



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:15 pm BST

PDB ID : 1OGY
Title : Crystal structure of the heterodimeric nitrate reductase from *Rhodobacter sphaeroides*
Authors : Arnoux, P.; Sabaty, M.; Alric, J.; Frangioni, B.; Guigliarelli, B.; Adriano, J.-M.; Pignol, D.
Deposited on : 2003-05-19
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

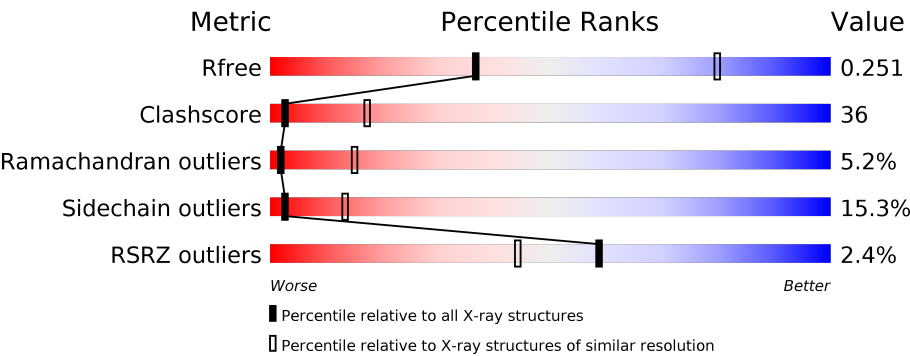
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 ≥ 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	802	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>49%39%11%..</div></div>
1	C	802	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>46%41%11%..</div></div>
1	E	802	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>48%40%10%..</div></div>
1	G	802	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>46%41%11%..</div></div>
1	I	802	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>44%42%12%..</div></div>
1	K	802	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>45%41%11%..</div></div>

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Mol	Chain	Length	Quality of chain
1	M	802	
1	O	802	
2	B	130	
2	D	130	
2	F	130	
2	H	130	
2	J	130	
2	L	130	
2	N	130	
2	P	130	

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
6	HEC	D	1129	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59336 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 PERIPLASMIC NITRATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	C	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	E	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	G	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	I	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	K	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	M	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	O	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			

- Molecule 2 is a protein called DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE.

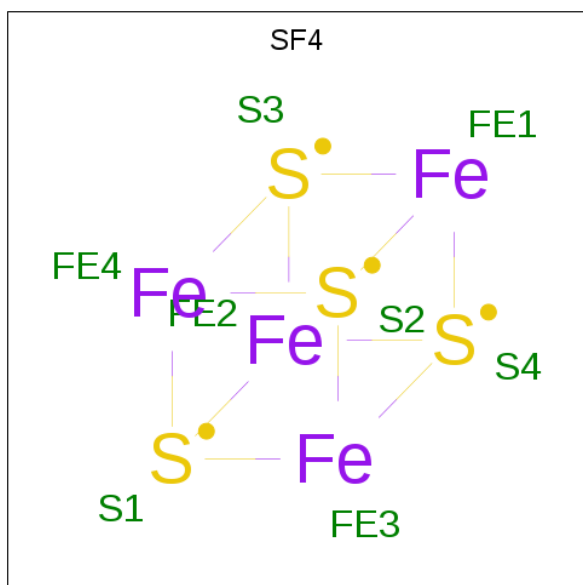
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	D	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	F	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	H	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	J	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	L	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	P	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

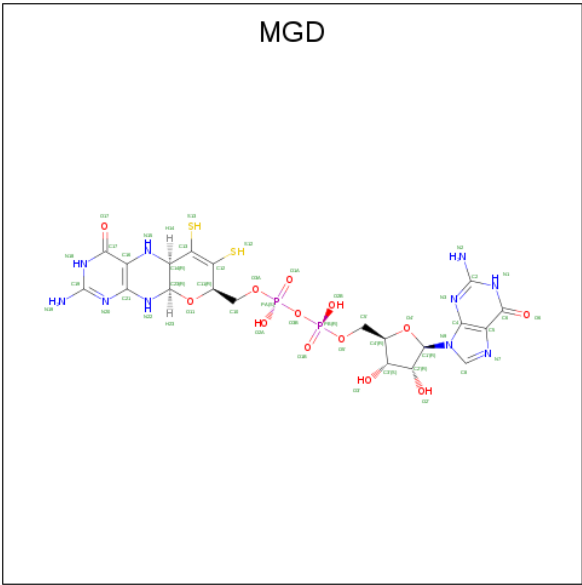


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		
3	I	1	Total	Fe	S	0	0
			8	4	4		
3	K	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mo 1 1	0	0
4	K	1	Total Mo 1 1	0	0
4	E	1	Total Mo 1 1	0	0
4	I	1	Total Mo 1 1	0	0
4	C	1	Total Mo 1 1	0	0
4	A	1	Total Mo 1 1	0	0
4	O	1	Total Mo 1 1	0	0
4	M	1	Total Mo 1 1	0	0

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



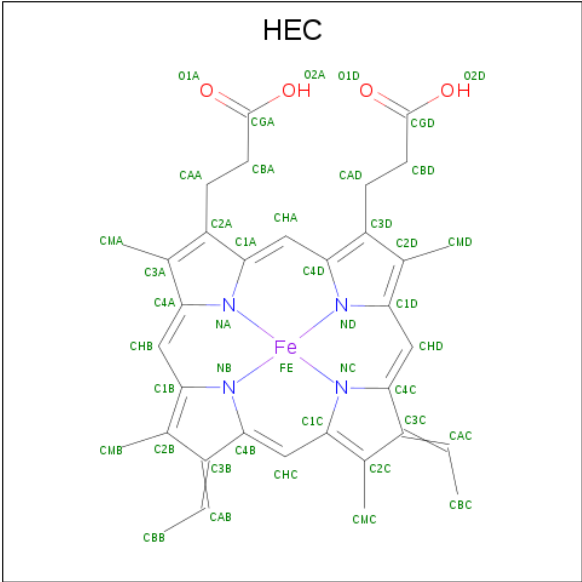
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P S 47 20 10 13 2 2	0	0
5	A	1	Total C N O P S 47 20 10 13 2 2	0	0
5	C	1	Total C N O P S 47 20 10 13 2 2	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	C	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	G	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	G	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	I	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	I	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	K	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	K	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	M	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	M	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	O	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	O	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 6 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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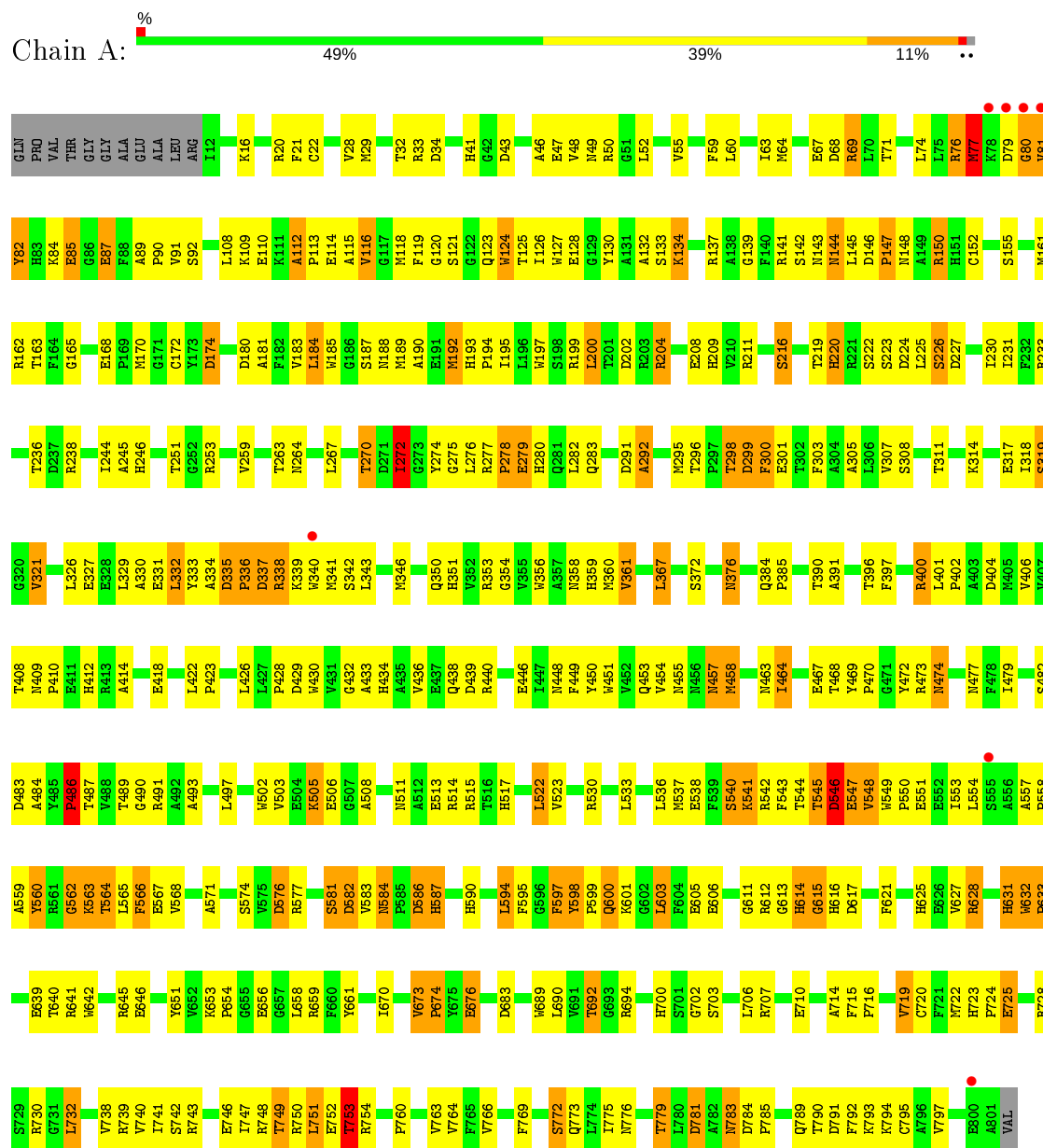
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

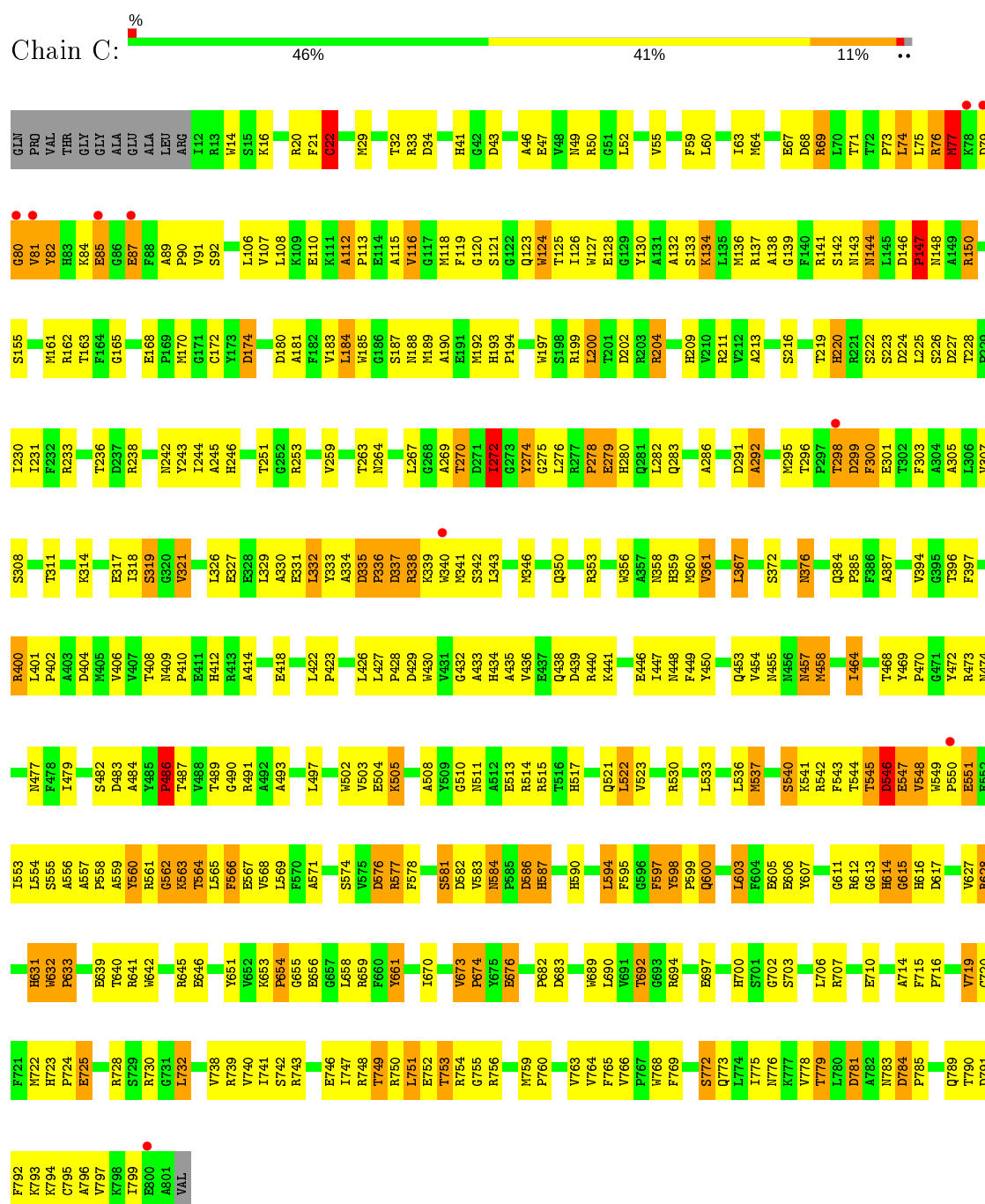
3 Residue-property plots

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.

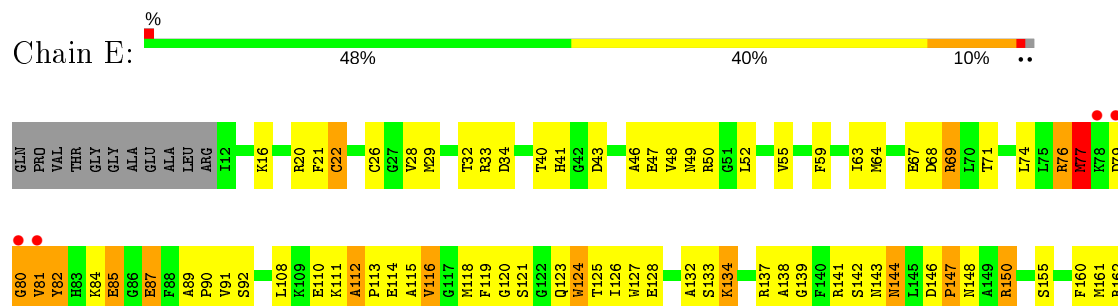
• Molecule 1: PERIPLASMIC NITRATE REDUCTASE

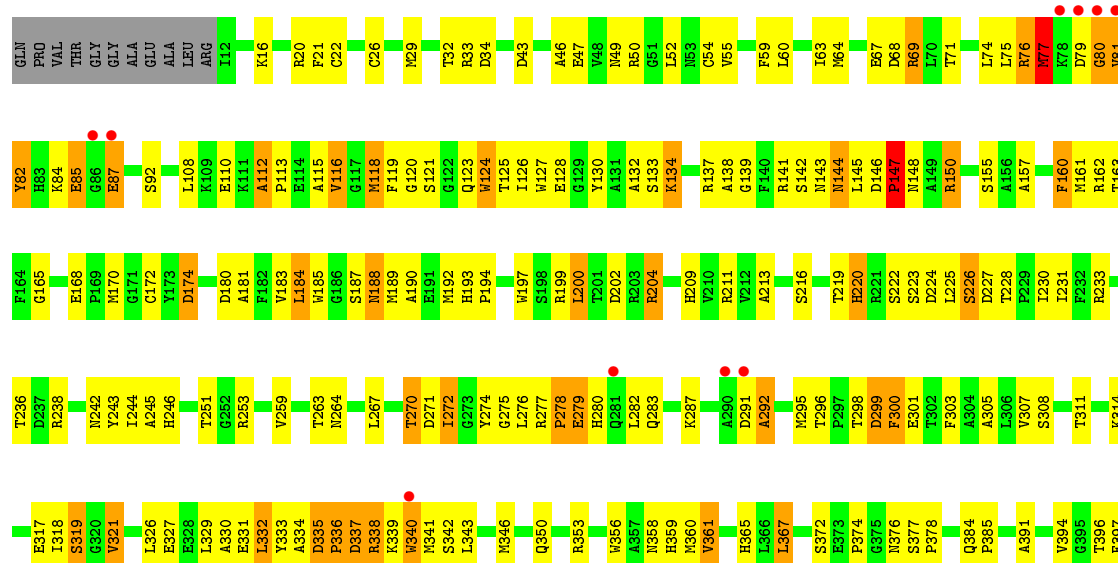


• Molecule 1: PERIPLASMIC NITRATE REDUCTASE

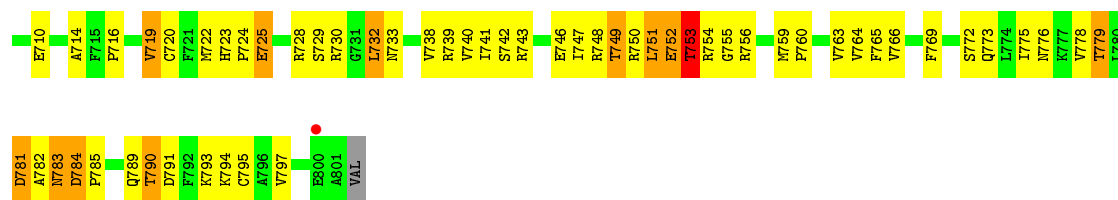


- Molecule 1: PERIPLASMIC NITRATE REDUCTASE

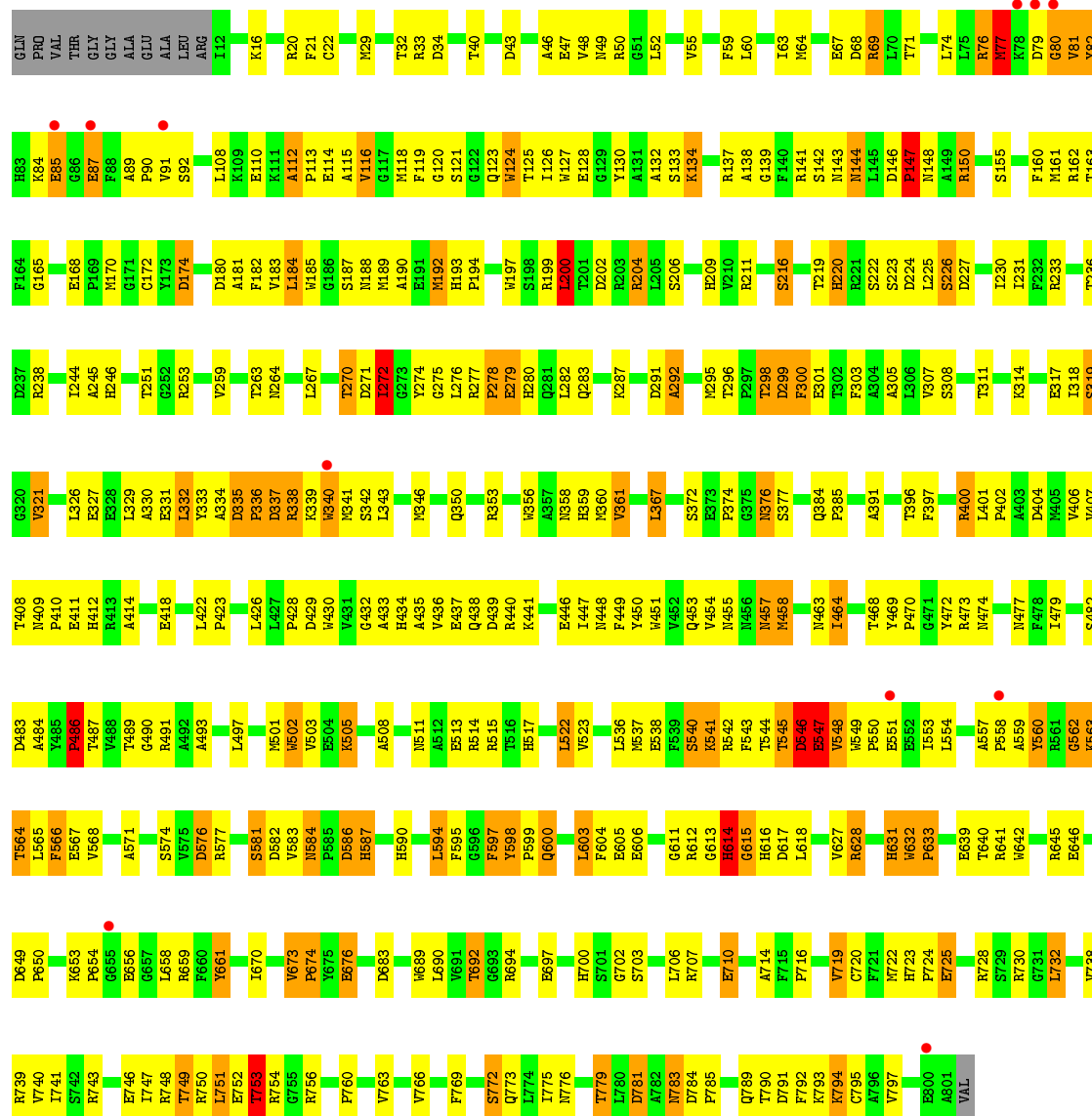




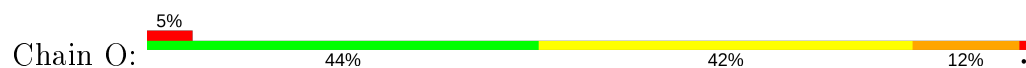


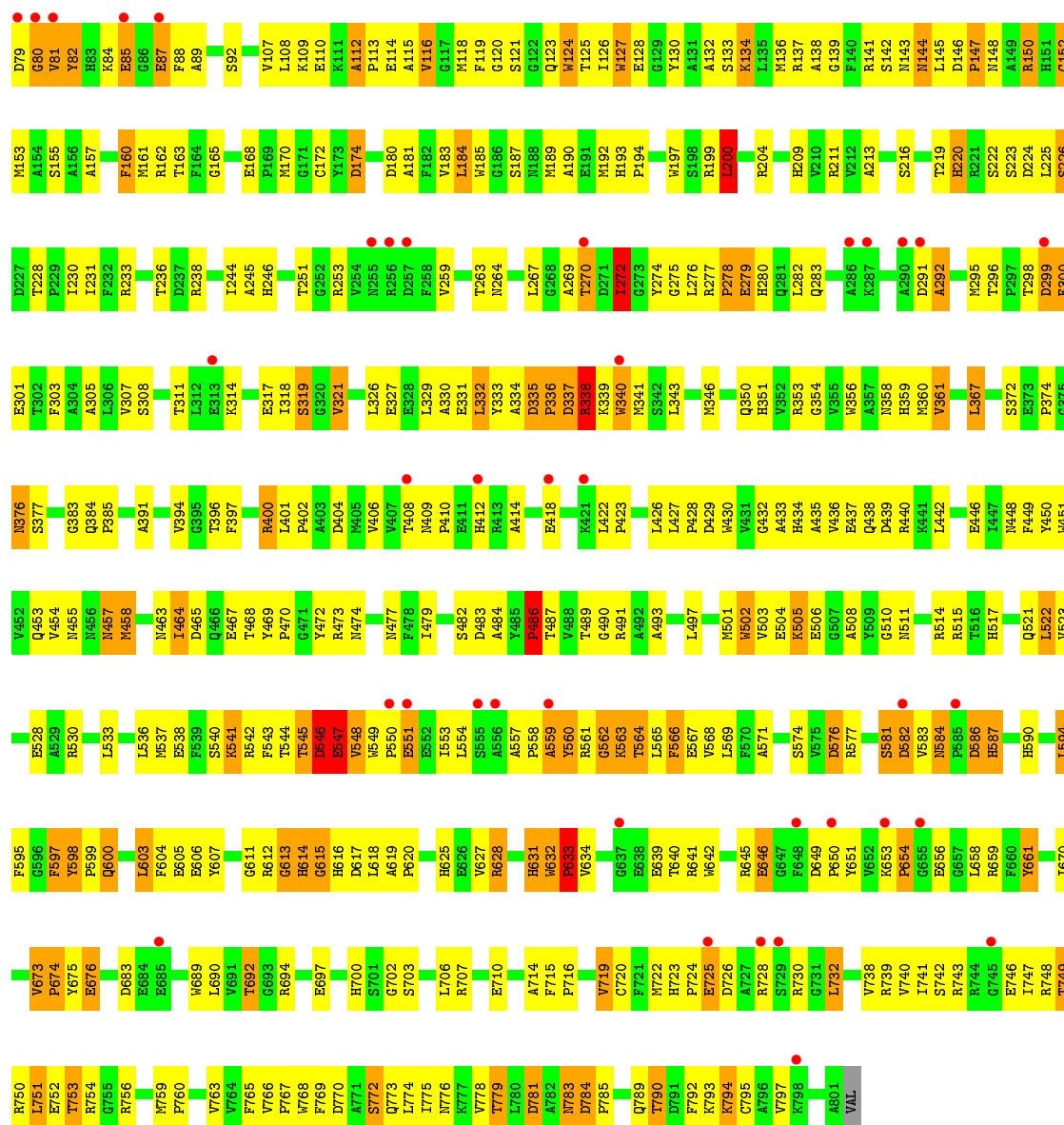


● Molecule 1: PERIPLASMIC NITRATE REDUCTASE

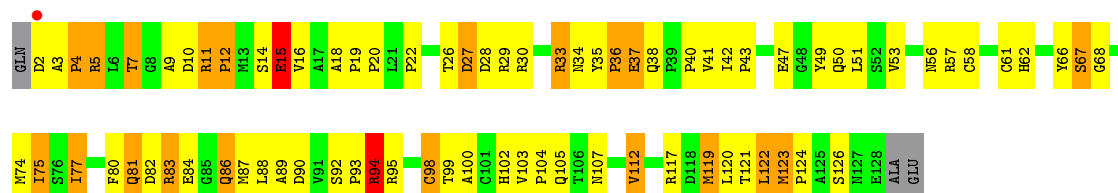


● Molecule 1: PERIPLASMIC NITRATE REDUCTASE



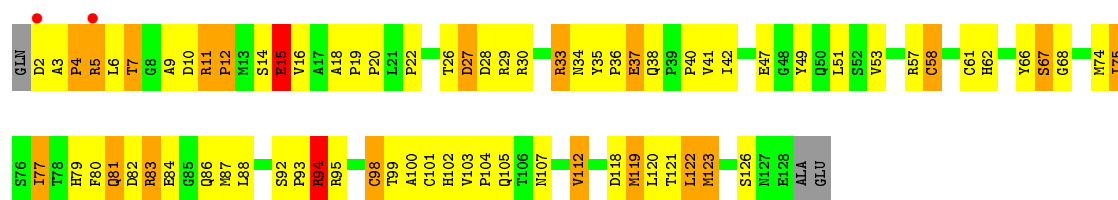


• Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE

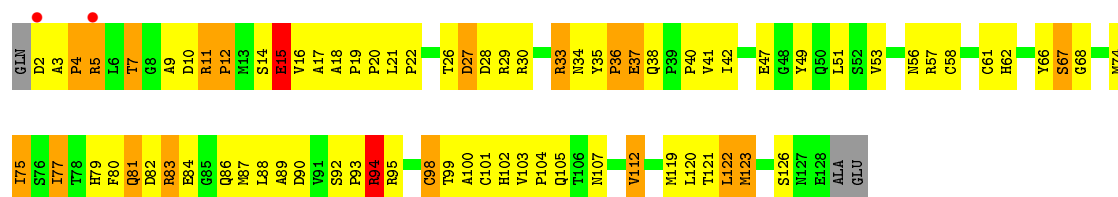


• Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE

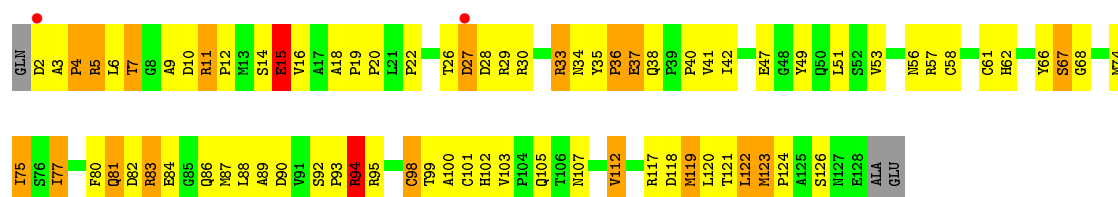




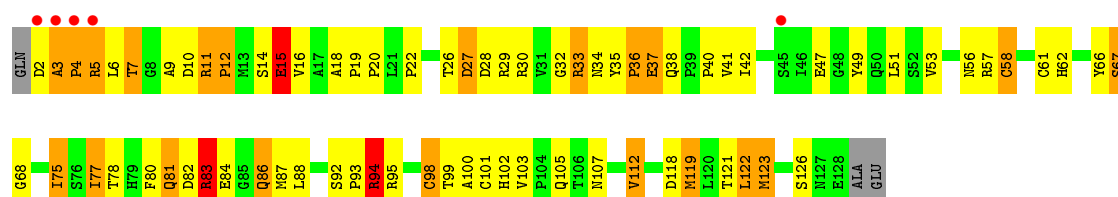
- Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE



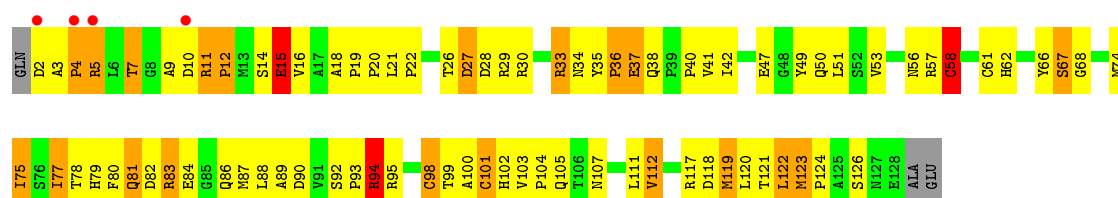
- Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE



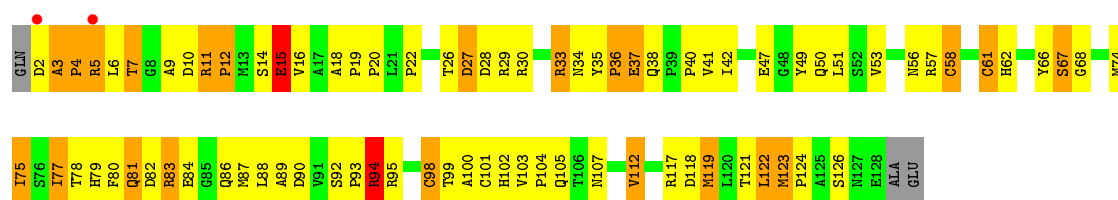
- Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE



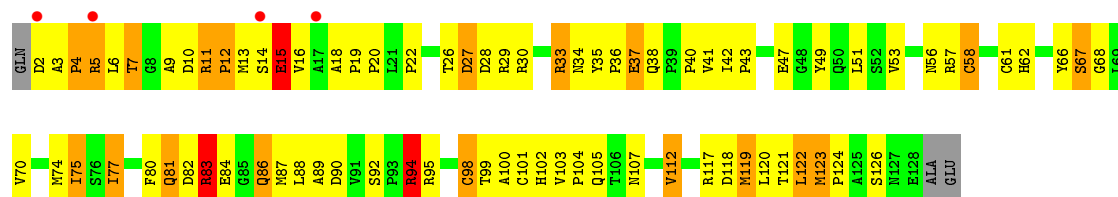
- Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE



- Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE



● Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.00Å 225.20Å 154.60Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 29.94 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-3.20) 97.0 (29.94-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.269 0.235 , 0.251	Depositor DCC
R_{free} test set	1348 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	59336	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SF4, HEC, MO, MGD

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	0.70	2/6433 (0.0%)	0.89	13/8741 (0.1%)
1	C	0.67	1/6433 (0.0%)	0.90	13/8741 (0.1%)
1	E	0.70	3/6433 (0.0%)	0.89	13/8741 (0.1%)
1	G	0.70	1/6433 (0.0%)	0.92	12/8741 (0.1%)
1	I	0.82	2/6433 (0.0%)	0.92	13/8741 (0.1%)
1	K	0.68	2/6433 (0.0%)	0.91	16/8741 (0.2%)
1	M	0.66	1/6433 (0.0%)	0.89	13/8741 (0.1%)
1	O	0.76	1/6433 (0.0%)	0.92	16/8741 (0.2%)
2	B	0.74	0/1001	0.94	1/1368 (0.1%)
2	D	0.72	0/1001	0.93	1/1368 (0.1%)
2	F	0.75	0/1001	0.94	1/1368 (0.1%)
2	H	0.76	0/1001	0.95	1/1368 (0.1%)
2	J	0.73	0/1001	0.96	2/1368 (0.1%)
2	L	0.75	2/1001 (0.2%)	0.95	1/1368 (0.1%)
2	N	0.78	1/1001 (0.1%)	0.95	1/1368 (0.1%)
2	P	0.73	0/1001	0.94	2/1368 (0.1%)
All	All	0.72	16/59472 (0.0%)	0.91	119/80872 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	22	CYS	CB-SG	-9.02	1.67	1.82
1	G	54	CYS	CB-SG	-7.57	1.69	1.82
1	K	22	CYS	CB-SG	-7.20	1.70	1.82
1	I	19	CYS	CB-SG	7.16	1.94	1.82
1	O	152	CYS	CB-SG	6.88	1.94	1.82
1	E	26	CYS	CB-SG	-6.79	1.70	1.82
2	L	58	CYS	CB-SG	-6.61	1.71	1.82
1	C	22	CYS	CB-SG	-6.21	1.71	1.82
2	N	61	CYS	CB-SG	-5.91	1.72	1.81
1	E	192	MET	SD-CE	-5.83	1.45	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	684	GLU	CG-CD	5.46	1.60	1.51
2	L	101	CYS	CB-SG	-5.34	1.73	1.81
1	A	192	MET	SD-CE	-5.30	1.48	1.77
1	I	152	CYS	CB-SG	5.28	1.91	1.82
1	A	208	GLU	CB-CG	5.07	1.61	1.52
1	M	192	MET	SD-CE	-5.03	1.49	1.77

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	632	TRP	C-N-CD	-24.39	66.94	120.60
1	K	632	TRP	C-N-CD	-22.20	71.75	120.60
1	O	632	TRP	C-N-CD	-21.86	72.50	120.60
1	I	632	TRP	C-N-CD	-21.10	74.19	120.60
1	E	632	TRP	C-N-CD	-17.95	81.12	120.60
1	A	632	TRP	C-N-CD	-17.56	81.97	120.60
1	C	632	TRP	C-N-CD	-17.30	82.54	120.60
1	M	632	TRP	C-N-CD	-16.23	84.90	120.60
1	K	632	TRP	C-N-CA	12.72	175.44	122.00
1	I	632	TRP	C-N-CA	11.67	171.02	122.00
1	A	632	TRP	C-N-CA	11.06	168.45	122.00
1	G	632	TRP	C-N-CA	11.01	168.25	122.00
1	E	632	TRP	C-N-CA	10.88	167.70	122.00
1	C	632	TRP	C-N-CA	10.86	167.62	122.00
1	O	632	TRP	C-N-CA	10.73	167.06	122.00
1	M	632	TRP	C-N-CA	9.09	160.19	122.00
2	J	94	ARG	N-CA-C	-8.05	89.26	111.00
2	D	94	ARG	N-CA-C	-7.69	90.23	111.00
2	F	94	ARG	N-CA-C	-7.69	90.24	111.00
1	K	613	GLY	N-CA-C	-7.67	93.92	113.10
2	P	94	ARG	N-CA-C	-7.67	90.29	111.00
2	B	94	ARG	N-CA-C	-7.64	90.38	111.00
1	G	613	GLY	N-CA-C	-7.62	94.05	113.10
1	C	613	GLY	N-CA-C	-7.59	94.13	113.10
1	E	613	GLY	N-CA-C	-7.59	94.13	113.10
1	M	613	GLY	N-CA-C	-7.54	94.26	113.10
1	O	200	LEU	CA-CB-CG	7.49	132.52	115.30
2	L	94	ARG	N-CA-C	-7.48	90.80	111.00
2	N	94	ARG	N-CA-C	-7.47	90.84	111.00
1	G	200	LEU	CA-CB-CG	7.41	132.35	115.30
2	H	94	ARG	N-CA-C	-7.41	91.00	111.00
1	I	613	GLY	N-CA-C	-7.25	94.98	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	613	GLY	N-CA-C	-7.22	95.06	113.10
1	I	200	LEU	CA-CB-CG	7.19	131.83	115.30
1	E	200	LEU	CA-CB-CG	7.17	131.78	115.30
1	A	613	GLY	N-CA-C	-7.16	95.20	113.10
1	A	80	GLY	N-CA-C	-7.11	95.32	113.10
1	G	80	GLY	N-CA-C	-7.10	95.36	113.10
1	C	200	LEU	CA-CB-CG	7.05	131.51	115.30
1	K	80	GLY	N-CA-C	-7.03	95.54	113.10
1	A	200	LEU	CA-CB-CG	7.00	131.39	115.30
1	M	200	LEU	CA-CB-CG	6.96	131.31	115.30
1	I	80	GLY	N-CA-C	-6.91	95.83	113.10
1	C	80	GLY	N-CA-C	-6.84	96.01	113.10
1	E	80	GLY	N-CA-C	-6.82	96.06	113.10
1	M	80	GLY	N-CA-C	-6.80	96.09	113.10
1	I	633	PRO	CA-N-CD	-6.79	101.99	111.50
1	I	594	LEU	N-CA-C	-6.68	92.97	111.00
1	O	80	GLY	N-CA-C	-6.57	96.67	113.10
1	K	200	LEU	CA-CB-CG	6.53	130.31	115.30
1	G	594	LEU	N-CA-C	-6.33	93.92	111.00
1	K	594	LEU	N-CA-C	-6.30	93.99	111.00
1	O	594	LEU	N-CA-C	-6.28	94.05	111.00
1	O	633	PRO	CA-N-CD	-6.21	102.80	111.50
1	E	594	LEU	N-CA-C	-6.12	94.49	111.00
1	M	594	LEU	N-CA-C	-6.07	94.62	111.00
1	C	594	LEU	N-CA-C	-6.04	94.69	111.00
1	E	749	THR	N-CA-C	-6.02	94.73	111.00
1	O	749	THR	N-CA-C	-5.87	95.16	111.00
1	I	632	TRP	CB-CA-C	-5.85	98.70	110.40
1	E	278	PRO	N-CA-C	-5.83	96.93	112.10
1	K	278	PRO	N-CA-C	-5.83	96.94	112.10
1	O	632	TRP	N-CA-C	5.82	126.71	111.00
1	I	632	TRP	N-CA-C	5.79	126.62	111.00
1	A	594	LEU	N-CA-C	-5.78	95.38	111.00
1	M	278	PRO	N-CA-C	-5.77	97.09	112.10
1	G	749	THR	N-CA-C	-5.75	95.46	111.00
1	K	338	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	G	278	PRO	N-CA-C	-5.63	97.46	112.10
1	O	278	PRO	N-CA-C	-5.61	97.51	112.10
1	A	749	THR	N-CA-C	-5.58	95.95	111.00
1	C	278	PRO	N-CA-C	-5.57	97.61	112.10
1	C	749	THR	N-CA-C	-5.56	95.98	111.00
1	A	562	GLY	N-CA-C	-5.55	99.21	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	546	ASP	N-CA-C	-5.53	96.07	111.00
1	I	278	PRO	N-CA-C	-5.52	97.75	112.10
1	M	546	ASP	N-CA-C	-5.51	96.11	111.00
1	E	562	GLY	N-CA-C	-5.50	99.36	113.10
1	I	749	THR	N-CA-C	-5.48	96.21	111.00
1	K	270	THR	N-CA-C	5.48	125.79	111.00
1	M	749	THR	N-CA-C	-5.47	96.23	111.00
1	K	749	THR	N-CA-C	-5.46	96.25	111.00
1	M	581	SER	N-CA-C	-5.46	96.26	111.00
1	A	278	PRO	N-CA-C	-5.44	97.95	112.10
1	O	546	ASP	N-CA-C	-5.44	96.31	111.00
1	I	546	ASP	N-CA-C	-5.43	96.34	111.00
1	A	581	SER	N-CA-C	-5.41	96.40	111.00
1	K	562	GLY	N-CA-C	-5.40	99.59	113.10
1	C	546	ASP	N-CA-C	-5.40	96.42	111.00
1	M	562	GLY	N-CA-C	-5.38	99.65	113.10
1	K	581	SER	N-CA-C	-5.38	96.48	111.00
2	P	83	ARG	N-CA-C	-5.28	96.73	111.00
1	M	270	THR	N-CA-C	5.28	125.26	111.00
1	E	546	ASP	N-CA-C	-5.28	96.75	111.00
1	G	546	ASP	N-CA-C	-5.26	96.80	111.00
1	C	581	SER	N-CA-C	-5.24	96.85	111.00
1	K	546	ASP	N-CA-C	-5.22	96.90	111.00
1	O	562	GLY	N-CA-C	-5.22	100.06	113.10
1	K	632	TRP	N-CA-C	5.16	124.93	111.00
1	G	562	GLY	N-CA-C	-5.16	100.21	113.10
2	J	83	ARG	N-CA-C	-5.15	97.10	111.00
1	E	581	SER	N-CA-C	-5.14	97.11	111.00
1	M	753	THR	N-CA-C	-5.14	97.12	111.00
1	K	753	THR	N-CA-C	-5.14	97.13	111.00
1	O	581	SER	N-CA-C	-5.13	97.14	111.00
1	G	270	THR	N-CA-C	5.13	124.86	111.00
1	O	338	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	I	581	SER	N-CA-C	-5.11	97.20	111.00
1	A	753	THR	N-CA-C	-5.11	97.20	111.00
1	A	270	THR	N-CA-C	5.10	124.77	111.00
1	E	753	THR	N-CA-C	-5.10	97.23	111.00
1	E	270	THR	N-CA-C	5.08	124.71	111.00
1	K	784	ASP	N-CA-C	-5.07	97.31	111.00
1	O	784	ASP	N-CA-C	-5.06	97.33	111.00
1	C	270	THR	N-CA-C	5.04	124.60	111.00
1	C	562	GLY	N-CA-C	-5.01	100.57	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	784	ASP	N-CA-C	-5.01	97.47	111.00
1	O	270	THR	N-CA-C	5.01	124.52	111.00
1	G	633	PRO	N-CA-C	-5.00	99.10	112.10

There are no chirality outliers.

There are no planarity outliers.

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	6251	0	5967	418	2
1	C	6251	0	5966	441	3
1	E	6251	0	5968	421	1
1	G	6251	0	5966	430	0
1	I	6251	0	5967	466	0
1	K	6251	0	5966	449	3
1	M	6251	0	5966	427	1
1	O	6251	0	5967	470	0
2	B	977	0	937	92	0
2	D	977	0	941	107	0
2	F	977	0	941	95	0
2	H	977	0	941	113	0
2	J	977	0	941	103	0
2	L	977	0	941	107	0
2	N	977	0	941	111	0
2	P	977	0	941	114	0
3	A	8	0	0	0	0
3	C	8	0	0	1	0
3	E	8	0	0	1	0
3	G	8	0	0	0	0
3	I	8	0	0	0	0
3	K	8	0	0	1	0
3	M	8	0	0	0	0
3	O	8	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
5	A	94	0	44	15	0
5	C	94	0	44	14	0
5	E	94	0	44	15	0
5	G	94	0	44	13	0
5	I	94	0	44	13	0
5	K	94	0	44	15	0
5	M	94	0	44	15	0
5	O	94	0	44	15	0
6	B	86	0	60	15	0
6	D	86	0	64	33	0
6	F	86	0	64	23	0
6	H	86	0	64	27	0
6	J	86	0	64	27	0
6	L	86	0	64	26	0
6	N	86	0	64	30	0
6	P	86	0	64	25	0
All	All	59336	0	56117	4193	5

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 36.

All (4193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:58:CYS:SG	6:N:1128:HEC:HAB	1.34	1.64
2:F:98:CYS:SG	6:F:1129:HEC:HAB	1.39	1.61
2:J:98:CYS:SG	6:J:1129:HEC:HAB	1.38	1.61
2:H:58:CYS:SG	6:H:1128:HEC:HAB	1.41	1.60
2:D:98:CYS:SG	6:D:1129:HEC:HAB	1.45	1.57
2:J:58:CYS:SG	6:J:1128:HEC:HAB	1.44	1.56
2:H:98:CYS:SG	6:H:1129:HEC:HAB	1.43	1.55
2:L:98:CYS:SG	6:L:1129:HEC:HAB	1.47	1.53
1:I:405:MET:CE	1:I:405:MET:SD	2.01	1.47
2:N:98:CYS:SG	6:N:1129:HEC:HAB	1.51	1.46
2:D:58:CYS:SG	6:D:1128:HEC:HAB	1.57	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:61:CYS:SG	6:F:1128:HEC:HAC	1.55	1.44
2:H:61:CYS:SG	6:H:1128:HEC:HAC	1.59	1.42
2:F:58:CYS:SG	6:F:1128:HEC:HAB	1.61	1.41
2:L:58:CYS:SG	6:L:1128:HEC:HAB	1.61	1.40
2:P:98:CYS:SG	6:P:1129:HEC:HAB	1.62	1.39
2:J:61:CYS:SG	6:J:1128:HEC:HAC	1.63	1.36
2:H:58:CYS:SG	6:H:1128:HEC:CAB	2.17	1.32
2:P:58:CYS:SG	6:P:1128:HEC:HAB	1.69	1.30
2:L:61:CYS:SG	6:L:1128:HEC:HAC	1.73	1.28
2:D:98:CYS:SG	6:D:1129:HEC:CAB	2.24	1.26
1:G:181:ALA:HB3	1:G:340:TRP:CZ3	1.70	1.24
2:D:58:CYS:SG	6:D:1128:HEC:CAB	2.26	1.23
2:F:58:CYS:SG	6:F:1128:HEC:CAB	2.25	1.23
2:P:98:CYS:SG	6:P:1129:HEC:CAB	2.28	1.21
1:I:181:ALA:HB3	1:I:340:TRP:CZ3	1.76	1.21
2:N:58:CYS:SG	6:N:1128:HEC:CAB	2.28	1.20
2:P:3:ALA:HB1	2:P:4:PRO:HD2	1.24	1.19
2:F:98:CYS:SG	6:F:1129:HEC:CAB	2.31	1.19
2:P:61:CYS:SG	6:P:1128:HEC:HAC	1.83	1.19
1:M:181:ALA:HB3	1:M:340:TRP:CZ3	1.77	1.18
1:I:550:PRO:HG2	1:I:553:ILE:HD12	1.21	1.18
2:L:98:CYS:SG	6:L:1129:HEC:CAB	2.30	1.18
2:D:3:ALA:HB1	2:D:4:PRO:HD2	1.24	1.18
1:K:181:ALA:HB3	1:K:340:TRP:CZ3	1.79	1.17
1:O:181:ALA:HB3	1:O:340:TRP:CZ3	1.80	1.17
1:I:747:ILE:HD11	1:I:775:ILE:HA	1.22	1.17
1:C:181:ALA:HB3	1:C:340:TRP:CZ3	1.78	1.16
1:G:747:ILE:HD11	1:G:775:ILE:HA	1.23	1.16
1:O:550:PRO:HG2	1:O:553:ILE:HD12	1.19	1.16
1:C:747:ILE:HD11	1:C:775:ILE:HA	1.27	1.16
1:A:181:ALA:HB3	1:A:340:TRP:CZ3	1.79	1.16
2:H:98:CYS:SG	6:H:1129:HEC:CAB	2.33	1.16
1:M:112:ALA:HB1	1:M:113:PRO:HD2	1.23	1.16
1:K:550:PRO:HG2	1:K:553:ILE:HD12	1.26	1.16
2:J:3:ALA:HB1	2:J:4:PRO:HD2	1.23	1.15
2:J:98:CYS:SG	6:J:1129:HEC:CAB	2.34	1.15
1:M:550:PRO:HG2	1:M:553:ILE:HD12	1.29	1.15
1:A:550:PRO:HG2	1:A:553:ILE:HD12	1.27	1.15
2:H:3:ALA:HB1	2:H:4:PRO:HD2	1.26	1.15
1:E:181:ALA:HB3	1:E:340:TRP:CZ3	1.81	1.15
1:E:550:PRO:HG2	1:E:553:ILE:HD12	1.27	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:747:ILE:HD11	1:M:775:ILE:HA	1.25	1.13
2:D:61:CYS:SG	6:D:1128:HEC:HAC	1.87	1.13
2:F:3:ALA:HB1	2:F:4:PRO:HD2	1.25	1.13
1:G:550:PRO:HG2	1:G:553:ILE:HD12	1.25	1.13
1:I:112:ALA:HB1	1:I:113:PRO:HD2	1.20	1.12
1:E:112:ALA:HB1	1:E:113:PRO:HD2	1.21	1.12
1:G:112:ALA:HB1	1:G:113:PRO:HD2	1.17	1.12
1:O:747:ILE:HD11	1:O:775:ILE:HA	1.25	1.11
1:A:747:ILE:HD11	1:A:775:ILE:HA	1.30	1.11
1:C:550:PRO:HG2	1:C:553:ILE:HD12	1.24	1.11
1:O:192:MET:HE2	1:O:694:ARG:HB2	1.29	1.11
2:L:3:ALA:HB1	2:L:4:PRO:HD2	1.26	1.10
2:P:4:PRO:HG3	2:P:16:VAL:HG11	1.31	1.10
2:L:58:CYS:SG	6:L:1128:HEC:CAB	2.39	1.10
2:F:61:CYS:SG	6:F:1128:HEC:CAC	2.38	1.10
1:A:112:ALA:HB1	1:A:113:PRO:HD2	1.18	1.09
1:K:112:ALA:HB1	1:K:113:PRO:HD2	1.13	1.09
1:E:747:ILE:HD11	1:E:775:ILE:HA	1.27	1.09
1:C:112:ALA:HB1	1:C:113:PRO:HD2	1.15	1.09
2:H:61:CYS:SG	6:H:1128:HEC:CAC	2.39	1.09
2:P:58:CYS:SG	6:P:1128:HEC:CAB	2.39	1.09
2:B:3:ALA:HB1	2:B:4:PRO:HD2	1.28	1.09
2:L:4:PRO:HG3	2:L:16:VAL:HG11	1.35	1.09
2:N:98:CYS:SG	6:N:1129:HEC:CAB	2.41	1.08
2:B:4:PRO:HG3	2:B:16:VAL:HG11	1.34	1.08
1:K:747:ILE:HD11	1:K:775:ILE:HA	1.22	1.08
2:N:61:CYS:SG	6:N:1128:HEC:HAC	1.92	1.08
2:J:4:PRO:HG3	2:J:16:VAL:HG11	1.34	1.08
1:I:192:MET:HE2	1:I:694:ARG:HB2	1.32	1.08
2:J:58:CYS:SG	6:J:1128:HEC:CAB	2.41	1.08
1:O:112:ALA:HB1	1:O:113:PRO:HD2	1.19	1.08
2:D:4:PRO:HG3	2:D:16:VAL:HG11	1.32	1.07
1:E:192:MET:HE2	1:E:694:ARG:HB2	1.36	1.07
2:N:4:PRO:HG3	2:N:16:VAL:HG11	1.35	1.07
1:G:192:MET:HE2	1:G:694:ARG:HB2	1.29	1.07
2:F:4:PRO:HG3	2:F:16:VAL:HG11	1.35	1.07
1:M:192:MET:HE2	1:M:694:ARG:HB2	1.34	1.06
2:N:3:ALA:HB1	2:N:4:PRO:HD2	1.28	1.06
2:H:4:PRO:HG3	2:H:16:VAL:HG11	1.36	1.06
2:N:101:CYS:SG	6:N:1129:HEC:CAC	2.44	1.05
1:O:716:PRO:HG3	2:P:22:PRO:HG2	1.38	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:61:CYS:SG	6:J:1128:HEC:CAC	2.46	1.03
1:K:192:MET:HE2	1:K:694:ARG:HB2	1.36	1.03
2:D:101:CYS:SG	6:D:1129:HEC:CAC	2.47	1.03
1:K:692:THR:HG21	5:K:1803:MGD:H191	1.23	1.03
1:O:749:THR:HG22	1:O:773:GLN:OE1	1.57	1.03
1:I:448:ASN:HD22	1:I:477:ASN:HD21	1.07	1.02
1:M:749:THR:HG22	1:M:773:GLN:OE1	1.59	1.02
1:E:749:THR:HG22	1:E:773:GLN:OE1	1.60	1.02
1:O:192:MET:CE	1:O:694:ARG:HB2	1.88	1.02
2:H:101:CYS:SG	6:H:1129:HEC:CAC	2.47	1.02
1:A:716:PRO:HG3	2:B:22:PRO:HG2	1.41	1.01
1:I:192:MET:CE	1:I:694:ARG:HB2	1.89	1.01
1:C:749:THR:HG22	1:C:773:GLN:OE1	1.61	1.01
1:G:192:MET:CE	1:G:694:ARG:HB2	1.89	1.01
1:O:448:ASN:HD22	1:O:477:ASN:ND2	1.58	1.01
1:A:192:MET:HE2	1:A:694:ARG:HB2	1.40	1.00
1:M:716:PRO:HG3	2:N:22:PRO:HG2	1.43	1.00
1:E:716:PRO:HG3	2:F:22:PRO:HG2	1.41	1.00
1:I:749:THR:HG22	1:I:773:GLN:OE1	1.62	1.00
1:K:125:THR:HB	1:K:128:GLU:HG3	1.42	1.00
1:I:448:ASN:HD22	1:I:477:ASN:ND2	1.60	1.00
1:O:112:ALA:HB1	1:O:113:PRO:CD	1.92	1.00
1:I:112:ALA:HB1	1:I:113:PRO:CD	1.92	0.99
1:M:692:THR:HG21	5:M:1803:MGD:H191	1.23	0.99
2:L:61:CYS:SG	6:L:1128:HEC:CAC	2.51	0.99
2:L:98:CYS:CB	6:L:1129:HEC:HAB	1.92	0.99
1:A:749:THR:HG22	1:A:773:GLN:OE1	1.63	0.99
1:C:192:MET:HE2	1:C:694:ARG:HB2	1.41	0.98
1:E:692:THR:HG21	5:E:1803:MGD:H191	1.28	0.98
1:G:448:ASN:HD22	1:G:477:ASN:HD21	1.10	0.98
1:G:181:ALA:CB	1:G:340:TRP:CZ3	2.47	0.98
1:A:692:THR:HG21	5:A:1803:MGD:H191	1.30	0.97
1:C:716:PRO:HG3	2:D:22:PRO:HG2	1.47	0.97
1:K:448:ASN:HD22	1:K:477:ASN:ND2	1.62	0.97
1:K:749:THR:HG22	1:K:773:GLN:OE1	1.64	0.97
2:P:3:ALA:CB	2:P:4:PRO:HD2	1.95	0.97
1:K:112:ALA:HB1	1:K:113:PRO:CD	1.95	0.97
1:K:134:LYS:HE3	1:K:606:GLU:OE2	1.64	0.97
1:M:125:THR:HB	1:M:128:GLU:HG3	1.44	0.97
1:O:134:LYS:HE3	1:O:606:GLU:OE2	1.64	0.97
2:H:3:ALA:CB	2:H:4:PRO:HD2	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:749:THR:HG22	1:G:773:GLN:OE1	1.65	0.96
1:I:766:VAL:HG23	1:I:775:ILE:HD13	1.45	0.96
1:E:112:ALA:HB1	1:E:113:PRO:CD	1.94	0.96
1:I:134:LYS:HE3	1:I:606:GLU:OE2	1.64	0.96
1:I:716:PRO:HG3	2:J:22:PRO:HG2	1.47	0.96
1:M:192:MET:CE	1:M:694:ARG:HB2	1.95	0.96
2:F:3:ALA:HB1	2:F:4:PRO:CD	1.96	0.96
2:H:98:CYS:CB	6:H:1129:HEC:HAB	1.96	0.96
1:C:692:THR:HG21	5:C:1803:MGD:H191	1.31	0.95
1:G:716:PRO:HG3	2:H:22:PRO:HG2	1.44	0.95
1:M:112:ALA:HB1	1:M:113:PRO:CD	1.96	0.95
1:E:84:LYS:O	1:E:85:GLU:HB2	1.64	0.95
1:K:716:PRO:HG3	2:L:22:PRO:HG2	1.47	0.95
2:L:3:ALA:CB	2:L:4:PRO:HD2	1.94	0.95
1:O:692:THR:HG21	5:O:1803:MGD:H191	1.31	0.95
1:K:448:ASN:HD22	1:K:477:ASN:HD21	1.14	0.95
2:P:3:ALA:HB1	2:P:4:PRO:CD	1.97	0.95
1:G:112:ALA:HB1	1:G:113:PRO:CD	1.97	0.95
2:D:3:ALA:CB	2:D:4:PRO:HD2	1.96	0.95
1:C:740:VAL:HG13	1:C:797:VAL:HG11	1.49	0.95
2:L:3:ALA:HB1	2:L:4:PRO:CD	1.97	0.95
2:N:98:CYS:CB	6:N:1129:HEC:HAB	1.96	0.95
2:F:101:CYS:SG	6:F:1129:HEC:CAC	2.55	0.95
2:F:3:ALA:CB	2:F:4:PRO:HD2	1.96	0.95
2:N:3:ALA:CB	2:N:4:PRO:HD2	1.96	0.94
1:A:112:ALA:HB1	1:A:113:PRO:CD	1.98	0.94
1:A:192:MET:CE	1:A:694:ARG:HB2	1.97	0.94
1:I:181:ALA:CB	1:I:340:TRP:CZ3	2.51	0.94
2:B:3:ALA:CB	2:B:4:PRO:HD2	1.96	0.94
1:O:84:LYS:O	1:O:85:GLU:HB2	1.66	0.94
2:J:3:ALA:CB	2:J:4:PRO:HD2	1.97	0.94
2:P:61:CYS:SG	6:P:1128:HEC:CAC	2.55	0.94
1:G:134:LYS:HE3	1:G:606:GLU:OE2	1.68	0.94
2:J:3:ALA:HB1	2:J:4:PRO:CD	1.98	0.94
1:C:112:ALA:HB1	1:C:113:PRO:CD	1.98	0.94
2:N:3:ALA:HB1	2:N:4:PRO:CD	1.98	0.94
2:B:3:ALA:HB1	2:B:4:PRO:CD	1.97	0.93
1:G:448:ASN:HD22	1:G:477:ASN:ND2	1.65	0.93
1:K:567:GLU:HA	1:K:571:ALA:HB3	1.48	0.93
1:K:192:MET:CE	1:K:694:ARG:HB2	1.97	0.93
1:M:181:ALA:CB	1:M:340:TRP:CZ3	2.52	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:98:CYS:CB	6:D:1129:HEC:HAB	1.98	0.93
1:A:448:ASN:HD22	1:A:477:ASN:ND2	1.66	0.93
1:O:163:THR:HG23	1:O:359:HIS:CE1	2.03	0.93
1:I:319:SER:HB2	1:I:321:VAL:HG22	1.51	0.93
2:J:101:CYS:SG	6:J:1129:HEC:CAC	2.57	0.93
1:O:125:THR:HB	1:O:128:GLU:HG3	1.48	0.93
1:C:544:THR:HG22	1:C:547:GLU:HB2	1.51	0.93
2:F:83:ARG:O	2:F:84:GLU:HB2	1.67	0.93
1:M:766:VAL:HG23	1:M:775:ILE:HD13	1.51	0.93
1:K:740:VAL:HG13	1:K:797:VAL:HG11	1.50	0.93
1:I:544:THR:HG22	1:I:547:GLU:HB2	1.51	0.92
2:D:3:ALA:HB1	2:D:4:PRO:CD	1.97	0.92
1:E:766:VAL:HG23	1:E:775:ILE:HD13	1.51	0.92
1:O:319:SER:HB2	1:O:321:VAL:HG22	1.51	0.92
2:H:3:ALA:HB1	2:H:4:PRO:CD	1.98	0.92
1:K:544:THR:HG22	1:K:547:GLU:HB2	1.50	0.92
1:O:544:THR:HG22	1:O:547:GLU:HB2	1.50	0.92
1:C:766:VAL:HG23	1:C:775:ILE:HD13	1.51	0.92
1:C:125:THR:HB	1:C:128:GLU:HG3	1.49	0.92
1:O:230:ILE:HG23	1:O:321:VAL:HG11	1.51	0.92
1:C:448:ASN:HD22	1:C:477:ASN:ND2	1.67	0.92
1:G:692:THR:HG21	5:G:1803:MGD:H191	1.32	0.92
1:C:84:LYS:O	1:C:85:GLU:HB2	1.68	0.92
1:E:29:MET:HE3	1:E:628:ARG:HH12	1.34	0.92
1:M:544:THR:HG22	1:M:547:GLU:HB2	1.50	0.92
1:A:134:LYS:HE3	1:A:606:GLU:OE2	1.71	0.91
1:C:181:ALA:CB	1:C:340:TRP:CZ3	2.53	0.91
1:G:544:THR:HG22	1:G:547:GLU:HB2	1.52	0.91
1:A:181:ALA:CB	1:A:340:TRP:CZ3	2.54	0.91
1:E:319:SER:HB2	1:E:321:VAL:HG22	1.52	0.91
1:M:567:GLU:HA	1:M:571:ALA:HB3	1.51	0.91
1:O:550:PRO:CG	1:O:553:ILE:HD12	1.99	0.91
1:E:192:MET:CE	1:E:694:ARG:HB2	2.00	0.91
1:K:181:ALA:CB	1:K:340:TRP:CZ3	2.53	0.91
1:K:230:ILE:HG23	1:K:321:VAL:HG11	1.52	0.91
2:N:58:CYS:HG	6:N:1128:HEC:HAB	1.22	0.91
1:E:448:ASN:HD22	1:E:477:ASN:HD21	1.17	0.91
1:E:448:ASN:HD22	1:E:477:ASN:ND2	1.67	0.91
1:O:448:ASN:HD22	1:O:477:ASN:HD21	1.11	0.91
1:A:84:LYS:O	1:A:85:GLU:HB2	1.68	0.91
1:E:125:THR:HB	1:E:128:GLU:HG3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:ALA:HA	1:A:576:ASP:OD2	1.72	0.90
1:K:766:VAL:HG23	1:K:775:ILE:HD13	1.50	0.90
1:O:550:PRO:HG2	1:O:553:ILE:CD1	2.01	0.90
1:A:125:THR:HB	1:A:128:GLU:HG3	1.53	0.90
1:K:163:THR:HG23	1:K:359:HIS:CE1	2.06	0.90
1:M:230:ILE:HG23	1:M:321:VAL:HG11	1.53	0.90
1:G:766:VAL:HG23	1:G:775:ILE:HD13	1.52	0.90
1:I:144:ASN:ND2	1:I:433:ALA:H	1.69	0.90
1:I:84:LYS:O	1:I:85:GLU:HB2	1.70	0.90
2:J:61:CYS:HG	6:J:1128:HEC:HAC	1.31	0.90
1:K:319:SER:HB2	1:K:321:VAL:HG22	1.53	0.90
1:A:319:SER:HB2	1:A:321:VAL:HG22	1.53	0.90
2:D:83:ARG:O	2:D:84:GLU:HB2	1.70	0.90
1:E:181:ALA:CB	1:E:340:TRP:CZ3	2.55	0.90
1:C:448:ASN:HD22	1:C:477:ASN:HD21	1.14	0.90
1:C:192:MET:CE	1:C:694:ARG:HB2	2.02	0.90
1:K:84:LYS:O	1:K:85:GLU:HB2	1.71	0.89
1:M:740:VAL:HG13	1:M:797:VAL:HG11	1.54	0.89
1:C:319:SER:HB2	1:C:321:VAL:HG22	1.55	0.89
1:G:319:SER:HB2	1:G:321:VAL:HG22	1.54	0.89
1:I:740:VAL:HG13	1:I:797:VAL:HG11	1.53	0.89
1:M:84:LYS:O	1:M:85:GLU:HB2	1.70	0.89
1:O:766:VAL:HG23	1:O:775:ILE:HD13	1.52	0.89
1:A:544:THR:HG22	1:A:547:GLU:HB2	1.53	0.89
1:I:567:GLU:HA	1:I:571:ALA:HB3	1.53	0.89
1:O:181:ALA:CB	1:O:340:TRP:CZ3	2.54	0.89
1:O:567:GLU:HA	1:O:571:ALA:HB3	1.53	0.89
1:G:125:THR:HB	1:G:128:GLU:HG3	1.53	0.89
1:G:772:SER:HB2	2:H:4:PRO:HG2	1.53	0.89
2:J:95:ARG:HA	6:J:1129:HEC:HMC2	1.55	0.89
1:M:163:THR:HG23	1:M:359:HIS:CE1	2.08	0.89
1:E:544:THR:HG22	1:E:547:GLU:HB2	1.53	0.89
1:I:550:PRO:HG2	1:I:553:ILE:CD1	2.03	0.89
1:I:747:ILE:HD11	1:I:775:ILE:CA	2.03	0.89
1:G:84:LYS:O	1:G:85:GLU:HB2	1.69	0.89
2:H:83:ARG:O	2:H:84:GLU:HB2	1.71	0.89
1:E:740:VAL:HG13	1:E:797:VAL:HG11	1.55	0.88
2:L:101:CYS:SG	6:L:1129:HEC:CAC	2.61	0.88
1:G:740:VAL:HG13	1:G:797:VAL:HG11	1.53	0.88
1:A:448:ASN:HD22	1:A:477:ASN:HD21	1.20	0.88
1:A:272:ILE:HG23	1:A:785:PRO:HG3	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:VAL:HG23	1:A:775:ILE:HD13	1.53	0.88
2:D:58:CYS:HG	6:D:1128:HEC:HAB	1.33	0.88
1:G:567:GLU:HA	1:G:571:ALA:HB3	1.54	0.88
1:I:571:ALA:HA	1:I:576:ASP:OD2	1.73	0.88
1:O:183:VAL:CG2	1:O:340:TRP:HE1	1.87	0.88
1:K:747:ILE:HD11	1:K:775:ILE:CA	2.02	0.88
1:C:550:PRO:HG2	1:C:553:ILE:CD1	2.03	0.88
1:O:740:VAL:HG13	1:O:797:VAL:HG11	1.56	0.88
1:A:183:VAL:CG2	1:A:340:TRP:HE1	1.87	0.88
2:L:83:ARG:O	2:L:84:GLU:HB2	1.71	0.88
1:M:747:ILE:HD11	1:M:775:ILE:CA	2.03	0.88
1:G:550:PRO:HG2	1:G:553:ILE:CD1	2.04	0.87
1:I:692:THR:HG21	5:I:1803:MGD:H191	1.36	0.87
1:C:571:ALA:HA	1:C:576:ASP:OD2	1.75	0.87
1:M:319:SER:HB2	1:M:321:VAL:HG22	1.56	0.87
1:O:772:SER:HB2	2:P:4:PRO:HG2	1.53	0.87
1:I:163:THR:HG23	1:I:359:HIS:CE1	2.08	0.87
1:O:272:ILE:HG23	1:O:785:PRO:HG3	1.53	0.87
1:G:571:ALA:HA	1:G:576:ASP:OD2	1.75	0.87
1:O:571:ALA:HA	1:O:576:ASP:OD2	1.74	0.87
1:E:144:ASN:ND2	1:E:433:ALA:H	1.73	0.87
1:C:567:GLU:HA	1:C:571:ALA:HB3	1.54	0.87
1:K:272:ILE:HG23	1:K:785:PRO:HG3	1.56	0.87
1:M:571:ALA:HA	1:M:576:ASP:OD2	1.74	0.87
1:I:230:ILE:HG23	1:I:321:VAL:HG11	1.56	0.86
1:I:125:THR:HB	1:I:128:GLU:HG3	1.56	0.86
1:E:567:GLU:HA	1:E:571:ALA:HB3	1.55	0.86
2:P:121:THR:O	2:P:123:MET:N	2.07	0.86
1:A:567:GLU:HA	1:A:571:ALA:HB3	1.57	0.86
2:B:83:ARG:O	2:B:84:GLU:HB2	1.74	0.86
1:E:747:ILE:HD11	1:E:775:ILE:CA	2.06	0.86
1:G:747:ILE:HD11	1:G:775:ILE:CA	2.03	0.86
1:M:144:ASN:ND2	1:M:433:ALA:H	1.72	0.86
1:M:723:HIS:HD2	1:M:725:GLU:H	1.20	0.86
2:N:83:ARG:O	2:N:84:GLU:HB2	1.72	0.86
1:E:183:VAL:CG2	1:E:340:TRP:HE1	1.89	0.86
1:C:723:HIS:HD2	1:C:725:GLU:H	1.24	0.85
1:G:230:ILE:HG23	1:G:321:VAL:HG11	1.57	0.85
1:G:272:ILE:HG23	1:G:785:PRO:HG3	1.55	0.85
1:O:723:HIS:HD2	1:O:725:GLU:H	1.23	0.85
1:O:144:ASN:ND2	1:O:433:ALA:H	1.73	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:ILE:HG23	1:E:785:PRO:HG3	1.56	0.85
1:G:181:ALA:HB3	1:G:340:TRP:HZ3	1.39	0.85
1:G:144:ASN:ND2	1:G:433:ALA:H	1.73	0.85
1:A:163:THR:HG23	1:A:359:HIS:CE1	2.11	0.85
1:C:747:ILE:HD11	1:C:775:ILE:CA	2.07	0.85
1:K:183:VAL:CG2	1:K:340:TRP:HE1	1.89	0.85
1:M:180:ASP:OD2	1:M:339:LYS:HG3	1.77	0.85
1:M:486:PRO:O	1:M:487:THR:HB	1.76	0.85
2:N:61:CYS:SG	6:N:1128:HEC:CAC	2.64	0.85
1:A:723:HIS:HD2	1:A:725:GLU:H	1.21	0.85
1:C:230:ILE:HG23	1:C:321:VAL:HG11	1.57	0.85
1:C:633:PRO:HD2	1:C:640:THR:HB	1.58	0.85
2:F:61:CYS:HG	6:F:1128:HEC:HAC	1.41	0.85
1:I:180:ASP:HB2	1:I:339:LYS:H	1.42	0.85
1:O:335:ASP:OD2	1:O:338:ARG:HB2	1.77	0.85
1:C:163:THR:HG23	1:C:359:HIS:CE1	2.12	0.84
1:I:550:PRO:CG	1:I:553:ILE:HD12	2.04	0.84
1:M:448:ASN:HD22	1:M:477:ASN:HD21	1.18	0.84
2:D:61:CYS:SG	6:D:1128:HEC:CAC	2.64	0.84
1:A:740:VAL:HG13	1:A:797:VAL:HG11	1.56	0.84
1:M:448:ASN:HD22	1:M:477:ASN:ND2	1.74	0.84
2:P:5:ARG:C	2:P:7:THR:H	1.81	0.84
1:E:230:ILE:HG23	1:E:321:VAL:HG11	1.59	0.84
2:P:83:ARG:O	2:P:84:GLU:HB2	1.75	0.84
2:B:61:CYS:SG	6:B:1128:HEC:C3C	2.65	0.84
1:C:144:ASN:ND2	1:C:433:ALA:H	1.75	0.84
1:M:537:MET:O	1:M:540:SER:HB2	1.77	0.84
1:C:134:LYS:HE3	1:C:606:GLU:OE2	1.77	0.84
1:I:125:THR:HG23	1:I:508:ALA:H	1.41	0.84
2:J:101:CYS:SG	6:J:1129:HEC:HAC	2.17	0.84
1:M:272:ILE:HG23	1:M:785:PRO:HG3	1.59	0.84
2:P:98:CYS:CB	6:P:1129:HEC:HAB	2.08	0.84
1:E:571:ALA:HA	1:E:576:ASP:OD2	1.76	0.84
1:I:372:SER:O	1:I:645:ARG:HG3	1.77	0.84
1:M:134:LYS:HE3	1:M:606:GLU:OE2	1.78	0.83
1:C:537:MET:O	1:C:540:SER:HB2	1.78	0.83
1:G:550:PRO:CG	1:G:553:ILE:HD12	2.07	0.83
1:K:723:HIS:HD2	1:K:725:GLU:H	1.24	0.83
1:I:692:THR:CG2	5:I:1803:MGD:H18	1.91	0.83
1:O:747:ILE:HD11	1:O:775:ILE:CA	2.06	0.83
1:E:772:SER:HB2	2:F:4:PRO:HG2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:THR:HG23	1:G:508:ALA:H	1.44	0.83
2:L:95:ARG:HA	6:L:1129:HEC:HMC2	1.59	0.83
1:G:335:ASP:OD2	1:G:338:ARG:HB2	1.77	0.83
1:K:571:ALA:HA	1:K:576:ASP:OD2	1.79	0.83
1:G:163:THR:HG23	1:G:359:HIS:CE1	2.14	0.83
1:I:723:HIS:HD2	1:I:725:GLU:H	1.27	0.83
1:K:112:ALA:CB	1:K:113:PRO:HD2	2.05	0.83
1:E:550:PRO:HG2	1:E:553:ILE:CD1	2.08	0.83
1:A:633:PRO:HD2	1:A:640:THR:HB	1.60	0.83
1:I:181:ALA:HB3	1:I:340:TRP:HZ3	1.43	0.83
1:A:491:ARG:NH2	2:B:11:ARG:H	1.77	0.82
1:C:272:ILE:HG23	1:C:785:PRO:HG3	1.58	0.82
1:O:183:VAL:HG21	1:O:340:TRP:HE1	1.42	0.82
1:E:723:HIS:HD2	1:E:725:GLU:H	1.23	0.82
2:F:30:ARG:HD2	6:F:1128:HEC:O1D	1.78	0.82
1:K:125:THR:HG23	1:K:508:ALA:H	1.44	0.82
1:K:550:PRO:HG2	1:K:553:ILE:CD1	2.09	0.82
2:N:121:THR:O	2:N:123:MET:N	2.11	0.82
1:C:339:LYS:HA	1:C:376:ASN:HD21	1.43	0.82
1:E:633:PRO:HD2	1:E:640:THR:HB	1.59	0.82
1:K:692:THR:CG2	5:K:1803:MGD:H18	1.93	0.82
2:L:5:ARG:C	2:L:7:THR:H	1.83	0.82
2:N:33:ARG:HH21	2:N:40:PRO:HG3	1.42	0.82
1:C:692:THR:CG2	5:C:1803:MGD:H18	1.93	0.82
1:I:150:ARG:HD3	1:I:434:HIS:HB2	1.62	0.82
1:C:550:PRO:CG	1:C:553:ILE:HD12	2.07	0.82
1:E:134:LYS:HE3	1:E:606:GLU:OE2	1.79	0.82
2:L:33:ARG:HH21	2:L:40:PRO:HG3	1.44	0.82
1:M:183:VAL:CG2	1:M:340:TRP:HE1	1.92	0.82
2:H:121:THR:O	2:H:123:MET:N	2.12	0.82
1:I:272:ILE:HG23	1:I:785:PRO:HG3	1.59	0.82
2:J:5:ARG:C	2:J:7:THR:H	1.81	0.82
1:A:332:LEU:HB3	1:A:340:TRP:CH2	2.16	0.81
1:E:163:THR:HG23	1:E:359:HIS:CE1	2.15	0.81
1:K:144:ASN:ND2	1:K:433:ALA:H	1.76	0.81
1:M:550:PRO:CG	1:M:553:ILE:HD12	2.09	0.81
1:C:486:PRO:O	1:C:487:THR:HB	1.81	0.81
1:M:29:MET:HE3	1:M:628:ARG:HH12	1.44	0.81
1:O:125:THR:HG23	1:O:508:ALA:H	1.45	0.81
1:O:491:ARG:NH2	2:P:11:ARG:H	1.76	0.81
2:P:95:ARG:HA	6:P:1129:HEC:HMC2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:PRO:HG2	1:A:553:ILE:CD1	2.10	0.81
1:I:180:ASP:OD2	1:I:339:LYS:HG3	1.80	0.81
1:A:144:ASN:ND2	1:A:433:ALA:H	1.79	0.81
2:F:5:ARG:C	2:F:7:THR:H	1.82	0.81
2:J:83:ARG:O	2:J:84:GLU:HB2	1.79	0.81
1:M:550:PRO:HG2	1:M:553:ILE:CD1	2.09	0.81
1:A:230:ILE:HG23	1:A:321:VAL:HG11	1.63	0.81
2:B:33:ARG:HH21	2:B:40:PRO:HG3	1.45	0.81
1:C:183:VAL:CG2	1:C:340:TRP:HE1	1.93	0.81
1:K:692:THR:HG22	5:K:1803:MGD:H18	1.46	0.81
2:H:5:ARG:C	2:H:7:THR:H	1.84	0.81
1:O:112:ALA:CB	1:O:113:PRO:HD2	2.09	0.81
1:K:537:MET:O	1:K:540:SER:HB2	1.80	0.81
1:K:550:PRO:CG	1:K:553:ILE:HD12	2.08	0.81
1:A:125:THR:HG23	1:A:508:ALA:H	1.44	0.80
1:I:760:PRO:HD2	1:I:763:VAL:HB	1.61	0.80
1:O:486:PRO:O	1:O:487:THR:HB	1.80	0.80
2:D:121:THR:O	2:D:123:MET:N	2.13	0.80
2:J:33:ARG:HH21	2:J:40:PRO:HG3	1.45	0.80
2:J:42:ILE:HD11	6:J:1128:HEC:HMB2	1.62	0.80
1:O:537:MET:O	1:O:540:SER:HB2	1.82	0.80
1:E:335:ASP:OD2	1:E:338:ARG:HB2	1.81	0.80
1:E:486:PRO:O	1:E:487:THR:HB	1.80	0.80
1:I:503:VAL:CG1	1:I:522:LEU:HB2	2.12	0.80
2:B:5:ARG:C	2:B:7:THR:H	1.83	0.80
1:C:112:ALA:CB	1:C:113:PRO:HD2	2.06	0.80
2:D:33:ARG:HH21	2:D:40:PRO:HG3	1.46	0.80
1:E:396:THR:HG22	1:E:396:THR:O	1.82	0.80
1:K:372:SER:O	1:K:645:ARG:HG3	1.81	0.80
1:M:181:ALA:HB3	1:M:340:TRP:HZ3	1.44	0.80
1:A:76:ARG:NH2	1:A:473:ARG:NH2	2.30	0.80
1:C:692:THR:HG22	5:C:1803:MGD:H18	1.47	0.80
2:F:95:ARG:HA	6:F:1129:HEC:HMC2	1.64	0.80
1:G:180:ASP:OD2	1:G:339:LYS:HG3	1.81	0.80
1:K:772:SER:HB2	2:L:4:PRO:HG2	1.64	0.80
1:C:339:LYS:HA	1:C:376:ASN:ND2	1.97	0.80
2:J:121:THR:O	2:J:123:MET:N	2.13	0.80
1:A:339:LYS:HA	1:A:376:ASN:HD21	1.47	0.79
1:G:183:VAL:CG2	1:G:340:TRP:HE1	1.94	0.79
1:C:180:ASP:OD2	1:C:339:LYS:HG3	1.81	0.79
1:G:183:VAL:HG23	1:G:340:TRP:CZ2	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:112:ALA:CB	1:I:113:PRO:HD2	2.09	0.79
1:O:150:ARG:HD3	1:O:434:HIS:HB2	1.64	0.79
1:E:692:THR:CG2	5:E:1803:MGD:H18	1.96	0.79
1:A:550:PRO:CG	1:A:553:ILE:HD12	2.11	0.79
1:C:332:LEU:HB3	1:C:340:TRP:CH2	2.17	0.79
2:D:95:ARG:HA	6:D:1129:HEC:HMC2	1.64	0.79
1:E:372:SER:O	1:E:645:ARG:HG3	1.82	0.79
1:G:723:HIS:HD2	1:G:725:GLU:H	1.29	0.79
2:L:42:ILE:HD11	6:L:1128:HEC:HMB2	1.62	0.79
1:G:29:MET:HE3	1:G:628:ARG:HH12	1.48	0.79
1:G:486:PRO:O	1:G:487:THR:HB	1.83	0.79
2:H:42:ILE:HD11	6:H:1128:HEC:HMB2	1.63	0.79
1:I:192:MET:HE2	1:I:694:ARG:CB	2.12	0.79
1:M:491:ARG:NH2	2:N:11:ARG:H	1.79	0.79
1:G:183:VAL:HG21	1:G:340:TRP:HE1	1.47	0.79
1:I:772:SER:HB2	2:J:4:PRO:HG2	1.64	0.79
1:M:692:THR:CG2	5:M:1803:MGD:H18	1.94	0.79
1:M:692:THR:HG22	5:M:1803:MGD:H18	1.47	0.79
1:M:332:LEU:HB3	1:M:340:TRP:CH2	2.18	0.79
1:A:29:MET:HE3	1:A:628:ARG:HH12	1.48	0.79
1:A:747:ILE:HD11	1:A:775:ILE:CA	2.10	0.79
1:E:183:VAL:HG23	1:E:340:TRP:CZ2	2.18	0.79
1:G:692:THR:CG2	5:G:1803:MGD:H18	1.96	0.79
1:A:760:PRO:HD2	1:A:763:VAL:HB	1.63	0.78
1:C:333:TYR:CE2	1:C:340:TRP:HD1	2.01	0.78
1:C:183:VAL:HG21	1:C:340:TRP:HE1	1.48	0.78
1:K:183:VAL:HG23	1:K:340:TRP:CZ2	2.18	0.78
1:O:750:ARG:CD	2:P:20:PRO:HA	2.13	0.78
2:P:4:PRO:HG3	2:P:16:VAL:CG1	2.13	0.78
1:I:692:THR:HG22	5:I:1803:MGD:H18	1.46	0.78
1:K:150:ARG:HD3	1:K:434:HIS:HB2	1.65	0.78
2:P:33:ARG:HH21	2:P:40:PRO:HG3	1.49	0.78
1:A:486:PRO:O	1:A:487:THR:HB	1.84	0.78
2:D:5:ARG:C	2:D:7:THR:H	1.85	0.78
1:E:125:THR:HG23	1:E:508:ALA:H	1.46	0.78
2:D:4:PRO:CG	2:D:16:VAL:HG11	2.13	0.78
1:M:692:THR:HG21	5:M:1803:MGD:N19	1.99	0.78
1:M:183:VAL:HG23	1:M:340:TRP:CZ2	2.18	0.78
1:A:112:ALA:CB	1:A:113:PRO:HD2	2.09	0.78
1:M:772:SER:HB2	2:N:4:PRO:HG2	1.64	0.78
1:E:332:LEU:HB3	1:E:340:TRP:CH2	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:238:ARG:NH1	1:I:353:ARG:HG3	1.98	0.78
1:M:125:THR:HG23	1:M:508:ALA:H	1.49	0.78
1:E:692:THR:HG22	5:E:1803:MGD:H18	1.46	0.78
1:M:372:SER:O	1:M:645:ARG:HG3	1.84	0.78
1:C:146:ASP:OD1	1:C:150:ARG:HD2	1.84	0.78
1:O:180:ASP:OD2	1:O:339:LYS:HG3	1.82	0.78
1:O:760:PRO:HD2	1:O:763:VAL:HB	1.63	0.78
1:O:716:PRO:CG	2:P:22:PRO:HG2	2.11	0.78
1:C:372:SER:O	1:C:645:ARG:HG3	1.83	0.78
1:I:146:ASP:OD1	1:I:150:ARG:HD2	1.84	0.78
1:K:332:LEU:HB3	1:K:340:TRP:CH2	2.19	0.78
1:M:423:PRO:HD3	1:M:560:TYR:CE1	2.19	0.78
2:N:5:ARG:C	2:N:7:THR:H	1.85	0.78
2:B:95:ARG:HA	6:B:1129:HEC:HMC2	1.64	0.77
1:K:21:PHE:CZ	1:K:63:ILE:HD11	2.19	0.77
1:K:692:THR:HG21	5:K:1803:MGD:N19	1.99	0.77
1:M:112:ALA:CB	1:M:113:PRO:HD2	2.11	0.77
1:M:633:PRO:HD2	1:M:640:THR:HB	1.65	0.77
1:G:339:LYS:HA	1:G:376:ASN:HD21	1.50	0.77
2:F:121:THR:O	2:F:123:MET:N	2.16	0.77
2:B:4:PRO:CG	2:B:16:VAL:HG11	2.14	0.77
1:C:150:ARG:HD3	1:C:434:HIS:HB2	1.67	0.77
1:K:335:ASP:OD2	1:K:338:ARG:HB2	1.84	0.77
2:P:5:ARG:C	2:P:7:THR:N	2.36	0.77
2:B:121:THR:O	2:B:123:MET:N	2.16	0.77
1:C:599:PRO:O	1:C:603:LEU:HD12	1.85	0.77
1:E:112:ALA:CB	1:E:113:PRO:HD2	2.11	0.77
2:F:33:ARG:HH21	2:F:40:PRO:HG3	1.47	0.77
1:M:335:ASP:OD2	1:M:338:ARG:HB2	1.84	0.77
1:O:183:VAL:HG23	1:O:340:TRP:CZ2	2.19	0.77
1:I:335:ASP:OD2	1:I:338:ARG:HB2	1.84	0.77
1:O:21:PHE:CZ	1:O:63:ILE:HD11	2.20	0.77
2:P:51:LEU:HD21	2:P:58:CYS:SG	2.24	0.77
1:A:183:VAL:HG21	1:A:340:TRP:HE1	1.49	0.77
2:J:5:ARG:C	2:J:7:THR:N	2.36	0.77
2:L:4:PRO:CG	2:L:16:VAL:HG11	2.15	0.77
2:D:4:PRO:HG3	2:D:16:VAL:CG1	2.15	0.77
1:I:183:VAL:HG23	1:I:340:TRP:CZ2	2.20	0.77
1:O:372:SER:O	1:O:645:ARG:HG3	1.85	0.77
1:O:192:MET:CE	1:O:694:ARG:CB	2.63	0.77
1:E:183:VAL:HG21	1:E:340:TRP:HE1	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:503:VAL:CG1	1:O:522:LEU:HB2	2.15	0.76
1:A:183:VAL:HG23	1:A:340:TRP:CZ2	2.19	0.76
1:I:455:ASN:ND2	1:I:457:ASN:HB2	1.99	0.76
1:O:692:THR:CG2	5:O:1803:MGD:H18	1.98	0.76
1:E:332:LEU:CG	1:E:340:TRP:CH2	2.68	0.76
1:O:238:ARG:NH1	1:O:353:ARG:HG3	2.00	0.76
1:O:723:HIS:CD2	1:O:725:GLU:H	2.04	0.76
1:A:335:ASP:OD2	1:A:338:ARG:HB2	1.86	0.76
2:B:5:ARG:C	2:B:7:THR:N	2.37	0.76
1:G:372:SER:O	1:G:645:ARG:HG3	1.85	0.76
1:C:183:VAL:HG23	1:C:340:TRP:CZ2	2.20	0.76
1:E:760:PRO:HD2	1:E:763:VAL:HB	1.67	0.76
2:H:33:ARG:HH21	2:H:40:PRO:HG3	1.51	0.76
1:I:238:ARG:HH11	1:I:353:ARG:HG3	1.50	0.76
1:K:486:PRO:O	1:K:487:THR:HB	1.86	0.76
1:O:692:THR:HG22	5:O:1803:MGD:H18	1.50	0.76
1:G:692:THR:HG22	5:G:1803:MGD:H18	1.50	0.76
1:G:750:ARG:CD	2:H:20:PRO:HA	2.16	0.76
2:P:4:PRO:CG	2:P:16:VAL:HG11	2.12	0.76
1:E:332:LEU:HG	1:E:340:TRP:CH2	2.21	0.76
2:F:4:PRO:HG3	2:F:16:VAL:CG1	2.15	0.76
1:K:238:ARG:HG2	1:K:360:MET:HE3	1.68	0.76
2:P:101:CYS:SG	6:P:1129:HEC:CAC	2.74	0.76
1:E:537:MET:O	1:E:540:SER:HB2	1.86	0.75
1:G:332:LEU:HG	1:G:340:TRP:CH2	2.21	0.75
1:G:537:MET:O	1:G:540:SER:HB2	1.86	0.75
1:I:333:TYR:CE2	1:I:340:TRP:HD1	2.04	0.75
1:M:150:ARG:HD3	1:M:434:HIS:HB2	1.68	0.75
1:O:332:LEU:HG	1:O:340:TRP:CH2	2.21	0.75
1:G:180:ASP:HB2	1:G:339:LYS:H	1.52	0.75
2:H:40:PRO:HD2	2:H:102:HIS:HE1	1.50	0.75
1:O:356:TRP:O	1:O:360:MET:HG3	1.87	0.75
2:D:5:ARG:C	2:D:7:THR:N	2.39	0.75
1:K:332:LEU:CG	1:K:340:TRP:CH2	2.69	0.75
1:O:332:LEU:HB3	1:O:340:TRP:CH2	2.22	0.75
1:A:692:THR:HG22	5:A:1803:MGD:H18	1.51	0.75
1:O:332:LEU:CG	1:O:340:TRP:CH2	2.69	0.75
1:E:550:PRO:CG	1:E:553:ILE:HD12	2.12	0.75
1:M:183:VAL:HG21	1:M:340:TRP:HE1	1.50	0.75
2:L:4:PRO:HG3	2:L:16:VAL:CG1	2.15	0.75
1:A:332:LEU:HG	1:A:340:TRP:CH2	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:THR:HG23	1:C:508:ALA:H	1.52	0.75
1:C:180:ASP:HB2	1:C:339:LYS:H	1.51	0.75
1:C:760:PRO:HD2	1:C:763:VAL:HB	1.66	0.75
1:G:150:ARG:HD3	1:G:434:HIS:HB2	1.69	0.75
1:I:503:VAL:HG13	1:I:522:LEU:HB2	1.69	0.75
1:I:741:ILE:HG12	1:I:746:GLU:HG2	1.68	0.75
1:M:750:ARG:CD	2:N:20:PRO:HA	2.17	0.75
2:N:33:ARG:NH2	2:N:40:PRO:HG3	2.02	0.75
1:C:181:ALA:HB3	1:C:340:TRP:HZ3	1.48	0.75
1:G:192:MET:HE2	1:G:694:ARG:CB	2.12	0.75
6:L:1129:HEC:HBC3	6:L:1129:HEC:HMC1	1.68	0.75
1:M:146:ASP:OD1	1:M:150:ARG:HD2	1.87	0.75
1:A:332:LEU:CG	1:A:340:TRP:CH2	2.69	0.75
1:I:238:ARG:HG2	1:I:360:MET:CE	2.17	0.75
1:M:760:PRO:HD2	1:M:763:VAL:HB	1.67	0.75
1:A:372:SER:O	1:A:645:ARG:HG3	1.85	0.74
2:F:4:PRO:CG	2:F:16:VAL:HG11	2.15	0.74
1:K:180:ASP:HB2	1:K:339:LYS:H	1.51	0.74
1:K:760:PRO:HD2	1:K:763:VAL:HB	1.68	0.74
2:L:121:THR:O	2:L:123:MET:N	2.19	0.74
1:C:776:ASN:HA	1:C:779:THR:OG1	1.87	0.74
1:E:180:ASP:HB2	1:E:339:LYS:H	1.51	0.74
2:F:33:ARG:HD3	6:F:1129:HEC:O2D	1.87	0.74
1:G:332:LEU:CG	1:G:340:TRP:CH2	2.70	0.74
1:I:332:LEU:CG	1:I:340:TRP:CH2	2.71	0.74
1:M:332:LEU:CG	1:M:340:TRP:CH2	2.69	0.74
1:C:491:ARG:NH2	2:D:11:ARG:H	1.85	0.74
1:G:487:THR:HG22	1:G:490:GLY:H	1.52	0.74
1:G:760:PRO:HD2	1:G:763:VAL:HB	1.67	0.74
2:H:61:CYS:HG	6:H:1128:HEC:HAC	1.51	0.74
2:N:40:PRO:HD2	2:N:102:HIS:HE1	1.52	0.74
1:A:537:MET:O	1:A:540:SER:HB2	1.88	0.74
1:C:335:ASP:OD2	1:C:338:ARG:HB2	1.87	0.74
2:J:51:LEU:HD21	2:J:58:CYS:SG	2.28	0.74
1:M:723:HIS:CD2	1:M:725:GLU:H	2.05	0.74
1:E:181:ALA:HB3	1:E:340:TRP:HZ3	1.51	0.74
1:G:112:ALA:CB	1:G:113:PRO:HD2	2.08	0.74
1:G:716:PRO:CG	2:H:22:PRO:HG2	2.16	0.74
1:M:332:LEU:HG	1:M:340:TRP:CH2	2.23	0.74
2:N:4:PRO:CG	2:N:16:VAL:HG11	2.15	0.74
1:I:633:PRO:CD	1:I:640:THR:HB	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:183:VAL:HG21	1:K:340:TRP:HE1	1.49	0.74
1:A:339:LYS:HA	1:A:376:ASN:ND2	2.01	0.74
1:G:339:LYS:HA	1:G:376:ASN:ND2	2.03	0.74
2:H:4:PRO:HG3	2:H:16:VAL:CG1	2.16	0.74
2:H:5:ARG:C	2:H:7:THR:N	2.39	0.74
1:O:747:ILE:HG22	1:O:748:ARG:N	2.03	0.74
1:A:180:ASP:OD2	1:A:339:LYS:HG3	1.88	0.74
2:H:4:PRO:CG	2:H:16:VAL:HG11	2.16	0.74
1:K:238:ARG:HH11	1:K:353:ARG:HG3	1.53	0.74
1:K:503:VAL:CG1	1:K:522:LEU:HB2	2.17	0.74
2:N:33:ARG:HD3	6:N:1129:HEC:O2D	1.88	0.74
1:O:146:ASP:OD1	1:O:150:ARG:HD2	1.87	0.74
1:O:68:ASP:HB2	1:O:707:ARG:NH1	2.03	0.74
1:A:692:THR:CG2	5:A:1803:MGD:H18	2.00	0.73
1:A:723:HIS:CD2	1:A:725:GLU:H	2.05	0.73
1:I:332:LEU:HB3	1:I:340:TRP:CH2	2.23	0.73
1:K:723:HIS:CD2	1:K:725:GLU:H	2.06	0.73
1:M:180:ASP:HB2	1:M:339:LYS:H	1.53	0.73
1:M:21:PHE:CZ	1:M:63:ILE:HD11	2.23	0.73
1:M:396:THR:HG22	1:M:396:THR:O	1.88	0.73
1:E:339:LYS:HA	1:E:376:ASN:HD21	1.53	0.73
1:O:339:LYS:HA	1:O:376:ASN:HD21	1.53	0.73
1:E:59:PHE:CZ	1:E:710:GLU:HG3	2.23	0.73
2:F:5:ARG:C	2:F:7:THR:N	2.37	0.73
1:O:272:ILE:CG2	1:O:785:PRO:HG3	2.18	0.73
1:A:772:SER:HB2	2:B:4:PRO:HG2	1.70	0.73
1:C:723:HIS:CD2	1:C:725:GLU:H	2.06	0.73
1:E:692:THR:HG21	5:E:1803:MGD:N19	2.04	0.73
1:G:59:PHE:CZ	1:G:710:GLU:HG3	2.23	0.73
1:I:332:LEU:HG	1:I:340:TRP:CH2	2.24	0.73
1:I:747:ILE:HG22	1:I:748:ARG:N	2.03	0.73
1:M:339:LYS:HA	1:M:376:ASN:HD21	1.54	0.73
1:A:21:PHE:CZ	1:A:63:ILE:HD11	2.23	0.73
2:F:98:CYS:CB	6:F:1129:HEC:HAB	2.18	0.73
1:O:333:TYR:CE2	1:O:340:TRP:HD1	2.06	0.73
1:O:720:CYS:HA	1:O:766:VAL:HG12	1.70	0.73
1:I:514:ARG:O	1:I:631:HIS:HA	1.88	0.73
1:K:400:ARG:NH2	1:K:404:ASP:H	1.85	0.73
1:K:168:GLU:HG3	1:K:632:TRP:HZ2	1.53	0.73
1:I:448:ASN:HA	1:I:477:ASN:ND2	2.04	0.73
2:L:61:CYS:HG	6:L:1128:HEC:HAC	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:HG12	1:A:408:THR:H	1.52	0.73
1:E:21:PHE:CZ	1:E:63:ILE:HD11	2.22	0.73
1:E:723:HIS:CD2	1:E:725:GLU:H	2.05	0.73
1:I:59:PHE:CZ	1:I:710:GLU:HG3	2.23	0.73
2:J:33:ARG:NH2	2:J:40:PRO:HG3	2.04	0.73
1:G:332:LEU:HB3	1:G:340:TRP:CH2	2.23	0.73
1:I:192:MET:CE	1:I:694:ARG:CB	2.65	0.73
1:K:750:ARG:CD	2:L:20:PRO:HA	2.19	0.73
2:L:33:ARG:NH2	2:L:40:PRO:HG3	2.03	0.73
1:K:747:ILE:HG22	1:K:748:ARG:N	2.04	0.72
1:O:272:ILE:HG23	1:O:785:PRO:CG	2.19	0.72
1:O:238:ARG:HH11	1:O:353:ARG:HG3	1.53	0.72
1:G:776:ASN:HA	1:G:779:THR:OG1	1.90	0.72
1:I:750:ARG:HD2	2:J:19:PRO:O	1.89	0.72
1:K:333:TYR:CE2	1:K:340:TRP:HD1	2.05	0.72
1:K:406:VAL:HG12	1:K:408:THR:H	1.53	0.72
1:O:180:ASP:HB2	1:O:339:LYS:H	1.53	0.72
1:O:400:ARG:NH2	1:O:404:ASP:H	1.87	0.72
2:B:33:ARG:NH2	2:B:40:PRO:HG3	2.04	0.72
1:C:772:SER:HB2	2:D:4:PRO:HG2	1.70	0.72
1:G:503:VAL:CG1	1:G:522:LEU:HB2	2.18	0.72
1:K:238:ARG:HG2	1:K:360:MET:CE	2.18	0.72
1:K:491:ARG:NH2	2:L:11:ARG:H	1.88	0.72
1:O:455:ASN:ND2	1:O:457:ASN:HB2	2.03	0.72
2:H:95:ARG:HA	6:H:1129:HEC:HMC2	1.71	0.72
1:K:76:ARG:O	1:K:77:MET:HB2	1.89	0.72
1:M:168:GLU:HG3	1:M:632:TRP:HZ2	1.54	0.72
2:P:33:ARG:NH2	2:P:40:PRO:HG3	2.04	0.72
1:C:184:LEU:HD11	1:C:189:MET:HE3	1.70	0.72
1:O:181:ALA:HB3	1:O:340:TRP:HZ3	1.51	0.72
1:C:332:LEU:HG	1:C:340:TRP:CH2	2.25	0.72
1:I:750:ARG:CD	2:J:20:PRO:HA	2.19	0.72
2:L:94:ARG:O	2:L:95:ARG:HB2	1.89	0.72
2:P:33:ARG:HD3	6:P:1129:HEC:O2D	1.90	0.72
1:C:692:THR:HG21	5:C:1803:MGD:N19	2.05	0.72
2:D:33:ARG:NH2	2:D:40:PRO:HG3	2.04	0.72
1:K:332:LEU:HG	1:K:340:TRP:CH2	2.24	0.72
1:K:76:ARG:NH2	1:K:473:ARG:NH2	2.37	0.72
1:O:163:THR:HG23	1:O:359:HIS:ND1	2.05	0.72
1:G:192:MET:CE	1:G:694:ARG:CB	2.66	0.72
1:G:272:ILE:HG23	1:G:785:PRO:CG	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:238:ARG:NH1	1:K:353:ARG:HG3	2.04	0.72
1:M:272:ILE:HG23	1:M:785:PRO:CG	2.19	0.72
1:C:332:LEU:CG	1:C:340:TRP:CH2	2.72	0.72
1:C:406:VAL:HG12	1:C:408:THR:H	1.53	0.72
1:E:747:ILE:HG22	1:E:748:ARG:N	2.05	0.72
1:G:396:THR:HG22	1:G:396:THR:O	1.90	0.72
2:P:40:PRO:HD2	2:P:102:HIS:HE1	1.54	0.72
1:C:238:ARG:NH1	1:C:353:ARG:HG3	2.05	0.71
1:C:559:ALA:O	1:C:560:TYR:CG	2.43	0.71
1:G:423:PRO:HD3	1:G:560:TYR:CE1	2.24	0.71
1:O:503:VAL:HG13	1:O:522:LEU:HB2	1.72	0.71
1:A:272:ILE:CG2	1:A:785:PRO:HG3	2.19	0.71
1:G:244:ILE:HD11	1:G:329:LEU:HD23	1.73	0.71
1:G:747:ILE:HG22	1:G:748:ARG:N	2.05	0.71
1:I:168:GLU:HG3	1:I:632:TRP:HZ2	1.56	0.71
2:L:5:ARG:C	2:L:7:THR:N	2.39	0.71
2:N:95:ARG:HA	6:N:1129:HEC:HMC2	1.70	0.71
1:O:633:PRO:CD	1:O:640:THR:HB	2.20	0.71
1:C:333:TYR:CE2	1:C:340:TRP:CD1	2.78	0.71
1:I:448:ASN:ND2	1:I:477:ASN:HD21	1.87	0.71
1:I:537:MET:O	1:I:540:SER:HB2	1.89	0.71
1:I:716:PRO:CG	2:J:22:PRO:HG2	2.20	0.71
2:N:4:PRO:HG3	2:N:16:VAL:CG1	2.15	0.71
1:C:511:ASN:OD1	1:C:515:ARG:HB3	1.91	0.71
1:C:59:PHE:CZ	1:C:710:GLU:HG3	2.25	0.71
1:C:741:ILE:HG12	1:C:746:GLU:HG2	1.71	0.71
1:E:183:VAL:CG2	1:E:340:TRP:NE1	2.54	0.71
1:G:146:ASP:OD1	1:G:150:ARG:HD2	1.89	0.71
1:I:21:PHE:CZ	1:I:63:ILE:HD11	2.26	0.71
2:J:4:PRO:CG	2:J:16:VAL:HG11	2.16	0.71
1:K:183:VAL:CG2	1:K:340:TRP:NE1	2.54	0.71
2:B:4:PRO:HG3	2:B:16:VAL:CG1	2.15	0.71
2:D:94:ARG:O	2:D:95:ARG:HB2	1.89	0.71
1:E:332:LEU:HD23	1:E:340:TRP:CH2	2.26	0.71
1:G:400:ARG:NH2	1:G:404:ASP:H	1.88	0.71
1:I:68:ASP:HB2	1:I:707:ARG:NH1	2.05	0.71
1:O:183:VAL:CG2	1:O:340:TRP:NE1	2.52	0.71
1:C:356:TRP:O	1:C:360:MET:HG3	1.91	0.71
1:K:155:SER:H	1:K:789:GLN:HE21	1.38	0.71
1:E:146:ASP:OD1	1:E:150:ARG:HD2	1.91	0.71
2:L:30:ARG:HD2	6:L:1128:HEC:O1D	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:406:VAL:HG12	1:M:408:THR:H	1.56	0.71
1:M:716:PRO:CG	2:N:22:PRO:HG2	2.20	0.71
1:C:238:ARG:HH11	1:C:353:ARG:HG3	1.54	0.71
2:D:33:ARG:HD3	6:D:1129:HEC:O2D	1.90	0.71
1:K:272:ILE:HG23	1:K:785:PRO:CG	2.21	0.71
1:A:184:LEU:HD11	1:A:189:MET:HE3	1.73	0.71
1:C:396:THR:HG22	1:C:396:THR:O	1.91	0.71
1:C:455:ASN:ND2	1:C:457:ASN:HB2	2.06	0.71
1:C:487:THR:HG22	1:C:490:GLY:H	1.54	0.71
1:I:183:VAL:CG2	1:I:340:TRP:HE1	2.04	0.71
1:K:455:ASN:ND2	1:K:457:ASN:HB2	2.06	0.71
1:K:59:PHE:CZ	1:K:710:GLU:HG3	2.26	0.71
1:C:168:GLU:HG3	1:C:632:TRP:HZ2	1.56	0.71
1:M:238:ARG:NH1	1:M:353:ARG:HG3	2.05	0.71
1:O:406:VAL:HG12	1:O:408:THR:H	1.55	0.71
1:A:716:PRO:CG	2:B:22:PRO:HG2	2.19	0.70
2:D:101:CYS:SG	6:D:1129:HEC:HAC	2.31	0.70
1:E:406:VAL:HG12	1:E:408:THR:H	1.55	0.70
1:M:339:LYS:HA	1:M:376:ASN:ND2	2.06	0.70
1:M:776:ASN:HA	1:M:779:THR:OG1	1.91	0.70
1:O:692:THR:HG21	5:O:1803:MGD:N19	2.06	0.70
1:E:559:ALA:O	1:E:560:TYR:CG	2.44	0.70
2:H:94:ARG:O	2:H:95:ARG:HB2	1.91	0.70
1:K:183:VAL:HG23	1:K:340:TRP:CE2	2.27	0.70
1:M:747:ILE:HG22	1:M:748:ARG:N	2.05	0.70
1:O:76:ARG:NH2	1:O:473:ARG:NH2	2.38	0.70
2:J:94:ARG:O	2:J:95:ARG:HB2	1.90	0.70
1:K:396:THR:O	1:K:396:THR:HG22	1.90	0.70
1:E:180:ASP:OD2	1:E:339:LYS:HG3	1.91	0.70
1:K:180:ASP:OD2	1:K:339:LYS:HG3	1.90	0.70
2:N:5:ARG:C	2:N:7:THR:N	2.41	0.70
1:A:168:GLU:HG3	1:A:632:TRP:HZ2	1.55	0.70
1:G:168:GLU:HG3	1:G:632:TRP:HZ2	1.56	0.70
1:G:333:TYR:CE2	1:G:340:TRP:HD1	2.09	0.70
1:I:723:HIS:CD2	1:I:725:GLU:H	2.09	0.70
1:O:184:LEU:HD11	1:O:189:MET:HE3	1.74	0.70
1:O:741:ILE:HG12	1:O:746:GLU:HG2	1.74	0.70
1:C:272:ILE:CG2	1:C:785:PRO:HG3	2.22	0.70
1:G:406:VAL:HG12	1:G:408:THR:H	1.56	0.70
2:L:4:PRO:O	2:L:5:ARG:C	2.30	0.70
1:A:183:VAL:CG2	1:A:340:TRP:NE1	2.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:720:CYS:HA	1:I:766:VAL:HG12	1.73	0.70
1:K:155:SER:H	1:K:789:GLN:NE2	1.89	0.70
1:O:339:LYS:HA	1:O:376:ASN:ND2	2.06	0.70
1:O:487:THR:HG22	1:O:490:GLY:H	1.55	0.70
1:O:599:PRO:O	1:O:603:LEU:HD12	1.92	0.70
1:A:559:ALA:O	1:A:560:TYR:CG	2.44	0.70
1:A:150:ARG:HD3	1:A:434:HIS:HB2	1.74	0.70
1:C:21:PHE:CZ	1:C:63:ILE:HD11	2.27	0.70
1:E:750:ARG:CD	2:F:20:PRO:HA	2.22	0.70
1:G:155:SER:H	1:G:789:GLN:HE21	1.38	0.70
1:I:486:PRO:O	1:I:487:THR:HB	1.92	0.70
1:K:719:VAL:HG11	1:K:752:GLU:HB2	1.73	0.70
2:L:33:ARG:HD3	6:L:1129:HEC:O2D	1.91	0.70
1:E:150:ARG:HD3	1:E:434:HIS:HB2	1.73	0.70
1:E:720:CYS:HA	1:E:766:VAL:HG12	1.72	0.70
2:F:33:ARG:NH2	2:F:40:PRO:HG3	2.07	0.70
1:G:448:ASN:HA	1:G:477:ASN:ND2	2.07	0.70
2:H:4:PRO:O	2:H:5:ARG:C	2.30	0.70
1:I:76:ARG:O	1:I:77:MET:HB2	1.89	0.70
1:M:76:ARG:NH2	1:M:473:ARG:NH2	2.40	0.70
1:C:272:ILE:HG23	1:C:785:PRO:CG	2.22	0.69
1:C:338:ARG:HG2	1:C:340:TRP:CE3	2.27	0.69
1:E:741:ILE:HG12	1:E:746:GLU:HG2	1.72	0.69
1:E:272:ILE:CG2	1:E:785:PRO:HG3	2.22	0.69
1:C:68:ASP:HB2	1:C:707:ARG:NH1	2.06	0.69
1:E:168:GLU:HG3	1:E:632:TRP:HZ2	1.56	0.69
1:I:184:LEU:HD11	1:I:189:MET:CE	2.21	0.69
1:I:356:TRP:O	1:I:360:MET:HG3	1.92	0.69
1:I:16:LYS:HD2	1:I:628:ARG:HG3	1.72	0.69
1:I:776:ASN:HA	1:I:779:THR:OG1	1.91	0.69
1:O:155:SER:H	1:O:789:GLN:HE21	1.39	0.69
1:A:238:ARG:NH1	1:A:353:ARG:HG3	2.07	0.69
1:G:720:CYS:HA	1:G:766:VAL:HG12	1.73	0.69
1:G:272:ILE:CG2	1:G:785:PRO:HG3	2.22	0.69
1:O:230:ILE:HG23	1:O:321:VAL:CG1	2.23	0.69
2:P:94:ARG:O	2:P:95:ARG:HB2	1.92	0.69
2:J:4:PRO:HG3	2:J:16:VAL:CG1	2.18	0.69
1:K:146:ASP:OD1	1:K:150:ARG:HD2	1.92	0.69
1:O:59:PHE:CZ	1:O:710:GLU:HG3	2.28	0.69
1:C:503:VAL:CG1	1:C:522:LEU:HB2	2.22	0.69
2:F:4:PRO:O	2:F:5:ARG:C	2.31	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:155:SER:H	1:I:789:GLN:HE21	1.41	0.69
1:K:716:PRO:CG	2:L:22:PRO:HG2	2.20	0.69
1:M:192:MET:CE	1:M:694:ARG:CB	2.70	0.69
1:C:155:SER:H	1:C:789:GLN:NE2	1.89	0.69
1:C:423:PRO:HD3	1:C:560:TYR:CE1	2.27	0.69
2:D:58:CYS:CB	6:D:1128:HEC:HAB	2.22	0.69
1:E:272:ILE:HG23	1:E:785:PRO:CG	2.21	0.69
2:J:118:ASP:OD1	2:P:67:SER:HA	1.92	0.69
1:M:333:TYR:CE2	1:M:340:TRP:HD1	2.10	0.69
1:M:653:LYS:O	1:M:656:GLU:HB2	1.93	0.69
1:O:776:ASN:HA	1:O:779:THR:OG1	1.93	0.69
1:E:400:ARG:NH2	1:E:404:ASP:H	1.91	0.69
1:E:599:PRO:O	1:E:603:LEU:HD12	1.93	0.69
1:G:356:TRP:O	1:G:360:MET:HG3	1.91	0.69
1:G:76:ARG:O	1:G:77:MET:HB2	1.91	0.69
1:I:333:TYR:CE2	1:I:340:TRP:CD1	2.80	0.69
1:K:339:LYS:HA	1:K:376:ASN:HD21	1.56	0.69
1:K:332:LEU:HD23	1:K:340:TRP:CH2	2.27	0.69
1:M:321:VAL:HG21	1:M:326:LEU:HD11	1.75	0.69
2:N:4:PRO:O	2:N:5:ARG:C	2.30	0.69
1:A:599:PRO:O	1:A:603:LEU:HD12	1.92	0.69
1:C:76:ARG:NH2	1:C:473:ARG:NH2	2.40	0.69
2:H:37:GLU:HA	6:H:1129:HEC:HMD1	1.73	0.69
1:K:76:ARG:HA	1:K:87:GLU:O	1.92	0.69
1:M:503:VAL:CG1	1:M:522:LEU:HB2	2.22	0.69
1:A:741:ILE:HG12	1:A:746:GLU:HG2	1.74	0.69
1:E:339:LYS:HA	1:E:376:ASN:ND2	2.07	0.69
1:I:543:PHE:O	1:I:564:THR:HA	1.93	0.69
1:M:43:ASP:OD2	1:M:628:ARG:NH1	2.26	0.69
1:A:611:GLY:O	1:A:612:ARG:HB2	1.92	0.69
1:C:238:ARG:HG2	1:C:360:MET:CE	2.23	0.69
1:G:155:SER:H	1:G:789:GLN:NE2	1.91	0.69
1:K:181:ALA:HB3	1:K:340:TRP:HZ3	1.51	0.69
1:K:740:VAL:CG1	1:K:797:VAL:HG11	2.22	0.69
1:O:220:HIS:CE1	1:O:222:SER:HB2	2.28	0.69
1:A:487:THR:HG22	1:A:490:GLY:H	1.57	0.69
1:A:80:GLY:O	1:A:81:VAL:HB	1.93	0.69
2:B:94:ARG:O	2:B:95:ARG:HB2	1.92	0.69
1:C:253:ARG:NH2	1:C:331:GLU:OE1	2.26	0.69
1:E:487:THR:HG22	1:E:490:GLY:H	1.57	0.69
1:E:503:VAL:CG1	1:E:522:LEU:HB2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:272:ILE:CG2	1:I:785:PRO:HG3	2.23	0.69
2:J:98:CYS:CB	6:J:1129:HEC:HAB	2.22	0.69
1:M:183:VAL:CG2	1:M:340:TRP:NE1	2.56	0.69
1:M:59:PHE:CZ	1:M:710:GLU:HG3	2.28	0.69
1:O:396:THR:HG22	1:O:396:THR:O	1.93	0.69
1:C:740:VAL:CG1	1:C:797:VAL:HG11	2.23	0.68
1:G:692:THR:HG21	5:G:1803:MGD:N19	2.08	0.68
1:G:76:ARG:HA	1:G:87:GLU:O	1.93	0.68
1:M:184:LEU:HD11	1:M:189:MET:HE3	1.75	0.68
1:O:338:ARG:HG2	1:O:340:TRP:CE3	2.27	0.68
1:A:118:MET:HE1	1:A:132:ALA:HB1	1.76	0.68
1:E:183:VAL:HG23	1:E:340:TRP:CE2	2.27	0.68
1:E:491:ARG:NH2	2:F:11:ARG:H	1.91	0.68
1:E:750:ARG:HD2	2:F:19:PRO:O	1.92	0.68
1:G:723:HIS:CD2	1:G:725:GLU:H	2.11	0.68
1:K:184:LEU:HD11	1:K:189:MET:HE3	1.75	0.68
1:C:776:ASN:HA	1:C:779:THR:HG1	1.57	0.68
2:F:42:ILE:HD11	6:F:1128:HEC:HMB2	1.74	0.68
1:I:43:ASP:OD2	1:I:628:ARG:NH1	2.27	0.68
1:M:338:ARG:HG2	1:M:340:TRP:CE3	2.29	0.68
1:G:21:PHE:CZ	1:G:63:ILE:HD11	2.28	0.68
1:I:400:ARG:NH2	1:I:404:ASP:H	1.89	0.68
1:M:455:ASN:ND2	1:M:457:ASN:HB2	2.07	0.68
1:O:147:PRO:HD3	1:O:396:THR:O	1.93	0.68
1:O:448:ASN:ND2	1:O:477:ASN:HD21	1.88	0.68
1:I:272:ILE:HG23	1:I:785:PRO:CG	2.23	0.68
1:I:339:LYS:HA	1:I:376:ASN:HD21	1.58	0.68
1:K:333:TYR:CE2	1:K:340:TRP:CD1	2.81	0.68
2:L:42:ILE:CD1	6:L:1128:HEC:HMB2	2.23	0.68
1:O:338:ARG:HG2	1:O:340:TRP:CZ3	2.29	0.68
1:K:272:ILE:CG2	1:K:785:PRO:HG3	2.22	0.68
1:K:339:LYS:HA	1:K:376:ASN:ND2	2.08	0.68
1:M:168:GLU:HG3	1:M:632:TRP:CZ2	2.29	0.68
1:O:238:ARG:HG2	1:O:360:MET:CE	2.24	0.68
1:O:43:ASP:OD2	1:O:628:ARG:NH1	2.27	0.68
1:O:76:ARG:O	1:O:77:MET:HB2	1.93	0.68
1:A:155:SER:H	1:A:789:GLN:NE2	1.92	0.68
1:K:720:CYS:HA	1:K:766:VAL:HG12	1.75	0.68
1:O:163:THR:CG2	1:O:359:HIS:HD1	2.06	0.68
1:A:192:MET:CE	1:A:694:ARG:CB	2.71	0.68
1:C:400:ARG:NH2	1:C:404:ASP:H	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:SER:H	1:E:789:GLN:NE2	1.91	0.68
1:I:406:VAL:HG12	1:I:408:THR:H	1.58	0.68
1:I:487:THR:HG22	1:I:490:GLY:H	1.58	0.68
1:I:692:THR:HG21	5:I:1803:MGD:N19	2.08	0.68
1:K:503:VAL:HG13	1:K:522:LEU:HB2	1.75	0.68
1:M:400:ARG:NH2	1:M:404:ASP:H	1.92	0.68
1:O:750:ARG:HD2	2:P:19:PRO:O	1.93	0.68
1:K:244:ILE:HD11	1:K:329:LEU:HD23	1.76	0.68
1:K:599:PRO:O	1:K:603:LEU:HD12	1.94	0.68
1:O:653:LYS:O	1:O:656:GLU:HB2	1.94	0.68
1:K:192:MET:CE	1:K:694:ARG:CB	2.71	0.68
1:K:168:GLU:HG3	1:K:632:TRP:CZ2	2.29	0.68
1:O:76:ARG:HA	1:O:87:GLU:O	1.94	0.68
1:A:747:ILE:HG22	1:A:748:ARG:N	2.08	0.67
1:A:76:ARG:O	1:A:77:MET:HB2	1.94	0.67
1:E:80:GLY:O	1:E:81:VAL:HB	1.94	0.67
1:G:168:GLU:HG3	1:G:632:TRP:CZ2	2.29	0.67
1:G:238:ARG:HG2	1:G:360:MET:CE	2.24	0.67
1:K:356:TRP:O	1:K:360:MET:HG3	1.93	0.67
1:K:776:ASN:HA	1:K:779:THR:OG1	1.94	0.67
1:A:68:ASP:HB2	1:A:707:ARG:NH1	2.07	0.67
2:D:4:PRO:O	2:D:5:ARG:C	2.32	0.67
1:E:253:ARG:NH2	1:E:331:GLU:OE1	2.26	0.67
1:G:455:ASN:ND2	1:G:457:ASN:HB2	2.10	0.67
1:G:503:VAL:HG13	1:G:522:LEU:HB2	1.77	0.67
2:H:98:CYS:O	2:H:100:ALA:N	2.27	0.67
1:O:29:MET:HE3	1:O:628:ARG:HH12	1.60	0.67
1:C:183:VAL:CG2	1:C:340:TRP:NE1	2.57	0.67
2:H:33:ARG:NH2	2:H:40:PRO:HG3	2.09	0.67
1:K:559:ALA:O	1:K:560:TYR:CG	2.47	0.67
1:K:68:ASP:HB2	1:K:707:ARG:NH1	2.08	0.67
1:O:438:GLN:HE21	1:O:450:TYR:HE1	1.42	0.67
1:C:747:ILE:HG22	1:C:748:ARG:N	2.09	0.67
1:E:776:ASN:HA	1:E:779:THR:OG1	1.94	0.67
1:G:653:LYS:O	1:G:656:GLU:HB2	1.94	0.67
1:I:339:LYS:HA	1:I:376:ASN:ND2	2.09	0.67
1:K:741:ILE:HG12	1:K:746:GLU:HG2	1.76	0.67
1:M:184:LEU:HD11	1:M:189:MET:CE	2.24	0.67
1:O:52:LEU:HG	6:P:1129:HEC:CBC	2.24	0.67
2:P:42:ILE:HD11	6:P:1128:HEC:HMB2	1.75	0.67
1:A:238:ARG:HH11	1:A:353:ARG:HG3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:O	1:C:77:MET:HB2	1.93	0.67
1:G:321:VAL:HG21	1:G:326:LEU:HD11	1.75	0.67
1:K:423:PRO:HD3	1:K:560:TYR:CE1	2.30	0.67
1:M:720:CYS:HA	1:M:766:VAL:HG12	1.75	0.67
1:O:183:VAL:HG23	1:O:340:TRP:CE2	2.28	0.67
1:A:272:ILE:HG23	1:A:785:PRO:CG	2.24	0.67
1:C:653:LYS:O	1:C:656:GLU:HB2	1.95	0.67
1:M:238:ARG:HH11	1:M:353:ARG:HG3	1.58	0.67
2:N:94:ARG:O	2:N:95:ARG:HB2	1.94	0.67
1:O:184:LEU:HD11	1:O:189:MET:CE	2.23	0.67
1:O:423:PRO:HD3	1:O:560:TYR:CE1	2.29	0.67
1:A:146:ASP:OD1	1:A:150:ARG:HD2	1.95	0.67
1:A:278:PRO:O	1:A:279:GLU:CB	2.43	0.67
1:A:338:ARG:HG2	1:A:340:TRP:CZ3	2.29	0.67
2:D:51:LEU:HD21	2:D:58:CYS:SG	2.34	0.67
1:I:155:SER:H	1:I:789:GLN:NE2	1.92	0.67
1:K:750:ARG:HD2	2:L:19:PRO:O	1.94	0.67
1:M:270:THR:HG22	1:M:674:PRO:HG3	1.77	0.67
2:N:42:ILE:HD11	6:N:1128:HEC:HMB2	1.76	0.67
2:P:49:TYR:CE1	6:P:1128:HEC:HMC2	2.30	0.67
1:A:396:THR:O	1:A:396:THR:HG22	1.94	0.67
1:A:400:ARG:NH2	1:A:404:ASP:H	1.93	0.67
1:G:68:ASP:HB2	1:G:707:ARG:NH1	2.09	0.67
1:I:633:PRO:HD2	1:I:640:THR:HB	1.75	0.67
1:M:511:ASN:OD1	1:M:515:ARG:HB3	1.94	0.67
1:O:633:PRO:HD2	1:O:640:THR:HB	1.76	0.67
1:A:76:ARG:HA	1:A:87:GLU:O	1.94	0.67
1:E:184:LEU:HD11	1:E:189:MET:HE3	1.77	0.67
1:O:511:ASN:OD1	1:O:515:ARG:HB3	1.95	0.67
1:A:776:ASN:HA	1:A:779:THR:OG1	1.95	0.67
1:C:611:GLY:O	1:C:612:ARG:HB2	1.95	0.67
1:E:333:TYR:CE2	1:E:340:TRP:HD1	2.13	0.67
1:E:155:SER:H	1:E:789:GLN:HE21	1.43	0.67
1:I:396:THR:HG22	1:I:396:THR:O	1.95	0.67
1:M:183:VAL:HG23	1:M:340:TRP:CE2	2.30	0.67
1:M:68:ASP:OD2	1:M:707:ARG:NH1	2.28	0.67
1:M:80:GLY:O	1:M:81:VAL:HB	1.93	0.67
1:O:448:ASN:HA	1:O:477:ASN:ND2	2.10	0.67
2:B:33:ARG:HD3	6:B:1129:HEC:O2D	1.94	0.66
1:C:155:SER:H	1:C:789:GLN:HE21	1.42	0.66
1:C:338:ARG:HG2	1:C:340:TRP:CZ3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:ARG:O	1:E:77:MET:HB2	1.93	0.66
1:G:68:ASP:OD2	1:G:707:ARG:NH1	2.29	0.66
1:M:332:LEU:HD23	1:M:340:TRP:CH2	2.30	0.66
1:I:338:ARG:HG2	1:I:340:TRP:CE3	2.29	0.66
1:M:741:ILE:HG12	1:M:746:GLU:HG2	1.76	0.66
1:M:750:ARG:HD2	2:N:19:PRO:O	1.96	0.66
1:O:155:SER:H	1:O:789:GLN:NE2	1.93	0.66
1:A:338:ARG:HG2	1:A:340:TRP:CE3	2.30	0.66
2:B:4:PRO:O	2:B:5:ARG:C	2.33	0.66
1:C:76:ARG:HA	1:C:87:GLU:O	1.95	0.66
1:G:183:VAL:CG2	1:G:340:TRP:NE1	2.57	0.66
1:I:338:ARG:HG2	1:I:340:TRP:CZ3	2.30	0.66
1:I:653:LYS:O	1:I:656:GLU:HB2	1.95	0.66
1:O:332:LEU:HD23	1:O:340:TRP:CH2	2.31	0.66
1:A:333:TYR:CE2	1:A:340:TRP:HD1	2.14	0.66
1:G:559:ALA:O	1:G:560:TYR:CG	2.49	0.66
1:G:631:HIS:ND1	1:G:639:GLU:OE2	2.28	0.66
2:N:58:CYS:CB	6:N:1128:HEC:HAB	2.24	0.66
1:O:632:TRP:CE3	1:O:632:TRP:O	2.48	0.66
1:A:455:ASN:ND2	1:A:457:ASN:HB2	2.10	0.66
2:D:83:ARG:O	2:D:84:GLU:CB	2.44	0.66
1:E:702:GLY:O	1:E:706:LEU:HB2	1.95	0.66
2:P:37:GLU:HA	6:P:1129:HEC:HMD1	1.76	0.66
1:K:448:ASN:ND2	1:K:477:ASN:HD21	1.90	0.66
1:E:238:ARG:NH1	1:E:353:ARG:HG3	2.10	0.66
1:G:183:VAL:HG23	1:G:340:TRP:CE2	2.30	0.66
1:I:163:THR:HG23	1:I:359:HIS:ND1	2.11	0.66
1:I:245:ALA:HB3	1:I:307:VAL:HG11	1.78	0.66
1:I:565:LEU:O	1:I:566:PHE:HB2	1.95	0.66
1:O:333:TYR:CE2	1:O:340:TRP:CD1	2.83	0.66
1:A:163:THR:HG23	1:A:359:HIS:ND1	2.10	0.66
1:E:338:ARG:HG2	1:E:340:TRP:CZ3	2.30	0.66
1:K:487:THR:HG22	1:K:490:GLY:H	1.60	0.66
1:M:76:ARG:O	1:M:77:MET:HB2	1.95	0.66
1:A:180:ASP:HB2	1:A:339:LYS:H	1.59	0.66
1:A:168:GLU:HG3	1:A:632:TRP:CZ2	2.31	0.66
1:C:448:ASN:HA	1:C:477:ASN:ND2	2.11	0.66
1:C:546:ASP:O	1:C:548:VAL:N	2.29	0.66
2:J:4:PRO:O	2:J:5:ARG:C	2.33	0.66
1:M:338:ARG:HG2	1:M:340:TRP:CZ3	2.31	0.66
1:M:559:ALA:O	1:M:560:TYR:CG	2.49	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:253:ARG:NH2	1:O:331:GLU:OE1	2.29	0.66
1:A:181:ALA:HB3	1:A:340:TRP:HZ3	1.57	0.66
1:E:455:ASN:ND2	1:E:457:ASN:HB2	2.11	0.66
1:E:631:HIS:ND1	1:E:639:GLU:OE2	2.27	0.66
2:H:42:ILE:CD1	6:H:1128:HEC:HMB2	2.26	0.66
1:I:172:CYS:SG	1:I:174:ASP:HB2	2.35	0.66
1:M:253:ARG:NH2	1:M:331:GLU:OE1	2.28	0.66
1:O:168:GLU:HG3	1:O:632:TRP:HZ2	1.60	0.66
1:O:321:VAL:HG21	1:O:326:LEU:HD11	1.78	0.66
1:A:719:VAL:HG11	1:A:752:GLU:HB2	1.76	0.65
1:C:20:ARG:HG3	1:C:20:ARG:O	1.96	0.65
1:C:80:GLY:O	1:C:81:VAL:HB	1.96	0.65
1:G:220:HIS:CE1	1:G:222:SER:HB2	2.31	0.65
1:A:43:ASP:OD2	1:A:628:ARG:NH1	2.29	0.65
1:A:720:CYS:HA	1:A:766:VAL:HG12	1.77	0.65
2:B:30:ARG:HD2	6:B:1128:HEC:O1D	1.95	0.65
1:C:633:PRO:CD	1:C:640:THR:HB	2.24	0.65
2:F:94:ARG:O	2:F:95:ARG:HB2	1.95	0.65
1:I:793:LYS:HE3	5:I:1804:MGD:H5'2	1.78	0.65
1:I:184:LEU:HD11	1:I:189:MET:HE3	1.78	0.65
1:I:225:LEU:HG	1:I:225:LEU:O	1.96	0.65
1:I:546:ASP:O	1:I:548:VAL:N	2.29	0.65
1:M:230:ILE:HG23	1:M:321:VAL:CG1	2.27	0.65
1:O:384:GLN:HB3	1:O:385:PRO:HD2	1.76	0.65
1:A:59:PHE:CZ	1:A:710:GLU:HG3	2.31	0.65
2:B:40:PRO:HD3	6:B:1129:HEC:HBD2	1.77	0.65
1:C:147:PRO:HD3	1:C:396:THR:O	1.97	0.65
1:C:168:GLU:HG3	1:C:632:TRP:CZ2	2.31	0.65
2:H:34:ASN:H	2:H:38:GLN:NE2	1.94	0.65
1:I:448:ASN:HA	1:I:477:ASN:HD22	1.62	0.65
1:I:168:GLU:HG3	1:I:632:TRP:CZ2	2.31	0.65
1:K:230:ILE:HG23	1:K:321:VAL:CG1	2.26	0.65
1:M:163:THR:HG23	1:M:359:HIS:ND1	2.11	0.65
1:M:633:PRO:CD	1:M:640:THR:HB	2.25	0.65
1:O:753:THR:O	1:O:754:ARG:HB2	1.96	0.65
1:C:720:CYS:HA	1:C:766:VAL:HG12	1.77	0.65
1:E:503:VAL:HG13	1:E:522:LEU:HB2	1.79	0.65
1:M:448:ASN:HA	1:M:477:ASN:ND2	2.10	0.65
1:M:155:SER:H	1:M:789:GLN:NE2	1.94	0.65
1:O:565:LEU:O	1:O:566:PHE:HB2	1.95	0.65
1:A:183:VAL:HG23	1:A:340:TRP:CE2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:PRO:CD	1:A:640:THR:HB	2.25	0.65
1:E:43:ASP:OD2	1:E:628:ARG:NH1	2.29	0.65
1:G:238:ARG:HH11	1:G:353:ARG:HG3	1.61	0.65
1:I:253:ARG:NH2	1:I:331:GLU:OE1	2.29	0.65
2:J:42:ILE:CD1	6:J:1128:HEC:HMB2	2.26	0.65
1:K:20:ARG:HG3	1:K:20:ARG:O	1.95	0.65
1:M:238:ARG:HG2	1:M:360:MET:CE	2.27	0.65
1:C:750:ARG:CD	2:D:20:PRO:HA	2.27	0.65
1:C:184:LEU:HD11	1:C:189:MET:CE	2.26	0.65
1:I:118:MET:HE1	1:I:132:ALA:HB1	1.77	0.65
1:I:423:PRO:HD3	1:I:560:TYR:CE1	2.32	0.65
1:K:714:ALA:HB2	2:L:103:VAL:HG11	1.77	0.65
1:M:333:TYR:CE2	1:M:340:TRP:CD1	2.85	0.65
1:M:272:ILE:CG2	1:M:785:PRO:HG3	2.26	0.65
1:C:346:MET:HB3	1:C:350:GLN:HG3	1.79	0.65
1:C:68:ASP:O	1:C:69:ARG:C	2.35	0.65
1:E:68:ASP:HB2	1:E:707:ARG:NH1	2.11	0.65
1:I:80:GLY:O	1:I:81:VAL:HB	1.97	0.65
1:K:184:LEU:HD11	1:K:189:MET:CE	2.27	0.65
1:K:253:ARG:NH2	1:K:331:GLU:OE1	2.28	0.65
1:M:545:THR:OG1	1:M:563:LYS:HB2	1.97	0.65
1:O:543:PHE:O	1:O:564:THR:HA	1.96	0.65
1:O:559:ALA:O	1:O:560:TYR:CG	2.49	0.65
1:C:183:VAL:HG23	1:C:340:TRP:CE2	2.32	0.65
1:E:168:GLU:HG3	1:E:632:TRP:CZ2	2.32	0.65
1:K:125:THR:HG21	1:K:127:TRP:NE1	2.12	0.65
1:K:80:GLY:O	1:K:81:VAL:HB	1.96	0.65
1:M:68:ASP:HB2	1:M:707:ARG:NH1	2.12	0.65
1:E:653:LYS:O	1:E:656:GLU:HB2	1.96	0.64
1:E:68:ASP:O	1:E:69:ARG:C	2.35	0.64
1:A:750:ARG:CD	2:B:20:PRO:HA	2.27	0.64
1:G:491:ARG:NH2	2:H:11:ARG:H	1.95	0.64
1:I:137:ARG:O	1:I:141:ARG:HA	1.97	0.64
1:I:559:ALA:O	1:I:560:TYR:CG	2.50	0.64
1:I:719:VAL:HG11	1:I:752:GLU:HB2	1.77	0.64
1:A:321:VAL:HG21	1:A:326:LEU:HD11	1.78	0.64
1:A:332:LEU:HD23	1:A:340:TRP:CH2	2.32	0.64
1:E:238:ARG:HH11	1:E:353:ARG:HG3	1.62	0.64
1:I:68:ASP:O	1:I:69:ARG:C	2.35	0.64
1:I:714:ALA:HB2	2:J:103:VAL:HG11	1.78	0.64
1:K:163:THR:HG23	1:K:359:HIS:ND1	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:583:VAL:HG13	1:M:583:VAL:O	1.97	0.64
1:M:631:HIS:ND1	1:M:639:GLU:OE2	2.29	0.64
1:O:514:ARG:O	1:O:631:HIS:HA	1.98	0.64
1:E:192:MET:CE	1:E:694:ARG:CB	2.74	0.64
1:E:76:ARG:HA	1:E:87:GLU:O	1.96	0.64
1:I:220:HIS:CE1	1:I:222:SER:HB2	2.32	0.64
1:K:29:MET:HE3	1:K:628:ARG:HH12	1.62	0.64
1:O:628:ARG:HH11	1:O:628:ARG:HG2	1.62	0.64
1:A:253:ARG:NH2	1:A:331:GLU:OE1	2.30	0.64
1:A:753:THR:O	1:A:754:ARG:HB2	1.98	0.64
1:C:753:THR:O	1:C:754:ARG:HB2	1.97	0.64
1:E:338:ARG:HG2	1:E:340:TRP:CE3	2.33	0.64
1:E:611:GLY:O	1:E:612:ARG:HB2	1.97	0.64
1:M:278:PRO:O	1:M:279:GLU:CB	2.45	0.64
2:N:37:GLU:HA	6:N:1129:HEC:HAD2	1.79	0.64
2:P:40:PRO:HD3	6:P:1129:HEC:HBD2	1.79	0.64
1:C:172:CYS:SG	1:C:174:ASP:HB2	2.38	0.64
1:C:321:VAL:HG21	1:C:326:LEU:HD11	1.79	0.64
1:E:583:VAL:O	1:E:583:VAL:HG13	1.96	0.64
1:K:346:MET:HG2	5:K:1804:MGD:H101	1.80	0.64
1:E:633:PRO:CD	1:E:640:THR:HB	2.27	0.64
1:G:303:PHE:O	1:G:307:VAL:HG23	1.97	0.64
1:G:253:ARG:NH2	1:G:331:GLU:OE1	2.31	0.64
1:G:238:ARG:NH1	1:G:353:ARG:HG3	2.13	0.64
1:G:76:ARG:NH2	1:G:473:ARG:NH2	2.45	0.64
1:O:750:ARG:HD3	2:P:20:PRO:HA	1.80	0.64
2:P:4:PRO:O	2:P:5:ARG:C	2.34	0.64
1:A:511:ASN:OD1	1:A:515:ARG:HB3	1.97	0.64
1:E:565:LEU:O	1:E:566:PHE:HB2	1.97	0.64
1:G:184:LEU:HD11	1:G:189:MET:HE3	1.80	0.64
1:I:332:LEU:HD23	1:I:340:TRP:CH2	2.31	0.64
1:I:384:GLN:HB3	1:I:385:PRO:HD2	1.79	0.64
2:J:58:CYS:CB	6:J:1128:HEC:HAB	2.27	0.64
1:M:487:THR:HG22	1:M:490:GLY:H	1.62	0.64
1:M:599:PRO:O	1:M:603:LEU:HD12	1.97	0.64
2:N:37:GLU:HA	6:N:1129:HEC:HMD1	1.80	0.64
1:O:719:VAL:HG11	1:O:752:GLU:HB2	1.80	0.64
1:A:21:PHE:O	1:A:385:PRO:HD3	1.98	0.64
1:C:750:ARG:HD2	2:D:19:PRO:O	1.97	0.64
1:I:511:ASN:OD1	1:I:515:ARG:HB3	1.97	0.64
1:M:346:MET:HG2	5:M:1804:MGD:H101	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:714:ALA:HB2	2:N:103:VAL:HG11	1.80	0.64
1:A:333:TYR:CE2	1:A:340:TRP:CD1	2.86	0.64
1:A:423:PRO:HD3	1:A:560:TYR:CE1	2.33	0.64
1:C:543:PHE:O	1:C:564:THR:HA	1.97	0.64
1:K:225:LEU:O	1:K:225:LEU:HG	1.96	0.64
1:G:448:ASN:ND2	1:G:477:ASN:HD21	1.90	0.63
1:G:702:GLY:O	1:G:706:LEU:HB2	1.98	0.63
1:M:546:ASP:O	1:M:548:VAL:N	2.31	0.63
2:N:51:LEU:HD21	2:N:58:CYS:SG	2.39	0.63
1:A:565:LEU:O	1:A:566:PHE:HB2	1.97	0.63
1:A:692:THR:HG21	5:A:1803:MGD:N19	2.06	0.63
1:A:81:VAL:HG12	1:A:82:TYR:N	2.13	0.63
1:C:47:GLU:OE1	1:C:50:ARG:NH2	2.29	0.63
1:E:184:LEU:HD11	1:E:189:MET:CE	2.29	0.63
1:G:332:LEU:HD23	1:G:340:TRP:CH2	2.33	0.63
2:H:41:VAL:CG1	2:H:105:GLN:HG3	2.28	0.63
1:I:180:ASP:HB2	1:I:339:LYS:N	2.12	0.63
1:I:180:ASP:O	1:I:181:ALA:HB2	1.98	0.63
1:I:244:ILE:HD11	1:I:329:LEU:HD23	1.81	0.63
1:K:543:PHE:O	1:K:564:THR:HA	1.98	0.63
1:O:458:MET:O	1:O:464:ILE:HG21	1.97	0.63
1:O:546:ASP:O	1:O:548:VAL:N	2.31	0.63
1:E:244:ILE:HD11	1:E:329:LEU:HD23	1.80	0.63
1:E:511:ASN:OD1	1:E:515:ARG:HB3	1.98	0.63
1:G:543:PHE:O	1:G:564:THR:HA	1.98	0.63
1:I:270:THR:HG22	1:I:674:PRO:HG3	1.79	0.63
1:I:76:ARG:HA	1:I:87:GLU:O	1.98	0.63
2:J:98:CYS:O	2:J:100:ALA:N	2.31	0.63
1:O:125:THR:HG21	1:O:127:TRP:NE1	2.12	0.63
1:O:225:LEU:HG	1:O:225:LEU:O	1.98	0.63
1:A:653:LYS:O	1:A:656:GLU:HB2	1.97	0.63
1:G:125:THR:HG21	1:G:127:TRP:NE1	2.13	0.63
1:G:338:ARG:HG2	1:G:340:TRP:CE3	2.33	0.63
1:I:458:MET:O	1:I:464:ILE:HG21	1.98	0.63
1:C:43:ASP:OD2	1:C:628:ARG:NH1	2.31	0.63
1:E:545:THR:OG1	1:E:563:LYS:HB2	1.99	0.63
1:E:716:PRO:CG	2:F:22:PRO:HG2	2.24	0.63
1:G:184:LEU:HD11	1:G:189:MET:CE	2.28	0.63
2:H:83:ARG:O	2:H:84:GLU:CB	2.45	0.63
1:K:511:ASN:OD1	1:K:515:ARG:HB3	1.98	0.63
1:M:793:LYS:HE3	5:M:1804:MGD:H5'2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:225:LEU:HG	1:M:225:LEU:O	1.99	0.63
1:M:483:ASP:OD1	1:M:484:ALA:N	2.28	0.63
1:M:753:THR:O	1:M:754:ARG:HB2	1.98	0.63
1:O:453:GLN:HG2	1:O:482:SER:HB2	1.80	0.63
1:A:155:SER:H	1:A:789:GLN:HE21	1.46	0.63
1:C:514:ARG:O	1:C:631:HIS:HA	1.99	0.63
1:G:314:LYS:O	1:G:318:ILE:HG13	1.99	0.63
1:I:702:GLY:O	1:I:706:LEU:HB2	1.96	0.63
1:K:43:ASP:OD2	1:K:628:ARG:NH1	2.32	0.63
2:P:41:VAL:CG1	2:P:105:GLN:HG3	2.28	0.63
1:C:220:HIS:CE1	1:C:222:SER:HB2	2.33	0.63
1:E:321:VAL:HG21	1:E:326:LEU:HD11	1.80	0.63
1:G:611:GLY:O	1:G:612:ARG:HB2	1.99	0.63
1:I:438:GLN:HE21	1:I:450:TYR:HE1	1.46	0.63
1:I:491:ARG:NH2	2:J:11:ARG:H	1.96	0.63
1:I:52:LEU:HG	6:J:1129:HEC:CBC	2.29	0.63
1:K:753:THR:O	1:K:754:ARG:HB2	1.99	0.63
1:M:356:TRP:O	1:M:360:MET:HG3	1.97	0.63
1:M:68:ASP:O	1:M:69:ARG:C	2.37	0.63
1:M:740:VAL:CG1	1:M:797:VAL:HG11	2.28	0.63
1:O:80:GLY:O	1:O:81:VAL:HB	1.98	0.63
2:P:10:ASP:O	2:P:11:ARG:C	2.36	0.63
1:C:458:MET:O	1:C:464:ILE:HG21	1.99	0.63
1:C:716:PRO:CG	2:D:22:PRO:HG2	2.24	0.63
1:E:76:ARG:NH2	1:E:473:ARG:NH2	2.46	0.63
1:G:118:MET:HE1	1:G:132:ALA:HB1	1.80	0.63
1:G:632:TRP:O	1:G:632:TRP:CE3	2.51	0.63
1:I:321:VAL:HG21	1:I:326:LEU:HD11	1.80	0.63
1:I:238:ARG:HG2	1:I:360:MET:HE3	1.81	0.63
1:O:137:ARG:O	1:O:141:ARG:HA	1.99	0.63
1:E:544:THR:HA	1:E:564:THR:HA	1.81	0.63
1:G:238:ARG:HG2	1:G:360:MET:HE3	1.80	0.63
1:G:511:ASN:OD1	1:G:515:ARG:HB3	1.98	0.63
1:G:546:ASP:O	1:G:548:VAL:N	2.32	0.63
1:I:544:THR:HA	1:I:564:THR:HA	1.80	0.63
1:K:554:LEU:HD22	1:K:560:TYR:O	1.99	0.63
1:M:503:VAL:HG13	1:M:522:LEU:HB2	1.81	0.63
1:C:503:VAL:CG1	1:C:503:VAL:O	2.47	0.62
1:K:702:GLY:O	1:K:706:LEU:HB2	1.98	0.62
1:M:244:ILE:HD11	1:M:329:LEU:HD23	1.81	0.62
1:M:155:SER:H	1:M:789:GLN:HE21	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:34:ASN:H	2:N:38:GLN:NE2	1.97	0.62
1:O:47:GLU:OE1	1:O:50:ARG:NH2	2.30	0.62
2:D:40:PRO:HD3	6:D:1129:HEC:HBD2	1.79	0.62
1:E:333:TYR:CE2	1:E:340:TRP:CD1	2.86	0.62
1:E:356:TRP:O	1:E:360:MET:HG3	1.98	0.62
2:F:37:GLU:HA	6:F:1129:HEC:HMD1	1.81	0.62
1:G:338:ARG:HG2	1:G:340:TRP:CZ3	2.34	0.62
1:K:147:PRO:HD3	1:K:396:THR:O	1.98	0.62
1:K:21:PHE:HZ	1:K:63:ILE:HD11	1.65	0.62
1:O:180:ASP:O	1:O:181:ALA:HB2	1.99	0.62
1:O:189:MET:HE1	1:O:343:LEU:HD13	1.82	0.62
1:O:702:GLY:O	1:O:706:LEU:HB2	1.99	0.62
1:A:332:LEU:CB	1:A:340:TRP:CH2	2.81	0.62
1:A:76:ARG:NH2	1:A:473:ARG:CZ	2.61	0.62
1:C:270:THR:HG22	1:C:674:PRO:HG3	1.80	0.62
1:G:21:PHE:O	1:G:385:PRO:HD3	1.98	0.62
1:K:220:HIS:CE1	1:K:222:SER:HB2	2.33	0.62
2:N:98:CYS:HB3	6:N:1129:HEC:HAB	1.80	0.62
1:A:503:VAL:HG13	1:A:522:LEU:HB2	1.80	0.62
1:C:332:LEU:HD23	1:C:340:TRP:CH2	2.34	0.62
2:D:94:ARG:O	2:D:95:ARG:CB	2.47	0.62
1:E:332:LEU:CB	1:E:340:TRP:CH2	2.82	0.62
1:E:543:PHE:O	1:E:564:THR:HA	1.99	0.62
1:G:333:TYR:CE2	1:G:340:TRP:CD1	2.86	0.62
1:G:47:GLU:OE1	1:G:50:ARG:NH2	2.31	0.62
1:K:338:ARG:HG2	1:K:340:TRP:CZ3	2.35	0.62
1:K:653:LYS:O	1:K:656:GLU:HB2	1.98	0.62
2:P:98:CYS:HG	6:P:1129:HEC:CAB	2.08	0.62
2:B:10:ASP:O	2:B:11:ARG:C	2.38	0.62
1:C:52:LEU:HG	6:D:1129:HEC:CBC	2.29	0.62
2:J:41:VAL:CG1	2:J:105:GLN:HG3	2.28	0.62
2:L:34:ASN:H	2:L:38:GLN:NE2	1.98	0.62
1:O:314:LYS:O	1:O:318:ILE:HG13	2.00	0.62
1:A:543:PHE:O	1:A:564:THR:HA	2.00	0.62
1:A:776:ASN:HA	1:A:779:THR:HG1	1.65	0.62
1:C:278:PRO:O	1:C:279:GLU:CB	2.47	0.62
1:I:76:ARG:NH2	1:I:473:ARG:NH2	2.47	0.62
1:K:321:VAL:HG21	1:K:326:LEU:HD11	1.81	0.62
1:O:168:GLU:HG3	1:O:632:TRP:CZ2	2.34	0.62
1:O:76:ARG:NH2	1:O:473:ARG:CZ	2.63	0.62
6:F:1129:HEC:HMC1	6:F:1129:HEC:HBC3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:183:VAL:HG21	1:I:340:TRP:HE1	1.64	0.62
1:I:81:VAL:HG12	1:I:82:TYR:N	2.15	0.62
1:K:448:ASN:HA	1:K:477:ASN:ND2	2.15	0.62
1:M:314:LYS:O	1:M:318:ILE:HG13	1.98	0.62
1:E:546:ASP:O	1:E:548:VAL:N	2.33	0.62
1:E:540:SER:HB3	1:E:565:LEU:O	2.00	0.62
1:I:453:GLN:HG2	1:I:482:SER:HB2	1.81	0.62
1:K:68:ASP:O	1:K:69:ARG:C	2.37	0.62
1:M:332:LEU:CB	1:M:340:TRP:CH2	2.82	0.62
1:M:76:ARG:HA	1:M:87:GLU:O	1.99	0.62
1:O:163:THR:CG2	1:O:359:HIS:ND1	2.62	0.62
1:E:278:PRO:O	1:E:279:GLU:CB	2.47	0.62
1:G:267:LEU:O	1:G:295:MET:O	2.18	0.62
1:I:346:MET:HB3	1:I:350:GLN:HG3	1.81	0.62
1:K:183:VAL:HG23	1:K:340:TRP:NE1	2.15	0.62
1:K:278:PRO:O	1:K:279:GLU:CB	2.47	0.62
1:M:565:LEU:O	1:M:566:PHE:HB2	1.98	0.62
1:M:238:ARG:CZ	1:M:676:GLU:O	2.47	0.62
1:O:554:LEU:HD22	1:O:560:TYR:O	2.00	0.62
1:A:184:LEU:HD11	1:A:189:MET:CE	2.28	0.62
1:C:219:THR:OG1	1:C:231:ILE:HD11	1.99	0.62
1:C:544:THR:HA	1:C:564:THR:HA	1.81	0.62
1:C:29:MET:HE3	1:C:628:ARG:HH12	1.64	0.62
2:D:10:ASP:O	2:D:11:ARG:C	2.38	0.62
1:G:68:ASP:O	1:G:69:ARG:C	2.38	0.62
1:G:80:GLY:O	1:G:81:VAL:HB	1.99	0.62
1:I:346:MET:HG2	5:I:1804:MGD:H101	1.81	0.62
1:I:238:ARG:HG2	1:I:360:MET:HE1	1.81	0.62
1:A:503:VAL:CG1	1:A:522:LEU:HB2	2.29	0.61
1:A:740:VAL:CG1	1:A:797:VAL:HG11	2.30	0.61
1:E:448:ASN:HA	1:E:477:ASN:ND2	2.15	0.61
1:E:423:PRO:HD3	1:E:560:TYR:CE1	2.35	0.61
2:B:50:GLN:HB3	2:H:123:MET:HG3	1.82	0.61
1:O:631:HIS:ND1	1:O:639:GLU:OE2	2.33	0.61
1:A:68:ASP:OD2	1:A:707:ARG:NH1	2.33	0.61
1:G:741:ILE:HG12	1:G:746:GLU:HG2	1.81	0.61
1:I:314:LYS:O	1:I:318:ILE:HG13	2.00	0.61
1:I:690:LEU:HD22	1:I:797:VAL:HG21	1.83	0.61
1:K:332:LEU:CB	1:K:340:TRP:CH2	2.83	0.61
1:K:400:ARG:HH21	1:K:404:ASP:H	1.48	0.61
1:K:631:HIS:ND1	1:K:639:GLU:OE2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:628:ARG:HG2	1:M:628:ARG:HH11	1.65	0.61
1:O:33:ARG:HD3	2:P:122:LEU:HD21	1.81	0.61
1:G:565:LEU:O	1:G:566:PHE:HB2	2.00	0.61
1:M:192:MET:HE2	1:M:694:ARG:CB	2.20	0.61
1:O:68:ASP:HB2	1:O:707:ARG:HH12	1.65	0.61
1:A:68:ASP:O	1:A:69:ARG:C	2.38	0.61
1:C:503:VAL:HG13	1:C:522:LEU:HB2	1.82	0.61
1:E:29:MET:HE3	1:E:628:ARG:NH1	2.11	0.61
1:G:346:MET:HB3	1:G:350:GLN:HG3	1.81	0.61
1:I:278:PRO:O	1:I:279:GLU:CB	2.47	0.61
1:I:632:TRP:CE3	1:I:632:TRP:O	2.53	0.61
2:J:49:TYR:CE1	6:J:1128:HEC:HMC2	2.35	0.61
1:O:270:THR:HG22	1:O:674:PRO:HG3	1.81	0.61
1:C:332:LEU:CB	1:C:340:TRP:CH2	2.83	0.61
1:C:163:THR:HG23	1:C:359:HIS:ND1	2.15	0.61
1:I:753:THR:O	1:I:754:ARG:HB2	2.00	0.61
1:O:793:LYS:HE3	5:O:1804:MGD:H5'2	1.82	0.61
1:G:793:LYS:HE3	5:G:1804:MGD:H5'2	1.83	0.61
1:G:574:SER:O	1:G:577:ARG:HB2	2.01	0.61
1:G:750:ARG:HD2	2:H:19:PRO:O	2.00	0.61
1:K:540:SER:HB3	1:K:565:LEU:O	2.01	0.61
1:O:346:MET:HG2	5:O:1804:MGD:H101	1.82	0.61
1:O:544:THR:HA	1:O:564:THR:HA	1.81	0.61
1:C:565:LEU:O	1:C:566:PHE:HB2	2.01	0.61
1:I:740:VAL:CG1	1:I:797:VAL:HG11	2.29	0.61
1:K:338:ARG:HG2	1:K:340:TRP:CE3	2.35	0.61
2:L:10:ASP:O	2:L:11:ARG:C	2.39	0.61
1:C:690:LEU:HB3	1:C:795:CYS:SG	2.40	0.61
1:E:238:ARG:NH1	1:E:676:GLU:O	2.34	0.61
1:G:225:LEU:O	1:G:225:LEU:HG	1.99	0.61
1:M:189:MET:HE1	1:M:343:LEU:HD13	1.82	0.61
1:M:719:VAL:HG11	1:M:752:GLU:HB2	1.82	0.61
1:C:225:LEU:HG	1:C:225:LEU:O	2.00	0.61
1:C:545:THR:OG1	1:C:563:LYS:HB2	2.01	0.61
1:C:702:GLY:O	1:C:706:LEU:HB2	2.00	0.61
1:E:448:ASN:ND2	1:E:477:ASN:HD21	1.96	0.61
1:M:163:THR:CG2	1:M:359:HIS:HD1	2.13	0.61
1:O:172:CYS:SG	1:O:174:ASP:HB2	2.41	0.61
1:O:244:ILE:HD11	1:O:329:LEU:HD23	1.82	0.61
1:A:491:ARG:NH2	2:B:11:ARG:N	2.47	0.61
1:C:314:LYS:O	1:C:318:ILE:HG13	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:VAL:CG1	2:D:105:GLN:HG3	2.31	0.61
1:K:514:ARG:O	1:K:631:HIS:HA	2.00	0.61
1:M:491:ARG:NH2	2:N:11:ARG:N	2.49	0.61
1:C:118:MET:HE1	1:C:132:ALA:HB1	1.81	0.60
1:E:753:THR:O	1:E:754:ARG:HB2	2.00	0.60
1:I:267:LEU:O	1:I:295:MET:O	2.19	0.60
1:I:47:GLU:OE1	1:I:50:ARG:NH2	2.30	0.60
1:M:543:PHE:O	1:M:564:THR:HA	2.00	0.60
1:M:81:VAL:HG12	1:M:82:TYR:N	2.16	0.60
2:D:42:ILE:HD11	6:D:1128:HEC:HMB2	1.82	0.60
1:G:270:THR:HG22	1:G:674:PRO:HG3	1.82	0.60
1:I:52:LEU:HG	6:J:1129:HEC:HBC1	1.83	0.60
1:K:81:VAL:HG12	1:K:82:TYR:N	2.16	0.60
2:L:98:CYS:CB	6:L:1129:HEC:CAB	2.74	0.60
1:O:278:PRO:O	1:O:279:GLU:CB	2.49	0.60
1:O:26:CYS:HB3	1:O:49:ASN:CG	2.22	0.60
1:C:76:ARG:NH2	1:C:473:ARG:CZ	2.65	0.60
1:E:21:PHE:HZ	1:E:63:ILE:HD11	1.66	0.60
2:F:10:ASP:O	2:F:11:ARG:C	2.39	0.60
1:G:43:ASP:OD2	1:G:628:ARG:NH1	2.34	0.60
1:G:719:VAL:HG11	1:G:752:GLU:HB2	1.81	0.60
1:I:230:ILE:HG23	1:I:321:VAL:CG1	2.30	0.60
1:K:16:LYS:HD2	1:K:628:ARG:HG3	1.83	0.60
1:K:303:PHE:O	1:K:307:VAL:HG23	2.01	0.60
1:K:628:ARG:HG2	1:K:628:ARG:HH11	1.67	0.60
1:A:280:HIS:CE1	1:A:282:LEU:HD12	2.37	0.60
1:A:702:GLY:O	1:A:706:LEU:HB2	2.00	0.60
1:C:358:ASN:O	1:C:361:VAL:HG23	2.01	0.60
1:E:147:PRO:HD3	1:E:396:THR:O	2.01	0.60
1:G:163:THR:HG23	1:G:359:HIS:ND1	2.16	0.60
1:G:453:GLN:HG2	1:G:482:SER:HB2	1.83	0.60
2:H:33:ARG:HD3	6:H:1129:HEC:O2D	2.02	0.60
1:K:565:LEU:O	1:K:566:PHE:HB2	2.01	0.60
2:L:98:CYS:HB3	6:L:1129:HEC:HAB	1.80	0.60
1:M:384:GLN:HB3	1:M:385:PRO:HD2	1.82	0.60
1:O:267:LEU:O	1:O:295:MET:O	2.19	0.60
1:O:16:LYS:HD2	1:O:628:ARG:HG3	1.83	0.60
1:O:367:LEU:HD13	1:O:670:ILE:HD13	1.83	0.60
1:G:583:VAL:HG13	1:G:583:VAL:O	2.02	0.60
1:G:753:THR:O	1:G:754:ARG:HB2	2.01	0.60
1:I:505:LYS:HG2	1:I:505:LYS:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:503:VAL:CG1	1:K:503:VAL:O	2.48	0.60
1:K:545:THR:OG1	1:K:563:LYS:HB2	2.02	0.60
2:L:41:VAL:CG1	2:L:105:GLN:HG3	2.31	0.60
1:M:574:SER:O	1:M:577:ARG:HB2	2.02	0.60
1:A:76:ARG:NH2	1:A:473:ARG:HH22	2.00	0.60
1:C:453:GLN:HG2	1:C:482:SER:HB2	1.82	0.60
1:E:439:ASP:OD1	1:E:468:THR:HG23	2.02	0.60
1:G:278:PRO:O	1:G:279:GLU:CB	2.50	0.60
1:K:633:PRO:CD	1:K:640:THR:HB	2.31	0.60
1:M:219:THR:OG1	1:M:231:ILE:HD11	2.02	0.60
1:O:68:ASP:CB	1:O:707:ARG:HH12	2.15	0.60
2:P:41:VAL:HG13	2:P:105:GLN:HG3	1.84	0.60
1:A:453:GLN:HG2	1:A:482:SER:HB2	1.84	0.60
1:E:81:VAL:HG12	1:E:82:TYR:N	2.17	0.60
1:G:617:ASP:HB2	1:G:633:PRO:HA	1.83	0.60
2:J:10:ASP:O	2:J:11:ARG:C	2.39	0.60
2:J:92:SER:O	2:J:94:ARG:O	2.19	0.60
1:K:163:THR:CG2	1:K:359:HIS:HD1	2.15	0.60
1:A:278:PRO:O	1:A:279:GLU:HB2	2.00	0.60
2:B:94:ARG:O	2:B:95:ARG:CB	2.49	0.60
2:H:94:ARG:O	2:H:95:ARG:CB	2.49	0.60
1:I:631:HIS:ND1	1:I:639:GLU:OE2	2.31	0.60
1:O:52:LEU:HG	6:P:1129:HEC:HBC1	1.84	0.60
1:C:267:LEU:O	1:C:295:MET:O	2.20	0.60
1:E:163:THR:HG23	1:E:359:HIS:ND1	2.17	0.60
2:L:94:ARG:O	2:L:95:ARG:CB	2.48	0.60
2:N:10:ASP:O	2:N:11:ARG:C	2.40	0.60
2:N:83:ARG:O	2:N:84:GLU:CB	2.46	0.60
1:O:332:LEU:CB	1:O:340:TRP:CH2	2.85	0.60
1:C:346:MET:HG2	5:C:1804:MGD:H101	1.82	0.59
1:E:483:ASP:OD1	1:E:484:ALA:N	2.35	0.59
1:I:68:ASP:CB	1:I:707:ARG:HH12	2.15	0.59
2:J:35:TYR:C	2:J:36:PRO:O	2.35	0.59
1:O:192:MET:HE1	1:O:694:ARG:CB	2.32	0.59
1:C:583:VAL:HG13	1:C:583:VAL:O	2.03	0.59
1:G:81:VAL:HG12	1:G:82:TYR:N	2.18	0.59
1:I:76:ARG:NH2	1:I:493:ALA:O	2.35	0.59
1:K:458:MET:O	1:K:464:ILE:HG21	2.02	0.59
1:K:617:ASP:HB2	1:K:633:PRO:HA	1.82	0.59
1:K:76:ARG:NH2	1:K:473:ARG:CZ	2.65	0.59
1:O:183:VAL:HG23	1:O:340:TRP:NE1	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:714:ALA:HB2	2:D:103:VAL:HG11	1.84	0.59
1:E:332:LEU:CD2	1:E:340:TRP:CH2	2.85	0.59
1:G:76:ARG:NH2	1:G:493:ALA:O	2.35	0.59
1:I:163:THR:CG2	1:I:359:HIS:HD1	2.15	0.59
1:I:59:PHE:CE2	1:I:710:GLU:HG3	2.37	0.59
1:M:47:GLU:OE1	1:M:50:ARG:NH2	2.32	0.59
1:O:690:LEU:HD22	1:O:797:VAL:HG21	1.84	0.59
2:B:83:ARG:O	2:B:84:GLU:CB	2.48	0.59
1:C:121:SER:HB2	1:C:148:ASN:ND2	2.17	0.59
2:F:42:ILE:CD1	6:F:1128:HEC:HMB2	2.32	0.59
1:G:245:ALA:HB3	1:G:307:VAL:HG11	1.84	0.59
2:H:35:TYR:C	2:H:36:PRO:O	2.37	0.59
1:K:793:LYS:HE3	5:K:1804:MGD:H5'2	1.84	0.59
2:L:83:ARG:O	2:L:84:GLU:CB	2.46	0.59
1:A:544:THR:HA	1:A:564:THR:HA	1.84	0.59
1:G:76:ARG:NH2	1:G:473:ARG:CZ	2.65	0.59
1:K:192:MET:HE2	1:K:694:ARG:CB	2.21	0.59
2:L:79:HIS:CD2	2:L:95:ARG:HD2	2.37	0.59
1:M:245:ALA:HB3	1:M:307:VAL:HG11	1.82	0.59
1:E:172:CYS:SG	1:E:174:ASP:HB2	2.42	0.59
1:E:33:ARG:HD3	2:F:122:LEU:HD21	1.84	0.59
1:I:356:TRP:HB3	1:I:673:VAL:HG11	1.85	0.59
2:J:81:GLN:HA	2:J:86:GLN:O	2.03	0.59
1:K:453:GLN:HG2	1:K:482:SER:HB2	1.85	0.59
1:K:47:GLU:OE1	1:K:50:ARG:NH2	2.34	0.59
1:O:118:MET:HE1	1:O:132:ALA:HB1	1.84	0.59
1:A:714:ALA:HB2	2:B:103:VAL:HG11	1.84	0.59
1:G:346:MET:HG2	5:G:1804:MGD:H101	1.83	0.59
1:I:540:SER:HB3	1:I:565:LEU:O	2.02	0.59
1:O:68:ASP:O	1:O:69:ARG:C	2.40	0.59
1:O:714:ALA:HB2	2:P:103:VAL:HG11	1.85	0.59
2:H:121:THR:O	2:H:121:THR:OG1	2.21	0.59
1:I:545:THR:OG1	1:I:563:LYS:HB2	2.02	0.59
2:J:94:ARG:O	2:J:95:ARG:CB	2.51	0.59
1:M:121:SER:HB2	1:M:148:ASN:ND2	2.18	0.59
1:M:611:GLY:O	1:M:612:ARG:HB2	2.02	0.59
1:E:238:ARG:CZ	1:E:676:GLU:O	2.51	0.59
1:G:367:LEU:CD1	1:G:670:ILE:HD13	2.32	0.59
1:G:448:ASN:HA	1:G:477:ASN:HD22	1.67	0.59
1:I:455:ASN:HD21	1:I:457:ASN:HB2	1.67	0.59
1:K:632:TRP:CE3	1:K:632:TRP:O	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:98:CYS:HG	6:L:1129:HEC:HAB	1.62	0.59
1:M:172:CYS:SG	1:M:174:ASP:HB2	2.42	0.59
1:M:438:GLN:HE21	1:M:450:TYR:HE1	1.49	0.59
1:M:702:GLY:O	1:M:706:LEU:HB2	2.02	0.59
1:O:238:ARG:HG2	1:O:360:MET:HE3	1.84	0.59
1:O:448:ASN:HA	1:O:477:ASN:HD22	1.66	0.59
1:O:740:VAL:CG1	1:O:797:VAL:HG11	2.32	0.59
1:A:367:LEU:CD1	1:A:670:ILE:HD13	2.32	0.59
1:A:47:GLU:OE1	1:A:50:ARG:NH2	2.35	0.59
1:A:67:GLU:HG2	2:B:112:VAL:HG13	1.85	0.59
1:K:314:LYS:O	1:K:318:ILE:HG13	2.02	0.59
1:O:121:SER:HA	1:O:148:ASN:OD1	2.03	0.59
2:P:83:ARG:O	2:P:84:GLU:CB	2.49	0.59
1:A:163:THR:CG2	1:A:359:HIS:HD1	2.16	0.58
1:C:448:ASN:ND2	1:C:477:ASN:HD21	1.93	0.58
1:I:700:HIS:O	1:I:769:PHE:HA	2.03	0.58
1:M:238:ARG:HG2	1:M:360:MET:HE3	1.85	0.58
1:A:540:SER:HB3	1:A:565:LEU:O	2.03	0.58
1:A:68:ASP:CB	1:A:707:ARG:HH12	2.16	0.58
2:D:27:ASP:OD2	2:D:29:ARG:HD3	2.04	0.58
1:K:180:ASP:O	1:K:181:ALA:HB2	2.03	0.58
1:O:233:ARG:HB3	1:O:236:THR:CG2	2.34	0.58
1:O:491:ARG:NH2	2:P:11:ARG:N	2.51	0.58
1:O:700:HIS:O	1:O:769:PHE:HA	2.03	0.58
1:C:562:GLY:O	1:C:564:THR:N	2.36	0.58
1:C:597:PHE:CD1	1:C:597:PHE:N	2.72	0.58
1:C:68:ASP:CB	1:C:707:ARG:HH12	2.15	0.58
1:G:438:GLN:HE21	1:G:450:TYR:HE1	1.50	0.58
1:G:59:PHE:CE2	1:G:710:GLU:HG3	2.38	0.58
1:I:147:PRO:HD3	1:I:396:THR:O	2.02	0.58
1:I:583:VAL:O	1:I:584:ASN:O	2.21	0.58
1:K:137:ARG:O	1:K:141:ARG:HA	2.03	0.58
1:K:68:ASP:CB	1:K:707:ARG:HH12	2.16	0.58
1:A:270:THR:HG22	1:A:674:PRO:HG3	1.84	0.58
1:A:537:MET:CE	1:A:595:PHE:CE2	2.86	0.58
1:A:628:ARG:HG2	1:A:628:ARG:HH11	1.68	0.58
1:E:314:LYS:O	1:E:318:ILE:HG13	2.03	0.58
1:I:358:ASN:O	1:I:361:VAL:HG23	2.03	0.58
1:I:554:LEU:HD22	1:I:560:TYR:O	2.03	0.58
1:I:597:PHE:CD1	1:I:597:PHE:N	2.71	0.58
1:K:219:THR:OG1	1:K:231:ILE:HD11	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:67:GLU:HG2	2:N:112:VAL:HG13	1.84	0.58
1:A:20:ARG:O	1:A:20:ARG:HG3	2.02	0.58
1:C:238:ARG:HG2	1:C:360:MET:HE1	1.84	0.58
1:C:68:ASP:HB2	1:C:707:ARG:HH12	1.67	0.58
1:E:793:LYS:HE3	5:E:1804:MGD:H5'2	1.85	0.58
1:G:16:LYS:HD2	1:G:628:ARG:HG3	1.85	0.58
1:I:332:LEU:CB	1:I:340:TRP:CH2	2.87	0.58
1:M:76:ARG:NH2	1:M:473:ARG:CZ	2.66	0.58
1:M:554:LEU:HD22	1:M:560:TYR:O	2.03	0.58
1:C:192:MET:CE	1:C:694:ARG:CB	2.78	0.58
1:E:267:LEU:O	1:E:295:MET:O	2.20	0.58
1:G:544:THR:HA	1:G:564:THR:HA	1.85	0.58
1:G:714:ALA:HB2	2:H:103:VAL:HG11	1.85	0.58
1:K:267:LEU:O	1:K:295:MET:O	2.21	0.58
1:M:16:LYS:HD2	1:M:628:ARG:HG3	1.85	0.58
1:M:180:ASP:O	1:M:181:ALA:HB2	2.04	0.58
1:M:597:PHE:N	1:M:597:PHE:CD1	2.70	0.58
1:A:690:LEU:HD22	1:A:797:VAL:HG21	1.85	0.58
1:C:631:HIS:ND1	1:C:639:GLU:OE2	2.36	0.58
1:C:81:VAL:HG12	1:C:82:TYR:N	2.18	0.58
1:E:554:LEU:HD22	1:E:560:TYR:O	2.03	0.58
1:I:367:LEU:CD1	1:I:670:ILE:HD13	2.33	0.58
1:K:633:PRO:HD2	1:K:640:THR:HB	1.86	0.58
1:M:272:ILE:CG2	1:M:785:PRO:CG	2.82	0.58
1:G:238:ARG:CZ	1:G:676:GLU:O	2.52	0.58
2:H:98:CYS:HB3	6:H:1129:HEC:HAB	1.83	0.58
1:I:121:SER:HA	1:I:148:ASN:OD1	2.04	0.58
1:I:150:ARG:HG2	1:I:435:ALA:HB3	1.85	0.58
1:I:611:GLY:O	1:I:612:ARG:HB2	2.02	0.58
1:A:367:LEU:HD13	1:A:670:ILE:HD13	1.85	0.58
1:G:230:ILE:HG23	1:G:321:VAL:CG1	2.31	0.58
1:I:219:THR:OG1	1:I:231:ILE:HD11	2.03	0.58
1:K:120:GLY:HA3	1:K:124:TRP:CZ3	2.39	0.58
1:K:59:PHE:CE2	1:K:710:GLU:HG3	2.38	0.58
1:M:121:SER:C	1:M:123:GLN:H	2.06	0.58
1:M:120:GLY:HA3	1:M:124:TRP:CZ3	2.39	0.58
1:O:722:MET:HG2	1:O:723:HIS:H	1.69	0.58
1:C:180:ASP:HB2	1:C:339:LYS:N	2.18	0.58
1:E:183:VAL:HG23	1:E:340:TRP:NE1	2.17	0.58
2:F:41:VAL:CG1	2:F:105:GLN:HG3	2.34	0.58
1:G:332:LEU:CB	1:G:340:TRP:CH2	2.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:766:VAL:CG2	1:I:775:ILE:HD13	2.27	0.58
1:K:121:SER:C	1:K:123:GLN:H	2.06	0.58
1:K:332:LEU:CD2	1:K:340:TRP:CH2	2.86	0.58
2:P:94:ARG:O	2:P:95:ARG:CB	2.51	0.58
1:E:346:MET:HG2	5:E:1804:MGD:H101	1.87	0.57
1:E:192:MET:HE2	1:E:694:ARG:CB	2.24	0.57
1:E:238:ARG:HG2	1:E:360:MET:CE	2.34	0.57
1:G:20:ARG:O	1:G:20:ARG:HG3	2.04	0.57
1:G:750:ARG:HD3	2:H:20:PRO:HA	1.86	0.57
1:I:714:ALA:CB	2:J:103:VAL:HG11	2.34	0.57
1:M:278:PRO:O	1:M:279:GLU:HB2	2.02	0.57
1:O:776:ASN:HA	1:O:779:THR:HG1	1.66	0.57
1:A:219:THR:OG1	1:A:231:ILE:HD11	2.04	0.57
1:A:238:ARG:HG2	1:A:360:MET:CE	2.33	0.57
1:A:546:ASP:O	1:A:548:VAL:N	2.38	0.57
1:E:180:ASP:HB2	1:E:339:LYS:N	2.19	0.57
1:G:400:ARG:HH21	1:G:404:ASP:H	1.52	0.57
1:G:458:MET:O	1:G:464:ILE:HG21	2.04	0.57
1:G:722:MET:HG2	1:G:723:HIS:H	1.69	0.57
1:I:189:MET:HE1	1:I:343:LEU:HD13	1.86	0.57
1:K:544:THR:HA	1:K:564:THR:HA	1.85	0.57
1:K:546:ASP:O	1:K:548:VAL:N	2.37	0.57
2:L:98:CYS:HB3	6:L:1129:HEC:CAB	2.34	0.57
1:M:147:PRO:HD3	1:M:396:THR:O	2.04	0.57
1:M:540:SER:O	1:M:542:ARG:N	2.37	0.57
1:O:367:LEU:CD1	1:O:670:ILE:HD13	2.35	0.57
1:A:46:ALA:O	1:A:50:ARG:HG2	2.05	0.57
1:C:540:SER:HB3	1:C:565:LEU:O	2.04	0.57
1:E:628:ARG:HH11	1:E:628:ARG:HG2	1.69	0.57
1:G:33:ARG:HD3	2:H:122:LEU:HD21	1.85	0.57
1:K:540:SER:O	1:K:542:ARG:N	2.37	0.57
1:M:121:SER:HA	1:M:148:ASN:OD1	2.05	0.57
1:A:192:MET:HB3	5:A:1804:MGD:N22	2.18	0.57
1:A:220:HIS:CE1	1:A:222:SER:HB2	2.39	0.57
1:A:358:ASN:O	1:A:361:VAL:HG23	2.04	0.57
1:A:356:TRP:O	1:A:360:MET:HG3	2.04	0.57
1:A:238:ARG:CZ	1:A:676:GLU:O	2.53	0.57
1:G:426:LEU:HD21	1:G:549:TRP:CZ2	2.40	0.57
1:K:121:SER:HA	1:K:148:ASN:OD1	2.04	0.57
1:K:627:VAL:HG12	1:K:628:ARG:N	2.19	0.57
1:M:267:LEU:O	1:M:295:MET:O	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:121:THR:OG1	2:P:121:THR:O	2.21	0.57
1:A:225:LEU:HG	1:A:225:LEU:O	2.04	0.57
1:A:458:MET:O	1:A:464:ILE:HG21	2.05	0.57
1:C:627:VAL:HG12	1:C:628:ARG:N	2.19	0.57
1:C:722:MET:HG2	1:C:723:HIS:H	1.69	0.57
1:E:537:MET:HE2	1:E:595:PHE:CE2	2.39	0.57
1:G:180:ASP:HB2	1:G:339:LYS:N	2.18	0.57
1:G:554:LEU:HD22	1:G:560:TYR:O	2.04	0.57
1:I:599:PRO:O	1:I:603:LEU:HD12	2.05	0.57
1:I:776:ASN:HA	1:I:779:THR:HG1	1.69	0.57
1:K:776:ASN:HA	1:K:779:THR:HG1	1.69	0.57
1:M:20:ARG:O	1:M:20:ARG:HG3	2.05	0.57
2:N:49:TYR:CE1	6:N:1128:HEC:HMC2	2.39	0.57
1:O:583:VAL:HG13	1:O:583:VAL:O	2.04	0.57
1:A:448:ASN:ND2	1:A:477:ASN:HD21	1.96	0.57
2:B:37:GLU:HA	6:B:1129:HEC:HMD1	1.86	0.57
1:C:16:LYS:HD2	1:C:628:ARG:HG3	1.84	0.57
1:C:628:ARG:HG2	1:C:628:ARG:HH11	1.70	0.57
1:E:125:THR:HG21	1:E:127:TRP:NE1	2.19	0.57
1:E:144:ASN:HD22	1:E:433:ALA:H	1.51	0.57
1:E:722:MET:HG2	1:E:723:HIS:H	1.69	0.57
1:G:120:GLY:HA3	1:G:124:TRP:CZ3	2.40	0.57
1:G:597:PHE:N	1:G:597:PHE:CD1	2.72	0.57
1:G:68:ASP:CB	1:G:707:ARG:HH12	2.17	0.57
1:G:740:VAL:CG1	1:G:797:VAL:HG11	2.31	0.57
1:I:583:VAL:O	1:I:583:VAL:HG13	2.04	0.57
1:K:180:ASP:HB2	1:K:339:LYS:N	2.19	0.57
1:M:238:ARG:NH1	1:M:676:GLU:O	2.37	0.57
2:N:94:ARG:O	2:N:95:ARG:CB	2.53	0.57
1:A:545:THR:OG1	1:A:563:LYS:HB2	2.05	0.57
2:D:30:ARG:HD2	6:D:1128:HEC:O1D	2.05	0.57
1:E:303:PHE:O	1:E:307:VAL:HG23	2.05	0.57
1:E:597:PHE:N	1:E:597:PHE:CD1	2.72	0.57
1:G:584:ASN:O	1:G:586:ASP:O	2.23	0.57
1:K:722:MET:CE	1:K:751:LEU:HD11	2.35	0.57
1:M:163:THR:CG2	1:M:359:HIS:ND1	2.68	0.57
1:O:332:LEU:HG	1:O:340:TRP:CZ3	2.39	0.57
2:D:41:VAL:HG13	2:D:105:GLN:HG3	1.87	0.57
1:I:76:ARG:NH2	1:I:473:ARG:CZ	2.67	0.57
1:K:245:ALA:HB3	1:K:307:VAL:HG11	1.86	0.57
1:M:458:MET:O	1:M:464:ILE:HG21	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:101:CYS:SG	6:N:1129:HEC:C3C	2.93	0.57
2:N:121:THR:OG1	2:N:121:THR:O	2.22	0.57
1:O:81:VAL:HG12	1:O:82:TYR:N	2.19	0.57
1:A:183:VAL:HG23	1:A:340:TRP:NE1	2.19	0.57
1:A:147:PRO:HD3	1:A:396:THR:O	2.05	0.57
1:A:750:ARG:HD2	2:B:19:PRO:O	2.04	0.57
1:E:719:VAL:HG11	1:E:752:GLU:HB2	1.85	0.57
1:I:278:PRO:O	1:I:279:GLU:HB2	2.05	0.57
1:K:172:CYS:SG	1:K:174:ASP:HB2	2.45	0.57
1:K:574:SER:O	1:K:577:ARG:HB2	2.05	0.57
2:L:40:PRO:HD2	2:L:102:HIS:HE1	1.70	0.57
1:M:183:VAL:HG23	1:M:340:TRP:NE1	2.20	0.57
1:O:400:ARG:HH21	1:O:404:ASP:H	1.52	0.57
2:P:66:TYR:O	2:P:68:GLY:N	2.38	0.57
1:A:267:LEU:O	1:A:295:MET:O	2.22	0.57
1:C:554:LEU:HD22	1:C:560:TYR:O	2.04	0.57
1:E:47:GLU:OE1	1:E:50:ARG:NH2	2.36	0.57
1:E:59:PHE:CE2	1:E:710:GLU:HG3	2.38	0.57
2:F:34:ASN:H	2:F:38:GLN:NE2	2.03	0.57
1:G:540:SER:HB3	1:G:565:LEU:O	2.05	0.57
1:G:633:PRO:CD	1:G:640:THR:HB	2.34	0.57
1:K:163:THR:CG2	1:K:359:HIS:ND1	2.67	0.57
1:K:690:LEU:HD22	1:K:797:VAL:HG21	1.87	0.57
1:M:144:ASN:HD22	1:M:433:ALA:H	1.51	0.57
1:O:180:ASP:HB2	1:O:339:LYS:N	2.19	0.57
1:O:358:ASN:O	1:O:361:VAL:HG23	2.04	0.57
1:C:230:ILE:HG23	1:C:321:VAL:CG1	2.30	0.56
1:E:180:ASP:O	1:E:181:ALA:HB2	2.05	0.56
1:E:225:LEU:HG	1:E:225:LEU:O	2.04	0.56
1:M:423:PRO:HD3	1:M:560:TYR:CZ	2.39	0.56
1:O:303:PHE:O	1:O:307:VAL:HG23	2.05	0.56
1:O:690:LEU:HB3	1:O:795:CYS:SG	2.45	0.56
1:C:438:GLN:HE21	1:C:450:TYR:HE1	1.53	0.56
1:E:458:MET:O	1:E:464:ILE:HG21	2.04	0.56
2:H:41:VAL:HG13	2:H:105:GLN:HG3	1.87	0.56
2:H:3:ALA:CB	2:H:4:PRO:CD	2.70	0.56
2:H:62:HIS:HA	2:H:74:MET:HB3	1.87	0.56
1:I:161:MET:O	1:I:165:GLY:N	2.36	0.56
2:J:40:PRO:HD3	6:J:1129:HEC:HBD2	1.86	0.56
2:L:37:GLU:HA	6:L:1129:HEC:HMD1	1.87	0.56
1:M:750:ARG:HD3	2:N:20:PRO:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:219:THR:OG1	1:O:231:ILE:HD11	2.05	0.56
1:O:272:ILE:CG2	1:O:785:PRO:CG	2.81	0.56
1:A:438:GLN:HE21	1:A:450:TYR:HE1	1.53	0.56
1:A:562:GLY:O	1:A:564:THR:N	2.39	0.56
1:A:16:LYS:HD2	1:A:628:ARG:HG3	1.86	0.56
1:C:540:SER:O	1:C:542:ARG:N	2.38	0.56
1:E:49:ASN:HB2	1:E:52:LEU:O	2.05	0.56
2:F:35:TYR:C	2:F:36:PRO:O	2.42	0.56
1:I:118:MET:CE	1:I:132:ALA:HB1	2.34	0.56
1:I:202:ASP:HA	2:J:93:PRO:HB2	1.87	0.56
1:I:356:TRP:CZ3	1:I:674:PRO:O	2.58	0.56
2:L:35:TYR:C	2:L:36:PRO:O	2.42	0.56
1:M:118:MET:HE1	1:M:132:ALA:HB1	1.86	0.56
2:N:62:HIS:HA	2:N:74:MET:HB3	1.87	0.56
1:C:577:ARG:HD3	1:C:578:PHE:CZ	2.41	0.56
2:N:30:ARG:HD2	6:N:1128:HEC:O1D	2.04	0.56
1:O:59:PHE:CE2	1:O:710:GLU:HG3	2.40	0.56
1:O:611:GLY:O	1:O:612:ARG:HB2	2.04	0.56
1:C:690:LEU:HD22	1:C:797:VAL:HG21	1.87	0.56
1:C:793:LYS:HE3	5:C:1804:MGD:H5'2	1.87	0.56
1:G:689:TRP:CZ3	1:G:794:LYS:HB2	2.40	0.56
1:K:33:ARG:HD3	2:L:122:LEU:HD21	1.88	0.56
1:O:455:ASN:HD21	1:O:457:ASN:HB2	1.68	0.56
2:B:27:ASP:OD2	2:B:29:ARG:HD3	2.04	0.56
1:C:272:ILE:CG2	1:C:785:PRO:CG	2.82	0.56
1:G:46:ALA:O	1:G:50:ARG:HG2	2.05	0.56
1:K:583:VAL:O	1:K:583:VAL:HG13	2.04	0.56
1:O:193:HIS:N	1:O:194:PRO:HD3	2.20	0.56
1:O:401:LEU:HB3	1:O:402:PRO:HD2	1.88	0.56
1:C:162:ARG:NH1	1:C:359:HIS:NE2	2.54	0.56
2:D:34:ASN:H	2:D:38:GLN:NE2	2.03	0.56
2:F:94:ARG:O	2:F:95:ARG:CB	2.52	0.56
1:G:503:VAL:O	1:G:503:VAL:CG1	2.54	0.56
1:G:356:TRP:HB3	1:G:673:VAL:HG11	1.88	0.56
1:I:562:GLY:O	1:I:564:THR:N	2.39	0.56
1:I:700:HIS:CE1	5:I:1804:MGD:S13	2.99	0.56
1:M:332:LEU:CD2	1:M:340:TRP:CH2	2.88	0.56
2:N:3:ALA:CB	2:N:4:PRO:CD	2.70	0.56
1:E:538:GLU:OE2	1:E:541:LYS:HD2	2.05	0.56
1:E:690:LEU:HD22	1:E:797:VAL:HG21	1.87	0.56
1:K:611:GLY:O	1:K:612:ARG:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:68:ASP:OD2	1:K:707:ARG:NH1	2.39	0.56
1:M:776:ASN:HA	1:M:779:THR:HG1	1.67	0.56
1:O:52:LEU:HG	6:P:1129:HEC:HBC2	1.87	0.56
1:O:583:VAL:O	1:O:584:ASN:O	2.23	0.56
1:A:346:MET:HB3	1:A:350:GLN:HG3	1.87	0.56
1:C:332:LEU:HB3	1:C:340:TRP:CZ2	2.40	0.56
1:E:137:ARG:O	1:E:141:ARG:HA	2.06	0.56
1:E:332:LEU:HG	1:E:340:TRP:CZ3	2.41	0.56
1:E:533:LEU:O	1:E:537:MET:HG3	2.06	0.56
1:I:605:GLU:OE1	1:I:612:ARG:NH2	2.37	0.56
1:M:303:PHE:O	1:M:307:VAL:HG23	2.06	0.56
1:M:59:PHE:CE2	1:M:710:GLU:HG3	2.41	0.56
1:O:562:GLY:O	1:O:564:THR:N	2.39	0.56
1:A:533:LEU:O	1:A:537:MET:HG3	2.06	0.56
1:E:562:GLY:O	1:E:564:THR:N	2.39	0.56
1:G:137:ARG:O	1:G:141:ARG:HA	2.06	0.56
1:G:538:GLU:OE2	1:G:541:LYS:HD2	2.04	0.56
2:J:75:ILE:CD1	2:J:80:PHE:HE2	2.18	0.56
1:M:125:THR:HG21	1:M:127:TRP:NE1	2.21	0.56
1:O:545:THR:HG22	1:O:549:TRP:CE3	2.41	0.56
1:A:189:MET:HE1	1:A:343:LEU:HD13	1.88	0.56
1:A:21:PHE:HZ	1:A:63:ILE:HD11	1.71	0.56
1:A:144:ASN:HD22	1:A:433:ALA:H	1.54	0.56
1:A:59:PHE:CE2	1:A:710:GLU:HG3	2.41	0.56
1:C:144:ASN:HD22	1:C:433:ALA:H	1.50	0.56
1:C:719:VAL:HG11	1:C:752:GLU:HB2	1.87	0.56
1:E:76:ARG:NH2	1:E:473:ARG:CZ	2.68	0.56
1:E:776:ASN:HA	1:E:779:THR:HG1	1.69	0.56
1:E:740:VAL:CG1	1:E:797:VAL:HG11	2.30	0.56
1:G:219:THR:OG1	1:G:231:ILE:HD11	2.05	0.56
1:I:183:VAL:CG2	1:I:340:TRP:NE1	2.68	0.56
1:M:766:VAL:CG2	1:M:775:ILE:HD13	2.32	0.56
1:O:121:SER:HB2	1:O:148:ASN:ND2	2.21	0.56
1:O:332:LEU:CD2	1:O:340:TRP:CH2	2.89	0.56
1:O:356:TRP:HB3	1:O:673:VAL:HG11	1.88	0.56
2:P:42:ILE:CD1	6:P:1128:HEC:HMB2	2.35	0.56
1:A:137:ARG:O	1:A:141:ARG:HA	2.07	0.55
2:B:92:SER:O	2:B:94:ARG:O	2.24	0.55
1:C:439:ASP:OD1	1:C:468:THR:HG23	2.06	0.55
2:D:121:THR:O	2:D:121:THR:OG1	2.23	0.55
1:G:633:PRO:HD2	1:G:640:THR:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:211:ARG:HB2	1:I:338:ARG:HH12	1.71	0.55
1:K:68:ASP:HB2	1:K:707:ARG:HH12	1.70	0.55
1:K:766:VAL:CG2	1:K:775:ILE:HD13	2.29	0.55
2:L:121:THR:O	2:L:121:THR:OG1	2.21	0.55
1:M:414:ALA:O	1:M:418:GLU:HG2	2.07	0.55
1:M:627:VAL:HG12	1:M:628:ARG:N	2.21	0.55
1:M:68:ASP:CB	1:M:707:ARG:HH12	2.19	0.55
2:N:35:TYR:C	2:N:36:PRO:O	2.40	0.55
1:O:545:THR:OG1	1:O:563:LYS:HB2	2.06	0.55
1:O:722:MET:HG2	1:O:723:HIS:N	2.21	0.55
1:O:722:MET:CE	1:O:751:LEU:HD11	2.37	0.55
1:A:192:MET:HE2	1:A:694:ARG:CB	2.24	0.55
2:B:86:GLN:HE21	2:B:86:GLN:HA	1.71	0.55
1:E:192:MET:HB3	5:E:1804:MGD:N22	2.21	0.55
1:E:722:MET:HG2	1:E:723:HIS:N	2.21	0.55
2:H:82:ASP:HB3	2:H:88:LEU:HD11	1.88	0.55
1:I:750:ARG:HD3	2:J:20:PRO:HA	1.89	0.55
2:J:40:PRO:HD2	2:J:102:HIS:HE1	1.70	0.55
1:M:21:PHE:HZ	1:M:63:ILE:HD11	1.70	0.55
1:A:455:ASN:HD22	1:A:457:ASN:H	1.53	0.55
2:B:41:VAL:CG1	2:B:105:GLN:HG3	2.36	0.55
2:B:3:ALA:CB	2:B:4:PRO:CD	2.69	0.55
1:C:49:ASN:HB2	1:C:52:LEU:O	2.06	0.55
1:E:121:SER:HB2	1:E:148:ASN:ND2	2.20	0.55
1:G:545:THR:OG1	1:G:563:LYS:HB2	2.06	0.55
1:I:183:VAL:HG23	1:I:340:TRP:CE2	2.40	0.55
2:J:37:GLU:HA	6:J:1129:HEC:HMD1	1.87	0.55
1:M:455:ASN:HD22	1:M:457:ASN:H	1.52	0.55
1:O:49:ASN:HB2	1:O:52:LEU:O	2.07	0.55
1:A:230:ILE:HG23	1:A:321:VAL:CG1	2.36	0.55
2:B:35:TYR:C	2:B:36:PRO:O	2.40	0.55
2:D:82:ASP:HB3	2:D:88:LEU:HD11	1.88	0.55
1:G:722:MET:HG2	1:G:723:HIS:N	2.22	0.55
2:J:121:THR:OG1	2:J:121:THR:O	2.21	0.55
2:N:81:GLN:HA	2:N:86:GLN:O	2.07	0.55
1:O:540:SER:HB3	1:O:565:LEU:O	2.06	0.55
1:A:554:LEU:HD22	1:A:560:TYR:O	2.05	0.55
1:A:728:ARG:HD3	2:H:5:ARG:HE	1.71	0.55
1:C:163:THR:CG2	1:C:359:HIS:HD1	2.19	0.55
1:C:356:TRP:HB3	1:C:673:VAL:HG11	1.88	0.55
1:C:67:GLU:HG2	2:D:112:VAL:HG13	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:HG	6:D:1129:HEC:HBC2	1.87	0.55
1:G:628:ARG:HH11	1:G:628:ARG:HG2	1.71	0.55
2:H:10:ASP:O	2:H:11:ARG:C	2.45	0.55
1:I:617:ASP:HB2	1:I:633:PRO:HA	1.87	0.55
1:A:332:LEU:HG	1:A:340:TRP:CZ3	2.41	0.55
1:C:180:ASP:O	1:C:181:ALA:HB2	2.06	0.55
1:E:584:ASN:O	1:E:586:ASP:O	2.23	0.55
1:E:627:VAL:HG12	1:E:628:ARG:N	2.21	0.55
1:G:514:ARG:O	1:G:631:HIS:HA	2.07	0.55
1:I:192:MET:HB3	5:I:1804:MGD:N22	2.22	0.55
1:K:144:ASN:HD22	1:K:433:ALA:H	1.53	0.55
1:K:455:ASN:HD22	1:K:457:ASN:H	1.54	0.55
1:K:272:ILE:CG2	1:K:785:PRO:CG	2.82	0.55
1:M:346:MET:HB3	1:M:350:GLN:HG3	1.87	0.55
1:M:448:ASN:HA	1:M:477:ASN:HD22	1.70	0.55
2:N:98:CYS:HB3	6:N:1129:HEC:CAB	2.36	0.55
2:P:62:HIS:HA	2:P:74:MET:HB3	1.88	0.55
2:P:92:SER:O	2:P:94:ARG:O	2.25	0.55
1:C:245:ALA:HB3	1:C:307:VAL:HG11	1.88	0.55
1:C:238:ARG:HG2	1:C:360:MET:HE3	1.88	0.55
1:C:483:ASP:OD1	1:C:484:ALA:N	2.33	0.55
1:E:720:CYS:SG	1:E:764:VAL:HG13	2.47	0.55
2:F:51:LEU:HD21	2:F:58:CYS:SG	2.46	0.55
1:G:540:SER:O	1:G:542:ARG:N	2.40	0.55
1:G:367:LEU:HD13	1:G:670:ILE:HD13	1.89	0.55
2:H:66:TYR:O	2:H:68:GLY:N	2.40	0.55
1:I:332:LEU:CD2	1:I:340:TRP:CH2	2.89	0.55
1:I:722:MET:HG2	1:I:723:HIS:H	1.71	0.55
2:J:41:VAL:HG13	2:J:105:GLN:HG3	1.89	0.55
1:K:700:HIS:O	1:K:769:PHE:HA	2.07	0.55
1:O:33:ARG:NH1	2:P:119:MET:O	2.37	0.55
1:A:233:ARG:HB3	1:A:236:THR:CG2	2.37	0.55
1:A:503:VAL:O	1:A:503:VAL:CG1	2.55	0.55
1:A:612:ARG:HA	1:A:617:ASP:OD1	2.07	0.55
1:G:26:CYS:HB3	1:G:49:ASN:CG	2.27	0.55
1:G:599:PRO:O	1:G:603:LEU:HD12	2.07	0.55
1:I:121:SER:C	1:I:123:GLN:H	2.09	0.55
1:I:183:VAL:HG12	1:I:185:TRP:CD1	2.41	0.55
1:K:278:PRO:O	1:K:279:GLU:HB2	2.06	0.55
1:K:605:GLU:OE1	1:K:612:ARG:NH2	2.39	0.55
1:M:192:MET:HB3	5:M:1804:MGD:N22	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:584:ASN:O	1:O:586:ASP:O	2.25	0.55
1:E:280:HIS:CE1	1:E:282:LEU:HD12	2.42	0.55
1:G:562:GLY:O	1:G:564:THR:N	2.39	0.55
2:D:118:ASP:OD1	2:H:67:SER:HA	2.05	0.55
1:I:537:MET:CE	1:I:595:PHE:CE2	2.90	0.55
1:I:367:LEU:HD13	1:I:670:ILE:HD13	1.89	0.55
1:K:583:VAL:O	1:K:584:ASN:O	2.25	0.55
1:K:738:VAL:HG21	1:K:751:LEU:HD13	1.89	0.55
1:M:202:ASP:HA	2:N:93:PRO:HB2	1.89	0.55
2:N:14:SER:O	2:N:15:GLU:HB3	2.07	0.55
1:O:628:ARG:HH11	1:O:628:ARG:CG	2.20	0.55
2:P:3:ALA:CB	2:P:4:PRO:CD	2.69	0.55
2:B:121:THR:O	2:B:121:THR:OG1	2.24	0.55
1:C:137:ARG:O	1:C:141:ARG:HA	2.06	0.55
1:C:202:ASP:HA	2:D:93:PRO:HB2	1.89	0.55
2:D:49:TYR:CE1	6:D:1128:HEC:HMC2	2.41	0.55
1:I:439:ASP:OD1	1:I:468:THR:HG23	2.07	0.55
1:I:574:SER:O	1:I:577:ARG:HB2	2.07	0.55
1:M:220:HIS:CE1	1:M:222:SER:HB2	2.43	0.55
1:O:21:PHE:HZ	1:O:63:ILE:HD11	1.69	0.55
1:A:583:VAL:O	1:A:584:ASN:O	2.25	0.54
1:E:245:ALA:HB3	1:E:307:VAL:HG11	1.87	0.54
1:E:278:PRO:O	1:E:279:GLU:HB2	2.06	0.54
1:E:21:PHE:O	1:E:385:PRO:HD3	2.07	0.54
1:E:68:ASP:CB	1:E:707:ARG:HH12	2.20	0.54
1:I:16:LYS:CA	1:I:29:MET:HE1	2.36	0.54
1:I:540:SER:O	1:I:542:ARG:N	2.40	0.54
1:K:332:LEU:HG	1:K:340:TRP:CZ3	2.42	0.54
1:K:750:ARG:HD3	2:L:20:PRO:HA	1.88	0.54
1:M:180:ASP:HB2	1:M:339:LYS:N	2.20	0.54
1:O:332:LEU:HB3	1:O:340:TRP:CZ2	2.42	0.54
1:O:46:ALA:O	1:O:50:ARG:HG2	2.06	0.54
1:A:793:LYS:HE3	5:A:1804:MGD:H5'2	1.89	0.54
1:A:574:SER:O	1:A:577:ARG:HB2	2.06	0.54
1:C:76:ARG:NH2	1:C:493:ALA:O	2.40	0.54
2:F:58:CYS:CB	6:F:1128:HEC:HAB	2.37	0.54
1:G:332:LEU:HB3	1:G:340:TRP:CZ2	2.42	0.54
1:G:423:PRO:HD3	1:G:560:TYR:CZ	2.42	0.54
1:G:700:HIS:O	1:G:769:PHE:HA	2.08	0.54
1:I:68:ASP:HB2	1:I:707:ARG:HH12	1.69	0.54
1:I:689:TRP:CZ3	1:I:794:LYS:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:66:TYR:O	2:J:68:GLY:N	2.41	0.54
1:O:479:ILE:HG22	1:O:493:ALA:HB1	1.90	0.54
1:A:346:MET:HG2	5:A:1804:MGD:H101	1.90	0.54
1:A:305:ALA:HA	1:A:308:SER:OG	2.07	0.54
1:A:332:LEU:HB3	1:A:340:TRP:CZ2	2.41	0.54
1:A:33:ARG:HD3	2:B:122:LEU:HD21	1.88	0.54
1:C:367:LEU:HD13	1:C:670:ILE:HD13	1.90	0.54
1:G:118:MET:CE	1:G:132:ALA:HB1	2.37	0.54
1:G:29:MET:CE	1:G:628:ARG:HH12	2.19	0.54
1:G:720:CYS:SG	1:G:764:VAL:HG13	2.47	0.54
1:I:233:ARG:HB3	1:I:236:THR:CG2	2.38	0.54
2:J:34:ASN:H	2:J:38:GLN:NE2	2.04	0.54
1:K:455:ASN:HD21	1:K:457:ASN:HB2	1.71	0.54
1:O:118:MET:CE	1:O:132:ALA:HB1	2.36	0.54
1:O:401:LEU:HB3	1:O:402:PRO:CD	2.36	0.54
2:H:61:CYS:SG	6:H:1128:HEC:C3C	2.95	0.54
2:H:27:ASP:OD2	2:H:29:ARG:HD3	2.07	0.54
1:I:332:LEU:HG	1:I:340:TRP:CZ3	2.42	0.54
1:I:356:TRP:HZ3	1:I:674:PRO:O	1.91	0.54
1:K:562:GLY:O	1:K:564:THR:N	2.41	0.54
2:L:41:VAL:HG13	2:L:105:GLN:HG3	1.90	0.54
1:M:332:LEU:HB3	1:M:340:TRP:CZ2	2.42	0.54
6:N:1129:HEC:HMC1	6:N:1129:HEC:HBC3	1.88	0.54
2:N:33:ARG:HH21	2:N:40:PRO:CG	2.15	0.54
1:O:209:HIS:C	1:O:209:HIS:CD2	2.81	0.54
1:O:245:ALA:HB3	1:O:307:VAL:HG11	1.89	0.54
1:O:238:ARG:CZ	1:O:676:GLU:O	2.55	0.54
1:O:689:TRP:CZ3	1:O:794:LYS:HB2	2.43	0.54
1:C:448:ASN:HA	1:C:477:ASN:HD22	1.73	0.54
1:E:332:LEU:HD23	1:E:340:TRP:HH2	1.69	0.54
1:E:702:GLY:HA3	1:E:706:LEU:HD12	1.89	0.54
1:G:180:ASP:O	1:G:181:ALA:HB2	2.06	0.54
1:G:29:MET:HE3	1:G:628:ARG:NH1	2.21	0.54
1:I:455:ASN:HD22	1:I:457:ASN:H	1.54	0.54
1:K:108:LEU:HD21	1:K:548:VAL:HG13	1.90	0.54
1:M:137:ARG:O	1:M:141:ARG:HA	2.07	0.54
1:M:332:LEU:HG	1:M:340:TRP:CZ3	2.42	0.54
1:M:426:LEU:HD21	1:M:549:TRP:CZ2	2.43	0.54
1:M:537:MET:CE	1:M:595:PHE:CE2	2.91	0.54
1:M:724:PRO:O	1:M:728:ARG:HG3	2.08	0.54
1:O:238:ARG:HG2	1:O:360:MET:HE1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:414:ALA:O	1:O:418:GLU:HG2	2.08	0.54
1:A:332:LEU:CD2	1:A:340:TRP:CH2	2.90	0.54
1:A:400:ARG:HH21	1:A:404:ASP:H	1.55	0.54
1:A:627:VAL:HG12	1:A:628:ARG:N	2.23	0.54
2:B:41:VAL:HG13	2:B:105:GLN:HG3	1.89	0.54
1:G:332:LEU:CD2	1:G:340:TRP:CH2	2.90	0.54
1:G:332:LEU:HG	1:G:340:TRP:CZ3	2.42	0.54
1:G:163:THR:CG2	1:G:359:HIS:HD1	2.19	0.54
1:G:118:MET:HG2	1:G:451:TRP:HB3	1.90	0.54
2:H:101:CYS:SG	6:H:1129:HEC:C3C	2.96	0.54
1:I:690:LEU:HB3	1:I:795:CYS:SG	2.47	0.54
2:L:82:ASP:HB3	2:L:88:LEU:HD11	1.90	0.54
1:M:76:ARG:NH2	1:M:493:ALA:O	2.40	0.54
1:O:233:ARG:HB3	1:O:236:THR:HG21	1.90	0.54
1:C:189:MET:HE1	1:C:343:LEU:HD13	1.90	0.54
1:C:537:MET:HE2	1:C:595:PHE:CE2	2.43	0.54
1:E:272:ILE:CG2	1:E:785:PRO:CG	2.83	0.54
2:J:82:ASP:HB3	2:J:88:LEU:HD11	1.89	0.54
2:L:98:CYS:O	2:L:100:ALA:N	2.41	0.54
2:N:27:ASP:OD2	2:N:29:ARG:HD3	2.07	0.54
1:O:439:ASP:OD1	1:O:468:THR:HG23	2.08	0.54
2:P:81:GLN:HA	2:P:86:GLN:O	2.07	0.54
1:A:202:ASP:HA	2:B:93:PRO:HB2	1.88	0.54
1:A:314:LYS:O	1:A:318:ILE:HG13	2.07	0.54
1:C:183:VAL:HG23	1:C:340:TRP:NE1	2.23	0.54
1:I:163:THR:CG2	1:I:359:HIS:ND1	2.70	0.54
1:K:545:THR:HG22	1:K:549:TRP:CE3	2.42	0.54
1:K:597:PHE:N	1:K:597:PHE:CD1	2.75	0.54
1:K:739:ARG:HA	1:K:747:ILE:O	2.07	0.54
1:M:714:ALA:CB	2:N:103:VAL:HG11	2.38	0.54
1:O:108:LEU:HD21	1:O:548:VAL:HG13	1.90	0.54
1:O:192:MET:HB3	5:O:1804:MGD:N22	2.23	0.54
1:O:574:SER:O	1:O:577:ARG:HB2	2.07	0.54
2:P:58:CYS:CB	6:P:1128:HEC:HAB	2.37	0.54
1:C:511:ASN:CG	1:C:515:ARG:HB3	2.28	0.54
1:G:272:ILE:CG2	1:G:785:PRO:CG	2.83	0.54
2:H:75:ILE:CD1	2:H:80:PHE:HE2	2.21	0.54
1:I:120:GLY:HA3	1:I:124:TRP:CZ3	2.42	0.54
1:K:346:MET:HB3	1:K:350:GLN:HG3	1.89	0.54
1:M:545:THR:HG22	1:M:549:TRP:CE3	2.43	0.54
1:M:690:LEU:HD22	1:M:797:VAL:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:PRO:HD3	1:C:560:TYR:CZ	2.43	0.54
1:C:367:LEU:CD1	1:C:670:ILE:HD13	2.37	0.54
2:D:81:GLN:HA	2:D:86:GLN:O	2.07	0.54
1:G:714:ALA:CB	2:H:103:VAL:HG11	2.38	0.54
1:G:776:ASN:HA	1:G:779:THR:HG1	1.71	0.54
1:I:537:MET:HE2	1:I:595:PHE:CE2	2.42	0.54
1:I:627:VAL:HG12	1:I:628:ARG:N	2.23	0.54
1:K:270:THR:HG22	1:K:674:PRO:HG3	1.89	0.54
2:P:98:CYS:O	2:P:100:ALA:N	2.41	0.54
1:A:448:ASN:HA	1:A:477:ASN:ND2	2.22	0.53
1:C:21:PHE:O	1:C:385:PRO:HD3	2.07	0.53
1:E:291:ASP:O	1:E:292:ALA:HB3	2.08	0.53
1:E:514:ARG:O	1:E:631:HIS:HA	2.07	0.53
1:E:722:MET:CE	1:E:751:LEU:HD11	2.39	0.53
2:F:101:CYS:SG	6:F:1129:HEC:CBC	2.95	0.53
1:G:139:GLY:HA2	1:G:565:LEU:HD22	1.90	0.53
1:I:20:ARG:O	1:I:20:ARG:HG3	2.08	0.53
1:I:506:GLU:OE1	1:I:625:HIS:HE1	1.91	0.53
2:J:41:VAL:HG11	2:J:105:GLN:HG3	1.90	0.53
1:K:714:ALA:HB2	2:L:103:VAL:CG1	2.39	0.53
1:O:747:ILE:CG2	1:O:748:ARG:N	2.71	0.53
1:O:772:SER:HB2	2:P:4:PRO:CG	2.33	0.53
1:A:121:SER:C	1:A:123:GLN:H	2.11	0.53
1:A:597:PHE:N	1:A:597:PHE:CD1	2.75	0.53
1:C:211:ARG:HB2	1:C:338:ARG:HH12	1.72	0.53
1:C:244:ILE:HD11	1:C:329:LEU:HD23	1.90	0.53
1:C:68:ASP:OD2	1:C:707:ARG:NH1	2.41	0.53
1:E:220:HIS:CE1	1:E:222:SER:HB2	2.44	0.53
1:E:367:LEU:CD1	1:E:670:ILE:HD13	2.39	0.53
1:I:29:MET:CE	1:I:628:ARG:HH12	2.21	0.53
1:I:722:MET:HG2	1:I:723:HIS:N	2.24	0.53
1:K:335:ASP:O	1:K:337:ASP:N	2.39	0.53
2:L:3:ALA:CB	2:L:4:PRO:CD	2.69	0.53
1:O:423:PRO:HD3	1:O:560:TYR:CZ	2.43	0.53
1:O:738:VAL:HG21	1:O:751:LEU:HD13	1.90	0.53
1:A:766:VAL:CG2	1:A:775:ILE:HD13	2.33	0.53
1:C:400:ARG:HH21	1:C:404:ASP:H	1.55	0.53
1:C:722:MET:HG2	1:C:723:HIS:N	2.24	0.53
2:H:98:CYS:CB	6:H:1129:HEC:CAB	2.79	0.53
1:K:291:ASP:O	1:K:292:ALA:HB3	2.08	0.53
2:L:14:SER:O	2:L:15:GLU:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:233:ARG:HB3	1:M:236:THR:CG2	2.39	0.53
1:M:628:ARG:CG	1:M:628:ARG:HH11	2.22	0.53
1:O:346:MET:HB3	1:O:350:GLN:HG3	1.89	0.53
1:A:303:PHE:O	1:A:307:VAL:HG23	2.09	0.53
1:A:211:ARG:HB2	1:A:338:ARG:HH12	1.74	0.53
1:A:583:VAL:O	1:A:583:VAL:HG13	2.07	0.53
1:C:414:ALA:O	1:C:418:GLU:HG2	2.07	0.53
2:D:35:TYR:C	2:D:36:PRO:O	2.43	0.53
1:E:628:ARG:HH11	1:E:628:ARG:CG	2.22	0.53
1:E:641:ARG:HD2	1:E:642:TRP:CZ3	2.44	0.53
1:I:133:SER:OG	1:I:137:ARG:NH1	2.42	0.53
1:I:16:LYS:HA	1:I:29:MET:HE1	1.90	0.53
2:J:27:ASP:OD2	2:J:29:ARG:HD3	2.09	0.53
1:K:448:ASN:HA	1:K:477:ASN:HD22	1.74	0.53
2:N:78:THR:O	2:N:81:GLN:HG3	2.09	0.53
1:O:20:ARG:O	1:O:20:ARG:HG3	2.08	0.53
1:A:68:ASP:HB2	1:A:707:ARG:HH12	1.73	0.53
1:C:702:GLY:HA3	1:C:706:LEU:HD12	1.91	0.53
1:G:238:ARG:NH1	1:G:676:GLU:O	2.42	0.53
1:K:118:MET:CE	1:K:132:ALA:HB1	2.38	0.53
1:K:659:ARG:O	1:K:661:TYR:N	2.41	0.53
1:K:367:LEU:CD1	1:K:670:ILE:HD13	2.39	0.53
1:M:714:ALA:HB2	2:N:103:VAL:CG1	2.38	0.53
1:O:617:ASP:HB2	1:O:633:PRO:HA	1.91	0.53
2:P:34:ASN:H	2:P:38:GLN:NE2	2.06	0.53
1:A:52:LEU:HG	6:B:1129:HEC:HBC2	1.91	0.53
2:B:42:ILE:HD11	6:B:1128:HEC:HMB2	1.91	0.53
1:E:583:VAL:O	1:E:584:ASN:O	2.26	0.53
1:G:189:MET:HE1	1:G:343:LEU:HD13	1.91	0.53
2:H:14:SER:O	2:H:15:GLU:HB3	2.08	0.53
1:I:299:ASP:OD1	1:I:301:GLU:HG2	2.09	0.53
1:I:144:ASN:HD22	1:I:433:ALA:H	1.53	0.53
1:K:384:GLN:HB3	1:K:385:PRO:HD2	1.89	0.53
2:L:27:ASP:OD2	2:L:29:ARG:HD3	2.08	0.53
2:N:101:CYS:SG	6:N:1129:HEC:CBC	2.96	0.53
2:N:41:VAL:CG1	2:N:105:GLN:HG3	2.39	0.53
1:O:143:ASN:O	1:O:432:GLY:HA3	2.09	0.53
1:O:161:MET:O	1:O:165:GLY:N	2.42	0.53
1:O:597:PHE:N	1:O:597:PHE:CD1	2.76	0.53
1:A:245:ALA:HB3	1:A:307:VAL:HG11	1.90	0.53
1:A:631:HIS:ND1	1:A:639:GLU:OE2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:ALA:HA	1:E:308:SER:OG	2.09	0.53
1:G:291:ASP:O	1:G:292:ALA:HB3	2.08	0.53
1:G:162:ARG:NH1	1:G:359:HIS:NE2	2.57	0.53
1:K:67:GLU:HG2	2:L:112:VAL:HG13	1.91	0.53
1:K:719:VAL:CG1	1:K:752:GLU:HB2	2.38	0.53
1:K:714:ALA:CB	2:L:103:VAL:HG11	2.38	0.53
1:O:280:HIS:CE1	1:O:282:LEU:HD12	2.44	0.53
2:P:14:SER:O	2:P:15:GLU:HB3	2.09	0.53
1:A:272:ILE:CG2	1:A:785:PRO:CG	2.85	0.53
1:A:426:LEU:HD13	1:A:553:ILE:HG21	1.90	0.53
1:C:278:PRO:O	1:C:279:GLU:CG	2.57	0.53
1:C:455:ASN:HD21	1:C:457:ASN:HB2	1.73	0.53
1:C:59:PHE:CE2	1:C:710:GLU:HG3	2.43	0.53
2:D:67:SER:HA	2:H:118:ASP:OD1	2.09	0.53
1:E:16:LYS:HD2	1:E:628:ARG:HG3	1.90	0.53
1:E:455:ASN:HD22	1:E:457:ASN:H	1.57	0.53
1:G:147:PRO:HD3	1:G:396:THR:O	2.09	0.53
1:G:545:THR:HG22	1:G:549:TRP:CE3	2.44	0.53
2:H:101:CYS:SG	6:H:1129:HEC:CBC	2.97	0.53
1:I:436:VAL:CG1	1:I:440:ARG:CZ	2.87	0.53
1:I:116:VAL:HG12	1:I:449:PHE:HB3	1.90	0.53
1:I:714:ALA:HB2	2:J:103:VAL:CG1	2.38	0.53
1:I:750:ARG:NH1	2:J:18:ALA:O	2.41	0.53
1:K:192:MET:HB3	5:K:1804:MGD:N22	2.23	0.53
1:K:689:TRP:CZ3	1:K:794:LYS:HB2	2.43	0.53
1:C:791:ASP:OD2	1:C:794:LYS:HE2	2.09	0.53
1:E:396:THR:O	1:E:396:THR:CG2	2.54	0.53
1:G:121:SER:HB2	1:G:148:ASN:ND2	2.24	0.53
2:H:51:LEU:HD21	2:H:58:CYS:SG	2.49	0.53
1:I:332:LEU:HB3	1:I:340:TRP:CZ2	2.44	0.53
2:L:81:GLN:HA	2:L:86:GLN:O	2.09	0.53
1:M:455:ASN:HD21	1:M:457:ASN:HB2	1.73	0.53
1:A:52:LEU:HG	6:B:1129:HEC:CBC	2.39	0.53
1:C:278:PRO:O	1:C:279:GLU:HB2	2.07	0.53
1:E:68:ASP:HB2	1:E:707:ARG:HH12	1.73	0.53
1:E:766:VAL:CG2	1:E:775:ILE:HD13	2.33	0.53
2:F:40:PRO:HD2	2:F:102:HIS:HE1	1.74	0.53
1:I:584:ASN:O	1:I:586:ASP:O	2.27	0.53
1:M:189:MET:CE	1:M:343:LEU:HD13	2.39	0.53
1:M:540:SER:HB3	1:M:565:LEU:O	2.08	0.53
1:M:583:VAL:O	1:M:584:ASN:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:ILE:HG23	2:B:87:MET:CE	2.39	0.52
1:E:438:GLN:HE21	1:E:450:TYR:HE1	1.57	0.52
1:G:113:PRO:C	1:G:115:ALA:H	2.13	0.52
1:G:439:ASP:OD1	1:G:468:THR:HG23	2.09	0.52
1:G:690:LEU:HD22	1:G:797:VAL:HG21	1.91	0.52
1:I:68:ASP:OD2	1:I:707:ARG:NH1	2.42	0.52
1:K:118:MET:HE1	1:K:132:ALA:HB1	1.91	0.52
1:K:358:ASN:O	1:K:361:VAL:HG23	2.10	0.52
1:K:690:LEU:HB3	1:K:795:CYS:SG	2.50	0.52
1:M:537:MET:HE2	1:M:595:PHE:CE2	2.43	0.52
1:A:537:MET:HE2	1:A:595:PHE:CE2	2.43	0.52
2:D:101:CYS:SG	6:D:1129:HEC:C3C	2.96	0.52
1:G:192:MET:HB3	5:G:1804:MGD:N22	2.25	0.52
1:G:144:ASN:HD22	1:G:433:ALA:H	1.50	0.52
1:I:233:ARG:HB3	1:I:236:THR:HG21	1.92	0.52
1:I:400:ARG:HH21	1:I:404:ASP:H	1.54	0.52
1:I:724:PRO:O	1:I:728:ARG:HG3	2.09	0.52
1:K:332:LEU:HD23	1:K:340:TRP:HH2	1.71	0.52
1:K:49:ASN:HB2	1:K:52:LEU:O	2.09	0.52
1:M:544:THR:HA	1:M:564:THR:HA	1.90	0.52
1:A:414:ALA:O	1:A:418:GLU:HG2	2.09	0.52
2:B:14:SER:O	2:B:15:GLU:HB3	2.09	0.52
2:B:66:TYR:O	2:B:68:GLY:N	2.42	0.52
1:C:125:THR:HG21	1:C:127:TRP:NE1	2.24	0.52
1:E:125:THR:HG22	1:E:126:ILE:N	2.23	0.52
1:E:540:SER:O	1:E:542:ARG:N	2.42	0.52
1:K:305:ALA:HA	1:K:308:SER:OG	2.09	0.52
1:K:332:LEU:HB3	1:K:340:TRP:CZ2	2.43	0.52
1:K:463:ASN:HD22	1:K:781:ASP:HB2	1.75	0.52
1:M:49:ASN:HB2	1:M:52:LEU:O	2.10	0.52
2:N:75:ILE:CD1	2:N:80:PHE:HE2	2.21	0.52
2:N:92:SER:O	2:N:94:ARG:O	2.27	0.52
1:O:121:SER:C	1:O:123:GLN:H	2.13	0.52
1:C:147:PRO:HD3	1:C:397:PHE:HA	1.91	0.52
1:E:121:SER:HA	1:E:148:ASN:OD1	2.10	0.52
1:E:700:HIS:CE1	5:E:1804:MGD:S13	3.02	0.52
1:G:121:SER:C	1:G:123:GLN:H	2.13	0.52
1:G:183:VAL:HG23	1:G:340:TRP:NE1	2.23	0.52
1:K:76:ARG:NH2	1:K:493:ALA:O	2.41	0.52
1:O:540:SER:O	1:O:542:ARG:N	2.42	0.52
1:A:76:ARG:HH22	1:A:473:ARG:CZ	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:NH1	1:A:676:GLU:O	2.42	0.52
2:B:40:PRO:HD2	2:B:102:HIS:HE1	1.74	0.52
1:C:118:MET:CE	1:C:132:ALA:HB1	2.40	0.52
1:E:346:MET:HB3	1:E:350:GLN:HG3	1.91	0.52
1:G:533:LEU:O	1:G:537:MET:HG3	2.10	0.52
1:G:722:MET:CE	1:G:751:LEU:HD11	2.40	0.52
1:I:272:ILE:CG2	1:I:785:PRO:CG	2.83	0.52
1:K:438:GLN:HE21	1:K:450:TYR:HE1	1.57	0.52
1:K:505:LYS:HG2	1:K:505:LYS:O	2.08	0.52
1:K:628:ARG:CG	1:K:628:ARG:HH11	2.23	0.52
2:L:40:PRO:HD3	6:L:1129:HEC:HBD2	1.91	0.52
1:O:291:ASP:O	1:O:292:ALA:HB3	2.10	0.52
1:A:163:THR:CG2	1:A:359:HIS:ND1	2.71	0.52
1:C:617:ASP:OD2	1:C:651:TYR:OH	2.28	0.52
1:C:714:ALA:HB2	2:D:103:VAL:CG1	2.40	0.52
2:F:77:ILE:HG23	2:F:87:MET:CE	2.40	0.52
1:I:426:LEU:HD13	1:I:553:ILE:HG21	1.91	0.52
1:I:700:HIS:HE1	5:I:1804:MGD:S13	2.33	0.52
1:K:540:SER:C	1:K:542:ARG:H	2.13	0.52
1:K:356:TRP:CZ3	1:K:674:PRO:O	2.63	0.52
1:M:455:ASN:ND2	1:M:457:ASN:H	2.08	0.52
2:N:42:ILE:CD1	6:N:1128:HEC:HMB2	2.38	0.52
1:O:162:ARG:NH1	1:O:359:HIS:NE2	2.58	0.52
1:A:121:SER:HB2	1:A:148:ASN:ND2	2.25	0.52
1:E:400:ARG:HH21	1:E:404:ASP:H	1.54	0.52
1:G:278:PRO:O	1:G:279:GLU:HB2	2.08	0.52
1:G:384:GLN:HB3	1:G:385:PRO:HD2	1.90	0.52
1:I:483:ASP:OD1	1:I:484:ALA:N	2.37	0.52
1:I:598:TYR:CE1	1:I:600:GLN:HG2	2.44	0.52
2:J:33:ARG:HH21	2:J:40:PRO:CG	2.21	0.52
2:B:34:ASN:H	2:B:38:GLN:NE2	2.08	0.52
2:D:66:TYR:O	2:D:68:GLY:N	2.43	0.52
1:E:270:THR:HG22	1:E:674:PRO:HG3	1.91	0.52
1:E:46:ALA:O	1:E:50:ARG:HG2	2.10	0.52
2:H:30:ARG:HD2	6:H:1128:HEC:O1D	2.09	0.52
1:I:503:VAL:HG12	1:I:523:VAL:HG22	1.91	0.52
2:J:95:ARG:CA	6:J:1129:HEC:HMC2	2.35	0.52
1:K:581:SER:OG	1:K:582:ASP:N	2.43	0.52
1:M:29:MET:HE3	1:M:628:ARG:NH1	2.18	0.52
2:P:75:ILE:CD1	2:P:80:PHE:HE2	2.23	0.52
2:P:5:ARG:O	2:P:7:THR:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:MET:CE	1:A:145:LEU:HD13	2.40	0.52
1:A:233:ARG:HB3	1:A:236:THR:HG21	1.90	0.52
1:A:278:PRO:O	1:A:279:GLU:CG	2.58	0.52
1:C:138:ALA:HB1	1:C:422:LEU:HD11	1.91	0.52
1:C:730:ARG:HB2	1:C:732:LEU:HD22	1.92	0.52
1:E:120:GLY:HA3	1:E:124:TRP:CZ3	2.45	0.52
1:E:617:ASP:HB2	1:E:633:PRO:HA	1.92	0.52
2:F:27:ASP:OD2	2:F:29:ARG:HD3	2.09	0.52
1:G:299:ASP:OD1	1:G:301:GLU:HG2	2.10	0.52
2:H:41:VAL:HG11	2:H:105:GLN:HG3	1.91	0.52
2:H:98:CYS:C	2:H:100:ALA:H	2.13	0.52
1:I:33:ARG:HD3	2:J:122:LEU:HD21	1.91	0.52
1:M:514:ARG:O	1:M:631:HIS:HA	2.09	0.52
1:M:689:TRP:CZ3	1:M:794:LYS:HB2	2.45	0.52
1:A:29:MET:HE3	1:A:628:ARG:NH1	2.22	0.52
1:C:738:VAL:HG21	1:C:751:LEU:HD13	1.91	0.52
1:C:491:ARG:NH2	2:D:11:ARG:N	2.54	0.52
1:E:230:ILE:HG23	1:E:321:VAL:CG1	2.35	0.52
1:E:332:LEU:HB3	1:E:340:TRP:CZ2	2.44	0.52
1:E:537:MET:CE	1:E:595:PHE:CE2	2.93	0.52
1:E:750:ARG:HD3	2:F:20:PRO:HA	1.92	0.52
1:I:68:ASP:CB	1:I:707:ARG:NH1	2.73	0.52
2:J:77:ILE:HG23	2:J:87:MET:CE	2.40	0.52
2:L:3:ALA:HB2	2:L:19:PRO:CG	2.40	0.52
1:M:426:LEU:HD21	1:M:549:TRP:CE2	2.45	0.52
1:O:299:ASP:OD1	1:O:301:GLU:HG2	2.10	0.52
1:A:722:MET:HG2	1:A:723:HIS:H	1.75	0.51
1:C:163:THR:CG2	1:C:359:HIS:ND1	2.73	0.51
1:C:332:LEU:HG	1:C:340:TRP:CZ3	2.44	0.51
1:E:163:THR:CG2	1:E:359:HIS:HD1	2.23	0.51
1:E:202:ASP:HA	2:F:93:PRO:HB2	1.92	0.51
1:E:694:ARG:HH22	5:E:1803:MGD:H15	1.58	0.51
1:G:627:VAL:HG12	1:G:628:ARG:N	2.25	0.51
6:H:1129:HEC:HBC3	6:H:1129:HEC:HMC1	1.91	0.51
2:H:66:TYR:OH	2:H:77:ILE:HD11	2.11	0.51
2:J:83:ARG:O	2:J:84:GLU:CB	2.53	0.51
1:M:632:TRP:O	1:M:632:TRP:CE3	2.63	0.51
1:O:448:ASN:ND2	1:O:477:ASN:ND2	2.42	0.51
1:O:581:SER:OG	1:O:582:ASP:N	2.43	0.51
1:O:612:ARG:HA	1:O:617:ASP:OD1	2.10	0.51
1:A:722:MET:CE	1:A:751:LEU:HD11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:VAL:CG2	1:C:775:ILE:HD13	2.31	0.51
1:E:113:PRO:C	1:E:115:ALA:H	2.12	0.51
2:F:121:THR:OG1	2:F:121:THR:O	2.24	0.51
2:F:83:ARG:O	2:F:84:GLU:CB	2.41	0.51
2:J:86:GLN:HA	2:J:86:GLN:HE21	1.74	0.51
1:K:367:LEU:HD13	1:K:670:ILE:HD13	1.91	0.51
1:K:139:GLY:HA2	1:K:565:LEU:HD22	1.92	0.51
1:K:584:ASN:O	1:K:586:ASP:O	2.27	0.51
1:M:605:GLU:OE1	1:M:612:ARG:NH2	2.41	0.51
1:O:436:VAL:CG1	1:O:440:ARG:CZ	2.89	0.51
1:C:14:TRP:HZ2	2:H:89:ALA:HB2	1.75	0.51
1:C:455:ASN:HD22	1:C:457:ASN:H	1.58	0.51
1:E:540:SER:C	1:E:542:ARG:H	2.14	0.51
2:F:75:ILE:CD1	2:F:80:PHE:HE2	2.24	0.51
1:G:49:ASN:HB2	1:G:52:LEU:O	2.10	0.51
1:I:303:PHE:O	1:I:307:VAL:HG23	2.10	0.51
1:M:299:ASP:OD1	1:M:301:GLU:HG2	2.10	0.51
1:M:143:ASN:O	1:M:432:GLY:HA3	2.10	0.51
1:M:448:ASN:ND2	1:M:477:ASN:HD21	1.98	0.51
1:O:133:SER:OG	1:O:137:ARG:NH1	2.44	0.51
1:O:60:LEU:HD23	1:O:63:ILE:HD12	1.92	0.51
1:O:76:ARG:NH2	1:O:493:ALA:O	2.42	0.51
1:A:423:PRO:HD3	1:A:560:TYR:CZ	2.46	0.51
1:C:192:MET:HB3	5:C:1804:MGD:N22	2.25	0.51
1:C:540:SER:C	1:C:542:ARG:H	2.14	0.51
1:E:358:ASN:O	1:E:361:VAL:HG23	2.10	0.51
1:E:545:THR:HG22	1:E:549:TRP:CE3	2.45	0.51
1:E:700:HIS:O	1:E:769:PHE:HA	2.11	0.51
1:E:749:THR:CG2	1:E:773:GLN:OE1	2.48	0.51
1:G:479:ILE:HG22	1:G:493:ALA:HB1	1.93	0.51
2:H:98:CYS:HB3	6:H:1129:HEC:CAB	2.39	0.51
1:I:426:LEU:HD21	1:I:549:TRP:CZ2	2.46	0.51
1:I:545:THR:HG22	1:I:549:TRP:CE3	2.44	0.51
1:K:332:LEU:CD2	1:K:340:TRP:HH2	2.24	0.51
1:K:455:ASN:ND2	1:K:457:ASN:H	2.08	0.51
1:M:453:GLN:HG2	1:M:482:SER:HB2	1.92	0.51
1:M:700:HIS:O	1:M:769:PHE:HA	2.10	0.51
1:O:505:LYS:HG2	1:O:505:LYS:O	2.11	0.51
1:A:791:ASP:OD2	1:A:794:LYS:HE2	2.10	0.51
1:C:332:LEU:CD2	1:C:340:TRP:CH2	2.92	0.51
1:E:20:ARG:HG3	1:E:20:ARG:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:GLN:H	2:H:123:MET:CE	2.24	0.51
1:I:238:ARG:CZ	1:I:676:GLU:O	2.58	0.51
1:K:202:ASP:HA	2:L:93:PRO:HB2	1.92	0.51
1:K:426:LEU:HD21	1:K:549:TRP:CZ2	2.46	0.51
1:K:84:LYS:HE2	1:K:473:ARG:C	2.31	0.51
1:M:118:MET:CE	1:M:132:ALA:HB1	2.40	0.51
1:M:291:ASP:O	1:M:292:ALA:HB3	2.10	0.51
1:M:511:ASN:CG	1:M:515:ARG:HB3	2.31	0.51
1:M:730:ARG:HB2	1:M:732:LEU:HD22	1.92	0.51
2:P:26:THR:HG22	2:P:26:THR:O	2.10	0.51
1:A:125:THR:HG21	1:A:127:TRP:NE1	2.26	0.51
1:A:180:ASP:O	1:A:181:ALA:HB2	2.10	0.51
1:A:259:VAL:O	1:A:263:THR:HB	2.10	0.51
1:A:332:LEU:HD23	1:A:340:TRP:HH2	1.73	0.51
1:A:690:LEU:HB3	1:A:795:CYS:SG	2.51	0.51
1:C:21:PHE:HZ	1:C:63:ILE:HD11	1.73	0.51
1:G:738:VAL:HG21	1:G:751:LEU:HD13	1.91	0.51
1:I:730:ARG:HB2	1:I:732:LEU:HD22	1.92	0.51
2:J:35:TYR:O	2:J:36:PRO:O	2.28	0.51
1:M:540:SER:C	1:M:542:ARG:H	2.14	0.51
1:M:558:PRO:O	1:M:560:TYR:N	2.44	0.51
2:N:66:TYR:OH	2:N:77:ILE:HD11	2.11	0.51
2:P:35:TYR:C	2:P:36:PRO:O	2.46	0.51
2:B:33:ARG:HH21	2:B:40:PRO:CG	2.21	0.51
2:B:66:TYR:OH	2:B:77:ILE:HD11	2.11	0.51
1:C:280:HIS:CE1	1:C:282:LEU:HD12	2.46	0.51
1:C:583:VAL:O	1:C:584:ASN:O	2.29	0.51
1:E:332:LEU:CD2	1:E:340:TRP:HH2	2.21	0.51
1:G:690:LEU:HB3	1:G:795:CYS:SG	2.51	0.51
1:I:793:LYS:CE	5:I:1804:MGD:H5'2	2.40	0.51
1:K:448:ASN:ND2	1:K:477:ASN:ND2	2.46	0.51
1:K:423:PRO:HD3	1:K:560:TYR:CZ	2.46	0.51
1:M:513:GLU:OE2	1:M:515:ARG:NH1	2.44	0.51
1:M:562:GLY:O	1:M:564:THR:N	2.44	0.51
1:M:40:THR:HG21	1:M:60:LEU:HB2	1.93	0.51
6:P:1129:HEC:HMC1	6:P:1129:HEC:HBC3	1.92	0.51
2:P:27:ASP:OD2	2:P:29:ARG:HD3	2.11	0.51
1:C:384:GLN:HB3	1:C:385:PRO:HD2	1.92	0.51
2:D:40:PRO:HD2	2:D:102:HIS:HE1	1.75	0.51
1:E:367:LEU:HD13	1:E:670:ILE:HD13	1.92	0.51
1:E:581:SER:OG	1:E:582:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:ALA:HB1	1:G:211:ARG:O	2.10	0.51
2:H:49:TYR:CD2	2:H:57:ARG:HG2	2.45	0.51
1:I:143:ASN:O	1:I:432:GLY:HA3	2.11	0.51
1:I:586:ASP:O	1:I:587:HIS:HB2	2.11	0.51
1:I:738:VAL:O	1:I:748:ARG:HA	2.11	0.51
1:K:278:PRO:O	1:K:279:GLU:CG	2.59	0.51
6:L:1129:HEC:HMC1	6:L:1129:HEC:CBC	2.40	0.51
1:M:367:LEU:CD1	1:M:670:ILE:HD13	2.41	0.51
1:O:278:PRO:O	1:O:279:GLU:HB2	2.09	0.51
1:O:549:TRP:CH2	1:O:568:VAL:HG11	2.45	0.51
1:O:714:ALA:CB	2:P:103:VAL:HG11	2.41	0.51
1:C:333:TYR:CZ	1:C:340:TRP:CD1	2.99	0.51
1:E:335:ASP:O	1:E:337:ASP:N	2.40	0.51
1:E:68:ASP:OD2	1:E:707:ARG:NH1	2.43	0.51
1:G:628:ARG:HH11	1:G:628:ARG:CG	2.23	0.51
1:I:209:HIS:C	1:I:209:HIS:CD2	2.83	0.51
1:I:394:VAL:HG22	1:I:607:TYR:CE1	2.46	0.51
1:K:116:VAL:HG12	1:K:449:PHE:HB3	1.92	0.51
2:L:89:ALA:O	2:L:90:ASP:HB2	2.10	0.51
1:M:278:PRO:O	1:M:279:GLU:CG	2.59	0.51
1:O:119:PHE:HA	1:O:146:ASP:O	2.11	0.51
1:O:192:MET:HE2	1:O:694:ARG:CB	2.19	0.51
1:O:426:LEU:HD13	1:O:553:ILE:HG21	1.93	0.51
1:O:543:PHE:HB2	1:O:565:LEU:HD12	1.92	0.51
1:A:714:ALA:HB2	2:B:103:VAL:CG1	2.41	0.51
1:C:233:ARG:HB3	1:C:236:THR:HG21	1.93	0.51
1:C:426:LEU:HD21	1:C:549:TRP:CZ2	2.46	0.51
1:E:436:VAL:CG1	1:E:440:ARG:CZ	2.89	0.51
1:E:689:TRP:CZ3	1:E:794:LYS:HB2	2.46	0.51
1:G:724:PRO:O	1:G:728:ARG:HG3	2.11	0.51
1:I:291:ASP:O	1:I:292:ALA:HB3	2.09	0.51
2:J:14:SER:O	2:J:15:GLU:HB3	2.11	0.51
1:K:332:LEU:HB3	1:K:340:TRP:CZ3	2.46	0.51
1:K:472:TYR:HA	1:K:479:ILE:CD1	2.41	0.51
1:K:722:MET:HG2	1:K:723:HIS:H	1.76	0.51
1:M:332:LEU:HD23	1:M:340:TRP:HH2	1.72	0.51
1:M:396:THR:CG2	1:M:396:THR:O	2.59	0.51
1:M:33:ARG:HD3	2:N:122:LEU:HD21	1.93	0.51
1:O:511:ASN:CG	1:O:515:ARG:HB3	2.31	0.51
1:A:120:GLY:HA3	1:A:124:TRP:CZ3	2.46	0.50
1:A:694:ARG:HH22	5:A:1803:MGD:H15	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HB3	1:A:340:TRP:CZ3	2.46	0.50
1:A:571:ALA:HA	1:A:576:ASP:CG	2.31	0.50
1:A:605:GLU:OE1	1:A:612:ARG:NH2	2.40	0.50
1:C:722:MET:CE	1:C:751:LEU:HD11	2.41	0.50
2:D:79:HIS:CD2	2:D:95:ARG:HD2	2.46	0.50
1:G:401:LEU:HB3	1:G:402:PRO:CD	2.41	0.50
1:G:67:GLU:HG2	2:H:112:VAL:HG13	1.92	0.50
1:I:21:PHE:O	1:I:385:PRO:HD3	2.11	0.50
1:I:374:PRO:HB3	1:I:642:TRP:CZ2	2.47	0.50
1:K:20:ARG:O	1:K:20:ARG:CG	2.60	0.50
1:M:722:MET:CE	1:M:751:LEU:HD11	2.41	0.50
2:N:3:ALA:HB2	2:N:19:PRO:CG	2.41	0.50
1:O:192:MET:HE1	1:O:694:ARG:HB3	1.92	0.50
1:A:291:ASP:O	1:A:292:ALA:HB3	2.11	0.50
2:B:75:ILE:CD1	2:B:80:PHE:HE2	2.25	0.50
1:C:33:ARG:HD3	2:D:122:LEU:HD21	1.92	0.50
2:D:66:TYR:OH	2:D:77:ILE:HD11	2.11	0.50
1:E:750:ARG:NH1	2:F:18:ALA:O	2.44	0.50
2:F:27:ASP:O	2:F:27:ASP:CG	2.49	0.50
1:G:163:THR:CG2	1:G:359:HIS:ND1	2.74	0.50
1:G:305:ALA:HA	1:G:308:SER:OG	2.12	0.50
1:G:581:SER:OG	1:G:582:ASP:N	2.43	0.50
1:G:738:VAL:O	1:G:748:ARG:HA	2.12	0.50
1:I:162:ARG:NH1	1:I:359:HIS:NE2	2.59	0.50
1:O:426:LEU:HD21	1:O:549:TRP:CZ2	2.46	0.50
2:P:66:TYR:OH	2:P:77:ILE:HD11	2.11	0.50
1:A:180:ASP:HB2	1:A:339:LYS:N	2.25	0.50
2:B:82:ASP:HB3	2:B:88:LEU:HD11	1.93	0.50
1:C:161:MET:O	1:C:165:GLY:N	2.44	0.50
1:C:29:MET:CE	1:C:628:ARG:HH12	2.24	0.50
1:C:689:TRP:CZ3	1:C:794:LYS:HB2	2.46	0.50
1:C:750:ARG:NH1	2:D:18:ALA:O	2.45	0.50
1:E:188:ASN:ND2	1:E:222:SER:OG	2.40	0.50
1:E:453:GLN:HG2	1:E:482:SER:HB2	1.93	0.50
2:F:41:VAL:HG13	2:F:105:GLN:HG3	1.94	0.50
2:F:81:GLN:HA	2:F:86:GLN:O	2.11	0.50
1:G:121:SER:HA	1:G:148:ASN:OD1	2.11	0.50
1:G:455:ASN:HD21	1:G:457:ASN:HB2	1.75	0.50
2:H:81:GLN:HA	2:H:86:GLN:O	2.11	0.50
1:I:305:ALA:HA	1:I:308:SER:OG	2.11	0.50
1:M:209:HIS:CD2	1:M:209:HIS:C	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:305:ALA:HA	1:M:308:SER:OG	2.11	0.50
2:N:77:ILE:HG23	2:N:87:MET:CE	2.41	0.50
1:O:147:PRO:HD3	1:O:397:PHE:HA	1.94	0.50
1:O:739:ARG:HA	1:O:747:ILE:O	2.11	0.50
2:P:82:ASP:HB3	2:P:88:LEU:HD11	1.93	0.50
1:A:537:MET:HE3	1:A:595:PHE:CE2	2.46	0.50
2:B:51:LEU:HD21	2:B:58:CYS:SG	2.51	0.50
1:C:233:ARG:HB3	1:C:236:THR:CG2	2.42	0.50
2:D:14:SER:O	2:D:15:GLU:HB3	2.11	0.50
1:E:384:GLN:HB3	1:E:385:PRO:HD2	1.93	0.50
1:G:233:ARG:HB3	1:G:236:THR:CG2	2.42	0.50
1:G:76:ARG:NH2	1:G:473:ARG:NH1	2.59	0.50
2:H:49:TYR:CE1	6:H:1128:HEC:HMC2	2.46	0.50
1:K:750:ARG:NH1	2:L:18:ALA:O	2.44	0.50
1:K:76:ARG:NH2	1:K:473:ARG:HH22	2.09	0.50
2:L:92:SER:O	2:L:94:ARG:O	2.28	0.50
1:M:793:LYS:CE	5:M:1804:MGD:H5'2	2.41	0.50
1:M:469:TYR:N	1:M:470:PRO:HD2	2.26	0.50
1:A:299:ASP:OD1	1:A:301:GLU:HG2	2.12	0.50
1:C:300:PHE:CD1	1:C:300:PHE:O	2.65	0.50
1:C:730:ARG:CB	1:C:732:LEU:HD22	2.41	0.50
2:D:3:ALA:HB2	2:D:19:PRO:CG	2.41	0.50
1:I:125:THR:HG21	1:I:127:TRP:NE1	2.26	0.50
1:I:340:TRP:HA	1:I:340:TRP:CE3	2.46	0.50
1:I:144:ASN:HD21	1:I:433:ALA:H	1.57	0.50
1:I:441:LYS:HB3	1:I:447:ILE:HG13	1.94	0.50
1:K:615:GLY:O	1:K:617:ASP:N	2.44	0.50
2:P:3:ALA:HB2	2:P:19:PRO:CG	2.42	0.50
1:A:113:PRO:C	1:A:115:ALA:H	2.15	0.50
1:A:628:ARG:CG	1:A:628:ARG:HH11	2.25	0.50
1:A:720:CYS:SG	1:A:764:VAL:HG13	2.52	0.50
2:B:98:CYS:O	2:B:100:ALA:N	2.44	0.50
1:C:332:LEU:HD23	1:C:340:TRP:HH2	1.75	0.50
1:C:563:LYS:O	1:C:564:THR:OG1	2.30	0.50
1:C:584:ASN:O	1:C:586:ASP:O	2.30	0.50
2:D:77:ILE:HG23	2:D:87:MET:CE	2.42	0.50
1:E:278:PRO:O	1:E:279:GLU:CG	2.60	0.50
1:G:280:HIS:CE1	1:G:282:LEU:HD12	2.46	0.50
1:G:540:SER:C	1:G:542:ARG:H	2.15	0.50
1:I:183:VAL:CG1	1:I:185:TRP:NE1	2.75	0.50
1:I:571:ALA:HA	1:I:576:ASP:CG	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:113:PRO:C	1:K:115:ALA:H	2.15	0.50
1:M:549:TRP:CH2	1:M:568:VAL:HG11	2.46	0.50
1:O:305:ALA:HA	1:O:308:SER:OG	2.11	0.50
1:O:700:HIS:CE1	5:O:1804:MGD:S13	3.05	0.50
1:O:67:GLU:HG2	2:P:112:VAL:HG13	1.92	0.50
1:A:540:SER:O	1:A:542:ARG:N	2.44	0.50
1:C:238:ARG:CZ	1:C:676:GLU:O	2.60	0.50
1:E:222:SER:C	1:E:224:ASP:H	2.15	0.50
1:G:483:ASP:OD1	1:G:484:ALA:N	2.40	0.50
1:G:356:TRP:CZ3	1:G:674:PRO:O	2.65	0.50
2:J:5:ARG:O	2:J:7:THR:N	2.45	0.50
1:K:26:CYS:HB3	1:K:49:ASN:CG	2.31	0.50
2:L:41:VAL:HG11	2:L:105:GLN:HG3	1.94	0.50
2:L:49:TYR:CD2	2:L:57:ARG:HG2	2.47	0.50
1:O:558:PRO:O	1:O:560:TYR:N	2.45	0.50
1:O:491:ARG:NH1	2:P:10:ASP:HA	2.26	0.50
1:A:483:ASP:OD1	1:A:484:ALA:N	2.41	0.50
1:A:540:SER:C	1:A:542:ARG:H	2.16	0.50
1:A:738:VAL:HG21	1:A:751:LEU:HD13	1.92	0.50
1:C:246:HIS:HB2	1:C:307:VAL:HG12	1.93	0.50
1:C:333:TYR:CD2	1:C:340:TRP:CD1	2.99	0.50
1:C:503:VAL:HG12	1:C:523:VAL:HG22	1.93	0.50
2:D:98:CYS:CB	6:D:1129:HEC:CAB	2.81	0.50
1:E:121:SER:C	1:E:123:GLN:H	2.15	0.50
1:G:68:ASP:CB	1:G:707:ARG:NH1	2.75	0.50
1:I:118:MET:HG2	1:I:451:TRP:HB3	1.93	0.50
2:J:49:TYR:CD2	2:J:57:ARG:HG2	2.46	0.50
1:K:340:TRP:CE3	1:K:340:TRP:HA	2.46	0.50
2:L:104:PRO:O	2:L:105:GLN:HG2	2.12	0.50
2:L:78:THR:O	2:L:81:GLN:HG3	2.12	0.50
1:A:463:ASN:HD22	1:A:781:ASP:HB2	1.77	0.50
2:B:81:GLN:HA	2:B:86:GLN:O	2.12	0.50
1:C:121:SER:C	1:C:123:GLN:H	2.13	0.50
1:C:209:HIS:CD2	1:C:209:HIS:C	2.85	0.50
1:C:138:ALA:CB	1:C:422:LEU:HD11	2.42	0.50
1:C:605:GLU:OE1	1:C:612:ARG:NH2	2.42	0.50
1:E:340:TRP:CE3	1:E:340:TRP:HA	2.47	0.50
1:E:423:PRO:HD3	1:E:560:TYR:CZ	2.46	0.50
1:E:29:MET:CE	1:E:628:ARG:HH12	2.13	0.50
1:G:793:LYS:CE	5:G:1804:MGD:H5'2	2.42	0.50
1:G:209:HIS:CD2	1:G:209:HIS:C	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:209:HIS:C	1:K:209:HIS:CD2	2.84	0.50
2:N:62:HIS:HA	2:N:74:MET:CB	2.42	0.50
1:O:335:ASP:O	1:O:337:ASP:N	2.41	0.50
1:O:356:TRP:CZ3	1:O:674:PRO:O	2.65	0.50
2:P:51:LEU:HD22	2:P:56:ASN:ND2	2.27	0.50
1:A:193:HIS:N	1:A:194:PRO:HD3	2.26	0.49
1:C:700:HIS:O	1:C:769:PHE:HA	2.12	0.49
1:E:356:TRP:HB3	1:E:673:VAL:HG11	1.93	0.49
1:G:119:PHE:HA	1:G:146:ASP:O	2.12	0.49
1:G:358:ASN:O	1:G:361:VAL:HG23	2.11	0.49
1:G:543:PHE:HB2	1:G:565:LEU:HD12	1.92	0.49
1:G:583:VAL:O	1:G:584:ASN:O	2.29	0.49
1:I:192:MET:SD	1:I:192:MET:N	2.85	0.49
1:I:783:ASN:HD22	1:I:790:THR:HA	1.77	0.49
2:L:75:ILE:CD1	2:L:80:PHE:HE2	2.25	0.49
2:L:86:GLN:HA	2:L:86:GLN:HE21	1.76	0.49
1:M:108:LEU:HD21	1:M:548:VAL:HG13	1.94	0.49
1:O:29:MET:CE	1:O:628:ARG:HH12	2.25	0.49
1:A:118:MET:CE	1:A:132:ALA:HB1	2.42	0.49
1:C:586:ASP:O	1:C:587:HIS:HB2	2.12	0.49
1:C:615:GLY:O	1:C:617:ASP:N	2.45	0.49
1:E:112:ALA:CB	1:E:113:PRO:CD	2.74	0.49
2:F:14:SER:O	2:F:15:GLU:HB3	2.12	0.49
1:G:246:HIS:HB2	1:G:307:VAL:HG12	1.93	0.49
1:G:340:TRP:HA	1:G:340:TRP:CE3	2.47	0.49
1:I:21:PHE:HZ	1:I:63:ILE:HD11	1.76	0.49
1:I:455:ASN:ND2	1:I:457:ASN:H	2.10	0.49
1:I:423:PRO:HD3	1:I:560:TYR:CZ	2.47	0.49
1:I:628:ARG:HH11	1:I:628:ARG:HG2	1.77	0.49
2:J:3:ALA:HB2	2:J:19:PRO:CG	2.42	0.49
1:K:161:MET:O	1:K:165:GLY:N	2.41	0.49
1:K:233:ARG:HB3	1:K:236:THR:CG2	2.42	0.49
1:K:238:ARG:CZ	1:K:676:GLU:O	2.60	0.49
2:N:58:CYS:HG	6:N:1128:HEC:CAB	2.03	0.49
2:P:77:ILE:HG23	2:P:87:MET:CE	2.42	0.49
1:A:332:LEU:CD2	1:A:340:TRP:HH2	2.25	0.49
1:A:339:LYS:CA	1:A:376:ASN:ND2	2.74	0.49
1:C:299:ASP:OD1	1:C:301:GLU:HG2	2.11	0.49
1:C:469:TYR:N	1:C:470:PRO:HD2	2.27	0.49
1:C:76:ARG:NH2	1:C:473:ARG:HH22	2.11	0.49
2:D:75:ILE:CD1	2:D:80:PHE:HE2	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:ALA:O	1:E:418:GLU:HG2	2.12	0.49
1:E:574:SER:O	1:E:577:ARG:HB2	2.13	0.49
2:F:92:SER:O	2:F:94:ARG:O	2.29	0.49
1:G:747:ILE:CG2	1:G:748:ARG:N	2.73	0.49
2:H:89:ALA:O	2:H:90:ASP:HB2	2.13	0.49
1:I:29:MET:HE3	1:I:628:ARG:HH12	1.78	0.49
1:I:333:TYR:CD2	1:I:340:TRP:CD1	3.00	0.49
1:I:549:TRP:CH2	1:I:568:VAL:HG11	2.47	0.49
1:K:491:ARG:NH2	2:L:11:ARG:N	2.57	0.49
2:L:26:THR:HG22	2:L:26:THR:O	2.12	0.49
1:M:139:GLY:HA2	1:M:565:LEU:HD22	1.93	0.49
1:M:193:HIS:N	1:M:194:PRO:HD3	2.27	0.49
1:M:439:ASP:OD1	1:M:468:THR:HG23	2.13	0.49
1:O:230:ILE:CG2	1:O:321:VAL:HG11	2.32	0.49
1:O:472:TYR:HA	1:O:479:ILE:CD1	2.43	0.49
2:P:86:GLN:HA	2:P:86:GLN:HE21	1.77	0.49
1:A:181:ALA:HB3	1:A:340:TRP:CE3	2.44	0.49
1:A:181:ALA:HB1	1:A:211:ARG:O	2.13	0.49
1:A:223:SER:HA	1:A:226:SER:OG	2.12	0.49
2:D:40:PRO:HD2	2:D:102:HIS:CE1	2.48	0.49
1:E:329:LEU:O	1:E:330:ALA:C	2.50	0.49
1:E:448:ASN:HA	1:E:477:ASN:HD22	1.76	0.49
1:E:714:ALA:HB2	2:F:103:VAL:HG11	1.93	0.49
1:E:76:ARG:NH2	1:E:493:ALA:O	2.45	0.49
2:F:86:GLN:HA	2:F:86:GLN:HE21	1.78	0.49
2:H:92:SER:O	2:H:94:ARG:O	2.30	0.49
1:I:19:CYS:SG	1:I:21:PHE:HB2	2.52	0.49
1:I:426:LEU:HD21	1:I:549:TRP:CE2	2.47	0.49
6:J:1129:HEC:HBC3	6:J:1129:HEC:HMC1	1.94	0.49
1:K:230:ILE:CG2	1:K:321:VAL:HG11	2.35	0.49
1:K:692:THR:CG2	5:K:1803:MGD:N18	2.71	0.49
1:M:730:ARG:CB	1:M:732:LEU:HD22	2.42	0.49
2:N:38:GLN:O	6:N:1129:HEC:HBD1	2.12	0.49
1:A:722:MET:HG2	1:A:723:HIS:N	2.28	0.49
1:E:543:PHE:HB2	1:E:565:LEU:HD12	1.94	0.49
2:F:3:ALA:HB2	2:F:19:PRO:CG	2.43	0.49
1:G:172:CYS:SG	1:G:174:ASP:HB2	2.52	0.49
1:G:714:ALA:HB2	2:H:103:VAL:CG1	2.42	0.49
2:H:62:HIS:HA	2:H:74:MET:CB	2.43	0.49
1:I:738:VAL:HG21	1:I:751:LEU:HD13	1.93	0.49
1:K:189:MET:HE1	1:K:343:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:60:LEU:HD23	1:K:63:ILE:HD12	1.94	0.49
1:K:724:PRO:O	1:K:728:ARG:HG3	2.12	0.49
1:M:586:ASP:O	1:M:587:HIS:HB2	2.11	0.49
1:M:747:ILE:CG2	1:M:748:ARG:N	2.73	0.49
1:O:223:SER:HA	1:O:226:SER:OG	2.12	0.49
1:O:510:GLY:HA2	1:O:515:ARG:O	2.13	0.49
1:O:742:SER:HB2	1:O:778:VAL:HG13	1.93	0.49
1:A:586:ASP:O	1:A:587:HIS:HB2	2.12	0.49
1:A:719:VAL:CG1	1:A:752:GLU:HB2	2.43	0.49
1:E:700:HIS:HE1	5:E:1804:MGD:S13	2.36	0.49
1:E:332:LEU:HB3	1:E:340:TRP:CZ3	2.47	0.49
1:I:246:HIS:HB2	1:I:307:VAL:HG12	1.94	0.49
1:I:414:ALA:O	1:I:418:GLU:HG2	2.12	0.49
1:I:747:ILE:CG2	1:I:748:ARG:N	2.72	0.49
1:K:439:ASP:OD1	1:K:468:THR:HG23	2.13	0.49
1:K:483:ASP:OD1	1:K:484:ALA:N	2.36	0.49
1:K:722:MET:HG2	1:K:723:HIS:N	2.28	0.49
1:M:246:HIS:HB2	1:M:307:VAL:HG12	1.93	0.49
1:M:659:ARG:O	1:M:661:TYR:N	2.45	0.49
1:O:138:ALA:CB	1:O:422:LEU:HD11	2.43	0.49
1:O:138:ALA:HB1	1:O:422:LEU:HD11	1.94	0.49
1:O:767:PRO:O	1:O:775:ILE:HD11	2.12	0.49
1:A:222:SER:C	1:A:224:ASP:H	2.16	0.49
1:A:244:ILE:HD11	1:A:329:LEU:HD23	1.93	0.49
1:A:514:ARG:O	1:A:631:HIS:HA	2.11	0.49
1:C:133:SER:OG	1:C:137:ARG:NH1	2.46	0.49
1:C:20:ARG:CG	1:C:20:ARG:O	2.59	0.49
1:C:332:LEU:HB3	1:C:340:TRP:CZ3	2.48	0.49
1:G:271:ASP:HB3	1:G:287:LYS:O	2.13	0.49
1:G:426:LEU:HD21	1:G:549:TRP:CE2	2.47	0.49
1:I:147:PRO:HD3	1:I:397:PHE:HA	1.95	0.49
1:I:714:ALA:CB	2:J:103:VAL:CG1	2.90	0.49
2:L:66:TYR:OH	2:L:77:ILE:HD11	2.13	0.49
1:O:723:HIS:HD2	1:O:725:GLU:N	2.02	0.49
1:O:749:THR:CG2	1:O:773:GLN:OE1	2.46	0.49
1:A:738:VAL:O	1:A:748:ARG:HA	2.12	0.49
1:C:305:ALA:HA	1:C:308:SER:OG	2.13	0.49
1:C:543:PHE:HB2	1:C:565:LEU:HD12	1.94	0.49
1:C:537:MET:CE	1:C:595:PHE:CE2	2.96	0.49
1:E:139:GLY:HA2	1:E:565:LEU:HD22	1.93	0.49
1:E:683:ASP:OD2	1:E:743:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:LEU:HD21	1:G:548:VAL:HG13	1.95	0.49
1:I:125:THR:HG22	1:I:126:ILE:N	2.28	0.49
1:K:193:HIS:N	1:K:194:PRO:HD3	2.27	0.49
1:K:747:ILE:CG2	1:K:748:ARG:N	2.72	0.49
1:M:113:PRO:C	1:M:115:ALA:H	2.16	0.49
1:M:233:ARG:HB3	1:M:236:THR:HG21	1.95	0.49
1:M:280:HIS:CE1	1:M:282:LEU:HD12	2.48	0.49
1:M:332:LEU:HB3	1:M:340:TRP:CZ3	2.47	0.49
1:M:584:ASN:O	1:M:586:ASP:O	2.30	0.49
1:M:84:LYS:HE2	1:M:473:ARG:C	2.33	0.49
1:O:222:SER:C	1:O:224:ASP:H	2.16	0.49
1:O:211:ARG:HB2	1:O:338:ARG:HH12	1.78	0.49
1:O:340:TRP:HA	1:O:340:TRP:CE3	2.47	0.49
1:O:598:TYR:CE1	1:O:600:GLN:HG2	2.47	0.49
1:C:113:PRO:C	1:C:115:ALA:H	2.16	0.49
1:E:513:GLU:O	1:E:514:ARG:HB2	2.11	0.49
2:F:82:ASP:HB3	2:F:88:LEU:HD11	1.94	0.49
1:G:238:ARG:HG2	1:G:360:MET:HE1	1.93	0.49
1:G:766:VAL:CG2	1:G:775:ILE:HD13	2.32	0.49
1:I:139:GLY:HA2	1:I:565:LEU:HD22	1.93	0.49
1:I:183:VAL:HG23	1:I:340:TRP:HZ2	1.74	0.49
1:I:581:SER:OG	1:I:582:ASP:N	2.46	0.49
1:K:538:GLU:OE2	1:K:541:LYS:HD2	2.13	0.49
1:M:332:LEU:CD2	1:M:340:TRP:HH2	2.25	0.49
1:M:238:ARG:HG2	1:M:360:MET:HE1	1.94	0.49
1:M:400:ARG:HH21	1:M:404:ASP:H	1.57	0.49
1:M:60:LEU:HD23	1:M:63:ILE:HD12	1.94	0.49
1:O:571:ALA:HA	1:O:576:ASP:CG	2.32	0.49
1:O:605:GLU:OE1	1:O:612:ARG:NH2	2.45	0.49
1:C:545:THR:HG22	1:C:549:TRP:CE3	2.46	0.49
2:D:98:CYS:HB3	6:D:1129:HEC:HAB	1.92	0.49
1:E:67:GLU:HG2	2:F:112:VAL:HG13	1.94	0.49
1:G:463:ASN:HD22	1:G:781:ASP:HB2	1.78	0.49
1:G:730:ARG:HB2	1:G:732:LEU:HD22	1.93	0.49
1:M:615:GLY:O	1:M:617:ASP:N	2.46	0.49
2:N:41:VAL:HG13	2:N:105:GLN:HG3	1.95	0.49
1:O:540:SER:C	1:O:542:ARG:H	2.16	0.49
1:O:730:ARG:HB2	1:O:732:LEU:HD22	1.94	0.49
1:C:571:ALA:HA	1:C:576:ASP:CG	2.32	0.48
1:C:581:SER:OG	1:C:582:ASP:N	2.46	0.48
1:C:628:ARG:HH11	1:C:628:ARG:CG	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:749:THR:CG2	1:C:773:GLN:OE1	2.48	0.48
1:E:163:THR:CG2	1:E:359:HIS:ND1	2.76	0.48
1:E:391:ALA:HA	1:E:396:THR:HB	1.94	0.48
1:E:356:TRP:CZ3	1:E:674:PRO:O	2.66	0.48
1:G:116:VAL:HG12	1:G:449:PHE:HB3	1.94	0.48
1:I:503:VAL:O	1:I:503:VAL:CG1	2.60	0.48
1:I:540:SER:C	1:I:542:ARG:H	2.16	0.48
1:I:108:LEU:HD21	1:I:548:VAL:HG13	1.95	0.48
1:I:719:VAL:CG1	1:I:752:GLU:HB2	2.43	0.48
1:K:333:TYR:CD2	1:K:340:TRP:CD1	3.01	0.48
1:K:414:ALA:O	1:K:418:GLU:HG2	2.12	0.48
2:L:118:ASP:OD1	2:N:67:SER:HA	2.13	0.48
1:M:401:LEU:HB3	1:M:402:PRO:CD	2.44	0.48
1:M:463:ASN:HD22	1:M:781:ASP:HB2	1.78	0.48
1:M:503:VAL:O	1:M:503:VAL:CG1	2.60	0.48
1:M:739:ARG:HA	1:M:747:ILE:O	2.13	0.48
1:C:436:VAL:CG1	1:C:440:ARG:CZ	2.91	0.48
1:C:724:PRO:O	1:C:728:ARG:HG3	2.13	0.48
1:E:659:ARG:O	1:E:661:TYR:N	2.46	0.48
2:F:66:TYR:OH	2:F:77:ILE:HD11	2.13	0.48
1:G:396:THR:O	1:G:396:THR:CG2	2.60	0.48
2:H:98:CYS:C	2:H:100:ALA:N	2.64	0.48
1:I:189:MET:HE1	1:I:200:LEU:HD23	1.95	0.48
1:M:356:TRP:CZ3	1:M:674:PRO:O	2.66	0.48
2:N:89:ALA:O	2:N:90:ASP:HB2	2.13	0.48
1:O:278:PRO:O	1:O:279:GLU:CG	2.61	0.48
1:O:537:MET:CE	1:O:595:PHE:CE2	2.96	0.48
1:O:766:VAL:CG2	1:O:775:ILE:HD13	2.33	0.48
1:A:68:ASP:CB	1:A:707:ARG:NH1	2.74	0.48
1:C:409:ASN:HB3	1:C:412:HIS:CD2	2.48	0.48
1:E:335:ASP:C	1:E:337:ASP:H	2.16	0.48
1:G:193:HIS:N	1:G:194:PRO:HD3	2.29	0.48
1:K:426:LEU:HD13	1:K:553:ILE:HG21	1.94	0.48
1:M:321:VAL:CG2	1:M:326:LEU:HD11	2.41	0.48
1:M:563:LYS:O	1:M:567:GLU:HG3	2.13	0.48
2:N:35:TYR:O	2:N:36:PRO:O	2.30	0.48
1:O:134:LYS:NZ	1:O:569:LEU:O	2.46	0.48
1:O:300:PHE:C	1:O:300:PHE:CD1	2.87	0.48
1:A:172:CYS:SG	1:A:174:ASP:HB2	2.53	0.48
1:A:448:ASN:ND2	1:A:477:ASN:ND2	2.49	0.48
1:A:617:ASP:HB2	1:A:633:PRO:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:NH2	1:C:473:ARG:NH1	2.60	0.48
2:H:66:TYR:O	2:H:67:SER:C	2.52	0.48
1:I:223:SER:HA	1:I:226:SER:OG	2.12	0.48
1:I:409:ASN:HB3	1:I:412:HIS:CD2	2.48	0.48
1:K:280:HIS:CE1	1:K:282:LEU:HD12	2.49	0.48
1:O:503:VAL:CG1	1:O:503:VAL:O	2.60	0.48
1:O:659:ARG:O	1:O:661:TYR:N	2.46	0.48
2:P:104:PRO:O	2:P:105:GLN:HG2	2.12	0.48
1:A:139:GLY:HA2	1:A:565:LEU:HD22	1.95	0.48
1:A:335:ASP:O	1:A:337:ASP:N	2.43	0.48
1:A:439:ASP:OD1	1:A:468:THR:HG23	2.14	0.48
1:C:300:PHE:CD1	1:C:300:PHE:C	2.87	0.48
1:E:119:PHE:HA	1:E:146:ASP:O	2.14	0.48
1:E:739:ARG:HA	1:E:747:ILE:O	2.13	0.48
2:F:30:ARG:CD	6:F:1128:HEC:O1D	2.57	0.48
1:G:739:ARG:HA	1:G:747:ILE:O	2.13	0.48
1:I:67:GLU:HG2	2:J:112:VAL:HG13	1.95	0.48
1:I:76:ARG:NH2	1:I:473:ARG:NH1	2.61	0.48
1:K:233:ARG:HB3	1:K:236:THR:HG21	1.93	0.48
1:K:401:LEU:HB3	1:K:402:PRO:CD	2.44	0.48
1:M:367:LEU:HD13	1:M:670:ILE:HD13	1.94	0.48
1:M:46:ALA:O	1:M:50:ARG:HG2	2.13	0.48
1:M:270:THR:CG2	1:M:674:PRO:HG3	2.43	0.48
1:O:300:PHE:O	1:O:300:PHE:CD1	2.67	0.48
1:O:730:ARG:CB	1:O:732:LEU:HD22	2.43	0.48
2:B:3:ALA:HB2	2:B:19:PRO:CG	2.44	0.48
1:C:120:GLY:HA3	1:C:124:TRP:CZ3	2.49	0.48
1:C:84:LYS:HE2	1:C:473:ARG:C	2.34	0.48
2:F:40:PRO:HD2	2:F:102:HIS:CE1	2.48	0.48
1:G:700:HIS:CE1	5:G:1804:MGD:S13	3.06	0.48
2:H:40:PRO:HD3	6:H:1129:HEC:HBD2	1.94	0.48
1:I:49:ASN:HB2	1:I:52:LEU:O	2.14	0.48
1:I:270:THR:CG2	1:I:674:PRO:HG3	2.43	0.48
1:I:71:THR:O	1:I:528:GLU:HB2	2.14	0.48
1:I:739:ARG:HA	1:I:747:ILE:O	2.13	0.48
1:K:138:ALA:HB1	1:K:422:LEU:HD11	1.94	0.48
1:K:426:LEU:HD21	1:K:549:TRP:CE2	2.48	0.48
1:K:563:LYS:O	1:K:567:GLU:HG3	2.13	0.48
1:K:598:TYR:CE1	1:K:600:GLN:CG	2.97	0.48
1:M:358:ASN:O	1:M:361:VAL:HG23	2.14	0.48
1:M:598:TYR:CE1	1:M:600:GLN:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:793:LYS:CE	5:O:1804:MGD:H5'2	2.43	0.48
1:O:632:TRP:CE3	1:O:632:TRP:C	2.87	0.48
1:A:125:THR:HG22	1:A:126:ILE:N	2.27	0.48
1:A:714:ALA:CB	2:B:103:VAL:HG11	2.43	0.48
1:C:222:SER:C	1:C:224:ASP:H	2.15	0.48
1:C:454:VAL:HG22	5:C:1803:MGD:C2	2.43	0.48
1:G:750:ARG:NH1	2:H:18:ALA:O	2.46	0.48
2:H:3:ALA:HB2	2:H:19:PRO:CG	2.43	0.48
2:H:77:ILE:HG23	2:H:87:MET:CE	2.44	0.48
1:I:278:PRO:O	1:I:279:GLU:CG	2.61	0.48
1:I:84:LYS:HE2	1:I:473:ARG:C	2.33	0.48
1:K:118:MET:HE2	1:K:145:LEU:HD13	1.96	0.48
1:K:125:THR:HG22	1:K:126:ILE:N	2.27	0.48
1:K:558:PRO:O	1:K:560:TYR:N	2.47	0.48
1:K:702:GLY:HA3	1:K:706:LEU:HD12	1.94	0.48
1:M:738:VAL:HG21	1:M:751:LEU:HD13	1.94	0.48
1:O:144:ASN:HD22	1:O:433:ALA:H	1.57	0.48
1:O:565:LEU:O	1:O:566:PHE:CB	2.62	0.48
1:O:738:VAL:O	1:O:748:ARG:HA	2.14	0.48
1:A:545:THR:HG22	1:A:549:TRP:CE3	2.49	0.48
1:A:739:ARG:HA	1:A:747:ILE:O	2.14	0.48
1:E:211:ARG:HB2	1:E:338:ARG:HH12	1.79	0.48
1:E:558:PRO:O	1:E:560:TYR:N	2.47	0.48
1:E:605:GLU:OE1	1:E:612:ARG:NH2	2.43	0.48
1:G:233:ARG:HB3	1:G:236:THR:HG21	1.95	0.48
1:G:278:PRO:O	1:G:279:GLU:CG	2.62	0.48
1:G:558:PRO:O	1:G:560:TYR:N	2.47	0.48
1:I:222:SER:C	1:I:224:ASP:H	2.17	0.48
1:I:332:LEU:HB3	1:I:340:TRP:CZ3	2.49	0.48
1:I:557:ALA:HA	1:I:558:PRO:HD2	1.63	0.48
1:M:300:PHE:CD1	1:M:300:PHE:O	2.66	0.48
1:M:68:ASP:HB2	1:M:707:ARG:HH12	1.74	0.48
1:M:722:MET:HG2	1:M:723:HIS:H	1.79	0.48
1:M:772:SER:HB3	2:N:6:LEU:HD22	1.96	0.48
1:O:120:GLY:HA3	1:O:124:TRP:CZ3	2.48	0.48
1:O:533:LEU:O	1:O:537:MET:HG3	2.13	0.48
1:O:675:TYR:CE1	1:O:676:GLU:O	2.67	0.48
1:A:300:PHE:C	1:A:300:PHE:CD1	2.86	0.48
1:A:300:PHE:O	1:A:300:PHE:CD1	2.66	0.48
1:A:238:ARG:HG2	1:A:360:MET:HE1	1.95	0.48
2:B:49:TYR:CD2	2:B:57:ARG:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:VAL:HG12	1:C:449:PHE:HB3	1.95	0.48
1:C:710:GLU:HA	2:D:105:GLN:OE1	2.14	0.48
2:D:92:SER:O	2:D:94:ARG:O	2.31	0.48
1:G:455:ASN:HD22	1:G:457:ASN:H	1.62	0.48
1:G:730:ARG:CB	1:G:732:LEU:HD22	2.44	0.48
2:H:86:GLN:HA	2:H:86:GLN:HE21	1.78	0.48
1:I:436:VAL:HG11	1:I:440:ARG:NH2	2.28	0.48
2:J:78:THR:O	2:J:81:GLN:HG3	2.12	0.48
1:K:455:ASN:HD22	1:K:457:ASN:N	2.12	0.48
1:M:750:ARG:NH1	2:N:18:ALA:O	2.47	0.48
2:N:40:PRO:HD2	2:N:102:HIS:CE1	2.41	0.48
1:O:116:VAL:HG12	1:O:449:PHE:HB3	1.96	0.48
1:O:384:GLN:CB	1:O:385:PRO:HD2	2.42	0.48
1:O:455:ASN:HD22	1:O:457:ASN:H	1.60	0.48
1:O:455:ASN:ND2	1:O:457:ASN:H	2.12	0.48
2:P:41:VAL:HG11	2:P:105:GLN:HG3	1.95	0.48
1:C:291:ASP:O	1:C:292:ALA:HB3	2.13	0.48
1:E:633:PRO:HD2	1:E:640:THR:CB	2.39	0.48
1:G:143:ASN:O	1:G:432:GLY:HA3	2.14	0.48
1:G:615:GLY:O	1:G:617:ASP:N	2.47	0.48
2:H:40:PRO:HD2	2:H:102:HIS:CE1	2.40	0.48
1:I:189:MET:CE	1:I:200:LEU:HD23	2.44	0.48
1:I:300:PHE:CD1	1:I:300:PHE:O	2.67	0.48
1:K:503:VAL:HG12	1:K:523:VAL:HG22	1.96	0.48
1:K:738:VAL:O	1:K:748:ARG:HA	2.14	0.48
2:L:27:ASP:O	2:L:27:ASP:CG	2.52	0.48
1:M:694:ARG:HH22	5:M:1803:MGD:H15	1.62	0.48
1:O:183:VAL:HG12	1:O:185:TRP:CD1	2.49	0.48
1:O:259:VAL:O	1:O:263:THR:HB	2.13	0.48
1:O:463:ASN:HD22	1:O:781:ASP:HB2	1.79	0.48
1:O:714:ALA:HB2	2:P:103:VAL:CG1	2.43	0.48
1:O:724:PRO:O	1:O:728:ARG:HG3	2.13	0.48
2:P:62:HIS:HA	2:P:74:MET:CB	2.44	0.48
2:B:5:ARG:O	2:B:7:THR:N	2.47	0.47
1:E:189:MET:HE1	1:E:343:LEU:HD13	1.96	0.47
1:E:747:ILE:CG2	1:E:748:ARG:N	2.73	0.47
1:E:84:LYS:HE2	1:E:473:ARG:C	2.34	0.47
2:F:61:CYS:SG	6:F:1128:HEC:C3C	3.01	0.47
1:G:441:LYS:HB3	1:G:447:ILE:HG13	1.95	0.47
1:G:469:TYR:N	1:G:470:PRO:HD2	2.28	0.47
1:G:571:ALA:HA	1:G:576:ASP:CG	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:335:ASP:O	1:I:337:ASP:N	2.46	0.47
1:I:409:ASN:HA	1:I:410:PRO:HD3	1.75	0.47
1:I:60:LEU:HD23	1:I:63:ILE:HD12	1.96	0.47
1:K:163:THR:CG2	1:K:359:HIS:CE1	2.90	0.47
1:O:333:TYR:CD2	1:O:340:TRP:CD1	3.02	0.47
2:J:67:SER:HA	2:P:118:ASP:OD1	2.13	0.47
1:A:49:ASN:HB2	1:A:52:LEU:O	2.14	0.47
2:D:120:LEU:O	2:D:121:THR:OG1	2.31	0.47
1:E:793:LYS:CE	5:E:1804:MGD:H5'2	2.43	0.47
1:E:463:ASN:HD22	1:E:781:ASP:HB2	1.78	0.47
1:E:730:ARG:HB2	1:E:732:LEU:HD22	1.96	0.47
1:E:791:ASP:OD2	1:E:794:LYS:HE2	2.14	0.47
2:F:38:GLN:O	6:F:1129:HEC:HBD1	2.14	0.47
1:I:479:ILE:HG22	1:I:493:ALA:HB1	1.96	0.47
1:K:162:ARG:NH1	1:K:359:HIS:NE2	2.62	0.47
1:K:728:ARG:HD3	2:P:5:ARG:HE	1.78	0.47
1:K:742:SER:HB2	1:K:778:VAL:HG13	1.96	0.47
1:M:133:SER:OG	1:M:137:ARG:NH1	2.46	0.47
1:M:138:ALA:HB1	1:M:422:LEU:HD11	1.96	0.47
1:M:714:ALA:CB	2:N:103:VAL:CG1	2.92	0.47
1:M:722:MET:HG2	1:M:723:HIS:N	2.28	0.47
2:N:98:CYS:CB	6:N:1129:HEC:CAB	2.80	0.47
1:O:190:ALA:HA	1:O:197:TRP:CD1	2.48	0.47
1:A:436:VAL:CG1	1:A:440:ARG:CZ	2.92	0.47
1:A:730:ARG:HB2	1:A:732:LEU:HD22	1.96	0.47
1:A:749:THR:CG2	1:A:773:GLN:OE1	2.51	0.47
1:C:356:TRP:CZ3	1:C:674:PRO:O	2.67	0.47
1:E:219:THR:OG1	1:E:231:ILE:HD11	2.14	0.47
1:E:455:ASN:HD21	1:E:457:ASN:HB2	1.80	0.47
1:E:617:ASP:OD2	1:E:651:TYR:OH	2.31	0.47
2:F:40:PRO:HD3	6:F:1129:HEC:HBD2	1.96	0.47
1:G:161:MET:O	1:G:165:GLY:N	2.45	0.47
1:G:772:SER:HB2	2:H:4:PRO:CG	2.36	0.47
1:K:300:PHE:O	1:K:300:PHE:CD1	2.66	0.47
1:K:76:ARG:NH2	1:K:473:ARG:NH1	2.62	0.47
1:M:216:SER:OG	5:M:1804:MGD:O2'	2.33	0.47
1:M:222:SER:C	1:M:224:ASP:H	2.17	0.47
1:E:571:ALA:HA	1:E:576:ASP:CG	2.35	0.47
1:G:222:SER:C	1:G:224:ASP:H	2.17	0.47
1:G:147:PRO:HD3	1:G:397:PHE:HA	1.96	0.47
1:I:144:ASN:ND2	1:I:433:ALA:N	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:259:VAL:O	1:I:263:THR:HB	2.14	0.47
1:I:175:ASP:HB2	1:I:341:MET:HE2	1.97	0.47
1:I:692:THR:CG2	5:I:1803:MGD:N18	2.69	0.47
2:J:66:TYR:OH	2:J:77:ILE:HD11	2.15	0.47
1:K:333:TYR:CZ	1:K:340:TRP:CD1	3.02	0.47
1:M:692:THR:CG2	5:M:1803:MGD:N18	2.72	0.47
1:O:551:GLU:HG2	1:O:551:GLU:H	1.32	0.47
1:O:563:LYS:O	1:O:567:GLU:HG3	2.14	0.47
1:A:143:ASN:O	1:A:432:GLY:HA3	2.15	0.47
1:A:181:ALA:HB1	1:A:340:TRP:CH2	2.49	0.47
1:A:116:VAL:HG12	1:A:449:PHE:HB3	1.95	0.47
1:A:584:ASN:O	1:A:586:ASP:O	2.32	0.47
1:A:689:TRP:CZ3	1:A:794:LYS:HB2	2.49	0.47
2:B:50:GLN:H	2:H:123:MET:HE3	1.80	0.47
1:C:482:SER:HA	1:C:497:LEU:O	2.14	0.47
1:C:52:LEU:HG	6:D:1129:HEC:HBC1	1.96	0.47
1:E:238:ARG:HG2	1:E:360:MET:HE1	1.96	0.47
1:E:612:ARG:HA	1:E:617:ASP:OD1	2.15	0.47
1:G:414:ALA:O	1:G:418:GLU:HG2	2.15	0.47
1:I:189:MET:CE	1:I:343:LEU:HD13	2.45	0.47
1:I:558:PRO:O	1:I:560:TYR:N	2.47	0.47
1:K:211:ARG:HB2	1:K:338:ARG:HH12	1.79	0.47
1:K:356:TRP:HB3	1:K:673:VAL:HG11	1.95	0.47
2:L:38:GLN:O	6:L:1129:HEC:HBD1	2.14	0.47
1:M:455:ASN:HD22	1:M:457:ASN:N	2.13	0.47
1:M:571:ALA:HA	1:M:576:ASP:CG	2.35	0.47
1:O:335:ASP:C	1:O:337:ASP:H	2.17	0.47
1:O:590:HIS:O	1:O:594:LEU:HG	2.14	0.47
1:O:627:VAL:HG12	1:O:628:ARG:N	2.30	0.47
1:A:750:ARG:HD3	2:B:20:PRO:HA	1.95	0.47
1:C:472:TYR:HA	1:C:479:ILE:CD1	2.45	0.47
1:C:479:ILE:HG22	1:C:493:ALA:HB1	1.97	0.47
1:C:598:TYR:HE1	1:C:600:GLN:HG3	1.80	0.47
2:D:3:ALA:CB	2:D:4:PRO:CD	2.70	0.47
1:E:118:MET:CE	1:E:132:ALA:HB1	2.45	0.47
1:E:259:VAL:O	1:E:263:THR:HB	2.14	0.47
1:E:469:TYR:N	1:E:470:PRO:HD2	2.29	0.47
1:E:503:VAL:CG1	1:E:503:VAL:O	2.61	0.47
1:E:738:VAL:HG21	1:E:751:LEU:HD13	1.95	0.47
1:I:119:PHE:HA	1:I:146:ASP:O	2.15	0.47
1:K:557:ALA:HA	1:K:558:PRO:HD2	1.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:300:PHE:CD1	1:M:300:PHE:C	2.87	0.47
1:M:749:THR:CG2	1:M:773:GLN:OE1	2.48	0.47
1:O:321:VAL:CG2	1:O:326:LEU:HD11	2.43	0.47
1:O:503:VAL:HG12	1:O:523:VAL:HG22	1.96	0.47
1:O:697:GLU:CD	1:O:756:ARG:HH22	2.18	0.47
2:P:33:ARG:HH21	2:P:40:PRO:CG	2.25	0.47
1:A:590:HIS:O	1:A:594:LEU:HG	2.14	0.47
1:C:340:TRP:CE3	1:C:340:TRP:HA	2.50	0.47
1:C:739:ARG:HA	1:C:747:ILE:O	2.14	0.47
1:E:426:LEU:HD21	1:E:549:TRP:CZ2	2.50	0.47
1:E:632:TRP:CE3	1:E:632:TRP:O	2.67	0.47
1:G:659:ARG:O	1:G:661:TYR:N	2.47	0.47
1:I:138:ALA:HB1	1:I:422:LEU:HD11	1.97	0.47
1:I:469:TYR:N	1:I:470:PRO:HD2	2.29	0.47
1:M:543:PHE:HB2	1:M:565:LEU:HD12	1.96	0.47
1:M:581:SER:OG	1:M:582:ASP:N	2.46	0.47
1:O:113:PRO:C	1:O:115:ALA:H	2.18	0.47
1:A:340:TRP:CE3	1:A:340:TRP:HA	2.50	0.47
1:C:334:ALA:O	1:C:335:ASP:C	2.52	0.47
1:C:426:LEU:HD21	1:C:549:TRP:CE2	2.50	0.47
1:C:427:LEU:HA	1:C:428:PRO:HD3	1.71	0.47
1:E:183:VAL:CG2	1:E:340:TRP:CZ2	2.94	0.47
1:E:143:ASN:O	1:E:432:GLY:HA3	2.15	0.47
1:I:543:PHE:HB2	1:I:565:LEU:HD12	1.95	0.47
1:I:741:ILE:O	1:I:797:VAL:HG13	2.14	0.47
1:I:41:HIS:CD2	2:J:37:GLU:HB2	2.50	0.47
1:K:598:TYR:HE1	1:K:600:GLN:HG3	1.79	0.47
1:K:747:ILE:HG22	1:K:748:ARG:H	1.77	0.47
1:K:783:ASN:ND2	1:K:783:ASN:N	2.62	0.47
2:L:62:HIS:HA	2:L:74:MET:HB3	1.96	0.47
1:M:543:PHE:N	1:M:543:PHE:CD1	2.82	0.47
1:O:21:PHE:O	1:O:385:PRO:HD3	2.14	0.47
1:A:426:LEU:HD21	1:A:549:TRP:CZ2	2.50	0.47
1:A:565:LEU:O	1:A:566:PHE:CB	2.63	0.47
1:A:356:TRP:HB3	1:A:673:VAL:HG11	1.96	0.47
1:E:233:ARG:HB3	1:E:236:THR:CG2	2.45	0.47
1:E:238:ARG:HG2	1:E:360:MET:HE3	1.97	0.47
1:G:537:MET:HE2	1:G:595:PHE:CE2	2.49	0.47
1:I:138:ALA:CB	1:I:422:LEU:HD11	2.45	0.47
1:I:659:ARG:O	1:I:661:TYR:N	2.48	0.47
1:K:299:ASP:OD1	1:K:301:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:586:ASP:O	1:K:587:HIS:HB2	2.14	0.47
1:K:394:VAL:HG22	1:K:607:TYR:CE1	2.50	0.47
1:M:116:VAL:HG12	1:M:449:PHE:HB3	1.96	0.47
1:M:119:PHE:HA	1:M:146:ASP:O	2.15	0.47
1:M:741:ILE:O	1:M:797:VAL:HG13	2.14	0.47
1:O:332:LEU:CD2	1:O:340:TRP:HH2	2.27	0.47
1:O:469:TYR:N	1:O:470:PRO:HD2	2.29	0.47
1:O:68:ASP:OD2	1:O:707:ARG:NH1	2.48	0.47
1:A:581:SER:OG	1:A:582:ASP:N	2.48	0.47
1:C:144:ASN:ND2	1:C:433:ALA:N	2.55	0.47
1:C:659:ARG:O	1:C:661:TYR:N	2.48	0.47
1:E:108:LEU:HD21	1:E:548:VAL:HG13	1.96	0.47
1:E:209:HIS:C	1:E:209:HIS:CD2	2.87	0.47
1:E:299:ASP:OD1	1:E:301:GLU:HG2	2.14	0.47
1:G:130:TYR:HD1	1:G:603:LEU:HD23	1.79	0.47
1:G:321:VAL:CG2	1:G:326:LEU:HD11	2.44	0.47
1:I:683:ASP:OD2	1:I:743:ARG:NH1	2.47	0.47
1:K:147:PRO:HD3	1:K:397:PHE:HA	1.95	0.47
1:K:436:VAL:CG1	1:K:440:ARG:CZ	2.93	0.47
1:K:469:TYR:N	1:K:470:PRO:HD2	2.29	0.47
2:L:120:LEU:O	2:L:121:THR:OG1	2.28	0.47
1:M:479:ILE:HG22	1:M:493:ALA:HB1	1.97	0.47
1:M:505:LYS:O	1:M:505:LYS:HG2	2.12	0.47
2:N:33:ARG:NH2	6:N:1129:HEC:HAA1	2.30	0.47
2:N:82:ASP:HB3	2:N:88:LEU:HD11	1.97	0.47
1:O:125:THR:HG22	1:O:126:ILE:N	2.29	0.47
1:O:332:LEU:HB3	1:O:340:TRP:CZ3	2.50	0.47
1:O:617:ASP:OD2	1:O:651:TYR:OH	2.33	0.47
2:P:102:HIS:CD2	6:P:1129:HEC:NB	2.82	0.47
1:C:181:ALA:HB1	1:C:211:ARG:O	2.15	0.47
1:C:334:ALA:O	1:C:336:PRO:N	2.48	0.47
1:C:401:LEU:HB3	1:C:402:PRO:CD	2.45	0.47
1:E:263:THR:CG2	1:E:264:ASN:N	2.78	0.47
1:E:537:MET:HE2	1:E:595:PHE:HE2	1.78	0.47
1:G:259:VAL:O	1:G:263:THR:HB	2.15	0.47
1:G:401:LEU:HB3	1:G:402:PRO:HD2	1.97	0.47
2:H:35:TYR:O	2:H:36:PRO:O	2.32	0.47
1:I:455:ASN:HD22	1:I:457:ASN:N	2.13	0.47
1:I:722:MET:CE	1:I:751:LEU:HD11	2.45	0.47
1:K:513:GLU:OE2	1:K:515:ARG:NH1	2.48	0.47
1:K:730:ARG:HB2	1:K:732:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:409:ASN:HB3	1:M:412:HIS:CD2	2.50	0.47
2:N:104:PRO:O	2:N:105:GLN:HG2	2.14	0.47
2:P:98:CYS:C	2:P:100:ALA:H	2.19	0.47
1:A:455:ASN:HD21	1:A:457:ASN:HB2	1.81	0.46
1:A:633:PRO:HD2	1:A:640:THR:CB	2.37	0.46
1:C:563:LYS:O	1:C:567:GLU:HG3	2.15	0.46
2:D:26:THR:O	2:D:26:THR:HG22	2.14	0.46
2:D:66:TYR:O	2:D:67:SER:C	2.54	0.46
1:E:138:ALA:HB1	1:E:422:LEU:HD11	1.97	0.46
1:E:406:VAL:H	1:E:412:HIS:HD2	1.63	0.46
1:E:738:VAL:O	1:E:748:ARG:HA	2.15	0.46
2:F:41:VAL:HG11	2:F:105:GLN:HG3	1.97	0.46
1:G:202:ASP:HA	2:H:93:PRO:HB2	1.97	0.46
1:I:271:ASP:HB3	1:I:287:LYS:O	2.15	0.46
1:K:121:SER:HB2	1:K:148:ASN:ND2	2.29	0.46
1:K:356:TRP:HZ3	1:K:674:PRO:O	1.98	0.46
1:K:40:THR:HG21	1:K:60:LEU:HB2	1.97	0.46
1:K:742:SER:OG	1:K:797:VAL:HG22	2.15	0.46
1:M:263:THR:CG2	1:M:264:ASN:N	2.79	0.46
1:M:335:ASP:O	1:M:337:ASP:N	2.45	0.46
1:O:263:THR:CG2	1:O:264:ASN:N	2.76	0.46
2:B:37:GLU:N	6:B:1129:HEC:O1D	2.48	0.46
1:G:211:ARG:HB2	1:G:338:ARG:HH12	1.80	0.46
1:G:537:MET:CE	1:G:595:PHE:CE2	2.99	0.46
1:G:605:GLU:OE1	1:G:612:ARG:NH2	2.47	0.46
1:I:428:PRO:HB3	1:I:430:TRP:NE1	2.30	0.46
1:K:511:ASN:CG	1:K:515:ARG:HB3	2.36	0.46
1:M:118:MET:HG2	1:M:451:TRP:HB3	1.97	0.46
1:M:21:PHE:O	1:M:385:PRO:HD3	2.15	0.46
1:M:401:LEU:HB3	1:M:402:PRO:HD2	1.97	0.46
1:M:617:ASP:HB2	1:M:633:PRO:HA	1.97	0.46
1:O:557:ALA:HA	1:O:558:PRO:HD2	1.66	0.46
1:O:192:MET:CE	1:O:694:ARG:HD2	2.45	0.46
1:O:192:MET:HE3	1:O:694:ARG:HD2	1.98	0.46
1:C:41:HIS:CD2	2:D:37:GLU:HB2	2.51	0.46
1:E:20:ARG:HB2	1:E:502:TRP:CD1	2.51	0.46
1:G:84:LYS:HE2	1:G:473:ARG:C	2.36	0.46
1:I:118:MET:HE3	1:I:124:TRP:HH2	1.80	0.46
1:I:730:ARG:CB	1:I:732:LEU:HD22	2.45	0.46
1:I:742:SER:HB2	1:I:778:VAL:HG13	1.96	0.46
2:J:51:LEU:HD22	2:J:56:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:409:ASN:HB3	1:K:412:HIS:CD2	2.50	0.46
1:K:143:ASN:O	1:K:432:GLY:HA3	2.15	0.46
1:K:598:TYR:CE1	1:K:600:GLN:HG2	2.50	0.46
1:K:730:ARG:CB	1:K:732:LEU:HD22	2.45	0.46
2:N:36:PRO:O	2:N:38:GLN:N	2.48	0.46
1:O:76:ARG:NH2	1:O:473:ARG:NH1	2.64	0.46
1:O:71:THR:O	1:O:528:GLU:HB2	2.16	0.46
1:A:263:THR:CG2	1:A:264:ASN:N	2.78	0.46
1:A:558:PRO:O	1:A:560:TYR:N	2.48	0.46
1:A:783:ASN:N	1:A:783:ASN:ND2	2.63	0.46
1:C:119:PHE:HA	1:C:146:ASP:O	2.15	0.46
1:C:183:VAL:HG12	1:C:185:TRP:CD1	2.50	0.46
1:C:426:LEU:HD13	1:C:553:ILE:HG21	1.97	0.46
1:G:426:LEU:HD13	1:G:553:ILE:HG21	1.98	0.46
1:I:52:LEU:HG	6:J:1129:HEC:HBC2	1.98	0.46
1:K:33:ARG:NH1	2:L:119:MET:O	2.44	0.46
1:M:223:SER:HA	1:M:226:SER:OG	2.15	0.46
1:M:142:SER:HA	1:M:430:TRP:CZ2	2.51	0.46
1:M:441:LYS:HB3	1:M:447:ILE:HG13	1.97	0.46
1:M:454:VAL:HG22	5:M:1803:MGD:C2	2.45	0.46
1:M:76:ARG:NH2	1:M:473:ARG:HH22	2.12	0.46
1:O:139:GLY:HA2	1:O:565:LEU:HD22	1.95	0.46
2:P:40:PRO:HD2	2:P:102:HIS:CE1	2.43	0.46
1:A:238:ARG:HG2	1:A:360:MET:HE3	1.97	0.46
1:A:615:GLY:O	1:A:617:ASP:N	2.49	0.46
2:B:38:GLN:O	6:B:1129:HEC:HBD1	2.15	0.46
1:C:121:SER:HA	1:C:148:ASN:OD1	2.16	0.46
1:C:303:PHE:O	1:C:307:VAL:HG23	2.14	0.46
1:C:738:VAL:O	1:C:748:ARG:HA	2.16	0.46
2:D:37:GLU:HA	6:D:1129:HEC:HMD1	1.97	0.46
1:E:300:PHE:CD1	1:E:300:PHE:O	2.68	0.46
1:E:479:ILE:HG22	1:E:493:ALA:HB1	1.98	0.46
1:E:692:THR:CG2	5:E:1803:MGD:N18	2.73	0.46
2:F:30:ARG:HD2	6:F:1128:HEC:CGD	2.44	0.46
1:G:356:TRP:HZ3	1:G:674:PRO:O	1.98	0.46
1:G:142:SER:HA	1:G:430:TRP:CZ2	2.51	0.46
1:G:557:ALA:HA	1:G:558:PRO:HD2	1.63	0.46
1:I:554:LEU:HD13	1:I:561:ARG:HG2	1.96	0.46
1:K:396:THR:CG2	1:K:396:THR:O	2.62	0.46
1:K:543:PHE:HB2	1:K:565:LEU:HD12	1.98	0.46
2:L:66:TYR:O	2:L:68:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:340:TRP:CE3	1:M:340:TRP:HA	2.49	0.46
1:O:332:LEU:HD23	1:O:340:TRP:HH2	1.76	0.46
1:O:394:VAL:HG22	1:O:607:TYR:CE1	2.51	0.46
1:O:615:GLY:O	1:O:617:ASP:N	2.48	0.46
1:C:193:HIS:N	1:C:194:PRO:HD3	2.31	0.46
1:E:142:SER:HA	1:E:430:TRP:CZ2	2.51	0.46
1:E:692:THR:HB	1:E:792:PHE:O	2.16	0.46
1:I:335:ASP:C	1:I:337:ASP:H	2.19	0.46
1:K:119:PHE:HA	1:K:146:ASP:O	2.15	0.46
1:M:80:GLY:O	1:M:81:VAL:CB	2.62	0.46
1:O:333:TYR:CZ	1:O:340:TRP:CD1	3.04	0.46
1:A:119:PHE:HA	1:A:146:ASP:O	2.16	0.46
1:A:333:TYR:CZ	1:A:340:TRP:CD1	3.04	0.46
1:C:339:LYS:CA	1:C:376:ASN:ND2	2.74	0.46
1:E:730:ARG:CB	1:E:732:LEU:HD22	2.46	0.46
1:G:335:ASP:C	1:G:337:ASP:H	2.19	0.46
1:G:436:VAL:CG1	1:G:440:ARG:CZ	2.94	0.46
1:G:472:TYR:HA	1:G:479:ILE:CD1	2.46	0.46
1:G:586:ASP:O	1:G:587:HIS:HB2	2.15	0.46
1:G:749:THR:CG2	1:G:773:GLN:OE1	2.52	0.46
1:I:184:LEU:HD11	1:I:189:MET:HE2	1.97	0.46
1:I:384:GLN:CB	1:I:385:PRO:HD2	2.46	0.46
1:I:501:MET:HG2	1:I:502:TRP:N	2.31	0.46
1:I:700:HIS:HB3	1:I:768:TRP:CH2	2.51	0.46
1:K:300:PHE:C	1:K:300:PHE:CD1	2.86	0.46
1:K:41:HIS:CD2	2:L:37:GLU:HB2	2.51	0.46
2:L:98:CYS:C	2:L:100:ALA:H	2.19	0.46
1:M:598:TYR:CE1	1:M:600:GLN:CG	2.99	0.46
1:M:356:TRP:HB3	1:M:673:VAL:HG11	1.98	0.46
1:O:514:ARG:NH2	1:O:641:ARG:O	2.42	0.46
2:P:89:ALA:O	2:P:90:ASP:HB2	2.15	0.46
1:A:700:HIS:CE1	5:A:1804:MGD:S13	3.09	0.46
2:D:38:GLN:O	6:D:1129:HEC:HBD1	2.15	0.46
1:E:144:ASN:HA	1:E:144:ASN:HD22	1.56	0.46
1:E:557:ALA:HA	1:E:558:PRO:HD2	1.68	0.46
1:E:491:ARG:NH2	2:F:11:ARG:N	2.61	0.46
1:G:332:LEU:HD23	1:G:340:TRP:HH2	1.77	0.46
2:H:120:LEU:O	2:H:121:THR:OG1	2.32	0.46
1:I:263:THR:CG2	1:I:264:ASN:N	2.79	0.46
1:I:579:PRO:O	1:I:581:SER:O	2.32	0.46
1:I:632:TRP:CE3	1:I:632:TRP:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:222:SER:C	1:K:224:ASP:H	2.19	0.46
1:M:121:SER:O	1:M:124:TRP:HB2	2.16	0.46
1:M:563:LYS:O	1:M:567:GLU:CD	2.54	0.46
1:O:40:THR:HG21	1:O:60:LEU:HB2	1.98	0.46
1:A:538:GLU:OE2	1:A:541:LYS:HD2	2.16	0.46
1:A:724:PRO:O	1:A:728:ARG:HG3	2.16	0.46
1:A:84:LYS:HE2	1:A:473:ARG:C	2.37	0.46
1:C:564:THR:OG1	1:C:567:GLU:HG3	2.15	0.46
1:C:270:THR:CG2	1:C:674:PRO:HG3	2.45	0.46
1:E:422:LEU:HD13	1:E:426:LEU:HD23	1.98	0.46
1:E:455:ASN:ND2	1:E:457:ASN:H	2.14	0.46
1:G:183:VAL:HG12	1:G:185:TRP:CD1	2.50	0.46
1:G:543:PHE:CD1	1:G:543:PHE:N	2.84	0.46
1:G:791:ASP:OD2	1:G:794:LYS:HE2	2.16	0.46
1:K:54:CYS:O	1:K:55:VAL:C	2.53	0.46
1:M:335:ASP:C	1:M:337:ASP:H	2.18	0.46
1:M:147:PRO:HD3	1:M:397:PHE:HA	1.96	0.46
1:M:426:LEU:HD13	1:M:553:ILE:HG21	1.96	0.46
1:O:189:MET:CE	1:O:343:LEU:HD13	2.46	0.46
1:A:118:MET:HE2	1:A:145:LEU:HD13	1.98	0.46
1:A:617:ASP:OD2	1:A:651:TYR:OH	2.32	0.46
1:A:80:GLY:O	1:A:81:VAL:CB	2.63	0.46
1:A:33:ARG:NH1	2:B:119:MET:O	2.42	0.46
1:E:125:THR:CG2	1:E:126:ILE:N	2.78	0.46
1:G:700:HIS:HE1	5:G:1804:MGD:S13	2.39	0.46
1:G:33:ARG:NH1	2:H:119:MET:O	2.43	0.46
2:H:82:ASP:O	2:H:83:ARG:C	2.54	0.46
1:I:533:LEU:O	1:I:537:MET:HG3	2.15	0.46
2:J:66:TYR:O	2:J:67:SER:C	2.53	0.46
1:M:76:ARG:NH2	1:M:473:ARG:NH1	2.63	0.46
1:M:791:ASP:OD2	1:M:794:LYS:HE2	2.16	0.46
1:O:183:VAL:CG1	1:O:185:TRP:NE1	2.80	0.46
1:O:246:HIS:HB2	1:O:307:VAL:HG12	1.97	0.46
1:O:76:ARG:HH22	1:O:473:ARG:CZ	2.29	0.46
1:A:20:ARG:O	1:A:20:ARG:CG	2.64	0.45
1:A:511:ASN:CG	1:A:515:ARG:HB3	2.37	0.45
1:A:692:THR:HB	1:A:792:PHE:O	2.16	0.45
1:C:137:ARG:HG2	1:C:143:ASN:OD1	2.16	0.45
1:C:321:VAL:CG2	1:C:326:LEU:HD11	2.46	0.45
1:C:49:ASN:O	1:C:50:ARG:HB2	2.15	0.45
1:E:565:LEU:O	1:E:566:PHE:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:ARG:HB2	1:I:502:TRP:CD1	2.52	0.45
1:I:276:LEU:HD13	1:I:280:HIS:CG	2.50	0.45
1:I:244:ILE:HG23	1:I:330:ALA:HA	1.97	0.45
1:I:334:ALA:O	1:I:335:ASP:C	2.54	0.45
1:I:491:ARG:NH2	2:J:11:ARG:N	2.64	0.45
1:K:216:SER:OG	5:K:1804:MGD:O2'	2.32	0.45
1:M:333:TYR:CZ	1:M:340:TRP:CD1	3.04	0.45
1:M:537:MET:HE2	1:M:595:PHE:HE2	1.81	0.45
1:O:702:GLY:HA3	1:O:706:LEU:HD12	1.98	0.45
1:A:409:ASN:HA	1:A:410:PRO:HD3	1.71	0.45
1:A:598:TYR:HE1	1:A:600:GLN:HG3	1.80	0.45
1:A:641:ARG:HD2	1:A:642:TRP:CZ3	2.52	0.45
1:A:700:HIS:O	1:A:769:PHE:HA	2.15	0.45
1:A:76:ARG:NH2	1:A:473:ARG:NH1	2.64	0.45
1:C:125:THR:HG22	1:C:126:ILE:N	2.31	0.45
1:C:46:ALA:O	1:C:50:ARG:HG2	2.16	0.45
1:C:139:GLY:HA2	1:C:565:LEU:HD22	1.97	0.45
1:C:692:THR:CG2	5:C:1803:MGD:N18	2.72	0.45
1:G:270:THR:CG2	1:G:674:PRO:HG3	2.46	0.45
1:G:714:ALA:CB	2:H:103:VAL:CG1	2.93	0.45
1:I:448:ASN:ND2	1:I:477:ASN:ND2	2.45	0.45
1:K:125:THR:CG2	1:K:126:ILE:N	2.79	0.45
1:K:181:ALA:HB1	1:K:211:ARG:O	2.16	0.45
1:K:537:MET:CE	1:K:595:PHE:CE2	2.99	0.45
1:M:20:ARG:HB2	1:M:502:TRP:CD1	2.51	0.45
1:M:740:VAL:O	1:M:746:GLU:HA	2.16	0.45
2:D:123:MET:HG3	2:N:50:GLN:HB3	1.97	0.45
1:O:719:VAL:CG1	1:O:752:GLU:HB2	2.46	0.45
2:B:26:THR:O	2:B:26:THR:HG22	2.15	0.45
2:B:62:HIS:HA	2:B:74:MET:HB3	1.99	0.45
1:C:332:LEU:CD2	1:C:340:TRP:HH2	2.29	0.45
1:C:747:ILE:CG2	1:C:748:ARG:N	2.78	0.45
1:C:714:ALA:CB	2:D:103:VAL:HG11	2.44	0.45
1:E:194:PRO:HD2	3:E:1801:SF4:S4	2.57	0.45
1:E:724:PRO:O	1:E:728:ARG:HG3	2.17	0.45
1:G:181:ALA:CB	1:G:340:TRP:CH2	2.99	0.45
1:G:300:PHE:O	1:G:300:PHE:CD1	2.70	0.45
1:G:458:MET:HB2	1:G:489:THR:OG1	2.16	0.45
1:G:513:GLU:O	1:G:514:ARG:HB2	2.16	0.45
1:G:84:LYS:O	1:G:85:GLU:CB	2.53	0.45
2:J:27:ASP:CG	2:J:27:ASP:O	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:683:ASP:OD2	1:K:743:ARG:NH1	2.50	0.45
1:M:130:TYR:HD1	1:M:603:LEU:HD23	1.82	0.45
2:N:49:TYR:CD2	2:N:57:ARG:HG2	2.51	0.45
2:P:98:CYS:C	2:P:100:ALA:N	2.69	0.45
1:A:181:ALA:CB	1:A:340:TRP:CH2	2.99	0.45
1:C:441:LYS:HB3	1:C:447:ILE:HG13	1.98	0.45
1:C:76:ARG:HH22	1:C:473:ARG:CZ	2.29	0.45
1:E:133:SER:OG	1:E:137:ARG:NH1	2.48	0.45
1:E:426:LEU:HD13	1:E:553:ILE:HG21	1.97	0.45
2:F:82:ASP:O	2:F:83:ARG:C	2.53	0.45
1:I:513:GLU:OE2	1:I:515:ARG:NH1	2.49	0.45
1:I:702:GLY:HA3	1:I:706:LEU:HD12	1.99	0.45
1:I:759:MET:HE1	1:I:765:PHE:HB2	1.98	0.45
1:K:793:LYS:CE	5:K:1804:MGD:H5'2	2.46	0.45
1:K:246:HIS:HB2	1:K:307:VAL:HG12	1.98	0.45
1:K:422:LEU:HD13	1:K:426:LEU:HD23	1.99	0.45
1:K:714:ALA:CB	2:L:103:VAL:CG1	2.94	0.45
1:K:738:VAL:CG1	1:K:751:LEU:HD22	2.47	0.45
2:L:82:ASP:O	2:L:83:ARG:C	2.54	0.45
1:M:144:ASN:ND2	1:M:433:ALA:N	2.54	0.45
1:M:138:ALA:CB	1:M:422:LEU:HD11	2.46	0.45
1:M:750:ARG:HD2	2:N:20:PRO:HA	1.96	0.45
2:N:40:PRO:HD3	6:N:1129:HEC:HBD1	1.98	0.45
1:O:118:MET:HG2	1:O:451:TRP:HB3	1.98	0.45
2:P:30:ARG:HD2	6:P:1128:HEC:O1D	2.16	0.45
1:A:714:ALA:CB	2:B:103:VAL:CG1	2.95	0.45
1:C:597:PHE:HB2	1:C:598:TYR:H	1.66	0.45
2:D:49:TYR:CD2	2:D:57:ARG:HG2	2.52	0.45
2:D:62:HIS:HA	2:D:74:MET:HB3	1.99	0.45
2:F:36:PRO:O	2:F:38:GLN:N	2.49	0.45
1:G:333:TYR:CD2	1:G:340:TRP:CD1	3.04	0.45
1:G:181:ALA:HB1	1:G:340:TRP:CH2	2.51	0.45
1:G:391:ALA:HA	1:G:396:THR:HB	1.98	0.45
1:I:675:TYR:CE1	1:I:676:GLU:O	2.69	0.45
1:K:175:ASP:HB2	1:K:341:MET:HE2	1.98	0.45
1:K:138:ALA:CB	1:K:422:LEU:HD11	2.47	0.45
1:K:441:LYS:HB3	1:K:447:ILE:HG13	1.99	0.45
2:L:101:CYS:SG	6:L:1129:HEC:HAC	2.55	0.45
1:O:150:ARG:HG2	1:O:435:ALA:HB3	1.97	0.45
1:O:597:PHE:HB2	1:O:598:TYR:H	1.66	0.45
1:A:209:HIS:C	1:A:209:HIS:CD2	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:ASP:OD1	1:A:781:ASP:O	2.34	0.45
2:B:82:ASP:O	2:B:83:ARG:C	2.54	0.45
1:C:557:ALA:HA	1:C:558:PRO:HD2	1.64	0.45
1:C:549:TRP:CH2	1:C:568:VAL:HG11	2.51	0.45
1:E:455:ASN:HD22	1:E:457:ASN:N	2.15	0.45
1:E:787:SER:O	1:E:788:ARG:HB2	2.17	0.45
2:H:58:CYS:CB	6:H:1128:HEC:HAB	2.38	0.45
1:I:157:ALA:O	1:I:160:PHE:HB2	2.17	0.45
1:K:401:LEU:HB3	1:K:402:PRO:HD2	1.98	0.45
2:L:77:ILE:HG23	2:L:87:MET:CE	2.46	0.45
1:M:538:GLU:OE2	1:M:541:LYS:HD2	2.17	0.45
1:M:690:LEU:HB3	1:M:795:CYS:SG	2.57	0.45
1:O:163:THR:CG2	1:O:359:HIS:CE1	2.89	0.45
1:O:586:ASP:O	1:O:587:HIS:HB2	2.16	0.45
1:A:659:ARG:O	1:A:661:TYR:N	2.50	0.45
1:C:244:ILE:HG23	1:C:330:ALA:HA	1.98	0.45
1:C:537:MET:HE2	1:C:595:PHE:HE2	1.82	0.45
1:E:549:TRP:CH2	1:E:568:VAL:HG11	2.52	0.45
1:E:80:GLY:O	1:E:81:VAL:CB	2.62	0.45
1:G:335:ASP:O	1:G:337:ASP:N	2.45	0.45
1:G:394:VAL:HG22	1:G:607:TYR:CE1	2.52	0.45
1:I:332:LEU:CD2	1:I:340:TRP:HH2	2.29	0.45
1:I:391:ALA:HA	1:I:396:THR:HB	1.98	0.45
1:I:401:LEU:HB3	1:I:402:PRO:HD2	1.98	0.45
1:I:598:TYR:CE1	1:I:600:GLN:CG	2.99	0.45
1:K:76:ARG:HH22	1:K:473:ARG:CZ	2.30	0.45
1:K:604:PHE:CZ	1:K:618:LEU:HD13	2.51	0.45
2:L:98:CYS:C	2:L:100:ALA:N	2.70	0.45
2:L:33:ARG:HH21	2:L:40:PRO:CG	2.24	0.45
1:M:683:ASP:OD2	1:M:743:ARG:NH1	2.49	0.45
2:L:67:SER:HA	2:N:118:ASP:OD1	2.17	0.45
1:A:133:SER:OG	1:A:137:ARG:NH1	2.50	0.45
1:A:384:GLN:HB3	1:A:385:PRO:HD2	1.98	0.45
1:C:189:MET:CE	1:C:343:LEU:HD13	2.47	0.45
1:C:422:LEU:HD13	1:C:426:LEU:HD23	1.99	0.45
1:C:472:TYR:HA	1:C:479:ILE:HD13	1.99	0.45
1:C:543:PHE:CD1	1:C:543:PHE:N	2.84	0.45
1:C:598:TYR:CE1	1:C:600:GLN:HG3	2.52	0.45
1:C:60:LEU:HD23	1:C:63:ILE:HD12	1.98	0.45
1:E:300:PHE:CD1	1:E:300:PHE:C	2.87	0.45
1:G:719:VAL:CG1	1:G:752:GLU:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:401:LEU:HB3	1:I:402:PRO:CD	2.47	0.45
1:K:133:SER:OG	1:K:137:ARG:NH1	2.50	0.45
1:M:772:SER:HB3	2:N:6:LEU:CD2	2.47	0.45
1:O:537:MET:HE2	1:O:595:PHE:CE2	2.51	0.45
1:O:544:THR:CG2	1:O:547:GLU:HB2	2.35	0.45
1:A:598:TYR:CE1	1:A:600:GLN:HG3	2.52	0.45
1:A:356:TRP:CZ3	1:A:674:PRO:O	2.70	0.45
1:C:617:ASP:HB2	1:C:633:PRO:HA	1.98	0.45
2:D:41:VAL:HG11	2:D:105:GLN:HG3	1.98	0.45
1:E:144:ASN:ND2	1:E:433:ALA:N	2.53	0.45
1:E:321:VAL:CG2	1:E:326:LEU:HD11	2.47	0.45
1:E:426:LEU:HD21	1:E:549:TRP:CE2	2.52	0.45
1:I:472:TYR:HA	1:I:479:ILE:CD1	2.47	0.45
2:J:33:ARG:NH2	6:J:1129:HEC:HAA1	2.31	0.45
1:M:188:ASN:ND2	1:M:222:SER:OG	2.45	0.45
1:M:29:MET:CE	1:M:628:ARG:HH12	2.21	0.45
1:M:783:ASN:N	1:M:783:ASN:ND2	2.63	0.45
2:N:86:GLN:HE21	2:N:86:GLN:HA	1.82	0.45
1:O:396:THR:CG2	1:O:396:THR:O	2.65	0.45
1:O:422:LEU:HD13	1:O:426:LEU:HD23	1.99	0.45
2:P:10:ASP:O	2:P:12:PRO:N	2.50	0.45
1:I:14:TRP:HZ2	2:P:89:ALA:HB2	1.82	0.45
2:B:27:ASP:CG	2:B:27:ASP:O	2.56	0.45
1:C:692:THR:CG2	5:C:1803:MGD:H191	2.16	0.45
1:C:143:ASN:O	1:C:432:GLY:HA3	2.16	0.45
1:C:458:MET:HB2	1:C:489:THR:OG1	2.17	0.45
1:E:554:LEU:O	1:E:557:ALA:N	2.48	0.45
2:F:5:ARG:O	2:F:7:THR:N	2.49	0.45
1:G:329:LEU:O	1:G:330:ALA:C	2.55	0.45
1:G:617:ASP:OD2	1:G:651:TYR:OH	2.34	0.45
1:G:781:ASP:OD1	1:G:781:ASP:O	2.35	0.45
1:I:510:GLY:HA2	1:I:515:ARG:O	2.16	0.45
1:I:641:ARG:HD2	1:I:642:TRP:CZ3	2.52	0.45
1:M:125:THR:HG22	1:M:126:ILE:N	2.32	0.45
1:M:190:ALA:HA	1:M:197:TRP:CD1	2.52	0.45
1:M:719:VAL:CG1	1:M:752:GLU:HB2	2.47	0.45
1:O:144:ASN:HD21	1:O:433:ALA:H	1.62	0.45
1:O:700:HIS:HE1	5:O:1804:MGD:S13	2.39	0.45
1:A:276:LEU:HD13	1:A:280:HIS:CG	2.52	0.44
1:A:321:VAL:CG2	1:A:326:LEU:HD11	2.46	0.44
1:A:335:ASP:C	1:A:337:ASP:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:HIS:CE1	5:C:1804:MGD:S13	3.10	0.44
1:C:335:ASP:O	1:C:337:ASP:N	2.46	0.44
2:D:5:ARG:O	2:D:7:THR:N	2.50	0.44
1:G:144:ASN:ND2	1:G:433:ALA:N	2.53	0.44
1:G:223:SER:HA	1:G:226:SER:OG	2.17	0.44
1:G:332:LEU:CD2	1:G:340:TRP:HH2	2.29	0.44
1:G:740:VAL:O	1:G:746:GLU:HA	2.17	0.44
1:I:46:ALA:O	1:I:50:ARG:HG2	2.17	0.44
1:I:739:ARG:O	1:I:799:ILE:HA	2.17	0.44
1:K:335:ASP:C	1:K:337:ASP:H	2.18	0.44
1:K:571:ALA:HA	1:K:576:ASP:CG	2.36	0.44
1:K:675:TYR:CE1	1:K:676:GLU:O	2.70	0.44
1:K:80:GLY:O	1:K:81:VAL:CB	2.65	0.44
2:L:50:GLN:H	2:P:123:MET:HE3	1.81	0.44
1:M:150:ARG:HG2	1:M:435:ALA:HB3	1.99	0.44
1:M:183:VAL:HG12	1:M:185:TRP:CD1	2.52	0.44
1:M:422:LEU:HD13	1:M:426:LEU:HD23	1.99	0.44
1:O:426:LEU:HD21	1:O:549:TRP:CE2	2.51	0.44
1:A:513:GLU:O	1:A:514:ARG:HB2	2.16	0.44
2:B:66:TYR:O	2:B:67:SER:C	2.55	0.44
1:C:108:LEU:HD21	1:C:548:VAL:HG13	2.00	0.44
1:C:356:TRP:HZ3	1:C:674:PRO:O	2.01	0.44
2:D:104:PRO:O	2:D:105:GLN:HG2	2.18	0.44
1:E:193:HIS:N	1:E:194:PRO:HD3	2.32	0.44
1:E:298:THR:HB	1:E:299:ASP:H	1.40	0.44
1:E:76:ARG:NH2	1:E:473:ARG:NH1	2.65	0.44
1:E:458:MET:HB2	1:E:489:THR:HA	1.99	0.44
1:E:49:ASN:O	1:E:50:ARG:HB2	2.16	0.44
2:F:98:CYS:O	2:F:100:ALA:N	2.50	0.44
1:G:332:LEU:HB3	1:G:340:TRP:CZ3	2.53	0.44
1:G:21:PHE:HZ	1:G:63:ILE:HD11	1.76	0.44
1:I:740:VAL:O	1:I:746:GLU:HA	2.17	0.44
1:K:46:ALA:O	1:K:50:ARG:HG2	2.17	0.44
1:K:759:MET:HE2	1:K:765:PHE:N	2.32	0.44
1:M:356:TRP:HZ3	1:M:674:PRO:O	2.00	0.44
1:O:276:LEU:HD13	1:O:280:HIS:CG	2.51	0.44
1:O:455:ASN:HD22	1:O:457:ASN:N	2.15	0.44
1:A:183:VAL:HG23	1:A:340:TRP:HZ2	1.76	0.44
1:A:338:ARG:HG2	1:A:340:TRP:HZ3	1.81	0.44
1:A:426:LEU:HD21	1:A:549:TRP:CE2	2.52	0.44
1:E:118:MET:HG2	1:E:451:TRP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:422:LEU:HD13	1:G:426:LEU:HD23	2.00	0.44
1:I:183:VAL:HG11	1:I:185:TRP:NE1	2.32	0.44
1:I:454:VAL:HG22	5:I:1803:MGD:C2	2.48	0.44
1:I:543:PHE:O	1:I:564:THR:CA	2.65	0.44
1:I:615:GLY:O	1:I:617:ASP:N	2.50	0.44
1:I:463:ASN:HD22	1:I:781:ASP:HB2	1.81	0.44
1:K:694:ARG:HH22	5:K:1803:MGD:H15	1.65	0.44
1:K:384:GLN:HB2	1:K:387:ALA:HB2	1.98	0.44
1:K:391:ALA:HA	1:K:396:THR:HB	1.99	0.44
1:K:537:MET:HE2	1:K:595:PHE:CE2	2.51	0.44
1:M:472:TYR:HA	1:M:479:ILE:CD1	2.47	0.44
2:N:14:SER:O	2:N:15:GLU:CB	2.65	0.44
1:O:183:VAL:HG11	1:O:185:TRP:NE1	2.32	0.44
1:O:269:ALA:O	1:O:272:ILE:HD12	2.17	0.44
1:O:270:THR:CG2	1:O:674:PRO:HG3	2.47	0.44
1:O:238:ARG:NH1	1:O:676:GLU:O	2.51	0.44
1:A:211:ARG:HB2	1:A:338:ARG:NH1	2.32	0.44
1:A:409:ASN:HB3	1:A:412:HIS:CD2	2.53	0.44
1:C:455:ASN:ND2	1:C:457:ASN:H	2.16	0.44
1:C:503:VAL:O	1:C:503:VAL:HG12	2.16	0.44
1:C:692:THR:HB	1:C:792:PHE:O	2.18	0.44
1:C:80:GLY:O	1:C:81:VAL:CB	2.65	0.44
1:E:138:ALA:CB	1:E:422:LEU:HD11	2.47	0.44
1:E:747:ILE:HG22	1:E:748:ARG:H	1.80	0.44
1:G:138:ALA:HB1	1:G:422:LEU:HD11	1.98	0.44
1:G:300:PHE:C	1:G:300:PHE:CD1	2.90	0.44
1:G:544:THR:HG22	1:G:547:GLU:OE1	2.18	0.44
1:G:514:ARG:NH2	1:G:641:ARG:O	2.44	0.44
1:I:458:MET:HB2	1:I:489:THR:OG1	2.18	0.44
1:I:472:TYR:HA	1:I:479:ILE:HD13	2.00	0.44
1:I:501:MET:O	1:I:502:TRP:C	2.55	0.44
1:I:511:ASN:CG	1:I:515:ARG:HB3	2.38	0.44
2:J:42:ILE:HG12	6:J:1128:HEC:CHB	2.48	0.44
1:K:121:SER:O	1:K:124:TRP:HB2	2.17	0.44
1:K:544:THR:CG2	1:K:547:GLU:HB2	2.35	0.44
2:L:98:CYS:HB3	6:L:1129:HEC:C3B	2.48	0.44
1:M:641:ARG:HD2	1:M:642:TRP:CZ3	2.53	0.44
1:O:700:HIS:HB3	1:O:768:TRP:CH2	2.53	0.44
1:A:683:ASP:OD2	1:A:743:ARG:NH1	2.50	0.44
1:A:702:GLY:HA3	1:A:706:LEU:HD12	1.98	0.44
1:C:510:GLY:HA2	1:C:515:ARG:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:PRO:O	1:C:560:TYR:N	2.50	0.44
1:C:558:PRO:O	1:C:561:ARG:HB2	2.18	0.44
1:C:720:CYS:SG	1:C:764:VAL:HG13	2.58	0.44
1:E:162:ARG:NH1	1:E:359:HIS:NE2	2.65	0.44
1:E:406:VAL:H	1:E:412:HIS:CD2	2.36	0.44
1:G:213:ALA:CB	1:G:228:THR:HB	2.48	0.44
1:G:276:LEU:HD13	1:G:280:HIS:CG	2.52	0.44
1:I:300:PHE:CD1	1:I:300:PHE:C	2.88	0.44
1:K:21:PHE:CZ	1:K:63:ILE:CD1	2.97	0.44
1:K:543:PHE:N	1:K:543:PHE:CD1	2.86	0.44
1:K:130:TYR:HD1	1:K:603:LEU:HD23	1.82	0.44
1:K:791:ASP:OD2	1:K:794:LYS:HE2	2.17	0.44
1:M:333:TYR:CD2	1:M:340:TRP:CD1	3.06	0.44
1:M:723:HIS:HD2	1:M:725:GLU:N	2.02	0.44
1:A:469:TYR:N	1:A:470:PRO:HD2	2.32	0.44
2:B:10:ASP:O	2:B:12:PRO:N	2.51	0.44
2:D:98:CYS:HB3	6:D:1129:HEC:CAB	2.47	0.44
1:E:333:TYR:CZ	1:E:340:TRP:CD1	3.05	0.44
1:G:133:SER:OG	1:G:137:ARG:NH1	2.50	0.44
1:G:138:ALA:CB	1:G:422:LEU:HD11	2.48	0.44
1:G:20:ARG:HB2	1:G:502:TRP:CD1	2.52	0.44
1:G:783:ASN:HD22	1:G:790:THR:HA	1.83	0.44
1:I:543:PHE:CD1	1:I:543:PHE:N	2.86	0.44
1:I:590:HIS:O	1:I:594:LEU:HG	2.17	0.44
1:K:458:MET:HB2	1:K:489:THR:HA	1.99	0.44
1:M:121:SER:HB2	1:M:148:ASN:HD21	1.83	0.44
1:O:694:ARG:HH22	5:O:1803:MGD:H15	1.64	0.44
1:O:428:PRO:HB3	1:O:430:TRP:NE1	2.33	0.44
1:O:472:TYR:HA	1:O:479:ILE:HD13	1.98	0.44
2:P:117:ARG:HH11	2:P:124:PRO:HD3	1.82	0.44
1:A:750:ARG:NH1	2:B:18:ALA:O	2.49	0.44
1:C:598:TYR:CE1	1:C:600:GLN:CG	3.00	0.44
1:C:714:ALA:CB	2:D:103:VAL:CG1	2.96	0.44
2:D:27:ASP:O	2:D:27:ASP:CG	2.55	0.44
1:E:28:VAL:CG1	1:E:29:MET:N	2.80	0.44
1:E:356:TRP:HZ3	1:E:674:PRO:O	2.01	0.44
1:E:353:ARG:NH2	1:E:676:GLU:OE1	2.41	0.44
1:E:723:HIS:HB3	1:E:726:ASP:HB2	1.99	0.44
2:F:35:TYR:O	2:F:36:PRO:O	2.36	0.44
1:G:125:THR:HG22	1:G:126:ILE:N	2.32	0.44
1:G:505:LYS:O	1:G:505:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:689:TRP:CE3	1:G:794:LYS:HB2	2.53	0.44
1:I:181:ALA:HB1	1:I:340:TRP:CH2	2.51	0.44
1:I:142:SER:HA	1:I:430:TRP:CZ2	2.52	0.44
1:K:549:TRP:CH2	1:K:568:VAL:HG11	2.53	0.44
1:K:641:ARG:HD2	1:K:642:TRP:CZ3	2.53	0.44
1:M:597:PHE:HB2	1:M:598:TYR:H	1.59	0.44
1:M:192:MET:HE1	1:M:694:ARG:CB	2.46	0.44
1:O:334:ALA:O	1:O:335:ASP:C	2.54	0.44
1:O:483:ASP:OD1	1:O:484:ALA:N	2.45	0.44
1:A:406:VAL:H	1:A:412:HIS:HD2	1.66	0.44
1:C:719:VAL:HG12	1:C:750:ARG:O	2.18	0.44
1:E:353:ARG:HD2	1:E:356:TRP:CE3	2.53	0.44
1:G:263:THR:CG2	1:G:264:ASN:N	2.80	0.44
2:J:98:CYS:C	2:J:100:ALA:H	2.21	0.44
2:J:77:ILE:HG23	2:J:87:MET:SD	2.58	0.44
1:K:617:ASP:OD2	1:K:651:TYR:OH	2.35	0.44
2:L:14:SER:O	2:L:15:GLU:CB	2.66	0.44
1:M:161:MET:O	1:M:165:GLY:N	2.47	0.44
2:N:10:ASP:O	2:N:12:PRO:N	2.51	0.44
2:N:79:HIS:CD2	2:N:95:ARG:HD2	2.51	0.44
1:O:189:MET:CE	1:O:200:LEU:HD23	2.48	0.44
1:O:543:PHE:N	1:O:543:PHE:CD1	2.85	0.44
1:A:422:LEU:HD13	1:A:426:LEU:HD23	1.99	0.44
1:A:458:MET:HB2	1:A:489:THR:HA	2.00	0.44
1:A:474:ASN:HD22	1:A:474:ASN:HA	1.67	0.44
1:E:216:SER:OG	5:E:1804:MGD:O2'	2.34	0.44
1:E:334:ALA:O	1:E:335:ASP:C	2.55	0.44
1:G:190:ALA:HA	1:G:197:TRP:CD1	2.53	0.44
1:I:633:PRO:HD2	1:I:640:THR:CB	2.46	0.44
1:I:633:PRO:HG2	1:I:640:THR:CB	2.48	0.44
1:I:772:SER:HB3	2:J:6:LEU:HD22	2.00	0.44
1:M:162:ARG:NH1	1:M:359:HIS:NE2	2.66	0.44
1:O:554:LEU:HD13	1:O:561:ARG:HG2	2.00	0.44
1:A:216:SER:OG	5:A:1804:MGD:O2'	2.36	0.43
1:A:189:MET:CE	1:A:343:LEU:HD13	2.48	0.43
1:A:543:PHE:HB2	1:A:565:LEU:HD12	2.00	0.43
1:C:259:VAL:O	1:C:263:THR:HB	2.18	0.43
1:C:272:ILE:HG12	1:C:292:ALA:CB	2.48	0.43
1:C:683:ASP:OD2	1:C:743:ARG:NH1	2.51	0.43
2:F:66:TYR:O	2:F:68:GLY:N	2.50	0.43
2:F:79:HIS:CD2	2:F:95:ARG:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:ASN:ND2	1:G:222:SER:OG	2.42	0.43
1:G:60:LEU:HD23	1:G:63:ILE:HD12	1.99	0.43
1:I:125:THR:HG23	1:I:508:ALA:N	2.22	0.43
1:K:118:MET:HG2	1:K:451:TRP:HB3	1.98	0.43
1:K:238:ARG:NH1	1:K:676:GLU:O	2.51	0.43
1:M:334:ALA:O	1:M:335:ASP:C	2.55	0.43
1:M:334:ALA:O	1:M:336:PRO:N	2.51	0.43
1:M:374:PRO:HB3	1:M:642:TRP:CZ2	2.53	0.43
1:O:409:ASN:HB3	1:O:412:HIS:CD2	2.53	0.43
1:O:683:ASP:OD2	1:O:743:ARG:NH1	2.50	0.43
1:A:121:SER:HA	1:A:148:ASN:OD1	2.18	0.43
1:A:454:VAL:HG22	5:A:1803:MGD:C2	2.47	0.43
1:A:700:HIS:HE1	5:A:1804:MGD:S13	2.41	0.43
2:B:104:PRO:O	2:B:105:GLN:HG2	2.17	0.43
1:C:134:LYS:NZ	1:C:569:LEU:O	2.51	0.43
1:C:75:LEU:HD12	1:C:76:ARG:H	1.82	0.43
1:C:89:ALA:HA	1:C:90:PRO:HD3	1.92	0.43
2:D:37:GLU:HA	6:D:1129:HEC:HAD2	2.00	0.43
2:D:82:ASP:O	2:D:83:ARG:C	2.56	0.43
2:D:86:GLN:HA	2:D:86:GLN:HE21	1.83	0.43
2:F:33:ARG:HH21	2:F:40:PRO:CG	2.22	0.43
1:G:427:LEU:HA	1:G:428:PRO:HD3	1.77	0.43
1:I:216:SER:HB3	1:I:218:PHE:O	2.18	0.43
1:I:128:GLU:OE2	1:I:532:ASP:HB2	2.18	0.43
1:K:263:THR:CG2	1:K:264:ASN:N	2.81	0.43
1:K:474:ASN:HA	1:K:474:ASN:HD22	1.70	0.43
1:K:720:CYS:SG	1:K:764:VAL:HG13	2.57	0.43
1:M:409:ASN:OD1	1:M:411:GLU:N	2.51	0.43
1:M:702:GLY:HA3	1:M:706:LEU:HD12	1.99	0.43
1:O:538:GLU:OE2	1:O:541:LYS:HD2	2.18	0.43
1:O:759:MET:HE2	1:O:765:PHE:N	2.33	0.43
2:B:120:LEU:O	2:B:121:THR:OG1	2.30	0.43
1:C:384:GLN:HB2	1:C:387:ALA:HB2	2.00	0.43
1:E:147:PRO:HD3	1:E:397:PHE:HA	1.99	0.43
1:E:590:HIS:O	1:E:594:LEU:HG	2.18	0.43
1:G:464:ILE:HG22	1:G:468:THR:HB	2.00	0.43
1:I:181:ALA:HB1	1:I:211:ARG:O	2.17	0.43
1:K:752:GLU:OE1	1:K:755:GLY:CA	2.66	0.43
1:M:564:THR:HG1	1:M:567:GLU:HG3	1.82	0.43
1:O:613:GLY:O	1:O:615:GLY:N	2.51	0.43
1:O:783:ASN:N	1:O:783:ASN:ND2	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:793:LYS:CE	5:C:1804:MGD:H5'2	2.48	0.43
1:C:646:GLU:OE2	1:C:654:PRO:O	2.35	0.43
1:E:692:THR:CG2	5:E:1803:MGD:H191	2.14	0.43
1:E:21:PHE:CZ	1:E:63:ILE:CD1	2.99	0.43
1:E:401:LEU:HB3	1:E:402:PRO:HD2	2.00	0.43
1:G:242:ASN:O	1:G:243:TYR:C	2.57	0.43
1:G:183:VAL:CG2	1:G:340:TRP:CZ2	2.94	0.43
1:G:565:LEU:O	1:G:566:PHE:CB	2.66	0.43
1:I:183:VAL:HG12	1:I:185:TRP:NE1	2.33	0.43
1:K:692:THR:CG2	5:K:1803:MGD:H191	2.12	0.43
1:K:700:HIS:CE1	5:K:1804:MGD:S13	3.11	0.43
1:K:350:GLN:OE1	1:K:793:LYS:HE2	2.18	0.43
1:K:482:SER:HA	1:K:497:LEU:O	2.18	0.43
2:L:5:ARG:O	2:L:7:THR:N	2.50	0.43
1:M:700:HIS:CE1	5:M:1804:MGD:S13	3.11	0.43
1:O:543:PHE:HB3	1:O:548:VAL:HG21	2.00	0.43
1:O:689:TRP:CE3	1:O:794:LYS:HB2	2.54	0.43
6:B:1129:HEC:HMC1	6:B:1129:HEC:HBC3	2.00	0.43
2:B:14:SER:O	2:B:15:GLU:CB	2.66	0.43
2:B:37:GLU:HA	6:B:1129:HEC:HAD2	2.01	0.43
1:C:274:TYR:O	1:C:276:LEU:N	2.52	0.43
1:C:396:THR:CG2	1:C:396:THR:O	2.63	0.43
1:C:533:LEU:O	1:C:537:MET:HG3	2.19	0.43
1:C:740:VAL:O	1:C:746:GLU:HA	2.17	0.43
1:E:350:GLN:OE1	1:E:793:LYS:HE2	2.17	0.43
2:F:120:LEU:O	2:F:121:THR:OG1	2.34	0.43
1:G:20:ARG:O	1:G:20:ARG:CG	2.66	0.43
1:G:334:ALA:O	1:G:335:ASP:C	2.55	0.43
1:G:692:THR:CG2	5:G:1803:MGD:N18	2.75	0.43
2:H:33:ARG:HH21	2:H:40:PRO:CG	2.27	0.43
1:I:332:LEU:HD23	1:I:340:TRP:HH2	1.79	0.43
2:J:40:PRO:HD2	2:J:102:HIS:CE1	2.52	0.43
1:K:223:SER:HA	1:K:226:SER:OG	2.19	0.43
1:K:510:GLY:HA2	1:K:515:ARG:O	2.17	0.43
1:K:722:MET:HE3	1:K:751:LEU:HD11	2.01	0.43
1:M:204:ARG:NH1	1:M:227:ASP:OD1	2.51	0.43
1:M:329:LEU:O	1:M:330:ALA:C	2.56	0.43
1:M:564:THR:OG1	1:M:567:GLU:HG3	2.19	0.43
2:N:27:ASP:CG	2:N:27:ASP:O	2.57	0.43
1:O:649:ASP:OD2	1:O:650:PRO:HD2	2.19	0.43
2:B:89:ALA:O	2:B:90:ASP:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ARG:HB2	1:C:338:ARG:NH1	2.33	0.43
1:C:223:SER:HA	1:C:226:SER:OG	2.18	0.43
2:D:10:ASP:O	2:D:12:PRO:N	2.52	0.43
1:E:118:MET:HE1	1:E:132:ALA:HB1	2.00	0.43
1:E:436:VAL:HG11	1:E:440:ARG:NH2	2.33	0.43
1:E:543:PHE:N	1:E:543:PHE:CD1	2.86	0.43
1:E:76:ARG:HH22	1:E:473:ARG:CZ	2.31	0.43
2:F:62:HIS:HA	2:F:74:MET:HB3	2.01	0.43
1:G:694:ARG:HH22	5:G:1803:MGD:H15	1.66	0.43
1:I:113:PRO:C	1:I:115:ALA:H	2.21	0.43
1:I:384:GLN:HB2	1:I:387:ALA:HB2	2.00	0.43
2:J:95:ARG:HA	6:J:1129:HEC:CMC	2.37	0.43
1:K:20:ARG:HB2	1:K:502:TRP:CD1	2.53	0.43
1:K:238:ARG:HG2	1:K:360:MET:HE1	1.97	0.43
1:K:503:VAL:O	1:K:503:VAL:HG12	2.17	0.43
1:M:406:VAL:H	1:M:412:HIS:CD2	2.36	0.43
1:M:563:LYS:O	1:M:567:GLU:CG	2.67	0.43
2:N:66:TYR:O	2:N:68:GLY:N	2.51	0.43
1:O:501:MET:HG2	1:O:502:TRP:N	2.33	0.43
1:O:774:LEU:HD12	2:P:13:MET:HG2	2.01	0.43
2:P:27:ASP:O	2:P:27:ASP:CG	2.56	0.43
1:A:329:LEU:O	1:A:330:ALA:C	2.56	0.43
1:C:554:LEU:O	1:C:557:ALA:N	2.52	0.43
1:C:738:VAL:CG1	1:C:751:LEU:HD22	2.48	0.43
2:D:3:ALA:O	2:D:4:PRO:C	2.57	0.43
1:C:772:SER:HB3	2:D:6:LEU:HD22	2.01	0.43
1:E:116:VAL:HG12	1:E:449:PHE:HB3	2.00	0.43
1:G:277:ARG:HH21	1:G:467:GLU:HG2	1.83	0.43
1:G:491:ARG:NH2	2:H:11:ARG:N	2.66	0.43
1:G:503:VAL:HG12	1:G:523:VAL:HG22	1.99	0.43
2:H:27:ASP:CG	2:H:27:ASP:O	2.57	0.43
1:I:334:ALA:O	1:I:336:PRO:N	2.51	0.43
1:I:791:ASP:OD2	1:I:794:LYS:HE2	2.18	0.43
1:I:692:THR:HB	1:I:792:PHE:O	2.18	0.43
1:K:188:ASN:ND2	1:K:222:SER:OG	2.44	0.43
1:K:472:TYR:HA	1:K:479:ILE:HD13	2.00	0.43
1:K:598:TYR:CE1	1:K:600:GLN:HG3	2.53	0.43
1:M:259:VAL:O	1:M:263:THR:HB	2.19	0.43
1:M:590:HIS:O	1:M:594:LEU:HG	2.19	0.43
1:M:76:ARG:HH22	1:M:473:ARG:CZ	2.31	0.43
1:O:598:TYR:CE1	1:O:600:GLN:CG	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:633:PRO:HG2	1:O:640:THR:CB	2.48	0.43
1:O:84:LYS:HE2	1:O:473:ARG:C	2.39	0.43
1:O:750:ARG:HD2	2:P:20:PRO:HA	1.97	0.43
1:A:300:PHE:O	1:A:300:PHE:HD1	2.02	0.43
1:A:554:LEU:O	1:A:557:ALA:N	2.51	0.43
1:C:338:ARG:HG2	1:C:340:TRP:HE3	1.81	0.43
1:C:455:ASN:HD22	1:C:457:ASN:N	2.17	0.43
1:C:513:GLU:O	1:C:514:ARG:HB2	2.19	0.43
1:C:590:HIS:O	1:C:594:LEU:HG	2.19	0.43
1:E:389:GLY:HA3	1:E:510:GLY:HA3	2.00	0.43
1:E:454:VAL:HG22	5:E:1803:MGD:C2	2.48	0.43
1:G:130:TYR:CD1	1:G:603:LEU:HD23	2.53	0.43
1:G:702:GLY:HA3	1:G:706:LEU:HD12	2.00	0.43
1:I:759:MET:HE2	1:I:765:PHE:N	2.33	0.43
1:I:771:ALA:HB3	2:J:6:LEU:O	2.18	0.43
2:J:98:CYS:C	2:J:100:ALA:N	2.72	0.43
2:J:82:ASP:O	2:J:83:ARG:C	2.55	0.43
1:K:427:LEU:HA	1:K:428:PRO:HD3	1.74	0.43
1:K:520:HIS:O	1:K:522:LEU:HD13	2.18	0.43
1:M:747:ILE:HG22	1:M:748:ARG:H	1.80	0.43
1:M:697:GLU:CD	1:M:756:ARG:HH22	2.22	0.43
2:N:117:ARG:HH11	2:N:124:PRO:HD3	1.84	0.43
1:O:374:PRO:HB3	1:O:642:TRP:CZ2	2.54	0.43
1:O:722:MET:HE3	1:O:751:LEU:HD11	2.01	0.43
1:A:401:LEU:HB3	1:A:402:PRO:CD	2.49	0.43
1:A:503:VAL:O	1:A:503:VAL:HG13	2.19	0.43
1:A:730:ARG:CB	1:A:732:LEU:HD22	2.48	0.43
1:A:41:HIS:CD2	2:B:37:GLU:HB2	2.54	0.43
1:C:574:SER:O	1:C:577:ARG:HB2	2.19	0.43
1:C:238:ARG:NH1	1:C:676:GLU:O	2.52	0.43
2:D:14:SER:O	2:D:15:GLU:CB	2.66	0.43
1:E:16:LYS:HA	1:E:29:MET:HE2	2.01	0.43
2:F:89:ALA:O	2:F:90:ASP:HB2	2.19	0.43
1:G:752:GLU:OE1	1:G:755:GLY:CA	2.67	0.43
1:I:193:HIS:N	1:I:194:PRO:HD3	2.33	0.43
1:I:280:HIS:CE1	1:I:282:LEU:HD12	2.54	0.43
1:I:333:TYR:CZ	1:I:340:TRP:CD1	3.06	0.43
1:I:604:PHE:CZ	1:I:618:LEU:HD13	2.53	0.43
1:O:118:MET:HE2	1:O:145:LEU:HD13	2.00	0.43
1:O:436:VAL:HG11	1:O:440:ARG:NH2	2.34	0.43
1:A:125:THR:CG2	1:A:126:ILE:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLN:OE1	1:A:793:LYS:HE2	2.19	0.43
1:C:401:LEU:HB3	1:C:402:PRO:HD2	2.01	0.43
1:C:409:ASN:HA	1:C:410:PRO:HD3	1.76	0.43
1:C:781:ASP:O	1:C:781:ASP:OD1	2.37	0.43
1:G:118:MET:HE2	1:G:145:LEU:HD13	2.00	0.43
1:G:683:ASP:OD2	1:G:743:ARG:NH1	2.51	0.43
1:G:80:GLY:O	1:G:81:VAL:CB	2.67	0.43
1:K:533:LEU:O	1:K:537:MET:HG3	2.18	0.43
1:M:181:ALA:HB1	1:M:340:TRP:CH2	2.54	0.43
1:M:49:ASN:O	1:M:50:ARG:HB2	2.19	0.43
1:O:29:MET:HE3	1:O:628:ARG:NH1	2.32	0.43
1:O:710:GLU:HA	2:P:105:GLN:OE1	2.19	0.43
1:A:108:LEU:HD21	1:A:548:VAL:HG13	1.99	0.42
1:A:719:VAL:HG12	1:A:750:ARG:O	2.19	0.42
1:A:710:GLU:HA	2:B:105:GLN:OE1	2.19	0.42
2:B:35:TYR:O	2:B:36:PRO:O	2.37	0.42
1:C:121:SER:O	1:C:124:TRP:HB2	2.19	0.42
1:C:551:GLU:HG2	1:C:551:GLU:H	1.42	0.42
1:E:409:ASN:HA	1:E:410:PRO:HD3	1.75	0.42
2:F:66:TYR:O	2:F:67:SER:C	2.57	0.42
1:G:183:VAL:CG2	1:G:340:TRP:CE2	3.00	0.42
1:G:374:PRO:HB3	1:G:642:TRP:CZ2	2.54	0.42
1:G:549:TRP:CH2	1:G:568:VAL:HG11	2.54	0.42
1:G:597:PHE:HB2	1:G:598:TYR:H	1.67	0.42
1:I:710:GLU:HA	2:J:105:GLN:OE1	2.19	0.42
1:I:33:ARG:NH1	2:J:119:MET:O	2.47	0.42
1:K:274:TYR:O	1:K:276:LEU:N	2.51	0.42
1:K:479:ILE:HG22	1:K:493:ALA:HB1	2.01	0.42
1:M:391:ALA:HA	1:M:396:THR:HB	2.01	0.42
1:O:130:TYR:HD1	1:O:603:LEU:HD23	1.84	0.42
1:O:192:MET:C	1:O:194:PRO:HD3	2.40	0.42
1:O:391:ALA:HA	1:O:396:THR:HB	2.01	0.42
1:O:142:SER:HA	1:O:430:TRP:CZ2	2.54	0.42
1:O:738:VAL:CG1	1:O:751:LEU:HD22	2.49	0.42
2:P:49:TYR:CD2	2:P:57:ARG:HG2	2.54	0.42
2:P:66:TYR:O	2:P:67:SER:C	2.57	0.42
1:A:204:ARG:NH1	1:A:227:ASP:OD1	2.52	0.42
1:A:401:LEU:HB3	1:A:402:PRO:HD2	2.00	0.42
1:A:455:ASN:ND2	1:A:457:ASN:H	2.15	0.42
1:A:479:ILE:HG22	1:A:493:ALA:HB1	2.02	0.42
1:C:16:LYS:CA	1:C:29:MET:HE1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:HIS:HE1	5:C:1804:MGD:S13	2.42	0.42
1:E:401:LEU:HB3	1:E:402:PRO:CD	2.49	0.42
1:G:454:VAL:HG22	5:G:1803:MGD:C2	2.49	0.42
1:G:339:LYS:CA	1:G:376:ASN:ND2	2.78	0.42
1:G:350:GLN:OE1	1:G:793:LYS:HE2	2.19	0.42
1:G:750:ARG:HD2	2:H:20:PRO:HA	1.96	0.42
1:I:125:THR:CG2	1:I:126:ILE:N	2.81	0.42
1:I:20:ARG:O	1:I:20:ARG:CG	2.67	0.42
1:I:565:LEU:O	1:I:566:PHE:CB	2.62	0.42
1:I:563:LYS:O	1:I:567:GLU:HG3	2.19	0.42
1:I:80:GLY:O	1:I:81:VAL:CB	2.65	0.42
1:K:150:ARG:HG2	1:K:435:ALA:HB3	2.01	0.42
1:K:791:ASP:OD1	1:K:791:ASP:C	2.57	0.42
1:M:33:ARG:NH1	2:N:119:MET:O	2.45	0.42
1:O:244:ILE:HG23	1:O:330:ALA:HA	2.01	0.42
1:O:80:GLY:O	1:O:81:VAL:CB	2.67	0.42
1:O:750:ARG:NH1	2:P:18:ALA:O	2.51	0.42
1:C:329:LEU:O	1:C:330:ALA:C	2.57	0.42
1:C:448:ASN:ND2	1:C:477:ASN:ND2	2.51	0.42
2:D:42:ILE:CD1	6:D:1128:HEC:HMB2	2.49	0.42
1:E:544:THR:CG2	1:E:547:GLU:HB2	2.38	0.42
1:G:472:TYR:HA	1:G:479:ILE:HD13	2.01	0.42
2:H:5:ARG:O	2:H:7:THR:N	2.51	0.42
1:I:269:ALA:O	1:I:272:ILE:HD12	2.19	0.42
1:I:353:ARG:HD2	1:I:356:TRP:CE3	2.54	0.42
1:K:329:LEU:O	1:K:330:ALA:C	2.57	0.42
1:K:564:THR:HG1	1:K:567:GLU:HG3	1.85	0.42
2:L:51:LEU:HD22	2:L:56:ASN:ND2	2.34	0.42
1:M:181:ALA:HB1	1:M:211:ARG:O	2.18	0.42
1:M:428:PRO:HB3	1:M:430:TRP:NE1	2.34	0.42
1:M:598:TYR:HE1	1:M:600:GLN:HG3	1.83	0.42
1:O:181:ALA:HB1	1:O:340:TRP:CH2	2.54	0.42
1:A:192:MET:HB3	5:A:1804:MGD:H22	1.84	0.42
1:A:406:VAL:H	1:A:412:HIS:CD2	2.38	0.42
1:C:130:TYR:HD1	1:C:603:LEU:HD23	1.85	0.42
1:C:181:ALA:HB1	1:C:340:TRP:CH2	2.54	0.42
1:C:213:ALA:CB	1:C:228:THR:HB	2.50	0.42
1:C:276:LEU:HD13	1:C:280:HIS:CG	2.54	0.42
1:C:513:GLU:OE2	1:C:515:ARG:NH1	2.52	0.42
1:C:697:GLU:CD	1:C:756:ARG:HH22	2.23	0.42
1:E:183:VAL:HG21	1:E:340:TRP:NE1	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:ALA:HB1	1:E:211:ARG:O	2.19	0.42
1:E:339:LYS:CA	1:E:376:ASN:ND2	2.81	0.42
1:E:586:ASP:O	1:E:587:HIS:HB2	2.18	0.42
1:E:68:ASP:CB	1:E:707:ARG:NH1	2.79	0.42
2:F:104:PRO:O	2:F:105:GLN:HG2	2.19	0.42
1:G:183:VAL:CG1	1:G:185:TRP:NE1	2.82	0.42
1:G:428:PRO:HB3	1:G:430:TRP:NE1	2.34	0.42
1:G:633:PRO:HG2	1:G:640:THR:CB	2.49	0.42
1:G:700:HIS:HB3	1:G:768:TRP:CH2	2.55	0.42
2:H:26:THR:HG22	2:H:26:THR:O	2.19	0.42
1:I:619:ALA:HB2	1:I:634:VAL:HG11	2.01	0.42
1:K:16:LYS:CA	1:K:29:MET:HE1	2.49	0.42
1:M:163:THR:CG2	1:M:359:HIS:CE1	2.92	0.42
1:M:554:LEU:O	1:M:557:ALA:N	2.50	0.42
1:O:125:THR:CG2	1:O:126:ILE:N	2.82	0.42
1:O:183:VAL:CG2	1:O:340:TRP:CE2	3.00	0.42
1:O:356:TRP:HZ3	1:O:674:PRO:O	2.03	0.42
1:O:692:THR:CG2	5:O:1803:MGD:N18	2.76	0.42
1:A:147:PRO:HD3	1:A:397:PHE:HA	2.01	0.42
1:A:162:ARG:NH1	1:A:359:HIS:NE2	2.67	0.42
1:A:396:THR:CG2	1:A:396:THR:O	2.64	0.42
2:B:117:ARG:HH11	2:B:124:PRO:HD3	1.85	0.42
1:C:503:VAL:HG13	1:C:503:VAL:O	2.19	0.42
2:D:102:HIS:CD2	6:D:1129:HEC:NB	2.87	0.42
1:E:181:ALA:HB3	1:E:340:TRP:CE3	2.47	0.42
1:E:20:ARG:CG	1:E:20:ARG:O	2.68	0.42
1:E:409:ASN:HB3	1:E:412:HIS:CD2	2.55	0.42
1:E:563:LYS:O	1:E:567:GLU:HG3	2.19	0.42
2:F:26:THR:HG22	2:F:26:THR:O	2.19	0.42
1:G:334:ALA:O	1:G:336:PRO:N	2.53	0.42
1:G:76:ARG:HH22	1:G:473:ARG:CZ	2.32	0.42
1:I:482:SER:HA	1:I:497:LEU:O	2.20	0.42
1:I:752:GLU:OE1	1:I:755:GLY:CA	2.67	0.42
2:J:82:ASP:C	2:J:94:ARG:NH1	2.73	0.42
1:K:276:LEU:HD13	1:K:280:HIS:CG	2.55	0.42
1:K:409:ASN:HA	1:K:410:PRO:HD3	1.75	0.42
1:M:183:VAL:CG1	1:M:185:TRP:NE1	2.82	0.42
1:M:271:ASP:HB3	1:M:287:LYS:O	2.19	0.42
1:M:473:ARG:HD2	1:M:473:ARG:HH11	1.74	0.42
2:N:26:THR:HG22	2:N:26:THR:O	2.19	0.42
1:O:465:ASP:HA	2:P:13:MET:HE1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:714:ALA:CB	2:P:103:VAL:CG1	2.97	0.42
1:A:195:ILE:HA	1:A:195:ILE:HD13	1.84	0.42
1:A:503:VAL:HG12	1:A:523:VAL:HG22	2.01	0.42
1:C:142:SER:HA	1:C:430:TRP:CZ2	2.55	0.42
1:C:491:ARG:NH1	2:D:10:ASP:HA	2.34	0.42
1:C:192:MET:HE1	1:C:694:ARG:CB	2.49	0.42
1:E:503:VAL:HG12	1:E:523:VAL:HG22	2.02	0.42
1:E:614:HIS:O	1:E:615:GLY:C	2.56	0.42
2:F:49:TYR:CD2	2:F:57:ARG:HG2	2.54	0.42
1:G:455:ASN:ND2	1:G:457:ASN:H	2.18	0.42
1:G:554:LEU:O	1:G:557:ALA:N	2.53	0.42
1:G:710:GLU:HA	2:H:105:GLN:OE1	2.19	0.42
1:I:458:MET:HB2	1:I:489:THR:HA	2.01	0.42
1:I:487:THR:HG22	1:I:489:THR:N	2.34	0.42
1:I:582:ASP:O	1:I:598:TYR:CE2	2.73	0.42
1:K:190:ALA:HA	1:K:197:TRP:CD1	2.55	0.42
1:K:298:THR:HB	1:K:299:ASP:H	1.42	0.42
1:K:590:HIS:O	1:K:594:LEU:HG	2.20	0.42
1:M:409:ASN:HA	1:M:410:PRO:HD3	1.76	0.42
1:M:472:TYR:HA	1:M:479:ILE:HD13	2.02	0.42
1:O:351:HIS:HB3	1:O:354:GLY:CA	2.50	0.42
1:O:747:ILE:HG22	1:O:748:ARG:H	1.78	0.42
2:L:50:GLN:HB3	2:P:123:MET:HG3	2.02	0.42
1:A:428:PRO:HB3	1:A:430:TRP:NE1	2.34	0.42
1:A:506:GLU:OE1	1:A:625:HIS:HE1	2.03	0.42
1:C:263:THR:CG2	1:C:264:ASN:N	2.83	0.42
1:C:350:GLN:OE1	1:C:793:LYS:HE2	2.20	0.42
1:C:740:VAL:HG13	1:C:797:VAL:CG1	2.35	0.42
1:E:134:LYS:NZ	1:E:569:LEU:O	2.53	0.42
1:E:161:MET:O	1:E:165:GLY:N	2.49	0.42
1:E:740:VAL:O	1:E:746:GLU:HA	2.20	0.42
1:G:554:LEU:HD13	1:G:561:ARG:HG2	2.01	0.42
1:I:100:MET:HG3	1:I:495:LEU:HD23	2.02	0.42
1:I:190:ALA:HA	1:I:197:TRP:CD1	2.54	0.42
1:I:747:ILE:HG22	1:I:748:ARG:H	1.79	0.42
1:K:433:ALA:HA	1:K:437:GLU:OE1	2.19	0.42
1:K:723:HIS:HD2	1:K:725:GLU:N	2.04	0.42
1:O:109:LYS:HD3	1:O:109:LYS:HA	1.83	0.42
1:O:118:MET:HE3	1:O:124:TRP:HH2	1.85	0.42
1:O:454:VAL:HG22	5:O:1803:MGD:C2	2.50	0.42
1:O:28:VAL:CG1	1:O:29:MET:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:383:GLY:HA3	5:O:1804:MGD:S12	2.59	0.42
1:O:564:THR:HG1	1:O:567:GLU:HG3	1.85	0.42
1:O:76:ARG:NH2	1:O:473:ARG:HH22	2.14	0.42
1:A:455:ASN:HD22	1:A:457:ASN:N	2.15	0.42
2:D:33:ARG:HH21	2:D:40:PRO:CG	2.22	0.42
1:E:233:ARG:HB3	1:E:236:THR:HG21	2.00	0.42
1:E:181:ALA:HB1	1:E:340:TRP:CH2	2.55	0.42
1:G:49:ASN:O	1:G:50:ARG:HB2	2.20	0.42
1:G:619:ALA:HB1	1:G:620:PRO:HD2	2.01	0.42
2:H:34:ASN:H	2:H:38:GLN:HE22	1.68	0.42
2:H:42:ILE:HG12	6:H:1128:HEC:CHB	2.50	0.42
1:I:181:ALA:CB	1:I:340:TRP:CH2	3.02	0.42
1:I:321:VAL:CG2	1:I:326:LEU:HD11	2.49	0.42
2:J:32:GLY:CA	2:P:70:VAL:HG22	2.50	0.42
1:K:130:TYR:CD1	1:K:603:LEU:HD23	2.54	0.42
1:K:181:ALA:HB3	1:K:340:TRP:CE3	2.45	0.42
1:K:565:LEU:O	1:K:566:PHE:CB	2.67	0.42
1:K:627:VAL:HG12	1:K:628:ARG:H	1.83	0.42
1:K:29:MET:CE	1:K:628:ARG:HH12	2.31	0.42
1:M:436:VAL:CG1	1:M:440:ARG:CZ	2.98	0.42
1:M:582:ASP:O	1:M:598:TYR:CE2	2.73	0.42
1:M:738:VAL:O	1:M:748:ARG:HA	2.19	0.42
1:M:722:MET:HE3	1:M:751:LEU:HD11	2.02	0.42
1:O:157:ALA:O	1:O:160:PHE:HB2	2.19	0.42
1:O:181:ALA:HB1	1:O:211:ARG:O	2.19	0.42
2:P:82:ASP:O	2:P:83:ARG:C	2.58	0.42
1:A:513:GLU:OE2	1:A:515:ARG:NH1	2.53	0.42
1:C:269:ALA:O	1:C:272:ILE:HD12	2.20	0.42
1:C:33:ARG:NH1	2:D:119:MET:O	2.41	0.42
1:C:750:ARG:HD3	2:D:20:PRO:HA	1.99	0.42
1:E:338:ARG:HG2	1:E:340:TRP:HZ3	1.82	0.42
1:E:183:VAL:CG2	1:E:340:TRP:CE2	2.99	0.42
1:E:557:ALA:HB3	1:E:560:TYR:HD1	1.85	0.42
1:E:615:GLY:O	1:E:617:ASP:N	2.53	0.42
1:G:157:ALA:O	1:G:160:PHE:HB2	2.20	0.42
1:G:513:GLU:OE2	1:G:515:ARG:NH1	2.53	0.42
1:I:238:ARG:NH1	1:I:676:GLU:O	2.53	0.42
1:M:183:VAL:HG11	1:M:185:TRP:NE1	2.35	0.42
1:M:458:MET:HB2	1:M:489:THR:HA	2.02	0.42
1:O:723:HIS:HB3	1:O:726:ASP:HB2	2.02	0.42
1:A:353:ARG:HD2	1:A:356:TRP:CE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:SER:HA	1:A:497:LEU:O	2.20	0.42
1:A:545:THR:O	1:A:546:ASP:O	2.38	0.42
1:A:747:ILE:HG22	1:A:748:ARG:H	1.82	0.42
2:B:86:GLN:HE21	2:B:86:GLN:CA	2.30	0.42
1:C:300:PHE:O	1:C:300:PHE:HD1	2.03	0.42
1:C:335:ASP:C	1:C:337:ASP:H	2.24	0.42
6:D:1129:HEC:HMC1	6:D:1129:HEC:HBC3	2.02	0.42
1:E:522:LEU:N	1:E:522:LEU:HD13	2.34	0.42
1:E:41:HIS:CD2	2:F:37:GLU:HB2	2.55	0.42
1:G:742:SER:OG	1:G:797:VAL:HG22	2.19	0.42
1:G:690:LEU:HD11	1:G:766:VAL:HG22	2.02	0.42
1:I:211:ARG:HB2	1:I:338:ARG:NH1	2.33	0.42
1:I:26:CYS:SG	1:I:49:ASN:HB3	2.59	0.42
1:I:613:GLY:O	1:I:615:GLY:N	2.53	0.42
1:K:242:ASN:O	1:K:243:TYR:C	2.59	0.42
1:K:259:VAL:O	1:K:263:THR:HB	2.19	0.42
2:L:66:TYR:O	2:L:67:SER:C	2.58	0.42
1:M:614:HIS:O	1:M:615:GLY:C	2.58	0.42
1:O:73:PRO:O	1:O:74:LEU:HD13	2.20	0.42
1:A:183:VAL:HG12	1:A:185:TRP:CD1	2.55	0.41
1:A:549:TRP:CH2	1:A:568:VAL:HG11	2.54	0.41
1:C:406:VAL:H	1:C:412:HIS:CD2	2.37	0.41
1:C:504:GLU:C	1:C:521:GLN:HG3	2.40	0.41
1:E:69:ARG:NH2	1:E:526:PRO:HD2	2.35	0.41
2:F:10:ASP:O	2:F:12:PRO:N	2.53	0.41
1:G:406:VAL:H	1:G:412:HIS:HD2	1.68	0.41
1:G:534:TRP:CD1	1:G:594:LEU:HD12	2.55	0.41
1:I:109:LYS:HD3	1:I:109:LYS:HA	1.84	0.41
1:I:183:VAL:HG23	1:I:340:TRP:NE1	2.33	0.41
1:I:298:THR:HB	1:I:299:ASP:H	1.41	0.41
1:I:551:GLU:HG2	1:I:551:GLU:H	1.36	0.41
1:I:537:MET:HE3	1:I:595:PHE:CE2	2.54	0.41
1:I:597:PHE:HB2	1:I:598:TYR:H	1.64	0.41
1:K:554:LEU:O	1:K:557:ALA:N	2.52	0.41
1:M:182:PHE:CD1	1:M:200:LEU:HD13	2.55	0.41
1:M:20:ARG:O	1:M:20:ARG:CG	2.66	0.41
1:M:211:ARG:HB2	1:M:338:ARG:HH12	1.85	0.41
1:M:353:ARG:HD2	1:M:356:TRP:CE3	2.55	0.41
1:M:503:VAL:HG12	1:M:523:VAL:HG22	2.01	0.41
1:M:600:GLN:HB3	1:M:600:GLN:HE21	1.66	0.41
1:O:213:ALA:CB	1:O:228:THR:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:272:ILE:HG12	1:O:292:ALA:CB	2.50	0.41
1:O:442:LEU:HA	1:O:442:LEU:HD12	1.92	0.41
2:P:14:SER:O	2:P:15:GLU:CB	2.68	0.41
1:O:41:HIS:CD2	2:P:37:GLU:HB2	2.55	0.41
1:A:391:ALA:HA	1:A:396:THR:HB	2.01	0.41
1:A:543:PHE:N	1:A:543:PHE:CD1	2.88	0.41
1:A:544:THR:CG2	1:A:547:GLU:HB2	2.39	0.41
1:C:204:ARG:NH1	1:C:227:ASP:OD1	2.53	0.41
1:C:428:PRO:HB3	1:C:430:TRP:NE1	2.35	0.41
1:C:555:SER:OG	1:C:556:ALA:N	2.53	0.41
2:D:33:ARG:NH2	6:D:1129:HEC:HAA1	2.35	0.41
1:E:246:HIS:HB2	1:E:307:VAL:HG12	2.01	0.41
1:E:271:ASP:HB3	1:E:287:LYS:O	2.20	0.41
1:E:722:MET:HE3	1:E:751:LEU:HD11	2.01	0.41
1:E:89:ALA:HA	1:E:90:PRO:HD3	1.91	0.41
1:G:511:ASN:CG	1:G:515:ARG:HB3	2.40	0.41
1:G:612:ARG:HA	1:G:617:ASP:OD1	2.20	0.41
1:G:76:ARG:NH2	1:G:473:ARG:HH22	2.17	0.41
1:G:772:SER:HB3	2:H:6:LEU:CD2	2.50	0.41
1:I:504:GLU:C	1:I:521:GLN:HG3	2.41	0.41
1:I:744:ARG:CZ	1:I:780:LEU:HB2	2.50	0.41
1:K:183:VAL:CG2	1:K:340:TRP:CZ2	2.97	0.41
1:K:454:VAL:HG22	5:K:1803:MGD:C2	2.50	0.41
1:K:514:ARG:NH2	1:K:641:ARG:O	2.50	0.41
2:L:62:HIS:HA	2:L:74:MET:CB	2.49	0.41
1:M:272:ILE:CG2	1:M:785:PRO:HG2	2.50	0.41
1:M:557:ALA:HA	1:M:558:PRO:HD2	1.64	0.41
1:M:604:PHE:CZ	1:M:618:LEU:HD13	2.55	0.41
1:O:329:LEU:O	1:O:330:ALA:C	2.58	0.41
1:O:604:PHE:CZ	1:O:618:LEU:HD13	2.55	0.41
1:O:613:GLY:O	1:O:651:TYR:CE2	2.73	0.41
1:C:694:ARG:HH22	5:C:1803:MGD:H15	1.67	0.41
1:C:458:MET:HB2	1:C:489:THR:HA	2.02	0.41
1:E:505:LYS:HG2	1:E:505:LYS:O	2.17	0.41
1:E:720:CYS:SG	1:E:764:VAL:CG1	3.08	0.41
1:G:204:ARG:NH1	1:G:227:ASP:OD1	2.53	0.41
1:G:409:ASN:HB3	1:G:412:HIS:CD2	2.56	0.41
1:G:458:MET:HB2	1:G:489:THR:HA	2.01	0.41
1:G:482:SER:HA	1:G:497:LEU:O	2.20	0.41
1:K:334:ALA:O	1:K:335:ASP:C	2.57	0.41
1:K:181:ALA:HB1	1:K:340:TRP:CH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:782:ALA:C	1:K:783:ASN:HD22	2.24	0.41
1:M:130:TYR:CD1	1:M:603:LEU:HD23	2.55	0.41
1:O:16:LYS:CA	1:O:29:MET:HE1	2.50	0.41
1:O:192:MET:HB3	5:O:1804:MGD:H22	1.85	0.41
1:O:482:SER:HA	1:O:497:LEU:O	2.20	0.41
1:A:464:ILE:HG22	1:A:468:THR:HB	2.02	0.41
1:A:601:LYS:HA	1:A:621:PHE:CD1	2.55	0.41
1:A:270:THR:CG2	1:A:674:PRO:HG3	2.50	0.41
1:A:192:MET:HE1	1:A:694:ARG:CB	2.48	0.41
1:A:723:HIS:HD2	1:A:725:GLU:N	2.03	0.41
1:C:125:THR:CG2	1:C:126:ILE:N	2.83	0.41
1:C:394:VAL:HG22	1:C:607:TYR:CE1	2.56	0.41
1:C:682:PRO:HA	1:C:796:ALA:CB	2.50	0.41
1:C:702:GLY:HA3	1:C:706:LEU:CD1	2.50	0.41
1:E:40:THR:O	1:E:40:THR:HG22	2.21	0.41
1:E:783:ASN:ND2	1:E:783:ASN:N	2.66	0.41
1:G:406:VAL:H	1:G:412:HIS:CD2	2.39	0.41
1:G:443:HIS:CD2	1:G:467:GLU:HG3	2.55	0.41
1:K:334:ALA:O	1:K:336:PRO:N	2.53	0.41
2:L:21:LEU:HA	2:L:22:PRO:HD3	1.91	0.41
1:M:272:ILE:HG12	1:M:292:ALA:CB	2.50	0.41
1:O:125:THR:HG22	1:O:127:TRP:H	1.85	0.41
1:O:152:CYS:SG	1:O:153:MET:SD	3.18	0.41
1:O:193:HIS:N	1:O:194:PRO:CD	2.84	0.41
1:O:338:ARG:HG2	1:O:340:TRP:HE3	1.83	0.41
1:O:427:LEU:HA	1:O:428:PRO:HD3	1.77	0.41
1:O:433:ALA:HB1	1:O:437:GLU:HG2	2.02	0.41
1:O:566:PHE:O	1:O:571:ALA:N	2.51	0.41
1:O:770:ASP:OD2	2:P:6:LEU:HB3	2.21	0.41
1:A:183:VAL:CG2	1:A:340:TRP:CZ2	2.99	0.41
2:B:102:HIS:CD2	6:B:1129:HEC:NB	2.88	0.41
1:C:118:MET:HE2	1:C:136:MET:HG3	2.02	0.41
1:C:564:THR:HG1	1:C:567:GLU:HG3	1.85	0.41
1:C:641:ARG:HD2	1:C:642:TRP:CZ3	2.56	0.41
1:E:28:VAL:HG12	1:E:29:MET:N	2.35	0.41
2:F:21:LEU:HA	2:F:22:PRO:HD3	1.90	0.41
1:G:272:ILE:HG12	1:G:292:ALA:CB	2.49	0.41
1:G:272:ILE:HG22	1:G:353:ARG:CZ	2.51	0.41
1:G:365:HIS:CD2	1:G:378:PRO:HB3	2.55	0.41
1:G:590:HIS:O	1:G:594:LEU:HG	2.20	0.41
1:I:119:PHE:CE2	1:I:457:ASN:CG	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:538:GLU:OE2	1:I:541:LYS:HD2	2.20	0.41
1:I:583:VAL:HG23	1:I:598:TYR:CZ	2.55	0.41
1:K:21:PHE:O	1:K:385:PRO:HD3	2.21	0.41
1:K:503:VAL:HG11	1:K:522:LEU:HB2	2.00	0.41
1:K:633:PRO:HG2	1:K:640:THR:CB	2.50	0.41
1:K:740:VAL:O	1:K:746:GLU:HA	2.19	0.41
1:K:782:ALA:C	1:K:783:ASN:ND2	2.74	0.41
2:N:33:ARG:CZ	2:N:40:PRO:HG3	2.51	0.41
1:O:543:PHE:O	1:O:564:THR:CA	2.67	0.41
1:O:692:THR:HB	1:O:792:PHE:O	2.20	0.41
1:A:161:MET:O	1:A:165:GLY:N	2.48	0.41
1:A:351:HIS:HB3	1:A:354:GLY:CA	2.51	0.41
1:C:436:VAL:HG11	1:C:440:ARG:NH2	2.36	0.41
1:C:505:LYS:O	1:C:505:LYS:HG2	2.18	0.41
2:D:82:ASP:HB3	2:D:88:LEU:CD1	2.50	0.41
1:E:511:ASN:CG	1:E:515:ARG:HB3	2.41	0.41
1:G:333:TYR:CZ	1:G:340:TRP:CD1	3.08	0.41
1:G:544:THR:CG2	1:G:547:GLU:HB2	2.38	0.41
6:H:1128:HEC:HHB	6:H:1128:HEC:HMA1	1.92	0.41
1:I:180:ASP:CB	1:I:339:LYS:H	2.22	0.41
1:I:738:VAL:CG1	1:I:751:LEU:HD22	2.49	0.41
2:J:62:HIS:HB3	6:J:1129:HEC:HMB2	2.02	0.41
1:K:109:LYS:HD3	1:K:109:LYS:HA	1.80	0.41
1:K:351:HIS:HB3	1:K:354:GLY:CA	2.50	0.41
2:L:42:ILE:HG12	6:L:1128:HEC:CHB	2.51	0.41
1:M:183:VAL:HG23	1:M:340:TRP:HZ2	1.78	0.41
1:M:338:ARG:HD3	1:M:338:ARG:HH11	1.73	0.41
2:N:40:PRO:HD3	6:N:1129:HEC:CBD	2.50	0.41
1:O:458:MET:HB2	1:O:489:THR:HA	2.03	0.41
2:P:49:TYR:N	2:P:49:TYR:CD2	2.89	0.41
1:A:188:ASN:ND2	1:A:222:SER:OG	2.48	0.41
1:A:740:VAL:HG13	1:A:797:VAL:CG1	2.40	0.41
1:A:747:ILE:CG2	1:A:748:ARG:N	2.77	0.41
1:A:690:LEU:HD11	1:A:766:VAL:HG22	2.03	0.41
1:A:76:ARG:NH2	1:A:493:ALA:O	2.53	0.41
1:C:742:SER:HB2	1:C:778:VAL:HG13	2.01	0.41
1:C:739:ARG:O	1:C:799:ILE:HA	2.21	0.41
1:E:238:ARG:NE	1:E:351:HIS:HE1	2.19	0.41
1:E:272:ILE:HG12	1:E:292:ALA:CB	2.51	0.41
1:E:286:ALA:O	1:E:287:LYS:C	2.58	0.41
1:E:428:PRO:HB3	1:E:430:TRP:NE1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:781:ASP:OD1	1:E:781:ASP:O	2.37	0.41
2:F:16:VAL:HG12	2:F:17:ALA:N	2.36	0.41
1:G:613:GLY:O	1:G:615:GLY:N	2.54	0.41
1:G:675:TYR:CE1	1:G:676:GLU:O	2.73	0.41
2:H:51:LEU:HD22	2:H:56:ASN:ND2	2.35	0.41
1:I:204:ARG:NH1	1:I:227:ASP:OD1	2.53	0.41
1:I:141:ARG:NE	1:I:426:LEU:O	2.47	0.41
1:I:781:ASP:O	1:I:781:ASP:OD1	2.38	0.41
1:I:783:ASN:ND2	1:I:783:ASN:N	2.68	0.41
1:K:271:ASP:HB3	1:K:287:LYS:O	2.21	0.41
1:K:338:ARG:HH11	1:K:338:ARG:HD3	1.63	0.41
1:K:741:ILE:O	1:K:797:VAL:HG13	2.20	0.41
1:M:781:ASP:O	1:M:781:ASP:OD1	2.38	0.41
2:N:51:LEU:HD22	2:N:56:ASN:ND2	2.35	0.41
1:O:107:VAL:C	1:O:109:LYS:H	2.24	0.41
1:O:277:ARG:HH21	1:O:467:GLU:HG2	1.86	0.41
1:O:506:GLU:OE1	1:O:625:HIS:HE1	2.03	0.41
1:O:68:ASP:CB	1:O:707:ARG:NH1	2.74	0.41
1:O:78:LYS:HB2	1:O:89:ALA:HB1	2.03	0.41
2:P:77:ILE:HG23	2:P:87:MET:SD	2.61	0.41
1:A:118:MET:HE3	1:A:124:TRP:HH2	1.86	0.41
1:A:334:ALA:O	1:A:336:PRO:N	2.54	0.41
1:A:28:VAL:HG21	1:A:60:LEU:HD12	2.02	0.41
1:C:118:MET:HE3	1:C:124:TRP:HH2	1.84	0.41
1:C:183:VAL:CG1	1:C:185:TRP:NE1	2.84	0.41
1:C:338:ARG:HG2	1:C:340:TRP:HZ3	1.84	0.41
1:C:150:ARG:HG2	1:C:435:ALA:HB3	2.02	0.41
1:E:223:SER:HA	1:E:226:SER:OG	2.21	0.41
1:E:560:TYR:HA	1:E:563:LYS:HG3	2.02	0.41
1:E:619:ALA:HB2	1:E:634:VAL:HG11	2.01	0.41
1:E:719:VAL:CG1	1:E:752:GLU:HB2	2.51	0.41
1:G:184:LEU:HD21	1:G:189:MET:HG3	2.03	0.41
1:G:246:HIS:ND1	1:G:308:SER:HA	2.36	0.41
1:G:403:ALA:O	1:G:404:ASP:HB2	2.21	0.41
2:H:14:SER:O	2:H:15:GLU:CB	2.67	0.41
1:I:719:VAL:HG12	1:I:750:ARG:O	2.21	0.41
2:J:10:ASP:O	2:J:12:PRO:N	2.54	0.41
1:K:106:LEU:HG	1:K:107:VAL:N	2.36	0.41
1:K:238:ARG:CZ	1:K:351:HIS:HE1	2.34	0.41
1:K:443:HIS:HD2	1:K:467:GLU:CG	2.33	0.41
1:K:503:VAL:O	1:K:503:VAL:HG13	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:749:THR:CG2	1:K:773:GLN:OE1	2.51	0.41
1:M:633:PRO:HD2	1:M:640:THR:CB	2.44	0.41
1:O:619:ALA:HB1	1:O:620:PRO:HD2	2.02	0.41
1:O:353:ARG:NH2	1:O:676:GLU:OE1	2.40	0.41
2:P:61:CYS:SG	6:P:1128:HEC:C3C	3.09	0.41
1:A:152:CYS:HB2	5:A:1803:MGD:S13	2.61	0.41
1:A:390:THR:O	1:A:391:ALA:C	2.58	0.41
1:A:747:ILE:HD13	1:A:747:ILE:HG21	1.78	0.41
1:C:190:ALA:HA	1:C:197:TRP:CD1	2.56	0.41
1:C:188:ASN:ND2	1:C:222:SER:OG	2.48	0.41
1:C:633:PRO:HD2	1:C:640:THR:CB	2.39	0.41
1:E:747:ILE:HG21	1:E:747:ILE:HD13	1.80	0.41
1:E:750:ARG:HD2	2:F:20:PRO:HA	2.00	0.41
1:G:409:ASN:OD1	1:G:411:GLU:N	2.54	0.41
1:G:438:GLN:O	1:G:442:LEU:HB2	2.20	0.41
1:G:455:ASN:HD22	1:G:457:ASN:N	2.19	0.41
1:G:563:LYS:O	1:G:567:GLU:HG3	2.20	0.41
1:I:245:ALA:CB	1:I:307:VAL:HG11	2.49	0.41
2:J:82:ASP:HB3	2:J:88:LEU:CD1	2.51	0.41
1:K:272:ILE:HG12	1:K:292:ALA:CB	2.51	0.41
1:K:750:ARG:HD2	2:L:20:PRO:HA	2.00	0.41
1:M:121:SER:C	1:M:123:GLN:N	2.72	0.41
1:M:181:ALA:HB1	1:M:340:TRP:CZ3	2.50	0.41
1:M:482:SER:HA	1:M:497:LEU:O	2.21	0.41
2:N:98:CYS:O	2:N:100:ALA:N	2.54	0.41
2:N:5:ARG:O	2:N:7:THR:N	2.53	0.41
2:N:75:ILE:HD12	2:N:80:PHE:HE2	1.86	0.41
1:O:334:ALA:O	1:O:336:PRO:N	2.53	0.41
1:O:406:VAL:H	1:O:412:HIS:CD2	2.39	0.41
1:O:78:LYS:HB2	1:O:89:ALA:CB	2.51	0.41
1:A:334:ALA:O	1:A:335:ASP:C	2.58	0.41
1:A:557:ALA:HA	1:A:558:PRO:HD2	1.64	0.41
1:A:560:TYR:HA	1:A:563:LYS:HG3	2.03	0.41
1:C:106:LEU:HG	1:C:107:VAL:N	2.35	0.41
1:C:183:VAL:CG2	1:C:340:TRP:CZ2	2.97	0.41
1:C:752:GLU:OE1	1:C:755:GLY:CA	2.69	0.41
1:E:482:SER:HA	1:E:497:LEU:O	2.20	0.41
1:E:579:PRO:O	1:E:581:SER:O	2.39	0.41
1:E:597:PHE:HB2	1:E:598:TYR:H	1.68	0.41
1:E:702:GLY:HA3	1:E:706:LEU:CD1	2.50	0.41
1:E:697:GLU:CD	1:E:756:ARG:HH22	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:MET:CE	1:G:343:LEU:HD13	2.50	0.41
1:G:75:LEU:HD12	1:G:76:ARG:H	1.86	0.41
1:G:772:SER:HB3	2:H:6:LEU:HD22	2.03	0.41
1:I:121:SER:HB2	1:I:148:ASN:ND2	2.36	0.41
1:I:694:ARG:HH22	5:I:1803:MGD:H15	1.69	0.41
1:I:243:TYR:CE1	1:I:312:LEU:HB2	2.56	0.41
1:I:245:ALA:HB3	1:I:307:VAL:CG1	2.48	0.41
2:J:14:SER:O	2:J:15:GLU:CB	2.69	0.41
1:K:121:SER:C	1:K:123:GLN:N	2.72	0.41
1:K:182:PHE:CD1	1:K:200:LEU:HD13	2.56	0.41
1:K:365:HIS:CD2	1:K:378:PRO:HB3	2.55	0.41
1:K:49:ASN:O	1:K:50:ARG:HB2	2.21	0.41
1:K:722:MET:HE1	1:K:751:LEU:HD11	2.02	0.41
1:M:276:LEU:HB3	1:M:277:ARG:H	1.76	0.41
1:M:491:ARG:NH1	2:N:10:ASP:HA	2.35	0.41
1:O:384:GLN:HB3	1:O:385:PRO:CD	2.47	0.41
1:O:619:ALA:HB2	1:O:634:VAL:HG11	2.03	0.41
1:O:783:ASN:HD22	1:O:790:THR:HA	1.86	0.41
1:A:793:LYS:CE	5:A:1804:MGD:H5'2	2.51	0.41
1:A:21:PHE:CZ	1:A:63:ILE:CD1	3.01	0.41
1:A:246:HIS:HB2	1:A:307:VAL:HG12	2.02	0.41
1:A:277:ARG:HH21	1:A:467:GLU:HG2	1.86	0.41
1:A:76:ARG:HH21	1:A:473:ARG:HH22	1.67	0.41
2:B:40:PRO:HD2	2:B:102:HIS:CE1	2.55	0.41
1:C:682:PRO:HA	1:C:796:ALA:HB2	2.01	0.41
1:C:759:MET:HE2	1:C:765:PHE:N	2.37	0.41
1:E:559:ALA:O	1:E:560:TYR:CD1	2.74	0.41
1:E:791:ASP:C	1:E:791:ASP:OD1	2.60	0.41
2:F:98:CYS:C	2:F:100:ALA:H	2.24	0.41
2:F:77:ILE:HG23	2:F:87:MET:SD	2.61	0.41
1:G:436:VAL:HG11	1:G:440:ARG:NH2	2.36	0.41
2:H:117:ARG:HH11	2:H:124:PRO:HD3	1.86	0.41
1:I:646:GLU:OE2	1:I:654:PRO:O	2.38	0.41
1:K:613:GLY:O	1:K:651:TYR:CE2	2.74	0.41
1:K:729:SER:OG	1:K:730:ARG:N	2.54	0.41
1:K:697:GLU:CD	1:K:756:ARG:HH22	2.24	0.41
1:M:125:THR:CG2	1:M:126:ILE:N	2.84	0.41
1:M:244:ILE:HG23	1:M:330:ALA:HA	2.03	0.41
1:M:433:ALA:HA	1:M:437:GLU:OE1	2.21	0.41
1:M:649:ASP:OD2	1:M:650:PRO:HD2	2.21	0.41
1:O:646:GLU:OE2	1:O:654:PRO:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:98:CYS:CB	6:P:1129:HEC:CAB	2.85	0.41
1:A:130:TYR:HD1	1:A:603:LEU:HD23	1.87	0.40
1:A:16:LYS:HB2	1:A:29:MET:HE1	2.03	0.40
1:A:28:VAL:CG1	1:A:29:MET:N	2.84	0.40
1:A:211:ARG:CG	1:A:338:ARG:HH12	2.34	0.40
1:A:505:LYS:HG2	1:A:505:LYS:O	2.20	0.40
1:C:594:LEU:O	1:C:595:PHE:HB2	2.20	0.40
1:C:73:PRO:O	1:C:74:LEU:HD13	2.21	0.40
2:D:98:CYS:O	2:D:100:ALA:N	2.54	0.40
1:E:111:LYS:O	1:E:112:ALA:HB3	2.22	0.40
1:E:274:TYR:O	1:E:276:LEU:N	2.55	0.40
1:E:334:ALA:O	1:E:336:PRO:N	2.53	0.40
1:E:192:MET:HE1	1:E:694:ARG:CB	2.50	0.40
2:F:51:LEU:HD22	2:F:56:ASN:ND2	2.35	0.40
1:G:598:TYR:CE1	1:G:600:GLN:CG	3.04	0.40
2:H:82:ASP:HB3	2:H:88:LEU:CD1	2.51	0.40
1:I:274:TYR:O	1:I:276:LEU:N	2.53	0.40
1:I:427:LEU:HA	1:I:428:PRO:HD3	1.78	0.40
2:J:26:THR:O	2:J:26:THR:HG22	2.21	0.40
2:J:30:ARG:HD2	6:J:1128:HEC:O1D	2.21	0.40
1:K:132:ALA:HB2	1:K:536:LEU:HD21	2.03	0.40
1:K:194:PRO:HD2	3:K:1801:SF4:S4	2.61	0.40
1:K:286:ALA:O	1:K:287:LYS:C	2.58	0.40
1:K:563:LYS:O	1:K:564:THR:OG1	2.38	0.40
1:K:700:HIS:HE1	5:K:1804:MGD:S13	2.44	0.40
2:L:117:ARG:HH11	2:L:124:PRO:HD3	1.86	0.40
1:M:326:LEU:CD1	1:M:326:LEU:N	2.84	0.40
1:M:406:VAL:H	1:M:412:HIS:HD2	1.68	0.40
1:M:144:ASN:HD21	1:M:433:ALA:H	1.62	0.40
1:M:692:THR:HB	1:M:792:PHE:O	2.20	0.40
2:N:37:GLU:N	6:N:1129:HEC:O1D	2.54	0.40
1:O:504:GLU:C	1:O:521:GLN:HG3	2.42	0.40
1:O:544:THR:HG22	1:O:547:GLU:OE1	2.21	0.40
1:A:791:ASP:C	1:A:791:ASP:OD1	2.60	0.40
1:A:89:ALA:HA	1:A:90:PRO:HD3	1.91	0.40
2:B:51:LEU:HD22	2:B:56:ASN:ND2	2.35	0.40
1:C:242:ASN:O	1:C:243:TYR:C	2.59	0.40
1:E:443:HIS:HD2	1:E:467:GLU:CG	2.34	0.40
1:E:558:PRO:O	1:E:561:ARG:HB2	2.21	0.40
1:E:738:VAL:CG1	1:E:751:LEU:HD22	2.50	0.40
1:G:673:VAL:HA	1:G:674:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:767:PRO:O	1:G:775:ILE:HD11	2.21	0.40
2:H:5:ARG:HA	2:H:5:ARG:HD3	1.94	0.40
1:I:238:ARG:NH1	1:I:353:ARG:CG	2.79	0.40
1:I:242:ASN:O	1:I:243:TYR:C	2.59	0.40
1:I:28:VAL:CG1	1:I:29:MET:N	2.84	0.40
1:I:49:ASN:O	1:I:50:ARG:HB2	2.21	0.40
1:I:543:PHE:HB3	1:I:548:VAL:HG21	2.03	0.40
1:I:723:HIS:HB3	1:I:726:ASP:HB2	2.02	0.40
1:I:759:MET:HA	1:I:760:PRO:HD3	1.92	0.40
1:K:515:ARG:HH11	1:K:515:ARG:HD2	1.70	0.40
1:M:202:ASP:O	1:M:206:SER:HB2	2.22	0.40
1:M:700:HIS:HE1	5:M:1804:MGD:S13	2.44	0.40
1:O:20:ARG:O	1:O:20:ARG:CG	2.68	0.40
1:O:409:ASN:HA	1:O:410:PRO:HD3	1.73	0.40
1:O:563:LYS:O	1:O:567:GLU:CD	2.60	0.40
2:P:66:TYR:C	2:P:68:GLY:N	2.75	0.40
1:O:772:SER:HB3	2:P:6:LEU:CD2	2.51	0.40
1:A:16:LYS:HA	1:A:29:MET:HE2	2.03	0.40
1:A:190:ALA:HA	1:A:197:TRP:CD1	2.57	0.40
1:C:291:ASP:HB3	1:C:292:ALA:H	1.77	0.40
1:C:627:VAL:HG12	1:C:628:ARG:H	1.86	0.40
6:D:1128:HEC:HMA1	6:D:1128:HEC:HHB	1.95	0.40
1:C:491:ARG:HH22	2:D:11:ARG:H	1.68	0.40
1:G:501:MET:O	1:G:502:TRP:C	2.59	0.40
1:K:269:ALA:O	1:K:272:ILE:HD12	2.20	0.40
1:K:181:ALA:HB1	1:K:340:TRP:CZ3	2.51	0.40
1:K:646:GLU:OE2	1:K:654:PRO:O	2.38	0.40
2:L:10:ASP:O	2:L:12:PRO:N	2.55	0.40
2:N:98:CYS:C	2:N:100:ALA:N	2.74	0.40
1:O:353:ARG:HD2	1:O:356:TRP:CE3	2.56	0.40
1:O:710:GLU:CD	1:O:710:GLU:H	2.25	0.40
1:A:278:PRO:O	1:A:279:GLU:CD	2.60	0.40
1:A:142:SER:HA	1:A:430:TRP:CZ2	2.56	0.40
1:A:118:MET:HG2	1:A:451:TRP:HB3	2.01	0.40
1:A:472:TYR:HA	1:A:479:ILE:CD1	2.52	0.40
1:A:598:TYR:CE1	1:A:600:GLN:CG	3.05	0.40
2:B:33:ARG:NH2	6:B:1129:HEC:HAA1	2.37	0.40
2:B:75:ILE:HD12	2:B:80:PHE:HE2	1.86	0.40
2:B:98:CYS:C	2:B:100:ALA:N	2.75	0.40
1:C:194:PRO:HD2	3:C:1801:SF4:S4	2.61	0.40
1:C:700:HIS:HB3	1:C:768:TRP:CH2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:GLU:N	6:D:1129:HEC:O1D	2.55	0.40
1:E:454:VAL:HG12	1:E:454:VAL:O	2.21	0.40
1:E:694:ARG:NH1	1:E:700:HIS:CE1	2.89	0.40
1:E:719:VAL:HG12	1:E:750:ARG:O	2.21	0.40
1:G:697:GLU:CD	1:G:756:ARG:HH22	2.24	0.40
1:I:319:SER:CB	1:I:321:VAL:HG22	2.36	0.40
1:I:422:LEU:HD13	1:I:426:LEU:HD23	2.04	0.40
1:I:474:ASN:HA	1:I:474:ASN:HD22	1.63	0.40
1:K:472:TYR:HA	1:K:479:ILE:HD11	2.04	0.40
1:K:540:SER:C	1:K:542:ARG:N	2.75	0.40
1:K:564:THR:OG1	1:K:567:GLU:HG3	2.22	0.40
1:K:84:LYS:HD3	1:K:475:PRO:HA	2.03	0.40
2:L:111:LEU:HG	2:L:111:LEU:H	1.72	0.40
2:L:82:ASP:HB3	2:L:88:LEU:CD1	2.51	0.40
1:M:314:LYS:HG2	1:M:318:ILE:HD11	2.04	0.40
1:M:89:ALA:HA	1:M:90:PRO:HD3	1.93	0.40
1:O:118:MET:HE2	1:O:136:MET:HG3	2.03	0.40
1:O:125:THR:HG21	1:O:127:TRP:CD1	2.57	0.40
1:O:181:ALA:HB3	1:O:340:TRP:CE3	2.48	0.40
1:O:545:THR:O	1:O:546:ASP:O	2.39	0.40
2:P:120:LEU:O	2:P:121:THR:OG1	2.36	0.40
2:B:86:GLN:NE2	2:B:86:GLN:HA	2.35	0.40
1:C:543:PHE:HB3	1:C:548:VAL:HG21	2.04	0.40
1:E:384:GLN:HB2	1:E:387:ALA:HB2	2.02	0.40
1:E:759:MET:HE2	1:E:765:PHE:N	2.37	0.40
1:G:144:ASN:HA	1:G:144:ASN:HD22	1.60	0.40
1:I:191:GLU:C	1:I:192:MET:SD	3.00	0.40
1:I:329:LEU:O	1:I:330:ALA:C	2.60	0.40
1:I:339:LYS:CA	1:I:376:ASN:ND2	2.83	0.40
1:I:68:ASP:HB3	1:I:486:PRO:CD	2.52	0.40
1:I:697:GLU:CD	1:I:756:ARG:HH22	2.25	0.40
1:I:52:LEU:HD21	2:J:94:ARG:HG3	2.04	0.40
1:K:144:ASN:ND2	1:K:433:ALA:N	2.57	0.40
1:K:555:SER:OG	1:K:556:ALA:N	2.53	0.40
1:K:783:ASN:HD22	1:K:790:THR:HA	1.87	0.40
1:M:16:LYS:HB2	1:M:29:MET:HE1	2.04	0.40
1:M:501:MET:HG3	5:M:1803:MGD:N7	2.37	0.40
1:M:545:THR:O	1:M:546:ASP:O	2.39	0.40
1:O:21:PHE:CZ	1:O:63:ILE:CD1	2.99	0.40
1:O:272:ILE:HG22	1:O:353:ARG:CZ	2.51	0.40
2:P:3:ALA:O	2:P:4:PRO:C	2.59	0.40

All (5) 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:109:LYS:CG	1:C:655:GLY:O[2_556]	1.82	0.38
1:C:577:ARG:CB	1:K:287:LYS:NZ[2_545]	1.90	0.30
1:C:577:ARG:CG	1:K:287:LYS:NZ[2_545]	1.97	0.23
1:E:411:GLU:OE2	1:M:410:PRO:CG[1_556]	2.06	0.14
1:A:410:PRO:CB	1:K:411:GLU:OE2[1_556]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	788/802 (98%)	669 (85%)	85 (11%)	34 (4%)	2	20
1	C	788/802 (98%)	658 (84%)	94 (12%)	36 (5%)	2	18
1	E	788/802 (98%)	671 (85%)	82 (10%)	35 (4%)	2	19
1	G	788/802 (98%)	666 (84%)	90 (11%)	32 (4%)	3	21
1	I	788/802 (98%)	656 (83%)	99 (13%)	33 (4%)	3	20
1	K	788/802 (98%)	665 (84%)	89 (11%)	34 (4%)	2	20
1	M	788/802 (98%)	665 (84%)	87 (11%)	36 (5%)	2	18
1	O	788/802 (98%)	662 (84%)	92 (12%)	34 (4%)	2	20
2	B	125/130 (96%)	98 (78%)	14 (11%)	13 (10%)	0	3
2	D	125/130 (96%)	100 (80%)	13 (10%)	12 (10%)	0	3
2	F	125/130 (96%)	98 (78%)	14 (11%)	13 (10%)	0	3
2	H	125/130 (96%)	98 (78%)	14 (11%)	13 (10%)	0	3
2	J	125/130 (96%)	100 (80%)	11 (9%)	14 (11%)	0	2
2	L	125/130 (96%)	98 (78%)	14 (11%)	13 (10%)	0	3
2	N	125/130 (96%)	97 (78%)	14 (11%)	14 (11%)	0	2
2	P	125/130 (96%)	99 (79%)	14 (11%)	12 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7304/7456 (98%)	6100 (84%)	826 (11%)	378 (5%)	2	15

All (378) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	CYS
1	A	81	VAL
1	A	85	GLU
1	A	274	TYR
1	A	275	GLY
1	A	486	PRO
1	A	546	ASP
1	A	547	GLU
1	A	560	TYR
1	A	566	PHE
1	A	584	ASN
1	A	616	HIS
2	B	15	GLU
2	B	67	SER
2	B	122	LEU
1	C	22	CYS
1	C	81	VAL
1	C	85	GLU
1	C	274	TYR
1	C	275	GLY
1	C	486	PRO
1	C	541	LYS
1	C	546	ASP
1	C	547	GLU
1	C	560	TYR
1	C	566	PHE
1	C	584	ASN
1	C	616	HIS
2	D	15	GLU
2	D	67	SER
2	D	122	LEU
1	E	22	CYS
1	E	81	VAL
1	E	85	GLU
1	E	274	TYR
1	E	275	GLY
1	E	486	PRO

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Mol	Chain	Res	Type
1	E	541	LYS
1	E	546	ASP
1	E	547	GLU
1	E	560	TYR
1	E	566	PHE
1	E	584	ASN
1	E	616	HIS
2	F	15	GLU
2	F	67	SER
2	F	122	LEU
1	G	81	VAL
1	G	85	GLU
1	G	274	TYR
1	G	275	GLY
1	G	486	PRO
1	G	541	LYS
1	G	546	ASP
1	G	547	GLU
1	G	560	TYR
1	G	566	PHE
1	G	584	ASN
1	G	616	HIS
1	G	633	PRO
2	H	12	PRO
2	H	15	GLU
2	H	67	SER
2	H	122	LEU
1	I	22	CYS
1	I	81	VAL
1	I	85	GLU
1	I	274	TYR
1	I	275	GLY
1	I	486	PRO
1	I	502	TRP
1	I	541	LYS
1	I	546	ASP
1	I	547	GLU
1	I	560	TYR
1	I	566	PHE
1	I	584	ASN
1	I	616	HIS
1	I	633	PRO

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Mol	Chain	Res	Type
2	J	15	GLU
2	J	37	GLU
2	J	67	SER
2	J	122	LEU
1	K	22	CYS
1	K	81	VAL
1	K	85	GLU
1	K	274	TYR
1	K	275	GLY
1	K	486	PRO
1	K	541	LYS
1	K	546	ASP
1	K	547	GLU
1	K	560	TYR
1	K	566	PHE
1	K	584	ASN
1	K	616	HIS
1	K	633	PRO
2	L	15	GLU
2	L	47	GLU
2	L	67	SER
2	L	122	LEU
1	M	22	CYS
1	M	81	VAL
1	M	85	GLU
1	M	274	TYR
1	M	275	GLY
1	M	486	PRO
1	M	541	LYS
1	M	546	ASP
1	M	547	GLU
1	M	560	TYR
1	M	566	PHE
1	M	584	ASN
1	M	616	HIS
2	N	12	PRO
2	N	15	GLU
2	N	37	GLU
2	N	67	SER
2	N	122	LEU
1	O	81	VAL
1	O	85	GLU

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Mol	Chain	Res	Type
1	O	274	TYR
1	O	275	GLY
1	O	486	PRO
1	O	541	LYS
1	O	546	ASP
1	O	547	GLU
1	O	560	TYR
1	O	566	PHE
1	O	584	ASN
1	O	616	HIS
1	O	633	PRO
2	P	15	GLU
2	P	67	SER
2	P	122	LEU
1	A	77	MET
1	A	82	TYR
1	A	279	GLU
1	A	502	TRP
1	A	541	LYS
1	A	563	LYS
2	B	5	ARG
2	B	9	ALA
2	B	12	PRO
2	B	37	GLU
2	B	47	GLU
1	C	77	MET
1	C	82	TYR
1	C	279	GLU
1	C	502	TRP
1	C	563	LYS
1	C	614	HIS
1	C	781	ASP
2	D	5	ARG
2	D	9	ALA
2	D	12	PRO
2	D	28	ASP
2	D	37	GLU
2	D	47	GLU
1	E	77	MET
1	E	82	TYR
1	E	279	GLU
1	E	502	TRP

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Mol	Chain	Res	Type
1	E	563	LYS
2	F	5	ARG
2	F	9	ALA
2	F	12	PRO
2	F	28	ASP
2	F	37	GLU
2	F	47	GLU
2	F	99	THR
1	G	22	CYS
1	G	77	MET
1	G	82	TYR
1	G	112	ALA
1	G	279	GLU
1	G	502	TRP
1	G	563	LYS
1	G	614	HIS
2	H	5	ARG
2	H	9	ALA
2	H	28	ASP
2	H	37	GLU
2	H	47	GLU
2	H	99	THR
1	I	77	MET
1	I	82	TYR
1	I	279	GLU
1	I	563	LYS
1	I	614	HIS
2	J	5	ARG
2	J	9	ALA
2	J	12	PRO
2	J	28	ASP
2	J	47	GLU
2	J	99	THR
1	K	77	MET
1	K	82	TYR
1	K	279	GLU
1	K	502	TRP
1	K	563	LYS
1	K	614	HIS
1	K	781	ASP
2	L	5	ARG
2	L	9	ALA

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Mol	Chain	Res	Type
2	L	12	PRO
2	L	28	ASP
2	L	37	GLU
1	M	77	MET
1	M	82	TYR
1	M	279	GLU
1	M	502	TRP
1	M	563	LYS
2	N	5	ARG
2	N	9	ALA
2	N	28	ASP
2	N	47	GLU
1	O	77	MET
1	O	82	TYR
1	O	112	ALA
1	O	279	GLU
1	O	502	TRP
1	O	563	LYS
1	O	614	HIS
2	P	5	ARG
2	P	9	ALA
2	P	12	PRO
2	P	28	ASP
2	P	37	GLU
2	P	47	GLU
1	A	69	ARG
1	A	112	ALA
1	A	564	THR
1	A	614	HIS
1	A	615	GLY
1	A	781	ASP
2	B	4	PRO
2	B	28	ASP
2	B	99	THR
1	C	69	ARG
1	C	112	ALA
1	C	564	THR
2	D	4	PRO
1	E	69	ARG
1	E	112	ALA
1	E	114	GLU
1	E	564	THR

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Mol	Chain	Res	Type
1	E	614	HIS
1	E	615	GLY
1	E	633	PRO
1	E	661	TYR
1	E	781	ASP
2	F	4	PRO
1	G	69	ARG
1	G	564	THR
1	G	661	TYR
1	G	781	ASP
2	H	4	PRO
1	I	69	ARG
1	I	112	ALA
1	I	781	ASP
1	K	69	ARG
1	K	112	ALA
1	K	661	TYR
2	L	4	PRO
2	L	99	THR
1	M	69	ARG
1	M	112	ALA
1	M	564	THR
1	M	614	HIS
1	O	69	ARG
1	O	781	ASP
2	P	99	THR
1	A	292	ALA
1	A	296	THR
1	C	292	ALA
1	C	296	THR
1	C	587	HIS
1	C	633	PRO
1	E	296	THR
1	E	587	HIS
1	G	296	THR
1	G	587	HIS
1	I	296	THR
1	I	564	THR
2	J	4	PRO
1	K	296	THR
1	K	564	THR
1	K	587	HIS

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Mol	Chain	Res	Type
1	M	114	GLU
1	M	296	THR
1	M	633	PRO
1	M	781	ASP
2	N	4	PRO
1	O	564	THR
1	O	587	HIS
1	O	661	TYR
2	P	4	PRO
1	A	114	GLU
1	A	587	HIS
1	A	633	PRO
1	C	661	TYR
2	D	99	THR
1	E	292	ALA
1	G	292	ALA
1	G	559	ALA
1	I	292	ALA
1	I	559	ALA
1	I	587	HIS
1	K	292	ALA
1	K	565	LEU
1	M	292	ALA
1	M	587	HIS
1	M	615	GLY
1	M	661	TYR
2	N	36	PRO
2	N	99	THR
1	O	114	GLU
1	O	292	ALA
1	O	296	THR
1	A	298	THR
1	A	336	PRO
2	B	11	ARG
1	C	286	ALA
1	C	298	THR
1	C	336	PRO
1	C	577	ARG
2	D	11	ARG
1	E	272	ILE
1	E	298	THR
2	F	11	ARG

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Mol	Chain	Res	Type
2	F	36	PRO
2	H	11	ARG
1	I	298	THR
1	I	661	TYR
2	J	11	ARG
2	J	36	PRO
1	K	298	THR
1	K	336	PRO
2	L	11	ARG
1	M	298	THR
1	M	336	PRO
2	N	11	ARG
1	O	559	ALA
2	P	11	ARG
2	B	36	PRO
1	C	615	GLY
1	E	336	PRO
1	G	615	GLY
1	A	48	VAL
1	G	336	PRO
1	I	336	PRO
1	K	615	GLY
2	L	36	PRO
1	M	48	VAL
1	O	336	PRO
1	C	147	PRO
1	E	48	VAL
2	H	36	PRO
1	I	615	GLY
1	M	654	PRO
1	O	615	GLY
1	A	272	ILE
1	E	654	PRO
1	K	272	ILE
1	K	654	PRO
1	M	147	PRO
1	M	272	ILE
2	N	3	ALA
1	O	48	VAL
1	O	272	ILE
1	O	654	PRO
1	A	654	PRO

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Mol	Chain	Res	Type
1	C	272	ILE
1	C	654	PRO
1	G	147	PRO
1	I	272	ILE
2	J	3	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	641/651 (98%)	546 (85%)	95 (15%)	3	14
1	C	641/651 (98%)	548 (86%)	93 (14%)	3	15
1	E	641/651 (98%)	546 (85%)	95 (15%)	3	14
1	G	641/651 (98%)	543 (85%)	98 (15%)	2	13
1	I	641/651 (98%)	542 (85%)	99 (15%)	2	13
1	K	641/651 (98%)	547 (85%)	94 (15%)	3	14
1	M	641/651 (98%)	543 (85%)	98 (15%)	2	13
1	O	641/651 (98%)	543 (85%)	98 (15%)	2	13
2	B	108/113 (96%)	89 (82%)	19 (18%)	2	9
2	D	108/113 (96%)	90 (83%)	18 (17%)	2	10
2	F	108/113 (96%)	91 (84%)	17 (16%)	2	12
2	H	108/113 (96%)	91 (84%)	17 (16%)	2	12
2	J	108/113 (96%)	89 (82%)	19 (18%)	2	9
2	L	108/113 (96%)	90 (83%)	18 (17%)	2	10
2	N	108/113 (96%)	90 (83%)	18 (17%)	2	10
2	P	108/113 (96%)	88 (82%)	20 (18%)	1	8
All	All	5992/6112 (98%)	5076 (85%)	916 (15%)	2	13

All (916) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	34	ASP
1	A	55	VAL
1	A	64	MET
1	A	71	THR
1	A	74	LEU
1	A	76	ARG
1	A	77	MET
1	A	79	ASP
1	A	87	GLU
1	A	91	VAL
1	A	92	SER
1	A	110	GLU
1	A	116	VAL
1	A	124	TRP
1	A	134	LYS
1	A	144	ASN
1	A	147	PRO
1	A	150	ARG
1	A	170	MET
1	A	174	ASP
1	A	184	LEU
1	A	187	SER
1	A	199	ARG
1	A	200	LEU
1	A	204	ARG
1	A	216	SER
1	A	220	HIS
1	A	226	SER
1	A	251	THR
1	A	272	ILE
1	A	283	GLN
1	A	298	THR
1	A	299	ASP
1	A	300	PHE
1	A	311	THR
1	A	317	GLU
1	A	319	SER
1	A	321	VAL
1	A	327	GLU
1	A	332	LEU
1	A	335	ASP
1	A	337	ASP

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Mol	Chain	Res	Type
1	A	338	ARG
1	A	341	MET
1	A	342	SER
1	A	361	VAL
1	A	367	LEU
1	A	376	ASN
1	A	400	ARG
1	A	429	ASP
1	A	446	GLU
1	A	457	ASN
1	A	458	MET
1	A	464	ILE
1	A	474	ASN
1	A	486	PRO
1	A	505	LYS
1	A	517	HIS
1	A	522	LEU
1	A	530	ARG
1	A	536	LEU
1	A	540	SER
1	A	545	THR
1	A	548	VAL
1	A	551	GLU
1	A	576	ASP
1	A	582	ASP
1	A	586	ASP
1	A	597	PHE
1	A	598	TYR
1	A	600	GLN
1	A	603	LEU
1	A	614	HIS
1	A	628	ARG
1	A	631	HIS
1	A	646	GLU
1	A	658	LEU
1	A	673	VAL
1	A	674	PRO
1	A	676	GLU
1	A	692	THR
1	A	703	SER
1	A	715	PHE
1	A	719	VAL

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Mol	Chain	Res	Type
1	A	725	GLU
1	A	732	LEU
1	A	742	SER
1	A	751	LEU
1	A	753	THR
1	A	772	SER
1	A	779	THR
1	A	783	ASN
1	A	784	ASP
1	A	790	THR
2	B	2	ASP
2	B	7	THR
2	B	15	GLU
2	B	27	ASP
2	B	33	ARG
2	B	43	PRO
2	B	53	VAL
2	B	75	ILE
2	B	77	ILE
2	B	81	GLN
2	B	83	ARG
2	B	86	GLN
2	B	94	ARG
2	B	98	CYS
2	B	107	ASN
2	B	112	VAL
2	B	119	MET
2	B	123	MET
2	B	126	SER
1	C	22	CYS
1	C	32	THR
1	C	34	ASP
1	C	55	VAL
1	C	64	MET
1	C	71	THR
1	C	74	LEU
1	C	76	ARG
1	C	77	MET
1	C	79	ASP
1	C	87	GLU
1	C	91	VAL
1	C	92	SER

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Mol	Chain	Res	Type
1	C	110	GLU
1	C	116	VAL
1	C	124	TRP
1	C	134	LYS
1	C	144	ASN
1	C	147	PRO
1	C	150	ARG
1	C	170	MET
1	C	174	ASP
1	C	184	LEU
1	C	187	SER
1	C	199	ARG
1	C	200	LEU
1	C	204	ARG
1	C	216	SER
1	C	220	HIS
1	C	251	THR
1	C	272	ILE
1	C	283	GLN
1	C	298	THR
1	C	299	ASP
1	C	300	PHE
1	C	311	THR
1	C	317	GLU
1	C	319	SER
1	C	321	VAL
1	C	327	GLU
1	C	332	LEU
1	C	335	ASP
1	C	337	ASP
1	C	338	ARG
1	C	341	MET
1	C	342	SER
1	C	361	VAL
1	C	367	LEU
1	C	376	ASN
1	C	400	ARG
1	C	429	ASP
1	C	446	GLU
1	C	457	ASN
1	C	458	MET
1	C	464	ILE

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Mol	Chain	Res	Type
1	C	474	ASN
1	C	486	PRO
1	C	505	LYS
1	C	517	HIS
1	C	522	LEU
1	C	530	ARG
1	C	536	LEU
1	C	537	MET
1	C	540	SER
1	C	545	THR
1	C	548	VAL
1	C	551	GLU
1	C	576	ASP
1	C	586	ASP
1	C	597	PHE
1	C	598	TYR
1	C	600	GLN
1	C	603	LEU
1	C	614	HIS
1	C	628	ARG
1	C	631	HIS
1	C	658	LEU
1	C	673	VAL
1	C	674	PRO
1	C	676	GLU
1	C	692	THR
1	C	703	SER
1	C	715	PHE
1	C	719	VAL
1	C	725	GLU
1	C	732	LEU
1	C	751	LEU
1	C	753	THR
1	C	772	SER
1	C	779	THR
1	C	783	ASN
1	C	784	ASP
1	C	790	THR
2	D	2	ASP
2	D	7	THR
2	D	15	GLU
2	D	27	ASP

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Mol	Chain	Res	Type
2	D	33	ARG
2	D	53	VAL
2	D	58	CYS
2	D	75	ILE
2	D	77	ILE
2	D	81	GLN
2	D	83	ARG
2	D	94	ARG
2	D	98	CYS
2	D	107	ASN
2	D	112	VAL
2	D	119	MET
2	D	123	MET
2	D	126	SER
1	E	32	THR
1	E	34	ASP
1	E	55	VAL
1	E	64	MET
1	E	71	THR
1	E	74	LEU
1	E	76	ARG
1	E	77	MET
1	E	79	ASP
1	E	87	GLU
1	E	91	VAL
1	E	92	SER
1	E	110	GLU
1	E	116	VAL
1	E	124	TRP
1	E	134	LYS
1	E	144	ASN
1	E	147	PRO
1	E	150	ARG
1	E	160	PHE
1	E	170	MET
1	E	174	ASP
1	E	184	LEU
1	E	187	SER
1	E	200	LEU
1	E	204	ARG
1	E	216	SER
1	E	220	HIS

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Mol	Chain	Res	Type
1	E	226	SER
1	E	251	THR
1	E	272	ILE
1	E	283	GLN
1	E	298	THR
1	E	299	ASP
1	E	300	PHE
1	E	311	THR
1	E	317	GLU
1	E	319	SER
1	E	321	VAL
1	E	327	GLU
1	E	332	LEU
1	E	335	ASP
1	E	337	ASP
1	E	338	ARG
1	E	341	MET
1	E	342	SER
1	E	361	VAL
1	E	367	LEU
1	E	376	ASN
1	E	377	SER
1	E	400	ARG
1	E	429	ASP
1	E	446	GLU
1	E	458	MET
1	E	464	ILE
1	E	474	ASN
1	E	486	PRO
1	E	505	LYS
1	E	517	HIS
1	E	522	LEU
1	E	530	ARG
1	E	536	LEU
1	E	537	MET
1	E	545	THR
1	E	547	GLU
1	E	548	VAL
1	E	551	GLU
1	E	576	ASP
1	E	586	ASP
1	E	597	PHE

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Mol	Chain	Res	Type
1	E	598	TYR
1	E	600	GLN
1	E	603	LEU
1	E	614	HIS
1	E	628	ARG
1	E	631	HIS
1	E	646	GLU
1	E	658	LEU
1	E	673	VAL
1	E	674	PRO
1	E	676	GLU
1	E	692	THR
1	E	703	SER
1	E	719	VAL
1	E	725	GLU
1	E	732	LEU
1	E	733	ASN
1	E	742	SER
1	E	751	LEU
1	E	753	THR
1	E	772	SER
1	E	779	THR
1	E	783	ASN
1	E	784	ASP
1	E	790	THR
2	F	2	ASP
2	F	7	THR
2	F	15	GLU
2	F	27	ASP
2	F	33	ARG
2	F	53	VAL
2	F	75	ILE
2	F	77	ILE
2	F	81	GLN
2	F	83	ARG
2	F	94	ARG
2	F	98	CYS
2	F	107	ASN
2	F	112	VAL
2	F	119	MET
2	F	123	MET
2	F	126	SER

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Mol	Chain	Res	Type
1	G	32	THR
1	G	34	ASP
1	G	55	VAL
1	G	64	MET
1	G	71	THR
1	G	74	LEU
1	G	76	ARG
1	G	77	MET
1	G	79	ASP
1	G	87	GLU
1	G	92	SER
1	G	110	GLU
1	G	116	VAL
1	G	118	MET
1	G	124	TRP
1	G	134	LYS
1	G	144	ASN
1	G	147	PRO
1	G	150	ARG
1	G	160	PHE
1	G	170	MET
1	G	174	ASP
1	G	184	LEU
1	G	187	SER
1	G	188	ASN
1	G	199	ARG
1	G	200	LEU
1	G	204	ARG
1	G	216	SER
1	G	220	HIS
1	G	226	SER
1	G	251	THR
1	G	272	ILE
1	G	283	GLN
1	G	298	THR
1	G	299	ASP
1	G	300	PHE
1	G	311	THR
1	G	317	GLU
1	G	319	SER
1	G	321	VAL
1	G	327	GLU

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Mol	Chain	Res	Type
1	G	332	LEU
1	G	335	ASP
1	G	337	ASP
1	G	338	ARG
1	G	340	TRP
1	G	341	MET
1	G	342	SER
1	G	361	VAL
1	G	367	LEU
1	G	377	SER
1	G	400	ARG
1	G	407	VAL
1	G	429	ASP
1	G	446	GLU
1	G	458	MET
1	G	464	ILE
1	G	474	ASN
1	G	486	PRO
1	G	505	LYS
1	G	517	HIS
1	G	522	LEU
1	G	530	ARG
1	G	536	LEU
1	G	545	THR
1	G	547	GLU
1	G	548	VAL
1	G	551	GLU
1	G	576	ASP
1	G	582	ASP
1	G	586	ASP
1	G	591	GLU
1	G	597	PHE
1	G	600	GLN
1	G	603	LEU
1	G	614	HIS
1	G	628	ARG
1	G	631	HIS
1	G	646	GLU
1	G	658	LEU
1	G	673	VAL
1	G	674	PRO
1	G	676	GLU

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Mol	Chain	Res	Type
1	G	692	THR
1	G	703	SER
1	G	715	PHE
1	G	719	VAL
1	G	725	GLU
1	G	732	LEU
1	G	751	LEU
1	G	753	THR
1	G	772	SER
1	G	779	THR
1	G	783	ASN
1	G	784	ASP
1	G	790	THR
1	G	794	LYS
2	H	2	ASP
2	H	7	THR
2	H	15	GLU
2	H	27	ASP
2	H	33	ARG
2	H	53	VAL
2	H	75	ILE
2	H	77	ILE
2	H	81	GLN
2	H	83	ARG
2	H	94	ARG
2	H	98	CYS
2	H	107	ASN
2	H	112	VAL
2	H	119	MET
2	H	123	MET
2	H	126	SER
1	I	32	THR
1	I	34	ASP
1	I	55	VAL
1	I	64	MET
1	I	71	THR
1	I	74	LEU
1	I	76	ARG
1	I	77	MET
1	I	79	ASP
1	I	87	GLU
1	I	91	VAL

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Mol	Chain	Res	Type
1	I	92	SER
1	I	110	GLU
1	I	116	VAL
1	I	118	MET
1	I	124	TRP
1	I	134	LYS
1	I	144	ASN
1	I	147	PRO
1	I	150	ARG
1	I	160	PHE
1	I	168	GLU
1	I	170	MET
1	I	174	ASP
1	I	184	LEU
1	I	187	SER
1	I	188	ASN
1	I	199	ARG
1	I	200	LEU
1	I	204	ARG
1	I	216	SER
1	I	220	HIS
1	I	226	SER
1	I	251	THR
1	I	272	ILE
1	I	283	GLN
1	I	298	THR
1	I	299	ASP
1	I	300	PHE
1	I	311	THR
1	I	317	GLU
1	I	319	SER
1	I	321	VAL
1	I	327	GLU
1	I	332	LEU
1	I	335	ASP
1	I	337	ASP
1	I	338	ARG
1	I	340	TRP
1	I	341	MET
1	I	342	SER
1	I	361	VAL
1	I	367	LEU

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Mol	Chain	Res	Type
1	I	376	ASN
1	I	377	SER
1	I	400	ARG
1	I	429	ASP
1	I	446	GLU
1	I	457	ASN
1	I	458	MET
1	I	464	ILE
1	I	474	ASN
1	I	486	PRO
1	I	505	LYS
1	I	517	HIS
1	I	522	LEU
1	I	530	ARG
1	I	536	LEU
1	I	545	THR
1	I	547	GLU
1	I	548	VAL
1	I	551	GLU
1	I	576	ASP
1	I	586	ASP
1	I	597	PHE
1	I	598	TYR
1	I	600	GLN
1	I	603	LEU
1	I	614	HIS
1	I	628	ARG
1	I	631	HIS
1	I	646	GLU
1	I	658	LEU
1	I	673	VAL
1	I	674	PRO
1	I	676	GLU
1	I	692	THR
1	I	703	SER
1	I	715	PHE
1	I	719	VAL
1	I	725	GLU
1	I	732	LEU
1	I	751	LEU
1	I	753	THR
1	I	772	SER

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Mol	Chain	Res	Type
1	I	779	THR
1	I	783	ASN
1	I	784	ASP
1	I	790	THR
2	J	2	ASP
2	J	7	THR
2	J	15	GLU
2	J	27	ASP
2	J	33	ARG
2	J	53	VAL
2	J	58	CYS
2	J	75	ILE
2	J	77	ILE
2	J	81	GLN
2	J	83	ARG
2	J	86	GLN
2	J	94	ARG
2	J	98	CYS
2	J	107	ASN
2	J	112	VAL
2	J	119	MET
2	J	123	MET
2	J	126	SER
1	K	32	THR
1	K	34	ASP
1	K	55	VAL
1	K	64	MET
1	K	71	THR
1	K	74	LEU
1	K	76	ARG
1	K	77	MET
1	K	79	ASP
1	K	87	GLU
1	K	91	VAL
1	K	92	SER
1	K	110	GLU
1	K	116	VAL
1	K	124	TRP
1	K	134	LYS
1	K	144	ASN
1	K	147	PRO
1	K	150	ARG

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Mol	Chain	Res	Type
1	K	170	MET
1	K	174	ASP
1	K	184	LEU
1	K	187	SER
1	K	188	ASN
1	K	199	ARG
1	K	200	LEU
1	K	204	ARG
1	K	216	SER
1	K	220	HIS
1	K	226	SER
1	K	251	THR
1	K	272	ILE
1	K	283	GLN
1	K	298	THR
1	K	300	PHE
1	K	311	THR
1	K	317	GLU
1	K	319	SER
1	K	321	VAL
1	K	327	GLU
1	K	332	LEU
1	K	335	ASP
1	K	337	ASP
1	K	338	ARG
1	K	340	TRP
1	K	341	MET
1	K	342	SER
1	K	361	VAL
1	K	367	LEU
1	K	376	ASN
1	K	377	SER
1	K	400	ARG
1	K	429	ASP
1	K	446	GLU
1	K	457	ASN
1	K	458	MET
1	K	464	ILE
1	K	474	ASN
1	K	486	PRO
1	K	505	LYS
1	K	517	HIS

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Mol	Chain	Res	Type
1	K	522	LEU
1	K	530	ARG
1	K	536	LEU
1	K	545	THR
1	K	547	GLU
1	K	548	VAL
1	K	551	GLU
1	K	576	ASP
1	K	586	ASP
1	K	597	PHE
1	K	598	TYR
1	K	600	GLN
1	K	614	HIS
1	K	628	ARG
1	K	631	HIS
1	K	646	GLU
1	K	658	LEU
1	K	673	VAL
1	K	674	PRO
1	K	676	GLU
1	K	692	THR
1	K	703	SER
1	K	719	VAL
1	K	725	GLU
1	K	732	LEU
1	K	733	ASN
1	K	751	LEU
1	K	752	GLU
1	K	753	THR
1	K	779	THR
1	K	783	ASN
1	K	784	ASP
1	K	790	THR
2	L	2	ASP
2	L	7	THR
2	L	15	GLU
2	L	27	ASP
2	L	33	ARG
2	L	53	VAL
2	L	58	CYS
2	L	75	ILE
2	L	77	ILE

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Mol	Chain	Res	Type
2	L	81	GLN
2	L	83	ARG
2	L	94	ARG
2	L	98	CYS
2	L	107	ASN
2	L	112	VAL
2	L	119	MET
2	L	123	MET
2	L	126	SER
1	M	32	THR
1	M	34	ASP
1	M	55	VAL
1	M	64	MET
1	M	71	THR
1	M	74	LEU
1	M	76	ARG
1	M	77	MET
1	M	79	ASP
1	M	87	GLU
1	M	91	VAL
1	M	92	SER
1	M	110	GLU
1	M	116	VAL
1	M	124	TRP
1	M	134	LYS
1	M	144	ASN
1	M	147	PRO
1	M	150	ARG
1	M	160	PHE
1	M	170	MET
1	M	174	ASP
1	M	184	LEU
1	M	187	SER
1	M	199	ARG
1	M	200	LEU
1	M	204	ARG
1	M	216	SER
1	M	220	HIS
1	M	226	SER
1	M	251	THR
1	M	272	ILE
1	M	283	GLN

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Mol	Chain	Res	Type
1	M	298	THR
1	M	299	ASP
1	M	300	PHE
1	M	311	THR
1	M	317	GLU
1	M	319	SER
1	M	321	VAL
1	M	327	GLU
1	M	332	LEU
1	M	335	ASP
1	M	337	ASP
1	M	338	ARG
1	M	340	TRP
1	M	341	MET
1	M	342	SER
1	M	361	VAL
1	M	367	LEU
1	M	376	ASN
1	M	377	SER
1	M	400	ARG
1	M	407	VAL
1	M	429	ASP
1	M	446	GLU
1	M	457	ASN
1	M	458	MET
1	M	464	ILE
1	M	474	ASN
1	M	486	PRO
1	M	505	LYS
1	M	517	HIS
1	M	522	LEU
1	M	536	LEU
1	M	540	SER
1	M	545	THR
1	M	547	GLU
1	M	548	VAL
1	M	551	GLU
1	M	576	ASP
1	M	586	ASP
1	M	597	PHE
1	M	598	TYR
1	M	600	GLN

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Mol	Chain	Res	Type
1	M	603	LEU
1	M	614	HIS
1	M	628	ARG
1	M	631	HIS
1	M	646	GLU
1	M	658	LEU
1	M	673	VAL
1	M	674	PRO
1	M	676	GLU
1	M	692	THR
1	M	703	SER
1	M	710	GLU
1	M	719	VAL
1	M	725	GLU
1	M	732	LEU
1	M	751	LEU
1	M	753	THR
1	M	772	SER
1	M	779	THR
1	M	783	ASN
1	M	784	ASP
1	M	790	THR
1	M	794	LYS
2	N	2	ASP
2	N	7	THR
2	N	15	GLU
2	N	27	ASP
2	N	33	ARG
2	N	53	VAL
2	N	58	CYS
2	N	75	ILE
2	N	77	ILE
2	N	81	GLN
2	N	83	ARG
2	N	94	ARG
2	N	98	CYS
2	N	107	ASN
2	N	112	VAL
2	N	119	MET
2	N	123	MET
2	N	126	SER
1	O	32	THR

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Mol	Chain	Res	Type
1	O	34	ASP
1	O	55	VAL
1	O	64	MET
1	O	71	THR
1	O	74	LEU
1	O	76	ARG
1	O	77	MET
1	O	79	ASP
1	O	87	GLU
1	O	88	PHE
1	O	92	SER
1	O	110	GLU
1	O	116	VAL
1	O	124	TRP
1	O	127	TRP
1	O	134	LYS
1	O	144	ASN
1	O	147	PRO
1	O	150	ARG
1	O	160	PHE
1	O	170	MET
1	O	174	ASP
1	O	184	LEU
1	O	187	SER
1	O	199	ARG
1	O	200	LEU
1	O	204	ARG
1	O	216	SER
1	O	220	HIS
1	O	226	SER
1	O	251	THR
1	O	272	ILE
1	O	283	GLN
1	O	298	THR
1	O	299	ASP
1	O	300	PHE
1	O	311	THR
1	O	317	GLU
1	O	319	SER
1	O	321	VAL
1	O	327	GLU
1	O	332	LEU

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Mol	Chain	Res	Type
1	O	335	ASP
1	O	337	ASP
1	O	338	ARG
1	O	340	TRP
1	O	341	MET
1	O	361	VAL
1	O	367	LEU
1	O	376	ASN
1	O	377	SER
1	O	400	ARG
1	O	429	ASP
1	O	446	GLU
1	O	457	ASN
1	O	458	MET
1	O	464	ILE
1	O	474	ASN
1	O	486	PRO
1	O	505	LYS
1	O	517	HIS
1	O	522	LEU
1	O	530	ARG
1	O	536	LEU
1	O	545	THR
1	O	547	GLU
1	O	548	VAL
1	O	551	GLU
1	O	576	ASP
1	O	582	ASP
1	O	586	ASP
1	O	597	PHE
1	O	598	TYR
1	O	600	GLN
1	O	603	LEU
1	O	614	HIS
1	O	628	ARG
1	O	631	HIS
1	O	646	GLU
1	O	658	LEU
1	O	673	VAL
1	O	674	PRO
1	O	676	GLU
1	O	692	THR

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Mol	Chain	Res	Type
1	O	703	SER
1	O	715	PHE
1	O	719	VAL
1	O	725	GLU
1	O	732	LEU
1	O	751	LEU
1	O	753	THR
1	O	772	SER
1	O	779	THR
1	O	783	ASN
1	O	784	ASP
1	O	790	THR
1	O	794	LYS
2	P	2	ASP
2	P	7	THR
2	P	15	GLU
2	P	27	ASP
2	P	33	ARG
2	P	43	PRO
2	P	53	VAL
2	P	58	CYS
2	P	75	ILE
2	P	77	ILE
2	P	81	GLN
2	P	83	ARG
2	P	86	GLN
2	P	94	ARG
2	P	98	CYS
2	P	107	ASN
2	P	112	VAL
2	P	119	MET
2	P	123	MET
2	P	126	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (197) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	144	ASN
1	A	188	ASN
1	A	242	ASN
1	A	280	HIS

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Mol	Chain	Res	Type
1	A	281	GLN
1	A	376	ASN
1	A	412	HIS
1	A	443	HIS
1	A	455	ASN
1	A	457	ASN
1	A	474	ASN
1	A	477	ASN
1	A	625	HIS
1	A	700	HIS
1	A	723	HIS
1	A	733	ASN
1	A	783	ASN
1	A	789	GLN
2	B	34	ASN
2	B	38	GLN
2	B	50	GLN
2	B	86	GLN
2	B	127	ASN
1	C	53	ASN
1	C	144	ASN
1	C	188	ASN
1	C	242	ASN
1	C	281	GLN
1	C	376	ASN
1	C	412	HIS
1	C	443	HIS
1	C	455	ASN
1	C	457	ASN
1	C	474	ASN
1	C	477	ASN
1	C	625	HIS
1	C	700	HIS
1	C	723	HIS
1	C	733	ASN
1	C	783	ASN
1	C	789	GLN
2	D	34	ASN
2	D	38	GLN
2	D	50	GLN
2	D	86	GLN
2	D	127	ASN

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Mol	Chain	Res	Type
1	E	53	ASN
1	E	144	ASN
1	E	188	ASN
1	E	280	HIS
1	E	281	GLN
1	E	376	ASN
1	E	412	HIS
1	E	443	HIS
1	E	455	ASN
1	E	457	ASN
1	E	459	GLN
1	E	463	ASN
1	E	474	ASN
1	E	477	ASN
1	E	520	HIS
1	E	625	HIS
1	E	700	HIS
1	E	723	HIS
1	E	733	ASN
1	E	783	ASN
1	E	789	GLN
2	F	34	ASN
2	F	38	GLN
2	F	50	GLN
2	F	86	GLN
2	F	127	ASN
1	G	53	ASN
1	G	144	ASN
1	G	188	ASN
1	G	242	ASN
1	G	281	GLN
1	G	376	ASN
1	G	412	HIS
1	G	443	HIS
1	G	455	ASN
1	G	457	ASN
1	G	459	GLN
1	G	466	GLN
1	G	474	ASN
1	G	477	ASN
1	G	520	HIS
1	G	625	HIS

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Mol	Chain	Res	Type
1	G	700	HIS
1	G	723	HIS
1	G	733	ASN
1	G	783	ASN
1	G	789	GLN
2	H	34	ASN
2	H	38	GLN
2	H	50	GLN
2	H	86	GLN
2	H	127	ASN
1	I	53	ASN
1	I	144	ASN
1	I	188	ASN
1	I	207	HIS
1	I	209	HIS
1	I	242	ASN
1	I	281	GLN
1	I	376	ASN
1	I	412	HIS
1	I	443	HIS
1	I	455	ASN
1	I	457	ASN
1	I	459	GLN
1	I	474	ASN
1	I	477	ASN
1	I	625	HIS
1	I	700	HIS
1	I	723	HIS
1	I	733	ASN
1	I	783	ASN
1	I	789	GLN
2	J	34	ASN
2	J	38	GLN
2	J	50	GLN
2	J	86	GLN
2	J	127	ASN
1	K	53	ASN
1	K	144	ASN
1	K	188	ASN
1	K	242	ASN
1	K	281	GLN
1	K	376	ASN

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Mol	Chain	Res	Type
1	K	412	HIS
1	K	443	HIS
1	K	455	ASN
1	K	457	ASN
1	K	459	GLN
1	K	474	ASN
1	K	477	ASN
1	K	625	HIS
1	K	700	HIS
1	K	723	HIS
1	K	733	ASN
1	K	783	ASN
1	K	789	GLN
2	L	34	ASN
2	L	38	GLN
2	L	50	GLN
2	L	86	GLN
2	L	127	ASN
1	M	53	ASN
1	M	144	ASN
1	M	188	ASN
1	M	242	ASN
1	M	281	GLN
1	M	376	ASN
1	M	412	HIS
1	M	443	HIS
1	M	455	ASN
1	M	457	ASN
1	M	466	GLN
1	M	474	ASN
1	M	477	ASN
1	M	625	HIS
1	M	700	HIS
1	M	723	HIS
1	M	733	ASN
1	M	783	ASN
1	M	789	GLN
2	N	34	ASN
2	N	38	GLN
2	N	50	GLN
2	N	86	GLN
2	N	127	ASN

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Mol	Chain	Res	Type
1	O	53	ASN
1	O	144	ASN
1	O	188	ASN
1	O	242	ASN
1	O	281	GLN
1	O	376	ASN
1	O	412	HIS
1	O	443	HIS
1	O	455	ASN
1	O	457	ASN
1	O	459	GLN
1	O	474	ASN
1	O	477	ASN
1	O	625	HIS
1	O	700	HIS
1	O	723	HIS
1	O	733	ASN
1	O	783	ASN
1	O	789	GLN
2	P	34	ASN
2	P	38	GLN
2	P	50	GLN
2	P	86	GLN
2	P	127	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 8 are monoatomic - leaving 40 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
3	SF4	M	1801	1	0,12,12	0.00	-	-		
5	MGD	K	1804	4	41,52,52	2.40	14 (34%)	43,81,81	2.82	19 (44%)
5	MGD	M	1804	4	41,52,52	2.35	14 (34%)	43,81,81	2.69	18 (41%)
5	MGD	A	1803	4	41,52,52	2.63	17 (41%)	43,81,81	2.35	16 (37%)
6	HEC	P	1129	2	26,50,50	2.05	8 (30%)	18,82,82	2.96	10 (55%)
5	MGD	E	1804	4	41,52,52	2.40	16 (39%)	43,81,81	2.67	20 (46%)
5	MGD	G	1804	4	41,52,52	2.53	18 (43%)	43,81,81	2.73	17 (39%)
6	HEC	L	1129	2	26,50,50	2.55	5 (19%)	18,82,82	3.01	10 (55%)
3	SF4	E	1801	1	0,12,12	0.00	-	-		
6	HEC	F	1129	2	26,50,50	2.23	6 (23%)	18,82,82	2.74	9 (50%)
6	HEC	P	1128	2	26,50,50	2.34	10 (38%)	18,82,82	2.35	6 (33%)
5	MGD	O	1804	4	41,52,52	2.64	19 (46%)	43,81,81	2.75	18 (41%)
5	MGD	O	1803	4	41,52,52	3.07	17 (41%)	43,81,81	2.37	16 (37%)
5	MGD	C	1804	4	41,52,52	2.40	14 (34%)	43,81,81	2.76	18 (41%)
6	HEC	L	1128	2	26,50,50	2.45	10 (38%)	18,82,82	2.64	10 (55%)
6	HEC	B	1128	2	26,50,50	3.00	10 (38%)	18,82,82	2.89	7 (38%)
6	HEC	F	1128	2	26,50,50	2.40	5 (19%)	18,82,82	2.79	8 (44%)
5	MGD	M	1803	4	41,52,52	2.36	14 (34%)	43,81,81	2.30	15 (34%)
3	SF4	G	1801	1	0,12,12	0.00	-	-		
6	HEC	J	1128	2	26,50,50	2.90	9 (34%)	18,82,82	2.80	6 (33%)
6	HEC	H	1128	2	26,50,50	2.69	8 (30%)	18,82,82	2.96	9 (50%)
3	SF4	O	1801	1	0,12,12	0.00	-	-		
3	SF4	I	1801	1	0,12,12	0.00	-	-		
6	HEC	N	1129	2	26,50,50	2.72	9 (34%)	18,82,82	2.79	9 (50%)
6	HEC	D	1128	2	26,50,50	2.58	10 (38%)	18,82,82	3.03	10 (55%)
5	MGD	K	1803	4	41,52,52	2.36	16 (39%)	43,81,81	2.25	15 (34%)
6	HEC	D	1129	2	26,50,50	2.50	6 (23%)	18,82,82	2.86	10 (55%)
6	HEC	B	1129	2	26,50,50	2.43	7 (26%)	18,82,82	2.55	8 (44%)
5	MGD	E	1803	4	41,52,52	2.37	16 (39%)	43,81,81	2.34	12 (27%)
5	MGD	C	1803	4	41,52,52	2.42	15 (36%)	43,81,81	2.28	15 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SF4	A	1801	1	0,12,12	0.00	-	-		
5	MGD	A	1804	4	41,52,52	2.28	14 (34%)	43,81,81	2.80	19 (44%)
3	SF4	K	1801	1	0,12,12	0.00	-	-		
6	HEC	N	1128	2	26,50,50	2.77	11 (42%)	18,82,82	2.94	9 (50%)
5	MGD	G	1803	4	41,52,52	2.54	16 (39%)	43,81,81	2.36	14 (32%)
6	HEC	H	1129	2	26,50,50	2.71	7 (26%)	18,82,82	2.67	8 (44%)
5	MGD	I	1804	4	41,52,52	2.70	16 (39%)	43,81,81	2.72	18 (41%)
5	MGD	I	1803	4	41,52,52	3.19	18 (43%)	43,81,81	2.39	19 (44%)
6	HEC	J	1129	2	26,50,50	2.50	9 (34%)	18,82,82	3.14	11 (61%)
3	SF4	C	1801	1	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MGD	K	1804	4	-	6/18/66/66	0/6/6/6
3	SF4	M	1801	1	-	-	0/6/5/5
5	MGD	M	1804	4	-	6/18/66/66	0/6/6/6
5	MGD	A	1803	4	-	6/18/66/66	0/6/6/6
6	HEC	P	1129	2	-	0/6/54/54	-
5	MGD	E	1804	4	-	6/18/66/66	0/6/6/6
5	MGD	G	1804	4	-	6/18/66/66	0/6/6/6
6	HEC	L	1129	2	-	0/6/54/54	-
3	SF4	E	1801	1	-	-	0/6/5/5
6	HEC	F	1129	2	-	0/6/54/54	-
6	HEC	P	1128	2	-	0/6/54/54	-
5	MGD	O	1804	4	-	5/18/66/66	0/6/6/6
5	MGD	O	1803	4	-	5/18/66/66	0/6/6/6
5	MGD	C	1804	4	-	5/18/66/66	0/6/6/6
6	HEC	L	1128	2	-	0/6/54/54	-
6	HEC	B	1128	2	-	0/6/54/54	-
6	HEC	F	1128	2	-	0/6/54/54	-
5	MGD	M	1803	4	-	6/18/66/66	0/6/6/6
3	SF4	G	1801	1	-	-	0/6/5/5
6	HEC	J	1128	2	-	0/6/54/54	-
6	HEC	H	1128	2	-	0/6/54/54	-
3	SF4	O	1801	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	I	1801	1	-	-	0/6/5/5
6	HEC	N	1129	2	-	2/6/54/54	-
6	HEC	D	1128	2	-	0/6/54/54	-
5	MGD	K	1803	4	-	6/18/66/66	0/6/6/6
6	HEC	D	1129	2	-	0/6/54/54	-
6	HEC	B	1129	2	-	0/6/54/54	-
5	MGD	E	1803	4	-	6/18/66/66	0/6/6/6
5	MGD	C	1803	4	-	6/18/66/66	0/6/6/6
3	SF4	A	1801	1	-	-	0/6/5/5
3	SF4	K	1801	1	-	-	0/6/5/5
5	MGD	A	1804	4	-	5/18/66/66	0/6/6/6
6	HEC	N	1128	2	-	0/6/54/54	-
5	MGD	G	1803	4	-	5/18/66/66	0/6/6/6
6	HEC	H	1129	2	-	0/6/54/54	-
3	SF4	C	1801	1	-	-	0/6/5/5
5	MGD	I	1803	4	-	6/18/66/66	0/6/6/6
6	HEC	J	1129	2	-	0/6/54/54	-
5	MGD	I	1804	4	-	7/18/66/66	0/6/6/6

All (384) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	1803	MGD	C23-C14	10.24	1.61	1.53
6	N	1129	HEC	C3B-C2B	-10.07	1.30	1.40
6	H	1129	HEC	C3B-C2B	-9.83	1.30	1.40
6	N	1128	HEC	C3B-C2B	-9.22	1.31	1.40
6	B	1128	HEC	C3B-C2B	-9.20	1.31	1.40
6	J	1128	HEC	C3B-C2B	-9.07	1.31	1.40
6	B	1128	HEC	C3C-C2C	-8.81	1.31	1.40
6	B	1129	HEC	C3B-C2B	-8.40	1.32	1.40
5	I	1803	MGD	C23-C14	8.28	1.60	1.53
6	L	1129	HEC	C3B-C2B	-8.27	1.32	1.40
6	H	1128	HEC	C3B-C2B	-8.21	1.32	1.40
6	D	1129	HEC	C3B-C2B	-8.18	1.32	1.40
6	H	1128	HEC	C3C-C2C	-7.97	1.32	1.40
6	D	1128	HEC	C3B-C2B	-7.77	1.32	1.40
6	F	1128	HEC	C3B-C2B	-7.77	1.32	1.40
5	I	1803	MGD	C17-N18	7.37	1.45	1.33
6	L	1128	HEC	C3B-C2B	-7.37	1.33	1.40
5	A	1803	MGD	C17-N18	7.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1803	MGD	O4'-C1'	7.18	1.51	1.41
6	J	1128	HEC	C3C-C2C	-7.14	1.33	1.40
5	G	1804	MGD	C17-N18	7.10	1.45	1.33
5	K	1804	MGD	C6-N1	7.02	1.45	1.33
6	F	1129	HEC	C3B-C2B	-6.95	1.33	1.40
6	L	1129	HEC	C3C-C2C	-6.90	1.33	1.40
6	D	1128	HEC	C3C-C2C	-6.87	1.33	1.40
6	D	1129	HEC	C3C-C2C	-6.80	1.33	1.40
5	I	1804	MGD	C17-N18	6.79	1.44	1.33
5	O	1804	MGD	C17-N18	6.71	1.44	1.33
5	K	1803	MGD	C17-N18	6.71	1.44	1.33
5	K	1804	MGD	C17-N18	6.54	1.44	1.33
5	G	1804	MGD	C6-N1	6.51	1.44	1.33
5	C	1803	MGD	C6-N1	6.50	1.44	1.33
6	J	1129	HEC	C3B-C2B	-6.49	1.34	1.40
5	E	1803	MGD	C17-N18	6.41	1.44	1.33
5	C	1804	MGD	C17-N18	6.33	1.44	1.33
5	I	1804	MGD	C6-N1	6.32	1.44	1.33
6	F	1128	HEC	C3C-C2C	-6.29	1.34	1.40
5	O	1804	MGD	C6-N1	6.28	1.44	1.33
5	E	1804	MGD	C6-N1	6.24	1.43	1.33
5	E	1804	MGD	C17-N18	6.23	1.43	1.33
5	O	1803	MGD	C6-N1	6.18	1.43	1.33
6	J	1129	HEC	C3C-C2C	-6.09	1.34	1.40
5	M	1804	MGD	C17-N18	6.07	1.43	1.33
5	I	1804	MGD	C14-N15	6.06	1.53	1.45
5	G	1803	MGD	C6-N1	6.05	1.43	1.33
5	O	1803	MGD	C17-N18	6.03	1.43	1.33
5	G	1803	MGD	C17-N18	6.01	1.43	1.33
5	M	1803	MGD	C17-N18	5.99	1.43	1.33
5	M	1804	MGD	C14-N15	5.92	1.53	1.45
5	C	1804	MGD	C14-N15	5.91	1.53	1.45
5	O	1803	MGD	C14-N15	5.88	1.53	1.45
5	C	1803	MGD	C17-N18	5.78	1.43	1.33
5	A	1803	MGD	C23-C14	5.78	1.58	1.53
5	M	1804	MGD	C6-N1	5.77	1.43	1.33
5	A	1804	MGD	C14-N15	5.68	1.53	1.45
5	A	1804	MGD	C6-N1	5.67	1.42	1.33
5	E	1803	MGD	C6-N1	5.64	1.42	1.33
6	P	1128	HEC	C3B-C2B	-5.61	1.34	1.40
6	N	1128	HEC	C3C-C2C	-5.60	1.34	1.40
6	L	1128	HEC	C3C-C2C	-5.59	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1803	MGD	C2'-C3'	5.58	1.68	1.53
5	M	1803	MGD	C6-N1	5.46	1.42	1.33
5	A	1804	MGD	C17-N18	5.43	1.42	1.33
5	A	1803	MGD	C6-N1	5.41	1.42	1.33
5	I	1803	MGD	C6-N1	5.41	1.42	1.33
6	H	1129	HEC	C3C-C2C	-5.36	1.35	1.40
5	C	1804	MGD	C6-N1	5.31	1.42	1.33
5	I	1803	MGD	C14-N15	5.29	1.52	1.45
5	G	1804	MGD	C14-N15	5.28	1.52	1.45
5	K	1804	MGD	C14-N15	5.20	1.52	1.45
5	E	1803	MGD	O4'-C1'	5.19	1.48	1.41
5	O	1804	MGD	C14-N15	5.16	1.52	1.45
5	G	1803	MGD	C14-N15	5.13	1.52	1.45
6	P	1129	HEC	C3B-C2B	-5.11	1.35	1.40
5	E	1804	MGD	C14-N15	4.96	1.52	1.45
6	N	1129	HEC	C3C-C2C	-4.91	1.35	1.40
5	O	1803	MGD	C2-N1	4.90	1.44	1.35
6	P	1128	HEC	C3C-C2C	-4.80	1.35	1.40
6	F	1129	HEC	C3C-C2C	-4.79	1.35	1.40
6	B	1129	HEC	C3C-C2C	-4.76	1.35	1.40
5	C	1803	MGD	C23-C14	4.74	1.57	1.53
5	K	1803	MGD	C6-N1	4.62	1.41	1.33
5	I	1804	MGD	C2-N1	4.54	1.43	1.35
5	O	1804	MGD	C16-N15	4.53	1.47	1.38
5	C	1804	MGD	C21-N20	4.52	1.43	1.34
5	O	1803	MGD	C16-N15	4.50	1.47	1.38
5	M	1803	MGD	C23-C14	4.48	1.57	1.53
5	I	1804	MGD	C16-N15	4.48	1.47	1.38
5	K	1803	MGD	C23-C14	4.47	1.57	1.53
6	P	1129	HEC	C3C-C2C	-4.39	1.36	1.40
5	A	1803	MGD	PB-O2B	-4.36	1.34	1.55
5	M	1803	MGD	C14-N15	4.34	1.51	1.45
5	I	1803	MGD	C2-N1	4.34	1.43	1.35
5	I	1803	MGD	C16-N15	4.31	1.46	1.38
5	O	1804	MGD	C23-C14	4.25	1.57	1.53
5	M	1804	MGD	C16-N15	4.22	1.46	1.38
5	K	1803	MGD	C14-N15	4.21	1.51	1.45
5	G	1804	MGD	C16-N15	4.21	1.46	1.38
5	G	1803	MGD	C2-N1	4.18	1.42	1.35
6	J	1129	HEC	CMD-C2D	4.16	1.60	1.51
5	K	1804	MGD	C16-N15	4.14	1.46	1.38
5	I	1803	MGD	C19-N18	4.13	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1803	MGD	C16-N15	4.12	1.46	1.38
5	A	1803	MGD	C21-N20	4.11	1.42	1.34
6	J	1128	HEC	C3B-C4B	4.11	1.50	1.43
5	M	1803	MGD	C16-N15	4.10	1.46	1.38
5	G	1803	MGD	C16-N15	4.07	1.46	1.38
5	C	1804	MGD	C16-N15	4.05	1.46	1.38
5	O	1804	MGD	C21-N20	4.04	1.42	1.34
5	I	1804	MGD	C2-N2	4.01	1.41	1.33
5	G	1803	MGD	C23-C14	4.00	1.56	1.53
5	I	1804	MGD	C23-C14	4.00	1.56	1.53
5	C	1804	MGD	C2'-C1'	-3.89	1.47	1.53
5	C	1804	MGD	C19-N18	3.88	1.42	1.35
5	E	1804	MGD	C16-N15	3.87	1.45	1.38
6	P	1128	HEC	C3B-C4B	3.86	1.50	1.43
5	O	1803	MGD	O11-C11	3.86	1.48	1.43
5	C	1803	MGD	C14-N15	3.83	1.50	1.45
5	E	1803	MGD	C16-N15	3.81	1.45	1.38
5	A	1804	MGD	C16-N15	3.81	1.45	1.38
5	O	1804	MGD	C19-N18	3.79	1.42	1.35
5	O	1803	MGD	C19-N18	3.78	1.42	1.35
6	J	1128	HEC	CAD-C3D	-3.76	1.46	1.52
5	E	1803	MGD	C21-N20	3.75	1.41	1.34
5	O	1804	MGD	C2'-C3'	3.74	1.63	1.53
5	K	1803	MGD	C2'-C3'	3.74	1.63	1.53
5	K	1804	MGD	C21-N20	3.71	1.41	1.34
6	H	1128	HEC	C3C-C4C	3.71	1.49	1.43
5	A	1804	MGD	C8-N7	-3.70	1.28	1.34
5	I	1804	MGD	C2'-C3'	3.70	1.63	1.53
5	G	1804	MGD	C21-N20	3.67	1.41	1.34
5	G	1803	MGD	O11-C11	3.66	1.48	1.43
5	E	1804	MGD	C23-C14	3.66	1.56	1.53
6	B	1129	HEC	CMD-C2D	3.64	1.59	1.51
5	I	1803	MGD	O11-C11	3.63	1.48	1.43
5	A	1803	MGD	C14-N15	3.62	1.50	1.45
6	N	1128	HEC	C3C-C4C	3.61	1.49	1.43
5	K	1803	MGD	C16-N15	3.60	1.45	1.38
6	J	1129	HEC	C1B-NB	3.60	1.43	1.36
5	K	1803	MGD	O4'-C1'	3.56	1.46	1.41
6	N	1129	HEC	C3B-C4B	3.52	1.49	1.43
5	M	1804	MGD	C23-C14	3.51	1.56	1.53
5	K	1803	MGD	C2-N1	3.51	1.41	1.35
5	A	1803	MGD	O11-C11	3.51	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1803	MGD	C21-N20	3.51	1.41	1.34
5	E	1803	MGD	C23-C14	3.51	1.56	1.53
5	O	1803	MGD	C2'-C3'	3.46	1.62	1.53
5	C	1803	MGD	C21-N20	3.44	1.41	1.34
5	M	1804	MGD	C21-N20	3.44	1.41	1.34
6	H	1129	HEC	C3B-C4B	3.43	1.49	1.43
5	M	1804	MGD	C2'-C3'	3.42	1.62	1.53
6	F	1129	HEC	C1B-NB	3.41	1.43	1.36
5	K	1803	MGD	C21-N20	3.41	1.41	1.34
5	G	1804	MGD	C4-N3	3.40	1.41	1.35
5	C	1803	MGD	C2-N1	3.40	1.41	1.35
5	A	1803	MGD	C16-N15	3.39	1.45	1.38
5	G	1803	MGD	C2'-C3'	3.38	1.62	1.53
5	I	1804	MGD	C21-N20	3.37	1.40	1.34
5	A	1804	MGD	C2'-C3'	3.37	1.62	1.53
5	M	1803	MGD	C2'-C3'	3.35	1.62	1.53
5	G	1803	MGD	O4'-C1'	3.35	1.45	1.41
5	G	1803	MGD	PB-O2B	-3.34	1.39	1.55
5	A	1803	MGD	PB-O1B	-3.31	1.39	1.50
5	K	1804	MGD	C2-N1	3.27	1.41	1.35
5	C	1804	MGD	C2'-C3'	3.27	1.62	1.53
5	O	1804	MGD	C4-N3	3.26	1.40	1.35
5	E	1803	MGD	C2'-C3'	3.25	1.62	1.53
5	O	1803	MGD	C21-N20	3.24	1.40	1.34
5	O	1804	MGD	C2-N1	3.23	1.41	1.35
5	E	1804	MGD	C19-N18	3.23	1.41	1.35
5	O	1803	MGD	O4'-C1'	3.21	1.45	1.41
5	M	1803	MGD	PB-O2B	-3.19	1.40	1.55
5	A	1803	MGD	C2-N2	3.17	1.40	1.33
5	G	1803	MGD	C2-N2	3.17	1.40	1.33
5	I	1804	MGD	C19-N18	3.17	1.41	1.35
5	A	1804	MGD	C21-N20	3.15	1.40	1.34
5	M	1803	MGD	O4'-C1'	3.14	1.45	1.41
6	J	1128	HEC	C1B-CHB	-3.14	1.32	1.41
6	N	1128	HEC	C1B-NB	3.13	1.42	1.36
6	P	1128	HEC	C1B-NB	3.13	1.42	1.36
5	O	1803	MGD	C4-N3	3.13	1.40	1.35
6	N	1128	HEC	CMD-C2D	3.12	1.58	1.51
5	G	1804	MGD	C2-N1	3.10	1.40	1.35
5	C	1803	MGD	PB-O2B	-3.10	1.40	1.55
5	E	1803	MGD	PB-O2B	-3.09	1.40	1.55
5	E	1804	MGD	C21-N20	3.08	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1129	HEC	CMD-C2D	3.08	1.58	1.51
5	I	1803	MGD	C4-N3	3.05	1.40	1.35
5	I	1803	MGD	C2-N2	3.05	1.40	1.33
5	I	1804	MGD	C10-C11	3.05	1.56	1.52
6	P	1129	HEC	C1B-NB	3.04	1.42	1.36
5	C	1803	MGD	O11-C11	3.04	1.47	1.43
6	B	1128	HEC	C1D-ND	3.04	1.42	1.36
5	E	1804	MGD	C8-N7	-3.04	1.29	1.34
5	K	1804	MGD	C3'-C4'	3.02	1.60	1.53
5	M	1803	MGD	C2-N1	3.02	1.40	1.35
5	I	1804	MGD	O11-C11	3.02	1.47	1.43
5	O	1804	MGD	C2-N2	3.01	1.39	1.33
5	I	1803	MGD	C21-N20	3.01	1.40	1.34
6	P	1129	HEC	CMD-C2D	3.01	1.57	1.51
5	A	1804	MGD	PB-O2B	-3.01	1.41	1.55
5	E	1803	MGD	PB-O1B	-2.99	1.40	1.50
5	I	1804	MGD	C4-N3	2.96	1.40	1.35
5	G	1803	MGD	C8-N7	-2.96	1.29	1.34
5	O	1803	MGD	C2-N2	2.95	1.39	1.33
5	O	1803	MGD	C23-N22	2.95	1.50	1.44
6	N	1129	HEC	C1B-NB	2.94	1.42	1.36
5	E	1804	MGD	C2'-C1'	-2.93	1.49	1.53
6	D	1128	HEC	CAD-C3D	-2.93	1.47	1.52
6	H	1129	HEC	C1B-NB	2.92	1.42	1.36
6	D	1129	HEC	CMD-C2D	2.92	1.57	1.51
5	G	1804	MGD	C2'-C3'	2.89	1.61	1.53
5	A	1804	MGD	C23-C14	2.89	1.55	1.53
5	M	1804	MGD	C4-N3	2.89	1.40	1.35
6	J	1129	HEC	C3B-C4B	2.88	1.48	1.43
6	B	1129	HEC	C1B-NB	2.87	1.42	1.36
5	G	1803	MGD	C21-N20	2.87	1.40	1.34
6	H	1129	HEC	CMD-C2D	2.85	1.57	1.51
6	B	1128	HEC	C3C-C4C	2.85	1.48	1.43
5	I	1804	MGD	C3'-C4'	2.83	1.60	1.53
6	J	1129	HEC	CBB-CAB	2.82	1.60	1.49
6	H	1128	HEC	C1B-CHB	-2.82	1.33	1.41
5	O	1803	MGD	O2'-C2'	2.81	1.49	1.43
5	C	1803	MGD	C4-N3	2.81	1.40	1.35
5	G	1803	MGD	C4-N3	2.81	1.40	1.35
5	A	1804	MGD	C19-N18	2.81	1.40	1.35
5	E	1803	MGD	C14-N15	2.80	1.49	1.45
5	A	1803	MGD	O11-C23	-2.80	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1803	MGD	C23-N22	2.80	1.50	1.44
6	B	1128	HEC	CMD-C2D	2.80	1.57	1.51
6	J	1128	HEC	C1D-ND	2.79	1.41	1.36
5	I	1803	MGD	O2'-C2'	2.76	1.49	1.43
5	M	1803	MGD	C2-N2	2.74	1.39	1.33
6	L	1128	HEC	C1B-CHB	-2.74	1.33	1.41
5	G	1804	MGD	O4'-C4'	-2.74	1.38	1.45
6	N	1129	HEC	CMD-C2D	2.73	1.57	1.51
5	M	1804	MGD	C3'-C4'	2.72	1.59	1.53
6	J	1128	HEC	C1B-NB	2.72	1.41	1.36
5	K	1803	MGD	O11-C11	2.72	1.47	1.43
5	G	1804	MGD	C19-N18	2.72	1.40	1.35
5	K	1804	MGD	C4-N3	2.71	1.39	1.35
5	O	1803	MGD	PB-O2B	-2.70	1.42	1.55
5	C	1803	MGD	O4'-C1'	2.70	1.44	1.41
5	O	1804	MGD	C3'-C4'	2.70	1.59	1.53
6	P	1129	HEC	C3B-C4B	2.70	1.47	1.43
5	K	1803	MGD	C2-N2	2.69	1.39	1.33
5	E	1803	MGD	O11-C11	2.69	1.47	1.43
5	A	1803	MGD	C2-N1	2.69	1.40	1.35
6	P	1128	HEC	C4A-C3A	2.68	1.48	1.42
5	C	1803	MGD	C2-N2	2.68	1.39	1.33
6	F	1129	HEC	C3B-C4B	2.67	1.47	1.43
5	G	1804	MGD	O11-C11	2.67	1.47	1.43
6	N	1128	HEC	C1D-ND	2.66	1.41	1.36
6	D	1128	HEC	C1D-CHD	-2.64	1.33	1.41
5	E	1804	MGD	C2'-C3'	2.63	1.60	1.53
5	G	1804	MGD	C3'-C4'	2.63	1.59	1.53
6	P	1128	HEC	C1D-CHD	-2.61	1.33	1.41
5	I	1803	MGD	PB-O2B	-2.61	1.43	1.55
5	M	1803	MGD	O11-C11	2.59	1.47	1.43
6	D	1129	HEC	C1B-NB	2.59	1.41	1.36
6	L	1129	HEC	C4A-C3A	2.59	1.48	1.42
5	E	1804	MGD	C4-N3	2.58	1.39	1.35
6	D	1129	HEC	C1D-CHD	-2.58	1.33	1.41
5	A	1803	MGD	C2'-C3'	2.56	1.60	1.53
6	P	1128	HEC	CMD-C2D	2.55	1.57	1.51
6	F	1129	HEC	CMD-C2D	2.54	1.56	1.51
5	K	1803	MGD	C8-N7	-2.54	1.30	1.34
5	C	1803	MGD	C19-N18	2.52	1.39	1.35
6	B	1128	HEC	CAA-C2A	2.52	1.56	1.52
5	G	1804	MGD	C2'-C1'	-2.52	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1128	HEC	C3B-C4B	2.52	1.47	1.43
5	M	1804	MGD	C8-N7	-2.52	1.30	1.34
5	I	1803	MGD	C19-N19	2.52	1.38	1.33
6	N	1128	HEC	C2A-C3A	-2.49	1.30	1.37
5	I	1804	MGD	O2'-C2'	2.48	1.48	1.43
6	H	1129	HEC	C1D-ND	2.48	1.41	1.36
6	N	1128	HEC	CAD-C3D	-2.48	1.48	1.52
6	D	1128	HEC	C1B-CHB	-2.46	1.34	1.41
5	A	1803	MGD	O4'-C1'	2.46	1.44	1.41
5	O	1804	MGD	C10-C11	2.45	1.55	1.52
5	C	1803	MGD	C2'-C3'	2.45	1.60	1.53
5	G	1803	MGD	C19-N18	2.45	1.39	1.35
5	K	1804	MGD	C2'-C3'	2.44	1.60	1.53
5	K	1803	MGD	PB-O2B	-2.44	1.43	1.55
5	E	1803	MGD	C2-N1	2.43	1.39	1.35
5	E	1804	MGD	PB-O2B	-2.43	1.43	1.55
5	A	1803	MGD	C17-C16	-2.41	1.38	1.41
5	G	1804	MGD	C2-N2	2.41	1.38	1.33
6	P	1129	HEC	CBB-CAB	2.40	1.58	1.49
6	F	1128	HEC	C1B-CHB	-2.38	1.34	1.41
6	N	1129	HEC	C1D-ND	2.38	1.41	1.36
6	J	1129	HEC	C4A-C3A	2.38	1.47	1.42
5	A	1804	MGD	O11-C11	2.37	1.46	1.43
6	L	1128	HEC	CBB-CAB	2.37	1.58	1.49
6	P	1128	HEC	C3C-C4C	2.36	1.47	1.43
6	J	1129	HEC	C1B-CHB	-2.36	1.34	1.41
6	L	1128	HEC	CAD-C3D	-2.36	1.48	1.52
6	N	1129	HEC	C1B-CHB	-2.35	1.34	1.41
5	C	1804	MGD	C8-N7	-2.35	1.30	1.34
5	K	1804	MGD	C2-N2	2.35	1.38	1.33
6	P	1129	HEC	C1D-ND	2.34	1.41	1.36
6	L	1129	HEC	C1D-CHD	-2.33	1.34	1.41
5	C	1804	MGD	PB-O2B	-2.33	1.44	1.55
6	B	1128	HEC	C1B-CHB	-2.32	1.34	1.41
5	G	1804	MGD	C23-C14	2.32	1.55	1.53
5	E	1803	MGD	O11-C23	-2.31	1.40	1.43
5	K	1804	MGD	C8-N7	-2.31	1.30	1.34
5	E	1803	MGD	C2-N2	2.30	1.38	1.33
5	A	1803	MGD	C5-C4	-2.30	1.34	1.40
5	M	1804	MGD	C2-N1	2.30	1.39	1.35
5	O	1804	MGD	C19-N19	2.30	1.38	1.33
6	D	1128	HEC	CBB-CAB	2.30	1.58	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	1804	MGD	PB-O2B	-2.28	1.44	1.55
5	G	1804	MGD	C17-C16	-2.28	1.38	1.41
6	N	1128	HEC	CBB-CAB	2.28	1.58	1.49
6	L	1128	HEC	CAA-C2A	2.28	1.56	1.52
5	E	1803	MGD	C8-N7	-2.28	1.30	1.34
5	K	1803	MGD	C4-N3	2.28	1.39	1.35
5	O	1804	MGD	C2'-C1'	-2.28	1.50	1.53
5	A	1804	MGD	C2'-C1'	-2.27	1.50	1.53
6	J	1128	HEC	CBB-CAB	2.27	1.58	1.49
6	D	1129	HEC	C1B-CHB	-2.26	1.34	1.41
5	O	1804	MGD	C8-N7	-2.25	1.30	1.34
5	G	1803	MGD	C5-C4	-2.25	1.35	1.40
6	B	1128	HEC	CBB-CAB	2.25	1.58	1.49
6	B	1128	HEC	CAD-C3D	-2.24	1.48	1.52
6	H	1128	HEC	C1B-NB	2.24	1.40	1.36
5	O	1803	MGD	C16-C21	2.24	1.45	1.41
6	L	1128	HEC	C1A-C2A	2.24	1.47	1.42
5	K	1803	MGD	O2'-C2'	2.24	1.48	1.43
6	P	1128	HEC	CAA-C2A	2.23	1.56	1.52
5	C	1804	MGD	O11-C11	2.21	1.46	1.43
6	P	1128	HEC	CBB-CAB	2.19	1.57	1.49
6	P	1129	HEC	CAD-C3D	2.18	1.55	1.52
5	O	1804	MGD	O11-C11	2.18	1.46	1.43
6	B	1129	HEC	C1B-CHB	-2.17	1.35	1.41
6	F	1128	HEC	C3D-C2D	-2.17	1.31	1.37
6	N	1128	HEC	C1A-C2A	2.17	1.47	1.42
6	D	1128	HEC	C3D-C2D	-2.16	1.31	1.37
6	D	1128	HEC	C1D-ND	2.15	1.40	1.36
5	K	1804	MGD	C17-C16	-2.15	1.38	1.41
6	J	1129	HEC	C4D-CHA	-2.15	1.35	1.41
5	E	1804	MGD	C10-C11	2.14	1.54	1.52
5	K	1804	MGD	O11-C11	2.13	1.46	1.43
6	B	1128	HEC	C4A-C3A	2.13	1.47	1.42
5	E	1803	MGD	C5-C4	-2.12	1.35	1.40
5	E	1804	MGD	C3'-C4'	2.11	1.58	1.53
6	H	1128	HEC	CBB-CAB	2.11	1.57	1.49
5	E	1804	MGD	O11-C11	2.11	1.46	1.43
5	M	1804	MGD	PB-O2B	-2.10	1.45	1.55
5	I	1803	MGD	C8-N7	-2.10	1.31	1.34
6	D	1128	HEC	CMD-C2D	2.10	1.56	1.51
5	O	1804	MGD	PB-O2B	-2.10	1.45	1.55
5	E	1804	MGD	C2-N1	2.10	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1804	MGD	O11-C11	2.09	1.46	1.43
6	H	1129	HEC	CBB-CAB	2.09	1.57	1.49
5	A	1804	MGD	O3A-C10	2.09	1.52	1.44
6	N	1128	HEC	C4A-C3A	2.09	1.47	1.42
5	C	1804	MGD	O4'-C4'	-2.08	1.40	1.45
6	J	1128	HEC	C3C-C4C	2.08	1.46	1.43
5	C	1804	MGD	C2-N1	2.07	1.39	1.35
6	F	1129	HEC	C1D-ND	2.06	1.40	1.36
6	H	1128	HEC	CMD-C2D	2.06	1.55	1.51
5	C	1803	MGD	C8-N7	-2.05	1.31	1.34
6	D	1128	HEC	C3B-C4B	2.05	1.46	1.43
5	A	1803	MGD	PB-O5'	-2.05	1.51	1.59
6	L	1128	HEC	C3C-C4C	2.04	1.46	1.43
5	M	1804	MGD	C2-N2	2.04	1.38	1.33
6	N	1129	HEC	C1D-CHD	-2.04	1.35	1.41
6	H	1128	HEC	CAA-C2A	2.04	1.55	1.52
6	B	1129	HEC	C4A-C3A	2.04	1.47	1.42
5	I	1804	MGD	C2'-C1'	-2.03	1.50	1.53
5	O	1804	MGD	O3A-C10	2.03	1.52	1.44
5	G	1804	MGD	O3A-C10	2.03	1.52	1.44
6	F	1128	HEC	C2A-C3A	-2.03	1.31	1.37
6	L	1128	HEC	CMD-C2D	2.03	1.55	1.51
5	G	1804	MGD	C10-C11	2.02	1.54	1.52
6	B	1129	HEC	CBB-CAB	2.02	1.57	1.49
5	M	1803	MGD	C4-N3	2.02	1.38	1.35
5	M	1803	MGD	O2'-C2'	2.01	1.47	1.43
5	A	1804	MGD	C5-C4	-2.01	1.35	1.40
6	N	1129	HEC	CBC-CAC	2.00	1.57	1.49
5	C	1804	MGD	C16-C21	2.00	1.45	1.41
5	K	1803	MGD	C17-C16	-2.00	1.38	1.41

All (409) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1804	MGD	O11-C23-N22	-8.54	99.79	108.57
5	O	1804	MGD	O11-C23-N22	-8.34	100.00	108.57
5	K	1804	MGD	O11-C23-N22	-8.28	100.06	108.57
5	A	1804	MGD	O11-C23-N22	-8.11	100.23	108.57
5	E	1804	MGD	O11-C23-N22	-7.95	100.40	108.57
5	M	1804	MGD	O11-C23-N22	-7.89	100.46	108.57
5	G	1804	MGD	O11-C23-N22	-7.46	100.90	108.57
6	D	1128	HEC	CBD-CAD-C3D	-7.36	98.91	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1804	MGD	O11-C23-N22	-7.34	101.03	108.57
5	G	1803	MGD	C5-C6-N1	-6.98	113.89	123.43
5	I	1803	MGD	C5-C6-N1	-6.85	114.06	123.43
6	L	1129	HEC	C1D-C2D-C3D	6.82	111.74	107.00
6	B	1128	HEC	CBD-CAD-C3D	-6.76	100.01	112.49
6	N	1129	HEC	C1D-C2D-C3D	6.55	111.55	107.00
5	C	1803	MGD	C5-C6-N1	-6.50	114.54	123.43
5	G	1804	MGD	O11-C23-C14	-6.46	104.65	108.96
5	O	1803	MGD	C5-C6-N1	-6.36	114.73	123.43
5	E	1803	MGD	C5-C6-N1	-6.32	114.79	123.43
5	M	1803	MGD	C5-C6-N1	-6.31	114.81	123.43
6	J	1128	HEC	C1D-C2D-C3D	6.27	111.36	107.00
5	A	1803	MGD	C5-C6-N1	-6.27	114.86	123.43
6	F	1129	HEC	C1D-C2D-C3D	6.16	111.28	107.00
6	D	1129	HEC	CMD-C2D-C1D	-6.13	119.04	128.46
6	J	1128	HEC	CBD-CAD-C3D	-6.13	101.18	112.49
5	C	1804	MGD	C5-C6-N1	-6.13	115.05	123.43
5	I	1804	MGD	C5-C6-N1	-6.13	115.05	123.43
6	J	1129	HEC	CMD-C2D-C1D	-6.07	119.14	128.46
5	K	1804	MGD	C5-C6-N1	-6.06	115.15	123.43
5	A	1804	MGD	C5-C6-N1	-6.05	115.16	123.43
6	N	1128	HEC	CMD-C2D-C1D	-6.01	119.22	128.46
5	K	1804	MGD	O11-C23-C14	-6.00	104.97	108.96
5	K	1803	MGD	C5-C6-N1	-5.92	115.34	123.43
6	H	1128	HEC	C1D-C2D-C3D	5.91	111.11	107.00
6	F	1128	HEC	C1D-C2D-C3D	5.85	111.07	107.00
5	M	1803	MGD	O4'-C1'-C2'	-5.85	98.38	106.93
6	N	1128	HEC	CBD-CAD-C3D	-5.84	101.71	112.49
5	O	1804	MGD	O11-C23-C14	-5.79	105.10	108.96
5	G	1803	MGD	C17-C16-C21	5.75	119.68	114.57
6	D	1129	HEC	C1D-C2D-C3D	5.73	110.98	107.00
5	E	1804	MGD	C5-C6-N1	-5.73	115.60	123.43
5	E	1803	MGD	O4'-C1'-C2'	-5.64	98.69	106.93
5	O	1804	MGD	C5-C6-N1	-5.63	115.73	123.43
5	G	1804	MGD	C5-C6-N1	-5.59	115.78	123.43
6	H	1128	HEC	CMD-C2D-C1D	-5.58	119.88	128.46
6	F	1128	HEC	CBD-CAD-C3D	-5.56	102.23	112.49
6	P	1129	HEC	C1D-C2D-C3D	5.55	110.86	107.00
6	H	1129	HEC	C1D-C2D-C3D	5.55	110.86	107.00
6	P	1129	HEC	CMD-C2D-C1D	-5.53	119.97	128.46
5	M	1804	MGD	C5-C6-N1	-5.45	115.98	123.43
5	I	1803	MGD	C17-C16-C21	5.44	119.40	114.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1129	HEC	CMD-C2D-C1D	-5.40	120.16	128.46
5	A	1804	MGD	O4'-C1'-C2'	-5.40	99.04	106.93
5	C	1804	MGD	O11-C23-C14	-5.36	105.39	108.96
5	I	1804	MGD	O11-C23-C14	-5.33	105.41	108.96
6	B	1128	HEC	C1D-C2D-C3D	5.31	110.69	107.00
5	M	1804	MGD	O11-C23-C14	-5.29	105.43	108.96
6	B	1129	HEC	C1D-C2D-C3D	5.29	110.68	107.00
6	P	1128	HEC	CMD-C2D-C1D	-5.29	120.33	128.46
6	D	1128	HEC	C1D-C2D-C3D	5.29	110.67	107.00
6	L	1128	HEC	C1D-C2D-C3D	5.27	110.66	107.00
6	L	1128	HEC	CMD-C2D-C1D	-5.14	120.57	128.46
6	J	1129	HEC	CBA-CAA-C2A	-5.12	103.04	112.48
5	O	1803	MGD	C17-C16-C21	5.12	119.11	114.57
6	B	1129	HEC	CMD-C2D-C1D	-5.08	120.66	128.46
6	H	1129	HEC	CMD-C2D-C1D	-5.04	120.71	128.46
6	J	1128	HEC	CMD-C2D-C1D	-5.02	120.75	128.46
5	A	1803	MGD	C17-C16-C21	5.00	119.01	114.57
5	K	1803	MGD	C17-C16-C21	4.96	118.98	114.57
6	P	1129	HEC	CBD-CAD-C3D	4.90	121.52	112.49
5	M	1803	MGD	C17-C16-C21	4.87	118.90	114.57
6	N	1129	HEC	CMD-C2D-C1D	-4.87	120.97	128.46
6	J	1129	HEC	C1D-C2D-C3D	4.87	110.38	107.00
5	C	1803	MGD	C17-C16-C21	4.85	118.88	114.57
6	F	1129	HEC	CBD-CAD-C3D	4.84	121.41	112.49
5	E	1804	MGD	O11-C23-C14	-4.78	105.77	108.96
5	A	1804	MGD	C17-N18-C19	4.76	123.49	115.93
5	E	1803	MGD	O11-C23-C14	4.73	112.12	108.96
5	C	1804	MGD	C17-N18-C19	4.72	123.42	115.93
5	E	1803	MGD	C17-C16-C21	4.71	118.76	114.57
5	O	1803	MGD	O4'-C1'-C2'	-4.67	100.11	106.93
6	H	1128	HEC	CAD-CBD-CGD	4.64	120.46	112.67
5	K	1804	MGD	C17-N18-C19	4.63	123.29	115.93
6	P	1128	HEC	C1D-C2D-C3D	4.62	110.21	107.00
5	K	1804	MGD	O4'-C1'-C2'	-4.61	100.19	106.93
6	F	1128	HEC	CMD-C2D-C1D	-4.61	121.39	128.46
5	O	1804	MGD	C6-C5-C4	-4.59	116.42	120.80
5	A	1803	MGD	C17-N18-C19	4.58	123.21	115.93
5	A	1804	MGD	C17-C16-C21	4.58	118.64	114.57
5	C	1804	MGD	O4'-C1'-C2'	-4.56	100.26	106.93
6	D	1128	HEC	CAD-CBD-CGD	4.56	120.32	112.67
5	E	1804	MGD	C17-N18-C19	4.54	123.14	115.93
5	I	1804	MGD	C17-C16-C21	4.52	118.58	114.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1128	HEC	CBD-CAD-C3D	-4.51	104.17	112.49
5	I	1804	MGD	C17-N18-C19	4.51	123.09	115.93
6	N	1128	HEC	C1D-C2D-C3D	4.50	110.13	107.00
5	A	1803	MGD	O4'-C1'-C2'	-4.48	100.37	106.93
5	G	1804	MGD	C17-N18-C19	4.47	123.04	115.93
5	G	1803	MGD	C6-N1-C2	4.47	123.04	115.93
5	I	1804	MGD	C6-N1-C2	4.47	123.03	115.93
6	B	1128	HEC	CAD-CBD-CGD	4.44	120.12	112.67
5	M	1804	MGD	C17-C16-C21	4.43	118.50	114.57
5	E	1804	MGD	C17-C16-C21	4.40	118.48	114.57
5	O	1804	MGD	C17-C16-C21	4.40	118.47	114.57
5	A	1804	MGD	O11-C23-C14	-4.40	106.03	108.96
6	J	1129	HEC	CBD-CAD-C3D	4.37	120.55	112.49
5	M	1804	MGD	O4'-C1'-C2'	-4.37	100.54	106.93
5	O	1803	MGD	C17-N18-C19	4.37	122.87	115.93
5	M	1804	MGD	C17-N18-C19	4.36	122.86	115.93
5	G	1804	MGD	C6-C5-C4	-4.35	116.64	120.80
6	F	1129	HEC	CMD-C2D-C1D	-4.35	121.78	128.46
6	P	1128	HEC	CBD-CAD-C3D	-4.35	104.47	112.49
5	O	1804	MGD	C17-N18-C19	4.34	122.83	115.93
5	G	1804	MGD	C17-C16-C21	4.34	118.42	114.57
5	O	1804	MGD	O4'-C1'-C2'	-4.28	100.67	106.93
6	B	1128	HEC	CMD-C2D-C1D	-4.26	121.92	128.46
5	I	1803	MGD	C6-N1-C2	4.24	122.67	115.93
5	A	1804	MGD	C6-C5-C4	-4.20	116.78	120.80
5	I	1804	MGD	O4'-C1'-C2'	-4.17	100.84	106.93
5	G	1804	MGD	C6-N1-C2	4.15	122.53	115.93
5	A	1804	MGD	C6-N1-C2	4.15	122.53	115.93
5	E	1803	MGD	C17-N18-C19	4.15	122.53	115.93
5	I	1803	MGD	C17-N18-C19	4.13	122.49	115.93
5	C	1804	MGD	C17-C16-C21	4.11	118.22	114.57
5	C	1803	MGD	C17-N18-C19	4.10	122.45	115.93
5	C	1803	MGD	C6-N1-C2	4.10	122.44	115.93
5	K	1804	MGD	C6-N1-C2	4.10	122.44	115.93
6	H	1128	HEC	CBD-CAD-C3D	-4.09	104.94	112.49
6	J	1129	HEC	CAA-CBA-CGA	4.08	119.51	112.67
5	O	1803	MGD	C6-N1-C2	4.07	122.39	115.93
5	K	1803	MGD	O4'-C1'-C2'	-4.05	101.00	106.93
5	O	1804	MGD	C6-N1-C2	4.05	122.36	115.93
5	K	1804	MGD	C6-C5-C4	-4.03	116.95	120.80
5	G	1803	MGD	C17-N18-C19	4.02	122.32	115.93
6	F	1128	HEC	CAD-CBD-CGD	4.00	119.38	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1803	MGD	C17-N18-C19	4.00	122.28	115.93
5	A	1803	MGD	C6-N1-C2	3.99	122.28	115.93
5	C	1804	MGD	C6-N1-C2	3.99	122.28	115.93
6	D	1128	HEC	CMD-C2D-C1D	-3.99	122.33	128.46
5	G	1804	MGD	O4'-C1'-C2'	-3.98	101.11	106.93
6	B	1129	HEC	CBD-CAD-C3D	3.95	119.77	112.49
5	C	1803	MGD	O4'-C1'-C2'	-3.93	101.18	106.93
5	K	1804	MGD	C17-C16-C21	3.93	118.06	114.57
5	M	1804	MGD	C6-C5-C4	-3.92	117.06	120.80
5	M	1804	MGD	C6-N1-C2	3.90	122.13	115.93
5	K	1803	MGD	C17-N18-C19	3.90	122.13	115.93
5	M	1803	MGD	C6-N1-C2	3.89	122.11	115.93
5	C	1804	MGD	C6-C5-C4	-3.89	117.09	120.80
5	K	1803	MGD	C6-C5-C4	-3.89	117.09	120.80
6	N	1128	HEC	CAD-CBD-CGD	3.84	119.11	112.67
6	N	1129	HEC	CMC-C2C-C3C	3.83	130.32	125.82
6	H	1129	HEC	CMA-C3A-C2A	3.76	132.03	124.94
5	K	1803	MGD	C6-N1-C2	3.74	121.87	115.93
6	P	1129	HEC	CMC-C2C-C3C	3.73	130.21	125.82
5	E	1803	MGD	C6-N1-C2	3.72	121.84	115.93
5	E	1803	MGD	C6-C5-C4	-3.70	117.27	120.80
5	O	1803	MGD	C6-C5-C4	-3.68	117.28	120.80
5	I	1803	MGD	C2-N3-C4	-3.68	111.16	115.36
5	I	1804	MGD	C6-C5-C4	-3.67	117.29	120.80
5	K	1804	MGD	C4-C5-N7	3.67	113.23	109.40
6	J	1129	HEC	CMB-C2B-C1B	-3.66	122.83	128.46
5	E	1804	MGD	C6-C5-C4	-3.66	117.31	120.80
5	A	1803	MGD	C6-C5-C4	-3.65	117.31	120.80
5	C	1803	MGD	C6-C5-C4	-3.65	117.32	120.80
6	L	1129	HEC	CBA-CAA-C2A	-3.64	105.76	112.48
5	E	1804	MGD	C6-N1-C2	3.64	121.72	115.93
5	E	1804	MGD	O4'-C1'-C2'	-3.64	101.61	106.93
6	P	1129	HEC	CMA-C3A-C2A	3.60	131.74	124.94
5	I	1804	MGD	N3-C2-N1	-3.60	122.43	127.22
5	K	1803	MGD	C2-N3-C4	-3.57	111.28	115.36
5	K	1804	MGD	C2-N3-C4	-3.57	111.28	115.36
5	G	1803	MGD	C6-C5-C4	-3.55	117.41	120.80
5	M	1803	MGD	C6-C5-C4	-3.54	117.41	120.80
6	L	1129	HEC	CMC-C2C-C3C	3.52	129.96	125.82
5	O	1803	MGD	C2-N3-C4	-3.52	111.34	115.36
5	I	1804	MGD	C2-N3-C4	-3.52	111.34	115.36
6	D	1129	HEC	CMA-C3A-C2A	3.51	131.56	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1803	MGD	O11-C23-C14	3.49	111.29	108.96
5	A	1803	MGD	O11-C23-C14	3.48	111.29	108.96
6	H	1129	HEC	CMC-C2C-C3C	3.48	129.91	125.82
5	I	1803	MGD	C3'-C2'-C1'	-3.45	95.78	100.98
6	L	1129	HEC	CMB-C2B-C1B	-3.44	123.17	128.46
5	G	1803	MGD	O4'-C1'-C2'	-3.43	101.91	106.93
6	H	1129	HEC	CBD-CAD-C3D	3.42	118.79	112.49
6	D	1129	HEC	CBD-CAD-C3D	3.40	118.75	112.49
6	D	1129	HEC	CAA-CBA-CGA	3.37	118.33	112.67
5	G	1803	MGD	N3-C2-N1	-3.37	122.73	127.22
6	L	1129	HEC	CBD-CAD-C3D	3.30	118.57	112.49
5	G	1804	MGD	N3-C2-N1	-3.27	122.86	127.22
6	N	1129	HEC	CMA-C3A-C2A	3.26	131.09	124.94
6	N	1129	HEC	CMC-C2C-C1C	-3.23	123.50	128.46
5	O	1804	MGD	N3-C2-N1	-3.23	122.92	127.22
6	F	1129	HEC	CMC-C2C-C3C	3.23	129.62	125.82
6	H	1128	HEC	CMB-C2B-C1B	-3.22	123.51	128.46
6	H	1128	HEC	CMA-C3A-C2A	3.22	131.01	124.94
5	A	1804	MGD	C4-C5-N7	3.22	112.75	109.40
6	D	1128	HEC	CMA-C3A-C2A	3.18	130.94	124.94
5	G	1804	MGD	O5'-C5'-C4'	-3.18	98.04	108.99
5	A	1803	MGD	N3-C2-N1	-3.18	122.98	127.22
5	I	1804	MGD	C16-C17-N18	-3.14	115.09	124.01
5	C	1803	MGD	N3-C2-N1	-3.12	123.06	127.22
5	G	1803	MGD	C2-N3-C4	-3.12	111.80	115.36
6	F	1129	HEC	CMA-C3A-C2A	3.11	130.81	124.94
5	I	1803	MGD	C16-C17-N18	-3.11	115.17	124.01
5	A	1804	MGD	C16-C17-N18	-3.11	115.18	124.01
6	B	1129	HEC	CMC-C2C-C3C	3.09	129.46	125.82
5	O	1803	MGD	C16-C17-N18	-3.09	115.23	124.01
5	A	1803	MGD	C16-C17-N18	-3.09	115.24	124.01
5	O	1803	MGD	C16-C21-N22	3.08	120.95	118.13
5	G	1803	MGD	C16-C17-N18	-3.08	115.26	124.01
5	I	1804	MGD	O5'-C5'-C4'	-3.08	98.40	108.99
6	H	1128	HEC	CAA-CBA-CGA	3.07	117.82	112.67
5	M	1804	MGD	N3-C2-N1	-3.07	123.13	127.22
5	I	1804	MGD	C4-C5-N7	3.06	112.59	109.40
6	N	1129	HEC	CBA-CAA-C2A	-3.06	106.84	112.48
5	G	1804	MGD	C16-C17-N18	-3.04	115.36	124.01
5	E	1804	MGD	C16-C17-N18	-3.04	115.37	124.01
5	K	1804	MGD	C16-C17-N18	-3.03	115.39	124.01
6	N	1128	HEC	CMD-C2D-C3D	3.03	130.65	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1803	MGD	C1'-N9-C4	-3.02	121.33	126.64
6	L	1129	HEC	CMA-C3A-C2A	3.02	130.64	124.94
6	J	1129	HEC	CMC-C2C-C3C	3.01	129.36	125.82
5	A	1804	MGD	N3-C2-N1	-3.00	123.22	127.22
6	P	1129	HEC	CMC-C2C-C1C	-3.00	123.86	128.46
5	G	1804	MGD	C4-C5-N7	3.00	112.52	109.40
5	K	1803	MGD	O11-C23-C14	3.00	110.96	108.96
5	C	1804	MGD	O4'-C4'-C3'	-3.00	99.18	105.11
5	I	1803	MGD	C2'-C3'-C4'	3.00	108.46	102.64
6	N	1129	HEC	CBD-CAD-C3D	2.99	118.01	112.49
5	M	1804	MGD	O5'-C5'-C4'	-2.98	98.73	108.99
5	E	1804	MGD	O5'-C5'-C4'	-2.97	98.75	108.99
5	C	1804	MGD	C16-C17-N18	-2.97	115.56	124.01
5	M	1804	MGD	C16-C17-N18	-2.97	115.57	124.01
5	A	1804	MGD	O4'-C4'-C3'	-2.94	99.29	105.11
5	E	1803	MGD	C2-N3-C4	-2.94	112.00	115.36
6	L	1128	HEC	CAD-CBD-CGD	2.93	117.59	112.67
6	J	1129	HEC	CMD-C2D-C3D	2.93	130.47	124.94
6	F	1129	HEC	CMB-C2B-C1B	-2.93	123.96	128.46
6	B	1129	HEC	CAA-CBA-CGA	2.92	117.57	112.67
5	M	1804	MGD	O4'-C4'-C3'	-2.92	99.34	105.11
5	M	1804	MGD	C2-N3-C4	-2.90	112.04	115.36
5	A	1804	MGD	C2-N3-C4	-2.90	112.04	115.36
5	I	1803	MGD	C6-C5-C4	-2.90	118.03	120.80
5	O	1804	MGD	C4-C5-N7	2.90	112.42	109.40
5	C	1803	MGD	C16-C17-N18	-2.89	115.80	124.01
6	J	1128	HEC	CMA-C3A-C2A	2.88	130.38	124.94
6	B	1128	HEC	CMB-C2B-C1B	-2.88	124.04	128.46
5	O	1804	MGD	C16-C17-N18	-2.87	115.84	124.01
5	K	1804	MGD	N3-C2-N1	-2.87	123.40	127.22
6	P	1128	HEC	CAD-CBD-CGD	2.87	117.48	112.67
6	F	1128	HEC	CMB-C2B-C1B	-2.86	124.06	128.46
5	E	1804	MGD	C16-C21-N22	2.86	120.74	118.13
6	P	1129	HEC	CMB-C2B-C1B	-2.85	124.08	128.46
5	I	1803	MGD	O11-C23-C14	2.85	110.87	108.96
5	O	1804	MGD	O5'-C5'-C4'	-2.85	99.18	108.99
5	E	1803	MGD	C16-C17-N18	-2.84	115.93	124.01
6	N	1128	HEC	CMB-C2B-C1B	-2.84	124.10	128.46
6	F	1128	HEC	CMA-C3A-C2A	2.83	130.28	124.94
6	P	1129	HEC	CAA-CBA-CGA	2.83	117.42	112.67
5	E	1804	MGD	O4'-C4'-C3'	-2.83	99.52	105.11
5	M	1803	MGD	N3-C2-N1	-2.82	123.46	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1129	HEC	CMC-C2C-C1C	-2.82	124.13	128.46
6	D	1129	HEC	CMC-C2C-C3C	2.82	129.13	125.82
5	O	1803	MGD	C1'-N9-C4	-2.80	121.72	126.64
6	L	1128	HEC	CMC-C2C-C1C	-2.79	124.17	128.46
5	E	1804	MGD	N3-C2-N1	-2.79	123.51	127.22
6	D	1128	HEC	CBA-CAA-C2A	-2.78	107.35	112.48
5	K	1803	MGD	C16-C17-N18	-2.78	116.11	124.01
6	N	1128	HEC	CBA-CAA-C2A	-2.78	107.36	112.48
5	C	1804	MGD	C4-C5-N7	2.77	112.28	109.40
5	K	1803	MGD	C3'-C2'-C1'	-2.76	96.82	100.98
5	M	1804	MGD	C4-C5-N7	2.75	112.27	109.40
6	H	1128	HEC	CMB-C2B-C3B	2.75	129.06	125.82
5	A	1804	MGD	C16-C21-N22	2.75	120.65	118.13
5	C	1804	MGD	C2-N3-C4	-2.75	112.22	115.36
5	C	1804	MGD	N3-C2-N1	-2.74	123.57	127.22
5	I	1803	MGD	O3'-C3'-C4'	-2.74	103.12	111.05
5	I	1803	MGD	C16-C21-N22	2.73	120.63	118.13
5	O	1804	MGD	O2B-PB-O5'	-2.72	95.11	107.75
6	F	1129	HEC	CBA-CAA-C2A	-2.72	107.47	112.48
5	A	1804	MGD	O2B-PB-O5'	-2.71	95.15	107.75
5	O	1803	MGD	N3-C2-N1	-2.70	123.62	127.22
6	J	1128	HEC	CAD-CBD-CGD	2.68	117.17	112.67
5	M	1803	MGD	C16-C17-N18	-2.68	116.40	124.01
5	E	1803	MGD	N3-C2-N1	-2.67	123.66	127.22
6	L	1129	HEC	CMB-C2B-C3B	2.67	128.96	125.82
6	D	1129	HEC	CMD-C2D-C3D	2.67	129.97	124.94
5	G	1804	MGD	O4'-C4'-C3'	-2.66	99.85	105.11
6	L	1128	HEC	CMB-C2B-C1B	-2.65	124.39	128.46
5	G	1803	MGD	C16-C21-N22	2.65	120.55	118.13
5	I	1803	MGD	N3-C2-N1	-2.64	123.69	127.22
6	N	1129	HEC	CMB-C2B-C1B	-2.63	124.42	128.46
5	O	1803	MGD	C3'-C2'-C1'	-2.62	97.03	100.98
6	D	1129	HEC	CMB-C2B-C1B	-2.61	124.45	128.46
5	O	1804	MGD	C16-N15-C14	-2.61	110.52	120.00
5	I	1803	MGD	O4'-C1'-C2'	-2.61	103.11	106.93
6	J	1129	HEC	CMA-C3A-C2A	2.61	129.86	124.94
5	E	1804	MGD	C4-C5-N7	2.60	112.11	109.40
6	J	1129	HEC	CMC-C2C-C1C	-2.60	124.47	128.46
5	K	1803	MGD	C1'-N9-C4	-2.60	122.07	126.64
5	C	1803	MGD	C2-N3-C4	-2.60	112.39	115.36
5	I	1804	MGD	C16-N15-C14	-2.60	110.58	120.00
5	A	1803	MGD	C1'-N9-C4	-2.59	122.10	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1804	MGD	O2B-PB-O5'	-2.57	95.80	107.75
5	M	1804	MGD	C3'-C2'-C1'	-2.56	97.13	100.98
5	O	1804	MGD	C2-N3-C4	-2.55	112.44	115.36
5	O	1804	MGD	O4'-C4'-C3'	-2.55	100.07	105.11
6	H	1129	HEC	CMB-C2B-C1B	-2.55	124.55	128.46
5	O	1803	MGD	O11-C23-C14	2.55	110.66	108.96
6	F	1128	HEC	CMB-C2B-C3B	2.54	128.81	125.82
6	D	1128	HEC	CAA-CBA-CGA	2.54	116.94	112.67
5	K	1804	MGD	C3'-C2'-C1'	-2.54	97.15	100.98
5	I	1804	MGD	O4'-C4'-C3'	-2.53	100.10	105.11
6	L	1129	HEC	CMC-C2C-C1C	-2.52	124.59	128.46
6	B	1128	HEC	CMA-C3A-C2A	2.50	129.66	124.94
6	L	1129	HEC	CAA-CBA-CGA	2.50	116.87	112.67
5	M	1803	MGD	C16-N15-C14	-2.50	110.91	120.00
5	M	1804	MGD	C16-C21-N22	2.50	120.42	118.13
5	G	1804	MGD	C2-N3-C4	-2.50	112.50	115.36
5	G	1803	MGD	C3'-C2'-C1'	-2.48	97.25	100.98
5	A	1803	MGD	C2-N3-C4	-2.47	112.54	115.36
5	K	1804	MGD	C16-N15-C14	-2.46	111.07	120.00
5	G	1804	MGD	C16-N15-C14	-2.45	111.11	120.00
6	L	1128	HEC	CBA-CAA-C2A	-2.44	107.97	112.48
5	K	1804	MGD	O2B-PB-O5'	-2.44	96.40	107.75
5	C	1803	MGD	C1'-N9-C4	-2.44	122.35	126.64
6	D	1129	HEC	CMC-C2C-C1C	-2.44	124.72	128.46
5	K	1804	MGD	O4'-C4'-C3'	-2.44	100.29	105.11
5	E	1804	MGD	C2-N3-C4	-2.44	112.58	115.36
5	K	1803	MGD	C16-N15-C14	-2.43	111.17	120.00
6	F	1129	HEC	CMC-C2C-C1C	-2.43	124.72	128.46
5	C	1804	MGD	C3'-C2'-C1'	-2.43	97.32	100.98
5	M	1803	MGD	C2-N3-C4	-2.43	112.58	115.36
5	O	1803	MGD	O11-C23-N22	-2.42	106.08	108.57
5	O	1804	MGD	C16-C21-N22	2.42	120.34	118.13
5	K	1804	MGD	O5'-C5'-C4'	-2.41	100.69	108.99
5	M	1803	MGD	C16-C21-N22	2.41	120.33	118.13
6	B	1128	HEC	CAA-CBA-CGA	2.40	116.69	112.67
6	P	1128	HEC	CMD-C2D-C3D	2.39	129.46	124.94
5	A	1803	MGD	C16-N15-C14	-2.39	111.32	120.00
5	C	1804	MGD	C17-C16-N15	2.39	121.13	119.12
5	K	1803	MGD	N3-C2-N1	-2.39	124.04	127.22
5	M	1804	MGD	C16-N15-C14	-2.38	111.35	120.00
6	N	1128	HEC	C4B-C3B-C2B	2.36	108.90	106.35
6	H	1129	HEC	CMC-C2C-C1C	-2.35	124.85	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1803	MGD	C16-N15-C14	-2.35	111.48	120.00
5	I	1803	MGD	C16-N15-C14	-2.35	111.48	120.00
6	N	1129	HEC	CAA-CBA-CGA	2.34	116.60	112.67
6	J	1129	HEC	CMB-C2B-C3B	2.34	128.57	125.82
6	D	1128	HEC	CMB-C2B-C1B	-2.33	124.89	128.46
6	H	1129	HEC	CAA-CBA-CGA	2.32	116.57	112.67
5	A	1803	MGD	C3'-C2'-C1'	-2.31	97.49	100.98
5	A	1803	MGD	C16-C21-N22	2.31	120.24	118.13
6	B	1129	HEC	CMB-C2B-C1B	-2.30	124.92	128.46
5	C	1804	MGD	O5'-C5'-C4'	-2.30	101.08	108.99
5	I	1804	MGD	C3'-C2'-C1'	-2.29	97.52	100.98
5	G	1804	MGD	C3'-C2'-C1'	-2.29	97.53	100.98
5	G	1803	MGD	C16-N15-C14	-2.28	111.73	120.00
6	L	1128	HEC	CMA-C3A-C2A	2.24	129.16	124.94
5	M	1803	MGD	C3'-C2'-C1'	-2.24	97.61	100.98
6	P	1129	HEC	CMD-C2D-C3D	2.23	129.15	124.94
5	I	1804	MGD	C16-C21-N22	2.23	120.17	118.13
5	A	1804	MGD	O5'-C5'-C4'	-2.22	101.34	108.99
6	P	1128	HEC	CMA-C3A-C2A	2.21	129.11	124.94
5	C	1803	MGD	C16-N15-C14	-2.21	111.97	120.00
6	P	1129	HEC	CMB-C2B-C3B	2.21	128.42	125.82
5	E	1803	MGD	C16-N15-C14	-2.21	112.00	120.00
5	E	1804	MGD	C16-N15-C14	-2.19	112.04	120.00
6	N	1128	HEC	CMB-C2B-C3B	2.19	128.40	125.82
6	F	1129	HEC	CMB-C2B-C3B	2.18	128.39	125.82
5	I	1803	MGD	C1'-N9-C4	-2.18	122.80	126.64
6	L	1128	HEC	CMC-C2C-C3C	2.18	128.38	125.82
5	C	1804	MGD	C16-N15-C14	-2.18	112.10	120.00
5	G	1803	MGD	O11-C23-N22	-2.16	106.35	108.57
5	M	1804	MGD	O2A-PA-O1A	2.16	122.92	112.24
5	M	1803	MGD	C1'-N9-C4	-2.16	122.85	126.64
6	H	1128	HEC	CMD-C2D-C3D	2.16	129.01	124.94
5	E	1804	MGD	N18-C19-N20	-2.15	122.05	125.42
6	J	1128	HEC	CMC-C2C-C1C	-2.15	125.16	128.46
5	O	1804	MGD	C3'-C2'-C1'	-2.15	97.75	100.98
5	O	1803	MGD	O4'-C4'-C5'	-2.14	102.33	109.37
6	B	1129	HEC	CMA-C3A-C2A	2.13	128.96	124.94
5	A	1803	MGD	O4'-C4'-C5'	-2.13	102.36	109.37
5	K	1803	MGD	O11-C23-N22	-2.13	106.38	108.57
5	E	1804	MGD	O5'-PB-O1B	2.12	117.35	109.07
5	K	1803	MGD	C2'-C3'-C4'	2.12	106.76	102.64
5	E	1803	MGD	C1'-N9-C4	-2.11	122.93	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1803	MGD	O2A-PA-O1A	2.11	122.68	112.24
5	K	1804	MGD	O2A-PA-O1A	2.11	122.68	112.24
6	D	1128	HEC	CMC-C2C-C3C	2.10	128.29	125.82
5	C	1803	MGD	O11-C23-N22	-2.10	106.41	108.57
5	A	1804	MGD	C16-N15-C14	-2.10	112.38	120.00
5	I	1803	MGD	N18-C19-N20	-2.10	122.13	125.42
5	C	1803	MGD	O4'-C4'-C5'	-2.09	102.50	109.37
5	G	1804	MGD	O2A-PA-O1A	2.08	122.52	112.24
5	M	1803	MGD	O4'-C4'-C5'	-2.08	102.54	109.37
5	M	1803	MGD	O4'-C4'-C3'	-2.07	101.02	105.11
5	E	1804	MGD	PA-O3B-PB	2.07	139.91	132.83
6	D	1129	HEC	CAD-CBD-CGD	2.06	116.13	112.67
5	A	1804	MGD	C3'-C2'-C1'	-2.06	97.87	100.98
5	K	1804	MGD	O5'-PB-O1B	2.06	117.11	109.07
5	A	1803	MGD	C2'-C3'-C4'	2.04	106.61	102.64
5	A	1804	MGD	C17-C16-N15	2.04	120.83	119.12
5	I	1803	MGD	O11-C23-N22	-2.04	106.47	108.57
6	L	1128	HEC	CMD-C2D-C3D	2.03	128.77	124.94
6	D	1128	HEC	CMB-C2B-C3B	2.02	128.20	125.82
5	C	1804	MGD	O2B-PB-O5'	-2.00	98.44	107.75
6	F	1128	HEC	CMC-C2C-C1C	-2.00	125.39	128.46
5	I	1804	MGD	O2A-PA-O1A	2.00	122.13	112.24
5	C	1803	MGD	C16-C21-N22	2.00	119.96	118.13

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1804	MGD	C5'-O5'-PB-O1B
5	K	1804	MGD	C5'-O5'-PB-O2B
5	M	1804	MGD	C5'-O5'-PB-O1B
5	M	1804	MGD	C5'-O5'-PB-O2B
5	A	1803	MGD	PA-O3B-PB-O5'
5	A	1803	MGD	C5'-O5'-PB-O1B
5	A	1803	MGD	C5'-O5'-PB-O2B
5	E	1804	MGD	C5'-O5'-PB-O1B
5	G	1804	MGD	C5'-O5'-PB-O1B
5	O	1804	MGD	C5'-O5'-PB-O1B
5	O	1804	MGD	C5'-O5'-PB-O2B
5	O	1803	MGD	PA-O3B-PB-O5'
5	O	1803	MGD	C5'-O5'-PB-O1B
5	O	1803	MGD	C5'-O5'-PB-O2B

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Mol	Chain	Res	Type	Atoms
5	C	1804	MGD	C5'-O5'-PB-O1B
5	M	1803	MGD	C5'-O5'-PB-O1B
5	M	1803	MGD	C5'-O5'-PB-O2B
6	N	1129	HEC	C4D-C3D-CAD-CBD
5	K	1803	MGD	PA-O3B-PB-O5'
5	K	1803	MGD	C5'-O5'-PB-O1B
5	K	1803	MGD	C5'-O5'-PB-O2B
5	E	1803	MGD	PA-O3B-PB-O5'
5	E	1803	MGD	C5'-O5'-PB-O1B
5	E	1803	MGD	C5'-O5'-PB-O2B
5	C	1803	MGD	PA-O3B-PB-O5'
5	C	1803	MGD	C5'-O5'-PB-O1B
5	C	1803	MGD	C5'-O5'-PB-O2B
5	A	1804	MGD	C5'-O5'-PB-O1B
5	A	1804	MGD	C5'-O5'-PB-O2B
5	G	1803	MGD	PA-O3B-PB-O5'
5	G	1803	MGD	C5'-O5'-PB-O1B
5	G	1803	MGD	C5'-O5'-PB-O2B
5	I	1804	MGD	C5'-O5'-PB-O1B
5	I	1804	MGD	C5'-O5'-PB-O2B
5	I	1803	MGD	PA-O3B-PB-O5'
5	I	1803	MGD	C5'-O5'-PB-O1B
5	I	1803	MGD	C5'-O5'-PB-O2B
5	K	1804	MGD	PA-O3B-PB-O5'
5	M	1804	MGD	PA-O3B-PB-O5'
5	E	1804	MGD	PA-O3B-PB-O5'
5	G	1804	MGD	PA-O3B-PB-O5'
5	O	1804	MGD	PA-O3B-PB-O5'
5	C	1804	MGD	PA-O3B-PB-O5'
5	M	1803	MGD	PA-O3B-PB-O5'
5	A	1804	MGD	PA-O3B-PB-O5'
5	I	1804	MGD	PA-O3B-PB-O5'
5	E	1804	MGD	C5'-O5'-PB-O2B
5	G	1804	MGD	C5'-O5'-PB-O2B
5	C	1804	MGD	C5'-O5'-PB-O2B
6	N	1129	HEC	C2D-C3D-CAD-CBD
5	C	1803	MGD	O4'-C4'-C5'-O5'
5	G	1803	MGD	O4'-C4'-C5'-O5'
5	I	1803	MGD	O4'-C4'-C5'-O5'
5	I	1804	MGD	PA-O3B-PB-O1B
5	K	1803	MGD	O4'-C4'-C5'-O5'
5	A	1803	MGD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	O	1803	MGD	O4'-C4'-C5'-O5'
5	M	1803	MGD	O4'-C4'-C5'-O5'
5	E	1803	MGD	O4'-C4'-C5'-O5'
5	K	1804	MGD	C5'-O5'-PB-O3B
5	M	1804	MGD	C5'-O5'-PB-O3B
5	A	1803	MGD	C5'-O5'-PB-O3B
5	E	1804	MGD	C5'-O5'-PB-O3B
5	G	1804	MGD	C5'-O5'-PB-O3B
5	O	1804	MGD	C5'-O5'-PB-O3B
5	O	1803	MGD	C5'-O5'-PB-O3B
5	C	1804	MGD	C5'-O5'-PB-O3B
5	M	1803	MGD	C5'-O5'-PB-O3B
5	K	1803	MGD	C5'-O5'-PB-O3B
5	E	1803	MGD	C5'-O5'-PB-O3B
5	C	1803	MGD	C5'-O5'-PB-O3B
5	A	1804	MGD	C5'-O5'-PB-O3B
5	G	1803	MGD	C5'-O5'-PB-O3B
5	I	1804	MGD	C5'-O5'-PB-O3B
5	I	1803	MGD	C5'-O5'-PB-O3B
5	K	1804	MGD	O4'-C4'-C5'-O5'
5	M	1804	MGD	O4'-C4'-C5'-O5'
5	G	1804	MGD	O4'-C4'-C5'-O5'
5	O	1804	MGD	O4'-C4'-C5'-O5'
5	C	1804	MGD	O4'-C4'-C5'-O5'
5	A	1804	MGD	O4'-C4'-C5'-O5'
5	I	1804	MGD	O4'-C4'-C5'-O5'
5	K	1804	MGD	PA-O3B-PB-O1B
5	M	1804	MGD	PA-O3B-PB-O1B
5	A	1803	MGD	PA-O3B-PB-O1B
5	E	1804	MGD	PA-O3B-PB-O1B
5	G	1804	MGD	PA-O3B-PB-O1B
5	M	1803	MGD	PA-O3B-PB-O1B
5	K	1803	MGD	PA-O3B-PB-O1B
5	E	1803	MGD	PA-O3B-PB-O1B
5	C	1803	MGD	PA-O3B-PB-O1B
5	I	1804	MGD	PA-O3B-PB-O2B
5	I	1803	MGD	PA-O3B-PB-O1B
5	E	1804	MGD	O4'-C4'-C5'-O5'

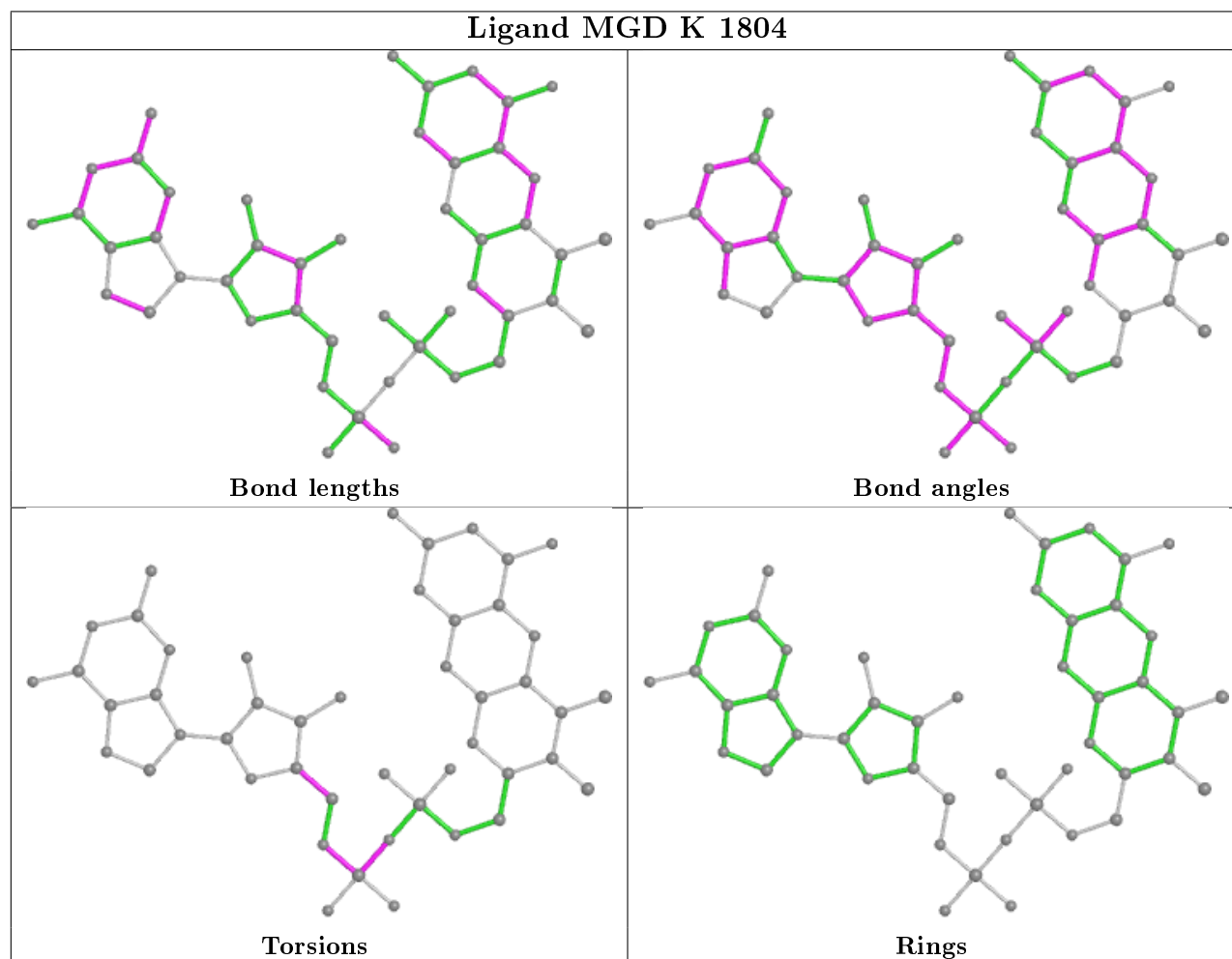
There are no ring outliers.

35 monomers are involved in 324 short contacts:

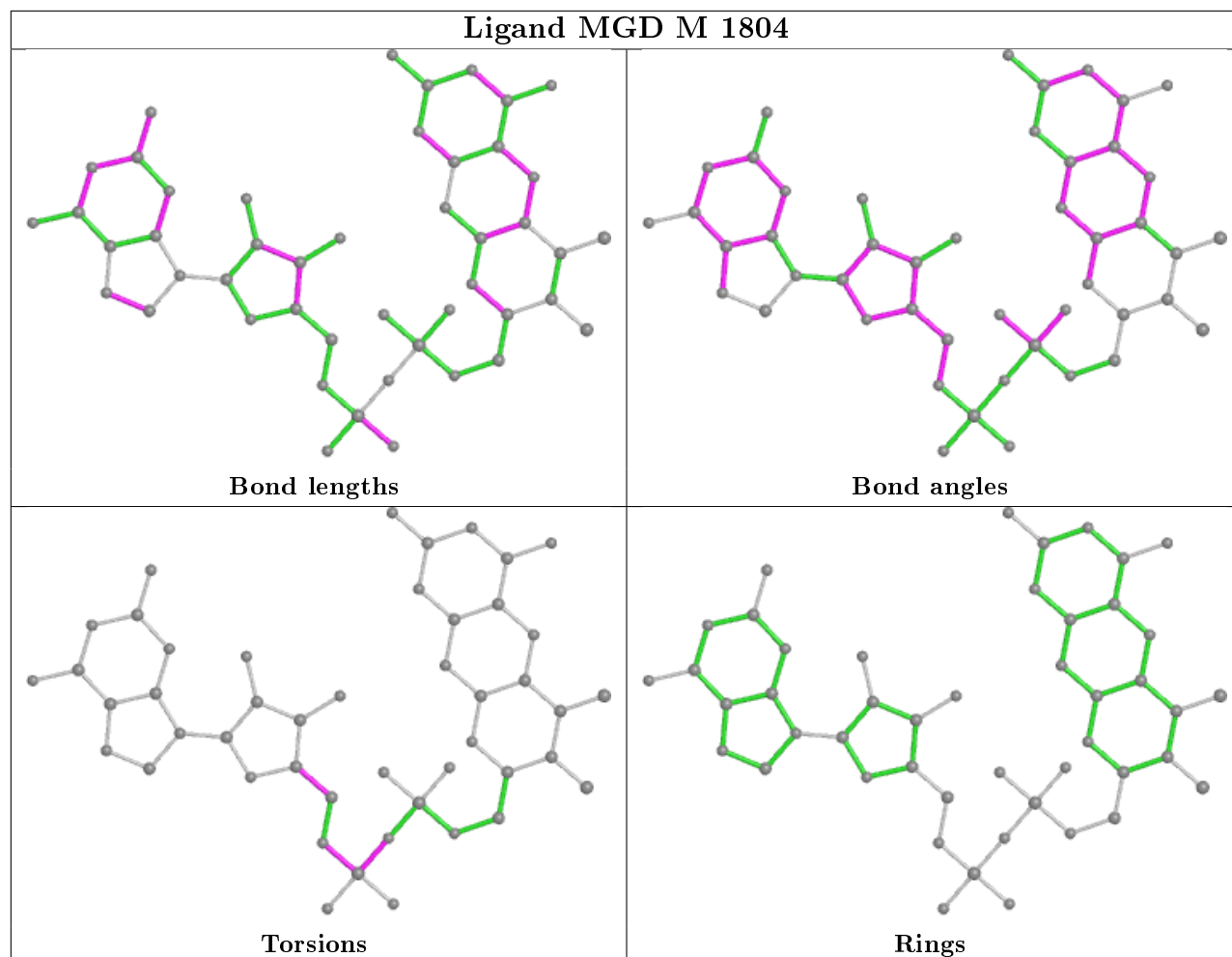
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1804	MGD	7	0
5	M	1804	MGD	7	0
5	A	1803	MGD	7	0
6	P	1129	HEC	15	0
5	E	1804	MGD	7	0
5	G	1804	MGD	6	0
6	L	1129	HEC	17	0
3	E	1801	SF4	1	0
6	F	1129	HEC	11	0
6	P	1128	HEC	10	0
5	O	1804	MGD	8	0
5	O	1803	MGD	7	0
5	C	1804	MGD	6	0
6	L	1128	HEC	9	0
6	B	1128	HEC	3	0
6	F	1128	HEC	12	0
5	M	1803	MGD	8	0
6	J	1128	HEC	11	0
6	H	1128	HEC	13	0
6	N	1129	HEC	19	0
6	D	1128	HEC	11	0
5	K	1803	MGD	8	0
6	D	1129	HEC	22	0
6	B	1129	HEC	12	0
5	E	1803	MGD	8	0
5	C	1803	MGD	8	0
5	A	1804	MGD	8	0
3	K	1801	SF4	1	0
6	N	1128	HEC	11	0
5	G	1803	MGD	7	0
6	H	1129	HEC	14	0
5	I	1804	MGD	6	0
5	I	1803	MGD	7	0
6	J	1129	HEC	16	0
3	C	1801	SF4	1	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

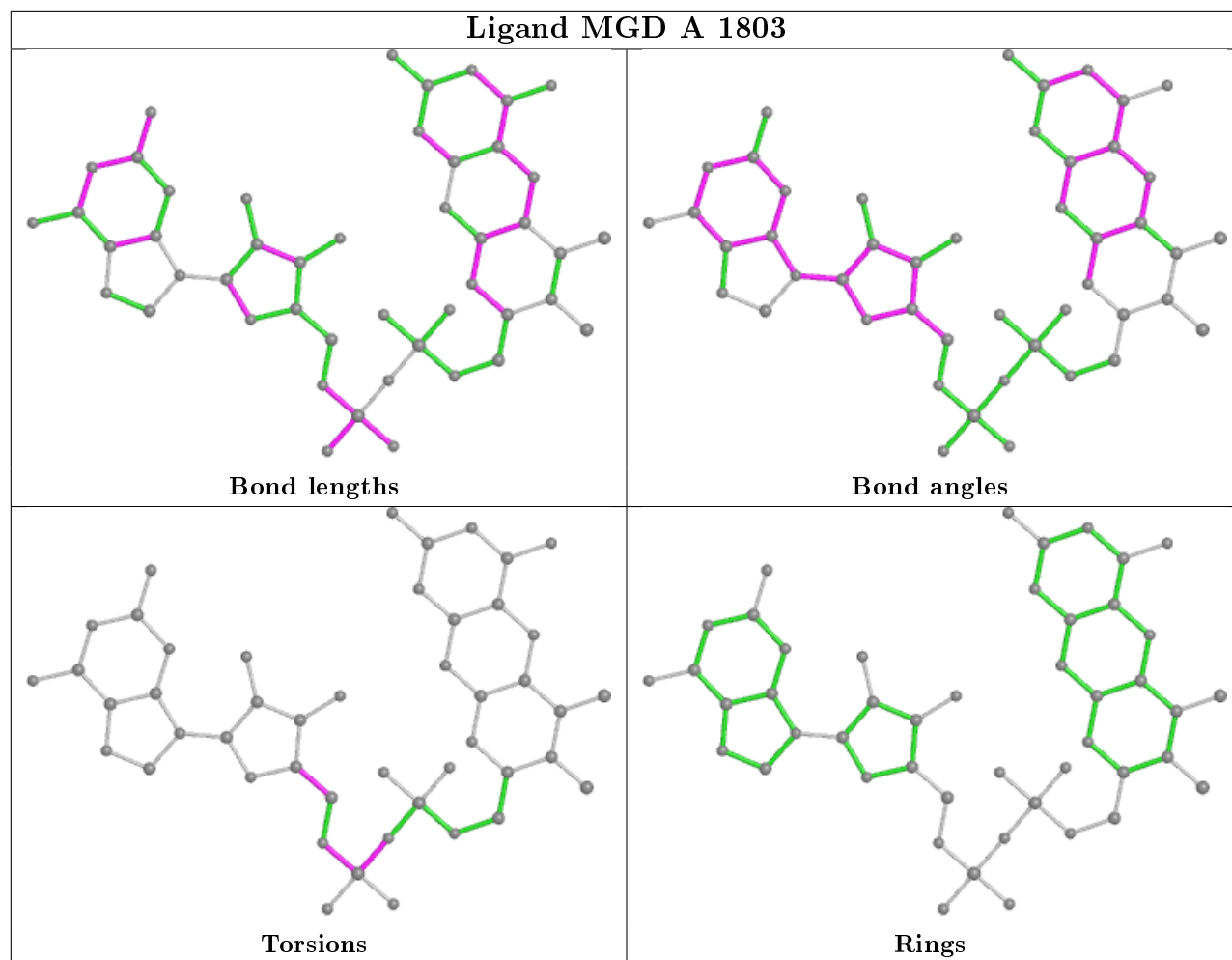
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



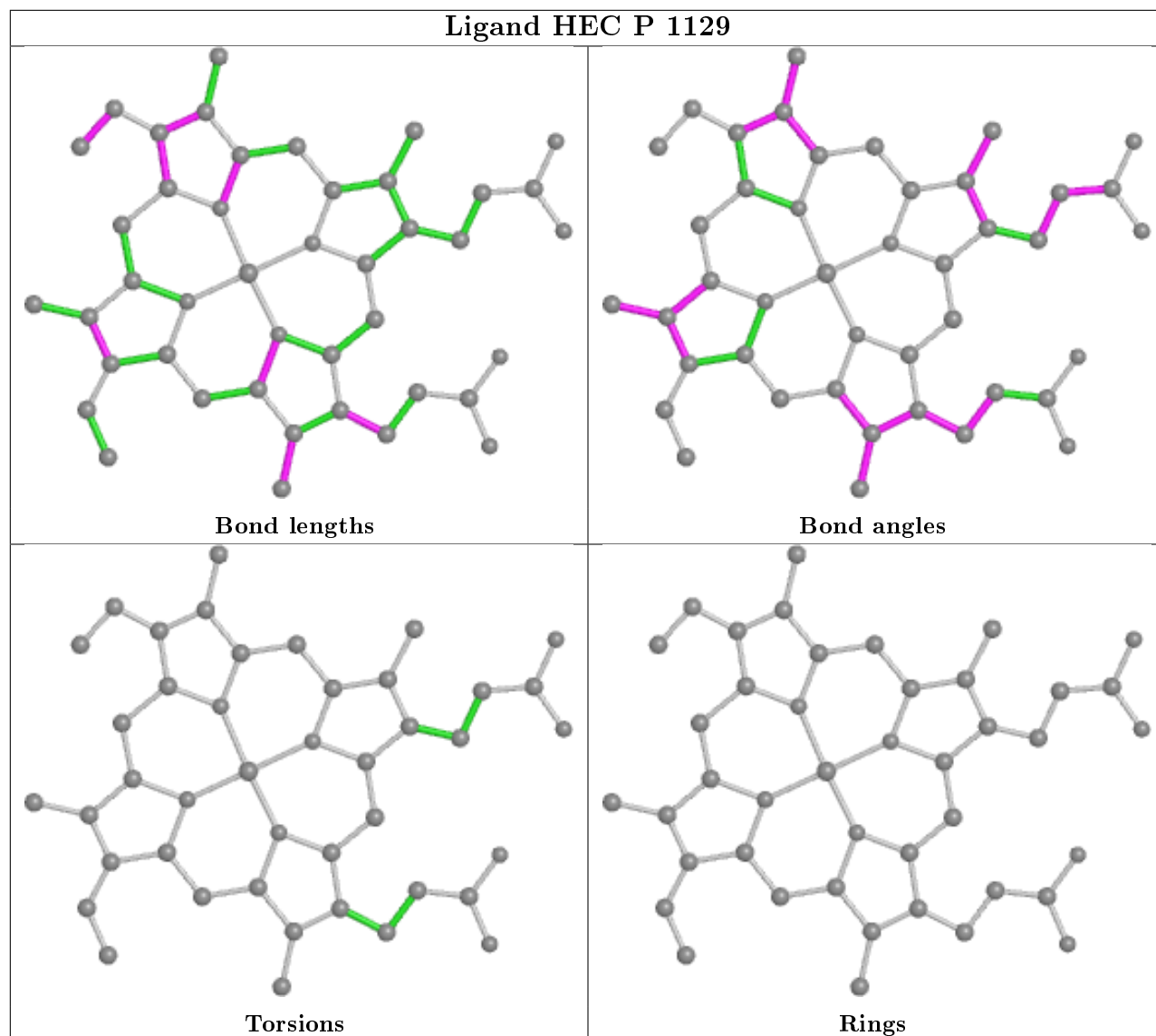
Ligand MGD M 1804



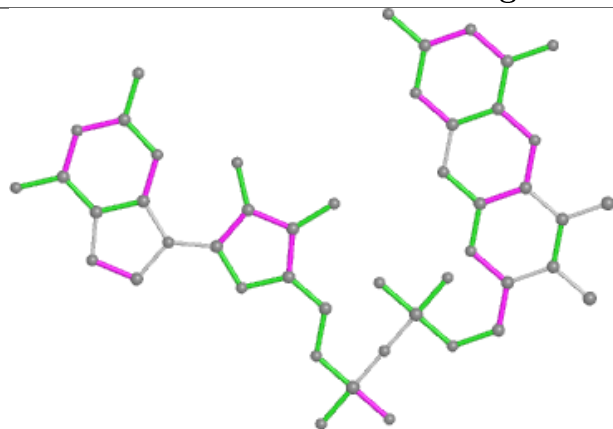
Ligand MGD A 1803



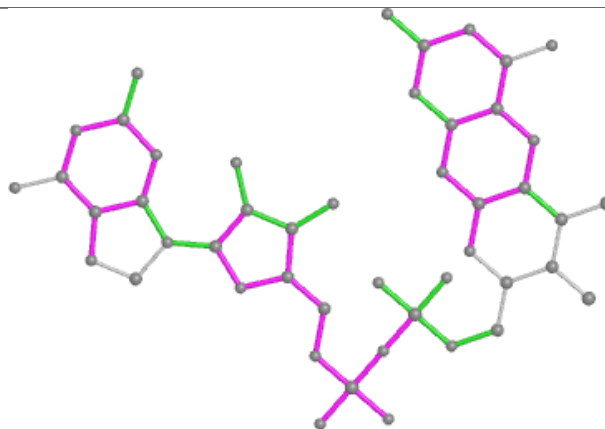
Ligand HEC P 1129



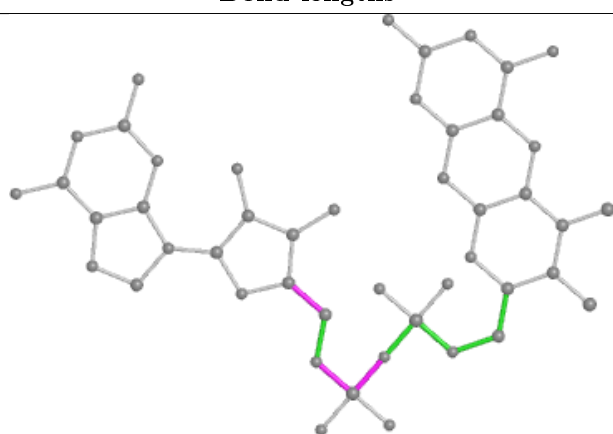
Ligand MGD E 1804



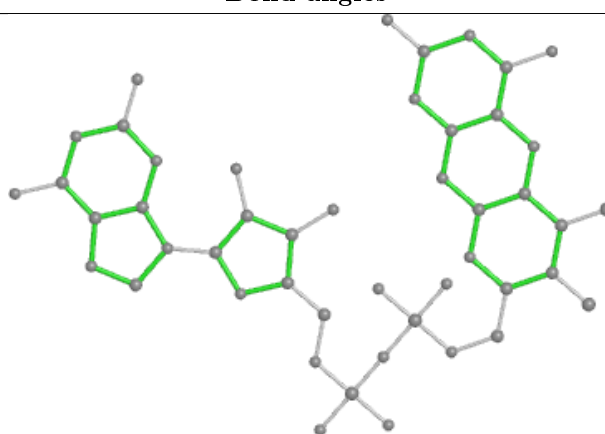
Bond lengths



Bond angles

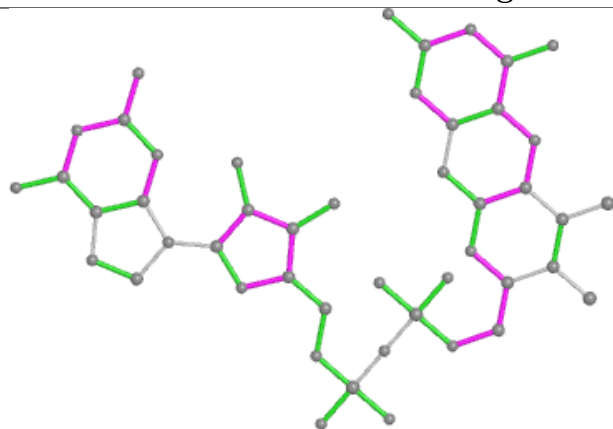


Torsions

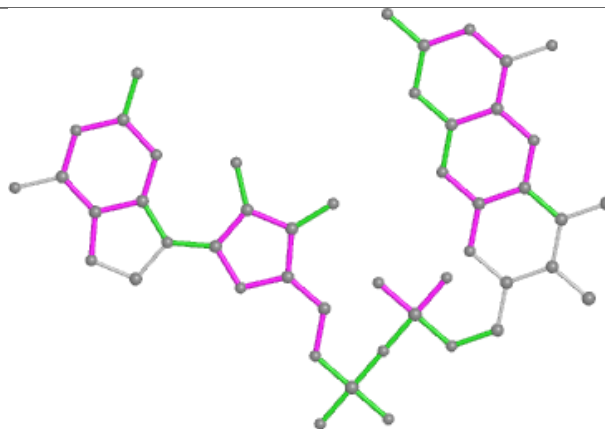


Rings

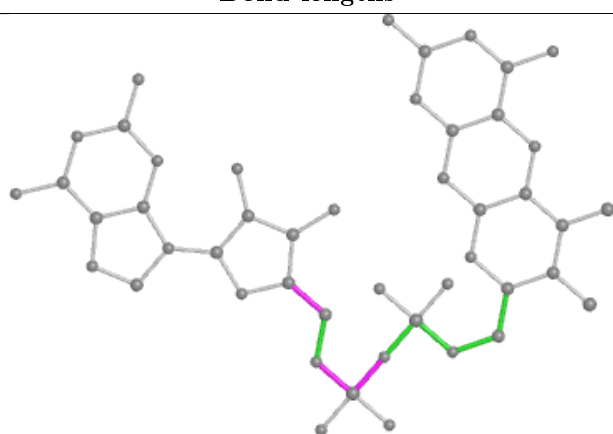
Ligand MGD G 1804



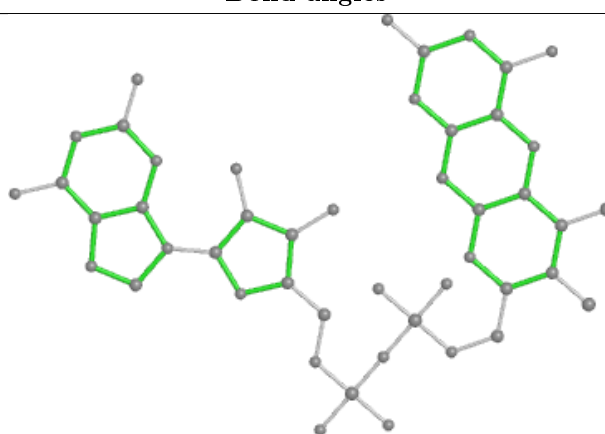
Bond lengths



Bond angles

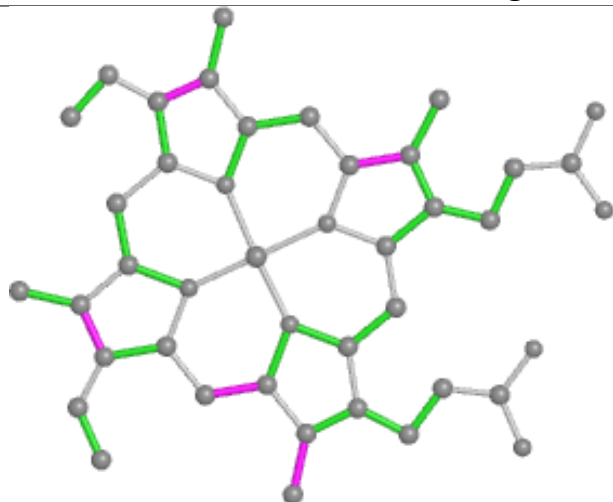


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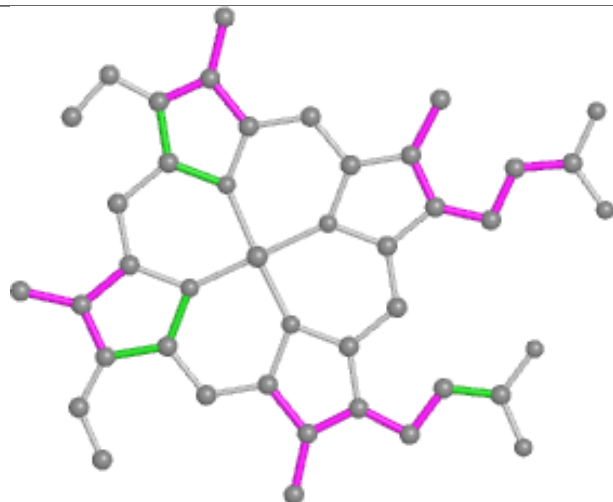


Rings

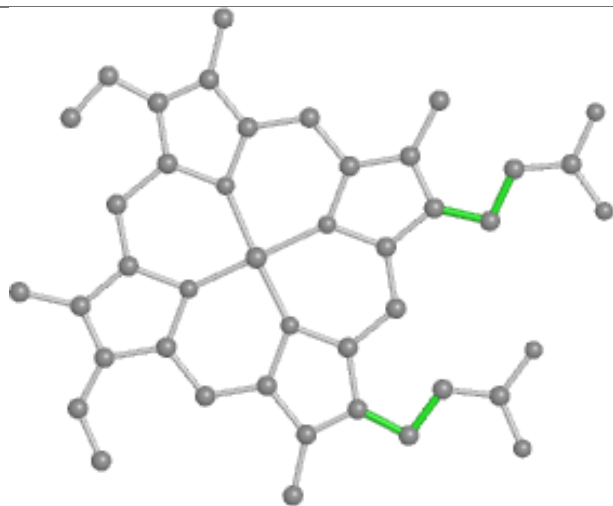
Ligand HEC L 1129



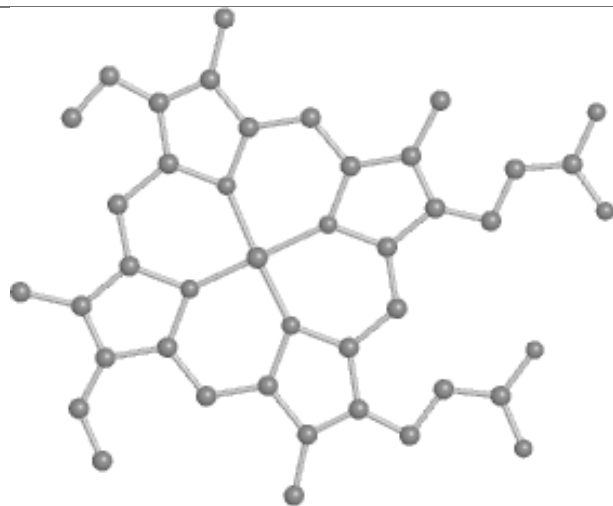
Bond lengths



Bond angles

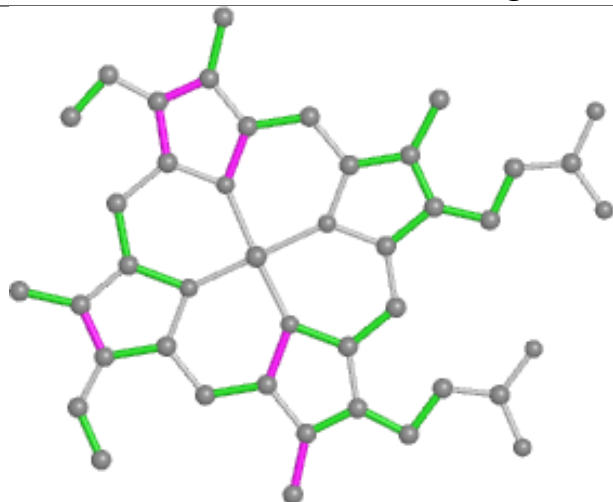


Torsions

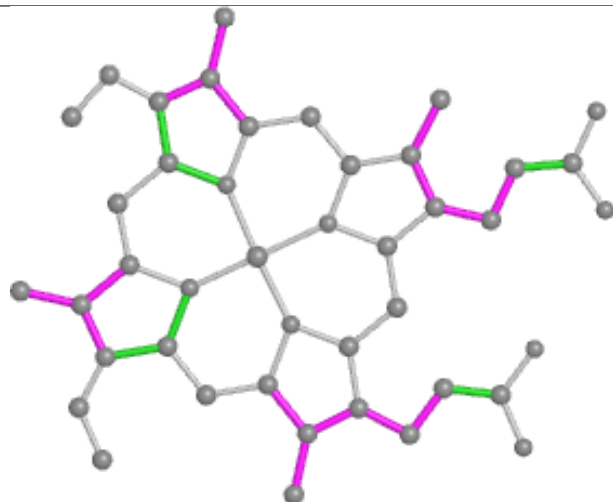


Rings

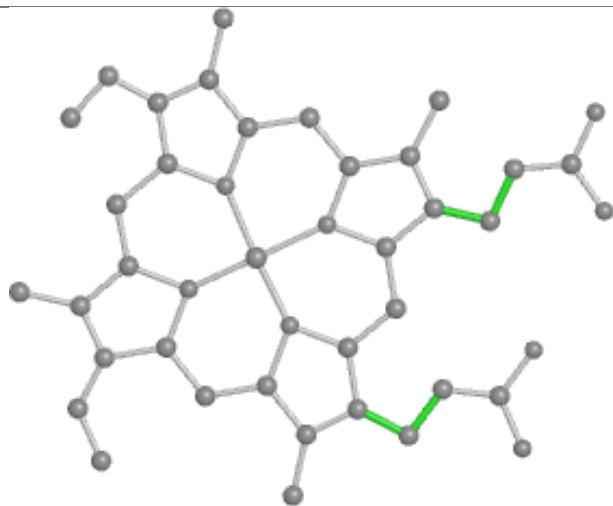
Ligand HEC F 1129



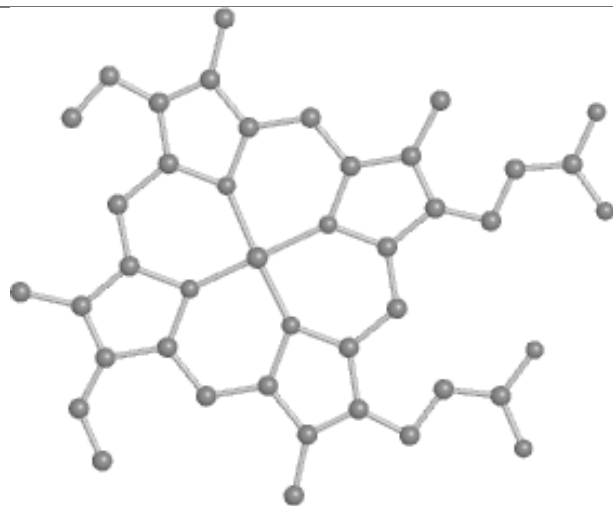
Bond lengths



Bond angles

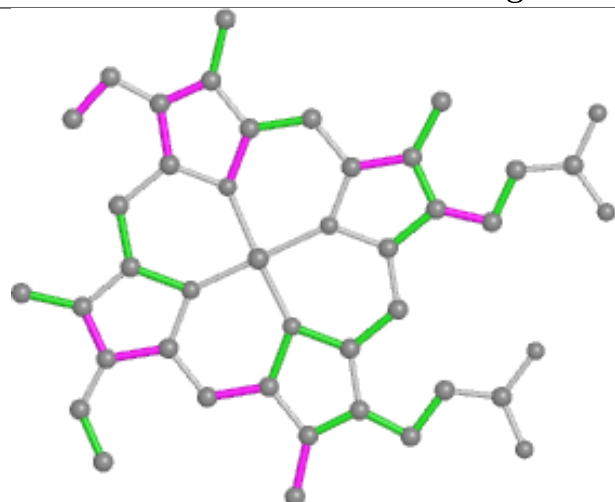


Torsions

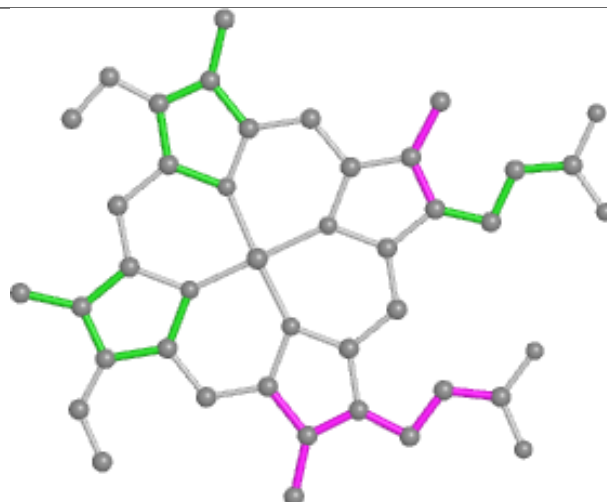


Rings

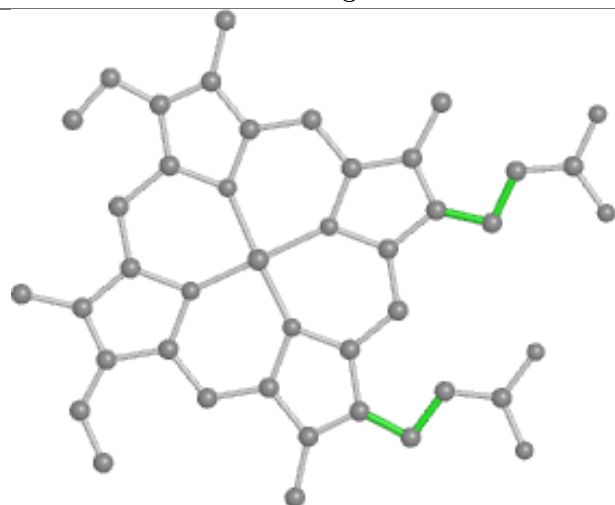
Ligand HEC P 1128



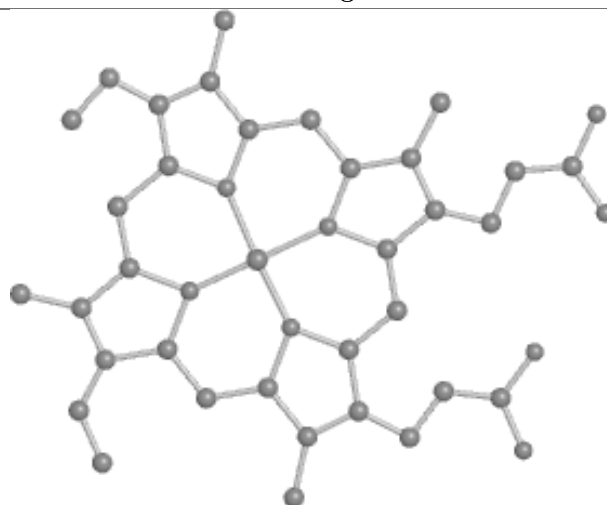
Bond lengths



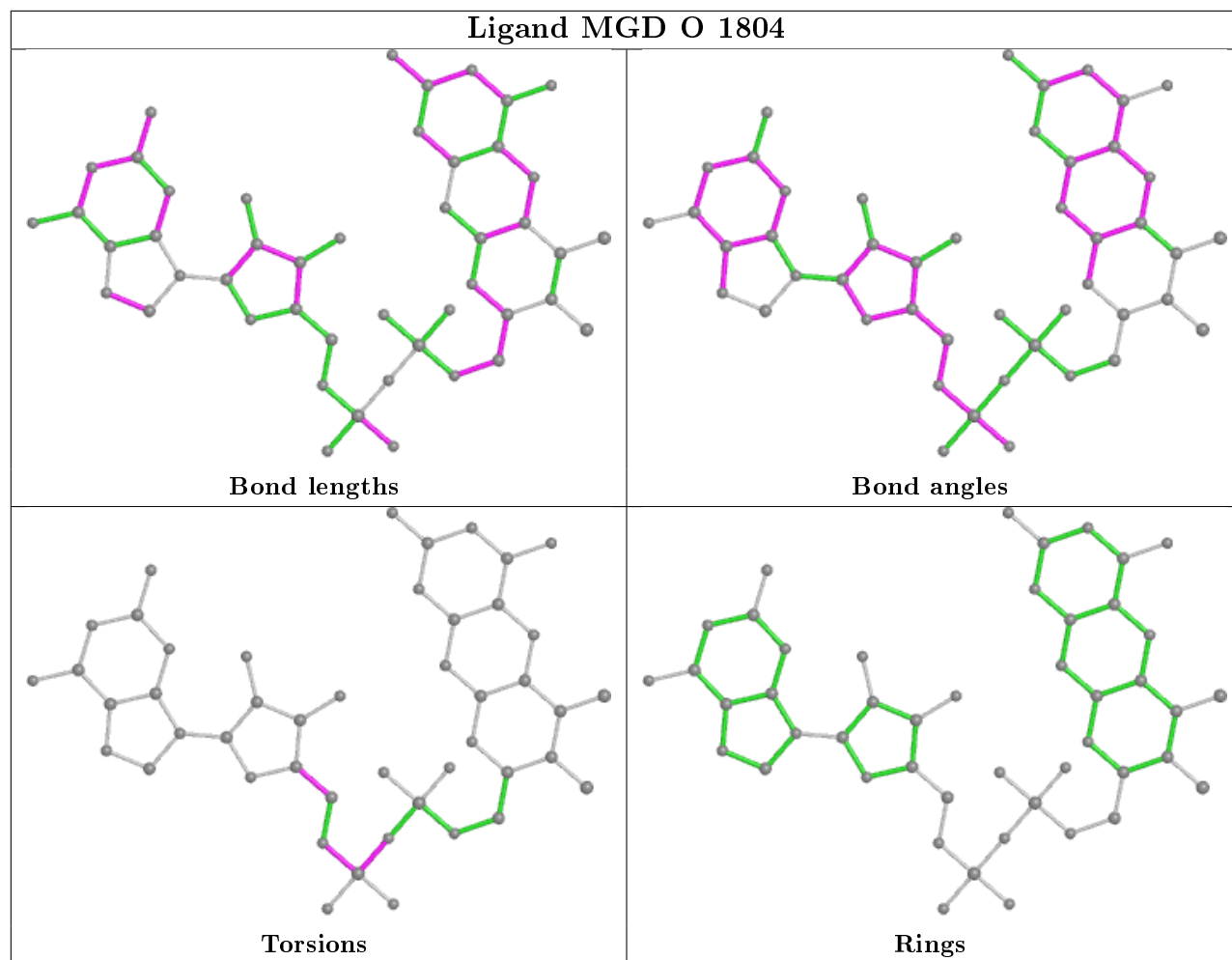
Bond angles



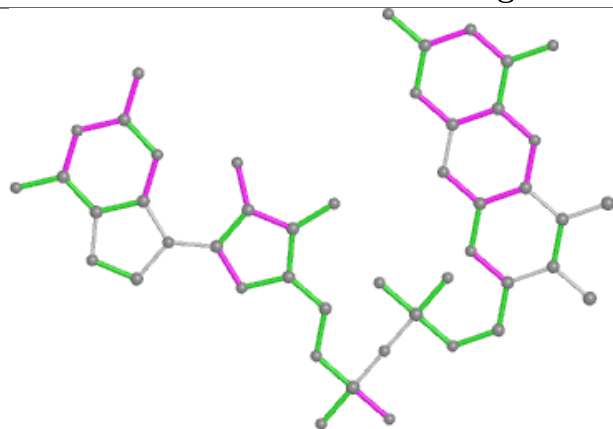
Torsions



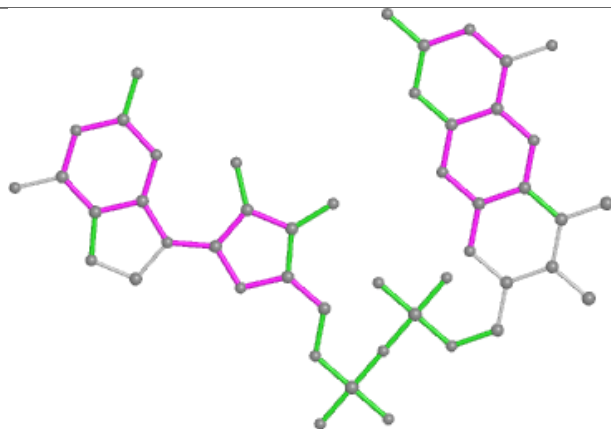
Rings



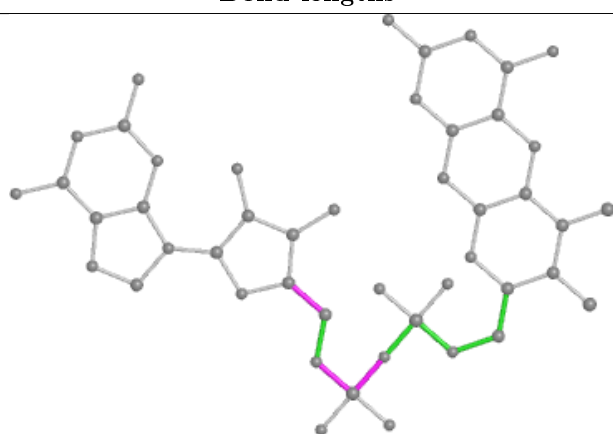
Ligand MGD O 1803



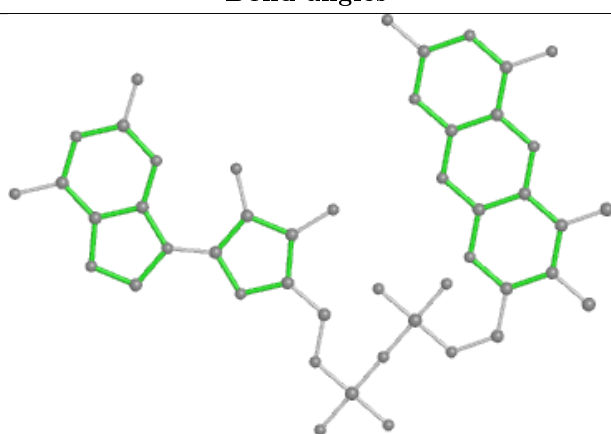
Bond lengths



Bond angles

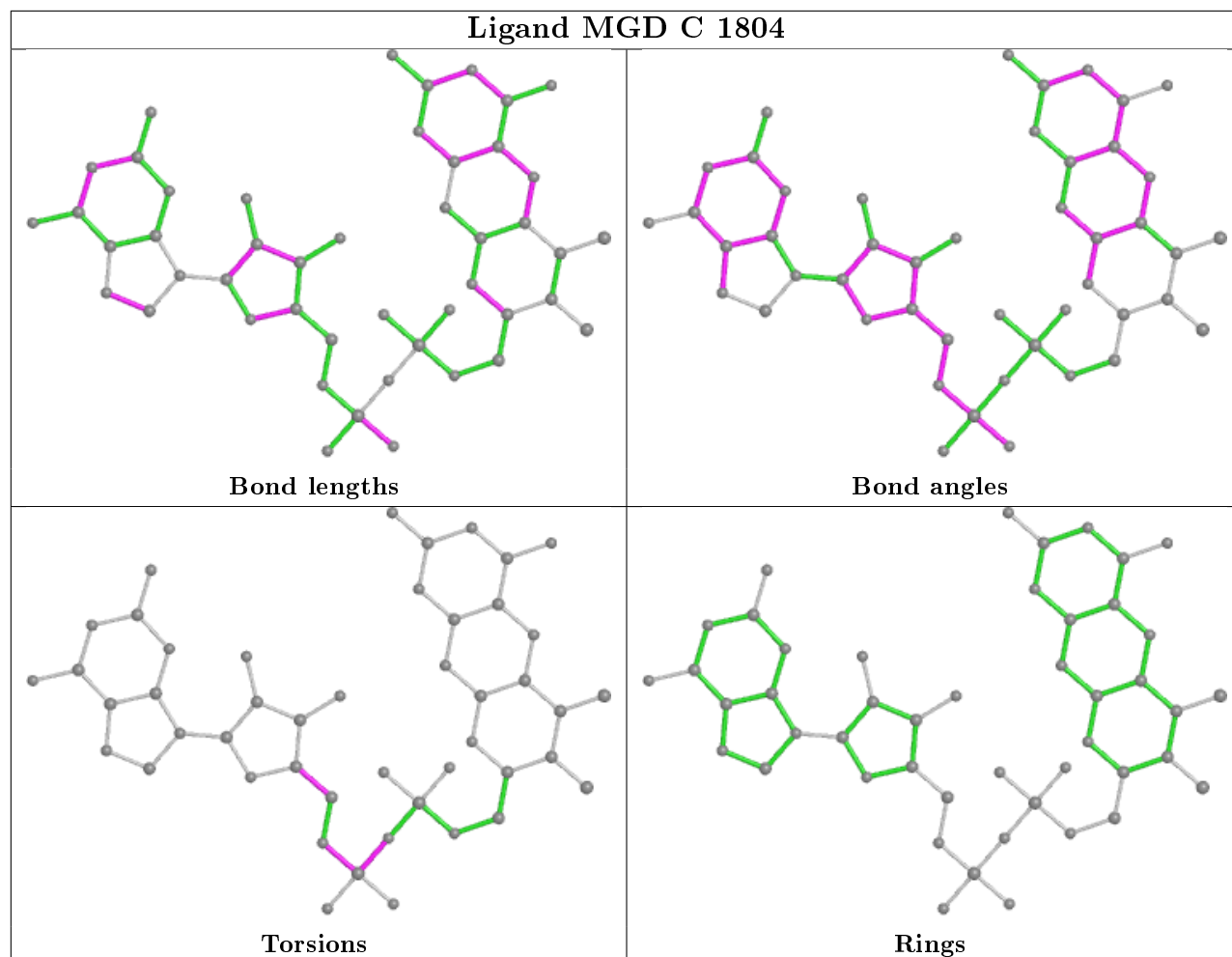


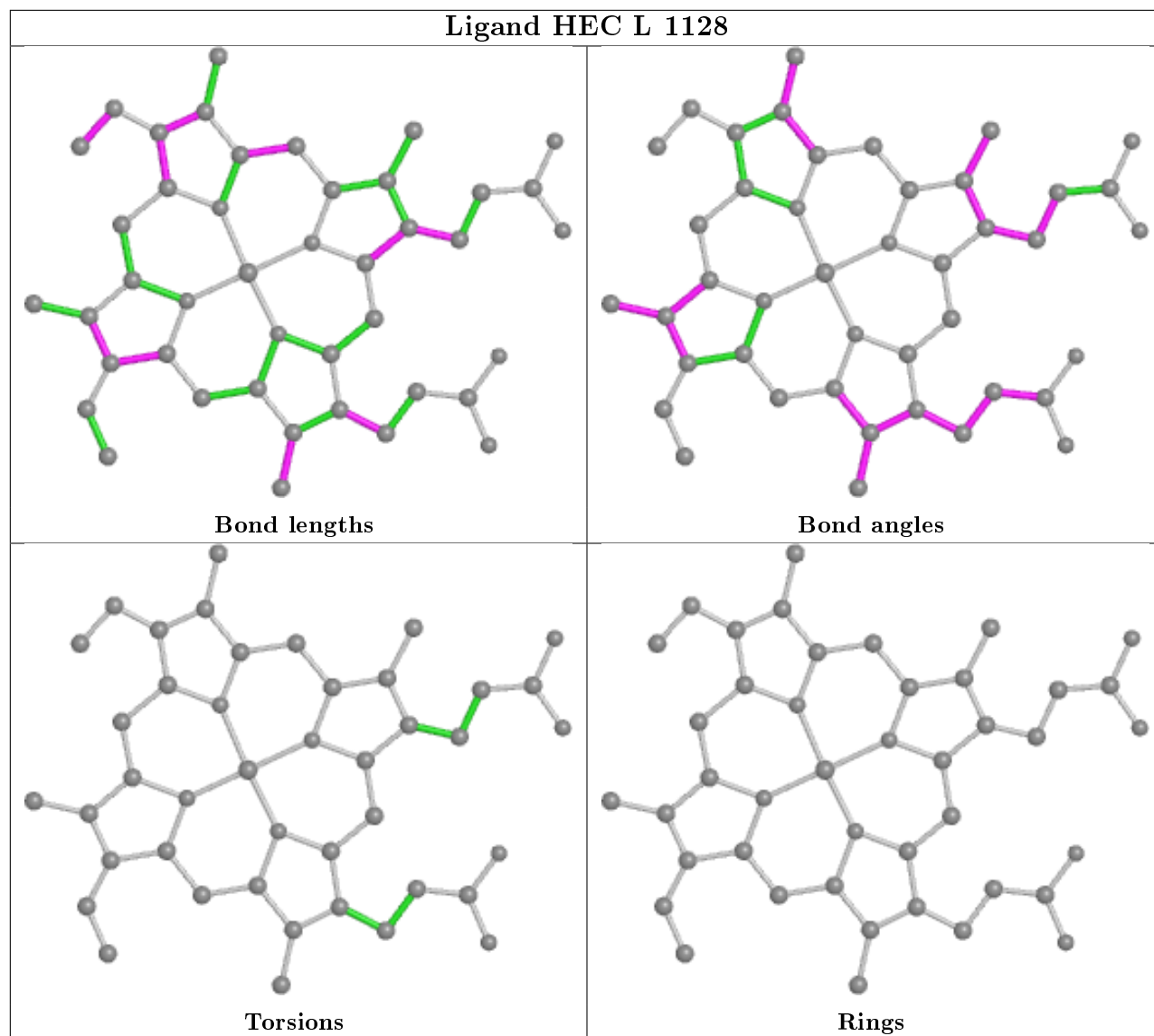
Torsions



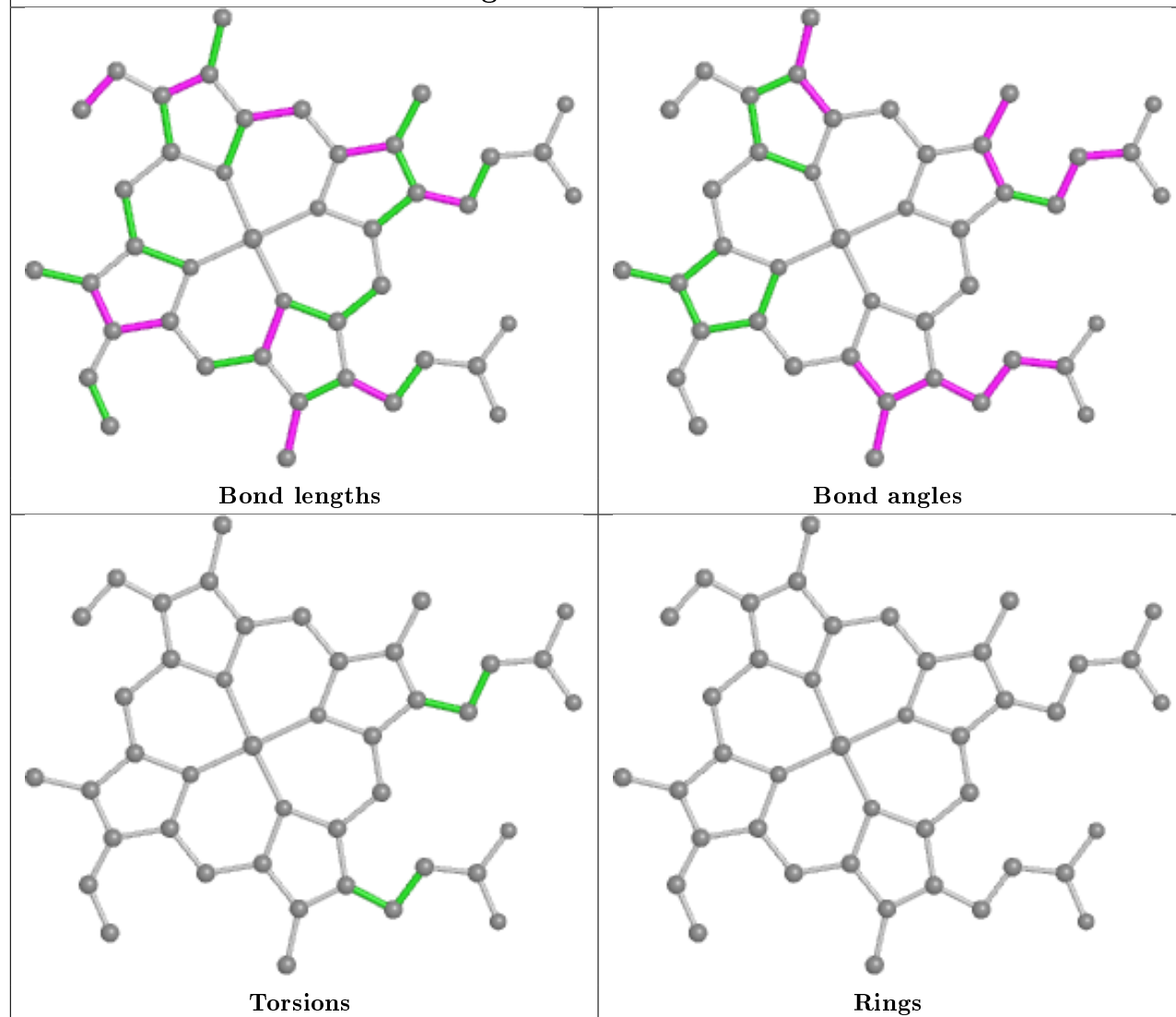
Rings

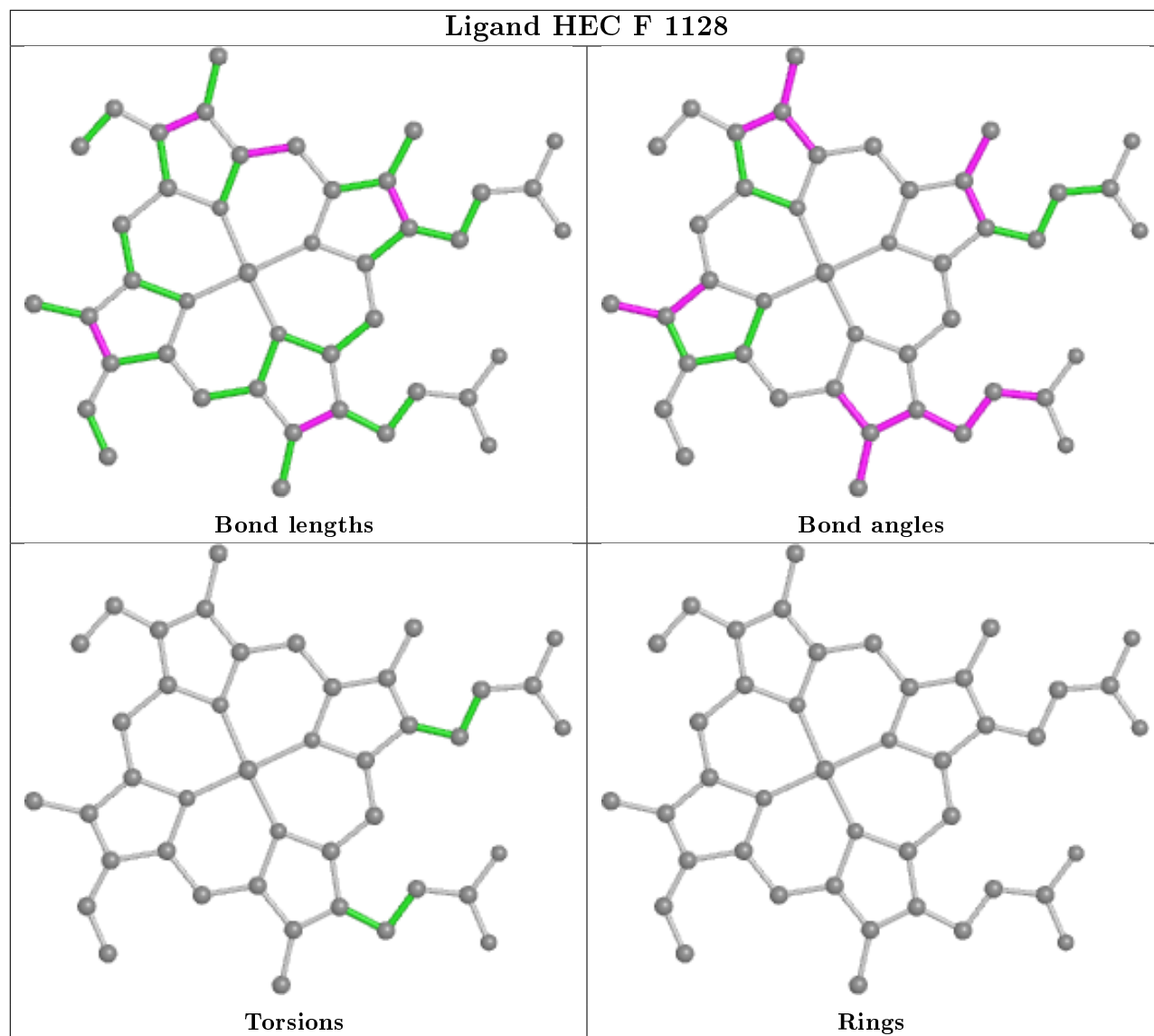
Ligand MGD C 1804



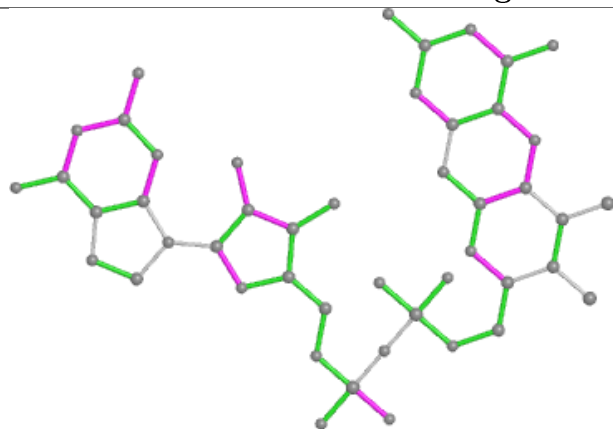


Ligand HEC B 1128

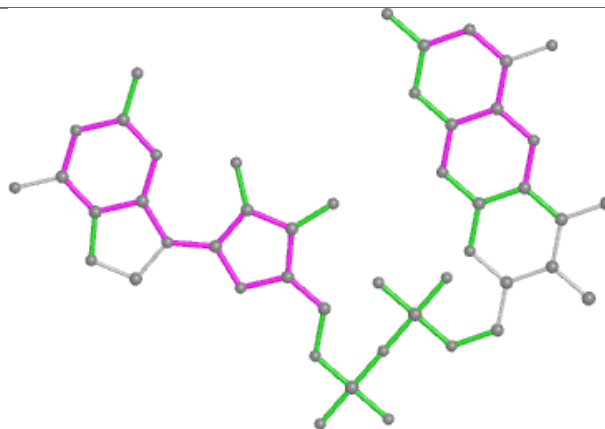




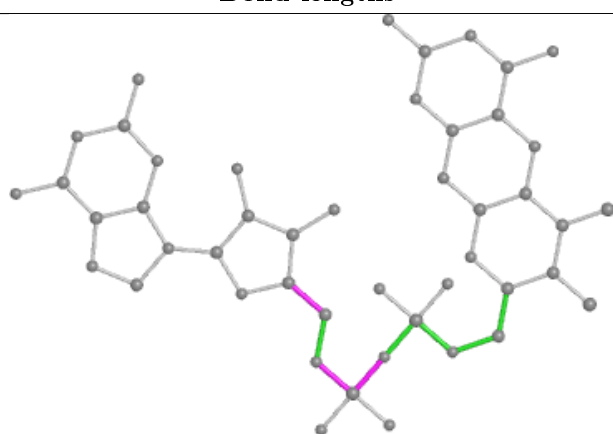
Ligand MGD M 1803



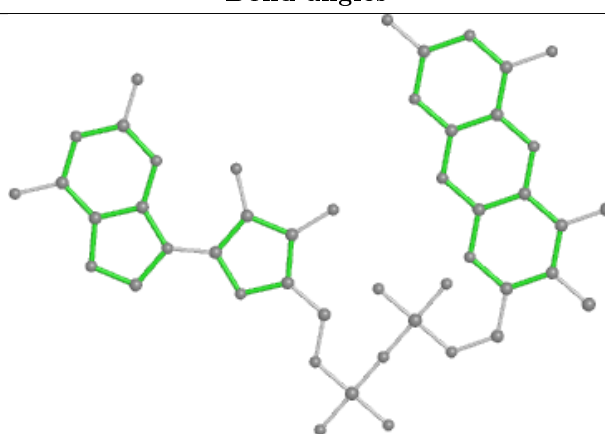
Bond lengths



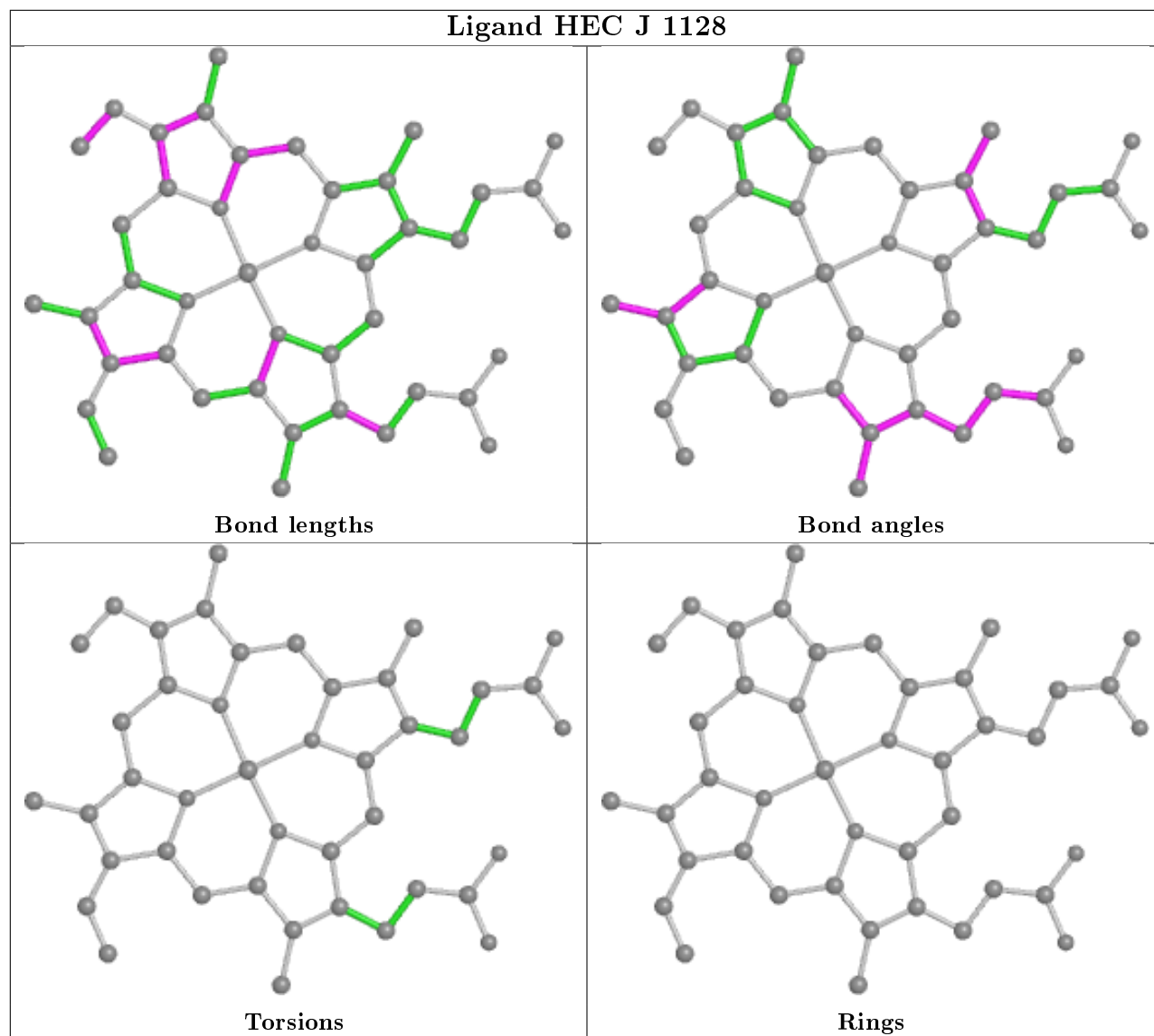
Bond angles



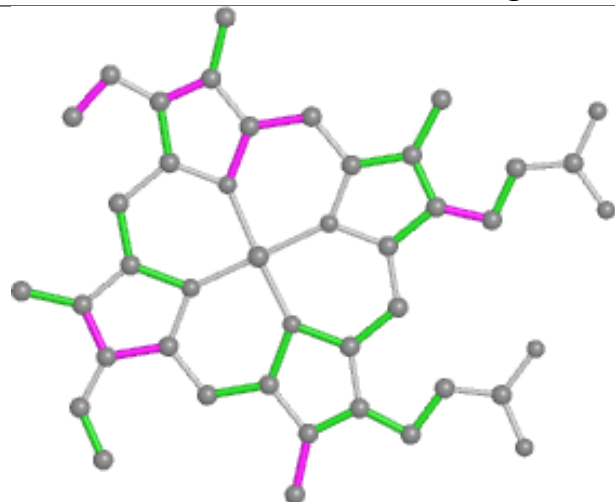
Torsions



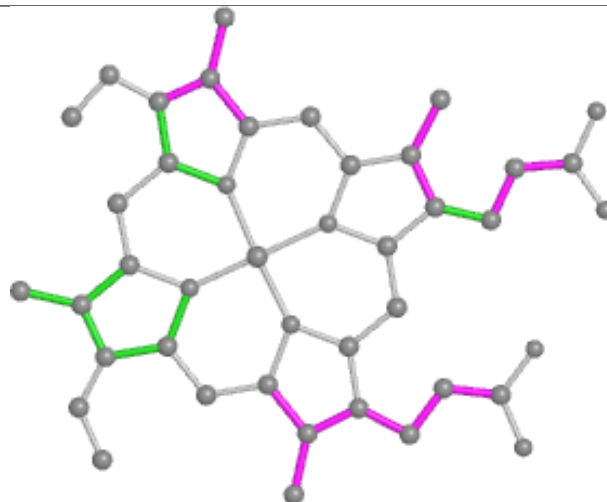
Rings



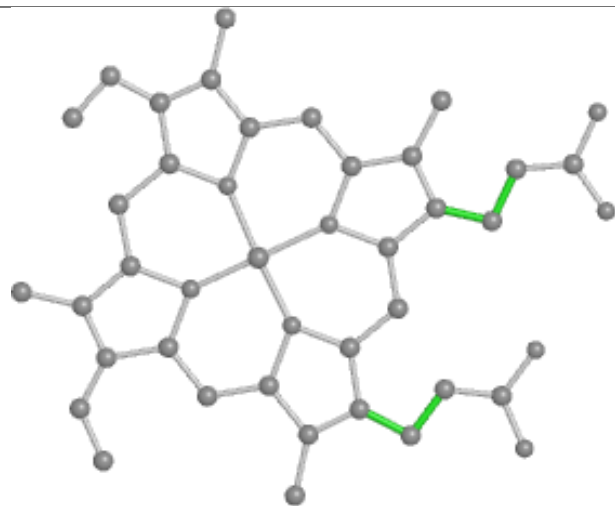
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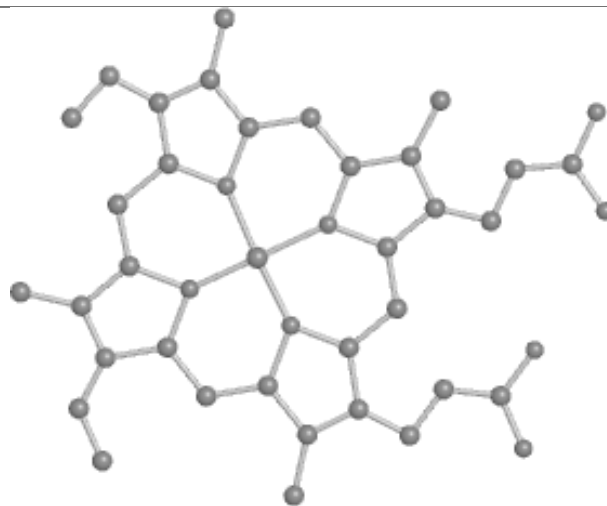
Bond lengths



Bond angles

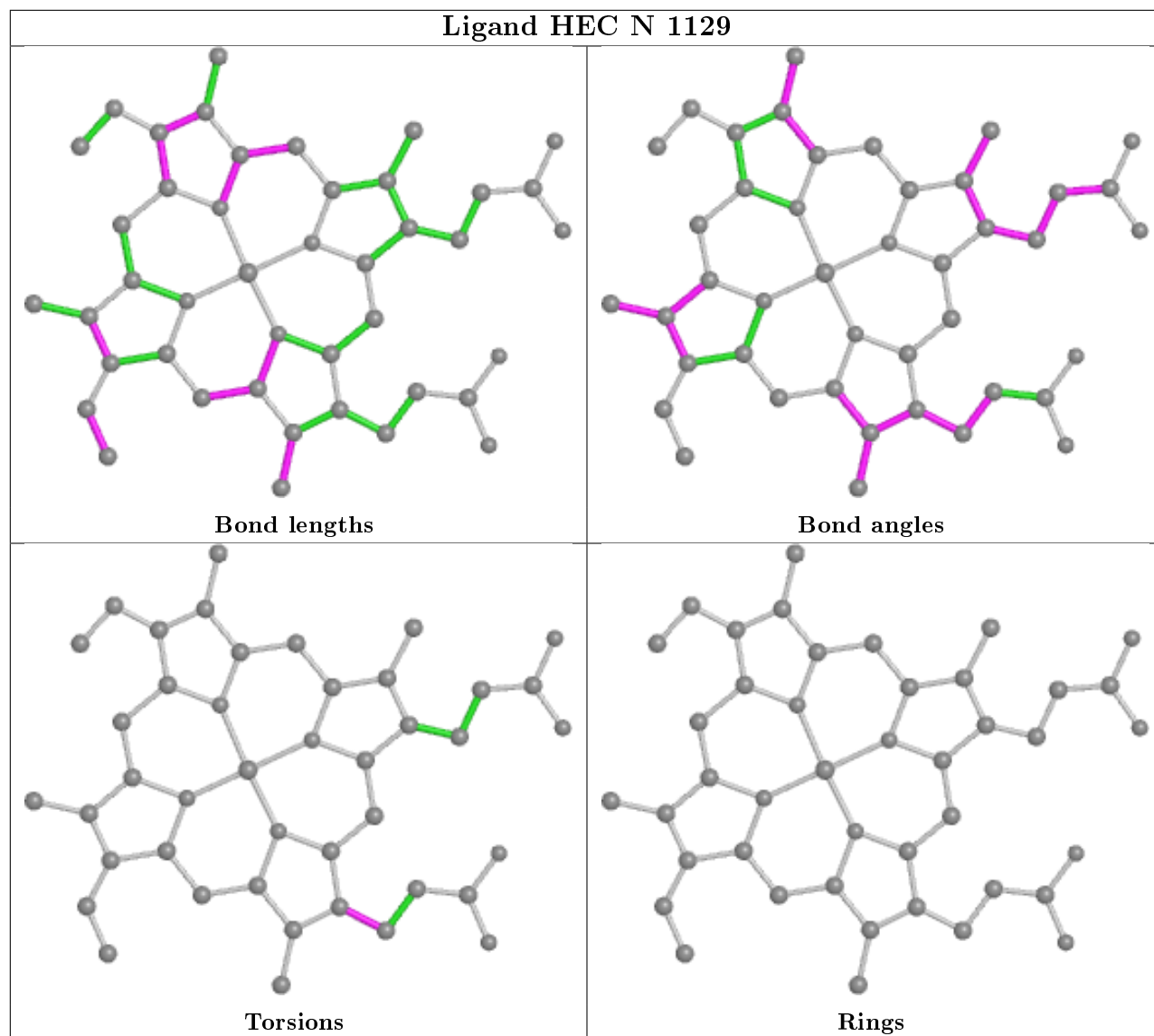


Torsions

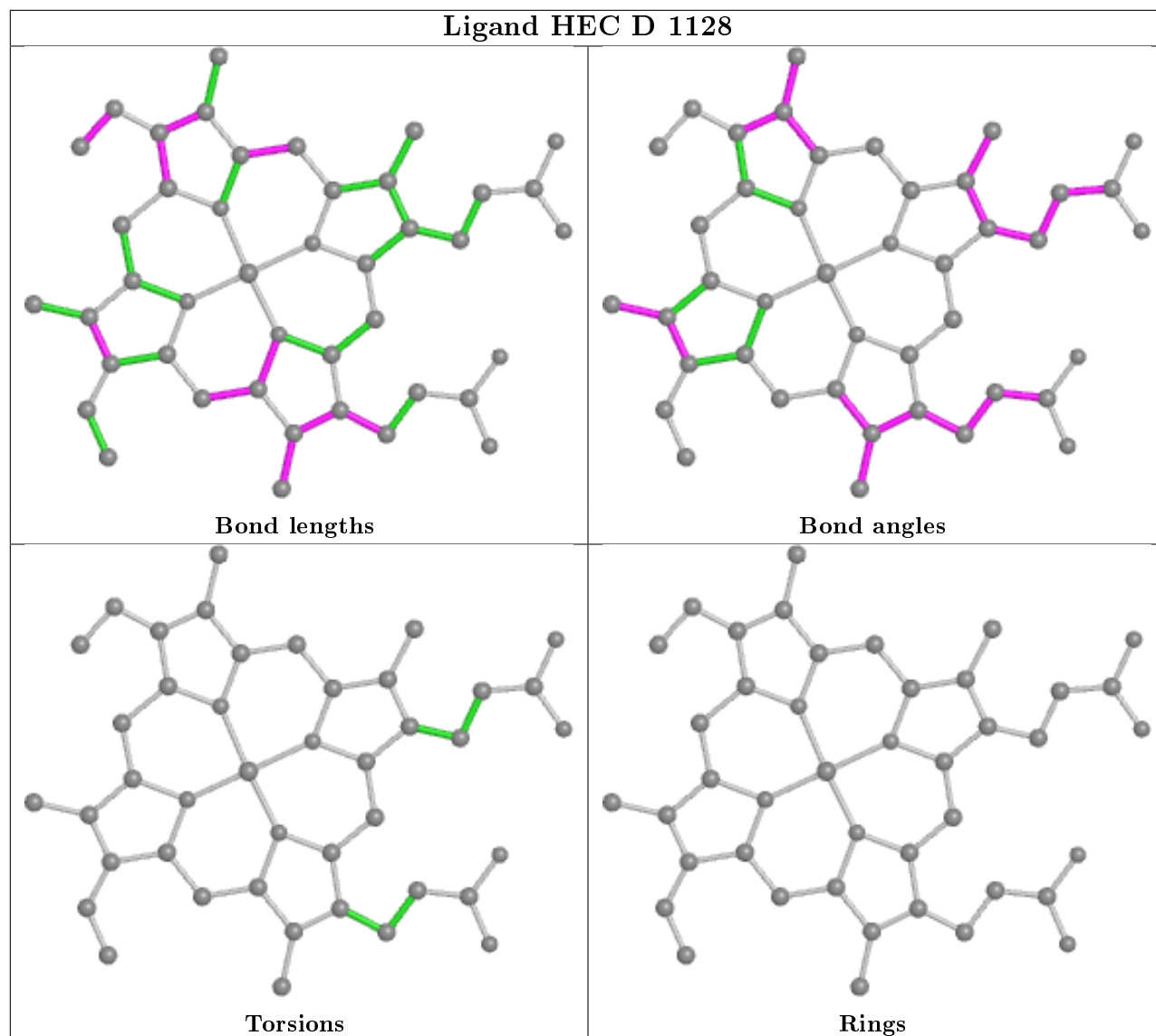


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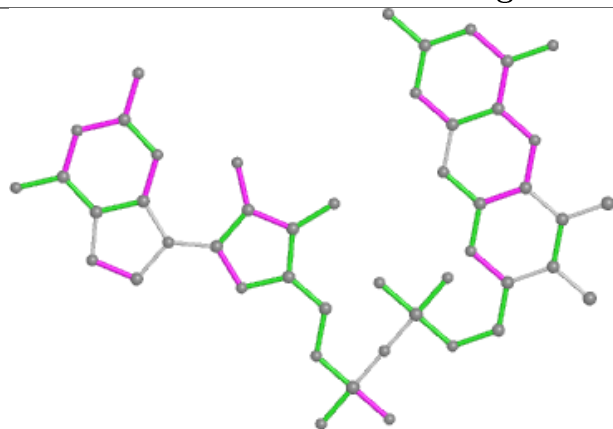
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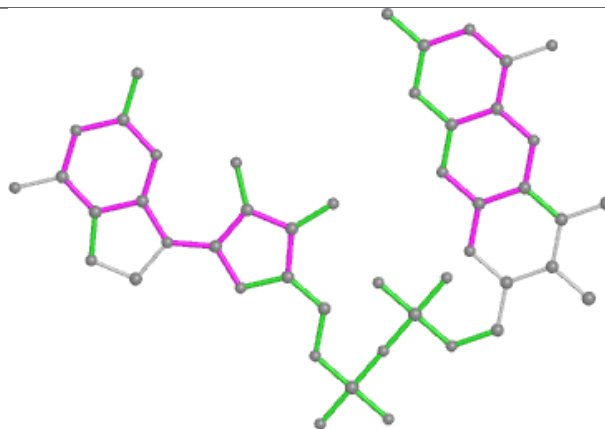
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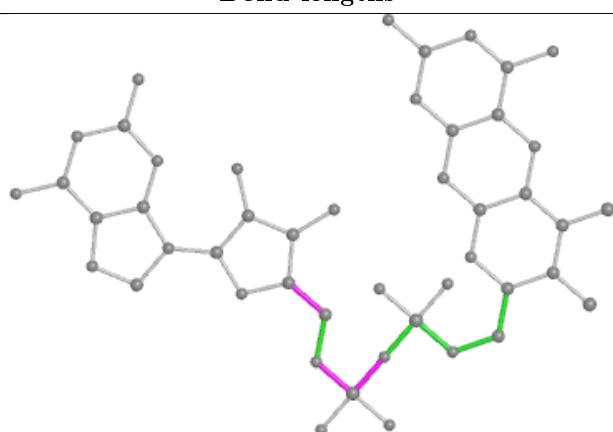
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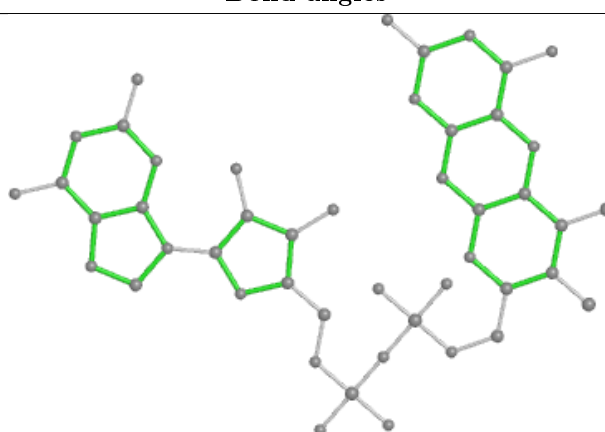
Bond lengths



Bond angles

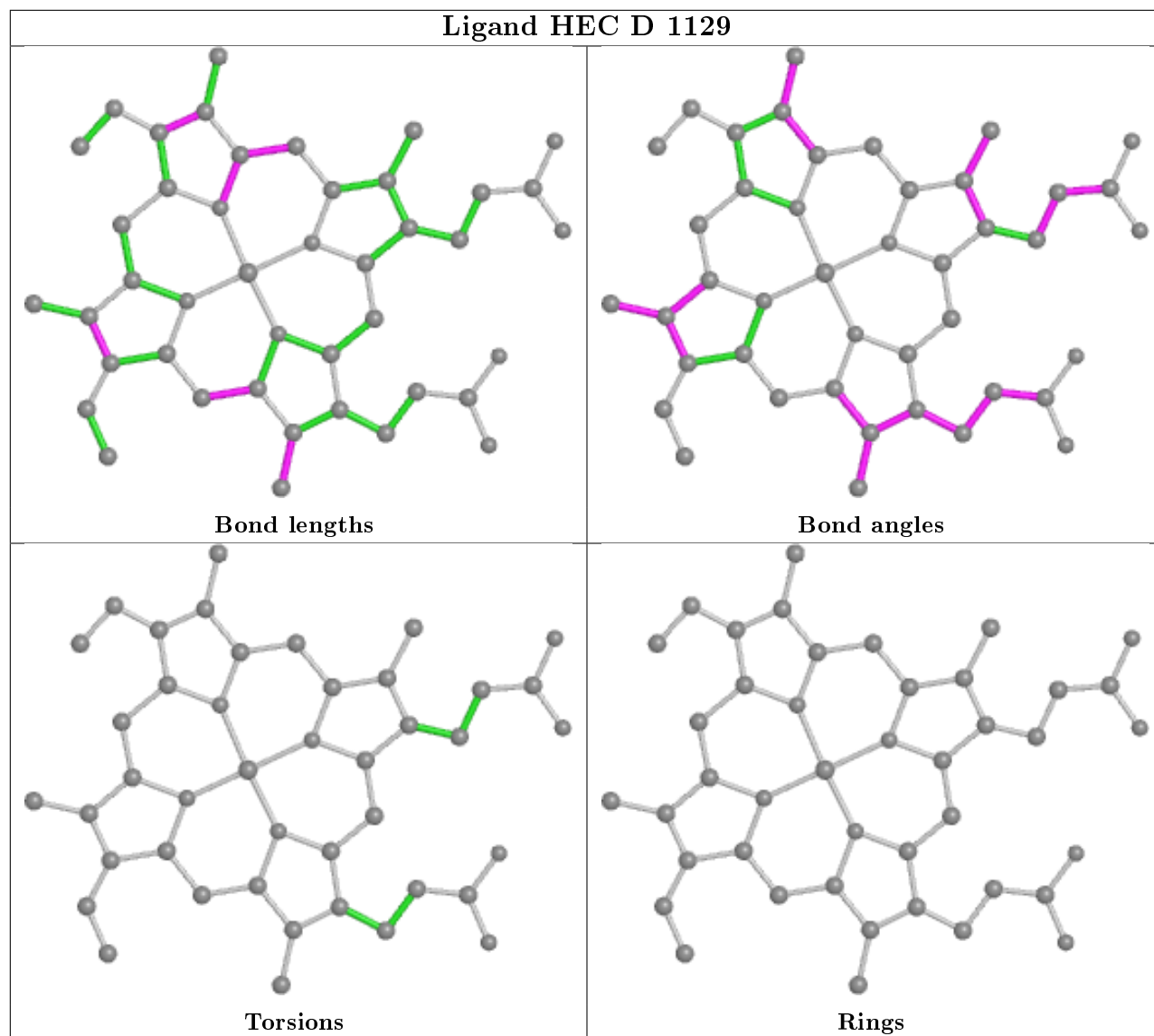


Torsions

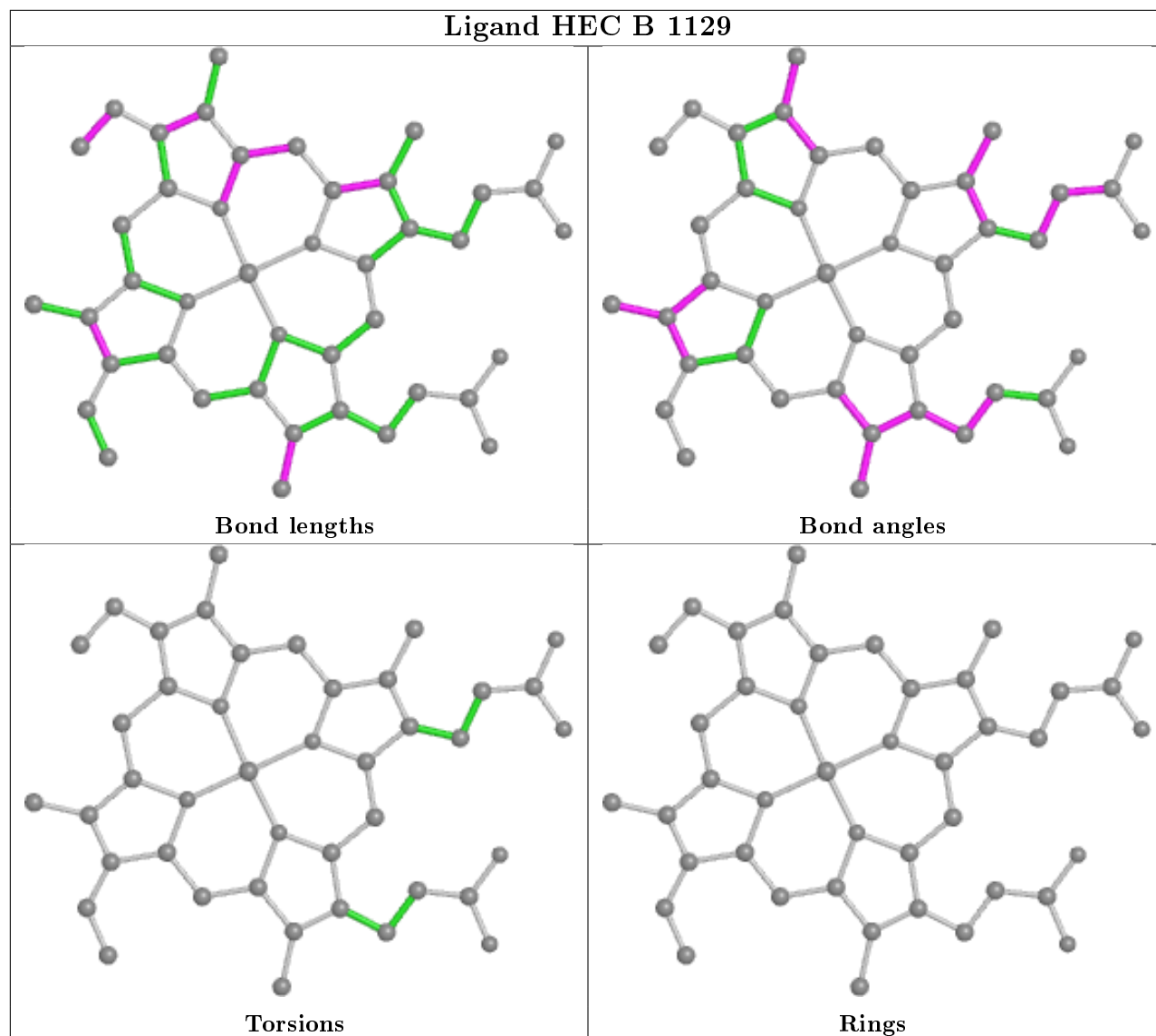


Rings

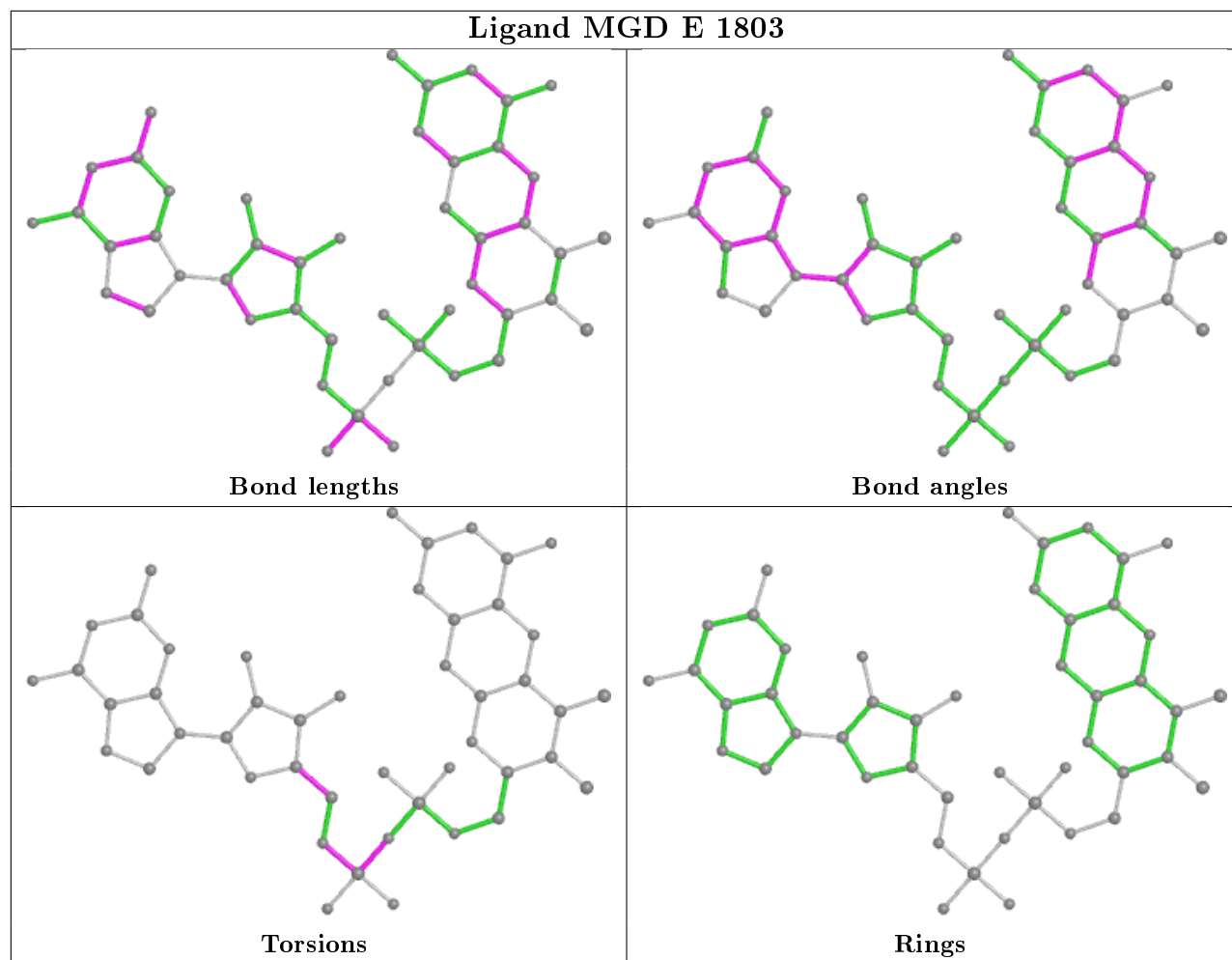
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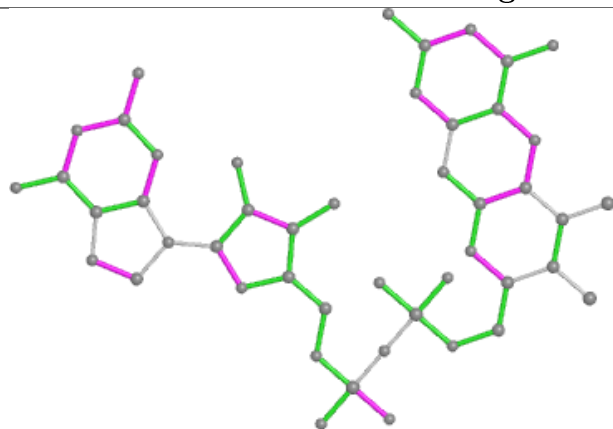
Ligand HEC B 1129



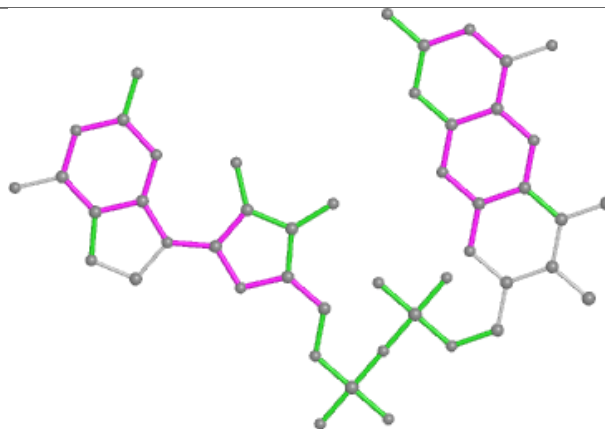
Ligand MGD E 1803



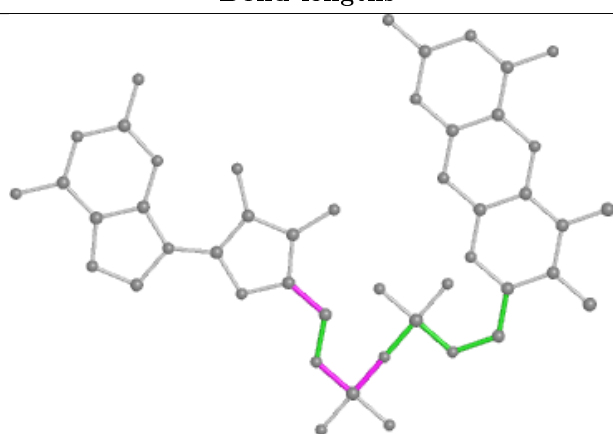
Ligand MGD C 1803



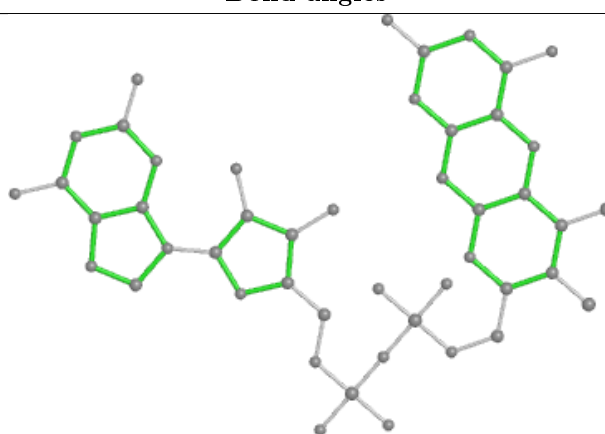
Bond lengths



Bond angles

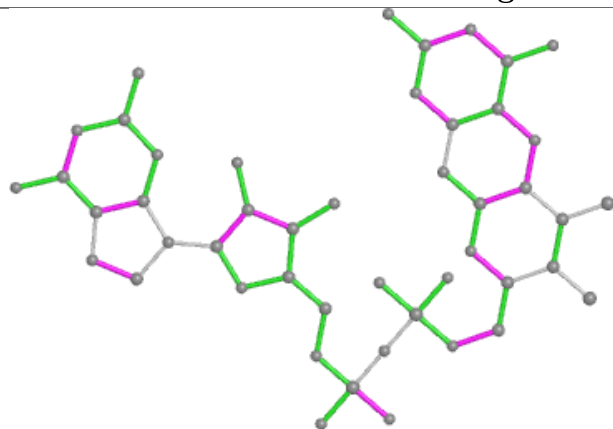


Torsions

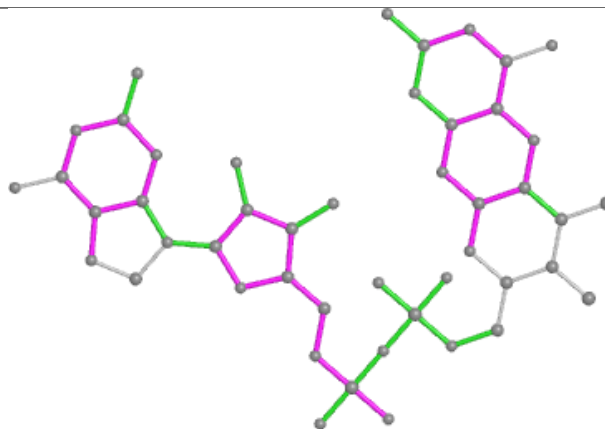


Rings

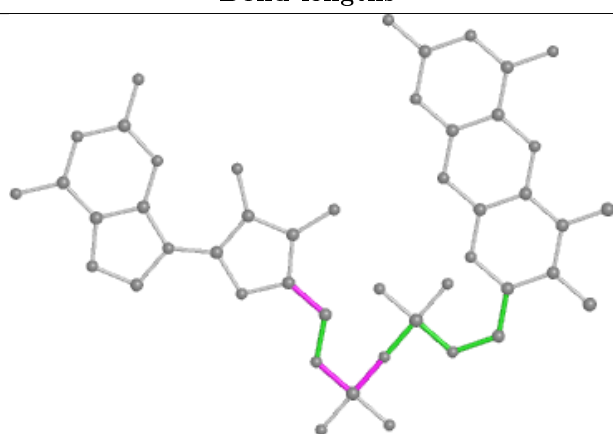
Ligand MGD A 1804



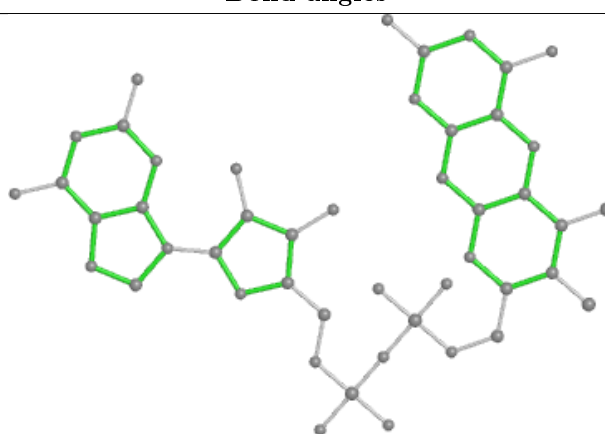
Bond lengths



Bond angles

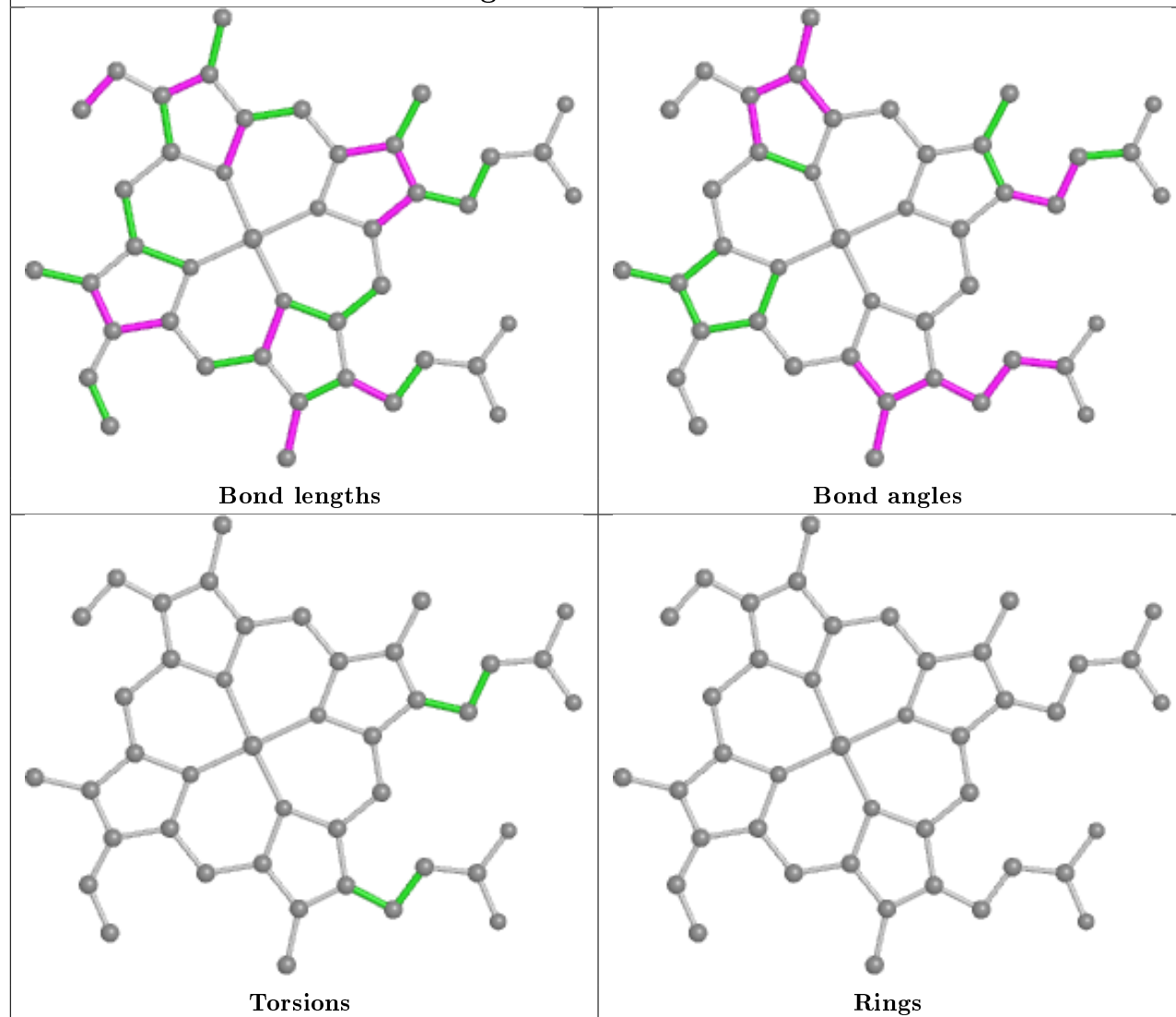


Torsions

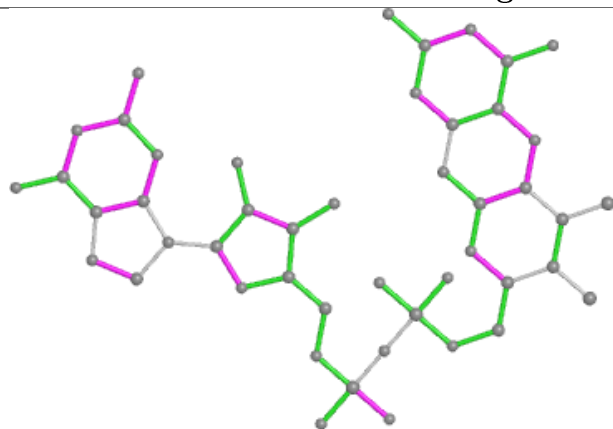


Rings

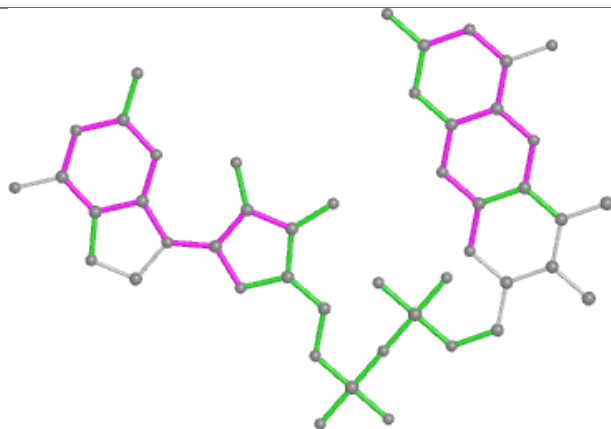
Ligand HEC N 1128



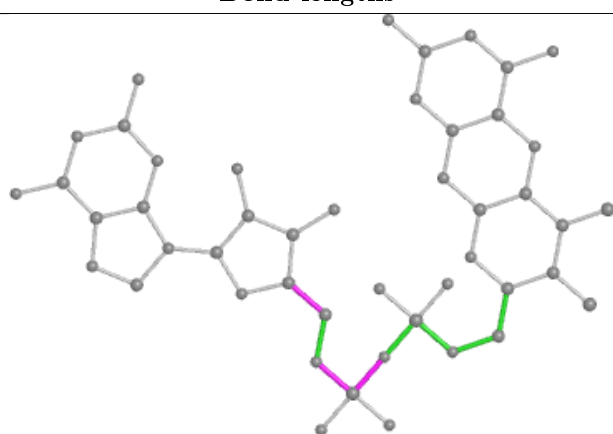
Ligand MGD G 1803



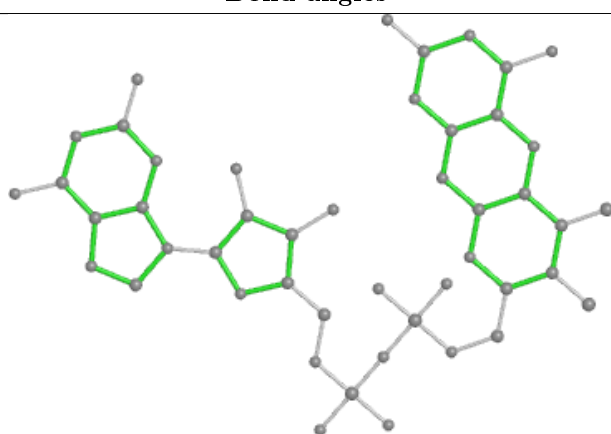
Bond lengths



Bond angles

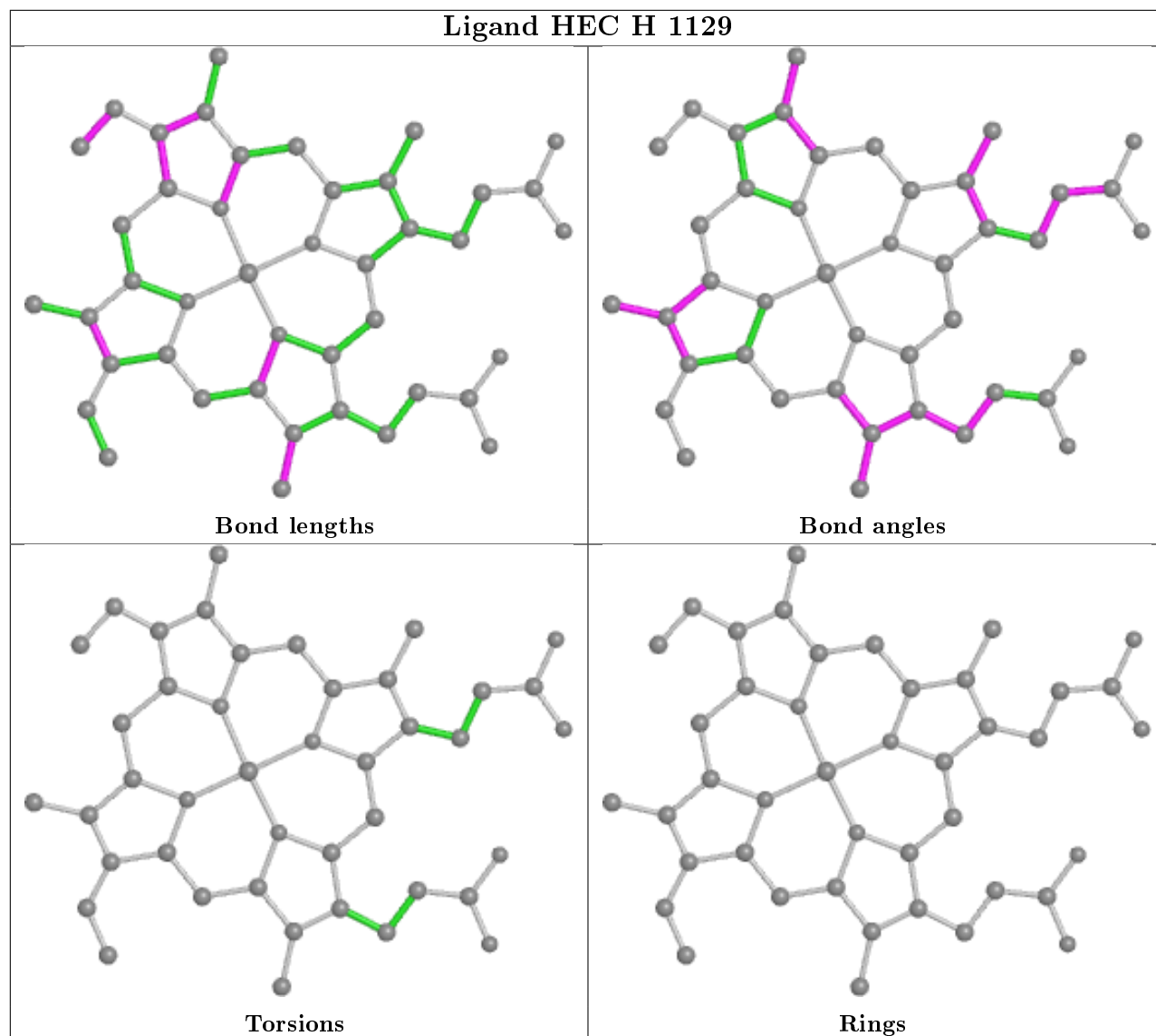


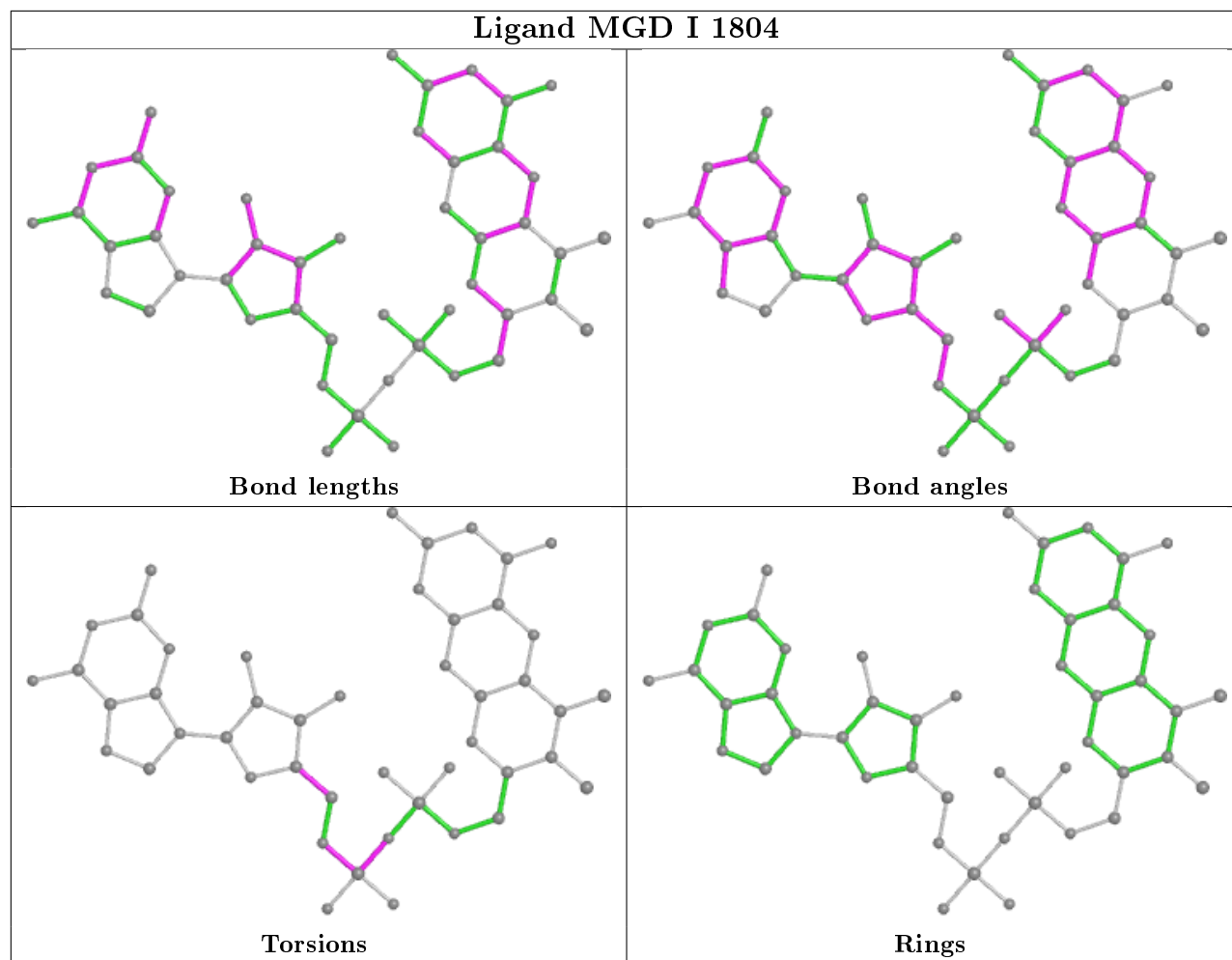
Torsions

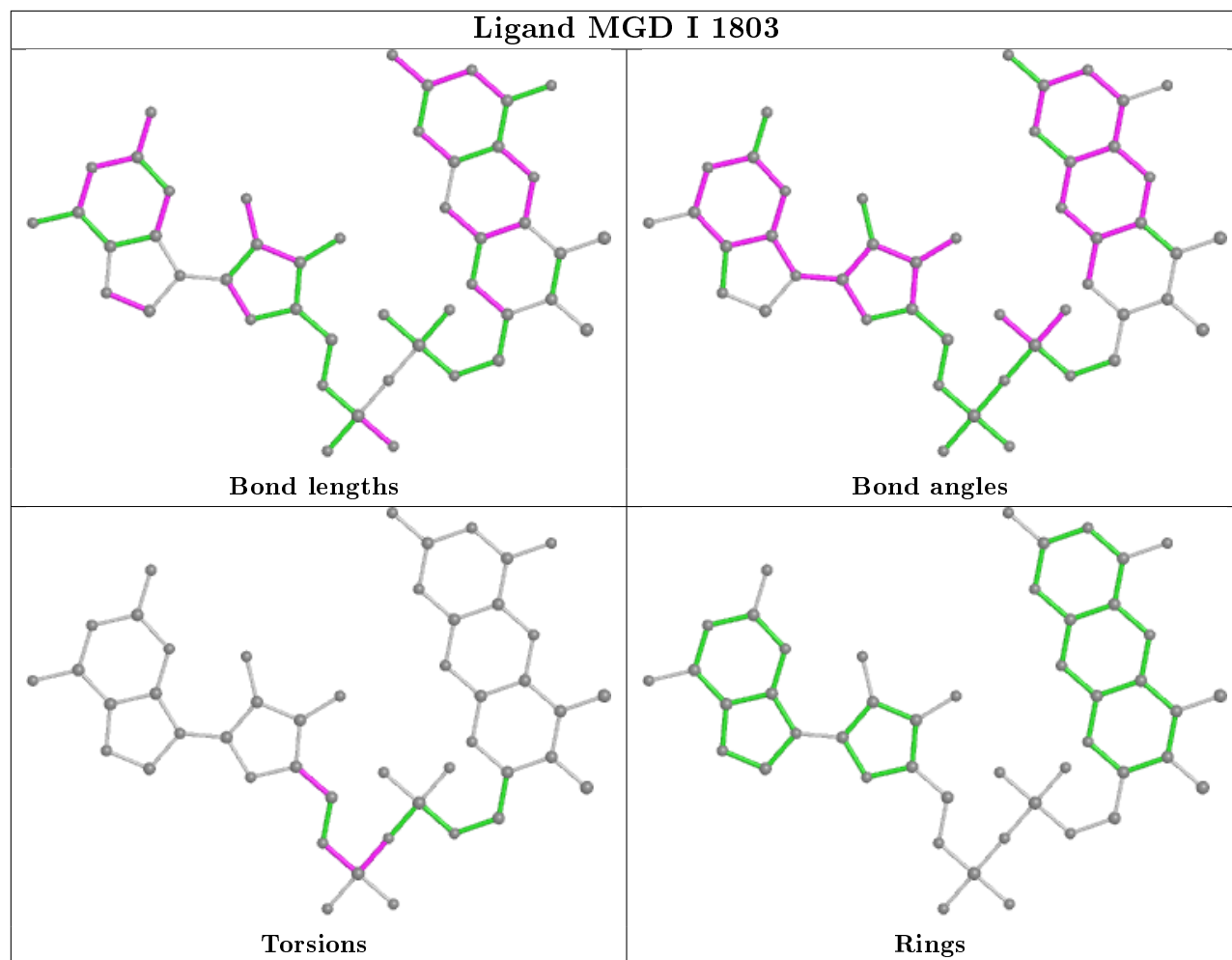


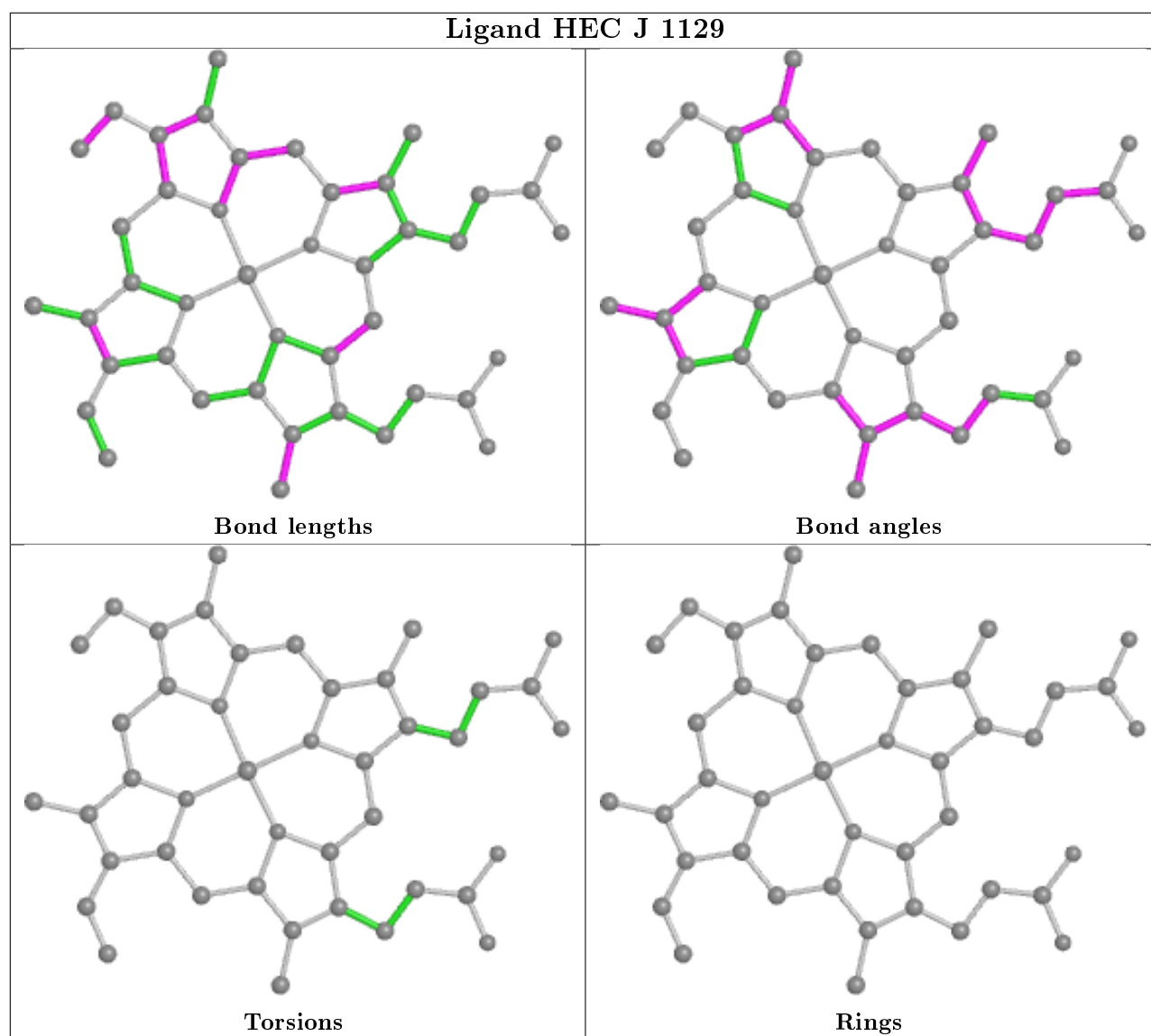
Rings

Ligand HEC H 1129









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, 95th 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 ²)	Q<0.9
1	A	790/802 (98%)	-0.32	7 (0%) 84 75	10, 24, 60, 88	0
1	C	790/802 (98%)	-0.18	10 (1%) 77 65	12, 38, 70, 92	0
1	E	790/802 (98%)	-0.29	6 (0%) 86 78	10, 30, 63, 88	0
1	G	790/802 (98%)	-0.05	16 (2%) 65 51	12, 44, 73, 92	0
1	I	790/802 (98%)	0.47	51 (6%) 18 11	23, 58, 77, 92	0
1	K	790/802 (98%)	-0.12	12 (1%) 73 61	17, 43, 70, 90	0
1	M	790/802 (98%)	-0.14	11 (1%) 75 63	13, 42, 70, 91	0
1	O	790/802 (98%)	0.34	39 (4%) 29 17	25, 53, 76, 95	0
2	B	127/130 (97%)	-0.22	1 (0%) 86 78	10, 33, 70, 83	0
2	D	127/130 (97%)	-0.07	2 (1%) 72 59	14, 38, 75, 87	0
2	F	127/130 (97%)	-0.17	2 (1%) 72 59	11, 34, 70, 85	0
2	H	127/130 (97%)	-0.09	2 (1%) 72 59	11, 39, 76, 86	0
2	J	127/130 (97%)	0.12	5 (3%) 39 25	18, 47, 82, 93	0
2	L	127/130 (97%)	-0.12	4 (3%) 49 32	15, 38, 75, 96	0
2	N	127/130 (97%)	-0.11	2 (1%) 72 59	12, 39, 75, 90	0
2	P	127/130 (97%)	-0.01	4 (3%) 49 32	19, 44, 76, 89	0
All	All	7336/7456 (98%)	-0.04	174 (2%) 59 44	10, 43, 73, 96	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	2	ASP	7.0
1	M	79	ASP	6.8
1	E	79	ASP	6.5
2	L	2	ASP	6.2
1	O	79	ASP	6.1

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Mol	Chain	Res	Type	RSRZ
1	M	78	LYS	6.0
1	C	79	ASP	5.9
1	I	79	ASP	5.5
2	H	2	ASP	5.0
1	O	637	GLY	4.9
1	O	290	ALA	4.8
1	A	79	ASP	4.6
1	O	291	ASP	4.4
1	I	655	GLY	4.3
1	O	81	VAL	4.3
1	K	79	ASP	4.1
1	O	85	GLU	4.0
1	O	80	GLY	3.9
1	O	408	THR	3.9
1	K	85	GLU	3.9
1	O	78	LYS	3.8
1	I	278	PRO	3.7
1	C	78	LYS	3.7
1	O	550	PRO	3.6
1	G	81	VAL	3.6
1	O	340	TRP	3.6
1	I	550	PRO	3.5
1	G	79	ASP	3.5
1	A	78	LYS	3.5
1	K	282	LEU	3.5
1	I	654	PRO	3.4
1	E	81	VAL	3.4
1	M	87	GLU	3.4
1	G	80	GLY	3.4
1	I	646	GLU	3.4
1	C	340	TRP	3.3
1	K	340	TRP	3.3
2	N	2	ASP	3.3
1	M	655	GLY	3.3
1	I	742	SER	3.3
1	I	798	LYS	3.3
1	I	340	TRP	3.2
1	I	408	THR	3.2
1	G	290	ALA	3.2
1	O	648	PHE	3.2
1	I	424	ALA	3.2
1	C	550	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	80	GLY	3.1
1	G	86	GLY	3.1
1	I	418	GLU	3.1
1	E	80	GLY	3.1
1	O	585	PRO	3.1
1	O	255	ASN	3.1
2	P	17	ALA	3.1
1	G	555	SER	3.1
1	O	559	ALA	3.0
1	I	279	GLU	3.0
2	D	2	ASP	3.0
1	O	418	GLU	3.0
1	O	555	SER	2.9
1	A	80	GLY	2.9
1	G	87	GLU	2.9
1	I	557	ALA	2.9
1	I	549	TRP	2.9
1	O	582	ASP	2.9
1	K	252	GLY	2.8
1	G	291	ASP	2.8
1	C	298	THR	2.8
1	O	798	LYS	2.8
1	K	80	GLY	2.8
1	M	340	TRP	2.8
1	I	745	GLY	2.8
1	I	85	GLU	2.7
1	A	340	TRP	2.7
1	O	729	SER	2.7
1	I	559	ALA	2.7
1	M	800	GLU	2.7
1	I	87	GLU	2.7
1	I	280	HIS	2.7
1	C	85	GLU	2.6
1	O	728	ARG	2.6
1	C	81	VAL	2.6
1	M	80	GLY	2.6
1	G	340	TRP	2.6
1	I	301	GLU	2.6
1	I	622	ASP	2.6
1	O	650	PRO	2.6
1	I	291	ASP	2.5
2	P	2	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	412	HIS	2.5
1	I	407	VAL	2.5
2	B	2	ASP	2.5
1	G	281	GLN	2.5
1	I	441	LYS	2.5
1	M	551	GLU	2.5
1	I	78	LYS	2.5
2	L	10	ASP	2.5
2	P	5	ARG	2.5
1	I	423	PRO	2.4
1	A	555	SER	2.4
1	K	655	GLY	2.4
1	O	270	THR	2.4
1	I	741	ILE	2.4
1	I	656	GLU	2.4
1	K	109	LYS	2.4
1	E	559	ALA	2.3
1	A	800	GLU	2.3
1	K	78	LYS	2.3
1	C	87	GLU	2.3
1	I	13	ARG	2.3
1	G	424	ALA	2.3
1	G	78	LYS	2.3
1	O	421	LYS	2.3
1	K	418	GLU	2.3
1	I	582	ASP	2.3
1	I	80	GLY	2.3
1	I	476	GLU	2.3
1	E	340	TRP	2.3
2	D	5	ARG	2.3
1	M	85	GLU	2.3
1	I	555	SER	2.3
1	O	287	LYS	2.3
1	O	653	LYS	2.3
1	O	685	GLU	2.2
2	F	5	ARG	2.2
1	I	416	ALA	2.2
1	I	551	GLU	2.2
2	L	5	ARG	2.2
1	I	274	TYR	2.2
2	P	14	SER	2.2
1	I	688	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	256	ARG	2.2
2	J	45	SER	2.2
1	K	800	GLU	2.2
2	F	2	ASP	2.2
1	I	399	HIS	2.2
1	I	725	GLU	2.2
1	I	553	ILE	2.2
1	O	87	GLU	2.2
1	I	629	GLY	2.2
1	M	558	PRO	2.2
2	J	3	ALA	2.2
1	A	81	VAL	2.2
1	O	745	GLY	2.2
1	G	801	ALA	2.1
1	I	431	VAL	2.1
1	K	684	GLU	2.1
1	I	104	ALA	2.1
2	J	4	PRO	2.1
2	J	5	ARG	2.1
1	G	729	SER	2.1
1	I	444	ASP	2.1
1	O	286	ALA	2.1
1	O	725	GLU	2.1
2	L	4	PRO	2.1
1	I	34	ASP	2.1
2	N	5	ARG	2.1
1	O	551	GLU	2.1
1	I	86	GLY	2.1
1	I	560	TYR	2.1
1	O	556	ALA	2.1
1	G	406	VAL	2.1
1	I	277	ARG	2.1
1	C	800	GLU	2.1
1	O	257	ASP	2.1
1	O	299	ASP	2.1
1	I	801	ALA	2.0
2	H	27	ASP	2.0
1	O	313	GLU	2.0
1	G	429	ASP	2.0
1	I	81	VAL	2.0
1	E	78	LYS	2.0
1	M	91	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	O	655	GLY	2.0

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

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

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, 95th 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(\AA^2)	Q<0.9
5	MGD	I	1804	47/47	0.90	0.21	47,53,61,64	0
6	HEC	L	1129	43/43	0.92	0.25	10,29,44,46	0
6	HEC	P	1128	43/43	0.92	0.26	27,37,49,54	0
6	HEC	J	1128	43/43	0.92	0.27	31,37,50,56	0
6	HEC	H	1129	43/43	0.92	0.23	13,19,42,46	0
6	HEC	P	1129	43/43	0.92	0.22	23,40,42,43	0
5	MGD	I	1803	47/47	0.92	0.19	34,49,58,61	0
4	MO	I	1802	1/1	0.93	0.05	66,66,66,66	0
5	MGD	O	1804	47/47	0.93	0.20	46,50,53,54	0
6	HEC	H	1128	43/43	0.93	0.25	15,24,38,45	0
6	HEC	D	1128	43/43	0.93	0.24	20,29,44,52	0
6	HEC	N	1128	43/43	0.93	0.25	25,31,43,51	0
5	MGD	O	1803	47/47	0.93	0.18	37,45,56,57	0
6	HEC	L	1128	43/43	0.93	0.23	27,35,44,51	0
6	HEC	F	1128	43/43	0.93	0.25	14,23,47,56	0
6	HEC	J	1129	43/43	0.93	0.25	32,43,47,50	0
6	HEC	N	1129	43/43	0.94	0.21	18,27,41,44	0
5	MGD	K	1804	47/47	0.94	0.21	24,36,39,42	0
6	HEC	D	1129	43/43	0.94	0.22	14,19,48,55	0
6	HEC	F	1129	43/43	0.94	0.21	10,19,38,43	0
5	MGD	C	1804	47/47	0.95	0.19	21,27,39,40	0
5	MGD	E	1804	47/47	0.95	0.18	10,12,20,24	0

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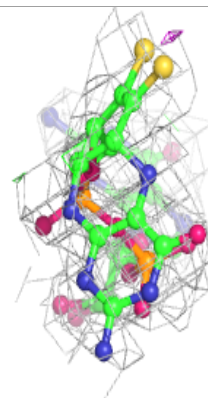
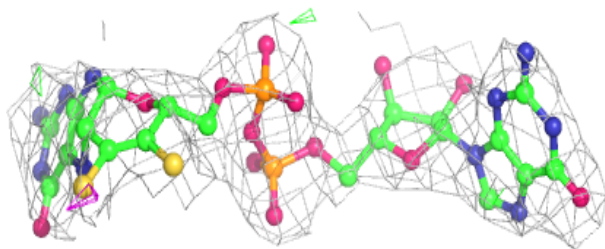
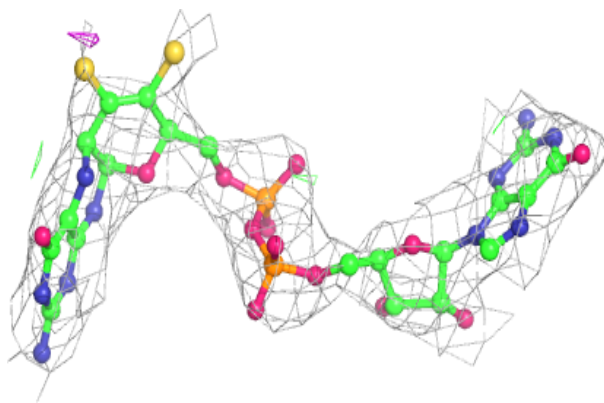
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	HEC	B	1128	43/43	0.95	0.20	12,15,38,45	0
5	MGD	A	1804	47/47	0.96	0.16	10,10,12,18	0
5	MGD	G	1804	47/47	0.96	0.17	28,35,39,42	0
5	MGD	A	1803	47/47	0.96	0.16	10,12,16,17	0
4	MO	O	1802	1/1	0.96	0.08	62,62,62,62	0
6	HEC	B	1129	43/43	0.96	0.18	10,16,36,41	0
5	MGD	C	1803	47/47	0.96	0.18	19,26,32,34	0
5	MGD	G	1803	47/47	0.97	0.15	23,26,36,37	0
5	MGD	E	1803	47/47	0.97	0.15	10,17,21,22	0
5	MGD	K	1803	47/47	0.97	0.17	31,34,36,40	0
5	MGD	M	1803	47/47	0.97	0.16	23,28,34,36	0
5	MGD	M	1804	47/47	0.97	0.16	23,26,30,34	0
3	SF4	O	1801	8/8	0.98	0.10	29,30,33,33	0
4	MO	C	1802	1/1	0.98	0.07	38,38,38,38	0
4	MO	E	1802	1/1	0.98	0.06	28,28,28,28	0
4	MO	A	1802	1/1	0.99	0.07	24,24,24,24	0
3	SF4	A	1801	8/8	0.99	0.10	10,10,10,12	0
3	SF4	I	1801	8/8	0.99	0.11	34,37,37,39	0
3	SF4	K	1801	8/8	0.99	0.11	10,10,11,12	0
4	MO	K	1802	1/1	0.99	0.09	40,40,40,40	0
3	SF4	M	1801	8/8	0.99	0.09	10,10,12,12	0
3	SF4	G	1801	8/8	0.99	0.09	10,10,12,12	0
4	MO	M	1802	1/1	0.99	0.07	39,39,39,39	0
4	MO	G	1802	1/1	0.99	0.09	35,35,35,35	0
3	SF4	E	1801	8/8	0.99	0.09	10,10,11,12	0
3	SF4	C	1801	8/8	0.99	0.09	10,10,11,12	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.

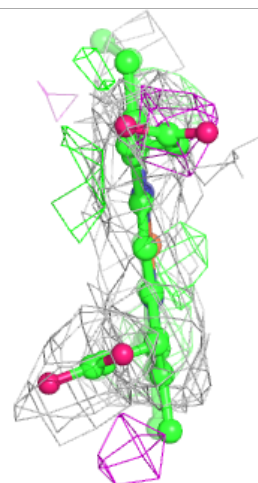
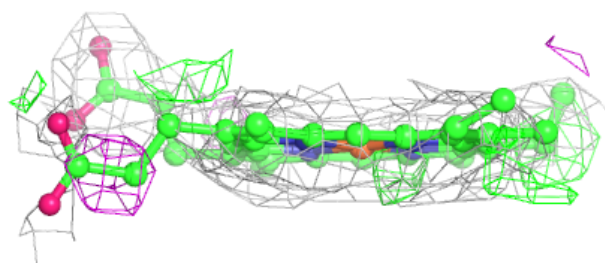
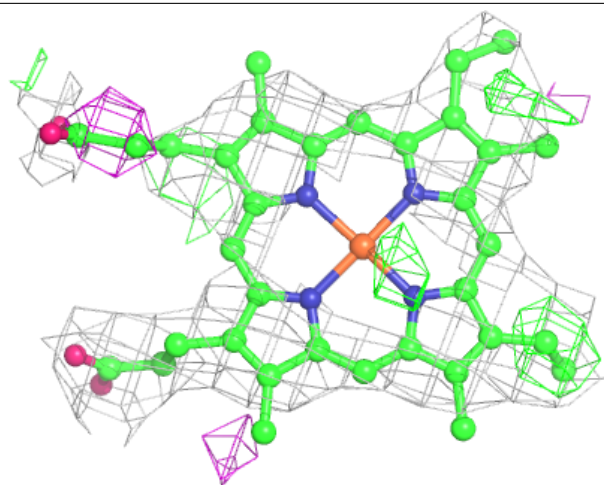
Electron density around MGD I 1804:

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



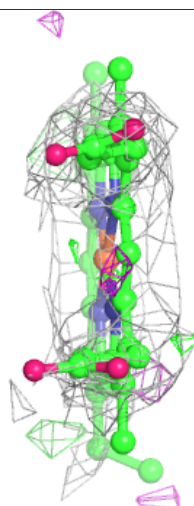
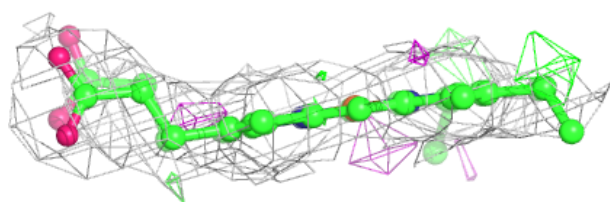
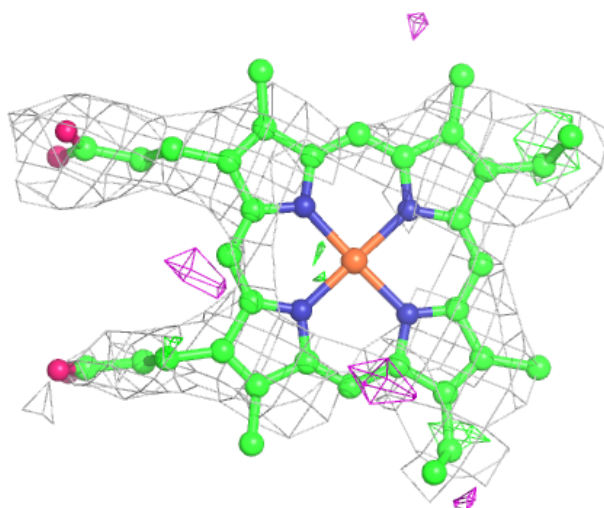
Electron density around HEC L 1129:

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



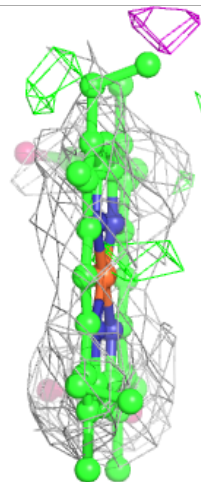
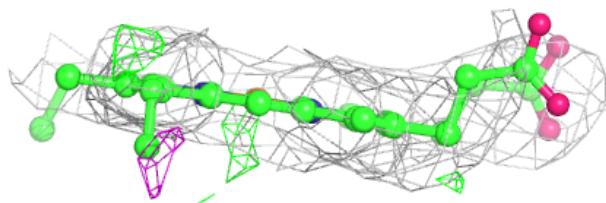
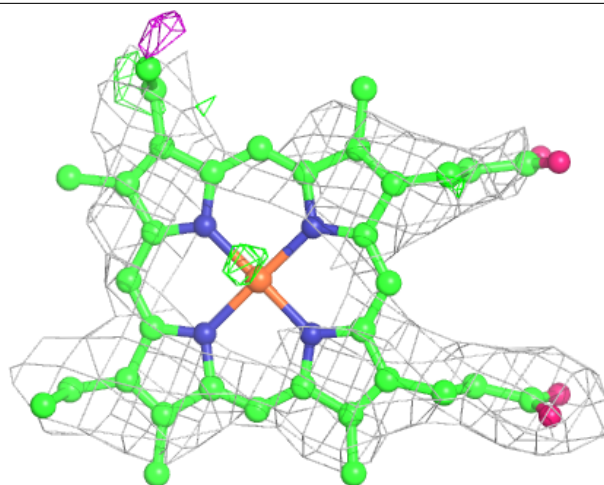
Electron density around HEC P 1128:

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



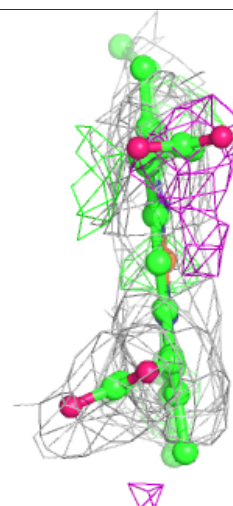
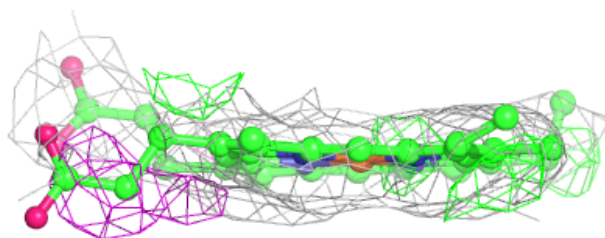
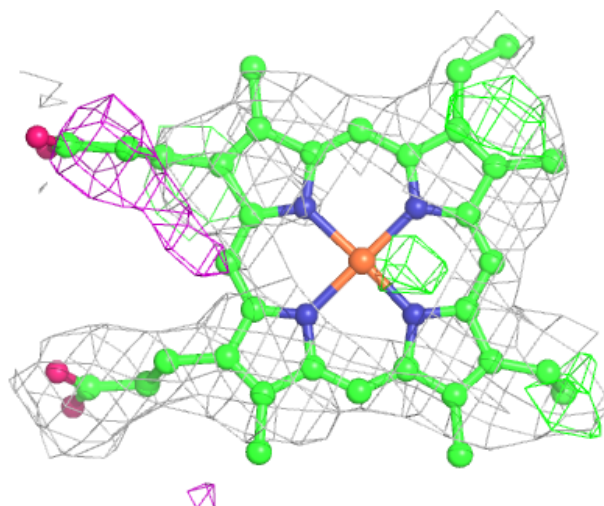
Electron density around HEC J 1128:

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



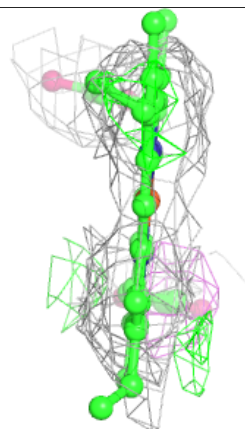
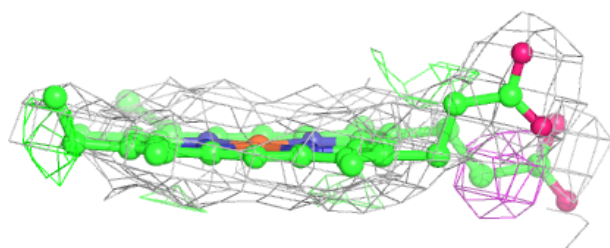
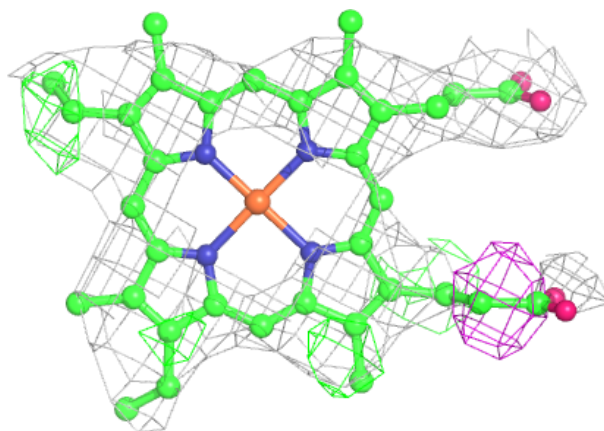
Electron density around HEC H 1129:

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

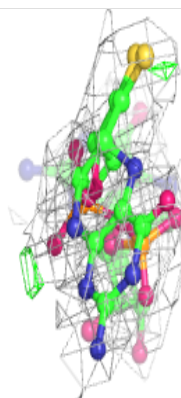
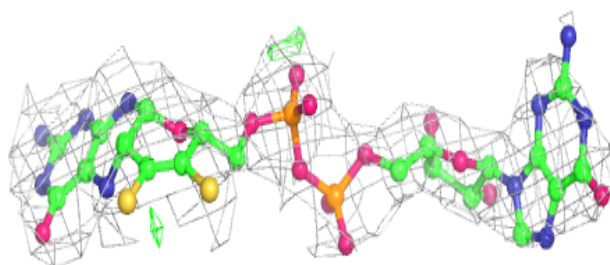
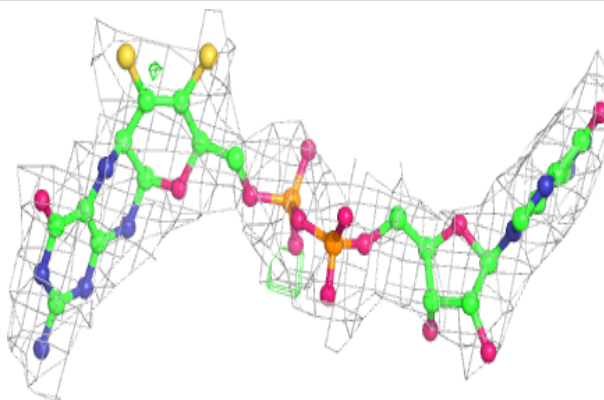


Electron density around HEC P 1129:

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

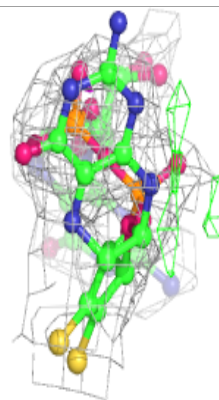
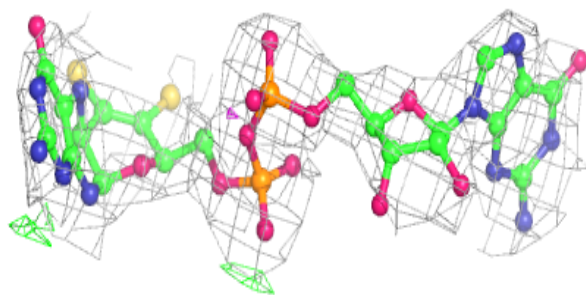
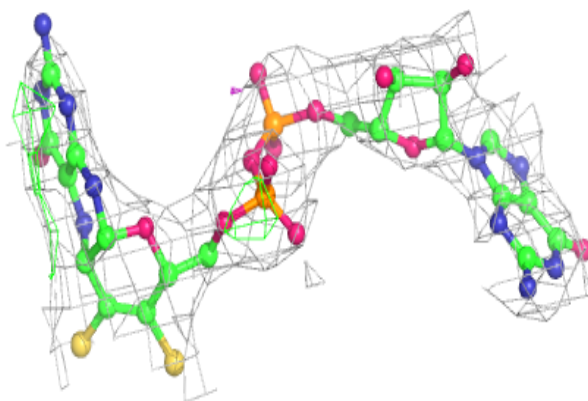
**Electron density around MGD I 1803:**

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



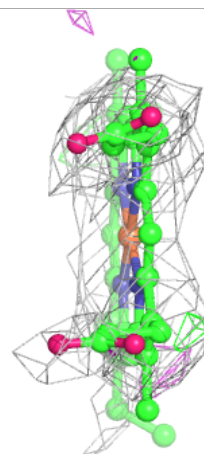
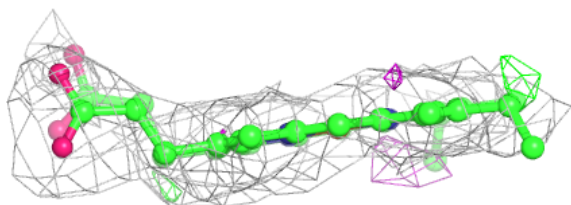
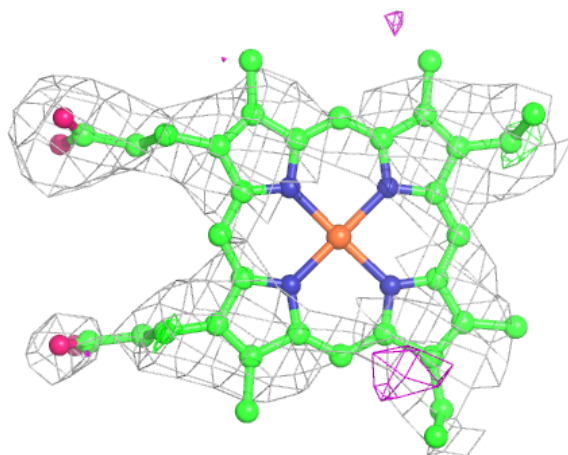
Electron density around MGD O 1804:

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



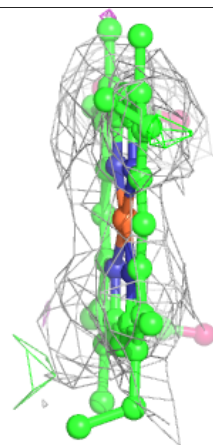
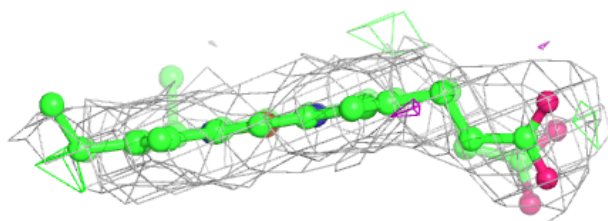
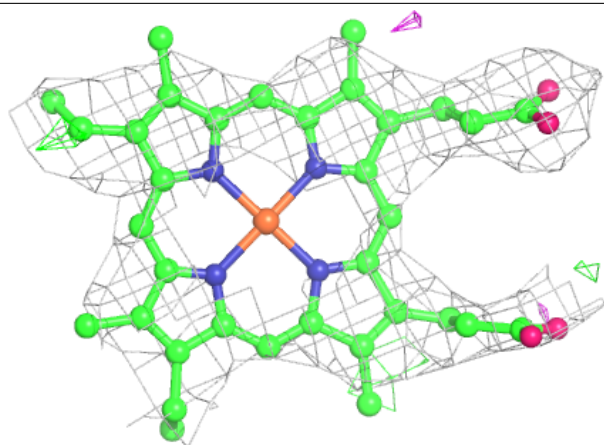
Electron density around HEC H 1128:

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



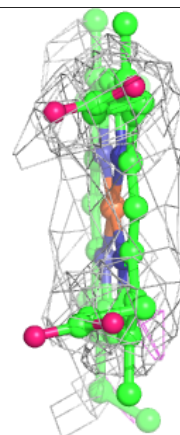
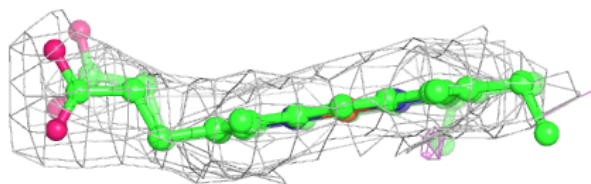
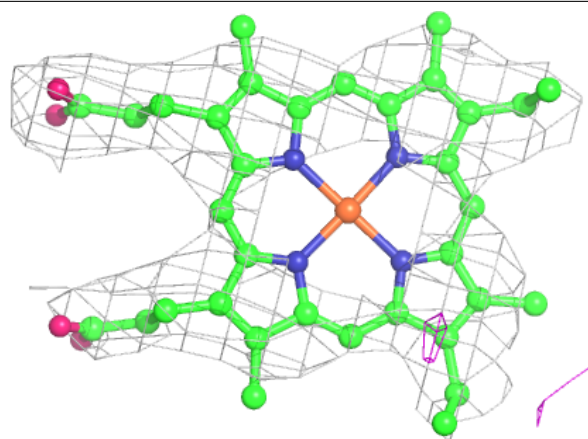
Electron density around HEC D 1128:

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

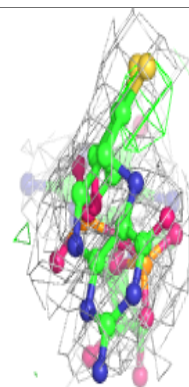
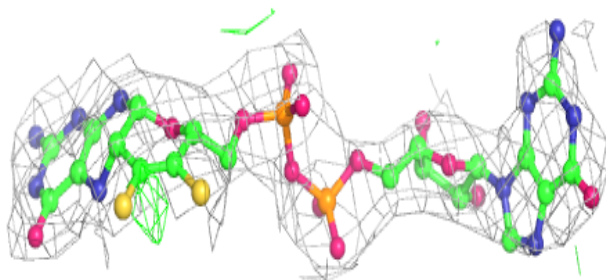
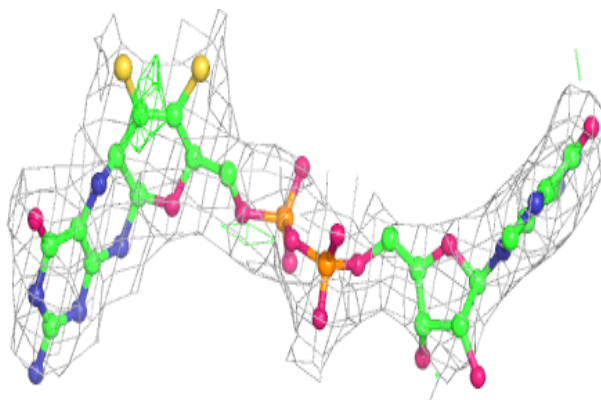


Electron density around HEC N 1128:

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

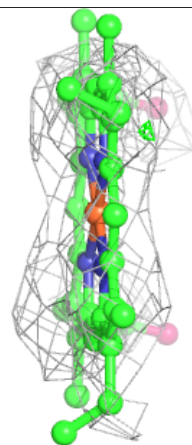
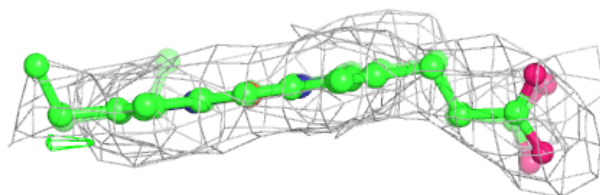
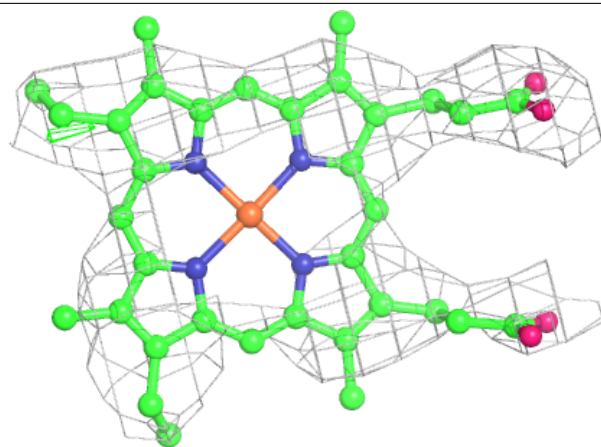
**Electron density around MGD O 1803:**

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



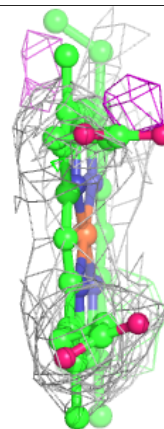
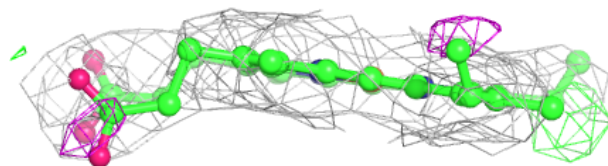
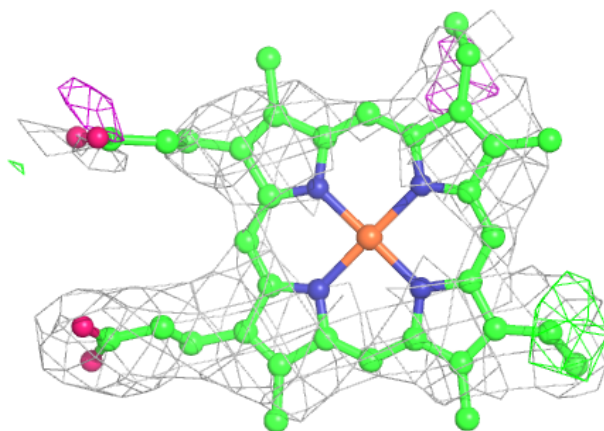
Electron density around HEC L 1128:

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



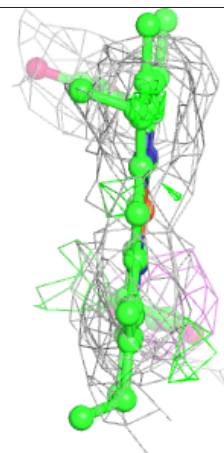
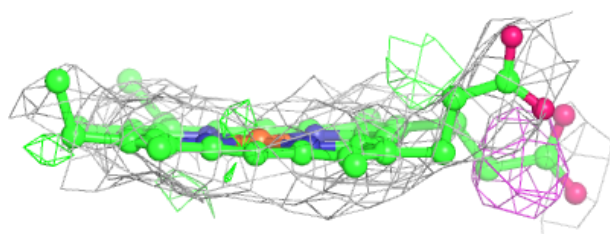
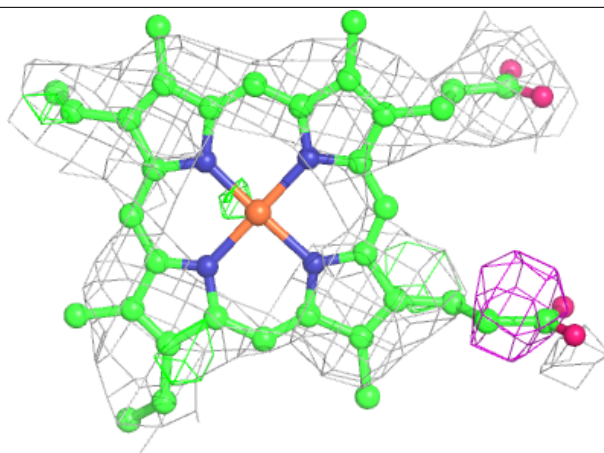
Electron density around HEC F 1128:

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



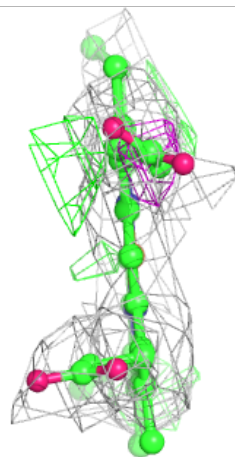
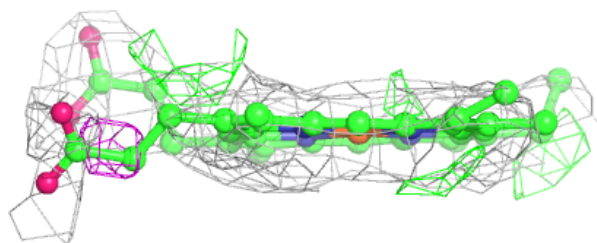
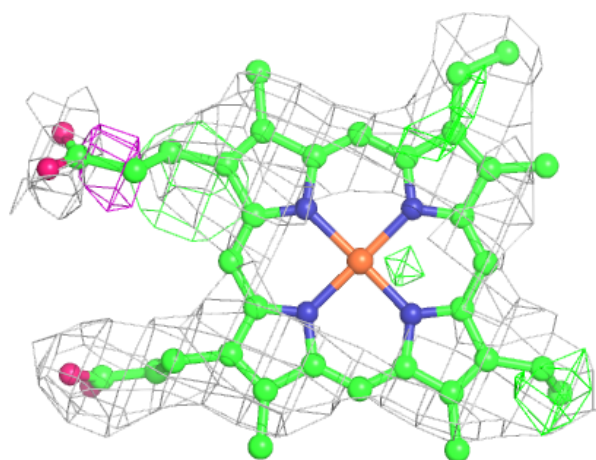
Electron density around HEC J 1129:

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



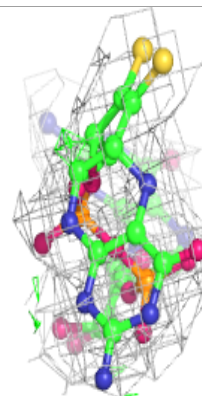
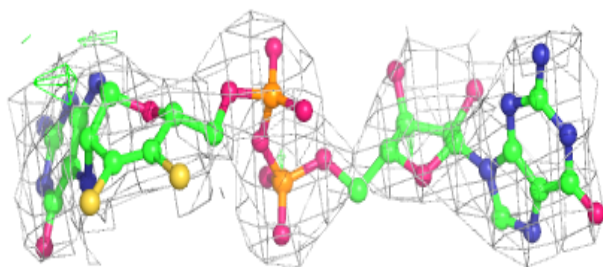
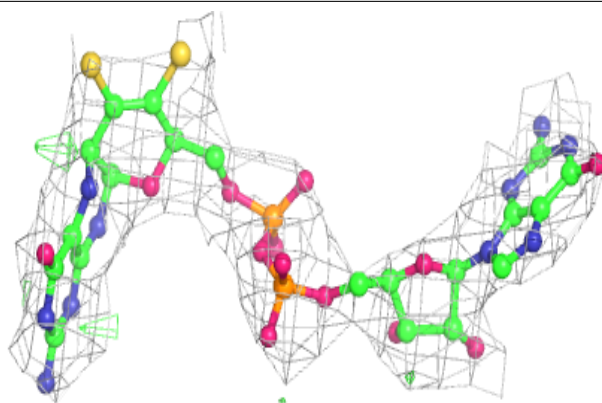
Electron density around HEC N 1129:

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



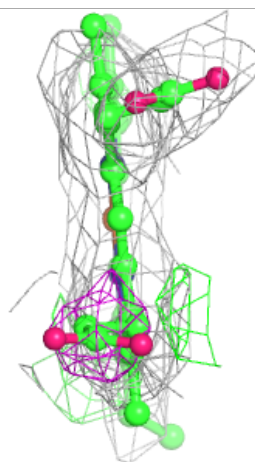
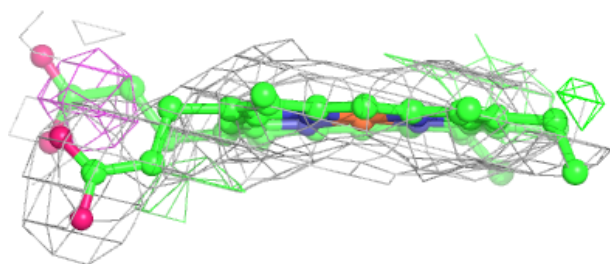
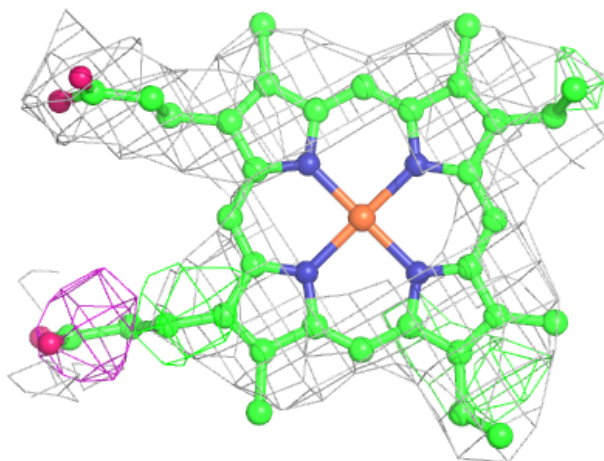
Electron density around MGD K 1804:

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



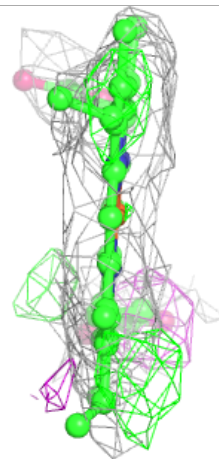
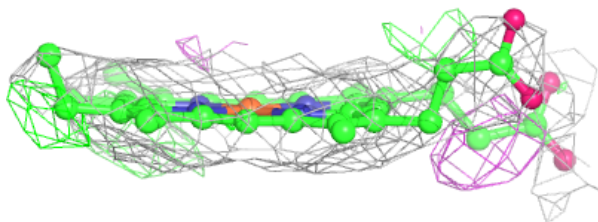
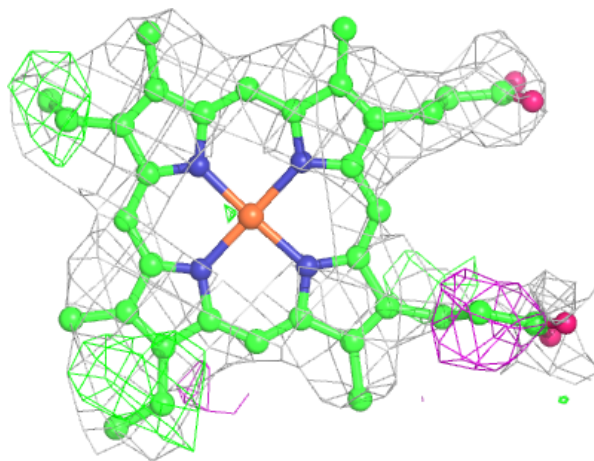
Electron density around HEC D 1129:

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



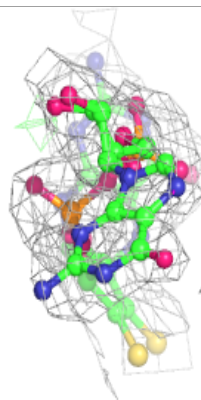
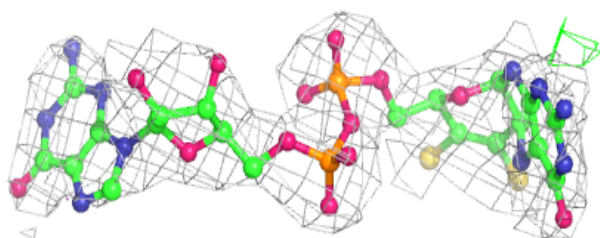
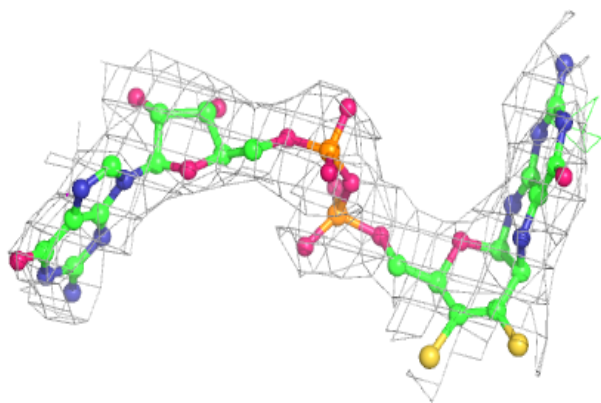
Electron density around HEC F 1129:

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

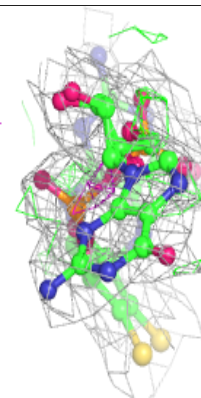
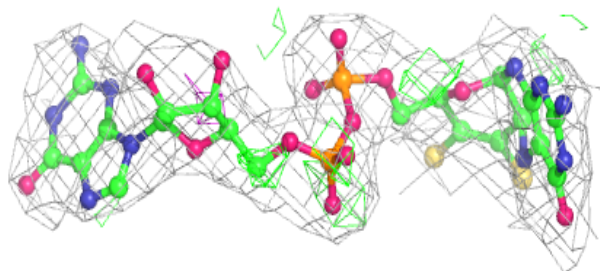
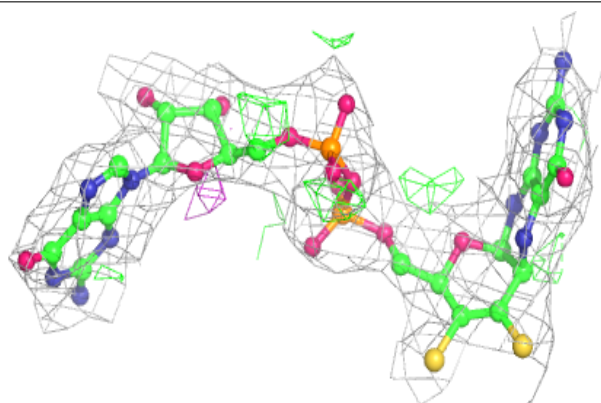


Electron density around MGD C 1804:

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

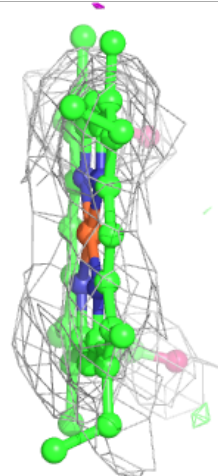
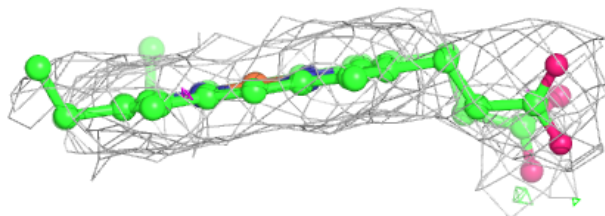
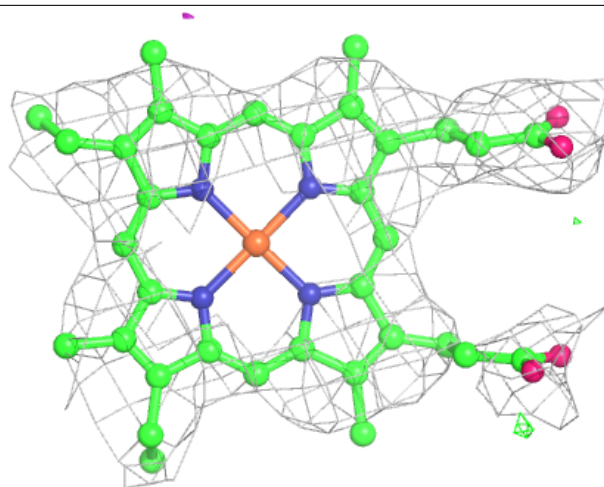
**Electron density around MGD E 1804:**

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



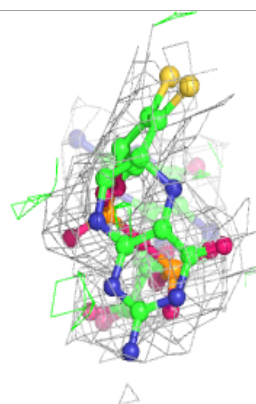
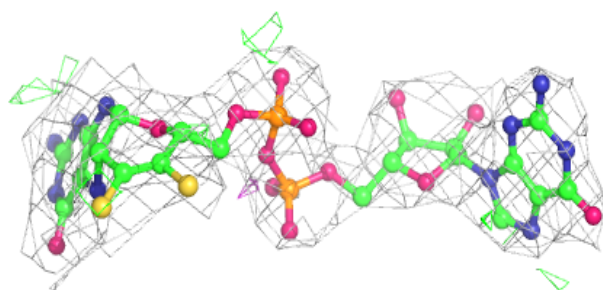
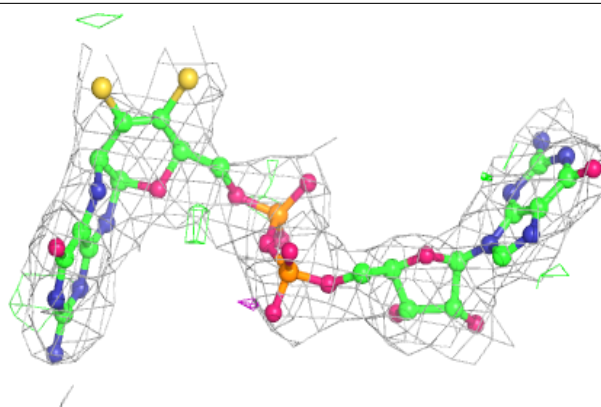
Electron density around HEC B 1128:

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

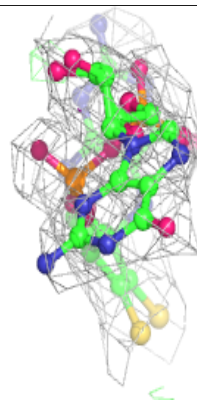
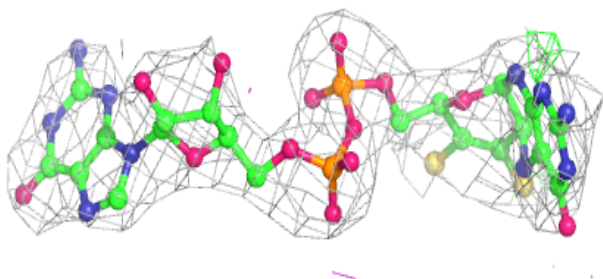
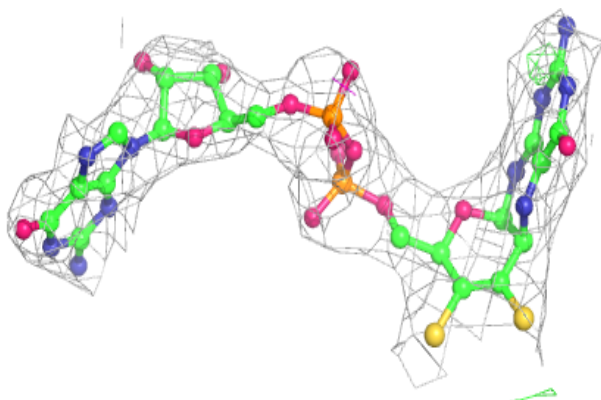


Electron density around MGD A 1804:

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

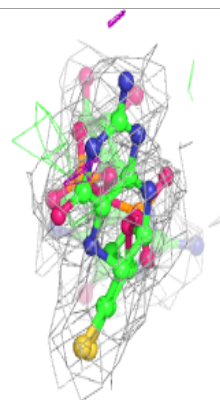
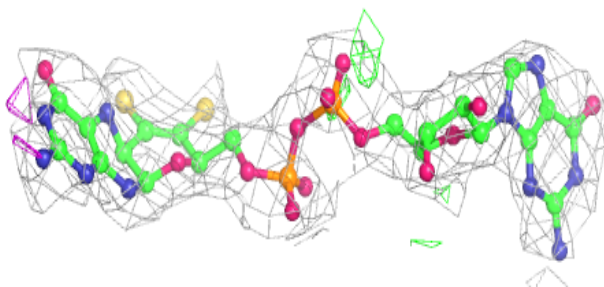
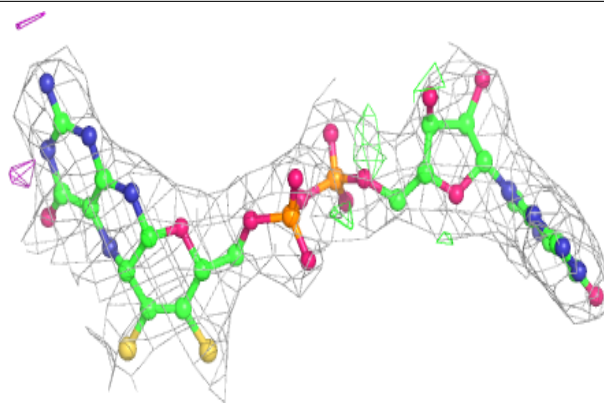
**Electron density around MGD G 1804:**

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



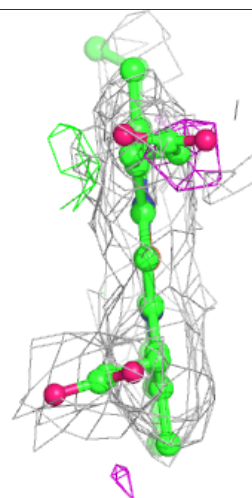
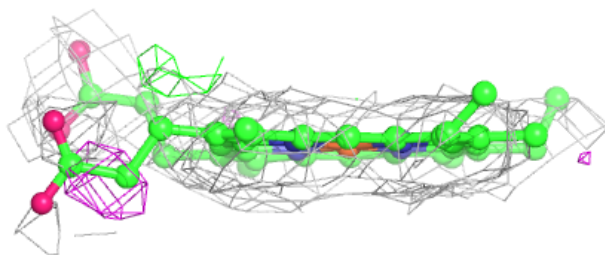
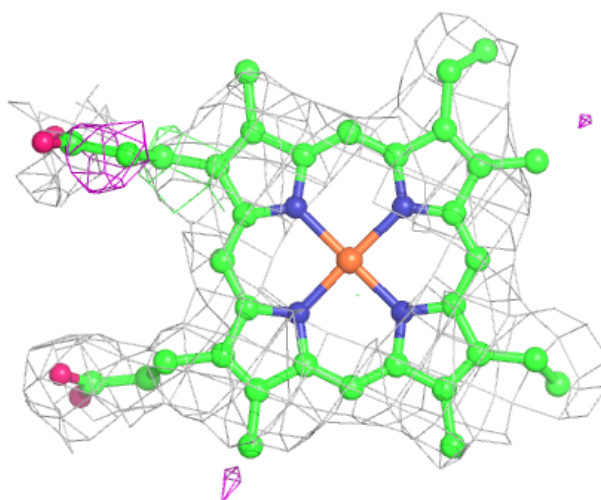
Electron density around MGD A 1803:

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



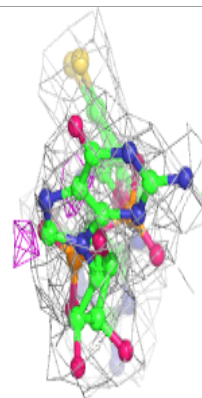
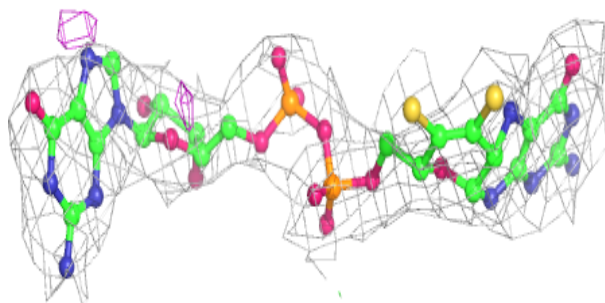
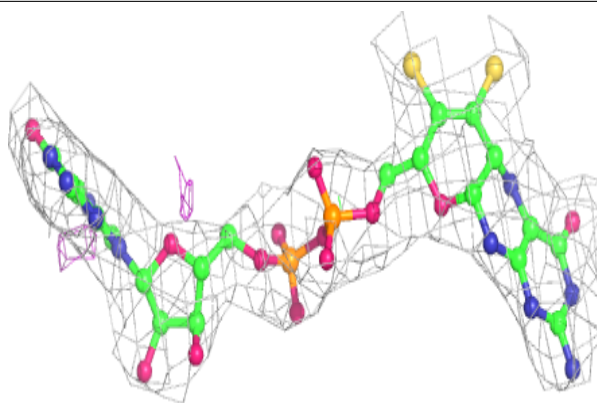
Electron density around HEC B 1129:

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

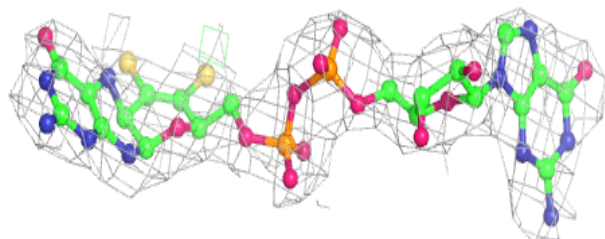
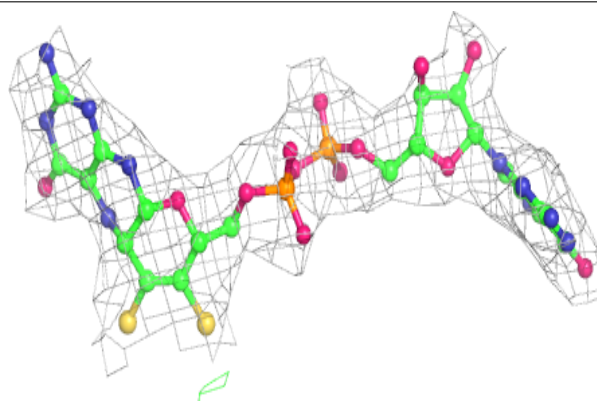


Electron density around MGD C 1803:

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

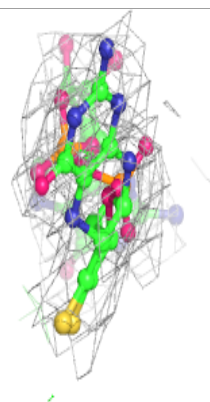
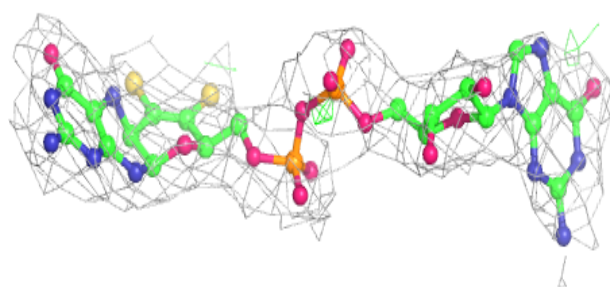
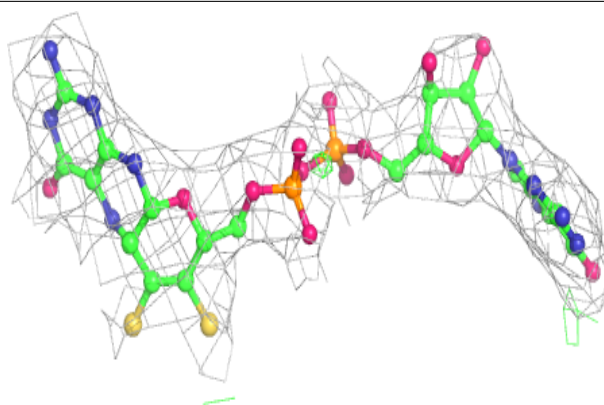
**Electron density around MGD G 1803:**

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

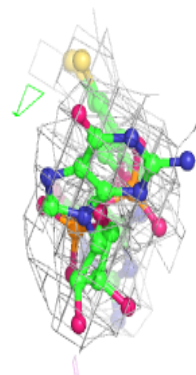
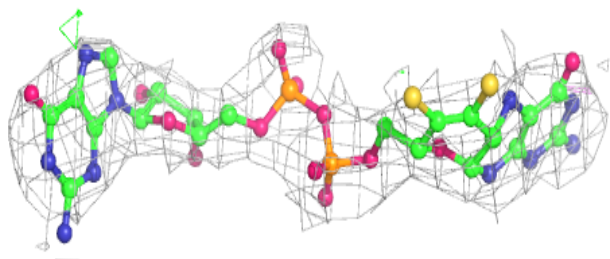
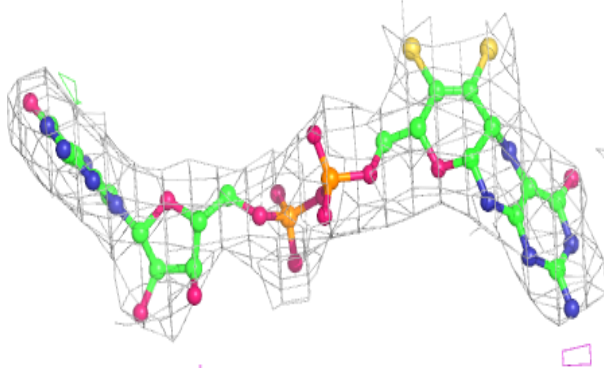


Electron density around MGD E 1803:

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

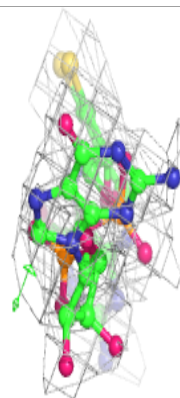
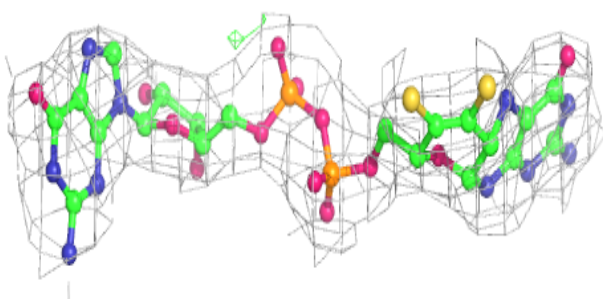
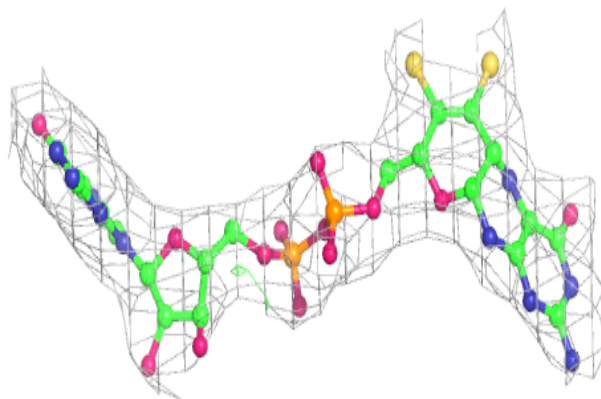
**Electron density around MGD K 1803:**

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

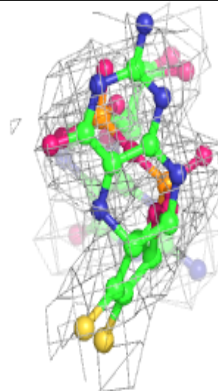
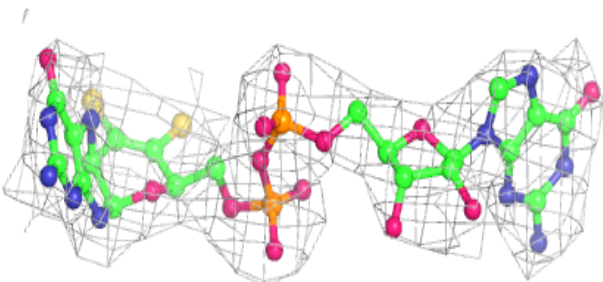
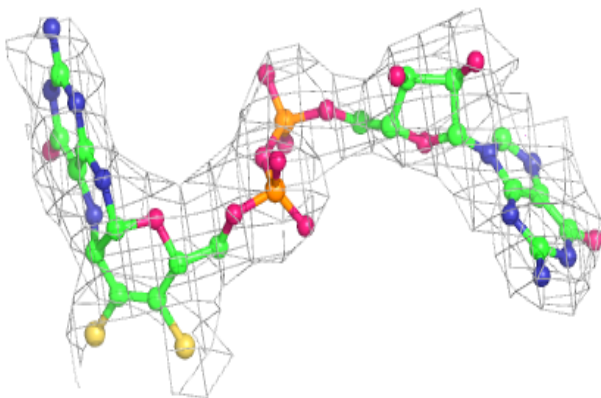


Electron density around MGD M 1803:

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

**Electron density around MGD M 1804:**

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



6.5 Other polymers

There are no such residues in this entry.