OD1	2.17	0.55
1:D:768:ILE:HD11	1:D:806:VAL:HG11	1.88	0.54
2:I:1709:ILE:HD11	2:I:1717:LEU:HD22	1.89	0.54
2:J:1709:ILE:HD11	2:J:1717:LEU:HD22	1.89	0.54
2:L:1808:SER:H	2:L:2013:ASN:HD21	1.54	0.54
2:G:1709:ILE:HD11	2:G:1717:LEU:HD22	1.89	0.54
2:G:1866:PHE:CE1	2:G:1870:ALA:HB1	2.42	0.54
2:I:106:ALA:HB2	2:I:545:GLN:HG2	1.88	0.54
2:K:1866:PHE:CE1	2:K:1870:ALA:HB1	2.42	0.54
1:C:768:ILE:HD11	1:C:806:VAL:HG11	1.88	0.54
1:D:940:THR:HG21	3:P:150:ILE:C	2.27	0.54
2:G:1610:CYS:SG	2:G:1651:LEU:HD22	2.46	0.54
2:I:615:TYR:OH	2:I:1075:ASP:OD1	2.17	0.54
2:K:1610:CYS:SG	2:K:1651:LEU:HD22	2.46	0.54
2:K:1709:ILE:HD11	2:K:1717:LEU:HD22	1.89	0.54
2:K:106:ALA:HB2	2:K:545:GLN:HG2	1.89	0.54
3:N:137:ASN:HB3	3:N:141:ASP:HA	1.89	0.54
2:H:1808:SER:H	2:H:2013:ASN:HD21	1.54	0.54
1:F:833:PHE:CZ	3:R:150:ILE:HG13	2.42	0.54
1:B:1153:ASP:OD2	1:C:359:ARG:NH1	2.41	0.54
1:F:1234:MET:HE3	1:F:1326:ILE:HG21	1.89	0.54
1:F:877:LEU:HD12	1:F:883:ILE:CG2	2.37	0.54
1:F:940:THR:HG21	3:R:150:ILE:C	2.28	0.54
2:L:106:ALA:HB2	2:L:545:GLN:HG2	1.89	0.54
1:A:221:LEU:O	1:A:225:SER:OG	2.23	0.54
1:B:877:LEU:HD12	1:B:883:ILE:CG2	2.37	0.54
2:J:1866:PHE:CE1	2:J:1870:ALA:HB1	2.42	0.54
3:R:137:ASN:HB3	3:R:141:ASP:HA	1.90	0.54
1:B:940:THR:HG21	3:N:150:ILE:C	2.28	0.54
1:A:359:ARG:NH1	1:C:1153:ASP:OD2	2.40	0.54
2:G:1808:SER:H	2:G:2013:ASN:HD21	1.53	0.54
2:J:1808:SER:H	2:J:2013:ASN:HD21	1.54	0.54
3:P:137:ASN:HB3	3:P:141:ASP:HA	1.89	0.54
2:I:1866:PHE:CE1	2:I:1870:ALA:HB1	2.42	0.54
3:M:137:ASN:HB3	3:M:141:ASP:HA	1.89	0.54
1:D:221:LEU:O	1:D:225:SER:OG	2.22	0.54
1:E:221:LEU:O	1:E:225:SER:OG	2.22	0.54
1:D:359:ARG:NH1	1:F:1153:ASP:OD2	2.41	0.54
2:H:432:LEU:HB3	2:H:484:ILE:HG23	1.89	0.54
2:J:432:LEU:HB3	2:J:484:ILE:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1709:ILE:HD11	2:L:1717:LEU:HD22	1.89	0.54
2:G:1177:SER:O	2:G:1180:MET:HG2	2.08	0.54
2:J:106:ALA:HB2	2:J:545:GLN:HG2	1.89	0.54
2:K:1177:SER:O	2:K:1180:MET:HG2	2.08	0.54
3:O:137:ASN:HB3	3:O:141:ASP:HA	1.90	0.54
1:C:833:PHE:CZ	3:O:150:ILE:HG13	2.42	0.54
2:I:1177:SER:O	2:I:1180:MET:HG2	2.08	0.53
2:I:218:TRP:HH2	2:I:236:ILE:HD11	1.71	0.53
1:A:877:LEU:HD12	1:A:883:ILE:CG2	2.37	0.53
2:H:1709:ILE:HD11	2:H:1717:LEU:HD22	1.90	0.53
2:K:498:ALA:O	2:K:525:VAL:HG22	2.09	0.53
3:Q:137:ASN:HB3	3:Q:141:ASP:HA	1.89	0.53
1:C:221:LEU:O	1:C:225:SER:OG	2.23	0.53
2:G:218:TRP:HH2	2:G:236:ILE:HD11	1.73	0.53
2:J:1177:SER:O	2:J:1180:MET:HG2	2.08	0.53
2:K:1808:SER:H	2:K:2013:ASN:HD21	1.54	0.53
1:D:1153:ASP:OD2	1:E:359:ARG:NH1	2.41	0.53
2:J:597:MET:HA	5:J:2101:FMN:N5	2.24	0.53
2:L:526:ARG:HH11	2:L:558:ASN:HD21	1.56	0.53
1:A:940:THR:HG21	3:M:150:ILE:C	2.29	0.53
1:E:940:THR:HG21	3:Q:150:ILE:C	2.29	0.53
2:H:526:ARG:HH11	2:H:558:ASN:HD21	1.57	0.53
2:I:1808:SER:H	2:I:2013:ASN:HD21	1.54	0.53
2:J:218:TRP:HH2	2:J:236:ILE:HD11	1.71	0.53
2:L:432:LEU:HB3	2:L:484:ILE:HG23	1.91	0.53
2:L:597:MET:HA	5:L:2101:FMN:N5	2.24	0.53
3:N:20:ILE:HD11	3:N:103:LEU:CD2	2.39	0.53
1:E:877:LEU:HD12	1:E:883:ILE:CG2	2.37	0.53
2:G:498:ALA:O	2:G:525:VAL:HG22	2.09	0.53
2:G:106:ALA:HB2	2:G:545:GLN:HG2	1.90	0.53
2:K:597:MET:HA	5:K:2101:FMN:N5	2.22	0.53
2:H:1177:SER:O	2:H:1180:MET:HG2	2.08	0.53
2:I:597:MET:HA	5:I:2101:FMN:N5	2.24	0.53
2:K:526:ARG:HH11	2:K:558:ASN:HD21	1.56	0.53
3:R:20:ILE:HD11	3:R:103:LEU:CD2	2.39	0.53
1:E:1153:ASP:OD2	1:F:359:ARG:NH1	2.41	0.53
2:I:143:SER:OG	2:I:547:ILE:O	2.23	0.53
2:J:146:PHE:HA	2:J:149:VAL:HG12	1.91	0.53
2:I:146:PHE:HA	2:I:149:VAL:HG12	1.91	0.52
2:I:432:LEU:HB3	2:I:484:ILE:HG23	1.91	0.52
2:L:1177:SER:O	2:L:1180:MET:HG2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD21	1:A:176:VAL:CG1	2.39	0.52
1:B:381:GLU:HG3	1:E:390:VAL:HG13	1.92	0.52
2:L:1774:THR:O	2:L:1778:GLN:HB2	2.09	0.52
3:P:20:ILE:HD11	3:P:103:LEU:CD2	2.39	0.52
2:G:526:ARG:HH11	2:G:558:ASN:HD21	1.57	0.52
1:A:1153:ASP:OD2	1:B:359:ARG:NH1	2.42	0.52
2:G:146:PHE:HA	2:G:149:VAL:HG12	1.91	0.52
2:H:1774:THR:O	2:H:1778:GLN:HB2	2.09	0.52
2:K:1774:THR:O	2:K:1778:GLN:HB2	2.09	0.52
1:D:871:TRP:CZ3	1:D:888:ILE:HD13	2.45	0.52
2:I:498:ALA:O	2:I:525:VAL:HG22	2.09	0.52
2:G:1774:THR:O	2:G:1778:GLN:HB2	2.09	0.52
2:H:498:ALA:O	2:H:525:VAL:HG22	2.09	0.52
2:I:1054:LEU:HB2	5:I:2101:FMN:HM72	1.90	0.52
2:I:526:ARG:HH11	2:I:558:ASN:HD21	1.56	0.52
2:K:146:PHE:HA	2:K:149:VAL:HG12	1.91	0.52
2:L:146:PHE:HA	2:L:149:VAL:HG12	1.91	0.52
1:C:871:TRP:CZ3	1:C:888:ILE:HD13	2.45	0.52
2:H:146:PHE:HA	2:H:149:VAL:HG12	1.91	0.52
2:J:1774:THR:O	2:J:1778:GLN:HB2	2.09	0.52
2:J:498:ALA:O	2:J:525:VAL:HG22	2.09	0.52
3:M:20:ILE:HD11	3:M:103:LEU:CD2	2.39	0.52
1:A:390:VAL:HG13	1:F:381:GLU:HG3	1.92	0.52
2:G:1956:ARG:O	2:G:1956:ARG:NE	2.43	0.52
2:G:432:LEU:HB3	2:G:484:ILE:HG23	1.90	0.52
2:H:309:ARG:NH1	2:H:442:ASP:OD2	2.43	0.52
2:L:309:ARG:NH1	2:L:442:ASP:OD2	2.43	0.52
3:O:20:ILE:HD11	3:O:103:LEU:CD2	2.39	0.52
1:D:159:LEU:HD21	1:D:176:VAL:CG1	2.40	0.52
1:E:871:TRP:CZ3	1:E:888:ILE:HD13	2.45	0.52
1:F:1531:LEU:HD21	1:F:1660:TYR:CZ	2.45	0.52
2:J:526:ARG:HH11	2:J:558:ASN:HD21	1.57	0.52
2:K:1956:ARG:NE	2:K:1956:ARG:O	2.43	0.52
2:K:432:LEU:HB3	2:K:484:ILE:HG23	1.90	0.52
2:L:498:ALA:O	2:L:525:VAL:HG22	2.09	0.52
3:Q:20:ILE:HD11	3:Q:103:LEU:CD2	2.39	0.52
1:A:871:TRP:CZ3	1:A:888:ILE:HD13	2.45	0.51
1:B:1531:LEU:HD21	1:B:1660:TYR:CZ	2.45	0.51
2:I:1040:LEU:HD21	2:I:1048:VAL:HG13	1.92	0.51
2:I:898:ASP:O	2:I:1050:ARG:HA	2.11	0.51
2:I:1774:THR:O	2:I:1778:GLN:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:330:ASN:HD22	2:J:394:ARG:CZ	2.24	0.51
1:F:773:ALA:HB3	3:R:142:VAL:HG23	1.92	0.51
1:E:529:MET:HE2	1:E:896:PHE:HE2	1.75	0.51
2:I:330:ASN:HD22	2:I:394:ARG:CZ	2.24	0.51
2:J:898:ASP:O	2:J:1050:ARG:HA	2.11	0.51
1:C:529:MET:HE2	1:C:896:PHE:HE2	1.75	0.51
2:H:1663:THR:HA	2:H:1803:THR:O	2.11	0.51
2:J:1040:LEU:HD21	2:J:1048:VAL:HG13	1.92	0.51
2:K:1040:LEU:HD21	2:K:1048:VAL:HG13	1.92	0.51
2:L:1663:THR:HA	2:L:1803:THR:O	2.11	0.51
1:C:1657:HIS:HD2	1:C:1659:ASP:H	1.58	0.51
1:C:159:LEU:HD21	1:C:176:VAL:CG1	2.40	0.51
1:D:1657:HIS:HD2	1:D:1659:ASP:H	1.58	0.51
2:I:706:LYS:NZ	5:I:2101:FMN:O2'	2.44	0.51
2:L:1339:PHE:N	2:L:1340:PRO:CD	2.74	0.51
1:C:773:ALA:HB3	3:O:142:VAL:HG23	1.92	0.51
1:E:159:LEU:HD21	1:E:176:VAL:CG1	2.40	0.51
2:J:1054:LEU:HB2	5:J:2101:FMN:HM72	1.92	0.51
1:B:1744:TYR:HB2	1:D:1432:HIS:CE1	2.46	0.51
1:B:871:TRP:CZ3	1:B:888:ILE:HD13	2.45	0.51
1:C:1531:LEU:HD21	1:C:1660:TYR:CZ	2.45	0.51
1:D:529:MET:HE2	1:D:896:PHE:HE2	1.76	0.51
1:E:773:ALA:HB3	3:Q:142:VAL:HG23	1.92	0.51
2:H:1339:PHE:N	2:H:1340:PRO:CD	2.74	0.51
2:L:898:ASP:O	2:L:1050:ARG:HA	2.11	0.51
1:A:529:MET:HE2	1:A:896:PHE:HE2	1.75	0.51
1:C:821:GLN:HE22	1:C:914:VAL:HG22	1.75	0.51
2:G:1663:THR:HA	2:G:1803:THR:O	2.11	0.51
2:G:330:ASN:HD22	2:G:394:ARG:CZ	2.23	0.51
2:H:898:ASP:O	2:H:1050:ARG:HA	2.11	0.51
2:K:1663:THR:HA	2:K:1803:THR:O	2.11	0.51
2:K:330:ASN:HD22	2:K:394:ARG:CZ	2.24	0.51
1:A:1531:LEU:HD21	1:A:1660:TYR:CZ	2.45	0.51
1:D:1531:LEU:HD21	1:D:1660:TYR:CZ	2.45	0.51
1:F:159:LEU:HD21	1:F:176:VAL:CG1	2.40	0.51
2:G:1040:LEU:HD21	2:G:1048:VAL:HG13	1.93	0.51
2:G:1054:LEU:HB2	5:G:2101:FMN:HM72	1.92	0.51
2:L:234:ILE:N	2:L:235:PRO:CD	2.74	0.51
1:B:159:LEU:HD21	1:B:176:VAL:CG1	2.41	0.51
1:D:865:CYS:HB2	1:D:917:CYS:SG	2.51	0.51
1:E:1531:LEU:HD21	1:E:1660:TYR:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:865:CYS:HB2	1:F:917:CYS:SG	2.51	0.51
2:G:597:MET:HA	5:G:2101:FMN:N5	2.25	0.51
2:H:1040:LEU:HD21	2:H:1048:VAL:HG13	1.92	0.51
2:J:1956:ARG:NE	2:J:1956:ARG:O	2.43	0.51
2:K:898:ASP:O	2:K:1050:ARG:HA	2.11	0.51
2:L:1040:LEU:HD21	2:L:1048:VAL:HG13	1.92	0.51
1:A:381:GLU:HG3	1:F:390:VAL:HG13	1.92	0.51
1:B:529:MET:HE2	1:B:896:PHE:HE2	1.75	0.51
1:C:865:CYS:HB2	1:C:917:CYS:SG	2.51	0.51
1:D:821:GLN:HE22	1:D:914:VAL:HG22	1.76	0.51
1:F:529:MET:HE2	1:F:896:PHE:HE2	1.75	0.51
1:F:871:TRP:CZ3	1:F:888:ILE:HD13	2.45	0.51
2:G:898:ASP:O	2:G:1050:ARG:HA	2.11	0.51
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.74	0.51
2:H:234:ILE:N	2:H:235:PRO:CD	2.74	0.51
2:I:1956:ARG:NE	2:I:1956:ARG:O	2.43	0.51
1:B:682:GLY:HA2	3:N:136:ASP:HA	1.93	0.50
1:B:865:CYS:HB2	1:B:917:CYS:SG	2.51	0.50
1:F:904:ASN:HB3	1:F:926:LEU:HD13	1.93	0.50
2:K:1339:PHE:N	2:K:1340:PRO:CD	2.74	0.50
1:B:1657:HIS:HD2	1:B:1659:ASP:H	1.58	0.50
1:E:821:GLN:HE22	1:E:914:VAL:HG22	1.75	0.50
1:F:1657:HIS:HD2	1:F:1659:ASP:H	1.58	0.50
1:F:682:GLY:HA2	3:R:136:ASP:HA	1.93	0.50
2:K:1665:VAL:HA	2:K:1805:ALA:O	2.11	0.50
2:L:615:TYR:OH	2:L:1075:ASP:OD1	2.17	0.50
1:B:904:ASN:HB3	1:B:926:LEU:HD13	1.93	0.50
1:C:505:LYS:O	1:C:954:ARG:HG2	2.12	0.50
1:D:1238:VAL:HG13	1:D:1242:GLU:HB2	1.94	0.50
1:D:682:GLY:HA2	3:P:136:ASP:HA	1.94	0.50
1:B:390:VAL:HG13	1:E:381:GLU:HG3	1.93	0.50
1:E:479:ASN:ND2	1:E:613:VAL:O	2.45	0.50
2:I:1751:ILE:HG23	2:I:1840:VAL:HG21	1.93	0.50
2:J:1339:PHE:N	2:J:1340:PRO:CD	2.74	0.50
2:K:517:HIS:CE1	2:K:540:ASP:HB3	2.46	0.50
1:A:821:GLN:HE22	1:A:914:VAL:HG22	1.76	0.50
2:G:1665:VAL:HA	2:G:1805:ALA:O	2.11	0.50
2:H:615:TYR:OH	2:H:1075:ASP:OD1	2.17	0.50
2:I:234:ILE:N	2:I:235:PRO:CD	2.74	0.50
2:J:1663:THR:HA	2:J:1803:THR:O	2.11	0.50
2:J:234:ILE:N	2:J:235:PRO:CD	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:GLY:HA2	3:O:136:ASP:HA	1.93	0.50
1:E:682:GLY:HA2	3:Q:136:ASP:HA	1.93	0.50
1:A:479:ASN:ND2	1:A:613:VAL:O	2.45	0.50
1:C:1238:VAL:HG13	1:C:1242:GLU:HB2	1.94	0.50
1:D:505:LYS:O	1:D:954:ARG:HG2	2.12	0.50
2:I:1339:PHE:N	2:I:1340:PRO:CD	2.74	0.50
2:I:1663:THR:HA	2:I:1803:THR:O	2.11	0.50
2:J:706:LYS:NZ	5:J:2101:FMN:O2'	2.45	0.50
2:K:1054:LEU:HB2	5:K:2101:FMN:HM72	1.93	0.50
2:L:1751:ILE:HG23	2:L:1840:VAL:HG21	1.94	0.50
1:A:682:GLY:HA2	3:M:136:ASP:HA	1.93	0.50
1:B:1238:VAL:HG13	1:B:1242:GLU:HB2	1.94	0.50
1:F:1238:VAL:HG13	1:F:1242:GLU:HB2	1.93	0.50
1:F:505:LYS:O	1:F:954:ARG:HG2	2.12	0.50
2:H:330:ASN:HD22	2:H:394:ARG:CZ	2.24	0.50
2:L:330:ASN:HD22	2:L:394:ARG:CZ	2.24	0.50
2:L:706:LYS:NZ	5:L:2101:FMN:O2'	2.45	0.50
1:C:390:VAL:HG13	1:D:381:GLU:HG3	1.92	0.50
1:C:381:GLU:HG3	1:D:390:VAL:HG13	1.92	0.50
2:G:234:ILE:N	2:G:235:PRO:CD	2.74	0.50
2:I:1665:VAL:HA	2:I:1805:ALA:O	2.11	0.50
2:J:1665:VAL:HA	2:J:1805:ALA:O	2.11	0.50
2:K:1751:ILE:HG23	2:K:1840:VAL:HG21	1.94	0.50
2:K:234:ILE:N	2:K:235:PRO:CD	2.74	0.50
2:K:706:LYS:NZ	5:K:2101:FMN:O2'	2.45	0.50
2:L:1054:LEU:HB2	5:L:2101:FMN:HM72	1.93	0.50
1:E:865:CYS:HB2	1:E:917:CYS:SG	2.51	0.50
2:I:517:HIS:CE1	2:I:540:ASP:HB3	2.46	0.50
2:I:99:ASN:HD21	2:I:550:VAL:H	1.60	0.50
1:B:505:LYS:O	1:B:954:ARG:HG2	2.12	0.50
1:D:1239:HIS:CE1	1:D:1717:ASP:O	2.65	0.50
1:E:1657:HIS:HD2	1:E:1659:ASP:H	1.58	0.50
2:H:706:LYS:NZ	5:H:2101:FMN:O2'	2.45	0.50
2:H:517:HIS:CE1	2:H:540:ASP:HB3	2.47	0.50
2:J:99:ASN:HD21	2:J:550:VAL:H	1.60	0.50
1:A:865:CYS:HB2	1:A:917:CYS:SG	2.51	0.49
1:A:904:ASN:HB3	1:A:926:LEU:HD13	1.93	0.49
1:B:773:ALA:HB3	3:N:142:VAL:HG23	1.94	0.49
1:C:1239:HIS:CE1	1:C:1717:ASP:O	2.65	0.49
1:E:505:LYS:O	1:E:954:ARG:HG2	2.12	0.49
1:A:1657:HIS:HD2	1:A:1659:ASP:H	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LYS:O	1:A:954:ARG:HG2	2.12	0.49
1:B:1280:ILE:HD12	1:D:1280:ILE:HD12	1.94	0.49
1:B:821:GLN:HE22	1:B:914:VAL:HG22	1.76	0.49
1:E:1238:VAL:HG13	1:E:1242:GLU:HB2	1.93	0.49
1:A:1744:TYR:HB2	1:E:1432:HIS:CE1	2.47	0.49
1:E:904:ASN:HB3	1:E:926:LEU:HD13	1.93	0.49
1:C:1280:ILE:HD12	1:F:1280:ILE:HD12	1.94	0.49
2:H:1665:VAL:HA	2:H:1805:ALA:O	2.11	0.49
2:K:1638:ILE:HG13	2:K:1657:ILE:HD12	1.94	0.49
2:K:309:ARG:NH1	2:K:442:ASP:OD2	2.43	0.49
2:L:1665:VAL:HA	2:L:1805:ALA:O	2.11	0.49
1:C:479:ASN:ND2	1:C:613:VAL:O	2.45	0.49
1:D:479:ASN:ND2	1:D:613:VAL:O	2.45	0.49
1:F:821:GLN:HE22	1:F:914:VAL:HG22	1.76	0.49
2:G:1638:ILE:HG13	2:G:1657:ILE:HD12	1.94	0.49
2:H:1470:THR:HA	2:H:1484:LYS:O	2.12	0.49
2:L:517:HIS:CE1	2:L:540:ASP:HB3	2.47	0.49
1:A:1238:VAL:HG13	1:A:1242:GLU:HB2	1.93	0.49
1:B:375:LEU:HD21	1:E:374:GLN:OE1	2.13	0.49
1:E:1239:HIS:CE1	1:E:1717:ASP:O	2.65	0.49
1:A:1432:HIS:CE1	1:E:1744:TYR:HB2	2.47	0.49
1:A:375:LEU:HD21	1:F:374:GLN:OE1	2.12	0.49
1:A:378:LEU:HD23	1:F:378:LEU:HD23	1.95	0.49
1:F:479:ASN:ND2	1:F:613:VAL:O	2.45	0.49
1:F:704:VAL:HG23	1:F:763:TRP:CZ3	2.48	0.49
2:G:1751:ILE:HG23	2:G:1840:VAL:HG21	1.95	0.49
2:G:330:ASN:ND2	2:G:394:ARG:CZ	2.76	0.49
2:G:99:ASN:HD21	2:G:550:VAL:H	1.60	0.49
2:J:1470:THR:HA	2:J:1484:LYS:O	2.12	0.49
2:K:330:ASN:ND2	2:K:394:ARG:CZ	2.76	0.49
2:L:330:ASN:ND2	2:L:394:ARG:CZ	2.76	0.49
1:A:1239:HIS:CE1	1:A:1717:ASP:O	2.65	0.49
1:C:704:VAL:HG23	1:C:763:TRP:CZ3	2.47	0.49
2:H:101:ILE:HD11	2:H:122:LEU:HD23	1.93	0.49
2:H:330:ASN:ND2	2:H:394:ARG:CZ	2.76	0.49
2:J:517:HIS:CE1	2:J:540:ASP:HB3	2.47	0.49
2:K:101:ILE:HD11	2:K:122:LEU:HD23	1.93	0.49
2:K:99:ASN:HD21	2:K:550:VAL:H	1.60	0.49
2:L:1470:THR:HA	2:L:1484:LYS:O	2.13	0.49
2:L:159:ILE:HA	2:L:271:THR:O	2.13	0.49
1:A:1280:ILE:HD12	1:E:1280:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:ASN:ND2	1:B:613:VAL:O	2.45	0.49
1:B:704:VAL:HG23	1:B:763:TRP:CZ3	2.48	0.49
1:C:871:TRP:HA	3:O:146:ASN:HD22	1.78	0.49
1:D:704:VAL:HG23	1:D:763:TRP:CZ3	2.48	0.49
1:B:378:LEU:HD23	1:E:378:LEU:HD23	1.95	0.49
1:E:704:VAL:HG23	1:E:763:TRP:CZ3	2.47	0.49
1:F:850:PHE:HZ	1:F:866:GLY:HA3	1.78	0.49
2:G:159:ILE:HA	2:G:271:THR:O	2.13	0.49
2:I:330:ASN:ND2	2:I:394:ARG:CZ	2.76	0.49
2:K:615:TYR:OH	2:K:1075:ASP:OD1	2.17	0.49
2:L:1638:ILE:HG13	2:L:1657:ILE:HD12	1.94	0.49
1:B:850:PHE:HZ	1:B:866:GLY:HA3	1.78	0.49
2:G:1470:THR:HA	2:G:1484:LYS:O	2.13	0.49
2:G:309:ARG:NH1	2:G:442:ASP:OD2	2.43	0.49
2:H:1956:ARG:NE	2:H:1956:ARG:O	2.43	0.49
2:H:159:ILE:HA	2:H:271:THR:O	2.13	0.49
2:I:1470:THR:HA	2:I:1484:LYS:O	2.13	0.49
2:I:309:ARG:NH1	2:I:442:ASP:OD2	2.43	0.49
2:J:330:ASN:ND2	2:J:394:ARG:CZ	2.76	0.49
2:K:1585:SER:HB3	2:K:1651:LEU:HD11	1.95	0.49
2:K:159:ILE:HA	2:K:271:THR:O	2.13	0.49
2:L:1956:ARG:O	2:L:1956:ARG:NE	2.43	0.49
1:A:374:GLN:OE1	1:F:375:LEU:HD21	2.13	0.49
1:C:821:GLN:NE2	1:C:914:VAL:HG22	2.28	0.49
1:C:833:PHE:CE2	3:O:150:ILE:HG13	2.47	0.49
1:D:821:GLN:NE2	1:D:914:VAL:HG22	2.28	0.49
2:G:517:HIS:CE1	2:G:540:ASP:HB3	2.48	0.49
2:J:309:ARG:NH1	2:J:442:ASP:OD2	2.43	0.49
2:K:1470:THR:HA	2:K:1484:LYS:O	2.13	0.49
1:A:704:VAL:HG23	1:A:763:TRP:CZ3	2.48	0.49
1:C:904:ASN:HB3	1:C:926:LEU:HD13	1.93	0.49
1:D:904:ASN:HB3	1:D:926:LEU:HD13	1.93	0.49
2:G:1585:SER:HB3	2:G:1651:LEU:HD11	1.95	0.49
2:H:1054:LEU:HB2	5:H:2101:FMN:HM72	1.94	0.49
2:I:101:ILE:HD11	2:I:122:LEU:HD23	1.93	0.49
3:P:146:ASN:HA	3:P:150:ILE:HG12	1.95	0.49
1:B:641:ARG:NH2	1:B:925:ASP:OD2	2.46	0.48
1:E:605:LEU:HG	1:E:612:GLU:HG3	1.95	0.48
1:E:641:ARG:NH2	1:E:925:ASP:OD2	2.46	0.48
1:E:850:PHE:HZ	1:E:866:GLY:HA3	1.77	0.48
1:F:1239:HIS:CE1	1:F:1717:ASP:O	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:821:GLN:NE2	1:F:914:VAL:HG22	2.28	0.48
2:H:1751:ILE:HG23	2:H:1840:VAL:HG21	1.95	0.48
2:J:101:ILE:HD11	2:J:122:LEU:HD23	1.93	0.48
1:F:833:PHE:CE2	3:R:150:ILE:HG13	2.48	0.48
1:B:1239:HIS:CE1	1:B:1717:ASP:O	2.65	0.48
1:B:821:GLN:NE2	1:B:914:VAL:HG22	2.28	0.48
1:C:850:PHE:HZ	1:C:866:GLY:HA3	1.78	0.48
1:D:850:PHE:HZ	1:D:866:GLY:HA3	1.78	0.48
1:F:641:ARG:NH2	1:F:925:ASP:OD2	2.46	0.48
2:H:1638:ILE:HG13	2:H:1657:ILE:HD12	1.95	0.48
1:A:641:ARG:NH2	1:A:925:ASP:OD2	2.46	0.48
2:J:1751:ILE:HG23	2:J:1840:VAL:HG21	1.95	0.48
2:L:101:ILE:HD11	2:L:122:LEU:HD23	1.94	0.48
1:B:374:GLN:OE1	1:E:375:LEU:HD21	2.13	0.48
2:I:59:GLU:HA	2:I:122:LEU:HD12	1.96	0.48
1:C:605:LEU:HG	1:C:612:GLU:HG3	1.95	0.48
1:C:374:GLN:OE1	1:D:375:LEU:HD21	2.13	0.48
2:G:101:ILE:HD11	2:G:122:LEU:HD23	1.94	0.48
1:A:773:ALA:HB3	3:M:142:VAL:HG23	1.95	0.48
1:A:821:GLN:NE2	1:A:914:VAL:HG22	2.28	0.48
1:A:850:PHE:HZ	1:A:866:GLY:HA3	1.78	0.48
1:C:378:LEU:HD23	1:D:378:LEU:HD23	1.95	0.48
1:B:1432:HIS:CE1	1:D:1744:TYR:HB2	2.49	0.48
1:E:833:PHE:CE2	3:Q:150:ILE:HG13	2.48	0.48
2:I:1638:ILE:HG13	2:I:1657:ILE:HD12	1.94	0.48
3:N:146:ASN:HA	3:N:150:ILE:HG12	1.95	0.48
1:A:605:LEU:HG	1:A:612:GLU:HG3	1.96	0.48
1:C:641:ARG:NH2	1:C:925:ASP:OD2	2.46	0.48
1:D:773:ALA:HB3	3:P:142:VAL:HG23	1.95	0.48
1:D:641:ARG:NH2	1:D:925:ASP:OD2	2.46	0.48
1:E:489:VAL:HG13	1:E:670:GLY:HA3	1.96	0.48
2:I:1127:PHE:CE1	2:I:1141:ALA:HB1	2.49	0.48
2:L:1808:SER:H	2:L:2013:ASN:ND2	2.12	0.48
2:L:99:ASN:HD21	2:L:550:VAL:H	1.60	0.48
1:E:1584:PRO:HG3	1:E:1591:TRP:CE3	2.49	0.48
2:G:370:LEU:HD21	2:G:428:HIS:CD2	2.49	0.48
2:J:1127:PHE:CE1	2:J:1141:ALA:HB1	2.49	0.48
1:A:489:VAL:HG13	1:A:670:GLY:HA3	1.96	0.48
1:B:489:VAL:HG13	1:B:670:GLY:HA3	1.96	0.48
1:C:1261:PHE:CD1	1:F:1338:GLU:HG2	2.49	0.48
1:E:821:GLN:NE2	1:E:914:VAL:HG22	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:605:LEU:HG	1:F:612:GLU:HG3	1.96	0.48
2:G:1496:LYS:HD3	2:G:2002:LYS:HG2	1.96	0.48
2:H:1808:SER:H	2:H:2013:ASN:ND2	2.12	0.48
2:H:99:ASN:HD21	2:H:550:VAL:H	1.60	0.48
2:I:1478:ASN:OD1	2:I:1478:ASN:N	2.47	0.48
2:I:159:ILE:HA	2:I:271:THR:O	2.13	0.48
2:J:1638:ILE:HG13	2:J:1657:ILE:HD12	1.94	0.48
2:J:59:GLU:HA	2:J:122:LEU:HD12	1.96	0.48
3:O:146:ASN:HA	3:O:150:ILE:HG12	1.96	0.48
3:R:146:ASN:HA	3:R:150:ILE:HG12	1.96	0.48
1:A:1584:PRO:HG3	1:A:1591:TRP:CE3	2.49	0.48
1:B:605:LEU:HG	1:B:612:GLU:HG3	1.96	0.48
1:F:1584:PRO:HG3	1:F:1591:TRP:CE3	2.49	0.48
1:F:489:VAL:HG13	1:F:670:GLY:HA3	1.96	0.48
2:G:706:LYS:NZ	5:G:2101:FMN:O2'	2.47	0.48
2:H:1855:ILE:HG22	2:H:1968:PRO:HA	1.96	0.48
2:J:1478:ASN:OD1	2:J:1478:ASN:N	2.47	0.48
1:C:489:VAL:HG13	1:C:670:GLY:HA3	1.96	0.47
1:D:605:LEU:HG	1:D:612:GLU:HG3	1.96	0.47
2:J:159:ILE:HA	2:J:271:THR:O	2.13	0.47
1:D:833:PHE:CE2	3:P:150:ILE:HG13	2.49	0.47
1:B:1584:PRO:HG3	1:B:1591:TRP:CE3	2.49	0.47
1:C:375:LEU:HD21	1:D:374:GLN:OE1	2.14	0.47
2:G:1808:SER:H	2:G:2013:ASN:ND2	2.12	0.47
2:G:1855:ILE:HG22	2:G:1968:PRO:HA	1.96	0.47
2:H:1585:SER:HB3	2:H:1651:LEU:HD11	1.95	0.47
2:I:1585:SER:HB3	2:I:1651:LEU:HD11	1.95	0.47
2:J:1808:SER:H	2:J:2013:ASN:ND2	2.12	0.47
2:K:370:LEU:HD21	2:K:428:HIS:CD2	2.49	0.47
2:K:663:ILE:HB	2:K:664:PRO:HD3	1.96	0.47
2:L:1585:SER:HB3	2:L:1651:LEU:HD11	1.95	0.47
1:C:1338:GLU:HG2	1:F:1261:PHE:CD1	2.49	0.47
1:C:1657:HIS:CD2	1:C:1658:PRO:HD2	2.50	0.47
1:B:1261:PHE:CD1	1:D:1338:GLU:HG2	2.49	0.47
1:A:1338:GLU:HG2	1:E:1261:PHE:CD1	2.49	0.47
2:H:1478:ASN:OD1	2:H:1478:ASN:N	2.47	0.47
2:I:1775:GLN:HG2	2:I:1836:MET:HE2	1.95	0.47
2:J:370:LEU:HD21	2:J:428:HIS:CD2	2.49	0.47
2:K:1855:ILE:HG22	2:K:1968:PRO:HA	1.97	0.47
3:M:146:ASN:HA	3:M:150:ILE:HG12	1.95	0.47
1:D:1107:GLU:OE1	1:D:1191:THR:OG1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1338:GLU:HG2	1:D:1261:PHE:CD1	2.50	0.47
1:A:1261:PHE:CD1	1:E:1338:GLU:HG2	2.49	0.47
2:I:1808:SER:H	2:I:2013:ASN:ND2	2.12	0.47
2:J:1585:SER:HB3	2:J:1651:LEU:HD11	1.95	0.47
2:K:1808:SER:H	2:K:2013:ASN:ND2	2.12	0.47
1:D:1584:PRO:HG3	1:D:1591:TRP:CE3	2.49	0.47
1:D:1657:HIS:CD2	1:D:1658:PRO:HD2	2.50	0.47
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.97	0.47
2:H:1775:GLN:HG2	2:H:1836:MET:HE2	1.95	0.47
2:H:598:THR:O	2:H:602:VAL:HB	2.15	0.47
2:K:1775:GLN:CG	2:K:1836:MET:HE2	2.44	0.47
2:L:1478:ASN:OD1	2:L:1478:ASN:N	2.47	0.47
1:C:1584:PRO:HG3	1:C:1591:TRP:CE3	2.49	0.47
1:D:489:VAL:HG13	1:D:670:GLY:HA3	1.96	0.47
2:J:1775:GLN:HG2	2:J:1836:MET:HE2	1.95	0.47
1:C:1107:GLU:OE1	1:C:1191:THR:OG1	2.29	0.47
2:G:1757:GLU:OE1	2:G:1757:GLU:N	2.38	0.47
2:H:370:LEU:HD21	2:H:428:HIS:CD2	2.49	0.47
2:L:1775:GLN:HG2	2:L:1836:MET:HE2	1.95	0.47
2:L:1496:LYS:HD3	2:L:2002:LYS:HG2	1.97	0.47
2:L:598:THR:O	2:L:602:VAL:HB	2.15	0.47
2:I:101:ILE:HD11	2:I:122:LEU:HD21	1.96	0.47
2:I:370:LEU:HD21	2:I:428:HIS:CD2	2.50	0.47
2:I:598:THR:O	2:I:602:VAL:HB	2.15	0.47
2:J:598:THR:O	2:J:602:VAL:HB	2.15	0.47
2:L:370:LEU:HD21	2:L:428:HIS:CD2	2.49	0.47
1:A:1657:HIS:CD2	1:A:1658:PRO:HD2	2.50	0.47
1:A:764:ASP:OD1	1:A:810:LYS:NZ	2.48	0.47
1:A:833:PHE:CE2	3:M:150:ILE:HG13	2.49	0.47
1:C:706:THR:HB	1:C:737:PHE:HB3	1.97	0.47
1:D:706:THR:HB	1:D:737:PHE:HB3	1.97	0.47
2:G:1478:ASN:N	2:G:1478:ASN:OD1	2.47	0.47
2:K:1757:GLU:OE1	2:K:1757:GLU:N	2.38	0.47
2:K:598:THR:O	2:K:602:VAL:HB	2.15	0.47
2:L:1855:ILE:HG22	2:L:1968:PRO:HA	1.97	0.47
1:E:764:ASP:OD1	1:E:810:LYS:NZ	2.48	0.47
1:F:1657:HIS:CD2	1:F:1658:PRO:HD2	2.50	0.47
2:H:1738:PHE:CZ	2:H:1840:VAL:HG12	2.50	0.47
2:J:1855:ILE:HG22	2:J:1968:PRO:HA	1.96	0.47
2:K:1478:ASN:N	2:K:1478:ASN:OD1	2.47	0.47
1:B:1657:HIS:CD2	1:B:1658:PRO:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1017:ARG:HG2	1:D:1510:ASN:ND2	2.31	0.47
1:E:1657:HIS:CD2	1:E:1658:PRO:HD2	2.50	0.47
2:G:1127:PHE:CE1	2:G:1141:ALA:HB1	2.49	0.47
2:G:598:THR:O	2:G:602:VAL:HB	2.15	0.47
3:Q:146:ASN:HA	3:Q:150:ILE:HG12	1.96	0.47
1:B:198:PRO:HG3	1:B:212:THR:HG21	1.96	0.46
1:C:1017:ARG:HG2	1:C:1510:ASN:ND2	2.31	0.46
2:I:1804:PHE:CZ	2:I:2010:TYR:HB2	2.51	0.46
2:J:1804:PHE:CZ	2:J:2010:TYR:HB2	2.50	0.46
2:L:59:GLU:HA	2:L:122:LEU:HD12	1.96	0.46
1:C:1432:HIS:CE1	1:F:1744:TYR:HB2	2.50	0.46
2:J:101:ILE:HD11	2:J:122:LEU:HD21	1.97	0.46
2:K:101:ILE:HD11	2:K:122:LEU:HD21	1.96	0.46
1:C:987:ASN:ND2	1:C:1685:TYR:OH	2.49	0.46
1:D:987:ASN:ND2	1:D:1685:TYR:OH	2.49	0.46
1:E:198:PRO:HG3	1:E:212:THR:HG21	1.97	0.46
2:H:1127:PHE:CE1	2:H:1141:ALA:HB1	2.49	0.46
2:J:1142:LEU:HD22	2:J:1182:VAL:HG11	1.97	0.46
2:J:1738:PHE:CZ	2:J:1840:VAL:HG12	2.50	0.46
2:K:1127:PHE:CE1	2:K:1141:ALA:HB1	2.49	0.46
2:K:59:GLU:HA	2:K:122:LEU:HD12	1.96	0.46
2:L:1127:PHE:CE1	2:L:1141:ALA:HB1	2.49	0.46
1:B:833:PHE:CE2	3:N:150:ILE:HG13	2.51	0.46
1:A:198:PRO:HG3	1:A:212:THR:HG21	1.97	0.46
1:A:706:THR:HB	1:A:737:PHE:HB3	1.97	0.46
1:E:706:THR:HB	1:E:737:PHE:HB3	1.97	0.46
2:G:101:ILE:HD11	2:G:122:LEU:HD21	1.96	0.46
2:G:1775:GLN:CG	2:G:1836:MET:HE2	2.45	0.46
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.50	0.46
2:H:59:GLU:HA	2:H:122:LEU:HD12	1.96	0.46
2:K:1804:PHE:CZ	2:K:2010:TYR:HB2	2.50	0.46
1:C:1310:GLU:OE1	1:C:1649:LYS:CE	2.64	0.46
1:A:1334:ASP:OD1	1:A:1380:GLN:NE2	2.49	0.46
1:B:764:ASP:OD1	1:B:810:LYS:NZ	2.48	0.46
1:D:1310:GLU:OE1	1:D:1649:LYS:CE	2.64	0.46
1:E:1334:ASP:OD1	1:E:1380:GLN:NE2	2.49	0.46
1:F:764:ASP:OD1	1:F:810:LYS:NZ	2.48	0.46
2:I:1855:ILE:HG22	2:I:1968:PRO:HA	1.97	0.46
1:B:881:ASN:ND2	3:N:146:ASN:O	2.48	0.46
1:D:881:ASN:ND2	3:P:146:ASN:O	2.48	0.46
1:F:1334:ASP:OD1	1:F:1380:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1142:LEU:HD22	2:G:1182:VAL:HG11	1.97	0.46
2:H:1804:PHE:CZ	2:H:2010:TYR:HB2	2.50	0.46
2:H:663:ILE:HB	2:H:664:PRO:HD3	1.96	0.46
2:L:101:ILE:HD11	2:L:122:LEU:HD21	1.96	0.46
2:L:868:PHE:CD1	2:L:872:ILE:HD12	2.51	0.46
1:B:1109:GLU:CD	1:B:1109:GLU:H	2.20	0.46
1:B:1334:ASP:OD1	1:B:1380:GLN:NE2	2.49	0.46
1:C:1334:ASP:OD1	1:C:1380:GLN:NE2	2.49	0.46
1:D:1334:ASP:OD1	1:D:1380:GLN:NE2	2.49	0.46
1:F:1109:GLU:CD	1:F:1109:GLU:H	2.20	0.46
1:F:198:PRO:HG3	1:F:212:THR:HG21	1.97	0.46
1:F:871:TRP:CZ3	3:R:150:ILE:HG21	2.51	0.46
2:H:868:PHE:CD1	2:H:872:ILE:HD12	2.51	0.46
2:I:868:PHE:CD1	2:I:872:ILE:HD12	2.51	0.46
2:L:663:ILE:HB	2:L:664:PRO:HD3	1.96	0.46
1:A:1249:SER:HB3	1:A:1280:ILE:HG23	1.98	0.46
1:C:764:ASP:OD1	1:C:810:LYS:NZ	2.48	0.46
1:D:764:ASP:OD1	1:D:810:LYS:NZ	2.48	0.46
1:E:1249:SER:HB3	1:E:1280:ILE:HG23	1.98	0.46
1:F:706:THR:HB	1:F:737:PHE:HB3	1.97	0.46
2:H:101:ILE:HD11	2:H:122:LEU:HD21	1.97	0.46
2:I:1142:LEU:HD22	2:I:1182:VAL:HG11	1.98	0.46
2:K:1496:LYS:HD3	2:K:2002:LYS:HG2	1.98	0.46
2:L:1738:PHE:CZ	2:L:1840:VAL:HG12	2.51	0.46
1:B:21:GLN:HE21	1:B:21:GLN:HB3	1.64	0.46
1:B:706:THR:HB	1:B:737:PHE:HB3	1.97	0.46
2:K:868:PHE:CD1	2:K:872:ILE:HD12	2.51	0.46
1:C:871:TRP:CZ3	3:O:150:ILE:HG21	2.51	0.46
1:A:1310:GLU:OE1	1:A:1649:LYS:CE	2.64	0.45
1:C:1744:TYR:HB2	1:F:1432:HIS:CE1	2.51	0.45
1:E:1304:ALA:O	1:E:1307:THR:HG23	2.17	0.45
2:G:1738:PHE:CZ	2:G:1840:VAL:HG12	2.51	0.45
2:G:868:PHE:CD1	2:G:872:ILE:HD12	2.51	0.45
2:I:663:ILE:HB	2:I:664:PRO:HD3	1.96	0.45
2:J:754:TYR:CD1	2:J:794:MET:HG2	2.51	0.45
2:L:1804:PHE:CZ	2:L:2010:TYR:HB2	2.51	0.45
1:A:1107:GLU:OE1	1:A:1191:THR:OG1	2.29	0.45
1:F:233:ILE:HG13	1:F:243:ILE:HD13	1.99	0.45
2:H:1149:TRP:CE2	2:H:1213:LEU:HD23	2.52	0.45
2:H:754:TYR:CD1	2:H:794:MET:HG2	2.52	0.45
2:L:754:TYR:CD1	2:L:794:MET:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:ASN:ND2	3:M:146:ASN:O	2.49	0.45
1:A:1304:ALA:O	1:A:1307:THR:HG23	2.17	0.45
1:A:233:ILE:HG13	1:A:243:ILE:HD13	1.99	0.45
1:E:1310:GLU:OE1	1:E:1649:LYS:CE	2.64	0.45
1:F:1017:ARG:HG2	1:F:1510:ASN:ND2	2.30	0.45
2:G:59:GLU:HA	2:G:122:LEU:HD12	1.97	0.45
2:H:230:TYR:CE2	2:H:236:ILE:HD13	2.52	0.45
2:J:1496:LYS:HD3	2:J:2002:LYS:HG2	1.98	0.45
2:J:868:PHE:CD1	2:J:872:ILE:HD12	2.51	0.45
2:L:1142:LEU:HD22	2:L:1182:VAL:HG11	1.97	0.45
2:L:249:TYR:CE2	2:L:283:ILE:HD12	2.52	0.45
1:B:1310:GLU:OE1	1:B:1649:LYS:CE	2.64	0.45
1:C:233:ILE:HG13	1:C:243:ILE:HD13	1.98	0.45
1:C:845:SER:HG	1:D:845:SER:HG	1.36	0.45
1:F:1107:GLU:OE1	1:F:1191:THR:OG1	2.29	0.45
2:H:1037:SER:HA	2:H:1051:THR:HG21	1.98	0.45
2:H:249:TYR:CE2	2:H:283:ILE:HD12	2.52	0.45
2:I:754:TYR:CD1	2:I:794:MET:HG2	2.52	0.45
2:J:1037:SER:HA	2:J:1051:THR:HG21	1.98	0.45
2:J:1330:GLY:HA2	2:J:1374:THR:HG21	1.99	0.45
2:K:1142:LEU:HD22	2:K:1182:VAL:HG11	1.97	0.45
2:K:9:LEU:HD21	2:K:34:GLN:HG3	1.98	0.45
2:L:1149:TRP:CE2	2:L:1213:LEU:HD23	2.52	0.45
1:B:1017:ARG:HG2	1:B:1510:ASN:ND2	2.30	0.45
1:E:233:ILE:HG13	1:E:243:ILE:HD13	1.99	0.45
1:F:1310:GLU:OE1	1:F:1649:LYS:CE	2.64	0.45
1:F:21:GLN:HE21	1:F:21:GLN:HB3	1.64	0.45
2:G:1330:GLY:HA2	2:G:1374:THR:HG21	1.99	0.45
2:G:754:TYR:CD1	2:G:794:MET:HG2	2.51	0.45
2:H:1142:LEU:HD22	2:H:1182:VAL:HG11	1.97	0.45
2:I:1081:HIS:O	2:I:1085:LEU:HB2	2.17	0.45
2:J:1081:HIS:O	2:J:1085:LEU:HB2	2.17	0.45
2:J:663:ILE:HB	2:J:664:PRO:HD3	1.97	0.45
2:L:1854:MET:HA	2:L:1907:LEU:HD21	1.98	0.45
2:L:398:ALA:HB2	2:L:413:LYS:HB2	1.99	0.45
1:A:1264:ARG:NH1	1:A:1270:VAL:HB	2.32	0.45
1:B:1304:ALA:O	1:B:1307:THR:HG23	2.17	0.45
1:B:233:ILE:HG13	1:B:243:ILE:HD13	1.99	0.45
1:D:1304:ALA:O	1:D:1307:THR:HG23	2.17	0.45
1:F:1304:ALA:O	1:F:1307:THR:HG23	2.17	0.45
1:F:1584:PRO:HG3	1:F:1591:TRP:CZ3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:499:THR:OG1	2:G:500:HIS:HD2	2.00	0.45
2:I:1037:SER:HA	2:I:1051:THR:HG21	1.98	0.45
2:I:1330:GLY:HA2	2:I:1374:THR:HG21	1.99	0.45
2:I:1738:PHE:CZ	2:I:1840:VAL:HG12	2.51	0.45
1:A:1109:GLU:H	1:A:1109:GLU:CD	2.20	0.45
1:B:1249:SER:HB3	1:B:1280:ILE:HG23	1.98	0.45
1:B:1584:PRO:HG3	1:B:1591:TRP:CZ3	2.52	0.45
1:C:198:PRO:HG3	1:C:212:THR:HG21	1.97	0.45
1:D:198:PRO:HG3	1:D:212:THR:HG21	1.97	0.45
1:E:1264:ARG:NH1	1:E:1270:VAL:HB	2.32	0.45
2:G:249:TYR:CE2	2:G:283:ILE:HD12	2.52	0.45
2:H:1081:HIS:O	2:H:1085:LEU:HB2	2.17	0.45
2:I:9:LEU:HD21	2:I:34:GLN:HG3	1.99	0.45
2:J:230:TYR:CE2	2:J:236:ILE:HD13	2.52	0.45
2:K:499:THR:OG1	2:K:500:HIS:HD2	2.00	0.45
2:K:754:TYR:CD1	2:K:794:MET:HG2	2.52	0.45
2:L:499:THR:OG1	2:L:500:HIS:HD2	2.00	0.45
1:C:1304:ALA:O	1:C:1307:THR:HG23	2.17	0.45
1:C:340:ARG:HH12	1:C:344:GLN:HE21	1.65	0.45
1:E:1109:GLU:CD	1:E:1109:GLU:H	2.20	0.45
1:E:400:ARG:HH11	1:E:715:THR:HG21	1.80	0.45
1:F:1249:SER:HB3	1:F:1280:ILE:HG23	1.98	0.45
2:G:1149:TRP:CE2	2:G:1213:LEU:HD23	2.52	0.45
2:G:1933:LEU:HD13	2:G:1933:LEU:N	2.32	0.45
2:I:1496:LYS:HD3	2:I:2002:LYS:HG2	1.98	0.45
2:J:249:TYR:CE2	2:J:283:ILE:HD12	2.52	0.45
2:K:1738:PHE:CZ	2:K:1840:VAL:HG12	2.51	0.45
2:L:1081:HIS:O	2:L:1085:LEU:HB2	2.17	0.45
1:A:871:TRP:CZ3	3:M:150:ILE:HG21	2.52	0.45
1:C:1264:ARG:NH1	1:C:1270:VAL:HB	2.32	0.45
1:E:1304:ALA:O	1:E:1307:THR:CG2	2.65	0.45
2:J:1757:GLU:N	2:J:1757:GLU:OE1	2.38	0.45
2:K:1037:SER:HA	2:K:1051:THR:HG21	1.98	0.45
2:K:249:TYR:CE2	2:K:283:ILE:HD12	2.52	0.45
2:L:1037:SER:HA	2:L:1051:THR:HG21	1.98	0.45
3:N:42:LEU:HD23	3:N:42:LEU:HA	1.89	0.45
1:E:871:TRP:CZ3	3:Q:150:ILE:HG21	2.52	0.45
3:R:42:LEU:HA	3:R:42:LEU:HD23	1.89	0.45
1:A:1304:ALA:O	1:A:1307:THR:CG2	2.65	0.45
1:A:400:ARG:HH11	1:A:715:THR:HG21	1.80	0.45
1:B:871:TRP:CZ3	3:N:150:ILE:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1264:ARG:NH1	1:D:1270:VAL:HB	2.32	0.45
1:F:1304:ALA:O	1:F:1307:THR:CG2	2.65	0.45
1:F:987:ASN:ND2	1:F:1685:TYR:OH	2.49	0.45
2:G:1037:SER:HA	2:G:1051:THR:HG21	1.98	0.45
2:G:679:LEU:HD21	2:G:681:ILE:HD11	1.99	0.45
2:H:1496:LYS:HD3	2:H:2002:LYS:HG2	1.99	0.45
2:H:7:ARG:HD3	2:H:27:PHE:CD1	2.53	0.45
2:H:499:THR:OG1	2:H:500:HIS:HD2	2.00	0.45
2:J:1149:TRP:CE2	2:J:1213:LEU:HD23	2.52	0.45
2:J:9:LEU:HD21	2:J:34:GLN:HG3	1.99	0.45
2:K:1330:GLY:HA2	2:K:1374:THR:HG21	1.99	0.45
2:L:741:HIS:CD2	2:L:855:HIS:ND1	2.85	0.45
1:A:1418:VAL:N	1:A:1419:PRO:HD2	2.32	0.44
1:B:1264:ARG:NH1	1:B:1270:VAL:HB	2.32	0.44
1:B:1304:ALA:O	1:B:1307:THR:CG2	2.66	0.44
1:B:987:ASN:ND2	1:B:1685:TYR:OH	2.49	0.44
1:C:1109:GLU:H	1:C:1109:GLU:CD	2.20	0.44
1:D:233:ILE:HG13	1:D:243:ILE:HD13	1.99	0.44
1:D:340:ARG:HH12	1:D:344:GLN:HE21	1.65	0.44
1:E:1584:PRO:HG3	1:E:1591:TRP:CZ3	2.52	0.44
1:E:987:ASN:ND2	1:E:1685:TYR:OH	2.49	0.44
1:F:1264:ARG:NH1	1:F:1270:VAL:HB	2.32	0.44
2:H:9:LEU:HD21	2:H:34:GLN:HG3	1.99	0.44
2:I:1854:MET:HA	2:I:1907:LEU:HD21	1.98	0.44
2:I:741:HIS:CD2	2:I:855:HIS:ND1	2.85	0.44
2:K:1081:HIS:O	2:K:1085:LEU:HB2	2.17	0.44
2:K:1933:LEU:N	2:K:1933:LEU:HD13	2.33	0.44
2:K:679:LEU:HD21	2:K:681:ILE:HD11	1.99	0.44
1:A:987:ASN:ND2	1:A:1685:TYR:OH	2.48	0.44
1:C:1418:VAL:N	1:C:1419:PRO:HD2	2.32	0.44
1:D:1109:GLU:H	1:D:1109:GLU:CD	2.20	0.44
1:E:1418:VAL:N	1:E:1419:PRO:HD2	2.32	0.44
2:G:398:ALA:HB2	2:G:413:LYS:HB2	1.98	0.44
2:G:741:HIS:CD2	2:G:855:HIS:ND1	2.85	0.44
1:A:984:PRO:HB3	2:G:959:THR:HG23	1.99	0.44
2:I:398:ALA:HB2	2:I:413:LYS:HB2	1.99	0.44
2:J:741:HIS:CD2	2:J:855:HIS:ND1	2.85	0.44
2:K:741:HIS:CD2	2:K:855:HIS:ND1	2.85	0.44
1:B:159:LEU:CD2	1:B:176:VAL:CG1	2.96	0.44
1:D:1418:VAL:N	1:D:1419:PRO:HD2	2.32	0.44
2:G:1081:HIS:O	2:G:1085:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:741:HIS:CD2	2:H:855:HIS:ND1	2.85	0.44
2:I:249:TYR:CE2	2:I:283:ILE:HD12	2.52	0.44
2:K:1149:TRP:CE2	2:K:1213:LEU:HD23	2.52	0.44
2:L:7:ARG:HD3	2:L:27:PHE:CD1	2.53	0.44
3:N:20:ILE:HD11	3:N:103:LEU:HD23	2.00	0.44
1:A:1584:PRO:HG3	1:A:1591:TRP:CZ3	2.52	0.44
1:C:1175:ILE:HG12	1:F:1173:LEU:CD2	2.48	0.44
1:C:1249:SER:HB3	1:C:1280:ILE:HG23	1.98	0.44
1:B:1173:LEU:CD2	1:D:1175:ILE:HG12	2.47	0.44
1:D:231:ARG:HH21	2:L:115:THR:HG21	1.83	0.44
1:D:871:TRP:CZ3	3:P:150:ILE:HG21	2.52	0.44
1:F:1418:VAL:N	1:F:1419:PRO:HD2	2.32	0.44
2:H:1854:MET:HA	2:H:1907:LEU:HD21	1.99	0.44
2:H:665:LEU:O	2:H:665:LEU:HD22	2.17	0.44
2:I:1852:TYR:HD1	2:I:1903:ASP:HA	1.82	0.44
2:K:1854:MET:HA	2:K:1907:LEU:HD21	1.98	0.44
2:L:1852:TYR:HD1	2:L:1903:ASP:HA	1.83	0.44
2:L:230:TYR:CE2	2:L:236:ILE:HD13	2.53	0.44
2:L:665:LEU:HD22	2:L:665:LEU:O	2.17	0.44
1:B:1418:VAL:N	1:B:1419:PRO:HD2	2.32	0.44
1:B:1146:HIS:HE1	1:D:1117:GLU:O	2.01	0.44
1:D:1249:SER:HB3	1:D:1280:ILE:HG23	1.98	0.44
1:E:529:MET:HE2	1:E:896:PHE:CE2	2.52	0.44
1:F:159:LEU:CD2	1:F:176:VAL:CG1	2.96	0.44
2:G:9:LEU:HD21	2:G:34:GLN:HG3	2.00	0.44
2:J:7:ARG:HD3	2:J:27:PHE:CD1	2.53	0.44
2:J:499:THR:OG1	2:J:500:HIS:HD2	2.00	0.44
2:L:1330:GLY:HA2	2:L:1374:THR:HG21	1.99	0.44
1:F:984:PRO:HB3	2:L:959:THR:HG23	2.00	0.44
1:A:986:ALA:HB2	1:A:1047:LEU:HD13	2.00	0.44
2:H:898:ASP:O	2:H:1050:ARG:HG2	2.18	0.44
2:I:1757:GLU:OE1	2:I:1757:GLU:N	2.38	0.44
2:J:398:ALA:HB2	2:J:413:LYS:HB2	1.99	0.44
2:L:9:LEU:HD21	2:L:34:GLN:HG3	1.99	0.44
2:L:679:LEU:HD21	2:L:681:ILE:HD11	1.99	0.44
3:O:141:ASP:OD1	3:O:143:VAL:HG12	2.18	0.44
1:A:529:MET:HE2	1:A:896:PHE:CE2	2.53	0.44
1:B:1303:GLY:H	1:B:1307:THR:HG22	1.83	0.44
1:C:1117:GLU:O	1:F:1146:HIS:HE1	2.01	0.44
2:H:1330:GLY:HA2	2:H:1374:THR:HG21	1.99	0.44
2:H:1852:TYR:HD1	2:H:1903:ASP:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1149:TRP:CE2	2:I:1213:LEU:HD23	2.52	0.44
2:I:499:THR:OG1	2:I:500:HIS:HD2	2.00	0.44
2:L:898:ASP:O	2:L:1050:ARG:HG2	2.18	0.44
1:C:1584:PRO:HG3	1:C:1591:TRP:CZ3	2.52	0.44
1:C:1173:LEU:CD2	1:F:1175:ILE:HG12	2.48	0.44
1:F:1303:GLY:H	1:F:1307:THR:HG22	1.83	0.44
2:G:230:TYR:CE2	2:G:236:ILE:HD13	2.52	0.44
2:H:679:LEU:HD21	2:H:681:ILE:HD11	1.99	0.44
2:I:230:TYR:CE2	2:I:236:ILE:HD13	2.53	0.44
2:I:7:ARG:HD3	2:I:27:PHE:CD1	2.53	0.44
2:K:1852:TYR:HD1	2:K:1903:ASP:HA	1.83	0.44
3:R:141:ASP:OD1	3:R:143:VAL:HG12	2.18	0.44
1:A:1017:ARG:HG2	1:A:1510:ASN:ND2	2.30	0.44
1:C:1585:LYS:HE3	1:C:1585:LYS:HB2	1.81	0.44
1:C:833:PHE:CZ	3:O:150:ILE:HG23	2.52	0.44
1:D:1584:PRO:HG3	1:D:1591:TRP:CZ3	2.52	0.44
1:E:986:ALA:HB2	1:E:1047:LEU:HD13	2.00	0.44
1:E:340:ARG:HH12	1:E:344:GLN:HE21	1.65	0.44
1:F:871:TRP:HA	3:R:146:ASN:HD22	1.79	0.44
1:F:881:ASN:ND2	3:R:146:ASN:O	2.51	0.44
2:G:1852:TYR:HD1	2:G:1903:ASP:HA	1.83	0.44
2:G:1854:MET:HA	2:G:1907:LEU:HD21	1.99	0.44
2:G:665:LEU:O	2:G:665:LEU:HD22	2.18	0.44
2:I:679:LEU:HD21	2:I:681:ILE:HD11	1.99	0.44
2:K:898:ASP:O	2:K:1050:ARG:HG2	2.17	0.44
2:K:665:LEU:HD22	2:K:665:LEU:O	2.17	0.44
2:L:1933:LEU:N	2:L:1933:LEU:HD13	2.32	0.44
1:A:159:LEU:CD2	1:A:176:VAL:CG1	2.95	0.43
1:C:1303:GLY:H	1:C:1307:THR:HG22	1.83	0.43
1:C:159:LEU:CD2	1:C:176:VAL:CG1	2.95	0.43
1:D:1426:LEU:HA	1:D:1426:LEU:HD23	1.90	0.43
1:D:1585:LYS:HE3	1:D:1585:LYS:HB2	1.81	0.43
1:E:1673:TYR:CZ	1:E:1677:VAL:HG21	2.53	0.43
1:F:59:ARG:HD2	2:L:1896:GLN:NE2	2.33	0.43
2:J:679:LEU:HD21	2:J:681:ILE:HD11	1.99	0.43
2:K:777:THR:HG23	2:K:1081:HIS:NE2	2.33	0.43
3:N:141:ASP:OD1	3:N:143:VAL:HG12	2.18	0.43
3:P:141:ASP:OD1	3:P:143:VAL:HG12	2.18	0.43
3:R:20:ILE:HD11	3:R:103:LEU:HD23	2.00	0.43
1:B:340:ARG:HH12	1:B:344:GLN:HE21	1.65	0.43
1:C:529:MET:HE2	1:C:896:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1303:GLY:H	1:D:1307:THR:HG22	1.83	0.43
1:F:1673:TYR:CZ	1:F:1677:VAL:HG21	2.53	0.43
1:A:381:GLU:OE1	1:F:793:ARG:NH2	2.51	0.43
2:G:898:ASP:O	2:G:1050:ARG:HG2	2.18	0.43
2:H:777:THR:HG23	2:H:1081:HIS:NE2	2.33	0.43
2:J:1852:TYR:HD1	2:J:1903:ASP:HA	1.83	0.43
2:J:898:ASP:O	2:J:1050:ARG:HG2	2.18	0.43
1:A:340:ARG:HH12	1:A:344:GLN:HE21	1.65	0.43
1:B:986:ALA:HB2	1:B:1047:LEU:HD13	2.00	0.43
1:B:1175:ILE:HG12	1:D:1173:LEU:CD2	2.48	0.43
1:C:1304:ALA:O	1:C:1307:THR:CG2	2.66	0.43
1:C:984:PRO:HB3	2:I:959:THR:HG23	2.01	0.43
1:C:793:ARG:NH2	1:D:381:GLU:OE1	2.51	0.43
1:E:159:LEU:CD2	1:E:176:VAL:CG1	2.95	0.43
1:F:986:ALA:HB2	1:F:1047:LEU:HD13	2.00	0.43
1:F:400:ARG:HH11	1:F:715:THR:HG21	1.80	0.43
2:G:777:THR:HG23	2:G:1081:HIS:NE2	2.33	0.43
2:H:398:ALA:HB2	2:H:413:LYS:HB2	2.00	0.43
2:I:898:ASP:O	2:I:1050:ARG:HG2	2.18	0.43
2:J:1854:MET:HA	2:J:1907:LEU:HD21	1.99	0.43
2:J:665:LEU:O	2:J:665:LEU:HD22	2.17	0.43
2:K:230:TYR:CE2	2:K:236:ILE:HD13	2.52	0.43
3:Q:141:ASP:OD1	3:Q:143:VAL:HG12	2.18	0.43
1:B:1673:TYR:CZ	1:B:1677:VAL:HG21	2.54	0.43
1:B:400:ARG:HH11	1:B:715:THR:HG21	1.80	0.43
1:D:1304:ALA:O	1:D:1307:THR:CG2	2.66	0.43
1:D:159:LEU:CD2	1:D:176:VAL:CG1	2.95	0.43
1:A:1173:LEU:CD2	1:E:1175:ILE:HG12	2.47	0.43
1:C:1146:HIS:HE1	1:F:1117:GLU:O	2.01	0.43
2:I:349:VAL:O	2:I:353:VAL:HG13	2.18	0.43
2:I:665:LEU:O	2:I:665:LEU:HD22	2.17	0.43
2:J:1933:LEU:HD13	2:J:1933:LEU:N	2.32	0.43
2:J:209:PHE:CD1	2:J:213:LEU:CD2	3.02	0.43
2:J:349:VAL:O	2:J:353:VAL:HG13	2.18	0.43
1:D:984:PRO:HB3	2:J:959:THR:HG23	2.01	0.43
2:L:1778:GLN:HG3	2:L:1809:LEU:HD22	2.00	0.43
1:A:1117:GLU:O	1:E:1146:HIS:HE1	2.01	0.43
1:A:1146:HIS:HE1	1:E:1117:GLU:O	2.01	0.43
1:A:1303:GLY:H	1:A:1307:THR:HG22	1.83	0.43
1:A:1673:TYR:CZ	1:A:1677:VAL:HG21	2.54	0.43
1:A:683:ALA:O	1:A:718:TYR:OH	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1302:VAL:HG23	1:D:1302:VAL:HG23	2.01	0.43
1:C:381:GLU:OE1	1:D:793:ARG:NH2	2.51	0.43
1:E:1303:GLY:H	1:E:1307:THR:HG22	1.83	0.43
1:E:1017:ARG:HG2	1:E:1510:ASN:ND2	2.31	0.43
1:C:1302:VAL:HG23	1:F:1302:VAL:HG23	2.01	0.43
2:I:1778:GLN:HG3	2:I:1809:LEU:HD22	2.00	0.43
2:I:1933:LEU:N	2:I:1933:LEU:HD13	2.33	0.43
2:I:777:THR:HG23	2:I:1081:HIS:NE2	2.33	0.43
2:J:777:THR:HG23	2:J:1081:HIS:NE2	2.33	0.43
2:K:426:PRO:O	2:K:429:SER:OG	2.37	0.43
2:K:7:ARG:HD3	2:K:27:PHE:CD1	2.53	0.43
1:C:644:THR:HG22	1:C:648:ASP:O	2.19	0.43
1:B:1117:GLU:O	1:D:1146:HIS:HE1	2.01	0.43
1:D:644:THR:HG22	1:D:648:ASP:O	2.19	0.43
1:D:529:MET:HE2	1:D:896:PHE:CE2	2.53	0.43
1:E:683:ALA:O	1:E:718:TYR:OH	2.34	0.43
1:E:881:ASN:ND2	3:Q:146:ASN:O	2.51	0.43
2:H:1933:LEU:N	2:H:1933:LEU:HD13	2.33	0.43
2:I:209:PHE:CD1	2:I:213:LEU:CD2	3.02	0.43
2:J:143:SER:OG	2:J:547:ILE:O	2.23	0.43
2:K:398:ALA:HB2	2:K:413:LYS:HB2	1.99	0.43
1:E:984:PRO:HB3	2:K:959:THR:HG23	2.01	0.43
1:A:1431:GLU:OE2	1:A:1523:ARG:NH1	2.52	0.43
1:C:400:ARG:HH11	1:C:715:THR:HG21	1.80	0.43
1:F:340:ARG:HH12	1:F:344:GLN:HE21	1.65	0.43
2:G:7:ARG:HD3	2:G:27:PHE:CD1	2.53	0.43
2:G:426:PRO:O	2:G:429:SER:OG	2.37	0.43
2:H:1778:GLN:HG3	2:H:1809:LEU:HD22	2.01	0.43
2:L:777:THR:HG23	2:L:1081:HIS:NE2	2.33	0.43
3:M:20:ILE:HD11	3:M:103:LEU:HD23	2.00	0.43
3:Q:20:ILE:HD11	3:Q:103:LEU:HD23	2.00	0.43
1:B:793:ARG:NH2	1:E:381:GLU:OE1	2.52	0.43
1:C:1776:ILE:HD12	1:C:1807:SER:HA	2.01	0.43
1:C:683:ALA:O	1:C:718:TYR:OH	2.34	0.43
1:D:1431:GLU:OE2	1:D:1523:ARG:NH1	2.52	0.43
1:E:907:GLY:O	1:E:910:THR:HG23	2.19	0.43
2:H:859:THR:HA	2:H:1049:GLN:HE22	1.84	0.43
2:K:349:VAL:O	2:K:353:VAL:HG13	2.18	0.43
2:L:426:PRO:O	2:L:429:SER:OG	2.37	0.43
3:M:141:ASP:OD1	3:M:143:VAL:HG12	2.18	0.43
3:Q:42:LEU:HA	3:Q:42:LEU:HD23	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:833:PHE:CZ	3:R:150:ILE:HG23	2.54	0.43
1:A:644:THR:HG22	1:A:648:ASP:O	2.19	0.43
1:C:986:ALA:HB2	1:C:1047:LEU:HD13	2.00	0.43
1:C:1673:TYR:CZ	1:C:1677:VAL:HG21	2.54	0.43
1:D:1776:ILE:HD12	1:D:1807:SER:HA	2.01	0.43
1:D:790:PHE:CE2	1:D:794:ILE:HD11	2.54	0.43
1:D:986:ALA:HB2	1:D:1047:LEU:HD13	2.00	0.43
1:E:790:PHE:CE2	1:E:794:ILE:HD11	2.54	0.43
2:G:349:VAL:O	2:G:353:VAL:HG13	2.18	0.43
2:H:1468:THR:CG2	2:H:1485:CYS:SG	3.07	0.43
2:J:1217:ASN:HA	2:J:1217:ASN:HD22	1.66	0.43
2:L:859:THR:HA	2:L:1049:GLN:HE22	1.84	0.43
1:A:790:PHE:CE2	1:A:794:ILE:HD11	2.54	0.43
1:C:1442:ASN:HA	1:C:1442:ASN:HD22	1.69	0.43
1:C:790:PHE:CE2	1:C:794:ILE:HD11	2.54	0.43
1:D:1673:TYR:CZ	1:D:1677:VAL:HG21	2.54	0.43
1:D:683:ALA:O	1:D:718:TYR:OH	2.34	0.43
1:D:400:ARG:HH11	1:D:715:THR:HG21	1.80	0.43
1:E:1431:GLU:OE2	1:E:1523:ARG:NH1	2.52	0.43
1:E:1776:ILE:HD12	1:E:1807:SER:HA	2.00	0.43
1:E:644:THR:HG22	1:E:648:ASP:O	2.19	0.43
1:F:907:GLY:O	1:F:910:THR:HG23	2.19	0.43
2:G:653:TYR:CD1	2:G:659:LEU:HD21	2.54	0.43
2:H:1217:ASN:HD22	2:H:1217:ASN:HA	1.66	0.43
2:H:426:PRO:O	2:H:429:SER:OG	2.37	0.43
2:K:209:PHE:CD1	2:K:213:LEU:CD2	3.02	0.43
2:K:653:TYR:CD1	2:K:659:LEU:HD21	2.54	0.43
1:A:907:GLY:O	1:A:910:THR:HG23	2.19	0.42
1:B:907:GLY:O	1:B:910:THR:HG23	2.19	0.42
1:C:1431:GLU:OE2	1:C:1523:ARG:NH1	2.52	0.42
1:C:907:GLY:O	1:C:910:THR:HG23	2.19	0.42
1:D:1303:GLY:HA2	1:D:1649:LYS:HE2	2.02	0.42
1:E:833:PHE:CZ	3:Q:150:ILE:HG23	2.53	0.42
2:G:973:LEU:HA	2:G:973:LEU:HD13	1.90	0.42
2:L:1217:ASN:HD22	2:L:1217:ASN:HA	1.67	0.42
3:M:42:LEU:HA	3:M:42:LEU:HD23	1.89	0.42
1:B:1431:GLU:OE2	1:B:1523:ARG:NH1	2.52	0.42
1:B:381:GLU:OE1	1:E:793:ARG:NH2	2.51	0.42
1:C:1303:GLY:HA2	1:C:1649:LYS:HE2	2.02	0.42
1:A:1302:VAL:HG23	1:E:1302:VAL:HG23	2.01	0.42
1:F:1431:GLU:OE2	1:F:1523:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:301:THR:HG21	2:G:448:VAL:HG21	2.01	0.42
2:H:1916:PHE:CE2	2:H:1943:ILE:HD12	2.55	0.42
2:H:209:PHE:CD1	2:H:213:LEU:CD2	3.02	0.42
2:H:349:VAL:O	2:H:353:VAL:HG13	2.18	0.42
2:H:330:ASN:HD22	2:H:394:ARG:NH1	2.18	0.42
2:I:653:TYR:CD1	2:I:659:LEU:HD21	2.54	0.42
2:J:653:TYR:CD1	2:J:659:LEU:HD21	2.54	0.42
2:L:349:VAL:O	2:L:353:VAL:HG13	2.18	0.42
1:A:793:ARG:NH2	1:F:381:GLU:OE1	2.51	0.42
1:C:853:TRP:CE3	1:C:921:PRO:HD3	2.54	0.42
1:C:881:ASN:ND2	3:O:146:ASN:O	2.51	0.42
2:G:271:THR:OG1	2:G:272:GLY:N	2.52	0.42
1:B:984:PRO:HB3	2:H:959:THR:HG23	2.01	0.42
2:I:1217:ASN:HD22	2:I:1217:ASN:HA	1.66	0.42
2:I:426:PRO:O	2:I:429:SER:OG	2.37	0.42
2:J:1468:THR:CG2	2:J:1485:CYS:SG	3.07	0.42
2:J:426:PRO:O	2:J:429:SER:OG	2.37	0.42
2:L:1468:THR:CG2	2:L:1485:CYS:SG	3.08	0.42
2:L:330:ASN:HD22	2:L:394:ARG:NH1	2.18	0.42
1:B:1776:ILE:HD12	1:B:1807:SER:HA	2.00	0.42
4:B:1901:PNS:H382	2:G:372:ASN:ND2	2.33	0.42
1:C:21:GLN:HE21	1:C:21:GLN:HB3	1.64	0.42
2:G:1468:THR:CG2	2:G:1485:CYS:SG	3.07	0.42
2:G:209:PHE:CD1	2:G:213:LEU:CD2	3.02	0.42
2:J:1778:GLN:HG3	2:J:1809:LEU:HD22	2.01	0.42
2:J:330:ASN:HD22	2:J:394:ARG:NH1	2.18	0.42
2:K:1778:GLN:HG3	2:K:1809:LEU:HD22	2.00	0.42
2:K:973:LEU:HA	2:K:973:LEU:HD13	1.90	0.42
2:L:271:THR:OG1	2:L:272:GLY:N	2.52	0.42
1:A:1776:ILE:HD12	1:A:1807:SER:HA	2.01	0.42
1:A:853:TRP:CE3	1:A:921:PRO:HD3	2.54	0.42
1:D:21:GLN:HE21	1:D:21:GLN:HB3	1.64	0.42
1:A:1175:ILE:HG12	1:E:1173:LEU:CD2	2.48	0.42
1:E:1303:GLY:HA2	1:E:1649:LYS:HE2	2.02	0.42
2:H:271:THR:OG1	2:H:272:GLY:N	2.52	0.42
2:I:330:ASN:HD22	2:I:394:ARG:NH1	2.18	0.42
2:J:754:TYR:CG	2:J:794:MET:HG2	2.55	0.42
2:K:1468:THR:CG2	2:K:1485:CYS:SG	3.08	0.42
2:K:1956:ARG:HB3	2:K:1957:PRO:HD3	2.02	0.42
2:K:271:THR:OG1	2:K:272:GLY:N	2.52	0.42
1:A:1303:GLY:HA2	1:A:1649:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:PHE:CE2	1:B:794:ILE:HD11	2.54	0.42
1:D:822:VAL:HG12	1:D:824:LEU:HD13	2.02	0.42
1:D:907:GLY:O	1:D:910:THR:HG23	2.19	0.42
1:D:853:TRP:CE3	1:D:921:PRO:HD3	2.54	0.42
1:E:337:VAL:HG12	1:E:341:GLN:NE2	2.35	0.42
1:E:853:TRP:CE3	1:E:921:PRO:HD3	2.54	0.42
2:G:330:ASN:HD22	2:G:394:ARG:NH1	2.18	0.42
2:L:209:PHE:CD1	2:L:213:LEU:CD2	3.02	0.42
3:O:42:LEU:HD23	3:O:42:LEU:HA	1.89	0.42
3:P:42:LEU:HA	3:P:42:LEU:HD23	1.89	0.42
1:A:337:VAL:HG12	1:A:341:GLN:NE2	2.35	0.42
1:C:822:VAL:HG12	1:C:824:LEU:HD13	2.02	0.42
1:D:337:VAL:HG12	1:D:341:GLN:NE2	2.35	0.42
1:F:1776:ILE:HD12	1:F:1807:SER:HA	2.01	0.42
2:G:1956:ARG:HB3	2:G:1957:PRO:HD3	2.02	0.42
3:P:20:ILE:HD11	3:P:103:LEU:HD23	2.00	0.42
1:A:864:VAL:HG22	1:A:921:PRO:HB3	2.02	0.42
1:D:1442:ASN:HD22	1:D:1442:ASN:HA	1.69	0.42
2:J:228:LYS:O	2:J:232:LEU:HD13	2.20	0.42
2:K:330:ASN:HD22	2:K:394:ARG:NH1	2.18	0.42
2:L:228:LYS:O	2:L:232:LEU:HD13	2.20	0.42
1:D:1298:ILE:HG23	1:D:1298:ILE:O	2.20	0.42
1:F:790:PHE:CE2	1:F:794:ILE:HD11	2.54	0.42
2:G:859:THR:HA	2:G:1049:GLN:HE22	1.84	0.42
2:H:754:TYR:CG	2:H:794:MET:HG2	2.55	0.42
2:I:1468:THR:CG2	2:I:1485:CYS:SG	3.08	0.42
2:I:271:THR:OG1	2:I:272:GLY:N	2.52	0.42
2:J:1916:PHE:CE2	2:J:1943:ILE:HD12	2.55	0.42
2:K:859:THR:HA	2:K:1049:GLN:HE22	1.84	0.42
2:L:653:TYR:CD1	2:L:659:LEU:HD21	2.54	0.42
1:B:644:THR:HG22	1:B:648:ASP:O	2.19	0.42
1:C:1298:ILE:HG23	1:C:1298:ILE:O	2.20	0.42
1:D:1367:ARG:HD2	1:D:1370:THR:HG21	2.02	0.42
1:E:864:VAL:HG22	1:E:921:PRO:HB3	2.02	0.42
1:F:644:THR:HG22	1:F:648:ASP:O	2.19	0.42
2:G:1778:GLN:HG3	2:G:1809:LEU:HD22	2.01	0.42
2:G:406:ARG:HG2	3:M:88:GLU:CG	2.49	0.42
2:H:228:LYS:O	2:H:232:LEU:HD13	2.20	0.42
2:I:228:LYS:O	2:I:232:LEU:HD13	2.20	0.42
2:I:754:TYR:CG	2:I:794:MET:HG2	2.55	0.42
2:L:1593:ILE:HG22	2:L:1657:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1426:LEU:HA	1:B:1426:LEU:HD23	1.90	0.41
1:B:1303:GLY:HA2	1:B:1649:LYS:HE2	2.02	0.41
1:C:1367:ARG:HD2	1:C:1370:THR:HG21	2.02	0.41
1:F:1303:GLY:HA2	1:F:1649:LYS:HE2	2.02	0.41
1:F:337:VAL:HG12	1:F:341:GLN:NE2	2.35	0.41
2:H:1757:GLU:N	2:H:1757:GLU:OE1	2.38	0.41
2:H:653:TYR:CD1	2:H:659:LEU:HD21	2.54	0.41
2:H:938:TRP:CH2	2:H:947:THR:HG21	2.55	0.41
2:I:1956:ARG:HE	2:I:1956:ARG:CA	2.33	0.41
2:J:1871:LEU:HA	2:J:1871:LEU:HD23	1.94	0.41
2:J:1956:ARG:HB3	2:J:1957:PRO:HD3	2.02	0.41
1:B:775:PRO:HA	3:N:142:VAL:HG11	2.02	0.41
1:C:337:VAL:HG12	1:C:341:GLN:NE2	2.35	0.41
1:B:1716:LEU:HD21	1:D:1426:LEU:HD22	2.02	0.41
1:E:1298:ILE:O	1:E:1298:ILE:HG23	2.20	0.41
2:G:228:LYS:O	2:G:232:LEU:HD13	2.19	0.41
2:I:1916:PHE:CE2	2:I:1943:ILE:HD12	2.56	0.41
2:J:271:THR:OG1	2:J:272:GLY:N	2.52	0.41
2:K:1956:ARG:CA	2:K:1956:ARG:HE	2.33	0.41
2:L:938:TRP:CH2	2:L:947:THR:HG21	2.55	0.41
3:O:20:ILE:HD11	3:O:103:LEU:HD23	2.00	0.41
1:A:1298:ILE:HG23	1:A:1298:ILE:O	2.20	0.41
1:B:337:VAL:HG12	1:B:341:GLN:NE2	2.35	0.41
1:B:853:TRP:CE3	1:B:921:PRO:HD3	2.54	0.41
1:B:1118:LYS:HE2	1:D:1146:HIS:O	2.20	0.41
1:F:853:TRP:CE3	1:F:921:PRO:HD3	2.54	0.41
2:G:1632:ILE:CG2	2:G:1637:LEU:HD23	2.50	0.41
2:G:1773:ALA:O	2:G:1775:GLN:N	2.47	0.41
2:H:1593:ILE:HG22	2:H:1657:ILE:HD11	2.02	0.41
2:H:301:THR:HG21	2:H:448:VAL:HG21	2.01	0.41
2:I:1956:ARG:HB3	2:I:1957:PRO:HD3	2.02	0.41
2:J:1593:ILE:HG22	2:J:1657:ILE:HD11	2.02	0.41
2:J:1956:ARG:CA	2:J:1956:ARG:HE	2.34	0.41
2:J:301:THR:HG21	2:J:448:VAL:HG21	2.01	0.41
2:J:938:TRP:CH2	2:J:947:THR:HG21	2.55	0.41
2:K:938:TRP:CH2	2:K:947:THR:HG21	2.55	0.41
2:L:143:SER:OG	2:L:547:ILE:O	2.23	0.41
1:A:1076:VAL:HG13	1:A:1081:LYS:HA	2.03	0.41
1:A:1754:LYS:HA	1:A:1754:LYS:HE2	2.03	0.41
1:B:1201:SER:OG	1:B:1203:ASP:OD1	2.29	0.41
1:B:871:TRP:HA	3:N:146:ASN:HD22	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1427:THR:O	1:E:1430:ARG:HD2	2.21	0.41
2:G:1956:ARG:HE	2:G:1956:ARG:CA	2.34	0.41
2:G:938:TRP:CH2	2:G:947:THR:HG21	2.55	0.41
2:H:1628:HIS:HE1	2:H:1630:GLY:O	2.03	0.41
2:H:1956:ARG:HB3	2:H:1957:PRO:HD3	2.01	0.41
2:I:1956:ARG:HE	2:I:1956:ARG:HA	1.86	0.41
2:I:938:TRP:CH2	2:I:947:THR:HG21	2.55	0.41
2:L:1757:GLU:OE1	2:L:1757:GLU:N	2.38	0.41
2:L:754:TYR:CG	2:L:794:MET:HG2	2.55	0.41
1:A:1367:ARG:HD2	1:A:1370:THR:HG21	2.02	0.41
1:A:1427:THR:O	1:A:1430:ARG:HD2	2.21	0.41
1:B:1146:HIS:O	1:D:1118:LYS:HE2	2.21	0.41
1:B:1298:ILE:HG23	1:B:1298:ILE:O	2.20	0.41
1:B:1442:ASN:HD22	1:B:1442:ASN:HA	1.69	0.41
1:B:719:GLN:HG3	1:B:1612:ASP:HA	2.03	0.41
1:E:1367:ARG:HD2	1:E:1370:THR:HG21	2.02	0.41
1:F:1076:VAL:HG13	1:F:1081:LYS:HA	2.03	0.41
1:F:1298:ILE:O	1:F:1298:ILE:HG23	2.20	0.41
1:F:1426:LEU:HD23	1:F:1426:LEU:HA	1.90	0.41
2:G:754:TYR:CG	2:G:794:MET:HG2	2.55	0.41
2:I:1871:LEU:HA	2:I:1871:LEU:HD23	1.94	0.41
2:K:1632:ILE:CG2	2:K:1637:LEU:HD23	2.50	0.41
2:K:228:LYS:O	2:K:232:LEU:HD13	2.20	0.41
2:L:1916:PHE:CE2	2:L:1943:ILE:HD12	2.56	0.41
1:A:775:PRO:HA	3:M:142:VAL:HG11	2.01	0.41
1:D:719:GLN:HG3	1:D:1612:ASP:HA	2.03	0.41
1:D:880:ALA:HA	3:P:147:SER:HA	2.02	0.41
1:E:1076:VAL:HG13	1:E:1081:LYS:HA	2.03	0.41
1:E:822:VAL:HG12	1:E:824:LEU:HD13	2.02	0.41
1:F:719:GLN:HG3	1:F:1612:ASP:HA	2.03	0.41
1:F:822:VAL:HG12	1:F:824:LEU:HD13	2.02	0.41
2:I:1593:ILE:HG22	2:I:1657:ILE:HD11	2.02	0.41
2:J:1148:ASN:HD22	2:J:1190:SER:HB3	1.86	0.41
2:K:1773:ALA:O	2:K:1775:GLN:N	2.47	0.41
2:L:1628:HIS:HE1	2:L:1630:GLY:O	2.04	0.41
1:A:1442:ASN:HD22	1:A:1442:ASN:HA	1.69	0.41
1:A:717:TYR:CZ	1:A:721:ILE:CD1	3.03	0.41
1:A:822:VAL:HG12	1:A:824:LEU:HD13	2.02	0.41
1:B:1076:VAL:HG13	1:B:1081:LYS:HA	2.03	0.41
1:B:683:ALA:O	1:B:718:TYR:OH	2.34	0.41
1:B:822:VAL:HG12	1:B:824:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1146:HIS:O	1:F:1118:LYS:HE2	2.21	0.41
1:C:719:GLN:HG3	1:C:1612:ASP:HA	2.03	0.41
1:C:237:MET:HB2	1:C:277:LEU:CD1	2.50	0.41
1:A:1118:LYS:HE2	1:E:1146:HIS:O	2.20	0.41
1:E:1463:VAL:HB	1:E:1773:VAL:HG21	2.03	0.41
1:E:1754:LYS:HE2	1:E:1754:LYS:HA	2.03	0.41
1:C:1076:VAL:HG13	1:C:1081:LYS:HA	2.03	0.41
1:C:1118:LYS:HE2	1:F:1146:HIS:O	2.21	0.41
1:D:1076:VAL:HG13	1:D:1081:LYS:HA	2.03	0.41
1:E:717:TYR:CZ	1:E:721:ILE:CD1	3.03	0.41
2:K:1916:PHE:CE2	2:K:1943:ILE:HD12	2.55	0.41
2:K:301:THR:HG21	2:K:448:VAL:HG21	2.02	0.41
2:K:754:TYR:CG	2:K:794:MET:HG2	2.55	0.41
2:L:1956:ARG:HB3	2:L:1957:PRO:HD3	2.02	0.41
1:B:1107:GLU:OE1	1:B:1191:THR:OG1	2.29	0.41
1:D:1754:LYS:HE2	1:D:1754:LYS:HA	2.03	0.41
1:F:1442:ASN:HD22	1:F:1442:ASN:HA	1.69	0.41
2:H:494:THR:HA	2:H:496:PHE:CE1	2.56	0.41
2:H:973:LEU:HD13	2:H:973:LEU:HA	1.90	0.41
2:J:859:THR:HA	2:J:1049:GLN:HE22	1.84	0.41
2:K:1484:LYS:HE3	2:K:1484:LYS:HB2	1.91	0.41
2:L:494:THR:HA	2:L:496:PHE:CE1	2.56	0.41
1:A:59:ARG:HD2	2:G:1896:GLN:NE2	2.36	0.41
1:B:529:MET:HE2	1:B:896:PHE:CE2	2.53	0.41
1:B:880:ALA:HA	3:N:147:SER:HA	2.02	0.41
1:C:1426:LEU:HD23	1:C:1426:LEU:HA	1.90	0.41
1:D:237:MET:HB2	1:D:277:LEU:CD1	2.51	0.41
1:E:1442:ASN:HA	1:E:1442:ASN:HD22	1.69	0.41
1:F:683:ALA:O	1:F:718:TYR:OH	2.34	0.41
2:G:1148:ASN:HD22	2:G:1190:SER:HB3	1.85	0.41
2:G:1484:LYS:HB2	2:G:1484:LYS:HE3	1.91	0.41
2:G:1628:HIS:HE1	2:G:1630:GLY:O	2.04	0.41
2:J:1865:SER:HB3	2:J:1923:ASP:OD1	2.21	0.41
2:J:1956:ARG:HE	2:J:1956:ARG:HA	1.86	0.41
2:L:864:LEU:HD11	2:L:868:PHE:CZ	2.56	0.41
1:A:390:VAL:O	1:A:390:VAL:HG13	2.22	0.41
1:C:1754:LYS:HA	1:C:1754:LYS:HE2	2.03	0.41
1:D:864:VAL:HG22	1:D:921:PRO:HB3	2.02	0.41
1:E:390:VAL:HG13	1:E:390:VAL:O	2.22	0.41
1:F:1367:ARG:O	1:F:1370:THR:HB	2.21	0.41
1:F:870:GLY:HA3	1:F:927:ASN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:100:ASP:OD1	2:G:101:ILE:N	2.53	0.41
2:H:1484:LYS:HE3	2:H:1484:LYS:HB2	1.90	0.41
2:H:864:LEU:HD11	2:H:868:PHE:CZ	2.56	0.41
2:I:690:VAL:O	2:I:693:GLU:N	2.54	0.41
2:J:1628:HIS:HE1	2:J:1630:GLY:O	2.03	0.41
2:K:1628:HIS:HE1	2:K:1630:GLY:O	2.03	0.41
2:L:1148:ASN:HD22	2:L:1190:SER:HB3	1.86	0.41
2:L:973:LEU:HD13	2:L:973:LEU:HA	1.90	0.41
1:B:1367:ARG:O	1:B:1370:THR:HB	2.21	0.40
1:B:1754:LYS:HA	1:B:1754:LYS:HE2	2.03	0.40
1:B:870:GLY:HA3	1:B:927:ASN:HA	2.03	0.40
1:F:1367:ARG:HD2	1:F:1370:THR:HG21	2.02	0.40
1:F:1754:LYS:HA	1:F:1754:LYS:HE2	2.03	0.40
2:G:494:THR:HA	2:G:496:PHE:CE1	2.56	0.40
2:I:859:THR:HA	2:I:1049:GLN:HE22	1.84	0.40
2:I:1628:HIS:HE1	2:I:1630:GLY:O	2.03	0.40
2:I:490:TRP:O	2:I:494:THR:HG22	2.21	0.40
2:J:1773:ALA:O	2:J:1775:GLN:N	2.47	0.40
1:C:1367:ARG:O	1:C:1370:THR:HB	2.21	0.40
1:C:823:ILE:HA	1:C:865:CYS:O	2.21	0.40
1:C:864:VAL:HG22	1:C:921:PRO:HB3	2.02	0.40
1:D:798:ASN:OD1	1:D:801:ARG:NH1	2.54	0.40
1:E:851:ASN:HA	1:E:851:ASN:HD22	1.77	0.40
1:F:529:MET:HE2	1:F:896:PHE:CE2	2.53	0.40
2:G:864:LEU:HD11	2:G:868:PHE:CZ	2.56	0.40
2:I:973:LEU:HA	2:I:973:LEU:HD13	1.90	0.40
2:J:690:VAL:O	2:J:693:GLU:N	2.54	0.40
2:K:100:ASP:OD1	2:K:101:ILE:N	2.53	0.40
1:B:1367:ARG:HD2	1:B:1370:THR:HG21	2.02	0.40
1:C:798:ASN:OD1	1:C:801:ARG:NH1	2.54	0.40
1:D:1367:ARG:O	1:D:1370:THR:HB	2.21	0.40
1:D:237:MET:CE	1:D:276:ARG:HA	2.51	0.40
1:D:823:ILE:HA	1:D:865:CYS:O	2.22	0.40
2:H:1148:ASN:HD22	2:H:1190:SER:HB3	1.86	0.40
2:H:1632:ILE:CG2	2:H:1637:LEU:HD23	2.50	0.40
2:I:1148:ASN:HD22	2:I:1190:SER:HB3	1.86	0.40
2:I:1773:ALA:O	2:I:1775:GLN:N	2.47	0.40
2:I:864:LEU:HD11	2:I:868:PHE:CZ	2.56	0.40
2:K:494:THR:HA	2:K:496:PHE:CE1	2.56	0.40
2:K:864:LEU:HD11	2:K:868:PHE:CZ	2.57	0.40
1:B:237:MET:N	1:B:238:PRO:CD	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:823:ILE:HA	1:B:865:CYS:O	2.21	0.40
1:C:1426:LEU:HD22	1:F:1716:LEU:HD21	2.03	0.40
1:A:1426:LEU:HD22	1:E:1716:LEU:HD21	2.02	0.40
2:G:1593:ILE:HG22	2:G:1657:ILE:HD11	2.02	0.40
2:G:1865:SER:HB3	2:G:1923:ASP:OD1	2.21	0.40
2:G:1916:PHE:CE2	2:G:1943:ILE:HD12	2.56	0.40
2:H:1628:HIS:CE1	2:H:1630:GLY:O	2.75	0.40
2:H:1963:GLY:O	2:H:1965:ALA:N	2.55	0.40
2:I:1551:GLU:N	2:I:1552:PRO:HD2	2.36	0.40
2:J:1551:GLU:N	2:J:1552:PRO:HD2	2.36	0.40
2:J:864:LEU:HD11	2:J:868:PHE:CZ	2.56	0.40
2:K:1551:GLU:N	2:K:1552:PRO:HD2	2.36	0.40
2:K:234:ILE:HG21	2:K:425:SER:HB3	2.03	0.40
1:A:823:ILE:HA	1:A:865:CYS:O	2.21	0.40
1:B:1427:THR:O	1:B:1430:ARG:HD2	2.22	0.40
1:B:864:VAL:HG22	1:B:921:PRO:HB3	2.02	0.40
1:C:870:GLY:HA3	1:C:927:ASN:HA	2.03	0.40
1:D:833:PHE:CZ	3:P:150:ILE:HG23	2.57	0.40
1:A:1146:HIS:O	1:E:1118:LYS:HE2	2.21	0.40
1:E:1243:VAL:O	1:E:1296:GLY:HA3	2.22	0.40
1:F:237:MET:N	1:F:238:PRO:CD	2.85	0.40
1:F:823:ILE:HA	1:F:865:CYS:O	2.21	0.40
2:G:1551:GLU:N	2:G:1552:PRO:HD2	2.36	0.40
2:H:1956:ARG:CA	2:H:1956:ARG:HE	2.34	0.40
2:H:2017:LYS:O	2:H:2018:PRO:C	2.59	0.40
2:I:1865:SER:HB3	2:I:1923:ASP:OD1	2.22	0.40
2:J:494:THR:HA	2:J:496:PHE:CE1	2.56	0.40
2:L:1628:HIS:CE1	2:L:1630:GLY:O	2.75	0.40
2:L:1956:ARG:CA	2:L:1956:ARG:HE	2.34	0.40
2:L:2017:LYS:O	2:L:2018:PRO:C	2.59	0.40
2:L:301:THR:HG21	2:L:448:VAL:HG21	2.03	0.40
2:L:406:ARG:HG2	3:R:88:GLU:CG	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM



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	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	24	57
1	B	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	24	57
1	C	1744/1887 (92%)	1612 (92%)	119 (7%)	13 (1%)	24	57
1	D	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	24	57
1	E	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	24	57
1	F	1744/1887 (92%)	1613 (92%)	119 (7%)	12 (1%)	24	57
2	G	2032/2040 (100%)	1843 (91%)	177 (9%)	12 (1%)	27	60
2	H	2032/2040 (100%)	1843 (91%)	176 (9%)	13 (1%)	27	60
2	I	2032/2040 (100%)	1844 (91%)	174 (9%)	14 (1%)	24	57
2	J	2032/2040 (100%)	1842 (91%)	178 (9%)	12 (1%)	27	60
2	K	2032/2040 (100%)	1844 (91%)	176 (9%)	12 (1%)	27	60
2	L	2032/2040 (100%)	1844 (91%)	176 (9%)	12 (1%)	27	60
3	M	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	9	28
3	N	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	9	28
3	O	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	9	28
3	P	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	9	28
3	Q	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	9	28
3	R	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	9	28
All	All	23292/24450 (95%)	21327 (92%)	1805 (8%)	160 (1%)	28	57

All (160) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1130	ASP
1	B	1130	ASP
1	C	1130	ASP
1	D	1130	ASP
1	E	1130	ASP
1	F	1130	ASP
2	G	1215	LYS
2	G	1845	ASP
2	H	1215	LYS

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Mol	Chain	Res	Type
2	H	1845	ASP
2	I	1215	LYS
2	I	1845	ASP
2	J	1215	LYS
2	J	1845	ASP
2	K	1215	LYS
2	K	1845	ASP
2	L	1215	LYS
2	L	1845	ASP
3	M	149	PHE
3	N	149	PHE
3	O	149	PHE
3	P	149	PHE
3	Q	149	PHE
3	R	149	PHE
1	A	178	GLY
1	A	875	THR
1	B	178	GLY
1	B	875	THR
1	C	178	GLY
1	C	875	THR
1	D	178	GLY
1	D	875	THR
1	E	178	GLY
1	E	875	THR
1	F	178	GLY
1	F	875	THR
2	G	185	GLY
2	G	769	SER
2	G	1874	VAL
2	H	185	GLY
2	H	769	SER
2	H	1874	VAL
2	I	185	GLY
2	I	769	SER
2	I	1874	VAL
2	J	185	GLY
2	J	769	SER
2	J	1874	VAL
2	K	185	GLY
2	K	769	SER
2	K	1874	VAL

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Mol	Chain	Res	Type
2	L	185	GLY
2	L	769	SER
2	L	1874	VAL
3	M	148	ILE
3	N	148	ILE
3	O	148	ILE
3	P	148	ILE
3	Q	148	ILE
3	R	148	ILE
1	A	198	PRO
1	A	238	PRO
1	A	618	ASN
1	B	238	PRO
1	B	618	ASN
1	C	238	PRO
1	C	618	ASN
1	D	198	PRO
1	D	238	PRO
1	D	618	ASN
1	E	238	PRO
1	E	618	ASN
1	F	198	PRO
1	F	238	PRO
1	F	618	ASN
2	G	1316	ASP
2	G	1774	THR
2	H	1316	ASP
2	H	1774	THR
2	H	1846	GLU
2	I	1316	ASP
2	I	1774	THR
2	J	1316	ASP
2	J	1774	THR
2	K	1316	ASP
2	K	1774	THR
2	L	1316	ASP
2	L	1774	THR
1	A	215	ASP
1	A	607	LYS
1	A	917	CYS
1	A	1267	ASP
1	A	1536	LEU

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Mol	Chain	Res	Type
1	B	198	PRO
1	B	215	ASP
1	B	607	LYS
1	B	917	CYS
1	B	1267	ASP
1	B	1536	LEU
1	C	198	PRO
1	C	215	ASP
1	C	917	CYS
1	C	1267	ASP
1	C	1536	LEU
1	D	215	ASP
1	D	607	LYS
1	D	917	CYS
1	D	1267	ASP
1	D	1536	LEU
1	E	198	PRO
1	E	215	ASP
1	E	917	CYS
1	E	1267	ASP
1	E	1536	LEU
1	F	215	ASP
1	F	607	LYS
1	F	917	CYS
1	F	1267	ASP
1	F	1536	LEU
2	G	134	LYS
2	G	1743	ASP
2	G	1846	GLU
2	H	134	LYS
2	H	1743	ASP
2	I	134	LYS
2	I	1743	ASP
2	I	1846	GLU
2	J	134	LYS
2	J	1743	ASP
2	J	1846	GLU
2	K	134	LYS
2	K	1743	ASP
2	K	1846	GLU
2	L	134	LYS
2	L	1743	ASP

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Mol	Chain	Res	Type
2	L	1846	GLU
1	C	607	LYS
1	E	607	LYS
2	G	140	LYS
2	G	772	GLY
2	H	140	LYS
2	H	772	GLY
2	I	140	LYS
2	I	772	GLY
2	J	140	LYS
2	J	772	GLY
2	K	140	LYS
2	K	772	GLY
2	L	140	LYS
2	L	772	GLY
1	C	538	GLU
2	H	1964	PHE
2	I	1820	ASP
2	I	1964	PHE
1	B	219	GLY
1	C	219	GLY
1	D	219	GLY
1	E	219	GLY
1	F	219	GLY
1	A	219	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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	1476/1566 (94%)	1381 (94%)	95 (6%)	19	48
1	B	1476/1566 (94%)	1380 (94%)	96 (6%)	19	48
1	C	1476/1566 (94%)	1380 (94%)	96 (6%)	19	48
1	D	1476/1566 (94%)	1379 (93%)	97 (7%)	18	47
1	E	1476/1566 (94%)	1381 (94%)	95 (6%)	19	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	1476/1566 (94%)	1378 (93%)	98 (7%)	18	47
2	G	1775/1779 (100%)	1660 (94%)	115 (6%)	19	48
2	H	1775/1779 (100%)	1660 (94%)	115 (6%)	19	48
2	I	1775/1779 (100%)	1661 (94%)	114 (6%)	19	48
2	J	1775/1779 (100%)	1660 (94%)	115 (6%)	19	48
2	K	1775/1779 (100%)	1661 (94%)	114 (6%)	19	48
2	L	1775/1779 (100%)	1660 (94%)	115 (6%)	19	48
3	M	97/129 (75%)	83 (86%)	14 (14%)	3	11
3	N	97/129 (75%)	83 (86%)	14 (14%)	3	11
3	O	97/129 (75%)	83 (86%)	14 (14%)	3	11
3	P	97/129 (75%)	83 (86%)	14 (14%)	3	11
3	Q	97/129 (75%)	83 (86%)	14 (14%)	3	11
3	R	97/129 (75%)	82 (84%)	15 (16%)	3	9
All	All	20088/20844 (96%)	18738 (93%)	1350 (7%)	22	46

All (1350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	22	PHE
1	A	35	PHE
1	A	38	ASP
1	A	44	VAL
1	A	52	THR
1	A	67	SER
1	A	179	LYS
1	A	182	VAL
1	A	184	ASN
1	A	202	GLU
1	A	217	PHE
1	A	221	LEU
1	A	237	MET
1	A	253	ARG
1	A	272	GLU
1	A	277	LEU
1	A	390	VAL
1	A	392	THR

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Mol	Chain	Res	Type
1	A	401	THR
1	A	416	LEU
1	A	435	GLU
1	A	447	LEU
1	A	458	THR
1	A	478	GLU
1	A	489	VAL
1	A	493	VAL
1	A	520	ARG
1	A	522	LEU
1	A	527	GLN
1	A	622	ILE
1	A	624	LYS
1	A	626	VAL
1	A	672	THR
1	A	719	GLN
1	A	731	THR
1	A	738	ASN
1	A	748	LEU
1	A	754	ASP
1	A	776	GLU
1	A	797	THR
1	A	806	VAL
1	A	823	ILE
1	A	826	MET
1	A	827	SER
1	A	862	LEU
1	A	864	VAL
1	A	901	MET
1	A	940	THR
1	A	999	LYS
1	A	1001	VAL
1	A	1020	VAL
1	A	1022	THR
1	A	1047	LEU
1	A	1050	CYS
1	A	1067	LEU
1	A	1073	THR
1	A	1079	LYS
1	A	1090	LYS
1	A	1096	SER
1	A	1166	LYS

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Mol	Chain	Res	Type
1	A	1183	ARG
1	A	1184	LEU
1	A	1197	THR
1	A	1208	VAL
1	A	1254	VAL
1	A	1262	LYS
1	A	1267	ASP
1	A	1283	MET
1	A	1298	ILE
1	A	1307	THR
1	A	1317	GLU
1	A	1327	CYS
1	A	1329	VAL
1	A	1332	TYR
1	A	1362	PRO
1	A	1366	SER
1	A	1370	THR
1	A	1392	LEU
1	A	1430	ARG
1	A	1432	HIS
1	A	1442	ASN
1	A	1501	LEU
1	A	1528	THR
1	A	1556	THR
1	A	1580	LEU
1	A	1585	LYS
1	A	1642	THR
1	A	1680	ARG
1	A	1722	VAL
1	A	1754	LYS
1	A	1756	ILE
1	A	1780	ASN
1	A	1842	VAL
1	A	1844	LYS
1	B	21	GLN
1	B	22	PHE
1	B	35	PHE
1	B	38	ASP
1	B	44	VAL
1	B	52	THR
1	B	67	SER
1	B	179	LYS

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Mol	Chain	Res	Type
1	B	182	VAL
1	B	184	ASN
1	B	202	GLU
1	B	217	PHE
1	B	221	LEU
1	B	237	MET
1	B	253	ARG
1	B	272	GLU
1	B	277	LEU
1	B	390	VAL
1	B	392	THR
1	B	401	THR
1	B	416	LEU
1	B	435	GLU
1	B	447	LEU
1	B	458	THR
1	B	478	GLU
1	B	489	VAL
1	B	493	VAL
1	B	520	ARG
1	B	522	LEU
1	B	527	GLN
1	B	622	ILE
1	B	624	LYS
1	B	626	VAL
1	B	672	THR
1	B	719	GLN
1	B	731	THR
1	B	738	ASN
1	B	748	LEU
1	B	754	ASP
1	B	776	GLU
1	B	797	THR
1	B	806	VAL
1	B	823	ILE
1	B	826	MET
1	B	827	SER
1	B	862	LEU
1	B	864	VAL
1	B	901	MET
1	B	915	GLU
1	B	940	THR

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Mol	Chain	Res	Type
1	B	999	LYS
1	B	1001	VAL
1	B	1020	VAL
1	B	1022	THR
1	B	1047	LEU
1	B	1050	CYS
1	B	1067	LEU
1	B	1073	THR
1	B	1079	LYS
1	B	1090	LYS
1	B	1096	SER
1	B	1166	LYS
1	B	1183	ARG
1	B	1184	LEU
1	B	1197	THR
1	B	1208	VAL
1	B	1254	VAL
1	B	1262	LYS
1	B	1267	ASP
1	B	1283	MET
1	B	1298	ILE
1	B	1307	THR
1	B	1317	GLU
1	B	1327	CYS
1	B	1329	VAL
1	B	1332	TYR
1	B	1362	PRO
1	B	1366	SER
1	B	1370	THR
1	B	1392	LEU
1	B	1430	ARG
1	B	1432	HIS
1	B	1442	ASN
1	B	1501	LEU
1	B	1528	THR
1	B	1556	THR
1	B	1580	LEU
1	B	1585	LYS
1	B	1642	THR
1	B	1680	ARG
1	B	1722	VAL
1	B	1754	LYS

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Mol	Chain	Res	Type
1	B	1756	ILE
1	B	1780	ASN
1	B	1842	VAL
1	B	1844	LYS
1	C	21	GLN
1	C	22	PHE
1	C	35	PHE
1	C	38	ASP
1	C	44	VAL
1	C	52	THR
1	C	67	SER
1	C	179	LYS
1	C	182	VAL
1	C	184	ASN
1	C	202	GLU
1	C	217	PHE
1	C	221	LEU
1	C	237	MET
1	C	253	ARG
1	C	272	GLU
1	C	277	LEU
1	C	390	VAL
1	C	392	THR
1	C	401	THR
1	C	416	LEU
1	C	435	GLU
1	C	447	LEU
1	C	458	THR
1	C	478	GLU
1	C	489	VAL
1	C	493	VAL
1	C	520	ARG
1	C	522	LEU
1	C	527	GLN
1	C	622	ILE
1	C	624	LYS
1	C	626	VAL
1	C	672	THR
1	C	719	GLN
1	C	731	THR
1	C	738	ASN
1	C	748	LEU

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Mol	Chain	Res	Type
1	C	754	ASP
1	C	776	GLU
1	C	797	THR
1	C	806	VAL
1	C	823	ILE
1	C	826	MET
1	C	827	SER
1	C	862	LEU
1	C	864	VAL
1	C	901	MET
1	C	915	GLU
1	C	940	THR
1	C	999	LYS
1	C	1001	VAL
1	C	1020	VAL
1	C	1022	THR
1	C	1047	LEU
1	C	1050	CYS
1	C	1067	LEU
1	C	1073	THR
1	C	1079	LYS
1	C	1090	LYS
1	C	1096	SER
1	C	1166	LYS
1	C	1183	ARG
1	C	1184	LEU
1	C	1197	THR
1	C	1208	VAL
1	C	1254	VAL
1	C	1262	LYS
1	C	1267	ASP
1	C	1283	MET
1	C	1298	ILE
1	C	1307	THR
1	C	1317	GLU
1	C	1327	CYS
1	C	1329	VAL
1	C	1332	TYR
1	C	1362	PRO
1	C	1366	SER
1	C	1370	THR
1	C	1392	LEU

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Mol	Chain	Res	Type
1	C	1430	ARG
1	C	1432	HIS
1	C	1442	ASN
1	C	1501	LEU
1	C	1528	THR
1	C	1556	THR
1	C	1580	LEU
1	C	1585	LYS
1	C	1642	THR
1	C	1680	ARG
1	C	1722	VAL
1	C	1754	LYS
1	C	1756	ILE
1	C	1780	ASN
1	C	1842	VAL
1	C	1844	LYS
1	D	21	GLN
1	D	22	PHE
1	D	35	PHE
1	D	38	ASP
1	D	44	VAL
1	D	52	THR
1	D	67	SER
1	D	179	LYS
1	D	182	VAL
1	D	184	ASN
1	D	202	GLU
1	D	217	PHE
1	D	221	LEU
1	D	237	MET
1	D	253	ARG
1	D	272	GLU
1	D	277	LEU
1	D	378	LEU
1	D	390	VAL
1	D	392	THR
1	D	401	THR
1	D	416	LEU
1	D	435	GLU
1	D	447	LEU
1	D	458	THR
1	D	478	GLU

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Mol	Chain	Res	Type
1	D	489	VAL
1	D	493	VAL
1	D	520	ARG
1	D	522	LEU
1	D	527	GLN
1	D	622	ILE
1	D	624	LYS
1	D	626	VAL
1	D	672	THR
1	D	719	GLN
1	D	731	THR
1	D	738	ASN
1	D	748	LEU
1	D	754	ASP
1	D	776	GLU
1	D	797	THR
1	D	806	VAL
1	D	823	ILE
1	D	826	MET
1	D	827	SER
1	D	862	LEU
1	D	864	VAL
1	D	901	MET
1	D	915	GLU
1	D	940	THR
1	D	999	LYS
1	D	1001	VAL
1	D	1020	VAL
1	D	1022	THR
1	D	1047	LEU
1	D	1050	CYS
1	D	1067	LEU
1	D	1073	THR
1	D	1079	LYS
1	D	1090	LYS
1	D	1096	SER
1	D	1166	LYS
1	D	1183	ARG
1	D	1184	LEU
1	D	1197	THR
1	D	1208	VAL
1	D	1254	VAL

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Mol	Chain	Res	Type
1	D	1262	LYS
1	D	1267	ASP
1	D	1283	MET
1	D	1298	ILE
1	D	1307	THR
1	D	1317	GLU
1	D	1327	CYS
1	D	1329	VAL
1	D	1332	TYR
1	D	1362	PRO
1	D	1366	SER
1	D	1370	THR
1	D	1392	LEU
1	D	1430	ARG
1	D	1432	HIS
1	D	1442	ASN
1	D	1501	LEU
1	D	1528	THR
1	D	1556	THR
1	D	1580	LEU
1	D	1585	LYS
1	D	1642	THR
1	D	1680	ARG
1	D	1722	VAL
1	D	1754	LYS
1	D	1756	ILE
1	D	1780	ASN
1	D	1842	VAL
1	D	1844	LYS
1	E	21	GLN
1	E	22	PHE
1	E	35	PHE
1	E	38	ASP
1	E	44	VAL
1	E	52	THR
1	E	67	SER
1	E	179	LYS
1	E	182	VAL
1	E	184	ASN
1	E	202	GLU
1	E	217	PHE
1	E	221	LEU

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Mol	Chain	Res	Type
1	E	237	MET
1	E	253	ARG
1	E	272	GLU
1	E	277	LEU
1	E	390	VAL
1	E	392	THR
1	E	401	THR
1	E	416	LEU
1	E	435	GLU
1	E	447	LEU
1	E	458	THR
1	E	478	GLU
1	E	489	VAL
1	E	493	VAL
1	E	520	ARG
1	E	522	LEU
1	E	527	GLN
1	E	622	ILE
1	E	624	LYS
1	E	626	VAL
1	E	672	THR
1	E	719	GLN
1	E	731	THR
1	E	738	ASN
1	E	748	LEU
1	E	754	ASP
1	E	776	GLU
1	E	797	THR
1	E	806	VAL
1	E	823	ILE
1	E	826	MET
1	E	827	SER
1	E	862	LEU
1	E	864	VAL
1	E	901	MET
1	E	940	THR
1	E	999	LYS
1	E	1001	VAL
1	E	1020	VAL
1	E	1022	THR
1	E	1047	LEU
1	E	1050	CYS

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Mol	Chain	Res	Type
1	E	1067	LEU
1	E	1073	THR
1	E	1079	LYS
1	E	1090	LYS
1	E	1096	SER
1	E	1166	LYS
1	E	1183	ARG
1	E	1184	LEU
1	E	1197	THR
1	E	1208	VAL
1	E	1254	VAL
1	E	1262	LYS
1	E	1267	ASP
1	E	1283	MET
1	E	1298	ILE
1	E	1307	THR
1	E	1317	GLU
1	E	1327	CYS
1	E	1329	VAL
1	E	1332	TYR
1	E	1362	PRO
1	E	1366	SER
1	E	1370	THR
1	E	1392	LEU
1	E	1430	ARG
1	E	1432	HIS
1	E	1442	ASN
1	E	1501	LEU
1	E	1528	THR
1	E	1556	THR
1	E	1580	LEU
1	E	1585	LYS
1	E	1642	THR
1	E	1680	ARG
1	E	1722	VAL
1	E	1754	LYS
1	E	1756	ILE
1	E	1780	ASN
1	E	1842	VAL
1	E	1844	LYS
1	F	21	GLN
1	F	22	PHE

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Mol	Chain	Res	Type
1	F	35	PHE
1	F	38	ASP
1	F	44	VAL
1	F	52	THR
1	F	67	SER
1	F	179	LYS
1	F	182	VAL
1	F	184	ASN
1	F	202	GLU
1	F	217	PHE
1	F	221	LEU
1	F	237	MET
1	F	253	ARG
1	F	272	GLU
1	F	277	LEU
1	F	378	LEU
1	F	390	VAL
1	F	392	THR
1	F	401	THR
1	F	416	LEU
1	F	435	GLU
1	F	447	LEU
1	F	458	THR
1	F	478	GLU
1	F	489	VAL
1	F	493	VAL
1	F	520	ARG
1	F	522	LEU
1	F	527	GLN
1	F	622	ILE
1	F	624	LYS
1	F	626	VAL
1	F	672	THR
1	F	719	GLN
1	F	731	THR
1	F	738	ASN
1	F	748	LEU
1	F	754	ASP
1	F	776	GLU
1	F	797	THR
1	F	806	VAL
1	F	823	ILE

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Mol	Chain	Res	Type
1	F	826	MET
1	F	827	SER
1	F	862	LEU
1	F	864	VAL
1	F	901	MET
1	F	915	GLU
1	F	940	THR
1	F	999	LYS
1	F	1001	VAL
1	F	1020	VAL
1	F	1022	THR
1	F	1047	LEU
1	F	1050	CYS
1	F	1067	LEU
1	F	1073	THR
1	F	1079	LYS
1	F	1090	LYS
1	F	1096	SER
1	F	1166	LYS
1	F	1183	ARG
1	F	1184	LEU
1	F	1197	THR
1	F	1208	VAL
1	F	1254	VAL
1	F	1262	LYS
1	F	1267	ASP
1	F	1283	MET
1	F	1298	ILE
1	F	1307	THR
1	F	1317	GLU
1	F	1327	CYS
1	F	1329	VAL
1	F	1332	TYR
1	F	1362	PRO
1	F	1366	SER
1	F	1370	THR
1	F	1372	THR
1	F	1392	LEU
1	F	1430	ARG
1	F	1432	HIS
1	F	1442	ASN
1	F	1501	LEU

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Mol	Chain	Res	Type
1	F	1528	THR
1	F	1556	THR
1	F	1580	LEU
1	F	1585	LYS
1	F	1642	THR
1	F	1680	ARG
1	F	1722	VAL
1	F	1754	LYS
1	F	1756	ILE
1	F	1780	ASN
1	F	1842	VAL
1	F	1844	LYS
2	G	38	ASN
2	G	52	ASP
2	G	99	ASN
2	G	111	GLU
2	G	119	THR
2	G	140	LYS
2	G	166	THR
2	G	173	LEU
2	G	197	GLU
2	G	213	LEU
2	G	246	LEU
2	G	264	ARG
2	G	279	THR
2	G	338	MET
2	G	339	LEU
2	G	340	SER
2	G	353	VAL
2	G	369	SER
2	G	377	LEU
2	G	453	LYS
2	G	462	THR
2	G	472	SER
2	G	497	LYS
2	G	576	LYS
2	G	593	LEU
2	G	598	THR
2	G	616	THR
2	G	659	LEU
2	G	665	LEU
2	G	670	ARG

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Mol	Chain	Res	Type
2	G	698	LEU
2	G	730	LEU
2	G	733	THR
2	G	777	THR
2	G	794	MET
2	G	805	VAL
2	G	845	THR
2	G	880	LEU
2	G	893	SER
2	G	910	GLN
2	G	953	ARG
2	G	972	LEU
2	G	973	LEU
2	G	1005	SER
2	G	1016	PRO
2	G	1023	ARG
2	G	1040	LEU
2	G	1048	VAL
2	G	1055	HIS
2	G	1110	ASP
2	G	1160	THR
2	G	1167	SER
2	G	1189	THR
2	G	1195	VAL
2	G	1211	LEU
2	G	1213	LEU
2	G	1217	ASN
2	G	1236	LEU
2	G	1265	MET
2	G	1313	SER
2	G	1317	ARG
2	G	1343	VAL
2	G	1347	LEU
2	G	1348	LEU
2	G	1375	THR
2	G	1408	SER
2	G	1439	LYS
2	G	1470	THR
2	G	1478	ASN
2	G	1482	SER
2	G	1485	CYS
2	G	1495	THR

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Mol	Chain	Res	Type
2	G	1499	VAL
2	G	1503	ILE
2	G	1530	LYS
2	G	1531	VAL
2	G	1549	THR
2	G	1585	SER
2	G	1586	SER
2	G	1590	ARG
2	G	1599	ASP
2	G	1609	THR
2	G	1610	CYS
2	G	1616	VAL
2	G	1629	VAL
2	G	1637	LEU
2	G	1639	LYS
2	G	1672	GLN
2	G	1679	ASP
2	G	1680	LEU
2	G	1750	LYS
2	G	1761	SER
2	G	1770	LEU
2	G	1774	THR
2	G	1775	GLN
2	G	1778	GLN
2	G	1782	THR
2	G	1795	LYS
2	G	1818	LEU
2	G	1847	LEU
2	G	1849	ARG
2	G	1914	LEU
2	G	1921	LYS
2	G	1930	SER
2	G	1933	LEU
2	G	1935	GLU
2	G	1946	GLU
2	G	1954	LYS
2	G	1956	ARG
2	G	1973	SER
2	G	1979	THR
2	G	1981	LEU
2	G	2002	LYS
2	G	2015	THR

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Mol	Chain	Res	Type
2	G	2033	THR
2	H	38	ASN
2	H	52	ASP
2	H	99	ASN
2	H	111	GLU
2	H	119	THR
2	H	140	LYS
2	H	166	THR
2	H	173	LEU
2	H	197	GLU
2	H	213	LEU
2	H	246	LEU
2	H	264	ARG
2	H	279	THR
2	H	338	MET
2	H	339	LEU
2	H	340	SER
2	H	353	VAL
2	H	369	SER
2	H	377	LEU
2	H	453	LYS
2	H	462	THR
2	H	472	SER
2	H	497	LYS
2	H	576	LYS
2	H	593	LEU
2	H	598	THR
2	H	616	THR
2	H	659	LEU
2	H	665	LEU
2	H	670	ARG
2	H	698	LEU
2	H	730	LEU
2	H	733	THR
2	H	777	THR
2	H	794	MET
2	H	805	VAL
2	H	845	THR
2	H	880	LEU
2	H	893	SER
2	H	910	GLN
2	H	953	ARG

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Mol	Chain	Res	Type
2	H	972	LEU
2	H	973	LEU
2	H	1005	SER
2	H	1016	PRO
2	H	1023	ARG
2	H	1040	LEU
2	H	1048	VAL
2	H	1055	HIS
2	H	1110	ASP
2	H	1160	THR
2	H	1167	SER
2	H	1189	THR
2	H	1195	VAL
2	H	1211	LEU
2	H	1213	LEU
2	H	1217	ASN
2	H	1236	LEU
2	H	1265	MET
2	H	1313	SER
2	H	1317	ARG
2	H	1343	VAL
2	H	1347	LEU
2	H	1348	LEU
2	H	1375	THR
2	H	1408	SER
2	H	1439	LYS
2	H	1470	THR
2	H	1478	ASN
2	H	1482	SER
2	H	1485	CYS
2	H	1495	THR
2	H	1499	VAL
2	H	1503	ILE
2	H	1530	LYS
2	H	1531	VAL
2	H	1549	THR
2	H	1585	SER
2	H	1586	SER
2	H	1590	ARG
2	H	1599	ASP
2	H	1609	THR
2	H	1610	CYS

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Mol	Chain	Res	Type
2	H	1616	VAL
2	H	1629	VAL
2	H	1637	LEU
2	H	1639	LYS
2	H	1672	GLN
2	H	1679	ASP
2	H	1680	LEU
2	H	1750	LYS
2	H	1761	SER
2	H	1770	LEU
2	H	1774	THR
2	H	1775	GLN
2	H	1778	GLN
2	H	1782	THR
2	H	1795	LYS
2	H	1818	LEU
2	H	1847	LEU
2	H	1914	LEU
2	H	1921	LYS
2	H	1930	SER
2	H	1933	LEU
2	H	1935	GLU
2	H	1946	GLU
2	H	1954	LYS
2	H	1956	ARG
2	H	1973	SER
2	H	1979	THR
2	H	1981	LEU
2	H	1986	LYS
2	H	2002	LYS
2	H	2015	THR
2	H	2033	THR
2	I	38	ASN
2	I	52	ASP
2	I	99	ASN
2	I	111	GLU
2	I	119	THR
2	I	140	LYS
2	I	166	THR
2	I	173	LEU
2	I	197	GLU
2	I	213	LEU

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Mol	Chain	Res	Type
2	I	246	LEU
2	I	264	ARG
2	I	279	THR
2	I	338	MET
2	I	339	LEU
2	I	340	SER
2	I	353	VAL
2	I	369	SER
2	I	377	LEU
2	I	453	LYS
2	I	462	THR
2	I	472	SER
2	I	497	LYS
2	I	576	LYS
2	I	593	LEU
2	I	598	THR
2	I	616	THR
2	I	659	LEU
2	I	665	LEU
2	I	670	ARG
2	I	698	LEU
2	I	730	LEU
2	I	733	THR
2	I	777	THR
2	I	794	MET
2	I	805	VAL
2	I	845	THR
2	I	880	LEU
2	I	893	SER
2	I	910	GLN
2	I	953	ARG
2	I	972	LEU
2	I	973	LEU
2	I	1005	SER
2	I	1016	PRO
2	I	1023	ARG
2	I	1040	LEU
2	I	1048	VAL
2	I	1055	HIS
2	I	1110	ASP
2	I	1160	THR
2	I	1167	SER

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Mol	Chain	Res	Type
2	I	1189	THR
2	I	1195	VAL
2	I	1211	LEU
2	I	1213	LEU
2	I	1217	ASN
2	I	1236	LEU
2	I	1265	MET
2	I	1313	SER
2	I	1317	ARG
2	I	1343	VAL
2	I	1347	LEU
2	I	1348	LEU
2	I	1375	THR
2	I	1408	SER
2	I	1439	LYS
2	I	1470	THR
2	I	1478	ASN
2	I	1482	SER
2	I	1485	CYS
2	I	1495	THR
2	I	1499	VAL
2	I	1503	ILE
2	I	1530	LYS
2	I	1531	VAL
2	I	1549	THR
2	I	1585	SER
2	I	1586	SER
2	I	1590	ARG
2	I	1599	ASP
2	I	1609	THR
2	I	1610	CYS
2	I	1616	VAL
2	I	1629	VAL
2	I	1637	LEU
2	I	1639	LYS
2	I	1672	GLN
2	I	1679	ASP
2	I	1680	LEU
2	I	1750	LYS
2	I	1761	SER
2	I	1770	LEU
2	I	1774	THR

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Mol	Chain	Res	Type
2	I	1775	GLN
2	I	1778	GLN
2	I	1782	THR
2	I	1795	LYS
2	I	1818	LEU
2	I	1847	LEU
2	I	1914	LEU
2	I	1921	LYS
2	I	1930	SER
2	I	1933	LEU
2	I	1935	GLU
2	I	1946	GLU
2	I	1954	LYS
2	I	1956	ARG
2	I	1973	SER
2	I	1979	THR
2	I	1981	LEU
2	I	2002	LYS
2	I	2015	THR
2	I	2033	THR
2	J	38	ASN
2	J	52	ASP
2	J	99	ASN
2	J	111	GLU
2	J	119	THR
2	J	140	LYS
2	J	166	THR
2	J	173	LEU
2	J	197	GLU
2	J	213	LEU
2	J	246	LEU
2	J	264	ARG
2	J	279	THR
2	J	338	MET
2	J	339	LEU
2	J	340	SER
2	J	353	VAL
2	J	369	SER
2	J	377	LEU
2	J	453	LYS
2	J	462	THR
2	J	472	SER

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Mol	Chain	Res	Type
2	J	497	LYS
2	J	576	LYS
2	J	593	LEU
2	J	598	THR
2	J	616	THR
2	J	659	LEU
2	J	665	LEU
2	J	670	ARG
2	J	698	LEU
2	J	730	LEU
2	J	733	THR
2	J	777	THR
2	J	794	MET
2	J	805	VAL
2	J	845	THR
2	J	880	LEU
2	J	893	SER
2	J	910	GLN
2	J	953	ARG
2	J	972	LEU
2	J	973	LEU
2	J	1005	SER
2	J	1016	PRO
2	J	1023	ARG
2	J	1040	LEU
2	J	1048	VAL
2	J	1055	HIS
2	J	1110	ASP
2	J	1160	THR
2	J	1167	SER
2	J	1189	THR
2	J	1195	VAL
2	J	1211	LEU
2	J	1213	LEU
2	J	1217	ASN
2	J	1236	LEU
2	J	1265	MET
2	J	1313	SER
2	J	1317	ARG
2	J	1343	VAL
2	J	1347	LEU
2	J	1348	LEU

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Mol	Chain	Res	Type
2	J	1375	THR
2	J	1408	SER
2	J	1439	LYS
2	J	1470	THR
2	J	1478	ASN
2	J	1482	SER
2	J	1485	CYS
2	J	1495	THR
2	J	1499	VAL
2	J	1503	ILE
2	J	1530	LYS
2	J	1531	VAL
2	J	1549	THR
2	J	1585	SER
2	J	1586	SER
2	J	1590	ARG
2	J	1599	ASP
2	J	1609	THR
2	J	1610	CYS
2	J	1616	VAL
2	J	1629	VAL
2	J	1637	LEU
2	J	1639	LYS
2	J	1672	GLN
2	J	1679	ASP
2	J	1680	LEU
2	J	1750	LYS
2	J	1761	SER
2	J	1770	LEU
2	J	1774	THR
2	J	1775	GLN
2	J	1778	GLN
2	J	1782	THR
2	J	1795	LYS
2	J	1818	LEU
2	J	1847	LEU
2	J	1914	LEU
2	J	1921	LYS
2	J	1930	SER
2	J	1933	LEU
2	J	1935	GLU
2	J	1946	GLU

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Mol	Chain	Res	Type
2	J	1954	LYS
2	J	1956	ARG
2	J	1973	SER
2	J	1979	THR
2	J	1981	LEU
2	J	1986	LYS
2	J	2002	LYS
2	J	2015	THR
2	J	2033	THR
2	K	38	ASN
2	K	52	ASP
2	K	99	ASN
2	K	111	GLU
2	K	119	THR
2	K	140	LYS
2	K	166	THR
2	K	173	LEU
2	K	197	GLU
2	K	213	LEU
2	K	246	LEU
2	K	264	ARG
2	K	279	THR
2	K	338	MET
2	K	339	LEU
2	K	340	SER
2	K	353	VAL
2	K	369	SER
2	K	377	LEU
2	K	453	LYS
2	K	462	THR
2	K	472	SER
2	K	497	LYS
2	K	576	LYS
2	K	593	LEU
2	K	598	THR
2	K	616	THR
2	K	659	LEU
2	K	665	LEU
2	K	670	ARG
2	K	698	LEU
2	K	730	LEU
2	K	733	THR

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Mol	Chain	Res	Type
2	K	777	THR
2	K	794	MET
2	K	805	VAL
2	K	845	THR
2	K	880	LEU
2	K	893	SER
2	K	910	GLN
2	K	953	ARG
2	K	972	LEU
2	K	973	LEU
2	K	1005	SER
2	K	1016	PRO
2	K	1023	ARG
2	K	1040	LEU
2	K	1048	VAL
2	K	1055	HIS
2	K	1110	ASP
2	K	1160	THR
2	K	1167	SER
2	K	1189	THR
2	K	1195	VAL
2	K	1211	LEU
2	K	1213	LEU
2	K	1217	ASN
2	K	1236	LEU
2	K	1265	MET
2	K	1313	SER
2	K	1317	ARG
2	K	1343	VAL
2	K	1347	LEU
2	K	1348	LEU
2	K	1375	THR
2	K	1408	SER
2	K	1439	LYS
2	K	1470	THR
2	K	1478	ASN
2	K	1482	SER
2	K	1485	CYS
2	K	1495	THR
2	K	1499	VAL
2	K	1503	ILE
2	K	1530	LYS

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Mol	Chain	Res	Type
2	K	1531	VAL
2	K	1549	THR
2	K	1585	SER
2	K	1586	SER
2	K	1590	ARG
2	K	1599	ASP
2	K	1609	THR
2	K	1610	CYS
2	K	1616	VAL
2	K	1629	VAL
2	K	1637	LEU
2	K	1639	LYS
2	K	1672	GLN
2	K	1679	ASP
2	K	1680	LEU
2	K	1750	LYS
2	K	1761	SER
2	K	1770	LEU
2	K	1774	THR
2	K	1775	GLN
2	K	1778	GLN
2	K	1782	THR
2	K	1795	LYS
2	K	1818	LEU
2	K	1847	LEU
2	K	1914	LEU
2	K	1921	LYS
2	K	1930	SER
2	K	1933	LEU
2	K	1935	GLU
2	K	1946	GLU
2	K	1954	LYS
2	K	1956	ARG
2	K	1973	SER
2	K	1979	THR
2	K	1981	LEU
2	K	2002	LYS
2	K	2015	THR
2	K	2033	THR
2	L	38	ASN
2	L	52	ASP
2	L	99	ASN

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Mol	Chain	Res	Type
2	L	111	GLU
2	L	119	THR
2	L	140	LYS
2	L	166	THR
2	L	173	LEU
2	L	197	GLU
2	L	213	LEU
2	L	246	LEU
2	L	264	ARG
2	L	279	THR
2	L	338	MET
2	L	339	LEU
2	L	340	SER
2	L	353	VAL
2	L	369	SER
2	L	377	LEU
2	L	453	LYS
2	L	462	THR
2	L	472	SER
2	L	497	LYS
2	L	576	LYS
2	L	593	LEU
2	L	598	THR
2	L	616	THR
2	L	659	LEU
2	L	665	LEU
2	L	670	ARG
2	L	698	LEU
2	L	730	LEU
2	L	733	THR
2	L	777	THR
2	L	794	MET
2	L	805	VAL
2	L	845	THR
2	L	880	LEU
2	L	893	SER
2	L	910	GLN
2	L	953	ARG
2	L	972	LEU
2	L	973	LEU
2	L	1005	SER
2	L	1016	PRO

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Mol	Chain	Res	Type
2	L	1023	ARG
2	L	1040	LEU
2	L	1048	VAL
2	L	1055	HIS
2	L	1110	ASP
2	L	1160	THR
2	L	1167	SER
2	L	1189	THR
2	L	1195	VAL
2	L	1211	LEU
2	L	1213	LEU
2	L	1217	ASN
2	L	1236	LEU
2	L	1265	MET
2	L	1313	SER
2	L	1317	ARG
2	L	1343	VAL
2	L	1347	LEU
2	L	1348	LEU
2	L	1375	THR
2	L	1408	SER
2	L	1439	LYS
2	L	1470	THR
2	L	1478	ASN
2	L	1482	SER
2	L	1485	CYS
2	L	1495	THR
2	L	1499	VAL
2	L	1503	ILE
2	L	1530	LYS
2	L	1531	VAL
2	L	1549	THR
2	L	1585	SER
2	L	1586	SER
2	L	1590	ARG
2	L	1599	ASP
2	L	1609	THR
2	L	1610	CYS
2	L	1616	VAL
2	L	1629	VAL
2	L	1637	LEU
2	L	1639	LYS

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Mol	Chain	Res	Type
2	L	1672	GLN
2	L	1679	ASP
2	L	1680	LEU
2	L	1750	LYS
2	L	1761	SER
2	L	1770	LEU
2	L	1774	THR
2	L	1775	GLN
2	L	1778	GLN
2	L	1782	THR
2	L	1795	LYS
2	L	1818	LEU
2	L	1847	LEU
2	L	1849	ARG
2	L	1914	LEU
2	L	1921	LYS
2	L	1930	SER
2	L	1933	LEU
2	L	1935	GLU
2	L	1946	GLU
2	L	1954	LYS
2	L	1956	ARG
2	L	1973	SER
2	L	1979	THR
2	L	1981	LEU
2	L	2002	LYS
2	L	2015	THR
2	L	2033	THR
3	M	3	SER
3	M	8	ARG
3	M	14	GLU
3	M	20	ILE
3	M	49	LEU
3	M	56	LEU
3	M	83	LYS
3	M	95	ASN
3	M	108	VAL
3	M	142	VAL
3	M	147	SER
3	M	148	ILE
3	M	149	PHE
3	M	150	ILE

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Mol	Chain	Res	Type
3	N	3	SER
3	N	8	ARG
3	N	14	GLU
3	N	20	ILE
3	N	49	LEU
3	N	56	LEU
3	N	83	LYS
3	N	95	ASN
3	N	108	VAL
3	N	142	VAL
3	N	147	SER
3	N	148	ILE
3	N	149	PHE
3	N	150	ILE
3	O	3	SER
3	O	8	ARG
3	O	14	GLU
3	O	20	ILE
3	O	49	LEU
3	O	56	LEU
3	O	83	LYS
3	O	95	ASN
3	O	108	VAL
3	O	142	VAL
3	O	147	SER
3	O	148	ILE
3	O	149	PHE
3	O	150	ILE
3	P	3	SER
3	P	8	ARG
3	P	14	GLU
3	P	20	ILE
3	P	49	LEU
3	P	56	LEU
3	P	83	LYS
3	P	95	ASN
3	P	108	VAL
3	P	142	VAL
3	P	147	SER
3	P	148	ILE
3	P	149	PHE
3	P	150	ILE

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Mol	Chain	Res	Type
3	Q	3	SER
3	Q	8	ARG
3	Q	14	GLU
3	Q	20	ILE
3	Q	49	LEU
3	Q	56	LEU
3	Q	83	LYS
3	Q	95	ASN
3	Q	108	VAL
3	Q	142	VAL
3	Q	147	SER
3	Q	148	ILE
3	Q	149	PHE
3	Q	150	ILE
3	R	3	SER
3	R	8	ARG
3	R	14	GLU
3	R	20	ILE
3	R	49	LEU
3	R	56	LEU
3	R	83	LYS
3	R	95	ASN
3	R	108	VAL
3	R	136	ASP
3	R	142	VAL
3	R	147	SER
3	R	148	ILE
3	R	149	PHE
3	R	150	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (420) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	261	GLN
1	A	335	HIS
1	A	344	GLN
1	A	379	ASN
1	A	438	ASN
1	A	719	GLN
1	A	738	ASN
1	A	851	ASN

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Mol	Chain	Res	Type
1	A	987	ASN
1	A	989	GLN
1	A	1064	ASN
1	A	1066	ASN
1	A	1146	HIS
1	A	1239	HIS
1	A	1271	GLN
1	A	1272	ASN
1	A	1288	ASN
1	A	1432	HIS
1	A	1442	ASN
1	A	1507	GLN
1	A	1510	ASN
1	A	1563	HIS
1	A	1610	ASN
1	A	1657	HIS
1	A	1690	ASN
1	A	1695	ASN
1	A	1780	ASN
1	B	21	GLN
1	B	261	GLN
1	B	344	GLN
1	B	379	ASN
1	B	438	ASN
1	B	719	GLN
1	B	738	ASN
1	B	851	ASN
1	B	987	ASN
1	B	989	GLN
1	B	1064	ASN
1	B	1066	ASN
1	B	1146	HIS
1	B	1239	HIS
1	B	1271	GLN
1	B	1288	ASN
1	B	1432	HIS
1	B	1442	ASN
1	B	1507	GLN
1	B	1510	ASN
1	B	1563	HIS
1	B	1610	ASN
1	B	1657	HIS

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Mol	Chain	Res	Type
1	B	1690	ASN
1	B	1695	ASN
1	B	1780	ASN
1	C	11	HIS
1	C	21	GLN
1	C	261	GLN
1	C	335	HIS
1	C	344	GLN
1	C	379	ASN
1	C	438	ASN
1	C	719	GLN
1	C	738	ASN
1	C	851	ASN
1	C	987	ASN
1	C	989	GLN
1	C	1064	ASN
1	C	1066	ASN
1	C	1146	HIS
1	C	1239	HIS
1	C	1271	GLN
1	C	1272	ASN
1	C	1288	ASN
1	C	1432	HIS
1	C	1442	ASN
1	C	1507	GLN
1	C	1510	ASN
1	C	1563	HIS
1	C	1610	ASN
1	C	1657	HIS
1	C	1690	ASN
1	C	1695	ASN
1	C	1780	ASN
1	D	21	GLN
1	D	261	GLN
1	D	335	HIS
1	D	344	GLN
1	D	379	ASN
1	D	438	ASN
1	D	719	GLN
1	D	738	ASN
1	D	851	ASN
1	D	987	ASN

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Mol	Chain	Res	Type
1	D	989	GLN
1	D	1066	ASN
1	D	1146	HIS
1	D	1239	HIS
1	D	1271	GLN
1	D	1288	ASN
1	D	1432	HIS
1	D	1442	ASN
1	D	1507	GLN
1	D	1510	ASN
1	D	1563	HIS
1	D	1610	ASN
1	D	1657	HIS
1	D	1690	ASN
1	D	1695	ASN
1	D	1780	ASN
1	E	21	GLN
1	E	261	GLN
1	E	335	HIS
1	E	344	GLN
1	E	379	ASN
1	E	438	ASN
1	E	719	GLN
1	E	738	ASN
1	E	851	ASN
1	E	987	ASN
1	E	989	GLN
1	E	1064	ASN
1	E	1066	ASN
1	E	1146	HIS
1	E	1239	HIS
1	E	1271	GLN
1	E	1288	ASN
1	E	1432	HIS
1	E	1442	ASN
1	E	1507	GLN
1	E	1510	ASN
1	E	1563	HIS
1	E	1610	ASN
1	E	1657	HIS
1	E	1690	ASN
1	E	1695	ASN

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Mol	Chain	Res	Type
1	E	1780	ASN
1	F	11	HIS
1	F	21	GLN
1	F	261	GLN
1	F	344	GLN
1	F	379	ASN
1	F	438	ASN
1	F	719	GLN
1	F	738	ASN
1	F	851	ASN
1	F	987	ASN
1	F	989	GLN
1	F	1064	ASN
1	F	1066	ASN
1	F	1146	HIS
1	F	1239	HIS
1	F	1271	GLN
1	F	1288	ASN
1	F	1432	HIS
1	F	1442	ASN
1	F	1507	GLN
1	F	1510	ASN
1	F	1563	HIS
1	F	1610	ASN
1	F	1657	HIS
1	F	1690	ASN
1	F	1695	ASN
1	F	1780	ASN
2	G	99	ASN
2	G	102	HIS
2	G	330	ASN
2	G	343	ASN
2	G	350	GLN
2	G	354	ASN
2	G	384	GLN
2	G	440	ASN
2	G	500	HIS
2	G	517	HIS
2	G	558	ASN
2	G	572	ASN
2	G	612	ASN
2	G	718	ASN

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Mol	Chain	Res	Type
2	G	747	HIS
2	G	910	GLN
2	G	993	GLN
2	G	1008	GLN
2	G	1049	GLN
2	G	1055	HIS
2	G	1217	ASN
2	G	1220	GLN
2	G	1302	HIS
2	G	1341	ASN
2	G	1383	ASN
2	G	1451	GLN
2	G	1476	ASN
2	G	1523	ASN
2	G	1529	GLN
2	G	1595	ASN
2	G	1628	HIS
2	G	1659	GLN
2	G	1669	GLN
2	G	1712	ASN
2	G	1775	GLN
2	G	1807	HIS
2	G	1890	ASN
2	G	1995	ASN
2	G	2013	ASN
2	G	2020	GLN
2	H	99	ASN
2	H	102	HIS
2	H	330	ASN
2	H	350	GLN
2	H	354	ASN
2	H	384	GLN
2	H	440	ASN
2	H	500	HIS
2	H	517	HIS
2	H	558	ASN
2	H	572	ASN
2	H	612	ASN
2	H	718	ASN
2	H	747	HIS
2	H	910	GLN
2	H	993	GLN

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Mol	Chain	Res	Type
2	H	1008	GLN
2	H	1049	GLN
2	H	1055	HIS
2	H	1217	ASN
2	H	1220	GLN
2	H	1302	HIS
2	H	1341	ASN
2	H	1383	ASN
2	H	1451	GLN
2	H	1476	ASN
2	H	1523	ASN
2	H	1529	GLN
2	H	1595	ASN
2	H	1628	HIS
2	H	1659	GLN
2	H	1669	GLN
2	H	1712	ASN
2	H	1775	GLN
2	H	1807	HIS
2	H	1890	ASN
2	H	1995	ASN
2	H	2013	ASN
2	H	2020	GLN
2	I	99	ASN
2	I	102	HIS
2	I	330	ASN
2	I	350	GLN
2	I	354	ASN
2	I	384	GLN
2	I	440	ASN
2	I	500	HIS
2	I	517	HIS
2	I	558	ASN
2	I	572	ASN
2	I	612	ASN
2	I	718	ASN
2	I	747	HIS
2	I	910	GLN
2	I	993	GLN
2	I	1008	GLN
2	I	1049	GLN
2	I	1055	HIS

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Mol	Chain	Res	Type
2	I	1217	ASN
2	I	1220	GLN
2	I	1302	HIS
2	I	1341	ASN
2	I	1383	ASN
2	I	1451	GLN
2	I	1476	ASN
2	I	1523	ASN
2	I	1529	GLN
2	I	1595	ASN
2	I	1628	HIS
2	I	1659	GLN
2	I	1669	GLN
2	I	1712	ASN
2	I	1775	GLN
2	I	1807	HIS
2	I	1890	ASN
2	I	1995	ASN
2	I	2013	ASN
2	I	2020	GLN
2	J	99	ASN
2	J	102	HIS
2	J	330	ASN
2	J	350	GLN
2	J	354	ASN
2	J	384	GLN
2	J	440	ASN
2	J	500	HIS
2	J	517	HIS
2	J	558	ASN
2	J	572	ASN
2	J	612	ASN
2	J	718	ASN
2	J	747	HIS
2	J	910	GLN
2	J	993	GLN
2	J	1008	GLN
2	J	1049	GLN
2	J	1055	HIS
2	J	1217	ASN
2	J	1220	GLN
2	J	1302	HIS

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Mol	Chain	Res	Type
2	J	1341	ASN
2	J	1383	ASN
2	J	1451	GLN
2	J	1476	ASN
2	J	1523	ASN
2	J	1529	GLN
2	J	1595	ASN
2	J	1628	HIS
2	J	1659	GLN
2	J	1669	GLN
2	J	1712	ASN
2	J	1775	GLN
2	J	1807	HIS
2	J	1890	ASN
2	J	1995	ASN
2	J	2013	ASN
2	J	2020	GLN
2	K	99	ASN
2	K	102	HIS
2	K	330	ASN
2	K	343	ASN
2	K	350	GLN
2	K	354	ASN
2	K	384	GLN
2	K	440	ASN
2	K	500	HIS
2	K	517	HIS
2	K	558	ASN
2	K	572	ASN
2	K	612	ASN
2	K	718	ASN
2	K	747	HIS
2	K	910	GLN
2	K	993	GLN
2	K	1008	GLN
2	K	1049	GLN
2	K	1055	HIS
2	K	1217	ASN
2	K	1220	GLN
2	K	1302	HIS
2	K	1341	ASN
2	K	1383	ASN

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Mol	Chain	Res	Type
2	K	1451	GLN
2	K	1476	ASN
2	K	1523	ASN
2	K	1529	GLN
2	K	1595	ASN
2	K	1628	HIS
2	K	1659	GLN
2	K	1669	GLN
2	K	1712	ASN
2	K	1775	GLN
2	K	1807	HIS
2	K	1890	ASN
2	K	1995	ASN
2	K	2013	ASN
2	K	2020	GLN
2	L	99	ASN
2	L	102	HIS
2	L	330	ASN
2	L	350	GLN
2	L	354	ASN
2	L	384	GLN
2	L	440	ASN
2	L	500	HIS
2	L	517	HIS
2	L	558	ASN
2	L	572	ASN
2	L	612	ASN
2	L	718	ASN
2	L	747	HIS
2	L	910	GLN
2	L	993	GLN
2	L	1008	GLN
2	L	1049	GLN
2	L	1055	HIS
2	L	1217	ASN
2	L	1220	GLN
2	L	1302	HIS
2	L	1341	ASN
2	L	1383	ASN
2	L	1451	GLN
2	L	1476	ASN
2	L	1523	ASN

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Mol	Chain	Res	Type
2	L	1529	GLN
2	L	1595	ASN
2	L	1628	HIS
2	L	1659	GLN
2	L	1669	GLN
2	L	1712	ASN
2	L	1716	ASN
2	L	1775	GLN
2	L	1807	HIS
2	L	1890	ASN
2	L	1995	ASN
2	L	2013	ASN
2	L	2020	GLN
3	M	94	ASN
3	M	95	ASN
3	M	146	ASN
3	N	40	ASN
3	N	94	ASN
3	N	95	ASN
3	N	146	ASN
3	O	94	ASN
3	O	95	ASN
3	O	146	ASN
3	P	94	ASN
3	P	95	ASN
3	P	146	ASN
3	Q	94	ASN
3	Q	95	ASN
3	Q	146	ASN
3	R	40	ASN
3	R	94	ASN
3	R	95	ASN
3	R	146	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PNS	A	1901	1	13,20,21	0.76	0	18,26,29	1.53	5 (27%)
4	PNS	B	1901	1	13,20,21	0.75	0	18,26,29	1.50	4 (22%)
4	PNS	C	1901	1	13,20,21	0.75	0	18,26,29	1.52	5 (27%)
4	PNS	D	1901	1	13,20,21	0.76	0	18,26,29	1.51	4 (22%)
4	PNS	E	1901	1	13,20,21	0.76	0	18,26,29	1.51	4 (22%)
4	PNS	F	1901	1	13,20,21	0.75	0	18,26,29	1.52	5 (27%)
5	FMN	G	2101	-	31,33,33	2.09	8 (25%)	40,50,50	2.59	12 (30%)
5	FMN	H	2101	-	31,33,33	2.10	7 (22%)	40,50,50	2.61	13 (32%)
5	FMN	I	2101	-	31,33,33	2.11	8 (25%)	40,50,50	2.60	13 (32%)
5	FMN	J	2101	-	31,33,33	2.10	8 (25%)	40,50,50	2.59	12 (30%)
5	FMN	K	2101	-	31,33,33	2.10	8 (25%)	40,50,50	2.60	13 (32%)
5	FMN	L	2101	-	31,33,33	2.08	8 (25%)	40,50,50	2.58	13 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PNS	A	1901	1	-	6/24/26/27	-
4	PNS	B	1901	1	-	7/24/26/27	-
4	PNS	C	1901	1	-	6/24/26/27	-
4	PNS	D	1901	1	-	7/24/26/27	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PNS	E	1901	1	-	6/24/26/27	-
4	PNS	F	1901	1	-	6/24/26/27	-
5	FMN	G	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	H	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	I	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	J	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	K	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	L	2101	-	-	6/18/18/18	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	2101	FMN	C4A-C10	8.44	1.47	1.38
5	I	2101	FMN	C4A-C10	8.40	1.47	1.38
5	H	2101	FMN	C4A-C10	8.39	1.47	1.38
5	J	2101	FMN	C4A-C10	8.34	1.47	1.38
5	G	2101	FMN	C4A-C10	8.34	1.47	1.38
5	L	2101	FMN	C4A-C10	8.19	1.47	1.38
5	G	2101	FMN	C1'-N10	-3.60	1.44	1.48
5	I	2101	FMN	C1'-N10	-3.49	1.44	1.48
5	K	2101	FMN	C1'-N10	-3.46	1.44	1.48
5	L	2101	FMN	C1'-N10	-3.44	1.44	1.48
5	H	2101	FMN	C1'-N10	-3.44	1.44	1.48
5	J	2101	FMN	C1'-N10	-3.43	1.44	1.48
5	G	2101	FMN	C6-C5A	-3.31	1.36	1.41
5	J	2101	FMN	C6-C5A	-3.24	1.36	1.41
5	L	2101	FMN	C6-C5A	-3.20	1.36	1.41
5	H	2101	FMN	C6-C5A	-3.16	1.36	1.41
5	I	2101	FMN	C6-C5A	-3.05	1.37	1.41
5	K	2101	FMN	C4-C4A	3.05	1.46	1.41
5	K	2101	FMN	C6-C5A	-3.05	1.37	1.41
5	H	2101	FMN	C4-C4A	2.99	1.46	1.41
5	I	2101	FMN	C4-C4A	2.98	1.46	1.41
5	L	2101	FMN	C4-C4A	2.91	1.46	1.41
5	J	2101	FMN	C4-C4A	2.80	1.46	1.41
5	G	2101	FMN	C4-C4A	2.62	1.46	1.41
5	J	2101	FMN	C9A-C5A	2.56	1.47	1.42
5	G	2101	FMN	C9A-C5A	2.55	1.47	1.42
5	I	2101	FMN	C9A-C5A	2.54	1.47	1.42
5	L	2101	FMN	C7M-C7	-2.53	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	2101	FMN	C7M-C7	-2.50	1.45	1.51
5	H	2101	FMN	C9A-C5A	2.50	1.47	1.42
5	L	2101	FMN	C9A-C5A	2.49	1.47	1.42
5	K	2101	FMN	C9A-C5A	2.47	1.47	1.42
5	J	2101	FMN	C7M-C7	-2.46	1.46	1.51
5	K	2101	FMN	C7M-C7	-2.38	1.46	1.51
5	I	2101	FMN	C8-C7	2.38	1.46	1.40
5	I	2101	FMN	C7M-C7	-2.37	1.46	1.51
5	K	2101	FMN	C8-C7	2.34	1.46	1.40
5	G	2101	FMN	C7M-C7	-2.33	1.46	1.51
5	J	2101	FMN	C8-C7	2.32	1.46	1.40
5	H	2101	FMN	C8-C7	2.32	1.46	1.40
5	L	2101	FMN	C8-C7	2.31	1.46	1.40
5	G	2101	FMN	C2-N1	-2.31	1.33	1.38
5	G	2101	FMN	C8-C7	2.28	1.46	1.40
5	K	2101	FMN	C2-N1	-2.10	1.34	1.38
5	L	2101	FMN	C2-N1	-2.10	1.34	1.38
5	I	2101	FMN	C2-N1	-2.09	1.34	1.38
5	J	2101	FMN	C2-N1	-2.08	1.34	1.38

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2101	FMN	C4-N3-C2	9.32	123.01	115.14
5	H	2101	FMN	C4-N3-C2	9.31	123.00	115.14
5	J	2101	FMN	C4-N3-C2	9.27	122.97	115.14
5	L	2101	FMN	C4-N3-C2	9.24	122.94	115.14
5	G	2101	FMN	C4-N3-C2	9.22	122.93	115.14
5	K	2101	FMN	C4-N3-C2	9.20	122.91	115.14
5	H	2101	FMN	C4-C4A-C10	-6.05	115.48	119.95
5	I	2101	FMN	C4-C4A-C10	-6.05	115.48	119.95
5	J	2101	FMN	C4-C4A-C10	-5.94	115.56	119.95
5	G	2101	FMN	C4-C4A-C10	-5.90	115.59	119.95
5	K	2101	FMN	C4-C4A-C10	-5.88	115.61	119.95
5	L	2101	FMN	C4-C4A-C10	-5.87	115.62	119.95
5	I	2101	FMN	C1'-N10-C9A	5.12	122.77	118.31
5	K	2101	FMN	C1'-N10-C9A	5.11	122.76	118.31
5	G	2101	FMN	C1'-N10-C9A	5.08	122.73	118.31
5	H	2101	FMN	C1'-N10-C9A	5.00	122.67	118.31
5	J	2101	FMN	C1'-N10-C9A	4.98	122.65	118.31
5	L	2101	FMN	C1'-N10-C9A	4.84	122.53	118.31
5	K	2101	FMN	C4-C4A-N5	4.39	123.43	118.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2101	FMN	C4-C4A-N5	4.32	123.35	118.59
5	G	2101	FMN	O3P-P-O5'	-4.29	95.31	106.73
5	H	2101	FMN	O3P-P-O5'	-4.22	95.51	106.73
5	H	2101	FMN	C4-C4A-N5	4.18	123.21	118.59
5	J	2101	FMN	O3P-P-O5'	-4.16	95.67	106.73
5	L	2101	FMN	O3P-P-O5'	-4.14	95.70	106.73
5	L	2101	FMN	C4-C4A-N5	4.13	123.15	118.59
5	G	2101	FMN	C4-C4A-N5	4.07	123.09	118.59
5	J	2101	FMN	C4-C4A-N5	4.07	123.08	118.59
5	K	2101	FMN	O3P-P-O5'	-4.02	96.03	106.73
5	I	2101	FMN	O3P-P-O5'	-3.87	96.43	106.73
5	K	2101	FMN	O5'-P-O1P	-3.44	96.83	106.47
5	I	2101	FMN	O5'-P-O1P	-3.42	96.89	106.47
5	L	2101	FMN	O5'-P-O1P	-3.26	97.33	106.47
5	J	2101	FMN	O5'-P-O1P	-3.25	97.35	106.47
5	G	2101	FMN	O5'-P-O1P	-3.23	97.41	106.47
5	H	2101	FMN	O5'-P-O1P	-3.21	97.47	106.47
5	K	2101	FMN	C4A-C4-N3	-3.10	119.15	123.47
5	G	2101	FMN	C4A-C4-N3	-3.10	119.15	123.47
4	A	1901	PNS	C37-C38-C39	-3.07	107.24	112.36
5	L	2101	FMN	C4A-C4-N3	-3.07	119.20	123.47
4	F	1901	PNS	C37-C38-C39	-3.06	107.27	112.36
4	B	1901	PNS	C37-C38-C39	-3.05	107.28	112.36
4	D	1901	PNS	C37-C38-C39	-3.04	107.29	112.36
4	E	1901	PNS	C37-C38-C39	-3.03	107.31	112.36
5	I	2101	FMN	C4A-C4-N3	-3.01	119.28	123.47
5	H	2101	FMN	C4A-C4-N3	-2.99	119.31	123.47
4	C	1901	PNS	C37-C38-C39	-2.98	107.39	112.36
5	J	2101	FMN	C4A-C4-N3	-2.98	119.33	123.47
5	G	2101	FMN	O2P-P-O5'	2.81	114.22	106.73
5	L	2101	FMN	O2P-P-O5'	2.80	114.18	106.73
5	H	2101	FMN	O2P-P-O5'	2.79	114.15	106.73
5	K	2101	FMN	O2P-P-O5'	2.73	114.00	106.73
5	J	2101	FMN	O2P-P-O5'	2.72	113.97	106.73
5	G	2101	FMN	O4'-C4'-C5'	-2.68	103.93	109.97
5	I	2101	FMN	O2P-P-O5'	2.68	113.87	106.73
5	J	2101	FMN	O4'-C4'-C5'	-2.67	103.96	109.97
5	K	2101	FMN	O4'-C4'-C5'	-2.61	104.09	109.97
5	J	2101	FMN	O4'-C4'-C3'	2.60	115.47	109.11
5	J	2101	FMN	C9A-N10-C10	-2.60	118.39	121.77
5	I	2101	FMN	C9A-N10-C10	-2.59	118.39	121.77
5	L	2101	FMN	O4'-C4'-C5'	-2.59	104.13	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2101	FMN	O4'-C4'-C5'	-2.56	104.21	109.97
5	G	2101	FMN	C9A-N10-C10	-2.55	118.44	121.77
5	I	2101	FMN	O4'-C4'-C3'	2.54	115.32	109.11
5	I	2101	FMN	O4'-C4'-C5'	-2.53	104.27	109.97
5	K	2101	FMN	C9A-N10-C10	-2.50	118.51	121.77
5	L	2101	FMN	C9A-N10-C10	-2.49	118.52	121.77
5	H	2101	FMN	C9A-N10-C10	-2.47	118.56	121.77
5	J	2101	FMN	C6-C5A-N5	-2.46	116.27	118.97
5	H	2101	FMN	O4'-C4'-C3'	2.44	115.07	109.11
5	L	2101	FMN	O4'-C4'-C3'	2.42	115.04	109.11
5	G	2101	FMN	O4'-C4'-C3'	2.42	115.03	109.11
5	H	2101	FMN	C6-C5A-N5	-2.40	116.33	118.97
5	G	2101	FMN	C6-C5A-N5	-2.39	116.34	118.97
5	K	2101	FMN	O4'-C4'-C3'	2.37	114.91	109.11
5	L	2101	FMN	C6-C5A-N5	-2.37	116.37	118.97
5	K	2101	FMN	C6-C5A-N5	-2.33	116.40	118.97
5	I	2101	FMN	C6-C5A-N5	-2.32	116.42	118.97
4	C	1901	PNS	C30-C29-C28	2.21	111.84	108.23
4	B	1901	PNS	C30-C29-C28	2.20	111.82	108.23
4	E	1901	PNS	C30-C29-C28	2.20	111.82	108.23
4	D	1901	PNS	C30-C29-C28	2.19	111.80	108.23
5	H	2101	FMN	C7M-C7-C6	-2.19	115.05	120.34
4	A	1901	PNS	C38-C39-N41	-2.18	112.75	116.45
4	D	1901	PNS	C38-C39-N41	-2.18	112.75	116.45
4	B	1901	PNS	C38-C39-N41	-2.17	112.77	116.45
4	E	1901	PNS	C38-C39-N41	-2.17	112.77	116.45
4	A	1901	PNS	C30-C29-C28	2.17	111.77	108.23
4	C	1901	PNS	C38-C39-N41	-2.16	112.78	116.45
5	L	2101	FMN	C7M-C7-C6	-2.15	115.15	120.34
4	F	1901	PNS	C30-C29-C28	2.14	111.72	108.23
4	A	1901	PNS	C43-C42-N41	2.12	117.28	112.33
4	F	1901	PNS	C38-C39-N41	-2.12	112.86	116.45
5	K	2101	FMN	C7M-C7-C6	-2.11	115.24	120.34
4	A	1901	PNS	O40-C39-N41	2.08	126.91	123.01
4	F	1901	PNS	C43-C42-N41	2.07	117.17	112.33
4	C	1901	PNS	C43-C42-N41	2.06	117.15	112.33
4	E	1901	PNS	O40-C39-N41	2.05	126.85	123.01
4	D	1901	PNS	O40-C39-N41	2.04	126.83	123.01
4	F	1901	PNS	O40-C39-N41	2.03	126.81	123.01
4	C	1901	PNS	O40-C39-N41	2.01	126.78	123.01
5	I	2101	FMN	C7M-C7-C6	-2.01	115.47	120.34
4	B	1901	PNS	O40-C39-N41	2.01	126.78	123.01

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1901	PNS	O27-C28-C29-C32
4	A	1901	PNS	N36-C37-C38-C39
4	A	1901	PNS	N41-C42-C43-S44
4	D	1901	PNS	O27-C28-C29-C32
4	D	1901	PNS	N36-C37-C38-C39
4	D	1901	PNS	N41-C42-C43-S44
4	B	1901	PNS	O27-C28-C29-C32
4	B	1901	PNS	N36-C37-C38-C39
4	B	1901	PNS	N41-C42-C43-S44
4	E	1901	PNS	O27-C28-C29-C32
4	E	1901	PNS	N36-C37-C38-C39
4	E	1901	PNS	N41-C42-C43-S44
4	F	1901	PNS	O27-C28-C29-C32
4	F	1901	PNS	N36-C37-C38-C39
4	F	1901	PNS	N41-C42-C43-S44
4	C	1901	PNS	O27-C28-C29-C32
4	C	1901	PNS	N36-C37-C38-C39
4	C	1901	PNS	N41-C42-C43-S44
4	A	1901	PNS	C38-C37-N36-C34
4	D	1901	PNS	C38-C37-N36-C34
4	B	1901	PNS	C38-C37-N36-C34
4	E	1901	PNS	C38-C37-N36-C34
4	F	1901	PNS	C38-C37-N36-C34
4	C	1901	PNS	C38-C37-N36-C34
5	G	2101	FMN	O3'-C3'-C4'-C5'
5	L	2101	FMN	O3'-C3'-C4'-C5'
5	H	2101	FMN	O3'-C3'-C4'-C5'
5	I	2101	FMN	O3'-C3'-C4'-C5'
5	J	2101	FMN	O3'-C3'-C4'-C5'
5	G	2101	FMN	C2'-C3'-C4'-C5'
5	L	2101	FMN	C2'-C3'-C4'-C5'
5	H	2101	FMN	C2'-C3'-C4'-C5'
5	I	2101	FMN	C2'-C3'-C4'-C5'
5	J	2101	FMN	C2'-C3'-C4'-C5'
5	K	2101	FMN	C2'-C3'-C4'-C5'
5	J	2101	FMN	C2'-C3'-C4'-O4'
5	K	2101	FMN	O3'-C3'-C4'-C5'
5	G	2101	FMN	C2'-C3'-C4'-O4'
5	L	2101	FMN	C2'-C3'-C4'-O4'
5	H	2101	FMN	C2'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
5	I	2101	FMN	C2'-C3'-C4'-O4'
5	K	2101	FMN	C2'-C3'-C4'-O4'
5	G	2101	FMN	C3'-C4'-C5'-O5'
5	J	2101	FMN	C3'-C4'-C5'-O5'
4	D	1901	PNS	O27-C28-C29-C31
5	J	2101	FMN	O3'-C3'-C4'-O4'
5	L	2101	FMN	C3'-C4'-C5'-O5'
5	H	2101	FMN	C3'-C4'-C5'-O5'
5	I	2101	FMN	C3'-C4'-C5'-O5'
5	G	2101	FMN	C4'-C5'-O5'-P
5	I	2101	FMN	C4'-C5'-O5'-P
5	K	2101	FMN	C4'-C5'-O5'-P
4	A	1901	PNS	O27-C28-C29-C31
4	B	1901	PNS	O27-C28-C29-C31
4	E	1901	PNS	O27-C28-C29-C31
4	C	1901	PNS	O27-C28-C29-C31
5	G	2101	FMN	O3'-C3'-C4'-O4'
5	L	2101	FMN	C4'-C5'-O5'-P
5	H	2101	FMN	C4'-C5'-O5'-P
5	J	2101	FMN	C4'-C5'-O5'-P
5	L	2101	FMN	O3'-C3'-C4'-O4'
5	H	2101	FMN	O3'-C3'-C4'-O4'
5	I	2101	FMN	O3'-C3'-C4'-O4'
4	A	1901	PNS	O27-C28-C29-C30
4	D	1901	PNS	O27-C28-C29-C30
4	B	1901	PNS	O27-C28-C29-C30
4	E	1901	PNS	O27-C28-C29-C30
4	F	1901	PNS	O27-C28-C29-C30
4	F	1901	PNS	O27-C28-C29-C31
4	C	1901	PNS	O27-C28-C29-C30
5	K	2101	FMN	C3'-C4'-C5'-O5'
5	K	2101	FMN	O3'-C3'-C4'-O4'
4	B	1901	PNS	C38-C39-N41-C42
4	D	1901	PNS	C38-C39-N41-C42

There are no ring outliers.

12 monomers are involved in 37 short contacts:

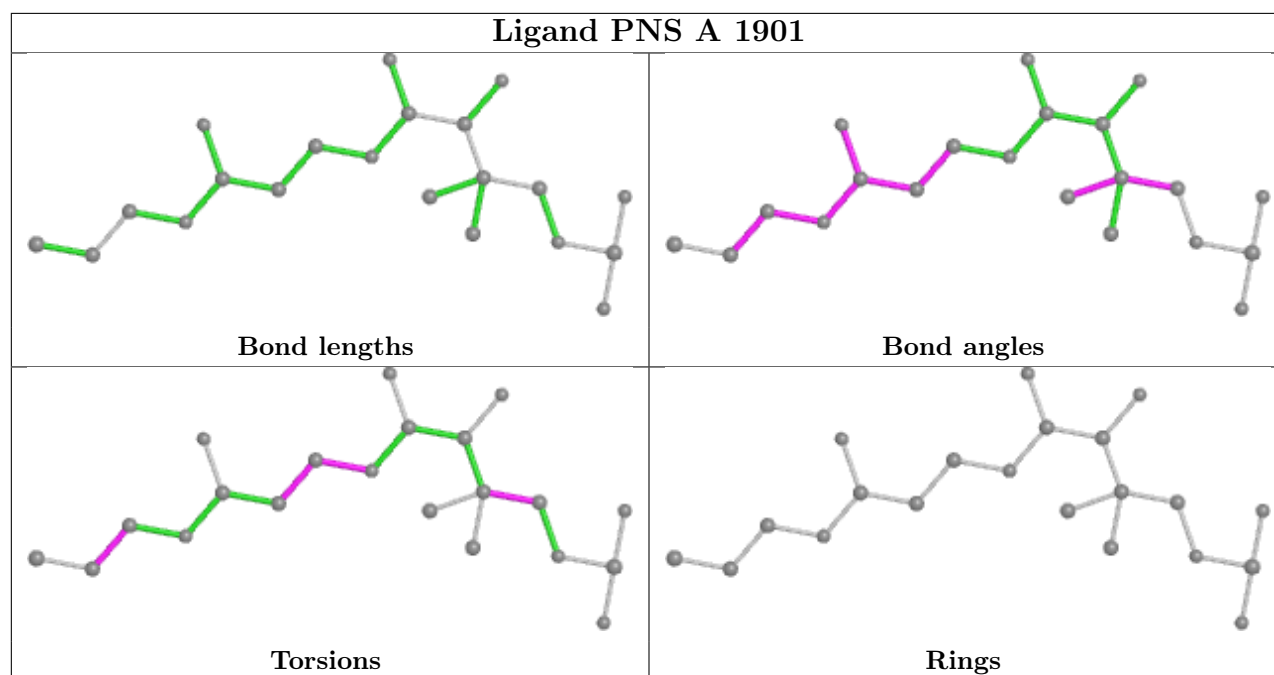
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1901	PNS	3	0
4	B	1901	PNS	4	0
4	C	1901	PNS	3	0

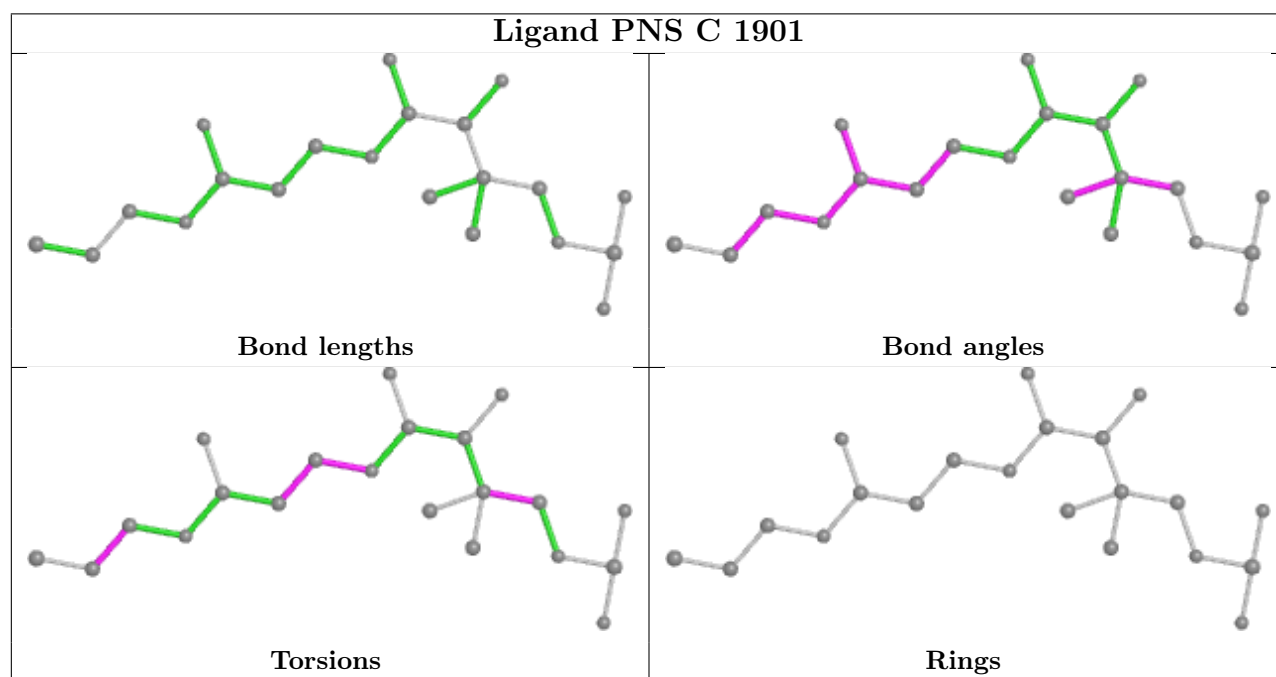
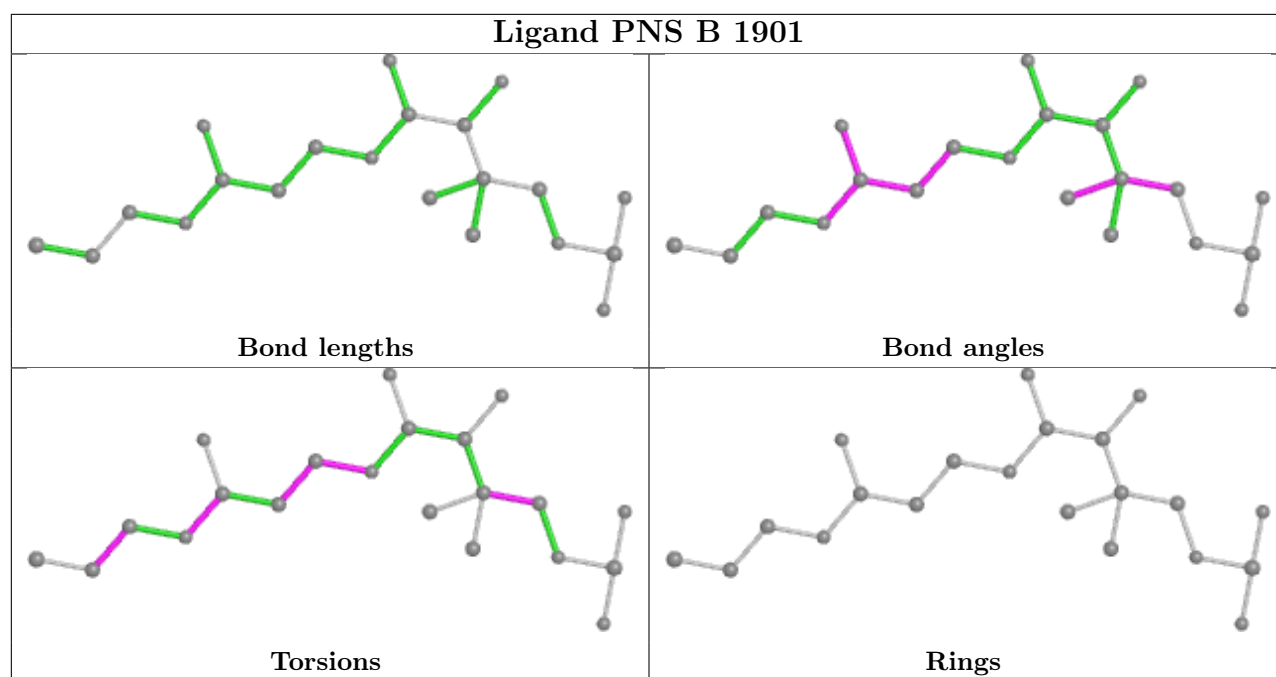
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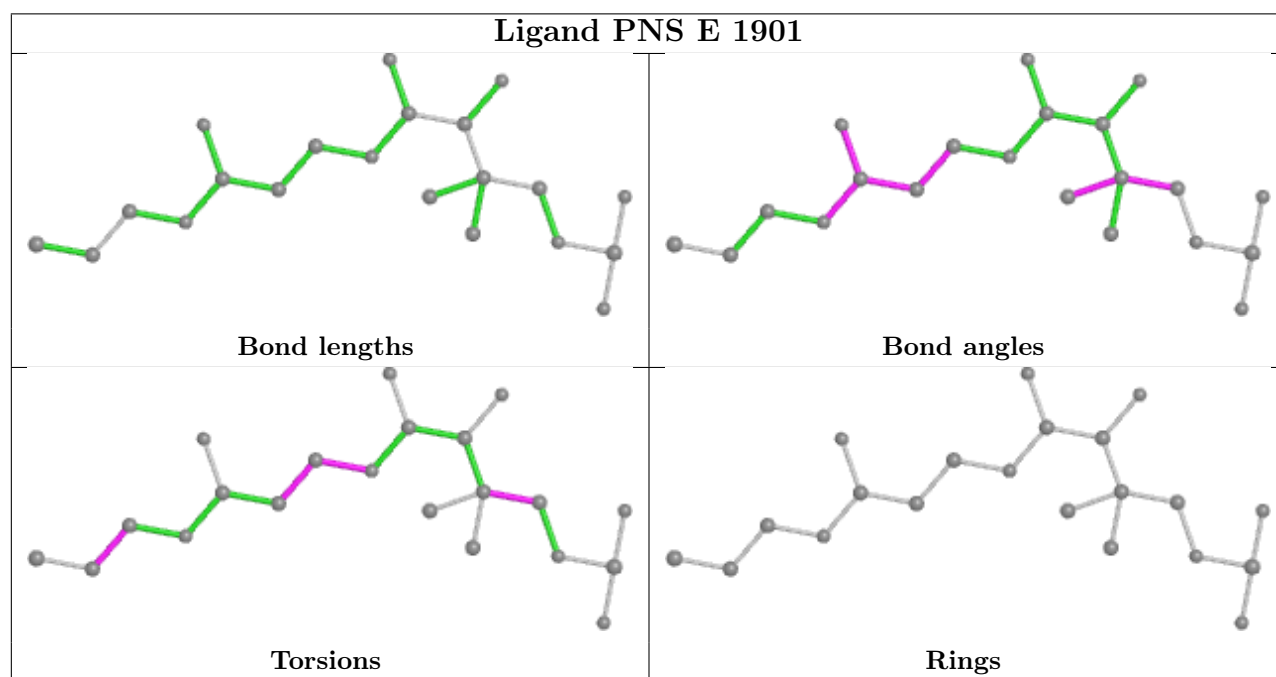
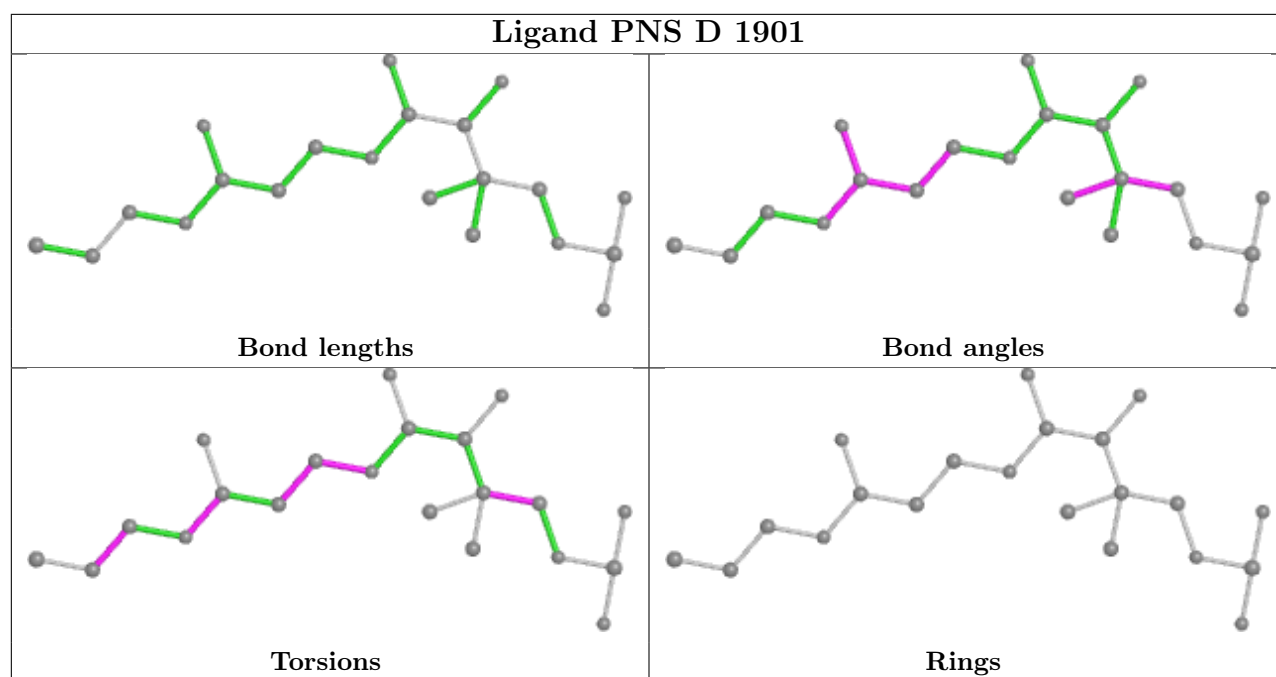
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1901	PNS	3	0
4	E	1901	PNS	3	0
4	F	1901	PNS	3	0
5	G	2101	FMN	3	0
5	H	2101	FMN	3	0
5	I	2101	FMN	3	0
5	J	2101	FMN	3	0
5	K	2101	FMN	3	0
5	L	2101	FMN	3	0

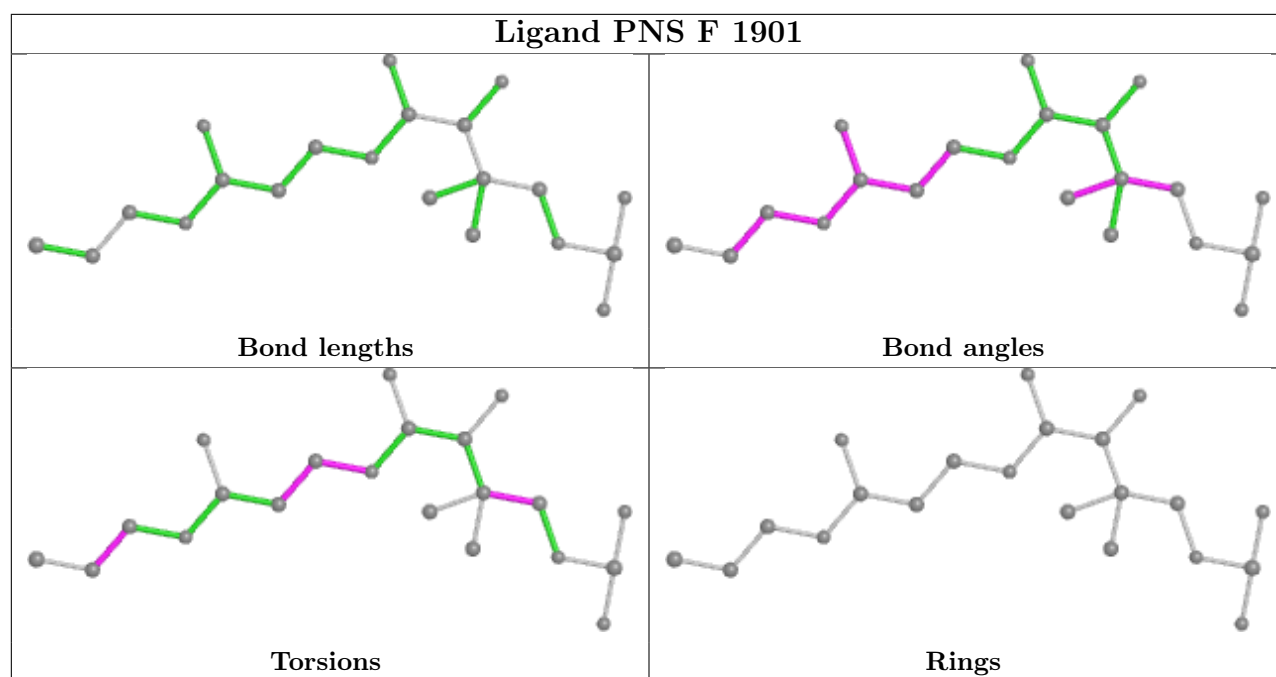
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



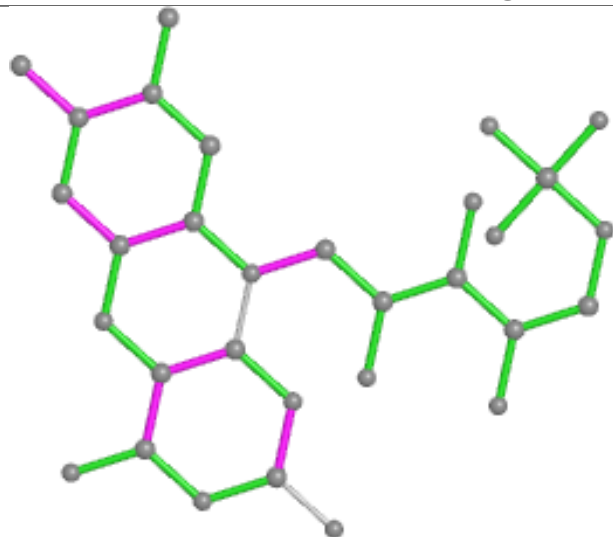




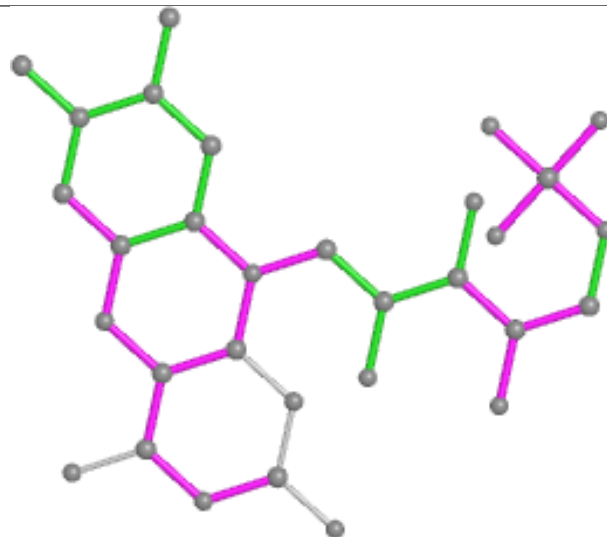




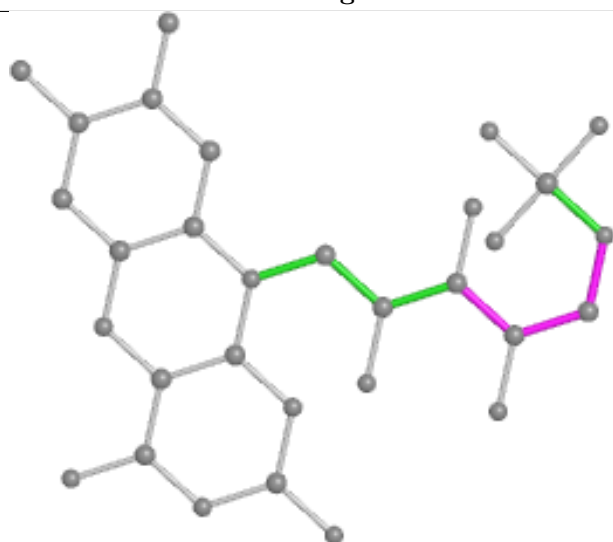
## Ligand FMN G 2101



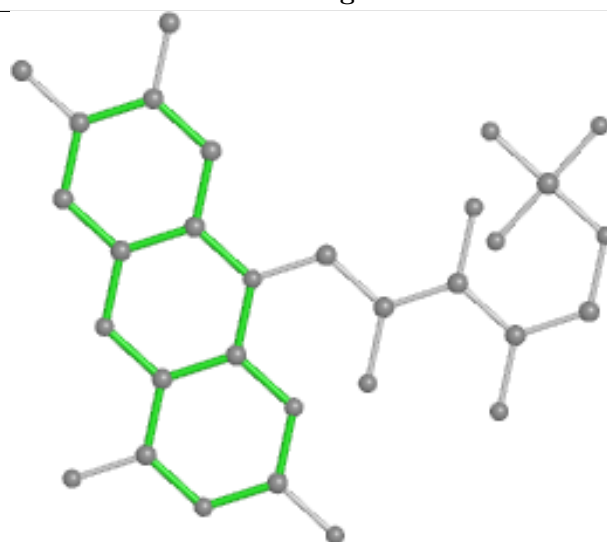
Bond lengths



Bond angles

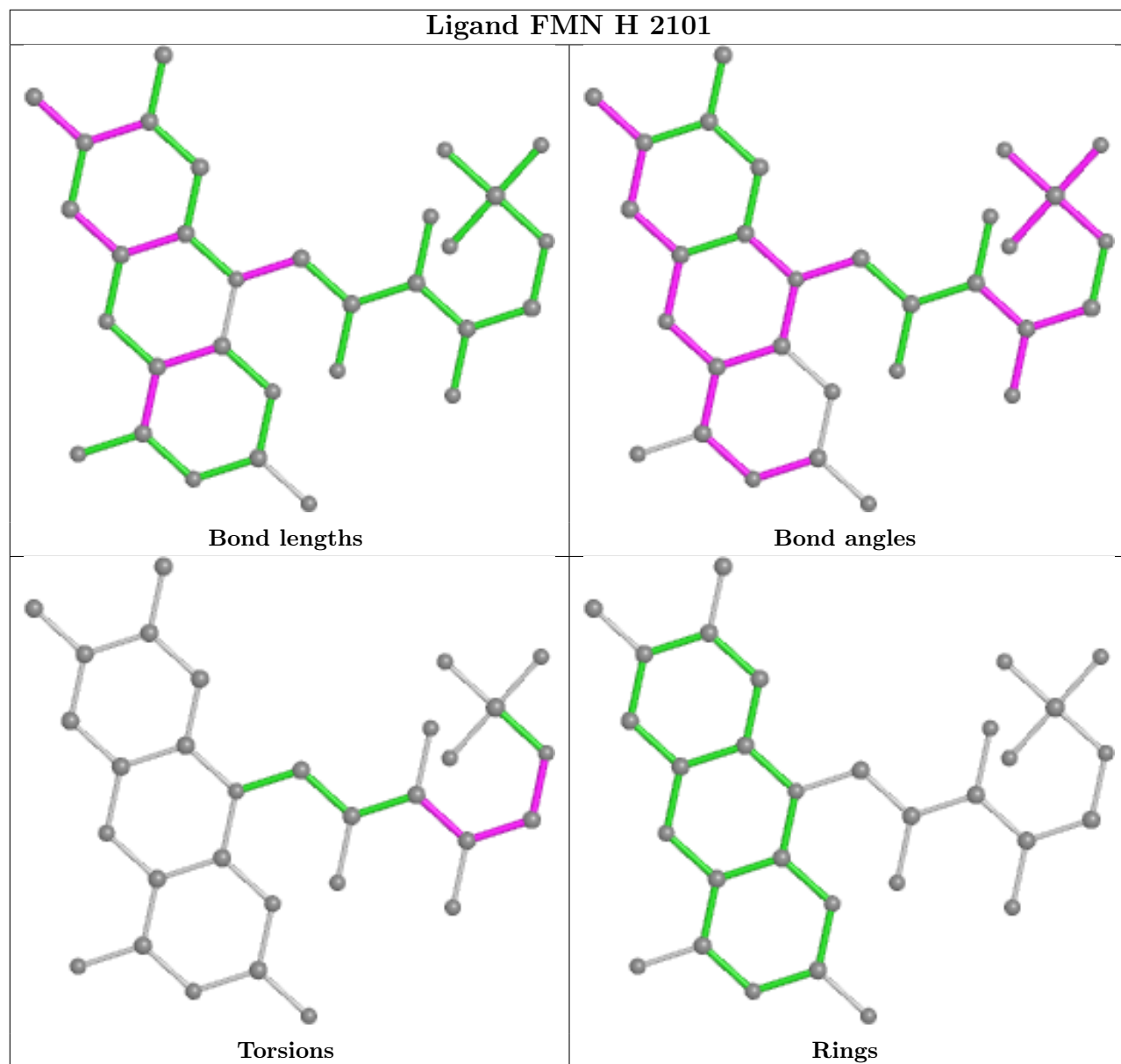


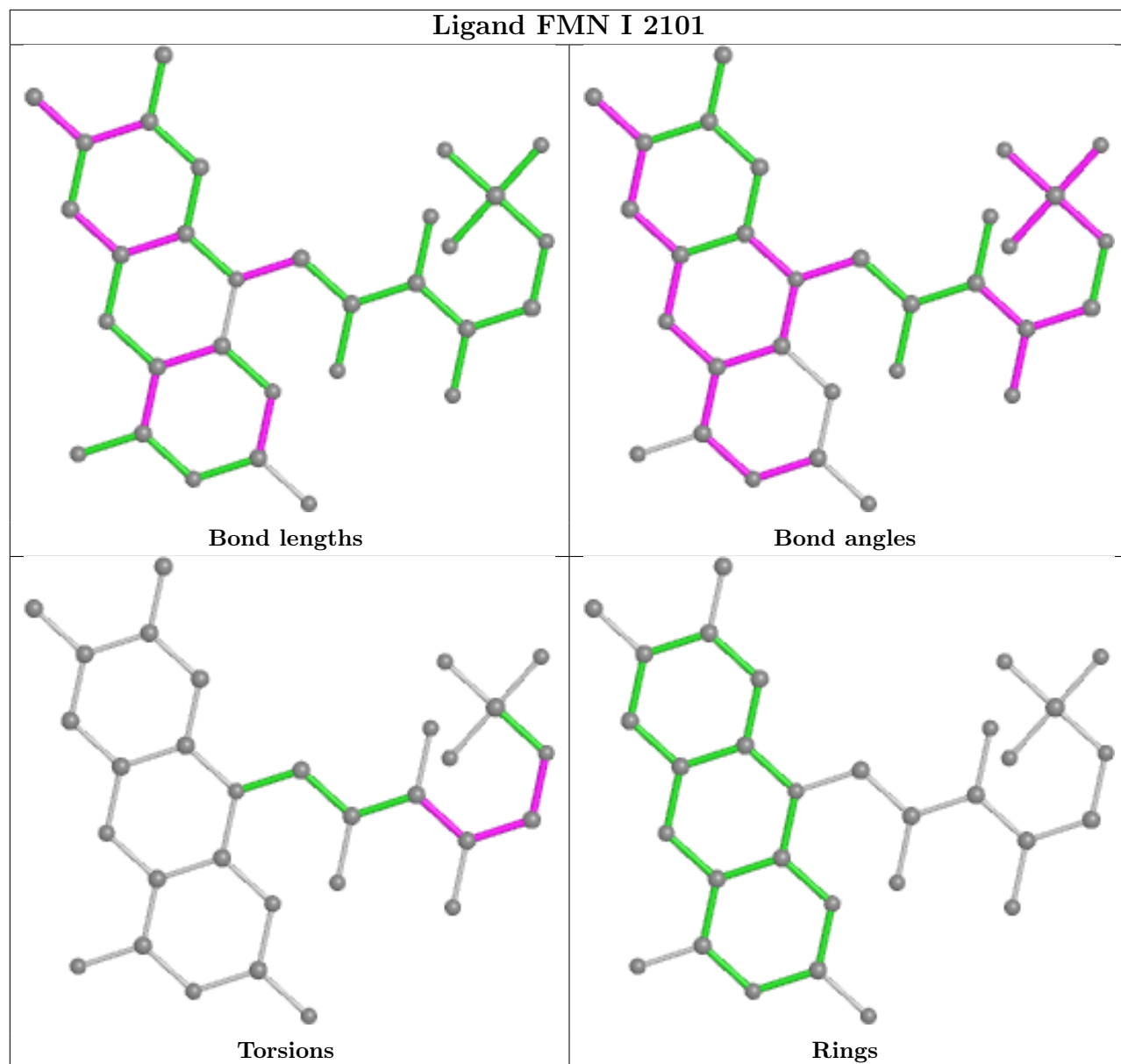
Torsions



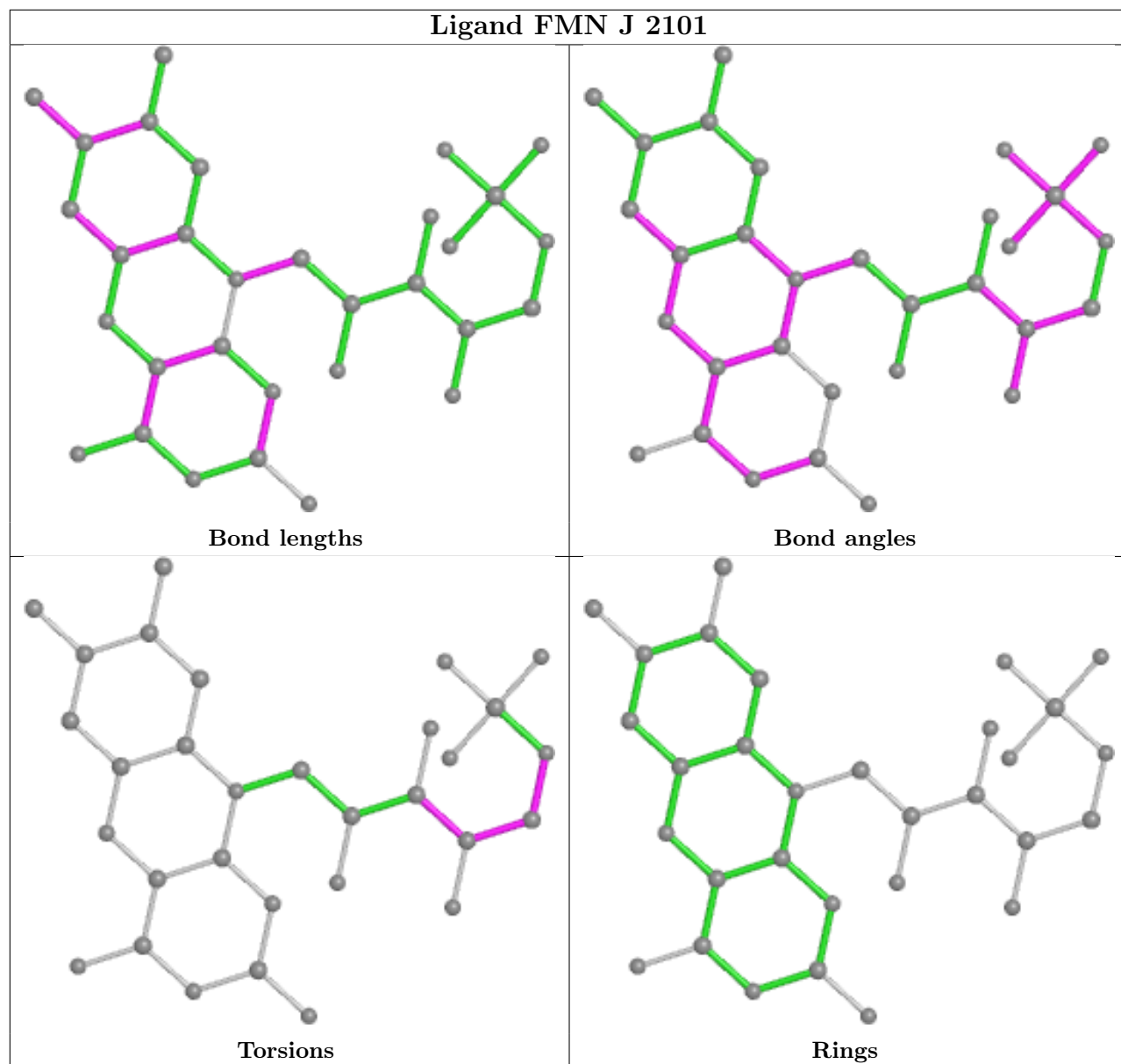
Rings

## Ligand FMN H 2101

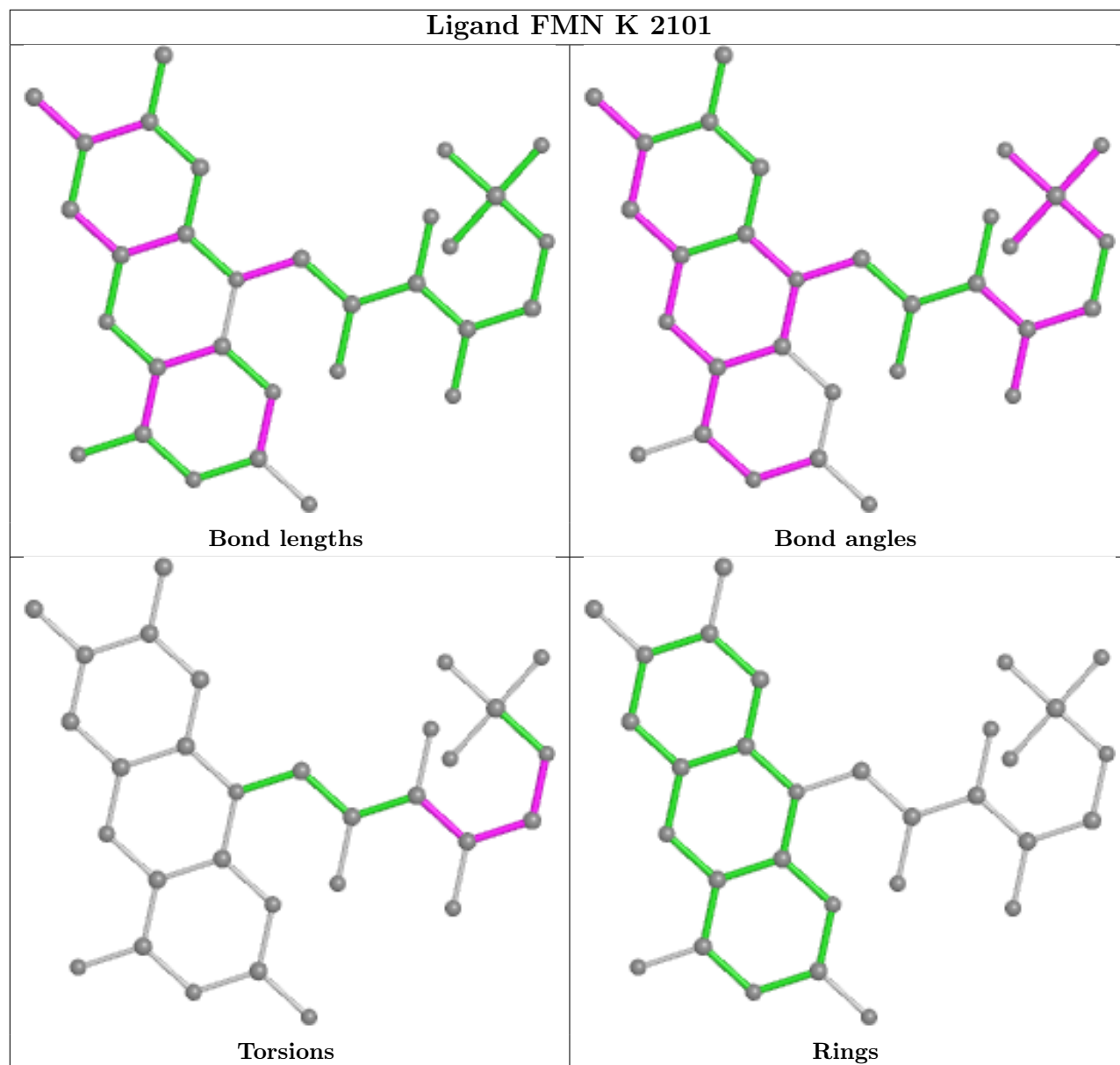


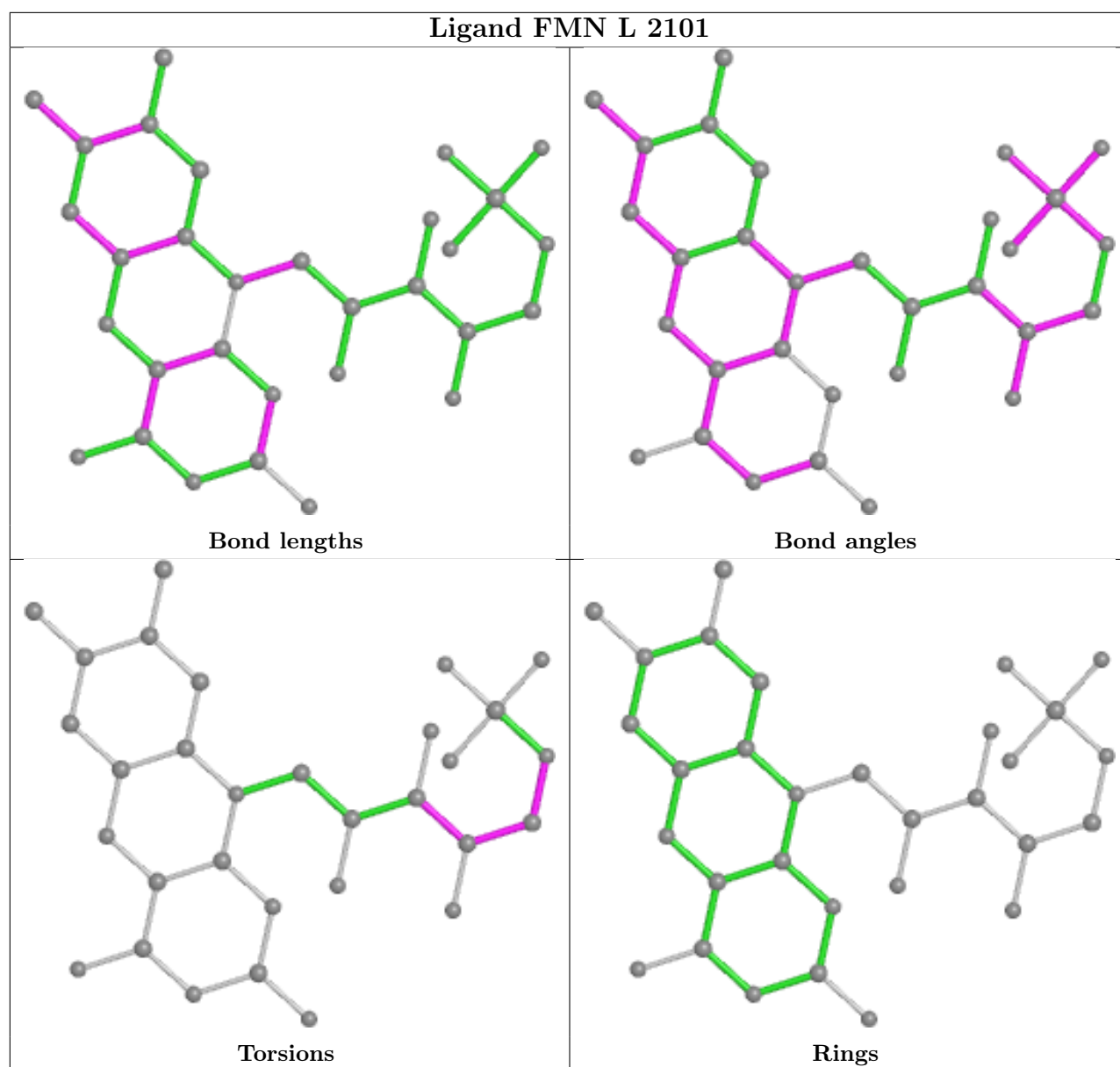


## Ligand FMN J 2101



## Ligand FMN K 2101





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.