



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:36 am BST

PDB ID : 6QL9  
Title : Structure of Fatty acid synthase complex from *Saccharomyces cerevisiae* at 2.9 Angstrom  
Authors : Singh, K.; Graf, B.; Linden, A.; Sautner, V.; Urlaub, H.; Tittmann, K.; Stark, H.; Chari, A.  
Deposited on : 2019-01-31  
Resolution : 2.82 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

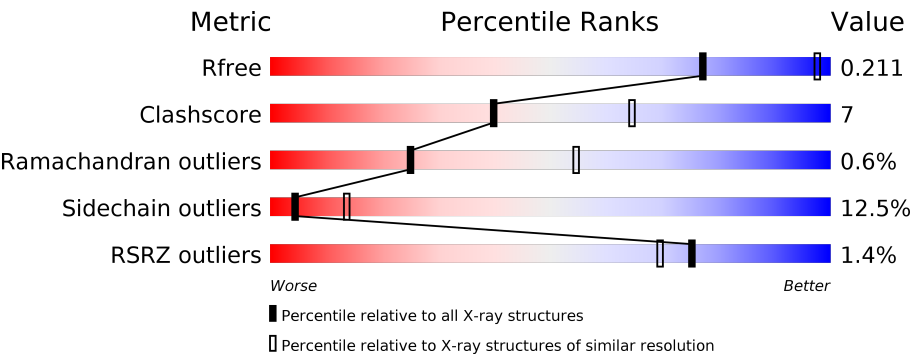
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1887	<div><div>2%</div><div><div></div><div>73%</div><div>18%</div><div>• 7%</div></div></div>
1	B	1887	<div><div>%</div><div><div></div><div>73%</div><div>17%</div><div>• 7%</div></div></div>
1	C	1887	<div><div>%</div><div><div></div><div>73%</div><div>18%</div><div>• 7%</div></div></div>
1	D	1887	<div><div>%</div><div><div></div><div>73%</div><div>17%</div><div>• 6%</div></div></div>
1	E	1887	<div><div>%</div><div><div></div><div>72%</div><div>18%</div><div>• 7%</div></div></div>
1	F	1887	<div><div>%</div><div><div></div><div>73%</div><div>17%</div><div>• 7%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	2051	
2	J	2051	
3	H	2051	
3	I	2051	
3	K	2051	
3	L	2051	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	MLI	J	2102	-	-	X	-
6	NA	C	1914	-	-	-	X
7	A2P	A	1918	-	-	-	X
7	A2P	B	1918	-	-	-	X
7	A2P	E	1917	-	-	-	X
7	A2P	F	1912	-	-	-	X
8	ACT	B	1902	-	-	-	X
8	ACT	C	1903	-	-	X	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 179453 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1760	Total	C	N	O	S	0	0	0
			13686	8661	2308	2665	52			
1	B	1759	Total	C	N	O	S	0	0	0
			13680	8658	2307	2663	52			
1	C	1759	Total	C	N	O	S	0	0	0
			13680	8658	2307	2663	52			
1	D	1765	Total	C	N	O	S	0	0	0
			13729	8688	2314	2675	52			
1	E	1759	Total	C	N	O	S	0	0	0
			13680	8658	2307	2663	52			
1	F	1759	Total	C	N	O	S	0	0	0
			13680	8658	2307	2663	52			

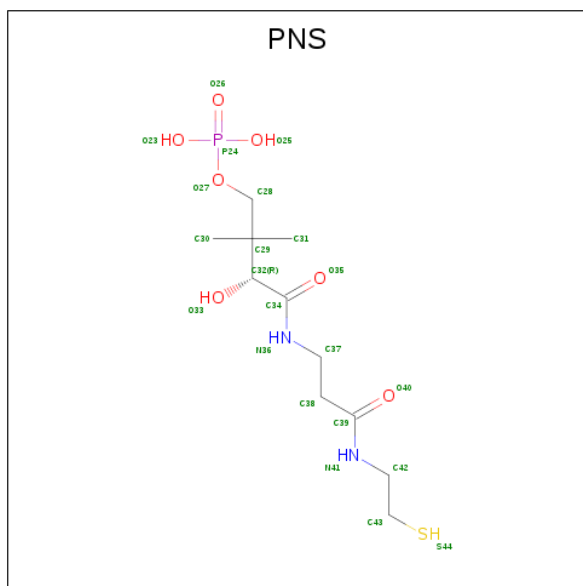
- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2036	Total	C	N	O	S	0	1	0
			16028	10271	2666	3035	56			
2	J	2035	Total	C	N	O	S	0	1	0
			16025	10272	2665	3032	56			

- Molecule 3 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	2035	Total	C	N	O	S	0	1	0
			16028	10274	2664	3034	56			
3	I	2034	Total	C	N	O	S	0	1	0
			16019	10266	2664	3033	56			
3	K	2035	Total	C	N	O	S	0	0	0
			16021	10269	2662	3034	56			
3	L	2036	Total	C	N	O	S	0	1	0
			16040	10280	2666	3038	56			

- Molecule 4 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula:  $C_{11}H_{23}N_2O_7PS$ ).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

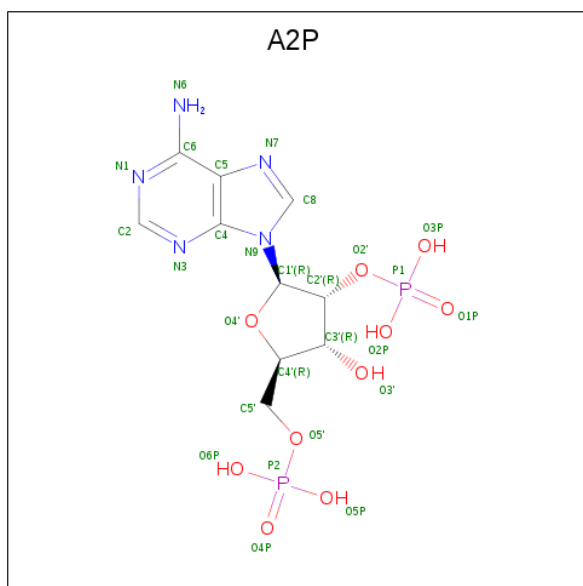
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	2	Total Na 2 2	0	0
6	J	2	Total Na 2 2	0	0
6	D	8	Total Na 8 8	0	0
6	K	2	Total Na 2 2	0	0
6	E	3	Total Na 3 3	0	0
6	H	2	Total Na 2 2	0	0
6	B	5	Total Na 5 5	0	0
6	I	1	Total Na 1 1	0	0

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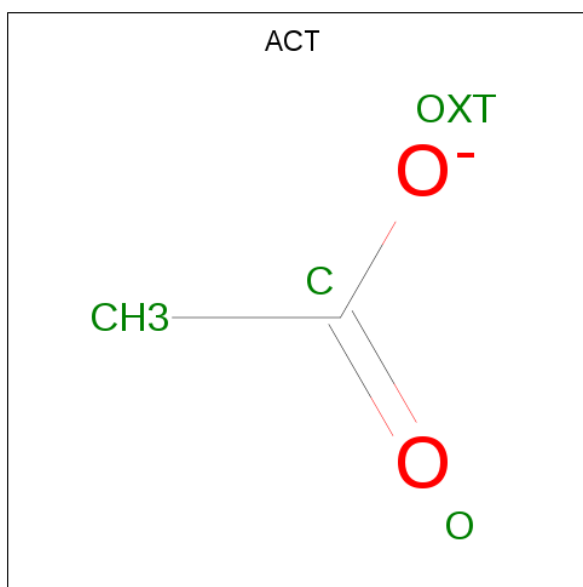
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	4	Total	Na	0	0
			4	4		
6	A	6	Total	Na	0	0
			6	6		
6	L	2	Total	Na	0	0
			2	2		
6	F	2	Total	Na	0	0
			2	2		

- Molecule 7 is ADENOSINE-2'-5'-DIPHOSPHATE (three-letter code: A2P) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



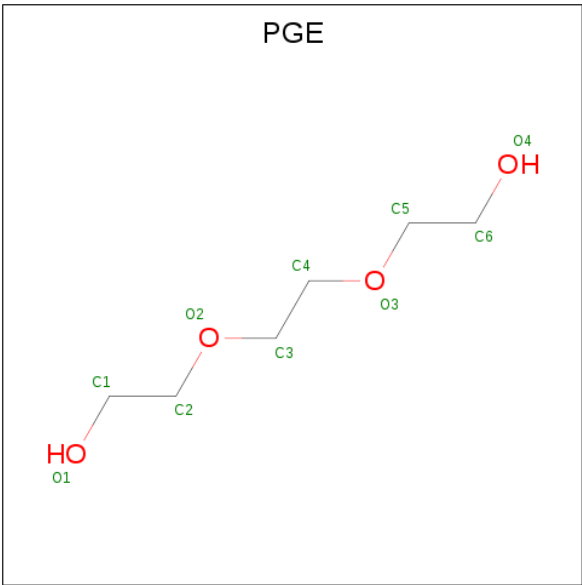
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



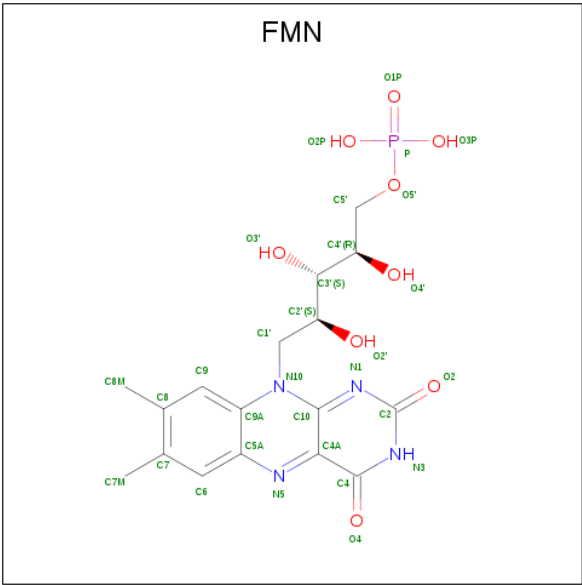
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



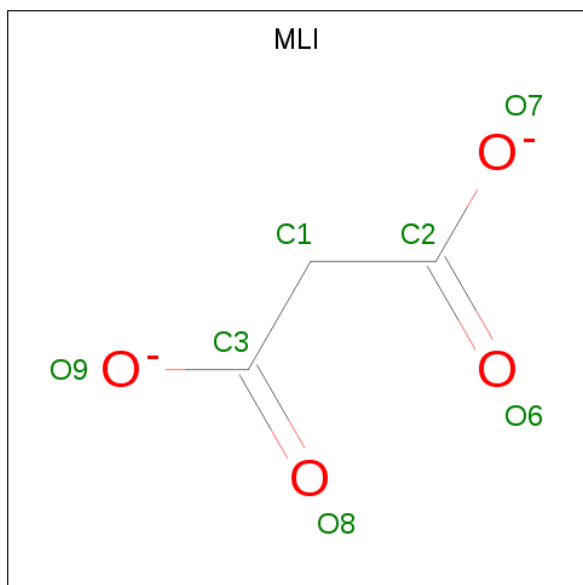
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	J	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	K	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	L	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 11 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	G	1	Total	C	O	0	0
			7	3	4		
11	J	1	Total	C	O	0	0
			7	3	4		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	42	Total	O	0	0
			42	42		
12	B	36	Total	O	0	0
			36	36		
12	C	42	Total	O	0	0
			42	42		
12	D	60	Total	O	0	0
			60	60		

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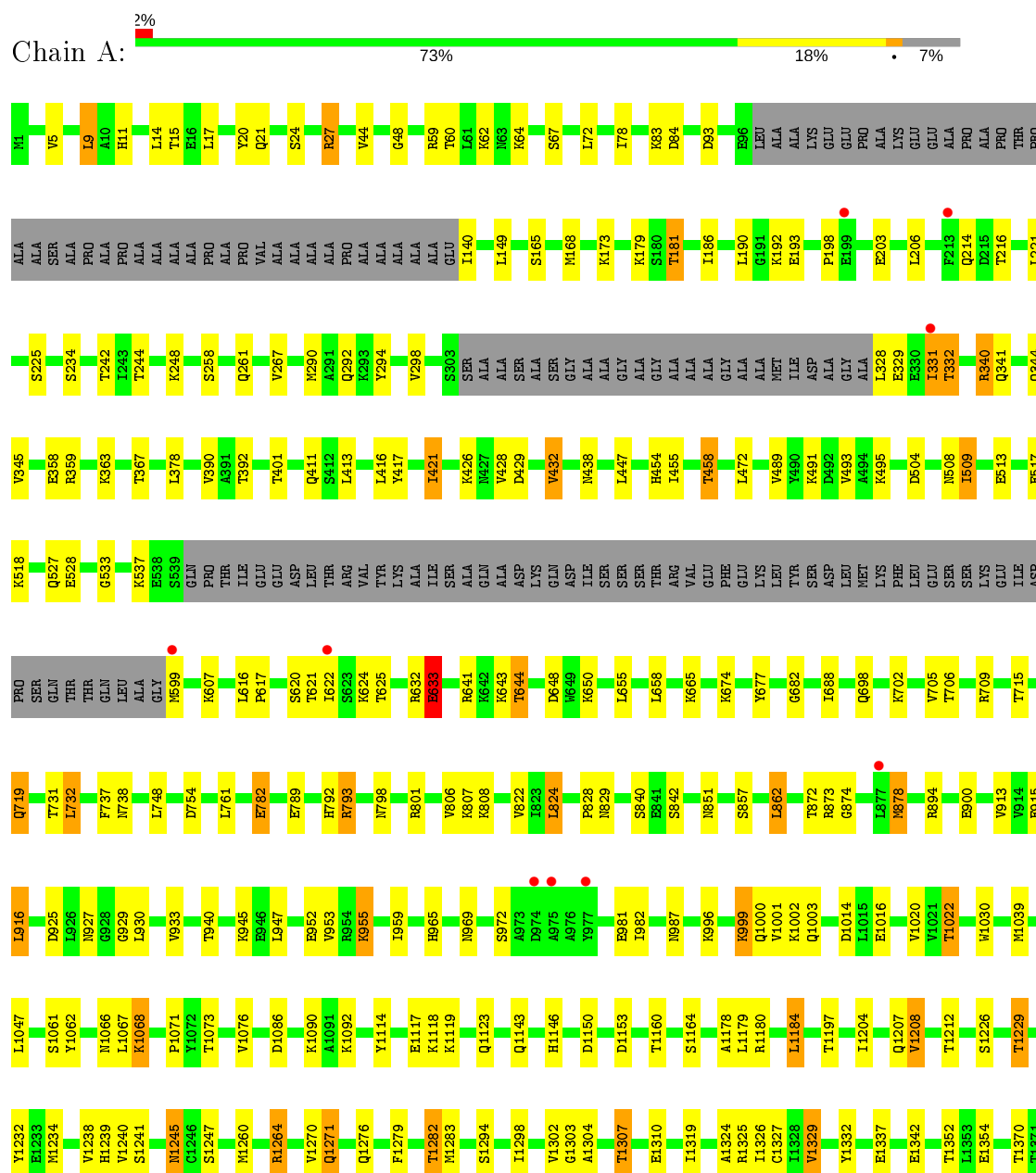
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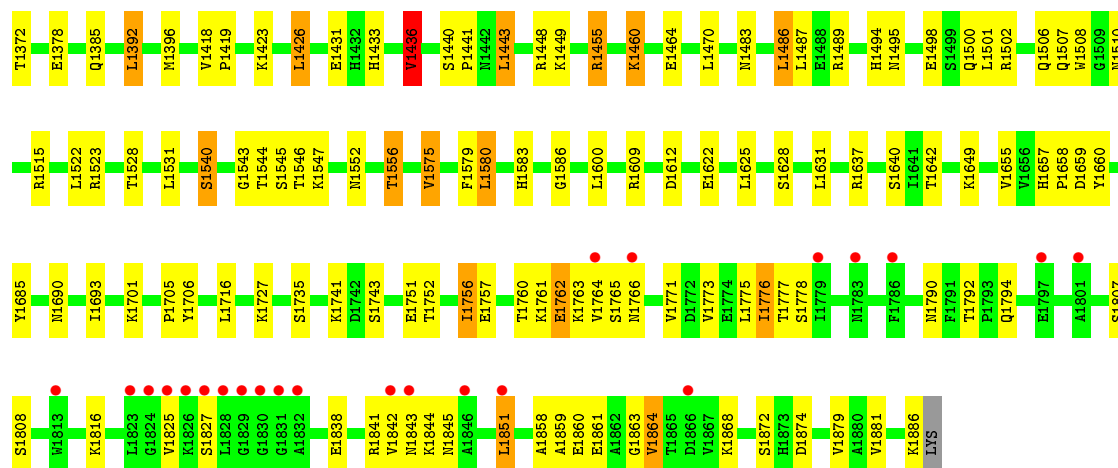
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	E	30	Total 30	O 30	0	0
12	F	24	Total 24	O 24	0	0
12	G	19	Total 19	O 19	0	0
12	H	24	Total 24	O 24	0	0
12	I	17	Total 17	O 17	0	0
12	J	17	Total 17	O 17	0	0
12	K	5	Total 5	O 5	0	0
12	L	12	Total 12	O 12	0	0

### 3 Residue-property plots

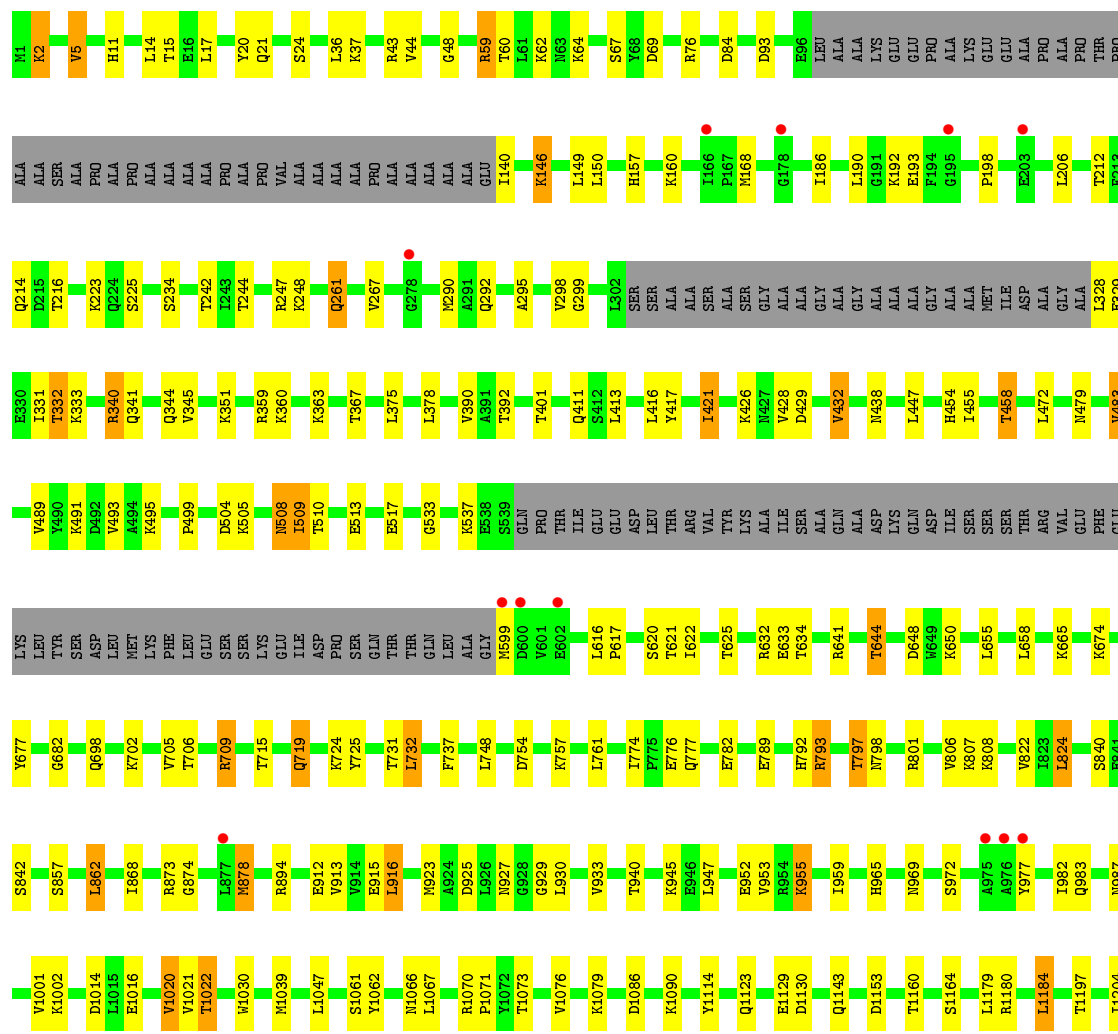
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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

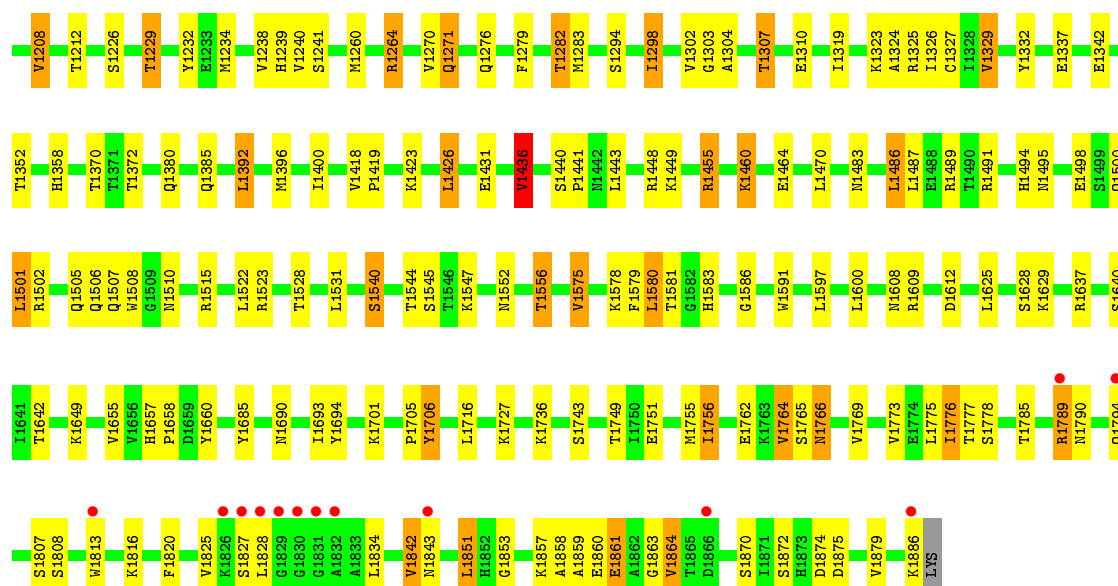




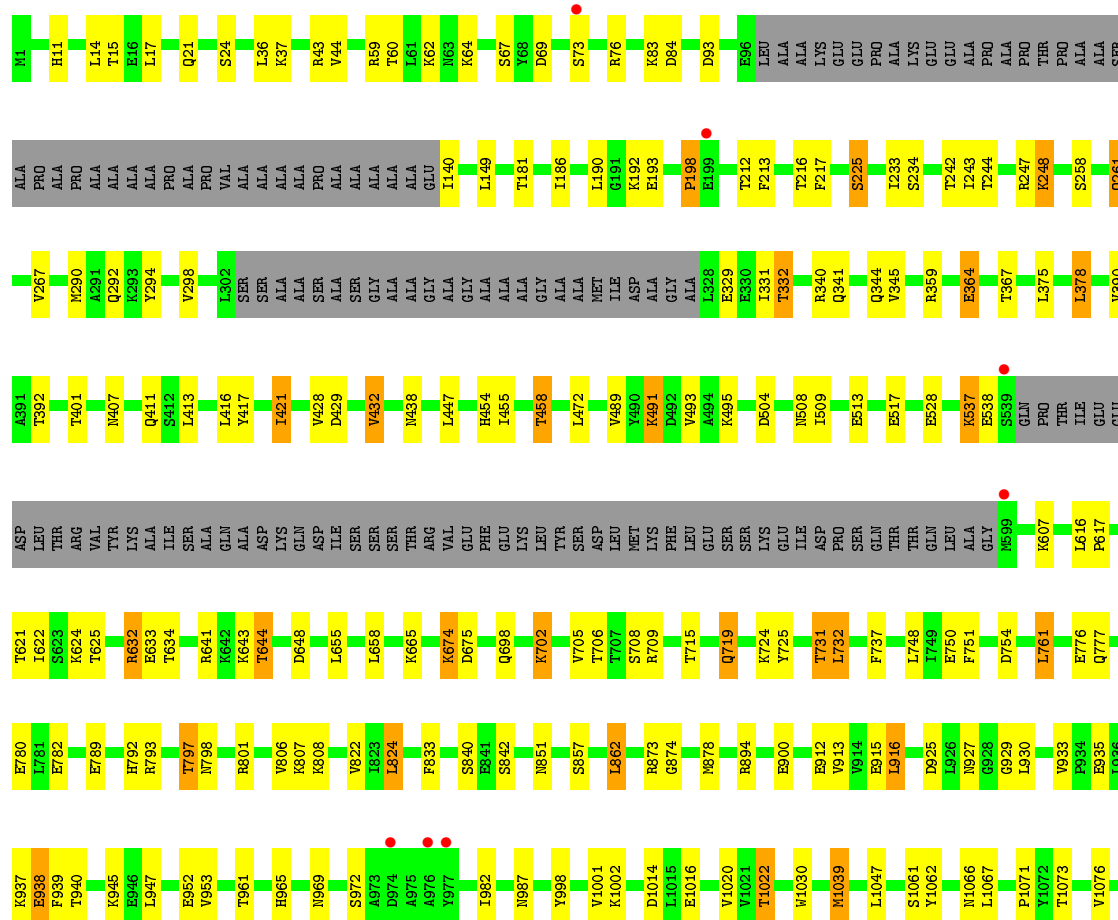
• Molecule 1: Fatty acid synthase subunit alpha

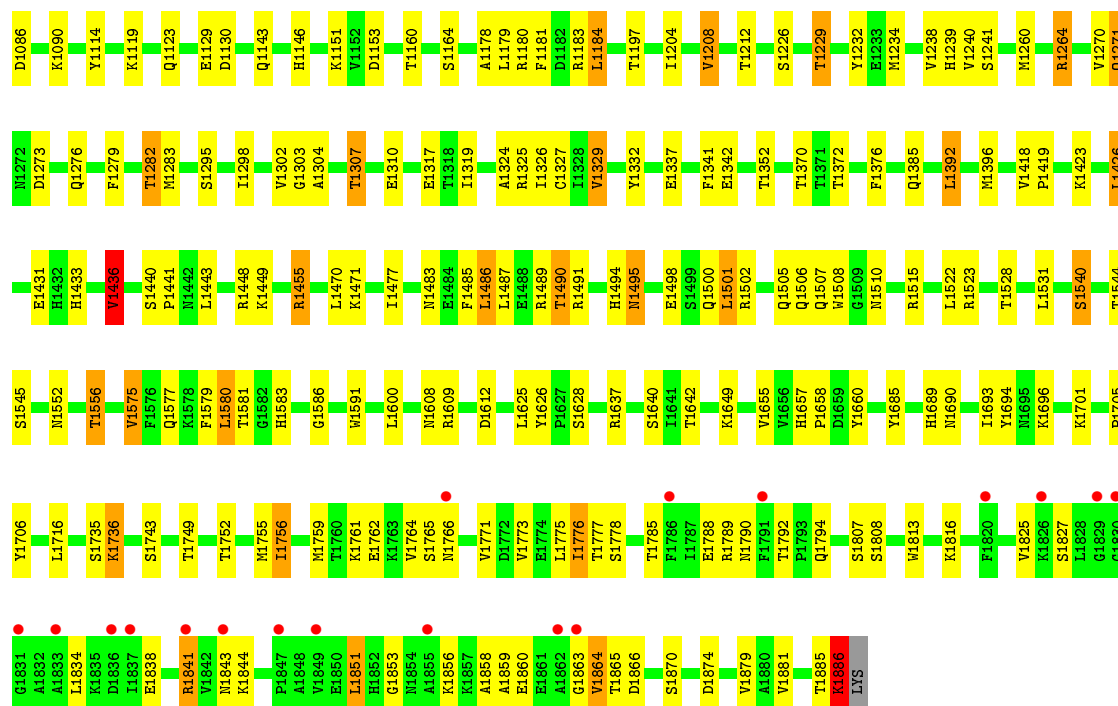


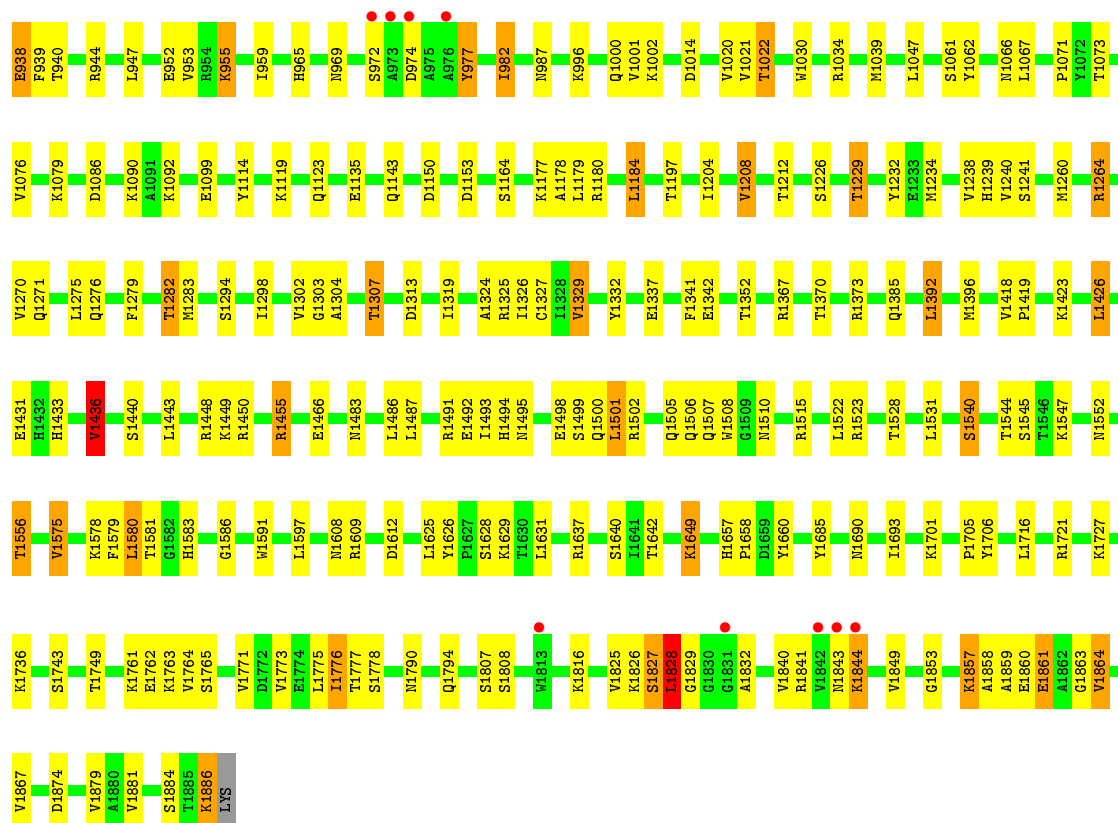




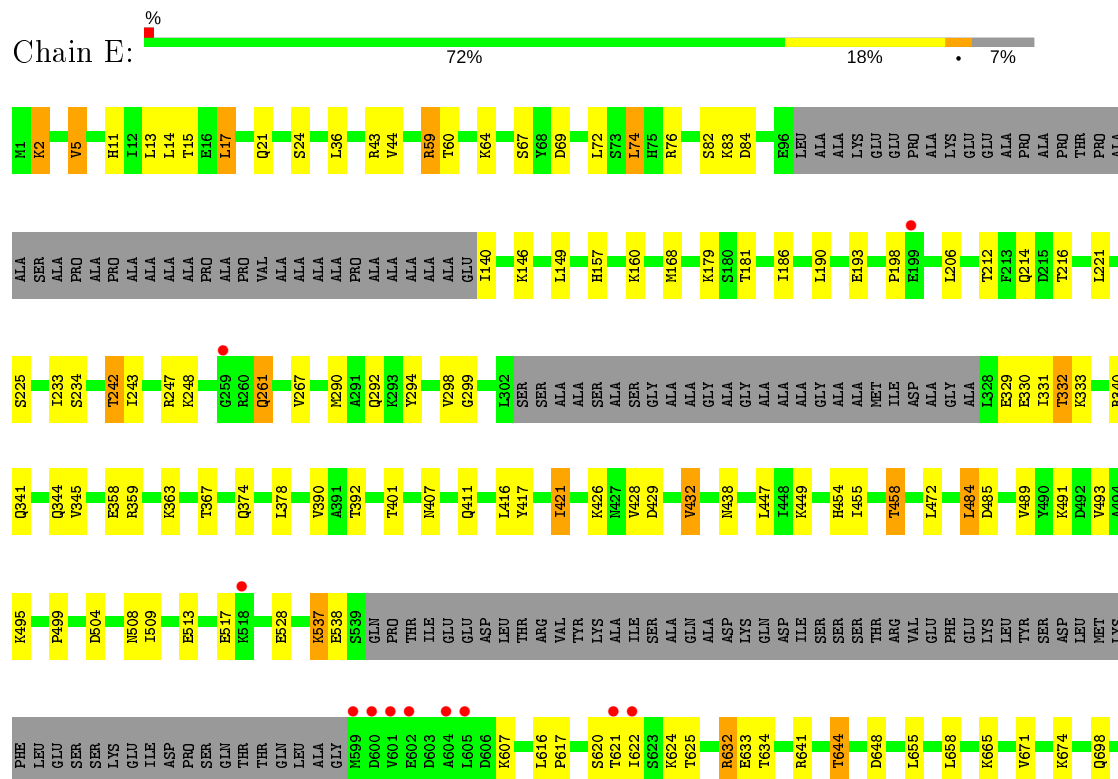
• Molecule 1: Fatty acid synthase subunit alpha

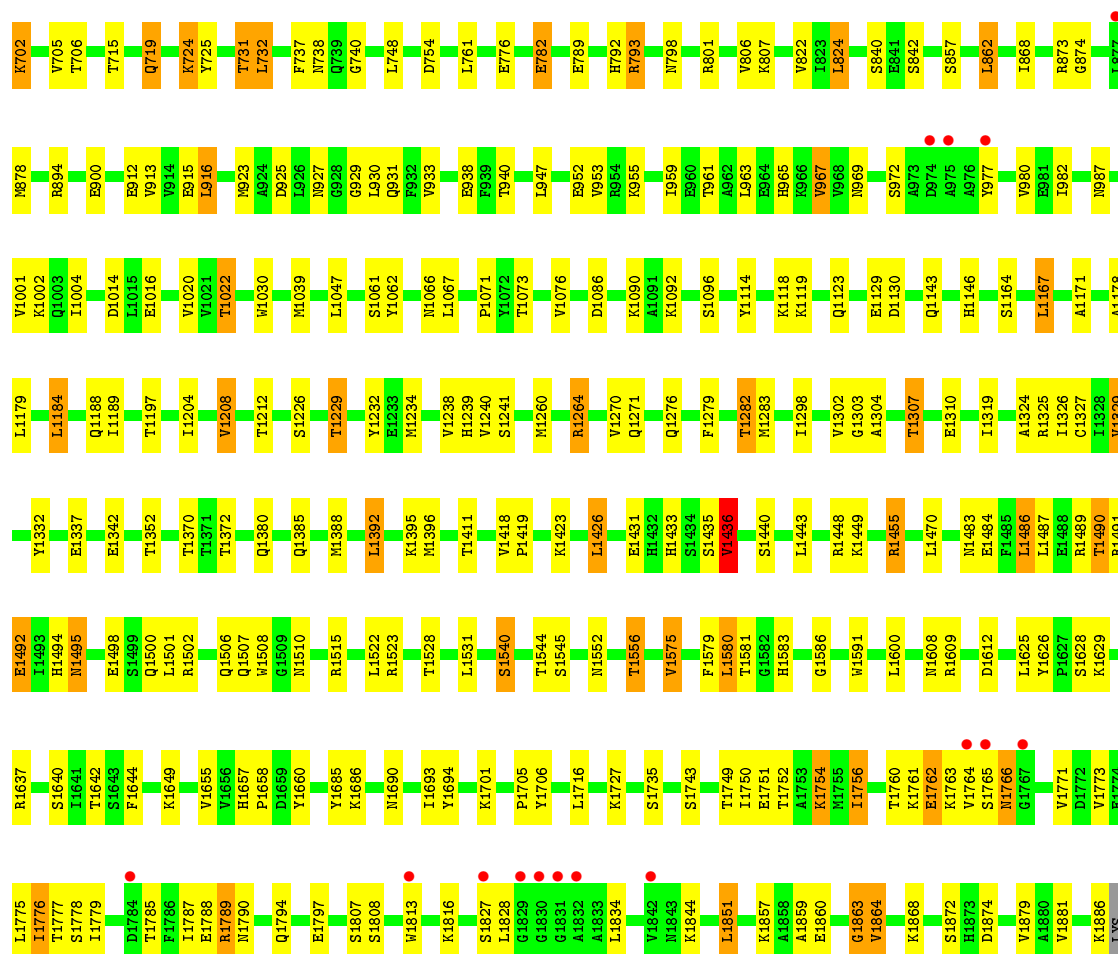




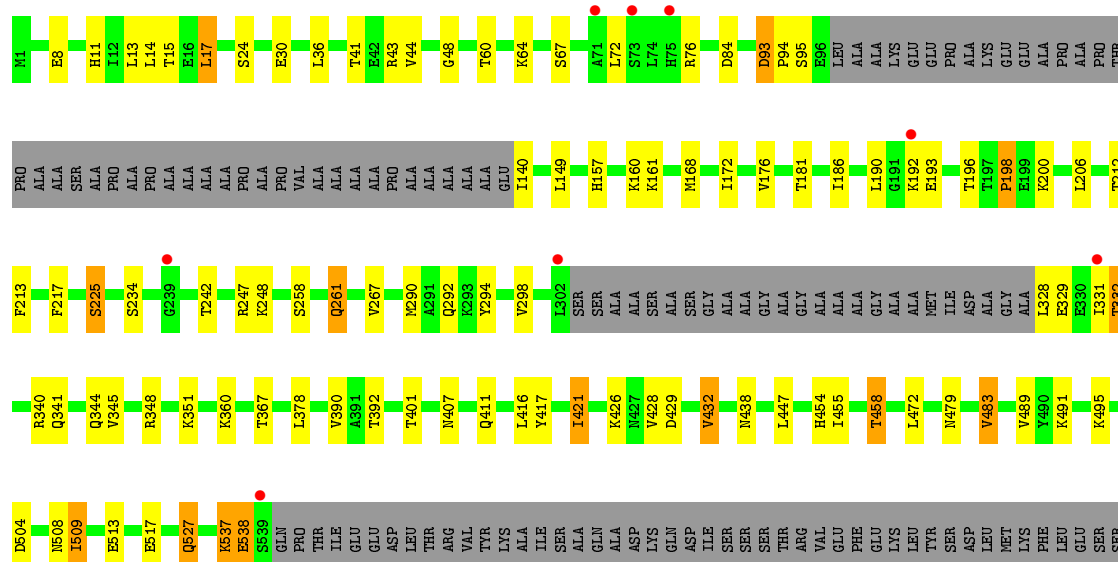
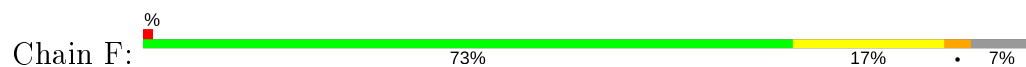


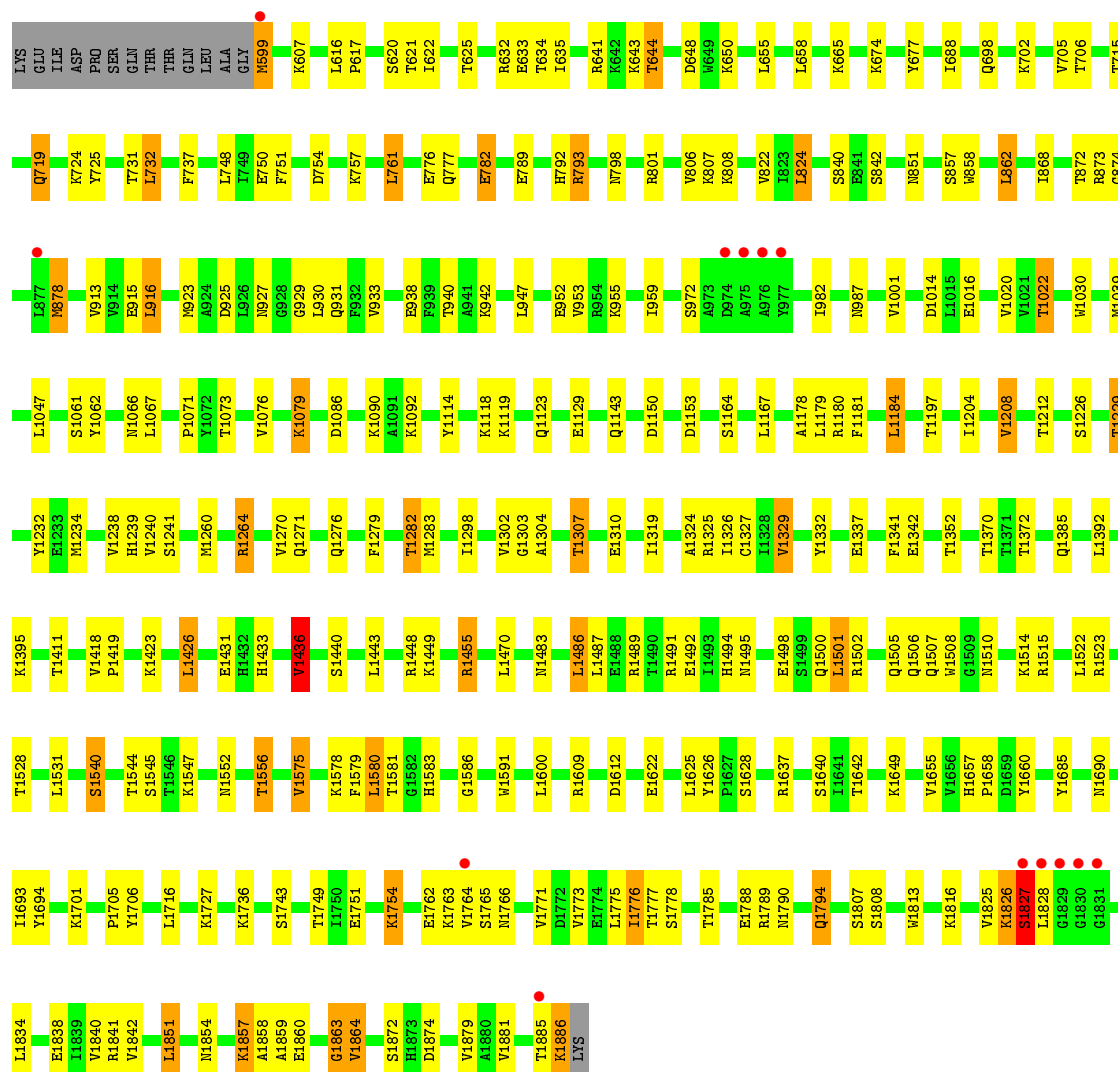
- Molecule 1: Fatty acid synthase subunit alpha



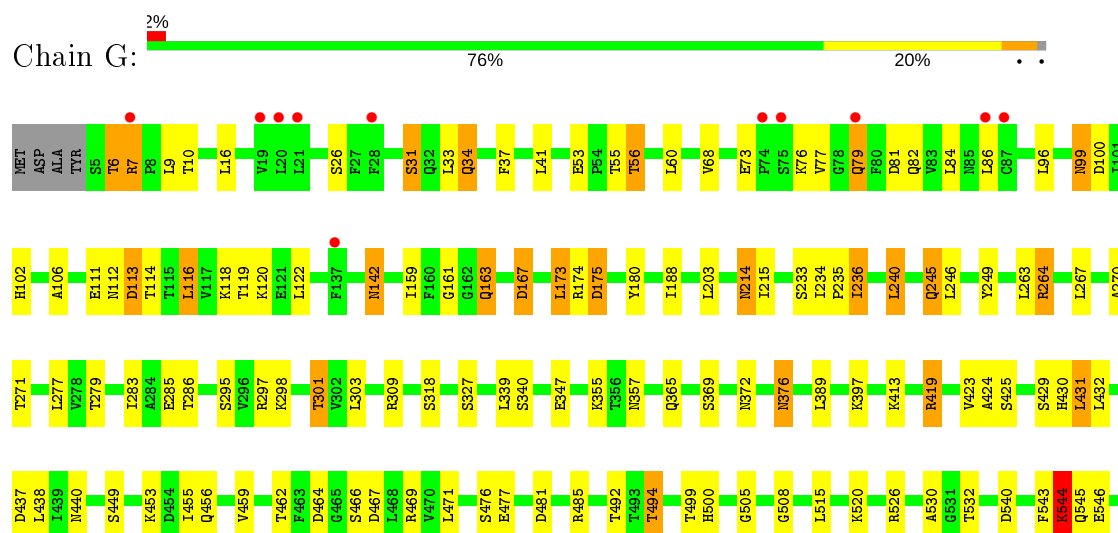


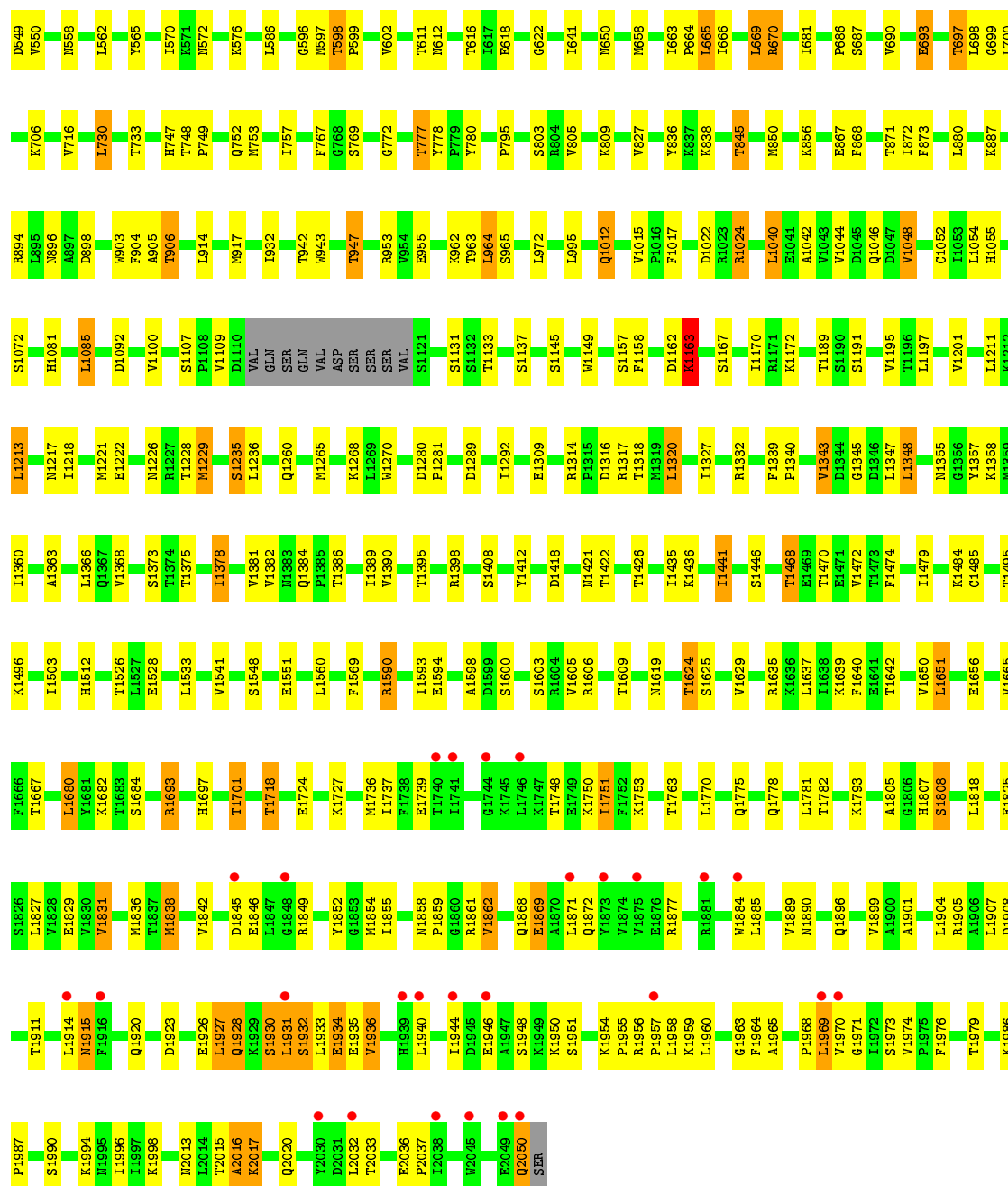
• Molecule 1: Fatty acid synthase subunit alpha



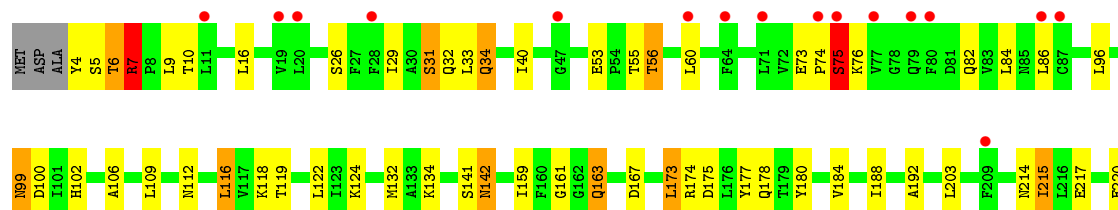
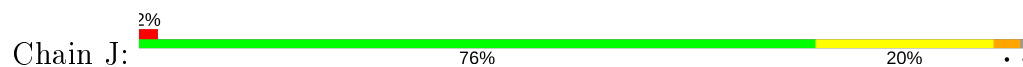


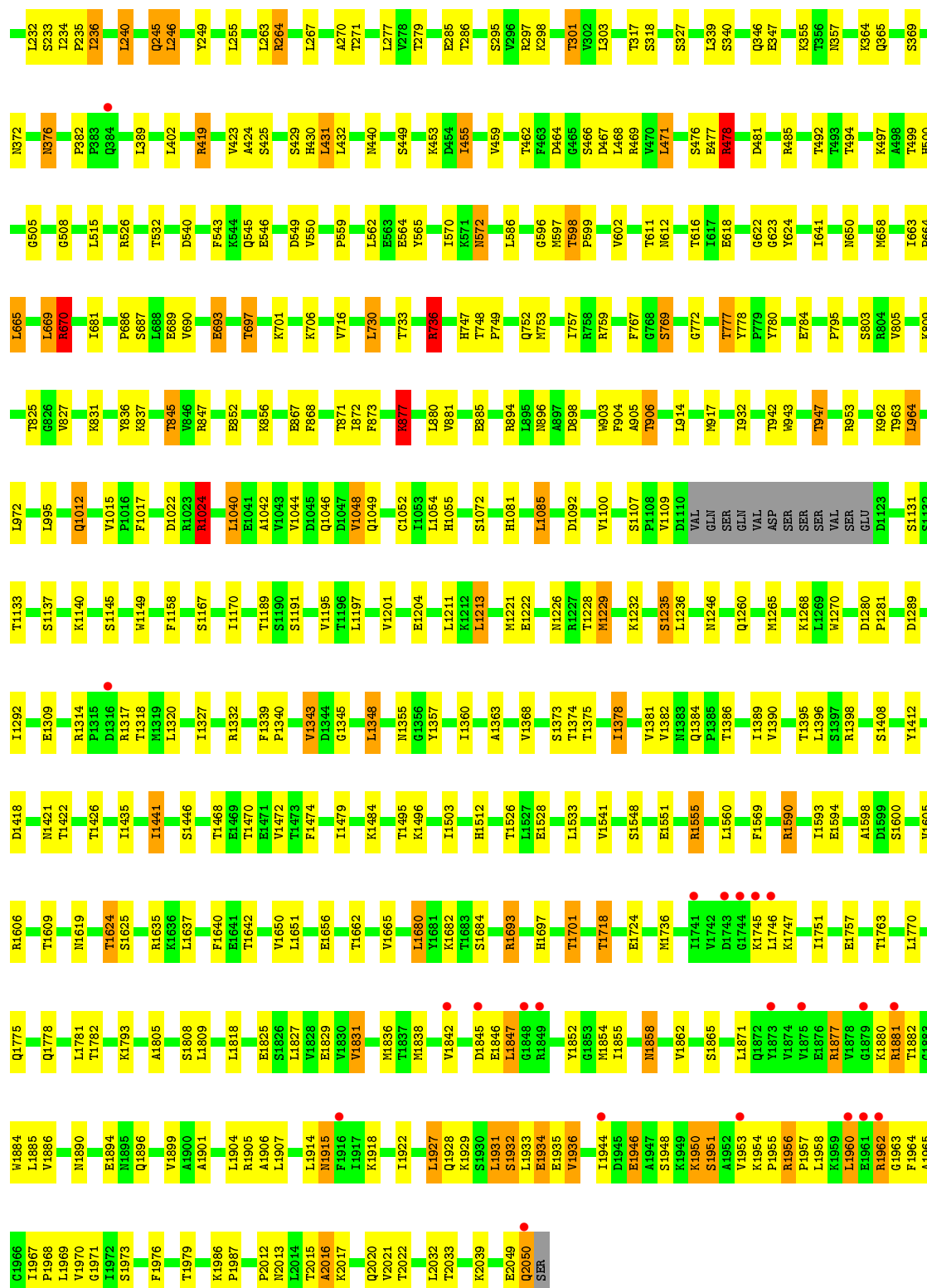
• Molecule 2: Fatty acid synthase subunit beta



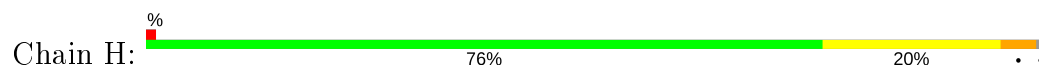


# Molecule 2: Fatty acid synthase subunit beta





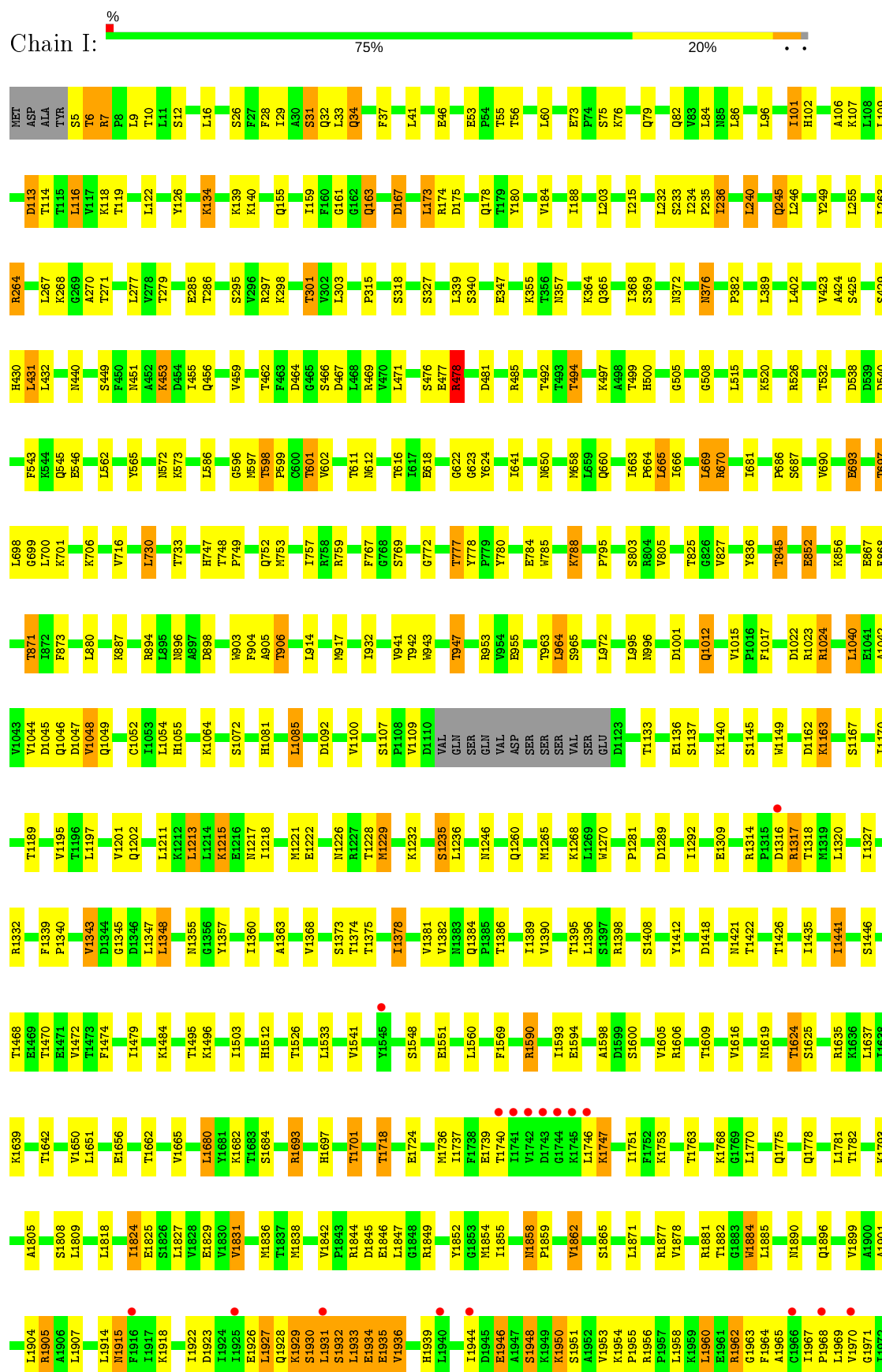
● Molecule 3: Fatty acid synthase subunit beta

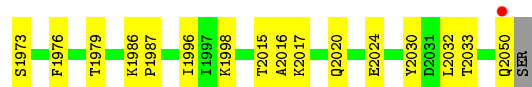




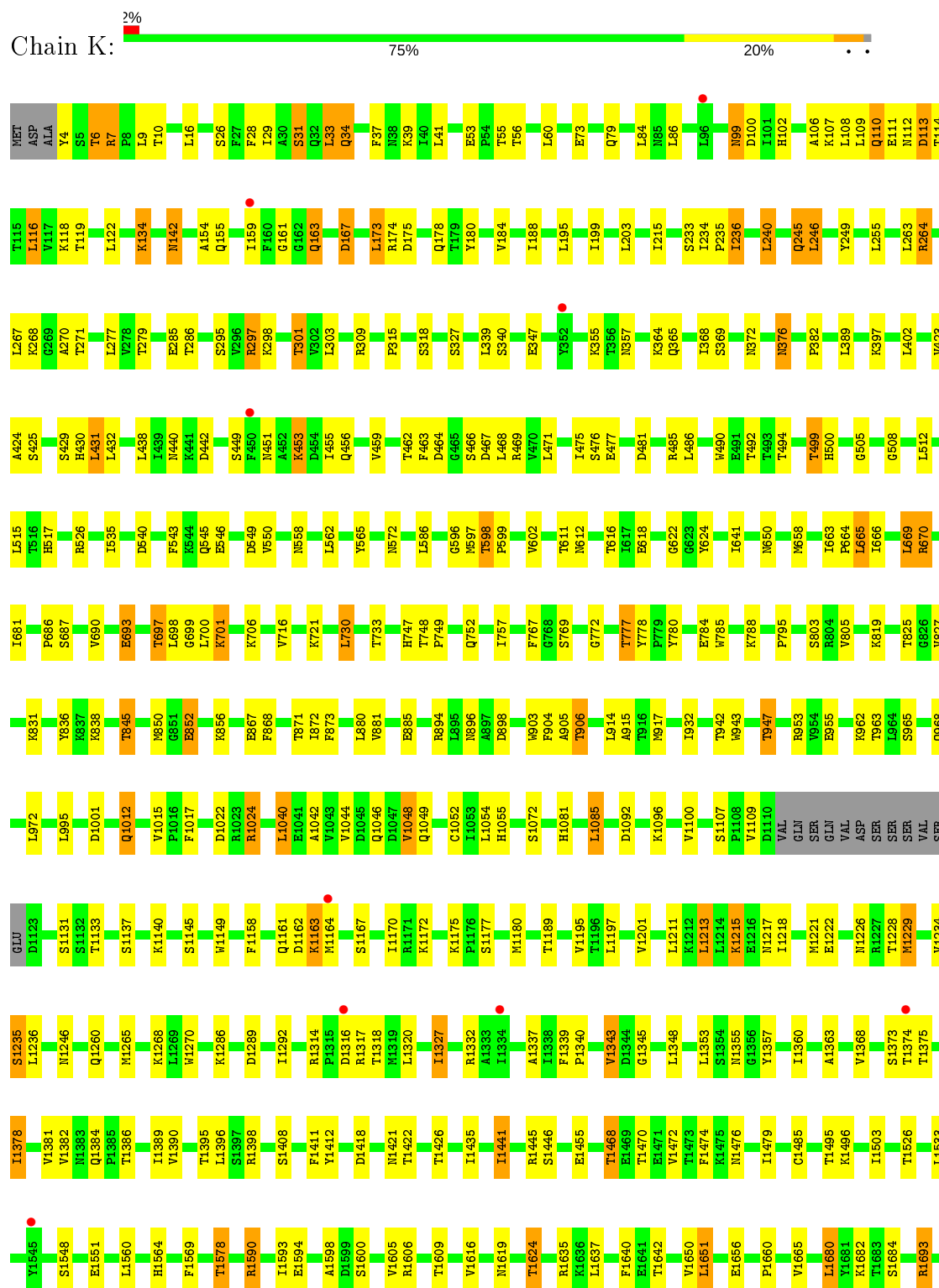


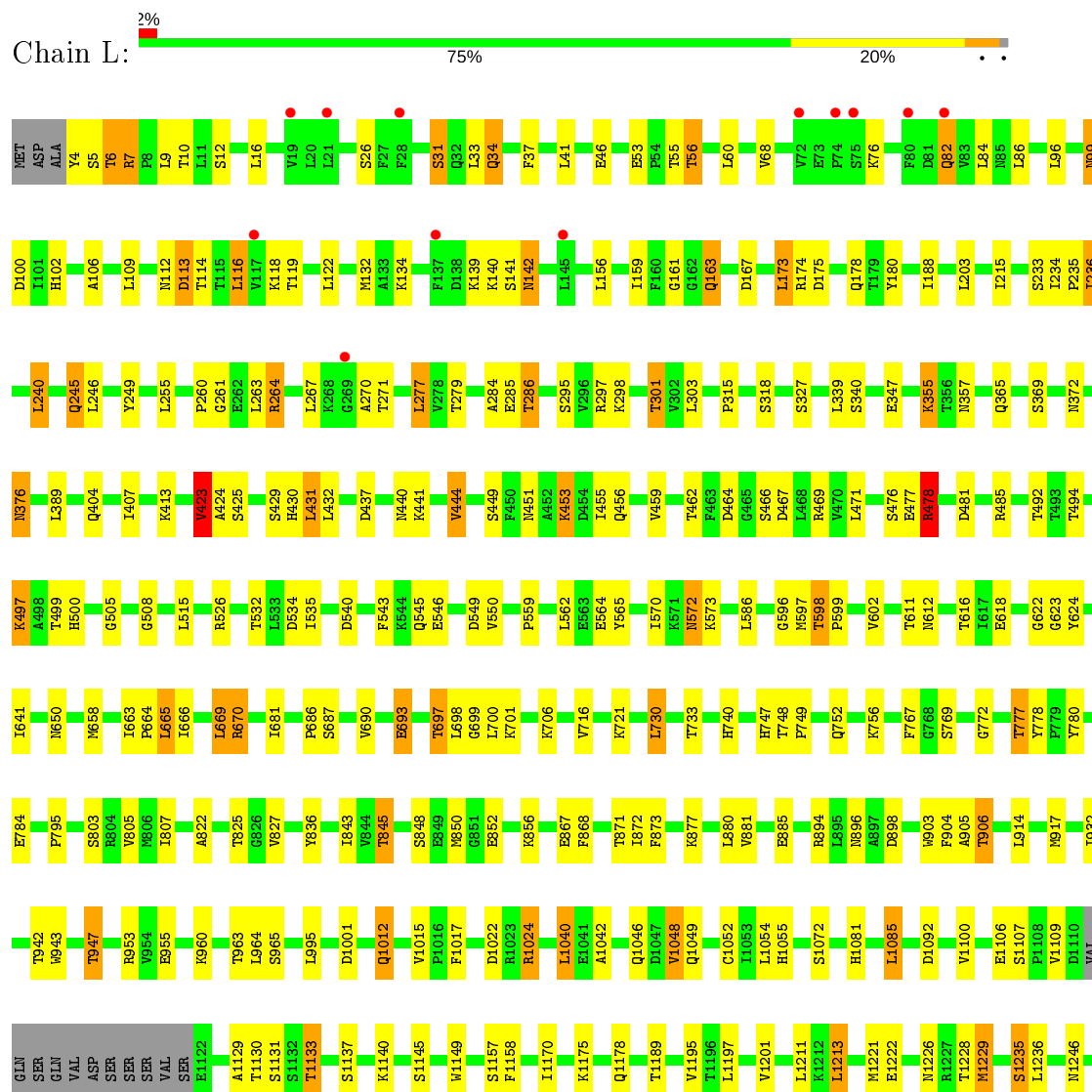
- Molecule 3: Fatty acid synthase subunit beta

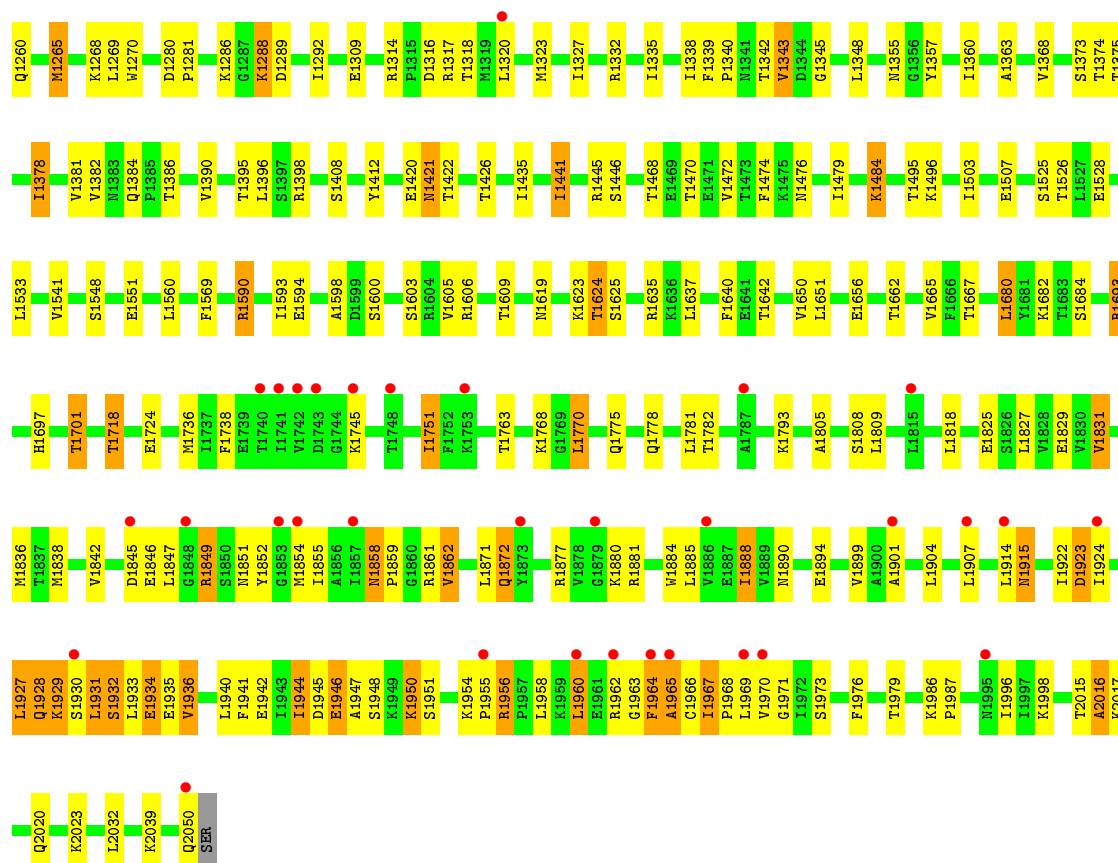




• Molecule 3: Fatty acid synthase subunit beta







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.62Å 347.60Å 265.27Å 90.00° 107.88° 90.00°	Depositor
Resolution (Å)	191.50 – 2.82 204.26 – 2.82	Depositor EDS
% Data completeness (in resolution range)	78.6 (191.50-2.82) 78.6 (204.26-2.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.192 , 0.211 0.194 , 0.211	Depositor DCC
$R_{free}$ test set	35171 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.8	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	179453	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A2P, PGE, J8W, NA, PNS, MLI, EDO, FMN, ACT

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	0.68	2/13939 (0.0%)	0.85	5/18837 (0.0%)
1	B	0.69	0/13933	0.85	4/18829 (0.0%)
1	C	0.69	1/13933 (0.0%)	0.84	3/18829 (0.0%)
1	D	0.69	0/13983	0.86	8/18898 (0.0%)
1	E	0.69	1/13933 (0.0%)	0.85	2/18829 (0.0%)
1	F	0.68	0/13933	0.83	2/18829 (0.0%)
2	G	0.67	0/16394	0.82	1/22244 (0.0%)
2	J	0.67	0/16392	0.83	4/22242 (0.0%)
3	H	0.67	1/16385 (0.0%)	0.82	0/22231
3	I	0.67	0/16372	0.82	1/22213 (0.0%)
3	K	0.67	0/16374	0.82	0/22216
3	L	0.67	0/16394	0.81	3/22243 (0.0%)
All	All	0.68	5/181965 (0.0%)	0.83	33/246440 (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	C	0	2
1	D	0	1
3	I	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1484	GLU	CD-OE2	6.00	1.32	1.25
3	H	852	GLU	CD-OE1	5.37	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1354	GLU	CD-OE1	5.29	1.31	1.25
1	A	1378	GLU	CD-OE1	5.19	1.31	1.25
1	C	1317	GLU	CD-OE1	5.05	1.31	1.25

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1886	LYS	CA-C-O	7.42	135.69	120.10
3	L	1964	PHE	CB-CA-C	7.13	124.66	110.40
1	E	1264	ARG	CG-CD-NE	-7.07	96.96	111.80
1	A	1264	ARG	CG-CD-NE	-7.04	97.01	111.80
1	B	1264	ARG	CG-CD-NE	-7.03	97.03	111.80
1	C	1264	ARG	CG-CD-NE	-6.91	97.28	111.80
1	D	1721	ARG	CG-CD-NE	-6.89	97.33	111.80
1	D	1264	ARG	CG-CD-NE	-6.72	97.68	111.80
2	J	478	ARG	CG-CD-NE	6.15	124.72	111.80
3	L	423	VAL	CA-CB-CG2	6.06	119.98	110.90
3	L	478	ARG	CG-CD-NE	6.04	124.49	111.80
1	A	1886	LYS	CA-C-O	5.88	132.45	120.10
1	F	1150	ASP	CB-CA-C	-5.87	98.66	110.40
1	D	1229	THR	CA-CB-OG1	-5.80	96.81	109.00
2	J	1024	ARG	CB-CG-CD	5.80	126.69	111.60
1	D	1886	LYS	CA-C-O	5.79	132.26	120.10
1	D	977	TYR	CA-CB-CG	5.78	124.38	113.40
1	B	1229	THR	CA-CB-OG1	-5.77	96.88	109.00
1	D	944	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	1150	ASP	CB-CA-C	-5.69	99.01	110.40
1	A	633	GLU	CB-CA-C	5.62	121.65	110.40
3	I	478	ARG	CG-CD-NE	5.60	123.57	111.80
1	A	1229	THR	CA-CB-OG1	-5.57	97.31	109.00
1	C	1229	THR	CA-CB-OG1	-5.57	97.31	109.00
1	D	1150	ASP	CB-CA-C	-5.54	99.31	110.40
1	E	1229	THR	CA-CB-OG1	-5.53	97.38	109.00
1	F	1229	THR	CA-CB-OG1	-5.50	97.45	109.00
1	B	1706	TYR	CB-CG-CD2	5.47	124.28	121.00
2	G	544	LYS	CA-CB-CG	5.32	125.10	113.40
2	J	670	ARG	CG-CD-NE	5.31	122.95	111.80
1	D	1034	ARG	CG-CD-NE	-5.06	101.17	111.80
2	J	736	ARG	CB-CG-CD	5.05	124.72	111.60
1	C	1886	LYS	CA-C-O	5.03	130.65	120.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1207	GLN	Peptide
1	C	1841	ARG	Peptide
1	C	538	GLU	Peptide
1	D	1828	LEU	Peptide
3	I	1844	ARG	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13686	0	13661	211	2
1	B	13680	0	13658	214	0
1	C	13680	0	13658	222	0
1	D	13729	0	13701	207	2
1	E	13680	0	13658	212	0
1	F	13680	0	13658	201	0
2	G	16028	0	15999	241	0
2	J	16025	0	15997	248	0
3	H	16028	0	15993	246	0
3	I	16019	0	15983	249	0
3	K	16021	0	15986	261	0
3	L	16040	0	15998	295	0
4	A	21	0	21	1	0
4	B	21	0	21	1	0
4	C	21	0	21	0	0
4	D	21	0	21	0	0
4	E	21	0	21	0	0
4	F	21	0	21	2	0
5	A	40	0	60	0	0
5	B	40	0	60	4	0
5	C	36	0	54	1	0
5	D	52	0	78	1	0
5	E	48	0	72	0	0
5	F	32	0	48	0	0
5	H	4	0	6	0	0
5	J	16	0	24	2	0
6	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	5	0	0	0	0
6	C	4	0	0	0	0
6	D	8	0	0	0	0
6	E	3	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
6	I	1	0	0	0	0
6	J	2	0	0	0	0
6	K	2	0	0	0	0
6	L	2	0	0	0	0
7	A	27	0	11	3	0
7	B	27	0	11	5	0
7	C	27	0	11	2	0
7	D	27	0	11	3	0
7	E	27	0	11	2	0
7	F	27	0	11	1	0
8	B	4	0	3	1	0
8	C	8	0	6	2	0
8	H	12	0	9	0	0
9	E	10	0	14	0	0
10	G	31	0	19	4	0
10	H	31	0	19	4	0
10	I	31	0	19	5	0
10	J	31	0	19	7	0
10	K	31	0	19	5	0
10	L	31	0	19	5	0
11	G	7	0	2	1	0
11	J	7	0	2	2	0
12	A	42	0	0	1	0
12	B	36	0	0	0	0
12	C	42	0	0	0	0
12	D	60	0	0	1	0
12	E	30	0	0	0	0
12	F	24	0	0	1	0
12	G	19	0	0	1	0
12	H	24	0	0	2	0
12	I	17	0	0	1	0
12	J	17	0	0	0	0
12	K	5	0	0	0	0
12	L	12	0	0	0	0
All	All	179453	0	178694	2594	2

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 7.

All (2594) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ASP:OD2	1:B:508:ASN:OD1	1.53	1.21
3:K:1904:LEU:HD22	3:K:1960:LEU:HD23	1.32	1.12
3:I:867:GLU:O	3:I:871:THR:OG1	1.69	1.08
1:C:1486:LEU:O	1:C:1490:THR:HG22	1.55	1.06
1:B:193:GLU:OE2	1:B:225:SER:OG	1.72	1.06
1:E:1486:LEU:O	1:E:1490:THR:HG22	1.56	1.05
1:B:508:ASN:HD22	1:B:508:ASN:C	1.61	1.04
3:I:1922:ILE:HB	3:I:1927:LEU:HD21	1.40	1.02
2:J:180:TYR:O	2:J:184:VAL:HG22	1.60	1.01
1:D:1135:GLU:OE2	1:E:242:THR:HG21	1.62	0.98
3:K:154:ALA:HA	3:K:499:THR:HG21	1.41	0.98
1:B:792:HIS:HE1	1:E:792:HIS:HE1	1.04	0.96
1:C:792:HIS:HE1	1:D:792:HIS:HE1	1.08	0.96
1:A:340:ARG:HH12	1:A:344:GLN:HE21	1.13	0.95
3:K:110:GLN:HG2	3:K:535:ILE:HD13	1.47	0.94
2:G:79:GLN:HE21	2:G:79:GLN:H	1.15	0.94
2:J:1946:GLU:O	2:J:1950:LYS:HD3	1.67	0.94
1:D:192:LYS:HG2	1:D:224:GLN:HB2	1.50	0.94
1:E:340:ARG:NH1	1:E:344:GLN:HE21	1.65	0.93
1:E:340:ARG:HH12	1:E:344:GLN:NE2	1.67	0.92
1:F:340:ARG:NH1	1:F:344:GLN:HE21	1.66	0.92
1:A:792:HIS:HE1	1:F:792:HIS:HE1	1.07	0.92
3:I:1946:GLU:O	3:I:1950:LYS:HD3	1.68	0.91
1:D:1119:LYS:HE3	1:D:1341:PHE:CD1	2.03	0.91
1:C:1486:LEU:O	1:C:1490:THR:CG2	2.17	0.91
1:A:340:ARG:NH1	1:A:344:GLN:HE21	1.69	0.90
1:C:340:ARG:NH1	1:C:344:GLN:HE21	1.68	0.90
1:F:340:ARG:HH12	1:F:344:GLN:NE2	1.68	0.90
1:E:1486:LEU:O	1:E:1490:THR:CG2	2.19	0.89
1:D:340:ARG:NH1	1:D:344:GLN:HE21	1.69	0.89
1:C:1851:LEU:HD22	1:C:1851:LEU:H	1.35	0.89
1:B:1851:LEU:H	1:B:1851:LEU:HD23	1.35	0.89
3:L:404:GLN:HA	3:L:407:ILE:HD13	1.50	0.89
1:B:508:ASN:O	1:B:508:ASN:ND2	2.03	0.89
3:L:261:GLY:O	3:L:264:ARG:NH1	2.04	0.89
1:B:340:ARG:HH12	1:B:344:GLN:HE21	1.20	0.88
1:B:340:ARG:NH1	1:B:344:GLN:HE21	1.70	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:438:LEU:O	3:K:442:ASP:OD1	1.92	0.88
2:G:964:LEU:H	2:G:964:LEU:HD23	1.38	0.88
1:C:340:ARG:HH12	1:C:344:GLN:HE21	0.88	0.88
1:C:340:ARG:HH12	1:C:344:GLN:NE2	1.71	0.87
3:I:964:LEU:H	3:I:964:LEU:HD23	1.40	0.87
3:K:2037:PRO:O	3:K:2041:ILE:HD12	1.75	0.86
3:L:1420:GLU:HG2	3:L:1421:ASN:ND2	1.88	0.86
3:L:1915:ASN:ND2	3:L:1964:PHE:H	1.74	0.86
2:G:856:LYS:NZ	2:G:1052:CYS:SG	2.49	0.86
1:D:340:ARG:HH12	1:D:344:GLN:HE21	1.19	0.85
1:B:1380:GLN:HE22	5:B:1906:EDO:H11	1.41	0.85
3:L:856:LYS:NZ	3:L:1052:CYS:SG	2.50	0.84
3:H:856:LYS:NZ	3:H:1052:CYS:SG	2.50	0.84
2:J:856:LYS:NZ	2:J:1052:CYS:SG	2.49	0.84
2:J:598:THR:HG22	2:J:622:GLY:HA3	1.59	0.84
3:K:598:THR:HG22	3:K:622:GLY:HA3	1.59	0.84
3:I:856:LYS:NZ	3:I:1052:CYS:SG	2.51	0.84
2:J:192:ALA:HB2	2:J:215:ILE:CD1	2.07	0.84
3:K:856:LYS:NZ	3:K:1052:CYS:SG	2.50	0.84
3:L:1922:ILE:HB	3:L:1927:LEU:HD11	1.58	0.84
3:I:597:MET:H	3:I:601:THR:CG2	1.90	0.83
3:I:598:THR:HG22	3:I:622:GLY:HA3	1.60	0.83
1:C:1471:LYS:HD3	1:C:1759:MET:CE	2.08	0.83
3:L:1421:ASN:HD22	3:L:1421:ASN:N	1.75	0.83
1:C:1471:LYS:HD3	1:C:1759:MET:HE2	1.62	0.82
3:H:598:THR:HG22	3:H:622:GLY:HA3	1.62	0.82
2:J:871:THR:HG22	2:J:872:ILE:HG13	1.61	0.82
2:G:598:THR:HG22	2:G:622:GLY:HA3	1.62	0.82
3:L:451:ASN:HD22	3:L:453:LYS:CE	1.93	0.82
3:H:871:THR:HG22	3:H:872:ILE:HG13	1.61	0.82
3:L:598:THR:HG22	3:L:622:GLY:HA3	1.63	0.81
1:D:1303:GLY:HA2	1:D:1649:LYS:CD	2.11	0.81
1:E:724:LYS:HG2	1:E:725:TYR:CD2	2.16	0.81
3:I:597:MET:H	3:I:601:THR:HG23	1.44	0.81
1:B:508:ASN:C	1:B:508:ASN:ND2	2.33	0.80
3:L:1861:ARG:HB2	3:L:1965:ALA:CB	2.11	0.80
1:A:738:ASN:HD22	7:A:1918:A2P:HN62	1.29	0.80
1:E:724:LYS:HG2	1:E:725:TYR:CE2	2.17	0.80
3:L:534:ASP:C	3:L:535:ILE:HD12	2.03	0.80
3:K:451:ASN:HD22	3:K:453:LYS:HE3	1.45	0.79
1:E:1279:PHE:HB2	1:E:1282:THR:HG23	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1279:PHE:HB2	1:B:1282:THR:HG23	1.65	0.79
2:G:1858:ASN:ND2	2:G:1861:ARG:HG2	1.97	0.79
1:C:1208:VAL:HG13	1:C:1212:THR:HB	1.65	0.78
3:K:195:LEU:O	3:K:199:ILE:HD12	1.83	0.78
3:K:297:ARG:O	3:K:301:THR:HG22	1.83	0.78
1:F:1208:VAL:HG13	1:F:1212:THR:HB	1.66	0.78
3:I:297:ARG:O	3:I:301:THR:HG22	1.84	0.78
1:B:1764:VAL:HG21	1:B:1769:VAL:HG13	1.63	0.78
1:F:1279:PHE:HB2	1:F:1282:THR:HG23	1.65	0.78
1:B:1208:VAL:HG13	1:B:1212:THR:HB	1.66	0.78
3:L:1942:GLU:O	3:L:1946:GLU:HG3	1.84	0.78
1:A:1208:VAL:HG13	1:A:1212:THR:HB	1.65	0.78
1:D:1279:PHE:HB2	1:D:1282:THR:HG23	1.66	0.78
1:C:935:GLU:HB3	1:C:938:GLU:HG2	1.66	0.78
1:D:1867:VAL:HG12	1:D:1884:SER:HB3	1.64	0.78
3:H:1916:PHE:CE2	3:H:1943:ILE:HD12	2.19	0.77
3:I:1170:ILE:HG12	3:I:1221:MET:CE	2.14	0.77
1:C:1426:LEU:HD22	1:F:1716:LEU:HD21	1.66	0.77
3:I:101:ILE:HD13	3:I:126:TYR:HB3	1.66	0.77
3:K:597:MET:HA	10:K:2101:FMN:N5	1.99	0.77
3:L:297:ARG:O	3:L:301:THR:HG22	1.84	0.77
1:A:1716:LEU:HD21	1:E:1426:LEU:HD22	1.66	0.77
3:L:871:THR:HG22	3:L:872:ILE:HG13	1.65	0.77
1:D:1208:VAL:HG13	1:D:1212:THR:HB	1.65	0.77
1:C:1716:LEU:HD21	1:F:1426:LEU:HD22	1.66	0.77
1:F:1303:GLY:HA2	1:F:1649:LYS:HE2	1.66	0.77
3:K:309:ARG:NH1	3:K:442:ASP:OD2	2.18	0.77
1:B:705:VAL:CG2	1:B:732:LEU:HD21	2.15	0.77
3:K:1170:ILE:HG12	3:K:1221:MET:CE	2.15	0.77
3:L:451:ASN:HD22	3:L:453:LYS:HE3	1.50	0.77
1:B:792:HIS:CE1	1:E:792:HIS:HE1	1.96	0.77
1:D:1466:GLU:HB3	1:D:1493:ILE:HD12	1.65	0.76
1:B:1303:GLY:HA2	1:B:1649:LYS:HE2	1.66	0.76
3:H:297:ARG:O	3:H:301:THR:HG22	1.85	0.76
1:B:1716:LEU:HD21	1:D:1426:LEU:HD22	1.67	0.76
2:J:53:GLU:O	2:J:118:LYS:HE2	1.86	0.76
3:K:871:THR:HG22	3:K:872:ILE:HG13	1.67	0.76
1:E:1208:VAL:HG13	1:E:1212:THR:HB	1.65	0.76
1:C:1279:PHE:HB2	1:C:1282:THR:HG23	1.67	0.76
3:I:597:MET:HA	10:I:2101:FMN:N5	2.01	0.75
1:B:1380:GLN:HE22	5:B:1906:EDO:C1	1.98	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:455:ILE:HD11	3:H:469:ARG:HG2	1.68	0.75
1:B:504:ASP:OD2	1:B:508:ASN:CG	2.24	0.75
2:G:297:ARG:O	2:G:301:THR:HG22	1.84	0.75
2:J:99:ASN:HD22	2:J:100:ASP:H	1.35	0.75
3:L:455:ILE:HD11	3:L:469:ARG:HG2	1.68	0.75
2:G:871:THR:HG22	2:G:872:ILE:HG13	1.69	0.75
3:I:455:ILE:HD11	3:I:469:ARG:HG2	1.68	0.75
1:A:1303:GLY:HA2	1:A:1649:LYS:HE2	1.66	0.75
2:G:455:ILE:HD11	2:G:469:ARG:HG2	1.67	0.75
1:A:1279:PHE:HB2	1:A:1282:THR:HG23	1.66	0.75
3:L:99:ASN:HD22	3:L:100:ASP:H	1.34	0.75
2:J:1314:ARG:NH2	3:L:315:PRO:O	2.19	0.75
1:A:1426:LEU:HD22	1:E:1716:LEU:HD21	1.67	0.75
2:J:1054:LEU:HB2	10:J:2101:FMN:HM72	1.69	0.75
2:J:297:ARG:O	2:J:301:THR:HG22	1.86	0.75
1:B:792:HIS:HE1	1:E:792:HIS:CE1	1.96	0.74
3:K:110:GLN:HG2	3:K:535:ILE:CD1	2.17	0.74
1:F:705:VAL:CG2	1:F:732:LEU:HD21	2.16	0.74
1:E:59:ARG:HG2	3:K:1896:GLN:HE22	1.51	0.74
1:B:774:ILE:HG22	7:B:1918:A2P:H2	1.69	0.74
3:L:1946:GLU:C	3:L:1950:LYS:HE3	2.07	0.74
1:C:1303:GLY:HA2	1:C:1649:LYS:HE2	1.67	0.74
2:J:1951:SER:HA	2:J:1954:LYS:HE2	1.70	0.74
2:J:376:ASN:C	2:J:376:ASN:HD22	1.91	0.74
1:B:1160:THR:CG2	1:C:244:THR:HG21	2.17	0.74
1:E:1303:GLY:HA2	1:E:1649:LYS:HE2	1.68	0.74
2:G:99:ASN:HD22	2:G:100:ASP:H	1.36	0.74
1:A:1276:GLN:O	1:A:1282:THR:HG21	1.87	0.74
1:D:705:VAL:CG2	1:D:732:LEU:HD21	2.18	0.74
1:E:1276:GLN:O	1:E:1282:THR:HG21	1.88	0.74
3:H:376:ASN:HD22	3:H:376:ASN:C	1.91	0.74
3:I:376:ASN:C	3:I:376:ASN:HD22	1.91	0.74
3:K:110:GLN:CG	3:K:535:ILE:HD13	2.17	0.74
1:C:1276:GLN:O	1:C:1282:THR:HG21	1.88	0.73
1:C:792:HIS:HE1	1:D:792:HIS:CE1	2.00	0.73
3:K:455:ILE:HD11	3:K:469:ARG:HG2	1.70	0.73
1:C:705:VAL:CG2	1:C:732:LEU:HD21	2.18	0.73
3:H:99:ASN:HD22	3:H:100:ASP:H	1.35	0.73
1:D:1276:GLN:O	1:D:1282:THR:HG21	1.87	0.73
3:K:451:ASN:ND2	3:K:453:LYS:HE3	2.02	0.73
1:D:1303:GLY:HA2	1:D:1649:LYS:HD3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1760:THR:HG23	1:A:1760:THR:O	1.89	0.73
2:G:376:ASN:C	2:G:376:ASN:HD22	1.91	0.73
1:D:59:ARG:HH11	2:J:1896:GLN:HE22	1.37	0.73
1:A:792:HIS:CE1	1:F:792:HIS:HE1	2.00	0.73
3:L:1054:LEU:HB2	10:L:2101:FMN:HM72	1.70	0.72
1:A:705:VAL:CG2	1:A:732:LEU:HD21	2.19	0.72
1:C:1865:THR:CB	1:C:1886:LYS:HG3	2.20	0.72
3:H:1054:LEU:HB2	10:H:2101:FMN:HM72	1.70	0.72
2:J:455:ILE:HD11	2:J:469:ARG:HG2	1.71	0.72
3:H:597:MET:HA	10:H:2101:FMN:N5	2.04	0.72
1:E:705:VAL:CG2	1:E:732:LEU:HD21	2.19	0.72
3:H:79:GLN:H	3:H:79:GLN:HE21	1.35	0.72
3:K:376:ASN:HD22	3:K:376:ASN:C	1.91	0.72
1:C:1785:THR:O	1:C:1789:ARG:HG2	1.90	0.72
1:F:1276:GLN:O	1:F:1282:THR:HG21	1.88	0.72
1:B:1276:GLN:O	1:B:1282:THR:HG21	1.88	0.72
1:C:789:GLU:OE1	1:D:801:ARG:NH2	2.23	0.72
1:C:792:HIS:CE1	1:D:792:HIS:HE1	2.01	0.71
3:L:1420:GLU:HG2	3:L:1421:ASN:HD22	1.53	0.71
3:L:264:ARG:HE	3:L:456:GLN:HB2	1.52	0.71
1:B:1279:PHE:HB2	1:B:1282:THR:CG2	2.21	0.71
3:K:110:GLN:CG	3:K:535:ILE:CD1	2.67	0.71
1:E:1279:PHE:HB2	1:E:1282:THR:CG2	2.20	0.71
3:I:1778:GLN:HB3	3:I:1831:VAL:HG13	1.73	0.71
3:L:376:ASN:HD22	3:L:376:ASN:C	1.91	0.71
1:A:792:HIS:HE1	1:F:792:HIS:CE1	2.00	0.71
3:L:1778:GLN:HB3	3:L:1831:VAL:HG13	1.73	0.71
7:C:1917:A2P:H1'	7:C:1917:A2P:O3P	1.91	0.71
3:H:1923:ASP:O	3:H:1927:LEU:HD22	1.91	0.71
2:J:597:MET:HA	10:J:2101:FMN:N5	2.05	0.71
3:L:597:MET:HA	10:L:2101:FMN:N5	2.05	0.71
1:A:1039:MET:O	1:A:1609:ARG:NH2	2.24	0.71
1:E:340:ARG:HH12	1:E:344:GLN:HE21	0.83	0.71
1:E:1039:MET:O	1:E:1609:ARG:NH2	2.24	0.71
1:F:1039:MET:O	1:F:1609:ARG:NH2	2.24	0.70
1:B:1039:MET:O	1:B:1609:ARG:NH2	2.24	0.70
1:C:1279:PHE:HB2	1:C:1282:THR:CG2	2.21	0.70
3:I:1878:VAL:O	3:I:1882:THR:HG22	1.91	0.70
3:K:1904:LEU:HD22	3:K:1960:LEU:CD2	2.15	0.70
1:A:454:HIS:O	1:A:458:THR:HG22	1.91	0.70
1:B:1426:LEU:HD22	1:D:1716:LEU:HD21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1778:GLN:HB3	2:G:1831:VAL:HG13	1.72	0.70
3:I:1217:ASN:O	3:I:1218:ILE:HD12	1.91	0.70
1:A:1279:PHE:HB2	1:A:1282:THR:CG2	2.21	0.70
1:F:340:ARG:HH12	1:F:344:GLN:HE21	0.83	0.70
3:H:1778:GLN:HB3	3:H:1831:VAL:HG13	1.73	0.70
3:K:1422:THR:HG22	3:K:1474:PHE:CD1	2.27	0.70
1:E:454:HIS:O	1:E:458:THR:HG22	1.92	0.70
2:G:597:MET:HA	10:G:2101:FMN:N5	2.07	0.70
2:J:1778:GLN:HB3	2:J:1831:VAL:HG13	1.73	0.70
3:K:1778:GLN:HB3	3:K:1831:VAL:HG13	1.72	0.70
1:D:1279:PHE:HB2	1:D:1282:THR:CG2	2.21	0.70
1:E:1167:LEU:HD12	1:E:1171:ALA:CB	2.21	0.70
1:D:454:HIS:O	1:D:458:THR:HG22	1.92	0.70
3:I:1422:THR:HG22	3:I:1474:PHE:CD1	2.26	0.69
1:A:1657:HIS:CD2	1:A:1658:PRO:HD2	2.27	0.69
3:K:315:PRO:O	3:L:1314:ARG:NH2	2.26	0.69
1:D:1039:MET:O	1:D:1609:ARG:NH2	2.24	0.69
3:L:1422:THR:HG22	3:L:1474:PHE:CD1	2.26	0.69
1:D:1119:LYS:HE3	1:D:1341:PHE:CG	2.27	0.69
3:H:315:PRO:O	3:I:1314:ARG:NH2	2.25	0.69
3:I:101:ILE:HD13	3:I:126:TYR:CB	2.22	0.69
1:A:1844:LYS:O	1:A:1844:LYS:HG3	1.92	0.69
1:C:1039:MET:O	1:C:1609:ARG:NH2	2.24	0.69
1:C:454:HIS:O	1:C:458:THR:HG22	1.92	0.69
1:E:1304:ALA:O	1:E:1307:THR:CG2	2.41	0.69
1:F:1279:PHE:HB2	1:F:1282:THR:CG2	2.21	0.69
3:H:1422:THR:HG22	3:H:1474:PHE:CD1	2.27	0.69
1:C:528:GLU:OE1	1:C:894:ARG:NH1	2.25	0.69
1:D:1304:ALA:O	1:D:1307:THR:CG2	2.41	0.69
1:D:1466:GLU:HB3	1:D:1493:ILE:CD1	2.23	0.69
1:D:528:GLU:OE1	1:D:894:ARG:NH1	2.26	0.69
1:F:13:LEU:O	1:F:17:LEU:HD12	1.92	0.69
2:G:1868:GLN:HG3	2:G:1872:GLN:NE2	2.08	0.69
3:K:99:ASN:HD22	3:K:100:ASP:H	1.39	0.69
1:C:1304:ALA:O	1:C:1307:THR:CG2	2.41	0.69
1:A:244:THR:HG21	1:C:1160:THR:CG2	2.23	0.69
1:B:454:HIS:O	1:B:458:THR:HG22	1.92	0.69
1:A:1304:ALA:O	1:A:1307:THR:CG2	2.41	0.69
1:D:1829:GLY:HA2	1:D:1832:ALA:HB3	1.74	0.69
1:E:982:ILE:HD12	3:K:965:SER:HA	1.74	0.69
2:G:1422:THR:HG22	2:G:1474:PHE:CD1	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:982:ILE:HD12	3:L:965:SER:HA	1.75	0.68
1:F:1304:ALA:O	1:F:1307:THR:CG2	2.42	0.68
3:L:1265:MET:O	3:L:1269:LEU:HD12	1.92	0.68
3:L:534:ASP:O	3:L:535:ILE:HD12	1.92	0.68
1:B:1304:ALA:O	1:B:1307:THR:CG2	2.41	0.68
3:K:1337:ALA:HB1	3:K:1378:ILE:HG13	1.74	0.68
1:B:793:ARG:HD2	1:E:789:GLU:OE2	1.93	0.68
2:J:1422:THR:HG22	2:J:1474:PHE:CD1	2.28	0.68
2:J:736:ARG:NH1	2:J:769:SER:O	2.25	0.68
1:D:1367:ARG:O	1:D:1370:THR:OG1	2.12	0.68
1:F:1303:GLY:HA2	1:F:1649:LYS:CE	2.24	0.68
3:K:154:ALA:HA	3:K:499:THR:CG2	2.20	0.68
3:K:155:GLN:H	3:K:499:THR:CG2	2.06	0.68
1:A:340:ARG:HH12	1:A:344:GLN:NE2	1.89	0.68
1:E:528:GLU:OE1	1:E:894:ARG:NH1	2.26	0.67
1:F:1854:ASN:O	1:F:1857:LYS:HG2	1.93	0.67
1:B:1500:GLN:HG2	1:D:1507:GLN:HE22	1.58	0.67
1:C:491:LYS:HE3	8:C:1903:ACT:H2	1.75	0.67
2:J:163:GLN:HG2	2:J:423:VAL:HG12	1.76	0.67
2:G:1217:ASN:C	2:G:1218:ILE:HD12	2.15	0.67
1:F:1826:LYS:O	1:F:1827:SER:O	2.13	0.67
3:I:1054:LEU:HB2	10:I:2101:FMN:HM72	1.76	0.67
3:K:730:LEU:C	3:K:730:LEU:HD12	2.15	0.67
1:A:1507:GLN:HE22	1:E:1500:GLN:HG2	1.59	0.67
1:F:1794:GLN:HG2	1:F:1838:GLU:OE2	1.94	0.67
3:L:163:GLN:HG2	3:L:423:VAL:HG13	1.77	0.67
1:F:454:HIS:O	1:F:458:THR:HG22	1.93	0.67
3:H:565:TYR:HB2	3:H:795:PRO:HG2	1.75	0.67
2:J:1881:ARG:C	2:J:1881:ARG:HD3	2.15	0.67
3:L:1923:ASP:O	3:L:1927:LEU:HG	1.93	0.67
1:A:789:GLU:OE1	1:F:801:ARG:NH2	2.28	0.67
1:B:682:GLY:HA2	7:B:1918:A2P:H1'	1.76	0.67
2:G:730:LEU:C	2:G:730:LEU:HD12	2.15	0.67
2:G:7:ARG:NH1	3:I:28:PHE:O	2.28	0.67
3:H:1933:LEU:O	3:H:1934:GLU:HG3	1.95	0.66
2:J:730:LEU:HD12	2:J:730:LEU:C	2.15	0.66
1:A:528:GLU:OE1	1:A:894:ARG:NH1	2.27	0.66
1:C:793:ARG:HA	1:C:797:THR:HG23	1.78	0.66
2:G:1149:TRP:CD1	2:G:1213:LEU:CD2	2.78	0.66
3:I:730:LEU:C	3:I:730:LEU:HD12	2.15	0.66
1:B:1303:GLY:HA2	1:B:1649:LYS:CE	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1303:GLY:HA2	1:D:1649:LYS:HD2	1.77	0.66
1:E:13:LEU:O	1:E:17:LEU:HD12	1.96	0.66
3:I:1635:ARG:NH1	3:I:1656:GLU:OE1	2.28	0.66
3:L:730:LEU:C	3:L:730:LEU:HD12	2.15	0.66
1:A:1303:GLY:HA2	1:A:1649:LYS:CE	2.25	0.66
3:H:1916:PHE:CE2	3:H:1943:ILE:CD1	2.78	0.66
3:L:1861:ARG:CB	3:L:1965:ALA:HB2	2.26	0.66
1:C:702:LYS:HE3	1:C:731:THR:HG23	1.78	0.66
2:J:214:ASN:OD1	2:J:217:GLU:HB2	1.95	0.66
1:B:1302:VAL:CG2	1:D:1302:VAL:CG2	2.74	0.66
3:L:843:ILE:HD11	3:L:1055:HIS:HB3	1.78	0.66
1:C:1303:GLY:HA2	1:C:1649:LYS:CE	2.25	0.66
1:E:1303:GLY:HA2	1:E:1649:LYS:CE	2.25	0.66
3:H:1635:ARG:NH1	3:H:1656:GLU:OE1	2.29	0.66
2:J:1149:TRP:CD1	2:J:1213:LEU:CD2	2.79	0.66
3:H:730:LEU:HD12	3:H:730:LEU:C	2.16	0.66
3:I:1217:ASN:C	3:I:1218:ILE:HD12	2.16	0.66
2:J:693:GLU:O	2:J:697:THR:OG1	2.14	0.66
3:L:1929:LYS:CE	3:L:1933:LEU:HD12	2.25	0.66
3:H:1170:ILE:HA	3:H:1221:MET:HE1	1.77	0.66
2:J:1933:LEU:O	2:J:1934:GLU:HG3	1.96	0.66
2:G:565:TYR:HB2	2:G:795:PRO:HG2	1.77	0.66
3:I:565:TYR:HB2	3:I:795:PRO:HG2	1.77	0.66
1:C:1785:THR:O	1:C:1789:ARG:CG	2.44	0.65
1:E:36:LEU:O	1:E:76:ARG:NH2	2.29	0.65
3:I:106:ALA:HB2	3:I:545:GLN:HG2	1.78	0.65
1:D:13:LEU:O	1:D:17:LEU:HD12	1.95	0.65
2:G:2050:GLN:O	2:G:2050:GLN:HG2	1.95	0.65
3:H:1149:TRP:CD1	3:H:1213:LEU:CD2	2.79	0.65
3:K:1149:TRP:CD1	3:K:1213:LEU:CD2	2.79	0.65
3:L:1635:ARG:NH1	3:L:1656:GLU:OE1	2.29	0.65
1:B:1380:GLN:NE2	5:B:1906:EDO:H11	2.12	0.65
1:B:793:ARG:HA	1:B:797:THR:HG23	1.78	0.65
1:F:411:GLN:HE22	1:F:1628:SER:H	1.44	0.65
2:J:1635:ARG:NH1	2:J:1656:GLU:OE1	2.28	0.65
1:D:36:LEU:O	1:D:76:ARG:NH2	2.30	0.65
2:J:565:TYR:HB2	2:J:795:PRO:HG2	1.77	0.65
3:L:1933:LEU:O	3:L:1934:GLU:HG3	1.96	0.65
3:L:565:TYR:HB2	3:L:795:PRO:HG2	1.78	0.65
1:A:1657:HIS:HD2	1:A:1659:ASP:H	1.45	0.65
2:G:1635:ARG:NH1	2:G:1656:GLU:OE1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1149:TRP:CD1	3:I:1213:LEU:CD2	2.79	0.65
3:L:1149:TRP:CD1	3:L:1213:LEU:CD2	2.79	0.65
1:C:36:LEU:O	1:C:76:ARG:NH2	2.30	0.65
1:C:1455:ARG:HD3	1:F:1455:ARG:NH2	2.12	0.65
3:K:1177:SER:OG	3:K:1180:MET:HE3	1.96	0.65
1:A:738:ASN:ND2	7:A:1918:A2P:HN62	1.94	0.65
1:B:1030:TRP:NE1	1:B:1580:LEU:HD22	2.12	0.65
3:K:468:LEU:O	3:K:475:ILE:CD1	2.45	0.65
1:A:5:VAL:O	1:A:9:LEU:HD12	1.97	0.65
1:B:36:LEU:O	1:B:76:ARG:NH2	2.30	0.65
3:I:163:GLN:HG2	3:I:423:VAL:HG12	1.78	0.65
3:K:1933:LEU:O	3:K:1934:GLU:HG3	1.97	0.65
3:K:565:TYR:HB2	3:K:795:PRO:HG2	1.78	0.65
2:G:163:GLN:HG2	2:G:423:VAL:HG12	1.79	0.64
3:L:1861:ARG:HB2	3:L:1965:ALA:HB3	1.79	0.64
1:A:1851:LEU:HD22	1:A:1851:LEU:H	1.61	0.64
3:I:1215:LYS:HE3	3:I:1218:ILE:HD13	1.79	0.64
2:J:964:LEU:H	2:J:964:LEU:HD22	1.63	0.64
1:B:774:ILE:CG2	7:B:1918:A2P:H2	2.27	0.64
1:E:1851:LEU:HD22	1:E:1851:LEU:H	1.62	0.64
1:F:655:LEU:HD22	1:F:916:LEU:HD11	1.79	0.64
2:J:598:THR:OG1	2:J:599:PRO:CD	2.45	0.64
3:K:108:LEU:HA	3:K:112:ASN:HD22	1.61	0.64
3:K:1635:ARG:NH1	3:K:1656:GLU:OE1	2.29	0.64
1:B:1304:ALA:O	1:B:1307:THR:HG22	1.98	0.64
1:E:1030:TRP:NE1	1:E:1580:LEU:HD22	2.12	0.64
2:G:693:GLU:O	2:G:697:THR:OG1	2.15	0.64
2:J:1886:VAL:HG23	2:J:1906:ALA:HB3	1.79	0.64
2:J:1904:LEU:HD23	2:J:1958:LEU:O	1.98	0.64
1:E:1304:ALA:O	1:E:1307:THR:HG22	1.98	0.64
3:K:693:GLU:O	3:K:697:THR:OG1	2.16	0.64
1:A:1304:ALA:O	1:A:1307:THR:HG22	1.98	0.64
1:B:411:GLN:HE22	1:B:1628:SER:H	1.44	0.64
1:C:1477:ILE:HD12	1:C:1485:PHE:CG	2.33	0.64
1:D:1014:ASP:H	1:D:1510:ASN:HD21	1.46	0.64
1:F:1030:TRP:NE1	1:F:1580:LEU:HD22	2.12	0.64
1:F:1310:GLU:OE1	1:F:1649:LYS:HE3	1.98	0.64
2:J:102:HIS:HE1	2:J:180:TYR:OH	1.80	0.64
3:L:843:ILE:HD12	3:L:1055:HIS:O	1.98	0.64
1:C:1030:TRP:NE1	1:C:1580:LEU:HD22	2.12	0.64
3:H:102:HIS:HE1	3:H:180:TYR:OH	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:102:HIS:HE1	3:I:180:TYR:OH	1.80	0.64
1:A:1030:TRP:NE1	1:A:1580:LEU:HD22	2.12	0.64
1:A:411:GLN:HE22	1:A:1628:SER:H	1.44	0.64
1:B:1014:ASP:H	1:B:1510:ASN:HD21	1.46	0.64
3:K:102:HIS:HE1	3:K:180:TYR:OH	1.80	0.64
3:L:407:ILE:N	3:L:407:ILE:HD12	2.13	0.64
1:D:411:GLN:HE22	1:D:1628:SER:H	1.45	0.63
2:G:598:THR:OG1	2:G:599:PRO:CD	2.46	0.63
3:L:102:HIS:HE1	3:L:180:TYR:OH	1.81	0.63
1:D:655:LEU:HD22	1:D:916:LEU:HD11	1.79	0.63
3:H:598:THR:OG1	3:H:599:PRO:CD	2.45	0.63
1:D:793:ARG:HA	1:D:797:THR:HG23	1.80	0.63
1:F:1014:ASP:H	1:F:1510:ASN:HD21	1.46	0.63
3:K:163:GLN:HG2	3:K:423:VAL:HG12	1.80	0.63
2:G:102:HIS:HE1	2:G:180:TYR:OH	1.81	0.63
3:I:693:GLU:O	3:I:697:THR:OG1	2.15	0.63
1:A:655:LEU:HD22	1:A:916:LEU:HD11	1.81	0.63
1:D:1030:TRP:NE1	1:D:1580:LEU:HD22	2.13	0.63
3:I:598:THR:OG1	3:I:599:PRO:CD	2.46	0.63
3:K:28:PHE:O	3:L:7:ARG:NH2	2.31	0.63
3:K:598:THR:OG1	3:K:599:PRO:CD	2.46	0.63
1:D:1232:TYR:CZ	1:D:1701:LYS:HD2	2.34	0.63
2:G:1838:MET:HE3	2:G:1976:PHE:CE1	2.34	0.63
3:L:1736:MET:HG2	3:L:1751:ILE:HG13	1.79	0.63
1:A:1310:GLU:OE1	1:A:1649:LYS:HE3	1.98	0.63
1:C:411:GLN:HE22	1:C:1628:SER:H	1.46	0.63
1:F:1232:TYR:CZ	1:F:1701:LYS:HD2	2.34	0.63
3:I:1170:ILE:CG1	3:I:1221:MET:CE	2.77	0.63
3:I:597:MET:N	3:I:601:THR:CG2	2.62	0.63
3:L:1851:ASN:ND2	3:L:1956:ARG:HH21	1.96	0.63
3:L:693:GLU:O	3:L:697:THR:OG1	2.16	0.63
1:B:789:GLU:OE2	1:E:793:ARG:HD2	1.99	0.63
3:H:163:GLN:HG2	3:H:423:VAL:HG12	1.81	0.63
1:F:36:LEU:O	1:F:76:ARG:NH2	2.32	0.63
3:L:1861:ARG:CB	3:L:1965:ALA:CB	2.77	0.63
1:B:1310:GLU:OE1	1:B:1649:LYS:HE3	1.99	0.62
1:D:1304:ALA:O	1:D:1307:THR:HG22	1.99	0.62
3:K:106:ALA:HB2	3:K:545:GLN:HG2	1.79	0.62
1:E:1232:TYR:CZ	1:E:1701:LYS:HD2	2.34	0.62
3:L:598:THR:OG1	3:L:599:PRO:CD	2.47	0.62
1:C:1014:ASP:H	1:C:1510:ASN:HD21	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1304:ALA:O	1:C:1307:THR:HG22	1.98	0.62
3:H:693:GLU:O	3:H:697:THR:OG1	2.16	0.62
3:K:1904:LEU:CD1	3:K:1958:LEU:O	2.47	0.62
1:E:655:LEU:HD22	1:E:916:LEU:HD11	1.82	0.62
2:J:1624:THR:HB	2:J:1642:THR:OG1	1.99	0.62
1:A:1757:GLU:O	1:A:1760:THR:HG22	1.98	0.62
1:A:1500:GLN:CG	1:E:1507:GLN:HE22	2.11	0.62
3:L:441:LYS:O	3:L:444:VAL:HG12	1.99	0.62
1:E:1014:ASP:H	1:E:1510:ASN:HD21	1.45	0.62
1:F:1304:ALA:O	1:F:1307:THR:HG22	1.99	0.62
1:B:1232:TYR:CZ	1:B:1701:LYS:HD2	2.34	0.62
3:L:109:LEU:HD21	3:L:116:LEU:HD22	1.81	0.62
1:E:1310:GLU:OE1	1:E:1649:LYS:HE3	2.00	0.62
3:I:1932:SER:HB3	3:I:1935:GLU:OE1	2.00	0.62
3:K:1904:LEU:CD2	3:K:1960:LEU:HD23	2.21	0.62
1:A:599:MET:N	1:A:624:LYS:HE2	2.15	0.62
1:E:738:ASN:HD22	7:E:1917:A2P:HN62	1.48	0.62
3:L:106:ALA:HB2	3:L:545:GLN:HG2	1.82	0.62
1:B:513:GLU:OE2	1:B:873:ARG:NH1	2.32	0.61
1:C:1500:GLN:HA	1:F:1507:GLN:HE22	1.65	0.61
1:C:1310:GLU:OE1	1:C:1649:LYS:HE3	1.99	0.61
1:E:411:GLN:HE22	1:E:1628:SER:H	1.46	0.61
3:I:1927:LEU:HA	3:I:1931:LEU:HB2	1.83	0.61
3:L:451:ASN:HD22	3:L:453:LYS:HE2	1.64	0.61
1:A:1160:THR:HB	1:B:244:THR:HG21	1.81	0.61
2:G:1054:LEU:HB2	10:G:2101:FMN:HM72	1.81	0.61
2:G:79:GLN:NE2	2:G:79:GLN:H	1.94	0.61
1:A:1232:TYR:CZ	1:A:1701:LYS:HD2	2.35	0.61
1:C:1302:VAL:CG2	1:F:1302:VAL:CG2	2.79	0.61
1:C:1471:LYS:HD3	1:C:1759:MET:HE3	1.82	0.61
3:K:110:GLN:HG3	3:K:535:ILE:CD1	2.31	0.61
2:J:877:LYS:H	2:J:877:LYS:HE2	1.65	0.61
3:K:1161:GLN:O	3:K:1164:MET:HG2	2.00	0.61
1:C:455:ILE:O	1:C:458:THR:HG23	2.01	0.61
1:A:1500:GLN:HG2	1:E:1507:GLN:HE22	1.65	0.61
2:G:1624:THR:HB	2:G:1642:THR:OG1	2.00	0.61
3:L:1915:ASN:HD21	3:L:1964:PHE:H	1.47	0.61
1:A:1160:THR:CG2	1:B:244:THR:HG21	2.30	0.61
1:A:1507:GLN:HE22	1:E:1500:GLN:CG	2.13	0.61
1:E:702:LYS:HE3	1:E:731:THR:HG23	1.81	0.61
3:I:599:PRO:O	3:I:602:VAL:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1838:MET:HE3	3:I:1976:PHE:CE1	2.35	0.61
3:K:1177:SER:OG	3:K:1180:MET:CE	2.49	0.61
3:K:1963:GLY:O	3:K:1965:ALA:N	2.34	0.61
1:F:11:HIS:ND1	3:L:1998:LYS:HA	2.15	0.61
1:D:1849:VAL:HB	1:D:1867:VAL:HG23	1.83	0.61
1:F:455:ILE:O	1:F:458:THR:HG23	2.00	0.61
3:H:1624:THR:HB	3:H:1642:THR:OG1	2.00	0.61
3:I:1624:THR:HB	3:I:1642:THR:OG1	2.01	0.61
3:K:1170:ILE:CG1	3:K:1221:MET:CE	2.79	0.61
3:H:1923:ASP:O	3:H:1927:LEU:CD2	2.49	0.60
3:I:601:THR:O	3:I:601:THR:OG1	2.16	0.60
3:K:1624:THR:HB	3:K:1642:THR:OG1	2.01	0.60
1:A:1014:ASP:H	1:A:1510:ASN:HD21	1.47	0.60
1:C:248:LYS:HE3	1:C:248:LYS:HA	1.82	0.60
2:J:1054:LEU:HB2	10:J:2101:FMN:C7M	2.30	0.60
3:K:599:PRO:O	3:K:602:VAL:HG12	2.01	0.60
1:A:455:ILE:O	1:A:458:THR:HG23	2.01	0.60
1:F:479:ASN:O	1:F:483:VAL:HG22	2.00	0.60
1:B:455:ILE:O	1:B:458:THR:HG23	2.02	0.60
3:I:1962:ARG:CZ	3:I:1962:ARG:HB3	2.30	0.60
1:E:982:ILE:HD13	3:K:955:GLU:CB	2.30	0.60
3:L:1476:ASN:HD21	3:L:1479:ILE:HD13	1.65	0.60
3:K:161:GLY:H	3:K:505:GLY:HA3	1.66	0.60
3:L:1054:LEU:HB2	10:L:2101:FMN:C7M	2.32	0.60
1:D:69:ASP:OD1	1:D:76:ARG:NH1	2.35	0.60
3:I:1904:LEU:HD23	3:I:1958:LEU:O	2.01	0.60
2:J:1946:GLU:O	2:J:1950:LYS:CD	2.47	0.60
1:F:705:VAL:HG23	1:F:732:LEU:HD21	1.83	0.60
1:A:793:ARG:HD2	1:F:789:GLU:OE2	2.02	0.60
1:C:11:HIS:ND1	3:I:1998:LYS:HA	2.17	0.60
3:L:599:PRO:O	3:L:602:VAL:HG12	2.02	0.60
1:B:479:ASN:O	1:B:483:VAL:HG22	2.01	0.60
1:C:1232:TYR:CZ	1:C:1701:LYS:HD2	2.37	0.60
1:D:455:ILE:O	1:D:458:THR:HG23	2.01	0.60
1:F:1857:LYS:HG3	1:F:1858:ALA:N	2.17	0.60
2:G:1868:GLN:O	2:G:1869:GLU:HG2	2.01	0.60
3:I:1854:MET:HB3	3:I:1901:ALA:HB2	1.84	0.60
1:C:801:ARG:NH2	1:D:789:GLU:OE1	2.35	0.60
1:E:513:GLU:OE2	1:E:873:ARG:NH1	2.32	0.60
2:J:1170:ILE:HA	2:J:1221:MET:HE1	1.82	0.60
2:J:1962:ARG:CZ	2:J:1962:ARG:HB3	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:2015:THR:HG23	3:K:2028:ASP:OD2	2.02	0.60
3:K:2015:THR:O	3:K:2017:LYS:N	2.35	0.60
3:L:1854:MET:HB3	3:L:1901:ALA:HB2	1.84	0.60
3:L:1904:LEU:HD23	3:L:1958:LEU:O	2.02	0.60
1:B:69:ASP:OD1	1:B:76:ARG:NH1	2.35	0.60
1:C:655:LEU:HD22	1:C:916:LEU:HD11	1.84	0.60
1:C:789:GLU:OE2	1:D:793:ARG:HD2	2.01	0.60
1:D:996:LYS:HD3	1:D:1000:GLN:NE2	2.17	0.60
2:G:142:ASN:HB3	2:G:550:VAL:HG13	1.83	0.60
3:K:1343:VAL:O	3:K:1343:VAL:HG22	2.02	0.60
3:L:1343:VAL:HG22	3:L:1343:VAL:O	2.02	0.60
3:L:1624:THR:HB	3:L:1642:THR:OG1	2.01	0.59
1:B:655:LEU:HD22	1:B:916:LEU:HD11	1.84	0.59
3:H:1838:MET:HE3	3:H:1976:PHE:CE1	2.36	0.59
2:J:142:ASN:HB3	2:J:550:VAL:HG13	1.83	0.59
3:K:1838:MET:HE3	3:K:1976:PHE:CE1	2.37	0.59
2:G:1933:LEU:O	2:G:1934:GLU:HG3	2.03	0.59
3:K:1476:ASN:HD21	3:K:1479:ILE:HD13	1.66	0.59
1:B:1859:ALA:O	1:B:1864:VAL:HG22	2.02	0.59
1:B:705:VAL:HG23	1:B:732:LEU:HD21	1.82	0.59
1:C:491:LYS:HE3	8:C:1903:ACT:CH3	2.31	0.59
1:F:1851:LEU:H	1:F:1851:LEU:CD2	2.14	0.59
2:G:161:GLY:H	2:G:505:GLY:HA3	1.67	0.59
3:H:1345:GLY:HA3	3:H:1412:TYR:CD1	2.38	0.59
3:H:1854:MET:HB3	3:H:1901:ALA:HB2	1.84	0.59
1:B:822:VAL:HG12	1:B:824:LEU:HD13	1.83	0.59
2:G:1343:VAL:HG22	2:G:1343:VAL:O	2.03	0.59
3:L:807:ILE:HD11	3:L:822:ALA:HB2	1.84	0.59
1:C:822:VAL:HG12	1:C:824:LEU:HD13	1.85	0.59
1:E:69:ASP:OD1	1:E:76:ARG:NH1	2.35	0.59
1:F:1470:LEU:HD13	1:F:1489:ARG:HG2	1.83	0.59
3:I:1922:ILE:HB	3:I:1927:LEU:CD2	2.26	0.59
3:I:1933:LEU:O	3:I:1934:GLU:HG3	2.03	0.59
1:B:150:LEU:HD11	1:B:225:SER:OG	2.03	0.59
1:F:822:VAL:HG12	1:F:824:LEU:HD13	1.83	0.59
3:I:1824:ILE:N	3:I:1824:ILE:HD13	2.18	0.59
2:J:599:PRO:O	2:J:602:VAL:HG12	2.01	0.59
1:A:5:VAL:HG12	1:A:9:LEU:CD1	2.33	0.59
2:G:1963:GLY:O	2:G:1965:ALA:N	2.34	0.59
3:H:2015:THR:O	3:H:2017:LYS:N	2.35	0.59
3:I:1963:GLY:O	3:I:1965:ALA:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1963:GLY:O	2:J:1965:ALA:N	2.34	0.59
3:K:1854:MET:HB3	3:K:1901:ALA:HB2	1.84	0.59
1:A:996:LYS:HD3	1:A:1000:GLN:NE2	2.17	0.59
3:H:599:PRO:O	3:H:602:VAL:HG12	2.01	0.59
3:I:1343:VAL:HG22	3:I:1343:VAL:O	2.03	0.59
2:J:161:GLY:H	2:J:505:GLY:HA3	1.67	0.59
1:A:1470:LEU:HD13	1:A:1489:ARG:HG2	1.85	0.59
3:H:161:GLY:H	3:H:505:GLY:HA3	1.68	0.59
1:C:1515:ARG:NH2	1:F:1016:GLU:OE1	2.36	0.58
2:G:1170:ILE:HA	2:G:1221:MET:HE1	1.83	0.58
3:I:1170:ILE:HG12	3:I:1221:MET:HE3	1.85	0.58
3:L:1838:MET:HE3	3:L:1976:PHE:CE1	2.38	0.58
3:L:1963:GLY:O	3:L:1965:ALA:N	2.35	0.58
1:B:1448:ARG:HD2	1:B:1508:TRP:O	2.03	0.58
1:E:455:ILE:O	1:E:458:THR:HG23	2.02	0.58
2:G:612:ASN:HD21	2:G:641:ILE:HA	1.68	0.58
3:I:161:GLY:H	3:I:505:GLY:HA3	1.68	0.58
2:J:214:ASN:OD1	2:J:217:GLU:CB	2.51	0.58
1:A:67:SER:HB3	3:I:355:LYS:HE3	1.85	0.58
1:B:1160:THR:HB	1:C:244:THR:HG21	1.85	0.58
1:D:513:GLU:OE2	1:D:873:ARG:NH1	2.32	0.58
2:G:1868:GLN:HG3	2:G:1872:GLN:HE21	1.66	0.58
3:H:1963:GLY:O	3:H:1965:ALA:N	2.34	0.58
3:I:236:ILE:HD12	3:I:240:LEU:HD22	1.85	0.58
2:J:2015:THR:O	2:J:2017:LYS:N	2.35	0.58
1:A:244:THR:HG21	1:C:1160:THR:HB	1.86	0.58
1:B:1764:VAL:HG21	1:B:1769:VAL:CG1	2.32	0.58
1:C:1448:ARG:HD2	1:C:1508:TRP:O	2.04	0.58
2:J:1838:MET:HE3	2:J:1976:PHE:CE1	2.37	0.58
2:J:236:ILE:HD12	2:J:240:LEU:HD22	1.85	0.58
3:K:1345:GLY:HA3	3:K:1412:TYR:CD1	2.39	0.58
1:B:411:GLN:NE2	1:B:1628:SER:H	2.01	0.58
1:E:1448:ARG:HD2	1:E:1508:TRP:O	2.03	0.58
2:G:1889:VAL:HG23	2:G:1899:VAL:HG12	1.85	0.58
3:H:236:ILE:HD12	3:H:240:LEU:HD22	1.86	0.58
3:L:1851:ASN:HD22	3:L:1956:ARG:HH21	1.49	0.58
1:A:1448:ARG:HD2	1:A:1508:TRP:O	2.04	0.58
1:A:411:GLN:NE2	1:A:1628:SER:H	2.01	0.58
1:C:69:ASP:OD1	1:C:76:ARG:NH1	2.36	0.58
2:J:1854:MET:HB3	2:J:1901:ALA:HB2	1.84	0.58
3:K:612:ASN:HD21	3:K:641:ILE:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1421:ASN:ND2	3:L:1421:ASN:N	2.48	0.58
1:D:1867:VAL:HG12	1:D:1884:SER:CB	2.32	0.58
1:D:340:ARG:HH12	1:D:344:GLN:NE2	1.95	0.58
3:H:1343:VAL:HG22	3:H:1343:VAL:O	2.04	0.58
3:K:1775:GLN:NE2	3:K:1839:GLN:HG3	2.19	0.58
1:A:1245:ASN:HD22	1:A:1245:ASN:C	2.07	0.58
1:D:411:GLN:NE2	1:D:1628:SER:H	2.01	0.58
1:E:705:VAL:HG23	1:E:732:LEU:HD21	1.85	0.58
3:K:142:ASN:HB3	3:K:550:VAL:HG13	1.86	0.58
3:L:1946:GLU:O	3:L:1950:LYS:CD	2.51	0.58
1:A:801:ARG:NH2	1:F:789:GLU:OE1	2.37	0.58
1:B:987:ASN:ND2	1:B:1685:TYR:OH	2.37	0.58
1:C:1470:LEU:HD13	1:C:1489:ARG:HG2	1.86	0.58
1:C:411:GLN:NE2	1:C:1628:SER:H	2.02	0.58
3:H:1852:TYR:N	3:H:1904:LEU:HD23	2.18	0.58
3:H:1907:LEU:HB3	3:H:1960:LEU:HD21	1.85	0.58
3:I:1946:GLU:O	3:I:1950:LYS:CD	2.48	0.58
2:J:1343:VAL:O	2:J:1343:VAL:HG22	2.04	0.58
1:A:1859:ALA:O	1:A:1864:VAL:HG22	2.04	0.58
1:C:513:GLU:OE2	1:C:873:ARG:NH1	2.32	0.58
1:F:172:ILE:O	1:F:176:VAL:HG22	2.04	0.58
2:G:1854:MET:HB3	2:G:1901:ALA:HB2	1.86	0.58
3:I:1345:GLY:HA3	3:I:1412:TYR:CD1	2.39	0.58
2:G:106:ALA:HB2	2:G:545:GLN:HG2	1.86	0.57
3:K:463:PHE:CG	3:K:486:LEU:HD23	2.39	0.57
1:D:822:VAL:HG12	1:D:824:LEU:HD13	1.85	0.57
1:E:1326:ILE:HG12	1:E:1388:MET:HG3	1.85	0.57
3:L:1922:ILE:HB	3:L:1927:LEU:CD1	2.32	0.57
1:C:1506:GLN:HA	1:C:1510:ASN:HD22	1.69	0.57
1:F:1794:GLN:HE22	1:F:1840:VAL:HA	1.67	0.57
3:H:142:ASN:HB3	3:H:550:VAL:HG13	1.85	0.57
3:K:1215:LYS:HE2	3:K:1218:ILE:HD12	1.87	0.57
3:L:264:ARG:HD2	3:L:284:ALA:O	2.05	0.57
3:L:161:GLY:H	3:L:505:GLY:HA3	1.68	0.57
1:C:644:THR:HG22	1:C:648:ASP:O	2.05	0.57
1:C:705:VAL:HG23	1:C:732:LEU:HD21	1.87	0.57
1:F:411:GLN:NE2	1:F:1628:SER:H	2.01	0.57
1:D:20:TYR:CE2	2:J:2033:THR:CG2	2.88	0.57
1:D:1448:ARG:HD2	1:D:1508:TRP:O	2.03	0.57
1:F:1448:ARG:HD2	1:F:1508:TRP:O	2.04	0.57
2:G:1807:HIS:ND1	2:G:1808:SER:OG	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:73:GLU:HG2	3:H:76:LYS:HB2	1.85	0.57
2:J:1345:GLY:HA3	2:J:1412:TYR:CD1	2.39	0.57
3:L:1345:GLY:HA3	3:L:1412:TYR:CD1	2.39	0.57
3:L:236:ILE:HD12	3:L:240:LEU:HD22	1.85	0.57
1:B:1160:THR:HG21	1:C:244:THR:HG21	1.85	0.57
3:K:236:ILE:HD12	3:K:240:LEU:HD22	1.85	0.57
3:H:612:ASN:HD21	3:H:641:ILE:HA	1.68	0.57
3:I:2015:THR:O	3:I:2017:LYS:N	2.35	0.57
3:I:612:ASN:HD21	3:I:641:ILE:HA	1.69	0.57
1:C:1307:THR:HG23	1:C:1586:GLY:HA2	1.86	0.57
2:G:1345:GLY:HA3	2:G:1412:TYR:CD1	2.39	0.57
1:B:1307:THR:HG23	1:B:1586:GLY:HA2	1.87	0.57
1:D:1307:THR:HG23	1:D:1586:GLY:HA2	1.86	0.57
3:H:106:ALA:HB2	3:H:545:GLN:HG2	1.86	0.57
2:J:1345:GLY:HA3	2:J:1412:TYR:CE1	2.40	0.57
3:K:1270:TRP:O	3:K:1332:ARG:NH1	2.38	0.57
1:A:67:SER:CB	3:I:355:LYS:HE3	2.35	0.57
1:C:11:HIS:HE1	3:I:1996:ILE:O	1.88	0.57
1:C:1507:GLN:HE22	1:F:1500:GLN:CG	2.18	0.57
1:A:1146:HIS:O	1:E:1118:LYS:HE2	2.05	0.57
1:F:1506:GLN:HA	1:F:1510:ASN:HD22	1.69	0.57
1:F:1307:THR:HG23	1:F:1586:GLY:HA2	1.86	0.57
1:F:719:GLN:HG3	1:F:1612:ASP:HA	1.87	0.57
2:J:612:ASN:HD21	2:J:641:ILE:HA	1.70	0.57
2:J:964:LEU:HD22	2:J:964:LEU:N	2.20	0.57
1:B:438:ASN:HD21	1:B:698:GLN:HE21	1.52	0.56
1:C:1859:ALA:O	1:C:1864:VAL:HG22	2.05	0.56
1:D:537:LYS:HE3	1:D:634:THR:OG1	2.04	0.56
1:F:927:ASN:O	1:F:929:GLY:N	2.37	0.56
2:G:964:LEU:CD2	2:G:964:LEU:H	2.14	0.56
3:H:1775:GLN:HB3	3:H:1836:MET:HE2	1.87	0.56
1:B:1470:LEU:HD13	1:B:1489:ARG:HG2	1.86	0.56
1:B:295:ALA:O	1:B:298:VAL:O	2.22	0.56
1:D:719:GLN:HG3	1:D:1612:ASP:HA	1.87	0.56
1:E:1307:THR:HG23	1:E:1586:GLY:HA2	1.86	0.56
1:E:1863:GLY:O	1:E:1886:LYS:C	2.43	0.56
2:G:1054:LEU:HB2	10:G:2101:FMN:C7M	2.36	0.56
1:A:1506:GLN:HA	1:A:1510:ASN:HD22	1.70	0.56
1:C:1431:GLU:OE2	1:C:1523:ARG:NH1	2.38	0.56
1:E:987:ASN:ND2	1:E:1685:TYR:OH	2.37	0.56
3:H:1693:ARG:NH1	3:H:1825:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:665:LEU:HD22	2:J:669:LEU:HD22	1.88	0.56
3:L:1946:GLU:O	3:L:1950:LYS:HE3	2.04	0.56
1:A:267:VAL:HG12	1:A:290:MET:HE3	1.86	0.56
1:D:935:GLU:HB3	1:D:938:GLU:HG2	1.86	0.56
1:E:411:GLN:NE2	1:E:1628:SER:H	2.03	0.56
3:K:1234:VAL:HG13	3:K:1268:LYS:HE3	1.87	0.56
3:K:1345:GLY:HA3	3:K:1412:TYR:CE1	2.40	0.56
3:L:612:ASN:HD21	3:L:641:ILE:HA	1.69	0.56
1:A:1319:ILE:HA	1:A:1324:ALA:O	2.06	0.56
1:A:1546:THR:HG21	4:F:1901:PNS:O40	2.05	0.56
1:D:542:THR:HG22	1:D:543:ILE:HG23	1.87	0.56
2:G:236:ILE:HD12	2:G:240:LEU:HD22	1.86	0.56
3:L:1944:ILE:HD13	3:L:1945:ASP:OD1	2.06	0.56
1:A:438:ASN:HD21	1:A:698:GLN:HE21	1.52	0.56
1:A:822:VAL:HG12	1:A:824:LEU:HD13	1.86	0.56
1:E:822:VAL:HG12	1:E:824:LEU:HD13	1.87	0.56
1:F:438:ASN:HD21	1:F:698:GLN:HE21	1.53	0.56
2:G:2015:THR:O	2:G:2017:LYS:N	2.35	0.56
2:G:598:THR:O	2:G:599:PRO:C	2.43	0.56
2:J:736:ARG:HD2	2:J:769:SER:OG	2.05	0.56
3:K:597:MET:HA	10:K:2101:FMN:C5A	2.36	0.56
1:C:267:VAL:HG12	1:C:290:MET:HE3	1.88	0.56
1:D:927:ASN:O	1:D:929:GLY:N	2.38	0.56
1:F:267:VAL:HG12	1:F:290:MET:HE3	1.87	0.56
1:F:93:ASP:HB2	1:F:94:PRO:HD2	1.86	0.56
2:J:192:ALA:HB2	2:J:215:ILE:HD13	1.85	0.56
3:K:1170:ILE:HG12	3:K:1221:MET:HE2	1.87	0.56
1:E:1486:LEU:HD11	1:E:1756:ILE:HD11	1.87	0.56
1:F:1319:ILE:HA	1:F:1324:ALA:O	2.06	0.56
3:I:1345:GLY:HA3	3:I:1412:TYR:CE1	2.40	0.56
2:J:1922:ILE:HD13	2:J:1927:LEU:HD11	1.88	0.56
3:L:1170:ILE:HA	3:L:1221:MET:HE1	1.87	0.56
3:L:1309:GLU:OE2	3:L:1314:ARG:NH1	2.39	0.56
3:L:1950:LYS:HE2	3:L:1950:LYS:H	1.70	0.56
3:L:2015:THR:O	3:L:2017:LYS:N	2.35	0.56
1:A:1016:GLU:OE1	1:E:1515:ARG:NH2	2.37	0.56
1:C:1184:LEU:HB2	1:C:1352:THR:HG21	1.88	0.56
1:C:1856:LYS:O	1:C:1860:GLU:HG2	2.06	0.56
1:C:927:ASN:O	1:C:929:GLY:N	2.37	0.56
1:E:1470:LEU:HD13	1:E:1489:ARG:HG2	1.87	0.56
1:E:267:VAL:HG12	1:E:290:MET:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1431:GLU:OE2	1:F:1523:ARG:NH1	2.38	0.56
1:D:1431:GLU:OE2	1:D:1523:ARG:NH1	2.38	0.56
1:A:1302:VAL:CG2	1:E:1302:VAL:CG2	2.83	0.56
1:E:1319:ILE:HA	1:E:1324:ALA:O	2.06	0.56
3:H:1345:GLY:HA3	3:H:1412:TYR:CE1	2.41	0.56
2:J:1886:VAL:CG2	2:J:1906:ALA:HB3	2.36	0.56
3:L:1345:GLY:HA3	3:L:1412:TYR:CE1	2.41	0.56
3:L:264:ARG:HE	3:L:456:GLN:CB	2.18	0.56
1:B:1486:LEU:HD11	1:B:1756:ILE:HD11	1.88	0.56
1:B:1431:GLU:OE2	1:B:1523:ARG:NH1	2.39	0.56
1:B:267:VAL:HG12	1:B:290:MET:HE3	1.87	0.56
1:C:1319:ILE:HA	1:C:1324:ALA:O	2.06	0.56
1:D:267:VAL:HG12	1:D:290:MET:HE3	1.87	0.56
1:E:1431:GLU:OE2	1:E:1523:ARG:NH1	2.39	0.56
2:G:1904:LEU:HD23	2:G:1958:LEU:O	2.06	0.56
3:I:778:TYR:HE1	3:I:1085:LEU:HD13	1.71	0.56
1:B:340:ARG:HH12	1:B:344:GLN:NE2	1.96	0.55
3:L:1929:LYS:HE3	3:L:1933:LEU:HD12	1.88	0.55
1:A:1431:GLU:OE2	1:A:1523:ARG:NH1	2.39	0.55
1:C:537:LYS:HE2	1:C:634:THR:OG1	2.05	0.55
1:D:1319:ILE:HA	1:D:1324:ALA:O	2.06	0.55
3:L:1942:GLU:O	3:L:1946:GLU:CG	2.52	0.55
1:B:705:VAL:HG23	1:B:732:LEU:CD2	2.36	0.55
1:B:1160:THR:CB	1:C:244:THR:HG21	2.36	0.55
1:F:1859:ALA:O	1:F:1864:VAL:HG22	2.06	0.55
2:G:1345:GLY:HA3	2:G:1412:TYR:CE1	2.41	0.55
3:I:1309:GLU:OE2	3:I:1314:ARG:NH1	2.39	0.55
2:J:903:TRP:O	2:J:906:THR:HG22	2.06	0.55
3:L:1130:THR:H	3:L:1133:THR:HG22	1.72	0.55
1:F:513:GLU:OE2	1:F:873:ARG:NH1	2.32	0.55
2:G:903:TRP:O	2:G:906:THR:HG22	2.06	0.55
3:L:404:GLN:CA	3:L:407:ILE:HD13	2.31	0.55
1:A:1153:ASP:OD2	1:B:359:ARG:NH1	2.39	0.55
1:B:1506:GLN:HA	1:B:1510:ASN:HD22	1.71	0.55
1:E:1552:ASN:O	1:E:1556:THR:HG23	2.07	0.55
3:I:1418:ASP:HB2	3:I:1421:ASN:HD22	1.72	0.55
1:A:1307:THR:HG23	1:A:1586:GLY:HA2	1.87	0.55
1:B:1319:ILE:HA	1:B:1324:ALA:O	2.06	0.55
1:B:1500:GLN:CG	1:D:1507:GLN:HE22	2.19	0.55
1:E:438:ASN:HD21	1:E:698:GLN:HE21	1.54	0.55
1:F:538:GLU:HG2	1:F:635:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:GLU:OE2	1:F:793:ARG:HD2	2.05	0.55
2:G:598:THR:OG1	2:G:599:PRO:HD3	2.07	0.55
3:I:1929:LYS:HD3	3:I:1929:LYS:O	2.05	0.55
3:K:451:ASN:HB3	3:K:453:LYS:HG2	1.89	0.55
3:L:1872:GLN:NE2	3:L:1888:ILE:HD11	2.21	0.55
1:A:1486:LEU:HD11	1:A:1756:ILE:HD11	1.89	0.55
1:C:1851:LEU:CD2	1:C:1851:LEU:H	2.15	0.55
1:C:438:ASN:HD21	1:C:698:GLN:HE21	1.55	0.55
1:D:705:VAL:HG23	1:D:732:LEU:HD21	1.87	0.55
2:G:777:THR:CG2	2:G:1081:HIS:NE2	2.70	0.55
2:G:1932:SER:HB2	2:G:1936:VAL:HG13	1.89	0.55
3:H:894:ARG:NH1	3:H:898:ASP:OD2	2.40	0.55
1:A:1460:LYS:NZ	1:A:1464:GLU:OE2	2.38	0.55
1:E:644:THR:HG22	1:E:648:ASP:O	2.06	0.55
1:B:801:ARG:NH2	1:E:789:GLU:OE1	2.39	0.55
3:K:73:GLU:O	3:K:134:LYS:NZ	2.39	0.55
3:K:1680:LEU:HD22	3:K:1684:SER:HB3	1.89	0.55
3:L:778:TYR:HE1	3:L:1085:LEU:HD13	1.71	0.55
1:A:719:GLN:HG3	1:A:1612:ASP:HA	1.88	0.55
1:B:927:ASN:O	1:B:929:GLY:N	2.37	0.55
1:C:793:ARG:HD2	1:D:789:GLU:OE2	2.06	0.55
1:E:963:LEU:O	1:E:967:VAL:HG12	2.07	0.55
3:L:777:THR:CG2	3:L:1081:HIS:NE2	2.70	0.55
1:B:417:TYR:OH	1:B:458:THR:HB	2.07	0.55
3:K:777:THR:CG2	3:K:1081:HIS:NE2	2.70	0.55
3:K:1855:ILE:HG22	3:K:1968:PRO:HA	1.89	0.55
1:A:705:VAL:HG23	1:A:732:LEU:HD21	1.88	0.54
1:E:1506:GLN:HA	1:E:1510:ASN:HD22	1.71	0.54
3:L:836:TYR:HA	3:L:845:THR:HG23	1.89	0.54
1:D:1450:ARG:NH1	12:D:2002:HOH:O	2.39	0.54
1:F:705:VAL:HG23	1:F:732:LEU:CD2	2.37	0.54
1:F:41:THR:O	1:F:76:ARG:HD3	2.07	0.54
1:C:982:ILE:HD13	3:I:955:GLU:CB	2.37	0.54
1:C:1486:LEU:HD11	1:C:1756:ILE:HD11	1.89	0.54
1:F:1329:VAL:HG12	1:F:1385:GLN:HB2	1.89	0.54
3:H:1680:LEU:HD22	3:H:1684:SER:HB3	1.88	0.54
2:J:777:THR:CG2	2:J:1081:HIS:NE2	2.70	0.54
3:K:903:TRP:O	3:K:906:THR:HG22	2.07	0.54
4:A:1901:PNS:H421	1:F:1544:THR:HG21	1.90	0.54
1:C:938:GLU:HG3	1:C:939:PHE:N	2.23	0.54
3:K:778:TYR:HE1	3:K:1085:LEU:HD13	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:53:GLU:O	3:L:118:LYS:HE2	2.08	0.54
1:B:644:THR:HG22	1:B:648:ASP:O	2.07	0.54
1:B:719:GLN:HG3	1:B:1612:ASP:HA	1.88	0.54
1:C:1329:VAL:HG12	1:C:1385:GLN:HB2	1.90	0.54
1:C:1552:ASN:O	1:C:1556:THR:HG23	2.07	0.54
1:D:644:THR:HG22	1:D:648:ASP:O	2.06	0.54
1:E:504:ASP:OD2	1:E:508:ASN:HB2	2.08	0.54
1:E:719:GLN:HG3	1:E:1612:ASP:HA	1.88	0.54
1:F:982:ILE:HD13	3:L:955:GLU:CB	2.38	0.54
2:G:1217:ASN:O	2:G:1218:ILE:HD12	2.06	0.54
1:B:11:HIS:HE1	3:H:1996:ILE:O	1.90	0.54
3:I:1923:ASP:O	3:I:1927:LEU:HG	2.08	0.54
3:I:894:ARG:NH1	3:I:898:ASP:OD2	2.40	0.54
2:J:1680:LEU:HD22	2:J:1684:SER:HB3	1.90	0.54
2:J:894:ARG:NH1	2:J:898:ASP:OD2	2.40	0.54
3:L:1693:ARG:NH1	3:L:1825:GLU:OE1	2.40	0.54
3:L:894:ARG:NH1	3:L:898:ASP:OD2	2.41	0.54
1:A:1851:LEU:HD22	1:A:1851:LEU:N	2.23	0.54
1:A:644:THR:HG22	1:A:648:ASP:O	2.06	0.54
1:F:1552:ASN:O	1:F:1556:THR:HG23	2.08	0.54
1:F:644:THR:HG22	1:F:648:ASP:O	2.07	0.54
2:G:297:ARG:O	2:G:301:THR:CG2	2.56	0.54
3:I:1317:ARG:O	3:I:1317:ARG:HG3	2.07	0.54
3:I:1693:ARG:NH1	3:I:1825:GLU:OE1	2.41	0.54
2:J:778:TYR:HE1	2:J:1085:LEU:HD13	1.73	0.54
3:L:142:ASN:HB3	3:L:550:VAL:HG13	1.90	0.54
1:A:244:THR:HG21	1:C:1160:THR:CB	2.38	0.54
2:G:778:TYR:HE1	2:G:1085:LEU:HD13	1.72	0.54
3:H:455:ILE:HG13	3:H:469:ARG:HD3	1.90	0.54
3:H:53:GLU:O	3:H:118:LYS:HE2	2.08	0.54
3:H:598:THR:OG1	3:H:599:PRO:HD3	2.07	0.54
3:H:665:LEU:HD22	3:H:669:LEU:HD22	1.90	0.54
3:I:777:THR:CG2	3:I:1081:HIS:NE2	2.70	0.54
3:I:53:GLU:O	3:I:118:LYS:HE2	2.08	0.54
2:J:903:TRP:O	2:J:906:THR:CG2	2.56	0.54
1:F:1863:GLY:O	1:F:1886:LYS:C	2.45	0.54
3:H:1130:THR:O	3:H:1133:THR:CG2	2.56	0.54
2:J:1855:ILE:HG22	2:J:1968:PRO:HA	1.90	0.54
3:K:451:ASN:HB3	3:K:453:LYS:CE	2.38	0.54
3:L:1420:GLU:HG2	3:L:1421:ASN:HD21	1.72	0.54
1:A:1552:ASN:O	1:A:1556:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ILE:HD12	1:C:332:THR:HB	1.90	0.54
1:D:1184:LEU:HB2	1:D:1352:THR:HG21	1.90	0.54
2:G:903:TRP:O	2:G:906:THR:CG2	2.56	0.54
3:K:53:GLU:O	3:K:118:LYS:HE2	2.08	0.54
1:A:417:TYR:OH	1:A:458:THR:HB	2.08	0.54
1:A:927:ASN:O	1:A:929:GLY:N	2.37	0.54
1:B:1515:ARG:HD2	1:D:1499:SER:OG	2.07	0.54
1:C:982:ILE:HD12	3:I:965:SER:HA	1.90	0.54
1:D:348:ARG:HD3	1:F:1129:GLU:OE1	2.07	0.54
1:D:417:TYR:OH	1:D:458:THR:HB	2.08	0.54
1:D:738:ASN:HD22	7:D:1923:A2P:HN62	1.56	0.54
1:E:1329:VAL:HG12	1:E:1385:GLN:HB2	1.90	0.54
3:H:1855:ILE:HG22	3:H:1968:PRO:HA	1.90	0.54
3:H:698:LEU:O	3:H:700:LEU:N	2.41	0.54
3:I:1932:SER:HB2	3:I:1936:VAL:HG13	1.89	0.54
3:K:896:ASN:HD21	3:K:906:THR:HG21	1.73	0.54
1:A:808:LYS:HE2	1:F:782:GLU:O	2.08	0.53
1:C:987:ASN:ND2	1:C:1685:TYR:OH	2.38	0.53
1:E:1851:LEU:N	1:E:1851:LEU:HD22	2.23	0.53
2:G:1838:MET:HE3	2:G:1976:PHE:CD1	2.43	0.53
3:H:777:THR:CG2	3:H:1081:HIS:NE2	2.70	0.53
3:K:598:THR:O	3:K:599:PRO:C	2.45	0.53
1:B:1552:ASN:O	1:B:1556:THR:HG23	2.09	0.53
1:C:1507:GLN:HE22	1:F:1500:GLN:HG2	1.73	0.53
1:E:1859:ALA:O	1:E:1864:VAL:HG22	2.08	0.53
3:K:485:ARG:NH1	3:K:486:LEU:CD1	2.71	0.53
1:A:1118:LYS:HE2	1:E:1146:HIS:O	2.09	0.53
1:B:1184:LEU:HB2	1:B:1352:THR:HG21	1.89	0.53
1:D:987:ASN:ND2	1:D:1685:TYR:OH	2.39	0.53
2:G:836:TYR:HA	2:G:845:THR:HG23	1.90	0.53
2:G:894:ARG:NH1	2:G:898:ASP:OD2	2.41	0.53
3:H:778:TYR:HE1	3:H:1085:LEU:HD13	1.72	0.53
2:J:106:ALA:HB2	2:J:545:GLN:HG2	1.89	0.53
2:J:836:TYR:HA	2:J:845:THR:HG23	1.91	0.53
3:L:1881:ARG:CG	3:L:1944:ILE:HD11	2.37	0.53
3:L:964:LEU:N	3:L:964:LEU:HD22	2.24	0.53
1:A:11:HIS:HE1	2:G:1996:ILE:O	1.92	0.53
1:A:1184:LEU:HB2	1:A:1352:THR:HG21	1.91	0.53
1:C:719:GLN:HG3	1:C:1612:ASP:HA	1.90	0.53
1:D:1153:ASP:OD1	1:E:359:ARG:NH1	2.42	0.53
1:D:504:ASP:OD2	1:D:508:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1304:ALA:O	1:F:1307:THR:HG23	2.09	0.53
2:G:1680:LEU:HD22	2:G:1684:SER:HB3	1.89	0.53
2:G:53:GLU:O	2:G:118:LYS:HE2	2.09	0.53
3:I:903:TRP:O	3:I:906:THR:HG22	2.08	0.53
3:L:598:THR:OG1	3:L:599:PRO:HD3	2.08	0.53
1:A:1825:VAL:HG11	1:A:1858:ALA:HB1	1.91	0.53
1:C:504:ASP:OD2	1:C:508:ASN:HB2	2.09	0.53
3:H:598:THR:O	3:H:599:PRO:C	2.44	0.53
3:I:903:TRP:O	3:I:906:THR:CG2	2.56	0.53
2:J:297:ARG:O	2:J:301:THR:CG2	2.56	0.53
3:K:155:GLN:H	3:K:499:THR:HG22	1.72	0.53
3:K:455:ILE:HG13	3:K:469:ARG:HD3	1.91	0.53
3:K:894:ARG:NH1	3:K:898:ASP:OD2	2.41	0.53
3:L:598:THR:O	3:L:599:PRO:C	2.46	0.53
3:L:903:TRP:O	3:L:906:THR:CG2	2.57	0.53
1:D:1303:GLY:CA	1:D:1649:LYS:HD3	2.37	0.53
2:G:455:ILE:HG13	2:G:469:ARG:HD3	1.89	0.53
3:I:1054:LEU:HB2	10:I:2101:FMN:C7M	2.37	0.53
3:I:73:GLU:O	3:I:134:LYS:NZ	2.41	0.53
3:I:298:LYS:NZ	3:I:449:SER:O	2.42	0.53
3:L:1940:LEU:O	3:L:1944:ILE:HG23	2.08	0.53
3:L:903:TRP:O	3:L:906:THR:HG22	2.08	0.53
3:H:1319:MET:HB3	3:H:1368:VAL:HG21	1.90	0.53
3:I:1882:THR:HG23	3:I:1884:TRP:H	1.73	0.53
2:J:598:THR:O	2:J:599:PRO:C	2.45	0.53
3:K:1378:ILE:O	3:K:1378:ILE:HG22	2.08	0.53
3:L:1881:ARG:HG3	3:L:1944:ILE:HD11	1.90	0.53
3:L:698:LEU:O	3:L:700:LEU:N	2.41	0.53
2:G:1309:GLU:OE2	2:G:1314:ARG:NH1	2.40	0.53
2:G:597:MET:HA	10:G:2101:FMN:C5A	2.39	0.53
3:H:903:TRP:O	3:H:906:THR:CG2	2.57	0.53
3:I:1775:GLN:HB3	3:I:1836:MET:HE2	1.90	0.53
3:I:297:ARG:O	3:I:301:THR:CG2	2.55	0.53
2:J:1418:ASP:HB2	2:J:1421:ASN:HD22	1.74	0.53
3:K:836:TYR:HA	3:K:845:THR:HG23	1.90	0.53
1:B:43:ARG:O	3:H:1662:THR:HA	2.09	0.53
3:H:903:TRP:O	3:H:906:THR:HG22	2.09	0.53
3:I:1680:LEU:HD22	3:I:1684:SER:HB3	1.90	0.53
2:J:1495:THR:O	2:J:1496:LYS:HB2	2.09	0.53
3:K:109:LEU:HD21	3:K:116:LEU:CD2	2.39	0.53
3:K:1170:ILE:HG12	3:K:1221:MET:HE3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:VAL:HG12	1:A:1385:GLN:HB2	1.91	0.53
1:A:513:GLU:OE2	1:A:873:ARG:NH1	2.33	0.53
1:C:982:ILE:HD13	3:I:955:GLU:HB2	1.90	0.53
1:D:1552:ASN:O	1:D:1556:THR:HG23	2.09	0.53
1:E:1189:ILE:H	1:E:1380:GLN:HE21	1.58	0.53
1:F:1825:VAL:HG11	1:F:1858:ALA:HB1	1.91	0.53
2:G:1149:TRP:CD1	2:G:1213:LEU:HD21	2.44	0.53
2:J:1309:GLU:OE2	2:J:1314:ARG:NH1	2.41	0.53
2:J:317:THR:HG23	3:K:1314:ARG:NH2	2.23	0.53
3:K:698:LEU:O	3:K:700:LEU:N	2.41	0.53
1:C:806:VAL:HG22	1:C:862:LEU:HD11	1.91	0.52
1:D:1859:ALA:O	1:D:1864:VAL:HG22	2.08	0.52
1:D:168:MET:HE2	1:D:206:LEU:CB	2.39	0.52
1:D:705:VAL:HG23	1:D:732:LEU:CD2	2.39	0.52
1:D:806:VAL:HG22	1:D:862:LEU:HD11	1.91	0.52
1:D:938:GLU:HG3	1:D:939:PHE:N	2.23	0.52
1:F:504:ASP:OD2	1:F:508:ASN:HB2	2.08	0.52
3:I:1022:ASP:OD2	3:I:1024:ARG:NH1	2.43	0.52
3:I:598:THR:OG1	3:I:599:PRO:HD3	2.09	0.52
3:K:1808:J8W:OG	3:K:1809:LEU:N	2.41	0.52
3:K:1962:ARG:HB3	3:K:1962:ARG:NH2	2.24	0.52
1:E:927:ASN:O	1:E:929:GLY:N	2.38	0.52
3:H:1916:PHE:CD2	3:H:1943:ILE:HD12	2.44	0.52
3:I:1170:ILE:HG12	3:I:1221:MET:HE2	1.89	0.52
3:I:1697:HIS:O	3:I:1701:THR:HG23	2.09	0.52
2:G:1314:ARG:NH2	3:I:315:PRO:O	2.42	0.52
3:K:297:ARG:O	3:K:301:THR:CG2	2.56	0.52
3:L:109:LEU:HD23	3:L:535:ILE:HD13	1.91	0.52
1:C:1016:GLU:OE1	1:F:1515:ARG:NH2	2.43	0.52
2:G:1548:SER:HB3	2:G:1619:ASN:HD21	1.75	0.52
3:I:1548:SER:HB3	3:I:1619:ASN:HD21	1.74	0.52
2:J:245:GLN:HE21	2:J:505:GLY:HA2	1.74	0.52
3:L:297:ARG:O	3:L:301:THR:CG2	2.56	0.52
1:C:1271:GLN:OE1	5:C:1907:EDO:H22	2.09	0.52
1:C:705:VAL:HG23	1:C:732:LEU:CD2	2.39	0.52
1:B:1441:PRO:HD2	1:D:1492:GLU:OE2	2.09	0.52
2:G:1022:ASP:OD1	2:G:1024:ARG:HG2	2.10	0.52
3:H:1548:SER:HB3	3:H:1619:ASN:HD21	1.74	0.52
2:J:1697:HIS:O	2:J:1701:THR:HG23	2.10	0.52
3:L:1680:LEU:HD22	3:L:1684:SER:HB3	1.90	0.52
1:A:705:VAL:HG23	1:A:732:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1304:ALA:O	1:E:1307:THR:HG23	2.09	0.52
2:G:1693:ARG:NH1	2:G:1825:GLU:OE1	2.43	0.52
3:I:598:THR:O	3:I:599:PRO:C	2.45	0.52
2:J:1932:SER:HB2	2:J:1936:VAL:HG13	1.92	0.52
2:J:1944:ILE:O	2:J:1948:SER:HB3	2.10	0.52
3:K:1418:ASP:HB2	3:K:1421:ASN:HD22	1.74	0.52
3:K:1693:ARG:NH1	3:K:1825:GLU:OE1	2.42	0.52
1:B:1329:VAL:HG12	1:B:1385:GLN:HB2	1.91	0.52
1:B:682:GLY:HA2	7:B:1918:A2P:C1'	2.39	0.52
1:D:1506:GLN:HA	1:D:1510:ASN:HD22	1.74	0.52
1:E:1167:LEU:CD1	1:E:1171:ALA:CB	2.88	0.52
1:A:982:ILE:HD13	2:G:955:GLU:HB2	1.92	0.52
3:H:1149:TRP:CD1	3:H:1213:LEU:HD21	2.44	0.52
3:H:245:GLN:HE21	3:H:505:GLY:HA2	1.74	0.52
2:J:1270:TRP:O	2:J:1332:ARG:NH1	2.42	0.52
1:D:21:GLN:HE21	2:J:2013:ASN:HD22	1.56	0.52
3:K:1054:LEU:HB2	10:K:2101:FMN:HM72	1.92	0.52
1:A:517:GLU:O	1:A:518:LYS:HB2	2.10	0.52
1:B:168:MET:HE2	1:B:206:LEU:CB	2.40	0.52
1:A:244:THR:HG21	1:C:1160:THR:HG21	1.90	0.52
3:I:1808:J8W:OG	3:I:1809:LEU:N	2.41	0.52
3:I:836:TYR:HA	3:I:845:THR:HG23	1.92	0.52
3:K:1697:HIS:O	3:K:1701:THR:HG23	2.09	0.52
3:L:298:LYS:NZ	3:L:449:SER:O	2.43	0.52
1:A:1245:ASN:ND2	1:A:1247:SER:H	2.07	0.52
1:D:27:ARG:HG3	2:J:2013:ASN:O	2.10	0.52
1:E:537:LYS:HE2	1:E:634:THR:OG1	2.10	0.52
3:H:1246:ASN:ND2	12:H:2201:HOH:O	2.43	0.52
3:H:1495:THR:O	3:H:1496:LYS:HB2	2.10	0.52
3:I:245:GLN:HE21	3:I:505:GLY:HA2	1.75	0.52
3:K:665:LEU:HD22	3:K:669:LEU:HD22	1.90	0.52
3:K:903:TRP:O	3:K:906:THR:CG2	2.57	0.52
3:L:1915:ASN:HD21	3:L:1964:PHE:N	2.06	0.52
1:A:329:GLU:HA	1:A:332:THR:CG2	2.40	0.52
1:F:632:ARG:O	1:F:633:GLU:HB2	2.10	0.52
3:K:1495:THR:O	3:K:1496:LYS:HB2	2.10	0.52
3:K:687:SER:OG	3:K:690:VAL:HG23	2.10	0.52
3:L:1129:ALA:HA	3:L:1133:THR:HG21	1.92	0.52
3:L:1270:TRP:O	3:L:1332:ARG:NH1	2.42	0.52
3:L:2015:THR:OG1	3:L:2015:THR:O	2.25	0.52
1:A:1304:ALA:O	1:A:1307:THR:HG23	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1577:GLN:HE22	1:C:1591:TRP:C	2.12	0.52
1:C:1792:THR:HG21	1:C:1838:GLU:OE2	2.10	0.52
1:D:1329:VAL:HG12	1:D:1385:GLN:HB2	1.92	0.52
1:B:1694:TYR:OH	3:H:1001:ASP:OD2	2.23	0.52
3:I:687:SER:OG	3:I:690:VAL:HG23	2.10	0.52
2:J:1548:SER:HB3	2:J:1619:ASN:HD21	1.75	0.52
2:J:1775:GLN:CG	2:J:1836:MET:HE3	2.40	0.52
2:J:896:ASN:HD21	2:J:906:THR:HG21	1.74	0.52
3:K:1229:MET:HE2	3:K:1268:LYS:O	2.10	0.52
3:L:1932:SER:HB2	3:L:1936:VAL:HG13	1.91	0.52
3:L:964:LEU:HD22	3:L:964:LEU:H	1.73	0.52
1:A:504:ASP:OD2	1:A:508:ASN:HB2	2.10	0.51
1:B:789:GLU:OE1	1:E:801:ARG:NH2	2.43	0.51
1:D:1304:ALA:O	1:D:1307:THR:HG23	2.08	0.51
1:D:59:ARG:HD3	2:J:1896:GLN:HE22	1.74	0.51
1:E:146:LYS:HG2	1:E:214:GLN:NE2	2.25	0.51
1:E:705:VAL:HG23	1:E:732:LEU:CD2	2.39	0.51
2:G:1418:ASP:HB2	2:G:1421:ASN:HD22	1.74	0.51
3:I:101:ILE:HD13	3:I:126:TYR:CG	2.45	0.51
3:I:1495:THR:O	3:I:1496:LYS:HB2	2.09	0.51
3:I:1855:ILE:HG22	3:I:1968:PRO:HA	1.91	0.51
2:J:1149:TRP:CD1	2:J:1213:LEU:HD21	2.44	0.51
1:E:982:ILE:HD12	3:K:965:SER:CA	2.41	0.51
3:L:1548:SER:HB3	3:L:1619:ASN:HD21	1.75	0.51
3:L:1950:LYS:HE2	3:L:1950:LYS:N	2.25	0.51
1:A:27:ARG:HG3	2:G:2013:ASN:O	2.10	0.51
3:K:1548:SER:HB3	3:K:1619:ASN:HD21	1.75	0.51
3:K:245:GLN:HE21	3:K:505:GLY:HA2	1.75	0.51
3:L:1855:ILE:HG22	3:L:1968:PRO:HA	1.92	0.51
3:L:2020:GLN:HA	3:L:2020:GLN:HE21	1.76	0.51
1:A:168:MET:HE2	1:A:206:LEU:CB	2.40	0.51
1:A:706:THR:HB	1:A:737:PHE:HB3	1.91	0.51
1:B:1302:VAL:HG22	1:D:1302:VAL:CG2	2.40	0.51
1:F:1184:LEU:HB2	1:F:1352:THR:HG21	1.92	0.51
3:I:1270:TRP:O	3:I:1332:ARG:NH1	2.43	0.51
2:J:298:LYS:NZ	2:J:449:SER:O	2.43	0.51
1:A:1066:ASN:HD22	1:A:1071:PRO:HA	1.76	0.51
1:A:987:ASN:ND2	1:A:1685:TYR:OH	2.40	0.51
1:B:1304:ALA:O	1:B:1307:THR:HG23	2.10	0.51
1:B:329:GLU:HA	1:B:332:THR:CG2	2.41	0.51
1:C:1304:ALA:O	1:C:1307:THR:HG23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1184:LEU:HB2	1:E:1352:THR:HG21	1.92	0.51
1:F:417:TYR:OH	1:F:458:THR:HB	2.09	0.51
3:H:687:SER:OG	3:H:690:VAL:HG23	2.11	0.51
3:I:698:LEU:O	3:I:700:LEU:N	2.41	0.51
2:J:1736:MET:HG2	2:J:1751:ILE:HD12	1.93	0.51
2:J:598:THR:OG1	2:J:599:PRO:HD3	2.09	0.51
3:L:455:ILE:HG13	3:L:469:ARG:HD3	1.92	0.51
3:L:665:LEU:HD22	3:L:669:LEU:HD22	1.91	0.51
1:A:1260:MET:HG2	1:E:1342:GLU:HG3	1.93	0.51
1:A:1792:THR:HG21	1:A:1838:GLU:OE2	2.09	0.51
1:B:706:THR:HB	1:B:737:PHE:HB3	1.92	0.51
3:H:836:TYR:HA	3:H:845:THR:HG23	1.93	0.51
3:I:455:ILE:HG13	3:I:469:ARG:HD3	1.92	0.51
3:I:665:LEU:HD22	3:I:669:LEU:HD22	1.92	0.51
2:J:1693:ARG:NH1	2:J:1825:GLU:OE1	2.43	0.51
2:J:1953:VAL:HG23	2:J:1953:VAL:O	2.10	0.51
3:K:1149:TRP:CD1	3:K:1213:LEU:HD21	2.45	0.51
3:K:1337:ALA:HB1	3:K:1378:ILE:CG1	2.40	0.51
3:K:1564:HIS:O	3:K:1578:THR:OG1	2.27	0.51
3:L:1149:TRP:CD1	3:L:1213:LEU:HD21	2.44	0.51
3:L:285:GLU:OE1	3:L:298:LYS:HE2	2.11	0.51
1:B:157:HIS:O	1:B:160:LYS:HD2	2.11	0.51
1:D:682:GLY:HA2	7:D:1923:A2P:H1'	1.93	0.51
1:E:706:THR:HB	1:E:737:PHE:HB3	1.91	0.51
2:G:1170:ILE:HA	2:G:1221:MET:CE	2.41	0.51
3:H:597:MET:HA	10:H:2101:FMN:C5A	2.41	0.51
1:D:20:TYR:CZ	2:J:2033:THR:CG2	2.93	0.51
2:J:877:LYS:N	2:J:877:LYS:HE2	2.25	0.51
3:K:1904:LEU:HD13	3:K:1958:LEU:O	2.10	0.51
3:K:285:GLU:OE1	3:K:298:LYS:HE2	2.11	0.51
1:A:1160:THR:CB	1:B:244:THR:HG21	2.40	0.51
1:C:1486:LEU:O	1:C:1490:THR:HG23	2.06	0.51
1:F:1851:LEU:H	1:F:1851:LEU:HD23	1.75	0.51
2:G:698:LEU:O	2:G:700:LEU:N	2.41	0.51
3:H:1054:LEU:HB2	10:H:2101:FMN:C7M	2.38	0.51
3:H:747:HIS:HE1	3:H:780:TYR:OH	1.93	0.51
1:B:1491:ARG:HD3	1:B:1749:THR:HG21	1.92	0.51
1:E:1686:LYS:HD2	3:K:915:ALA:HB1	1.92	0.51
3:I:1023:ARG:CZ	3:I:1023:ARG:HB3	2.41	0.51
3:K:298:LYS:NZ	3:K:449:SER:O	2.43	0.51
1:B:1507:GLN:HE22	1:D:1500:GLN:HA	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1066:ASN:HD22	1:C:1071:PRO:HA	1.76	0.51
1:C:1146:HIS:O	1:F:1118:LYS:HE2	2.10	0.51
1:D:632:ARG:O	1:D:633:GLU:HB2	2.11	0.51
1:E:193:GLU:OE2	1:E:225:SER:HB2	2.11	0.51
1:F:1234:MET:CE	1:F:1326:ILE:HG21	2.41	0.51
1:F:806:VAL:HG22	1:F:862:LEU:HD11	1.93	0.51
1:F:982:ILE:HD12	3:L:965:SER:CA	2.40	0.51
3:H:1150:ARG:HD2	3:H:1193:THR:HG21	1.93	0.51
3:H:1697:HIS:O	3:H:1701:THR:HG23	2.11	0.51
2:J:357:ASN:HB3	2:J:365:GLN:OE1	2.11	0.51
3:K:1337:ALA:O	3:K:1378:ILE:HD11	2.10	0.51
1:E:11:HIS:ND1	3:K:1998:LYS:HA	2.26	0.51
3:L:1697:HIS:O	3:L:1701:THR:HG23	2.11	0.51
3:L:747:HIS:HE1	3:L:780:TYR:OH	1.94	0.51
1:A:999:LYS:HE3	1:A:1003:GLN:HE21	1.76	0.51
1:A:1760:THR:HG23	1:A:1762:GLU:HG3	1.91	0.51
1:C:1866:ASP:HB3	1:C:1885:THR:HG22	1.92	0.51
1:C:417:TYR:OH	1:C:458:THR:HB	2.09	0.51
1:F:792:HIS:HD2	1:F:842:SER:OG	1.93	0.51
2:G:33:LEU:HD23	2:G:68:VAL:HG22	1.93	0.51
2:G:665:LEU:HD22	2:G:669:LEU:HD22	1.92	0.51
3:H:896:ASN:HD21	3:H:906:THR:HG21	1.76	0.51
1:C:193:GLU:OE2	1:C:225:SER:HB2	2.11	0.50
1:C:706:THR:HB	1:C:737:PHE:HB3	1.92	0.50
1:E:1637:ARG:HG2	1:E:1660:TYR:OH	2.11	0.50
1:F:168:MET:HE2	1:F:206:LEU:CB	2.41	0.50
1:A:11:HIS:ND1	2:G:1998:LYS:HA	2.25	0.50
3:I:896:ASN:HD21	3:I:906:THR:HG21	1.76	0.50
2:J:747:HIS:HE1	2:J:780:TYR:OH	1.94	0.50
1:F:67:SER:CB	3:K:355:LYS:HE2	2.41	0.50
3:L:1495:THR:O	3:L:1496:LYS:HB2	2.10	0.50
3:L:1946:GLU:O	3:L:1950:LYS:HD2	2.10	0.50
3:L:687:SER:OG	3:L:690:VAL:HG23	2.11	0.50
1:A:193:GLU:OE2	1:A:225:SER:HB2	2.11	0.50
1:B:792:HIS:HD2	1:B:842:SER:OG	1.94	0.50
1:D:706:THR:HB	1:D:737:PHE:HB3	1.92	0.50
1:D:792:HIS:HD2	1:D:842:SER:OG	1.94	0.50
1:E:1754:LYS:HA	1:E:1754:LYS:HE3	1.92	0.50
1:E:67:SER:HB3	2:J:355:LYS:HE3	1.92	0.50
1:F:1066:ASN:HD22	1:F:1071:PRO:HA	1.75	0.50
1:F:982:ILE:HD13	3:L:955:GLU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:2013:HOH:O	2:G:1727:LYS:HE3	2.11	0.50
2:G:357:ASN:HB3	2:G:365:GLN:OE1	2.12	0.50
1:A:982:ILE:HD13	2:G:955:GLU:CB	2.41	0.50
3:H:285:GLU:OE1	3:H:298:LYS:HE2	2.10	0.50
3:I:785:TRP:O	3:I:788:LYS:HD3	2.11	0.50
3:I:964:LEU:HD23	3:I:964:LEU:N	2.17	0.50
2:J:1170:ILE:HA	2:J:1221:MET:CE	2.42	0.50
3:K:1932:SER:HB2	3:K:1936:VAL:HG13	1.93	0.50
3:L:245:GLN:HE21	3:L:505:GLY:HA2	1.76	0.50
1:D:17:LEU:CD2	2:J:2012:PRO:HG2	2.41	0.50
2:G:1697:HIS:O	2:G:1701:THR:HG23	2.11	0.50
2:G:245:GLN:HE21	2:G:505:GLY:HA2	1.75	0.50
2:G:298:LYS:NZ	2:G:449:SER:O	2.42	0.50
3:H:1270:TRP:O	3:H:1332:ARG:NH1	2.43	0.50
2:J:687:SER:OG	2:J:690:VAL:HG23	2.12	0.50
1:A:792:HIS:HD2	1:A:842:SER:OG	1.94	0.50
3:H:298:LYS:NZ	3:H:449:SER:O	2.43	0.50
3:I:285:GLU:OE1	3:I:298:LYS:HE2	2.11	0.50
3:K:598:THR:OG1	3:K:599:PRO:HD3	2.12	0.50
3:L:1170:ILE:HA	3:L:1221:MET:CE	2.40	0.50
1:B:1298:ILE:HG13	1:D:1649:LYS:HE3	1.93	0.50
1:D:193:GLU:OE2	1:D:225:SER:HB2	2.10	0.50
1:F:417:TYR:CE2	1:F:421:ILE:CD1	2.94	0.50
2:G:1270:TRP:O	2:G:1332:ARG:NH1	2.41	0.50
2:G:1855:ILE:HG22	2:G:1968:PRO:HA	1.92	0.50
2:G:687:SER:OG	2:G:690:VAL:HG23	2.11	0.50
3:I:777:THR:HG23	3:I:1081:HIS:NE2	2.27	0.50
3:I:747:HIS:HE1	3:I:780:TYR:OH	1.94	0.50
3:L:777:THR:HG23	3:L:1081:HIS:NE2	2.27	0.50
3:L:1941:PHE:HA	3:L:1944:ILE:HD12	1.93	0.50
3:L:497:LYS:HD3	3:L:497:LYS:H	1.76	0.50
1:A:78:ILE:HD12	1:A:78:ILE:N	2.27	0.50
1:B:658:LEU:HD21	1:B:912:GLU:HB3	1.93	0.50
1:B:1302:VAL:CG2	1:D:1302:VAL:HG22	2.40	0.50
1:E:417:TYR:OH	1:E:458:THR:HB	2.10	0.50
2:J:1107:SER:OG	2:J:1109:VAL:HG22	2.12	0.50
2:J:2020:GLN:HE21	2:J:2020:GLN:HA	1.77	0.50
3:K:2020:GLN:HA	3:K:2020:GLN:HE21	1.76	0.50
1:F:1694:TYR:OH	3:L:1001:ASP:OD2	2.23	0.50
1:B:247:ARG:HD3	1:B:261:GLN:NE2	2.27	0.50
1:B:677:TYR:CZ	1:B:702:LYS:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1790:ASN:O	1:D:1816:LYS:NZ	2.42	0.50
1:E:1760:THR:O	1:E:1762:GLU:HG3	2.12	0.50
3:H:109:LEU:HD21	3:H:116:LEU:HD13	1.94	0.50
3:I:357:ASN:HB3	3:I:365:GLN:OE1	2.11	0.50
1:B:1066:ASN:HD22	1:B:1071:PRO:HA	1.77	0.50
1:B:1842:VAL:O	1:B:1842:VAL:HG22	2.12	0.50
1:E:982:ILE:HD13	3:K:955:GLU:HB2	1.93	0.50
2:G:747:HIS:HE1	2:G:780:TYR:OH	1.95	0.50
2:J:1881:ARG:HD3	2:J:1882:THR:N	2.27	0.50
3:L:357:ASN:HB3	3:L:365:GLN:OE1	2.12	0.50
1:A:1637:ARG:HG2	1:A:1660:TYR:OH	2.12	0.50
1:D:658:LEU:HD21	1:D:912:GLU:HB3	1.94	0.50
1:F:706:THR:HB	1:F:737:PHE:HB3	1.92	0.50
3:H:1170:ILE:HA	3:H:1221:MET:CE	2.41	0.50
3:I:1852:TYR:N	3:I:1904:LEU:HD13	2.27	0.50
1:B:793:ARG:HA	1:B:797:THR:CG2	2.42	0.49
1:C:792:HIS:HD2	1:C:842:SER:OG	1.94	0.49
1:E:168:MET:HE2	1:E:206:LEU:CB	2.42	0.49
1:F:193:GLU:OE2	1:F:225:SER:HB2	2.12	0.49
3:H:576:LYS:HE2	12:H:2219:HOH:O	2.12	0.49
3:K:1177:SER:N	3:K:1180:MET:HE1	2.27	0.49
3:K:1736:MET:HG2	3:K:1751:ILE:HD12	1.94	0.49
3:L:499:THR:OG1	3:L:500:HIS:HD2	1.95	0.49
1:A:267:VAL:HG12	1:A:290:MET:CE	2.42	0.49
1:A:417:TYR:CE2	1:A:421:ILE:CD1	2.95	0.49
2:G:1590:ARG:NH2	2:G:1594:GLU:OE2	2.44	0.49
2:G:1782:THR:HG21	2:G:1827:LEU:HG	1.94	0.49
2:G:419:ARG:HB2	2:G:419:ARG:CZ	2.43	0.49
1:C:1694:TYR:OH	3:I:1001:ASP:OD2	2.26	0.49
2:J:376:ASN:ND2	2:J:376:ASN:C	2.64	0.49
3:K:1946:GLU:O	3:K:1946:GLU:HG2	2.11	0.49
3:L:1107:SER:OG	3:L:1109:VAL:HG22	2.12	0.49
3:L:896:ASN:HD21	3:L:906:THR:HG21	1.76	0.49
1:A:1531:LEU:HD21	1:A:1660:TYR:CZ	2.47	0.49
1:B:1234:MET:CE	1:B:1326:ILE:HG21	2.42	0.49
1:B:1637:ARG:HG2	1:B:1660:TYR:OH	2.12	0.49
1:B:1851:LEU:CD2	1:B:1851:LEU:H	2.13	0.49
1:F:267:VAL:HG12	1:F:290:MET:CE	2.43	0.49
3:H:1418:ASP:HB2	3:H:1421:ASN:HD22	1.77	0.49
1:A:1245:ASN:HD22	1:A:1247:SER:H	1.60	0.49
1:A:1760:THR:O	1:A:1762:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1016:GLU:OE1	1:D:1515:ARG:NH2	2.46	0.49
1:B:417:TYR:CE2	1:B:421:ILE:CD1	2.95	0.49
1:D:417:TYR:CE2	1:D:421:ILE:CD1	2.95	0.49
1:C:780:GLU:OE1	1:D:857:SER:OG	2.29	0.49
1:E:806:VAL:HG22	1:E:862:LEU:HD11	1.94	0.49
2:G:1852:TYR:N	2:G:1904:LEU:HD13	2.27	0.49
2:G:2020:GLN:HE21	2:G:2020:GLN:HA	1.76	0.49
3:H:1890:ASN:HB2	3:H:1899:VAL:HB	1.94	0.49
3:H:297:ARG:O	3:H:301:THR:CG2	2.56	0.49
3:K:1107:SER:OG	3:K:1109:VAL:HG22	2.12	0.49
1:D:1857:LYS:O	1:D:1861:GLU:HG3	2.12	0.49
1:E:1066:ASN:HD22	1:E:1071:PRO:HA	1.77	0.49
2:G:2036:GLU:HB2	2:G:2037:PRO:HD3	1.94	0.49
2:G:467:ASP:OD1	2:G:469:ARG:HG3	2.12	0.49
3:H:357:ASN:HB3	3:H:365:GLN:OE1	2.12	0.49
3:I:2020:GLN:HA	3:I:2020:GLN:HE21	1.76	0.49
2:J:1852:TYR:N	2:J:1904:LEU:HD13	2.27	0.49
2:J:777:THR:HG23	2:J:1081:HIS:NE2	2.28	0.49
3:L:109:LEU:CD2	3:L:535:ILE:HD13	2.43	0.49
3:L:1852:TYR:N	3:L:1904:LEU:HD13	2.28	0.49
1:A:48:GLY:HA3	2:G:1667:THR:OG1	2.12	0.49
1:D:738:ASN:ND2	7:D:1923:A2P:HN62	2.10	0.49
1:E:1813:TRP:CZ3	1:E:1834:LEU:HD12	2.47	0.49
2:G:1990:SER:O	2:G:1994:LYS:HD3	2.13	0.49
3:H:1932:SER:HB2	3:H:1936:VAL:HG13	1.93	0.49
1:C:1264:ARG:NH1	1:C:1270:VAL:HB	2.28	0.49
1:C:1577:GLN:NE2	1:C:1591:TRP:HB3	2.27	0.49
1:C:793:ARG:HA	1:C:797:THR:CG2	2.43	0.49
1:D:1066:ASN:HD22	1:D:1071:PRO:HA	1.76	0.49
2:G:1944:ILE:O	2:G:1948:SER:HB3	2.12	0.49
3:H:376:ASN:ND2	3:H:376:ASN:C	2.65	0.49
3:I:1107:SER:OG	3:I:1109:VAL:HG22	2.12	0.49
3:I:1149:TRP:CD1	3:I:1213:LEU:HD21	2.46	0.49
3:I:1170:ILE:HA	3:I:1221:MET:CE	2.42	0.49
3:I:1953:VAL:HG23	3:I:1953:VAL:O	2.13	0.49
3:I:455:ILE:O	3:I:455:ILE:HG13	2.12	0.49
3:L:1590:ARG:NH2	3:L:1594:GLU:OE2	2.43	0.49
1:A:806:VAL:HG22	1:A:862:LEU:HD11	1.93	0.49
1:C:417:TYR:CE2	1:C:421:ILE:CD1	2.96	0.49
2:G:1107:SER:OG	2:G:1109:VAL:HG22	2.12	0.49
2:G:530:ALA:O	2:G:544:LYS:HE3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1339:PHE:N	3:H:1340:PRO:CD	2.76	0.49
3:H:173:LEU:HD21	3:H:188:ILE:HD12	1.95	0.49
3:H:1740:THR:OG1	3:H:1747:LYS:HE3	2.12	0.49
3:H:2020:GLN:HA	3:H:2020:GLN:HE21	1.77	0.49
3:I:499:THR:OG1	3:I:500:HIS:HD2	1.96	0.49
3:L:33:LEU:HD23	3:L:68:VAL:HG22	1.95	0.49
1:A:1234:MET:CE	1:A:1326:ILE:HG21	2.43	0.49
1:E:792:HIS:HD2	1:E:842:SER:OG	1.95	0.49
1:F:527:GLN:HE22	1:F:599:MET:HB2	1.77	0.49
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.76	0.49
3:H:1229:MET:HE2	3:H:1268:LYS:O	2.13	0.49
3:I:1590:ARG:NH2	3:I:1594:GLU:OE2	2.44	0.49
2:J:1339:PHE:N	2:J:1340:PRO:CD	2.75	0.49
3:K:357:ASN:HB3	3:K:365:GLN:OE1	2.12	0.49
3:L:1808:J8W:OG	3:L:1809:LEU:N	2.41	0.49
3:L:264:ARG:NE	3:L:456:GLN:HB2	2.26	0.49
1:A:1264:ARG:NH1	1:A:1270:VAL:HB	2.28	0.49
1:A:677:TYR:CZ	1:A:702:LYS:HD2	2.48	0.49
1:E:157:HIS:O	1:E:160:LYS:HD2	2.13	0.49
1:E:417:TYR:CE2	1:E:421:ILE:CD1	2.96	0.49
1:F:1303:GLY:C	1:F:1307:THR:HG22	2.33	0.49
1:F:247:ARG:HD3	1:F:261:GLN:NE2	2.28	0.49
2:G:1495:THR:O	2:G:1496:LYS:HB2	2.11	0.49
2:G:777:THR:HG23	2:G:1081:HIS:NE2	2.28	0.49
3:H:777:THR:HG23	3:H:1081:HIS:NE2	2.28	0.49
3:H:1953:VAL:O	3:H:1953:VAL:HG23	2.13	0.49
3:I:597:MET:HA	10:I:2101:FMN:C5A	2.43	0.49
3:L:1890:ASN:HB2	3:L:1899:VAL:HB	1.93	0.49
3:L:467:ASP:OD1	3:L:469:ARG:HG3	2.13	0.49
1:B:806:VAL:HG22	1:B:862:LEU:HD11	1.95	0.48
1:C:267:VAL:HG12	1:C:290:MET:CE	2.43	0.48
1:B:1323:LYS:NZ	1:D:1313:ASP:OD1	2.43	0.48
1:D:1373:ARG:O	1:D:1547:LYS:HE3	2.13	0.48
1:D:1637:ARG:HG2	1:D:1660:TYR:OH	2.12	0.48
1:D:509:ILE:O	1:D:878:MET:HE1	2.13	0.48
2:G:430:HIS:CE1	2:G:431:LEU:HD13	2.48	0.48
3:H:1129:ALA:HA	3:H:1133:THR:HG21	1.95	0.48
1:D:59:ARG:HD3	2:J:1896:GLN:NE2	2.27	0.48
3:K:467:ASP:OD1	3:K:469:ARG:HG3	2.13	0.48
3:K:747:HIS:HE1	3:K:780:TYR:OH	1.94	0.48
1:A:1544:THR:O	1:A:1545:SER:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1857:LYS:O	1:B:1861:GLU:HG3	2.13	0.48
1:C:1302:VAL:HG22	1:F:1302:VAL:CG2	2.43	0.48
1:C:1234:MET:CE	1:C:1326:ILE:HG21	2.43	0.48
1:C:1637:ARG:HG2	1:C:1660:TYR:OH	2.13	0.48
1:F:1540:SER:HA	1:F:1575:VAL:HG22	1.95	0.48
3:H:1107:SER:OG	3:H:1109:VAL:HG22	2.12	0.48
3:H:481:ASP:OD2	3:H:485:ARG:NH1	2.46	0.48
3:I:1339:PHE:N	3:I:1340:PRO:CD	2.76	0.48
3:I:1890:ASN:HB2	3:I:1899:VAL:HB	1.95	0.48
2:J:1890:ASN:HB2	2:J:1899:VAL:HB	1.93	0.48
2:J:499:THR:OG1	2:J:500:HIS:HD2	1.96	0.48
3:K:1022:ASP:OD2	3:K:1024:ARG:NH1	2.46	0.48
3:K:1170:ILE:HA	3:K:1221:MET:CE	2.43	0.48
1:E:17:LEU:CD2	3:K:2012:PRO:HG2	2.43	0.48
3:L:1738:PHE:CE1	3:L:1751:ILE:HD13	2.48	0.48
3:L:234:ILE:N	3:L:235:PRO:CD	2.76	0.48
1:A:782:GLU:O	1:F:808:LYS:HE2	2.13	0.48
1:B:1531:LEU:HD21	1:B:1660:TYR:CZ	2.48	0.48
1:F:1637:ARG:HG2	1:F:1660:TYR:OH	2.13	0.48
2:G:77:VAL:HG23	2:G:81:ASP:OD2	2.13	0.48
3:H:1590:ARG:NH2	3:H:1594:GLU:OE2	2.44	0.48
3:K:481:ASP:OD2	3:K:485:ARG:NH1	2.46	0.48
3:L:1265:MET:HE1	3:L:1569:PHE:CZ	2.47	0.48
1:B:632:ARG:O	1:B:633:GLU:HB2	2.14	0.48
1:D:1234:MET:CE	1:D:1326:ILE:HG21	2.42	0.48
1:D:267:VAL:HG12	1:D:290:MET:CE	2.42	0.48
2:G:499:THR:OG1	2:G:500:HIS:HD2	1.96	0.48
3:K:1775:GLN:CG	3:K:1836:MET:HE3	2.43	0.48
1:C:1657:HIS:ND1	1:C:1658:PRO:HD2	2.29	0.48
1:C:632:ARG:O	1:C:633:GLU:HB2	2.13	0.48
1:B:1342:GLU:HG3	1:D:1260:MET:HG2	1.95	0.48
3:I:964:LEU:H	3:I:964:LEU:CD2	2.18	0.48
2:J:1962:ARG:NH2	2:J:1962:ARG:HB3	2.28	0.48
3:L:1962:ARG:NH2	3:L:1967:ILE:HD12	2.28	0.48
3:L:455:ILE:O	3:L:455:ILE:HG13	2.13	0.48
1:B:267:VAL:HG12	1:B:290:MET:CE	2.43	0.48
1:D:1303:GLY:C	1:D:1307:THR:HG22	2.34	0.48
1:F:43:ARG:O	3:L:1662:THR:HA	2.14	0.48
2:G:1890:ASN:HB2	2:G:1899:VAL:HB	1.95	0.48
2:G:1976:PHE:CD2	11:G:2102:MLI:H12	2.48	0.48
3:H:455:ILE:HG13	3:H:455:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1886:VAL:HG23	2:J:1906:ALA:CB	2.42	0.48
3:K:159:ILE:HA	3:K:271:THR:O	2.14	0.48
3:L:481:ASP:OD2	3:L:485:ARG:NH1	2.46	0.48
1:D:67:SER:HB3	3:L:355:LYS:HE3	1.95	0.48
1:E:1531:LEU:HD21	1:E:1660:TYR:CZ	2.48	0.48
1:E:1544:THR:O	1:E:1545:SER:HB3	2.13	0.48
1:C:1302:VAL:CG2	1:F:1302:VAL:HG22	2.44	0.48
1:C:1507:GLN:HE22	1:F:1500:GLN:HA	1.79	0.48
1:F:1857:LYS:HG3	1:F:1858:ALA:H	1.77	0.48
1:B:67:SER:OG	2:G:355:LYS:HE3	2.14	0.48
2:G:376:ASN:ND2	2:G:376:ASN:C	2.64	0.48
3:H:467:ASP:OD1	3:H:469:ARG:HG3	2.13	0.48
3:I:1170:ILE:HA	3:I:1221:MET:HE2	1.96	0.48
3:I:1736:MET:HG2	3:I:1751:ILE:HD12	1.95	0.48
2:J:1808:SER:OG	2:J:1809:LEU:N	2.41	0.48
2:J:1886:VAL:CG2	2:J:1906:ALA:CB	2.91	0.48
2:J:285:GLU:OE1	2:J:298:LYS:HE2	2.13	0.48
2:J:467:ASP:OD1	2:J:469:ARG:HG3	2.13	0.48
1:A:1303:GLY:C	1:A:1307:THR:HG22	2.34	0.48
1:A:359:ARG:NH1	1:C:1153:ASP:OD2	2.46	0.48
1:E:1790:ASN:O	1:E:1816:LYS:NZ	2.40	0.48
2:G:494:THR:HG23	2:G:520:LYS:NZ	2.29	0.48
2:G:896:ASN:HD21	2:G:906:THR:HG21	1.78	0.48
3:H:234:ILE:N	3:H:235:PRO:CD	2.77	0.48
3:I:2015:THR:OG1	3:I:2015:THR:O	2.26	0.48
3:I:159:ILE:HA	3:I:271:THR:O	2.13	0.48
2:J:1590:ARG:NH2	2:J:1594:GLU:OE2	2.43	0.48
2:J:481:ASP:OD2	2:J:485:ARG:NH1	2.47	0.48
3:K:376:ASN:C	3:K:376:ASN:ND2	2.64	0.48
3:L:1697:HIS:HE1	3:L:1829:GLU:OE1	1.97	0.48
1:A:21:GLN:NE2	2:G:1808:SER:O	2.47	0.48
1:A:509:ILE:O	1:A:878:MET:HE1	2.13	0.48
1:B:1303:GLY:C	1:B:1307:THR:HG22	2.33	0.48
1:C:329:GLU:HB2	1:C:332:THR:CG2	2.44	0.48
2:G:1162:ASP:O	2:G:1163:LYS:HB2	2.13	0.48
2:G:455:ILE:HG13	2:G:455:ILE:O	2.13	0.48
3:H:159:ILE:HA	3:H:271:THR:O	2.14	0.48
3:K:777:THR:HG23	3:K:1081:HIS:NE2	2.27	0.48
3:K:1339:PHE:N	3:K:1340:PRO:CD	2.77	0.48
3:K:1593:ILE:HD11	3:K:1640:PHE:CD1	2.49	0.48
3:K:455:ILE:HG13	3:K:455:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:526:ARG:NH2	3:K:546:GLU:OE2	2.46	0.48
1:A:1271:GLN:HG2	12:A:2025:HOH:O	2.14	0.48
1:B:1657:HIS:ND1	1:B:1658:PRO:HD2	2.29	0.48
1:D:1544:THR:O	1:D:1545:SER:HB3	2.14	0.48
1:E:1234:MET:CE	1:E:1326:ILE:HG21	2.44	0.48
1:E:247:ARG:HD3	1:E:261:GLN:NE2	2.29	0.48
1:F:1544:THR:O	1:F:1545:SER:HB3	2.14	0.48
1:A:1546:THR:CG2	4:F:1901:PNS:O40	2.61	0.48
2:G:1697:HIS:HE1	2:G:1829:GLU:OE1	1.97	0.48
2:G:159:ILE:HA	2:G:271:THR:O	2.13	0.48
3:I:1932:SER:CB	3:I:1935:GLU:OE1	2.62	0.48
2:J:1808:SER:OG	11:J:2102:MLI:C2	2.61	0.48
2:J:177:TYR:OH	2:J:220:GLU:OE2	2.31	0.48
3:K:1162:ASP:O	3:K:1163:LYS:HB2	2.14	0.48
1:B:1271:GLN:OE1	5:B:1910:EDO:H11	2.13	0.47
1:D:329:GLU:HA	1:D:332:THR:CG2	2.44	0.47
1:C:808:LYS:HE2	1:D:782:GLU:O	2.13	0.47
1:A:1342:GLU:HG3	1:E:1260:MET:HG2	1.94	0.47
2:G:285:GLU:OE1	2:G:298:LYS:HE2	2.14	0.47
2:G:526:ARG:NH2	2:G:546:GLU:OE2	2.47	0.47
3:H:1881:ARG:NH2	3:H:1941:PHE:CG	2.82	0.47
3:H:99:ASN:HD21	3:H:549:ASP:HA	1.79	0.47
3:I:376:ASN:C	3:I:376:ASN:ND2	2.64	0.47
2:J:234:ILE:N	2:J:235:PRO:CD	2.77	0.47
3:K:1890:ASN:HB2	3:K:1899:VAL:HB	1.94	0.47
3:L:285:GLU:HG3	3:L:455:ILE:HG22	1.96	0.47
1:B:533:GLY:O	1:B:537:LYS:HE3	2.14	0.47
1:B:724:LYS:HD3	1:B:725:TYR:CZ	2.49	0.47
1:C:724:LYS:HD3	1:C:725:TYR:CZ	2.49	0.47
1:A:808:LYS:HE3	1:F:782:GLU:HB2	1.95	0.47
3:H:1697:HIS:HE1	3:H:1829:GLU:OE1	1.97	0.47
3:H:1927:LEU:HA	3:H:1931:LEU:HB2	1.96	0.47
3:I:467:ASP:OD1	3:I:469:ARG:HG3	2.13	0.47
1:A:1153:ASP:CG	1:B:359:ARG:NH1	2.67	0.47
1:C:1303:GLY:C	1:C:1307:THR:HG22	2.33	0.47
1:C:1260:MET:HG2	1:F:1342:GLU:HG3	1.95	0.47
3:H:1162:ASP:O	3:H:1163:LYS:HB2	2.14	0.47
3:H:1578:THR:O	3:H:1578:THR:OG1	2.28	0.47
2:J:1775:GLN:HG3	2:J:1836:MET:HE3	1.96	0.47
2:J:173:LEU:HD21	2:J:188:ILE:HD12	1.96	0.47
2:J:159:ILE:HA	2:J:271:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:681:ILE:HG21	2:J:686:PRO:HD3	1.95	0.47
3:K:785:TRP:O	3:K:788:LYS:HD3	2.13	0.47
3:L:1339:PHE:N	3:L:1340:PRO:CD	2.77	0.47
3:L:159:ILE:HA	3:L:271:THR:O	2.14	0.47
1:B:168:MET:HE2	1:B:206:LEU:HB2	1.97	0.47
1:E:1188:GLN:HA	1:E:1380:GLN:HE21	1.79	0.47
1:E:1303:GLY:C	1:E:1307:THR:HG22	2.34	0.47
1:E:267:VAL:HG12	1:E:290:MET:CE	2.44	0.47
1:A:11:HIS:CE1	2:G:1996:ILE:O	2.66	0.47
1:A:1436:VAL:HG13	1:A:1436:VAL:O	2.14	0.47
1:C:1544:THR:O	1:C:1545:SER:HB3	2.14	0.47
1:F:1531:LEU:HD21	1:F:1660:TYR:CZ	2.49	0.47
1:F:987:ASN:ND2	1:F:1685:TYR:OH	2.40	0.47
2:G:234:ILE:N	2:G:235:PRO:CD	2.77	0.47
3:H:1782:THR:HG21	3:H:1827:LEU:HG	1.96	0.47
3:H:681:ILE:HG21	3:H:686:PRO:HD3	1.97	0.47
2:J:430:HIS:CE1	2:J:431:LEU:HD13	2.50	0.47
1:C:1531:LEU:HD21	1:C:1660:TYR:CZ	2.49	0.47
1:C:364:GLU:OE2	1:D:365:LYS:HG3	2.14	0.47
1:D:1531:LEU:HD21	1:D:1660:TYR:CZ	2.49	0.47
1:F:1790:ASN:O	1:F:1816:LYS:NZ	2.43	0.47
1:F:1794:GLN:CG	1:F:1838:GLU:OE2	2.61	0.47
2:G:572:ASN:OD1	2:G:576:LYS:N	2.46	0.47
3:H:264:ARG:HA	3:H:267:LEU:HD22	1.96	0.47
2:J:1222:GLU:HG2	2:J:1235:SER:OG	2.14	0.47
3:K:1842:VAL:O	3:K:1842:VAL:HG23	2.14	0.47
3:K:670:ARG:HA	3:K:670:ARG:NE	2.30	0.47
3:K:905:ALA:HA	3:K:917:MET:SD	2.55	0.47
1:E:982:ILE:HD13	3:K:955:GLU:HB3	1.97	0.47
1:F:43:ARG:HB3	3:L:1662:THR:HG22	1.96	0.47
1:E:1657:HIS:ND1	1:E:1658:PRO:HD2	2.29	0.47
2:G:670:ARG:HA	2:G:670:ARG:NE	2.30	0.47
3:H:499:THR:OG1	3:H:500:HIS:HD2	1.96	0.47
2:J:1782:THR:HG21	2:J:1827:LEU:HG	1.96	0.47
2:J:99:ASN:HD21	2:J:549:ASP:HA	1.79	0.47
3:K:1177:SER:N	3:K:1180:MET:CE	2.77	0.47
3:K:1962:ARG:NH2	3:K:1967:ILE:HG12	2.29	0.47
3:K:234:ILE:N	3:K:235:PRO:CD	2.77	0.47
3:L:596:GLY:N	3:L:618:GLU:HB2	2.30	0.47
3:H:23:PRO:CD	3:H:86:LEU:CD1	2.93	0.47
2:J:1842:VAL:HG23	2:J:1842:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:596:GLY:N	2:J:618:GLU:HB2	2.30	0.47
3:K:1697:HIS:HE1	3:K:1829:GLU:OE1	1.98	0.47
3:K:430:HIS:CE1	3:K:431:LEU:HD13	2.50	0.47
1:B:1825:VAL:HG11	1:B:1858:ALA:HB1	1.97	0.47
1:F:1657:HIS:ND1	1:F:1658:PRO:HD2	2.30	0.47
2:G:543:PHE:HB2	2:G:545:GLN:OE1	2.14	0.47
2:G:596:GLY:N	2:G:618:GLU:HB2	2.30	0.47
3:H:1319:MET:HB3	3:H:1368:VAL:CG2	2.45	0.47
3:I:526:ARG:NH2	3:I:546:GLU:OE2	2.47	0.47
2:J:1697:HIS:HE1	2:J:1829:GLU:OE1	1.97	0.47
2:J:264:ARG:HA	2:J:267:LEU:HD22	1.97	0.47
3:L:99:ASN:HD21	3:L:549:ASP:HA	1.80	0.47
1:B:1540:SER:HA	1:B:1575:VAL:HG22	1.97	0.47
1:D:1494:HIS:HE1	1:D:1874:ASP:OD2	1.98	0.47
1:D:1657:HIS:ND1	1:D:1658:PRO:HD2	2.30	0.47
1:E:1436:VAL:O	1:E:1436:VAL:HG13	2.14	0.47
1:F:1494:HIS:HE1	1:F:1874:ASP:OD2	1.98	0.47
2:G:1222:GLU:HG2	2:G:1235:SER:OG	2.14	0.47
2:G:867:GLU:O	2:G:871:THR:HB	2.15	0.47
3:H:430:HIS:CE1	3:H:431:LEU:HD13	2.50	0.47
3:I:1697:HIS:HE1	3:I:1829:GLU:OE1	1.98	0.47
3:L:905:ALA:HA	3:L:917:MET:SD	2.55	0.47
1:A:1790:ASN:O	1:A:1816:LYS:NZ	2.42	0.47
1:C:1540:SER:HA	1:C:1575:VAL:HG22	1.96	0.47
1:C:247:ARG:HD3	1:C:261:GLN:NE2	2.30	0.47
1:D:1264:ARG:NH1	1:D:1270:VAL:HB	2.30	0.47
1:D:1436:VAL:O	1:D:1436:VAL:HG13	2.15	0.47
1:B:808:LYS:HE2	1:E:782:GLU:O	2.15	0.47
1:F:157:HIS:O	1:F:160:LYS:HD2	2.15	0.47
2:G:598:THR:O	2:G:602:VAL:HG23	2.14	0.47
3:I:481:ASP:OD2	3:I:485:ARG:NH1	2.47	0.47
2:J:543:PHE:HB2	2:J:545:GLN:OE1	2.15	0.47
3:K:167:ASP:OD1	3:K:167:ASP:N	2.45	0.47
3:L:1775:GLN:HB3	3:L:1836:MET:HE2	1.97	0.47
3:L:1946:GLU:CA	3:L:1950:LYS:HE3	2.44	0.47
3:L:597:MET:HA	10:L:2101:FMN:C5A	2.45	0.47
3:L:670:ARG:NE	3:L:670:ARG:HA	2.29	0.47
7:F:1912:A2P:H1'	7:F:1912:A2P:O1P	2.14	0.46
1:F:724:LYS:HD3	1:F:725:TYR:CZ	2.50	0.46
1:A:982:ILE:HD12	2:G:965:SER:HA	1.97	0.46
3:H:526:ARG:NH2	3:H:546:GLU:OE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:285:GLU:HG3	2:J:455:ILE:HG22	1.97	0.46
2:J:29:ILE:HD13	2:J:82:GLN:NE2	2.29	0.46
3:K:1054:LEU:HB2	10:K:2101:FMN:C7M	2.45	0.46
3:K:155:GLN:HG3	3:K:268:LYS:HE3	1.97	0.46
1:B:1436:VAL:HG13	1:B:1436:VAL:O	2.15	0.46
1:F:1436:VAL:O	1:F:1436:VAL:HG13	2.14	0.46
2:G:1775:GLN:CG	2:G:1836:MET:HE3	2.45	0.46
3:H:1736:MET:HG2	3:H:1751:ILE:HD12	1.96	0.46
3:I:543:PHE:HB2	3:I:545:GLN:OE1	2.15	0.46
2:J:1281:PRO:O	2:J:1378:ILE:HG23	2.15	0.46
2:J:881:VAL:O	2:J:885:GLU:HG3	2.15	0.46
3:K:1782:THR:HG21	3:K:1827:LEU:HG	1.97	0.46
3:L:1775:GLN:CG	3:L:1836:MET:HE3	2.45	0.46
3:L:543:PHE:HB2	3:L:545:GLN:OE1	2.15	0.46
1:B:1455:ARG:HD2	1:B:1455:ARG:HA	1.78	0.46
1:E:1264:ARG:NH1	1:E:1270:VAL:HB	2.30	0.46
1:B:789:GLU:OE1	1:E:793:ARG:NH1	2.48	0.46
1:F:294:TYR:CE1	1:F:298:VAL:HG21	2.51	0.46
3:H:1916:PHE:HE2	3:H:1943:ILE:CD1	2.26	0.46
3:I:234:ILE:N	3:I:235:PRO:CD	2.77	0.46
3:I:264:ARG:HA	3:I:267:LEU:HD22	1.98	0.46
3:I:670:ARG:HA	3:I:670:ARG:NE	2.30	0.46
2:J:1479:ILE:HD11	2:J:1512:HIS:CE1	2.51	0.46
1:B:1114:TYR:CE1	1:B:1337:GLU:HG3	2.50	0.46
1:B:1544:THR:O	1:B:1545:SER:HB3	2.14	0.46
1:B:2:LYS:HD3	3:H:2050:GLN:HA	1.96	0.46
1:C:1755:MET:HG2	1:C:1870:SER:HB3	1.97	0.46
1:D:247:ARG:HD3	1:D:261:GLN:NE2	2.30	0.46
1:D:793:ARG:HA	1:D:797:THR:CG2	2.44	0.46
1:E:1189:ILE:H	1:E:1380:GLN:NE2	2.12	0.46
1:E:1540:SER:HA	1:E:1575:VAL:HG22	1.96	0.46
2:G:1842:VAL:HG23	2:G:1842:VAL:O	2.15	0.46
3:H:1808:J8W:OG	3:H:1809:LEU:N	2.41	0.46
3:H:543:PHE:HB2	3:H:545:GLN:OE1	2.15	0.46
3:I:1162:ASP:O	3:I:1163:LYS:HB2	2.14	0.46
2:J:1593:ILE:HD11	2:J:1640:PHE:CD1	2.50	0.46
1:A:1540:SER:HA	1:A:1575:VAL:HG22	1.97	0.46
1:C:1455:ARG:HA	1:C:1455:ARG:HD2	1.77	0.46
3:H:1842:VAL:O	3:H:1842:VAL:HG23	2.16	0.46
3:H:596:GLY:N	3:H:618:GLU:HB2	2.30	0.46
3:K:110:GLN:HG3	3:K:535:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1927:LEU:HA	3:L:1931:LEU:HB2	1.97	0.46
1:A:1068:LYS:N	1:A:1068:LYS:CD	2.79	0.46
1:B:20:TYR:CE2	3:H:2033:THR:CG2	2.99	0.46
1:E:1167:LEU:CD1	1:E:1171:ALA:HB1	2.46	0.46
1:C:1500:GLN:CG	1:F:1507:GLN:HE22	2.28	0.46
3:H:670:ARG:NE	3:H:670:ARG:HA	2.30	0.46
3:I:596:GLY:N	3:I:618:GLU:HB2	2.30	0.46
2:J:526:ARG:NH2	2:J:546:GLU:OE2	2.48	0.46
2:J:905:ALA:HA	2:J:917:MET:SD	2.55	0.46
3:K:264:ARG:HA	3:K:267:LEU:HD22	1.98	0.46
1:B:1875:ASP:OD1	1:B:1875:ASP:N	2.45	0.46
1:D:1825:VAL:HG11	1:D:1858:ALA:HB1	1.98	0.46
1:E:1114:TYR:CE1	1:E:1337:GLU:HG3	2.51	0.46
2:G:173:LEU:HD21	2:G:188:ILE:HD12	1.98	0.46
2:G:481:ASP:OD2	2:G:485:ARG:NH1	2.48	0.46
3:H:663:ILE:HB	3:H:664:PRO:HD3	1.98	0.46
2:J:867:GLU:O	2:J:871:THR:HB	2.15	0.46
3:K:598:THR:OG1	3:K:599:PRO:HD2	2.15	0.46
3:K:867:GLU:O	3:K:871:THR:HB	2.16	0.46
3:L:663:ILE:HB	3:L:664:PRO:HD3	1.98	0.46
1:B:1500:GLN:HG2	1:D:1507:GLN:NE2	2.29	0.46
1:B:2:LYS:O	1:B:5:VAL:HG23	2.15	0.46
1:B:479:ASN:O	1:B:483:VAL:CG2	2.64	0.46
1:F:1232:TYR:CZ	1:F:1705:PRO:HD3	2.51	0.46
2:G:1915:ASN:HD22	2:G:1915:ASN:N	2.14	0.46
2:G:1927:LEU:HD13	2:G:1931:LEU:HD22	1.98	0.46
3:I:430:HIS:CE1	3:I:431:LEU:HD13	2.51	0.46
3:I:905:ALA:HA	3:I:917:MET:SD	2.56	0.46
3:L:430:HIS:CE1	3:L:431:LEU:HD13	2.50	0.46
1:B:1842:VAL:O	1:B:1842:VAL:CG2	2.64	0.46
1:E:724:LYS:CG	1:E:725:TYR:CD2	2.94	0.46
1:A:793:ARG:NH1	1:F:789:GLU:OE1	2.48	0.46
3:I:1435:ILE:CG2	3:I:1441:ILE:HG22	2.46	0.46
2:J:1954:LYS:HB3	2:J:1955:PRO:HD2	1.98	0.46
2:J:1955:PRO:O	2:J:1958:LEU:HB3	2.15	0.46
3:K:173:LEU:HD21	3:K:188:ILE:HD12	1.98	0.46
1:C:833:PHE:O	1:C:937:LYS:NZ	2.42	0.46
1:E:616:LEU:N	1:E:617:PRO:HD2	2.31	0.46
3:I:1718:THR:HB	3:I:1763:THR:OG1	2.16	0.46
3:I:1782:THR:HG21	3:I:1827:LEU:HG	1.97	0.46
3:K:681:ILE:HG21	3:K:686:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ARG:O	1:A:633:GLU:HB3	2.17	0.45
1:B:1358:HIS:NE2	8:B:1902:ACT:H3	2.31	0.45
1:B:20:TYR:CG	3:H:2033:THR:HG23	2.52	0.45
1:C:1204:ILE:O	1:C:1208:VAL:HB	2.16	0.45
1:C:658:LEU:HD21	1:C:912:GLU:HB3	1.97	0.45
2:G:1281:PRO:O	2:G:1378:ILE:HG23	2.16	0.45
2:G:1651:LEU:HD23	2:G:1651:LEU:HA	1.87	0.45
3:H:1040:LEU:HD21	3:H:1048:VAL:HG13	1.99	0.45
3:H:1926:GLU:O	3:H:1930:SER:OG	2.21	0.45
3:K:1775:GLN:HE22	3:K:1839:GLN:HG3	1.80	0.45
3:K:596:GLY:N	3:K:618:GLU:HB2	2.30	0.45
3:L:407:ILE:CD1	3:L:407:ILE:N	2.78	0.45
1:A:1494:HIS:HE1	1:A:1874:ASP:OD2	1.99	0.45
1:B:1264:ARG:NH1	1:B:1270:VAL:HB	2.31	0.45
2:G:264:ARG:HA	2:G:267:LEU:HD22	1.97	0.45
3:H:932:ILE:HD12	3:H:1042:ALA:HA	1.97	0.45
3:H:372:ASN:HB3	3:H:515:LEU:HD21	1.98	0.45
3:I:109:LEU:HD21	3:I:116:LEU:HD13	1.97	0.45
2:J:670:ARG:NE	2:J:670:ARG:HA	2.32	0.45
3:L:113:ASP:OD1	3:L:113:ASP:N	2.49	0.45
1:A:1776:ILE:HG13	1:A:1807:SER:HA	1.97	0.45
1:B:411:GLN:HE22	1:B:1628:SER:N	2.14	0.45
1:E:1494:HIS:HE1	1:E:1874:ASP:OD2	1.99	0.45
1:C:1342:GLU:HG3	1:F:1260:MET:HG2	1.97	0.45
3:I:904:PHE:HB2	3:I:1017:PHE:CD2	2.52	0.45
3:I:1229:MET:HE2	3:I:1268:LYS:O	2.16	0.45
3:I:6:THR:O	3:I:7:ARG:CB	2.65	0.45
3:I:943:TRP:O	3:I:947:THR:HG23	2.17	0.45
3:K:113:ASP:N	3:K:113:ASP:OD1	2.50	0.45
3:L:1022:ASP:OD2	3:L:1024:ARG:NH1	2.49	0.45
1:A:20:TYR:CD1	2:G:2033:THR:HG23	2.51	0.45
1:B:509:ILE:O	1:B:878:MET:HE1	2.15	0.45
1:C:1494:HIS:HE1	1:C:1874:ASP:OD2	2.00	0.45
1:D:1114:TYR:CE1	1:D:1337:GLU:HG3	2.51	0.45
1:D:1014:ASP:N	1:D:1510:ASN:HD21	2.14	0.45
1:D:1540:SER:HA	1:D:1575:VAL:HG22	1.99	0.45
1:A:1515:ARG:NH2	1:E:1016:GLU:OE1	2.47	0.45
1:E:1766:ASN:OD1	1:E:1766:ASN:N	2.50	0.45
1:B:360:LYS:NZ	1:E:358:GLU:OE2	2.45	0.45
3:H:867:GLU:O	3:H:871:THR:HB	2.16	0.45
3:H:905:ALA:HA	3:H:917:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:173:LEU:HD21	3:I:188:ILE:HD12	1.99	0.45
2:J:109:LEU:HD21	2:J:116:LEU:CD2	2.46	0.45
3:K:31:SER:HA	3:K:34:GLN:HB3	1.99	0.45
3:K:99:ASN:HD21	3:K:549:ASP:HA	1.81	0.45
3:L:1782:THR:HG21	3:L:1827:LEU:HG	1.97	0.45
3:L:376:ASN:C	3:L:376:ASN:ND2	2.64	0.45
1:A:168:MET:HE2	1:A:206:LEU:HB2	1.98	0.45
1:B:1483:ASN:HD21	1:B:1487:LEU:HD11	1.82	0.45
1:B:1766:ASN:N	1:B:1766:ASN:OD1	2.48	0.45
1:C:1436:VAL:HG13	1:C:1436:VAL:O	2.16	0.45
1:E:168:MET:HE2	1:E:206:LEU:HB2	1.99	0.45
3:H:23:PRO:HG2	3:H:86:LEU:HD11	1.99	0.45
2:J:602:VAL:HG23	2:J:624:TYR:CE2	2.51	0.45
3:K:1170:ILE:HA	3:K:1221:MET:HE1	1.99	0.45
3:K:701:LYS:HD2	3:K:701:LYS:O	2.16	0.45
3:L:1288:LYS:N	3:L:1288:LYS:HD3	2.32	0.45
3:L:526:ARG:NH2	3:L:546:GLU:OE2	2.48	0.45
3:L:848:SER:OG	3:L:852:GLU:HG2	2.16	0.45
3:L:867:GLU:O	3:L:871:THR:HB	2.16	0.45
1:A:1483:ASN:HD21	1:A:1487:LEU:HD11	1.81	0.45
1:C:1022:THR:CG2	1:C:1226:SER:OG	2.65	0.45
1:D:694:GLN:HE21	5:D:1910:EDO:C1	2.29	0.45
1:E:1239:HIS:HD2	1:E:1241:SER:OG	1.99	0.45
2:G:1593:ILE:HD11	2:G:1640:PHE:CD1	2.52	0.45
2:G:1782:THR:CG2	2:G:1827:LEU:HD21	2.46	0.45
1:A:981:GLU:CD	2:G:962:LYS:HE2	2.37	0.45
3:H:666:ILE:O	3:H:670:ARG:HB2	2.17	0.45
3:I:1842:VAL:O	3:I:1842:VAL:HG23	2.15	0.45
2:J:99:ASN:ND2	2:J:100:ASP:H	2.09	0.45
3:K:285:GLU:HG3	3:K:455:ILE:HG22	1.98	0.45
3:L:1947:ALA:HA	3:L:1950:LYS:HG2	1.99	0.45
3:L:666:ILE:O	3:L:670:ARG:HB2	2.17	0.45
1:B:616:LEU:N	1:B:617:PRO:HD2	2.32	0.45
1:D:1455:ARG:HA	1:D:1455:ARG:HD2	1.78	0.45
1:A:1441:PRO:HD2	1:E:1492:GLU:OE2	2.17	0.45
1:E:1776:ILE:HG13	1:E:1807:SER:HA	1.98	0.45
2:G:622:GLY:HA2	2:G:658:MET:HE1	1.99	0.45
3:I:1363:ALA:O	3:I:1606:ARG:NH2	2.50	0.45
2:J:2050:GLN:HE21	2:J:2050:GLN:HB2	1.59	0.45
3:K:1590:ARG:NH2	3:K:1594:GLU:OE2	2.43	0.45
3:K:1651:LEU:HD23	3:K:1651:LEU:HA	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1842:VAL:HG23	3:L:1842:VAL:O	2.16	0.45
3:L:681:ILE:HG21	3:L:686:PRO:HD3	1.97	0.45
1:A:1114:TYR:CE1	1:A:1337:GLU:HG3	2.52	0.45
1:B:1776:ILE:HG13	1:B:1807:SER:HA	1.99	0.45
1:C:1790:ASN:O	1:C:1816:LYS:NZ	2.43	0.45
1:D:1483:ASN:HD21	1:D:1487:LEU:HD11	1.81	0.45
1:F:1114:TYR:CE1	1:F:1337:GLU:HG3	2.51	0.45
2:G:270:ALA:O	2:G:459:VAL:HA	2.17	0.45
2:G:932:ILE:HD12	2:G:1042:ALA:HA	1.99	0.45
1:B:11:HIS:CE1	3:H:1996:ILE:O	2.69	0.45
2:J:109:LEU:HD21	2:J:116:LEU:HD22	1.99	0.45
2:J:1348:LEU:HA	2:J:1348:LEU:HD12	1.90	0.45
2:J:2020:GLN:HA	2:J:2020:GLN:NE2	2.32	0.45
3:K:543:PHE:HB2	3:K:545:GLN:OE1	2.17	0.45
3:K:881:VAL:O	3:K:885:GLU:HG3	2.17	0.45
3:L:1782:THR:CG2	3:L:1827:LEU:HD21	2.46	0.45
1:A:173:LYS:NZ	1:A:203:GLU:OE2	2.50	0.45
1:C:1483:ASN:HD21	1:C:1487:LEU:HD11	1.82	0.45
1:D:1239:HIS:HD2	1:D:1241:SER:OG	2.00	0.45
1:D:545:GLU:N	1:D:545:GLU:OE1	2.48	0.45
1:E:1491:ARG:HD3	1:E:1749:THR:HG21	1.99	0.45
1:E:1014:ASP:N	1:E:1510:ASN:HD21	2.14	0.45
2:G:1775:GLN:HB3	2:G:1836:MET:HE2	1.99	0.45
2:G:455:ILE:HD11	2:G:469:ARG:CG	2.43	0.45
2:G:285:GLU:HG3	2:G:455:ILE:HG22	1.98	0.45
3:H:904:PHE:HB2	3:H:1017:PHE:CD2	2.52	0.45
3:H:1040:LEU:O	3:H:1046:GLN:HA	2.17	0.45
3:H:1381:VAL:HG13	3:H:1390:VAL:HG22	1.99	0.45
3:H:285:GLU:HG3	3:H:455:ILE:HG22	1.99	0.45
3:H:943:TRP:O	3:H:947:THR:HG23	2.17	0.45
3:I:748:THR:HB	3:I:749:PRO:HD3	1.98	0.45
2:J:1229:MET:HE2	2:J:1268:LYS:O	2.17	0.45
2:J:1435:ILE:CG2	2:J:1441:ILE:HG22	2.47	0.45
2:J:1904:LEU:HG	2:J:1960:LEU:HD23	1.98	0.45
2:J:270:ALA:O	2:J:459:VAL:HA	2.17	0.45
2:J:943:TRP:O	2:J:947:THR:HG23	2.17	0.45
3:K:372:ASN:HB3	3:K:515:LEU:HD21	1.99	0.45
1:A:1232:TYR:CZ	1:A:1705:PRO:HD3	2.52	0.45
1:A:533:GLY:O	1:A:537:LYS:NZ	2.50	0.45
1:B:1204:ILE:O	1:B:1208:VAL:HB	2.17	0.45
1:B:1022:THR:CG2	1:B:1226:SER:OG	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LYS:HG2	1:B:214:GLN:NE2	2.32	0.45
1:D:1232:TYR:CZ	1:D:1705:PRO:HD3	2.51	0.45
1:D:168:MET:HE2	1:D:206:LEU:HB2	1.97	0.45
2:G:1363:ALA:O	2:G:1606:ARG:NH2	2.50	0.45
2:G:1775:GLN:HG3	2:G:1836:MET:HE3	1.98	0.45
3:H:1955:PRO:O	3:H:1958:LEU:HB3	2.17	0.45
3:H:2020:GLN:HA	3:H:2020:GLN:NE2	2.32	0.45
3:H:602:VAL:HG23	3:H:624:TYR:CE2	2.52	0.45
3:I:681:ILE:HG21	3:I:686:PRO:HD3	1.99	0.45
1:B:1232:TYR:CZ	1:B:1705:PRO:HD3	2.52	0.44
1:C:1491:ARG:HD3	1:C:1749:THR:HG21	1.98	0.44
1:E:1232:TYR:CZ	1:E:1705:PRO:HD3	2.52	0.44
1:E:658:LEU:HD21	1:E:912:GLU:HB3	1.99	0.44
1:F:1239:HIS:HD2	1:F:1241:SER:OG	2.00	0.44
2:G:1265:MET:HE1	2:G:1569:PHE:CZ	2.52	0.44
2:G:1736:MET:HG2	2:G:1751:ILE:HD12	1.99	0.44
2:G:2020:GLN:NE2	2:G:2020:GLN:HA	2.32	0.44
2:G:666:ILE:O	2:G:670:ARG:HB2	2.17	0.44
2:G:6:THR:OG1	2:G:7:ARG:N	2.50	0.44
3:H:1479:ILE:HD11	3:H:1512:HIS:CE1	2.52	0.44
3:H:1718:THR:HB	3:H:1763:THR:OG1	2.17	0.44
3:H:1782:THR:CG2	3:H:1827:LEU:HD21	2.47	0.44
3:H:270:ALA:O	3:H:459:VAL:HA	2.17	0.44
3:I:1955:PRO:O	3:I:1958:LEU:HB3	2.17	0.44
3:I:1962:ARG:HB3	3:I:1962:ARG:NH2	2.31	0.44
3:I:285:GLU:HG3	3:I:455:ILE:HG22	1.99	0.44
3:K:1363:ALA:O	3:K:1606:ARG:NH2	2.50	0.44
3:L:1422:THR:CG2	3:L:1474:PHE:CD1	2.99	0.44
3:L:1738:PHE:HE1	3:L:1751:ILE:HD13	1.82	0.44
3:L:270:ALA:O	3:L:459:VAL:HA	2.17	0.44
1:A:1204:ILE:O	1:A:1208:VAL:HB	2.17	0.44
1:C:1114:TYR:CE1	1:C:1337:GLU:HG3	2.52	0.44
1:D:894:ARG:NH2	1:D:900:GLU:OE1	2.50	0.44
1:E:67:SER:CB	2:J:355:LYS:HE3	2.47	0.44
1:F:1491:ARG:HD3	1:F:1749:THR:HG21	1.99	0.44
1:E:1129:GLU:OE1	1:F:348:ARG:HD3	2.18	0.44
2:G:1213:LEU:HD13	2:G:1213:LEU:HA	1.85	0.44
3:I:1213:LEU:HA	3:I:1213:LEU:HD13	1.85	0.44
2:J:1040:LEU:HD21	2:J:1048:VAL:HG13	1.99	0.44
2:J:1292:ILE:O	2:J:1368:VAL:O	2.36	0.44
2:J:372:ASN:HB3	2:J:515:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1222:GLU:HG2	3:K:1235:SER:OG	2.17	0.44
3:K:943:TRP:O	3:K:947:THR:HG23	2.17	0.44
3:L:1130:THR:O	3:L:1178:GLN:NE2	2.50	0.44
3:L:173:LEU:HD21	3:L:188:ILE:HD12	1.97	0.44
3:L:1946:GLU:O	3:L:1950:LYS:CE	2.65	0.44
1:A:1153:ASP:OD1	1:B:359:ARG:NH1	2.49	0.44
1:B:1239:HIS:HD2	1:B:1241:SER:OG	2.00	0.44
1:B:198:PRO:HG3	1:B:212:THR:HG21	1.99	0.44
1:C:248:LYS:HE3	1:C:248:LYS:CA	2.48	0.44
1:C:43:ARG:O	3:I:1662:THR:HA	2.17	0.44
1:C:641:ARG:NH2	1:C:925:ASP:OD2	2.51	0.44
1:E:1022:THR:CG2	1:E:1226:SER:OG	2.65	0.44
1:E:1204:ILE:O	1:E:1208:VAL:HB	2.17	0.44
1:E:198:PRO:HG3	1:E:212:THR:HG21	1.99	0.44
2:G:113:ASP:OD1	2:G:113:ASP:N	2.50	0.44
2:G:905:ALA:HA	2:G:917:MET:SD	2.58	0.44
3:H:1363:ALA:O	3:H:1606:ARG:NH2	2.50	0.44
1:B:20:TYR:CD1	3:H:2033:THR:HG23	2.52	0.44
3:H:31:SER:HA	3:H:34:GLN:HB3	2.00	0.44
3:I:2020:GLN:NE2	3:I:2020:GLN:HA	2.32	0.44
3:L:1363:ALA:O	3:L:1606:ARG:NH2	2.50	0.44
1:D:616:LEU:N	1:D:617:PRO:HD2	2.33	0.44
1:F:1022:THR:CG2	1:F:1226:SER:OG	2.65	0.44
2:G:31:SER:HA	2:G:34:GLN:HB3	1.99	0.44
3:H:2015:THR:O	3:H:2015:THR:OG1	2.26	0.44
3:H:622:GLY:HA2	3:H:658:MET:HE1	2.00	0.44
3:I:1292:ILE:O	3:I:1368:VAL:O	2.36	0.44
3:K:663:ILE:HB	3:K:664:PRO:HD3	1.99	0.44
3:L:701:LYS:HD3	3:L:701:LYS:O	2.17	0.44
1:A:1239:HIS:HD2	1:A:1241:SER:OG	2.00	0.44
1:D:1022:THR:CG2	1:D:1226:SER:OG	2.65	0.44
1:D:1776:ILE:HG13	1:D:1807:SER:HA	1.98	0.44
1:F:168:MET:HE2	1:F:206:LEU:HB2	1.98	0.44
2:G:1877:ARG:HG3	2:G:1940:LEU:HD23	1.99	0.44
2:G:1955:PRO:O	2:G:1958:LEU:HB3	2.17	0.44
3:H:1737:ILE:HG21	3:H:1748:THR:HG23	2.00	0.44
2:J:1555:ARG:N	2:J:1555:ARG:HD2	2.32	0.44
3:K:1718:THR:HB	3:K:1763:THR:OG1	2.17	0.44
3:K:1926:GLU:O	3:K:1930:SER:OG	2.21	0.44
3:K:2020:GLN:HA	3:K:2020:GLN:NE2	2.32	0.44
3:K:451:ASN:HB3	3:K:453:LYS:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:748:THR:HB	3:K:749:PRO:HD3	1.99	0.44
3:L:6:THR:OG1	3:L:7:ARG:N	2.50	0.44
1:A:1022:THR:CG2	1:A:1226:SER:OG	2.65	0.44
1:A:1741:LYS:HE3	1:E:1435:SER:OG	2.18	0.44
1:A:682:GLY:HA2	7:A:1918:A2P:H1'	2.00	0.44
1:C:1232:TYR:CZ	1:C:1705:PRO:HD3	2.52	0.44
1:D:20:TYR:CD1	2:J:2033:THR:HG23	2.53	0.44
1:D:543:ILE:HD12	1:D:543:ILE:O	2.17	0.44
1:E:1483:ASN:HD21	1:E:1487:LEU:HD11	1.83	0.44
1:F:1264:ARG:NH1	1:F:1270:VAL:HB	2.33	0.44
2:G:856:LYS:HD3	2:G:1052:CYS:SG	2.58	0.44
2:G:99:ASN:HD21	2:G:549:ASP:HA	1.82	0.44
3:I:270:ALA:O	3:I:459:VAL:HA	2.17	0.44
3:I:372:ASN:HB3	3:I:515:LEU:HD21	1.99	0.44
3:I:663:ILE:HB	3:I:664:PRO:HD3	1.99	0.44
2:J:1976:PHE:CD2	11:J:2102:MLI:H11	2.52	0.44
2:J:6:THR:OG1	2:J:7:ARG:N	2.48	0.44
2:J:904:PHE:HB2	2:J:1017:PHE:CD2	2.52	0.44
3:L:1222:GLU:HG2	3:L:1235:SER:OG	2.18	0.44
3:L:1718:THR:HB	3:L:1763:THR:OG1	2.17	0.44
3:L:264:ARG:HA	3:L:267:LEU:HD22	1.99	0.44
3:L:6:THR:O	3:L:7:ARG:CB	2.66	0.44
3:L:868:PHE:HB3	3:L:873:PHE:CE2	2.52	0.44
1:D:411:GLN:HE22	1:D:1628:SER:N	2.14	0.44
1:E:538:GLU:O	1:E:633:GLU:HG3	2.17	0.44
1:F:1204:ILE:O	1:F:1208:VAL:HB	2.18	0.44
3:H:559:PRO:HB3	3:H:564:GLU:HG3	1.99	0.44
3:I:602:VAL:HG23	3:I:624:TYR:CE2	2.53	0.44
3:I:666:ILE:O	3:I:670:ARG:HB2	2.18	0.44
2:J:1782:THR:CG2	2:J:1827:LEU:HD21	2.48	0.44
1:A:1022:THR:HG23	1:A:1226:SER:OG	2.18	0.44
1:A:181:THR:HG21	1:C:1273:ASP:HB3	2.00	0.44
1:B:1494:HIS:HE1	1:B:1874:ASP:OD2	2.01	0.44
2:G:1479:ILE:HD11	2:G:1512:HIS:CE1	2.52	0.44
2:G:558:ASN:HA	2:G:558:ASN:HD22	1.59	0.44
3:H:1680:LEU:HD22	3:H:1684:SER:CB	2.48	0.44
3:I:1782:THR:CG2	3:I:1827:LEU:HD21	2.48	0.44
3:I:31:SER:HA	3:I:34:GLN:HB3	2.00	0.44
3:I:464:ASP:HB3	3:I:466:SER:H	1.82	0.44
2:J:622:GLY:HA2	2:J:658:MET:HE1	2.00	0.44
3:K:1435:ILE:CG2	3:K:1441:ILE:HG22	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1908:ASP:OD2	3:K:1954:LYS:HE3	2.18	0.44
3:K:270:ALA:O	3:K:459:VAL:HA	2.17	0.44
3:K:6:THR:O	3:K:7:ARG:CB	2.65	0.44
3:L:1040:LEU:O	3:L:1046:GLN:HA	2.18	0.44
3:L:1381:VAL:HG13	3:L:1390:VAL:HG22	2.00	0.44
3:L:1736:MET:O	3:L:1751:ILE:HG13	2.17	0.44
3:L:1960:LEU:HA	3:L:1960:LEU:HD13	1.89	0.44
3:L:2020:GLN:HA	3:L:2020:GLN:NE2	2.32	0.44
1:A:1068:LYS:N	1:A:1068:LYS:HD2	2.33	0.44
1:A:1014:ASP:N	1:A:1510:ASN:HD21	2.15	0.44
1:D:20:TYR:CE1	2:J:2033:THR:HG23	2.53	0.44
1:D:624:LYS:O	1:D:624:LYS:CG	2.66	0.44
1:E:1418:VAL:N	1:E:1419:PRO:CD	2.81	0.44
1:E:1423:LYS:O	1:E:1426:LEU:HB2	2.18	0.44
3:H:1201:VAL:HG11	3:H:1226:ASN:HB2	2.00	0.44
3:H:1479:ILE:N	3:H:1479:ILE:HD13	2.33	0.44
2:J:1854:MET:HA	2:J:1907:LEU:HD21	1.99	0.44
2:J:598:THR:OG1	2:J:599:PRO:HD2	2.17	0.44
3:K:1172:LYS:HB2	3:K:1172:LYS:HE3	1.82	0.44
3:K:1854:MET:HA	3:K:1907:LEU:HD21	1.99	0.44
3:K:464:ASP:HB3	3:K:466:SER:H	1.83	0.44
1:A:1771:VAL:HG22	1:A:1881:VAL:HG22	2.00	0.43
1:C:1696:LYS:HE2	1:C:1696:LYS:HB3	1.79	0.43
1:C:411:GLN:HE22	1:C:1628:SER:N	2.14	0.43
1:C:894:ARG:NH2	1:C:900:GLU:OE1	2.51	0.43
1:D:1431:GLU:CG	1:D:1433:HIS:CE1	3.01	0.43
1:D:641:ARG:NH2	1:D:925:ASP:OD2	2.51	0.43
1:E:2:LYS:O	1:E:5:VAL:HG23	2.18	0.43
2:G:1858:ASN:OD1	2:G:1896:GLN:HA	2.18	0.43
2:G:681:ILE:HG21	2:G:686:PRO:HD3	2.00	0.43
2:G:748:THR:HB	2:G:749:PRO:HD3	1.99	0.43
3:H:455:ILE:HD11	3:H:469:ARG:CG	2.44	0.43
3:I:856:LYS:HD3	3:I:1052:CYS:SG	2.58	0.43
3:I:1201:VAL:HG11	3:I:1226:ASN:HB2	2.00	0.43
3:I:1479:ILE:HD11	3:I:1512:HIS:CE1	2.52	0.43
3:L:1229:MET:HE2	3:L:1268:LYS:O	2.17	0.43
3:L:1775:GLN:HG3	3:L:1836:MET:HE3	1.99	0.43
1:A:1431:GLU:CG	1:A:1433:HIS:CE1	3.01	0.43
1:B:429:ASP:O	1:B:432:VAL:HG13	2.18	0.43
1:C:1014:ASP:N	1:C:1510:ASN:HD21	2.15	0.43
1:F:1785:THR:O	1:F:1789:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:616:LEU:N	1:F:617:PRO:HD2	2.33	0.43
2:G:1292:ILE:O	2:G:1368:VAL:O	2.37	0.43
3:I:1265:MET:HE1	3:I:1569:PHE:CZ	2.54	0.43
2:J:1289:ASP:OD1	2:J:1373:SER:HB3	2.18	0.43
2:J:1422:THR:CG2	2:J:1474:PHE:CD1	2.99	0.43
2:J:440:ASN:HD21	2:J:477:GLU:HA	1.83	0.43
2:J:932:ILE:HD12	2:J:1042:ALA:HA	2.00	0.43
3:K:1040:LEU:O	3:K:1046:GLN:HA	2.19	0.43
3:K:1422:THR:CG2	3:K:1474:PHE:CD1	2.99	0.43
3:K:1265:MET:CE	3:K:1569:PHE:CZ	3.01	0.43
3:K:1927:LEU:HD13	3:K:1931:LEU:HD22	2.00	0.43
3:K:622:GLY:HA2	3:K:658:MET:HE1	2.00	0.43
3:L:881:VAL:O	3:L:885:GLU:HG2	2.18	0.43
1:B:641:ARG:NH2	1:B:925:ASP:OD2	2.51	0.43
1:D:677:TYR:CZ	1:D:702:LYS:HD2	2.52	0.43
1:F:429:ASP:O	1:F:432:VAL:HG13	2.18	0.43
1:F:479:ASN:O	1:F:483:VAL:CG2	2.65	0.43
2:G:120:LYS:HD3	2:G:175:ASP:OD2	2.18	0.43
2:G:1969:LEU:O	2:G:1971:GLY:N	2.51	0.43
2:G:464:ASP:HB3	2:G:466:SER:H	1.83	0.43
2:G:904:PHE:HB2	2:G:1017:PHE:CD2	2.53	0.43
3:H:1915:ASN:HD21	3:H:1963:GLY:HA3	1.83	0.43
3:H:701:LYS:O	3:H:701:LYS:HD2	2.18	0.43
3:I:1281:PRO:O	3:I:1378:ILE:HG23	2.19	0.43
3:I:455:ILE:HD11	3:I:469:ARG:CG	2.45	0.43
2:J:942:THR:HB	2:J:1012:GLN:HB2	2.00	0.43
2:J:1718:THR:HB	2:J:1763:THR:OG1	2.17	0.43
2:J:748:THR:HB	2:J:749:PRO:HD3	1.99	0.43
3:K:1680:LEU:HD22	3:K:1684:SER:CB	2.48	0.43
3:K:602:VAL:HG23	3:K:624:TYR:CE2	2.53	0.43
3:K:666:ILE:O	3:K:670:ARG:HB2	2.18	0.43
3:L:1915:ASN:ND2	3:L:1964:PHE:N	2.53	0.43
1:B:1153:ASP:OD2	1:C:359:ARG:NH1	2.50	0.43
1:B:1423:LYS:O	1:B:1426:LEU:HB2	2.18	0.43
1:B:1460:LYS:NZ	1:B:1464:GLU:OE2	2.39	0.43
1:B:983:GLN:HE22	3:H:962:LYS:HD2	1.82	0.43
1:D:1204:ILE:O	1:D:1208:VAL:HB	2.17	0.43
1:D:1022:THR:HG23	1:D:1226:SER:OG	2.18	0.43
1:E:1431:GLU:OE2	1:E:1433:HIS:HE1	2.01	0.43
1:F:1776:ILE:HG13	1:F:1807:SER:HA	1.99	0.43
2:G:1378:ILE:HD11	2:G:1381:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1435:ILE:CG2	2:G:1441:ILE:HG22	2.48	0.43
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.99	0.43
2:G:868:PHE:HB3	2:G:873:PHE:CE2	2.53	0.43
3:H:1281:PRO:O	3:H:1378:ILE:HG23	2.17	0.43
3:I:113:ASP:N	3:I:113:ASP:OD1	2.50	0.43
3:I:1265:MET:CE	3:I:1569:PHE:CZ	3.01	0.43
3:I:868:PHE:HB3	3:I:873:PHE:CE2	2.53	0.43
3:I:887:LYS:HE3	12:I:2215:HOH:O	2.18	0.43
2:J:249:TYR:CZ	2:J:263:LEU:HD23	2.54	0.43
2:J:868:PHE:HB3	2:J:873:PHE:CE2	2.53	0.43
3:K:1040:LEU:HD21	3:K:1048:VAL:HG13	2.01	0.43
3:L:904:PHE:HB2	3:L:1017:PHE:CD2	2.52	0.43
3:L:1736:MET:HG2	3:L:1751:ILE:CG1	2.47	0.43
3:L:1955:PRO:O	3:L:1958:LEU:HB3	2.18	0.43
10:L:2101:FMN:O1P	10:L:2101:FMN:O4'	2.30	0.43
1:A:1431:GLU:OE2	1:A:1433:HIS:HE1	2.02	0.43
1:A:1455:ARG:HA	1:A:1455:ARG:HD2	1.78	0.43
1:A:643:LYS:NZ	1:A:851:ASN:HD21	2.17	0.43
1:B:48:GLY:HA3	3:H:1667:THR:OG1	2.17	0.43
1:C:1498:GLU:O	1:C:1502:ARG:HG3	2.19	0.43
1:C:616:LEU:N	1:C:617:PRO:HD2	2.33	0.43
1:E:1486:LEU:HA	1:E:1486:LEU:HD12	1.85	0.43
1:E:738:ASN:ND2	7:E:1917:A2P:HN62	2.15	0.43
1:E:641:ARG:NH2	1:E:925:ASP:OD2	2.52	0.43
1:F:1418:VAL:N	1:F:1419:PRO:CD	2.81	0.43
1:F:641:ARG:NH2	1:F:925:ASP:OD2	2.51	0.43
2:G:2015:THR:O	2:G:2015:THR:OG1	2.25	0.43
3:I:1040:LEU:O	3:I:1046:GLN:HA	2.18	0.43
3:I:1381:VAL:HG13	3:I:1390:VAL:HG22	2.00	0.43
3:I:1915:ASN:N	3:I:1915:ASN:HD22	2.16	0.43
2:J:559:PRO:HB3	2:J:564:GLU:HG3	2.00	0.43
3:K:1775:GLN:HG3	3:K:1836:MET:HE3	2.01	0.43
3:K:233:SER:HA	3:K:424:ALA:CB	2.49	0.43
3:L:1040:LEU:HD21	3:L:1048:VAL:HG13	2.01	0.43
3:L:500:HIS:HA	3:L:526:ARG:O	2.19	0.43
3:L:932:ILE:HD12	3:L:1042:ALA:HA	2.01	0.43
1:A:807:LYS:HD3	1:A:807:LYS:C	2.39	0.43
1:C:429:ASP:O	1:C:432:VAL:HG13	2.18	0.43
1:D:1498:GLU:O	1:D:1502:ARG:HG3	2.17	0.43
1:F:509:ILE:O	1:F:878:MET:HE1	2.18	0.43
2:G:1265:MET:CE	2:G:1569:PHE:CZ	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:943:TRP:O	2:G:947:THR:HG23	2.18	0.43
3:H:1292:ILE:O	3:H:1368:VAL:O	2.35	0.43
3:H:1846:GLU:OE2	3:H:1957:PRO:HB3	2.19	0.43
3:H:233:SER:HA	3:H:424:ALA:CB	2.48	0.43
3:H:6:THR:OG1	3:H:7:ARG:N	2.50	0.43
3:I:1680:LEU:HD22	3:I:1684:SER:CB	2.48	0.43
2:J:1201:VAL:HG11	2:J:1226:ASN:HB2	1.99	0.43
2:J:1915:ASN:HD22	2:J:1915:ASN:N	2.15	0.43
3:K:1954:LYS:HB3	3:K:1955:PRO:HD2	2.00	0.43
3:K:558:ASN:HD22	3:K:558:ASN:HA	1.62	0.43
3:L:1281:PRO:O	3:L:1378:ILE:HG23	2.17	0.43
3:L:478:ARG:HD3	3:L:478:ARG:HA	1.92	0.43
3:L:372:ASN:HB3	3:L:515:LEU:HD21	2.01	0.43
1:A:294:TYR:CE1	1:A:298:VAL:HG21	2.54	0.43
1:C:341:GLN:O	1:C:345:VAL:HG13	2.18	0.43
1:D:1392:LEU:HD22	1:D:1396:MET:HG3	2.00	0.43
1:D:6:GLU:CG	2:J:2021:VAL:HG11	2.48	0.43
1:E:411:GLN:HE22	1:E:1628:SER:N	2.14	0.43
1:E:807:LYS:HD3	1:E:807:LYS:C	2.39	0.43
1:C:1495:ASN:HD22	1:F:1515:ARG:HG2	1.84	0.43
2:G:1680:LEU:HD22	2:G:1684:SER:CB	2.48	0.43
2:G:716:VAL:HG11	2:G:730:LEU:HD22	2.00	0.43
2:G:77:VAL:HG13	2:G:77:VAL:O	2.18	0.43
3:H:1265:MET:CE	3:H:1569:PHE:CZ	3.01	0.43
3:I:1775:GLN:CG	3:I:1836:MET:HE3	2.48	0.43
3:I:1944:ILE:O	3:I:1948:SER:HB3	2.19	0.43
3:I:2030:TYR:HA	3:I:2033:THR:OG1	2.19	0.43
1:E:1694:TYR:OH	3:K:1001:ASP:OD2	2.29	0.43
3:K:6:THR:OG1	3:K:7:ARG:N	2.51	0.43
3:L:740[A]:HIS:CD2	3:L:852:GLU:OE2	2.71	0.43
1:A:1302:VAL:HG22	1:E:1302:VAL:CG2	2.48	0.43
1:B:375:LEU:HD21	1:E:374:GLN:OE1	2.19	0.43
1:C:1776:ILE:HG13	1:C:1807:SER:HA	2.00	0.43
1:C:1865:THR:H	1:C:1886:LYS:HB2	1.84	0.43
1:D:1423:LYS:O	1:D:1426:LEU:HB2	2.19	0.43
2:G:116:LEU:HA	2:G:116:LEU:HD13	1.79	0.43
2:G:1343:VAL:CG2	2:G:1343:VAL:O	2.67	0.43
2:G:1541:VAL:HG22	2:G:1625:SER:HB2	2.01	0.43
3:H:1347:LEU:HD12	3:H:1347:LEU:HA	1.89	0.43
3:H:1422:THR:CG2	3:H:1474:PHE:CD1	3.00	0.43
3:H:868:PHE:HB3	3:H:873:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1222:GLU:HG2	3:I:1235:SER:OG	2.18	0.43
3:I:1904:LEU:HG	3:I:1960:LEU:HD23	2.01	0.43
3:I:1854:MET:HA	3:I:1907:LEU:HD21	2.01	0.43
3:I:602:VAL:HG21	3:I:623:GLY:HA3	2.01	0.43
3:I:852:GLU:H	3:I:852:GLU:HG3	1.71	0.43
3:I:942:THR:HB	3:I:1012:GLN:HB2	2.01	0.43
2:J:1374:THR:HG23	2:J:1396:LEU:HD12	2.01	0.43
3:L:1085:LEU:HA	3:L:1085:LEU:HD12	1.86	0.43
3:L:1292:ILE:O	3:L:1368:VAL:O	2.37	0.43
3:L:233:SER:HA	3:L:424:ALA:CB	2.49	0.43
3:L:82:GLN:H	3:L:82:GLN:HG3	1.71	0.43
1:A:1423:LYS:O	1:A:1426:LEU:HB2	2.19	0.43
1:B:341:GLN:O	1:B:345:VAL:HG13	2.19	0.43
1:C:1239:HIS:HD2	1:C:1241:SER:OG	2.01	0.43
1:C:1813:TRP:CZ3	1:C:1834:LEU:HD12	2.54	0.43
1:D:20:TYR:CZ	2:J:2033:THR:HG23	2.54	0.43
1:D:27:ARG:HB2	2:J:2016:ALA:HB2	2.01	0.43
1:B:793:ARG:NH1	1:E:789:GLU:OE1	2.52	0.43
1:C:1495:ASN:ND2	1:F:1515:ARG:HG2	2.33	0.43
2:G:1320:LEU:HD12	2:G:1366:LEU:O	2.19	0.43
2:G:1718:THR:HB	2:G:1763:THR:OG1	2.17	0.43
3:I:1045:ASP:HB2	3:I:1047:ASP:HB2	2.01	0.43
3:I:1422:THR:CG2	3:I:1474:PHE:CD1	3.00	0.43
3:I:155:GLN:HG3	3:I:268:LYS:HE3	2.01	0.43
3:I:440:ASN:HD21	3:I:477:GLU:HA	1.83	0.43
3:I:478:ARG:HD3	3:I:478:ARG:HA	1.93	0.43
3:I:6:THR:OG1	3:I:7:ARG:N	2.51	0.43
2:J:602:VAL:HG21	2:J:623:GLY:HA3	2.01	0.43
2:J:74:PRO:O	2:J:75:SER:HB3	2.17	0.43
2:J:99:ASN:HD22	2:J:100:ASP:N	2.10	0.43
3:K:1327:ILE:HA	3:K:1327:ILE:HD13	1.86	0.43
3:K:1343:VAL:CG2	3:K:1343:VAL:O	2.67	0.43
3:K:1381:VAL:HG13	3:K:1390:VAL:HG22	2.00	0.43
3:K:440:ASN:HD21	3:K:477:GLU:HA	1.84	0.43
3:L:1201:VAL:HG11	3:L:1226:ASN:HB2	2.01	0.43
3:L:1342:THR:HB	3:L:1421:ASN:OD1	2.18	0.43
3:L:1484:LYS:HG3	3:L:1507:GLU:HG3	2.01	0.43
1:F:11:HIS:CE1	3:L:1996:ILE:O	2.72	0.43
1:A:1062:TYR:CG	1:A:1693:ILE:HB	2.54	0.43
1:B:1418:VAL:N	1:B:1419:PRO:CD	2.82	0.43
1:B:186:ILE:O	1:B:190:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1418:VAL:N	1:C:1419:PRO:CD	2.81	0.43
1:D:1418:VAL:N	1:D:1419:PRO:CD	2.82	0.43
1:D:341:GLN:O	1:D:345:VAL:HG13	2.19	0.43
4:B:1901:PNS:H422	1:E:1644:PHE:O	2.19	0.43
1:E:186:ILE:O	1:E:190:LEU:HG	2.19	0.43
1:C:1295:SER:HA	1:F:1411:THR:O	2.19	0.43
1:F:1483:ASN:HD21	1:F:1487:LEU:HD11	1.83	0.43
1:F:1754:LYS:HA	1:F:1754:LYS:HE3	2.01	0.43
1:F:341:GLN:O	1:F:345:VAL:HG13	2.19	0.43
1:F:538:GLU:CG	1:F:635:ILE:HD11	2.48	0.43
1:F:807:LYS:HD3	1:F:807:LYS:C	2.40	0.43
2:G:249:TYR:CZ	2:G:263:LEU:HD23	2.54	0.43
2:G:99:ASN:HD22	2:G:100:ASP:N	2.11	0.43
3:H:748:THR:HB	3:H:749:PRO:HD3	2.00	0.43
3:I:1775:GLN:HG3	3:I:1836:MET:HE3	2.01	0.43
3:I:1852:TYR:C	3:I:1904:LEU:CD1	2.88	0.43
2:J:1378:ILE:HD11	2:J:1381:VAL:HG22	2.00	0.43
3:K:856:LYS:HD3	3:K:1052:CYS:SG	2.59	0.43
3:L:1593:ILE:HD11	3:L:1640:PHE:CD1	2.54	0.43
3:L:1854:MET:HA	3:L:1907:LEU:HD21	2.00	0.43
3:L:1944:ILE:CD1	3:L:1945:ASP:OD1	2.67	0.43
3:L:31:SER:HA	3:L:34:GLN:HB3	2.00	0.43
3:L:602:VAL:HG23	3:L:624:TYR:CE2	2.54	0.43
1:B:807:LYS:HD3	1:B:807:LYS:C	2.39	0.42
1:C:1431:GLU:OE2	1:C:1433:HIS:HE1	2.02	0.42
1:C:375:LEU:HD12	1:D:375:LEU:HD12	2.01	0.42
1:F:1431:GLU:OE2	1:F:1433:HIS:HE1	2.02	0.42
1:F:1600:LEU:CD1	1:F:1655:VAL:HG12	2.49	0.42
2:G:1347:LEU:HD12	2:G:1347:LEU:HA	1.87	0.42
2:G:1381:VAL:HG13	2:G:1390:VAL:HG22	2.01	0.42
2:G:1854:MET:HA	2:G:1907:LEU:HD21	2.00	0.42
3:H:1435:ILE:CG2	3:H:1441:ILE:HG22	2.50	0.42
3:H:803:SER:HB3	3:H:1055:HIS:CD2	2.54	0.42
2:J:233:SER:HA	2:J:424:ALA:CB	2.49	0.42
2:J:31:SER:HA	2:J:34:GLN:HB3	2.00	0.42
3:K:932:ILE:HD12	3:K:1042:ALA:HA	2.00	0.42
3:K:1838:MET:HE3	3:K:1976:PHE:CD1	2.54	0.42
3:K:730:LEU:C	3:K:730:LEU:CD1	2.87	0.42
3:L:1858:ASN:HB3	3:L:1965:ALA:HB1	2.01	0.42
1:A:1498:GLU:O	1:A:1502:ARG:HG3	2.19	0.42
1:A:358:GLU:OE2	1:F:360:LYS:NZ	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ASP:O	1:A:432:VAL:HG13	2.19	0.42
1:C:1423:LYS:O	1:C:1426:LEU:HB2	2.19	0.42
1:F:186:ILE:O	1:F:190:LEU:HG	2.19	0.42
1:F:537:LYS:NZ	1:F:634:THR:OG1	2.48	0.42
2:G:1040:LEU:O	2:G:1046:GLN:HA	2.18	0.42
2:G:1629:VAL:HG11	2:G:1639:LYS:HE2	2.01	0.42
2:G:6:THR:O	2:G:7:ARG:CB	2.66	0.42
3:H:1838:MET:HE3	3:H:1976:PHE:CD1	2.54	0.42
3:I:101:ILE:HD13	3:I:126:TYR:CD2	2.54	0.42
3:I:1289:ASP:OD1	3:I:1373:SER:HB3	2.19	0.42
3:I:1348:LEU:HD12	3:I:1348:LEU:HA	1.89	0.42
3:I:1594:GLU:O	3:I:1598:ALA:HB3	2.19	0.42
3:I:1740:THR:HB	3:I:1747:LYS:HD2	2.01	0.42
3:I:1954:LYS:HB3	3:I:1955:PRO:HD2	2.00	0.42
3:I:233:SER:HA	3:I:424:ALA:CB	2.48	0.42
3:I:730:LEU:C	3:I:730:LEU:CD1	2.87	0.42
3:I:932:ILE:HD12	3:I:1042:ALA:HA	2.01	0.42
2:J:1363:ALA:O	2:J:1606:ARG:NH2	2.51	0.42
3:K:1085:LEU:HD12	3:K:1085:LEU:HA	1.85	0.42
3:K:1096:LYS:HA	3:K:1096:LYS:HD2	1.88	0.42
3:K:1289:ASP:OD1	3:K:1373:SER:HB3	2.19	0.42
3:K:1782:THR:CG2	3:K:1827:LEU:HD21	2.49	0.42
3:K:517:HIS:O	3:K:517:HIS:CD2	2.72	0.42
3:L:455:ILE:HD11	3:L:469:ARG:CG	2.45	0.42
3:L:730:LEU:C	3:L:730:LEU:CD1	2.87	0.42
3:L:803:SER:HB3	3:L:1055:HIS:CD2	2.54	0.42
3:L:943:TRP:O	3:L:947:THR:HG23	2.19	0.42
1:B:1736:LYS:HD3	1:B:1736:LYS:HA	1.87	0.42
1:B:537:LYS:HE2	1:B:634:THR:OG1	2.19	0.42
1:B:709:ARG:HD3	7:B:1918:A2P:O1P	2.19	0.42
1:C:1392:LEU:HD22	1:C:1396:MET:HG3	2.01	0.42
1:D:1431:GLU:OE2	1:D:1433:HIS:HE1	2.01	0.42
1:D:1491:ARG:HD3	1:D:1749:THR:HG21	2.01	0.42
1:E:341:GLN:O	1:E:345:VAL:HG13	2.20	0.42
1:F:198:PRO:HG3	1:F:212:THR:HG21	2.01	0.42
2:G:942:THR:HB	2:G:1012:GLN:HB2	2.01	0.42
2:G:1040:LEU:HD21	2:G:1048:VAL:HG13	2.01	0.42
2:G:1229:MET:HE2	2:G:1268:LYS:O	2.19	0.42
2:G:372:ASN:HB3	2:G:515:LEU:HD21	2.00	0.42
2:G:440:ASN:HD21	2:G:477:GLU:HA	1.84	0.42
3:H:1854:MET:HB3	3:H:1901:ALA:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:6:THR:O	3:H:7:ARG:CB	2.67	0.42
3:H:896:ASN:ND2	3:H:906:THR:HG21	2.34	0.42
3:I:1040:LEU:HD21	3:I:1048:VAL:HG13	2.01	0.42
2:J:1852:TYR:C	2:J:1904:LEU:CD1	2.87	0.42
2:J:1969:LEU:O	2:J:1971:GLY:N	2.52	0.42
3:K:246:LEU:HD12	3:K:246:LEU:HA	1.89	0.42
3:K:803:SER:HB3	3:K:1055:HIS:CD2	2.55	0.42
3:L:1877:ARG:HG3	3:L:1940:LEU:HD23	2.01	0.42
3:L:896:ASN:ND2	3:L:906:THR:HG21	2.34	0.42
1:A:1418:VAL:N	1:A:1419:PRO:CD	2.82	0.42
1:A:1751:GLU:HG3	1:A:1872:SER:HB2	2.00	0.42
1:C:1022:THR:HG23	1:C:1226:SER:OG	2.19	0.42
1:E:632:ARG:O	1:E:633:GLU:CB	2.67	0.42
1:E:952:GLU:HA	1:E:952:GLU:OE1	2.18	0.42
1:F:407:ASN:ND2	1:F:1626:TYR:O	2.44	0.42
1:F:952:GLU:OE1	1:F:952:GLU:HA	2.19	0.42
2:G:1468:THR:HG23	2:G:1485:CYS:SG	2.60	0.42
1:B:59:ARG:HG2	3:H:1896:GLN:HE22	1.83	0.42
3:I:1838:MET:HE3	3:I:1976:PHE:CD1	2.55	0.42
3:I:597:MET:HB3	10:I:2101:FMN:C6	2.50	0.42
3:I:598:THR:OG1	3:I:599:PRO:HD2	2.18	0.42
2:J:856:LYS:HD3	2:J:1052:CYS:SG	2.58	0.42
2:J:1381:VAL:HG13	2:J:1390:VAL:HG22	2.00	0.42
2:J:598:THR:HG23	10:J:2101:FMN:O4	2.20	0.42
2:J:847:ARG:HG2	5:J:2104:EDO:C2	2.49	0.42
3:K:1292:ILE:O	3:K:1368:VAL:O	2.36	0.42
3:K:868:PHE:HB3	3:K:873:PHE:CE2	2.54	0.42
3:L:277:LEU:HD23	3:L:277:LEU:HA	1.88	0.42
3:L:602:VAL:HG21	3:L:623:GLY:HA3	2.02	0.42
1:A:616:LEU:N	1:A:617:PRO:HD2	2.33	0.42
1:A:641:ARG:NH2	1:A:925:ASP:OD2	2.52	0.42
1:B:1813:TRP:HZ3	1:B:1834:LEU:HD13	1.83	0.42
1:D:807:LYS:C	1:D:807:LYS:HD3	2.40	0.42
1:D:955:LYS:O	1:D:959:ILE:HG13	2.19	0.42
1:E:1431:GLU:CG	1:E:1433:HIS:CE1	3.02	0.42
1:E:1498:GLU:O	1:E:1502:ARG:HG3	2.20	0.42
1:E:407:ASN:ND2	1:E:1626:TYR:O	2.45	0.42
1:F:643:LYS:NZ	1:F:851:ASN:HD21	2.17	0.42
2:G:1358:LYS:HG3	12:G:2216:HOH:O	2.18	0.42
3:H:1265:MET:HE1	3:H:1569:PHE:CZ	2.55	0.42
3:H:1908:ASP:OD2	3:H:1954:LYS:HE3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:249:TYR:CZ	3:H:263:LEU:HD23	2.54	0.42
3:I:1347:LEU:HD12	3:I:1347:LEU:HA	1.90	0.42
10:J:2101:FMN:O4'	10:J:2101:FMN:O3P	2.30	0.42
2:J:468:LEU:HA	2:J:471:LEU:CD2	2.49	0.42
2:J:468:LEU:HA	2:J:471:LEU:HD21	2.01	0.42
3:K:942:THR:HB	3:K:1012:GLN:HB2	2.01	0.42
3:K:249:TYR:CZ	3:K:263:LEU:HD23	2.54	0.42
3:K:99:ASN:HD22	3:K:100:ASP:N	2.13	0.42
1:A:965:HIS:CE1	1:A:969:ASN:ND2	2.88	0.42
1:C:186:ILE:O	1:C:190:LEU:HG	2.19	0.42
1:C:438:ASN:HD21	1:C:698:GLN:HG3	1.84	0.42
1:D:1794:GLN:HE22	1:D:1840:VAL:HA	1.84	0.42
1:E:798:ASN:HA	1:E:801:ARG:HB2	2.01	0.42
1:D:359:ARG:NH1	1:F:1153:ASP:OD1	2.53	0.42
2:G:1348:LEU:HA	2:G:1348:LEU:HD12	1.90	0.42
2:G:1852:TYR:C	2:G:1904:LEU:CD1	2.88	0.42
2:G:1926:GLU:O	2:G:1930:SER:OG	2.24	0.42
2:G:803:SER:HB3	2:G:1055:HIS:CD2	2.55	0.42
3:H:856:LYS:HD3	3:H:1052:CYS:SG	2.59	0.42
3:H:1854:MET:HA	3:H:1907:LEU:HD21	2.01	0.42
3:I:1926:GLU:O	3:I:1930:SER:OG	2.23	0.42
3:I:249:TYR:CZ	3:I:263:LEU:HD23	2.54	0.42
2:J:1265:MET:CE	2:J:1569:PHE:CZ	3.02	0.42
2:J:6:THR:O	2:J:7:ARG:CB	2.67	0.42
2:J:852:GLU:HG2	2:J:852:GLU:H	1.71	0.42
3:K:904:PHE:HB2	3:K:1017:PHE:CD2	2.54	0.42
3:K:1468:THR:HG23	3:K:1485:CYS:SG	2.59	0.42
3:K:1955:PRO:O	3:K:1958:LEU:HB3	2.18	0.42
3:K:852:GLU:HG3	3:K:852:GLU:H	1.71	0.42
3:L:1343:VAL:CG2	3:L:1343:VAL:O	2.67	0.42
1:A:27:ARG:HB2	2:G:2016:ALA:HB2	2.01	0.42
1:A:341:GLN:O	1:A:345:VAL:HG13	2.19	0.42
1:B:1498:GLU:O	1:B:1502:ARG:HG3	2.19	0.42
1:B:1755:MET:HG2	1:B:1870:SER:HB3	2.01	0.42
1:C:1431:GLU:CG	1:C:1433:HIS:CE1	3.02	0.42
1:C:1600:LEU:CD1	1:C:1655:VAL:HG12	2.49	0.42
1:C:1689:HIS:CE1	3:I:996:ASN:HD21	2.38	0.42
1:D:43:ARG:O	2:J:1662:THR:HA	2.20	0.42
1:E:1062:TYR:CG	1:E:1693:ILE:HB	2.55	0.42
1:E:1486:LEU:O	1:E:1490:THR:HG23	2.09	0.42
1:F:495:LYS:HE3	1:F:495:LYS:HB3	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:ASP:O	1:F:95:SER:N	2.50	0.42
2:G:1908:ASP:OD2	2:G:1954:LYS:HE3	2.19	0.42
2:G:1928:GLN:HB2	2:G:1928:GLN:HE21	1.67	0.42
2:G:1954:LYS:HB3	2:G:1955:PRO:HD2	2.02	0.42
2:G:33:LEU:HD12	2:G:33:LEU:N	2.34	0.42
2:G:500:HIS:HA	2:G:526:ARG:O	2.19	0.42
3:H:1289:ASP:OD1	3:H:1373:SER:HB3	2.19	0.42
3:H:1877:ARG:HG3	3:H:1940:LEU:HD23	2.01	0.42
2:J:1877:ARG:HD2	2:J:1877:ARG:HA	1.84	0.42
3:K:500:HIS:HA	3:K:526:ARG:O	2.19	0.42
3:L:1541:VAL:HG22	3:L:1625:SER:HB2	2.02	0.42
3:L:464:ASP:HB3	3:L:466:SER:H	1.85	0.42
1:A:1119:LYS:O	1:A:1178:ALA:HA	2.20	0.42
1:A:1752:THR:O	1:A:1756:ILE:HG23	2.19	0.42
1:A:186:ILE:O	1:A:190:LEU:HG	2.19	0.42
1:B:952:GLU:HA	1:B:952:GLU:OE1	2.19	0.42
1:C:1736:LYS:HD2	1:C:1736:LYS:N	2.33	0.42
1:D:186:ILE:O	1:D:190:LEU:HG	2.19	0.42
1:E:72:LEU:HB2	1:E:74:LEU:HD23	2.02	0.42
2:G:730:LEU:C	2:G:730:LEU:CD1	2.87	0.42
3:H:1594:GLU:O	3:H:1598:ALA:HB3	2.20	0.42
3:H:285:GLU:OE1	3:H:298:LYS:CE	2.68	0.42
3:H:303:LEU:HD12	3:H:303:LEU:HA	1.93	0.42
3:I:1374:THR:HG23	3:I:1396:LEU:HD12	2.01	0.42
3:I:1859:PRO:O	3:I:1862:VAL:HG13	2.20	0.42
3:I:1969:LEU:O	3:I:1971:GLY:N	2.53	0.42
3:I:451:ASN:HB3	3:I:453:LYS:HG3	2.02	0.42
3:I:716:VAL:HG11	3:I:730:LEU:HD22	2.02	0.42
2:J:1040:LEU:O	2:J:1046:GLN:HA	2.18	0.42
2:J:1962:ARG:NH2	2:J:1967:ILE:HG12	2.34	0.42
2:J:716:VAL:HG11	2:J:730:LEU:HD22	2.01	0.42
2:J:803:SER:HB3	2:J:1055:HIS:CD2	2.55	0.42
3:K:1927:LEU:HA	3:K:1931:LEU:HB2	2.01	0.42
1:E:980:VAL:HB	3:K:968:GLN:OE1	2.20	0.42
3:L:1770:LEU:HD13	3:L:1770:LEU:HA	1.94	0.42
3:L:622:GLY:HA2	3:L:658:MET:HE1	2.01	0.42
1:A:1760:THR:O	1:A:1760:THR:CG2	2.58	0.42
1:B:17:LEU:O	1:B:21:GLN:HB2	2.20	0.42
1:C:1062:TYR:CG	1:C:1693:ILE:HB	2.55	0.42
1:A:359:ARG:NH1	1:C:1153:ASP:OD1	2.52	0.42
1:E:17:LEU:O	1:E:21:GLN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:798:ASN:HA	1:F:801:ARG:HB2	2.02	0.42
2:G:1594:GLU:O	2:G:1598:ALA:HB3	2.20	0.42
3:H:1468:THR:HG23	3:H:1485:CYS:SG	2.60	0.42
3:H:500:HIS:HA	3:H:526:ARG:O	2.20	0.42
3:I:101:ILE:CD1	3:I:126:TYR:HB3	2.44	0.42
2:J:246:LEU:HA	2:J:246:LEU:HD12	1.88	0.42
3:L:1852:TYR:C	3:L:1904:LEU:CD1	2.88	0.42
1:B:1500:GLN:CG	1:D:1507:GLN:NE2	2.81	0.42
1:B:1790:ASN:O	1:B:1816:LYS:NZ	2.43	0.42
1:D:1062:TYR:CG	1:D:1693:ILE:HB	2.55	0.42
1:E:438:ASN:HD21	1:E:698:GLN:HG3	1.85	0.42
1:F:1431:GLU:CG	1:F:1433:HIS:CE1	3.03	0.42
1:F:868:ILE:HD11	1:F:923:MET:HE3	2.02	0.42
2:G:233:SER:HA	2:G:424:ALA:CB	2.49	0.42
3:H:1343:VAL:CG2	3:H:1343:VAL:O	2.67	0.42
3:H:1859:PRO:O	3:H:1862:VAL:HG13	2.20	0.42
3:H:1944:ILE:O	3:H:1948:SER:HB3	2.20	0.42
3:H:419:ARG:HB3	3:H:419:ARG:CZ	2.49	0.42
3:I:1737:ILE:HD13	3:I:1739:GLU:HG2	2.02	0.42
3:I:1923:ASP:OD2	3:I:1926:GLU:HB2	2.20	0.42
2:J:1265:MET:HE1	2:J:1569:PHE:CZ	2.55	0.42
2:J:597:MET:HA	10:J:2101:FMN:C4A	2.50	0.42
2:J:663:ILE:HB	2:J:664:PRO:HD3	2.01	0.42
2:J:896:ASN:ND2	2:J:906:THR:HG21	2.34	0.42
3:K:1969:LEU:O	3:K:1971:GLY:N	2.52	0.42
3:L:1854:MET:HB3	3:L:1901:ALA:CB	2.49	0.42
3:L:1915:ASN:N	3:L:1915:ASN:HD22	2.16	0.42
3:L:1969:LEU:O	3:L:1971:GLY:N	2.53	0.42
1:B:11:HIS:ND1	3:H:1998:LYS:HA	2.34	0.41
1:B:1014:ASP:N	1:B:1510:ASN:HD21	2.14	0.41
1:C:294:TYR:CE1	1:C:298:VAL:HG21	2.55	0.41
1:C:952:GLU:HA	1:C:952:GLU:OE1	2.20	0.41
1:E:1022:THR:HG23	1:E:1226:SER:OG	2.20	0.41
1:E:894:ARG:NH2	1:E:900:GLU:OE1	2.52	0.41
1:F:1022:THR:HG23	1:F:1226:SER:OG	2.20	0.41
2:G:1280:ASP:OD1	2:G:1281:PRO:HD2	2.20	0.41
2:G:285:GLU:OE1	2:G:298:LYS:CE	2.68	0.41
3:I:500:HIS:HA	3:I:526:ARG:O	2.19	0.41
3:I:896:ASN:ND2	3:I:906:THR:HG21	2.34	0.41
2:J:478:ARG:HA	2:J:478:ARG:HD3	1.91	0.41
3:K:1915:ASN:HD21	3:K:1963:GLY:HA3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1872:GLN:HE21	3:L:1888:ILE:HD11	1.85	0.41
3:L:716:VAL:HG11	3:L:730:LEU:HD22	2.01	0.41
1:A:955:LYS:O	1:A:959:ILE:HG13	2.20	0.41
1:C:1752:THR:O	1:C:1756:ILE:HG23	2.20	0.41
1:C:807:LYS:HD3	1:C:807:LYS:C	2.39	0.41
1:D:688:ILE:HD11	1:D:872:THR:HG21	2.02	0.41
1:E:1392:LEU:HD22	1:E:1396:MET:HG3	2.01	0.41
1:E:1600:LEU:CD1	1:E:1655:VAL:HG12	2.50	0.41
1:E:329:GLU:HA	1:E:332:THR:HG22	2.01	0.41
1:F:1062:TYR:CG	1:F:1693:ILE:HB	2.55	0.41
1:F:1423:LYS:O	1:F:1426:LEU:HB2	2.19	0.41
1:F:1501:LEU:O	1:F:1505:GLN:HG3	2.21	0.41
2:G:214:ASN:C	2:G:214:ASN:HD22	2.22	0.41
2:G:79:GLN:HE21	2:G:79:GLN:N	1.98	0.41
2:J:464:ASP:HB3	2:J:466:SER:H	1.84	0.41
1:A:1515:ARG:HG2	1:E:1495:ASN:HD22	1.85	0.41
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.90	0.41
1:C:1716:LEU:HD21	1:F:1426:LEU:CD2	2.45	0.41
1:C:708:SER:OG	7:C:1917:A2P:O1P	2.31	0.41
2:G:56:THR:HG21	2:G:112:ASN:HD22	1.84	0.41
3:H:1222:GLU:HG2	3:H:1235:SER:OG	2.19	0.41
3:H:1374:THR:HG23	3:H:1396:LEU:HD12	2.02	0.41
3:H:1986:LYS:N	3:H:1987:PRO:HD2	2.35	0.41
3:H:998:GLN:HB3	3:H:998:GLN:HE21	1.65	0.41
3:I:1858:ASN:ND2	3:I:1896:GLN:HA	2.36	0.41
3:I:29:ILE:HD12	3:I:82:GLN:NE2	2.35	0.41
3:L:1265:MET:CE	3:L:1569:PHE:CZ	3.03	0.41
3:L:1929:LYS:CD	3:L:1933:LEU:HD12	2.50	0.41
3:L:559:PRO:HB3	3:L:564:GLU:HG3	2.02	0.41
1:B:20:TYR:CD2	3:H:2033:THR:HG23	2.55	0.41
1:C:1477:ILE:CD1	1:C:1485:PHE:CD1	3.03	0.41
1:C:674:LYS:O	1:C:675:ASP:HB2	2.20	0.41
1:C:67:SER:HB3	3:H:355:LYS:HE3	2.02	0.41
1:D:930:LEU:HA	1:D:930:LEU:HD23	1.94	0.41
1:E:484:LEU:HD22	1:E:485:ASP:N	2.35	0.41
1:F:1794:GLN:NE2	1:F:1840:VAL:HA	2.34	0.41
3:H:602:VAL:HG21	3:H:623:GLY:HA3	2.02	0.41
2:J:1541:VAL:HG22	2:J:1625:SER:HB2	2.02	0.41
2:J:1927:LEU:HB3	2:J:1931:LEU:HD13	2.02	0.41
2:J:730:LEU:C	2:J:730:LEU:CD1	2.87	0.41
3:K:1201:VAL:HG11	3:K:1226:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1280:ASP:OD1	3:L:1281:PRO:HD2	2.20	0.41
3:L:1881:ARG:HG2	3:L:1944:ILE:HD11	2.02	0.41
3:L:249:TYR:CZ	3:L:263:LEU:HD23	2.55	0.41
3:L:37:PHE:CZ	3:L:41:LEU:HD21	2.55	0.41
1:B:1260:MET:HG2	1:D:1342:GLU:HG3	2.01	0.41
1:F:1498:GLU:O	1:F:1502:ARG:HG3	2.21	0.41
2:G:167:ASP:OD1	2:G:167:ASP:N	2.45	0.41
2:G:753:MET:O	2:G:757:ILE:HG13	2.21	0.41
3:H:942:THR:HB	3:H:1012:GLN:HB2	2.03	0.41
3:H:1734:SER:O	3:H:1750:LYS:HE2	2.20	0.41
3:H:29:ILE:O	3:H:33:LEU:HD22	2.20	0.41
3:H:464:ASP:HB3	3:H:466:SER:H	1.84	0.41
3:I:1986:LYS:N	3:I:1987:PRO:HD2	2.36	0.41
2:J:1680:LEU:HD22	2:J:1684:SER:CB	2.50	0.41
2:J:1838:MET:HE3	2:J:1976:PHE:CD1	2.55	0.41
3:K:1353:LEU:HD11	3:K:1411:PHE:HB2	2.02	0.41
3:K:455:ILE:HD11	3:K:469:ARG:CG	2.46	0.41
1:A:1370:THR:HG22	1:A:1372:THR:H	1.85	0.41
1:A:894:ARG:NH2	1:A:900:GLU:OE1	2.52	0.41
1:A:952:GLU:HA	1:A:952:GLU:OE1	2.21	0.41
1:B:1022:THR:HG23	1:B:1226:SER:OG	2.20	0.41
1:C:1370:THR:HG22	1:C:1372:THR:H	1.86	0.41
1:C:1477:ILE:HD12	1:C:1485:PHE:CD1	2.56	0.41
1:C:1771:VAL:HG22	1:C:1881:VAL:HG22	2.02	0.41
1:C:798:ASN:HA	1:C:801:ARG:HB2	2.02	0.41
1:C:793:ARG:NH1	1:D:789:GLU:OE1	2.54	0.41
1:E:1785:THR:O	1:E:1789:ARG:HB2	2.20	0.41
1:E:294:TYR:CE1	1:E:298:VAL:HG21	2.55	0.41
1:D:359:ARG:NH1	1:F:1153:ASP:OD2	2.54	0.41
1:F:1486:LEU:HD12	1:F:1486:LEU:HA	1.90	0.41
1:F:751:PHE:CZ	1:F:761:LEU:HD13	2.55	0.41
2:G:1986:LYS:N	2:G:1987:PRO:HD2	2.36	0.41
3:H:1378:ILE:HD11	3:H:1381:VAL:HG22	2.02	0.41
3:I:1343:VAL:CG2	3:I:1343:VAL:O	2.68	0.41
2:J:285:GLU:OE1	2:J:298:LYS:CE	2.69	0.41
3:K:1594:GLU:O	3:K:1598:ALA:HB3	2.20	0.41
3:L:56:THR:HG21	3:L:112:ASN:HD22	1.85	0.41
3:L:1838:MET:HE3	3:L:1976:PHE:CD1	2.56	0.41
3:L:885:GLU:HA	3:L:885:GLU:OE1	2.20	0.41
1:A:688:ILE:HD11	1:A:872:THR:HG21	2.03	0.41
1:B:1062:TYR:CG	1:B:1693:ILE:HB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1020:VAL:HG22	1:B:1400:ILE:HG23	2.03	0.41
1:B:1785:THR:O	1:B:1789:ARG:HB2	2.21	0.41
1:B:798:ASN:HA	1:B:801:ARG:HB2	2.02	0.41
1:C:1581:THR:HB	1:C:1591:TRP:CZ3	2.56	0.41
1:C:1825:VAL:HG11	1:C:1858:ALA:HB1	2.03	0.41
1:C:198:PRO:HG3	1:C:212:THR:HG21	2.02	0.41
1:D:1119:LYS:O	1:D:1178:ALA:HA	2.21	0.41
1:D:1431:GLU:HG3	1:D:1433:HIS:CE1	2.55	0.41
1:D:407:ASN:ND2	1:D:1626:TYR:O	2.45	0.41
1:A:1117:GLU:O	1:E:1146:HIS:HE1	2.03	0.41
1:A:1507:GLN:NE2	1:E:1500:GLN:CG	2.83	0.41
1:E:868:ILE:HD11	1:E:923:MET:HE3	2.02	0.41
1:E:955:LYS:O	1:E:959:ILE:HG13	2.20	0.41
1:F:1766:ASN:N	1:F:1766:ASN:OD1	2.52	0.41
1:F:677:TYR:CZ	1:F:702:LYS:HD2	2.55	0.41
2:G:1201:VAL:HG11	2:G:1226:ASN:HB2	2.03	0.41
2:G:1289:ASP:OD1	2:G:1373:SER:HB3	2.20	0.41
2:G:1858:ASN:HD22	2:G:1861:ARG:HG2	1.77	0.41
3:H:1969:LEU:O	3:H:1971:GLY:N	2.53	0.41
3:I:1884:TRP:CZ3	3:I:1905:ARG:HB3	2.56	0.41
2:J:1280:ASP:OD1	2:J:1281:PRO:HD2	2.21	0.41
2:J:1854:MET:HB3	2:J:1901:ALA:CB	2.50	0.41
2:J:1858:ASN:ND2	2:J:1896:GLN:HA	2.35	0.41
2:J:500:HIS:HA	2:J:526:ARG:O	2.20	0.41
3:L:748:THR:HB	3:L:749:PRO:HD3	2.02	0.41
1:A:1443:LEU:HA	1:A:1443:LEU:HD23	1.94	0.41
1:A:17:LEU:O	1:A:21:GLN:HB2	2.21	0.41
1:B:1370:THR:HG22	1:B:1372:THR:H	1.86	0.41
1:C:1119:LYS:O	1:C:1178:ALA:HA	2.20	0.41
1:C:413:LEU:HD13	1:C:413:LEU:C	2.41	0.41
1:D:1771:VAL:HG22	1:D:1881:VAL:HG22	2.02	0.41
1:D:20:TYR:CG	2:J:2033:THR:HG23	2.55	0.41
1:E:1129:GLU:O	1:E:1130:ASP:C	2.59	0.41
1:E:1752:THR:O	1:E:1756:ILE:HG23	2.21	0.41
1:E:233:ILE:HG21	1:E:243:ILE:N	2.36	0.41
1:E:429:ASP:O	1:E:432:VAL:HG13	2.20	0.41
1:F:1119:LYS:O	1:F:1178:ALA:HA	2.21	0.41
2:G:1737:ILE:HD13	2:G:1739:GLU:HG2	2.03	0.41
3:H:1348:LEU:HA	3:H:1348:LEU:HD12	1.90	0.41
3:H:1737:ILE:HD13	3:H:1739:GLU:HG2	2.02	0.41
3:H:1858:ASN:ND2	3:H:1896:GLN:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:56:THR:HG21	3:H:112:ASN:HD22	1.86	0.41
3:H:99:ASN:HD22	3:H:100:ASP:N	2.10	0.41
3:I:167:ASP:OD1	3:I:167:ASP:N	2.45	0.41
3:I:1852:TYR:CA	3:I:1904:LEU:HD13	2.51	0.41
3:I:1962:ARG:NH2	3:I:1967:ILE:HG12	2.35	0.41
3:I:494:THR:HG23	3:I:520:LYS:HE3	2.03	0.41
2:J:29:ILE:O	2:J:32:GLN:HB3	2.21	0.41
2:J:6:THR:O	2:J:7:ARG:HB2	2.20	0.41
3:K:896:ASN:ND2	3:K:906:THR:HG21	2.34	0.41
3:L:109:LEU:HD21	3:L:116:LEU:CD2	2.50	0.41
3:L:1374:THR:HG23	3:L:1396:LEU:HD12	2.02	0.41
3:L:856:LYS:HD3	3:L:1052:CYS:SG	2.61	0.41
1:A:1762:GLU:OE1	1:A:1763:LYS:N	2.50	0.41
1:B:1501:LEU:O	1:B:1505:GLN:HG3	2.21	0.41
1:C:73:SER:HG	3:H:387:TYR:HD2	1.68	0.41
1:D:798:ASN:HA	1:D:801:ARG:HB2	2.02	0.41
1:E:1771:VAL:HG22	1:E:1881:VAL:HG22	2.01	0.41
1:F:11:HIS:HE1	3:L:1996:ILE:O	2.04	0.41
1:F:1014:ASP:N	1:F:1510:ASN:HD21	2.14	0.41
1:F:1771:VAL:HG22	1:F:1881:VAL:HG22	2.01	0.41
1:F:213:PHE:O	1:F:217:PHE:HB2	2.21	0.41
2:G:1859:PRO:O	2:G:1862:VAL:HG13	2.19	0.41
3:H:323:ILE:HG12	3:H:387:TYR:CE2	2.56	0.41
3:H:753:MET:O	3:H:757:ILE:HG13	2.21	0.41
3:I:1378:ILE:HD11	3:I:1381:VAL:HG22	2.03	0.41
3:I:1479:ILE:N	3:I:1479:ILE:HD13	2.36	0.41
2:J:1022:ASP:OD1	2:J:1024:ARG:HG3	2.21	0.41
2:J:346:GLN:HE22	5:J:2105:EDO:H22	1.84	0.41
2:J:364:LYS:HA	2:J:382:PRO:HG2	2.02	0.41
3:K:364:LYS:HA	3:K:382:PRO:HG2	2.02	0.41
3:L:1479:ILE:H	3:L:1479:ILE:HD12	1.86	0.41
3:L:1594:GLU:O	3:L:1598:ALA:HB3	2.20	0.41
3:L:1665:VAL:HA	3:L:1805:ALA:O	2.21	0.41
1:A:1600:LEU:CD1	1:A:1655:VAL:HG12	2.50	0.41
1:B:504:ASP:CG	1:B:508:ASN:CG	2.78	0.41
1:B:732:LEU:HD23	1:B:732:LEU:HA	1.90	0.41
1:B:499:PRO:HB3	1:B:873:ARG:HD3	2.02	0.41
1:C:1441:PRO:HD2	1:F:1492:GLU:OE2	2.20	0.41
1:C:1785:THR:O	1:C:1789:ARG:HG3	2.20	0.41
1:E:1370:THR:HG22	1:E:1372:THR:H	1.84	0.41
1:F:1813:TRP:CZ3	1:F:1834:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1422:THR:CG2	2:G:1474:PHE:CD1	3.00	0.41
2:G:1479:ILE:N	2:G:1479:ILE:HD13	2.35	0.41
3:H:1085:LEU:HD12	3:H:1085:LEU:HA	1.87	0.41
3:H:1541:VAL:HG22	3:H:1625:SER:CB	2.51	0.41
3:H:1907:LEU:HD23	3:H:1960:LEU:CD2	2.51	0.41
3:H:440:ASN:HD21	3:H:477:GLU:HA	1.84	0.41
1:D:20:TYR:CD2	2:J:2033:THR:HG23	2.56	0.41
2:J:964:LEU:CD2	2:J:964:LEU:H	2.33	0.41
3:K:1374:THR:HG23	3:K:1396:LEU:HD12	2.02	0.41
3:K:1479:ILE:HD12	3:K:1479:ILE:H	1.85	0.41
3:L:1289:ASP:OD1	3:L:1373:SER:HB3	2.20	0.41
1:F:48:GLY:HA3	3:L:1667:THR:OG1	2.21	0.41
1:A:438:ASN:HD21	1:A:698:GLN:HG3	1.86	0.41
1:A:828:PRO:HG2	1:A:829:ASN:ND2	2.36	0.41
1:C:407:ASN:ND2	1:C:1626:TYR:O	2.45	0.41
1:C:751:PHE:CZ	1:C:761:LEU:HD13	2.56	0.41
1:D:1827:SER:O	1:D:1828:LEU:HB2	2.21	0.41
1:D:982:ILE:O	2:J:962:LYS:HA	2.21	0.41
1:E:1167:LEU:HD11	1:E:1171:ALA:HB1	2.03	0.41
1:F:438:ASN:HD21	1:F:698:GLN:HG3	1.86	0.41
3:H:249:TYR:CE2	3:H:283:ILE:HD12	2.56	0.41
3:I:1541:VAL:HG22	3:I:1625:SER:CB	2.51	0.41
3:I:1665:VAL:HA	3:I:1805:ALA:O	2.21	0.41
3:I:37:PHE:CZ	3:I:41:LEU:HD21	2.56	0.41
3:I:622:GLY:HA2	3:I:658:MET:HE1	2.03	0.41
2:J:1594:GLU:O	2:J:1598:ALA:HB3	2.21	0.41
2:J:597:MET:HA	10:J:2101:FMN:C5A	2.49	0.41
3:K:1858:ASN:ND2	3:K:1896:GLN:HA	2.35	0.41
3:K:2030:TYR:HA	3:K:2033:THR:OG1	2.21	0.41
3:K:716:VAL:HG11	3:K:730:LEU:HD22	2.02	0.41
3:L:1954:LYS:HB3	3:L:1955:PRO:HD2	2.02	0.41
3:L:942:THR:HB	3:L:1012:GLN:HB2	2.03	0.41
1:A:1515:ARG:HG2	1:E:1495:ASN:ND2	2.36	0.40
1:A:798:ASN:HA	1:A:801:ARG:HB2	2.02	0.40
1:B:1021:VAL:HG11	1:B:1597:LEU:HD11	2.03	0.40
1:C:17:LEU:O	1:C:21:GLN:HB2	2.21	0.40
1:D:732:LEU:HA	1:D:732:LEU:HD23	1.90	0.40
1:E:221:LEU:HD23	1:E:221:LEU:HA	1.91	0.40
1:F:1079:LYS:HA	1:F:1079:LYS:HE3	2.03	0.40
1:F:1581:THR:HB	1:F:1591:TRP:CZ3	2.56	0.40
1:F:1826:LYS:C	1:F:1827:SER:O	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:329:GLU:HA	1:F:332:THR:HG22	2.03	0.40
1:F:688:ILE:HD11	1:F:872:THR:HG21	2.03	0.40
2:G:1911:THR:O	2:G:1915:ASN:ND2	2.54	0.40
2:G:37:PHE:CZ	2:G:41:LEU:HD21	2.56	0.40
2:G:896:ASN:ND2	2:G:906:THR:HG21	2.36	0.40
3:H:1130:THR:N	3:H:1133:THR:HG22	2.36	0.40
3:H:1665:VAL:HA	3:H:1805:ALA:O	2.21	0.40
3:H:1775:GLN:CG	3:H:1836:MET:HE3	2.50	0.40
3:H:1956:ARG:N	3:H:1957:PRO:HD2	2.36	0.40
3:H:37:PHE:CZ	3:H:41:LEU:HD21	2.56	0.40
3:I:285:GLU:OE1	3:I:298:LYS:CE	2.68	0.40
2:J:1956:ARG:N	2:J:1957:PRO:HD2	2.36	0.40
2:J:1986:LYS:N	2:J:1987:PRO:HD2	2.37	0.40
3:K:1986:LYS:N	3:K:1987:PRO:HD2	2.36	0.40
3:K:285:GLU:OE1	3:K:298:LYS:CE	2.68	0.40
3:L:1904:LEU:HG	3:L:1960:LEU:HD23	2.03	0.40
3:L:1861:ARG:HG3	3:L:1965:ALA:HB2	2.03	0.40
3:L:285:GLU:OE1	3:L:298:LYS:CE	2.68	0.40
3:L:740[B]:HIS:CE1	3:L:852:GLU:HB2	2.56	0.40
1:B:360:LYS:CE	1:E:358:GLU:OE2	2.69	0.40
1:B:965:HIS:CE1	1:B:969:ASN:ND2	2.89	0.40
1:C:965:HIS:CE1	1:C:969:ASN:ND2	2.89	0.40
1:D:1021:VAL:HG11	1:D:1597:LEU:HD11	2.04	0.40
1:D:378:LEU:HD12	1:D:378:LEU:HA	1.86	0.40
1:D:952:GLU:HA	1:D:952:GLU:OE1	2.20	0.40
1:E:1119:LYS:O	1:E:1178:ALA:HA	2.20	0.40
1:E:1600:LEU:HD11	1:E:1655:VAL:HG12	2.03	0.40
1:F:1751:GLU:HG3	1:F:1872:SER:HB2	2.02	0.40
2:G:1849:ARG:NH1	2:G:1957:PRO:HG3	2.36	0.40
3:H:1280:ASP:OD1	3:H:1281:PRO:HD2	2.21	0.40
3:H:1541:VAL:HG22	3:H:1625:SER:HB2	2.02	0.40
3:H:1740:THR:OG1	3:H:1747:LYS:CE	2.69	0.40
3:H:29:ILE:O	3:H:32:GLN:HB3	2.21	0.40
3:H:364:LYS:HA	3:H:382:PRO:HG2	2.03	0.40
3:H:852:GLU:H	3:H:852:GLU:HG3	1.75	0.40
3:H:883:THR:O	3:H:887:LYS:HG2	2.21	0.40
3:I:29:ILE:O	3:I:32:GLN:HB3	2.21	0.40
2:J:1541:VAL:HG22	2:J:1625:SER:CB	2.52	0.40
2:J:419:ARG:CZ	2:J:419:ARG:HB3	2.51	0.40
2:J:753:MET:O	2:J:757:ILE:HG13	2.21	0.40
3:K:1665:VAL:HA	3:K:1805:ALA:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1854:MET:HB3	3:K:1901:ALA:CB	2.49	0.40
3:K:1871:LEU:HD23	3:K:1871:LEU:HA	1.92	0.40
3:K:37:PHE:CZ	3:K:41:LEU:HD21	2.56	0.40
3:K:597:MET:HB3	10:K:2101:FMN:C6	2.51	0.40
3:L:1335:ILE:O	3:L:1338:ILE:HG12	2.22	0.40
3:L:1541:VAL:HG22	3:L:1625:SER:CB	2.52	0.40
3:L:1986:LYS:N	3:L:1987:PRO:HD2	2.36	0.40
1:B:1153:ASP:CG	1:C:359:ARG:NH1	2.75	0.40
1:B:413:LEU:C	1:B:413:LEU:HD13	2.42	0.40
1:B:955:LYS:O	1:B:959:ILE:HG13	2.21	0.40
1:C:998:TYR:CE2	1:C:1002:LYS:HD3	2.56	0.40
1:C:1181:PHE:CZ	1:C:1341:PHE:HA	2.56	0.40
1:C:1501:LEU:O	1:C:1505:GLN:HG3	2.21	0.40
1:C:213:PHE:O	1:C:217:PHE:HB2	2.22	0.40
1:B:1342:GLU:HB3	1:D:1275:LEU:HB2	2.04	0.40
1:D:1581:THR:HB	1:D:1591:TRP:CZ3	2.57	0.40
1:D:413:LEU:HD13	1:D:413:LEU:C	2.42	0.40
1:D:429:ASP:O	1:D:432:VAL:HG13	2.20	0.40
1:D:632:ARG:O	1:D:633:GLU:CB	2.69	0.40
1:E:1303:GLY:HA2	1:E:1649:LYS:HE3	2.02	0.40
1:E:1431:GLU:HG3	1:E:1433:HIS:CE1	2.56	0.40
1:E:1455:ARG:HD2	1:E:1455:ARG:HA	1.77	0.40
1:E:1581:THR:HB	1:E:1591:TRP:CZ3	2.56	0.40
1:E:738:ASN:ND2	1:E:740:GLY:H	2.20	0.40
1:F:30:GLU:HB2	3:L:2016:ALA:CB	2.51	0.40
2:G:1974:VAL:HB	2:G:1976:PHE:CE1	2.56	0.40
3:H:1775:GLN:HG3	3:H:1836:MET:HE3	2.03	0.40
3:H:598:THR:OG1	3:H:599:PRO:HD2	2.19	0.40
3:H:730:LEU:CD1	3:H:730:LEU:C	2.88	0.40
3:I:803:SER:HB3	3:I:1055:HIS:CD2	2.56	0.40
1:D:29:ILE:CD1	2:J:1894:GLU:N	2.85	0.40
3:L:1435:ILE:CG2	3:L:1441:ILE:HG22	2.51	0.40
3:L:1849:ARG:HD2	3:L:1849:ARG:N	2.36	0.40
1:A:1657:HIS:CD2	1:A:1658:PRO:CD	3.01	0.40
1:A:732:LEU:HA	1:A:732:LEU:HD23	1.91	0.40
1:B:1129:GLU:O	1:B:1130:ASP:C	2.59	0.40
1:C:1129:GLU:O	1:C:1130:ASP:C	2.59	0.40
1:C:329:GLU:HB2	1:C:332:THR:HG23	2.03	0.40
1:C:378:LEU:HA	1:C:378:LEU:HD12	1.87	0.40
1:C:643:LYS:NZ	1:C:851:ASN:HD21	2.19	0.40
1:D:1153:ASP:OD2	1:E:359:ARG:NH1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1501:LEU:O	1:D:1505:GLN:HG3	2.21	0.40
1:D:17:LEU:O	1:D:21:GLN:HB2	2.21	0.40
1:D:233:ILE:HG21	1:D:243:ILE:N	2.37	0.40
1:D:294:TYR:CE1	1:D:298:VAL:HG21	2.56	0.40
1:D:965:HIS:CE1	1:D:969:ASN:ND2	2.89	0.40
1:E:1751:GLU:HG3	1:E:1872:SER:HB2	2.03	0.40
1:E:43:ARG:HD3	3:K:1660:PRO:HG2	2.03	0.40
1:F:1181:PHE:CZ	1:F:1341:PHE:HA	2.57	0.40
1:F:1736:LYS:HA	1:F:1736:LYS:HD3	1.92	0.40
1:F:807:LYS:HG3	1:F:858:TRP:HB3	2.03	0.40
2:G:1085:LEU:HA	2:G:1085:LEU:HD12	1.86	0.40
3:H:1852:TYR:C	3:H:1904:LEU:CD2	2.90	0.40
3:H:716:VAL:HG11	3:H:730:LEU:HD22	2.02	0.40
3:I:1854:MET:HB3	3:I:1901:ALA:CB	2.49	0.40
3:I:753:MET:O	3:I:757:ILE:HG13	2.21	0.40
3:K:1217:ASN:HD22	3:K:1217:ASN:HA	1.62	0.40
3:K:2046:GLU:N	3:K:2046:GLU:CD	2.75	0.40
3:K:490:TRP:CH2	3:K:512:LEU:HD21	2.57	0.40
3:L:1323:MET:HE2	3:L:1590:ARG:HE	1.85	0.40
3:L:1924:ILE:O	3:L:1928:GLN:HB2	2.22	0.40
3:L:1966:CYS:C	3:L:1967:ILE:HD13	2.41	0.40
3:L:440:ASN:HD21	3:L:477:GLU:HA	1.86	0.40
1:A:1302:VAL:CG2	1:E:1302:VAL:HG22	2.51	0.40
1:A:1392:LEU:HD22	1:A:1396:MET:HG3	2.02	0.40
1:A:359:ARG:NH1	1:C:1153:ASP:CG	2.75	0.40
1:A:413:LEU:C	1:A:413:LEU:HD13	2.42	0.40
1:B:1392:LEU:HD22	1:B:1396:MET:HG3	2.03	0.40
1:B:1581:THR:HB	1:B:1591:TRP:CZ3	2.56	0.40
1:B:1600:LEU:CD1	1:B:1655:VAL:HG12	2.51	0.40
1:B:1751:GLU:HG3	1:B:1872:SER:HB2	2.04	0.40
1:B:868:ILE:HD11	1:B:923:MET:HE3	2.03	0.40
1:C:1181:PHE:CE2	1:C:1183:ARG:HB2	2.56	0.40
1:C:233:ILE:HG21	1:C:243:ILE:N	2.36	0.40
1:D:20:TYR:CE2	2:J:2033:THR:HG23	2.56	0.40
1:D:499:PRO:HB3	1:D:873:ARG:HD3	2.03	0.40
1:E:499:PRO:HB3	1:E:873:ARG:HD3	2.03	0.40
1:E:965:HIS:CE1	1:E:969:ASN:ND2	2.90	0.40
1:F:1167:LEU:HA	1:F:1167:LEU:HD12	1.94	0.40
1:F:1370:THR:HG22	1:F:1372:THR:H	1.86	0.40
1:F:1395:LYS:HB2	1:F:1395:LYS:HE3	1.93	0.40
1:F:955:LYS:O	1:F:959:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1665:VAL:HA	2:G:1805:ALA:O	2.21	0.40
2:G:249:TYR:CE2	2:G:283:ILE:HD12	2.57	0.40
3:H:1086:LEU:HG	3:H:1092:ASP:HA	2.03	0.40
3:H:1905:ARG:O	3:H:1909:THR:HG23	2.22	0.40
3:H:1954:LYS:HB3	3:H:1955:PRO:HD2	2.03	0.40
3:I:364:LYS:HA	3:I:382:PRO:HG2	2.03	0.40
2:J:1665:VAL:HA	2:J:1805:ALA:O	2.21	0.40
2:J:56:THR:HG21	2:J:112:ASN:HD22	1.86	0.40
3:K:1944:ILE:O	3:K:1948:SER:HB3	2.21	0.40
3:K:29:ILE:O	3:K:33:LEU:HD22	2.22	0.40
3:L:1778:GLN:CB	3:L:1831:VAL:HG13	2.49	0.40
3:L:1859:PRO:O	3:L:1862:VAL:HG13	2.21	0.40
3:L:1967:ILE:N	3:L:1967:ILE:HD13	2.36	0.40
3:L:260:PRO:HB2	3:L:286:THR:HG23	2.03	0.40
3:L:497:LYS:CD	3:L:497:LYS:H	2.35	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1843:ASN:O	1:D:1843:ASN:O[1_655]	1.70	0.50
1:A:1845:ASN:OD1	1:D:1844:LYS:O[1_655]	1.96	0.24

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1752/1887 (93%)	1667 (95%)	77 (4%)	8 (0%)	29	59
1	B	1751/1887 (93%)	1663 (95%)	77 (4%)	11 (1%)	25	54
1	C	1751/1887 (93%)	1661 (95%)	80 (5%)	10 (1%)	25	54
1	D	1757/1887 (93%)	1664 (95%)	81 (5%)	12 (1%)	22	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	1751/1887 (93%)	1667 (95%)	75 (4%)	9 (0%)	29	59
1	F	1751/1887 (93%)	1662 (95%)	79 (4%)	10 (1%)	25	54
2	G	2033/2051 (99%)	1915 (94%)	105 (5%)	13 (1%)	25	54
2	J	2032/2051 (99%)	1914 (94%)	101 (5%)	17 (1%)	19	47
3	H	2031/2051 (99%)	1913 (94%)	105 (5%)	13 (1%)	25	54
3	I	2030/2051 (99%)	1911 (94%)	106 (5%)	13 (1%)	25	54
3	K	2030/2051 (99%)	1909 (94%)	109 (5%)	12 (1%)	25	54
3	L	2032/2051 (99%)	1912 (94%)	107 (5%)	13 (1%)	25	54
All	All	22701/23628 (96%)	21458 (94%)	1102 (5%)	141 (1%)	25	54

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1843	ASN
1	D	539	SER
1	F	1827	SER
2	G	7	ARG
2	G	1869	GLU
2	G	1970	VAL
3	H	7	ARG
3	H	1865	SER
3	H	1970	VAL
3	I	7	ARG
3	I	1865	SER
3	I	1970	VAL
2	J	7	ARG
2	J	1865	SER
2	J	1970	VAL
3	K	7	ARG
3	K	1970	VAL
3	L	7	ARG
3	L	1970	VAL
1	A	874	GLY
1	A	1436	VAL
1	B	874	GLY
1	B	1436	VAL
1	B	1765	SER
1	C	874	GLY
1	C	1436	VAL

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Mol	Chain	Res	Type
1	D	874	GLY
1	D	1436	VAL
1	D	1828	LEU
1	E	874	GLY
1	E	1436	VAL
1	E	1765	SER
1	F	874	GLY
1	F	1436	VAL
1	F	1885	THR
2	G	769	SER
2	G	1092	ASP
2	G	1964	PHE
3	H	769	SER
3	H	1092	ASP
3	H	1964	PHE
3	I	769	SER
3	I	1092	ASP
3	I	1964	PHE
2	J	769	SER
2	J	1092	ASP
2	J	1928	GLN
2	J	1964	PHE
2	J	2049	GLU
3	K	769	SER
3	K	1092	ASP
3	K	1964	PHE
3	L	769	SER
3	L	1092	ASP
3	L	1965	ALA
1	B	517	GLU
1	C	517	GLU
1	C	1765	SER
1	D	517	GLU
1	D	1764	VAL
1	E	517	GLU
1	F	517	GLU
1	F	1764	VAL
1	F	1765	SER
2	G	2016	ALA
3	H	1928	GLN
3	I	1928	GLN
3	I	2016	ALA

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Mol	Chain	Res	Type
2	J	75	SER
2	J	2016	ALA
3	K	1928	GLN
3	L	1928	GLN
1	A	1764	VAL
1	A	1765	SER
1	C	1764	VAL
1	D	1765	SER
1	E	1764	VAL
2	G	203	LEU
2	G	598	THR
3	H	203	LEU
3	H	2016	ALA
3	I	203	LEU
3	I	598	THR
2	J	203	LEU
2	J	598	THR
3	K	203	LEU
3	K	598	THR
3	K	1864	ALA
3	L	598	THR
3	L	2016	ALA
1	C	1608	ASN
1	D	1608	ASN
2	G	508	GLY
2	G	699	GLY
3	H	598	THR
3	I	699	GLY
2	J	508	GLY
3	K	699	GLY
3	L	203	LEU
3	L	508	GLY
3	L	699	GLY
1	A	198	PRO
1	B	1608	ASN
1	E	1608	ASN
2	G	1163	LYS
3	H	699	GLY
3	I	508	GLY
2	J	572	ASN
2	J	877	LYS
2	J	1847	LEU

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Mol	Chain	Res	Type
3	L	572	ASN
1	A	1298	ILE
1	B	299	GLY
1	B	1298	ILE
1	B	1764	VAL
1	B	1863	GLY
1	C	1298	ILE
1	C	1863	GLY
1	D	1298	ILE
1	E	1298	ILE
1	E	1863	GLY
1	F	1298	ILE
3	H	508	GLY
3	K	508	GLY
1	D	198	PRO
1	F	198	PRO
1	A	1863	GLY
1	B	1853	GLY
1	C	198	PRO
1	C	1853	GLY
1	D	1853	GLY
1	E	299	GLY
1	F	1863	GLY
2	J	772	GLY
3	K	772	GLY
3	L	772	GLY
1	A	1543	GLY
1	D	1863	GLY
2	G	772	GLY
3	H	772	GLY
3	I	772	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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1484/1566 (95%)	1310 (88%)	174 (12%)	5	16
1	B	1483/1566 (95%)	1306 (88%)	177 (12%)	5	15
1	C	1483/1566 (95%)	1319 (89%)	164 (11%)	6	18
1	D	1489/1566 (95%)	1315 (88%)	174 (12%)	5	16
1	E	1483/1566 (95%)	1299 (88%)	184 (12%)	4	14
1	F	1483/1566 (95%)	1310 (88%)	173 (12%)	5	16
2	G	1776/1789 (99%)	1553 (87%)	223 (13%)	4	13
2	J	1775/1789 (99%)	1540 (87%)	235 (13%)	4	11
3	H	1774/1788 (99%)	1557 (88%)	217 (12%)	5	14
3	I	1773/1788 (99%)	1529 (86%)	244 (14%)	3	10
3	K	1773/1788 (99%)	1541 (87%)	232 (13%)	4	12
3	L	1775/1788 (99%)	1533 (86%)	242 (14%)	3	11
All	All	19551/20126 (97%)	17112 (88%)	2439 (12%)	4	14

All (2439) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	14	LEU
1	A	15	THR
1	A	24	SER
1	A	27	ARG
1	A	44	VAL
1	A	59	ARG
1	A	60	THR
1	A	62	LYS
1	A	64	LYS
1	A	72	LEU
1	A	83	LYS
1	A	84	ASP
1	A	93	ASP
1	A	140	ILE
1	A	149	LEU
1	A	165	SER
1	A	179	LYS
1	A	181	THR

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Mol	Chain	Res	Type
1	A	192	LYS
1	A	214	GLN
1	A	216	THR
1	A	234	SER
1	A	242	THR
1	A	248	LYS
1	A	258	SER
1	A	261	GLN
1	A	292	GLN
1	A	328	LEU
1	A	331	ILE
1	A	332	THR
1	A	340	ARG
1	A	363	LYS
1	A	367	THR
1	A	378	LEU
1	A	390	VAL
1	A	392	THR
1	A	401	THR
1	A	416	LEU
1	A	421	ILE
1	A	426	LYS
1	A	428	VAL
1	A	432	VAL
1	A	447	LEU
1	A	458	THR
1	A	472	LEU
1	A	489	VAL
1	A	491	LYS
1	A	493	VAL
1	A	495	LYS
1	A	509	ILE
1	A	527	GLN
1	A	607	LYS
1	A	620	SER
1	A	621	THR
1	A	622	ILE
1	A	625	THR
1	A	633	GLU
1	A	644	THR
1	A	650	LYS
1	A	658	LEU

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Mol	Chain	Res	Type
1	A	665	LYS
1	A	674	LYS
1	A	709	ARG
1	A	715	THR
1	A	719	GLN
1	A	731	THR
1	A	732	LEU
1	A	748	LEU
1	A	754	ASP
1	A	761	LEU
1	A	782	GLU
1	A	793	ARG
1	A	824	LEU
1	A	840	SER
1	A	857	SER
1	A	862	LEU
1	A	878	MET
1	A	913	VAL
1	A	915	GLU
1	A	916	LEU
1	A	930	LEU
1	A	933	VAL
1	A	940	THR
1	A	945	LYS
1	A	947	LEU
1	A	953	VAL
1	A	955	LYS
1	A	972	SER
1	A	999	LYS
1	A	1001	VAL
1	A	1002	LYS
1	A	1020	VAL
1	A	1022	THR
1	A	1047	LEU
1	A	1061	SER
1	A	1067	LEU
1	A	1068	LYS
1	A	1073	THR
1	A	1076	VAL
1	A	1086	ASP
1	A	1090	LYS
1	A	1092	LYS

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Mol	Chain	Res	Type
1	A	1123	GLN
1	A	1143	GLN
1	A	1164	SER
1	A	1179	LEU
1	A	1180	ARG
1	A	1184	LEU
1	A	1197	THR
1	A	1208	VAL
1	A	1229	THR
1	A	1238	VAL
1	A	1240	VAL
1	A	1245	ASN
1	A	1271	GLN
1	A	1282	THR
1	A	1283	MET
1	A	1294	SER
1	A	1307	THR
1	A	1325	ARG
1	A	1327	CYS
1	A	1329	VAL
1	A	1332	TYR
1	A	1392	LEU
1	A	1426	LEU
1	A	1436	VAL
1	A	1440	SER
1	A	1443	LEU
1	A	1449	LYS
1	A	1455	ARG
1	A	1460	LYS
1	A	1486	LEU
1	A	1495	ASN
1	A	1501	LEU
1	A	1522	LEU
1	A	1528	THR
1	A	1540	SER
1	A	1547	LYS
1	A	1556	THR
1	A	1575	VAL
1	A	1579	PHE
1	A	1580	LEU
1	A	1583	HIS
1	A	1622	GLU

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Mol	Chain	Res	Type
1	A	1625	LEU
1	A	1631	LEU
1	A	1640	SER
1	A	1642	THR
1	A	1690	ASN
1	A	1706	TYR
1	A	1727	LYS
1	A	1735	SER
1	A	1743	SER
1	A	1756	ILE
1	A	1761	LYS
1	A	1762	GLU
1	A	1766	ASN
1	A	1773	VAL
1	A	1775	LEU
1	A	1776	ILE
1	A	1777	THR
1	A	1778	SER
1	A	1794	GLN
1	A	1808	SER
1	A	1827	SER
1	A	1841	ARG
1	A	1842	VAL
1	A	1851	LEU
1	A	1860	GLU
1	A	1861	GLU
1	A	1864	VAL
1	A	1868	LYS
1	A	1879	VAL
1	B	2	LYS
1	B	5	VAL
1	B	14	LEU
1	B	15	THR
1	B	24	SER
1	B	37	LYS
1	B	44	VAL
1	B	59	ARG
1	B	60	THR
1	B	62	LYS
1	B	64	LYS
1	B	84	ASP
1	B	93	ASP

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Mol	Chain	Res	Type
1	B	140	ILE
1	B	146	LYS
1	B	149	LEU
1	B	192	LYS
1	B	216	THR
1	B	223	LYS
1	B	234	SER
1	B	242	THR
1	B	248	LYS
1	B	261	GLN
1	B	292	GLN
1	B	328	LEU
1	B	331	ILE
1	B	332	THR
1	B	333	LYS
1	B	340	ARG
1	B	351	LYS
1	B	363	LYS
1	B	367	THR
1	B	378	LEU
1	B	390	VAL
1	B	392	THR
1	B	401	THR
1	B	416	LEU
1	B	421	ILE
1	B	426	LYS
1	B	428	VAL
1	B	432	VAL
1	B	447	LEU
1	B	458	THR
1	B	472	LEU
1	B	483	VAL
1	B	489	VAL
1	B	491	LYS
1	B	493	VAL
1	B	495	LYS
1	B	505	LYS
1	B	508	ASN
1	B	509	ILE
1	B	510	THR
1	B	599	MET
1	B	620	SER

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Mol	Chain	Res	Type
1	B	621	THR
1	B	622	ILE
1	B	625	THR
1	B	644	THR
1	B	650	LYS
1	B	665	LYS
1	B	674	LYS
1	B	709	ARG
1	B	715	THR
1	B	719	GLN
1	B	731	THR
1	B	732	LEU
1	B	748	LEU
1	B	754	ASP
1	B	757	LYS
1	B	761	LEU
1	B	776	GLU
1	B	777	GLN
1	B	782	GLU
1	B	793	ARG
1	B	797	THR
1	B	824	LEU
1	B	840	SER
1	B	857	SER
1	B	862	LEU
1	B	878	MET
1	B	894	ARG
1	B	913	VAL
1	B	915	GLU
1	B	916	LEU
1	B	930	LEU
1	B	933	VAL
1	B	940	THR
1	B	945	LYS
1	B	947	LEU
1	B	953	VAL
1	B	955	LYS
1	B	972	SER
1	B	977	TYR
1	B	982	ILE
1	B	1001	VAL
1	B	1002	LYS

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Mol	Chain	Res	Type
1	B	1020	VAL
1	B	1022	THR
1	B	1047	LEU
1	B	1061	SER
1	B	1067	LEU
1	B	1070	ARG
1	B	1073	THR
1	B	1076	VAL
1	B	1079	LYS
1	B	1086	ASP
1	B	1090	LYS
1	B	1123	GLN
1	B	1143	GLN
1	B	1164	SER
1	B	1179	LEU
1	B	1180	ARG
1	B	1184	LEU
1	B	1197	THR
1	B	1208	VAL
1	B	1229	THR
1	B	1238	VAL
1	B	1240	VAL
1	B	1271	GLN
1	B	1282	THR
1	B	1283	MET
1	B	1294	SER
1	B	1307	THR
1	B	1325	ARG
1	B	1327	CYS
1	B	1329	VAL
1	B	1332	TYR
1	B	1392	LEU
1	B	1426	LEU
1	B	1436	VAL
1	B	1440	SER
1	B	1443	LEU
1	B	1449	LYS
1	B	1455	ARG
1	B	1460	LYS
1	B	1486	LEU
1	B	1495	ASN
1	B	1501	LEU

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Mol	Chain	Res	Type
1	B	1522	LEU
1	B	1528	THR
1	B	1540	SER
1	B	1547	LYS
1	B	1556	THR
1	B	1575	VAL
1	B	1578	LYS
1	B	1579	PHE
1	B	1580	LEU
1	B	1583	HIS
1	B	1625	LEU
1	B	1629	LYS
1	B	1640	SER
1	B	1642	THR
1	B	1690	ASN
1	B	1706	TYR
1	B	1727	LYS
1	B	1743	SER
1	B	1756	ILE
1	B	1762	GLU
1	B	1766	ASN
1	B	1773	VAL
1	B	1775	LEU
1	B	1776	ILE
1	B	1777	THR
1	B	1778	SER
1	B	1789	ARG
1	B	1794	GLN
1	B	1808	SER
1	B	1820	PHE
1	B	1827	SER
1	B	1828	LEU
1	B	1842	VAL
1	B	1851	LEU
1	B	1860	GLU
1	B	1861	GLU
1	B	1864	VAL
1	B	1879	VAL
1	C	14	LEU
1	C	15	THR
1	C	24	SER
1	C	37	LYS

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Mol	Chain	Res	Type
1	C	44	VAL
1	C	59	ARG
1	C	60	THR
1	C	62	LYS
1	C	64	LYS
1	C	83	LYS
1	C	84	ASP
1	C	93	ASP
1	C	140	ILE
1	C	149	LEU
1	C	181	THR
1	C	192	LYS
1	C	216	THR
1	C	225	SER
1	C	234	SER
1	C	242	THR
1	C	248	LYS
1	C	258	SER
1	C	261	GLN
1	C	292	GLN
1	C	331	ILE
1	C	332	THR
1	C	364	GLU
1	C	367	THR
1	C	378	LEU
1	C	390	VAL
1	C	392	THR
1	C	401	THR
1	C	416	LEU
1	C	421	ILE
1	C	428	VAL
1	C	432	VAL
1	C	447	LEU
1	C	458	THR
1	C	472	LEU
1	C	489	VAL
1	C	491	LYS
1	C	493	VAL
1	C	495	LYS
1	C	509	ILE
1	C	537	LYS
1	C	607	LYS

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Mol	Chain	Res	Type
1	C	621	THR
1	C	622	ILE
1	C	624	LYS
1	C	625	THR
1	C	632	ARG
1	C	644	THR
1	C	665	LYS
1	C	674	LYS
1	C	702	LYS
1	C	709	ARG
1	C	715	THR
1	C	719	GLN
1	C	731	THR
1	C	732	LEU
1	C	748	LEU
1	C	750	GLU
1	C	754	ASP
1	C	761	LEU
1	C	776	GLU
1	C	777	GLN
1	C	782	GLU
1	C	797	THR
1	C	824	LEU
1	C	840	SER
1	C	857	SER
1	C	862	LEU
1	C	878	MET
1	C	913	VAL
1	C	915	GLU
1	C	916	LEU
1	C	930	LEU
1	C	933	VAL
1	C	938	GLU
1	C	940	THR
1	C	945	LYS
1	C	947	LEU
1	C	953	VAL
1	C	961	THR
1	C	972	SER
1	C	1001	VAL
1	C	1020	VAL
1	C	1022	THR

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Mol	Chain	Res	Type
1	C	1039	MET
1	C	1047	LEU
1	C	1061	SER
1	C	1067	LEU
1	C	1073	THR
1	C	1076	VAL
1	C	1086	ASP
1	C	1090	LYS
1	C	1123	GLN
1	C	1143	GLN
1	C	1151	LYS
1	C	1164	SER
1	C	1179	LEU
1	C	1180	ARG
1	C	1184	LEU
1	C	1197	THR
1	C	1208	VAL
1	C	1229	THR
1	C	1238	VAL
1	C	1240	VAL
1	C	1271	GLN
1	C	1282	THR
1	C	1283	MET
1	C	1307	THR
1	C	1325	ARG
1	C	1327	CYS
1	C	1329	VAL
1	C	1332	TYR
1	C	1376	PHE
1	C	1392	LEU
1	C	1426	LEU
1	C	1436	VAL
1	C	1440	SER
1	C	1443	LEU
1	C	1449	LYS
1	C	1455	ARG
1	C	1486	LEU
1	C	1490	THR
1	C	1495	ASN
1	C	1501	LEU
1	C	1522	LEU
1	C	1528	THR

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Mol	Chain	Res	Type
1	C	1540	SER
1	C	1556	THR
1	C	1575	VAL
1	C	1579	PHE
1	C	1580	LEU
1	C	1583	HIS
1	C	1625	LEU
1	C	1640	SER
1	C	1642	THR
1	C	1690	ASN
1	C	1706	TYR
1	C	1735	SER
1	C	1736	LYS
1	C	1743	SER
1	C	1756	ILE
1	C	1761	LYS
1	C	1762	GLU
1	C	1766	ASN
1	C	1773	VAL
1	C	1775	LEU
1	C	1776	ILE
1	C	1777	THR
1	C	1778	SER
1	C	1788	GLU
1	C	1794	GLN
1	C	1808	SER
1	C	1827	SER
1	C	1841	ARG
1	C	1843	ASN
1	C	1844	LYS
1	C	1851	LEU
1	C	1864	VAL
1	C	1879	VAL
1	C	1886	LYS
1	D	14	LEU
1	D	15	THR
1	D	17	LEU
1	D	24	SER
1	D	27	ARG
1	D	44	VAL
1	D	60	THR
1	D	64	LYS

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Mol	Chain	Res	Type
1	D	83	LYS
1	D	84	ASP
1	D	93	ASP
1	D	140	ILE
1	D	149	LEU
1	D	176	VAL
1	D	181	THR
1	D	192	LYS
1	D	216	THR
1	D	234	SER
1	D	242	THR
1	D	261	GLN
1	D	292	GLN
1	D	328	LEU
1	D	331	ILE
1	D	332	THR
1	D	336	LYS
1	D	340	ARG
1	D	351	LYS
1	D	367	THR
1	D	378	LEU
1	D	390	VAL
1	D	392	THR
1	D	401	THR
1	D	416	LEU
1	D	421	ILE
1	D	428	VAL
1	D	432	VAL
1	D	447	LEU
1	D	458	THR
1	D	472	LEU
1	D	489	VAL
1	D	491	LYS
1	D	493	VAL
1	D	495	LYS
1	D	505	LYS
1	D	509	ILE
1	D	527	GLN
1	D	537	LYS
1	D	538	GLU
1	D	544	GLU
1	D	599	MET

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Mol	Chain	Res	Type
1	D	607	LYS
1	D	611	LYS
1	D	620	SER
1	D	622	ILE
1	D	624	LYS
1	D	625	THR
1	D	644	THR
1	D	674	LYS
1	D	715	THR
1	D	719	GLN
1	D	731	THR
1	D	732	LEU
1	D	748	LEU
1	D	754	ASP
1	D	761	LEU
1	D	776	GLU
1	D	777	GLN
1	D	782	GLU
1	D	793	ARG
1	D	797	THR
1	D	824	LEU
1	D	840	SER
1	D	857	SER
1	D	862	LEU
1	D	878	MET
1	D	913	VAL
1	D	915	GLU
1	D	916	LEU
1	D	930	LEU
1	D	933	VAL
1	D	935	GLU
1	D	938	GLU
1	D	940	THR
1	D	947	LEU
1	D	953	VAL
1	D	955	LYS
1	D	972	SER
1	D	974	ASP
1	D	977	TYR
1	D	982	ILE
1	D	1001	VAL
1	D	1002	LYS

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Mol	Chain	Res	Type
1	D	1020	VAL
1	D	1022	THR
1	D	1047	LEU
1	D	1061	SER
1	D	1067	LEU
1	D	1073	THR
1	D	1076	VAL
1	D	1079	LYS
1	D	1086	ASP
1	D	1090	LYS
1	D	1092	LYS
1	D	1099	GLU
1	D	1123	GLN
1	D	1143	GLN
1	D	1164	SER
1	D	1177	LYS
1	D	1179	LEU
1	D	1180	ARG
1	D	1184	LEU
1	D	1197	THR
1	D	1208	VAL
1	D	1229	THR
1	D	1238	VAL
1	D	1240	VAL
1	D	1271	GLN
1	D	1282	THR
1	D	1283	MET
1	D	1294	SER
1	D	1307	THR
1	D	1325	ARG
1	D	1327	CYS
1	D	1329	VAL
1	D	1332	TYR
1	D	1392	LEU
1	D	1426	LEU
1	D	1436	VAL
1	D	1440	SER
1	D	1443	LEU
1	D	1449	LYS
1	D	1455	ARG
1	D	1486	LEU
1	D	1495	ASN

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Mol	Chain	Res	Type
1	D	1501	LEU
1	D	1522	LEU
1	D	1528	THR
1	D	1540	SER
1	D	1556	THR
1	D	1575	VAL
1	D	1578	LYS
1	D	1579	PHE
1	D	1580	LEU
1	D	1583	HIS
1	D	1625	LEU
1	D	1629	LYS
1	D	1631	LEU
1	D	1640	SER
1	D	1642	THR
1	D	1649	LYS
1	D	1690	ASN
1	D	1706	TYR
1	D	1727	LYS
1	D	1736	LYS
1	D	1743	SER
1	D	1761	LYS
1	D	1762	GLU
1	D	1763	LYS
1	D	1773	VAL
1	D	1775	LEU
1	D	1776	ILE
1	D	1777	THR
1	D	1778	SER
1	D	1808	SER
1	D	1826	LYS
1	D	1827	SER
1	D	1841	ARG
1	D	1844	LYS
1	D	1857	LYS
1	D	1860	GLU
1	D	1861	GLU
1	D	1864	VAL
1	D	1879	VAL
1	D	1886	LYS
1	E	2	LYS
1	E	5	VAL

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Mol	Chain	Res	Type
1	E	14	LEU
1	E	15	THR
1	E	17	LEU
1	E	24	SER
1	E	44	VAL
1	E	59	ARG
1	E	60	THR
1	E	64	LYS
1	E	74	LEU
1	E	82	SER
1	E	83	LYS
1	E	84	ASP
1	E	140	ILE
1	E	149	LEU
1	E	179	LYS
1	E	181	THR
1	E	216	THR
1	E	234	SER
1	E	242	THR
1	E	248	LYS
1	E	261	GLN
1	E	292	GLN
1	E	330	GLU
1	E	331	ILE
1	E	332	THR
1	E	333	LYS
1	E	363	LYS
1	E	367	THR
1	E	378	LEU
1	E	390	VAL
1	E	392	THR
1	E	401	THR
1	E	416	LEU
1	E	421	ILE
1	E	426	LYS
1	E	428	VAL
1	E	432	VAL
1	E	447	LEU
1	E	449	LYS
1	E	458	THR
1	E	472	LEU
1	E	484	LEU

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Mol	Chain	Res	Type
1	E	489	VAL
1	E	491	LYS
1	E	493	VAL
1	E	495	LYS
1	E	509	ILE
1	E	537	LYS
1	E	607	LYS
1	E	620	SER
1	E	621	THR
1	E	622	ILE
1	E	624	LYS
1	E	625	THR
1	E	632	ARG
1	E	644	THR
1	E	665	LYS
1	E	671	VAL
1	E	674	LYS
1	E	702	LYS
1	E	715	THR
1	E	719	GLN
1	E	724	LYS
1	E	731	THR
1	E	732	LEU
1	E	748	LEU
1	E	754	ASP
1	E	761	LEU
1	E	776	GLU
1	E	782	GLU
1	E	793	ARG
1	E	824	LEU
1	E	840	SER
1	E	857	SER
1	E	862	LEU
1	E	878	MET
1	E	913	VAL
1	E	915	GLU
1	E	916	LEU
1	E	930	LEU
1	E	931	GLN
1	E	933	VAL
1	E	938	GLU
1	E	940	THR

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Mol	Chain	Res	Type
1	E	947	LEU
1	E	953	VAL
1	E	961	THR
1	E	967	VAL
1	E	972	SER
1	E	977	TYR
1	E	1001	VAL
1	E	1002	LYS
1	E	1004	ILE
1	E	1020	VAL
1	E	1022	THR
1	E	1047	LEU
1	E	1061	SER
1	E	1067	LEU
1	E	1073	THR
1	E	1076	VAL
1	E	1086	ASP
1	E	1090	LYS
1	E	1092	LYS
1	E	1096	SER
1	E	1123	GLN
1	E	1143	GLN
1	E	1164	SER
1	E	1167	LEU
1	E	1179	LEU
1	E	1184	LEU
1	E	1197	THR
1	E	1208	VAL
1	E	1229	THR
1	E	1238	VAL
1	E	1240	VAL
1	E	1271	GLN
1	E	1282	THR
1	E	1283	MET
1	E	1307	THR
1	E	1325	ARG
1	E	1327	CYS
1	E	1329	VAL
1	E	1332	TYR
1	E	1392	LEU
1	E	1395	LYS
1	E	1411	THR

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Mol	Chain	Res	Type
1	E	1426	LEU
1	E	1436	VAL
1	E	1440	SER
1	E	1443	LEU
1	E	1449	LYS
1	E	1455	ARG
1	E	1486	LEU
1	E	1490	THR
1	E	1492	GLU
1	E	1495	ASN
1	E	1501	LEU
1	E	1522	LEU
1	E	1528	THR
1	E	1540	SER
1	E	1556	THR
1	E	1575	VAL
1	E	1579	PHE
1	E	1580	LEU
1	E	1583	HIS
1	E	1625	LEU
1	E	1629	LYS
1	E	1640	SER
1	E	1642	THR
1	E	1690	ASN
1	E	1706	TYR
1	E	1727	LYS
1	E	1735	SER
1	E	1743	SER
1	E	1750	ILE
1	E	1754	LYS
1	E	1756	ILE
1	E	1761	LYS
1	E	1762	GLU
1	E	1763	LYS
1	E	1766	ASN
1	E	1773	VAL
1	E	1775	LEU
1	E	1776	ILE
1	E	1777	THR
1	E	1778	SER
1	E	1779	ILE
1	E	1787	ILE

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Mol	Chain	Res	Type
1	E	1788	GLU
1	E	1789	ARG
1	E	1794	GLN
1	E	1797	GLU
1	E	1808	SER
1	E	1827	SER
1	E	1828	LEU
1	E	1844	LYS
1	E	1851	LEU
1	E	1857	LYS
1	E	1860	GLU
1	E	1864	VAL
1	E	1868	LYS
1	E	1879	VAL
1	F	8	GLU
1	F	14	LEU
1	F	15	THR
1	F	17	LEU
1	F	24	SER
1	F	44	VAL
1	F	60	THR
1	F	64	LYS
1	F	72	LEU
1	F	84	ASP
1	F	93	ASP
1	F	140	ILE
1	F	149	LEU
1	F	161	LYS
1	F	181	THR
1	F	192	LYS
1	F	196	THR
1	F	200	LYS
1	F	225	SER
1	F	234	SER
1	F	242	THR
1	F	248	LYS
1	F	258	SER
1	F	261	GLN
1	F	292	GLN
1	F	328	LEU
1	F	331	ILE
1	F	332	THR

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Mol	Chain	Res	Type
1	F	351	LYS
1	F	367	THR
1	F	378	LEU
1	F	390	VAL
1	F	392	THR
1	F	401	THR
1	F	416	LEU
1	F	421	ILE
1	F	426	LYS
1	F	428	VAL
1	F	432	VAL
1	F	447	LEU
1	F	458	THR
1	F	472	LEU
1	F	483	VAL
1	F	489	VAL
1	F	491	LYS
1	F	509	ILE
1	F	527	GLN
1	F	537	LYS
1	F	538	GLU
1	F	599	MET
1	F	607	LYS
1	F	620	SER
1	F	621	THR
1	F	622	ILE
1	F	625	THR
1	F	644	THR
1	F	650	LYS
1	F	658	LEU
1	F	665	LYS
1	F	674	LYS
1	F	715	THR
1	F	719	GLN
1	F	731	THR
1	F	732	LEU
1	F	748	LEU
1	F	750	GLU
1	F	754	ASP
1	F	757	LYS
1	F	761	LEU
1	F	776	GLU

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Mol	Chain	Res	Type
1	F	777	GLN
1	F	782	GLU
1	F	793	ARG
1	F	824	LEU
1	F	840	SER
1	F	857	SER
1	F	862	LEU
1	F	878	MET
1	F	913	VAL
1	F	915	GLU
1	F	916	LEU
1	F	930	LEU
1	F	931	GLN
1	F	933	VAL
1	F	938	GLU
1	F	940	THR
1	F	942	LYS
1	F	947	LEU
1	F	953	VAL
1	F	972	SER
1	F	1001	VAL
1	F	1020	VAL
1	F	1022	THR
1	F	1047	LEU
1	F	1061	SER
1	F	1067	LEU
1	F	1073	THR
1	F	1076	VAL
1	F	1079	LYS
1	F	1086	ASP
1	F	1090	LYS
1	F	1092	LYS
1	F	1123	GLN
1	F	1143	GLN
1	F	1164	SER
1	F	1179	LEU
1	F	1180	ARG
1	F	1184	LEU
1	F	1197	THR
1	F	1208	VAL
1	F	1229	THR
1	F	1238	VAL

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Mol	Chain	Res	Type
1	F	1240	VAL
1	F	1264	ARG
1	F	1271	GLN
1	F	1282	THR
1	F	1283	MET
1	F	1307	THR
1	F	1325	ARG
1	F	1327	CYS
1	F	1329	VAL
1	F	1332	TYR
1	F	1392	LEU
1	F	1426	LEU
1	F	1436	VAL
1	F	1440	SER
1	F	1443	LEU
1	F	1449	LYS
1	F	1455	ARG
1	F	1486	LEU
1	F	1495	ASN
1	F	1501	LEU
1	F	1514	LYS
1	F	1522	LEU
1	F	1528	THR
1	F	1540	SER
1	F	1547	LYS
1	F	1556	THR
1	F	1575	VAL
1	F	1578	LYS
1	F	1579	PHE
1	F	1580	LEU
1	F	1583	HIS
1	F	1622	GLU
1	F	1625	LEU
1	F	1640	SER
1	F	1642	THR
1	F	1690	ASN
1	F	1706	TYR
1	F	1727	LYS
1	F	1743	SER
1	F	1754	LYS
1	F	1762	GLU
1	F	1763	LYS

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Mol	Chain	Res	Type
1	F	1773	VAL
1	F	1775	LEU
1	F	1776	ILE
1	F	1777	THR
1	F	1778	SER
1	F	1788	GLU
1	F	1794	GLN
1	F	1808	SER
1	F	1826	LYS
1	F	1827	SER
1	F	1828	LEU
1	F	1841	ARG
1	F	1842	VAL
1	F	1851	LEU
1	F	1857	LYS
1	F	1860	GLU
1	F	1864	VAL
1	F	1879	VAL
1	F	1886	LYS
2	G	6	THR
2	G	9	LEU
2	G	10	THR
2	G	16	LEU
2	G	26	SER
2	G	31	SER
2	G	34	GLN
2	G	55	THR
2	G	56	THR
2	G	60	LEU
2	G	73	GLU
2	G	76	LYS
2	G	79	GLN
2	G	82	GLN
2	G	84	LEU
2	G	86	LEU
2	G	96	LEU
2	G	99	ASN
2	G	111	GLU
2	G	113	ASP
2	G	114	THR
2	G	116	LEU
2	G	119	THR

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Mol	Chain	Res	Type
2	G	122	LEU
2	G	142	ASN
2	G	163	GLN
2	G	167	ASP
2	G	173	LEU
2	G	174	ARG
2	G	175	ASP
2	G	214	ASN
2	G	215	ILE
2	G	236	ILE
2	G	240	LEU
2	G	245	GLN
2	G	246	LEU
2	G	264	ARG
2	G	277	LEU
2	G	279	THR
2	G	286	THR
2	G	295	SER
2	G	301	THR
2	G	303	LEU
2	G	309	ARG
2	G	318	SER
2	G	327	SER
2	G	339	LEU
2	G	340	SER
2	G	347	GLU
2	G	369	SER
2	G	376	ASN
2	G	389	LEU
2	G	397	LYS
2	G	413	LYS
2	G	419	ARG
2	G	425	SER
2	G	429	SER
2	G	431	LEU
2	G	432	LEU
2	G	437	ASP
2	G	438	LEU
2	G	453	LYS
2	G	456	GLN
2	G	462	THR
2	G	471	LEU

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Mol	Chain	Res	Type
2	G	476	SER
2	G	492	THR
2	G	494	THR
2	G	532	THR
2	G	540	ASP
2	G	544	LYS
2	G	562	LEU
2	G	570	ILE
2	G	586	LEU
2	G	611	THR
2	G	616	THR
2	G	650	ASN
2	G	665	LEU
2	G	669	LEU
2	G	670	ARG
2	G	693	GLU
2	G	697	THR
2	G	706	LYS
2	G	730	LEU
2	G	733	THR
2	G	752	GLN
2	G	767	PHE
2	G	777	THR
2	G	805	VAL
2	G	809	LYS
2	G	827	VAL
2	G	838	LYS
2	G	845	THR
2	G	850	MET
2	G	880	LEU
2	G	887	LYS
2	G	906	THR
2	G	914	LEU
2	G	947	THR
2	G	953	ARG
2	G	963	THR
2	G	964	LEU
2	G	972	LEU
2	G	995	LEU
2	G	1012	GLN
2	G	1015	VAL
2	G	1024	ARG

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Mol	Chain	Res	Type
2	G	1040	LEU
2	G	1044	VAL
2	G	1048	VAL
2	G	1072	SER
2	G	1085	LEU
2	G	1100	VAL
2	G	1131	SER
2	G	1133	THR
2	G	1137	SER
2	G	1145	SER
2	G	1157	SER
2	G	1158	PHE
2	G	1163	LYS
2	G	1167	SER
2	G	1172	LYS
2	G	1189	THR
2	G	1191	SER
2	G	1195	VAL
2	G	1197	LEU
2	G	1211	LEU
2	G	1213	LEU
2	G	1228	THR
2	G	1229	MET
2	G	1235	SER
2	G	1236	LEU
2	G	1260	GLN
2	G	1316	ASP
2	G	1317	ARG
2	G	1318	THR
2	G	1320	LEU
2	G	1327	ILE
2	G	1343	VAL
2	G	1348	LEU
2	G	1355	ASN
2	G	1357	TYR
2	G	1360	ILE
2	G	1375	THR
2	G	1378	ILE
2	G	1382	VAL
2	G	1384	GLN
2	G	1386	THR
2	G	1389	ILE

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Mol	Chain	Res	Type
2	G	1395	THR
2	G	1398	ARG
2	G	1408	SER
2	G	1426	THR
2	G	1436	LYS
2	G	1441	ILE
2	G	1446	SER
2	G	1468	THR
2	G	1470	THR
2	G	1472	VAL
2	G	1484	LYS
2	G	1503	ILE
2	G	1526	THR
2	G	1528	GLU
2	G	1533	LEU
2	G	1551	GLU
2	G	1560	LEU
2	G	1590	ARG
2	G	1600	SER
2	G	1603	SER
2	G	1605	VAL
2	G	1609	THR
2	G	1624	THR
2	G	1637	LEU
2	G	1650	VAL
2	G	1651	LEU
2	G	1680	LEU
2	G	1682	LYS
2	G	1693	ARG
2	G	1701	THR
2	G	1718	THR
2	G	1724	GLU
2	G	1748	THR
2	G	1750	LYS
2	G	1751	ILE
2	G	1753	LYS
2	G	1770	LEU
2	G	1781	LEU
2	G	1793	LYS
2	G	1808	SER
2	G	1818	LEU
2	G	1831	VAL

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Mol	Chain	Res	Type
2	G	1838	MET
2	G	1845	ASP
2	G	1846	GLU
2	G	1862	VAL
2	G	1871	LEU
2	G	1884	TRP
2	G	1885	LEU
2	G	1905	ARG
2	G	1914	LEU
2	G	1915	ASN
2	G	1920	GLN
2	G	1923	ASP
2	G	1927	LEU
2	G	1928	GLN
2	G	1930	SER
2	G	1931	LEU
2	G	1932	SER
2	G	1934	GLU
2	G	1935	GLU
2	G	1936	VAL
2	G	1946	GLU
2	G	1950	LYS
2	G	1951	SER
2	G	1956	ARG
2	G	1959	LYS
2	G	1960	LEU
2	G	1969	LEU
2	G	1973	SER
2	G	1979	THR
2	G	2017	LYS
2	G	2032	LEU
2	G	2050	GLN
3	H	5	SER
3	H	6	THR
3	H	9	LEU
3	H	10	THR
3	H	16	LEU
3	H	26	SER
3	H	31	SER
3	H	33	LEU
3	H	34	GLN
3	H	55	THR

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Mol	Chain	Res	Type
3	H	56	THR
3	H	60	LEU
3	H	79	GLN
3	H	84	LEU
3	H	96	LEU
3	H	99	ASN
3	H	113	ASP
3	H	114	THR
3	H	116	LEU
3	H	119	THR
3	H	122	LEU
3	H	134	LYS
3	H	139	LYS
3	H	140	LYS
3	H	141	SER
3	H	142	ASN
3	H	163	GLN
3	H	167	ASP
3	H	173	LEU
3	H	174	ARG
3	H	175	ASP
3	H	178	GLN
3	H	184	VAL
3	H	215	ILE
3	H	236	ILE
3	H	240	LEU
3	H	245	GLN
3	H	246	LEU
3	H	255	LEU
3	H	264	ARG
3	H	277	LEU
3	H	279	THR
3	H	286	THR
3	H	295	SER
3	H	297	ARG
3	H	301	THR
3	H	303	LEU
3	H	318	SER
3	H	327	SER
3	H	339	LEU
3	H	340	SER
3	H	347	GLU

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Mol	Chain	Res	Type
3	H	369	SER
3	H	376	ASN
3	H	389	LEU
3	H	400	SER
3	H	402	LEU
3	H	406	ARG
3	H	419	ARG
3	H	425	SER
3	H	429	SER
3	H	431	LEU
3	H	432	LEU
3	H	453	LYS
3	H	456	GLN
3	H	462	THR
3	H	492	THR
3	H	494	THR
3	H	497	LYS
3	H	532	THR
3	H	540	ASP
3	H	562	LEU
3	H	572	ASN
3	H	586	LEU
3	H	611	THR
3	H	616	THR
3	H	650	ASN
3	H	665	LEU
3	H	669	LEU
3	H	670	ARG
3	H	693	GLU
3	H	697	THR
3	H	701	LYS
3	H	706	LYS
3	H	730	LEU
3	H	733	THR
3	H	752	GLN
3	H	767	PHE
3	H	777	THR
3	H	784	GLU
3	H	805	VAL
3	H	827	VAL
3	H	837	LYS
3	H	845	THR

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Mol	Chain	Res	Type
3	H	852	GLU
3	H	877	LYS
3	H	880	LEU
3	H	887	LYS
3	H	906	THR
3	H	914	LEU
3	H	941	VAL
3	H	947	THR
3	H	953	ARG
3	H	960	LYS
3	H	963	THR
3	H	972	LEU
3	H	995	LEU
3	H	1012	GLN
3	H	1015	VAL
3	H	1040	LEU
3	H	1044	VAL
3	H	1048	VAL
3	H	1049	GLN
3	H	1072	SER
3	H	1085	LEU
3	H	1100	VAL
3	H	1131	SER
3	H	1133	THR
3	H	1137	SER
3	H	1145	SER
3	H	1158	PHE
3	H	1163	LYS
3	H	1167	SER
3	H	1189	THR
3	H	1191	SER
3	H	1195	VAL
3	H	1197	LEU
3	H	1211	LEU
3	H	1213	LEU
3	H	1215	LYS
3	H	1218	ILE
3	H	1228	THR
3	H	1229	MET
3	H	1232	LYS
3	H	1235	SER
3	H	1236	LEU

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Mol	Chain	Res	Type
3	H	1246	ASN
3	H	1260	GLN
3	H	1265	MET
3	H	1316	ASP
3	H	1317	ARG
3	H	1320	LEU
3	H	1327	ILE
3	H	1343	VAL
3	H	1348	LEU
3	H	1355	ASN
3	H	1357	TYR
3	H	1360	ILE
3	H	1375	THR
3	H	1378	ILE
3	H	1382	VAL
3	H	1384	GLN
3	H	1386	THR
3	H	1389	ILE
3	H	1395	THR
3	H	1398	ARG
3	H	1408	SER
3	H	1426	THR
3	H	1441	ILE
3	H	1446	SER
3	H	1468	THR
3	H	1470	THR
3	H	1472	VAL
3	H	1484	LYS
3	H	1503	ILE
3	H	1526	THR
3	H	1533	LEU
3	H	1551	GLU
3	H	1560	LEU
3	H	1578	THR
3	H	1590	ARG
3	H	1593	ILE
3	H	1600	SER
3	H	1605	VAL
3	H	1609	THR
3	H	1616	VAL
3	H	1624	THR
3	H	1637	LEU

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Mol	Chain	Res	Type
3	H	1639	LYS
3	H	1650	VAL
3	H	1651	LEU
3	H	1680	LEU
3	H	1693	ARG
3	H	1701	THR
3	H	1718	THR
3	H	1724	GLU
3	H	1746	LEU
3	H	1770	LEU
3	H	1781	LEU
3	H	1818	LEU
3	H	1831	VAL
3	H	1845	ASP
3	H	1846	GLU
3	H	1847	LEU
3	H	1858	ASN
3	H	1862	VAL
3	H	1871	LEU
3	H	1877	ARG
3	H	1884	TRP
3	H	1885	LEU
3	H	1914	LEU
3	H	1927	LEU
3	H	1930	SER
3	H	1931	LEU
3	H	1932	SER
3	H	1934	GLU
3	H	1936	VAL
3	H	1946	GLU
3	H	1948	SER
3	H	1950	LYS
3	H	1951	SER
3	H	1956	ARG
3	H	1962	ARG
3	H	1973	SER
3	H	1979	THR
3	H	1993	LYS
3	H	2032	LEU
3	I	5	SER
3	I	6	THR
3	I	9	LEU

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Mol	Chain	Res	Type
3	I	10	THR
3	I	12	SER
3	I	16	LEU
3	I	26	SER
3	I	31	SER
3	I	33	LEU
3	I	34	GLN
3	I	46	GLU
3	I	55	THR
3	I	56	THR
3	I	60	LEU
3	I	75	SER
3	I	76	LYS
3	I	79	GLN
3	I	84	LEU
3	I	86	LEU
3	I	96	LEU
3	I	101	ILE
3	I	107	LYS
3	I	113	ASP
3	I	114	THR
3	I	116	LEU
3	I	119	THR
3	I	122	LEU
3	I	134	LYS
3	I	139	LYS
3	I	140	LYS
3	I	163	GLN
3	I	167	ASP
3	I	173	LEU
3	I	174	ARG
3	I	175	ASP
3	I	178	GLN
3	I	184	VAL
3	I	215	ILE
3	I	232	LEU
3	I	236	ILE
3	I	240	LEU
3	I	245	GLN
3	I	246	LEU
3	I	255	LEU
3	I	264	ARG

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Mol	Chain	Res	Type
3	I	277	LEU
3	I	279	THR
3	I	286	THR
3	I	295	SER
3	I	301	THR
3	I	303	LEU
3	I	318	SER
3	I	327	SER
3	I	339	LEU
3	I	340	SER
3	I	347	GLU
3	I	368	ILE
3	I	369	SER
3	I	376	ASN
3	I	389	LEU
3	I	402	LEU
3	I	425	SER
3	I	429	SER
3	I	431	LEU
3	I	432	LEU
3	I	453	LYS
3	I	456	GLN
3	I	462	THR
3	I	471	LEU
3	I	476	SER
3	I	478	ARG
3	I	492	THR
3	I	494	THR
3	I	497	LYS
3	I	532	THR
3	I	538	ASP
3	I	540	ASP
3	I	562	LEU
3	I	572	ASN
3	I	573	LYS
3	I	586	LEU
3	I	601	THR
3	I	611	THR
3	I	616	THR
3	I	650	ASN
3	I	660	GLN
3	I	665	LEU

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Mol	Chain	Res	Type
3	I	669	LEU
3	I	670	ARG
3	I	693	GLU
3	I	697	THR
3	I	701	LYS
3	I	706	LYS
3	I	730	LEU
3	I	733	THR
3	I	752	GLN
3	I	759	ARG
3	I	767	PHE
3	I	777	THR
3	I	784	GLU
3	I	788	LYS
3	I	805	VAL
3	I	825	THR
3	I	827	VAL
3	I	845	THR
3	I	852	GLU
3	I	871	THR
3	I	880	LEU
3	I	906	THR
3	I	914	LEU
3	I	941	VAL
3	I	947	THR
3	I	953	ARG
3	I	963	THR
3	I	964	LEU
3	I	972	LEU
3	I	995	LEU
3	I	1012	GLN
3	I	1015	VAL
3	I	1024	ARG
3	I	1040	LEU
3	I	1044	VAL
3	I	1048	VAL
3	I	1049	GLN
3	I	1064	LYS
3	I	1072	SER
3	I	1085	LEU
3	I	1100	VAL
3	I	1133	THR

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Mol	Chain	Res	Type
3	I	1136	GLU
3	I	1137	SER
3	I	1140	LYS
3	I	1145	SER
3	I	1163	LYS
3	I	1167	SER
3	I	1189	THR
3	I	1195	VAL
3	I	1197	LEU
3	I	1202	GLN
3	I	1211	LEU
3	I	1213	LEU
3	I	1215	LYS
3	I	1228	THR
3	I	1229	MET
3	I	1232	LYS
3	I	1235	SER
3	I	1236	LEU
3	I	1246	ASN
3	I	1260	GLN
3	I	1316	ASP
3	I	1317	ARG
3	I	1318	THR
3	I	1320	LEU
3	I	1327	ILE
3	I	1343	VAL
3	I	1348	LEU
3	I	1355	ASN
3	I	1357	TYR
3	I	1360	ILE
3	I	1375	THR
3	I	1378	ILE
3	I	1382	VAL
3	I	1384	GLN
3	I	1386	THR
3	I	1389	ILE
3	I	1395	THR
3	I	1398	ARG
3	I	1408	SER
3	I	1426	THR
3	I	1441	ILE
3	I	1446	SER

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Mol	Chain	Res	Type
3	I	1468	THR
3	I	1470	THR
3	I	1472	VAL
3	I	1484	LYS
3	I	1503	ILE
3	I	1526	THR
3	I	1533	LEU
3	I	1551	GLU
3	I	1560	LEU
3	I	1590	ARG
3	I	1593	ILE
3	I	1600	SER
3	I	1605	VAL
3	I	1609	THR
3	I	1616	VAL
3	I	1624	THR
3	I	1637	LEU
3	I	1639	LYS
3	I	1650	VAL
3	I	1651	LEU
3	I	1680	LEU
3	I	1682	LYS
3	I	1693	ARG
3	I	1701	THR
3	I	1718	THR
3	I	1724	GLU
3	I	1746	LEU
3	I	1747	LYS
3	I	1753	LYS
3	I	1768	LYS
3	I	1770	LEU
3	I	1781	LEU
3	I	1793	LYS
3	I	1818	LEU
3	I	1824	ILE
3	I	1831	VAL
3	I	1845	ASP
3	I	1846	GLU
3	I	1847	LEU
3	I	1849	ARG
3	I	1858	ASN
3	I	1862	VAL

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Mol	Chain	Res	Type
3	I	1871	LEU
3	I	1877	ARG
3	I	1881	ARG
3	I	1884	TRP
3	I	1885	LEU
3	I	1905	ARG
3	I	1914	LEU
3	I	1915	ASN
3	I	1918	LYS
3	I	1927	LEU
3	I	1929	LYS
3	I	1930	SER
3	I	1931	LEU
3	I	1932	SER
3	I	1933	LEU
3	I	1934	GLU
3	I	1935	GLU
3	I	1936	VAL
3	I	1939	HIS
3	I	1946	GLU
3	I	1948	SER
3	I	1950	LYS
3	I	1951	SER
3	I	1956	ARG
3	I	1960	LEU
3	I	1962	ARG
3	I	1973	SER
3	I	1979	THR
3	I	2024	GLU
3	I	2032	LEU
3	I	2050	GLN
2	J	4	TYR
2	J	5	SER
2	J	6	THR
2	J	7	ARG
2	J	9	LEU
2	J	10	THR
2	J	16	LEU
2	J	26	SER
2	J	31	SER
2	J	33	LEU
2	J	34	GLN

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Mol	Chain	Res	Type
2	J	40	ILE
2	J	55	THR
2	J	56	THR
2	J	60	LEU
2	J	73	GLU
2	J	75	SER
2	J	76	LYS
2	J	84	LEU
2	J	86	LEU
2	J	96	LEU
2	J	99	ASN
2	J	116	LEU
2	J	119	THR
2	J	122	LEU
2	J	124	LYS
2	J	132	MET
2	J	134	LYS
2	J	141	SER
2	J	142	ASN
2	J	163	GLN
2	J	167	ASP
2	J	173	LEU
2	J	174	ARG
2	J	175	ASP
2	J	178	GLN
2	J	215	ILE
2	J	232	LEU
2	J	236	ILE
2	J	240	LEU
2	J	245	GLN
2	J	246	LEU
2	J	255	LEU
2	J	264	ARG
2	J	277	LEU
2	J	279	THR
2	J	286	THR
2	J	295	SER
2	J	301	THR
2	J	303	LEU
2	J	318	SER
2	J	327	SER
2	J	339	LEU

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Mol	Chain	Res	Type
2	J	340	SER
2	J	347	GLU
2	J	369	SER
2	J	376	ASN
2	J	389	LEU
2	J	402	LEU
2	J	419	ARG
2	J	425	SER
2	J	429	SER
2	J	431	LEU
2	J	432	LEU
2	J	453	LYS
2	J	455	ILE
2	J	462	THR
2	J	471	LEU
2	J	476	SER
2	J	478	ARG
2	J	492	THR
2	J	494	THR
2	J	497	LYS
2	J	532	THR
2	J	540	ASP
2	J	562	LEU
2	J	570	ILE
2	J	572	ASN
2	J	586	LEU
2	J	611	THR
2	J	616	THR
2	J	650	ASN
2	J	665	LEU
2	J	669	LEU
2	J	670	ARG
2	J	689	GLU
2	J	693	GLU
2	J	697	THR
2	J	701	LYS
2	J	706	LYS
2	J	730	LEU
2	J	733	THR
2	J	736	ARG
2	J	752	GLN
2	J	759	ARG

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Mol	Chain	Res	Type
2	J	767	PHE
2	J	777	THR
2	J	784	GLU
2	J	805	VAL
2	J	809	LYS
2	J	825	THR
2	J	827	VAL
2	J	831	LYS
2	J	837	LYS
2	J	845	THR
2	J	877	LYS
2	J	880	LEU
2	J	906	THR
2	J	914	LEU
2	J	947	THR
2	J	953	ARG
2	J	963	THR
2	J	964	LEU
2	J	972	LEU
2	J	995	LEU
2	J	1012	GLN
2	J	1015	VAL
2	J	1024	ARG
2	J	1040	LEU
2	J	1044	VAL
2	J	1048	VAL
2	J	1049	GLN
2	J	1072	SER
2	J	1085	LEU
2	J	1100	VAL
2	J	1131	SER
2	J	1133	THR
2	J	1137	SER
2	J	1140	LYS
2	J	1145	SER
2	J	1158	PHE
2	J	1167	SER
2	J	1189	THR
2	J	1191	SER
2	J	1195	VAL
2	J	1197	LEU
2	J	1204	GLU

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Mol	Chain	Res	Type
2	J	1211	LEU
2	J	1213	LEU
2	J	1228	THR
2	J	1229	MET
2	J	1232	LYS
2	J	1235	SER
2	J	1236	LEU
2	J	1246	ASN
2	J	1260	GLN
2	J	1317	ARG
2	J	1318	THR
2	J	1320	LEU
2	J	1327	ILE
2	J	1343	VAL
2	J	1348	LEU
2	J	1355	ASN
2	J	1357	TYR
2	J	1360	ILE
2	J	1375	THR
2	J	1378	ILE
2	J	1382	VAL
2	J	1384	GLN
2	J	1386	THR
2	J	1389	ILE
2	J	1395	THR
2	J	1398	ARG
2	J	1408	SER
2	J	1426	THR
2	J	1441	ILE
2	J	1446	SER
2	J	1468	THR
2	J	1470	THR
2	J	1472	VAL
2	J	1484	LYS
2	J	1503	ILE
2	J	1526	THR
2	J	1528	GLU
2	J	1533	LEU
2	J	1551	GLU
2	J	1555	ARG
2	J	1560	LEU
2	J	1590	ARG

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Mol	Chain	Res	Type
2	J	1600	SER
2	J	1605	VAL
2	J	1609	THR
2	J	1624	THR
2	J	1637	LEU
2	J	1650	VAL
2	J	1651	LEU
2	J	1680	LEU
2	J	1682	LYS
2	J	1693	ARG
2	J	1701	THR
2	J	1718	THR
2	J	1724	GLU
2	J	1745	LYS
2	J	1746	LEU
2	J	1747	LYS
2	J	1757	GLU
2	J	1770	LEU
2	J	1781	LEU
2	J	1793	LYS
2	J	1818	LEU
2	J	1831	VAL
2	J	1845	ASP
2	J	1846	GLU
2	J	1847	LEU
2	J	1858	ASN
2	J	1862	VAL
2	J	1871	LEU
2	J	1877	ARG
2	J	1880	LYS
2	J	1881	ARG
2	J	1884	TRP
2	J	1885	LEU
2	J	1905	ARG
2	J	1914	LEU
2	J	1915	ASN
2	J	1918	LYS
2	J	1927	LEU
2	J	1929	LYS
2	J	1931	LEU
2	J	1932	SER
2	J	1934	GLU

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Mol	Chain	Res	Type
2	J	1935	GLU
2	J	1936	VAL
2	J	1946	GLU
2	J	1950	LYS
2	J	1951	SER
2	J	1956	ARG
2	J	1960	LEU
2	J	1962	ARG
2	J	1973	SER
2	J	1979	THR
2	J	2022	THR
2	J	2032	LEU
2	J	2039	LYS
2	J	2050	GLN
3	K	4	TYR
3	K	6	THR
3	K	9	LEU
3	K	10	THR
3	K	16	LEU
3	K	26	SER
3	K	31	SER
3	K	33	LEU
3	K	34	GLN
3	K	39	LYS
3	K	55	THR
3	K	56	THR
3	K	60	LEU
3	K	79	GLN
3	K	84	LEU
3	K	86	LEU
3	K	99	ASN
3	K	107	LYS
3	K	110	GLN
3	K	111	GLU
3	K	113	ASP
3	K	114	THR
3	K	116	LEU
3	K	119	THR
3	K	122	LEU
3	K	134	LYS
3	K	142	ASN
3	K	163	GLN

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Mol	Chain	Res	Type
3	K	167	ASP
3	K	173	LEU
3	K	174	ARG
3	K	175	ASP
3	K	178	GLN
3	K	184	VAL
3	K	215	ILE
3	K	236	ILE
3	K	240	LEU
3	K	245	GLN
3	K	246	LEU
3	K	255	LEU
3	K	264	ARG
3	K	277	LEU
3	K	279	THR
3	K	286	THR
3	K	295	SER
3	K	297	ARG
3	K	301	THR
3	K	303	LEU
3	K	318	SER
3	K	327	SER
3	K	339	LEU
3	K	340	SER
3	K	347	GLU
3	K	368	ILE
3	K	369	SER
3	K	376	ASN
3	K	389	LEU
3	K	397	LYS
3	K	402	LEU
3	K	425	SER
3	K	429	SER
3	K	431	LEU
3	K	432	LEU
3	K	453	LYS
3	K	456	GLN
3	K	462	THR
3	K	471	LEU
3	K	476	SER
3	K	492	THR
3	K	494	THR

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Mol	Chain	Res	Type
3	K	499	THR
3	K	540	ASP
3	K	562	LEU
3	K	572	ASN
3	K	586	LEU
3	K	611	THR
3	K	616	THR
3	K	650	ASN
3	K	665	LEU
3	K	669	LEU
3	K	670	ARG
3	K	693	GLU
3	K	697	THR
3	K	701	LYS
3	K	706	LYS
3	K	721	LYS
3	K	730	LEU
3	K	733	THR
3	K	752	GLN
3	K	757	ILE
3	K	767	PHE
3	K	777	THR
3	K	784	GLU
3	K	805	VAL
3	K	819	LYS
3	K	825	THR
3	K	827	VAL
3	K	831	LYS
3	K	838	LYS
3	K	845	THR
3	K	850	MET
3	K	852	GLU
3	K	880	LEU
3	K	906	THR
3	K	914	LEU
3	K	947	THR
3	K	953	ARG
3	K	962	LYS
3	K	963	THR
3	K	972	LEU
3	K	995	LEU
3	K	1012	GLN

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Mol	Chain	Res	Type
3	K	1015	VAL
3	K	1024	ARG
3	K	1040	LEU
3	K	1044	VAL
3	K	1048	VAL
3	K	1049	GLN
3	K	1072	SER
3	K	1085	LEU
3	K	1100	VAL
3	K	1131	SER
3	K	1133	THR
3	K	1137	SER
3	K	1140	LYS
3	K	1145	SER
3	K	1158	PHE
3	K	1163	LYS
3	K	1167	SER
3	K	1175	LYS
3	K	1189	THR
3	K	1195	VAL
3	K	1197	LEU
3	K	1211	LEU
3	K	1213	LEU
3	K	1215	LYS
3	K	1228	THR
3	K	1229	MET
3	K	1235	SER
3	K	1236	LEU
3	K	1246	ASN
3	K	1260	GLN
3	K	1286	LYS
3	K	1316	ASP
3	K	1317	ARG
3	K	1318	THR
3	K	1320	LEU
3	K	1327	ILE
3	K	1343	VAL
3	K	1348	LEU
3	K	1355	ASN
3	K	1357	TYR
3	K	1360	ILE
3	K	1375	THR

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Mol	Chain	Res	Type
3	K	1378	ILE
3	K	1382	VAL
3	K	1384	GLN
3	K	1386	THR
3	K	1389	ILE
3	K	1395	THR
3	K	1398	ARG
3	K	1408	SER
3	K	1426	THR
3	K	1441	ILE
3	K	1445	ARG
3	K	1446	SER
3	K	1455	GLU
3	K	1468	THR
3	K	1470	THR
3	K	1472	VAL
3	K	1503	ILE
3	K	1526	THR
3	K	1533	LEU
3	K	1551	GLU
3	K	1560	LEU
3	K	1578	THR
3	K	1590	ARG
3	K	1600	SER
3	K	1605	VAL
3	K	1609	THR
3	K	1616	VAL
3	K	1624	THR
3	K	1637	LEU
3	K	1650	VAL
3	K	1651	LEU
3	K	1680	LEU
3	K	1682	LYS
3	K	1693	ARG
3	K	1701	THR
3	K	1718	THR
3	K	1724	GLU
3	K	1741	ILE
3	K	1770	LEU
3	K	1775	GLN
3	K	1781	LEU
3	K	1818	LEU

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Mol	Chain	Res	Type
3	K	1831	VAL
3	K	1845	ASP
3	K	1846	GLU
3	K	1847	LEU
3	K	1858	ASN
3	K	1862	VAL
3	K	1871	LEU
3	K	1877	ARG
3	K	1881	ARG
3	K	1884	TRP
3	K	1885	LEU
3	K	1904	LEU
3	K	1914	LEU
3	K	1918	LYS
3	K	1921	LYS
3	K	1923	ASP
3	K	1926	GLU
3	K	1927	LEU
3	K	1929	LYS
3	K	1931	LEU
3	K	1932	SER
3	K	1934	GLU
3	K	1936	VAL
3	K	1946	GLU
3	K	1948	SER
3	K	1949	LYS
3	K	1950	LYS
3	K	1951	SER
3	K	1953	VAL
3	K	1956	ARG
3	K	1960	LEU
3	K	1962	ARG
3	K	1979	THR
3	K	2032	LEU
3	K	2041	ILE
3	K	2050	GLN
3	L	4	TYR
3	L	5	SER
3	L	6	THR
3	L	9	LEU
3	L	10	THR
3	L	12	SER

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Mol	Chain	Res	Type
3	L	16	LEU
3	L	26	SER
3	L	31	SER
3	L	34	GLN
3	L	46	GLU
3	L	55	THR
3	L	56	THR
3	L	60	LEU
3	L	76	LYS
3	L	82	GLN
3	L	84	LEU
3	L	86	LEU
3	L	96	LEU
3	L	99	ASN
3	L	113	ASP
3	L	114	THR
3	L	116	LEU
3	L	119	THR
3	L	122	LEU
3	L	132	MET
3	L	134	LYS
3	L	139	LYS
3	L	140	LYS
3	L	141	SER
3	L	142	ASN
3	L	156	LEU
3	L	163	GLN
3	L	167	ASP
3	L	173	LEU
3	L	174	ARG
3	L	175	ASP
3	L	178	GLN
3	L	215	ILE
3	L	236	ILE
3	L	240	LEU
3	L	245	GLN
3	L	246	LEU
3	L	255	LEU
3	L	264	ARG
3	L	277	LEU
3	L	279	THR
3	L	286	THR

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Mol	Chain	Res	Type
3	L	295	SER
3	L	301	THR
3	L	303	LEU
3	L	318	SER
3	L	327	SER
3	L	339	LEU
3	L	340	SER
3	L	347	GLU
3	L	355	LYS
3	L	369	SER
3	L	376	ASN
3	L	389	LEU
3	L	413	LYS
3	L	423	VAL
3	L	425	SER
3	L	429	SER
3	L	431	LEU
3	L	432	LEU
3	L	437	ASP
3	L	444	VAL
3	L	453	LYS
3	L	462	THR
3	L	471	LEU
3	L	476	SER
3	L	478	ARG
3	L	492	THR
3	L	494	THR
3	L	497	LYS
3	L	532	THR
3	L	540	ASP
3	L	562	LEU
3	L	570	ILE
3	L	572	ASN
3	L	573	LYS
3	L	586	LEU
3	L	611	THR
3	L	616	THR
3	L	650	ASN
3	L	665	LEU
3	L	669	LEU
3	L	670	ARG
3	L	693	GLU

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Mol	Chain	Res	Type
3	L	697	THR
3	L	706	LYS
3	L	721	LYS
3	L	730	LEU
3	L	733	THR
3	L	752	GLN
3	L	756	LYS
3	L	767	PHE
3	L	777	THR
3	L	784	GLU
3	L	805	VAL
3	L	825	THR
3	L	827	VAL
3	L	845	THR
3	L	850	MET
3	L	877	LYS
3	L	880	LEU
3	L	906	THR
3	L	914	LEU
3	L	947	THR
3	L	953	ARG
3	L	960	LYS
3	L	963	THR
3	L	995	LEU
3	L	1012	GLN
3	L	1015	VAL
3	L	1024	ARG
3	L	1040	LEU
3	L	1048	VAL
3	L	1049	GLN
3	L	1072	SER
3	L	1085	LEU
3	L	1100	VAL
3	L	1106	GLU
3	L	1131	SER
3	L	1133	THR
3	L	1137	SER
3	L	1140	LYS
3	L	1145	SER
3	L	1157	SER
3	L	1158	PHE
3	L	1175	LYS

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Mol	Chain	Res	Type
3	L	1189	THR
3	L	1195	VAL
3	L	1197	LEU
3	L	1211	LEU
3	L	1213	LEU
3	L	1228	THR
3	L	1229	MET
3	L	1235	SER
3	L	1236	LEU
3	L	1246	ASN
3	L	1260	GLN
3	L	1265	MET
3	L	1286	LYS
3	L	1288	LYS
3	L	1316	ASP
3	L	1317	ARG
3	L	1318	THR
3	L	1320	LEU
3	L	1327	ILE
3	L	1343	VAL
3	L	1348	LEU
3	L	1355	ASN
3	L	1357	TYR
3	L	1360	ILE
3	L	1375	THR
3	L	1378	ILE
3	L	1382	VAL
3	L	1384	GLN
3	L	1386	THR
3	L	1395	THR
3	L	1398	ARG
3	L	1408	SER
3	L	1421	ASN
3	L	1426	THR
3	L	1441	ILE
3	L	1445	ARG
3	L	1446	SER
3	L	1468	THR
3	L	1470	THR
3	L	1472	VAL
3	L	1484	LYS
3	L	1503	ILE

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Mol	Chain	Res	Type
3	L	1525	SER
3	L	1526	THR
3	L	1528	GLU
3	L	1533	LEU
3	L	1551	GLU
3	L	1560	LEU
3	L	1590	ARG
3	L	1600	SER
3	L	1603	SER
3	L	1605	VAL
3	L	1609	THR
3	L	1623	LYS
3	L	1624	THR
3	L	1637	LEU
3	L	1650	VAL
3	L	1651	LEU
3	L	1680	LEU
3	L	1682	LYS
3	L	1693	ARG
3	L	1701	THR
3	L	1718	THR
3	L	1724	GLU
3	L	1745	LYS
3	L	1751	ILE
3	L	1768	LYS
3	L	1770	LEU
3	L	1781	LEU
3	L	1793	LYS
3	L	1818	LEU
3	L	1831	VAL
3	L	1845	ASP
3	L	1846	GLU
3	L	1847	LEU
3	L	1849	ARG
3	L	1858	ASN
3	L	1862	VAL
3	L	1871	LEU
3	L	1872	GLN
3	L	1880	LYS
3	L	1884	TRP
3	L	1885	LEU
3	L	1888	ILE

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Mol	Chain	Res	Type
3	L	1894	GLU
3	L	1914	LEU
3	L	1915	ASN
3	L	1923	ASP
3	L	1927	LEU
3	L	1929	LYS
3	L	1930	SER
3	L	1931	LEU
3	L	1932	SER
3	L	1934	GLU
3	L	1935	GLU
3	L	1936	VAL
3	L	1944	ILE
3	L	1946	GLU
3	L	1948	SER
3	L	1950	LYS
3	L	1951	SER
3	L	1956	ARG
3	L	1960	LEU
3	L	1967	ILE
3	L	1973	SER
3	L	1979	THR
3	L	2023	LYS
3	L	2032	LEU
3	L	2039	LYS
3	L	2050	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (458) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	32	GLN
1	A	292	GLN
1	A	335	HIS
1	A	344	GLN
1	A	411	GLN
1	A	422	HIS
1	A	438	ASN
1	A	506	ASN
1	A	719	GLN
1	A	738	ASN
1	A	743	GLN

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Mol	Chain	Res	Type
1	A	792	HIS
1	A	829	ASN
1	A	851	ASN
1	A	965	HIS
1	A	969	ASN
1	A	987	ASN
1	A	989	GLN
1	A	1000	GLN
1	A	1003	GLN
1	A	1064	ASN
1	A	1066	ASN
1	A	1123	GLN
1	A	1146	HIS
1	A	1239	HIS
1	A	1245	ASN
1	A	1272	ASN
1	A	1432	HIS
1	A	1433	HIS
1	A	1442	ASN
1	A	1444	ASN
1	A	1483	ASN
1	A	1494	HIS
1	A	1507	GLN
1	A	1510	ASN
1	A	1610	ASN
1	A	1657	HIS
1	A	1690	ASN
1	A	1748	ASN
1	B	11	HIS
1	B	32	GLN
1	B	261	GLN
1	B	335	HIS
1	B	344	GLN
1	B	411	GLN
1	B	422	HIS
1	B	438	ASN
1	B	506	ASN
1	B	508	ASN
1	B	719	GLN
1	B	738	ASN
1	B	792	HIS
1	B	829	ASN

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Mol	Chain	Res	Type
1	B	851	ASN
1	B	965	HIS
1	B	969	ASN
1	B	1000	GLN
1	B	1064	ASN
1	B	1066	ASN
1	B	1123	GLN
1	B	1146	HIS
1	B	1239	HIS
1	B	1272	ASN
1	B	1380	GLN
1	B	1432	HIS
1	B	1442	ASN
1	B	1444	ASN
1	B	1483	ASN
1	B	1494	HIS
1	B	1507	GLN
1	B	1510	ASN
1	B	1610	ASN
1	B	1690	ASN
1	B	1748	ASN
1	B	1780	ASN
1	B	1852	HIS
1	C	11	HIS
1	C	32	GLN
1	C	261	GLN
1	C	335	HIS
1	C	344	GLN
1	C	411	GLN
1	C	438	ASN
1	C	506	ASN
1	C	719	GLN
1	C	738	ASN
1	C	743	GLN
1	C	792	HIS
1	C	829	ASN
1	C	851	ASN
1	C	965	HIS
1	C	969	ASN
1	C	1000	GLN
1	C	1066	ASN
1	C	1123	GLN

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Mol	Chain	Res	Type
1	C	1146	HIS
1	C	1239	HIS
1	C	1272	ASN
1	C	1432	HIS
1	C	1433	HIS
1	C	1442	ASN
1	C	1444	ASN
1	C	1482	GLN
1	C	1483	ASN
1	C	1494	HIS
1	C	1507	GLN
1	C	1510	ASN
1	C	1577	GLN
1	C	1610	ASN
1	C	1690	ASN
1	C	1766	ASN
1	D	32	GLN
1	D	261	GLN
1	D	335	HIS
1	D	342	GLN
1	D	344	GLN
1	D	411	GLN
1	D	438	ASN
1	D	694	GLN
1	D	698	GLN
1	D	719	GLN
1	D	738	ASN
1	D	783	HIS
1	D	792	HIS
1	D	829	ASN
1	D	851	ASN
1	D	965	HIS
1	D	969	ASN
1	D	979	GLN
1	D	1000	GLN
1	D	1064	ASN
1	D	1066	ASN
1	D	1146	HIS
1	D	1239	HIS
1	D	1432	HIS
1	D	1433	HIS
1	D	1442	ASN

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Mol	Chain	Res	Type
1	D	1444	ASN
1	D	1483	ASN
1	D	1494	HIS
1	D	1507	GLN
1	D	1510	ASN
1	D	1610	ASN
1	D	1690	ASN
1	D	1748	ASN
1	D	1794	GLN
1	D	1852	HIS
1	E	32	GLN
1	E	261	GLN
1	E	335	HIS
1	E	342	GLN
1	E	344	GLN
1	E	411	GLN
1	E	422	HIS
1	E	438	ASN
1	E	506	ASN
1	E	719	GLN
1	E	738	ASN
1	E	792	HIS
1	E	829	ASN
1	E	851	ASN
1	E	965	HIS
1	E	969	ASN
1	E	987	ASN
1	E	989	GLN
1	E	1064	ASN
1	E	1066	ASN
1	E	1123	GLN
1	E	1146	HIS
1	E	1239	HIS
1	E	1272	ASN
1	E	1380	GLN
1	E	1432	HIS
1	E	1433	HIS
1	E	1442	ASN
1	E	1483	ASN
1	E	1494	HIS
1	E	1507	GLN
1	E	1510	ASN

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Mol	Chain	Res	Type
1	E	1610	ASN
1	E	1690	ASN
1	E	1748	ASN
1	E	1780	ASN
1	E	1852	HIS
1	F	32	GLN
1	F	261	GLN
1	F	335	HIS
1	F	344	GLN
1	F	411	GLN
1	F	422	HIS
1	F	438	ASN
1	F	506	ASN
1	F	527	GLN
1	F	719	GLN
1	F	738	ASN
1	F	743	GLN
1	F	792	HIS
1	F	829	ASN
1	F	851	ASN
1	F	965	HIS
1	F	969	ASN
1	F	1000	GLN
1	F	1064	ASN
1	F	1066	ASN
1	F	1123	GLN
1	F	1146	HIS
1	F	1239	HIS
1	F	1432	HIS
1	F	1433	HIS
1	F	1442	ASN
1	F	1444	ASN
1	F	1483	ASN
1	F	1494	HIS
1	F	1507	GLN
1	F	1510	ASN
1	F	1610	ASN
1	F	1690	ASN
1	F	1748	ASN
1	F	1780	ASN
1	F	1794	GLN
1	F	1852	HIS

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Mol	Chain	Res	Type
2	G	79	GLN
2	G	99	ASN
2	G	102	HIS
2	G	214	ASN
2	G	354	ASN
2	G	376	ASN
2	G	404	GLN
2	G	440	ASN
2	G	500	HIS
2	G	553	ASN
2	G	558	ASN
2	G	612	ASN
2	G	650	ASN
2	G	718	ASN
2	G	747	HIS
2	G	936	ASN
2	G	993	GLN
2	G	998	GLN
2	G	1049	GLN
2	G	1055	HIS
2	G	1178	GLN
2	G	1217	ASN
2	G	1220	GLN
2	G	1355	ASN
2	G	1383	ASN
2	G	1421	ASN
2	G	1512	HIS
2	G	1595	ASN
2	G	1619	ASN
2	G	1697	HIS
2	G	1712	ASN
2	G	1872	GLN
2	G	1890	ASN
2	G	1915	ASN
2	G	1928	GLN
2	G	2020	GLN
3	H	79	GLN
3	H	99	ASN
3	H	102	HIS
3	H	178	GLN
3	H	354	ASN
3	H	359	HIS

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Mol	Chain	Res	Type
3	H	376	ASN
3	H	404	GLN
3	H	440	ASN
3	H	500	HIS
3	H	517	HIS
3	H	553	ASN
3	H	558	ASN
3	H	572	ASN
3	H	612	ASN
3	H	718	ASN
3	H	747	HIS
3	H	936	ASN
3	H	998	GLN
3	H	1049	GLN
3	H	1055	HIS
3	H	1178	GLN
3	H	1217	ASN
3	H	1220	GLN
3	H	1246	ASN
3	H	1355	ASN
3	H	1367	GLN
3	H	1383	ASN
3	H	1421	ASN
3	H	1512	HIS
3	H	1595	ASN
3	H	1619	ASN
3	H	1697	HIS
3	H	1712	ASN
3	H	1858	ASN
3	H	1890	ASN
3	H	1896	GLN
3	H	2020	GLN
3	I	82	GLN
3	I	102	HIS
3	I	354	ASN
3	I	376	ASN
3	I	404	GLN
3	I	440	ASN
3	I	500	HIS
3	I	517	HIS
3	I	553	ASN
3	I	558	ASN

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Mol	Chain	Res	Type
3	I	572	ASN
3	I	612	ASN
3	I	650	ASN
3	I	718	ASN
3	I	747	HIS
3	I	936	ASN
3	I	998	GLN
3	I	1049	GLN
3	I	1055	HIS
3	I	1178	GLN
3	I	1217	ASN
3	I	1220	GLN
3	I	1246	ASN
3	I	1355	ASN
3	I	1383	ASN
3	I	1421	ASN
3	I	1512	HIS
3	I	1595	ASN
3	I	1619	ASN
3	I	1697	HIS
3	I	1712	ASN
3	I	1858	ASN
3	I	1890	ASN
3	I	1896	GLN
3	I	1915	ASN
3	I	1928	GLN
3	I	2013	ASN
3	I	2020	GLN
2	J	34	GLN
2	J	82	GLN
2	J	99	ASN
2	J	102	HIS
2	J	346	GLN
2	J	354	ASN
2	J	359	HIS
2	J	376	ASN
2	J	404	GLN
2	J	440	ASN
2	J	500	HIS
2	J	517	HIS
2	J	553	ASN
2	J	558	ASN

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Mol	Chain	Res	Type
2	J	572	ASN
2	J	612	ASN
2	J	650	ASN
2	J	718	ASN
2	J	747	HIS
2	J	936	ASN
2	J	998	GLN
2	J	1049	GLN
2	J	1055	HIS
2	J	1178	GLN
2	J	1217	ASN
2	J	1220	GLN
2	J	1246	ASN
2	J	1355	ASN
2	J	1383	ASN
2	J	1421	ASN
2	J	1512	HIS
2	J	1595	ASN
2	J	1619	ASN
2	J	1697	HIS
2	J	1712	ASN
2	J	1858	ASN
2	J	1890	ASN
2	J	1896	GLN
2	J	1915	ASN
2	J	2013	ASN
2	J	2020	GLN
2	J	2050	GLN
3	K	82	GLN
3	K	99	ASN
3	K	102	HIS
3	K	112	ASN
3	K	178	GLN
3	K	354	ASN
3	K	359	HIS
3	K	376	ASN
3	K	404	GLN
3	K	440	ASN
3	K	451	ASN
3	K	500	HIS
3	K	517	HIS
3	K	553	ASN

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Mol	Chain	Res	Type
3	K	558	ASN
3	K	572	ASN
3	K	612	ASN
3	K	650	ASN
3	K	718	ASN
3	K	747	HIS
3	K	834	GLN
3	K	936	ASN
3	K	993	GLN
3	K	998	GLN
3	K	1049	GLN
3	K	1055	HIS
3	K	1178	GLN
3	K	1217	ASN
3	K	1220	GLN
3	K	1246	ASN
3	K	1355	ASN
3	K	1383	ASN
3	K	1421	ASN
3	K	1595	ASN
3	K	1619	ASN
3	K	1697	HIS
3	K	1712	ASN
3	K	1775	GLN
3	K	1858	ASN
3	K	1890	ASN
3	K	1896	GLN
3	K	2020	GLN
3	L	79	GLN
3	L	99	ASN
3	L	102	HIS
3	L	354	ASN
3	L	359	HIS
3	L	376	ASN
3	L	404	GLN
3	L	440	ASN
3	L	451	ASN
3	L	500	HIS
3	L	517	HIS
3	L	553	ASN
3	L	558	ASN
3	L	572	ASN

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Mol	Chain	Res	Type
3	L	612	ASN
3	L	650	ASN
3	L	718	ASN
3	L	747	HIS
3	L	936	ASN
3	L	998	GLN
3	L	1049	GLN
3	L	1055	HIS
3	L	1178	GLN
3	L	1217	ASN
3	L	1220	GLN
3	L	1246	ASN
3	L	1355	ASN
3	L	1383	ASN
3	L	1421	ASN
3	L	1595	ASN
3	L	1619	ASN
3	L	1697	HIS
3	L	1712	ASN
3	L	1851	ASN
3	L	1858	ASN
3	L	1872	GLN
3	L	1890	ASN
3	L	1915	ASN
3	L	2013	ASN
3	L	2020	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
3	J8W	I	1808	3	7,11,12	2.22	1 (14%)	5,13,15	2.47	2 (40%)
3	J8W	L	1808	3	7,11,12	2.04	1 (14%)	5,13,15	2.63	2 (40%)
3	J8W	H	1808	3	7,11,12	1.95	1 (14%)	5,13,15	2.27	2 (40%)
3	J8W	K	1808	3	7,11,12	2.11	1 (14%)	5,13,15	2.55	2 (40%)

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
3	J8W	I	1808	3	-	4/7/11/13	-
3	J8W	L	1808	3	-	4/7/11/13	-
3	J8W	H	1808	3	-	4/7/11/13	-
3	J8W	K	1808	3	-	4/7/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1808	J8W	OG-C2	5.59	1.49	1.33
3	K	1808	J8W	OG-C2	5.35	1.49	1.33
3	L	1808	J8W	OG-C2	5.16	1.48	1.33
3	H	1808	J8W	OG-C2	4.94	1.47	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1808	J8W	OG-C2-C1	4.29	118.34	111.07
3	K	1808	J8W	OG-C2-C1	3.85	117.60	111.07
3	I	1808	J8W	OG-C2-C1	3.80	117.52	111.07
3	H	1808	J8W	CB-OG-C2	3.78	131.14	117.12
3	K	1808	J8W	CB-OG-C2	3.75	131.00	117.12
3	I	1808	J8W	CB-OG-C2	3.56	130.29	117.12
3	L	1808	J8W	CB-OG-C2	3.46	129.93	117.12
3	H	1808	J8W	OG-C2-C1	2.96	116.09	111.07

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1808	J8W	N-CA-CB-OG
3	I	1808	J8W	C-CA-CB-OG
3	L	1808	J8W	N-CA-CB-OG
3	L	1808	J8W	C-CA-CB-OG
3	H	1808	J8W	N-CA-CB-OG
3	H	1808	J8W	C-CA-CB-OG
3	K	1808	J8W	N-CA-CB-OG
3	K	1808	J8W	C-CA-CB-OG
3	I	1808	J8W	O7-C2-OG-CB
3	L	1808	J8W	O7-C2-OG-CB
3	H	1808	J8W	O7-C2-OG-CB
3	K	1808	J8W	O7-C2-OG-CB
3	I	1808	J8W	C1-C2-OG-CB
3	L	1808	J8W	C1-C2-OG-CB
3	H	1808	J8W	C1-C2-OG-CB
3	K	1808	J8W	C1-C2-OG-CB

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1808	J8W	1	0
3	L	1808	J8W	1	0
3	H	1808	J8W	1	0
3	K	1808	J8W	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 133 ligands modelled in this entry, 39 are monoatomic - leaving 94 for Mogul analysis.

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
9	PGE	E	1918	-	9,9,9	0.23	0	8,8,8	0.16	0
7	A2P	D	1923	-	25,29,29	0.71	0	31,45,45	0.85	1 (3%)
5	EDO	E	1909	-	3,3,3	0.17	0	2,2,2	0.41	0
5	EDO	F	1905	-	3,3,3	0.19	0	2,2,2	0.41	0
10	FMN	H	2101	-	31,33,33	2.26	4 (12%)	40,50,50	2.36	10 (25%)
8	ACT	B	1902	-	1,3,3	5.32	1 (100%)	0,3,3	0.00	-
10	FMN	J	2101	-	31,33,33	2.24	5 (16%)	40,50,50	2.34	10 (25%)
7	A2P	A	1918	-	25,29,29	0.65	0	31,45,45	0.70	0
5	EDO	B	1909	-	3,3,3	0.30	0	2,2,2	0.45	0
5	EDO	C	1909	-	3,3,3	0.22	0	2,2,2	0.41	0
5	EDO	B	1905	-	3,3,3	0.07	0	2,2,2	0.25	0
10	FMN	L	2101	-	31,33,33	2.23	6 (19%)	40,50,50	2.30	11 (27%)
5	EDO	B	1908	-	3,3,3	0.13	0	2,2,2	0.29	0
5	EDO	J	2106	-	3,3,3	0.07	0	2,2,2	0.35	0
10	FMN	K	2101	-	31,33,33	2.50	7 (22%)	40,50,50	2.67	11 (27%)
5	EDO	A	1911	-	3,3,3	0.19	0	2,2,2	0.45	0
5	EDO	C	1911	-	3,3,3	0.43	0	2,2,2	0.50	0
8	ACT	C	1902	-	1,3,3	3.82	1 (100%)	0,3,3	0.00	-
5	EDO	B	1903	-	3,3,3	0.10	0	2,2,2	0.18	0
8	ACT	H	2103	-	1,3,3	5.12	1 (100%)	0,3,3	0.00	-
5	EDO	A	1904	-	3,3,3	0.13	0	2,2,2	0.29	0
5	EDO	J	2105	-	3,3,3	0.08	0	2,2,2	0.17	0
5	EDO	E	1908	-	3,3,3	0.10	0	2,2,2	0.29	0
5	EDO	B	1907	-	3,3,3	0.15	0	2,2,2	0.25	0
5	EDO	D	1913	-	3,3,3	0.13	0	2,2,2	0.07	0
5	EDO	C	1904	-	3,3,3	0.15	0	2,2,2	0.36	0
5	EDO	C	1910	-	3,3,3	0.11	0	2,2,2	0.23	0
5	EDO	A	1906	-	3,3,3	0.05	0	2,2,2	0.12	0
5	EDO	C	1906	-	3,3,3	0.32	0	2,2,2	0.57	0
4	PNS	B	1901	1	13,20,21	0.61	0	18,26,29	1.23	2 (11%)
5	EDO	B	1904	-	3,3,3	0.12	0	2,2,2	0.16	0
5	EDO	E	1907	-	3,3,3	0.13	0	2,2,2	0.28	0
8	ACT	C	1903	-	1,3,3	3.55	1 (100%)	0,3,3	0.00	-
5	EDO	E	1913	-	3,3,3	0.16	0	2,2,2	0.34	0
5	EDO	A	1903	-	3,3,3	0.27	0	2,2,2	0.48	0
5	EDO	D	1905	-	3,3,3	0.11	0	2,2,2	0.13	0
5	EDO	A	1907	-	3,3,3	0.20	0	2,2,2	0.31	0
4	PNS	E	1901	1	13,20,21	0.64	0	18,26,29	1.21	1 (5%)
5	EDO	B	1911	-	3,3,3	0.18	0	2,2,2	0.39	0
5	EDO	D	1910	-	3,3,3	0.13	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	D	1903	-	3,3,3	0.32	0	2,2,2	0.51	0
5	EDO	F	1908	-	3,3,3	0.09	0	2,2,2	0.23	0
5	EDO	F	1903	-	3,3,3	0.10	0	2,2,2	0.20	0
8	ACT	H	2102	-	1,3,3	4.95	1 (100%)	0,3,3	0.00	-
5	EDO	B	1912	-	3,3,3	0.11	0	2,2,2	0.22	0
5	EDO	E	1910	-	3,3,3	0.15	0	2,2,2	0.36	0
5	EDO	E	1902	-	3,3,3	0.09	0	2,2,2	0.23	0
5	EDO	F	1902	-	3,3,3	0.09	0	2,2,2	0.13	0
5	EDO	J	2103	-	3,3,3	0.08	0	2,2,2	0.14	0
7	A2P	F	1912	-	25,29,29	0.69	0	31,45,45	0.75	1 (3%)
5	EDO	D	1912	-	3,3,3	0.11	0	2,2,2	0.23	0
5	EDO	D	1911	-	3,3,3	0.19	0	2,2,2	0.32	0
5	EDO	B	1906	-	3,3,3	0.16	0	2,2,2	0.49	0
5	EDO	E	1905	-	3,3,3	0.12	0	2,2,2	0.36	0
5	EDO	D	1914	-	3,3,3	0.24	0	2,2,2	0.45	0
5	EDO	C	1908	-	3,3,3	0.29	0	2,2,2	0.55	0
7	A2P	C	1917	-	25,29,29	0.73	0	31,45,45	0.80	1 (3%)
4	PNS	F	1901	1	13,20,21	0.86	0	18,26,29	2.65	7 (38%)
5	EDO	F	1907	-	3,3,3	0.13	0	2,2,2	0.33	0
5	EDO	C	1912	-	3,3,3	0.29	0	2,2,2	0.64	0
5	EDO	B	1910	-	3,3,3	0.15	0	2,2,2	0.33	0
5	EDO	D	1904	-	3,3,3	0.11	0	2,2,2	0.29	0
5	EDO	J	2104	-	3,3,3	0.10	0	2,2,2	0.34	0
5	EDO	E	1912	-	3,3,3	0.09	0	2,2,2	0.14	0
5	EDO	A	1908	-	3,3,3	0.10	0	2,2,2	0.28	0
4	PNS	C	1901	1	13,20,21	0.61	0	18,26,29	1.15	1 (5%)
4	PNS	A	1901	1	13,20,21	0.68	0	18,26,29	1.03	1 (5%)
5	EDO	C	1905	-	3,3,3	0.18	0	2,2,2	0.39	0
5	EDO	F	1904	-	3,3,3	0.31	0	2,2,2	0.49	0
5	EDO	E	1904	-	3,3,3	0.07	0	2,2,2	0.20	0
5	EDO	E	1906	-	3,3,3	0.05	0	2,2,2	0.10	0
5	EDO	A	1910	-	3,3,3	0.37	0	2,2,2	0.63	0
5	EDO	D	1907	-	3,3,3	0.13	0	2,2,2	0.32	0
5	EDO	D	1902	-	3,3,3	0.17	0	2,2,2	0.49	0
10	FMN	G	2101	-	31,33,33	2.17	6 (19%)	40,50,50	2.35	13 (32%)
11	MLI	G	2102	-	0,6,6	0.00	-	0,7,7	0.00	-
5	EDO	H	2105	-	3,3,3	0.11	0	2,2,2	0.18	0
5	EDO	A	1902	-	3,3,3	0.18	0	2,2,2	0.41	0
5	EDO	E	1903	-	3,3,3	0.13	0	2,2,2	0.24	0
4	PNS	D	1901	1	13,20,21	0.60	0	18,26,29	1.08	1 (5%)
5	EDO	D	1908	-	3,3,3	0.10	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	D	1909	-	3,3,3	0.28	0	2,2,2	0.64	0
5	EDO	C	1907	-	3,3,3	0.10	0	2,2,2	0.21	0
5	EDO	E	1911	-	3,3,3	0.19	0	2,2,2	0.41	0
11	MLI	J	2102	-	0,6,6	0.00	-	0,7,7	0.00	-
5	EDO	D	1906	-	3,3,3	0.43	0	2,2,2	0.65	0
8	ACT	H	2104	-	1,3,3	4.79	1 (100%)	0,3,3	0.00	-
5	EDO	A	1905	-	3,3,3	0.29	0	2,2,2	0.48	0
5	EDO	A	1909	-	3,3,3	0.32	0	2,2,2	0.51	0
5	EDO	F	1909	-	3,3,3	0.23	0	2,2,2	0.52	0
7	A2P	E	1917	-	25,29,29	0.68	0	31,45,45	0.81	1 (3%)
10	FMN	I	2101	-	31,33,33	2.08	5 (16%)	40,50,50	2.32	10 (25%)
5	EDO	F	1906	-	3,3,3	0.23	0	2,2,2	0.38	0
7	A2P	B	1918	-	25,29,29	0.70	0	31,45,45	0.96	1 (3%)

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
9	PGE	E	1918	-	-	3/7/7/7	-
7	A2P	D	1923	-	-	4/11/31/31	0/3/3/3
5	EDO	E	1909	-	-	1/1/1/1	-
5	EDO	F	1905	-	-	1/1/1/1	-
10	FMN	H	2101	-	-	2/18/18/18	0/3/3/3
10	FMN	J	2101	-	-	5/18/18/18	0/3/3/3
7	A2P	A	1918	-	-	5/11/31/31	0/3/3/3
5	EDO	B	1909	-	-	0/1/1/1	-
5	EDO	C	1909	-	-	1/1/1/1	-
5	EDO	B	1905	-	-	0/1/1/1	-
10	FMN	L	2101	-	-	3/18/18/18	0/3/3/3
5	EDO	B	1908	-	-	0/1/1/1	-
5	EDO	J	2106	-	-	1/1/1/1	-
10	FMN	K	2101	-	-	3/18/18/18	0/3/3/3
5	EDO	A	1911	-	-	1/1/1/1	-
5	EDO	C	1911	-	-	1/1/1/1	-
5	EDO	B	1903	-	-	1/1/1/1	-
5	EDO	A	1904	-	-	0/1/1/1	-
5	EDO	J	2105	-	-	0/1/1/1	-
5	EDO	E	1908	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	1907	-	-	0/1/1/1	-
5	EDO	D	1913	-	-	0/1/1/1	-
5	EDO	C	1904	-	-	1/1/1/1	-
5	EDO	C	1910	-	-	1/1/1/1	-
5	EDO	A	1906	-	-	1/1/1/1	-
5	EDO	C	1906	-	-	1/1/1/1	-
4	PNS	B	1901	1	-	1/24/26/27	-
5	EDO	B	1904	-	-	1/1/1/1	-
5	EDO	E	1907	-	-	1/1/1/1	-
5	EDO	E	1913	-	-	1/1/1/1	-
5	EDO	A	1903	-	-	1/1/1/1	-
5	EDO	D	1905	-	-	1/1/1/1	-
5	EDO	A	1907	-	-	1/1/1/1	-
4	PNS	E	1901	1	-	1/24/26/27	-
5	EDO	B	1911	-	-	1/1/1/1	-
5	EDO	D	1910	-	-	0/1/1/1	-
5	EDO	D	1903	-	-	1/1/1/1	-
5	EDO	F	1908	-	-	0/1/1/1	-
5	EDO	F	1903	-	-	0/1/1/1	-
5	EDO	B	1912	-	-	1/1/1/1	-
5	EDO	E	1910	-	-	0/1/1/1	-
5	EDO	E	1902	-	-	0/1/1/1	-
5	EDO	F	1902	-	-	0/1/1/1	-
5	EDO	J	2103	-	-	0/1/1/1	-
7	A2P	F	1912	-	-	9/11/31/31	0/3/3/3
5	EDO	D	1912	-	-	1/1/1/1	-
5	EDO	D	1911	-	-	1/1/1/1	-
5	EDO	B	1906	-	-	0/1/1/1	-
5	EDO	E	1905	-	-	1/1/1/1	-
5	EDO	D	1914	-	-	1/1/1/1	-
5	EDO	C	1908	-	-	1/1/1/1	-
7	A2P	C	1917	-	-	6/11/31/31	0/3/3/3
4	PNS	F	1901	1	-	3/24/26/27	-
5	EDO	F	1907	-	-	0/1/1/1	-
5	EDO	C	1912	-	-	1/1/1/1	-
5	EDO	B	1910	-	-	1/1/1/1	-
5	EDO	D	1904	-	-	1/1/1/1	-
5	EDO	J	2104	-	-	0/1/1/1	-
5	EDO	E	1912	-	-	0/1/1/1	-
5	EDO	A	1908	-	-	1/1/1/1	-
4	PNS	C	1901	1	-	1/24/26/27	-
4	PNS	A	1901	1	-	1/24/26/27	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	1905	-	-	1/1/1/1	-
5	EDO	F	1904	-	-	0/1/1/1	-
5	EDO	E	1904	-	-	0/1/1/1	-
5	EDO	E	1906	-	-	1/1/1/1	-
5	EDO	A	1910	-	-	1/1/1/1	-
5	EDO	D	1907	-	-	1/1/1/1	-
5	EDO	D	1902	-	-	1/1/1/1	-
10	FMN	G	2101	-	-	5/18/18/18	0/3/3/3
11	MLI	G	2102	-	-	0/0/4/4	-
5	EDO	H	2105	-	-	1/1/1/1	-
5	EDO	A	1902	-	-	1/1/1/1	-
5	EDO	E	1903	-	-	1/1/1/1	-
4	PNS	D	1901	1	-	0/24/26/27	-
5	EDO	D	1908	-	-	1/1/1/1	-
5	EDO	D	1909	-	-	1/1/1/1	-
5	EDO	C	1907	-	-	1/1/1/1	-
5	EDO	E	1911	-	-	1/1/1/1	-
11	MLI	J	2102	-	-	0/0/4/4	-
5	EDO	D	1906	-	-	1/1/1/1	-
5	EDO	A	1905	-	-	1/1/1/1	-
5	EDO	A	1909	-	-	0/1/1/1	-
5	EDO	F	1909	-	-	0/1/1/1	-
7	A2P	E	1917	-	-	6/11/31/31	0/3/3/3
10	FMN	I	2101	-	-	6/18/18/18	0/3/3/3
5	EDO	F	1906	-	-	1/1/1/1	-
7	A2P	B	1918	-	-	5/11/31/31	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	2101	FMN	C4A-C10	10.44	1.49	1.38
10	J	2101	FMN	C4A-C10	9.83	1.48	1.38
10	H	2101	FMN	C4A-C10	9.82	1.48	1.38
10	L	2101	FMN	C4A-C10	9.62	1.48	1.38
10	G	2101	FMN	C4A-C10	9.13	1.47	1.38
10	I	2101	FMN	C4A-C10	8.38	1.47	1.38
10	K	2101	FMN	C4-C4A	5.41	1.50	1.41
8	B	1902	ACT	CH3-C	5.32	1.55	1.48
8	H	2103	ACT	CH3-C	5.12	1.55	1.48
8	H	2102	ACT	CH3-C	4.95	1.55	1.48
10	G	2101	FMN	C4-C4A	4.82	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	2104	ACT	CH3-C	4.79	1.54	1.48
10	J	2101	FMN	C4-C4A	4.42	1.49	1.41
10	I	2101	FMN	C4-C4A	4.33	1.48	1.41
10	H	2101	FMN	C4-C4A	4.12	1.48	1.41
10	L	2101	FMN	C4-C4A	3.91	1.48	1.41
8	C	1902	ACT	CH3-C	3.82	1.53	1.48
10	I	2101	FMN	C8-C7	3.62	1.49	1.40
10	K	2101	FMN	C9A-C5A	3.60	1.49	1.42
10	L	2101	FMN	C9A-C5A	3.56	1.49	1.42
8	C	1903	ACT	CH3-C	3.55	1.53	1.48
10	H	2101	FMN	C9A-C5A	3.44	1.49	1.42
10	I	2101	FMN	C9A-C5A	3.36	1.49	1.42
10	K	2101	FMN	C8-C7	3.22	1.48	1.40
10	L	2101	FMN	C8-C7	3.20	1.48	1.40
10	G	2101	FMN	C9A-C5A	3.17	1.48	1.42
10	J	2101	FMN	C9A-C5A	3.10	1.48	1.42
10	G	2101	FMN	C8-C7	2.86	1.48	1.40
10	H	2101	FMN	C8-C7	2.80	1.47	1.40
10	J	2101	FMN	C8-C7	2.78	1.47	1.40
10	G	2101	FMN	C6-C5A	-2.48	1.38	1.41
10	K	2101	FMN	C9A-N10	2.38	1.41	1.38
10	I	2101	FMN	C9A-N10	2.38	1.41	1.38
10	J	2101	FMN	C6-C5A	-2.26	1.38	1.41
10	L	2101	FMN	C9A-N10	2.23	1.41	1.38
10	L	2101	FMN	C6-C5A	-2.23	1.38	1.41
10	K	2101	FMN	C2-N1	-2.21	1.33	1.38
10	G	2101	FMN	C2-N1	-2.15	1.33	1.38
10	K	2101	FMN	C6-C5A	-2.09	1.38	1.41

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	2101	FMN	C4-N3-C2	9.37	123.05	115.14
10	J	2101	FMN	C4-N3-C2	9.37	123.05	115.14
10	H	2101	FMN	C4-N3-C2	9.21	122.92	115.14
10	L	2101	FMN	C4-N3-C2	8.65	122.45	115.14
10	G	2101	FMN	C4-N3-C2	8.52	122.34	115.14
10	I	2101	FMN	C4-N3-C2	8.05	121.94	115.14
10	K	2101	FMN	C1'-N10-C9A	6.38	123.32	118.29
4	F	1901	PNS	C38-C39-N41	6.24	126.93	116.42
10	J	2101	FMN	C4A-C4-N3	-5.87	115.40	123.43
10	K	2101	FMN	C4A-C4-N3	-5.58	115.80	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1901	PNS	C43-C42-N41	-5.51	99.72	112.31
10	G	2101	FMN	C4A-C4-N3	-5.26	116.24	123.43
10	I	2101	FMN	C4A-N5-C5A	5.17	121.94	116.77
10	I	2101	FMN	C1'-N10-C9A	5.13	122.33	118.29
10	H	2101	FMN	C4-C4A-C10	-5.03	116.62	119.95
10	L	2101	FMN	C4A-C4-N3	-4.92	116.70	123.43
10	K	2101	FMN	C4-C4A-C10	-4.87	116.73	119.95
10	K	2101	FMN	C4-C4A-N5	4.72	123.99	118.60
10	H	2101	FMN	C4A-C4-N3	-4.63	117.09	123.43
10	I	2101	FMN	C4A-C4-N3	-4.49	117.29	123.43
10	L	2101	FMN	O3P-P-O5'	-4.37	95.10	106.73
10	H	2101	FMN	C4-C4A-N5	4.35	123.57	118.60
10	J	2101	FMN	C4A-N5-C5A	4.30	121.07	116.77
10	H	2101	FMN	C1'-N10-C9A	4.26	121.65	118.29
4	F	1901	PNS	O40-C39-N41	-4.18	115.12	123.01
10	K	2101	FMN	C4A-N5-C5A	4.16	120.93	116.77
10	G	2101	FMN	C1'-N10-C10	4.01	122.00	118.41
10	H	2101	FMN	C4A-N5-C5A	3.97	120.74	116.77
10	I	2101	FMN	C4-C4A-N5	3.89	123.04	118.60
10	G	2101	FMN	C4A-N5-C5A	3.89	120.66	116.77
10	L	2101	FMN	C1'-N10-C9A	3.81	121.29	118.29
10	G	2101	FMN	C4-C4A-N5	3.68	122.80	118.60
10	L	2101	FMN	C4A-N5-C5A	3.52	120.28	116.77
10	I	2101	FMN	C4-C4A-C10	-3.49	117.64	119.95
10	J	2101	FMN	C1'-N10-C9A	3.39	120.96	118.29
4	F	1901	PNS	C42-N41-C39	3.38	129.12	122.84
10	L	2101	FMN	C4-C4A-C10	-3.30	117.76	119.95
10	G	2101	FMN	C9A-N10-C10	-3.28	117.61	121.91
10	J	2101	FMN	C4-C4A-N5	3.19	122.24	118.60
4	F	1901	PNS	C31-C29-C32	3.07	114.15	108.82
4	B	1901	PNS	C31-C29-C32	3.03	114.08	108.82
10	L	2101	FMN	C9A-N10-C10	-3.02	117.95	121.91
10	G	2101	FMN	C4-C4A-C10	-2.99	117.97	119.95
10	G	2101	FMN	C10-C4A-N5	-2.94	119.22	121.26
4	E	1901	PNS	C31-C29-C32	2.91	113.87	108.82
4	C	1901	PNS	C31-C29-C32	2.90	113.85	108.82
10	K	2101	FMN	C10-C4A-N5	-2.86	119.28	121.26
10	I	2101	FMN	C10-C4A-N5	-2.80	119.32	121.26
10	L	2101	FMN	C4-C4A-N5	2.79	121.79	118.60
10	J	2101	FMN	C9A-N10-C10	-2.75	118.30	121.91
7	B	1918	A2P	C5-C6-N6	2.74	124.52	120.35
4	A	1901	PNS	C31-C29-C32	2.73	113.56	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1901	PNS	C31-C29-C32	2.71	113.52	108.82
10	K	2101	FMN	C9A-N10-C10	-2.69	118.38	121.91
10	K	2101	FMN	O5'-P-O1P	-2.68	98.97	106.47
4	F	1901	PNS	C37-C38-C39	-2.67	107.91	112.36
10	J	2101	FMN	C10-C4A-N5	-2.66	119.42	121.26
10	I	2101	FMN	C9A-N10-C10	-2.65	118.43	121.91
10	G	2101	FMN	C1'-N10-C9A	2.62	120.36	118.29
10	L	2101	FMN	C1'-N10-C10	2.61	120.75	118.41
10	L	2101	FMN	P-O5'-C5'	2.60	125.45	118.30
10	H	2101	FMN	O3P-P-O5'	-2.55	99.96	106.73
10	K	2101	FMN	O3'-C3'-C4'	2.53	114.93	108.81
10	K	2101	FMN	O2'-C2'-C1'	2.52	115.67	109.59
10	H	2101	FMN	C9A-N10-C10	-2.49	118.65	121.91
10	J	2101	FMN	C1'-N10-C10	2.46	120.61	118.41
10	J	2101	FMN	C4-C4A-C10	-2.44	118.33	119.95
10	G	2101	FMN	O3P-P-O5'	-2.32	100.55	106.73
10	G	2101	FMN	O4'-C4'-C3'	2.32	114.75	109.10
10	I	2101	FMN	O5'-P-O1P	-2.32	99.97	106.47
10	G	2101	FMN	C5'-C4'-C3'	-2.31	107.75	112.20
7	D	1923	A2P	C5-C6-N6	2.30	123.85	120.35
10	G	2101	FMN	O3P-P-O2P	2.24	116.21	107.64
7	E	1917	A2P	C5-C6-N6	2.23	123.75	120.35
4	F	1901	PNS	O40-C39-C38	-2.23	117.94	122.02
7	F	1912	A2P	C5-C6-N6	2.21	123.70	120.35
10	J	2101	FMN	O2P-P-O5'	-2.12	101.09	106.73
10	L	2101	FMN	O2P-P-O5'	2.12	112.36	106.73
10	H	2101	FMN	C10-C4A-N5	-2.10	119.80	121.26
4	B	1901	PNS	C43-C42-N41	2.04	116.96	112.31
10	I	2101	FMN	O4'-C4'-C5'	-2.02	105.37	109.92
7	C	1917	A2P	C5-C6-N6	2.01	123.40	120.35
10	H	2101	FMN	C5'-C4'-C3'	-2.01	108.33	112.20

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1918	A2P	C5'-O5'-P2-O4P
7	A	1918	A2P	C5'-O5'-P2-O6P
7	D	1923	A2P	C5'-O5'-P2-O5P
7	D	1923	A2P	C5'-O5'-P2-O6P
10	L	2101	FMN	C3'-C4'-C5'-O5'
10	L	2101	FMN	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
10	L	2101	FMN	C4'-C5'-O5'-P
7	F	1912	A2P	C5'-O5'-P2-O5P
7	F	1912	A2P	O4'-C4'-C5'-O5'
7	F	1912	A2P	C1'-C2'-O2'-P1
7	C	1917	A2P	C2'-O2'-P1-O3P
7	C	1917	A2P	C5'-O5'-P2-O4P
7	C	1917	A2P	C5'-O5'-P2-O5P
7	C	1917	A2P	C5'-O5'-P2-O6P
4	F	1901	PNS	C38-C39-N41-C42
4	F	1901	PNS	O40-C39-N41-C42
5	A	1910	EDO	O1-C1-C2-O2
7	B	1918	A2P	C5'-O5'-P2-O5P
7	B	1918	A2P	C5'-O5'-P2-O6P
7	B	1918	A2P	O4'-C4'-C5'-O5'
7	A	1918	A2P	O4'-C4'-C5'-O5'
7	B	1918	A2P	C3'-C4'-C5'-O5'
7	C	1917	A2P	C1'-C2'-O2'-P1
7	E	1917	A2P	C1'-C2'-O2'-P1
7	F	1912	A2P	C3'-C4'-C5'-O5'
7	E	1917	A2P	O4'-C4'-C5'-O5'
7	E	1917	A2P	C3'-C4'-C5'-O5'
5	A	1906	EDO	O1-C1-C2-O2
9	E	1918	PGE	O2-C3-C4-O3
7	A	1918	A2P	C3'-C4'-C5'-O5'
9	E	1918	PGE	O3-C5-C6-O4
7	F	1912	A2P	C3'-C2'-O2'-P1
10	K	2101	FMN	O2'-C2'-C3'-C4'
5	E	1909	EDO	O1-C1-C2-O2
5	J	2106	EDO	O1-C1-C2-O2
5	C	1911	EDO	O1-C1-C2-O2
5	E	1908	EDO	O1-C1-C2-O2
5	C	1904	EDO	O1-C1-C2-O2
5	C	1906	EDO	O1-C1-C2-O2
5	A	1903	EDO	O1-C1-C2-O2
5	A	1907	EDO	O1-C1-C2-O2
5	D	1903	EDO	O1-C1-C2-O2
5	C	1908	EDO	O1-C1-C2-O2
5	D	1912	EDO	O1-C1-C2-O2
5	D	1911	EDO	O1-C1-C2-O2
5	D	1914	EDO	O1-C1-C2-O2
5	B	1910	EDO	O1-C1-C2-O2
5	D	1904	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	1908	EDO	O1-C1-C2-O2
5	D	1909	EDO	O1-C1-C2-O2
10	J	2101	FMN	C2'-C3'-C4'-O4'
7	D	1923	A2P	C5'-O5'-P2-O4P
7	B	1918	A2P	C5'-O5'-P2-O4P
5	B	1912	EDO	O1-C1-C2-O2
5	F	1906	EDO	O1-C1-C2-O2
10	I	2101	FMN	O2'-C2'-C3'-C4'
10	K	2101	FMN	C4'-C5'-O5'-P
5	B	1904	EDO	O1-C1-C2-O2
5	E	1907	EDO	O1-C1-C2-O2
5	E	1905	EDO	O1-C1-C2-O2
5	D	1906	EDO	O1-C1-C2-O2
10	I	2101	FMN	C2'-C3'-C4'-C5'
7	A	1918	A2P	C5'-O5'-P2-O5P
7	F	1912	A2P	C5'-O5'-P2-O6P
7	E	1917	A2P	C2'-O2'-P1-O1P
10	G	2101	FMN	C2'-C3'-C4'-O4'
10	H	2101	FMN	C4'-C5'-O5'-P
10	G	2101	FMN	C4'-C5'-O5'-P
7	E	1917	A2P	C4'-C5'-O5'-P2
9	E	1918	PGE	C3-C4-O3-C5
10	J	2101	FMN	C4'-C5'-O5'-P
5	F	1905	EDO	O1-C1-C2-O2
5	C	1909	EDO	O1-C1-C2-O2
5	B	1903	EDO	O1-C1-C2-O2
5	A	1905	EDO	O1-C1-C2-O2
5	D	1908	EDO	O1-C1-C2-O2
10	I	2101	FMN	C4'-C5'-O5'-P
7	F	1912	A2P	C5'-O5'-P2-O4P
5	C	1910	EDO	O1-C1-C2-O2
5	C	1912	EDO	O1-C1-C2-O2
5	C	1905	EDO	O1-C1-C2-O2
5	A	1902	EDO	O1-C1-C2-O2
5	E	1911	EDO	O1-C1-C2-O2
10	I	2101	FMN	C2'-C3'-C4'-O4'
10	K	2101	FMN	O2'-C2'-C3'-O3'
10	J	2101	FMN	C2'-C3'-C4'-C5'
5	B	1911	EDO	O1-C1-C2-O2
5	E	1906	EDO	O1-C1-C2-O2
10	I	2101	FMN	O3'-C3'-C4'-C5'
10	G	2101	FMN	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
7	C	1917	A2P	O4'-C4'-C5'-O5'
5	D	1905	EDO	O1-C1-C2-O2
5	E	1903	EDO	O1-C1-C2-O2
5	C	1907	EDO	O1-C1-C2-O2
4	B	1901	PNS	O33-C32-C34-O35
4	E	1901	PNS	O33-C32-C34-O35
4	F	1901	PNS	O33-C32-C34-O35
4	C	1901	PNS	O33-C32-C34-O35
4	A	1901	PNS	O33-C32-C34-O35
7	F	1912	A2P	C2'-O2'-P1-O1P
7	E	1917	A2P	C3'-C2'-O2'-P1
10	I	2101	FMN	O2'-C2'-C3'-O3'
5	E	1913	EDO	O1-C1-C2-O2
5	D	1902	EDO	O1-C1-C2-O2
5	H	2105	EDO	O1-C1-C2-O2
7	F	1912	A2P	C2'-O2'-P1-O3P
10	J	2101	FMN	O3'-C3'-C4'-O4'
10	J	2101	FMN	O3'-C3'-C4'-C5'
10	G	2101	FMN	O3'-C3'-C4'-C5'
7	D	1923	A2P	O4'-C4'-C5'-O5'
10	G	2101	FMN	O3'-C3'-C4'-O4'
5	A	1911	EDO	O1-C1-C2-O2
5	D	1907	EDO	O1-C1-C2-O2
10	H	2101	FMN	O3'-C3'-C4'-C5'

There are no ring outliers.

25 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1923	A2P	3	0
10	H	2101	FMN	4	0
8	B	1902	ACT	1	0
10	J	2101	FMN	7	0
7	A	1918	A2P	3	0
10	L	2101	FMN	5	0
10	K	2101	FMN	5	0
5	J	2105	EDO	1	0
4	B	1901	PNS	1	0
8	C	1903	ACT	2	0
5	D	1910	EDO	1	0
7	F	1912	A2P	1	0
5	B	1906	EDO	3	0

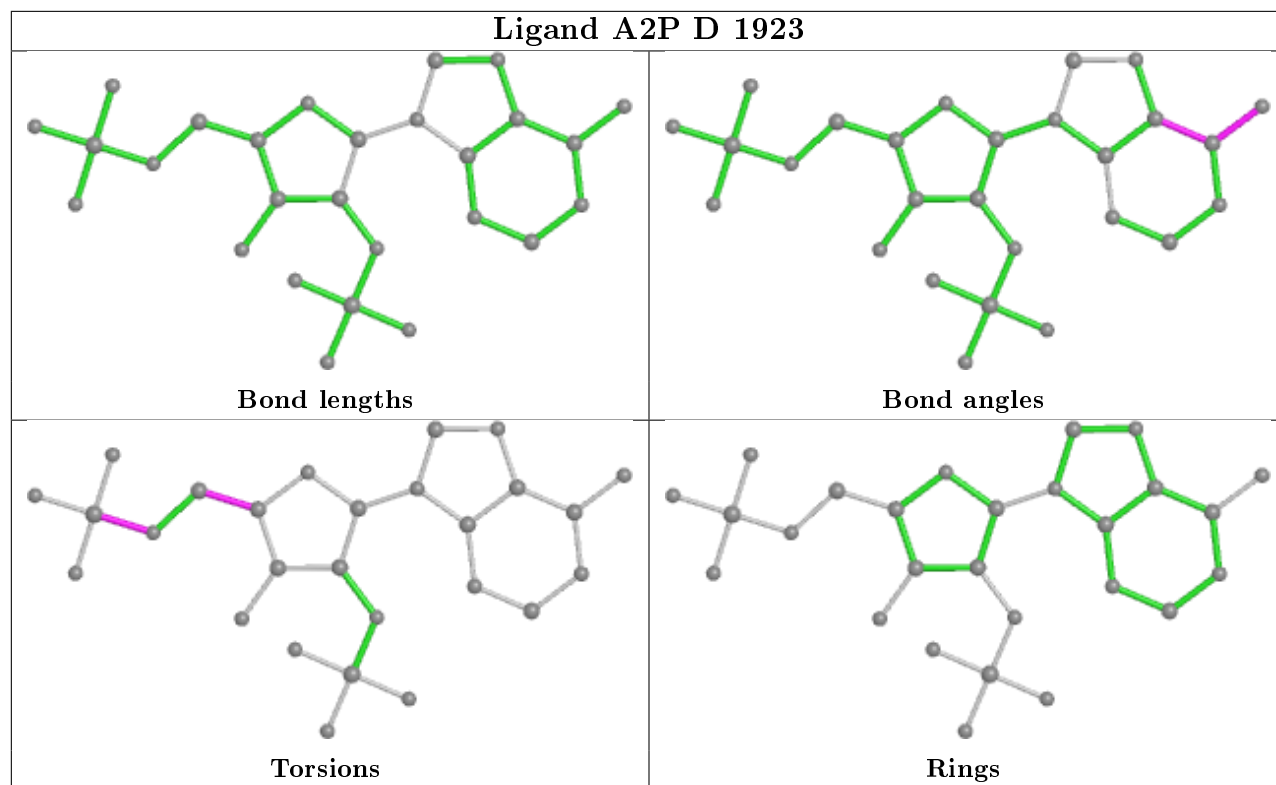
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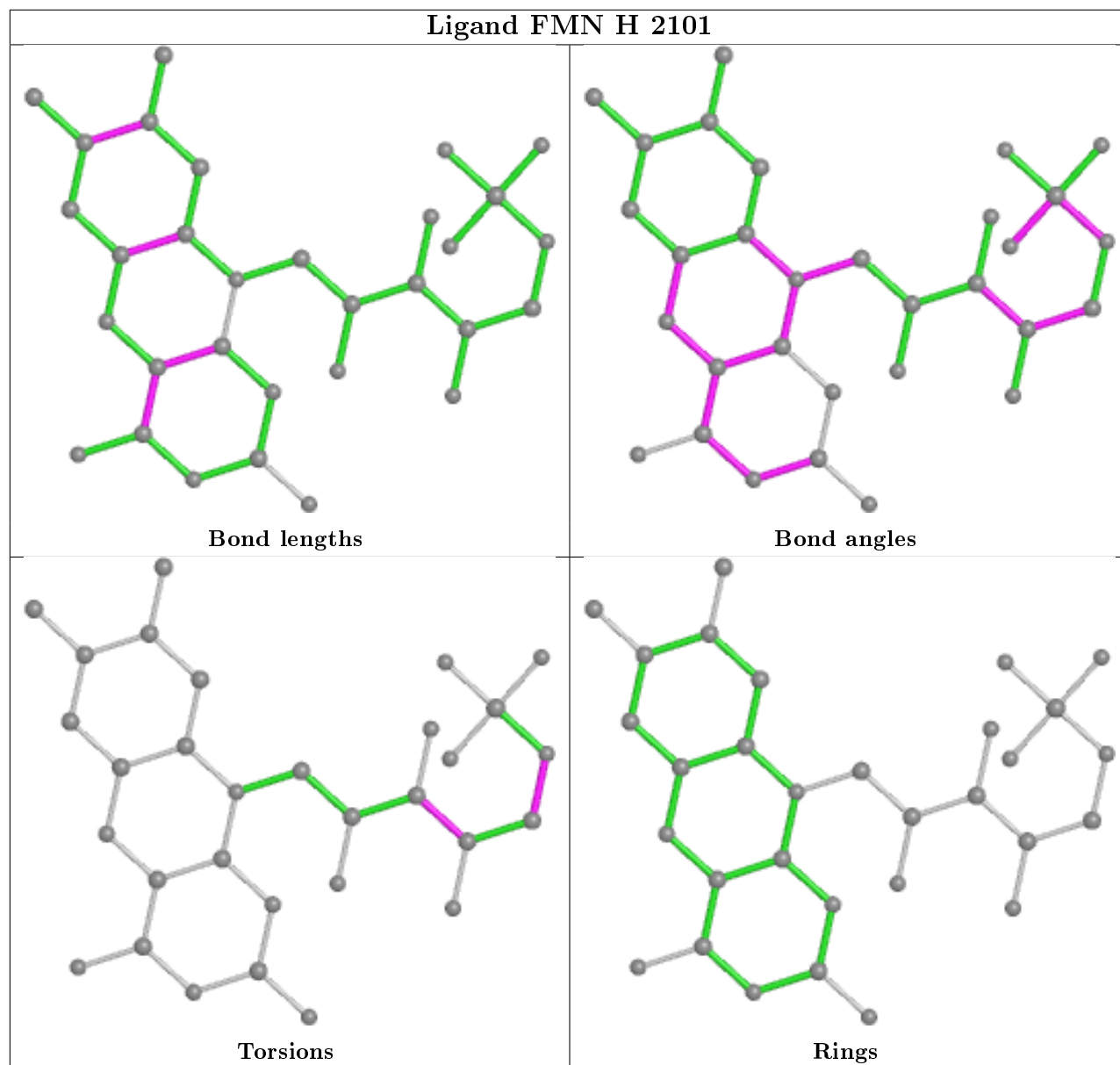
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1917	A2P	2	0
4	F	1901	PNS	2	0
5	B	1910	EDO	1	0
5	J	2104	EDO	1	0
4	A	1901	PNS	1	0
10	G	2101	FMN	4	0
11	G	2102	MLI	1	0
5	C	1907	EDO	1	0
11	J	2102	MLI	2	0
7	E	1917	A2P	2	0
10	I	2101	FMN	5	0
7	B	1918	A2P	5	0

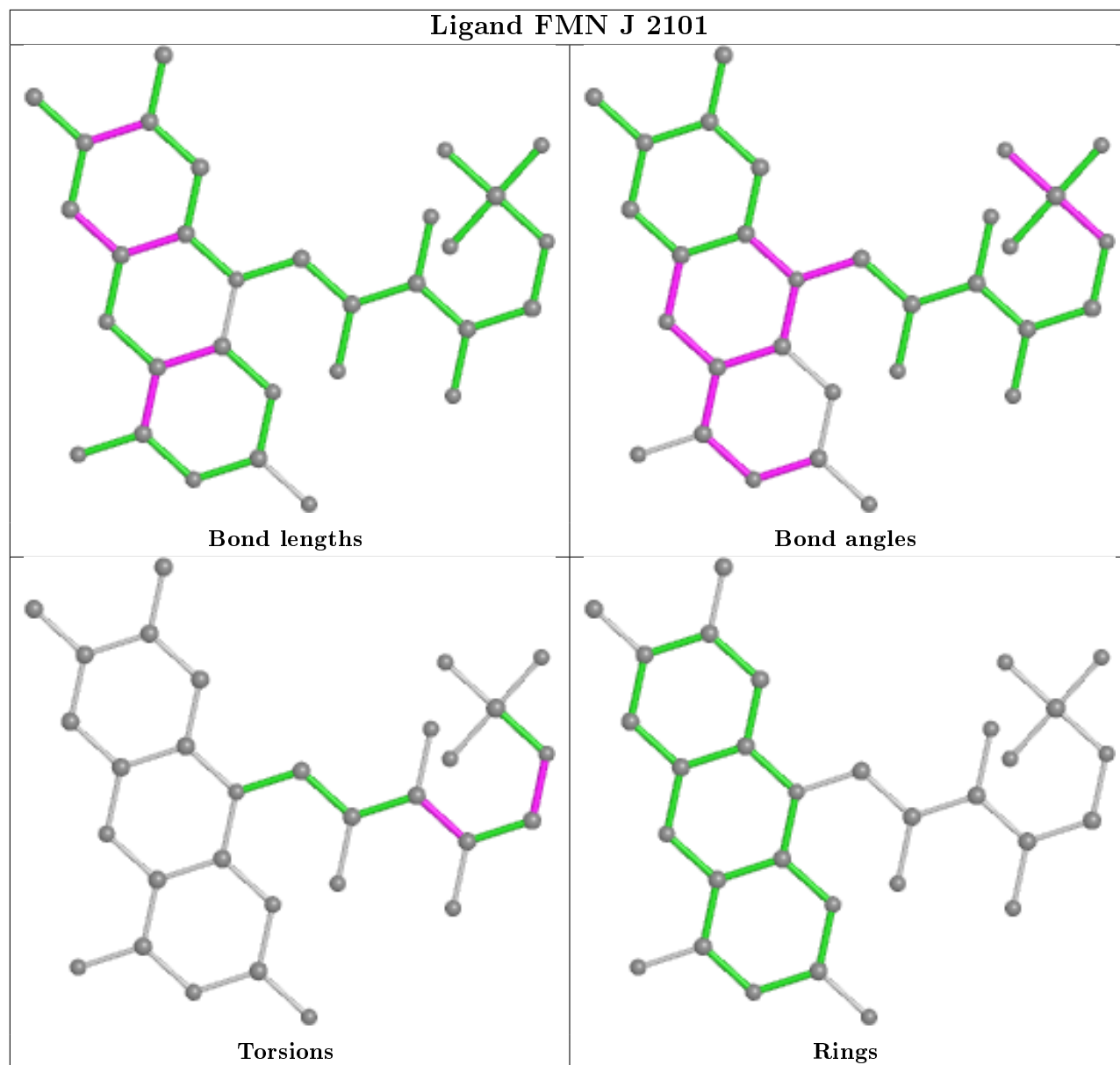
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

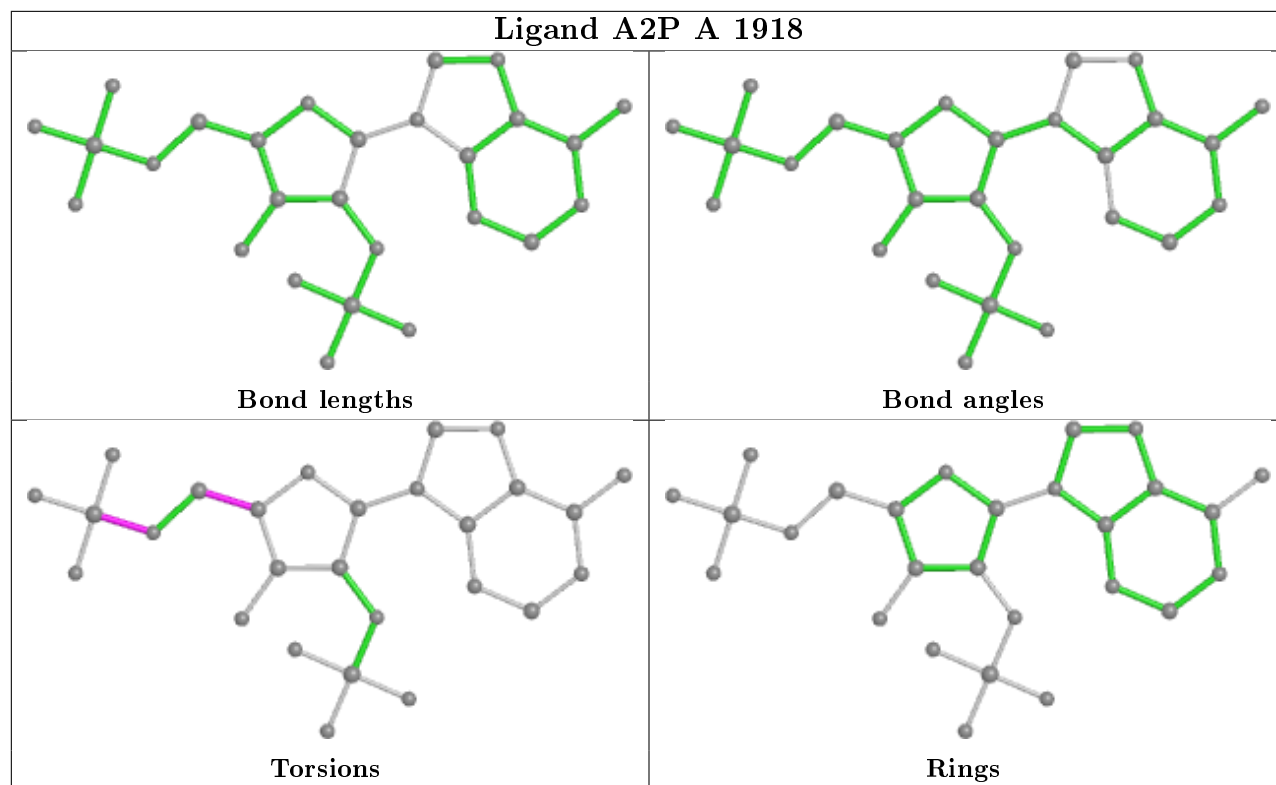


## Ligand FMN H 2101

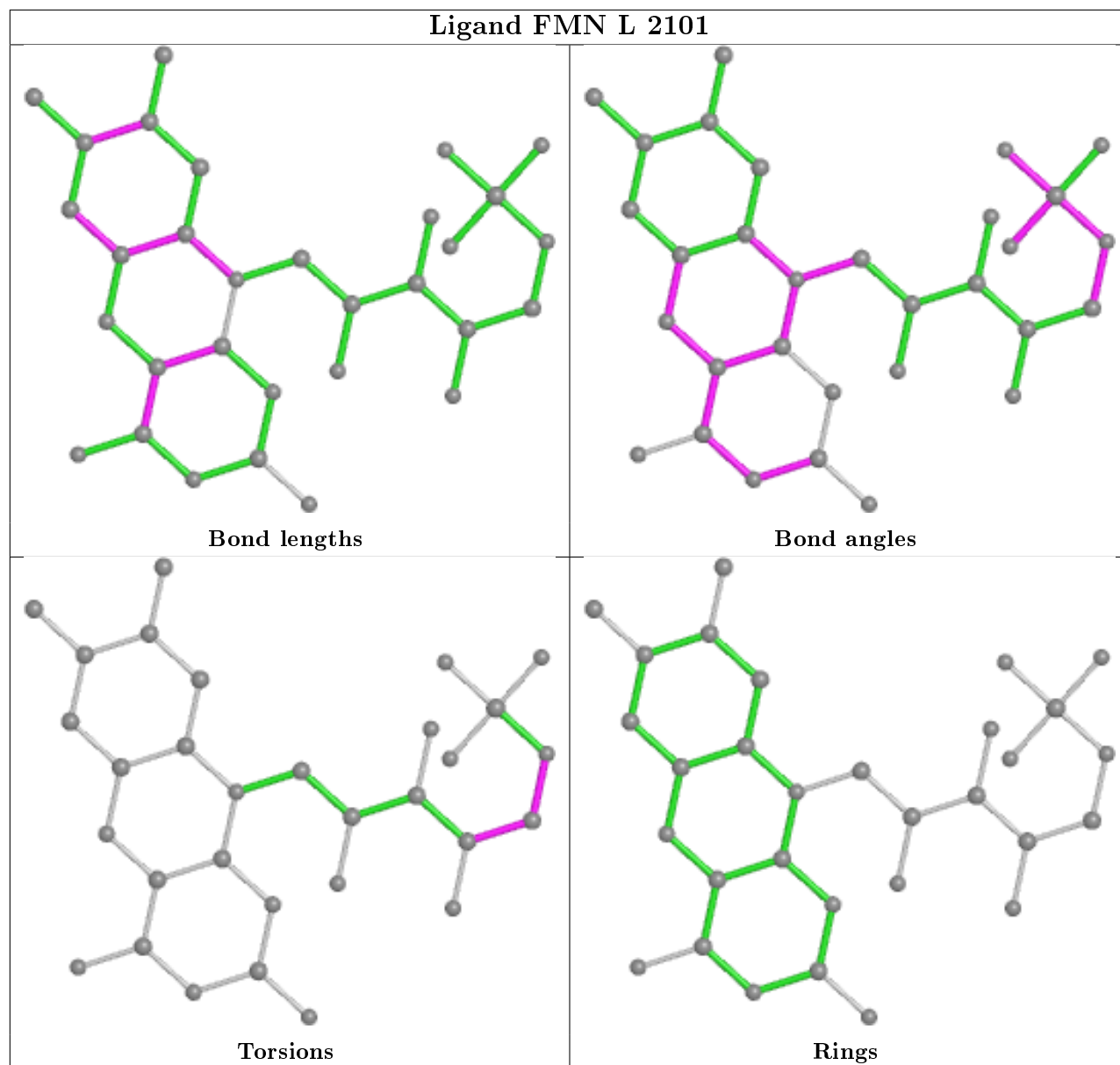


## Ligand FMN J 2101

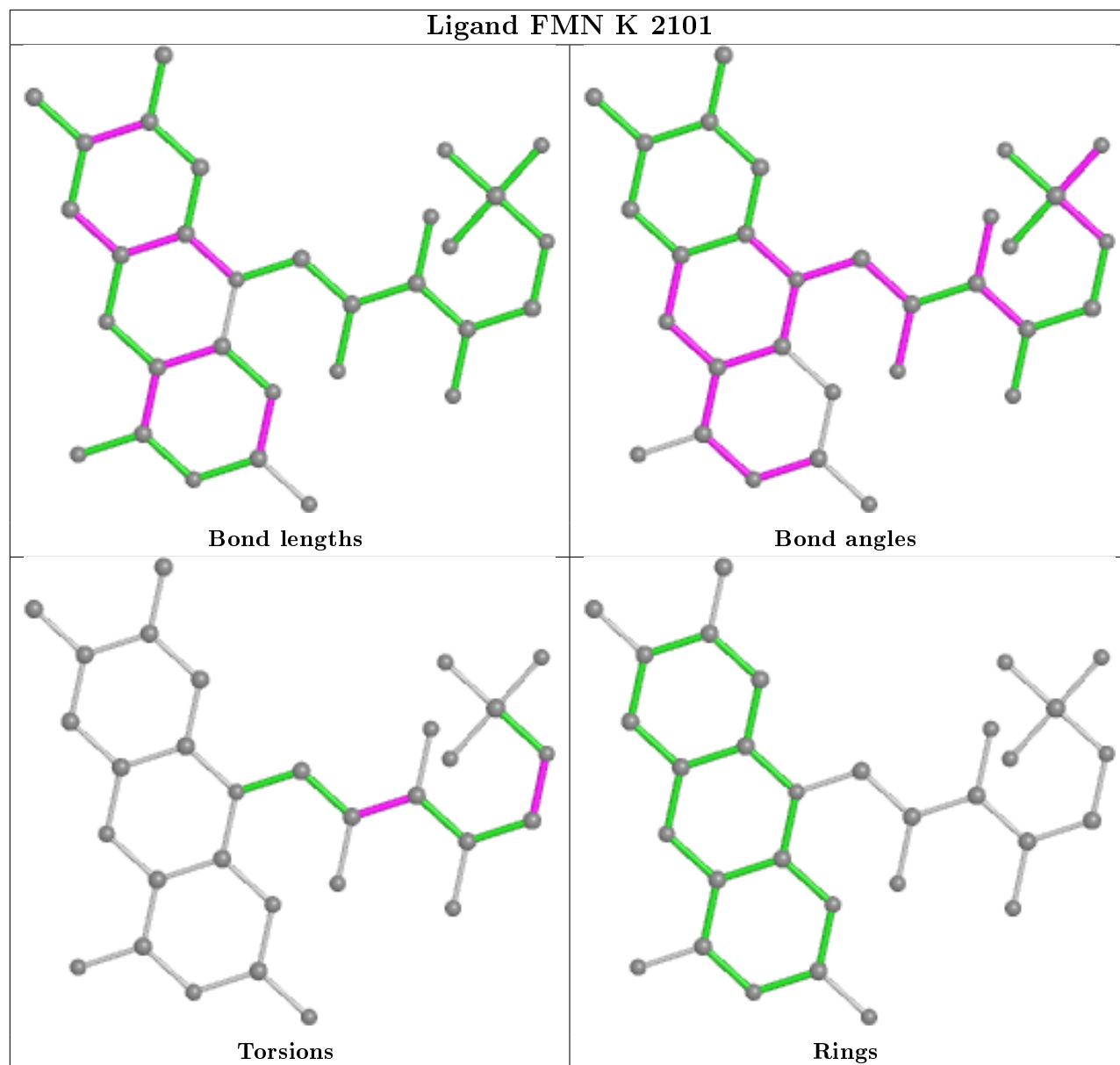




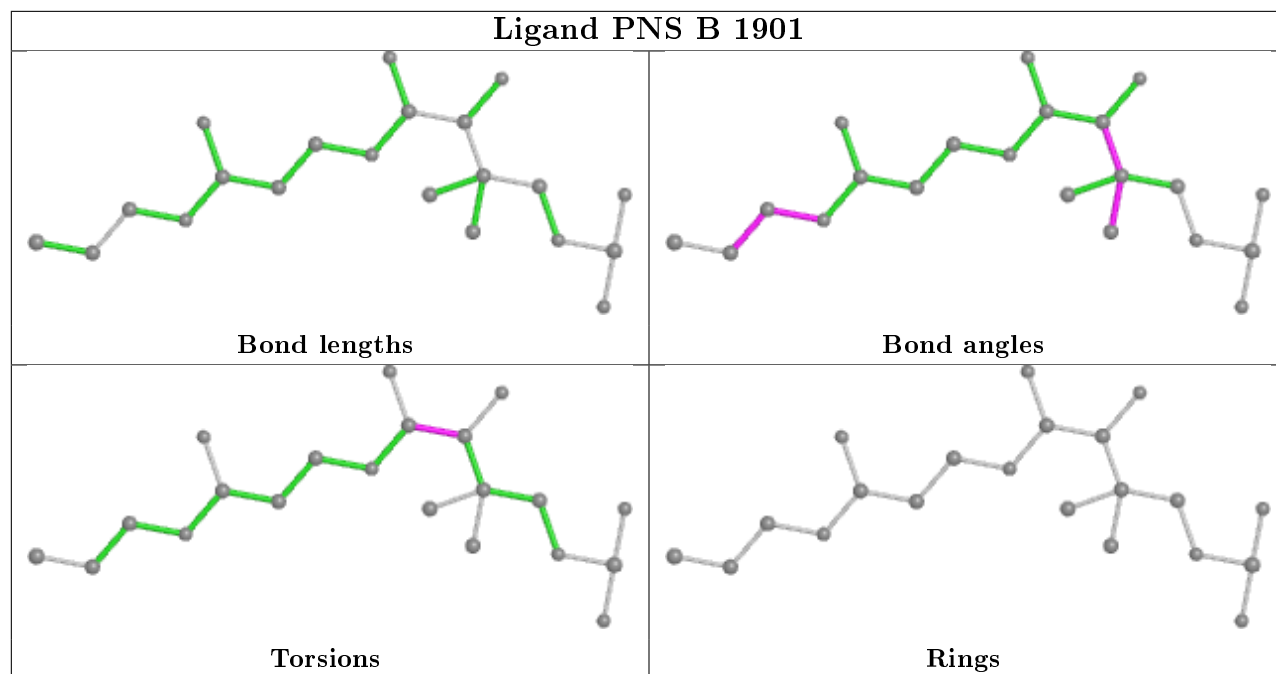
## Ligand FMN L 2101



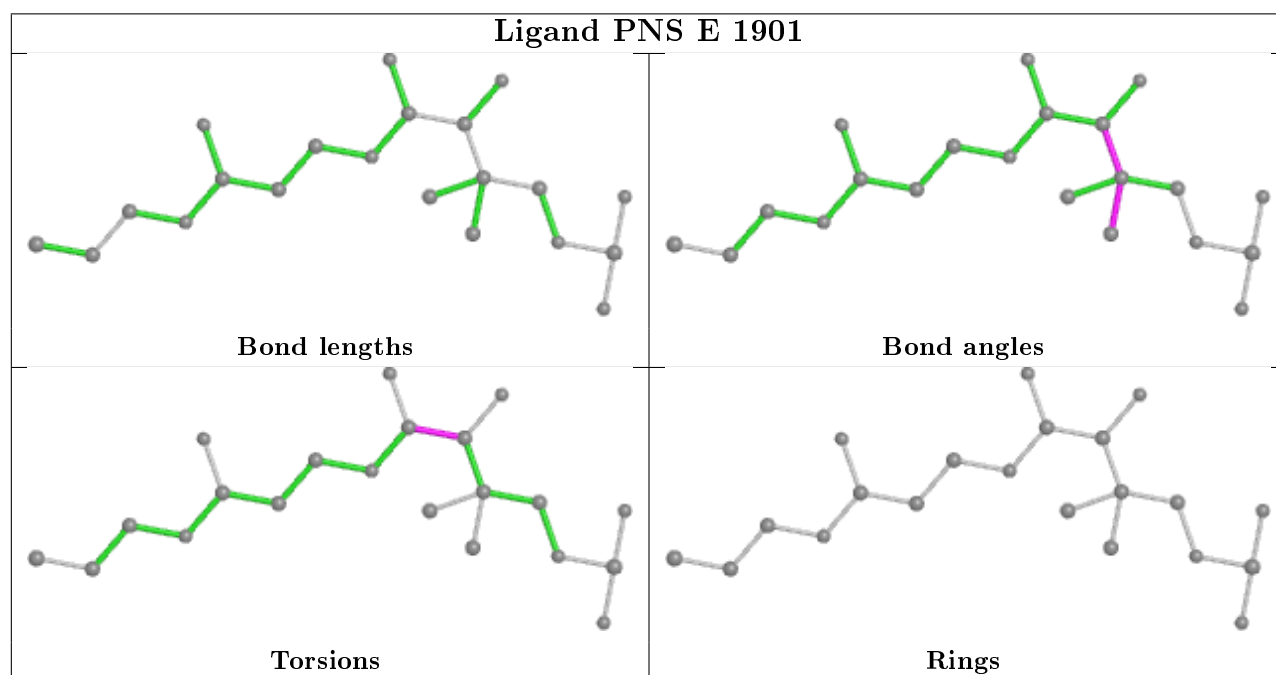
## Ligand FMN K 2101



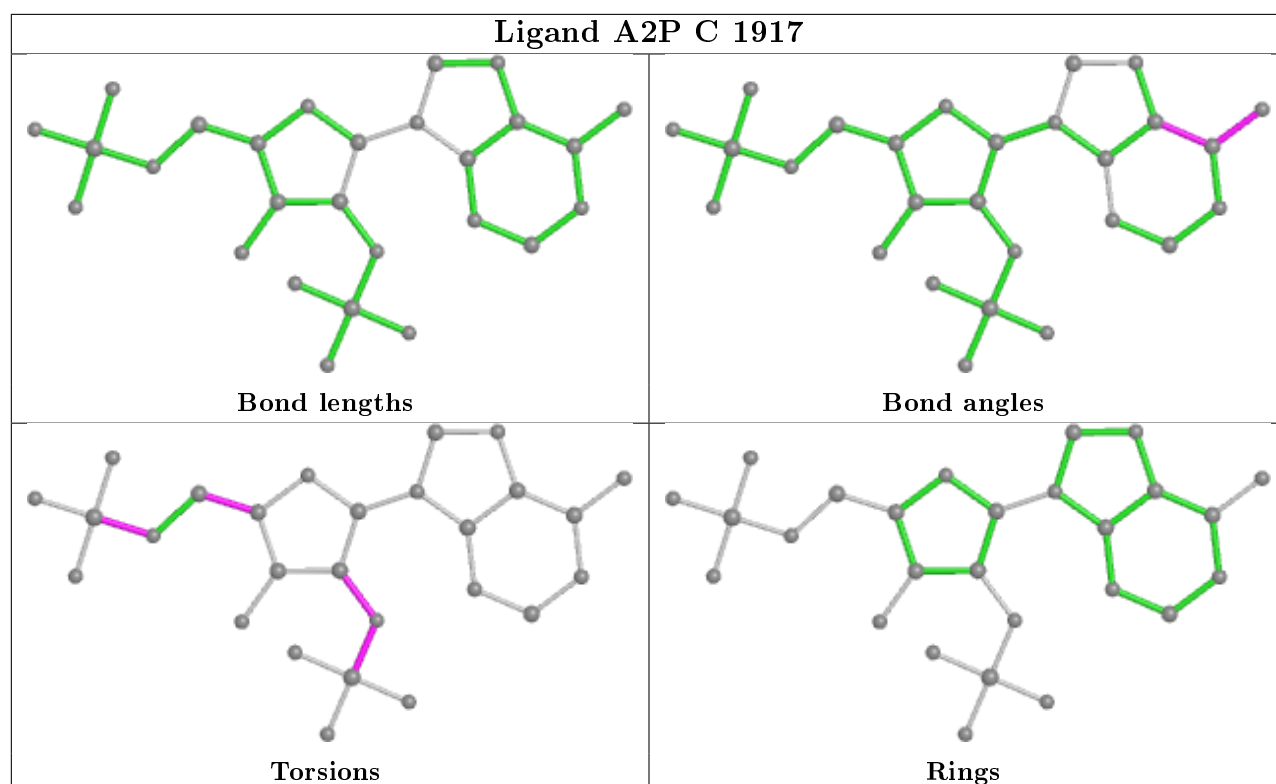
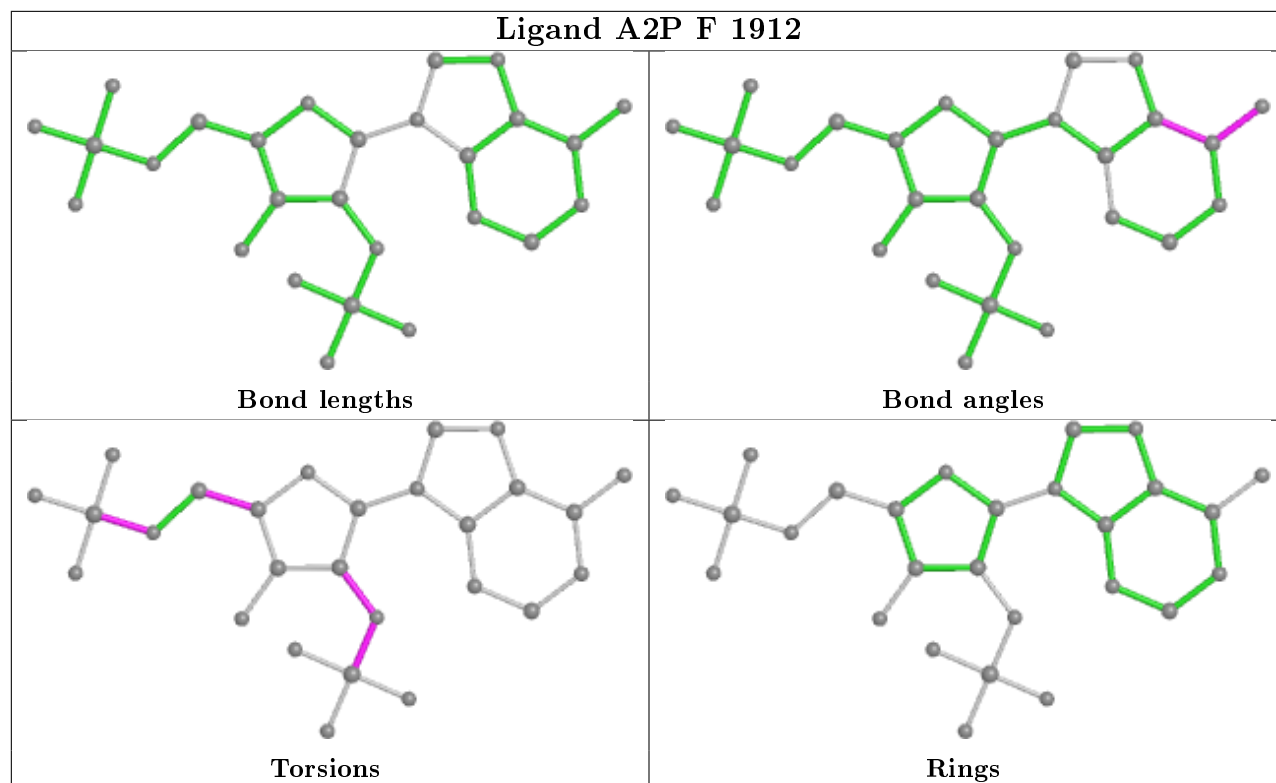
## Ligand PNS B 1901



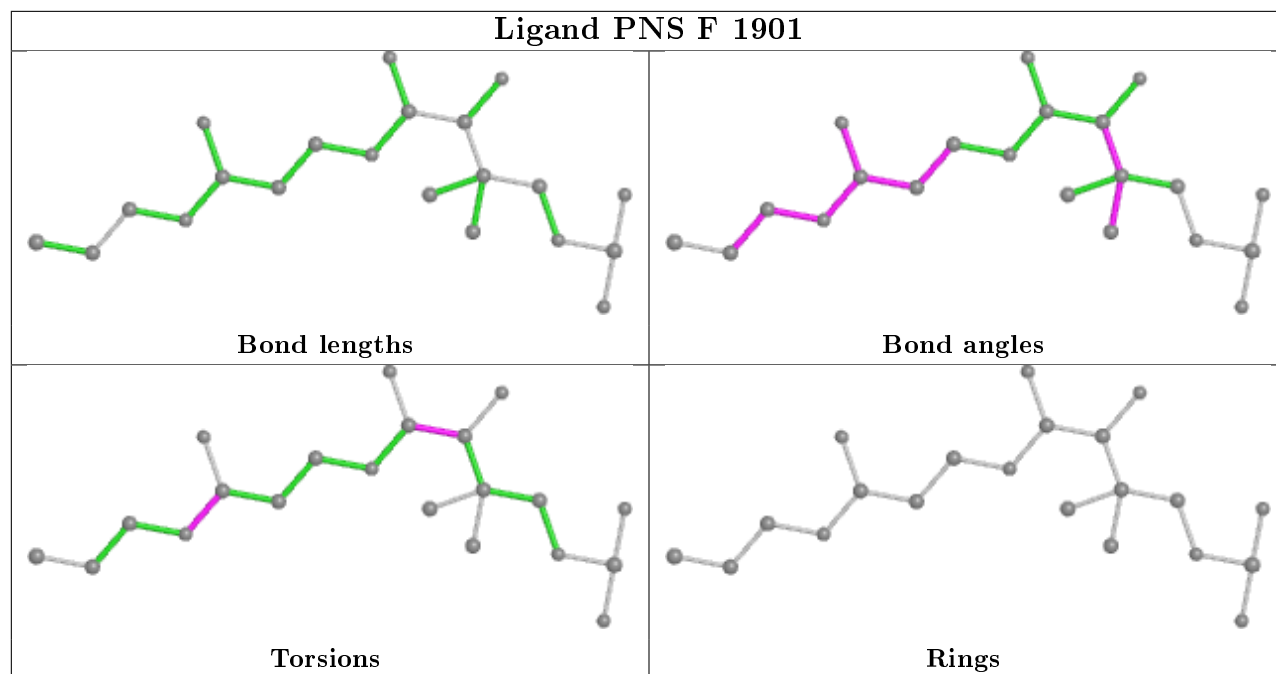
## Ligand PNS E 1901



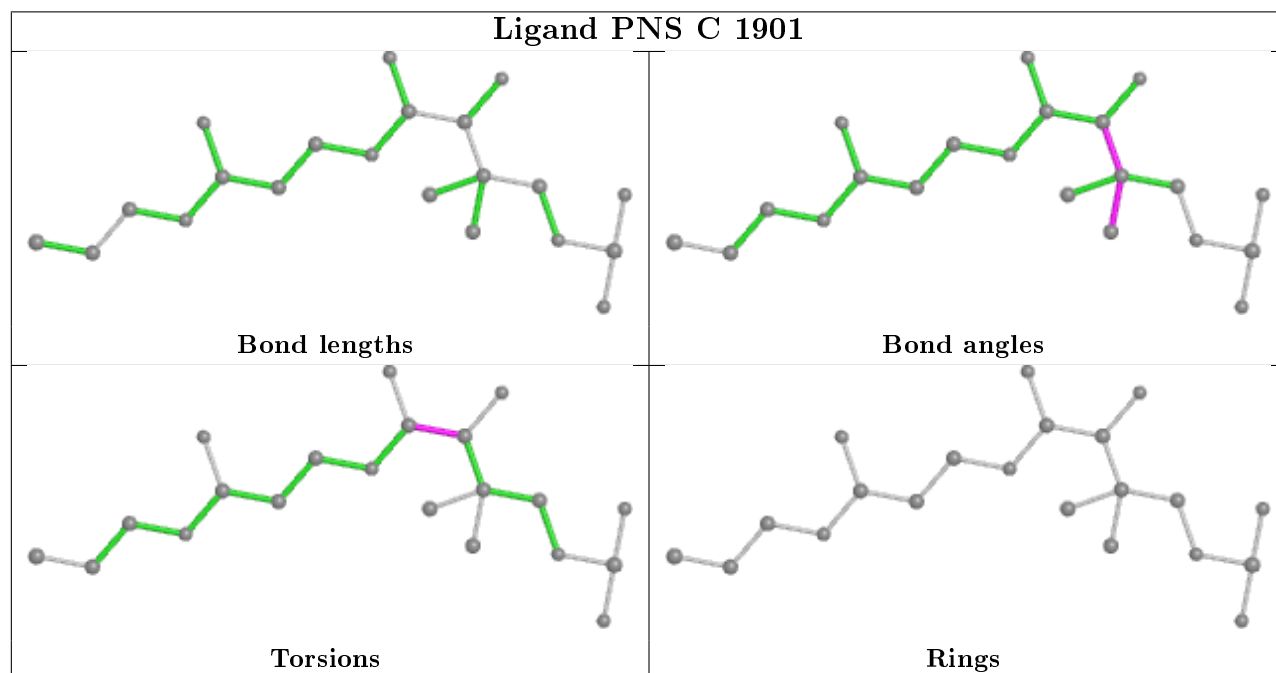


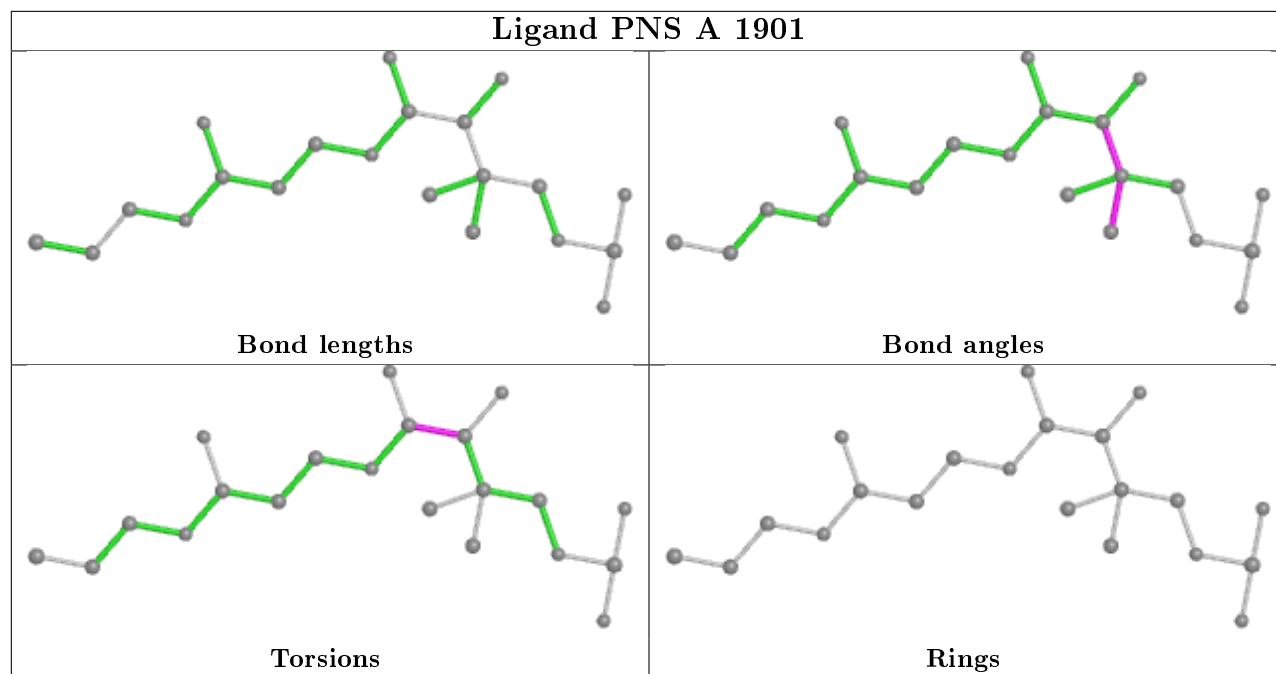


## Ligand PNS F 1901

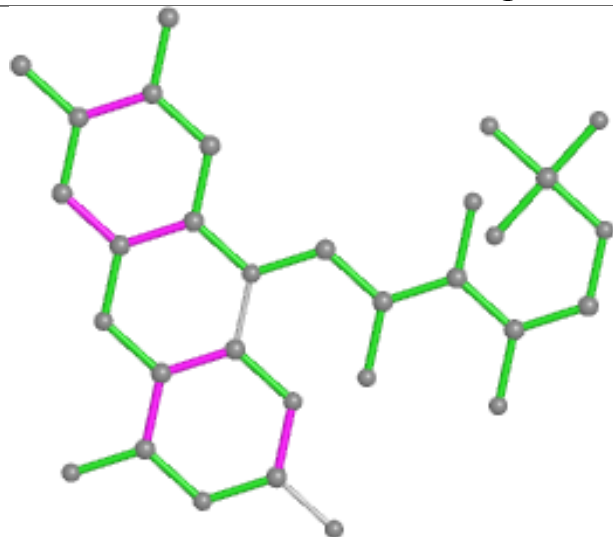


## Ligand PNS C 1901

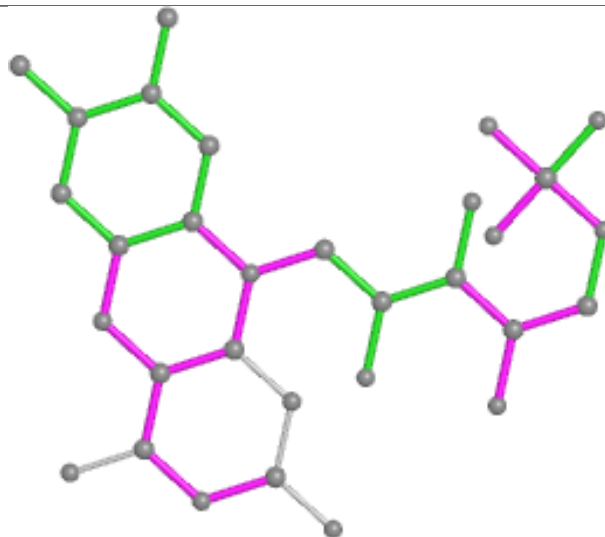




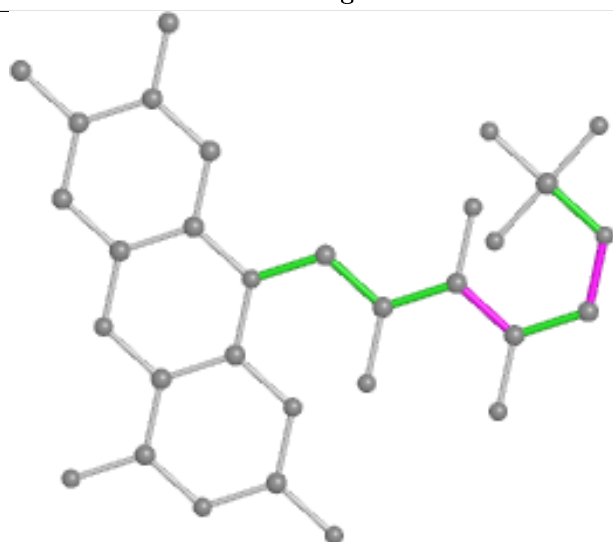
## Ligand FMN G 2101



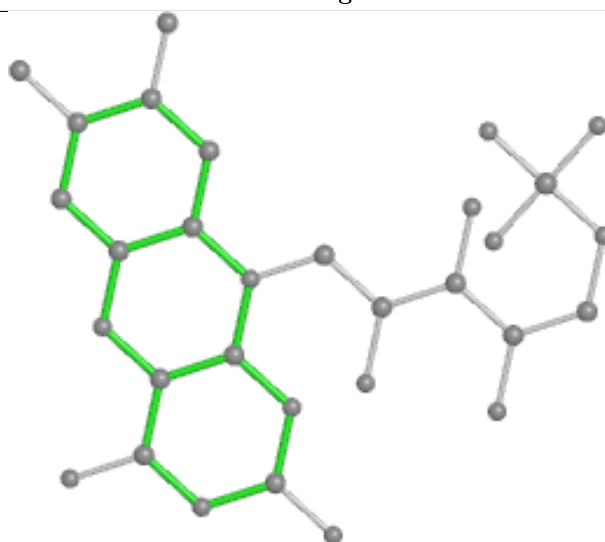
Bond lengths



Bond angles

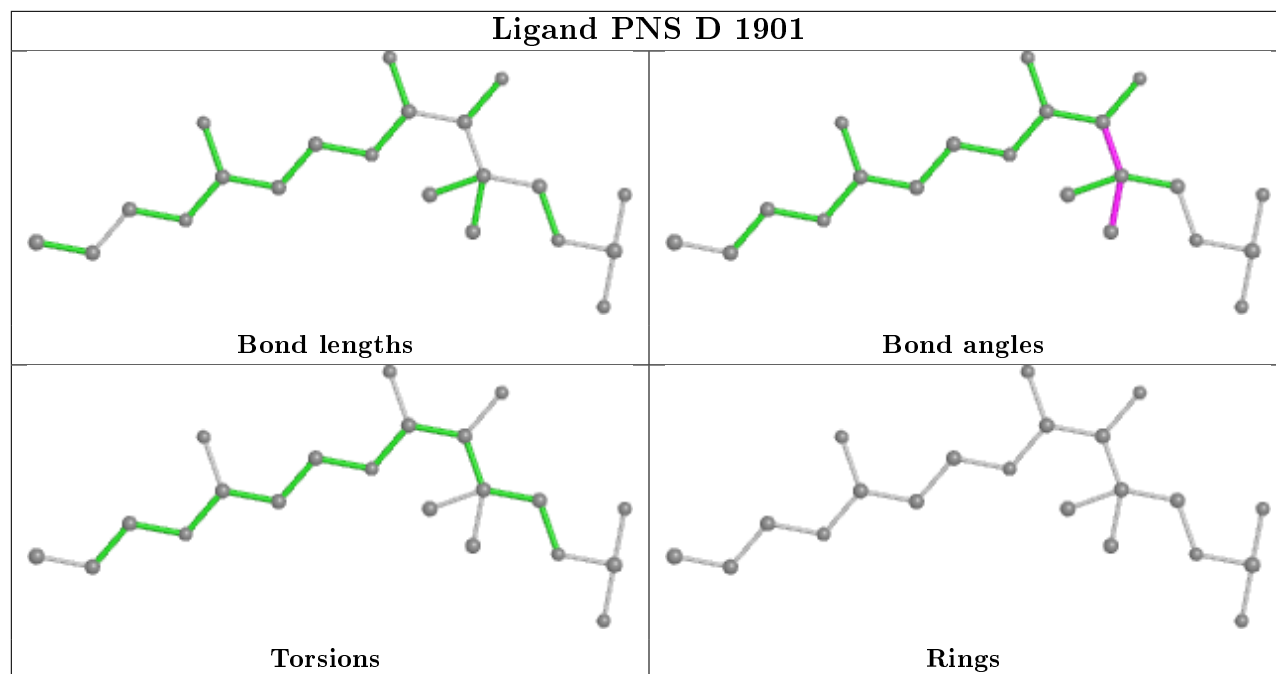


Torsions

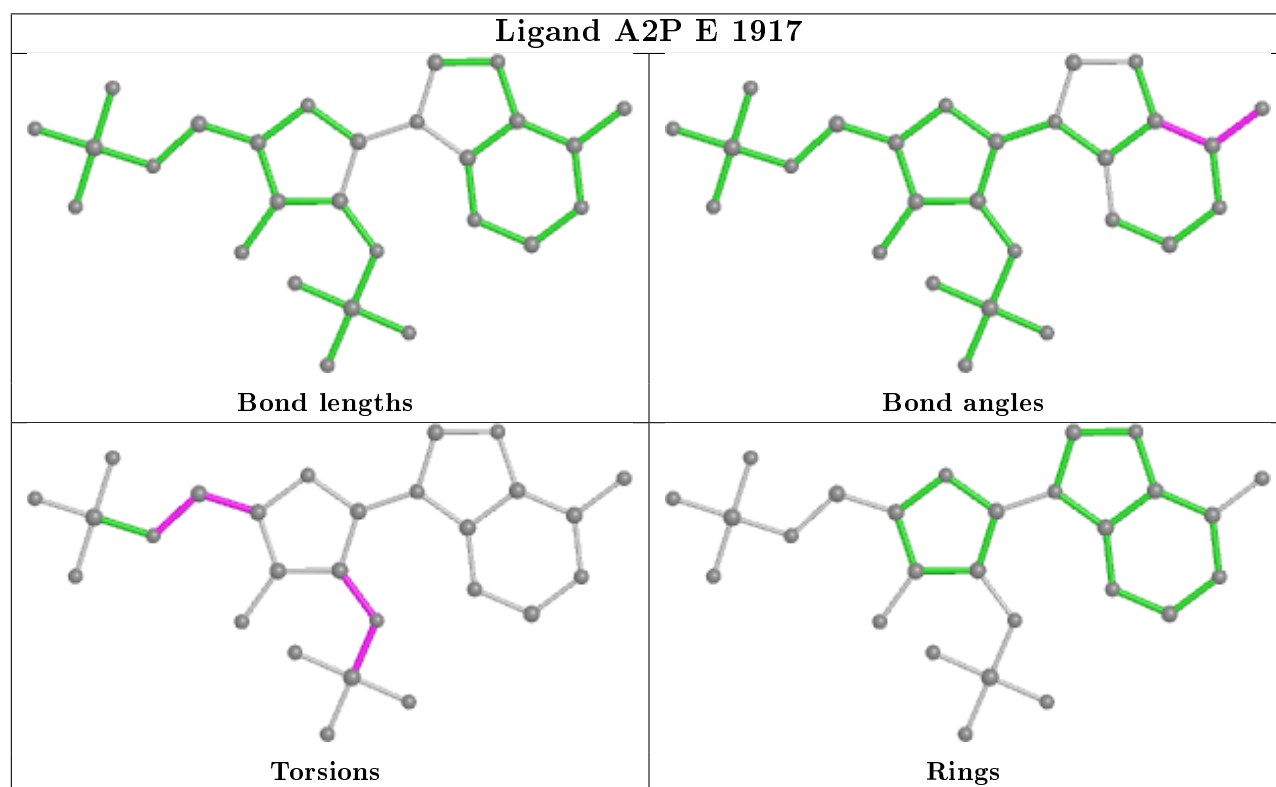


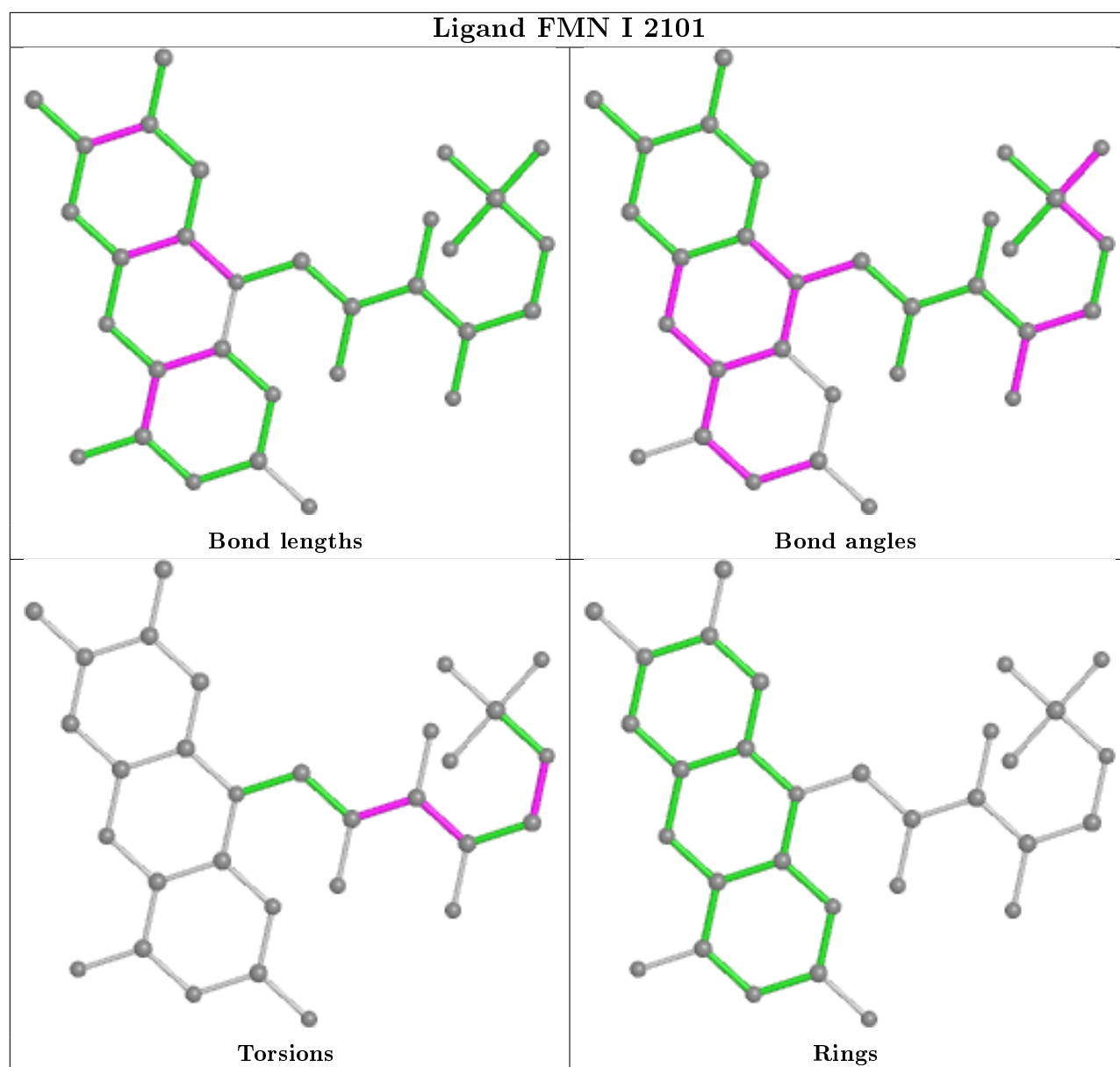
Rings

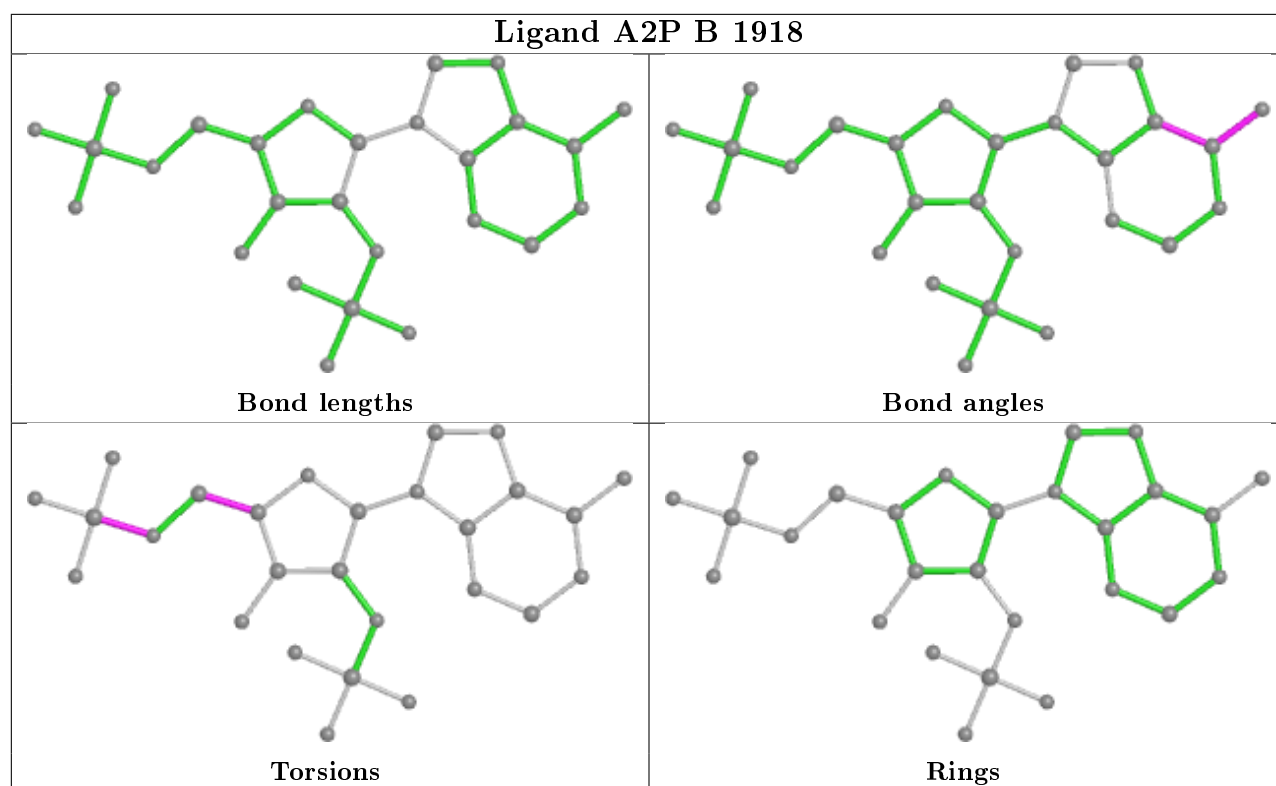
## Ligand PNS D 1901



## Ligand A2P E 1917







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1760/1887 (93%)	0.23	32 (1%) 68 61	32, 54, 115, 158	0
1	B	1759/1887 (93%)	0.23	25 (1%) 75 69	29, 53, 108, 154	0
1	C	1759/1887 (93%)	0.19	25 (1%) 75 69	31, 53, 112, 166	0
1	D	1765/1887 (93%)	0.21	12 (0%) 87 84	27, 47, 111, 154	0
1	E	1759/1887 (93%)	0.20	26 (1%) 73 67	35, 57, 109, 162	0
1	F	1759/1887 (93%)	0.19	21 (1%) 79 73	34, 59, 117, 172	0
2	G	2036/2051 (99%)	0.18	38 (1%) 66 59	42, 70, 130, 175	0
2	J	2035/2051 (99%)	0.22	38 (1%) 66 59	37, 69, 135, 189	0
3	H	2034/2051 (99%)	0.15	12 (0%) 89 86	39, 67, 119, 162	0
3	I	2033/2051 (99%)	0.17	18 (0%) 84 80	48, 79, 124, 167	0
3	K	2034/2051 (99%)	0.23	32 (1%) 72 65	57, 87, 129, 175	0
3	L	2035/2051 (99%)	0.27	44 (2%) 62 52	56, 84, 137, 191	0
All	All	22768/23628 (96%)	0.21	323 (1%) 75 69	27, 71, 122, 191	0

All (323) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1830	GLY	10.0
1	E	599	MET	8.9
1	B	1831	GLY	8.7
1	F	1830	GLY	8.3
1	A	1829	GLY	8.1
3	I	2050	GLN	8.0
1	A	1830	GLY	6.3
1	E	600	ASP	6.0
1	A	1831	GLY	5.6
3	K	1746	LEU	5.4
1	D	974	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	976	ALA	5.1
1	B	975	ALA	5.0
1	B	977	TYR	5.0
3	H	1743	ASP	4.8
3	K	1745	LYS	4.8
2	J	79	GLN	4.7
1	F	974	ASP	4.6
3	H	2050	GLN	4.6
3	L	1740	THR	4.6
2	G	1875	VAL	4.5
3	I	1741	ILE	4.4
3	L	1743	ASP	4.3
2	G	1744	GLY	4.2
1	C	1836	ASP	4.1
3	H	74	PRO	4.0
1	E	1764	VAL	4.0
1	A	1843	ASN	4.0
1	D	1843	ASN	4.0
1	F	1831	GLY	4.0
1	A	599	MET	4.0
1	F	975	ALA	4.0
1	A	622	ILE	3.9
1	E	1829	GLY	3.9
1	B	1828	LEU	3.9
2	J	1848	GLY	3.9
2	J	1745	LYS	3.9
1	F	599	MET	3.9
2	G	1873	TYR	3.9
1	D	1844	LYS	3.8
3	H	75	SER	3.8
1	C	1843	ASN	3.7
1	C	539	SER	3.7
1	E	1830	GLY	3.7
1	B	599	MET	3.7
3	L	1853	GLY	3.7
3	L	74	PRO	3.7
3	H	1740	THR	3.7
3	L	1924	ILE	3.7
2	G	1931	LEU	3.7
1	D	199	GLU	3.7
1	D	1842	VAL	3.7
1	C	599	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	1885	THR	3.6
1	E	601	VAL	3.6
3	L	1965	ALA	3.6
3	I	1743	ASP	3.6
1	A	1827	SER	3.6
2	G	1939	HIS	3.5
1	B	1826	LYS	3.5
1	B	1829	GLY	3.4
2	G	1916	PHE	3.4
1	A	1832	ALA	3.4
2	J	74	PRO	3.4
1	E	622	ILE	3.4
1	A	1824	GLY	3.4
2	G	28	PHE	3.3
1	F	977	TYR	3.3
1	E	199	GLU	3.3
3	H	71	LEU	3.3
2	J	1746	LEU	3.3
1	C	1829	GLY	3.3
3	K	1741	ILE	3.2
2	G	74	PRO	3.2
2	J	1743	ASP	3.2
2	J	384	GLN	3.2
1	E	974	ASP	3.2
1	E	1831	GLY	3.2
2	J	1881	ARG	3.2
1	A	977	TYR	3.2
3	L	1753	LYS	3.2
1	D	599	MET	3.2
3	I	1940	LEU	3.2
1	A	199	GLU	3.2
3	L	2050	GLN	3.2
2	J	87	CYS	3.2
1	A	1826	LYS	3.1
2	J	86	LEU	3.1
2	G	1957	PRO	3.1
1	B	1832	ALA	3.1
1	C	1855	ALA	3.1
2	G	1881	ARG	3.1
3	L	1879	GLY	3.1
3	L	1886	VAL	3.1
3	L	1901	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
3	L	28	PHE	3.0
1	B	877	LEU	3.0
3	I	1746	LEU	3.0
2	J	1316	ASP	3.0
3	I	1745	LYS	3.0
2	J	77	VAL	3.0
3	L	1970	VAL	3.0
2	G	1740	THR	3.0
1	B	1827	SER	3.0
1	C	1863	GLY	3.0
3	H	1741	ILE	3.0
1	F	1764	VAL	3.0
1	A	1846	ALA	3.0
3	I	1916	PHE	2.9
2	G	1845	ASP	2.9
3	K	1164	MET	2.9
3	L	1742	VAL	2.9
2	G	75	SER	2.9
1	B	976	ALA	2.9
1	D	1831	GLY	2.9
3	L	1964	PHE	2.9
2	G	79	GLN	2.9
1	F	1828	LEU	2.9
2	J	1741	ILE	2.9
2	G	1940	LEU	2.9
2	J	1849	ARG	2.9
3	K	1981	LEU	2.9
1	F	302	LEU	2.8
1	A	1813	TRP	2.8
2	J	47	GLY	2.8
3	I	1316	ASP	2.8
3	L	80	PHE	2.8
3	K	1966	CYS	2.8
2	G	1946	GLU	2.8
1	A	974	ASP	2.8
1	E	602	GLU	2.8
1	A	975	ALA	2.8
1	F	73	SER	2.8
1	A	1828	LEU	2.8
1	C	199	GLU	2.8
2	G	2050	GLN	2.8
3	K	1545	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	1766	ASN	2.7
2	G	2049	GLU	2.7
1	A	1866	ASP	2.7
3	L	1873	TYR	2.7
2	G	1848	GLY	2.7
1	C	974	ASP	2.7
3	K	1740	THR	2.7
3	K	1744	GLY	2.7
1	A	1842	VAL	2.7
3	H	1744	GLY	2.7
3	K	450	PHE	2.7
1	F	877	LEU	2.7
2	G	2030	TYR	2.7
3	L	1962	ARG	2.7
3	L	1748	THR	2.7
1	E	1842	VAL	2.7
2	G	1970	VAL	2.7
2	J	1744	GLY	2.7
1	B	602	GLU	2.6
1	E	605	LEU	2.6
3	L	1745	LYS	2.6
2	J	1879	GLY	2.6
2	J	75	SER	2.6
2	G	19	VAL	2.6
2	J	1961	GLU	2.6
3	K	1965	ALA	2.6
1	B	600	ASP	2.6
3	I	1944	ILE	2.6
2	J	1916	PHE	2.6
2	J	71	LEU	2.5
3	K	1748	THR	2.5
3	L	269	GLY	2.5
3	H	1742	VAL	2.5
3	I	1742	VAL	2.5
1	E	1832	ALA	2.5
1	E	1765	SER	2.5
1	E	1827	SER	2.5
3	K	1866	PHE	2.5
1	F	331	ILE	2.5
1	A	1823	LEU	2.5
3	K	1885	LEU	2.5
2	G	86	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	20	LEU	2.5
2	G	1746	LEU	2.5
3	H	83	VAL	2.5
1	B	195	GLY	2.5
1	F	192	LYS	2.5
2	J	20	LEU	2.5
1	A	1825	VAL	2.5
3	K	1743	ASP	2.5
3	I	1740	THR	2.5
3	K	1960	LEU	2.5
3	I	1970	VAL	2.5
3	K	1873	TYR	2.5
3	L	1320	LEU	2.5
2	G	7	ARG	2.4
1	C	1862	ALA	2.4
1	A	1764	VAL	2.4
2	G	1969	LEU	2.4
2	J	11	LEU	2.4
1	B	1843	ASN	2.4
1	B	1789	ARG	2.4
1	B	1813	TRP	2.4
2	J	1845	ASP	2.4
2	J	1944	ILE	2.4
2	J	1960	LEU	2.4
3	L	1960	LEU	2.4
1	E	621	THR	2.4
2	J	19	VAL	2.4
3	K	1930	SER	2.4
2	J	1962	ARG	2.4
1	C	1831	GLY	2.4
2	J	1875	VAL	2.4
1	E	1813	TRP	2.4
3	K	1984	GLY	2.4
3	K	159	ILE	2.4
3	K	1334	ILE	2.4
3	L	1969	LEU	2.4
1	A	1786	PHE	2.3
1	B	178	GLY	2.3
1	F	1829	GLY	2.3
2	J	1953	VAL	2.3
3	L	137	PHE	2.3
3	H	1931	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	K	1316	ASP	2.3
1	F	239	GLY	2.3
2	G	1884	TRP	2.3
2	G	1871	LEU	2.3
2	G	2032	LEU	2.3
2	J	1842	VAL	2.3
3	I	1968	PRO	2.3
3	L	1845	ASP	2.3
1	A	877	LEU	2.3
1	E	877	LEU	2.3
2	J	60	LEU	2.3
1	E	1767	GLY	2.3
3	I	1744	GLY	2.3
3	K	1976	PHE	2.3
3	L	1995	ASN	2.3
1	B	1886	LYS	2.3
3	K	2045	TRP	2.3
2	G	21	LEU	2.3
1	A	213	PHE	2.3
1	E	604	ALA	2.2
2	J	80	PHE	2.2
3	I	1545	TYR	2.2
1	A	1797	GLU	2.2
3	K	1970	VAL	2.2
3	L	75	SER	2.2
3	K	1914	LEU	2.2
3	L	21	LEU	2.2
3	K	1374	THR	2.2
1	E	975	ALA	2.2
2	G	1944	ILE	2.2
2	J	64	PHE	2.2
3	L	1854	MET	2.2
1	D	1813	TRP	2.2
1	A	1766	ASN	2.2
1	A	1801	ALA	2.2
1	C	1820	PHE	2.2
1	D	973	ALA	2.2
1	E	518	LYS	2.2
3	L	19	VAL	2.2
1	D	160	LYS	2.2
2	G	2038	ILE	2.2
2	J	28	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
3	L	1741	ILE	2.2
3	L	1955	PRO	2.2
1	B	203	GLU	2.2
3	H	1971	GLY	2.2
2	G	1914	LEU	2.2
3	I	1931	LEU	2.2
3	K	96	LEU	2.2
3	K	1888	ILE	2.2
1	F	75	HIS	2.2
1	C	1849	VAL	2.2
2	G	2045	TRP	2.2
1	A	1783	ASN	2.2
1	C	1837	ILE	2.2
2	J	2050	GLN	2.2
3	K	1747	LYS	2.2
3	L	117	VAL	2.2
1	F	976	ALA	2.1
1	C	1826	LYS	2.1
1	A	331	ILE	2.1
1	D	976	ALA	2.1
1	D	972	SER	2.1
3	K	2029	VAL	2.1
1	C	977	TYR	2.1
1	E	977	TYR	2.1
3	K	352	TYR	2.1
1	E	1784	ASP	2.1
2	G	137	PHE	2.1
1	C	1847	PRO	2.1
3	L	72	VAL	2.1
2	J	1873	TYR	2.1
3	L	1815	LEU	2.1
1	F	71	ALA	2.1
3	L	1857	ILE	2.1
3	L	1914	LEU	2.1
3	L	1848	GLY	2.1
1	B	1866	ASP	2.1
1	C	1830	GLY	2.1
1	E	259	GLY	2.1
1	C	73	SER	2.1
3	I	1966	CYS	2.1
1	C	1786	PHE	2.1
1	C	1791	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	L	82	GLN	2.1
1	A	1779	ILE	2.1
3	L	1907	LEU	2.1
2	G	87	CYS	2.1
1	C	1833	ALA	2.1
3	I	1925	ILE	2.1
3	L	1787	ALA	2.1
3	L	145	LEU	2.0
1	F	1827	SER	2.0
1	B	278	GLY	2.0
1	B	1794	GLN	2.0
1	A	1851	LEU	2.0
2	J	209	PHE	2.0
1	B	166	ILE	2.0
1	F	539	SER	2.0
2	G	1741	ILE	2.0
3	L	1930	SER	2.0
1	C	1841	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	J8W	I	1808	12/13	0.88	0.23	79,93,103,106	0
3	J8W	L	1808	12/13	0.88	0.23	97,105,108,110	0
3	J8W	K	1808	12/13	0.91	0.21	83,92,98,98	0
3	J8W	H	1808	12/13	0.94	0.22	66,82,88,89	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	E	1908	4/4	0.61	0.28	76,79,81,82	0
5	EDO	F	1904	4/4	0.64	0.27	68,73,77,78	0
7	A2P	B	1918	27/27	0.68	0.43	87,126,138,145	0
5	EDO	F	1902	4/4	0.72	0.39	75,80,85,89	0
8	ACT	B	1902	4/4	0.73	0.41	68,72,75,76	0
5	EDO	J	2104	4/4	0.74	0.22	68,70,71,71	0
6	NA	J	2108	1/1	0.74	0.13	60,60,60,60	0
8	ACT	H	2102	4/4	0.74	0.31	80,82,86,89	0
5	EDO	C	1910	4/4	0.74	0.30	79,83,84,86	0
7	A2P	F	1912	27/27	0.77	0.43	86,121,152,158	0
7	A2P	A	1918	27/27	0.77	0.48	87,121,166,169	0
5	EDO	E	1912	4/4	0.77	0.37	91,93,93,97	0
6	NA	C	1914	1/1	0.77	0.52	60,60,60,60	0
9	PGE	E	1918	10/10	0.77	0.39	88,99,106,107	0
5	EDO	C	1908	4/4	0.77	0.27	60,69,73,74	0
5	EDO	D	1912	4/4	0.79	0.27	79,81,81,82	0
5	EDO	C	1907	4/4	0.79	0.32	75,78,80,81	0
5	EDO	A	1909	4/4	0.79	0.38	64,64,71,71	0
7	A2P	D	1923	27/27	0.79	0.35	74,107,137,145	0
5	EDO	D	1906	4/4	0.80	0.24	51,52,58,59	0
6	NA	G	2104	1/1	0.80	0.18	59,59,59,59	0
7	A2P	E	1917	27/27	0.80	0.45	83,114,130,138	0
5	EDO	F	1906	4/4	0.80	0.27	71,74,76,77	0
5	EDO	J	2105	4/4	0.80	0.33	73,77,78,79	0
8	ACT	C	1903	4/4	0.82	0.49	59,69,73,75	0
8	ACT	H	2104	4/4	0.82	0.29	81,84,84,85	0
6	NA	E	1915	1/1	0.82	0.09	50,50,50,50	0
6	NA	I	2102	1/1	0.83	0.17	84,84,84,84	0
5	EDO	A	1907	4/4	0.83	0.39	69,71,74,75	0
5	EDO	C	1911	4/4	0.83	0.40	64,65,71,71	0
5	EDO	B	1903	4/4	0.83	0.17	70,76,77,79	0
8	ACT	H	2103	4/4	0.84	0.31	66,66,70,73	0
6	NA	D	1918	1/1	0.84	0.34	56,56,56,56	0
6	NA	B	1915	1/1	0.84	0.13	49,49,49,49	0
5	EDO	C	1909	4/4	0.84	0.28	72,78,79,80	0
7	A2P	C	1917	27/27	0.84	0.34	66,97,150,153	0
6	NA	H	2107	1/1	0.85	0.12	49,49,49,49	0
6	NA	F	1910	1/1	0.85	0.67	65,65,65,65	0
5	EDO	F	1905	4/4	0.85	0.36	65,67,67,67	0
5	EDO	H	2105	4/4	0.86	0.20	68,72,74,76	0
5	EDO	F	1909	4/4	0.86	0.29	54,54,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	B	1910	4/4	0.86	0.25	69,72,76,78	0
5	EDO	A	1908	4/4	0.86	0.21	59,60,60,60	0
5	EDO	B	1911	4/4	0.86	0.36	55,57,58,59	0
6	NA	D	1920	1/1	0.87	0.26	45,45,45,45	0
5	EDO	A	1911	4/4	0.87	0.25	83,84,90,91	0
5	EDO	B	1912	4/4	0.87	0.21	74,78,78,80	0
5	EDO	A	1903	4/4	0.87	0.22	56,60,60,61	0
6	NA	A	1916	1/1	0.87	0.47	51,51,51,51	0
5	EDO	E	1910	4/4	0.88	0.32	80,82,84,85	0
5	EDO	A	1905	4/4	0.88	0.17	57,60,60,61	0
5	EDO	C	1906	4/4	0.88	0.21	67,68,72,74	0
5	EDO	D	1902	4/4	0.89	0.30	58,59,59,60	0
5	EDO	D	1911	4/4	0.89	0.18	60,61,61,62	0
5	EDO	B	1906	4/4	0.89	0.32	52,54,58,65	0
5	EDO	E	1911	4/4	0.89	0.25	69,69,72,72	0
6	NA	C	1916	1/1	0.89	0.70	61,61,61,61	0
5	EDO	D	1903	4/4	0.89	0.21	46,52,55,56	0
5	EDO	B	1907	4/4	0.90	0.36	57,58,58,59	0
5	EDO	J	2106	4/4	0.90	0.33	72,72,73,73	0
5	EDO	A	1910	4/4	0.90	0.32	64,69,70,70	0
5	EDO	E	1905	4/4	0.90	0.41	64,68,70,72	0
6	NA	A	1915	1/1	0.90	0.09	51,51,51,51	0
5	EDO	D	1907	4/4	0.90	0.25	56,63,70,70	0
5	EDO	E	1909	4/4	0.91	0.22	69,70,71,72	0
5	EDO	D	1913	4/4	0.91	0.14	61,61,63,66	0
6	NA	F	1911	1/1	0.91	0.14	62,62,62,62	0
6	NA	A	1913	1/1	0.91	0.38	42,42,42,42	0
5	EDO	C	1904	4/4	0.91	0.46	74,76,78,79	0
5	EDO	D	1909	4/4	0.91	0.27	60,61,62,63	0
5	EDO	E	1906	4/4	0.91	0.14	68,75,75,75	0
6	NA	D	1916	1/1	0.91	0.10	55,55,55,55	0
6	NA	K	2103	1/1	0.92	0.16	69,69,69,69	0
5	EDO	C	1905	4/4	0.92	0.34	54,57,61,62	0
5	EDO	B	1909	4/4	0.92	0.22	50,53,54,55	0
5	EDO	C	1912	4/4	0.92	0.41	50,52,53,54	0
6	NA	G	2103	1/1	0.92	0.12	37,37,37,37	0
6	NA	B	1917	1/1	0.92	0.44	47,47,47,47	0
6	NA	J	2107	1/1	0.92	0.17	38,38,38,38	0
11	MLI	J	2102	7/7	0.92	0.25	83,86,87,96	0
6	NA	A	1912	1/1	0.93	0.14	65,65,65,65	0
6	NA	E	1914	1/1	0.93	0.16	62,62,62,62	0
5	EDO	F	1908	4/4	0.93	0.45	83,88,92,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NA	C	1915	1/1	0.93	0.74	62,62,62,62	0
4	PNS	B	1901	21/22	0.93	0.33	91,95,106,107	0
5	EDO	D	1914	4/4	0.93	0.29	49,52,54,56	0
10	FMN	K	2101	31/31	0.93	0.20	64,75,80,88	0
5	EDO	D	1904	4/4	0.93	0.22	58,63,66,68	0
5	EDO	E	1907	4/4	0.93	0.18	69,72,73,74	0
5	EDO	B	1908	4/4	0.94	0.17	58,62,62,62	0
5	EDO	E	1913	4/4	0.94	0.54	78,81,86,86	0
11	MLI	G	2102	7/7	0.94	0.27	78,86,91,92	0
5	EDO	E	1904	4/4	0.94	0.30	67,70,72,74	0
5	EDO	A	1904	4/4	0.94	0.37	59,63,65,65	0
4	PNS	F	1901	21/22	0.94	0.29	89,92,102,103	0
5	EDO	J	2103	4/4	0.94	0.22	69,71,71,71	0
4	PNS	C	1901	21/22	0.94	0.25	75,78,88,89	0
6	NA	A	1914	1/1	0.94	0.36	55,55,55,55	0
5	EDO	A	1906	4/4	0.95	0.30	53,58,58,59	0
6	NA	C	1913	1/1	0.95	0.07	56,56,56,56	0
6	NA	D	1921	1/1	0.95	0.15	52,52,52,52	0
5	EDO	D	1905	4/4	0.95	0.24	45,46,47,49	0
8	ACT	C	1902	4/4	0.95	0.24	59,62,63,65	0
4	PNS	E	1901	21/22	0.95	0.29	86,88,91,92	0
5	EDO	E	1902	4/4	0.95	0.40	51,51,51,52	0
6	NA	L	2103	1/1	0.95	0.17	66,66,66,66	0
6	NA	L	2102	1/1	0.95	0.10	46,46,46,46	0
5	EDO	B	1905	4/4	0.95	0.32	65,66,67,67	0
5	EDO	D	1910	4/4	0.95	0.23	59,63,64,64	0
5	EDO	B	1904	4/4	0.95	0.24	51,53,56,62	0
10	FMN	I	2101	31/31	0.95	0.21	66,73,78,79	0
4	PNS	D	1901	21/22	0.95	0.35	90,93,101,103	0
5	EDO	D	1908	4/4	0.95	0.30	54,56,58,58	0
6	NA	B	1914	1/1	0.96	0.15	43,43,43,43	0
6	NA	E	1916	1/1	0.96	0.23	51,51,51,51	0
4	PNS	A	1901	21/22	0.96	0.27	86,90,101,101	0
6	NA	A	1917	1/1	0.96	0.34	53,53,53,53	0
10	FMN	L	2101	31/31	0.96	0.20	54,62,68,81	0
6	NA	D	1922	1/1	0.96	0.54	46,46,46,46	0
5	EDO	A	1902	4/4	0.96	0.18	47,51,54,54	0
6	NA	B	1916	1/1	0.96	0.31	52,52,52,52	0
5	EDO	E	1903	4/4	0.97	0.24	50,54,55,56	0
6	NA	D	1915	1/1	0.97	0.11	49,49,49,49	0
10	FMN	J	2101	31/31	0.97	0.19	43,46,50,55	0
6	NA	K	2102	1/1	0.97	0.11	53,53,53,53	0

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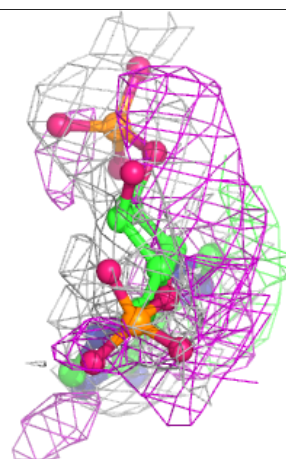
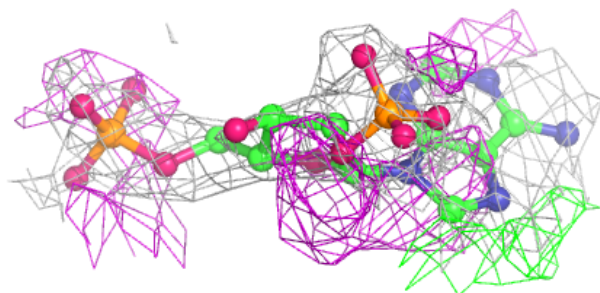
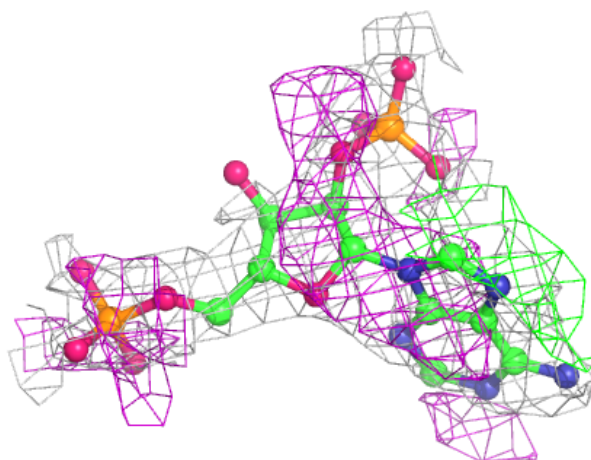
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	FMN	G	2101	31/31	0.97	0.21	46,49,53,56	0
5	EDO	F	1907	4/4	0.97	0.43	54,58,61,63	0
10	FMN	H	2101	31/31	0.97	0.21	43,50,54,61	0
6	NA	D	1917	1/1	0.97	0.46	46,46,46,46	0
5	EDO	F	1903	4/4	0.97	0.23	65,66,70,70	0
6	NA	H	2106	1/1	0.98	0.13	34,34,34,34	0
6	NA	D	1919	1/1	0.98	0.65	46,46,46,46	0
6	NA	B	1913	1/1	0.98	0.12	43,43,43,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

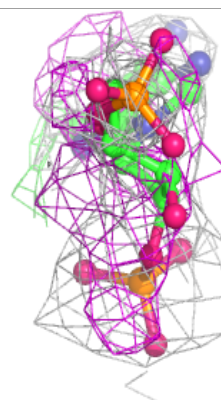
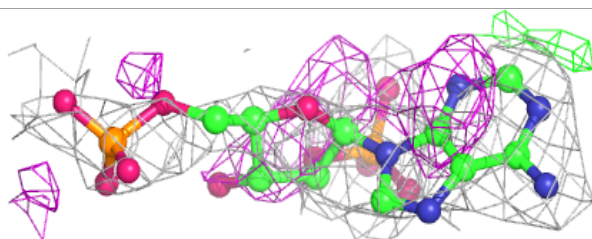
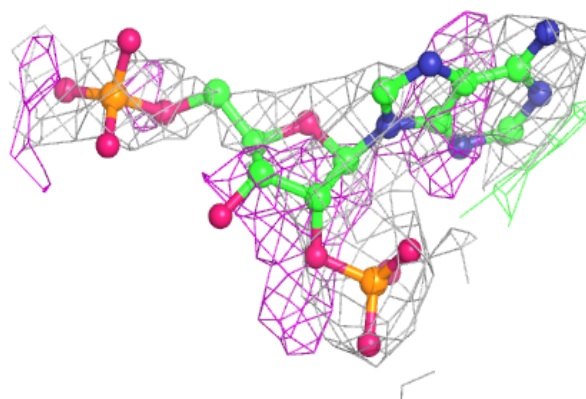
**Electron density around A2P B 1918:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

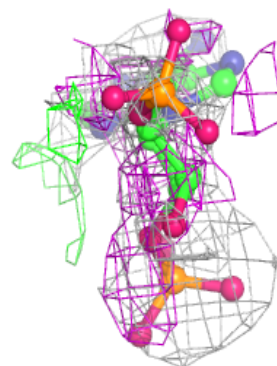
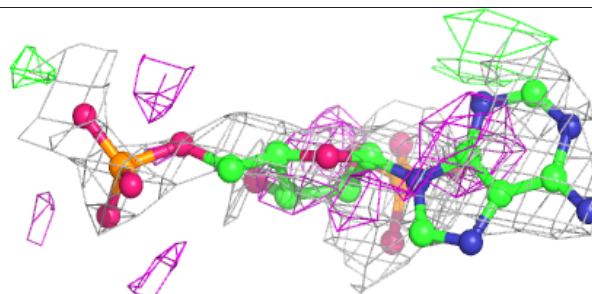
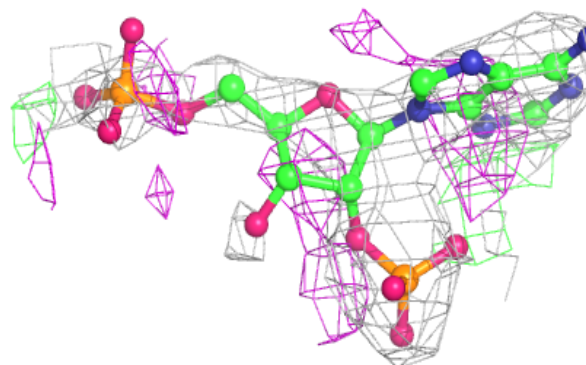


**Electron density around A2P F 1912:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

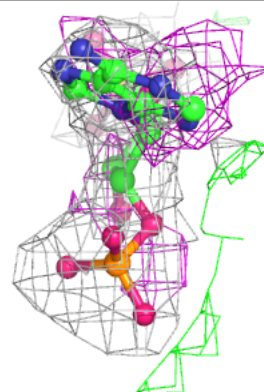
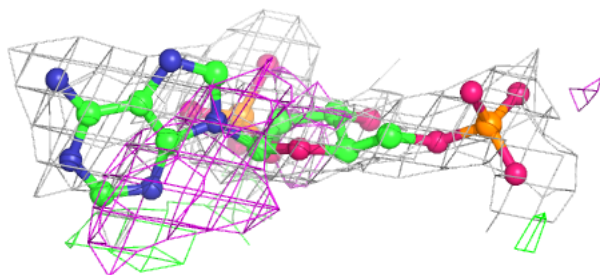
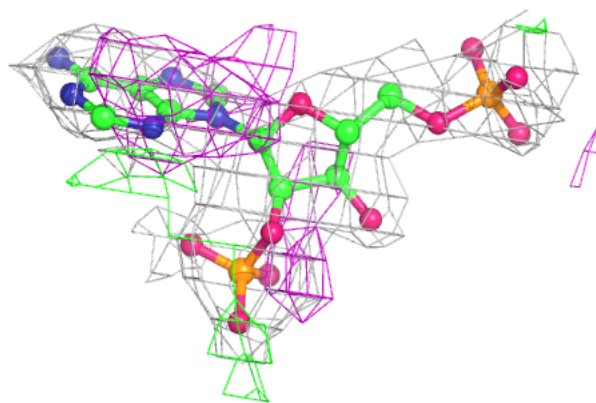
**Electron density around A2P A 1918:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

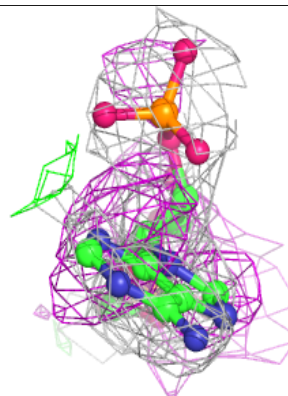
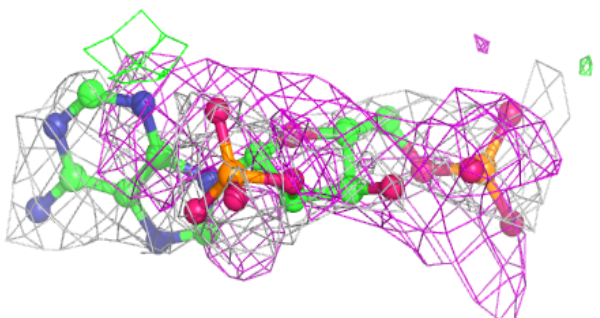
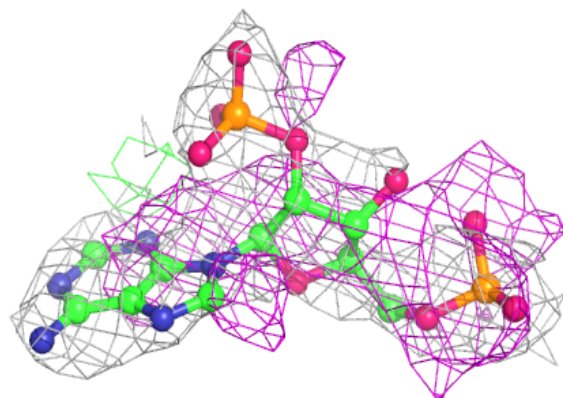


**Electron density around A2P D 1923:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around A2P E 1917:**

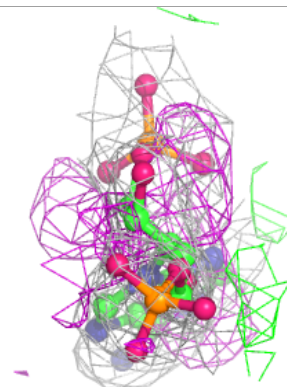
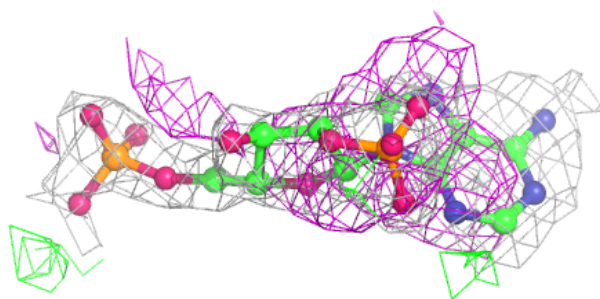
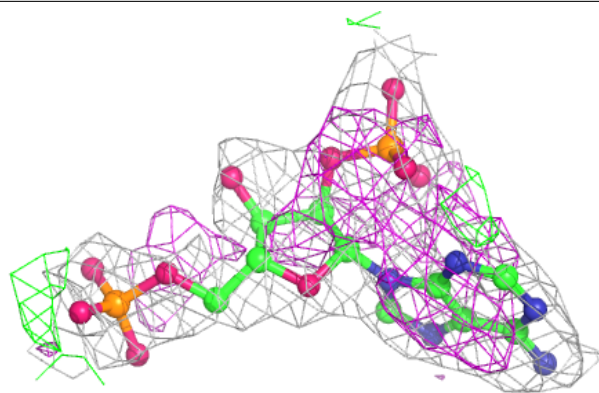
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



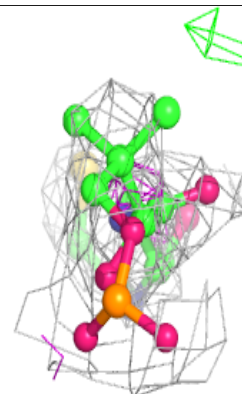
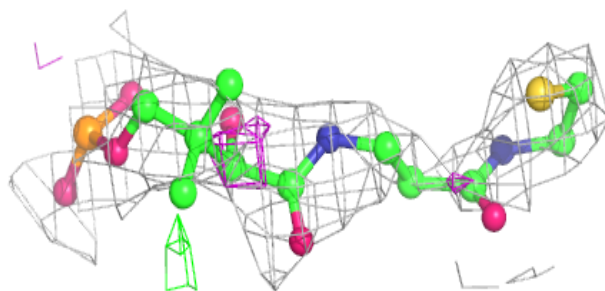
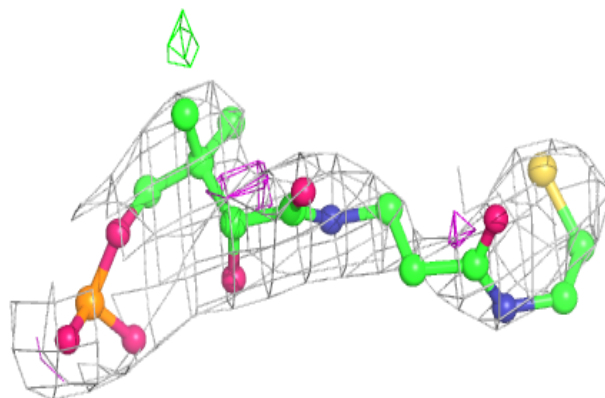


**Electron density around A2P C 1917:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

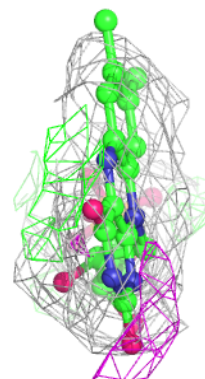
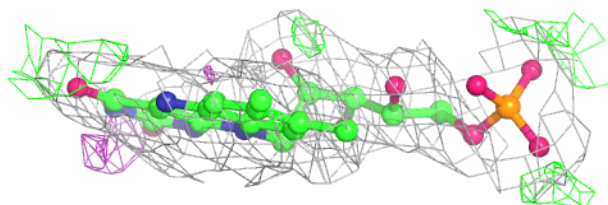
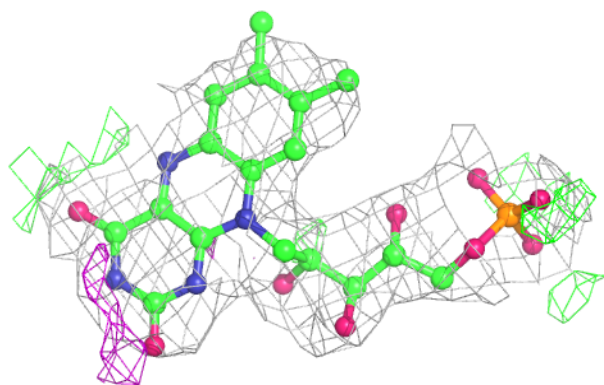
**Electron density around PNS B 1901:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

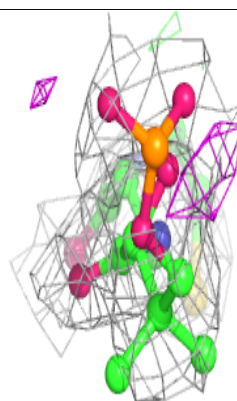
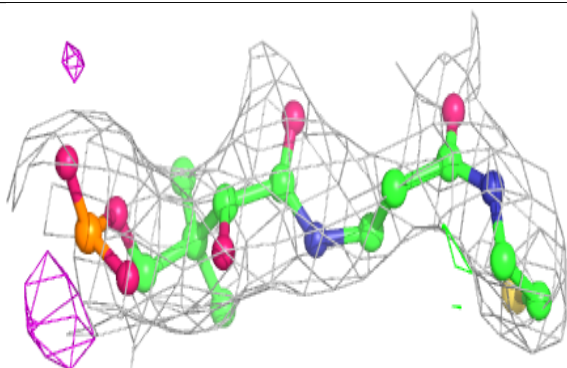
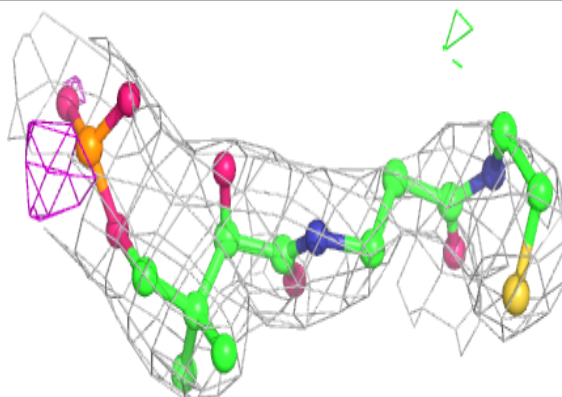


**Electron density around FMN K 2101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PNS F 1901:**

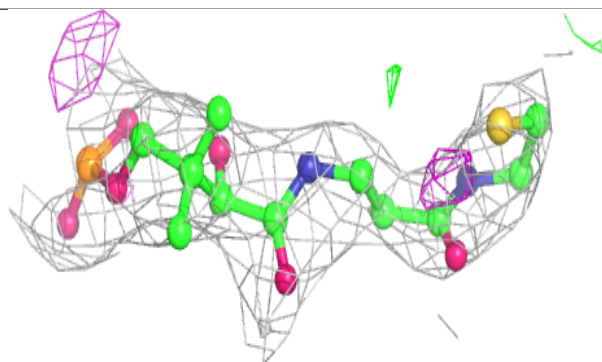
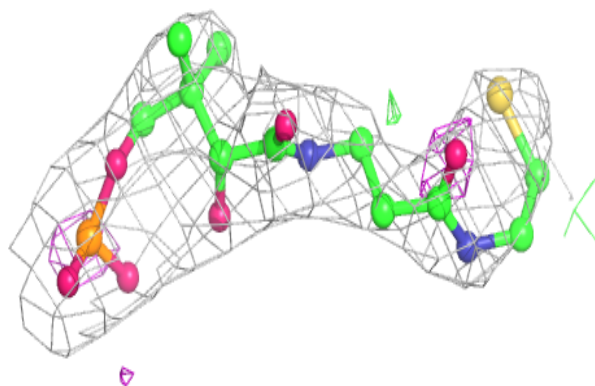
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



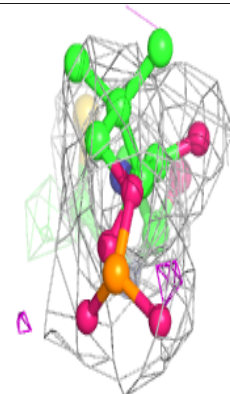
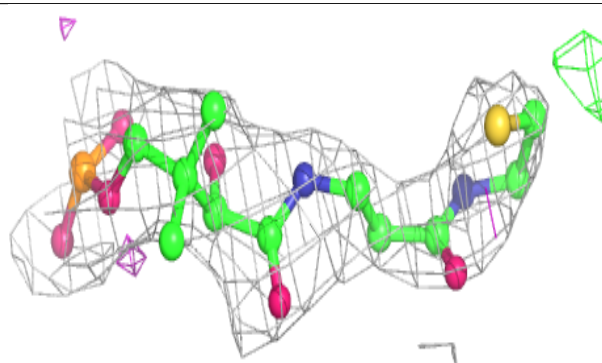
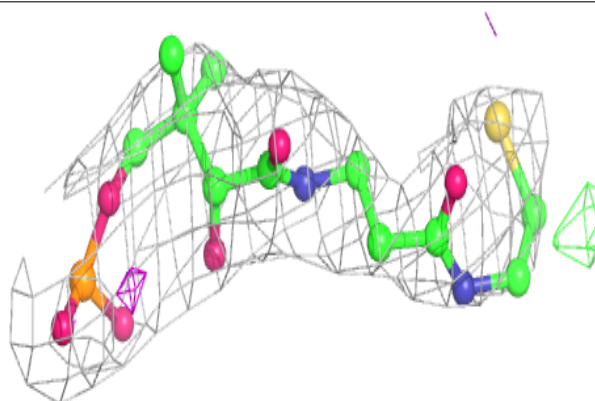


**Electron density around PNS C 1901:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

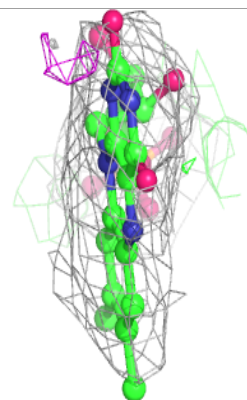
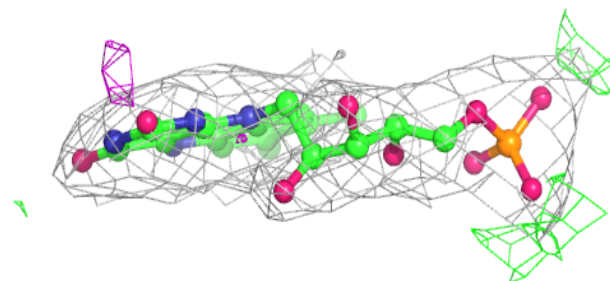
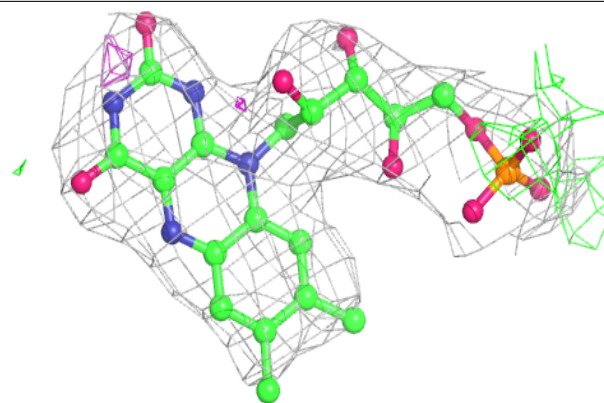
**Electron density around PNS E 1901:**

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and green (positive)

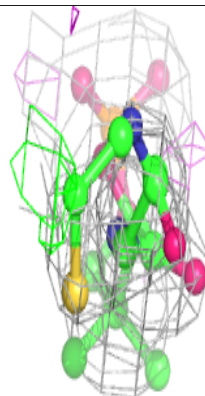
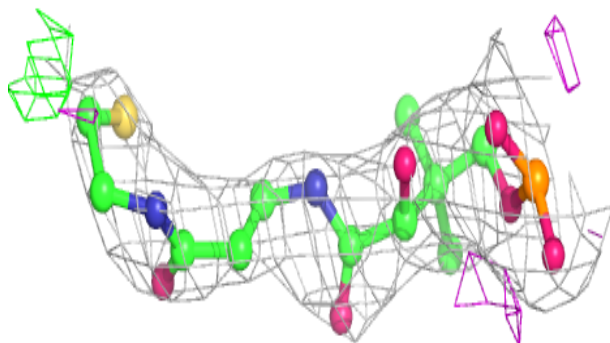
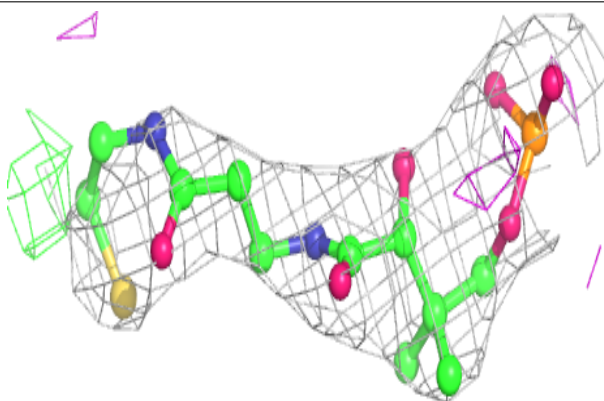


**Electron density around FMN I 2101:**

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and green (positive)

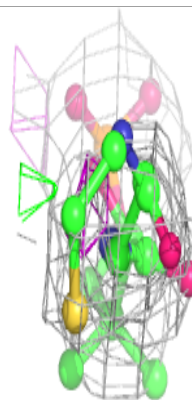
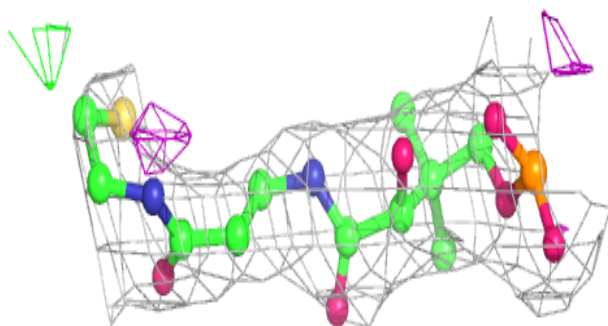
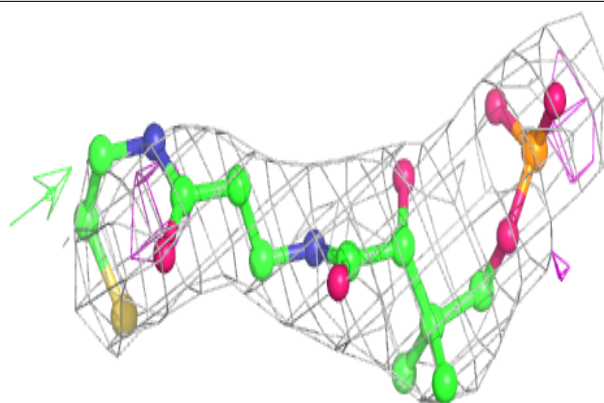
**Electron density around PNS D 1901:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

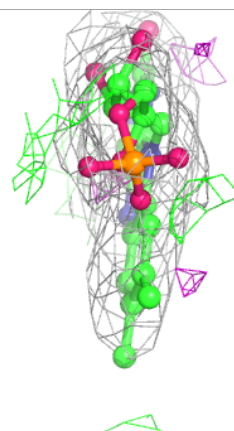
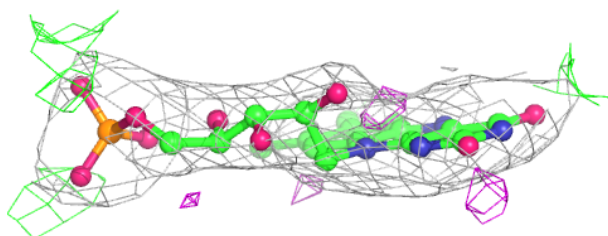
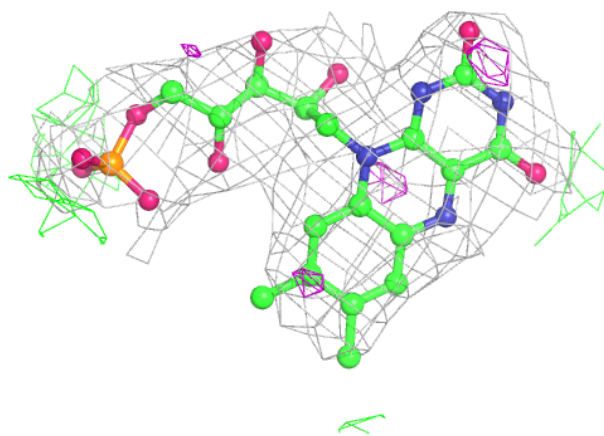


**Electron density around PNS A 1901:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
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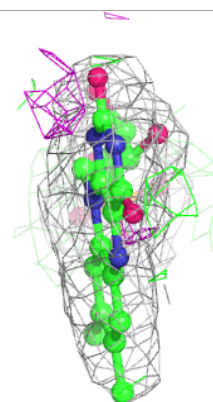
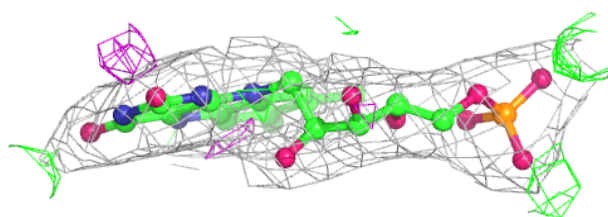
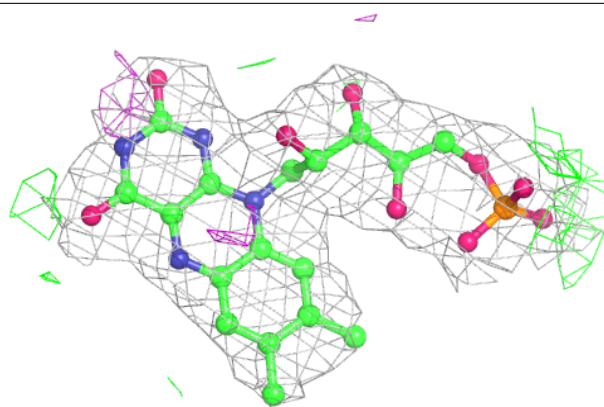
**Electron density around FMN L 2101:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

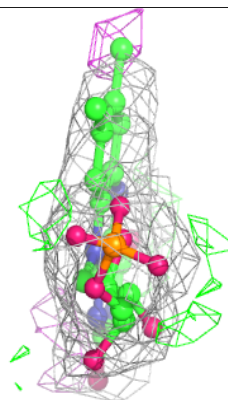
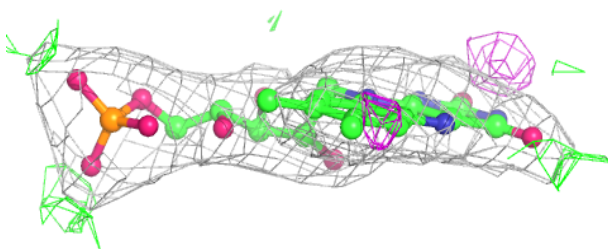
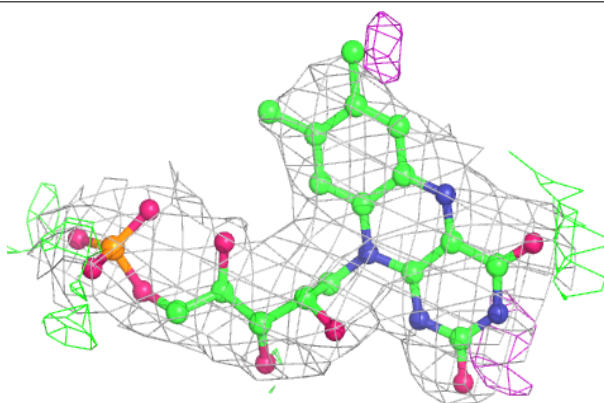


**Electron density around FMN J 2101:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

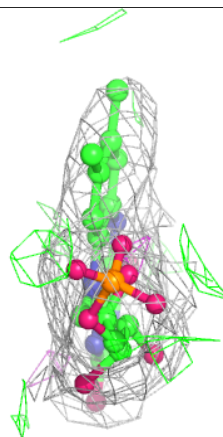
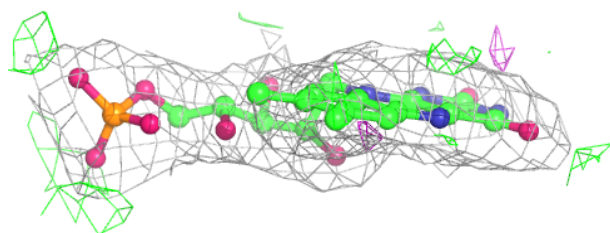
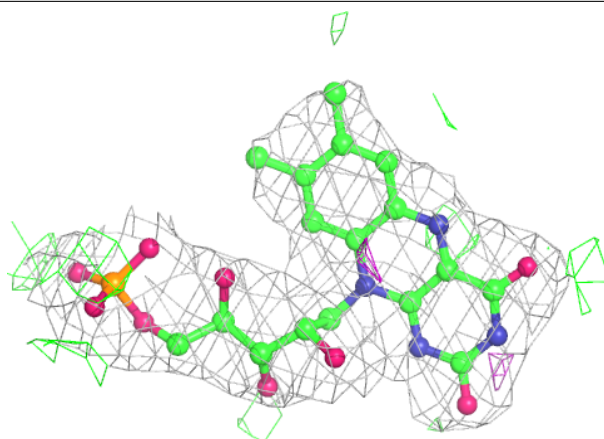
**Electron density around FMN G 2101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN H 2101:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.