



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 10:28 AM EDT

PDB ID : 5JUY / pdb_00005juy
EMDB ID : EMD-8178
Title : Active human apoptosome with procaspase-9
Authors : Cheng, T.C.; Hong, C.; Akey, I.V.; Yuan, S.; Akey, C.W.
Deposited on : 2016-05-10
Resolution : 4.10 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

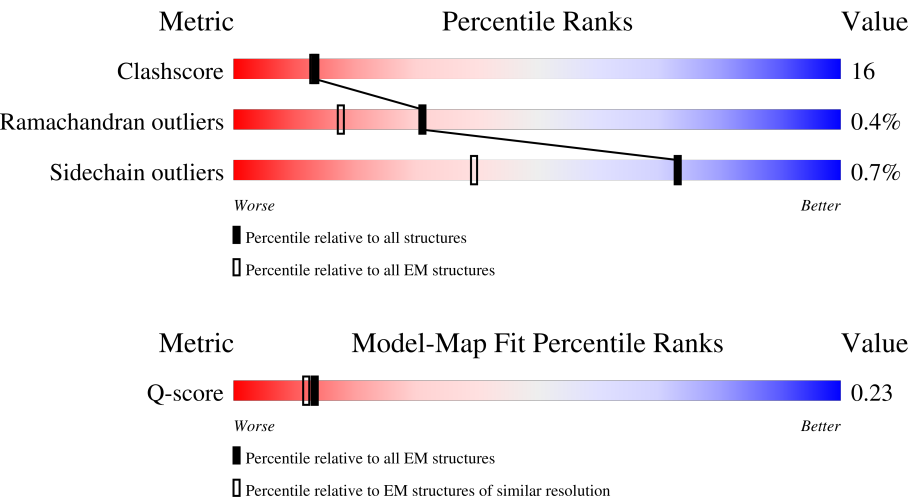
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1248	39% 63% 27% 9%
1	B	1248	46% 70% 28% ..
1	C	1248	39% 63% 27% 9%
1	D	1248	46% 70% 28% ..

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Mol	Chain	Length	Quality of chain
1	E	1248	
1	F	1248	
1	G	1248	
2	H	104	
2	I	104	
2	J	104	
2	K	104	
2	L	104	
2	M	104	
2	N	104	
3	O	95	
3	P	95	
3	Q	95	
3	R	95	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 76058 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Apoptotic protease-activating factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	B	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	C	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	D	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	E	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	F	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	G	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		

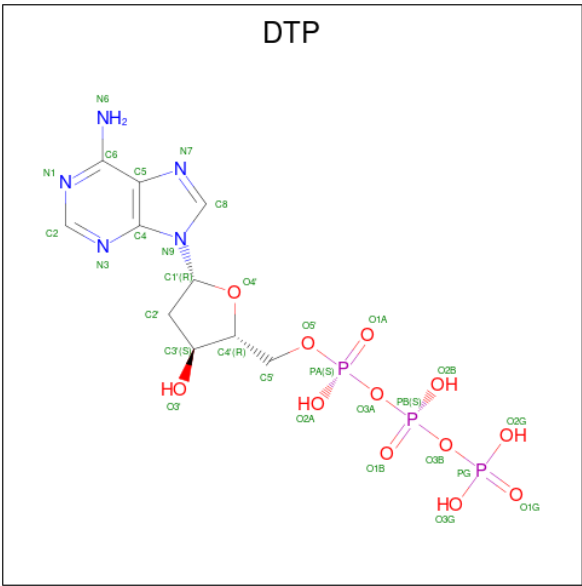
- Molecule 2 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	I	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	J	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	K	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	L	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	M	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	N	104	Total	C	N	O	S	0	0
			814	517	143	150	4		

- Molecule 3 is a protein called Caspase-9.

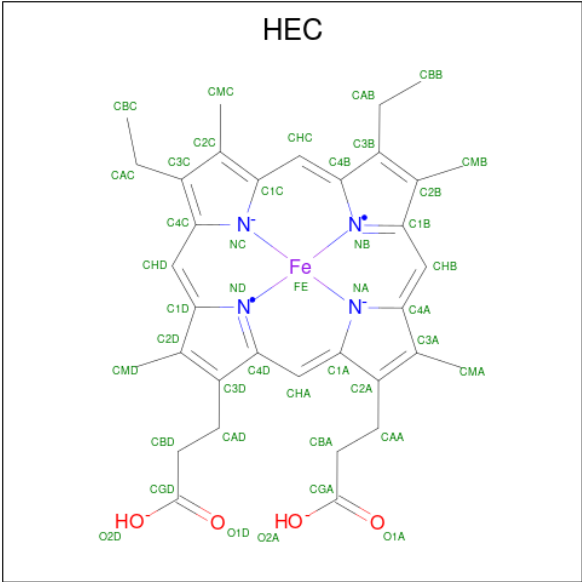
Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	P	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	Q	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	R	95	Total	C	N	O	S	0	0
			777	475	152	145	5		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	B	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	C	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	D	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	E	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	F	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	G	1	Total	C	N	O	P	0
			30	10	5	12	3	

- Molecule 5 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).

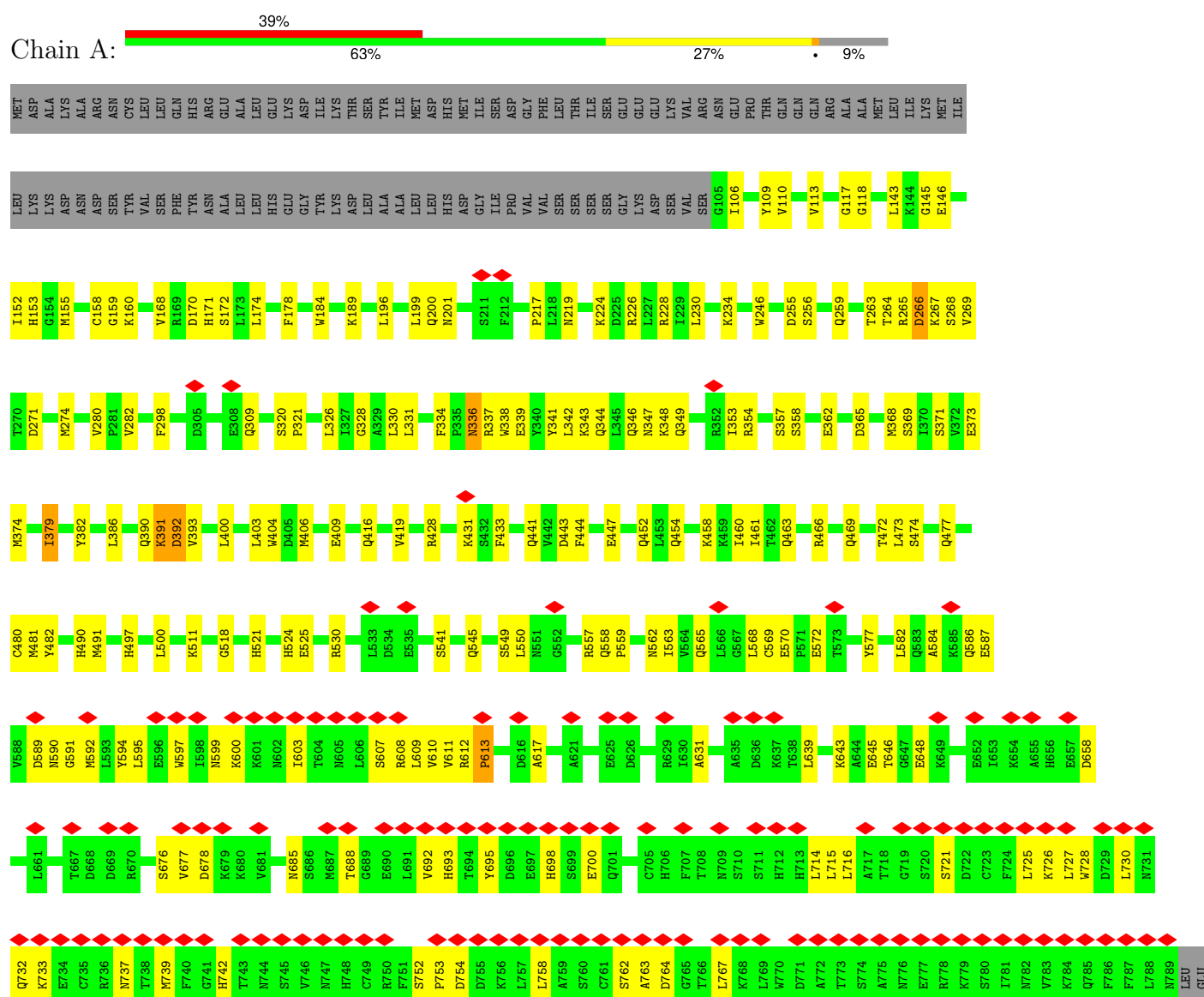


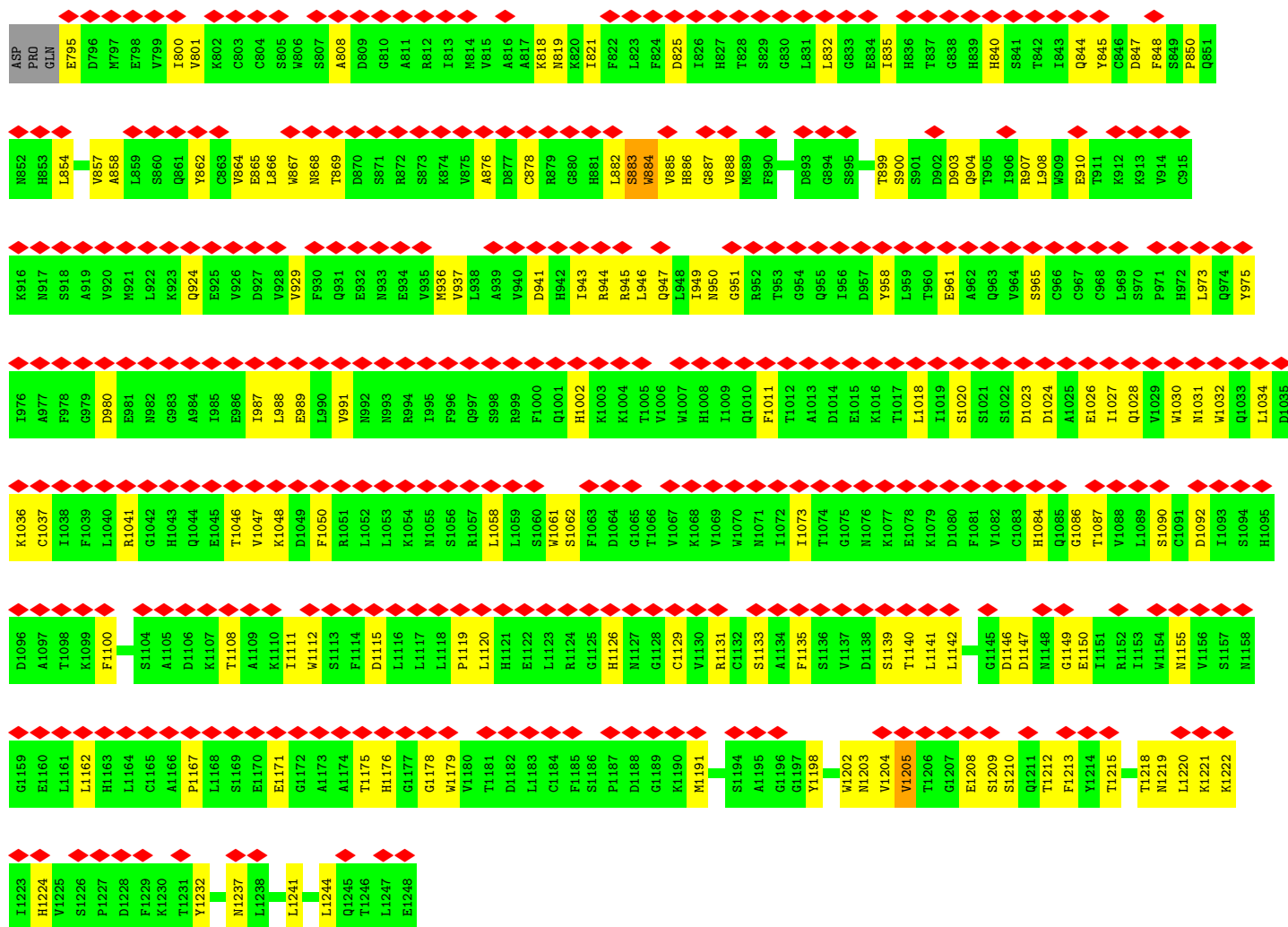
Mol	Chain	Residues	Atoms					AltConf
5	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	M	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

3 Residue-property plots

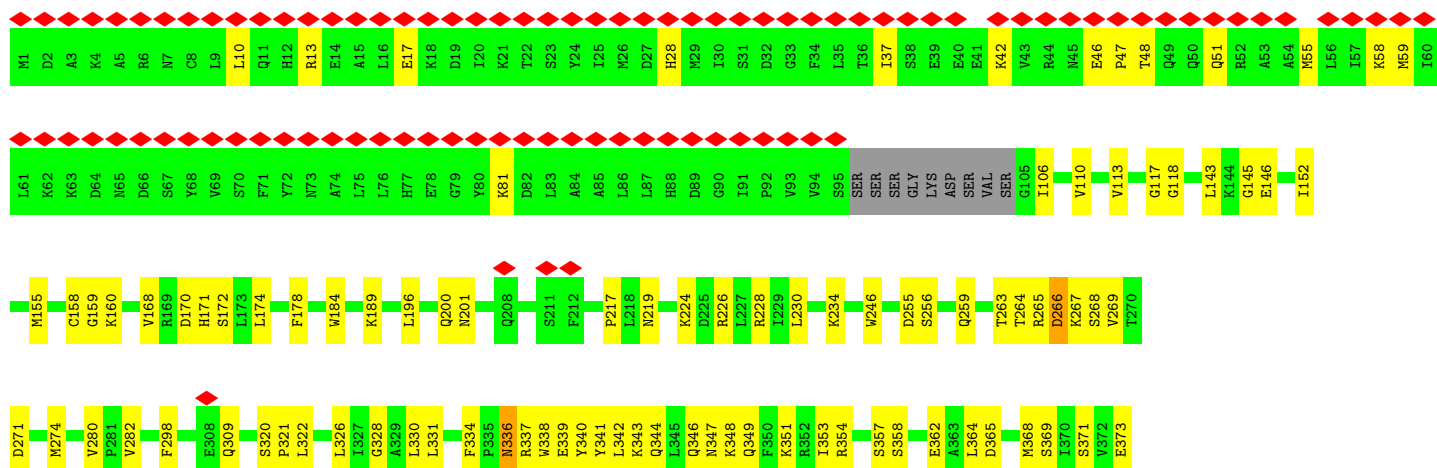
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

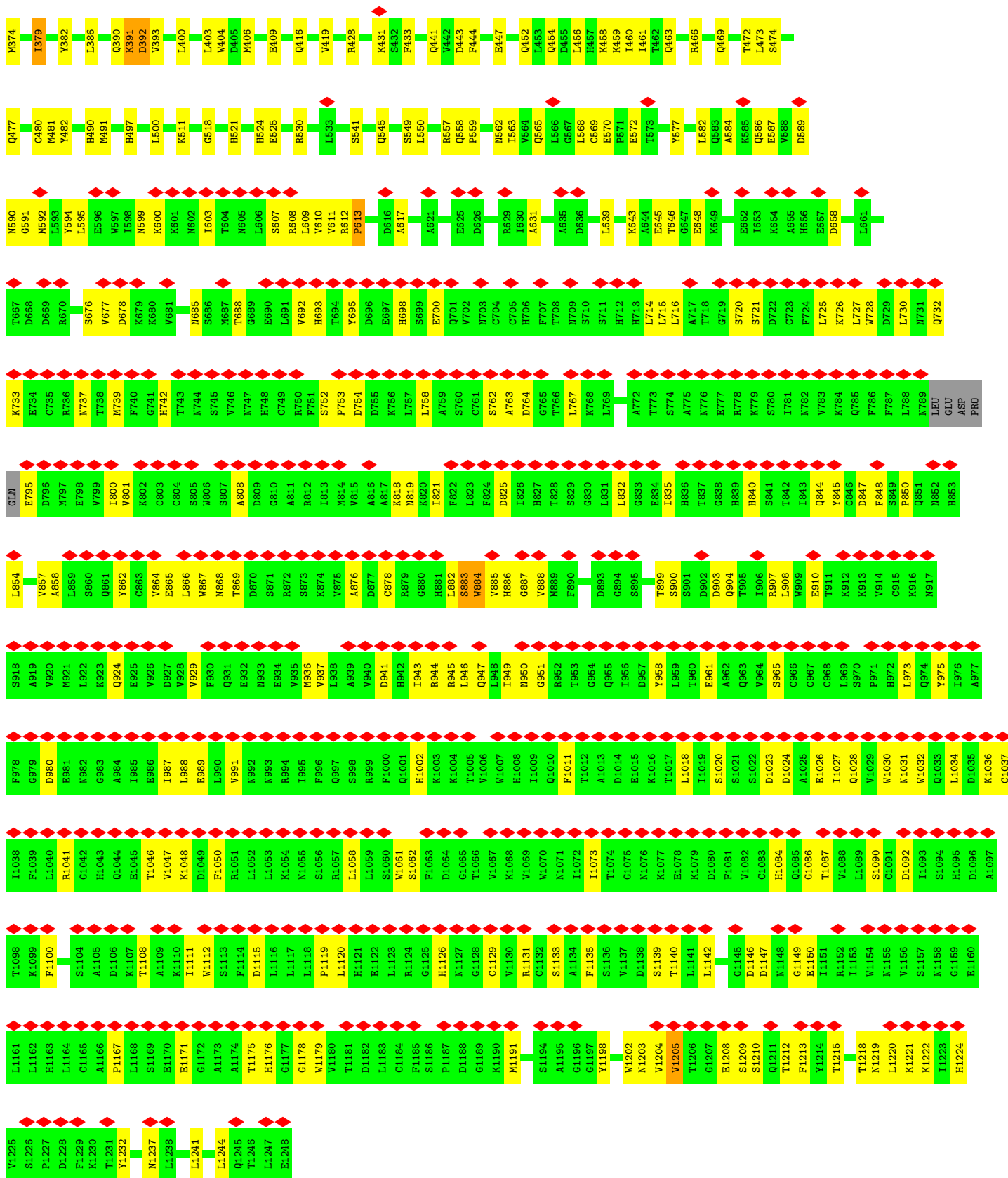
- Molecule 1: Apoptotic protease-activating factor 1



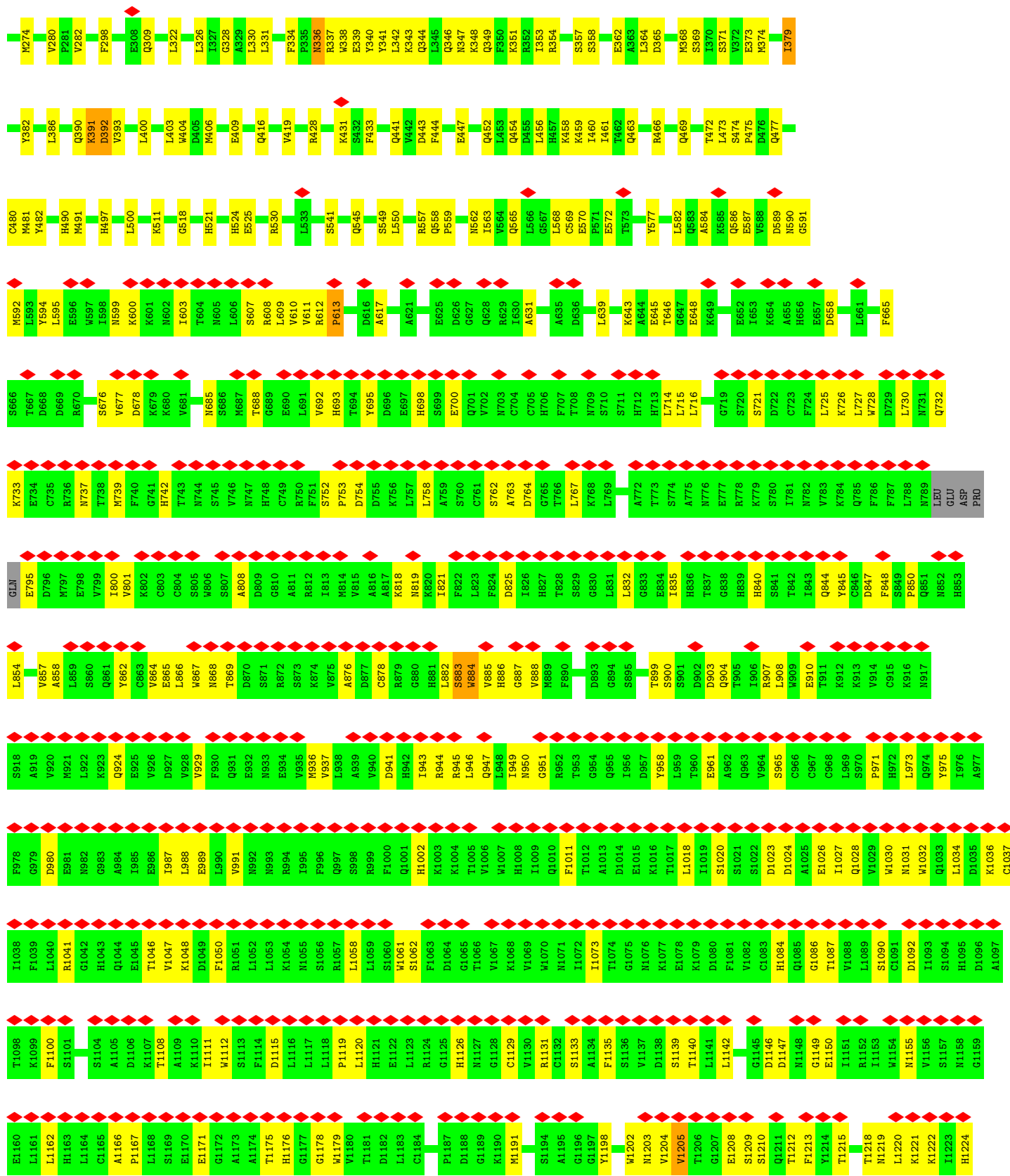


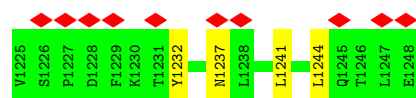
• Molecule 1: Apoptotic protease-activating factor 1



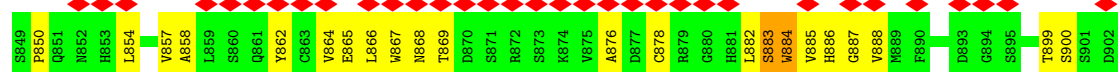
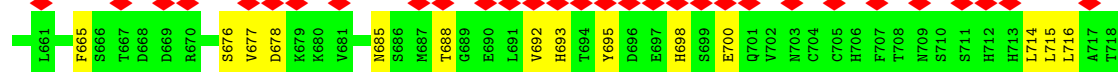
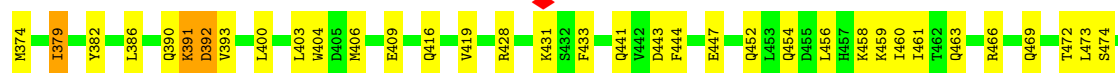
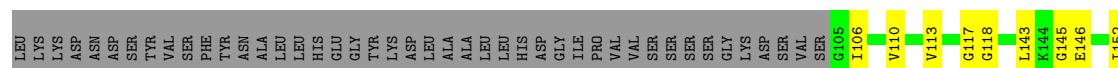
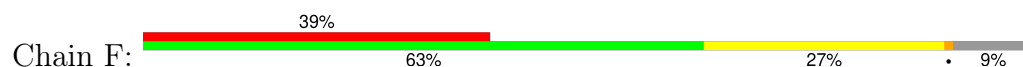


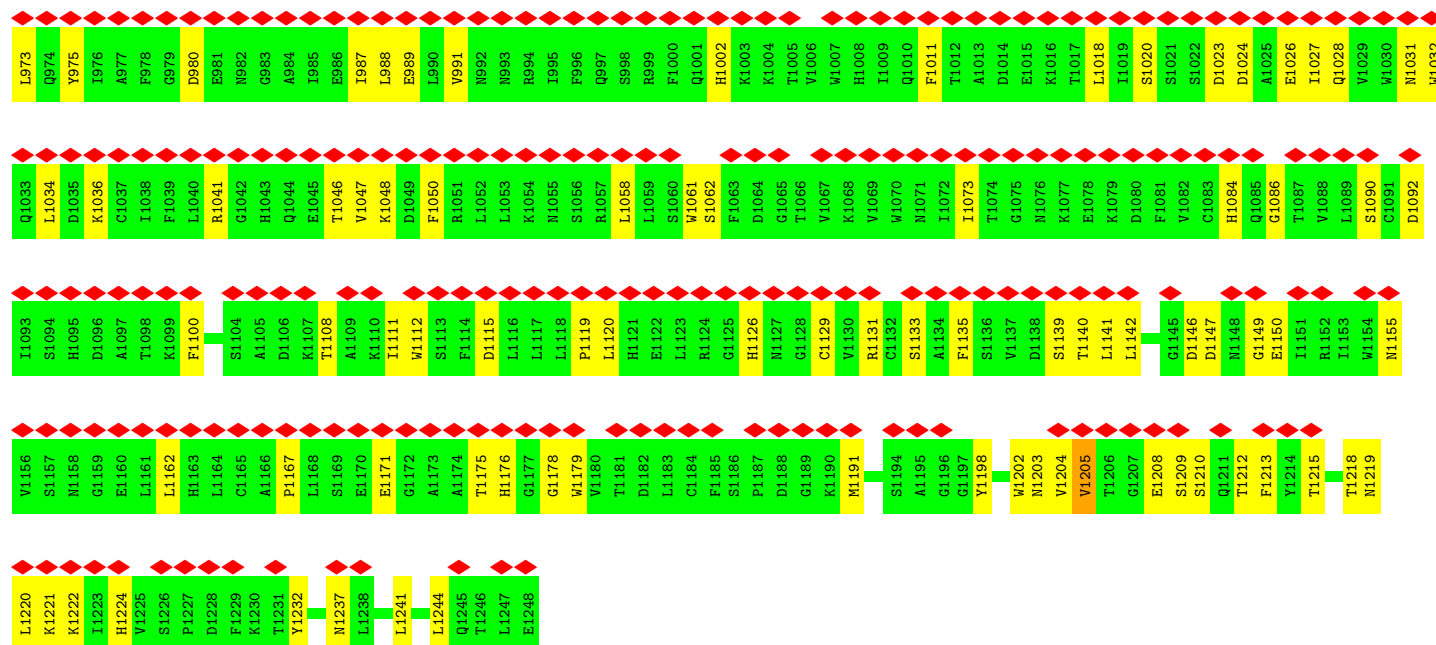




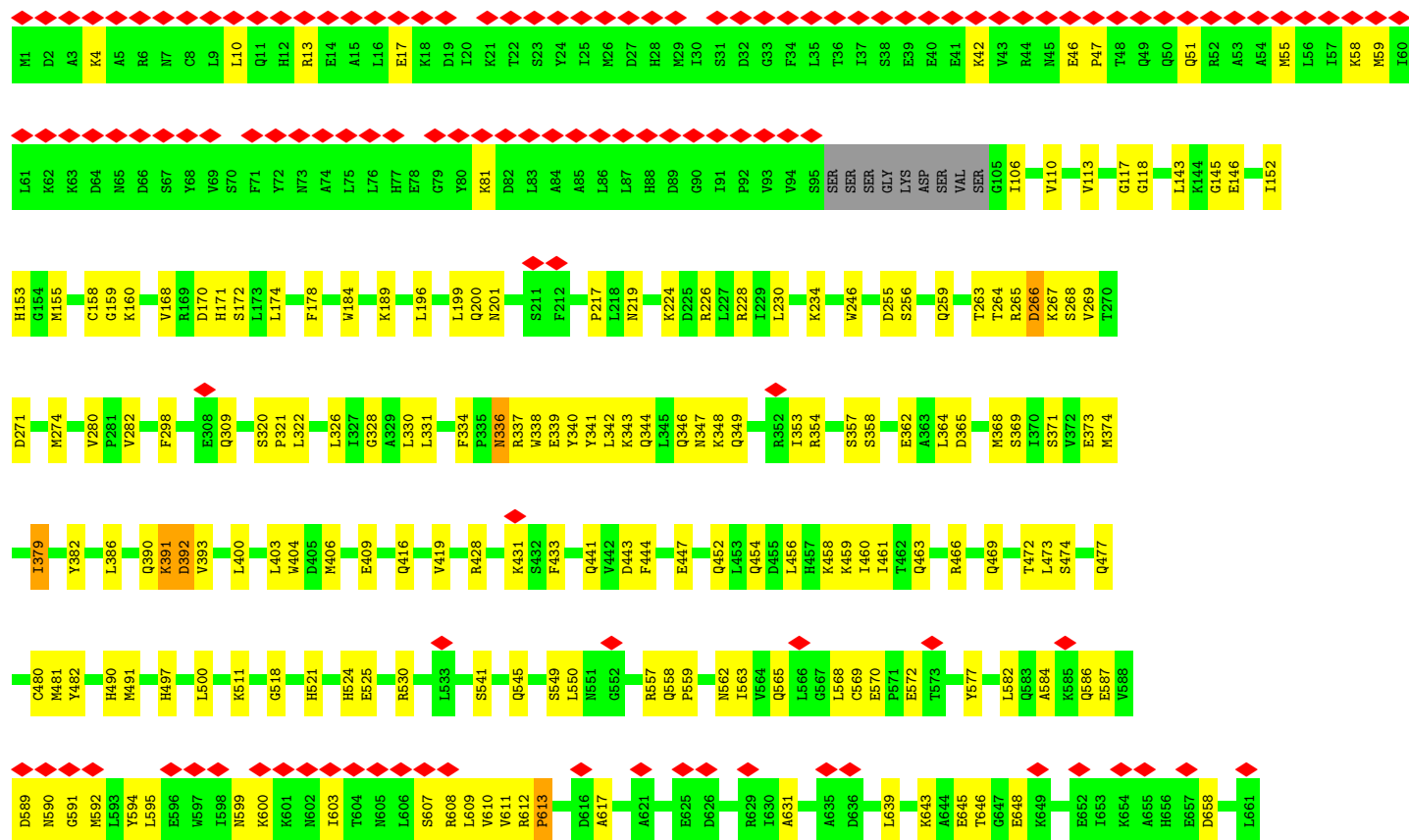


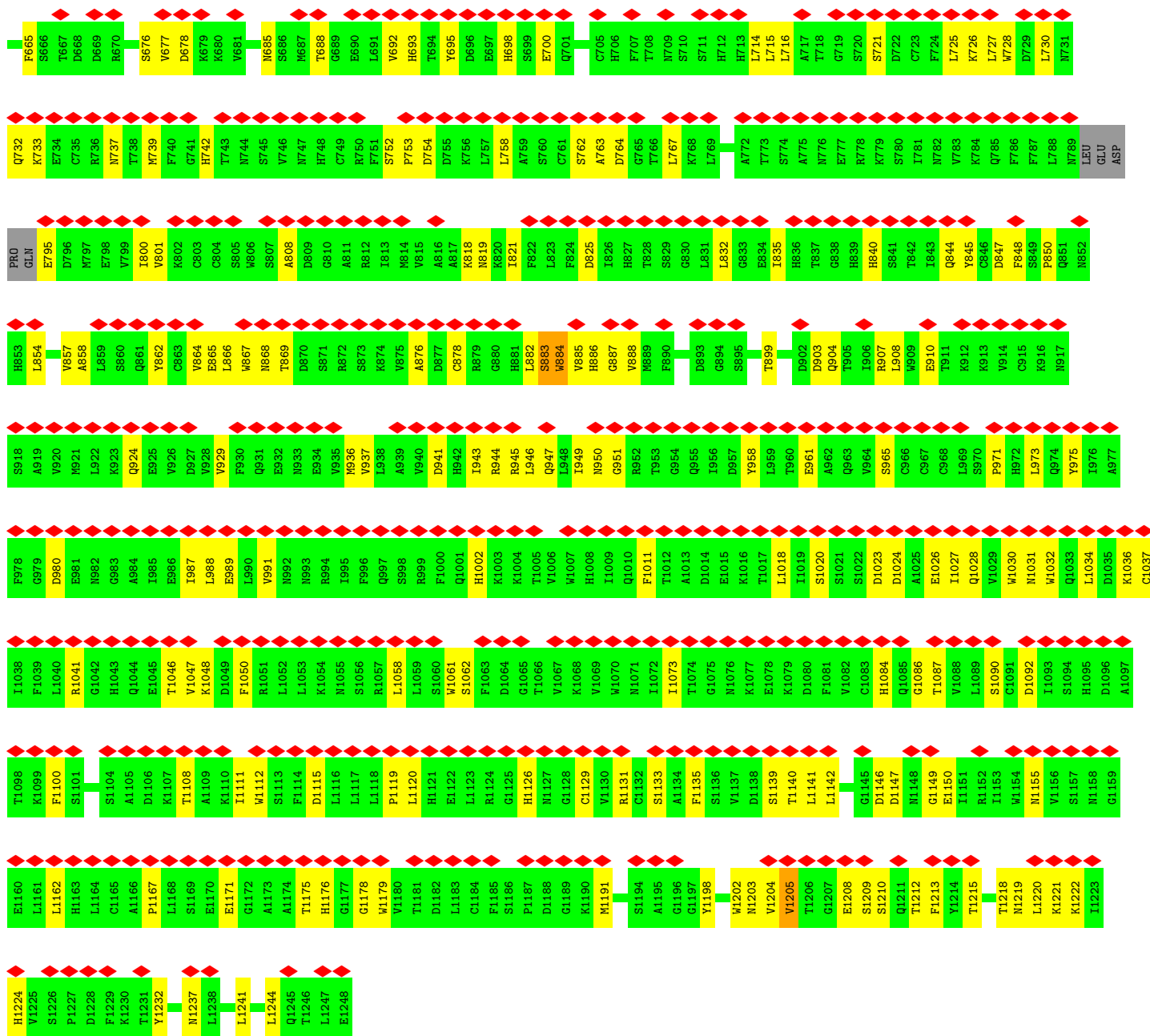
● Molecule 1: Apoptotic protease-activating factor 1

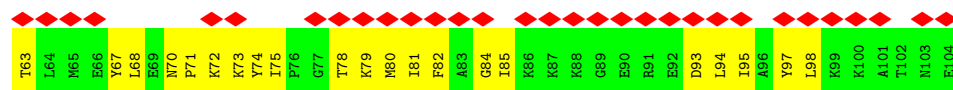
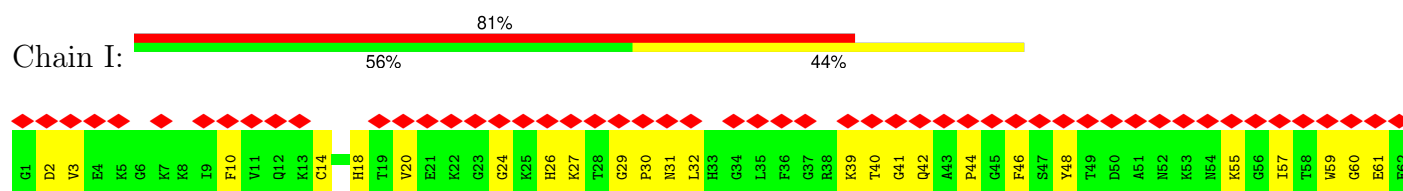




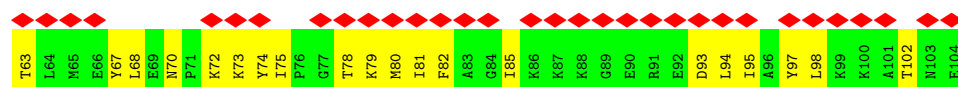
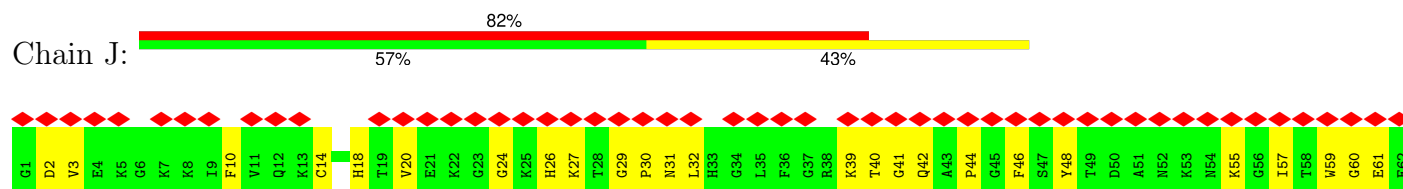
• Molecule 1: Apoptotic protease-activating factor 1



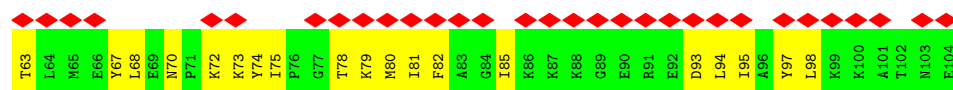
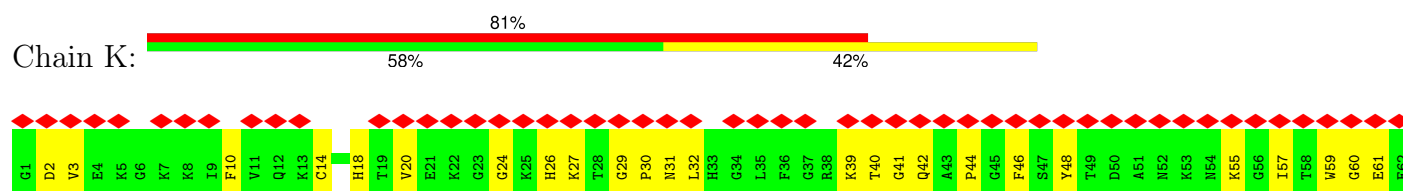




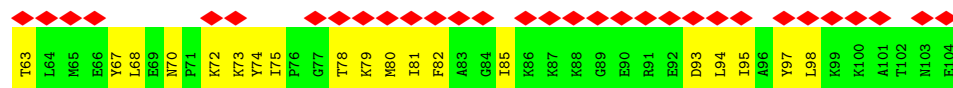
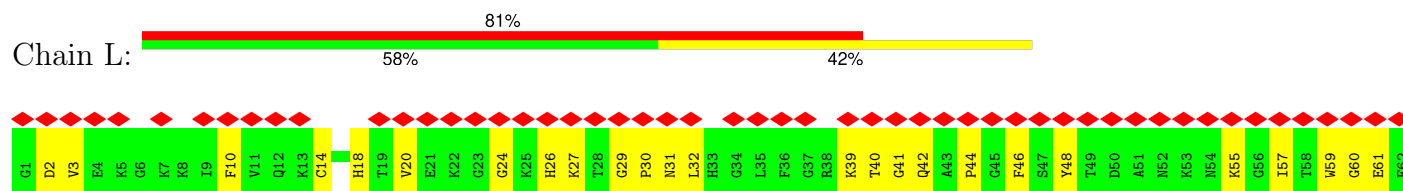
• Molecule 2: Cytochrome c



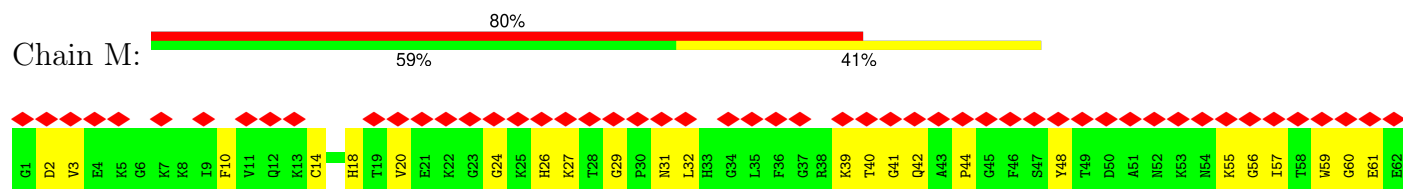
• Molecule 2: Cytochrome c

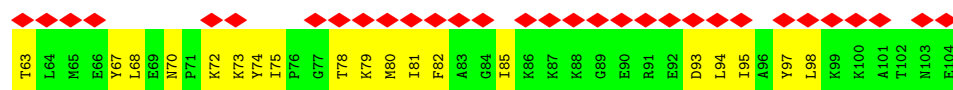


• Molecule 2: Cytochrome c

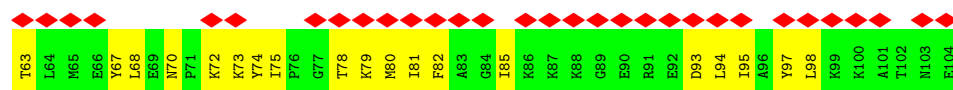
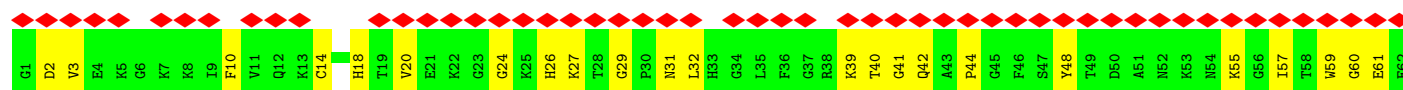
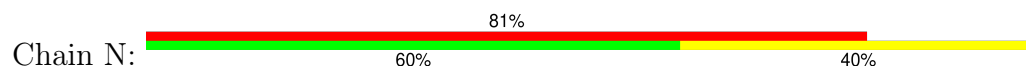


• Molecule 2: Cytochrome c

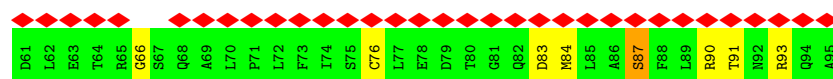
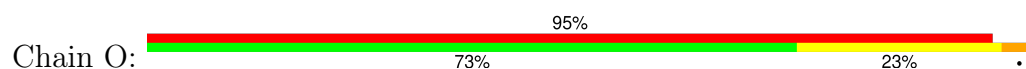




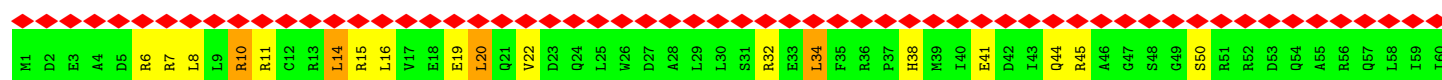
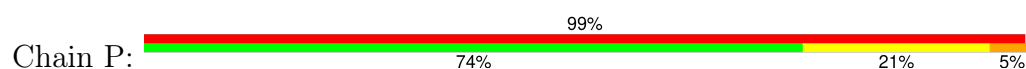
• Molecule 2: Cytochrome c



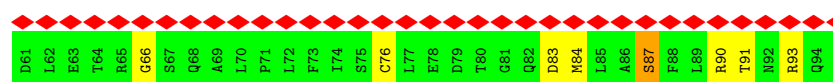
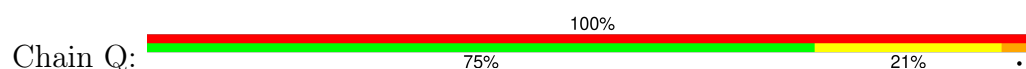
• Molecule 3: Caspase-9



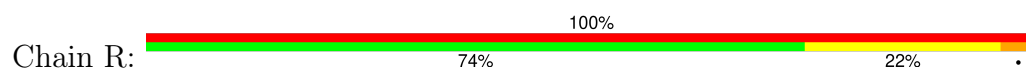
• Molecule 3: Caspase-9



• Molecule 3: Caspase-9



• Molecule 3: Caspase-9





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	92867	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	437.76, 437.76, 437.76	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.368, 1.368, 1.368	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.42	1/9295 (0.0%)	0.80	14/12575 (0.1%)
1	B	0.49	1/10068 (0.0%)	0.80	14/13613 (0.1%)
1	C	0.42	1/9295 (0.0%)	0.80	14/12575 (0.1%)
1	D	0.48	1/10068 (0.0%)	0.80	14/13613 (0.1%)
1	E	0.49	1/10068 (0.0%)	0.80	14/13613 (0.1%)
1	F	0.42	1/9295 (0.0%)	0.80	14/12575 (0.1%)
1	G	0.49	1/10068 (0.0%)	0.80	14/13613 (0.1%)
2	H	0.31	0/830	0.73	0/1105
2	I	0.31	0/830	0.73	0/1105
2	J	0.31	0/830	0.73	0/1105
2	K	0.31	0/830	0.73	0/1105
2	L	0.31	0/830	0.73	0/1105
2	M	0.31	0/830	0.73	0/1105
2	N	0.31	0/830	0.73	0/1105
3	O	0.87	0/784	0.88	2/1051 (0.2%)
3	P	0.87	0/784	0.88	2/1051 (0.2%)
3	Q	0.87	0/784	0.88	1/1051 (0.1%)
3	R	0.87	0/784	0.88	2/1051 (0.2%)
All	All	0.47	7/77103 (0.0%)	0.80	105/104116 (0.1%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	G	0	1
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	168	VAL	C-N	11.07	1.50	1.33
1	B	168	VAL	C-N	11.04	1.50	1.33
1	A	168	VAL	C-N	11.04	1.50	1.33
1	E	168	VAL	C-N	11.04	1.50	1.33
1	D	168	VAL	C-N	11.02	1.50	1.33
1	G	168	VAL	C-N	11.00	1.50	1.33
1	C	168	VAL	C-N	10.99	1.50	1.33

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	178	PHE	CA-C-N	-8.62	112.95	121.65
1	G	178	PHE	C-N-CA	-8.62	112.95	121.65
1	E	178	PHE	CA-C-N	-8.60	112.97	121.65
1	E	178	PHE	C-N-CA	-8.60	112.97	121.65
1	B	178	PHE	CA-C-N	-8.58	112.98	121.65
1	B	178	PHE	C-N-CA	-8.58	112.98	121.65
1	A	178	PHE	CA-C-N	-8.55	113.01	121.65
1	A	178	PHE	C-N-CA	-8.55	113.01	121.65
1	C	178	PHE	CA-C-N	-8.54	113.02	121.65
1	C	178	PHE	C-N-CA	-8.54	113.02	121.65
1	F	178	PHE	CA-C-N	-8.54	113.03	121.65
1	F	178	PHE	C-N-CA	-8.54	113.03	121.65
1	D	178	PHE	CA-C-N	-8.52	113.04	121.65
1	D	178	PHE	C-N-CA	-8.52	113.04	121.65
1	G	146	GLU	CA-C-N	-8.40	111.37	119.85
1	G	146	GLU	C-N-CA	-8.40	111.37	119.85
1	F	146	GLU	CA-C-N	-8.39	111.38	119.85
1	F	146	GLU	C-N-CA	-8.39	111.38	119.85
1	E	146	GLU	CA-C-N	-8.38	111.38	119.85
1	E	146	GLU	C-N-CA	-8.38	111.38	119.85
1	B	146	GLU	CA-C-N	-8.34	111.42	119.85
1	B	146	GLU	C-N-CA	-8.34	111.42	119.85
1	A	146	GLU	CA-C-N	-8.34	111.43	119.85
1	A	146	GLU	C-N-CA	-8.34	111.43	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	GLU	CA-C-N	-8.30	111.46	119.85
1	C	146	GLU	C-N-CA	-8.30	111.46	119.85
1	D	146	GLU	CA-C-N	-8.29	111.48	119.85
1	D	146	GLU	C-N-CA	-8.29	111.48	119.85
1	D	117	GLY	N-CA-C	-6.58	105.44	114.64
1	C	117	GLY	N-CA-C	-6.57	105.44	114.64
1	G	117	GLY	N-CA-C	-6.57	105.44	114.64
1	A	117	GLY	N-CA-C	-6.56	105.45	114.64
1	B	117	GLY	N-CA-C	-6.55	105.47	114.64
1	E	117	GLY	N-CA-C	-6.55	105.47	114.64
1	F	117	GLY	N-CA-C	-6.54	105.48	114.64
1	E	883	SER	N-CA-C	6.28	118.49	109.14
1	G	883	SER	N-CA-C	6.26	118.47	109.14
1	D	883	SER	N-CA-C	6.25	118.46	109.14
1	A	883	SER	N-CA-C	6.25	118.45	109.14
1	B	883	SER	N-CA-C	6.25	118.45	109.14
1	C	883	SER	N-CA-C	6.23	118.43	109.14
1	F	883	SER	N-CA-C	6.22	118.41	109.14
1	F	518	GLY	CA-C-N	6.20	125.61	118.85
1	F	518	GLY	C-N-CA	6.20	125.61	118.85
1	E	518	GLY	CA-C-N	6.20	125.61	118.85
1	E	518	GLY	C-N-CA	6.20	125.61	118.85
1	D	518	GLY	CA-C-N	6.19	125.60	118.85
1	D	518	GLY	C-N-CA	6.19	125.60	118.85
1	G	518	GLY	CA-C-N	6.18	125.58	118.85
1	G	518	GLY	C-N-CA	6.18	125.58	118.85
1	A	518	GLY	CA-C-N	6.17	125.58	118.85
1	A	518	GLY	C-N-CA	6.17	125.58	118.85
1	B	518	GLY	CA-C-N	6.14	125.54	118.85
1	B	518	GLY	C-N-CA	6.14	125.54	118.85
1	C	518	GLY	CA-C-N	6.14	125.54	118.85
1	C	518	GLY	C-N-CA	6.14	125.54	118.85
1	C	246	TRP	N-CA-C	6.01	119.09	111.69
1	F	246	TRP	N-CA-C	6.01	119.09	111.69
1	B	246	TRP	N-CA-C	6.00	119.07	111.69
1	A	246	TRP	N-CA-C	5.99	119.05	111.69
1	D	246	TRP	N-CA-C	5.99	119.05	111.69
1	G	246	TRP	N-CA-C	5.97	119.03	111.69
1	E	246	TRP	N-CA-C	5.97	119.03	111.69
3	R	66	GLY	N-CA-C	5.65	117.84	111.85
1	D	168	VAL	O-C-N	-5.64	115.52	122.57
1	C	886	HIS	N-CA-C	-5.64	105.21	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	886	HIS	N-CA-C	-5.64	105.22	111.36
1	A	886	HIS	N-CA-C	-5.63	105.23	111.36
1	F	886	HIS	N-CA-C	-5.63	105.23	111.36
1	A	168	VAL	O-C-N	-5.62	115.55	122.57
1	E	168	VAL	O-C-N	-5.62	115.55	122.57
1	F	168	VAL	O-C-N	-5.62	115.55	122.57
1	E	886	HIS	N-CA-C	-5.62	105.24	111.36
1	B	168	VAL	O-C-N	-5.62	115.55	122.57
1	B	886	HIS	N-CA-C	-5.62	105.24	111.36
1	G	168	VAL	O-C-N	-5.62	115.55	122.57
3	O	66	GLY	N-CA-C	5.60	117.79	111.85
1	C	168	VAL	O-C-N	-5.59	115.58	122.57
1	D	886	HIS	N-CA-C	-5.58	105.27	111.36
3	Q	66	GLY	N-CA-C	5.57	117.76	111.85
3	P	66	GLY	N-CA-C	5.54	117.72	111.85
1	G	589	ASP	N-CA-C	-5.30	105.45	112.24
1	F	589	ASP	N-CA-C	-5.29	105.46	112.24
1	B	589	ASP	N-CA-C	-5.29	105.46	112.24
1	C	589	ASP	N-CA-C	-5.29	105.47	112.24
1	A	589	ASP	N-CA-C	-5.29	105.47	112.24
1	E	589	ASP	N-CA-C	-5.29	105.47	112.24
1	D	589	ASP	N-CA-C	-5.26	105.51	112.24
3	O	22	VAL	N-CA-C	5.23	116.31	111.81
3	R	22	VAL	N-CA-C	5.23	116.31	111.81
3	P	22	VAL	N-CA-C	5.18	116.27	111.81
1	G	379	ILE	CA-C-N	5.13	127.87	120.38
1	G	379	ILE	C-N-CA	5.13	127.87	120.38
1	D	379	ILE	CA-C-N	5.13	127.86	120.38
1	D	379	ILE	C-N-CA	5.13	127.86	120.38
1	E	379	ILE	CA-C-N	5.12	127.86	120.38
1	E	379	ILE	C-N-CA	5.12	127.86	120.38
1	A	379	ILE	CA-C-N	5.12	127.85	120.38
1	A	379	ILE	C-N-CA	5.12	127.85	120.38
1	C	379	ILE	CA-C-N	5.11	127.84	120.38
1	C	379	ILE	C-N-CA	5.11	127.84	120.38
1	B	379	ILE	CA-C-N	5.11	127.84	120.38
1	B	379	ILE	C-N-CA	5.11	127.84	120.38
1	F	379	ILE	CA-C-N	5.10	127.83	120.38
1	F	379	ILE	C-N-CA	5.10	127.83	120.38

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ASN	Peptide
1	B	336	ASN	Peptide
1	C	336	ASN	Peptide
1	D	336	ASN	Peptide
1	E	336	ASN	Peptide
1	F	336	ASN	Peptide
1	G	336	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9099	0	8967	309	0
1	B	9861	0	9736	317	0
1	C	9099	0	8968	306	0
1	D	9861	0	9736	324	0
1	E	9861	0	9736	329	0
1	F	9099	0	8968	317	0
1	G	9861	0	9736	319	0
2	H	814	0	833	58	0
2	I	814	0	833	58	0
2	J	814	0	833	59	0
2	K	814	0	833	56	0
2	L	814	0	833	57	0
2	M	814	0	833	58	0
2	N	814	0	833	55	0
3	O	777	0	787	21	0
3	P	777	0	787	28	0
3	Q	777	0	786	39	0
3	R	777	0	787	29	0
4	A	30	0	9	3	0
4	B	30	0	9	3	0
4	C	30	0	9	3	0
4	D	30	0	9	3	0
4	E	30	0	9	3	0
4	F	30	0	9	3	0
4	G	30	0	9	3	0
5	H	43	0	32	2	0
5	I	43	0	32	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	43	0	32	2	0
5	K	43	0	32	2	0
5	L	43	0	32	2	0
5	M	43	0	32	2	0
5	N	43	0	32	2	0
All	All	76058	0	75112	2427	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (2427) 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)
3:Q:52:ARG:HD3	3:R:38:HIS:CE1	1.20	1.66
3:Q:52:ARG:CD	3:R:38:HIS:CE1	2.01	1.40
1:E:884:TRP:CH2	2:L:79:LYS:HA	1.68	1.28
1:D:884:TRP:CH2	2:K:79:LYS:HA	1.68	1.28
1:G:884:TRP:CH2	2:N:79:LYS:HA	1.68	1.28
1:A:884:TRP:CH2	2:H:79:LYS:HA	1.68	1.27
1:E:7:ASN:HB2	1:F:236:PRO:CG	1.63	1.26
1:C:884:TRP:CH2	2:J:79:LYS:HA	1.68	1.26
1:F:884:TRP:CH2	2:M:79:LYS:HA	1.68	1.26
1:B:884:TRP:CH2	2:I:79:LYS:HA	1.68	1.26
1:C:884:TRP:CZ3	2:J:79:LYS:HD2	1.74	1.22
1:B:884:TRP:CZ3	2:I:79:LYS:HD2	1.74	1.22
1:D:884:TRP:CZ3	2:K:79:LYS:HD2	1.74	1.21
1:A:884:TRP:CZ3	2:H:79:LYS:HD2	1.74	1.21
1:E:884:TRP:CZ3	2:L:79:LYS:HD2	1.74	1.21
1:F:884:TRP:CZ3	2:M:79:LYS:HD2	1.74	1.21
1:G:884:TRP:CZ3	2:N:79:LYS:HD2	1.74	1.21
1:B:884:TRP:CZ3	2:I:79:LYS:HA	1.82	1.15
1:A:884:TRP:CZ3	2:H:79:LYS:HA	1.82	1.15
1:C:884:TRP:CZ3	2:J:79:LYS:HA	1.82	1.15
1:G:884:TRP:CZ3	2:N:79:LYS:HA	1.81	1.14
1:D:884:TRP:CZ3	2:K:79:LYS:HA	1.82	1.14
1:E:884:TRP:CZ3	2:L:79:LYS:HA	1.82	1.14
1:F:884:TRP:CZ3	2:M:79:LYS:HA	1.82	1.13
1:F:1086:GLY:HA2	2:M:39:LYS:HZ1	1.16	1.11
1:E:7:ASN:HB2	1:F:236:PRO:HG3	1.28	1.10
1:G:1086:GLY:HA2	2:N:39:LYS:HZ1	1.22	1.04
1:E:7:ASN:HB2	1:F:236:PRO:HG2	1.36	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1086:GLY:HA2	2:L:39:LYS:HZ1	1.20	1.01
1:G:569:CYS:SG	1:G:1213:PHE:HE1	1.85	0.99
1:A:565:GLN:NE2	1:A:1213:PHE:H	1.60	0.99
1:F:569:CYS:SG	1:F:1213:PHE:CE1	2.56	0.99
1:B:569:CYS:SG	1:B:600:LYS:NZ	2.36	0.99
1:C:565:GLN:NE2	1:C:1213:PHE:H	1.60	0.99
1:G:569:CYS:SG	1:G:1213:PHE:CE1	2.56	0.99
1:D:569:CYS:SG	1:D:1213:PHE:HE1	1.85	0.99
1:E:569:CYS:SG	1:E:600:LYS:NZ	2.36	0.99
1:F:569:CYS:SG	1:F:600:LYS:NZ	2.36	0.99
1:B:569:CYS:SG	1:B:1213:PHE:CE1	2.56	0.99
1:B:569:CYS:SG	1:B:1213:PHE:HE1	1.85	0.99
1:E:565:GLN:CD	1:E:1213:PHE:H	1.71	0.99
1:F:565:GLN:CD	1:F:1213:PHE:H	1.71	0.99
1:C:569:CYS:SG	1:C:1213:PHE:CE1	2.56	0.99
1:C:569:CYS:SG	1:C:1213:PHE:HE1	1.85	0.99
1:C:569:CYS:SG	1:C:600:LYS:NZ	2.36	0.99
1:E:569:CYS:SG	1:E:1213:PHE:CE1	2.56	0.99
1:G:569:CYS:SG	1:G:600:LYS:NZ	2.36	0.99
1:A:569:CYS:SG	1:A:1213:PHE:CE1	2.56	0.99
1:B:565:GLN:NE2	1:B:1213:PHE:H	1.60	0.99
1:D:565:GLN:CD	1:D:1213:PHE:H	1.71	0.99
1:F:569:CYS:SG	1:F:1213:PHE:HE1	1.85	0.99
1:G:565:GLN:CD	1:G:1213:PHE:H	1.71	0.98
1:E:569:CYS:SG	1:E:1213:PHE:HE1	1.85	0.98
1:G:565:GLN:NE2	1:G:1213:PHE:H	1.60	0.98
1:G:884:TRP:HH2	2:N:79:LYS:HA	1.28	0.98
1:D:569:CYS:SG	1:D:1213:PHE:CE1	2.56	0.98
1:C:565:GLN:CD	1:C:1213:PHE:H	1.71	0.98
1:A:569:CYS:SG	1:A:1213:PHE:HE1	1.85	0.98
1:A:569:CYS:SG	1:A:600:LYS:NZ	2.36	0.98
1:C:1086:GLY:HA2	2:J:39:LYS:HZ1	1.27	0.98
1:A:565:GLN:CD	1:A:1213:PHE:H	1.71	0.98
1:B:565:GLN:CD	1:B:1213:PHE:H	1.71	0.97
1:E:565:GLN:NE2	1:E:1213:PHE:H	1.60	0.97
1:D:569:CYS:SG	1:D:600:LYS:NZ	2.36	0.97
1:F:565:GLN:NE2	1:F:1213:PHE:H	1.60	0.97
1:A:109:TYR:HE1	1:G:4:LYS:NZ	1.34	0.97
1:A:884:TRP:HH2	2:H:79:LYS:HA	1.28	0.97
1:D:565:GLN:NE2	1:D:1213:PHE:H	1.60	0.97
3:O:52:ARG:CB	3:P:38:HIS:CE1	2.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:52:ARG:HD3	3:R:38:HIS:ND1	1.79	0.96
1:E:884:TRP:HH2	2:L:79:LYS:HA	1.28	0.95
1:E:7:ASN:CB	1:F:236:PRO:HG2	1.97	0.94
1:D:884:TRP:HH2	2:K:79:LYS:HA	1.28	0.93
1:C:884:TRP:HH2	2:J:79:LYS:HA	1.28	0.93
1:B:1086:GLY:HA2	2:I:39:LYS:HZ1	1.30	0.93
1:D:30:ILE:CG2	3:Q:10:ARG:HB3	1.97	0.93
1:F:884:TRP:HH2	2:M:79:LYS:HA	1.28	0.93
1:E:7:ASN:CB	1:F:236:PRO:CG	2.46	0.92
1:E:550:LEU:CD2	1:E:607:SER:HB2	2.00	0.92
1:G:550:LEU:CD2	1:G:607:SER:HB2	2.00	0.92
1:B:884:TRP:HH2	2:I:79:LYS:HA	1.28	0.92
1:B:550:LEU:CD2	1:B:607:SER:HB2	2.00	0.92
1:F:550:LEU:CD2	1:F:607:SER:HB2	2.00	0.92
1:D:1086:GLY:HA2	2:K:39:LYS:HZ1	1.32	0.92
1:A:550:LEU:CD2	1:A:607:SER:HB2	2.00	0.91
1:A:1086:GLY:HA2	2:H:39:LYS:HZ1	1.32	0.91
1:D:524:HIS:HB2	1:D:646:THR:HG21	1.52	0.91
1:C:550:LEU:CD2	1:C:607:SER:HB2	2.00	0.91
1:C:1086:GLY:HA2	2:J:39:LYS:NZ	1.85	0.91
1:B:1086:GLY:HA2	2:I:39:LYS:NZ	1.86	0.91
1:C:524:HIS:HB2	1:C:646:THR:HG21	1.52	0.91
1:D:1086:GLY:HA2	2:K:39:LYS:NZ	1.85	0.91
1:A:1086:GLY:HA2	2:H:39:LYS:NZ	1.86	0.90
3:O:52:ARG:HB2	3:P:38:HIS:CE1	2.06	0.90
1:E:524:HIS:HB2	1:E:646:THR:HG21	1.52	0.90
1:D:550:LEU:CD2	1:D:607:SER:HB2	2.00	0.90
3:O:52:ARG:HB3	3:P:38:HIS:CE1	2.07	0.90
1:B:524:HIS:HB2	1:B:646:THR:HG21	1.52	0.90
1:E:1086:GLY:HA2	2:L:39:LYS:NZ	1.85	0.90
1:G:1086:GLY:HA2	2:N:39:LYS:NZ	1.85	0.90
1:G:524:HIS:HB2	1:G:646:THR:HG21	1.52	0.89
1:F:1086:GLY:HA2	2:M:39:LYS:NZ	1.85	0.89
1:A:524:HIS:HB2	1:A:646:THR:HG21	1.52	0.89
1:F:524:HIS:HB2	1:F:646:THR:HG21	1.52	0.88
1:F:884:TRP:CZ3	2:M:79:LYS:CD	2.57	0.88
1:B:884:TRP:CZ3	2:I:79:LYS:CD	2.57	0.88
1:A:884:TRP:CZ3	2:H:79:LYS:CD	2.57	0.88
1:E:884:TRP:CZ3	2:L:79:LYS:CD	2.57	0.88
1:C:884:TRP:CZ3	2:J:79:LYS:CD	2.57	0.87
1:A:109:TYR:CE1	1:G:4:LYS:NZ	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:884:TRP:CZ3	2:K:79:LYS:CD	2.57	0.87
1:A:109:TYR:CE1	1:G:4:LYS:HD2	2.11	0.86
3:Q:52:ARG:CD	3:R:38:HIS:HE1	1.89	0.86
3:Q:52:ARG:CB	3:R:38:HIS:HE1	1.88	0.86
3:P:50:SER:CB	3:Q:45:ARG:HH12	1.89	0.85
1:A:884:TRP:CH2	2:H:79:LYS:CA	2.59	0.85
3:Q:52:ARG:HD3	3:R:38:HIS:NE2	1.88	0.85
1:B:884:TRP:CH2	2:I:79:LYS:CA	2.59	0.85
1:E:885:VAL:HG11	1:E:888:VAL:HG13	1.59	0.85
1:G:885:VAL:HG11	1:G:888:VAL:HG13	1.59	0.85
1:G:884:TRP:CH2	2:N:79:LYS:CA	2.59	0.85
1:G:884:TRP:CZ3	2:N:79:LYS:CD	2.57	0.85
1:A:885:VAL:HG11	1:A:888:VAL:HG13	1.59	0.85
1:D:885:VAL:HG11	1:D:888:VAL:HG13	1.59	0.85
1:F:885:VAL:HG11	1:F:888:VAL:HG13	1.59	0.85
1:B:882:LEU:HB2	1:B:903:ASP:HB3	1.59	0.84
1:A:882:LEU:HB2	1:A:903:ASP:HB3	1.59	0.84
1:B:885:VAL:HG11	1:B:888:VAL:HG13	1.59	0.84
1:C:884:TRP:CH2	2:J:79:LYS:CA	2.58	0.84
1:G:550:LEU:HD21	1:G:607:SER:HB2	1.60	0.84
1:C:885:VAL:HG11	1:C:888:VAL:HG13	1.59	0.84
1:A:550:LEU:HD21	1:A:607:SER:HB2	1.60	0.83
1:F:884:TRP:CH2	2:M:79:LYS:CA	2.59	0.83
1:F:550:LEU:HD21	1:F:607:SER:HB2	1.60	0.83
1:G:882:LEU:HB2	1:G:903:ASP:HB3	1.59	0.83
1:C:882:LEU:HB2	1:C:903:ASP:HB3	1.59	0.83
1:F:565:GLN:NE2	1:F:1213:PHE:N	2.27	0.82
1:C:550:LEU:HD21	1:C:607:SER:HB2	1.60	0.82
1:E:550:LEU:HD21	1:E:607:SER:HB2	1.60	0.82
1:B:565:GLN:NE2	1:B:1213:PHE:N	2.27	0.82
1:E:565:GLN:NE2	1:E:1213:PHE:N	2.27	0.82
1:E:882:LEU:HB2	1:E:903:ASP:HB3	1.59	0.82
1:B:550:LEU:HD21	1:B:607:SER:HB2	1.60	0.82
1:D:358:SER:HB3	1:E:274:MET:HE2	1.62	0.82
1:D:550:LEU:HD21	1:D:607:SER:HB2	1.60	0.82
1:A:565:GLN:NE2	1:A:1213:PHE:N	2.27	0.82
1:C:565:GLN:NE2	1:C:1213:PHE:N	2.27	0.82
1:F:882:LEU:HB2	1:F:903:ASP:HB3	1.59	0.82
1:D:565:GLN:NE2	1:D:1213:PHE:N	2.27	0.81
1:F:1086:GLY:CA	2:M:39:LYS:HZ1	1.91	0.81
1:D:884:TRP:CH2	2:K:79:LYS:CA	2.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:MET:HE2	1:G:358:SER:HB3	1.62	0.81
1:G:565:GLN:NE2	1:G:1213:PHE:N	2.27	0.81
1:G:584:ALA:HA	1:G:594:TYR:CE2	2.16	0.81
1:E:584:ALA:HA	1:E:594:TYR:CE2	2.16	0.81
1:D:882:LEU:HB2	1:D:903:ASP:HB3	1.59	0.81
1:D:584:ALA:HA	1:D:594:TYR:CE2	2.16	0.81
1:E:358:SER:HB3	1:F:274:MET:HE2	1.63	0.81
1:A:862:TYR:CA	1:A:884:TRP:HA	2.11	0.80
1:B:584:ALA:HA	1:B:594:TYR:CE2	2.16	0.80
1:F:584:ALA:HA	1:F:594:TYR:CE2	2.16	0.80
1:F:862:TYR:CA	1:F:884:TRP:HA	2.11	0.80
1:B:358:SER:HB3	1:C:274:MET:HE2	1.64	0.80
1:C:862:TYR:HA	1:C:884:TRP:HA	1.63	0.80
1:E:7:ASN:CG	1:F:236:PRO:HG2	2.06	0.80
1:E:862:TYR:CA	1:E:884:TRP:HA	2.11	0.80
1:E:884:TRP:CH2	2:L:79:LYS:CA	2.59	0.80
1:A:584:ALA:HA	1:A:594:TYR:CE2	2.16	0.80
1:B:862:TYR:HA	1:B:884:TRP:HA	1.63	0.80
1:D:862:TYR:HA	1:D:884:TRP:HA	1.63	0.80
1:E:862:TYR:HA	1:E:884:TRP:HA	1.63	0.80
1:C:358:SER:HB3	1:D:274:MET:HE2	1.64	0.80
1:E:7:ASN:CB	1:F:236:PRO:HG3	2.11	0.80
1:A:862:TYR:HA	1:A:884:TRP:HA	1.63	0.80
3:Q:52:ARG:CD	3:R:38:HIS:ND1	2.40	0.80
1:D:862:TYR:CA	1:D:884:TRP:HA	2.11	0.79
1:E:6:ARG:NH2	1:F:232:LEU:O	2.15	0.79
1:G:862:TYR:CA	1:G:884:TRP:HA	2.11	0.79
1:F:862:TYR:HA	1:F:884:TRP:HA	1.64	0.79
1:F:882:LEU:HD13	1:F:1176:HIS:NE2	1.98	0.79
3:O:15:ARG:CD	3:O:19:GLU:OE2	2.30	0.79
1:A:358:SER:HB3	1:B:274:MET:HE2	1.64	0.79
1:B:862:TYR:CA	1:B:884:TRP:HA	2.11	0.79
1:C:584:ALA:HA	1:C:594:TYR:CE2	2.16	0.79
1:B:882:LEU:HD13	1:B:1176:HIS:NE2	1.98	0.79
1:E:1084:HIS:HE2	1:E:1108:THR:HG1	1.30	0.79
1:G:862:TYR:HA	1:G:884:TRP:HA	1.63	0.79
3:Q:15:ARG:CD	3:Q:19:GLU:OE2	2.30	0.79
1:C:862:TYR:CA	1:C:884:TRP:HA	2.11	0.79
3:P:15:ARG:CD	3:P:19:GLU:OE2	2.30	0.79
3:R:15:ARG:CD	3:R:19:GLU:OE2	2.30	0.79
1:C:1084:HIS:HE2	1:C:1108:THR:HG1	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:882:LEU:HD13	1:D:1176:HIS:NE2	1.98	0.78
1:C:882:LEU:HD13	1:C:1176:HIS:NE2	1.98	0.78
1:E:1086:GLY:CA	2:L:39:LYS:HZ1	1.96	0.78
1:F:1084:HIS:HE2	1:F:1108:THR:HG1	1.30	0.78
1:A:882:LEU:HD13	1:A:1176:HIS:NE2	1.98	0.78
1:G:882:LEU:HD13	1:G:1176:HIS:NE2	1.98	0.78
1:E:882:LEU:HD13	1:E:1176:HIS:NE2	1.98	0.77
3:P:50:SER:HB2	3:Q:45:ARG:HH12	1.48	0.77
1:D:1084:HIS:HE2	1:D:1108:THR:HG1	1.30	0.77
1:A:565:GLN:HE22	1:A:1213:PHE:H	1.33	0.77
1:E:349:GLN:HA	1:E:447:GLU:OE2	1.86	0.76
1:A:349:GLN:HA	1:A:447:GLU:OE2	1.85	0.76
1:B:884:TRP:HH2	2:I:79:LYS:CA	1.97	0.76
1:B:349:GLN:HA	1:B:447:GLU:OE2	1.85	0.76
1:F:884:TRP:HH2	2:M:79:LYS:CA	1.97	0.76
1:G:47:PRO:HG2	1:G:51:GLN:HE22	1.51	0.76
1:G:1086:GLY:CA	2:N:39:LYS:HZ1	1.98	0.76
1:C:565:GLN:HE22	1:C:1213:PHE:H	1.33	0.76
1:G:884:TRP:HH2	2:N:79:LYS:CA	1.97	0.76
1:F:349:GLN:HA	1:F:447:GLU:OE2	1.85	0.76
1:E:47:PRO:HG2	1:E:51:GLN:HE22	1.51	0.76
1:B:565:GLN:HE22	1:B:1213:PHE:H	1.33	0.75
1:D:349:GLN:HA	1:D:447:GLU:OE2	1.85	0.75
1:C:1112:TRP:HB3	1:C:1119:PRO:HA	1.68	0.75
1:A:882:LEU:CD1	1:A:1176:HIS:NE2	2.50	0.75
3:Q:7:ARG:O	3:Q:11:ARG:HG3	1.87	0.75
1:A:557:ARG:NH2	1:A:1175:THR:HG23	2.02	0.75
1:E:882:LEU:CD1	1:E:1176:HIS:NE2	2.50	0.75
1:G:882:LEU:CD1	1:G:1176:HIS:NE2	2.50	0.75
1:A:1084:HIS:HE2	1:A:1108:THR:HG1	1.31	0.75
1:B:47:PRO:HG2	1:B:51:GLN:HE22	1.51	0.75
1:B:557:ARG:NH2	1:B:1175:THR:HG23	2.01	0.75
1:E:884:TRP:HH2	2:L:79:LYS:CA	1.97	0.75
1:C:349:GLN:HA	1:C:447:GLU:OE2	1.85	0.75
1:D:1112:TRP:HB3	1:D:1119:PRO:HA	1.68	0.75
1:F:358:SER:HB3	1:G:274:MET:HE2	1.69	0.75
3:R:7:ARG:O	3:R:11:ARG:HG3	1.87	0.75
1:B:882:LEU:CD1	1:B:1176:HIS:NE2	2.50	0.75
1:F:882:LEU:CD1	1:F:1176:HIS:NE2	2.50	0.75
2:N:24:GLY:O	2:N:31:ASN:ND2	2.20	0.75
1:D:404:TRP:HB3	1:D:406:MET:HE3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1112:TRP:HB3	1:E:1119:PRO:HA	1.68	0.75
1:F:1112:TRP:HB3	1:F:1119:PRO:HA	1.68	0.74
1:G:565:GLN:HE22	1:G:1213:PHE:H	1.33	0.74
2:H:24:GLY:O	2:H:31:ASN:ND2	2.20	0.74
1:B:884:TRP:HZ3	2:I:79:LYS:HD2	1.51	0.74
1:D:309:GLN:NE2	1:D:339:GLU:OE1	2.21	0.74
1:E:309:GLN:NE2	1:E:339:GLU:OE1	2.21	0.74
1:F:557:ARG:NH2	1:F:1175:THR:HG23	2.01	0.74
1:G:349:GLN:HA	1:G:447:GLU:OE2	1.85	0.74
1:G:557:ARG:NH2	1:G:1175:THR:HG23	2.01	0.74
3:P:7:ARG:O	3:P:11:ARG:HG3	1.87	0.74
1:B:339:GLU:OE2	1:B:343:LYS:NZ	2.20	0.74
1:C:404:TRP:HB3	1:C:406:MET:HE3	1.69	0.74
1:F:941:ASP:H	1:F:946:LEU:HA	1.53	0.74
1:A:884:TRP:HH2	2:H:79:LYS:CA	1.97	0.74
1:C:309:GLN:NE2	1:C:339:GLU:OE1	2.21	0.74
1:D:882:LEU:CD1	1:D:1176:HIS:NE2	2.50	0.74
1:F:309:GLN:NE2	1:F:339:GLU:OE1	2.21	0.74
1:A:1112:TRP:HB3	1:A:1119:PRO:HA	1.68	0.74
1:C:339:GLU:OE2	1:C:343:LYS:NZ	2.20	0.74
1:E:404:TRP:HB3	1:E:406:MET:HE3	1.69	0.74
2:L:24:GLY:O	2:L:31:ASN:ND2	2.20	0.74
1:C:557:ARG:NH2	1:C:1175:THR:HG23	2.01	0.74
1:C:882:LEU:CD1	1:C:1176:HIS:NE2	2.50	0.74
1:D:47:PRO:HG2	1:D:51:GLN:HE22	1.51	0.74
1:D:557:ARG:NH2	1:D:1175:THR:HG23	2.01	0.74
1:D:941:ASP:H	1:D:946:LEU:HA	1.53	0.74
1:F:565:GLN:HE22	1:F:1213:PHE:H	1.33	0.74
2:I:24:GLY:O	2:I:31:ASN:ND2	2.20	0.74
1:C:884:TRP:HH2	2:J:79:LYS:CA	1.97	0.74
1:C:941:ASP:H	1:C:946:LEU:HA	1.53	0.74
1:E:565:GLN:HE22	1:E:1213:PHE:H	1.33	0.74
1:E:884:TRP:HZ3	2:L:79:LYS:HD2	1.51	0.74
1:G:1112:TRP:HB3	1:G:1119:PRO:HA	1.68	0.74
2:K:24:GLY:O	2:K:31:ASN:ND2	2.20	0.74
2:M:24:GLY:O	2:M:31:ASN:ND2	2.20	0.74
3:Q:52:ARG:HD2	3:R:38:HIS:CE1	2.17	0.74
1:A:274:MET:CE	1:G:358:SER:HB3	2.17	0.74
1:B:1112:TRP:HB3	1:B:1119:PRO:HA	1.68	0.74
1:D:339:GLU:OE2	1:D:343:LYS:NZ	2.20	0.73
1:G:941:ASP:H	1:G:946:LEU:HA	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:7:ARG:O	3:O:11:ARG:HG3	1.87	0.73
1:D:884:TRP:HH2	2:K:79:LYS:CA	1.97	0.73
1:E:557:ARG:NH2	1:E:1175:THR:HG23	2.01	0.73
2:J:24:GLY:O	2:J:31:ASN:ND2	2.20	0.73
1:A:309:GLN:NE2	1:A:339:GLU:OE1	2.21	0.73
1:C:590:ASN:C	1:C:592:MET:H	1.97	0.73
1:B:309:GLN:NE2	1:B:339:GLU:OE1	2.21	0.73
1:B:404:TRP:HB3	1:B:406:MET:HE3	1.69	0.73
1:C:884:TRP:HZ3	2:J:79:LYS:HD2	1.51	0.73
1:E:339:GLU:OE2	1:E:343:LYS:NZ	2.20	0.73
1:G:309:GLN:NE2	1:G:339:GLU:OE1	2.21	0.73
3:Q:52:ARG:CB	3:R:38:HIS:CE1	2.72	0.73
1:B:590:ASN:C	1:B:592:MET:H	1.97	0.73
1:A:339:GLU:OE2	1:A:343:LYS:NZ	2.20	0.73
1:D:590:ASN:C	1:D:592:MET:H	1.97	0.73
1:D:884:TRP:HZ3	2:K:79:LYS:HD2	1.52	0.73
3:R:87:SER:O	3:R:91:THR:HG23	1.89	0.73
1:B:1084:HIS:HE2	1:B:1108:THR:HG1	1.34	0.73
1:F:404:TRP:HB3	1:F:406:MET:HE3	1.69	0.72
3:Q:87:SER:O	3:Q:91:THR:HG23	1.89	0.72
1:A:404:TRP:HB3	1:A:406:MET:HE3	1.69	0.72
1:E:941:ASP:H	1:E:946:LEU:HA	1.53	0.72
1:G:339:GLU:OE2	1:G:343:LYS:NZ	2.20	0.72
1:A:941:ASP:H	1:A:946:LEU:HA	1.53	0.72
1:C:358:SER:HB3	1:D:274:MET:CE	2.19	0.72
1:B:941:ASP:H	1:B:946:LEU:HA	1.53	0.72
3:P:87:SER:O	3:P:91:THR:HG23	1.89	0.72
1:G:404:TRP:HB3	1:G:406:MET:HE3	1.69	0.72
1:B:609:LEU:HB3	1:B:908:LEU:HB2	1.71	0.72
1:C:609:LEU:HB3	1:C:908:LEU:HB2	1.71	0.72
1:D:565:GLN:HE22	1:D:1213:PHE:H	1.33	0.72
2:K:26:HIS:NE2	2:K:44:PRO:O	2.23	0.72
1:E:565:GLN:CD	1:E:1213:PHE:N	2.48	0.72
1:A:590:ASN:C	1:A:592:MET:H	1.97	0.71
1:B:882:LEU:HB2	1:B:903:ASP:CB	2.20	0.71
1:F:339:GLU:OE2	1:F:343:LYS:NZ	2.20	0.71
1:G:882:LEU:HB2	1:G:903:ASP:CB	2.20	0.71
1:G:1084:HIS:HE2	1:G:1108:THR:HG1	1.35	0.71
2:I:26:HIS:NE2	2:I:44:PRO:O	2.23	0.71
1:D:609:LEU:HB3	1:D:908:LEU:HB2	1.71	0.71
1:E:590:ASN:C	1:E:592:MET:H	1.97	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:26:HIS:NE2	2:H:44:PRO:O	2.23	0.71
2:J:26:HIS:NE2	2:J:44:PRO:O	2.23	0.71
2:L:26:HIS:NE2	2:L:44:PRO:O	2.23	0.71
1:D:565:GLN:CD	1:D:1213:PHE:N	2.48	0.71
1:D:1034:LEU:HB3	1:D:1036:LYS:HD3	1.73	0.71
1:E:609:LEU:HB3	1:E:908:LEU:HB2	1.71	0.71
3:O:87:SER:O	3:O:91:THR:HG23	1.89	0.71
1:C:1034:LEU:HB3	1:C:1036:LYS:HD3	1.73	0.71
1:D:358:SER:HB3	1:E:274:MET:CE	2.19	0.71
2:M:26:HIS:NE2	2:M:44:PRO:O	2.23	0.71
1:A:609:LEU:HB3	1:A:908:LEU:HB2	1.71	0.71
1:F:590:ASN:C	1:F:592:MET:H	1.97	0.71
1:G:565:GLN:HE22	1:G:1213:PHE:N	1.89	0.71
1:A:1034:LEU:HB3	1:A:1036:LYS:HD3	1.73	0.71
1:D:30:ILE:HG23	3:Q:10:ARG:HB3	1.73	0.71
1:G:549:SER:O	1:G:610:VAL:HB	1.91	0.71
1:A:549:SER:O	1:A:610:VAL:HB	1.91	0.71
1:D:882:LEU:HB2	1:D:903:ASP:CB	2.20	0.71
1:E:549:SER:O	1:E:610:VAL:HB	1.91	0.71
2:N:26:HIS:NE2	2:N:44:PRO:O	2.23	0.71
3:P:41:GLU:HB3	3:P:45:ARG:HH12	1.56	0.71
1:B:28:HIS:CE1	3:P:14:LEU:HD21	2.26	0.71
1:B:346:GLN:O	1:B:348:LYS:HG3	1.91	0.71
1:B:549:SER:O	1:B:610:VAL:HB	1.91	0.71
1:B:1034:LEU:HB3	1:B:1036:LYS:HD3	1.73	0.71
1:F:609:LEU:HB3	1:F:908:LEU:HB2	1.71	0.71
1:G:1034:LEU:HB3	1:G:1036:LYS:HD3	1.73	0.71
1:C:346:GLN:O	1:C:348:LYS:HG3	1.91	0.70
1:D:47:PRO:HG2	1:D:51:GLN:NE2	2.07	0.70
1:E:882:LEU:HB2	1:E:903:ASP:CB	2.20	0.70
1:F:346:GLN:O	1:F:348:LYS:HG3	1.91	0.70
1:C:565:GLN:CD	1:C:1213:PHE:N	2.48	0.70
1:G:609:LEU:HB3	1:G:908:LEU:HB2	1.71	0.70
1:A:882:LEU:HB2	1:A:903:ASP:CB	2.20	0.70
1:C:549:SER:O	1:C:610:VAL:HB	1.91	0.70
1:D:346:GLN:O	1:D:348:LYS:HG3	1.91	0.70
1:D:403:LEU:HD13	1:D:460:ILE:HG22	1.73	0.70
1:D:569:CYS:SG	1:D:1213:PHE:CZ	2.85	0.70
1:E:47:PRO:HG2	1:E:51:GLN:NE2	2.07	0.70
1:F:549:SER:O	1:F:610:VAL:HB	1.91	0.70
1:A:569:CYS:SG	1:A:1213:PHE:CZ	2.85	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:565:GLN:HE22	1:C:1213:PHE:N	1.89	0.70
1:E:884:TRP:CE3	2:L:79:LYS:HD2	2.27	0.70
1:A:358:SER:HB3	1:B:274:MET:CE	2.20	0.70
1:E:346:GLN:O	1:E:348:LYS:HG3	1.91	0.70
1:E:1034:LEU:HB3	1:E:1036:LYS:HD3	1.73	0.70
1:E:189:LYS:NZ	1:E:374:MET:SD	2.65	0.70
1:E:403:LEU:HD13	1:E:460:ILE:HG22	1.73	0.70
1:G:569:CYS:SG	1:G:1213:PHE:CZ	2.85	0.70
1:G:590:ASN:C	1:G:592:MET:H	1.97	0.70
1:B:358:SER:HB3	1:C:274:MET:CE	2.21	0.70
1:C:403:LEU:HD13	1:C:460:ILE:HG22	1.73	0.70
1:C:569:CYS:SG	1:C:1213:PHE:CZ	2.85	0.70
1:D:189:LYS:NZ	1:D:374:MET:SD	2.65	0.70
1:D:854:LEU:HB3	1:D:866:LEU:HD11	1.74	0.70
1:A:854:LEU:HB3	1:A:866:LEU:HD11	1.74	0.70
1:G:346:GLN:O	1:G:348:LYS:HG3	1.91	0.70
1:B:565:GLN:CD	1:B:1213:PHE:N	2.48	0.70
1:C:854:LEU:HB3	1:C:866:LEU:HD11	1.74	0.70
1:C:882:LEU:HB2	1:C:903:ASP:CB	2.21	0.70
1:D:884:TRP:CE3	2:K:79:LYS:HD2	2.27	0.70
1:E:569:CYS:SG	1:E:1213:PHE:CZ	2.85	0.70
1:B:565:GLN:HE22	1:B:1213:PHE:N	1.89	0.69
1:B:884:TRP:CE3	2:I:79:LYS:HD2	2.27	0.69
1:G:854:LEU:HB3	1:G:866:LEU:HD11	1.74	0.69
1:A:346:GLN:O	1:A:348:LYS:HG3	1.91	0.69
1:A:565:GLN:CD	1:A:1213:PHE:N	2.48	0.69
1:E:854:LEU:HB3	1:E:866:LEU:HD11	1.74	0.69
1:F:882:LEU:HB2	1:F:903:ASP:CB	2.20	0.69
1:F:1034:LEU:HB3	1:F:1036:LYS:HD3	1.73	0.69
1:G:884:TRP:CE3	2:N:79:LYS:HD2	2.27	0.69
3:P:15:ARG:HD3	3:P:19:GLU:OE2	1.92	0.69
1:E:358:SER:HB3	1:F:274:MET:CE	2.21	0.69
1:G:47:PRO:HG2	1:G:51:GLN:NE2	2.07	0.69
1:A:844:GLN:HE22	2:H:79:LYS:NZ	1.91	0.69
1:B:854:LEU:HB3	1:B:866:LEU:HD11	1.74	0.69
1:E:844:GLN:HE22	2:L:79:LYS:NZ	1.91	0.69
1:B:569:CYS:SG	1:B:1213:PHE:CZ	2.85	0.69
1:C:844:GLN:HE22	2:J:79:LYS:NZ	1.91	0.69
1:D:549:SER:O	1:D:610:VAL:HB	1.91	0.69
1:G:565:GLN:CD	1:G:1213:PHE:N	2.48	0.69
3:Q:15:ARG:HD3	3:Q:19:GLU:OE2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:PRO:HG2	1:B:51:GLN:NE2	2.07	0.69
1:F:854:LEU:HB3	1:F:866:LEU:HD11	1.74	0.69
1:B:844:GLN:HE22	2:I:79:LYS:NZ	1.90	0.69
1:D:844:GLN:HE22	2:K:79:LYS:NZ	1.91	0.69
1:F:189:LYS:NZ	1:F:374:MET:SD	2.65	0.69
1:F:403:LEU:HD13	1:F:460:ILE:HG22	1.74	0.69
1:F:569:CYS:SG	1:F:1213:PHE:CZ	2.85	0.69
1:G:844:GLN:HE22	2:N:79:LYS:NZ	1.91	0.69
1:F:565:GLN:HE22	1:F:1213:PHE:N	1.89	0.68
1:B:403:LEU:HD13	1:B:460:ILE:HG22	1.73	0.68
1:F:844:GLN:HE22	2:M:79:LYS:NZ	1.91	0.68
1:A:403:LEU:HD13	1:A:460:ILE:HG22	1.73	0.68
1:B:37:ILE:HG13	3:P:10:ARG:NH1	2.08	0.68
1:C:189:LYS:NZ	1:C:374:MET:SD	2.65	0.68
1:G:403:LEU:HD13	1:G:460:ILE:HG22	1.74	0.68
2:I:61:GLU:HA	2:I:95:ILE:HG21	1.76	0.68
3:R:15:ARG:HD3	3:R:19:GLU:OE2	1.93	0.68
1:F:884:TRP:CE3	2:M:79:LYS:HD2	2.27	0.68
2:J:61:GLU:HA	2:J:95:ILE:HG21	1.76	0.68
1:B:611:VAL:HG12	1:B:613:PRO:HD3	1.75	0.68
2:H:61:GLU:HA	2:H:95:ILE:HG21	1.75	0.68
1:D:565:GLN:HE22	1:D:1213:PHE:N	1.89	0.68
1:F:611:VAL:HG12	1:F:613:PRO:HD3	1.75	0.68
1:G:611:VAL:HG12	1:G:613:PRO:HD3	1.75	0.68
1:D:1204:VAL:HG12	1:D:1205:VAL:HG23	1.76	0.68
1:F:565:GLN:CD	1:F:1213:PHE:N	2.48	0.68
1:G:189:LYS:NZ	1:G:374:MET:SD	2.65	0.68
1:E:565:GLN:HE22	1:E:1213:PHE:N	1.89	0.67
2:H:20:VAL:HG12	2:H:32:LEU:HB2	1.77	0.67
1:A:884:TRP:CE3	2:H:79:LYS:HD2	2.27	0.67
1:C:611:VAL:HG12	1:C:613:PRO:HD3	1.75	0.67
1:C:884:TRP:CE3	2:J:79:LYS:HD2	2.27	0.67
1:C:1204:VAL:HG12	1:C:1205:VAL:HG23	1.76	0.67
1:C:1086:GLY:HA2	2:J:39:LYS:CE	2.24	0.67
1:D:14:GLU:OE1	1:E:31:SER:OG	2.10	0.67
2:K:61:GLU:HA	2:K:95:ILE:HG21	1.75	0.67
2:N:61:GLU:HA	2:N:95:ILE:HG21	1.75	0.67
3:O:15:ARG:HD3	3:O:19:GLU:OE2	1.93	0.67
3:O:52:ARG:CB	3:P:38:HIS:HE1	2.07	0.67
2:I:20:VAL:HG12	2:I:32:LEU:HB2	1.77	0.67
1:E:1204:VAL:HG12	1:E:1205:VAL:HG23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:20:VAL:HG12	2:N:32:LEU:HB2	1.77	0.67
1:B:1086:GLY:HA2	2:I:39:LYS:CE	2.24	0.67
1:A:189:LYS:NZ	1:A:374:MET:SD	2.65	0.67
2:J:18:HIS:NE2	5:J:500:HEC:NB	2.43	0.67
2:K:18:HIS:NE2	5:K:500:HEC:NB	2.43	0.67
2:M:61:GLU:HA	2:M:95:ILE:HG21	1.76	0.67
3:O:6:ARG:O	3:O:10:ARG:HG2	1.95	0.67
1:A:611:VAL:HG12	1:A:613:PRO:HD3	1.75	0.67
2:L:61:GLU:HA	2:L:95:ILE:HG21	1.75	0.67
1:B:189:LYS:NZ	1:B:374:MET:SD	2.65	0.67
2:L:18:HIS:NE2	5:L:500:HEC:NB	2.43	0.67
1:B:1204:VAL:HG12	1:B:1205:VAL:HG23	1.76	0.66
1:D:611:VAL:HG12	1:D:613:PRO:HD3	1.75	0.66
2:N:18:HIS:NE2	5:N:500:HEC:NB	2.43	0.66
1:A:569:CYS:HG	1:A:1213:PHE:HE1	1.43	0.66
1:E:611:VAL:HG12	1:E:613:PRO:HD3	1.75	0.66
1:E:1086:GLY:HA2	2:L:39:LYS:CE	2.24	0.66
3:Q:6:ARG:O	3:Q:10:ARG:HG2	1.95	0.66
1:B:474:SER:HB2	1:B:477:GLN:HG2	1.78	0.66
1:A:1086:GLY:HA2	2:H:39:LYS:CE	2.24	0.66
1:F:1086:GLY:HA2	2:M:39:LYS:CE	2.25	0.66
2:H:18:HIS:NE2	5:H:500:HEC:NB	2.43	0.66
1:D:1027:ILE:HD11	1:D:1047:VAL:HG11	1.78	0.66
1:E:1027:ILE:HD11	1:E:1047:VAL:HG11	1.78	0.66
1:F:1027:ILE:HD11	1:F:1047:VAL:HG11	1.78	0.66
1:G:1086:GLY:HA2	2:N:39:LYS:CE	2.24	0.66
1:C:1086:GLY:CA	2:J:39:LYS:HZ1	2.04	0.66
1:A:474:SER:HB2	1:A:477:GLN:HG2	1.78	0.66
2:I:18:HIS:NE2	5:I:500:HEC:NB	2.43	0.66
2:L:20:VAL:HG12	2:L:32:LEU:HB2	1.77	0.66
1:E:844:GLN:NE2	2:L:79:LYS:HE3	2.11	0.66
1:F:1204:VAL:HG12	1:F:1205:VAL:HG23	1.77	0.66
3:R:6:ARG:O	3:R:10:ARG:HG2	1.95	0.66
1:D:1086:GLY:HA2	2:K:39:LYS:CE	2.24	0.66
2:J:20:VAL:HG12	2:J:32:LEU:HB2	1.77	0.66
1:F:844:GLN:NE2	2:M:79:LYS:HE3	2.11	0.66
3:P:6:ARG:O	3:P:10:ARG:HG2	1.95	0.66
1:D:844:GLN:NE2	2:K:79:LYS:HE3	2.11	0.65
1:F:354:ARG:NH1	1:F:362:GLU:OE1	2.30	0.65
1:G:844:GLN:NE2	2:N:79:LYS:HE3	2.11	0.65
1:G:1027:ILE:HD11	1:G:1047:VAL:HG11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:20:VAL:HG12	2:K:32:LEU:HB2	1.77	0.65
2:M:18:HIS:NE2	5:M:500:HEC:NB	2.43	0.65
1:E:391:LYS:O	1:E:392:ASP:HB2	1.96	0.65
1:F:391:LYS:O	1:F:392:ASP:HB2	1.96	0.65
1:A:1204:VAL:HG12	1:A:1205:VAL:HG23	1.76	0.65
1:B:354:ARG:NH1	1:B:362:GLU:OE1	2.30	0.65
1:C:474:SER:HB2	1:C:477:GLN:HG2	1.78	0.65
1:D:943:ILE:HG22	1:D:944:ARG:HG2	1.78	0.65
1:E:943:ILE:HG22	1:E:944:ARG:HG2	1.78	0.65
1:F:201:ASN:HD21	1:G:219:ASN:HD21	1.44	0.65
1:F:943:ILE:HG22	1:F:944:ARG:HG2	1.78	0.65
1:G:1204:VAL:HG12	1:G:1205:VAL:HG23	1.76	0.65
1:A:866:LEU:HB3	1:A:876:ALA:HB3	1.77	0.65
1:B:590:ASN:O	1:B:592:MET:N	2.30	0.65
1:C:1027:ILE:HD11	1:C:1047:VAL:HG11	1.78	0.65
1:E:569:CYS:HG	1:E:1213:PHE:HE1	1.42	0.65
1:C:590:ASN:O	1:C:592:MET:N	2.30	0.65
1:E:354:ARG:NH1	1:E:362:GLU:OE1	2.30	0.65
1:F:590:ASN:O	1:F:592:MET:N	2.30	0.65
1:G:354:ARG:NH1	1:G:362:GLU:OE1	2.30	0.65
1:C:844:GLN:NE2	2:J:79:LYS:HE3	2.11	0.65
1:C:943:ILE:HG22	1:C:944:ARG:HG2	1.78	0.65
1:G:866:LEU:HB3	1:G:876:ALA:HB3	1.77	0.65
1:G:943:ILE:HG22	1:G:944:ARG:HG2	1.78	0.65
1:F:358:SER:HB3	1:G:274:MET:CE	2.25	0.65
2:M:20:VAL:HG12	2:M:32:LEU:HB2	1.77	0.65
1:A:943:ILE:HG22	1:A:944:ARG:HG2	1.78	0.65
1:B:391:LYS:O	1:B:392:ASP:HB2	1.96	0.65
1:B:884:TRP:HZ3	2:I:79:LYS:HA	1.56	0.65
1:C:354:ARG:NH1	1:C:362:GLU:OE1	2.30	0.65
1:C:266:ASP:OD2	1:C:268:SER:OG	2.16	0.64
1:D:866:LEU:HB3	1:D:876:ALA:HB3	1.77	0.64
1:A:565:GLN:HE22	1:A:1213:PHE:N	1.89	0.64
1:B:943:ILE:HG22	1:B:944:ARG:HG2	1.78	0.64
1:D:160:LYS:N	4:D:1301:DTP:O1A	2.21	0.64
1:D:266:ASP:OD2	1:D:268:SER:OG	2.16	0.64
1:D:391:LYS:O	1:D:392:ASP:HB2	1.96	0.64
1:F:469:GLN:HB2	1:F:472:THR:HB	1.79	0.64
1:F:1133:SER:HB2	1:F:1142:LEU:HD11	1.79	0.64
1:G:474:SER:HB2	1:G:477:GLN:HG2	1.78	0.64
1:A:590:ASN:O	1:A:592:MET:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:SER:HB2	1:A:1142:LEU:HD11	1.79	0.64
1:C:866:LEU:HB3	1:C:876:ALA:HB3	1.77	0.64
1:D:643:LYS:HE3	1:D:645:GLU:HB3	1.79	0.64
1:D:715:LEU:HD13	1:D:727:LEU:HD21	1.79	0.64
1:G:1133:SER:HB2	1:G:1142:LEU:HD11	1.79	0.64
2:J:2:ASP:N	2:J:93:ASP:OD1	2.28	0.64
1:A:160:LYS:N	4:A:1301:DTP:O1A	2.21	0.64
1:A:643:LYS:HE3	1:A:645:GLU:HB3	1.79	0.64
1:B:266:ASP:OD2	1:B:268:SER:OG	2.16	0.64
1:D:590:ASN:O	1:D:592:MET:N	2.30	0.64
1:E:469:GLN:HB2	1:E:472:THR:HB	1.79	0.64
2:N:2:ASP:N	2:N:93:ASP:OD1	2.28	0.64
1:A:354:ARG:NH1	1:A:362:GLU:OE1	2.30	0.64
1:B:844:GLN:NE2	2:I:79:LYS:HE3	2.11	0.64
1:B:866:LEU:HB3	1:B:876:ALA:HB3	1.77	0.64
1:F:866:LEU:HB3	1:F:876:ALA:HB3	1.77	0.64
1:A:1027:ILE:HD11	1:A:1047:VAL:HG11	1.78	0.64
1:C:643:LYS:HE3	1:C:645:GLU:HB3	1.79	0.64
1:D:354:ARG:NH1	1:D:362:GLU:OE1	2.30	0.64
1:A:844:GLN:NE2	2:H:79:LYS:HE3	2.11	0.64
1:E:715:LEU:HD13	1:E:727:LEU:HD21	1.79	0.64
1:G:391:LYS:O	1:G:392:ASP:HB2	1.96	0.64
1:G:884:TRP:HZ3	2:N:79:LYS:HD2	1.52	0.64
1:A:884:TRP:HZ3	2:H:79:LYS:HA	1.56	0.64
1:A:1232:TYR:HB2	1:A:1244:LEU:HB2	1.80	0.64
1:B:1027:ILE:HD11	1:B:1047:VAL:HG11	1.78	0.64
1:B:1232:TYR:HB2	1:B:1244:LEU:HB2	1.80	0.64
1:C:1232:TYR:HB2	1:C:1244:LEU:HB2	1.80	0.64
1:E:160:LYS:N	4:E:1301:DTP:O1A	2.21	0.64
1:E:643:LYS:HE3	1:E:645:GLU:HB3	1.79	0.64
1:E:474:SER:HB2	1:E:477:GLN:HG2	1.78	0.64
2:I:2:ASP:N	2:I:93:ASP:OD1	2.28	0.64
1:B:643:LYS:HE3	1:B:645:GLU:HB3	1.79	0.64
1:D:474:SER:HB2	1:D:477:GLN:HG2	1.78	0.64
1:E:266:ASP:OD2	1:E:268:SER:OG	2.16	0.64
1:E:866:LEU:HB3	1:E:876:ALA:HB3	1.77	0.64
1:A:391:LYS:O	1:A:392:ASP:HB2	1.96	0.63
1:B:1133:SER:HB2	1:B:1142:LEU:HD11	1.79	0.63
1:C:715:LEU:HD13	1:C:727:LEU:HD21	1.79	0.63
1:G:469:GLN:HB2	1:G:472:THR:HB	1.79	0.63
1:G:643:LYS:HE3	1:G:645:GLU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1232:TYR:HB2	1:G:1244:LEU:HB2	1.80	0.63
1:D:469:GLN:HB2	1:D:472:THR:HB	1.79	0.63
1:E:945:ARG:HH22	1:E:988:LEU:HD22	1.64	0.63
1:E:1133:SER:HB2	1:E:1142:LEU:HD11	1.79	0.63
1:F:474:SER:HB2	1:F:477:GLN:HG2	1.78	0.63
1:C:391:LYS:O	1:C:392:ASP:HB2	1.96	0.63
1:C:1133:SER:HB2	1:C:1142:LEU:HD11	1.79	0.63
1:A:266:ASP:OD2	1:A:268:SER:OG	2.16	0.63
1:C:884:TRP:HZ3	2:J:79:LYS:HA	1.56	0.63
1:G:715:LEU:HD13	1:G:727:LEU:HD21	1.79	0.63
1:D:1133:SER:HB2	1:D:1142:LEU:HD11	1.79	0.63
1:D:1232:TYR:HB2	1:D:1244:LEU:HB2	1.80	0.63
1:A:109:TYR:HE1	1:G:4:LYS:HZ3	0.70	0.63
1:F:565:GLN:OE1	1:F:1213:PHE:N	2.32	0.63
1:F:715:LEU:HD13	1:F:727:LEU:HD21	1.79	0.63
1:F:1232:TYR:HB2	1:F:1244:LEU:HB2	1.80	0.63
1:G:565:GLN:OE1	1:G:1213:PHE:N	2.32	0.63
1:D:565:GLN:OE1	1:D:1213:PHE:N	2.32	0.63
1:A:715:LEU:HD13	1:A:727:LEU:HD21	1.79	0.62
1:D:945:ARG:HH22	1:D:988:LEU:HD22	1.64	0.62
1:E:590:ASN:O	1:E:592:MET:N	2.30	0.62
1:F:643:LYS:HE3	1:F:645:GLU:HB3	1.79	0.62
1:G:945:ARG:HH22	1:G:988:LEU:HD22	1.64	0.62
1:B:715:LEU:HD13	1:B:727:LEU:HD21	1.79	0.62
1:C:903:ASP:OD2	1:C:907:ARG:NH1	2.28	0.62
1:D:587:GLU:OE1	1:D:594:TYR:OH	2.18	0.62
1:E:1232:TYR:HB2	1:E:1244:LEU:HB2	1.80	0.62
1:G:590:ASN:O	1:G:592:MET:N	2.30	0.62
3:O:52:ARG:HB2	3:P:38:HIS:HE1	1.61	0.62
1:A:945:ARG:HH22	1:A:988:LEU:HD22	1.64	0.62
1:B:469:GLN:HB2	1:B:472:THR:HB	1.79	0.62
1:B:945:ARG:HH22	1:B:988:LEU:HD22	1.64	0.62
1:G:160:LYS:N	4:G:1301:DTP:O1A	2.21	0.62
2:K:2:ASP:N	2:K:93:ASP:OD1	2.28	0.62
1:A:565:GLN:OE1	1:A:1213:PHE:N	2.32	0.62
1:A:1031:ASN:HB2	1:A:1036:LYS:HB2	1.82	0.62
1:C:945:ARG:HH22	1:C:988:LEU:HD22	1.64	0.62
1:F:266:ASP:OD2	1:F:268:SER:OG	2.16	0.62
1:F:569:CYS:HG	1:F:1213:PHE:HE1	1.47	0.62
1:A:557:ARG:HH22	1:A:1175:THR:HG23	1.64	0.62
1:C:565:GLN:OE1	1:C:1213:PHE:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:945:ARG:HH22	1:F:988:LEU:HD22	1.64	0.62
2:M:2:ASP:N	2:M:93:ASP:OD1	2.28	0.62
1:A:469:GLN:HB2	1:A:472:THR:HB	1.79	0.62
1:B:924:GLN:NE2	1:B:965:SER:O	2.33	0.62
1:B:1031:ASN:HB2	1:B:1036:LYS:HB2	1.82	0.62
1:C:469:GLN:HB2	1:C:472:THR:HB	1.79	0.62
1:G:569:CYS:HG	1:G:1213:PHE:HE1	1.44	0.62
1:G:1031:ASN:HB2	1:G:1036:LYS:HB2	1.82	0.62
1:B:557:ARG:HH22	1:B:1175:THR:HG23	1.64	0.62
1:A:1086:GLY:CA	2:H:39:LYS:HZ1	2.10	0.62
1:B:565:GLN:OE1	1:B:1213:PHE:N	2.32	0.62
1:C:924:GLN:NE2	1:C:965:SER:O	2.33	0.62
1:D:862:TYR:HB3	1:D:884:TRP:HA	1.82	0.62
1:F:924:GLN:NE2	1:F:965:SER:O	2.33	0.62
1:A:924:GLN:NE2	1:A:965:SER:O	2.33	0.62
1:E:924:GLN:NE2	1:E:965:SER:O	2.33	0.62
1:E:587:GLU:OE1	1:E:594:TYR:OH	2.18	0.62
1:G:559:PRO:HD3	1:G:1171:GLU:OE1	2.00	0.62
1:G:714:LEU:HB3	1:G:730:LEU:HD12	1.82	0.62
1:A:145:GLY:HA2	1:A:259:GLN:NE2	2.15	0.61
1:D:569:CYS:HG	1:D:1213:PHE:HE1	1.48	0.61
1:E:565:GLN:OE1	1:E:1213:PHE:N	2.32	0.61
1:G:266:ASP:OD2	1:G:268:SER:OG	2.16	0.61
1:G:587:GLU:OE1	1:G:594:TYR:OH	2.17	0.61
1:C:1031:ASN:HB2	1:C:1036:LYS:HB2	1.82	0.61
1:G:557:ARG:HH22	1:G:1175:THR:HG23	1.64	0.61
1:D:559:PRO:HD3	1:D:1171:GLU:OE1	2.00	0.61
1:F:714:LEU:HB3	1:F:730:LEU:HD12	1.82	0.61
1:G:884:TRP:HZ3	2:N:79:LYS:HA	1.56	0.61
1:G:924:GLN:NE2	1:G:965:SER:O	2.33	0.61
2:L:2:ASP:N	2:L:93:ASP:OD1	2.28	0.61
1:A:274:MET:HG2	1:G:358:SER:OG	2.00	0.61
1:C:559:PRO:HD3	1:C:1171:GLU:OE1	2.00	0.61
1:C:862:TYR:HB3	1:C:884:TRP:HA	1.82	0.61
1:D:924:GLN:NE2	1:D:965:SER:O	2.33	0.61
1:E:145:GLY:HA2	1:E:259:GLN:NE2	2.15	0.61
1:F:559:PRO:HD3	1:F:1171:GLU:OE1	2.00	0.61
1:A:587:GLU:OE1	1:A:594:TYR:OH	2.18	0.61
1:A:884:TRP:HZ3	2:H:79:LYS:HD2	1.52	0.61
1:D:145:GLY:HA2	1:D:259:GLN:NE2	2.15	0.61
1:E:862:TYR:HB3	1:E:884:TRP:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:882:LEU:HD12	1:F:903:ASP:HB2	1.83	0.61
1:F:1031:ASN:HB2	1:F:1036:LYS:HB2	1.82	0.61
2:H:2:ASP:N	2:H:93:ASP:OD1	2.28	0.61
2:J:67:TYR:OH	2:J:80:MET:SD	2.57	0.61
1:A:862:TYR:HB3	1:A:884:TRP:HA	1.82	0.61
1:B:160:LYS:N	4:B:1301:DTP:O1A	2.21	0.61
1:B:882:LEU:HD13	1:B:1176:HIS:CE1	2.36	0.61
1:A:882:LEU:HD13	1:A:1176:HIS:CE1	2.36	0.61
1:A:882:LEU:HD12	1:A:903:ASP:HB2	1.83	0.61
1:D:599:ASN:ND2	1:D:1241:LEU:O	2.34	0.61
1:D:882:LEU:HD13	1:D:1176:HIS:CE1	2.36	0.61
1:E:714:LEU:HB3	1:E:730:LEU:HD12	1.82	0.61
1:E:882:LEU:HD12	1:E:903:ASP:HB2	1.83	0.61
1:F:145:GLY:HA2	1:F:259:GLN:NE2	2.15	0.61
1:F:862:TYR:CB	1:F:884:TRP:HA	2.31	0.61
1:F:1092:ASP:OD2	1:F:1133:SER:OG	2.17	0.61
1:G:145:GLY:HA2	1:G:259:GLN:NE2	2.16	0.61
1:A:752:SER:OG	1:A:754:ASP:O	2.19	0.61
1:B:145:GLY:HA2	1:B:259:GLN:NE2	2.16	0.61
1:B:599:ASN:ND2	1:B:1241:LEU:O	2.34	0.61
1:E:559:PRO:HD3	1:E:1171:GLU:OE1	2.00	0.61
1:G:599:ASN:ND2	1:G:1241:LEU:O	2.34	0.61
1:A:714:LEU:HB3	1:A:730:LEU:HD12	1.82	0.61
1:B:882:LEU:HD12	1:B:903:ASP:HB2	1.83	0.61
1:C:265:ARG:NH2	4:C:1301:DTP:O2G	2.31	0.61
1:F:844:GLN:HE22	2:M:79:LYS:CE	2.14	0.61
1:G:862:TYR:HB3	1:G:884:TRP:HA	1.82	0.61
1:B:844:GLN:HE22	2:I:79:LYS:CE	2.14	0.61
1:C:557:ARG:HH22	1:C:1175:THR:HG23	1.64	0.61
1:C:714:LEU:HB3	1:C:730:LEU:HD12	1.82	0.61
1:C:882:LEU:HD13	1:C:1176:HIS:CE1	2.36	0.61
1:D:844:GLN:HE22	2:K:79:LYS:CE	2.14	0.61
3:Q:52:ARG:HB2	3:R:38:HIS:HE1	1.65	0.61
1:C:160:LYS:N	4:C:1301:DTP:O1A	2.21	0.60
1:D:1031:ASN:HB2	1:D:1036:LYS:HB2	1.82	0.60
1:G:752:SER:OG	1:G:754:ASP:O	2.19	0.60
1:G:882:LEU:HD12	1:G:903:ASP:HB2	1.83	0.60
1:A:559:PRO:HD3	1:A:1171:GLU:OE1	2.00	0.60
1:B:714:LEU:HB3	1:B:730:LEU:HD12	1.82	0.60
1:D:844:GLN:NE2	2:K:79:LYS:CE	2.64	0.60
1:D:882:LEU:HD12	1:D:903:ASP:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1086:GLY:CA	2:K:39:LYS:HZ1	2.10	0.60
1:E:201:ASN:HD21	1:F:219:ASN:HD21	1.49	0.60
1:E:557:ARG:HH22	1:E:1175:THR:HG23	1.64	0.60
1:E:752:SER:OG	1:E:754:ASP:O	2.19	0.60
1:E:844:GLN:NE2	2:L:79:LYS:CE	2.64	0.60
1:E:1031:ASN:HB2	1:E:1036:LYS:HB2	1.82	0.60
1:G:265:ARG:NH2	4:G:1301:DTP:O2G	2.31	0.60
1:B:903:ASP:OD2	1:B:907:ARG:NH1	2.28	0.60
1:B:1086:GLY:CA	2:I:39:LYS:HZ1	2.07	0.60
1:D:1092:ASP:OD2	1:D:1133:SER:OG	2.17	0.60
1:E:143:LEU:C	1:E:145:GLY:H	2.09	0.60
1:E:844:GLN:HE22	2:L:79:LYS:CE	2.14	0.60
1:F:599:ASN:ND2	1:F:1241:LEU:O	2.34	0.60
1:G:844:GLN:HE22	2:N:79:LYS:CE	2.14	0.60
1:C:844:GLN:NE2	2:J:79:LYS:CE	2.65	0.60
1:C:862:TYR:CB	1:C:884:TRP:HA	2.31	0.60
1:C:882:LEU:HD12	1:C:903:ASP:HB2	1.83	0.60
1:D:884:TRP:HZ3	2:K:79:LYS:HA	1.56	0.60
1:F:143:LEU:C	1:F:145:GLY:H	2.09	0.60
1:G:844:GLN:NE2	2:N:79:LYS:CE	2.65	0.60
1:B:559:PRO:HD3	1:B:1171:GLU:OE1	2.00	0.60
1:B:862:TYR:HB3	1:B:884:TRP:HA	1.82	0.60
1:D:714:LEU:HB3	1:D:730:LEU:HD12	1.82	0.60
1:D:752:SER:OG	1:D:754:ASP:O	2.19	0.60
1:E:862:TYR:CB	1:E:884:TRP:HA	2.31	0.60
1:F:557:ARG:HH22	1:F:1175:THR:HG23	1.64	0.60
1:F:1210:SER:HB2	1:F:1212:THR:HG23	1.84	0.60
1:A:599:ASN:ND2	1:A:1241:LEU:O	2.34	0.60
1:B:569:CYS:HG	1:B:1213:PHE:HE1	1.50	0.60
1:B:862:TYR:CB	1:B:884:TRP:HA	2.31	0.60
1:C:145:GLY:HA2	1:C:259:GLN:NE2	2.15	0.60
1:D:557:ARG:HH22	1:D:1175:THR:HG23	1.64	0.60
1:E:882:LEU:HD13	1:E:1176:HIS:CE1	2.36	0.60
1:F:862:TYR:HB3	1:F:884:TRP:HA	1.82	0.60
1:F:884:TRP:HZ3	2:M:79:LYS:HD2	1.51	0.60
1:B:587:GLU:OE1	1:B:594:TYR:OH	2.18	0.60
1:B:752:SER:OG	1:B:754:ASP:O	2.19	0.60
1:D:862:TYR:CB	1:D:884:TRP:HA	2.31	0.60
1:A:844:GLN:HE22	2:H:79:LYS:CE	2.14	0.60
1:A:844:GLN:NE2	2:H:79:LYS:CE	2.65	0.60
1:A:862:TYR:CB	1:A:884:TRP:HA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:844:GLN:NE2	2:I:79:LYS:CE	2.65	0.60
1:G:1210:SER:HB2	1:G:1212:THR:HG23	1.84	0.60
1:E:265:ARG:NH2	4:E:1301:DTP:O2G	2.31	0.60
1:F:882:LEU:HD13	1:F:1176:HIS:CE1	2.36	0.60
1:G:862:TYR:CB	1:G:884:TRP:HA	2.31	0.60
1:G:882:LEU:HD13	1:G:1176:HIS:CE1	2.36	0.60
1:C:358:SER:OG	1:D:274:MET:HG2	2.02	0.60
1:D:1210:SER:HB2	1:D:1212:THR:HG23	1.84	0.60
1:E:599:ASN:ND2	1:E:1241:LEU:O	2.34	0.60
1:F:844:GLN:NE2	2:M:79:LYS:CE	2.64	0.60
1:C:599:ASN:ND2	1:C:1241:LEU:O	2.34	0.59
1:E:1115:ASP:HB2	1:E:1120:LEU:HD11	1.84	0.59
1:F:882:LEU:HD13	1:F:1176:HIS:CD2	2.37	0.59
1:A:903:ASP:OD2	1:A:907:ARG:NH1	2.28	0.59
1:A:1115:ASP:HB2	1:A:1120:LEU:HD11	1.84	0.59
1:B:201:ASN:HD21	1:C:219:ASN:HD21	1.50	0.59
1:E:1210:SER:HB2	1:E:1212:THR:HG23	1.84	0.59
1:F:752:SER:OG	1:F:754:ASP:O	2.19	0.59
1:F:903:ASP:OD2	1:F:907:ARG:NH1	2.28	0.59
3:R:8:LEU:HD23	3:R:8:LEU:C	2.27	0.59
1:B:1115:ASP:HB2	1:B:1120:LEU:HD11	1.84	0.59
1:G:903:ASP:OD2	1:G:907:ARG:NH1	2.28	0.59
3:P:8:LEU:C	3:P:8:LEU:HD23	2.27	0.59
1:A:201:ASN:HD21	1:B:219:ASN:HD21	1.50	0.59
1:A:882:LEU:HD13	1:A:1176:HIS:CD2	2.38	0.59
1:B:143:LEU:C	1:B:145:GLY:H	2.09	0.59
1:C:844:GLN:HE22	2:J:79:LYS:CE	2.14	0.59
1:D:143:LEU:C	1:D:145:GLY:H	2.09	0.59
1:F:587:GLU:OE1	1:F:594:TYR:OH	2.18	0.59
1:D:1115:ASP:HB2	1:D:1120:LEU:HD11	1.84	0.59
1:E:715:LEU:HB3	1:E:727:LEU:HD11	1.85	0.59
1:B:882:LEU:HD13	1:B:1176:HIS:CD2	2.38	0.59
1:C:143:LEU:C	1:C:145:GLY:H	2.09	0.59
1:C:752:SER:OG	1:C:754:ASP:O	2.19	0.59
1:C:1210:SER:HB2	1:C:1212:THR:HG23	1.84	0.59
1:D:715:LEU:HB3	1:D:727:LEU:HD11	1.85	0.59
1:D:1131:ARG:NH2	1:D:1147:ASP:OD1	2.36	0.59
1:E:903:ASP:OD2	1:E:907:ARG:NH1	2.28	0.59
1:F:1115:ASP:HB2	1:F:1120:LEU:HD11	1.84	0.59
2:N:67:TYR:OH	2:N:80:MET:SD	2.57	0.59
3:Q:52:ARG:CG	3:R:38:HIS:CE1	2.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:715:LEU:HB3	1:F:727:LEU:HD11	1.85	0.59
1:A:143:LEU:C	1:A:145:GLY:H	2.09	0.59
1:A:1210:SER:HB2	1:A:1212:THR:HG23	1.84	0.59
1:C:1131:ARG:NH2	1:C:1147:ASP:OD1	2.36	0.59
1:E:1131:ARG:NH2	1:E:1147:ASP:OD1	2.36	0.59
1:G:1115:ASP:HB2	1:G:1120:LEU:HD11	1.84	0.59
3:P:41:GLU:HB3	3:P:45:ARG:NH1	2.17	0.59
3:Q:8:LEU:HD23	3:Q:8:LEU:C	2.27	0.59
1:D:882:LEU:HD13	1:D:1176:HIS:CD2	2.37	0.59
1:C:521:HIS:NE2	1:C:525:GLU:OE2	2.36	0.59
1:C:1031:ASN:HB3	1:C:1034:LEU:HD12	1.85	0.59
1:E:882:LEU:HD13	1:E:1176:HIS:CD2	2.37	0.59
1:G:463:GLN:OE1	1:G:466:ARG:NH2	2.28	0.59
1:A:521:HIS:NE2	1:A:525:GLU:OE2	2.36	0.58
1:D:558:GLN:HA	1:D:559:PRO:C	2.28	0.58
1:F:160:LYS:N	4:F:1301:DTP:O1A	2.20	0.58
1:G:143:LEU:C	1:G:145:GLY:H	2.09	0.58
1:G:882:LEU:HD13	1:G:1176:HIS:CD2	2.38	0.58
1:D:358:SER:OG	1:E:274:MET:HG2	2.03	0.58
1:E:1202:TRP:HA	1:E:1208:GLU:HB2	1.85	0.58
1:F:482:TYR:OH	1:F:490:HIS:NE2	2.35	0.58
1:F:1202:TRP:HA	1:F:1208:GLU:HB2	1.85	0.58
1:A:558:GLN:HA	1:A:559:PRO:C	2.28	0.58
1:B:48:THR:HG22	1:D:45:ASN:OD1	2.04	0.58
1:B:1031:ASN:HB3	1:B:1034:LEU:HD12	1.85	0.58
1:B:1210:SER:HB2	1:B:1212:THR:HG23	1.84	0.58
1:C:201:ASN:HD21	1:D:219:ASN:HD21	1.51	0.58
1:C:715:LEU:HB3	1:C:727:LEU:HD11	1.85	0.58
1:C:1092:ASP:OD2	1:C:1133:SER:OG	2.17	0.58
1:C:1115:ASP:HB2	1:C:1120:LEU:HD11	1.84	0.58
1:D:903:ASP:OD2	1:D:907:ARG:NH1	2.28	0.58
1:E:4:LYS:HA	1:F:237:ARG:HH21	1.68	0.58
1:F:558:GLN:HA	1:F:559:PRO:C	2.28	0.58
1:F:884:TRP:HZ3	2:M:79:LYS:HA	1.56	0.58
3:Q:52:ARG:HB3	3:R:38:HIS:CE1	2.37	0.58
1:C:882:LEU:HD13	1:C:1176:HIS:CD2	2.38	0.58
1:C:1202:TRP:HA	1:C:1208:GLU:HB2	1.85	0.58
1:D:1202:TRP:HA	1:D:1208:GLU:HB2	1.85	0.58
1:B:1131:ARG:NH2	1:B:1147:ASP:OD1	2.36	0.58
1:C:558:GLN:HA	1:C:559:PRO:C	2.28	0.58
3:O:8:LEU:HD23	3:O:8:LEU:C	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:884:TRP:HZ3	2:L:79:LYS:HA	1.56	0.58
1:F:1131:ARG:NH2	1:F:1147:ASP:OD1	2.36	0.58
1:G:884:TRP:CZ3	2:N:79:LYS:CA	2.74	0.58
1:A:1031:ASN:HB3	1:A:1034:LEU:HD12	1.85	0.58
1:B:265:ARG:NH2	4:B:1301:DTP:O2G	2.31	0.58
1:B:482:TYR:HH	1:B:490:HIS:HE2	1.50	0.58
1:D:265:ARG:NH2	4:D:1301:DTP:O2G	2.31	0.58
1:E:558:GLN:HA	1:E:559:PRO:C	2.28	0.58
1:F:1031:ASN:HB3	1:F:1034:LEU:HD12	1.85	0.58
1:G:558:GLN:HA	1:G:559:PRO:C	2.28	0.58
1:G:1131:ARG:NH2	1:G:1147:ASP:OD1	2.36	0.58
1:A:1131:ARG:NH2	1:A:1147:ASP:OD1	2.36	0.58
1:C:884:TRP:CH2	2:J:78:THR:O	2.57	0.58
1:D:1031:ASN:HB3	1:D:1034:LEU:HD12	1.85	0.58
1:G:1048:LYS:H	1:G:1062:SER:HA	1.69	0.58
1:B:42:LYS:HB3	1:B:59:MET:HE1	1.86	0.58
1:B:1202:TRP:HA	1:B:1208:GLU:HB2	1.85	0.58
1:C:587:GLU:OE1	1:C:594:TYR:OH	2.18	0.58
1:F:1048:LYS:H	1:F:1062:SER:HA	1.69	0.58
1:G:715:LEU:HB3	1:G:727:LEU:HD11	1.85	0.58
1:B:521:HIS:NE2	1:B:525:GLU:OE2	2.36	0.57
1:D:521:HIS:NE2	1:D:525:GLU:OE2	2.36	0.57
1:F:521:HIS:NE2	1:F:525:GLU:OE2	2.36	0.57
1:G:482:TYR:OH	1:G:490:HIS:NE2	2.36	0.57
1:A:715:LEU:HB3	1:A:727:LEU:HD11	1.85	0.57
1:B:558:GLN:HA	1:B:559:PRO:C	2.28	0.57
1:B:884:TRP:CH2	2:I:78:THR:O	2.57	0.57
1:D:884:TRP:CH2	2:K:78:THR:O	2.57	0.57
1:G:1202:TRP:HA	1:G:1208:GLU:HB2	1.86	0.57
1:B:715:LEU:HB3	1:B:727:LEU:HD11	1.85	0.57
1:D:201:ASN:HD21	1:E:219:ASN:HD21	1.52	0.57
1:B:454:GLN:OE1	1:B:458:LYS:NZ	2.38	0.57
1:D:454:GLN:OE1	1:D:458:LYS:NZ	2.38	0.57
1:E:358:SER:OG	1:F:274:MET:HG2	2.04	0.57
1:E:521:HIS:NE2	1:E:525:GLU:OE2	2.36	0.57
1:B:1048:LYS:H	1:B:1062:SER:HA	1.69	0.57
1:C:454:GLN:OE1	1:C:458:LYS:NZ	2.38	0.57
1:E:454:GLN:OE1	1:E:458:LYS:NZ	2.38	0.57
1:F:884:TRP:CH2	2:M:78:THR:O	2.57	0.57
1:G:521:HIS:NE2	1:G:525:GLU:OE2	2.36	0.57
1:A:454:GLN:OE1	1:A:458:LYS:NZ	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:884:TRP:CZ3	2:I:79:LYS:CA	2.74	0.57
1:D:1048:LYS:H	1:D:1062:SER:HA	1.69	0.57
1:E:1048:LYS:H	1:E:1062:SER:HA	1.69	0.57
1:G:42:LYS:HB3	1:G:59:MET:HE1	1.86	0.57
1:G:884:TRP:CH2	2:N:78:THR:O	2.57	0.57
1:G:1031:ASN:HB3	1:G:1034:LEU:HD12	1.85	0.57
1:A:1202:TRP:HA	1:A:1208:GLU:HB2	1.85	0.57
1:B:358:SER:OG	1:C:274:MET:HG2	2.04	0.57
1:D:42:LYS:HB3	1:D:59:MET:HE1	1.86	0.57
1:G:454:GLN:OE1	1:G:458:LYS:NZ	2.38	0.57
1:A:884:TRP:CH2	2:H:78:THR:O	2.57	0.57
1:D:1139:SER:O	1:D:1140:THR:HG22	2.05	0.57
1:G:264:THR:OG1	1:G:265:ARG:N	2.37	0.57
1:A:358:SER:OG	1:B:274:MET:HG2	2.04	0.57
1:C:763:ALA:HA	1:C:801:VAL:H	1.70	0.57
1:C:1048:LYS:H	1:C:1062:SER:HA	1.69	0.57
1:D:264:THR:OG1	1:D:265:ARG:N	2.37	0.57
1:E:763:ALA:HA	1:E:801:VAL:H	1.70	0.57
1:E:1031:ASN:HB3	1:E:1034:LEU:HD12	1.85	0.57
1:F:265:ARG:NH2	4:F:1301:DTP:O2G	2.31	0.57
1:F:454:GLN:OE1	1:F:458:LYS:NZ	2.38	0.57
1:G:1092:ASP:OD2	1:G:1133:SER:OG	2.17	0.57
1:G:1139:SER:O	1:G:1140:THR:HG22	2.05	0.57
1:B:264:THR:OG1	1:B:265:ARG:N	2.37	0.56
1:B:524:HIS:HB2	1:B:646:THR:CG2	2.32	0.56
1:F:264:THR:OG1	1:F:265:ARG:N	2.38	0.56
1:A:1139:SER:O	1:A:1140:THR:HG22	2.05	0.56
1:C:1139:SER:O	1:C:1140:THR:HG22	2.05	0.56
1:E:1092:ASP:OD2	1:E:1133:SER:OG	2.17	0.56
1:B:1139:SER:O	1:B:1140:THR:HG22	2.05	0.56
1:E:524:HIS:HB2	1:E:646:THR:CG2	2.32	0.56
1:B:1023:ASP:OD1	1:B:1046:THR:OG1	2.24	0.56
1:C:590:ASN:C	1:C:592:MET:N	2.64	0.56
1:C:884:TRP:CZ3	2:J:79:LYS:CA	2.74	0.56
1:D:569:CYS:HB3	1:D:600:LYS:HZ3	1.71	0.56
1:E:42:LYS:HB3	1:E:59:MET:HE1	1.86	0.56
1:E:884:TRP:CH2	2:L:78:THR:O	2.57	0.56
1:A:264:THR:OG1	1:A:265:ARG:N	2.37	0.56
1:C:716:LEU:HB3	1:C:728:TRP:HB2	1.87	0.56
1:D:463:GLN:OE1	1:D:466:ARG:NH2	2.28	0.56
1:E:264:THR:OG1	1:E:265:ARG:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:HIS:HB2	1:A:646:THR:CG2	2.32	0.56
1:A:565:GLN:NE2	1:A:1213:PHE:CA	2.69	0.56
1:A:1048:LYS:H	1:A:1062:SER:HA	1.69	0.56
1:F:1139:SER:O	1:F:1140:THR:HG22	2.05	0.56
2:L:67:TYR:OH	2:L:80:MET:SD	2.57	0.56
1:C:1086:GLY:CA	2:J:39:LYS:NZ	2.66	0.56
1:G:565:GLN:NE2	1:G:1213:PHE:CA	2.69	0.56
1:G:716:LEU:HB3	1:G:728:TRP:HB2	1.87	0.56
1:A:844:GLN:HE22	2:H:79:LYS:HE3	1.71	0.56
1:A:1023:ASP:OD1	1:A:1046:THR:OG1	2.24	0.56
1:B:763:ALA:HA	1:B:801:VAL:H	1.70	0.56
1:D:716:LEU:HB3	1:D:728:TRP:HB2	1.87	0.56
1:E:1139:SER:O	1:E:1140:THR:HG22	2.05	0.56
2:M:67:TYR:OH	2:M:80:MET:SD	2.57	0.56
1:A:170:ASP:OD1	1:A:171:HIS:N	2.39	0.56
1:B:844:GLN:HE22	2:I:79:LYS:HE3	1.71	0.56
1:C:264:THR:OG1	1:C:265:ARG:N	2.37	0.56
1:C:326:LEU:HD13	1:C:353:ILE:CG2	2.37	0.56
1:D:326:LEU:HD13	1:D:353:ILE:CG2	2.36	0.56
3:P:50:SER:CB	3:Q:45:ARG:NH1	2.64	0.56
1:C:1023:ASP:OD1	1:C:1046:THR:OG1	2.24	0.55
1:D:884:TRP:CZ3	2:K:79:LYS:CA	2.74	0.55
1:E:326:LEU:HD13	1:E:353:ILE:CG2	2.36	0.55
1:F:336:ASN:HB2	1:G:431:LYS:HE3	1.87	0.55
1:G:844:GLN:HE22	2:N:79:LYS:HE3	1.71	0.55
1:A:463:GLN:OE1	1:A:466:ARG:NH2	2.28	0.55
1:B:170:ASP:OD1	1:B:171:HIS:N	2.39	0.55
1:B:326:LEU:HD13	1:B:353:ILE:CG2	2.37	0.55
1:B:1092:ASP:OD2	1:B:1133:SER:OG	2.17	0.55
1:G:170:ASP:OD1	1:G:171:HIS:N	2.39	0.55
1:A:326:LEU:HD13	1:A:353:ILE:CG2	2.37	0.55
1:A:716:LEU:HB3	1:A:728:TRP:HB2	1.87	0.55
1:A:884:TRP:CZ3	2:H:79:LYS:CA	2.74	0.55
1:B:845:TYR:HB3	1:B:858:ALA:HB3	1.89	0.55
1:C:217:PRO:HG3	1:C:226:ARG:HH12	1.72	0.55
1:C:844:GLN:HE22	2:J:79:LYS:HE3	1.71	0.55
1:D:217:PRO:HG3	1:D:226:ARG:HH12	1.71	0.55
1:A:763:ALA:HA	1:A:801:VAL:H	1.70	0.55
1:C:617:ALA:HA	1:C:904:GLN:HG2	1.89	0.55
1:C:845:TYR:HB3	1:C:858:ALA:HB3	1.89	0.55
1:D:572:GLU:HA	1:D:577:TYR:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:884:TRP:N	1:E:884:TRP:CD1	2.73	0.55
1:F:572:GLU:HA	1:F:577:TYR:CD2	2.42	0.55
1:F:716:LEU:HB3	1:F:728:TRP:HB2	1.87	0.55
1:F:763:ALA:HA	1:F:801:VAL:H	1.70	0.55
1:G:590:ASN:C	1:G:592:MET:N	2.64	0.55
1:G:763:ALA:HA	1:G:801:VAL:H	1.70	0.55
1:A:845:TYR:HB3	1:A:858:ALA:HB3	1.89	0.55
1:B:572:GLU:HA	1:B:577:TYR:CD2	2.42	0.55
1:C:170:ASP:OD1	1:C:171:HIS:N	2.39	0.55
1:C:463:GLN:OE1	1:C:466:ARG:NH2	2.28	0.55
1:C:572:GLU:HA	1:C:577:TYR:CD2	2.42	0.55
1:D:763:ALA:HA	1:D:801:VAL:H	1.70	0.55
1:E:572:GLU:HA	1:E:577:TYR:CD2	2.42	0.55
1:F:326:LEU:HD13	1:F:353:ILE:CG2	2.36	0.55
1:A:572:GLU:HA	1:A:577:TYR:CD2	2.42	0.55
1:B:28:HIS:CE1	3:P:14:LEU:CD2	2.90	0.55
1:B:565:GLN:NE2	1:B:1213:PHE:CA	2.69	0.55
1:B:1086:GLY:CA	2:I:39:LYS:NZ	2.66	0.55
1:C:565:GLN:NE2	1:C:1213:PHE:CA	2.69	0.55
1:D:617:ALA:HA	1:D:904:GLN:HG2	1.89	0.55
1:D:844:GLN:HE22	2:K:79:LYS:HE3	1.71	0.55
1:F:217:PRO:HG3	1:F:226:ARG:HH12	1.71	0.55
1:G:326:LEU:HD13	1:G:353:ILE:CG2	2.36	0.55
1:G:572:GLU:HA	1:G:577:TYR:CD2	2.42	0.55
1:E:716:LEU:HB3	1:E:728:TRP:HB2	1.87	0.55
3:O:27:ASP:OD1	3:R:13:ARG:HG2	2.06	0.55
1:A:1092:ASP:OD2	1:A:1133:SER:OG	2.17	0.55
1:D:170:ASP:OD1	1:D:171:HIS:N	2.39	0.55
1:D:565:GLN:NE2	1:D:1213:PHE:CA	2.69	0.55
1:E:565:GLN:NE2	1:E:1213:PHE:CA	2.69	0.55
1:F:844:GLN:HE22	2:M:79:LYS:HE3	1.71	0.55
1:G:845:TYR:HB3	1:G:858:ALA:HB3	1.89	0.55
3:R:15:ARG:HD2	3:R:19:GLU:OE2	2.07	0.55
1:D:1086:GLY:CA	2:K:39:LYS:NZ	2.66	0.55
1:F:170:ASP:OD1	1:F:171:HIS:N	2.39	0.55
2:N:60:GLY:N	2:N:63:THR:OG1	2.34	0.55
1:B:617:ALA:HA	1:B:904:GLN:HG2	1.89	0.55
1:D:845:TYR:HB3	1:D:858:ALA:HB3	1.89	0.55
1:D:884:TRP:N	1:D:884:TRP:CD1	2.73	0.55
1:F:524:HIS:HB2	1:F:646:THR:CG2	2.32	0.55
1:A:482:TYR:HH	1:A:490:HIS:HE2	1.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:565:GLN:NE2	1:F:1213:PHE:CA	2.69	0.54
1:A:550:LEU:HD21	1:A:607:SER:CB	2.35	0.54
1:B:716:LEU:HB3	1:B:728:TRP:HB2	1.87	0.54
1:B:1219:ASN:HB2	1:B:1237:ASN:HB3	1.89	0.54
1:E:170:ASP:OD1	1:E:171:HIS:N	2.39	0.54
1:E:844:GLN:HE22	2:L:79:LYS:HE3	1.71	0.54
1:G:265:ARG:HH11	1:G:371:SER:HG	1.52	0.54
1:G:1023:ASP:OD1	1:G:1046:THR:OG1	2.24	0.54
1:C:1219:ASN:HB2	1:C:1237:ASN:HB3	1.89	0.54
1:F:550:LEU:HD21	1:F:607:SER:CB	2.35	0.54
1:F:590:ASN:C	1:F:592:MET:N	2.64	0.54
1:F:884:TRP:N	1:F:884:TRP:CD1	2.73	0.54
1:B:482:TYR:OH	1:B:490:HIS:NE2	2.35	0.54
1:C:727:LEU:HB3	1:C:737:ASN:HB2	1.90	0.54
1:D:800:ILE:H	1:D:818:LYS:HE2	1.73	0.54
1:D:1087:THR:N	2:K:39:LYS:HZ3	2.06	0.54
1:E:217:PRO:HG3	1:E:226:ARG:HH12	1.71	0.54
1:E:617:ALA:HA	1:E:904:GLN:HG2	1.89	0.54
1:A:217:PRO:HG3	1:A:226:ARG:HH12	1.71	0.54
1:A:219:ASN:HD21	1:G:201:ASN:HD21	1.54	0.54
1:D:727:LEU:HB3	1:D:737:ASN:HB2	1.90	0.54
1:D:1023:ASP:OD1	1:D:1046:THR:OG1	2.24	0.54
1:F:800:ILE:H	1:F:818:LYS:HE2	1.73	0.54
1:B:800:ILE:H	1:B:818:LYS:HE2	1.73	0.54
1:C:1030:TRP:CD1	1:C:1037:CYS:HG	2.26	0.54
1:E:884:TRP:CZ3	2:L:79:LYS:CA	2.74	0.54
3:O:15:ARG:HD2	3:O:19:GLU:OE2	2.07	0.54
1:B:217:PRO:HG3	1:B:226:ARG:HH12	1.72	0.54
1:B:727:LEU:HB3	1:B:737:ASN:HB2	1.90	0.54
1:C:800:ILE:H	1:C:818:LYS:HE2	1.73	0.54
1:C:884:TRP:H	1:C:884:TRP:CD1	2.25	0.54
1:D:612:ARG:NH2	1:D:903:ASP:O	2.41	0.54
1:E:727:LEU:HB3	1:E:737:ASN:HB2	1.90	0.54
1:F:612:ARG:NH2	1:F:903:ASP:O	2.41	0.54
1:F:845:TYR:HB3	1:F:858:ALA:HB3	1.89	0.54
2:I:40:THR:HA	2:I:59:TRP:HE1	1.73	0.54
2:I:67:TYR:OH	2:I:80:MET:SD	2.57	0.54
1:A:800:ILE:H	1:A:818:LYS:HE2	1.73	0.54
1:A:1219:ASN:HB2	1:A:1237:ASN:HB3	1.89	0.54
1:C:265:ARG:NH1	1:C:371:SER:OG	2.37	0.54
1:D:30:ILE:CG2	3:Q:10:ARG:CB	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ASP:CG	1:E:268:SER:HG	2.16	0.54
1:F:266:ASP:CG	1:F:268:SER:HG	2.15	0.54
1:A:265:ARG:HH11	1:A:371:SER:HG	1.56	0.54
1:A:266:ASP:CG	1:A:268:SER:HG	2.15	0.54
1:G:482:TYR:HH	1:G:490:HIS:HE2	1.52	0.54
1:G:550:LEU:HD21	1:G:607:SER:CB	2.35	0.54
2:L:40:THR:HA	2:L:59:TRP:HE1	1.73	0.54
1:A:617:ALA:HA	1:A:904:GLN:HG2	1.89	0.54
1:A:864:VAL:CG2	1:A:885:VAL:HG21	2.38	0.54
1:B:336:ASN:HB2	1:C:431:LYS:HE3	1.90	0.54
1:D:884:TRP:CD1	1:D:884:TRP:H	2.25	0.54
1:D:1219:ASN:HB2	1:D:1237:ASN:HB3	1.89	0.54
1:F:265:ARG:HH11	1:F:371:SER:HG	1.55	0.54
1:F:987:ILE:HD11	1:F:1018:LEU:HD22	1.90	0.54
1:F:1219:ASN:HB2	1:F:1237:ASN:HB3	1.89	0.54
1:G:217:PRO:HG3	1:G:226:ARG:HH12	1.72	0.54
1:G:612:ARG:NH2	1:G:903:ASP:O	2.41	0.54
3:Q:15:ARG:HD2	3:Q:19:GLU:OE2	2.07	0.54
1:B:13:ARG:O	1:B:17:GLU:HG3	2.09	0.53
1:B:612:ARG:NH2	1:B:903:ASP:O	2.41	0.53
1:F:727:LEU:HB3	1:F:737:ASN:HB2	1.90	0.53
1:F:884:TRP:CD1	1:F:884:TRP:H	2.26	0.53
1:A:844:GLN:HE22	2:H:79:LYS:HZ2	1.55	0.53
1:D:524:HIS:HB2	1:D:646:THR:CG2	2.32	0.53
1:E:845:TYR:HB3	1:E:858:ALA:HB3	1.89	0.53
1:E:884:TRP:CD1	1:E:884:TRP:H	2.25	0.53
1:E:987:ILE:HD11	1:E:1018:LEU:HD22	1.90	0.53
1:F:266:ASP:OD1	1:F:267:LYS:N	2.41	0.53
1:G:800:ILE:H	1:G:818:LYS:HE2	1.73	0.53
1:A:266:ASP:OD1	1:A:267:LYS:N	2.41	0.53
1:B:884:TRP:CD1	1:B:884:TRP:H	2.25	0.53
1:C:266:ASP:OD1	1:C:267:LYS:N	2.42	0.53
1:C:1061:TRP:CE2	1:C:1090:SER:HA	2.43	0.53
1:E:266:ASP:OD1	1:E:267:LYS:N	2.42	0.53
1:E:612:ARG:NH2	1:E:903:ASP:O	2.41	0.53
1:E:1023:ASP:OD1	1:E:1046:THR:OG1	2.24	0.53
1:F:1023:ASP:OD1	1:F:1046:THR:OG1	2.24	0.53
2:K:40:THR:HA	2:K:59:TRP:HE1	1.73	0.53
2:N:40:THR:HA	2:N:59:TRP:HE1	1.73	0.53
1:C:864:VAL:CG2	1:C:885:VAL:HG21	2.38	0.53
1:D:13:ARG:O	1:D:17:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1061:TRP:CE2	1:D:1090:SER:HA	2.43	0.53
1:E:698:HIS:CE1	1:E:726:LYS:HD2	2.44	0.53
1:E:864:VAL:CG2	1:E:885:VAL:HG21	2.38	0.53
1:E:1061:TRP:CE2	1:E:1090:SER:HA	2.43	0.53
1:F:358:SER:OG	1:G:274:MET:HG2	2.09	0.53
1:G:266:ASP:OD1	1:G:267:LYS:N	2.41	0.53
1:G:864:VAL:CG2	1:G:885:VAL:HG21	2.38	0.53
1:G:987:ILE:HD11	1:G:1018:LEU:HD22	1.91	0.53
1:A:612:ARG:NH2	1:A:903:ASP:O	2.41	0.53
1:A:884:TRP:N	1:A:884:TRP:CD1	2.73	0.53
1:B:1061:TRP:CE2	1:B:1090:SER:HA	2.43	0.53
1:E:13:ARG:O	1:E:17:GLU:HG3	2.09	0.53
1:E:800:ILE:H	1:E:818:LYS:HE2	1.73	0.53
1:F:617:ALA:HA	1:F:904:GLN:HG2	1.89	0.53
1:G:1030:TRP:CD1	1:G:1037:CYS:HG	2.27	0.53
1:B:584:ALA:HB1	1:B:594:TYR:CD2	2.44	0.53
1:B:884:TRP:CD1	1:B:884:TRP:N	2.73	0.53
1:C:612:ARG:NH2	1:C:903:ASP:O	2.41	0.53
1:D:1149:GLY:HA3	1:D:1178:GLY:HA2	1.91	0.53
1:E:1149:GLY:HA3	1:E:1178:GLY:HA2	1.91	0.53
1:G:884:TRP:CD1	1:G:884:TRP:H	2.25	0.53
2:M:40:THR:HA	2:M:59:TRP:HE1	1.73	0.53
1:A:698:HIS:CE1	1:A:726:LYS:HD2	2.44	0.53
1:A:1086:GLY:CA	2:H:39:LYS:NZ	2.66	0.53
1:A:1087:THR:N	2:H:39:LYS:HZ3	2.06	0.53
1:B:463:GLN:OE1	1:B:466:ARG:NH2	2.28	0.53
1:C:884:TRP:CD1	1:C:884:TRP:N	2.73	0.53
1:D:864:VAL:CG2	1:D:885:VAL:HG21	2.38	0.53
1:D:987:ILE:HD11	1:D:1018:LEU:HD22	1.90	0.53
1:G:727:LEU:HB3	1:G:737:ASN:HB2	1.90	0.53
1:G:1149:GLY:HA3	1:G:1178:GLY:HA2	1.91	0.53
2:J:40:THR:HA	2:J:59:TRP:HE1	1.73	0.53
1:A:336:ASN:HB2	1:B:431:LYS:HE3	1.90	0.53
1:A:1149:GLY:HA3	1:A:1178:GLY:HA2	1.91	0.53
1:B:266:ASP:OD1	1:B:267:LYS:N	2.41	0.53
1:B:864:VAL:CG2	1:B:885:VAL:HG21	2.38	0.53
1:C:267:LYS:HZ1	1:C:419:VAL:HG12	1.74	0.53
1:F:864:VAL:CG2	1:F:885:VAL:HG21	2.38	0.53
1:G:524:HIS:HB2	1:G:646:THR:CG2	2.32	0.53
1:A:267:LYS:HZ1	1:A:419:VAL:HG12	1.74	0.53
1:A:727:LEU:HB3	1:A:737:ASN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:584:ALA:HB1	1:D:594:TYR:CD2	2.44	0.53
1:F:698:HIS:CE1	1:F:726:LYS:HD2	2.44	0.53
1:G:617:ALA:HA	1:G:904:GLN:HG2	1.89	0.53
1:G:698:HIS:CE1	1:G:726:LYS:HD2	2.44	0.53
1:G:1219:ASN:HB2	1:G:1237:ASN:HB3	1.90	0.53
1:C:524:HIS:HB2	1:C:646:THR:CG2	2.32	0.53
1:C:584:ALA:HB1	1:C:594:TYR:CD2	2.44	0.53
1:D:698:HIS:CE1	1:D:726:LYS:HD2	2.44	0.53
1:F:631:ALA:HB1	1:F:639:LEU:HD11	1.91	0.53
1:F:1061:TRP:CE2	1:F:1090:SER:HA	2.43	0.53
1:F:1149:GLY:HA3	1:F:1178:GLY:HA2	1.91	0.53
1:F:1191:MET:SD	1:F:1209:SER:OG	2.63	0.53
2:H:40:THR:HA	2:H:59:TRP:HE1	1.73	0.53
1:D:266:ASP:OD1	1:D:267:LYS:N	2.41	0.52
1:D:267:LYS:HZ1	1:D:419:VAL:HG12	1.74	0.52
1:E:1219:ASN:HB2	1:E:1237:ASN:HB3	1.89	0.52
1:G:13:ARG:O	1:G:17:GLU:HG3	2.08	0.52
1:G:884:TRP:CD1	1:G:884:TRP:N	2.73	0.52
1:A:884:TRP:CD1	1:A:884:TRP:H	2.25	0.52
1:A:1061:TRP:CE2	1:A:1090:SER:HA	2.43	0.52
1:C:1149:GLY:HA3	1:C:1178:GLY:HA2	1.91	0.52
1:D:609:LEU:HD23	1:D:908:LEU:HD13	1.91	0.52
1:E:336:ASN:HB2	1:F:431:LYS:HE3	1.91	0.52
1:G:584:ALA:HB1	1:G:594:TYR:CD2	2.44	0.52
1:A:987:ILE:HD11	1:A:1018:LEU:HD22	1.90	0.52
1:B:326:LEU:HD13	1:B:353:ILE:HG22	1.92	0.52
1:B:1126:HIS:CE1	1:B:1129:CYS:H	2.28	0.52
1:B:1149:GLY:HA3	1:B:1178:GLY:HA2	1.91	0.52
1:C:698:HIS:CE1	1:C:726:LYS:HD2	2.44	0.52
1:E:631:ALA:HB1	1:E:639:LEU:HD11	1.91	0.52
1:G:945:ARG:HD2	1:G:961:GLU:HB2	1.92	0.52
1:G:1061:TRP:CE2	1:G:1090:SER:HA	2.43	0.52
2:K:67:TYR:OH	2:K:80:MET:SD	2.57	0.52
1:A:365:ASP:OD1	1:A:444:PHE:CE1	2.63	0.52
1:B:265:ARG:HH11	1:B:371:SER:HG	1.55	0.52
1:B:1087:THR:N	2:I:39:LYS:HZ3	2.07	0.52
1:C:265:ARG:HH11	1:C:371:SER:HG	1.57	0.52
1:E:267:LYS:HZ1	1:E:419:VAL:HG12	1.74	0.52
1:E:609:LEU:HD23	1:E:908:LEU:HD13	1.91	0.52
1:G:365:ASP:OD1	1:G:444:PHE:CE1	2.63	0.52
3:P:50:SER:HB3	3:Q:45:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ALA:HB1	1:A:594:TYR:CD2	2.44	0.52
1:C:336:ASN:HB2	1:D:431:LYS:HE3	1.91	0.52
1:D:326:LEU:HD13	1:D:353:ILE:HG22	1.92	0.52
1:F:267:LYS:HZ1	1:F:419:VAL:HG12	1.74	0.52
1:F:945:ARG:HD2	1:F:961:GLU:HB2	1.92	0.52
2:M:60:GLY:N	2:M:63:THR:OG1	2.34	0.52
1:A:945:ARG:HD2	1:A:961:GLU:HB2	1.92	0.52
1:C:326:LEU:HD13	1:C:353:ILE:HG22	1.92	0.52
1:E:326:LEU:HD13	1:E:353:ILE:HG22	1.92	0.52
1:E:584:ALA:HB1	1:E:594:TYR:CD2	2.44	0.52
1:G:631:ALA:HB1	1:G:639:LEU:HD11	1.91	0.52
1:G:844:GLN:NE2	2:N:79:LYS:NZ	2.58	0.52
2:H:67:TYR:OH	2:H:80:MET:SD	2.57	0.52
1:B:267:LYS:HZ1	1:B:419:VAL:HG12	1.75	0.52
1:B:987:ILE:HD11	1:B:1018:LEU:HD22	1.90	0.52
1:C:987:ILE:HD11	1:C:1018:LEU:HD22	1.90	0.52
1:D:37:ILE:HG12	3:Q:10:ARG:CD	2.40	0.52
1:D:725:LEU:HB2	1:D:739:MET:HB2	1.92	0.52
1:F:365:ASP:OD1	1:F:444:PHE:CE1	2.63	0.52
1:A:326:LEU:HD13	1:A:353:ILE:HG22	1.92	0.52
1:A:609:LEU:HD23	1:A:908:LEU:HD13	1.91	0.52
1:A:882:LEU:HD12	1:A:1176:HIS:NE2	2.25	0.52
1:B:550:LEU:HD21	1:B:607:SER:CB	2.35	0.52
1:C:1126:HIS:CE1	1:C:1129:CYS:H	2.28	0.52
1:D:14:GLU:HB2	1:E:31:SER:OG	2.09	0.52
1:D:864:VAL:HG23	1:D:885:VAL:HG21	1.92	0.52
1:E:945:ARG:HD2	1:E:961:GLU:HB2	1.92	0.52
1:A:1126:HIS:CE1	1:A:1129:CYS:H	2.28	0.52
1:B:365:ASP:OD1	1:B:444:PHE:CE1	2.63	0.52
1:E:365:ASP:OD1	1:E:444:PHE:CE1	2.63	0.52
1:F:326:LEU:HD13	1:F:353:ILE:HG22	1.92	0.52
1:A:265:ARG:NH2	4:A:1301:DTP:O2G	2.31	0.52
1:A:416:GLN:HE21	1:G:334:PHE:HE1	1.57	0.52
1:A:530:ARG:HD2	1:A:545:GLN:HE22	1.75	0.52
1:B:698:HIS:CE1	1:B:726:LYS:HD2	2.44	0.52
1:B:945:ARG:HD2	1:B:961:GLU:HB2	1.92	0.52
1:C:864:VAL:HG23	1:C:885:VAL:HG21	1.92	0.52
1:D:844:GLN:NE2	2:K:79:LYS:NZ	2.57	0.52
1:D:882:LEU:HD12	1:D:1176:HIS:NE2	2.25	0.52
1:D:1126:HIS:CE1	1:D:1129:CYS:H	2.28	0.52
1:E:864:VAL:HG23	1:E:885:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:584:ALA:HB1	1:F:594:TYR:CD2	2.44	0.52
1:G:609:LEU:HD23	1:G:908:LEU:HD13	1.91	0.52
1:B:844:GLN:NE2	2:I:79:LYS:NZ	2.57	0.51
1:C:609:LEU:HD23	1:C:908:LEU:HD13	1.91	0.51
1:E:550:LEU:HD21	1:E:607:SER:CB	2.35	0.51
1:E:600:LYS:HZ1	1:E:1213:PHE:HZ	1.58	0.51
1:G:265:ARG:NH1	1:G:371:SER:OG	2.37	0.51
1:A:844:GLN:NE2	2:H:79:LYS:NZ	2.58	0.51
1:E:725:LEU:HB2	1:E:739:MET:HB2	1.92	0.51
1:F:882:LEU:HD12	1:F:1176:HIS:NE2	2.25	0.51
1:G:267:LYS:HZ1	1:G:419:VAL:HG12	1.74	0.51
2:J:60:GLY:N	2:J:63:THR:OG1	2.34	0.51
1:A:1030:TRP:CD1	1:A:1037:CYS:HG	2.28	0.51
1:C:550:LEU:HD21	1:C:607:SER:CB	2.35	0.51
1:C:725:LEU:HB2	1:C:739:MET:HB2	1.92	0.51
1:F:337:ARG:NH1	1:G:409:GLU:OE2	2.44	0.51
1:G:326:LEU:HD13	1:G:353:ILE:HG22	1.92	0.51
1:B:400:LEU:HB3	1:B:404:TRP:CZ3	2.46	0.51
1:C:334:PHE:HE1	1:D:416:GLN:HE21	1.57	0.51
1:C:400:LEU:HB3	1:C:404:TRP:CZ3	2.46	0.51
1:D:365:ASP:OD1	1:D:444:PHE:CE1	2.63	0.51
1:D:530:ARG:HD2	1:D:545:GLN:HE22	1.75	0.51
1:D:550:LEU:HD21	1:D:607:SER:CB	2.35	0.51
1:D:631:ALA:HB1	1:D:639:LEU:HD11	1.91	0.51
1:E:530:ARG:HD2	1:E:545:GLN:HE22	1.76	0.51
1:F:609:LEU:HD23	1:F:908:LEU:HD13	1.91	0.51
1:F:692:VAL:HG12	1:F:693:HIS:ND1	2.26	0.51
1:F:884:TRP:CZ3	2:M:79:LYS:CA	2.74	0.51
1:G:864:VAL:HG23	1:G:885:VAL:HG21	1.92	0.51
1:A:692:VAL:HG12	1:A:693:HIS:ND1	2.25	0.51
1:A:725:LEU:HB2	1:A:739:MET:HB2	1.92	0.51
1:B:609:LEU:HD23	1:B:908:LEU:HD13	1.91	0.51
1:B:762:SER:OG	1:B:764:ASP:OD1	2.26	0.51
1:D:1191:MET:SD	1:D:1209:SER:OG	2.63	0.51
1:E:882:LEU:HD12	1:E:1176:HIS:NE2	2.25	0.51
1:F:844:GLN:NE2	2:M:79:LYS:NZ	2.57	0.51
2:K:60:GLY:N	2:K:63:THR:OG1	2.34	0.51
3:P:50:SER:HB3	3:Q:45:ARG:HH12	1.74	0.51
1:B:692:VAL:HG12	1:B:693:HIS:ND1	2.26	0.51
1:B:1030:TRP:CD1	1:B:1037:CYS:HG	2.28	0.51
1:C:692:VAL:HG12	1:C:693:HIS:ND1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1086:GLY:HA2	2:L:39:LYS:HE2	1.92	0.51
1:F:530:ARG:HD2	1:F:545:GLN:HE22	1.75	0.51
1:F:1126:HIS:CE1	1:F:1129:CYS:H	2.28	0.51
1:C:365:ASP:OD1	1:C:444:PHE:CE1	2.63	0.51
1:G:1086:GLY:HA2	2:N:39:LYS:HE2	1.92	0.51
1:G:1086:GLY:CA	2:N:39:LYS:NZ	2.66	0.51
1:G:1126:HIS:CE1	1:G:1129:CYS:H	2.28	0.51
2:L:60:GLY:N	2:L:63:THR:OG1	2.34	0.51
1:A:400:LEU:HB3	1:A:404:TRP:CZ3	2.46	0.51
1:A:631:ALA:HB1	1:A:639:LEU:HD11	1.91	0.51
1:B:725:LEU:HB2	1:B:739:MET:HB2	1.92	0.51
1:B:864:VAL:HG23	1:B:885:VAL:HG21	1.92	0.51
1:C:945:ARG:HD2	1:C:961:GLU:HB2	1.92	0.51
1:D:336:ASN:HB2	1:E:431:LYS:HE3	1.93	0.51
1:D:400:LEU:HB3	1:D:404:TRP:CZ3	2.46	0.51
1:F:265:ARG:NH1	1:F:371:SER:OG	2.37	0.51
1:F:762:SER:OG	1:F:764:ASP:OD1	2.26	0.51
2:H:60:GLY:N	2:H:63:THR:OG1	2.34	0.51
1:C:530:ARG:HD2	1:C:545:GLN:HE22	1.76	0.51
1:E:1126:HIS:CE1	1:E:1129:CYS:H	2.28	0.51
1:G:152:ILE:HD11	1:G:263:THR:HG22	1.92	0.51
3:P:32:ARG:HD2	3:P:76:CYS:SG	2.51	0.51
1:B:530:ARG:HD2	1:B:545:GLN:HE22	1.76	0.51
1:B:1002:HIS:ND1	1:B:1024:ASP:OD2	2.44	0.51
1:C:562:ASN:HB2	1:C:565:GLN:HG2	1.93	0.51
1:C:762:SER:OG	1:C:764:ASP:OD1	2.26	0.51
1:F:334:PHE:HE1	1:G:416:GLN:HE21	1.58	0.51
1:F:725:LEU:HB2	1:F:739:MET:HB2	1.92	0.51
1:G:530:ARG:HD2	1:G:545:GLN:HE22	1.76	0.51
1:G:725:LEU:HB2	1:G:739:MET:HB2	1.92	0.51
1:G:882:LEU:HD12	1:G:1176:HIS:NE2	2.25	0.51
1:A:152:ILE:HD11	1:A:263:THR:HG22	1.92	0.50
1:A:864:VAL:HG23	1:A:885:VAL:HG21	1.92	0.50
1:B:608:ARG:HD2	1:B:910:GLU:HB2	1.94	0.50
1:C:844:GLN:NE2	2:J:79:LYS:NZ	2.57	0.50
1:D:562:ASN:HB2	1:D:565:GLN:HG2	1.94	0.50
1:D:945:ARG:HD2	1:D:961:GLU:HB2	1.92	0.50
1:E:692:VAL:HG12	1:E:693:HIS:ND1	2.26	0.50
1:F:864:VAL:HG23	1:F:885:VAL:HG21	1.92	0.50
2:I:60:GLY:N	2:I:63:THR:OG1	2.34	0.50
3:O:32:ARG:HD2	3:O:76:CYS:SG	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:GLU:HG3	1:B:721:SER:HB2	1.94	0.50
1:C:1002:HIS:ND1	1:C:1024:ASP:OD2	2.45	0.50
1:D:1002:HIS:ND1	1:D:1024:ASP:OD2	2.44	0.50
1:E:400:LEU:HB3	1:E:404:TRP:CZ3	2.46	0.50
1:E:844:GLN:HE22	2:L:79:LYS:HZ2	1.59	0.50
1:F:862:TYR:HB3	1:F:884:TRP:CA	2.42	0.50
1:F:1002:HIS:ND1	1:F:1024:ASP:OD2	2.44	0.50
1:A:334:PHE:HE1	1:B:416:GLN:HE21	1.58	0.50
1:A:608:ARG:HD2	1:A:910:GLU:HB2	1.94	0.50
1:A:1002:HIS:ND1	1:A:1024:ASP:OD2	2.44	0.50
1:B:344:GLN:OE1	1:B:349:GLN:NE2	2.44	0.50
1:B:562:ASN:HB2	1:B:565:GLN:HG2	1.94	0.50
1:C:1086:GLY:HA2	2:J:39:LYS:HE2	1.92	0.50
1:G:819:ASN:ND2	1:G:840:HIS:O	2.45	0.50
1:C:348:LYS:NZ	1:C:443:ASP:OD1	2.45	0.50
1:G:692:VAL:HG12	1:G:693:HIS:ND1	2.26	0.50
1:G:1002:HIS:ND1	1:G:1024:ASP:OD2	2.44	0.50
3:P:15:ARG:HD2	3:P:19:GLU:OE2	2.07	0.50
1:A:431:LYS:HE3	1:G:336:ASN:HB2	1.92	0.50
1:A:482:TYR:OH	1:A:490:HIS:NE2	2.35	0.50
1:A:762:SER:OG	1:A:764:ASP:OD1	2.26	0.50
1:B:631:ALA:HB1	1:B:639:LEU:HD11	1.91	0.50
1:D:155:MET:HE1	1:D:441:GLN:HG3	1.92	0.50
1:E:562:ASN:HB2	1:E:565:GLN:HG2	1.94	0.50
1:E:862:TYR:HB3	1:E:884:TRP:CA	2.42	0.50
1:E:1030:TRP:CD1	1:E:1037:CYS:HG	2.28	0.50
1:F:152:ILE:HD11	1:F:263:THR:HG22	1.92	0.50
1:G:400:LEU:HB3	1:G:404:TRP:CZ3	2.46	0.50
3:Q:52:ARG:HD2	3:R:38:HIS:ND1	2.22	0.50
1:B:152:ILE:HD11	1:B:263:THR:HG22	1.92	0.50
1:B:348:LYS:NZ	1:B:443:ASP:OD1	2.45	0.50
1:C:882:LEU:HD12	1:C:1176:HIS:NE2	2.25	0.50
1:D:265:ARG:NH1	1:D:371:SER:OG	2.37	0.50
1:D:348:LYS:NZ	1:D:443:ASP:OD1	2.45	0.50
1:E:463:GLN:OE1	1:E:466:ARG:NH2	2.28	0.50
1:F:562:ASN:HB2	1:F:565:GLN:HG2	1.93	0.50
1:F:819:ASN:ND2	1:F:840:HIS:O	2.45	0.50
1:G:646:THR:HG23	1:G:648:GLU:HG3	1.94	0.50
1:A:700:GLU:HG3	1:A:721:SER:HB2	1.94	0.50
1:A:819:ASN:ND2	1:A:840:HIS:O	2.45	0.50
1:C:631:ALA:HB1	1:C:639:LEU:HD11	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:GLU:HG3	1:C:721:SER:HB2	1.94	0.50
1:D:692:VAL:HG12	1:D:693:HIS:ND1	2.26	0.50
1:E:155:MET:HE1	1:E:441:GLN:HG3	1.92	0.50
1:F:862:TYR:OH	1:F:1237:ASN:O	2.30	0.50
3:R:32:ARG:HD2	3:R:76:CYS:SG	2.51	0.50
1:A:155:MET:HE1	1:A:441:GLN:HG3	1.92	0.50
1:C:152:ILE:HD11	1:C:263:THR:HG22	1.92	0.50
1:C:825:ASP:HB2	1:C:832:LEU:HD22	1.93	0.50
1:D:1086:GLY:HA2	2:K:39:LYS:HE2	1.92	0.50
1:D:1222:LYS:HB3	1:D:1224:HIS:HE1	1.77	0.50
1:E:1002:HIS:ND1	1:E:1024:ASP:OD2	2.44	0.50
1:F:400:LEU:HB3	1:F:404:TRP:CZ3	2.46	0.50
1:A:298:PHE:HD2	1:A:328:GLY:HA3	1.77	0.50
1:A:562:ASN:HB2	1:A:565:GLN:HG2	1.93	0.50
1:B:825:ASP:HB2	1:B:832:LEU:HD22	1.93	0.50
1:C:155:MET:HE1	1:C:441:GLN:HG3	1.92	0.50
1:C:608:ARG:HD2	1:C:910:GLU:HB2	1.94	0.50
1:C:819:ASN:ND2	1:C:840:HIS:O	2.45	0.50
1:D:819:ASN:ND2	1:D:840:HIS:O	2.45	0.50
1:E:348:LYS:NZ	1:E:443:ASP:OD1	2.45	0.50
1:E:862:TYR:OH	1:E:1237:ASN:O	2.30	0.50
1:A:365:ASP:OD1	1:A:444:PHE:HE1	1.95	0.49
1:A:646:THR:HG23	1:A:648:GLU:HG3	1.94	0.49
1:A:1222:LYS:HB3	1:A:1224:HIS:HE1	1.77	0.49
1:B:819:ASN:ND2	1:B:840:HIS:O	2.45	0.49
1:D:152:ILE:HD11	1:D:263:THR:HG22	1.92	0.49
1:D:365:ASP:OD1	1:D:444:PHE:HE1	1.95	0.49
1:F:646:THR:HG23	1:F:648:GLU:HG3	1.94	0.49
1:G:298:PHE:HD2	1:G:328:GLY:HA3	1.77	0.49
1:G:862:TYR:HB3	1:G:884:TRP:CA	2.42	0.49
1:G:862:TYR:OH	1:G:1237:ASN:O	2.30	0.49
2:I:41:GLY:HA2	2:I:48:TYR:CE1	2.47	0.49
2:J:41:GLY:HA2	2:J:48:TYR:CE1	2.47	0.49
3:Q:16:LEU:O	3:Q:20:LEU:HB2	2.12	0.49
1:A:1086:GLY:HA2	2:H:39:LYS:HE2	1.92	0.49
1:B:155:MET:HE1	1:B:441:GLN:HG3	1.92	0.49
1:B:1222:LYS:HB3	1:B:1224:HIS:HE1	1.77	0.49
1:E:819:ASN:ND2	1:E:840:HIS:O	2.45	0.49
1:E:884:TRP:CE3	2:L:81:ILE:HD11	2.48	0.49
1:F:155:MET:HE1	1:F:441:GLN:HG3	1.92	0.49
1:F:298:PHE:HD2	1:F:328:GLY:HA3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:463:GLN:OE1	1:F:466:ARG:NH2	2.28	0.49
1:F:1222:LYS:HB3	1:F:1224:HIS:HE1	1.77	0.49
1:G:155:MET:HE1	1:G:441:GLN:HG3	1.92	0.49
1:G:562:ASN:HB2	1:G:565:GLN:HG2	1.94	0.49
2:H:41:GLY:HA2	2:H:48:TYR:CE1	2.47	0.49
3:R:16:LEU:O	3:R:20:LEU:HB2	2.12	0.49
1:C:365:ASP:OD1	1:C:444:PHE:HE1	1.96	0.49
1:C:862:TYR:HB3	1:C:884:TRP:CA	2.42	0.49
1:C:884:TRP:CE3	2:J:81:ILE:HD11	2.48	0.49
1:D:762:SER:OG	1:D:764:ASP:OD1	2.26	0.49
1:E:762:SER:OG	1:E:764:ASP:OD1	2.26	0.49
1:F:884:TRP:CE3	2:M:81:ILE:HD11	2.47	0.49
1:G:1020:SER:HB2	1:G:1028:GLN:HE21	1.77	0.49
2:K:41:GLY:HA2	2:K:48:TYR:CE1	2.47	0.49
1:A:265:ARG:NH1	1:A:371:SER:OG	2.37	0.49
1:A:331:LEU:HD13	1:A:338:TRP:CH2	2.48	0.49
1:A:348:LYS:NZ	1:A:443:ASP:OD1	2.45	0.49
1:C:1087:THR:N	2:J:39:LYS:HZ3	2.10	0.49
1:C:1222:LYS:HB3	1:C:1224:HIS:HE1	1.77	0.49
1:D:825:ASP:HB2	1:D:832:LEU:HD22	1.93	0.49
1:E:152:ILE:HD11	1:E:263:THR:HG22	1.92	0.49
1:F:365:ASP:OD1	1:F:444:PHE:HE1	1.96	0.49
1:F:700:GLU:HG3	1:F:721:SER:HB2	1.94	0.49
2:N:41:GLY:HA2	2:N:48:TYR:CE1	2.47	0.49
3:Q:32:ARG:HD2	3:Q:76:CYS:SG	2.52	0.49
1:A:825:ASP:HB2	1:A:832:LEU:HD22	1.93	0.49
1:B:298:PHE:HD2	1:B:328:GLY:HA3	1.77	0.49
1:B:885:VAL:HG12	1:B:887:GLY:N	2.28	0.49
1:B:1086:GLY:HA2	2:I:39:LYS:HE2	1.92	0.49
1:D:646:THR:HG23	1:D:648:GLU:HG3	1.94	0.49
1:D:700:GLU:HG3	1:D:721:SER:HB2	1.94	0.49
1:D:862:TYR:OH	1:D:1237:ASN:O	2.30	0.49
1:D:884:TRP:CE3	2:K:81:ILE:HD11	2.47	0.49
1:E:700:GLU:HG3	1:E:721:SER:HB2	1.94	0.49
2:I:40:THR:HG22	2:I:59:TRP:CE2	2.48	0.49
1:B:118:GLY:O	1:B:184:TRP:HB2	2.13	0.49
1:B:862:TYR:HB3	1:B:884:TRP:CA	2.42	0.49
1:D:31:SER:HA	3:Q:11:ARG:HA	1.95	0.49
1:D:334:PHE:HE1	1:E:416:GLN:HE21	1.60	0.49
1:E:885:VAL:HG12	1:E:887:GLY:N	2.28	0.49
1:F:118:GLY:O	1:F:184:TRP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:348:LYS:NZ	1:F:443:ASP:OD1	2.45	0.49
1:F:825:ASP:HB2	1:F:832:LEU:HD22	1.93	0.49
1:G:608:ARG:HD2	1:G:910:GLU:HB2	1.94	0.49
1:A:862:TYR:HB3	1:A:884:TRP:CA	2.42	0.49
1:B:334:PHE:HE1	1:C:416:GLN:HE21	1.60	0.49
1:B:884:TRP:CE3	2:I:81:ILE:HD11	2.48	0.49
1:D:118:GLY:O	1:D:184:TRP:HB2	2.13	0.49
1:D:565:GLN:NE2	1:D:1213:PHE:HA	2.28	0.49
1:E:265:ARG:NH1	1:E:371:SER:OG	2.37	0.49
1:E:365:ASP:OD1	1:E:444:PHE:HE1	1.95	0.49
1:E:844:GLN:NE2	2:L:79:LYS:NZ	2.57	0.49
1:F:608:ARG:HD2	1:F:910:GLU:HB2	1.94	0.49
1:G:346:GLN:C	1:G:348:LYS:N	2.71	0.49
1:G:825:ASP:HB2	1:G:832:LEU:HD22	1.93	0.49
1:G:1222:LYS:HB3	1:G:1224:HIS:HE1	1.76	0.49
1:A:862:TYR:OH	1:A:1237:ASN:O	2.30	0.49
1:C:118:GLY:O	1:C:184:TRP:HB2	2.13	0.49
1:C:885:VAL:HG12	1:C:887:GLY:N	2.28	0.49
1:C:1020:SER:HB2	1:C:1028:GLN:HE21	1.77	0.49
1:D:1020:SER:HB2	1:D:1028:GLN:HE21	1.77	0.49
1:E:331:LEU:HD13	1:E:338:TRP:CH2	2.48	0.49
1:E:825:ASP:HB2	1:E:832:LEU:HD22	1.93	0.49
2:L:41:GLY:HA2	2:L:48:TYR:CE1	2.47	0.49
2:M:40:THR:HG22	2:M:59:TRP:CE2	2.48	0.49
3:O:16:LEU:O	3:O:20:LEU:HB2	2.12	0.49
1:B:365:ASP:OD1	1:B:444:PHE:HE1	1.96	0.49
1:B:929:VAL:HB	1:B:936:MET:HB2	1.95	0.49
1:D:569:CYS:CB	1:D:600:LYS:HZ3	2.25	0.49
1:D:862:TYR:HB3	1:D:884:TRP:CA	2.42	0.49
1:E:298:PHE:HD2	1:E:328:GLY:HA3	1.77	0.49
1:E:608:ARG:HD2	1:E:910:GLU:HB2	1.94	0.49
1:F:331:LEU:HD13	1:F:338:TRP:CH2	2.47	0.49
1:F:565:GLN:NE2	1:F:1213:PHE:HA	2.28	0.49
2:H:40:THR:HG22	2:H:59:TRP:CE2	2.48	0.49
2:J:40:THR:HG22	2:J:59:TRP:CE2	2.48	0.49
2:L:40:THR:HG22	2:L:59:TRP:CE2	2.48	0.49
1:A:885:VAL:HG12	1:A:887:GLY:N	2.28	0.49
1:B:265:ARG:NH1	1:B:371:SER:OG	2.37	0.49
1:B:1203:ASN:OD1	1:B:1204:VAL:N	2.46	0.49
1:C:331:LEU:HD13	1:C:338:TRP:CH2	2.47	0.49
1:C:646:THR:HG23	1:C:648:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1086:GLY:HA2	2:M:39:LYS:HE2	1.92	0.49
1:G:700:GLU:HG3	1:G:721:SER:HB2	1.94	0.49
1:B:646:THR:HG23	1:B:648:GLU:HG3	1.94	0.48
1:C:565:GLN:NE2	1:C:1213:PHE:HA	2.28	0.48
1:D:608:ARG:HD2	1:D:910:GLU:HB2	1.94	0.48
1:D:1026:GLU:HG3	1:D:1041:ARG:HG2	1.95	0.48
1:D:1203:ASN:OD1	1:D:1204:VAL:N	2.46	0.48
1:E:646:THR:HG23	1:E:648:GLU:HG3	1.94	0.48
1:E:1203:ASN:OD1	1:E:1204:VAL:N	2.46	0.48
1:G:118:GLY:O	1:G:184:TRP:HB2	2.13	0.48
1:G:565:GLN:NE2	1:G:1213:PHE:HA	2.28	0.48
1:G:884:TRP:CE3	2:N:81:ILE:HD11	2.47	0.48
1:A:346:GLN:C	1:A:348:LYS:N	2.71	0.48
1:A:565:GLN:NE2	1:A:1213:PHE:HA	2.28	0.48
1:A:884:TRP:CE3	2:H:81:ILE:HD11	2.47	0.48
1:B:346:GLN:C	1:B:348:LYS:N	2.71	0.48
1:B:565:GLN:NE2	1:B:1213:PHE:HA	2.28	0.48
1:B:862:TYR:OH	1:B:1237:ASN:O	2.30	0.48
1:D:113:VAL:HG11	1:D:174:LEU:HD21	1.95	0.48
1:D:885:VAL:HG12	1:D:887:GLY:N	2.28	0.48
1:E:568:LEU:HD13	1:E:595:LEU:O	2.13	0.48
1:E:1026:GLU:HG3	1:E:1041:ARG:HG2	1.95	0.48
1:E:1222:LYS:HB3	1:E:1224:HIS:HE1	1.77	0.48
1:F:752:SER:HB2	1:F:753:PRO:HD2	1.95	0.48
1:G:1026:GLU:HG3	1:G:1041:ARG:HG2	1.95	0.48
1:G:1203:ASN:OD1	1:G:1204:VAL:N	2.46	0.48
2:K:40:THR:HG22	2:K:59:TRP:CE2	2.48	0.48
2:M:41:GLY:HA2	2:M:48:TYR:CE1	2.47	0.48
3:P:16:LEU:O	3:P:20:LEU:HB2	2.12	0.48
1:A:118:GLY:O	1:A:184:TRP:HB2	2.13	0.48
1:A:568:LEU:HD13	1:A:595:LEU:O	2.13	0.48
1:A:929:VAL:HB	1:A:936:MET:HB2	1.95	0.48
1:C:346:GLN:C	1:C:348:LYS:N	2.71	0.48
1:E:113:VAL:HG11	1:E:174:LEU:HD21	1.95	0.48
1:E:1020:SER:HB2	1:E:1028:GLN:HE21	1.77	0.48
1:F:885:VAL:HG12	1:F:887:GLY:N	2.28	0.48
1:F:1179:TRP:NE1	1:F:1220:LEU:H	2.12	0.48
1:G:752:SER:HB2	1:G:753:PRO:HD2	1.95	0.48
1:A:196:LEU:HG	1:A:200:GLN:HE22	1.78	0.48
1:A:1026:GLU:HG3	1:A:1041:ARG:HG2	1.95	0.48
1:B:1198:TYR:HA	1:B:1215:THR:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:LEU:HD13	1:D:595:LEU:O	2.13	0.48
1:E:230:LEU:O	1:E:234:LYS:N	2.41	0.48
1:E:565:GLN:NE2	1:E:1213:PHE:HA	2.28	0.48
1:F:344:GLN:OE1	1:F:349:GLN:NE2	2.44	0.48
1:F:1026:GLU:HG3	1:F:1041:ARG:HG2	1.95	0.48
1:G:550:LEU:HD23	1:G:607:SER:HB2	1.91	0.48
1:B:331:LEU:HD13	1:B:338:TRP:CH2	2.48	0.48
1:B:1191:MET:SD	1:B:1209:SER:OG	2.63	0.48
1:C:113:VAL:HG11	1:C:174:LEU:HD21	1.95	0.48
1:C:862:TYR:OH	1:C:1237:ASN:O	2.30	0.48
1:C:929:VAL:HB	1:C:936:MET:HB2	1.95	0.48
1:C:1026:GLU:HG3	1:C:1041:ARG:HG2	1.95	0.48
1:C:1198:TYR:HA	1:C:1215:THR:HB	1.96	0.48
1:D:1198:TYR:HA	1:D:1215:THR:HB	1.96	0.48
1:E:1179:TRP:NE1	1:E:1220:LEU:H	2.12	0.48
1:F:569:CYS:HB3	1:F:600:LYS:HZ3	1.78	0.48
1:F:884:TRP:HH2	2:M:78:THR:C	2.22	0.48
1:G:331:LEU:HD13	1:G:338:TRP:CH2	2.48	0.48
1:G:885:VAL:HG12	1:G:887:GLY:N	2.28	0.48
2:N:40:THR:HG22	2:N:59:TRP:CE2	2.48	0.48
1:B:1020:SER:HB2	1:B:1028:GLN:HE21	1.77	0.48
1:C:298:PHE:HD2	1:C:328:GLY:HA3	1.77	0.48
1:D:298:PHE:HD2	1:D:328:GLY:HA3	1.77	0.48
1:F:196:LEU:HG	1:F:200:GLN:HE22	1.78	0.48
1:G:884:TRP:HH2	2:N:78:THR:C	2.22	0.48
1:A:113:VAL:HG11	1:A:174:LEU:HD21	1.95	0.48
1:A:1203:ASN:OD1	1:A:1204:VAL:N	2.46	0.48
1:B:113:VAL:HG11	1:B:174:LEU:HD21	1.95	0.48
1:B:752:SER:HB2	1:B:753:PRO:HD2	1.95	0.48
1:C:569:CYS:HB3	1:C:600:LYS:HZ3	1.78	0.48
1:D:331:LEU:HD13	1:D:338:TRP:CH2	2.48	0.48
1:D:752:SER:HB2	1:D:753:PRO:HD2	1.95	0.48
1:E:1198:TYR:HA	1:E:1215:THR:HB	1.96	0.48
1:F:1203:ASN:OD1	1:F:1204:VAL:N	2.46	0.48
1:A:266:ASP:CG	1:A:268:SER:H	2.20	0.48
1:C:170:ASP:OD2	1:C:172:SER:OG	2.32	0.48
1:D:326:LEU:HA	1:D:326:LEU:HD23	1.44	0.48
1:E:265:ARG:HH11	1:E:371:SER:HG	1.57	0.48
1:E:497:HIS:HA	1:E:500:LEU:HB3	1.96	0.48
1:F:113:VAL:HG11	1:F:174:LEU:HD21	1.95	0.48
1:F:497:HIS:HA	1:F:500:LEU:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1020:SER:HB2	1:F:1028:GLN:HE21	1.77	0.48
1:G:541:SER:O	1:G:545:GLN:HG3	2.14	0.48
1:G:929:VAL:HB	1:G:936:MET:HB2	1.95	0.48
1:A:884:TRP:HH2	2:H:78:THR:C	2.22	0.48
1:A:1198:TYR:HA	1:A:1215:THR:HB	1.96	0.48
1:B:497:HIS:HA	1:B:500:LEU:HB3	1.95	0.48
1:B:882:LEU:HD12	1:B:1176:HIS:NE2	2.25	0.48
1:B:1026:GLU:HG3	1:B:1041:ARG:HG2	1.95	0.48
1:D:14:GLU:OE1	1:E:31:SER:CB	2.62	0.48
1:D:929:VAL:HB	1:D:936:MET:HB2	1.95	0.48
1:E:118:GLY:O	1:E:184:TRP:HB2	2.13	0.48
1:E:170:ASP:OD2	1:E:172:SER:OG	2.32	0.48
1:E:346:GLN:C	1:E:348:LYS:N	2.71	0.48
1:E:884:TRP:HH2	2:L:78:THR:C	2.22	0.48
1:G:113:VAL:HG11	1:G:174:LEU:HD21	1.95	0.48
1:G:196:LEU:HG	1:G:200:GLN:HE22	1.78	0.48
1:G:568:LEU:HD13	1:G:595:LEU:O	2.13	0.48
1:G:762:SER:OG	1:G:764:ASP:OD1	2.26	0.48
1:G:1179:TRP:NE1	1:G:1220:LEU:H	2.12	0.48
1:A:330:LEU:HD13	1:A:341:TYR:OH	2.14	0.48
1:B:196:LEU:HG	1:B:200:GLN:HE22	1.78	0.48
1:C:541:SER:O	1:C:545:GLN:HG3	2.14	0.48
1:C:568:LEU:HD13	1:C:595:LEU:O	2.13	0.48
1:D:541:SER:O	1:D:545:GLN:HG3	2.14	0.48
1:D:550:LEU:HD23	1:D:607:SER:HB2	1.91	0.48
1:D:1179:TRP:NE1	1:D:1220:LEU:H	2.12	0.48
1:E:158:CYS:SG	1:E:159:GLY:N	2.87	0.48
1:E:196:LEU:HG	1:E:200:GLN:HE22	1.78	0.48
1:E:929:VAL:HB	1:E:936:MET:HB2	1.95	0.48
1:F:158:CYS:SG	1:F:159:GLY:N	2.87	0.48
1:F:346:GLN:C	1:F:348:LYS:N	2.71	0.48
1:F:550:LEU:HD23	1:F:607:SER:HB2	1.91	0.48
1:F:568:LEU:HD13	1:F:595:LEU:O	2.13	0.48
1:G:266:ASP:CG	1:G:268:SER:H	2.20	0.48
1:G:348:LYS:NZ	1:G:443:ASP:OD1	2.45	0.48
1:A:1179:TRP:NE1	1:A:1220:LEU:H	2.12	0.47
1:B:569:CYS:HB3	1:B:600:LYS:HZ3	1.79	0.47
1:D:330:LEU:HD13	1:D:341:TYR:OH	2.14	0.47
1:E:752:SER:HB2	1:E:753:PRO:HD2	1.95	0.47
1:G:365:ASP:OD1	1:G:444:PHE:HE1	1.95	0.47
1:A:344:GLN:OE1	1:A:349:GLN:NE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:SER:HB2	1:A:753:PRO:HD2	1.95	0.47
1:B:568:LEU:HD13	1:B:595:LEU:O	2.13	0.47
1:C:330:LEU:HD13	1:C:341:TYR:OH	2.14	0.47
1:C:884:TRP:HH2	2:J:78:THR:C	2.22	0.47
1:D:884:TRP:HH2	2:K:78:THR:C	2.22	0.47
1:A:541:SER:O	1:A:545:GLN:HG3	2.14	0.47
1:A:1020:SER:HB2	1:A:1028:GLN:HE21	1.77	0.47
1:B:884:TRP:HH2	2:I:78:THR:C	2.22	0.47
1:C:497:HIS:HA	1:C:500:LEU:HB3	1.96	0.47
1:C:1203:ASN:OD1	1:C:1204:VAL:N	2.46	0.47
1:D:344:GLN:OE1	1:D:349:GLN:NE2	2.44	0.47
1:F:330:LEU:HD13	1:F:341:TYR:OH	2.14	0.47
1:F:844:GLN:HE22	2:M:79:LYS:HZ2	1.61	0.47
1:F:1198:TYR:HA	1:F:1215:THR:HB	1.96	0.47
1:A:109:TYR:CE1	1:G:4:LYS:CD	2.58	0.47
1:B:821:ILE:HB	1:B:835:ILE:HB	1.97	0.47
1:C:155:MET:HE3	1:C:368:MET:HE1	1.97	0.47
1:C:344:GLN:OE1	1:C:349:GLN:NE2	2.44	0.47
1:D:196:LEU:HG	1:D:200:GLN:HE22	1.78	0.47
1:E:1131:ARG:H	1:E:1146:ASP:HA	1.80	0.47
1:G:158:CYS:SG	1:G:159:GLY:N	2.87	0.47
1:A:106:ILE:HA	1:A:110:VAL:HG21	1.97	0.47
1:A:155:MET:HE3	1:A:368:MET:HE1	1.97	0.47
1:B:155:MET:HE3	1:B:368:MET:HE1	1.97	0.47
1:B:170:ASP:OD2	1:B:172:SER:OG	2.32	0.47
1:B:266:ASP:CG	1:B:268:SER:H	2.20	0.47
1:C:752:SER:HB2	1:C:753:PRO:HD2	1.95	0.47
1:C:821:ILE:HB	1:C:835:ILE:HB	1.97	0.47
1:D:155:MET:HE3	1:D:368:MET:HE1	1.97	0.47
1:E:330:LEU:HD13	1:E:341:TYR:OH	2.14	0.47
1:F:541:SER:O	1:F:545:GLN:HG3	2.14	0.47
1:B:230:LEU:O	1:B:234:LYS:N	2.41	0.47
1:C:1131:ARG:H	1:C:1146:ASP:HA	1.80	0.47
1:C:1179:TRP:NE1	1:C:1220:LEU:H	2.12	0.47
1:E:160:LYS:HB3	4:E:1301:DTP:O1B	2.15	0.47
1:F:266:ASP:CG	1:F:268:SER:H	2.20	0.47
1:G:600:LYS:HZ1	1:G:1213:PHE:HZ	1.63	0.47
2:K:39:LYS:HB2	2:K:42:GLN:HG3	1.97	0.47
2:L:39:LYS:HB2	2:L:42:GLN:HG3	1.97	0.47
1:A:230:LEU:O	1:A:234:LYS:N	2.41	0.47
1:A:337:ARG:NH1	1:B:409:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:HIS:HA	1:A:500:LEU:HB3	1.96	0.47
1:A:550:LEU:HD23	1:A:607:SER:HB2	1.91	0.47
1:A:600:LYS:HZ1	1:A:1213:PHE:HZ	1.63	0.47
1:A:1032:TRP:C	1:A:1034:LEU:H	2.23	0.47
1:B:158:CYS:SG	1:B:159:GLY:N	2.87	0.47
1:B:330:LEU:HD13	1:B:341:TYR:OH	2.14	0.47
1:B:1179:TRP:NE1	1:B:1220:LEU:H	2.12	0.47
1:B:1221:LYS:HE3	1:B:1222:LYS:HE3	1.97	0.47
1:D:346:GLN:C	1:D:348:LYS:N	2.71	0.47
1:D:497:HIS:HA	1:D:500:LEU:HB3	1.96	0.47
1:D:821:ILE:HB	1:D:835:ILE:HB	1.97	0.47
1:D:1131:ARG:H	1:D:1146:ASP:HA	1.80	0.47
1:E:344:GLN:OE1	1:E:349:GLN:NE2	2.44	0.47
1:E:541:SER:O	1:E:545:GLN:HG3	2.14	0.47
1:F:106:ILE:HA	1:F:110:VAL:HG21	1.97	0.47
1:F:160:LYS:HB3	4:F:1301:DTP:O1B	2.15	0.47
1:F:1131:ARG:H	1:F:1146:ASP:HA	1.80	0.47
1:G:106:ILE:HA	1:G:110:VAL:HG21	1.97	0.47
1:G:497:HIS:HA	1:G:500:LEU:HB3	1.96	0.47
1:G:1198:TYR:HA	1:G:1215:THR:HB	1.96	0.47
2:I:39:LYS:HB2	2:I:42:GLN:HG3	1.97	0.47
1:A:158:CYS:SG	1:A:159:GLY:N	2.87	0.47
1:A:170:ASP:OD2	1:A:172:SER:OG	2.32	0.47
1:A:1221:LYS:HE3	1:A:1222:LYS:HE3	1.97	0.47
1:B:337:ARG:NH1	1:C:409:GLU:OE2	2.48	0.47
1:B:541:SER:O	1:B:545:GLN:HG3	2.14	0.47
1:C:158:CYS:SG	1:C:159:GLY:N	2.87	0.47
1:C:196:LEU:HG	1:C:200:GLN:HE22	1.78	0.47
1:D:158:CYS:SG	1:D:159:GLY:N	2.87	0.47
1:A:821:ILE:HB	1:A:835:ILE:HB	1.97	0.47
1:B:106:ILE:HA	1:B:110:VAL:HG21	1.97	0.47
1:B:1222:LYS:HB3	1:B:1224:HIS:CE1	2.50	0.47
1:D:170:ASP:OD2	1:D:172:SER:OG	2.32	0.47
1:D:230:LEU:O	1:D:234:LYS:N	2.41	0.47
1:F:929:VAL:HB	1:F:936:MET:HB2	1.95	0.47
1:A:1131:ARG:H	1:A:1146:ASP:HA	1.80	0.47
1:A:1222:LYS:HB3	1:A:1224:HIS:CE1	2.50	0.47
1:B:570:GLU:HB2	1:B:577:TYR:HB2	1.97	0.47
1:C:266:ASP:CG	1:C:268:SER:H	2.20	0.47
1:C:1222:LYS:HB3	1:C:1224:HIS:CE1	2.50	0.47
1:D:337:ARG:NH1	1:E:409:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1222:LYS:HB3	1:D:1224:HIS:CE1	2.50	0.47
1:E:155:MET:HE3	1:E:368:MET:HE1	1.97	0.47
1:E:1222:LYS:HB3	1:E:1224:HIS:CE1	2.50	0.47
2:J:39:LYS:HB2	2:J:42:GLN:HG3	1.97	0.47
1:A:570:GLU:HB2	1:A:577:TYR:HB2	1.97	0.46
1:B:844:GLN:HE22	2:I:79:LYS:HZ2	1.60	0.46
1:C:230:LEU:O	1:C:234:LYS:N	2.41	0.46
1:E:266:ASP:CG	1:E:268:SER:H	2.20	0.46
1:C:612:ARG:HG3	1:C:904:GLN:O	2.16	0.46
1:C:1221:LYS:HE3	1:C:1222:LYS:HE3	1.97	0.46
1:D:160:LYS:HB3	4:D:1301:DTP:O1B	2.15	0.46
1:E:152:ILE:HG22	1:E:280:VAL:HB	1.97	0.46
1:G:155:MET:HE3	1:G:368:MET:HE1	1.97	0.46
1:G:330:LEU:HD13	1:G:341:TYR:OH	2.14	0.46
2:H:39:LYS:HB2	2:H:42:GLN:HG3	1.97	0.46
1:A:862:TYR:HB3	1:A:883:SER:C	2.41	0.46
1:B:160:LYS:HB3	4:B:1301:DTP:O1B	2.15	0.46
1:C:337:ARG:NH1	1:D:409:GLU:OE2	2.49	0.46
1:E:524:HIS:CB	1:E:646:THR:HG21	2.36	0.46
1:E:612:ARG:HG3	1:E:904:GLN:O	2.16	0.46
1:E:1221:LYS:HE3	1:E:1222:LYS:HE3	1.97	0.46
1:F:862:TYR:HB3	1:F:883:SER:C	2.41	0.46
1:G:1222:LYS:HB3	1:G:1224:HIS:CE1	2.50	0.46
2:I:70:ASN:HD22	2:I:73:LYS:HB2	1.81	0.46
2:M:39:LYS:HB2	2:M:42:GLN:HG3	1.97	0.46
1:A:160:LYS:HB3	4:A:1301:DTP:O1B	2.15	0.46
1:B:695:TYR:OH	1:B:732:GLN:O	2.31	0.46
1:B:862:TYR:HB3	1:B:884:TRP:N	2.31	0.46
1:B:1032:TRP:C	1:B:1034:LEU:H	2.23	0.46
1:D:266:ASP:CG	1:D:268:SER:H	2.20	0.46
1:E:106:ILE:HA	1:E:110:VAL:HG21	1.97	0.46
1:E:862:TYR:HB3	1:E:884:TRP:N	2.31	0.46
1:F:152:ILE:HG22	1:F:280:VAL:HB	1.97	0.46
1:G:1131:ARG:H	1:G:1146:ASP:HA	1.80	0.46
2:L:70:ASN:HD22	2:L:73:LYS:HB2	1.81	0.46
1:A:472:THR:O	1:A:473:LEU:HD12	2.16	0.46
1:A:888:VAL:HG12	1:A:899:THR:HA	1.98	0.46
1:C:524:HIS:CB	1:C:646:THR:HG21	2.36	0.46
1:D:152:ILE:HG22	1:D:280:VAL:HB	1.97	0.46
1:D:265:ARG:HH11	1:D:371:SER:HG	1.57	0.46
1:D:862:TYR:HB3	1:D:884:TRP:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:ARG:NH1	1:F:409:GLU:OE2	2.48	0.46
1:E:472:THR:O	1:E:473:LEU:HD12	2.16	0.46
1:E:821:ILE:HB	1:E:835:ILE:HB	1.97	0.46
1:G:160:LYS:HB3	4:G:1301:DTP:O1B	2.15	0.46
1:B:269:VAL:C	1:B:271:ASP:H	2.24	0.46
1:C:950:ASN:OD1	1:C:951:GLY:N	2.49	0.46
1:D:950:ASN:OD1	1:D:951:GLY:N	2.49	0.46
1:F:155:MET:HE3	1:F:368:MET:HE1	1.97	0.46
1:G:821:ILE:HB	1:G:835:ILE:HB	1.97	0.46
1:G:888:VAL:HG12	1:G:899:THR:HA	1.98	0.46
2:H:10:PHE:HA	2:H:14:CYS:HB2	1.98	0.46
1:B:862:TYR:HB3	1:B:883:SER:C	2.41	0.46
1:C:570:GLU:HB2	1:C:577:TYR:HB2	1.97	0.46
1:C:862:TYR:HB3	1:C:884:TRP:N	2.31	0.46
1:D:14:GLU:HB2	1:E:31:SER:HG	1.81	0.46
1:E:862:TYR:HB3	1:E:883:SER:C	2.41	0.46
1:F:170:ASP:OD2	1:F:172:SER:OG	2.32	0.46
1:F:1221:LYS:HE3	1:F:1222:LYS:HE3	1.97	0.46
1:G:152:ILE:HG22	1:G:280:VAL:HB	1.97	0.46
1:G:170:ASP:OD2	1:G:172:SER:OG	2.32	0.46
1:G:1011:PHE:HE1	1:G:1018:LEU:HD13	1.81	0.46
2:N:39:LYS:HB2	2:N:42:GLN:HG3	1.97	0.46
1:A:643:LYS:HD3	1:A:646:THR:HG22	1.98	0.46
1:A:1011:PHE:HE1	1:A:1018:LEU:HD13	1.81	0.46
1:B:590:ASN:C	1:B:592:MET:N	2.64	0.46
1:B:888:VAL:HG12	1:B:899:THR:HA	1.98	0.46
1:B:950:ASN:OD1	1:B:951:GLY:N	2.49	0.46
1:D:1011:PHE:HE1	1:D:1018:LEU:HD13	1.81	0.46
1:G:862:TYR:HB3	1:G:883:SER:C	2.41	0.46
1:G:1191:MET:SD	1:G:1209:SER:OG	2.63	0.46
2:J:98:LEU:O	2:J:102:THR:OG1	2.30	0.46
1:B:472:THR:O	1:B:473:LEU:HD12	2.16	0.46
1:B:643:LYS:HD3	1:B:646:THR:HG22	1.98	0.46
1:C:862:TYR:HB3	1:C:883:SER:C	2.41	0.46
1:D:106:ILE:HA	1:D:110:VAL:HG21	1.97	0.46
1:E:950:ASN:OD1	1:E:951:GLY:N	2.49	0.46
1:F:269:VAL:C	1:F:271:ASP:H	2.24	0.46
1:F:570:GLU:HB2	1:F:577:TYR:HB2	1.97	0.46
1:F:821:ILE:HB	1:F:835:ILE:HB	1.97	0.46
1:F:1222:LYS:HB3	1:F:1224:HIS:CE1	2.50	0.46
1:G:570:GLU:HB2	1:G:577:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:862:TYR:HB3	1:G:884:TRP:N	2.31	0.46
1:G:1032:TRP:C	1:G:1034:LEU:H	2.23	0.46
2:M:10:PHE:HA	2:M:14:CYS:HB2	1.98	0.46
2:M:70:ASN:HD22	2:M:73:LYS:HB2	1.81	0.46
2:N:10:PHE:HA	2:N:14:CYS:HB2	1.98	0.46
3:R:90:ARG:NH2	3:R:90:ARG:HG2	2.31	0.46
1:A:612:ARG:HG3	1:A:904:GLN:O	2.16	0.46
1:B:152:ILE:HG22	1:B:280:VAL:HB	1.97	0.46
1:F:950:ASN:OD1	1:F:951:GLY:N	2.49	0.46
1:F:1215:THR:HG21	1:F:1220:LEU:HD21	1.98	0.46
1:G:1215:THR:HG21	1:G:1220:LEU:HD21	1.98	0.46
2:H:70:ASN:HD22	2:H:73:LYS:HB2	1.81	0.46
1:A:950:ASN:OD1	1:A:951:GLY:N	2.49	0.45
1:A:1215:THR:HG21	1:A:1220:LEU:HD21	1.98	0.45
1:B:1215:THR:HG21	1:B:1220:LEU:HD21	1.99	0.45
1:C:160:LYS:HB3	4:C:1301:DTP:O1B	2.15	0.45
1:C:269:VAL:C	1:C:271:ASP:H	2.24	0.45
1:C:472:THR:O	1:C:473:LEU:HD12	2.16	0.45
1:C:1215:THR:HG21	1:C:1220:LEU:HD21	1.98	0.45
1:D:862:TYR:HB3	1:D:883:SER:C	2.41	0.45
1:D:1221:LYS:HE3	1:D:1222:LYS:HE3	1.97	0.45
1:E:550:LEU:HD23	1:E:607:SER:HB2	1.91	0.45
1:E:1011:PHE:HE1	1:E:1018:LEU:HD13	1.81	0.45
1:E:1032:TRP:C	1:E:1034:LEU:H	2.23	0.45
1:F:862:TYR:HB3	1:F:884:TRP:N	2.31	0.45
1:G:266:ASP:CG	1:G:268:SER:HG	2.22	0.45
1:G:472:THR:O	1:G:473:LEU:HD12	2.16	0.45
1:C:106:ILE:HA	1:C:110:VAL:HG21	1.97	0.45
1:C:844:GLN:HE22	2:J:79:LYS:HZ2	1.62	0.45
1:C:1011:PHE:HE1	1:C:1018:LEU:HD13	1.81	0.45
1:D:472:THR:O	1:D:473:LEU:HD12	2.16	0.45
1:D:570:GLU:HB2	1:D:577:TYR:HB2	1.97	0.45
1:D:1032:TRP:C	1:D:1034:LEU:H	2.23	0.45
1:G:269:VAL:C	1:G:271:ASP:H	2.24	0.45
1:G:1221:LYS:HE3	1:G:1222:LYS:HE3	1.97	0.45
2:J:68:LEU:HB3	2:J:85:ILE:HD12	1.98	0.45
2:K:68:LEU:HB3	2:K:85:ILE:HD12	1.98	0.45
3:O:90:ARG:NH2	3:O:90:ARG:HG2	2.31	0.45
3:Q:90:ARG:NH2	3:Q:90:ARG:HG2	2.31	0.45
1:A:298:PHE:CD2	1:A:328:GLY:HA3	2.52	0.45
1:A:461:ILE:HD11	1:A:491:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:THR:CG2	1:D:45:ASN:OD1	2.64	0.45
1:C:152:ILE:HG22	1:C:280:VAL:HB	1.97	0.45
1:F:1011:PHE:HE1	1:F:1018:LEU:HD13	1.81	0.45
2:I:10:PHE:HA	2:I:14:CYS:HB2	1.98	0.45
1:A:862:TYR:HB3	1:A:884:TRP:N	2.31	0.45
1:D:1215:THR:HG21	1:D:1220:LEU:HD21	1.98	0.45
1:E:1215:THR:HG21	1:E:1220:LEU:HD21	1.99	0.45
1:F:612:ARG:HG3	1:F:904:GLN:O	2.16	0.45
1:F:1086:GLY:C	2:M:39:LYS:HZ1	2.24	0.45
1:G:612:ARG:HG3	1:G:904:GLN:O	2.16	0.45
2:H:68:LEU:HB3	2:H:85:ILE:HD12	1.98	0.45
1:A:1150:GLU:HB2	1:A:1167:PRO:HG2	1.99	0.45
1:B:461:ILE:HD11	1:B:491:MET:HA	1.99	0.45
1:C:482:TYR:OH	1:C:490:HIS:NE2	2.35	0.45
1:E:334:PHE:HE1	1:F:416:GLN:HE21	1.63	0.45
1:E:570:GLU:HB2	1:E:577:TYR:HB2	1.97	0.45
1:F:472:THR:O	1:F:473:LEU:HD12	2.16	0.45
1:F:1150:GLU:HB2	1:F:1167:PRO:HG2	1.99	0.45
1:G:950:ASN:OD1	1:G:951:GLY:N	2.49	0.45
1:G:1150:GLU:HB2	1:G:1167:PRO:HG2	1.99	0.45
2:J:70:ASN:HD22	2:J:73:LYS:HB2	1.81	0.45
2:L:10:PHE:HA	2:L:14:CYS:HB2	1.98	0.45
1:A:152:ILE:HG22	1:A:280:VAL:HB	1.97	0.45
1:B:1131:ARG:H	1:B:1146:ASP:HA	1.80	0.45
1:B:1150:GLU:HB2	1:B:1167:PRO:HG2	1.99	0.45
1:C:643:LYS:HD3	1:C:646:THR:HG22	1.98	0.45
1:C:1191:MET:SD	1:C:1209:SER:OG	2.63	0.45
1:D:612:ARG:HG3	1:D:904:GLN:O	2.16	0.45
1:F:461:ILE:HD11	1:F:491:MET:HA	1.99	0.45
1:G:461:ILE:HD11	1:G:491:MET:HA	1.99	0.45
1:B:266:ASP:CG	1:B:268:SER:HG	2.23	0.45
1:B:298:PHE:CD2	1:B:328:GLY:HA3	2.52	0.45
1:B:612:ARG:HG3	1:B:904:GLN:O	2.16	0.45
1:B:821:ILE:HD11	1:B:857:VAL:HG21	1.99	0.45
1:C:888:VAL:HG12	1:C:899:THR:HA	1.98	0.45
1:E:821:ILE:HD11	1:E:857:VAL:HG21	1.99	0.45
1:F:888:VAL:HG12	1:F:899:THR:HA	1.98	0.45
2:K:10:PHE:HA	2:K:14:CYS:HB2	1.98	0.45
1:C:216:LEU:HA	1:C:217:PRO:HD2	1.84	0.45
1:C:821:ILE:HD11	1:C:857:VAL:HG21	1.99	0.45
1:C:1032:TRP:C	1:C:1034:LEU:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:695:TYR:OH	1:D:732:GLN:O	2.30	0.45
1:D:868:ASN:OD1	1:D:869:THR:N	2.50	0.45
1:E:269:VAL:C	1:E:271:ASP:H	2.24	0.45
1:F:326:LEU:HD23	1:F:326:LEU:HA	1.44	0.45
1:F:821:ILE:HD11	1:F:857:VAL:HG21	1.99	0.45
1:A:868:ASN:OD1	1:A:869:THR:N	2.50	0.45
1:B:868:ASN:OD1	1:B:869:THR:N	2.50	0.45
1:E:326:LEU:HD23	1:E:326:LEU:HA	1.44	0.45
1:E:590:ASN:C	1:E:592:MET:N	2.64	0.45
1:E:1150:GLU:HB2	1:E:1167:PRO:HG2	1.99	0.45
1:F:868:ASN:OD1	1:F:869:THR:N	2.50	0.45
1:G:143:LEU:C	1:G:145:GLY:N	2.75	0.45
1:G:298:PHE:CD2	1:G:328:GLY:HA3	2.52	0.45
2:J:10:PHE:HA	2:J:14:CYS:HB2	1.98	0.45
2:K:70:ASN:HD22	2:K:73:LYS:HB2	1.81	0.45
2:N:68:LEU:HB3	2:N:85:ILE:HD12	1.98	0.45
3:P:90:ARG:NH2	3:P:90:ARG:HG2	2.31	0.45
1:A:409:GLU:OE2	1:G:337:ARG:NH1	2.49	0.45
1:A:480:CYS:SG	1:A:481:MET:N	2.90	0.45
1:B:1011:PHE:HE1	1:B:1018:LEU:HD13	1.81	0.45
1:C:1150:GLU:HB2	1:C:1167:PRO:HG2	1.99	0.45
1:E:390:GLN:HB2	1:E:393:VAL:HG21	1.99	0.45
1:E:461:ILE:HD11	1:E:491:MET:HA	1.99	0.45
1:G:643:LYS:HD3	1:G:646:THR:HG22	1.98	0.45
1:G:868:ASN:OD1	1:G:869:THR:N	2.50	0.45
2:N:70:ASN:HD22	2:N:73:LYS:HB2	1.81	0.45
1:A:269:VAL:C	1:A:271:ASP:H	2.24	0.44
1:B:600:LYS:HA	1:B:603:ILE:HG13	2.00	0.44
1:D:266:ASP:CG	1:D:268:SER:HG	2.23	0.44
1:D:821:ILE:HD11	1:D:857:VAL:HG21	1.99	0.44
1:E:643:LYS:HD3	1:E:646:THR:HG22	1.98	0.44
2:I:72:LYS:NZ	2:I:78:THR:O	2.51	0.44
3:Q:41:GLU:HA	3:Q:44:GLN:HE21	1.83	0.44
1:A:821:ILE:HD11	1:A:857:VAL:HG21	1.99	0.44
1:C:868:ASN:OD1	1:C:869:THR:N	2.50	0.44
1:D:357:SER:OG	1:D:358:SER:N	2.50	0.44
1:D:888:VAL:HG12	1:D:899:THR:HA	1.98	0.44
1:D:1150:GLU:HB2	1:D:1167:PRO:HG2	1.99	0.44
1:E:7:ASN:CG	1:F:236:PRO:CG	2.81	0.44
1:E:480:CYS:SG	1:E:481:MET:N	2.90	0.44
1:F:230:LEU:O	1:F:234:LYS:N	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:643:LYS:HD3	1:F:646:THR:HG22	1.98	0.44
1:F:1032:TRP:C	1:F:1034:LEU:H	2.23	0.44
1:G:1087:THR:N	2:N:39:LYS:HZ3	2.15	0.44
2:L:68:LEU:HB3	2:L:85:ILE:HD12	1.98	0.44
3:O:45:ARG:O	3:O:45:ARG:HG2	2.17	0.44
1:A:569:CYS:HB3	1:A:600:LYS:HZ3	1.82	0.44
1:B:357:SER:OG	1:B:358:SER:N	2.50	0.44
1:B:480:CYS:SG	1:B:481:MET:N	2.90	0.44
1:C:480:CYS:SG	1:C:481:MET:N	2.90	0.44
1:C:600:LYS:HA	1:C:603:ILE:HG13	2.00	0.44
1:D:143:LEU:C	1:D:145:GLY:N	2.75	0.44
1:D:298:PHE:CD2	1:D:328:GLY:HA3	2.52	0.44
1:D:643:LYS:HD3	1:D:646:THR:HG22	1.98	0.44
1:E:888:VAL:HG12	1:E:899:THR:HA	1.98	0.44
2:M:68:LEU:HB3	2:M:85:ILE:HD12	1.98	0.44
2:M:72:LYS:NZ	2:M:78:THR:O	2.51	0.44
1:A:600:LYS:HA	1:A:603:ILE:HG13	2.00	0.44
1:C:461:ILE:HD11	1:C:491:MET:HA	1.99	0.44
1:D:342:LEU:O	1:D:346:GLN:CG	2.66	0.44
1:D:480:CYS:SG	1:D:481:MET:N	2.90	0.44
1:E:530:ARG:NH1	1:E:545:GLN:OE1	2.51	0.44
1:E:1191:MET:SD	1:E:1209:SER:OG	2.63	0.44
1:F:342:LEU:O	1:F:346:GLN:CG	2.66	0.44
2:J:72:LYS:NZ	2:J:78:THR:O	2.51	0.44
3:R:10:ARG:HG2	3:R:10:ARG:H	1.60	0.44
1:A:357:SER:OG	1:A:358:SER:N	2.50	0.44
1:C:342:LEU:O	1:C:346:GLN:CG	2.66	0.44
1:D:269:VAL:C	1:D:271:ASP:H	2.24	0.44
1:D:390:GLN:HB2	1:D:393:VAL:HG21	1.99	0.44
1:E:357:SER:OG	1:E:358:SER:N	2.50	0.44
1:F:390:GLN:HB2	1:F:393:VAL:HG21	1.99	0.44
1:F:600:LYS:HZ1	1:F:1213:PHE:HZ	1.66	0.44
1:F:600:LYS:HA	1:F:603:ILE:HG13	2.00	0.44
1:G:342:LEU:O	1:G:346:GLN:CG	2.66	0.44
1:G:600:LYS:HA	1:G:603:ILE:HG13	2.00	0.44
1:G:695:TYR:HE1	1:G:733:LYS:HD2	1.83	0.44
1:G:821:ILE:HD11	1:G:857:VAL:HG21	1.99	0.44
2:I:68:LEU:HB3	2:I:85:ILE:HD12	1.98	0.44
2:J:3:VAL:O	2:J:97:TYR:HB2	2.18	0.44
2:N:3:VAL:O	2:N:97:TYR:HB2	2.18	0.44
1:A:143:LEU:C	1:A:145:GLY:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:GLN:HB2	1:B:393:VAL:HG21	1.99	0.44
1:B:550:LEU:HD23	1:B:607:SER:HB2	1.91	0.44
1:C:695:TYR:HE1	1:C:733:LYS:HD2	1.82	0.44
1:E:600:LYS:HA	1:E:603:ILE:HG13	2.00	0.44
1:E:868:ASN:OD1	1:E:869:THR:N	2.50	0.44
1:G:230:LEU:O	1:G:234:LYS:N	2.41	0.44
1:G:530:ARG:NH1	1:G:545:GLN:OE1	2.51	0.44
1:G:795:GLU:HG3	1:G:795:GLU:O	2.18	0.44
1:A:530:ARG:NH1	1:A:545:GLN:OE1	2.51	0.44
1:B:695:TYR:HE1	1:B:733:LYS:HD2	1.83	0.44
1:C:143:LEU:C	1:C:145:GLY:N	2.75	0.44
1:C:298:PHE:CD2	1:C:328:GLY:HA3	2.52	0.44
1:C:795:GLU:HG3	1:C:795:GLU:O	2.18	0.44
1:C:1135:PHE:CE1	1:C:1142:LEU:HD13	2.53	0.44
1:D:461:ILE:HD11	1:D:491:MET:HA	1.99	0.44
1:D:600:LYS:HA	1:D:603:ILE:HG13	2.00	0.44
1:D:685:ASN:HB3	1:D:688:THR:HB	1.99	0.44
1:F:143:LEU:C	1:F:145:GLY:N	2.75	0.44
1:F:298:PHE:CD2	1:F:328:GLY:HA3	2.52	0.44
1:G:344:GLN:OE1	1:G:349:GLN:NE2	2.44	0.44
1:G:390:GLN:HB2	1:G:393:VAL:HG21	1.99	0.44
2:K:3:VAL:O	2:K:97:TYR:HB2	2.18	0.44
2:L:3:VAL:O	2:L:97:TYR:HB2	2.18	0.44
2:M:70:ASN:ND2	2:M:73:LYS:HB2	2.33	0.44
1:A:342:LEU:O	1:A:346:GLN:CG	2.66	0.44
1:A:685:ASN:HB3	1:A:688:THR:HB	1.99	0.44
1:B:391:LYS:H	1:B:391:LYS:HG2	1.62	0.44
1:B:600:LYS:HZ1	1:B:1213:PHE:HZ	1.65	0.44
1:B:1135:PHE:CE1	1:B:1142:LEU:HD13	2.53	0.44
1:D:524:HIS:N	1:D:646:THR:OG1	2.51	0.44
2:K:72:LYS:NZ	2:K:78:THR:O	2.51	0.44
2:N:70:ASN:ND2	2:N:73:LYS:HB2	2.33	0.44
1:A:695:TYR:OH	1:A:732:GLN:O	2.31	0.44
1:B:685:ASN:HB3	1:B:688:THR:HB	1.99	0.44
1:C:530:ARG:NH1	1:C:545:GLN:OE1	2.51	0.44
1:C:847:ASP:OD1	1:C:848:PHE:N	2.51	0.44
1:D:530:ARG:NH1	1:D:545:GLN:OE1	2.51	0.44
1:D:695:TYR:HE1	1:D:733:LYS:HD2	1.83	0.44
1:D:847:ASP:OD1	1:D:848:PHE:N	2.51	0.44
1:E:685:ASN:HB3	1:E:688:THR:HB	2.00	0.44
1:G:480:CYS:SG	1:G:481:MET:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:LYS:NZ	2:H:78:THR:O	2.51	0.44
3:O:41:GLU:HA	3:O:44:GLN:HE21	1.83	0.44
1:A:795:GLU:HG3	1:A:795:GLU:O	2.18	0.43
1:B:326:LEU:HD23	1:B:326:LEU:HA	1.44	0.43
1:B:524:HIS:N	1:B:646:THR:OG1	2.51	0.43
1:C:390:GLN:HB2	1:C:393:VAL:HG21	1.99	0.43
1:E:342:LEU:O	1:E:346:GLN:CG	2.66	0.43
1:E:695:TYR:HE1	1:E:733:LYS:HD2	1.83	0.43
1:E:795:GLU:HG3	1:E:795:GLU:O	2.18	0.43
1:F:524:HIS:N	1:F:646:THR:OG1	2.51	0.43
1:F:795:GLU:HG3	1:F:795:GLU:O	2.18	0.43
1:G:685:ASN:HB3	1:G:688:THR:HB	1.99	0.43
2:L:18:HIS:CE1	2:L:29:GLY:HA3	2.53	0.43
2:L:72:LYS:NZ	2:L:78:THR:O	2.51	0.43
2:N:18:HIS:CE1	2:N:29:GLY:HA3	2.53	0.43
1:B:224:LYS:HE3	1:B:255:ASP:O	2.18	0.43
1:B:342:LEU:O	1:B:346:GLN:CG	2.66	0.43
1:B:530:ARG:NH1	1:B:545:GLN:OE1	2.51	0.43
1:B:795:GLU:HG3	1:B:795:GLU:O	2.18	0.43
1:C:334:PHE:HD2	1:C:337:ARG:HH11	1.66	0.43
1:E:298:PHE:CD2	1:E:328:GLY:HA3	2.52	0.43
1:F:480:CYS:SG	1:F:481:MET:N	2.90	0.43
1:G:224:LYS:HE3	1:G:255:ASP:O	2.18	0.43
1:G:357:SER:OG	1:G:358:SER:N	2.50	0.43
1:G:524:HIS:N	1:G:646:THR:OG1	2.51	0.43
2:H:18:HIS:CE1	2:H:29:GLY:HA3	2.53	0.43
2:J:70:ASN:ND2	2:J:73:LYS:HB2	2.33	0.43
1:A:524:HIS:N	1:A:646:THR:OG1	2.51	0.43
1:A:695:TYR:HE1	1:A:733:LYS:HD2	1.83	0.43
1:A:847:ASP:OD1	1:A:848:PHE:N	2.51	0.43
1:A:1135:PHE:CE1	1:A:1142:LEU:HD13	2.53	0.43
1:B:428:ARG:HG2	1:B:433:PHE:CE1	2.54	0.43
1:E:524:HIS:N	1:E:646:THR:OG1	2.51	0.43
1:F:357:SER:OG	1:F:358:SER:N	2.50	0.43
1:F:973:LEU:C	1:F:975:TYR:H	2.27	0.43
1:G:268:SER:O	1:G:271:ASP:N	2.51	0.43
1:G:844:GLN:HE22	2:N:79:LYS:HZ2	1.63	0.43
2:N:72:LYS:NZ	2:N:78:THR:O	2.51	0.43
3:R:41:GLU:HA	3:R:44:GLN:HE21	1.83	0.43
1:A:386:LEU:O	1:A:386:LEU:HD23	2.19	0.43
1:A:390:GLN:HB2	1:A:393:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:SER:H	1:A:980:ASP:HA	1.84	0.43
1:B:937:VAL:HB	1:B:949:ILE:HB	2.00	0.43
1:C:685:ASN:HB3	1:C:688:THR:HB	2.00	0.43
1:C:937:VAL:HB	1:C:949:ILE:HB	2.00	0.43
1:C:965:SER:H	1:C:980:ASP:HA	1.84	0.43
1:D:582:LEU:O	1:D:586:GLN:HG3	2.19	0.43
1:E:143:LEU:C	1:E:145:GLY:N	2.75	0.43
1:F:530:ARG:NH1	1:F:545:GLN:OE1	2.51	0.43
1:G:386:LEU:O	1:G:386:LEU:HD23	2.19	0.43
1:G:569:CYS:HB3	1:G:600:LYS:HZ3	1.83	0.43
2:H:70:ASN:ND2	2:H:73:LYS:HB2	2.33	0.43
2:M:26:HIS:O	2:M:27:LYS:HD2	2.19	0.43
1:A:224:LYS:HE3	1:A:255:ASP:O	2.18	0.43
1:B:334:PHE:HD2	1:B:337:ARG:HH11	1.66	0.43
1:B:582:LEU:O	1:B:586:GLN:HG3	2.19	0.43
1:E:973:LEU:C	1:E:975:TYR:H	2.27	0.43
1:E:1135:PHE:CE1	1:E:1142:LEU:HD13	2.53	0.43
1:F:965:SER:H	1:F:980:ASP:HA	1.84	0.43
1:G:1218:THR:H	1:G:1237:ASN:ND2	2.17	0.43
2:J:18:HIS:CE1	2:J:29:GLY:HA3	2.53	0.43
2:N:26:HIS:O	2:N:27:LYS:HD2	2.19	0.43
1:A:346:GLN:O	1:A:348:LYS:N	2.52	0.43
1:A:739:MET:HE1	1:A:758:LEU:HD23	2.00	0.43
1:C:428:ARG:HG2	1:C:433:PHE:CE1	2.54	0.43
1:C:524:HIS:N	1:C:646:THR:OG1	2.51	0.43
1:C:802:LYS:NZ	1:C:843:ILE:O	2.50	0.43
1:C:884:TRP:HH2	2:J:78:THR:O	2.02	0.43
1:D:224:LYS:HE3	1:D:255:ASP:O	2.18	0.43
1:D:386:LEU:O	1:D:386:LEU:HD23	2.19	0.43
1:D:937:VAL:HB	1:D:949:ILE:HB	2.00	0.43
1:E:224:LYS:HE3	1:E:255:ASP:O	2.18	0.43
1:E:428:ARG:HG2	1:E:433:PHE:CE1	2.54	0.43
1:E:1166:ALA:HA	1:E:1167:PRO:HD2	1.93	0.43
2:I:26:HIS:O	2:I:27:LYS:HD2	2.19	0.43
2:J:26:HIS:O	2:J:27:LYS:HD2	2.19	0.43
2:M:18:HIS:CE1	2:M:29:GLY:HA3	2.53	0.43
2:N:82:PHE:HE2	2:N:85:ILE:HG13	1.84	0.43
1:A:379:ILE:O	1:A:382:TYR:N	2.52	0.43
1:B:346:GLN:O	1:B:348:LYS:N	2.52	0.43
1:B:386:LEU:O	1:B:386:LEU:HD23	2.19	0.43
1:D:965:SER:H	1:D:980:ASP:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:SER:O	1:E:271:ASP:N	2.51	0.43
1:E:1100:PHE:HB3	1:E:1111:ILE:HD11	2.00	0.43
1:F:224:LYS:HE3	1:F:255:ASP:O	2.18	0.43
1:F:386:LEU:HD23	1:F:386:LEU:O	2.19	0.43
1:F:685:ASN:HB3	1:F:688:THR:HB	1.99	0.43
1:F:695:TYR:HE1	1:F:733:LYS:HD2	1.83	0.43
1:F:847:ASP:OD1	1:F:848:PHE:N	2.51	0.43
1:G:379:ILE:O	1:G:382:TYR:N	2.52	0.43
1:G:973:LEU:C	1:G:975:TYR:H	2.27	0.43
2:H:3:VAL:O	2:H:97:TYR:HB2	2.18	0.43
2:I:18:HIS:CE1	2:I:29:GLY:HA3	2.53	0.43
1:A:326:LEU:HA	1:A:326:LEU:HD23	1.44	0.43
1:A:973:LEU:C	1:A:975:TYR:H	2.27	0.43
1:B:973:LEU:C	1:B:975:TYR:H	2.27	0.43
1:C:379:ILE:O	1:C:382:TYR:N	2.52	0.43
1:D:428:ARG:HG2	1:D:433:PHE:CE1	2.54	0.43
1:E:695:TYR:OH	1:E:732:GLN:O	2.31	0.43
1:F:582:LEU:O	1:F:586:GLN:HG3	2.19	0.43
1:F:937:VAL:HB	1:F:949:ILE:HB	2.00	0.43
1:G:847:ASP:OD1	1:G:848:PHE:N	2.51	0.43
2:I:3:VAL:O	2:I:97:TYR:HB2	2.18	0.43
2:I:70:ASN:ND2	2:I:73:LYS:HB2	2.33	0.43
2:K:26:HIS:O	2:K:27:LYS:HD2	2.19	0.43
2:L:41:GLY:HA2	2:L:48:TYR:CZ	2.54	0.43
1:A:524:HIS:CB	1:A:646:THR:HG21	2.36	0.43
1:B:379:ILE:O	1:B:382:TYR:N	2.52	0.43
1:B:767:LEU:HD21	1:B:801:VAL:HG11	2.01	0.43
1:B:1100:PHE:HB3	1:B:1111:ILE:HD11	2.00	0.43
1:C:224:LYS:HE3	1:C:255:ASP:O	2.18	0.43
1:C:346:GLN:O	1:C:348:LYS:N	2.52	0.43
1:D:725:LEU:HD11	1:D:742:HIS:CD2	2.54	0.43
1:D:1100:PHE:HB3	1:D:1111:ILE:HD11	2.00	0.43
1:E:725:LEU:HD11	1:E:742:HIS:CD2	2.54	0.43
1:E:739:MET:HE1	1:E:758:LEU:HD23	2.00	0.43
1:E:847:ASP:OD1	1:E:848:PHE:N	2.51	0.43
1:E:965:SER:H	1:E:980:ASP:HA	1.84	0.43
1:F:379:ILE:O	1:F:382:TYR:N	2.52	0.43
1:G:428:ARG:HG2	1:G:433:PHE:CE1	2.54	0.43
1:G:739:MET:HE1	1:G:758:LEU:HD23	2.00	0.43
2:H:41:GLY:HA2	2:H:48:TYR:CZ	2.54	0.43
2:H:82:PHE:HE2	2:H:85:ILE:HG13	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:18:HIS:CE1	2:K:29:GLY:HA3	2.53	0.43
2:K:70:ASN:ND2	2:K:73:LYS:HB2	2.33	0.43
2:M:3:VAL:O	2:M:97:TYR:HB2	2.18	0.43
1:B:739:MET:HE1	1:B:758:LEU:HD23	2.00	0.43
1:B:965:SER:H	1:B:980:ASP:HA	1.84	0.43
1:C:582:LEU:O	1:C:586:GLN:HG3	2.19	0.43
1:C:767:LEU:HD21	1:C:801:VAL:HG11	2.01	0.43
1:D:334:PHE:HD2	1:D:337:ARG:HH11	1.66	0.43
1:D:795:GLU:O	1:D:795:GLU:HG3	2.18	0.43
1:D:973:LEU:C	1:D:975:TYR:H	2.27	0.43
1:D:1135:PHE:CE1	1:D:1142:LEU:HD13	2.53	0.43
1:E:1218:THR:H	1:E:1237:ASN:ND2	2.17	0.43
1:F:201:ASN:ND2	1:G:219:ASN:HD21	2.14	0.43
1:F:346:GLN:O	1:F:348:LYS:N	2.52	0.43
1:F:1100:PHE:HB3	1:F:1111:ILE:HD11	2.00	0.43
1:G:346:GLN:O	1:G:348:LYS:N	2.52	0.43
1:G:1050:PHE:CD1	1:G:1058:LEU:HD11	2.54	0.43
2:H:67:TYR:HD1	2:H:74:TYR:HB3	1.84	0.43
2:L:26:HIS:O	2:L:27:LYS:HD2	2.19	0.43
2:L:70:ASN:ND2	2:L:73:LYS:HB2	2.33	0.43
2:L:82:PHE:HE2	2:L:85:ILE:HG13	1.84	0.43
3:P:41:GLU:HA	3:P:44:GLN:HE21	1.83	0.43
1:C:676:SER:OG	1:C:678:ASP:OD1	2.37	0.42
1:D:767:LEU:HD21	1:D:801:VAL:HG11	2.01	0.42
1:E:658:ASP:HB3	1:E:677:VAL:HB	2.00	0.42
1:F:1135:PHE:CE1	1:F:1142:LEU:HD13	2.53	0.42
1:G:658:ASP:HB3	1:G:677:VAL:HB	2.00	0.42
1:G:937:VAL:HB	1:G:949:ILE:HB	2.00	0.42
2:I:82:PHE:HE2	2:I:85:ILE:HG13	1.84	0.42
2:N:41:GLY:HA2	2:N:48:TYR:CZ	2.54	0.42
3:P:90:ARG:HG2	3:P:90:ARG:HH21	1.84	0.42
1:A:658:ASP:HB3	1:A:677:VAL:HB	2.00	0.42
1:A:1050:PHE:CD1	1:A:1058:LEU:HD11	2.54	0.42
1:C:550:LEU:HD23	1:C:607:SER:HB2	1.91	0.42
1:C:1100:PHE:HB3	1:C:1111:ILE:HD11	2.00	0.42
1:D:658:ASP:HB3	1:D:677:VAL:HB	2.00	0.42
1:E:482:TYR:OH	1:E:490:HIS:NE2	2.35	0.42
1:E:767:LEU:HD21	1:E:801:VAL:HG11	2.01	0.42
1:F:569:CYS:CB	1:F:600:LYS:HZ3	2.32	0.42
1:F:808:ALA:HB2	1:F:850:PRO:HA	2.01	0.42
1:G:1135:PHE:CE1	1:G:1142:LEU:HD13	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:82:PHE:HE2	2:M:85:ILE:HG13	1.84	0.42
3:R:90:ARG:HG2	3:R:90:ARG:HH21	1.85	0.42
1:A:511:LYS:HB2	1:A:563:ILE:HG13	2.02	0.42
1:A:767:LEU:HD21	1:A:801:VAL:HG11	2.01	0.42
1:B:658:ASP:HB3	1:B:677:VAL:HB	2.00	0.42
1:B:1218:THR:H	1:B:1237:ASN:ND2	2.17	0.42
1:C:973:LEU:C	1:C:975:TYR:H	2.27	0.42
1:D:524:HIS:CB	1:D:646:THR:HG21	2.36	0.42
1:G:808:ALA:HB2	1:G:850:PRO:HA	2.02	0.42
2:J:14:CYS:SG	5:J:500:HEC:HBB3	2.59	0.42
2:J:82:PHE:HE2	2:J:85:ILE:HG13	1.84	0.42
2:N:14:CYS:SG	5:N:500:HEC:HBB3	2.59	0.42
3:O:90:ARG:HG2	3:O:90:ARG:HH21	1.85	0.42
1:A:428:ARG:HG2	1:A:433:PHE:CE1	2.54	0.42
1:A:865:GLU:CD	1:A:867:TRP:HE1	2.27	0.42
1:A:937:VAL:HB	1:A:949:ILE:HB	2.00	0.42
1:A:1100:PHE:HB3	1:A:1111:ILE:HD11	2.00	0.42
1:A:1218:THR:H	1:A:1237:ASN:ND2	2.17	0.42
1:D:739:MET:HE1	1:D:758:LEU:HD23	2.00	0.42
1:E:379:ILE:O	1:E:382:TYR:N	2.52	0.42
1:E:937:VAL:HB	1:E:949:ILE:HB	2.00	0.42
1:F:658:ASP:HB3	1:F:677:VAL:HB	2.00	0.42
1:F:725:LEU:HD11	1:F:742:HIS:CD2	2.54	0.42
1:F:739:MET:HE1	1:F:758:LEU:HD23	2.00	0.42
1:F:767:LEU:HD21	1:F:801:VAL:HG11	2.01	0.42
2:J:67:TYR:HD1	2:J:74:TYR:HB3	1.84	0.42
2:K:14:CYS:SG	5:K:500:HEC:HBB3	2.59	0.42
3:O:34:LEU:HD12	3:O:34:LEU:HA	1.93	0.42
3:Q:90:ARG:HG2	3:Q:90:ARG:HH21	1.84	0.42
1:B:511:LYS:HB2	1:B:563:ILE:HG13	2.02	0.42
1:B:847:ASP:OD1	1:B:848:PHE:N	2.51	0.42
1:B:865:GLU:CD	1:B:867:TRP:HE1	2.27	0.42
1:B:989:GLU:HG2	1:B:991:VAL:H	1.85	0.42
1:C:725:LEU:HD11	1:C:742:HIS:CD2	2.54	0.42
1:C:1135:PHE:HE1	1:C:1142:LEU:HD13	1.85	0.42
1:D:676:SER:OG	1:D:678:ASP:OD1	2.37	0.42
1:D:1218:THR:H	1:D:1237:ASN:ND2	2.17	0.42
1:E:346:GLN:O	1:E:348:LYS:N	2.52	0.42
1:E:808:ALA:HB2	1:E:850:PRO:HA	2.01	0.42
1:F:482:TYR:HH	1:F:490:HIS:HE2	1.55	0.42
1:G:145:GLY:HA2	1:G:259:GLN:HE21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:26:HIS:O	2:H:27:LYS:HD2	2.19	0.42
2:I:14:CYS:SG	5:I:500:HEC:HBB3	2.59	0.42
2:K:41:GLY:HA2	2:K:48:TYR:CZ	2.54	0.42
3:R:7:ARG:HA	3:R:10:ARG:HG3	2.02	0.42
1:A:344:GLN:CD	1:A:349:GLN:HE21	2.28	0.42
1:A:808:ALA:HB2	1:A:850:PRO:HA	2.01	0.42
1:C:658:ASP:HB3	1:C:677:VAL:HB	2.00	0.42
1:D:452:GLN:N	1:D:452:GLN:OE1	2.53	0.42
1:E:386:LEU:HD23	1:E:386:LEU:O	2.19	0.42
1:E:582:LEU:O	1:E:586:GLN:HG3	2.19	0.42
1:F:334:PHE:HD2	1:F:337:ARG:HH11	1.66	0.42
1:F:865:GLU:CD	1:F:867:TRP:HE1	2.27	0.42
1:F:1050:PHE:CD1	1:F:1058:LEU:HD11	2.54	0.42
1:G:865:GLU:CD	1:G:867:TRP:HE1	2.27	0.42
2:H:40:THR:HG23	2:H:57:ILE:HG13	2.02	0.42
2:K:82:PHE:HE2	2:K:85:ILE:HG13	1.84	0.42
2:N:67:TYR:HD1	2:N:74:TYR:HB3	1.84	0.42
1:A:320:SER:HA	1:A:321:PRO:HD3	1.87	0.42
1:C:386:LEU:HD23	1:C:386:LEU:O	2.19	0.42
1:C:400:LEU:HB3	1:C:404:TRP:HZ3	1.84	0.42
1:C:1050:PHE:CD1	1:C:1058:LEU:HD11	2.54	0.42
1:D:884:TRP:HH2	2:K:78:THR:O	2.02	0.42
1:G:10:LEU:CD2	1:G:13:ARG:NH2	2.83	0.42
1:G:170:ASP:CG	1:G:172:SER:HG	2.26	0.42
1:G:320:SER:HA	1:G:321:PRO:HD3	1.87	0.42
1:G:344:GLN:CD	1:G:349:GLN:HE21	2.28	0.42
1:G:511:LYS:HB2	1:G:563:ILE:HG13	2.02	0.42
1:G:582:LEU:O	1:G:586:GLN:HG3	2.19	0.42
2:I:94:LEU:O	2:I:98:LEU:HG	2.20	0.42
2:J:41:GLY:HA2	2:J:48:TYR:CZ	2.54	0.42
2:M:41:GLY:HA2	2:M:48:TYR:CZ	2.54	0.42
1:B:265:ARG:HG3	1:B:265:ARG:O	2.20	0.42
1:B:320:SER:HA	1:B:321:PRO:HD3	1.87	0.42
1:B:1050:PHE:CD1	1:B:1058:LEU:HD11	2.54	0.42
1:B:1135:PHE:HE1	1:B:1142:LEU:HD13	1.85	0.42
1:C:145:GLY:HA2	1:C:259:GLN:HE21	1.85	0.42
1:C:600:LYS:HZ1	1:C:1213:PHE:HZ	1.66	0.42
1:C:1218:THR:H	1:C:1237:ASN:ND2	2.17	0.42
1:D:10:LEU:CD2	1:D:13:ARG:NH2	2.83	0.42
1:D:265:ARG:HG3	1:D:265:ARG:O	2.20	0.42
1:D:379:ILE:O	1:D:382:TYR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1218:THR:H	1:F:1237:ASN:ND2	2.17	0.42
1:G:400:LEU:HB3	1:G:404:TRP:HZ3	1.85	0.42
1:G:767:LEU:HD21	1:G:801:VAL:HG11	2.01	0.42
1:G:1135:PHE:HE1	1:G:1142:LEU:HD13	1.85	0.42
2:H:14:CYS:SG	5:H:500:HEC:HBB3	2.59	0.42
2:L:14:CYS:SG	5:L:500:HEC:HBB3	2.59	0.42
2:N:40:THR:HG23	2:N:57:ILE:HG13	2.02	0.42
3:O:7:ARG:HA	3:O:10:ARG:HG3	2.02	0.42
1:A:265:ARG:HG3	1:A:265:ARG:O	2.20	0.42
1:B:268:SER:O	1:B:271:ASP:N	2.51	0.42
1:C:865:GLU:CD	1:C:867:TRP:HE1	2.27	0.42
1:D:346:GLN:O	1:D:348:LYS:N	2.52	0.42
1:D:865:GLU:CD	1:D:867:TRP:HE1	2.27	0.42
1:E:452:GLN:OE1	1:E:452:GLN:N	2.53	0.42
1:E:1050:PHE:CD1	1:E:1058:LEU:HD11	2.54	0.42
1:F:428:ARG:HG2	1:F:433:PHE:CE1	2.54	0.42
1:G:452:GLN:OE1	1:G:452:GLN:N	2.53	0.42
2:H:94:LEU:O	2:H:98:LEU:HG	2.20	0.42
2:M:40:THR:HG23	2:M:57:ILE:HG13	2.02	0.42
2:M:67:TYR:HD1	2:M:74:TYR:HB3	1.84	0.42
1:A:582:LEU:O	1:A:586:GLN:HG3	2.19	0.42
1:A:864:VAL:HB	1:A:878:CYS:HB2	2.02	0.42
1:B:10:LEU:CD2	1:B:13:ARG:NH2	2.83	0.42
1:B:452:GLN:OE1	1:B:452:GLN:N	2.53	0.42
1:C:265:ARG:O	1:C:265:ARG:HG3	2.20	0.42
1:C:268:SER:O	1:C:271:ASP:N	2.51	0.42
1:C:452:GLN:OE1	1:C:452:GLN:N	2.53	0.42
1:C:864:VAL:HB	1:C:878:CYS:HB2	2.02	0.42
1:D:346:GLN:C	1:D:348:LYS:H	2.28	0.42
1:D:864:VAL:HB	1:D:878:CYS:HB2	2.02	0.42
1:D:989:GLU:HG2	1:D:991:VAL:H	1.85	0.42
1:E:265:ARG:HG3	1:E:265:ARG:O	2.20	0.42
1:F:989:GLU:HG2	1:F:991:VAL:H	1.85	0.42
1:G:334:PHE:HD2	1:G:337:ARG:HH11	1.66	0.42
1:G:346:GLN:C	1:G:348:LYS:H	2.28	0.42
1:G:676:SER:OG	1:G:678:ASP:OD1	2.37	0.42
1:G:725:LEU:HD11	1:G:742:HIS:CD2	2.54	0.42
1:G:965:SER:H	1:G:980:ASP:HA	1.84	0.42
2:J:94:LEU:O	2:J:98:LEU:HG	2.20	0.42
2:L:67:TYR:HD1	2:L:74:TYR:HB3	1.84	0.42
2:M:14:CYS:SG	5:M:500:HEC:HBB3	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:GLN:N	1:A:452:GLN:OE1	2.53	0.41
1:A:989:GLU:HG2	1:A:991:VAL:H	1.85	0.41
1:B:346:GLN:C	1:B:348:LYS:H	2.28	0.41
1:F:947:GLN:HG2	1:F:958:TYR:HD1	1.85	0.41
1:B:456:LEU:O	1:B:459:LYS:HB3	2.20	0.41
1:D:1050:PHE:CD1	1:D:1058:LEU:HD11	2.54	0.41
1:E:865:GLU:CD	1:E:867:TRP:HE1	2.27	0.41
1:F:369:SER:O	1:F:373:GLU:HG2	2.21	0.41
1:F:511:LYS:HB2	1:F:563:ILE:HG13	2.01	0.41
1:F:864:VAL:HB	1:F:878:CYS:HB2	2.02	0.41
2:K:67:TYR:HD1	2:K:74:TYR:HB3	1.84	0.41
2:K:94:LEU:O	2:K:98:LEU:HG	2.20	0.41
2:L:94:LEU:O	2:L:98:LEU:HG	2.20	0.41
1:A:145:GLY:HA2	1:A:259:GLN:HE21	1.85	0.41
1:A:1191:MET:SD	1:A:1209:SER:OG	2.63	0.41
1:G:282:VAL:O	1:G:282:VAL:HG12	2.21	0.41
1:G:947:GLN:HG2	1:G:958:TYR:HD1	1.85	0.41
1:G:1100:PHE:HB3	1:G:1111:ILE:HD11	2.00	0.41
2:I:41:GLY:HA2	2:I:48:TYR:CZ	2.54	0.41
1:A:334:PHE:HD2	1:A:337:ARG:HH11	1.66	0.41
1:B:725:LEU:HD11	1:B:742:HIS:CD2	2.54	0.41
1:C:346:GLN:C	1:C:348:LYS:H	2.28	0.41
1:C:511:LYS:HB2	1:C:563:ILE:HG13	2.02	0.41
1:D:342:LEU:O	1:D:346:GLN:HG3	2.21	0.41
1:D:456:LEU:O	1:D:459:LYS:HB3	2.21	0.41
1:D:808:ALA:HB2	1:D:850:PRO:HA	2.02	0.41
1:D:885:VAL:HG13	1:D:900:SER:O	2.21	0.41
1:E:282:VAL:O	1:E:282:VAL:HG12	2.20	0.41
1:E:1135:PHE:HE1	1:E:1142:LEU:HD13	1.85	0.41
1:F:265:ARG:HG3	1:F:265:ARG:O	2.20	0.41
1:F:337:ARG:O	1:F:340:TYR:N	2.54	0.41
1:G:265:ARG:HG3	1:G:265:ARG:O	2.20	0.41
1:G:369:SER:O	1:G:373:GLU:HG2	2.20	0.41
2:I:40:THR:HG23	2:I:57:ILE:HG13	2.02	0.41
2:K:40:THR:HG23	2:K:57:ILE:HG13	2.02	0.41
1:A:676:SER:OG	1:A:678:ASP:OD1	2.37	0.41
1:B:808:ALA:HB2	1:B:850:PRO:HA	2.01	0.41
1:C:456:LEU:O	1:C:459:LYS:HB3	2.21	0.41
1:C:739:MET:HE1	1:C:758:LEU:HD23	2.00	0.41
1:C:808:ALA:HB2	1:C:850:PRO:HA	2.01	0.41
1:D:30:ILE:HG21	3:Q:10:ARG:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:SER:O	1:D:271:ASP:N	2.51	0.41
1:D:565:GLN:CD	1:D:1213:PHE:CA	2.94	0.41
1:E:369:SER:O	1:E:373:GLU:HG2	2.20	0.41
1:E:474:SER:HA	1:E:475:PRO:HD2	1.91	0.41
1:F:452:GLN:OE1	1:F:452:GLN:N	2.53	0.41
2:N:94:LEU:O	2:N:98:LEU:HG	2.20	0.41
3:Q:7:ARG:HA	3:Q:10:ARG:HG3	2.02	0.41
1:A:884:TRP:HH2	2:H:78:THR:O	2.02	0.41
1:C:369:SER:O	1:C:373:GLU:HG2	2.20	0.41
1:D:14:GLU:CB	1:E:31:SER:HG	2.34	0.41
1:D:358:SER:CB	1:E:274:MET:HE2	2.44	0.41
1:D:400:LEU:HB3	1:D:404:TRP:HZ3	1.84	0.41
1:D:947:GLN:HG2	1:D:958:TYR:HD1	1.85	0.41
1:E:337:ARG:O	1:E:340:TYR:N	2.54	0.41
1:E:565:GLN:CD	1:E:1213:PHE:CA	2.94	0.41
1:E:1087:THR:N	2:L:39:LYS:HZ3	2.17	0.41
1:F:268:SER:O	1:F:271:ASP:N	2.51	0.41
1:F:282:VAL:O	1:F:282:VAL:HG12	2.20	0.41
1:F:456:LEU:O	1:F:459:LYS:HB3	2.21	0.41
1:F:695:TYR:OH	1:F:732:GLN:O	2.31	0.41
1:F:884:TRP:HH2	2:M:79:LYS:N	2.18	0.41
1:F:884:TRP:HH2	2:M:78:THR:O	2.02	0.41
1:G:337:ARG:O	1:G:340:TYR:N	2.54	0.41
1:G:695:TYR:OH	1:G:732:GLN:O	2.31	0.41
1:G:989:GLU:HG2	1:G:991:VAL:H	1.85	0.41
2:J:40:THR:HG23	2:J:57:ILE:HG13	2.02	0.41
2:L:40:THR:HG23	2:L:57:ILE:HG13	2.02	0.41
2:M:94:LEU:O	2:M:98:LEU:HG	2.20	0.41
1:A:342:LEU:O	1:A:346:GLN:HG3	2.21	0.41
1:A:947:GLN:HG2	1:A:958:TYR:HD1	1.85	0.41
1:B:282:VAL:O	1:B:282:VAL:HG12	2.21	0.41
1:C:569:CYS:CB	1:C:600:LYS:HZ3	2.32	0.41
1:C:700:GLU:HB2	1:C:720:SER:HB2	2.03	0.41
1:D:216:LEU:HA	1:D:217:PRO:HD2	1.84	0.41
1:E:344:GLN:CD	1:E:349:GLN:HE21	2.28	0.41
1:F:971:PRO:C	1:F:973:LEU:H	2.29	0.41
1:G:342:LEU:O	1:G:346:GLN:HG3	2.21	0.41
1:A:725:LEU:HD11	1:A:742:HIS:CD2	2.54	0.41
1:A:1135:PHE:HE1	1:A:1142:LEU:HD13	1.85	0.41
1:B:145:GLY:HA2	1:B:259:GLN:HE21	1.85	0.41
1:B:569:CYS:CB	1:B:600:LYS:HZ3	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:885:VAL:HG13	1:B:900:SER:O	2.21	0.41
1:C:153:HIS:HA	1:C:264:THR:O	2.21	0.41
1:C:344:GLN:CD	1:C:349:GLN:HE21	2.28	0.41
1:C:358:SER:HB3	1:D:274:MET:HE3	2.00	0.41
1:C:584:ALA:CA	1:C:594:TYR:CE2	2.98	0.41
1:D:46:GLU:OE2	1:D:55:MET:HE2	2.21	0.41
1:D:196:LEU:O	1:D:199:LEU:HB2	2.21	0.41
1:D:348:LYS:NZ	1:D:443:ASP:CG	2.79	0.41
1:E:334:PHE:HD2	1:E:337:ARG:HH11	1.66	0.41
1:E:864:VAL:HB	1:E:878:CYS:HB2	2.02	0.41
1:E:971:PRO:C	1:E:973:LEU:H	2.29	0.41
1:F:322:LEU:HD23	1:F:364:LEU:HD13	2.03	0.41
1:F:676:SER:OG	1:F:678:ASP:OD1	2.37	0.41
1:F:885:VAL:HG13	1:F:900:SER:O	2.21	0.41
1:G:864:VAL:HB	1:G:878:CYS:HB2	2.02	0.41
2:I:30:PRO:HB3	2:I:46:PHE:CD2	2.56	0.41
2:K:30:PRO:HB3	2:K:46:PHE:CD2	2.56	0.41
2:M:55:LYS:HG2	2:M:75:ILE:HG12	2.03	0.41
1:A:400:LEU:HB3	1:A:404:TRP:HZ3	1.84	0.41
1:A:565:GLN:CD	1:A:1213:PHE:CA	2.94	0.41
1:B:46:GLU:OE2	1:B:55:MET:HE2	2.21	0.41
1:B:143:LEU:C	1:B:145:GLY:N	2.75	0.41
1:B:369:SER:O	1:B:373:GLU:HG2	2.21	0.41
1:B:400:LEU:HB3	1:B:404:TRP:HZ3	1.84	0.41
1:B:700:GLU:HB2	1:B:720:SER:HB2	2.03	0.41
1:B:864:VAL:HB	1:B:878:CYS:HB2	2.02	0.41
1:C:196:LEU:O	1:C:199:LEU:HB2	2.21	0.41
1:C:282:VAL:O	1:C:282:VAL:HG12	2.21	0.41
1:C:342:LEU:O	1:C:346:GLN:HG3	2.21	0.41
1:C:348:LYS:NZ	1:C:443:ASP:CG	2.79	0.41
1:C:565:GLN:CD	1:C:1213:PHE:CA	2.94	0.41
1:D:282:VAL:O	1:D:282:VAL:HG12	2.20	0.41
1:D:369:SER:O	1:D:373:GLU:HG2	2.21	0.41
1:D:530:ARG:HD2	1:D:545:GLN:NE2	2.36	0.41
1:E:10:LEU:CD2	1:E:13:ARG:NH2	2.83	0.41
1:E:322:LEU:HD23	1:E:364:LEU:HD13	2.03	0.41
1:E:346:GLN:C	1:E:348:LYS:H	2.28	0.41
1:E:456:LEU:O	1:E:459:LYS:HB3	2.21	0.41
1:E:511:LYS:HB2	1:E:563:ILE:HG13	2.02	0.41
1:E:530:ARG:HD2	1:E:545:GLN:NE2	2.36	0.41
1:E:565:GLN:OE1	1:E:1212:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:884:TRP:HH2	2:L:78:THR:O	2.02	0.41
1:F:565:GLN:OE1	1:F:1212:THR:HB	2.21	0.41
1:F:1141:LEU:HG	1:F:1155:ASN:HA	2.03	0.41
1:G:46:GLU:OE2	1:G:55:MET:HE2	2.21	0.41
1:G:228:ARG:HD3	1:G:256:SER:HB3	2.03	0.41
1:G:326:LEU:HA	1:G:326:LEU:HD23	1.44	0.41
1:G:456:LEU:O	1:G:459:LYS:HB3	2.21	0.41
1:G:565:GLN:OE1	1:G:1212:THR:HB	2.21	0.41
2:I:67:TYR:HD1	2:I:74:TYR:HB3	1.84	0.41
2:L:30:PRO:HB3	2:L:46:PHE:CD2	2.56	0.41
2:L:55:LYS:HG2	2:L:75:ILE:HG12	2.03	0.41
1:A:153:HIS:HA	1:A:264:THR:O	2.21	0.41
1:A:348:LYS:NZ	1:A:443:ASP:CG	2.79	0.41
1:B:160:LYS:NZ	1:B:264:THR:O	2.53	0.41
1:B:337:ARG:O	1:B:340:TYR:N	2.54	0.41
1:B:342:LEU:O	1:B:346:GLN:HG3	2.21	0.41
1:B:348:LYS:NZ	1:B:443:ASP:CG	2.79	0.41
1:B:676:SER:OG	1:B:678:ASP:OD1	2.37	0.41
1:D:474:SER:HA	1:D:475:PRO:HD2	1.91	0.41
1:D:511:LYS:HB2	1:D:563:ILE:HG13	2.02	0.41
1:D:700:GLU:HB2	1:D:720:SER:HB2	2.03	0.41
1:E:342:LEU:O	1:E:346:GLN:HG3	2.21	0.41
1:E:676:SER:OG	1:E:678:ASP:OD1	2.37	0.41
1:E:947:GLN:HG2	1:E:958:TYR:HD1	1.85	0.41
1:F:153:HIS:HA	1:F:264:THR:O	2.21	0.41
1:F:346:GLN:C	1:F:348:LYS:H	2.28	0.41
1:F:400:LEU:HB3	1:F:404:TRP:HZ3	1.85	0.41
2:J:30:PRO:HB3	2:J:46:PHE:CD2	2.56	0.41
1:A:346:GLN:C	1:A:348:LYS:H	2.28	0.40
1:A:1155:ASN:HB3	1:A:1162:LEU:HB2	2.04	0.40
1:B:351:LYS:NZ	1:B:365:ASP:OD2	2.54	0.40
1:C:322:LEU:HD23	1:C:364:LEU:HD13	2.03	0.40
1:C:326:LEU:HD23	1:C:326:LEU:HA	1.44	0.40
1:C:885:VAL:HG13	1:C:900:SER:O	2.21	0.40
1:C:1141:LEU:HG	1:C:1155:ASN:HA	2.03	0.40
1:D:37:ILE:HG12	3:Q:10:ARG:HD2	2.03	0.40
1:D:1141:LEU:HG	1:D:1155:ASN:HA	2.03	0.40
1:D:1166:ALA:HA	1:D:1167:PRO:HD2	1.93	0.40
1:E:153:HIS:HA	1:E:264:THR:O	2.21	0.40
1:E:885:VAL:HG13	1:E:900:SER:O	2.21	0.40
1:E:1086:GLY:CA	2:L:39:LYS:NZ	2.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:348:LYS:NZ	1:F:443:ASP:CG	2.79	0.40
1:F:631:ALA:H	1:F:665:PHE:HZ	1.69	0.40
1:F:1155:ASN:HB3	1:F:1162:LEU:HB2	2.04	0.40
1:G:322:LEU:HD23	1:G:364:LEU:HD13	2.03	0.40
1:G:1141:LEU:HG	1:G:1155:ASN:HA	2.03	0.40
1:G:1155:ASN:HB3	1:G:1162:LEU:HB2	2.04	0.40
2:N:55:LYS:HG2	2:N:75:ILE:HG12	2.03	0.40
3:R:14:LEU:HD13	3:R:14:LEU:HA	1.97	0.40
1:A:228:ARG:HD3	1:A:256:SER:HB3	2.03	0.40
1:A:282:VAL:O	1:A:282:VAL:HG12	2.21	0.40
1:D:153:HIS:HA	1:D:264:THR:O	2.21	0.40
1:D:565:GLN:OE1	1:D:1212:THR:HB	2.21	0.40
1:D:1135:PHE:HE1	1:D:1142:LEU:HD13	1.85	0.40
1:E:196:LEU:O	1:E:199:LEU:HB2	2.21	0.40
1:E:1155:ASN:HB3	1:E:1162:LEU:HB2	2.04	0.40
1:F:344:GLN:CD	1:F:349:GLN:HE21	2.28	0.40
1:F:530:ARG:HD2	1:F:545:GLN:NE2	2.36	0.40
1:F:584:ALA:CA	1:F:594:TYR:CE2	2.98	0.40
1:G:196:LEU:O	1:G:199:LEU:HB2	2.21	0.40
2:H:30:PRO:HB3	2:H:46:PHE:CD2	2.56	0.40
3:P:34:LEU:HD12	3:P:34:LEU:HA	1.93	0.40
1:A:885:VAL:HG13	1:A:900:SER:O	2.21	0.40
1:B:884:TRP:HH2	2:I:79:LYS:N	2.18	0.40
1:B:947:GLN:HG2	1:B:958:TYR:HD1	1.85	0.40
1:C:947:GLN:HG2	1:C:958:TYR:HD1	1.85	0.40
1:E:351:LYS:NZ	1:E:365:ASP:OD2	2.54	0.40
1:E:989:GLU:HG2	1:E:991:VAL:H	1.85	0.40
1:F:565:GLN:CD	1:F:1213:PHE:CA	2.94	0.40
1:G:153:HIS:HA	1:G:264:THR:O	2.21	0.40
1:G:348:LYS:NZ	1:G:443:ASP:CG	2.79	0.40
1:G:631:ALA:H	1:G:665:PHE:HZ	1.69	0.40
1:G:971:PRO:C	1:G:973:LEU:H	2.29	0.40
2:K:55:LYS:HG2	2:K:75:ILE:HG12	2.03	0.40
3:Q:14:LEU:HD13	3:Q:14:LEU:HA	1.98	0.40
1:A:196:LEU:O	1:A:199:LEU:HB2	2.21	0.40
1:A:274:MET:HE2	1:G:358:SER:CB	2.43	0.40
1:A:1141:LEU:HG	1:A:1155:ASN:HA	2.03	0.40
1:B:228:ARG:HD3	1:B:256:SER:HB3	2.03	0.40
1:B:1146:ASP:HB2	1:B:1150:GLU:HG2	2.04	0.40
1:C:337:ARG:O	1:C:340:TYR:N	2.54	0.40
1:C:351:LYS:NZ	1:C:365:ASP:OD2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:884:TRP:HH2	2:J:79:LYS:N	2.18	0.40
1:C:989:GLU:HG2	1:C:991:VAL:H	1.85	0.40
1:D:597:TRP:CD2	1:D:600:LYS:HE3	2.57	0.40
1:E:46:GLU:OE2	1:E:55:MET:HE2	2.21	0.40
1:E:348:LYS:NZ	1:E:443:ASP:CG	2.79	0.40
1:E:631:ALA:H	1:E:665:PHE:HZ	1.69	0.40
1:F:289:GLU:OE2	1:F:303:LYS:NZ	2.43	0.40
2:H:39:LYS:HD2	2:H:56:GLY:O	2.22	0.40
2:H:55:LYS:HG2	2:H:75:ILE:HG12	2.03	0.40
2:I:71:PRO:CD	2:I:84:GLY:HA2	2.52	0.40
2:J:55:LYS:HG2	2:J:75:ILE:HG12	2.03	0.40
2:M:39:LYS:HD2	2:M:56:GLY:O	2.22	0.40
1:A:217:PRO:HG3	1:A:226:ARG:NH1	2.36	0.40
1:A:369:SER:O	1:A:373:GLU:HG2	2.21	0.40
1:A:597:TRP:CD2	1:A:600:LYS:HE3	2.57	0.40
1:B:322:LEU:HD23	1:B:364:LEU:HD13	2.02	0.40
1:B:344:GLN:CD	1:B:349:GLN:HE21	2.28	0.40
1:D:145:GLY:HA2	1:D:259:GLN:HE21	1.85	0.40
1:E:400:LEU:HB3	1:E:404:TRP:HZ3	1.84	0.40
1:F:1086:GLY:CA	2:M:39:LYS:NZ	2.66	0.40
2:I:55:LYS:HG2	2:I:75:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	24	61
1	B	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	24	61
1	C	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	24	61
1	D	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	24	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	24	61
1	F	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	24	61
1	G	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	24	61
2	H	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	I	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	J	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	K	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	L	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	M	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	N	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
3	O	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	P	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	Q	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	R	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
All	All	9403/9844 (96%)	8741 (93%)	620 (7%)	42 (0%)	31	65

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1073	ILE
1	B	1073	ILE
1	C	1073	ILE
1	D	1073	ILE
1	E	1073	ILE
1	F	1073	ILE
1	G	1073	ILE
1	A	591	GLY
1	B	591	GLY
1	C	591	GLY
1	D	591	GLY
1	E	591	GLY
1	F	591	GLY
1	G	591	GLY
1	A	347	ASN
1	B	347	ASN
1	C	347	ASN
1	D	347	ASN

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Mol	Chain	Res	Type
1	E	347	ASN
1	F	347	ASN
1	G	347	ASN
1	A	266	ASP
1	B	266	ASP
1	C	266	ASP
1	D	266	ASP
1	E	266	ASP
1	F	266	ASP
1	G	266	ASP
1	A	613	PRO
1	B	613	PRO
1	C	613	PRO
1	D	613	PRO
1	E	613	PRO
1	F	613	PRO
1	G	613	PRO
1	A	1205	VAL
1	B	1205	VAL
1	C	1205	VAL
1	D	1205	VAL
1	E	1205	VAL
1	F	1205	VAL
1	G	1205	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1022/1119 (91%)	1019 (100%)	3 (0%)	86	85
1	B	1106/1119 (99%)	1101 (100%)	5 (0%)	81	82
1	C	1022/1119 (91%)	1019 (100%)	3 (0%)	86	85
1	D	1106/1119 (99%)	1101 (100%)	5 (0%)	81	82
1	E	1106/1119 (99%)	1101 (100%)	5 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	1022/1119 (91%)	1019 (100%)	3 (0%)	86	85
1	G	1106/1119 (99%)	1101 (100%)	5 (0%)	81	82
2	H	84/84 (100%)	84 (100%)	0	100	100
2	I	84/84 (100%)	84 (100%)	0	100	100
2	J	84/84 (100%)	84 (100%)	0	100	100
2	K	84/84 (100%)	84 (100%)	0	100	100
2	L	84/84 (100%)	84 (100%)	0	100	100
2	M	84/84 (100%)	84 (100%)	0	100	100
2	N	84/84 (100%)	84 (100%)	0	100	100
3	O	84/84 (100%)	76 (90%)	8 (10%)	8	27
3	P	84/84 (100%)	77 (92%)	7 (8%)	10	32
3	Q	84/84 (100%)	76 (90%)	8 (10%)	8	27
3	R	84/84 (100%)	76 (90%)	8 (10%)	8	27
All	All	8414/8757 (96%)	8354 (99%)	60 (1%)	73	79

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	391	LYS
1	A	392	ASP
1	A	884	TRP
1	B	58	LYS
1	B	81	LYS
1	B	391	LYS
1	B	392	ASP
1	B	884	TRP
1	C	391	LYS
1	C	392	ASP
1	C	884	TRP
1	D	58	LYS
1	D	81	LYS
1	D	391	LYS
1	D	392	ASP
1	D	884	TRP
1	E	58	LYS
1	E	81	LYS
1	E	391	LYS

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Mol	Chain	Res	Type
1	E	392	ASP
1	E	884	TRP
1	F	391	LYS
1	F	392	ASP
1	F	884	TRP
1	G	58	LYS
1	G	81	LYS
1	G	391	LYS
1	G	392	ASP
1	G	884	TRP
3	O	10	ARG
3	O	14	LEU
3	O	20	LEU
3	O	34	LEU
3	O	83	ASP
3	O	84	MET
3	O	87	SER
3	O	93	ARG
3	P	10	ARG
3	P	14	LEU
3	P	20	LEU
3	P	34	LEU
3	P	84	MET
3	P	87	SER
3	P	93	ARG
3	Q	10	ARG
3	Q	14	LEU
3	Q	20	LEU
3	Q	34	LEU
3	Q	83	ASP
3	Q	84	MET
3	Q	87	SER
3	Q	93	ARG
3	R	10	ARG
3	R	14	LEU
3	R	20	LEU
3	R	34	LEU
3	R	83	ASP
3	R	84	MET
3	R	87	SER
3	R	93	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (196)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	214	GLN
1	A	416	GLN
1	A	469	GLN
1	A	551	ASN
1	A	602	ASN
1	A	620	HIS
1	A	698	HIS
1	A	703	ASN
1	A	709	ASN
1	A	712	HIS
1	A	713	HIS
1	A	748	HIS
1	A	782	ASN
1	A	785	GLN
1	A	819	ASN
1	A	836	HIS
1	A	844	GLN
1	A	917	ASN
1	A	992	ASN
1	A	1076	ASN
1	A	1126	HIS
1	B	11	GLN
1	B	45	ASN
1	B	50	GLN
1	B	51	GLN
1	B	201	ASN
1	B	214	GLN
1	B	416	GLN
1	B	469	GLN
1	B	551	ASN
1	B	602	ASN
1	B	605	ASN
1	B	620	HIS
1	B	698	HIS
1	B	703	ASN
1	B	712	HIS
1	B	713	HIS
1	B	748	HIS
1	B	782	ASN
1	B	785	GLN
1	B	819	ASN

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Mol	Chain	Res	Type
1	B	827	HIS
1	B	836	HIS
1	B	844	GLN
1	B	917	ASN
1	B	963	GLN
1	B	992	ASN
1	B	1076	ASN
1	B	1126	HIS
1	C	121	GLN
1	C	201	ASN
1	C	214	GLN
1	C	416	GLN
1	C	469	GLN
1	C	551	ASN
1	C	602	ASN
1	C	620	HIS
1	C	703	ASN
1	C	709	ASN
1	C	712	HIS
1	C	713	HIS
1	C	748	HIS
1	C	782	ASN
1	C	785	GLN
1	C	819	ASN
1	C	827	HIS
1	C	836	HIS
1	C	844	GLN
1	C	917	ASN
1	C	992	ASN
1	C	1076	ASN
1	C	1126	HIS
1	D	11	GLN
1	D	51	GLN
1	D	201	ASN
1	D	214	GLN
1	D	416	GLN
1	D	469	GLN
1	D	551	ASN
1	D	602	ASN
1	D	605	ASN
1	D	620	HIS
1	D	698	HIS

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Mol	Chain	Res	Type
1	D	703	ASN
1	D	712	HIS
1	D	713	HIS
1	D	748	HIS
1	D	782	ASN
1	D	785	GLN
1	D	819	ASN
1	D	836	HIS
1	D	844	GLN
1	D	917	ASN
1	D	982	ASN
1	D	992	ASN
1	D	1076	ASN
1	D	1126	HIS
1	D	1158	ASN
1	E	11	GLN
1	E	45	ASN
1	E	51	GLN
1	E	201	ASN
1	E	214	GLN
1	E	416	GLN
1	E	469	GLN
1	E	551	ASN
1	E	602	ASN
1	E	620	HIS
1	E	703	ASN
1	E	709	ASN
1	E	712	HIS
1	E	713	HIS
1	E	748	HIS
1	E	782	ASN
1	E	785	GLN
1	E	819	ASN
1	E	827	HIS
1	E	836	HIS
1	E	844	GLN
1	E	917	ASN
1	E	963	GLN
1	E	982	ASN
1	E	992	ASN
1	E	1043	HIS
1	E	1076	ASN

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Mol	Chain	Res	Type
1	E	1126	HIS
1	F	201	ASN
1	F	214	GLN
1	F	416	GLN
1	F	469	GLN
1	F	551	ASN
1	F	602	ASN
1	F	605	ASN
1	F	620	HIS
1	F	703	ASN
1	F	709	ASN
1	F	712	HIS
1	F	713	HIS
1	F	748	HIS
1	F	782	ASN
1	F	785	GLN
1	F	819	ASN
1	F	827	HIS
1	F	836	HIS
1	F	844	GLN
1	F	886	HIS
1	F	917	ASN
1	F	992	ASN
1	F	1043	HIS
1	F	1076	ASN
1	F	1126	HIS
1	F	1158	ASN
1	G	11	GLN
1	G	45	ASN
1	G	51	GLN
1	G	121	GLN
1	G	201	ASN
1	G	214	GLN
1	G	416	GLN
1	G	469	GLN
1	G	551	ASN
1	G	602	ASN
1	G	605	ASN
1	G	620	HIS
1	G	703	ASN
1	G	712	HIS
1	G	713	HIS

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Mol	Chain	Res	Type
1	G	748	HIS
1	G	782	ASN
1	G	785	GLN
1	G	819	ASN
1	G	827	HIS
1	G	836	HIS
1	G	844	GLN
1	G	917	ASN
1	G	963	GLN
1	G	982	ASN
1	G	992	ASN
1	G	1043	HIS
1	G	1076	ASN
1	G	1126	HIS
2	I	70	ASN
2	J	70	ASN
2	K	70	ASN
2	M	70	ASN
2	N	70	ASN
3	O	44	GLN
3	O	92	ASN
3	P	44	GLN
3	P	92	ASN
3	Q	44	GLN
3	Q	92	ASN
3	R	38	HIS
3	R	44	GLN
3	R	92	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	HEC	L	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.54	5 (7%)
4	DTP	A	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
4	DTP	F	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	M	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.54	5 (7%)
4	DTP	B	1301	-	31,32,32	3.50	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	I	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.55	5 (7%)
4	DTP	G	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	J	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.54	5 (7%)
5	HEC	K	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.55	5 (7%)
4	DTP	D	1301	-	31,32,32	3.52	12 (38%)	46,50,50	2.02	11 (23%)
4	DTP	C	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	N	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.54	5 (7%)
5	HEC	H	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.53	5 (7%)
4	DTP	E	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.03	11 (23%)

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	HEC	L	500	2	-	5/14/54/54	-
4	DTP	A	1301	-	-	8/22/34/34	0/3/3/3
4	DTP	F	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	M	500	2	-	5/14/54/54	-
4	DTP	B	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	I	500	2	-	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	G	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	J	500	2	-	5/14/54/54	-
5	HEC	K	500	2	-	5/14/54/54	-
4	DTP	D	1301	-	-	8/22/34/34	0/3/3/3
4	DTP	C	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	N	500	2	-	5/14/54/54	-
5	HEC	H	500	2	-	5/14/54/54	-
4	DTP	E	1301	-	-	8/22/34/34	0/3/3/3

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1301	DTP	C2'-C3'	-12.34	1.21	1.52
4	G	1301	DTP	C2'-C3'	-12.33	1.21	1.52
4	F	1301	DTP	C2'-C3'	-12.33	1.21	1.52
4	A	1301	DTP	C2'-C3'	-12.31	1.21	1.52
4	E	1301	DTP	C2'-C3'	-12.31	1.21	1.52
4	C	1301	DTP	C2'-C3'	-12.31	1.21	1.52
4	B	1301	DTP	C2'-C3'	-12.29	1.21	1.52
4	G	1301	DTP	O4'-C4'	-8.29	1.26	1.45
4	D	1301	DTP	O4'-C4'	-8.28	1.26	1.45
4	F	1301	DTP	O4'-C4'	-8.27	1.26	1.45
4	A	1301	DTP	O4'-C4'	-8.27	1.26	1.45
4	E	1301	DTP	O4'-C4'	-8.27	1.26	1.45
4	C	1301	DTP	O4'-C4'	-8.27	1.26	1.45
4	B	1301	DTP	O4'-C4'	-8.25	1.26	1.45
4	E	1301	DTP	C1'-N9	-8.11	1.31	1.46
4	C	1301	DTP	C1'-N9	-8.09	1.31	1.46
4	F	1301	DTP	C1'-N9	-8.07	1.31	1.46
4	G	1301	DTP	C1'-N9	-8.07	1.31	1.46
4	B	1301	DTP	C1'-N9	-8.07	1.31	1.46
4	A	1301	DTP	C1'-N9	-8.07	1.31	1.46
4	D	1301	DTP	C1'-N9	-8.06	1.31	1.46
5	K	500	HEC	C3D-C2D	7.95	1.53	1.36
5	I	500	HEC	C3D-C2D	7.93	1.53	1.36
5	H	500	HEC	C3D-C2D	7.93	1.53	1.36
5	J	500	HEC	C3D-C2D	7.92	1.53	1.36
5	L	500	HEC	C3D-C2D	7.92	1.53	1.36
5	M	500	HEC	C3D-C2D	7.91	1.53	1.36
5	N	500	HEC	C3D-C2D	7.88	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1301	DTP	C3'-C4'	4.23	1.64	1.53
4	E	1301	DTP	C3'-C4'	4.23	1.64	1.53
4	G	1301	DTP	C3'-C4'	4.20	1.64	1.53
4	C	1301	DTP	C3'-C4'	4.20	1.64	1.53
4	B	1301	DTP	C3'-C4'	4.20	1.64	1.53
4	A	1301	DTP	C3'-C4'	4.20	1.64	1.53
4	F	1301	DTP	C3'-C4'	4.19	1.64	1.53
5	N	500	HEC	CBB-CAB	-4.10	1.34	1.51
5	H	500	HEC	CBB-CAB	-4.09	1.34	1.51
5	M	500	HEC	CBB-CAB	-4.09	1.34	1.51
5	L	500	HEC	CBB-CAB	-4.08	1.34	1.51
5	J	500	HEC	CBB-CAB	-4.08	1.34	1.51
5	K	500	HEC	CBB-CAB	-4.08	1.34	1.51
5	I	500	HEC	CBB-CAB	-4.08	1.34	1.51
5	H	500	HEC	CBC-CAC	-4.03	1.34	1.51
5	J	500	HEC	CBC-CAC	-4.03	1.34	1.51
5	N	500	HEC	CBC-CAC	-4.03	1.34	1.51
5	L	500	HEC	CBC-CAC	-4.02	1.34	1.51
5	K	500	HEC	CBC-CAC	-4.02	1.34	1.51
5	I	500	HEC	CBC-CAC	-4.02	1.34	1.51
5	M	500	HEC	CBC-CAC	-4.01	1.34	1.51
5	J	500	HEC	FE-NB	3.81	2.06	1.94
5	N	500	HEC	FE-NB	3.81	2.06	1.94
5	I	500	HEC	FE-NB	3.79	2.06	1.94
5	L	500	HEC	FE-NB	3.79	2.06	1.94
5	M	500	HEC	FE-NB	3.79	2.06	1.94
5	H	500	HEC	FE-NB	3.79	2.06	1.94
5	K	500	HEC	FE-NB	3.78	2.06	1.94
4	E	1301	DTP	O4'-C1'	3.37	1.49	1.42
4	D	1301	DTP	O4'-C1'	3.36	1.49	1.42
4	A	1301	DTP	O4'-C1'	3.35	1.49	1.42
4	G	1301	DTP	O4'-C1'	3.34	1.49	1.42
4	C	1301	DTP	O4'-C1'	3.33	1.49	1.42
4	B	1301	DTP	O4'-C1'	3.32	1.49	1.42
4	F	1301	DTP	O4'-C1'	3.32	1.49	1.42
5	K	500	HEC	FE-ND	3.30	2.05	1.94
5	I	500	HEC	FE-ND	3.29	2.05	1.94
5	N	500	HEC	FE-ND	3.26	2.04	1.94
5	M	500	HEC	FE-ND	3.26	2.04	1.94
5	L	500	HEC	FE-ND	3.26	2.04	1.94
5	J	500	HEC	FE-ND	3.25	2.04	1.94
5	H	500	HEC	FE-ND	3.24	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	500	HEC	FE-NA	3.21	2.05	1.95
5	K	500	HEC	FE-NA	3.21	2.05	1.95
5	J	500	HEC	FE-NA	3.21	2.05	1.95
5	I	500	HEC	FE-NA	3.20	2.05	1.95
5	L	500	HEC	FE-NA	3.20	2.05	1.95
5	N	500	HEC	FE-NA	3.19	2.05	1.95
5	H	500	HEC	FE-NA	3.19	2.05	1.95
5	I	500	HEC	FE-NC	3.01	2.05	1.95
5	H	500	HEC	FE-NC	3.01	2.05	1.95
5	K	500	HEC	FE-NC	3.00	2.05	1.95
5	N	500	HEC	FE-NC	3.00	2.05	1.95
5	L	500	HEC	FE-NC	3.00	2.05	1.95
5	M	500	HEC	FE-NC	3.00	2.05	1.95
5	J	500	HEC	FE-NC	2.99	2.05	1.95
4	E	1301	DTP	C6-N6	2.87	1.41	1.34
4	G	1301	DTP	C6-N6	2.87	1.41	1.34
4	C	1301	DTP	C6-N6	2.87	1.41	1.34
4	D	1301	DTP	C6-N6	2.87	1.41	1.34
4	B	1301	DTP	C6-N6	2.86	1.41	1.34
4	A	1301	DTP	C6-N6	2.86	1.41	1.34
4	F	1301	DTP	C6-N6	2.86	1.41	1.34
4	G	1301	DTP	O3'-C3'	2.80	1.49	1.43
4	F	1301	DTP	O3'-C3'	2.77	1.49	1.43
4	C	1301	DTP	C5-C4	-2.77	1.34	1.39
4	C	1301	DTP	O3'-C3'	2.76	1.49	1.43
4	A	1301	DTP	O3'-C3'	2.76	1.49	1.43
4	A	1301	DTP	C5-C4	-2.75	1.34	1.39
4	F	1301	DTP	C5-C4	-2.75	1.34	1.39
4	B	1301	DTP	C5-C4	-2.74	1.34	1.39
4	D	1301	DTP	C5-C4	-2.74	1.34	1.39
4	E	1301	DTP	C5-C4	-2.74	1.34	1.39
4	B	1301	DTP	O3'-C3'	2.74	1.49	1.43
4	D	1301	DTP	O3'-C3'	2.74	1.49	1.43
4	G	1301	DTP	C5-C4	-2.73	1.34	1.39
4	E	1301	DTP	O3'-C3'	2.73	1.49	1.43
4	C	1301	DTP	PB-O3B	-2.71	1.56	1.59
4	F	1301	DTP	PB-O3B	-2.66	1.56	1.59
4	G	1301	DTP	PB-O3B	-2.65	1.56	1.59
4	A	1301	DTP	PB-O3B	-2.63	1.56	1.59
4	D	1301	DTP	PB-O3B	-2.63	1.56	1.59
4	B	1301	DTP	PB-O3B	-2.62	1.56	1.59
4	E	1301	DTP	PB-O3B	-2.57	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1301	DTP	PA-O3A	-2.41	1.56	1.59
4	D	1301	DTP	PA-O3A	-2.40	1.56	1.59
4	F	1301	DTP	PA-O3A	-2.39	1.56	1.59
4	A	1301	DTP	PA-O3A	-2.38	1.56	1.59
4	C	1301	DTP	PA-O3A	-2.37	1.56	1.59
4	E	1301	DTP	PA-O3A	-2.37	1.56	1.59
4	G	1301	DTP	PA-O3A	-2.36	1.57	1.59
4	D	1301	DTP	PB-O3A	-2.34	1.57	1.59
4	B	1301	DTP	PB-O3A	-2.28	1.57	1.59
4	G	1301	DTP	PB-O3A	-2.27	1.57	1.59
4	A	1301	DTP	PB-O3A	-2.25	1.57	1.59
4	C	1301	DTP	PB-O3A	-2.24	1.57	1.59
4	F	1301	DTP	PB-O3A	-2.19	1.57	1.59
4	D	1301	DTP	C5-N7	-2.18	1.35	1.39
4	E	1301	DTP	PB-O3A	-2.17	1.57	1.59
4	G	1301	DTP	C5-N7	-2.16	1.35	1.39
4	E	1301	DTP	C5-N7	-2.16	1.35	1.39
4	A	1301	DTP	C5-N7	-2.15	1.35	1.39
4	B	1301	DTP	C5-N7	-2.15	1.35	1.39
4	C	1301	DTP	C5-N7	-2.15	1.35	1.39
4	F	1301	DTP	C5-N7	-2.14	1.35	1.39
5	I	500	HEC	CMC-C2C	2.11	1.55	1.50
5	K	500	HEC	CMC-C2C	2.11	1.55	1.50
5	L	500	HEC	CMC-C2C	2.11	1.55	1.50
5	H	500	HEC	CMC-C2C	2.11	1.55	1.50
5	J	500	HEC	CMC-C2C	2.09	1.55	1.50
5	M	500	HEC	CMC-C2C	2.09	1.55	1.50
5	N	500	HEC	CMC-C2C	2.08	1.55	1.50
5	I	500	HEC	CMA-C3A	2.05	1.55	1.50
5	K	500	HEC	CMA-C3A	2.05	1.55	1.50
5	H	500	HEC	CMA-C3A	2.04	1.55	1.50
5	L	500	HEC	CMA-C3A	2.02	1.54	1.50
5	J	500	HEC	CMA-C3A	2.01	1.54	1.50
5	M	500	HEC	CMA-C3A	2.01	1.54	1.50
5	N	500	HEC	CMA-C3A	2.01	1.54	1.50

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1301	DTP	N3-C2-N1	-5.67	120.00	128.58
4	G	1301	DTP	N3-C2-N1	-5.67	120.01	128.58
4	E	1301	DTP	N3-C2-N1	-5.66	120.01	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1301	DTP	N3-C2-N1	-5.64	120.04	128.58
4	A	1301	DTP	N3-C2-N1	-5.64	120.04	128.58
5	I	500	HEC	C1D-ND-C4D	5.63	111.87	105.21
4	B	1301	DTP	N3-C2-N1	-5.62	120.07	128.58
5	M	500	HEC	C1D-ND-C4D	5.62	111.86	105.21
5	K	500	HEC	C1D-ND-C4D	5.61	111.86	105.21
5	N	500	HEC	C1D-ND-C4D	5.61	111.85	105.21
4	F	1301	DTP	N3-C2-N1	-5.60	120.10	128.58
5	L	500	HEC	C1D-ND-C4D	5.58	111.81	105.21
5	J	500	HEC	C1D-ND-C4D	5.57	111.81	105.21
5	H	500	HEC	C1D-ND-C4D	5.55	111.78	105.21
4	D	1301	DTP	N6-C6-N1	-5.45	106.23	118.38
4	G	1301	DTP	N6-C6-N1	-5.45	106.24	118.38
4	E	1301	DTP	N6-C6-N1	-5.45	106.24	118.38
4	F	1301	DTP	N6-C6-N1	-5.45	106.24	118.38
4	A	1301	DTP	N6-C6-N1	-5.44	106.25	118.38
4	B	1301	DTP	N6-C6-N1	-5.44	106.25	118.38
4	C	1301	DTP	N6-C6-N1	-5.43	106.28	118.38
4	C	1301	DTP	C5-C4-N3	-4.98	119.86	126.72
4	E	1301	DTP	C5-C4-N3	-4.98	119.86	126.72
4	D	1301	DTP	C5-C4-N3	-4.96	119.88	126.72
4	F	1301	DTP	C5-C4-N3	-4.96	119.89	126.72
4	B	1301	DTP	C5-C4-N3	-4.96	119.89	126.72
4	A	1301	DTP	C5-C4-N3	-4.96	119.89	126.72
4	G	1301	DTP	C5-C4-N3	-4.93	119.93	126.72
5	I	500	HEC	CBC-CAC-C3C	4.69	125.14	112.42
5	H	500	HEC	CBC-CAC-C3C	4.69	125.14	112.42
5	L	500	HEC	CBC-CAC-C3C	4.68	125.11	112.42
5	J	500	HEC	CBC-CAC-C3C	4.68	125.11	112.42
5	M	500	HEC	CBC-CAC-C3C	4.68	125.10	112.42
5	N	500	HEC	CBC-CAC-C3C	4.67	125.09	112.42
5	K	500	HEC	CBC-CAC-C3C	4.67	125.07	112.42
5	M	500	HEC	CBB-CAB-C3B	4.63	124.97	112.42
5	H	500	HEC	CBB-CAB-C3B	4.62	124.95	112.42
5	J	500	HEC	CBB-CAB-C3B	4.62	124.95	112.42
5	I	500	HEC	CBB-CAB-C3B	4.61	124.92	112.42
5	L	500	HEC	CBB-CAB-C3B	4.61	124.91	112.42
5	K	500	HEC	CBB-CAB-C3B	4.60	124.89	112.42
5	N	500	HEC	CBB-CAB-C3B	4.59	124.86	112.42
4	E	1301	DTP	C5-C6-N6	4.34	134.02	123.29
4	F	1301	DTP	C5-C6-N6	4.32	133.98	123.29
4	B	1301	DTP	C5-C6-N6	4.32	133.98	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1301	DTP	C5-C6-N6	4.31	133.97	123.29
4	C	1301	DTP	C5-C6-N6	4.30	133.94	123.29
4	D	1301	DTP	C5-C6-N6	4.30	133.93	123.29
4	G	1301	DTP	C5-C6-N6	4.29	133.92	123.29
4	C	1301	DTP	N9-C8-N7	-4.04	108.20	113.94
4	F	1301	DTP	N9-C8-N7	-4.04	108.21	113.94
4	E	1301	DTP	N9-C8-N7	-4.04	108.21	113.94
4	D	1301	DTP	N9-C8-N7	-4.04	108.21	113.94
4	A	1301	DTP	N9-C8-N7	-4.02	108.23	113.94
4	G	1301	DTP	N9-C8-N7	-4.01	108.25	113.94
4	B	1301	DTP	N9-C8-N7	-4.00	108.26	113.94
4	D	1301	DTP	C2-N3-C4	3.30	119.89	111.83
4	E	1301	DTP	C2-N3-C4	3.29	119.87	111.83
4	C	1301	DTP	C2-N3-C4	3.28	119.84	111.83
4	G	1301	DTP	C2-N3-C4	3.28	119.84	111.83
4	A	1301	DTP	C2-N3-C4	3.28	119.84	111.83
4	B	1301	DTP	C2-N3-C4	3.27	119.83	111.83
4	F	1301	DTP	C2-N3-C4	3.26	119.80	111.83
4	D	1301	DTP	N3-C4-N9	2.77	131.88	127.17
4	B	1301	DTP	N3-C4-N9	2.76	131.86	127.17
4	E	1301	DTP	N3-C4-N9	2.75	131.85	127.17
4	A	1301	DTP	N3-C4-N9	2.74	131.83	127.17
4	C	1301	DTP	N3-C4-N9	2.74	131.83	127.17
4	F	1301	DTP	N3-C4-N9	2.74	131.83	127.17
4	G	1301	DTP	N3-C4-N9	2.73	131.81	127.17
4	C	1301	DTP	C5-N7-C8	2.70	107.70	103.45
4	G	1301	DTP	C5-N7-C8	2.70	107.69	103.45
4	F	1301	DTP	C5-N7-C8	2.70	107.69	103.45
4	E	1301	DTP	C5-N7-C8	2.70	107.69	103.45
4	D	1301	DTP	C5-N7-C8	2.69	107.68	103.45
4	A	1301	DTP	C5-N7-C8	2.68	107.67	103.45
4	B	1301	DTP	C5-N7-C8	2.67	107.65	103.45
4	E	1301	DTP	C6-C5-C4	2.44	120.51	117.18
4	C	1301	DTP	C6-C5-C4	2.44	120.50	117.18
4	F	1301	DTP	C6-C5-C4	2.42	120.49	117.18
4	B	1301	DTP	C6-C5-C4	2.42	120.48	117.18
4	A	1301	DTP	C6-C5-C4	2.41	120.47	117.18
5	J	500	HEC	C2A-C1A-NA	-2.41	108.00	110.32
5	M	500	HEC	C2A-C1A-NA	-2.41	108.00	110.32
4	D	1301	DTP	C6-C5-C4	2.39	120.44	117.18
5	L	500	HEC	C2A-C1A-NA	-2.38	108.02	110.32
4	G	1301	DTP	C6-C5-C4	2.37	120.42	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	500	HEC	C2A-C1A-NA	-2.35	108.05	110.32
5	I	500	HEC	C2A-C1A-NA	-2.34	108.06	110.32
5	N	500	HEC	C2A-C1A-NA	-2.34	108.06	110.32
5	H	500	HEC	C2A-C1A-NA	-2.32	108.09	110.32
4	C	1301	DTP	C5-C4-N9	2.29	108.30	105.81
5	J	500	HEC	CAB-C3B-C4B	-2.28	121.83	124.79
5	N	500	HEC	CAB-C3B-C4B	-2.27	121.84	124.79
4	E	1301	DTP	C5-C4-N9	2.27	108.28	105.81
4	F	1301	DTP	C5-C4-N9	2.26	108.28	105.81
5	K	500	HEC	CAB-C3B-C4B	-2.26	121.85	124.79
5	L	500	HEC	CAB-C3B-C4B	-2.26	121.85	124.79
4	A	1301	DTP	C5-C4-N9	2.26	108.27	105.81
4	G	1301	DTP	C5-C4-N9	2.25	108.26	105.81
5	I	500	HEC	CAB-C3B-C4B	-2.25	121.87	124.79
4	B	1301	DTP	C5-C4-N9	2.23	108.25	105.81
5	H	500	HEC	CAB-C3B-C4B	-2.23	121.89	124.79
5	M	500	HEC	CAB-C3B-C4B	-2.23	121.89	124.79
4	D	1301	DTP	C5-C4-N9	2.22	108.23	105.81
4	C	1301	DTP	C4-C5-N7	-2.07	108.22	110.58
4	F	1301	DTP	C4-C5-N7	-2.06	108.23	110.58
4	G	1301	DTP	C4-C5-N7	-2.05	108.24	110.58
4	A	1301	DTP	C4-C5-N7	-2.05	108.24	110.58
4	B	1301	DTP	C4-C5-N7	-2.05	108.24	110.58
4	E	1301	DTP	C4-C5-N7	-2.05	108.24	110.58
4	D	1301	DTP	C4-C5-N7	-2.02	108.27	110.58

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	DTP	C5'-O5'-PA-O1A
4	A	1301	DTP	C5'-O5'-PA-O2A
4	A	1301	DTP	C5'-O5'-PA-O3A
4	A	1301	DTP	O4'-C4'-C5'-O5'
4	B	1301	DTP	C5'-O5'-PA-O1A
4	B	1301	DTP	C5'-O5'-PA-O2A
4	B	1301	DTP	C5'-O5'-PA-O3A
4	B	1301	DTP	O4'-C4'-C5'-O5'
4	C	1301	DTP	C5'-O5'-PA-O1A
4	C	1301	DTP	C5'-O5'-PA-O2A
4	C	1301	DTP	C5'-O5'-PA-O3A
4	C	1301	DTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	D	1301	DTP	C5'-O5'-PA-O1A
4	D	1301	DTP	C5'-O5'-PA-O2A
4	D	1301	DTP	C5'-O5'-PA-O3A
4	D	1301	DTP	O4'-C4'-C5'-O5'
4	E	1301	DTP	C5'-O5'-PA-O1A
4	E	1301	DTP	C5'-O5'-PA-O2A
4	E	1301	DTP	C5'-O5'-PA-O3A
4	E	1301	DTP	O4'-C4'-C5'-O5'
4	F	1301	DTP	C5'-O5'-PA-O1A
4	F	1301	DTP	C5'-O5'-PA-O2A
4	F	1301	DTP	C5'-O5'-PA-O3A
4	F	1301	DTP	O4'-C4'-C5'-O5'
4	G	1301	DTP	C5'-O5'-PA-O1A
4	G	1301	DTP	C5'-O5'-PA-O2A
4	G	1301	DTP	C5'-O5'-PA-O3A
4	G	1301	DTP	O4'-C4'-C5'-O5'
5	H	500	HEC	C4C-C3C-CAC-CBC
5	I	500	HEC	C4C-C3C-CAC-CBC
5	J	500	HEC	C4C-C3C-CAC-CBC
5	K	500	HEC	C4C-C3C-CAC-CBC
5	L	500	HEC	C4C-C3C-CAC-CBC
5	M	500	HEC	C4C-C3C-CAC-CBC
5	N	500	HEC	C4C-C3C-CAC-CBC
5	H	500	HEC	C4B-C3B-CAB-CBB
5	I	500	HEC	C4B-C3B-CAB-CBB
5	J	500	HEC	C4B-C3B-CAB-CBB
5	K	500	HEC	C4B-C3B-CAB-CBB
5	L	500	HEC	C4B-C3B-CAB-CBB
5	M	500	HEC	C4B-C3B-CAB-CBB
5	N	500	HEC	C4B-C3B-CAB-CBB
5	H	500	HEC	C2B-C3B-CAB-CBB
5	I	500	HEC	C2B-C3B-CAB-CBB
5	J	500	HEC	C2B-C3B-CAB-CBB
5	K	500	HEC	C2B-C3B-CAB-CBB
5	L	500	HEC	C2B-C3B-CAB-CBB
5	M	500	HEC	C2B-C3B-CAB-CBB
5	N	500	HEC	C2B-C3B-CAB-CBB
5	H	500	HEC	C2C-C3C-CAC-CBC
5	I	500	HEC	C2C-C3C-CAC-CBC
5	J	500	HEC	C2C-C3C-CAC-CBC
5	K	500	HEC	C2C-C3C-CAC-CBC
5	L	500	HEC	C2C-C3C-CAC-CBC

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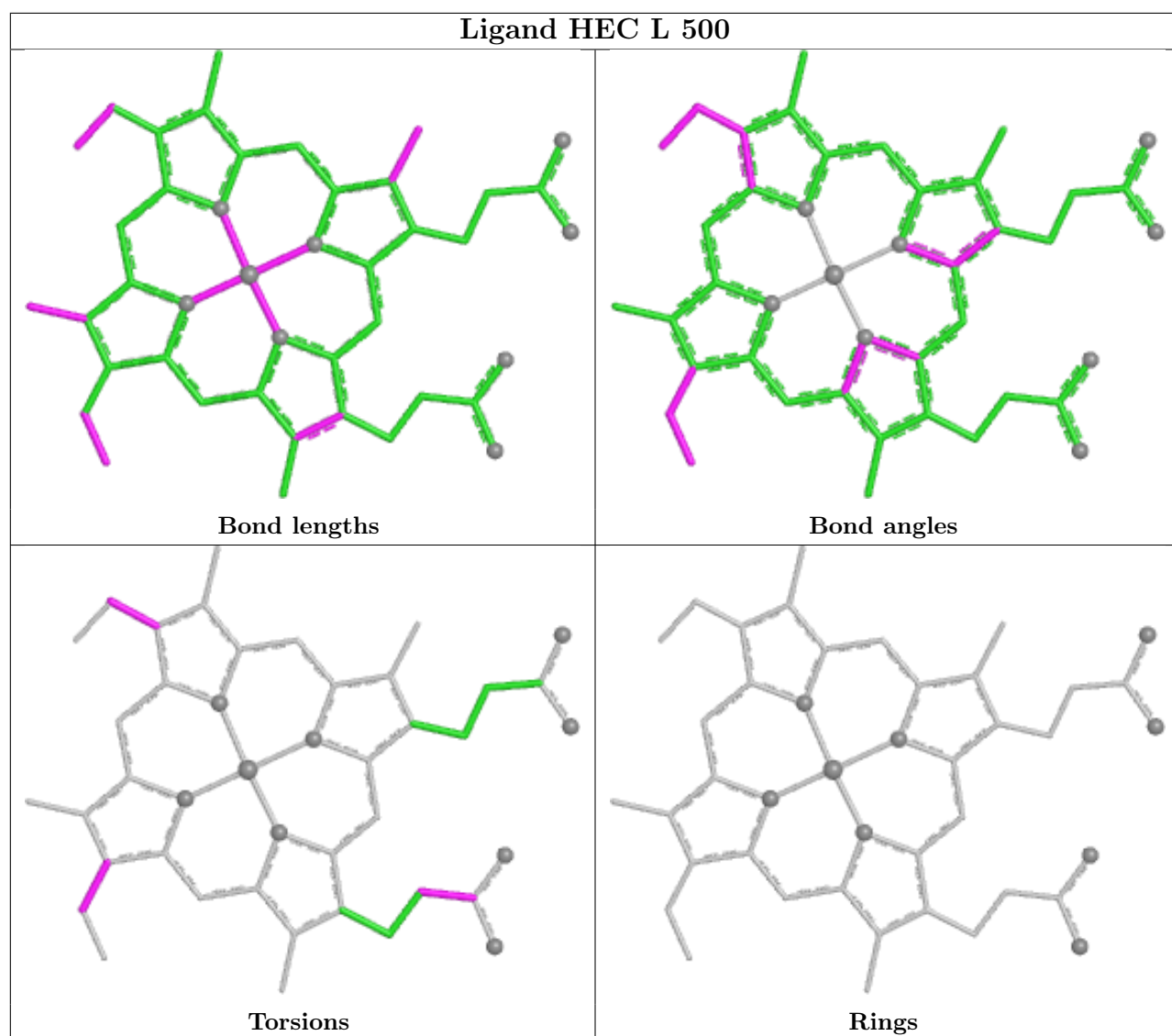
Mol	Chain	Res	Type	Atoms
5	M	500	HEC	C2C-C3C-CAC-CBC
5	N	500	HEC	C2C-C3C-CAC-CBC
4	A	1301	DTP	C3'-C4'-C5'-O5'
4	B	1301	DTP	C3'-C4'-C5'-O5'
4	C	1301	DTP	C3'-C4'-C5'-O5'
4	D	1301	DTP	C3'-C4'-C5'-O5'
4	E	1301	DTP	C3'-C4'-C5'-O5'
4	F	1301	DTP	C3'-C4'-C5'-O5'
4	G	1301	DTP	C3'-C4'-C5'-O5'
4	A	1301	DTP	O4'-C1'-N9-C8
4	B	1301	DTP	O4'-C1'-N9-C8
4	C	1301	DTP	O4'-C1'-N9-C8
4	D	1301	DTP	O4'-C1'-N9-C8
4	E	1301	DTP	O4'-C1'-N9-C8
4	F	1301	DTP	O4'-C1'-N9-C8
4	G	1301	DTP	O4'-C1'-N9-C8
4	A	1301	DTP	PG-O3B-PB-O2B
4	B	1301	DTP	PG-O3B-PB-O2B
4	C	1301	DTP	PG-O3B-PB-O2B
4	D	1301	DTP	PG-O3B-PB-O2B
4	E	1301	DTP	PG-O3B-PB-O2B
4	F	1301	DTP	PG-O3B-PB-O2B
4	G	1301	DTP	PG-O3B-PB-O2B
4	A	1301	DTP	O4'-C1'-N9-C4
4	B	1301	DTP	O4'-C1'-N9-C4
4	C	1301	DTP	O4'-C1'-N9-C4
4	D	1301	DTP	O4'-C1'-N9-C4
4	E	1301	DTP	O4'-C1'-N9-C4
4	F	1301	DTP	O4'-C1'-N9-C4
4	G	1301	DTP	O4'-C1'-N9-C4
5	N	500	HEC	CAD-CBD-CGD-O2D
5	H	500	HEC	CAD-CBD-CGD-O2D
5	I	500	HEC	CAD-CBD-CGD-O2D
5	J	500	HEC	CAD-CBD-CGD-O2D
5	K	500	HEC	CAD-CBD-CGD-O2D
5	L	500	HEC	CAD-CBD-CGD-O2D
5	M	500	HEC	CAD-CBD-CGD-O2D

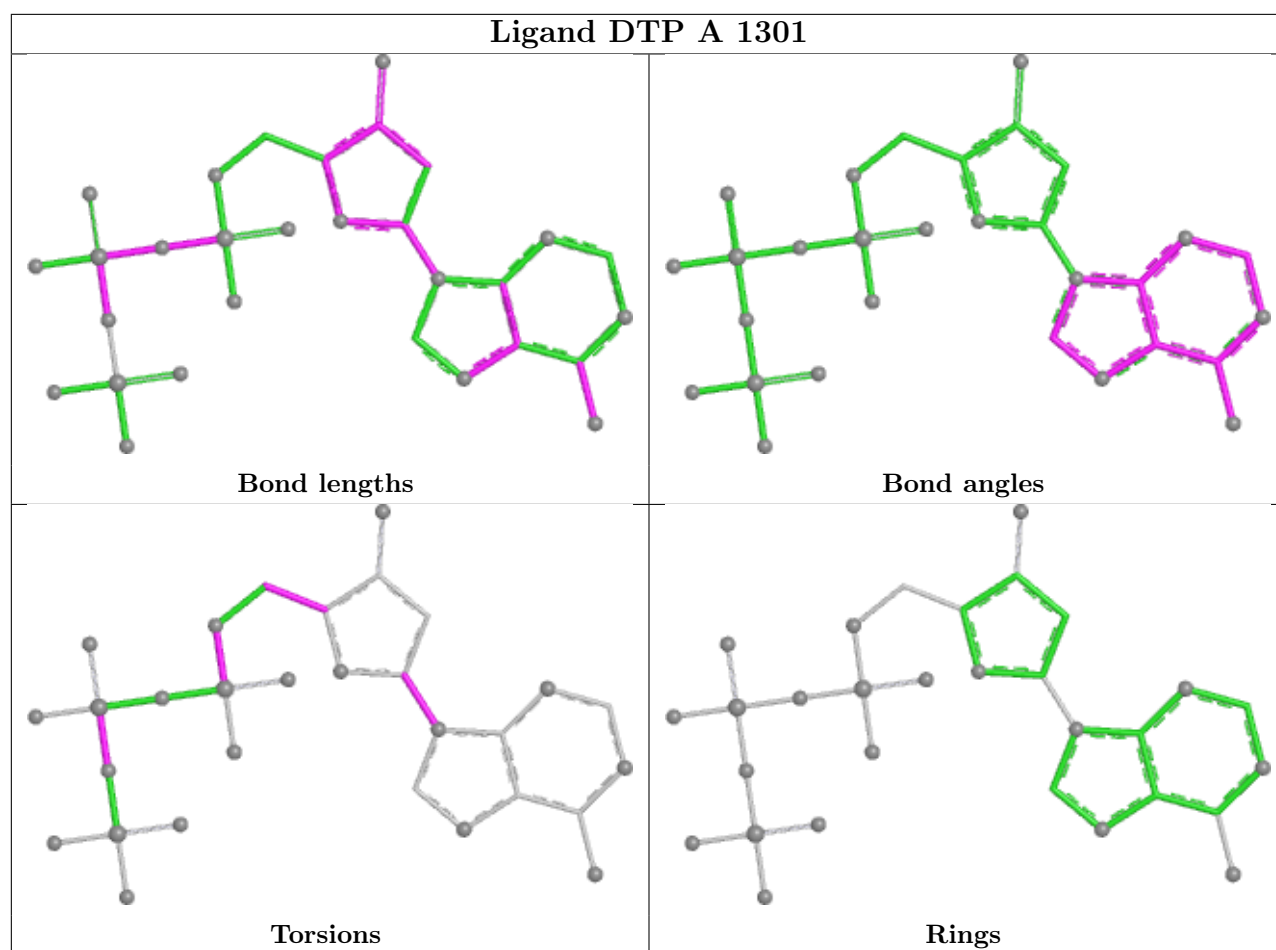
There are no ring outliers.

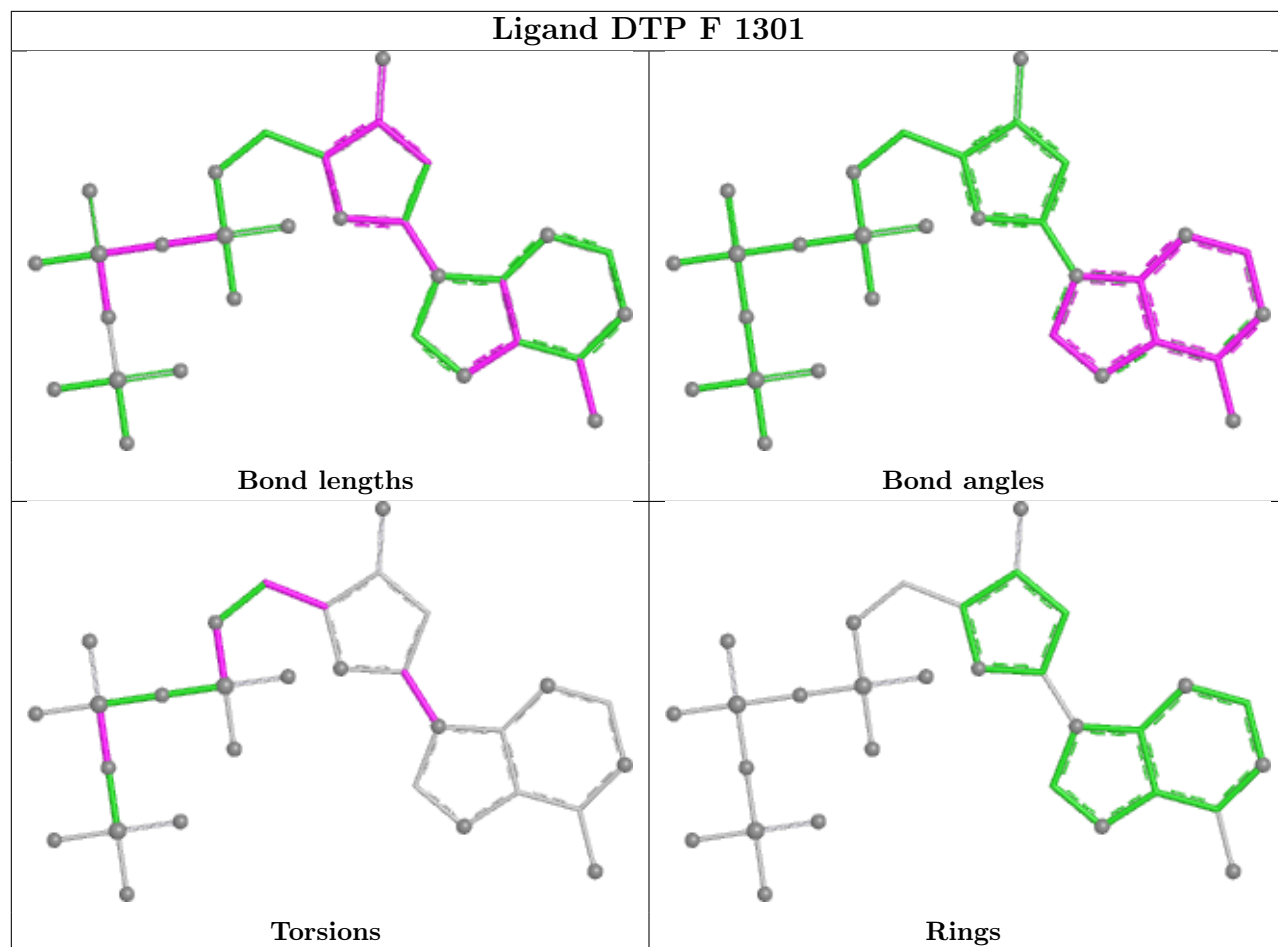
14 monomers are involved in 35 short contacts:

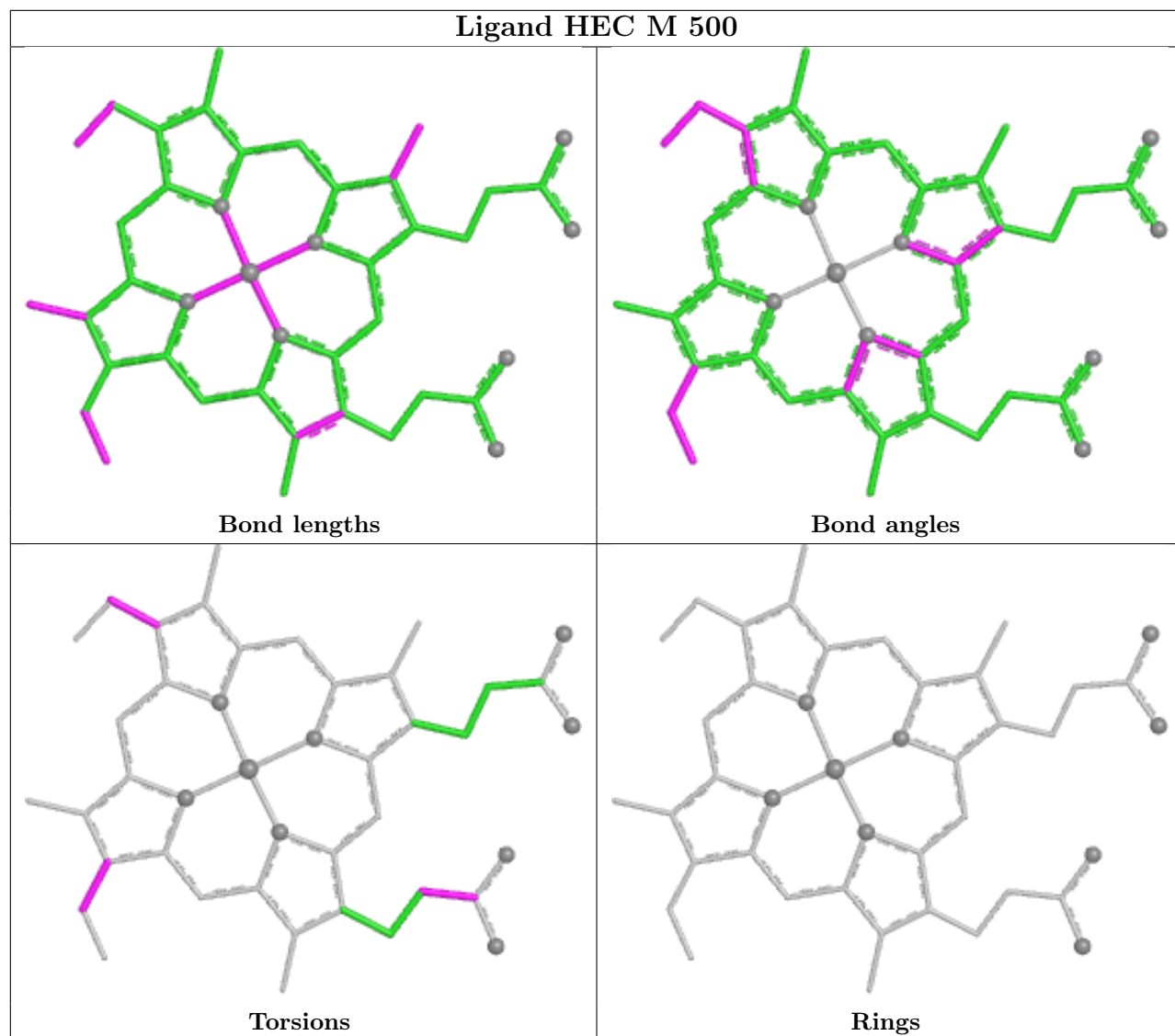
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	500	HEC	2	0
4	A	1301	DTP	3	0
4	F	1301	DTP	3	0
5	M	500	HEC	2	0
4	B	1301	DTP	3	0
5	I	500	HEC	2	0
4	G	1301	DTP	3	0
5	J	500	HEC	2	0
5	K	500	HEC	2	0
4	D	1301	DTP	3	0
4	C	1301	DTP	3	0
5	N	500	HEC	2	0
5	H	500	HEC	2	0
4	E	1301	DTP	3	0

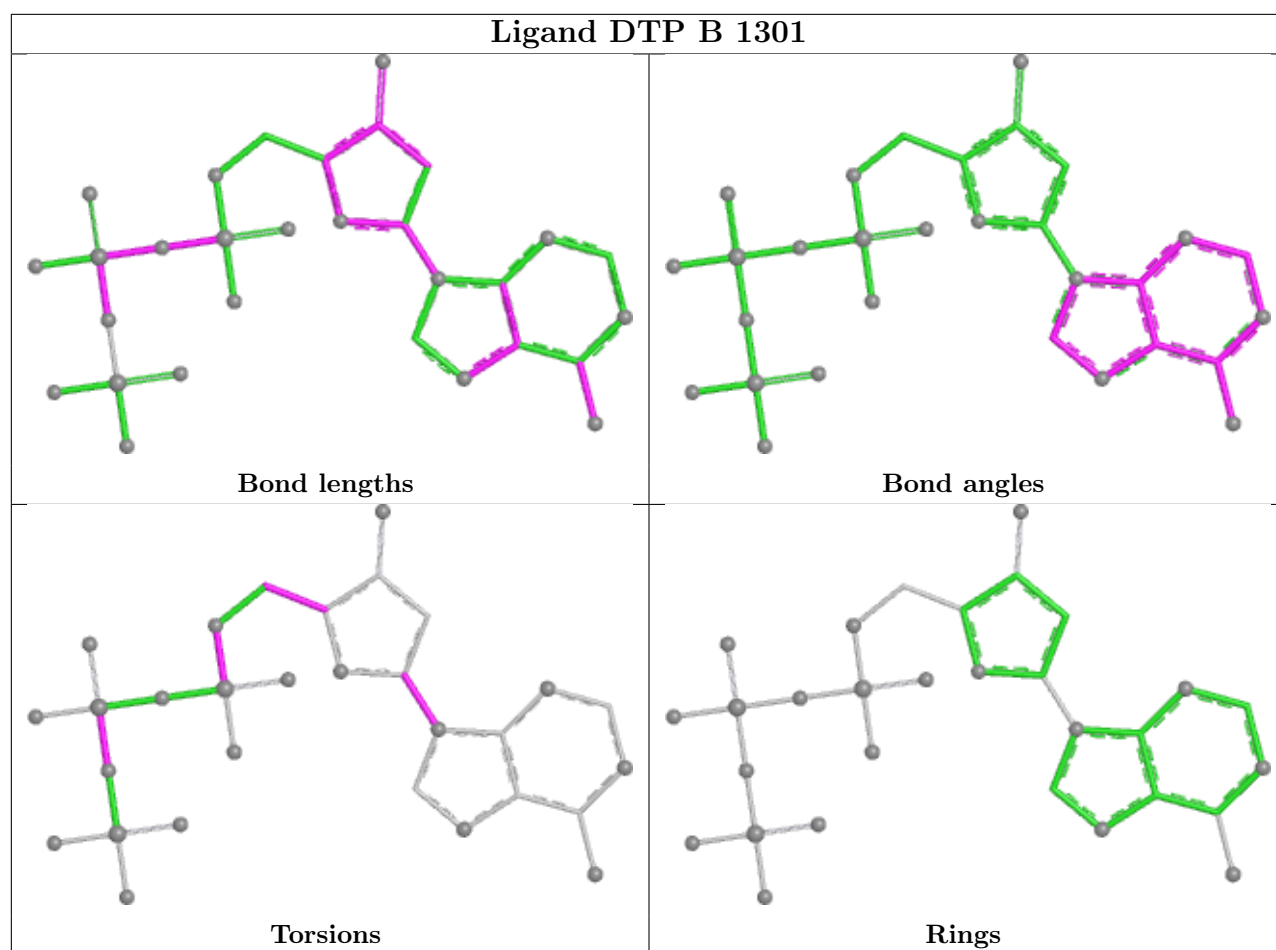
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



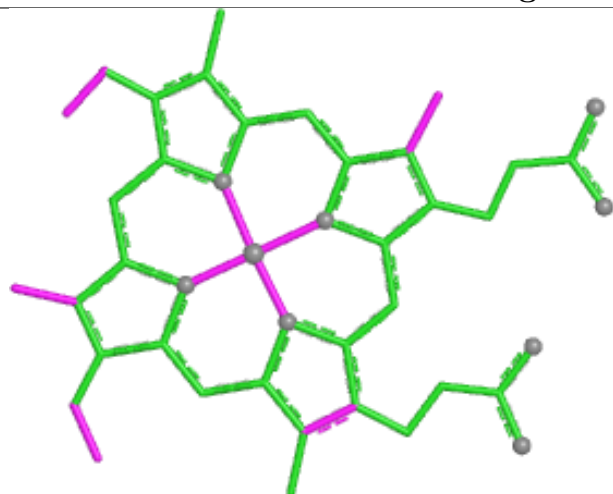




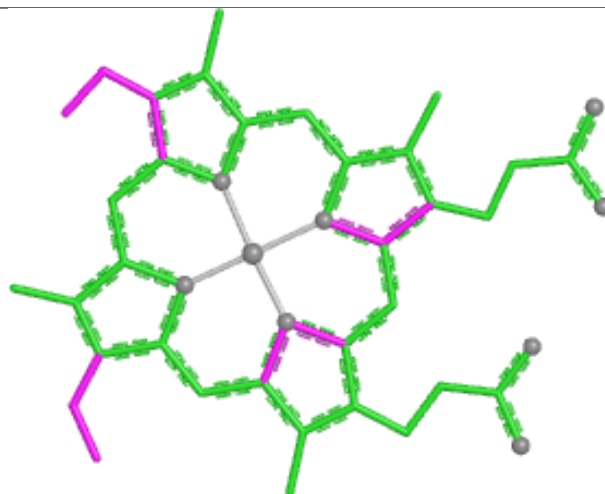




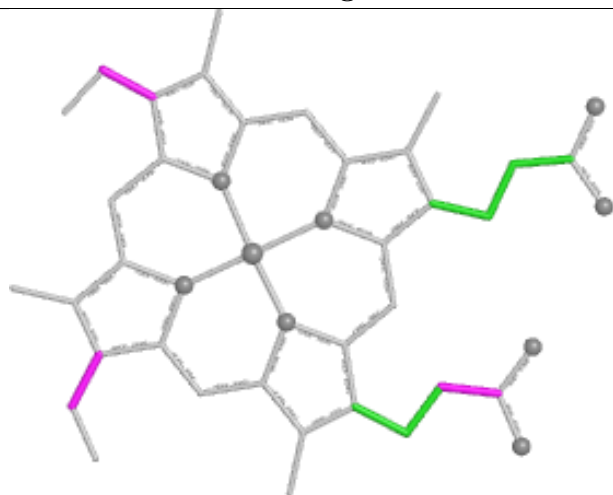
Ligand HEC I 500



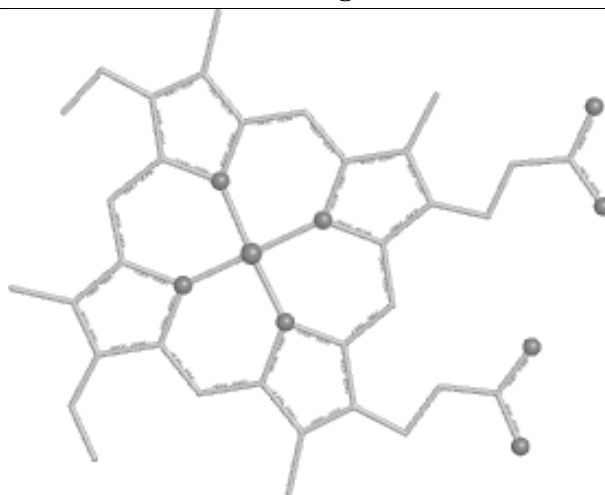
Bond lengths



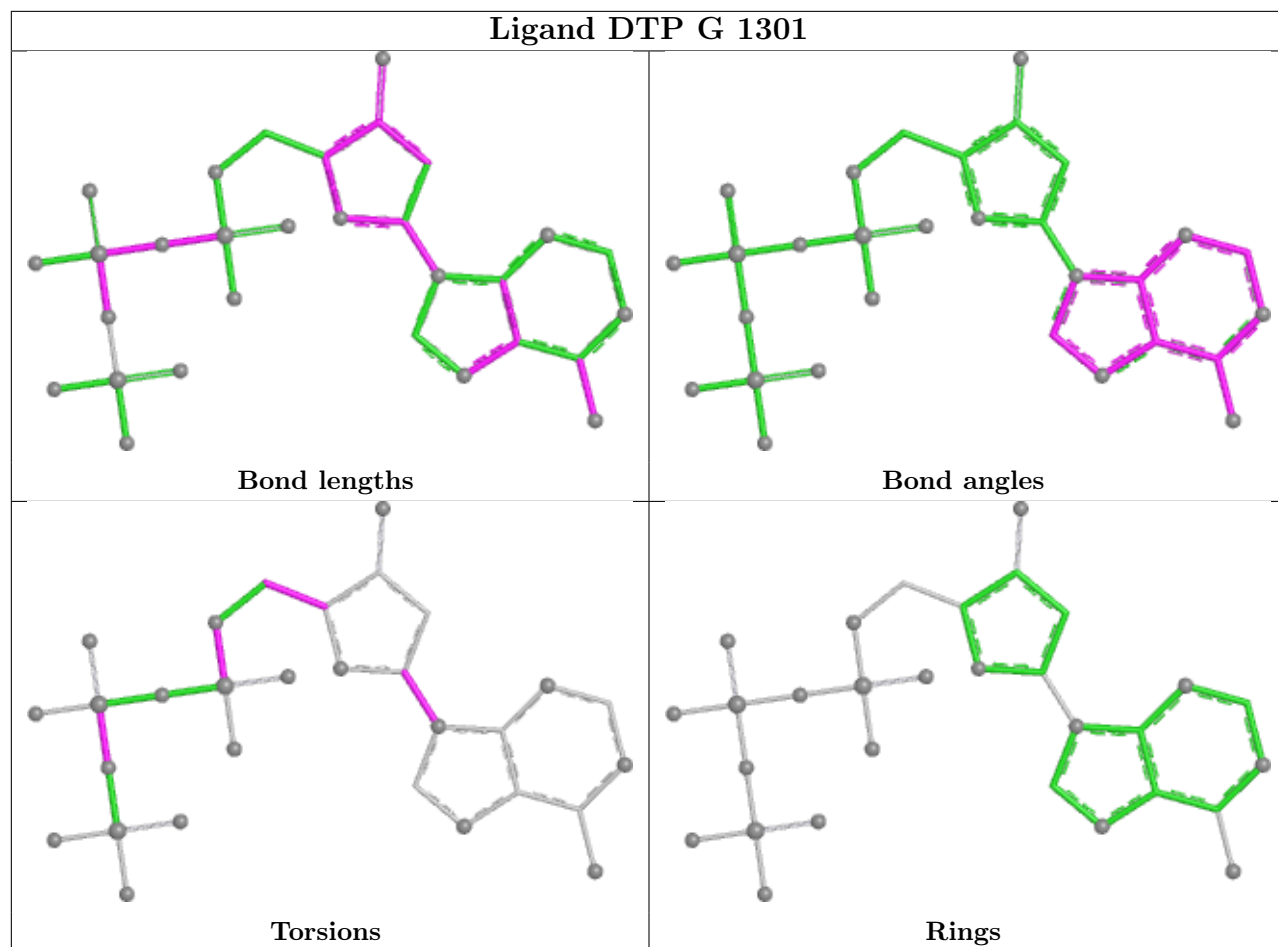
Bond angles



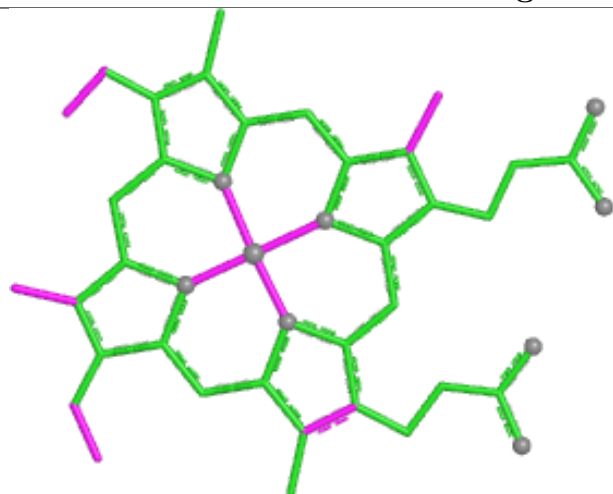
Torsions



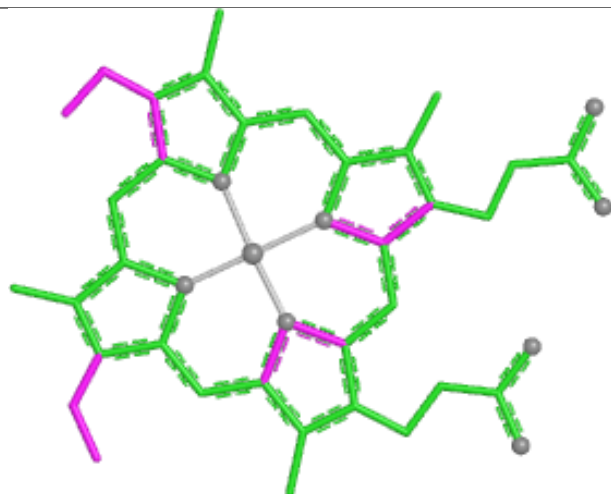
Rings



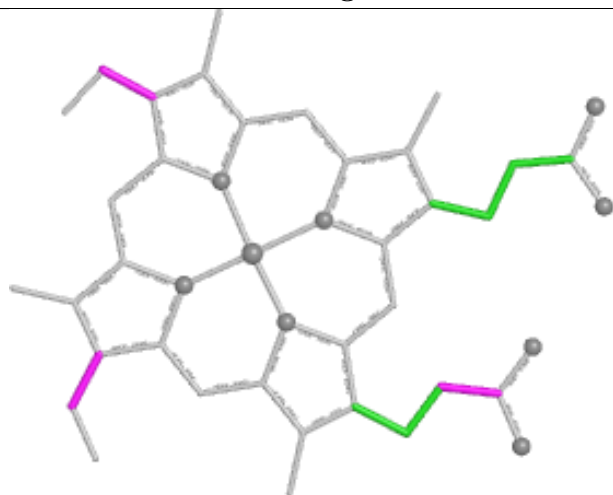
Ligand HEC J 500



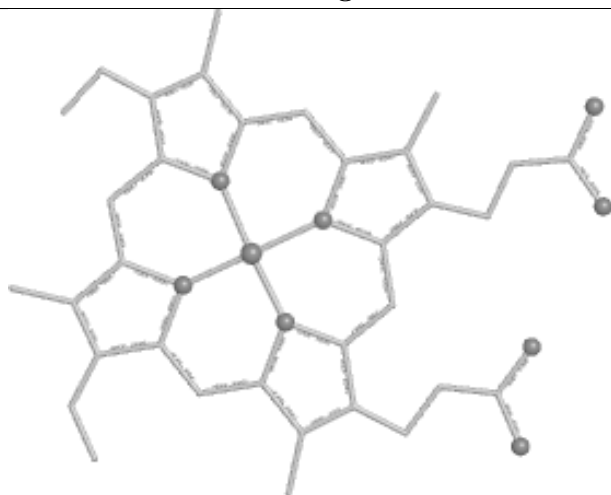
Bond lengths



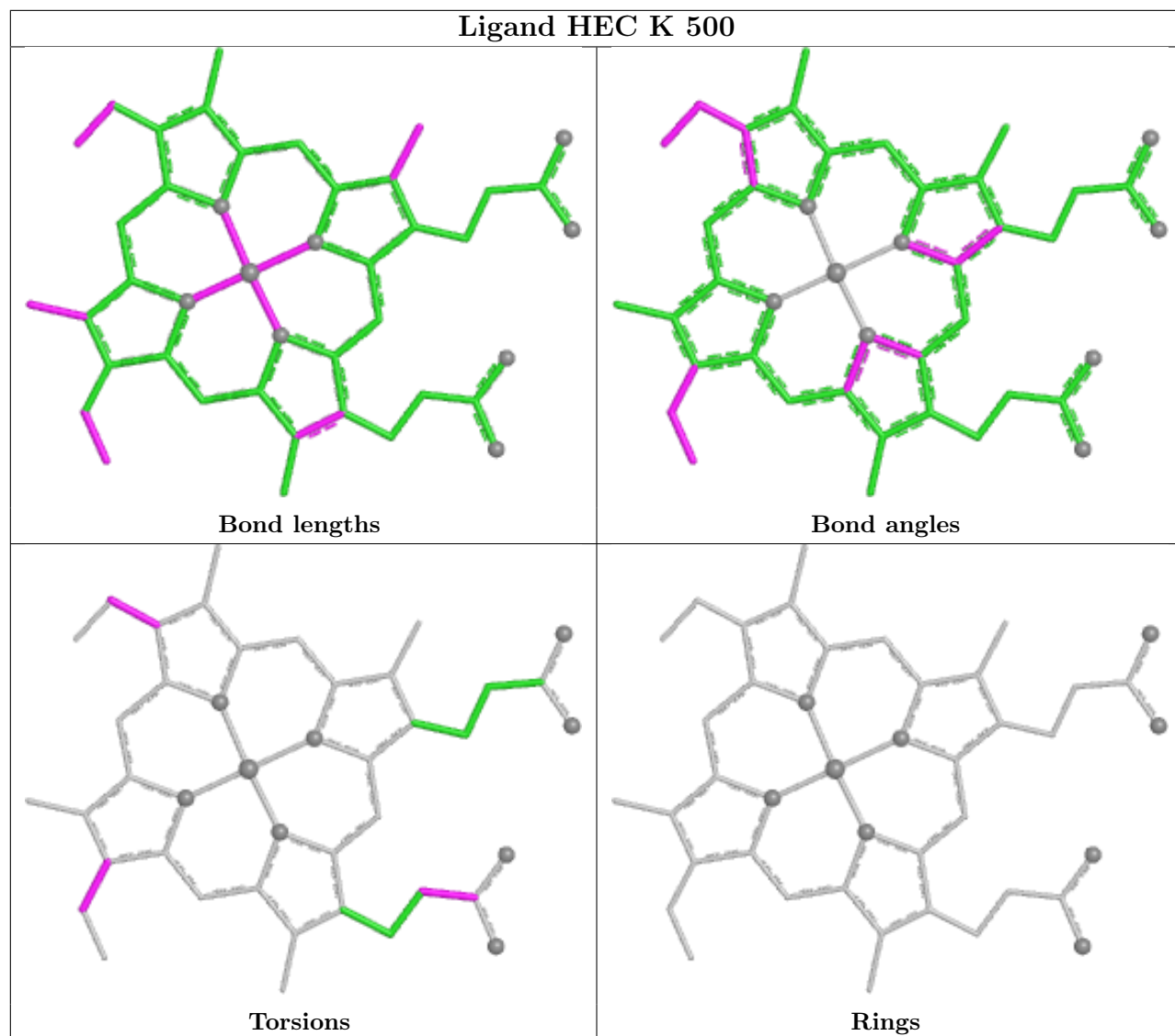
Bond angles

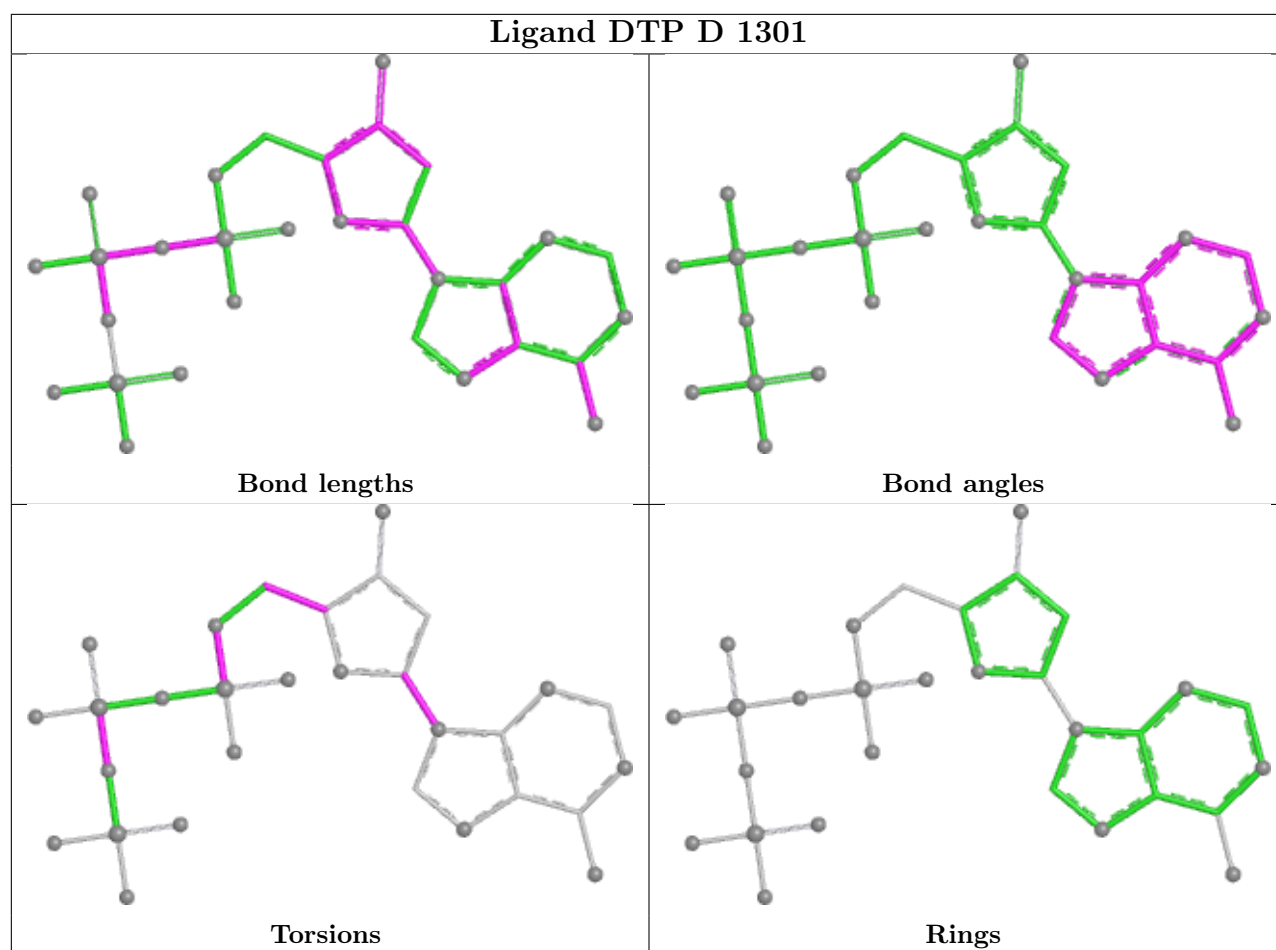


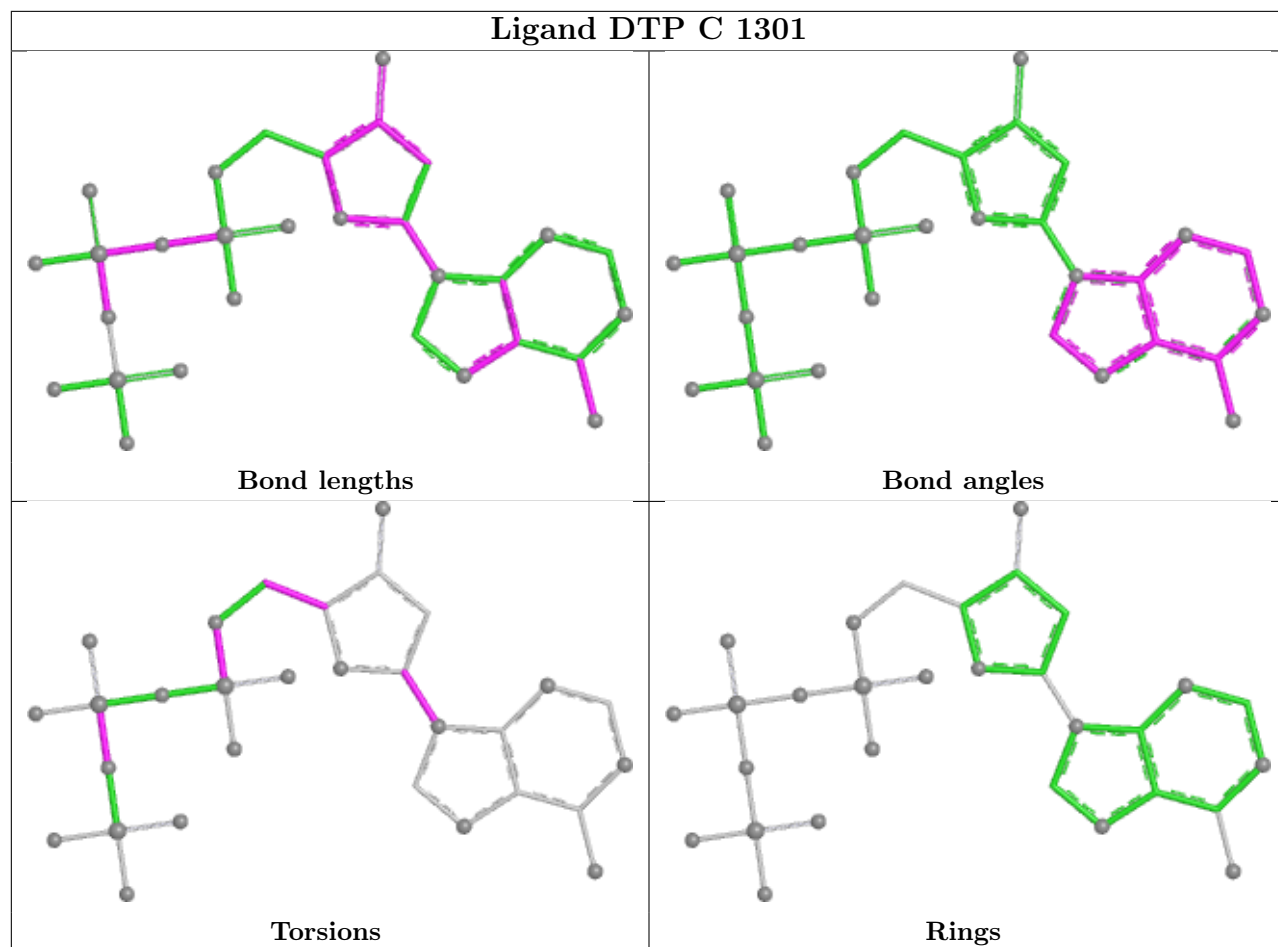
Torsions

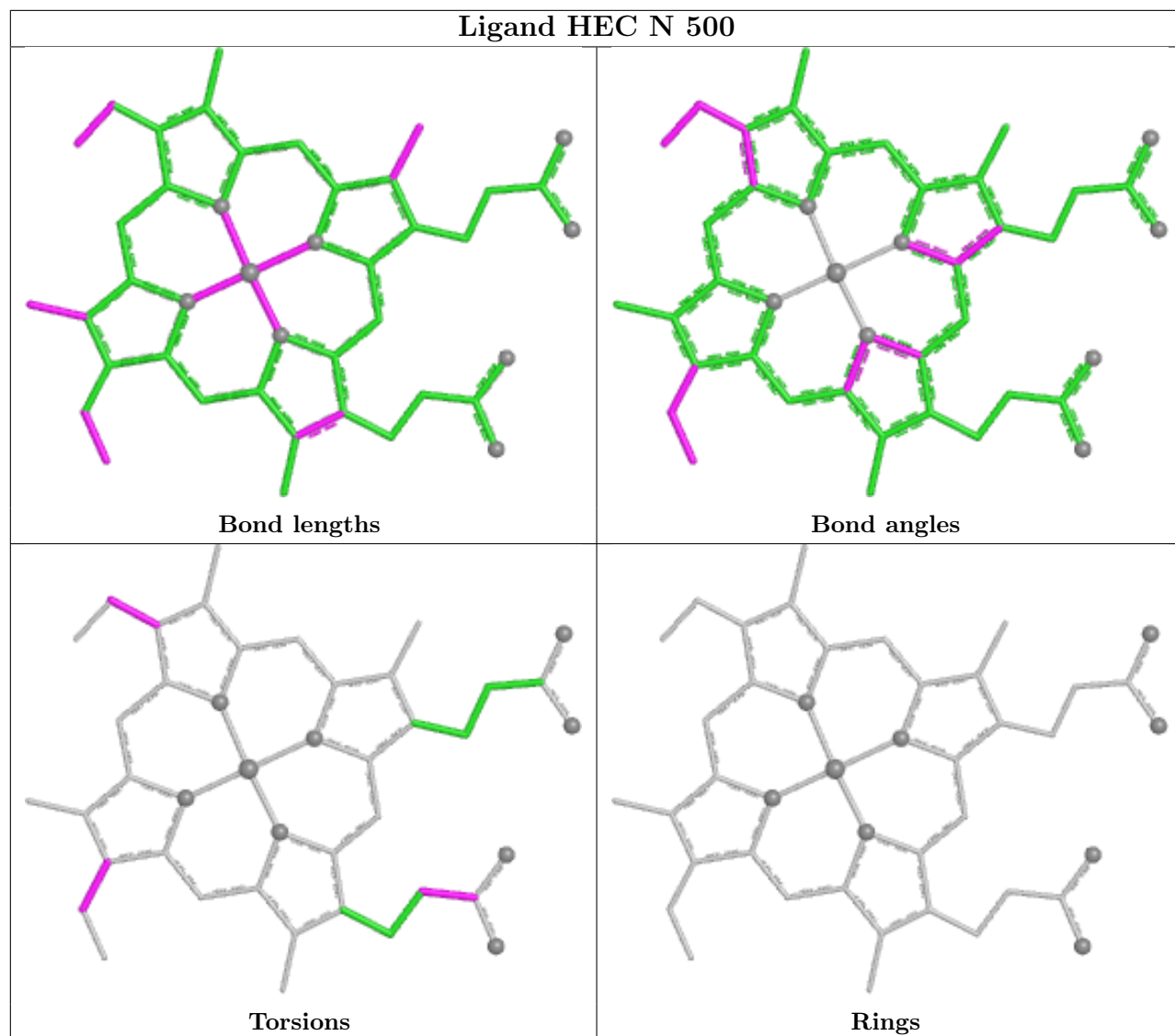


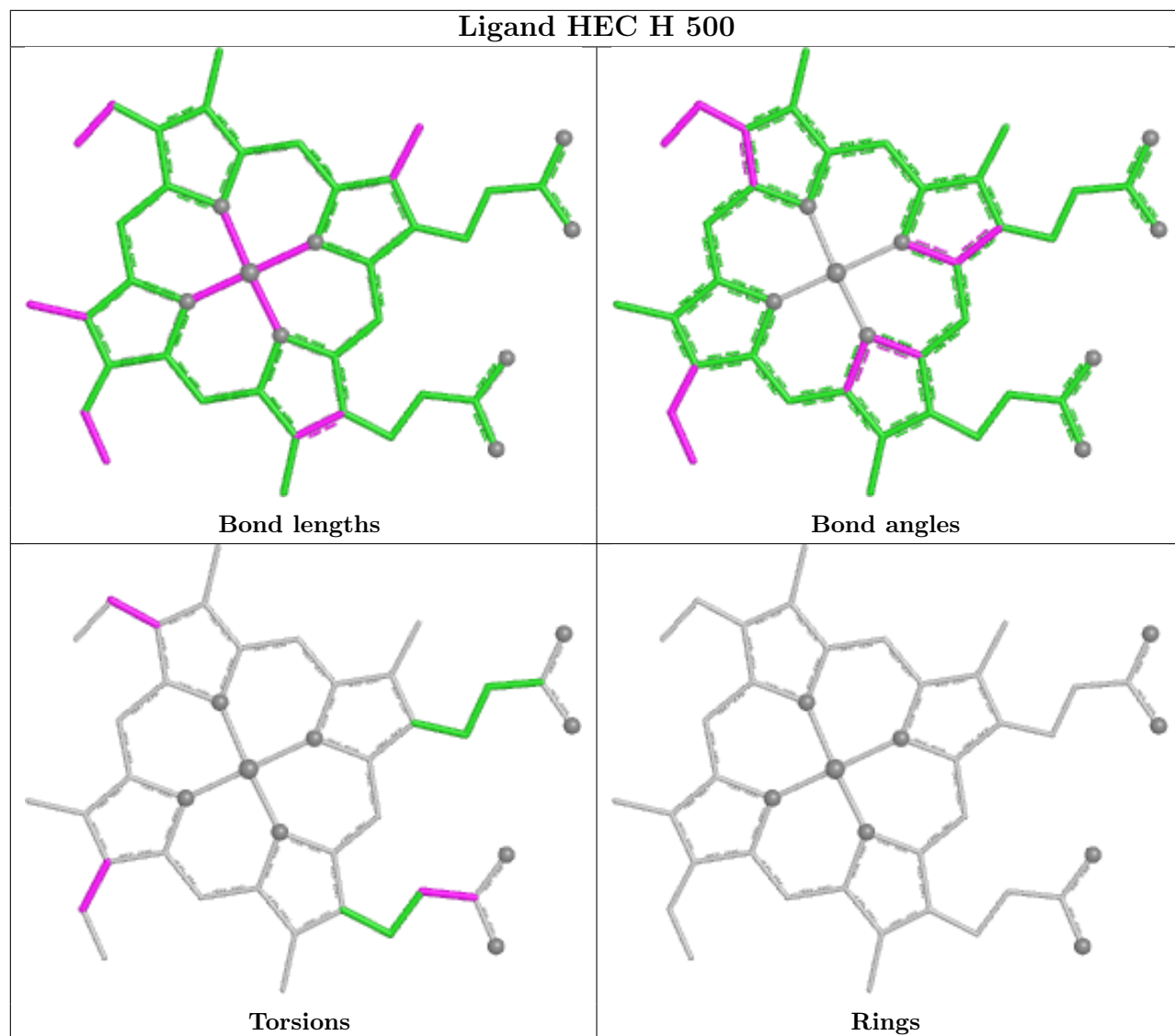
Rings

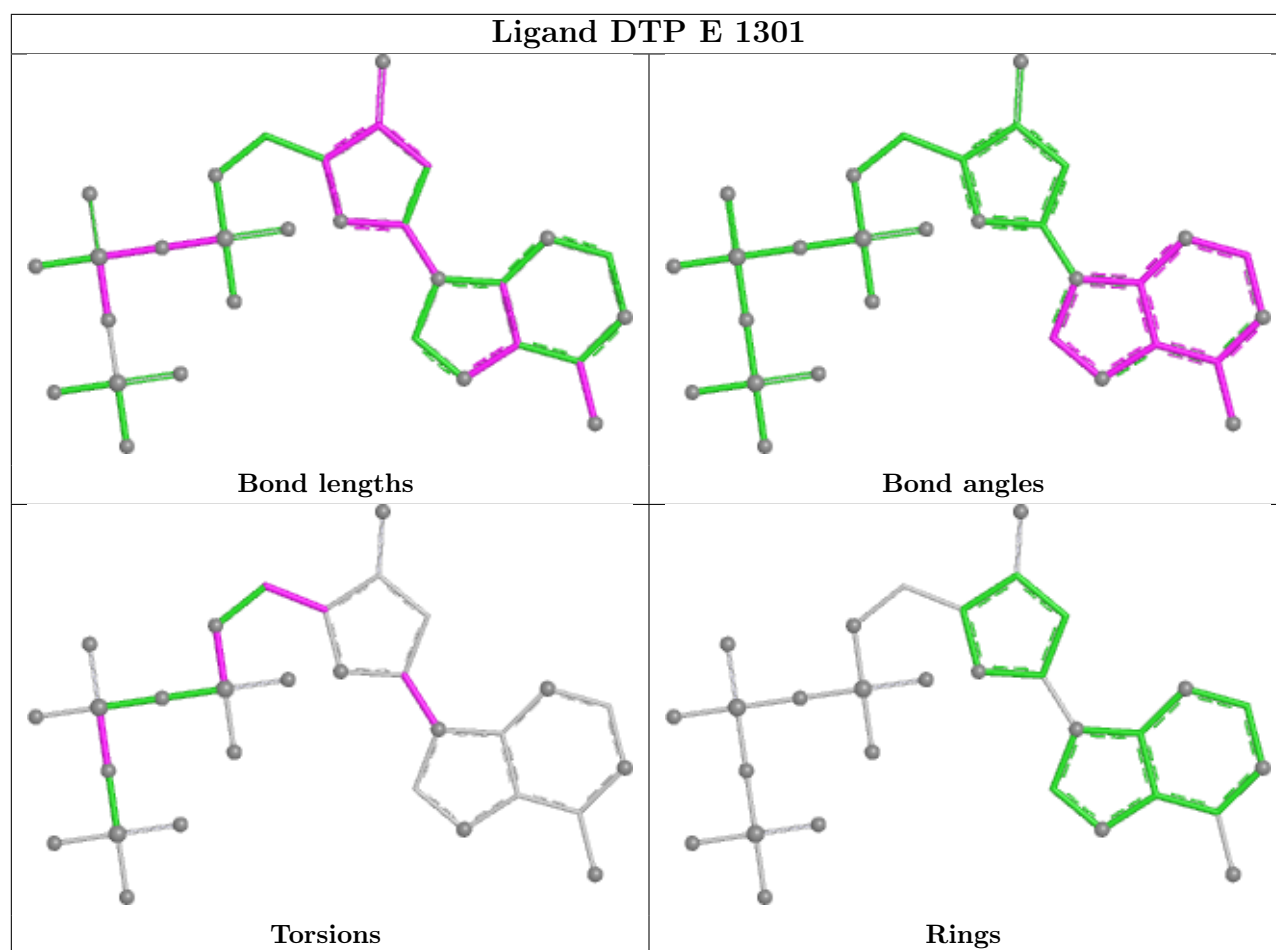












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

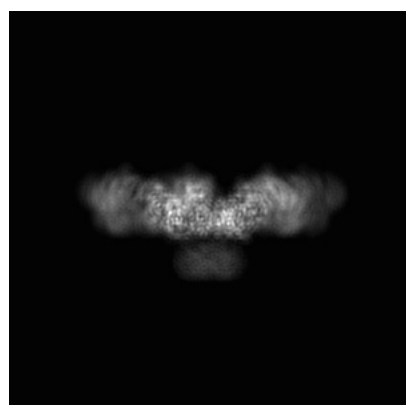
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8178. These allow visual inspection of the internal detail of the map and identification of artifacts.

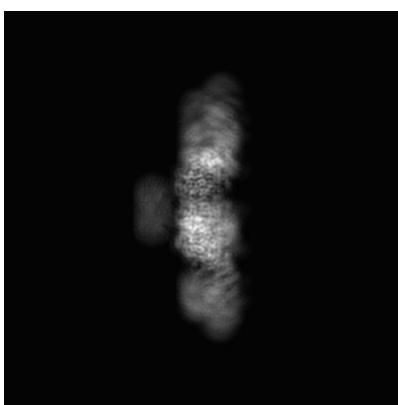
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

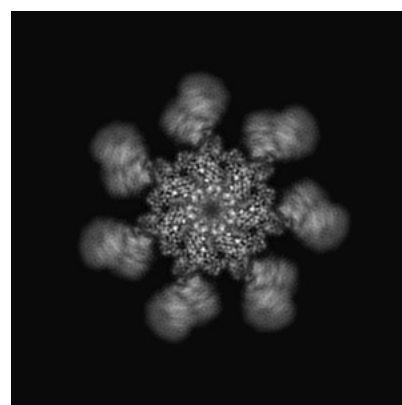
6.1.1 Primary map



X



Y

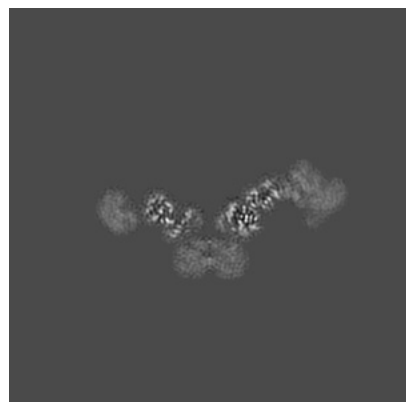


Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

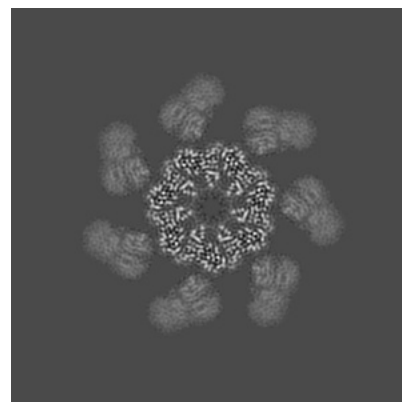
6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

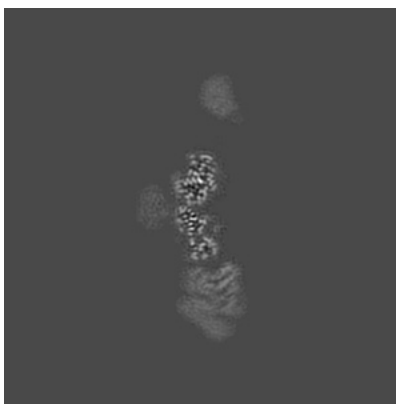
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

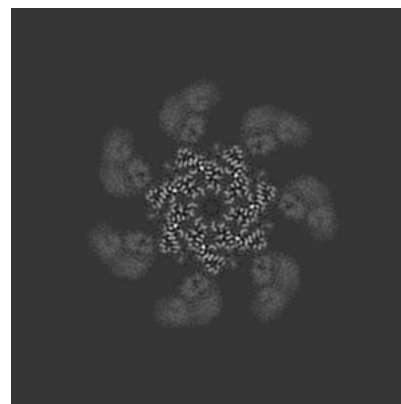
6.3.1 Primary map



X Index: 146



Y Index: 135

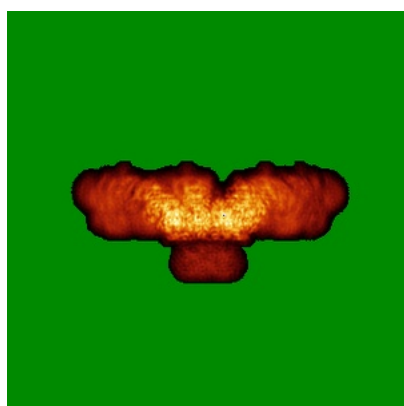


Z Index: 157

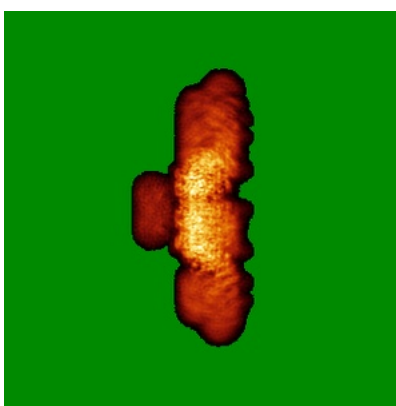
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

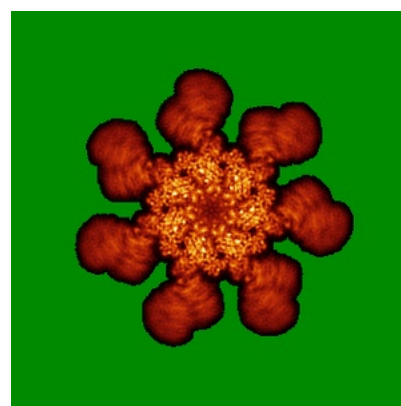
6.4.1 Primary map



X



Y

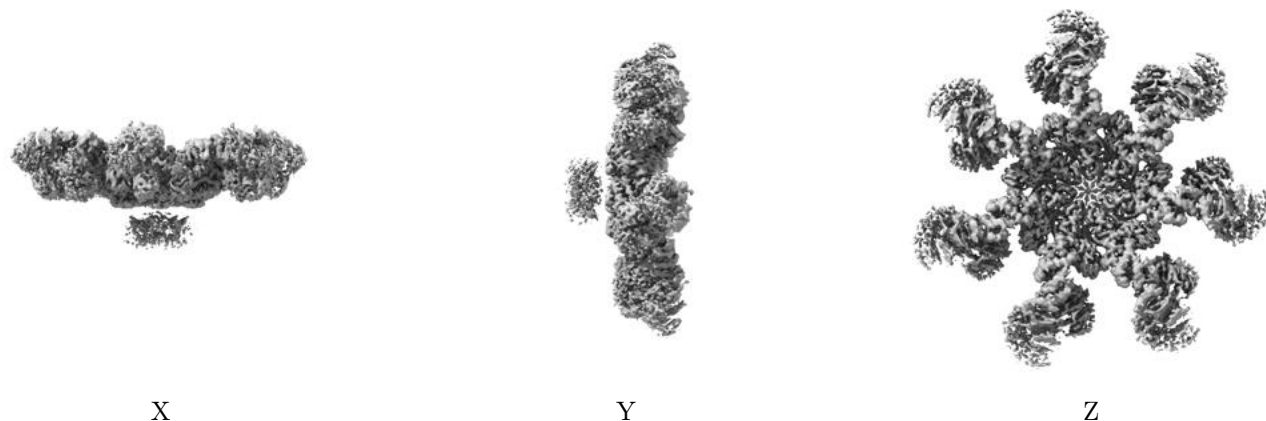


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

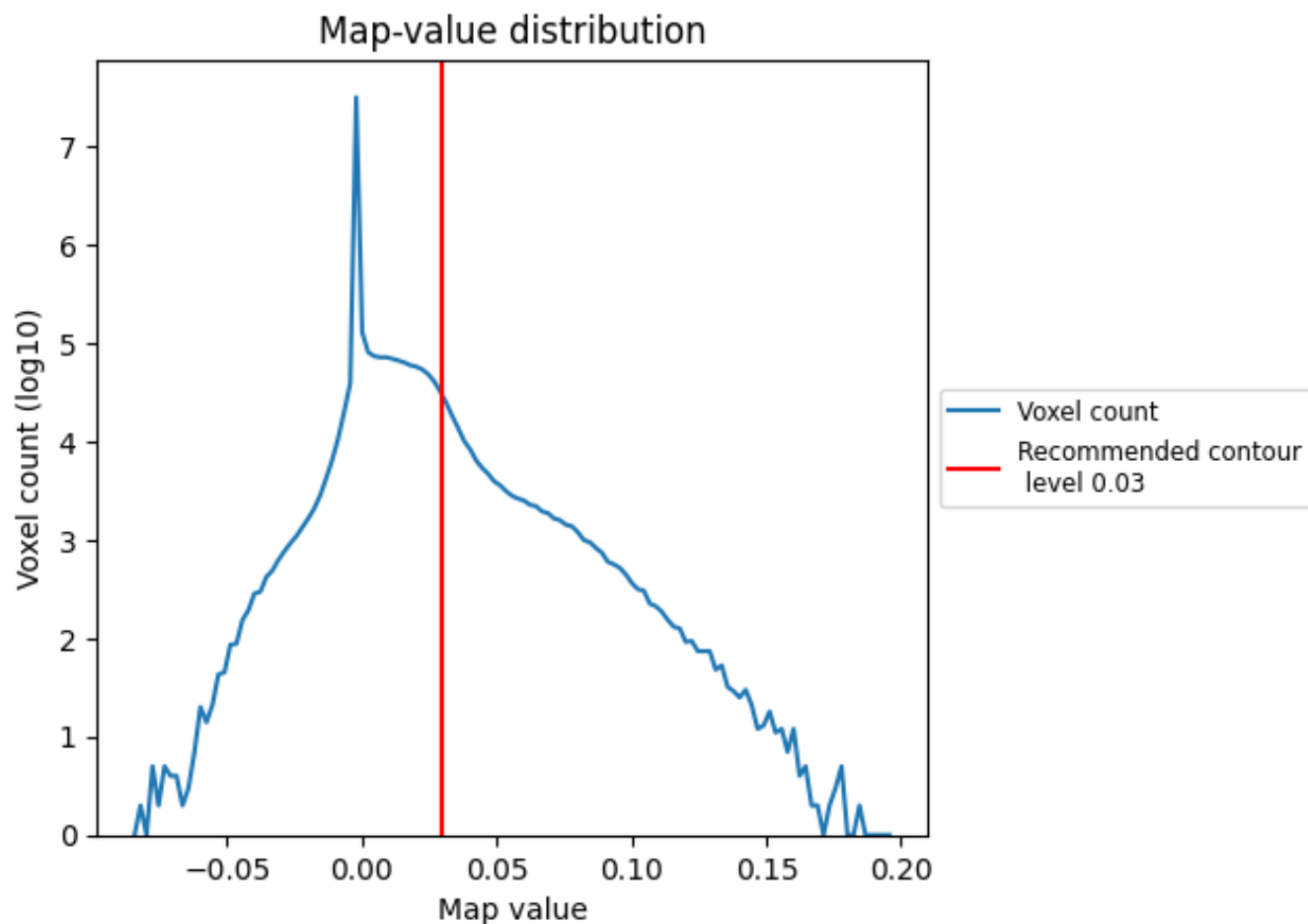
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

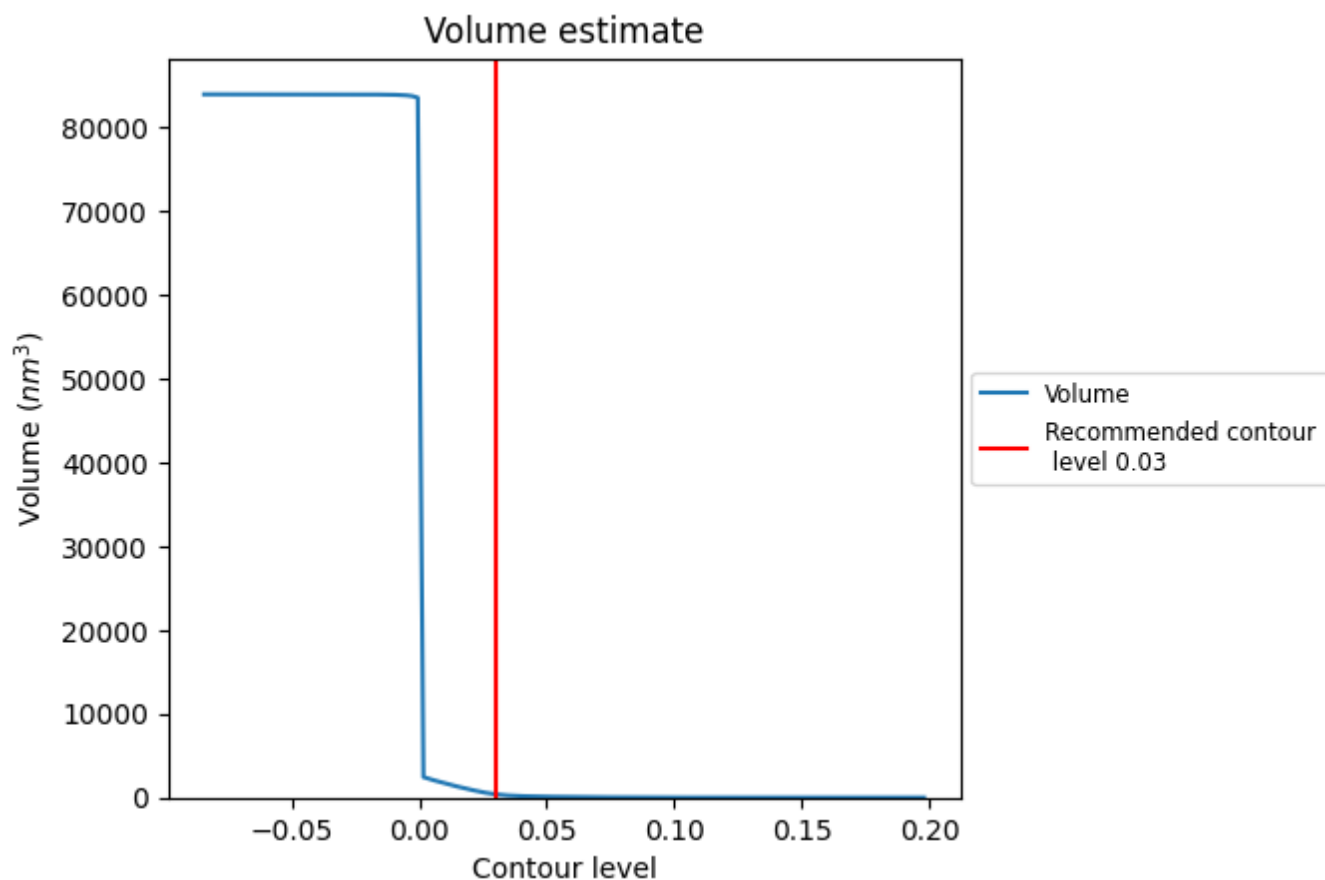
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

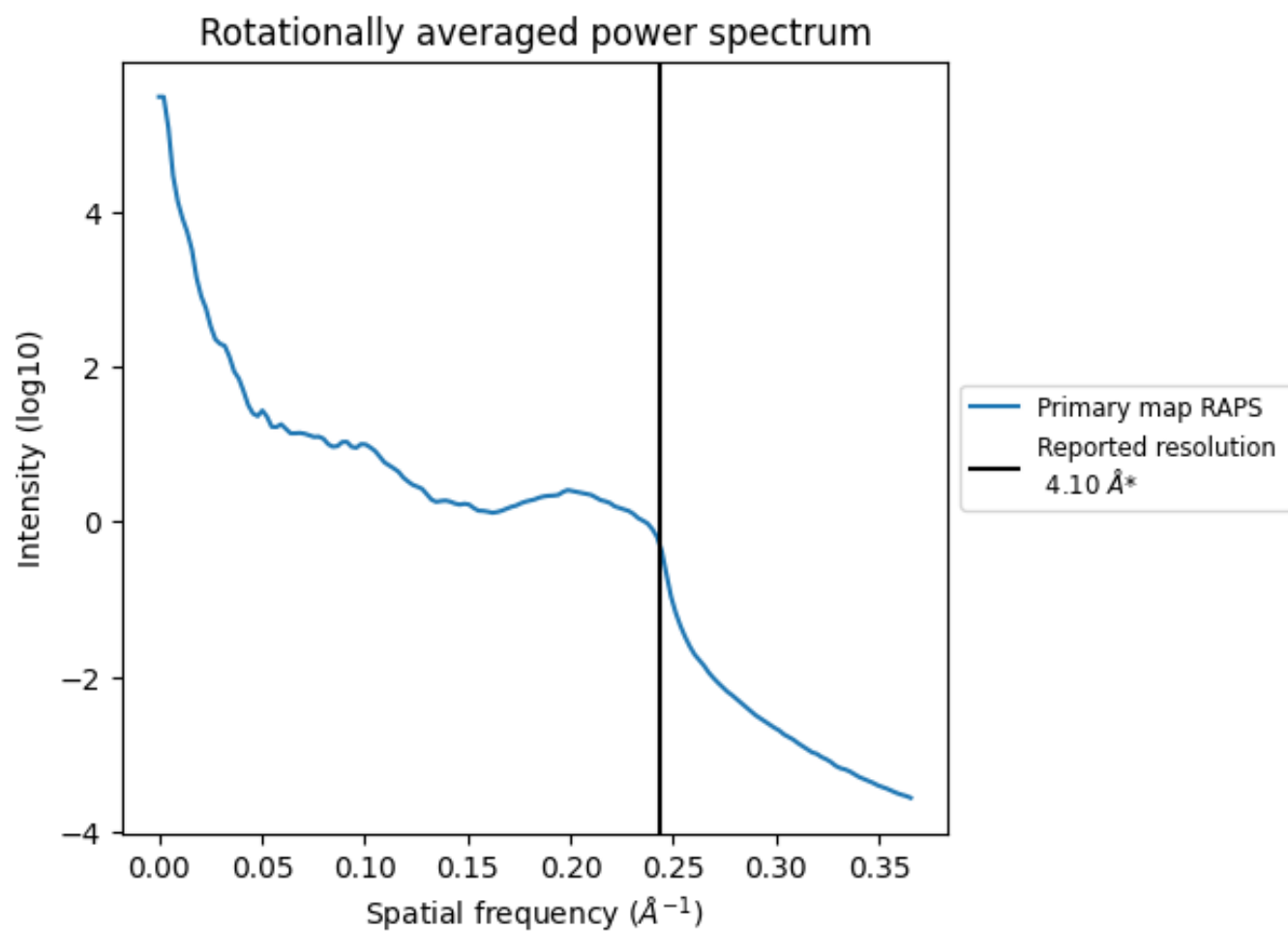
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 389 nm^3 ; this corresponds to an approximate mass of 352 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

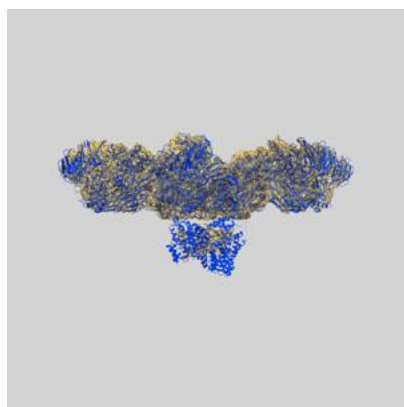
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

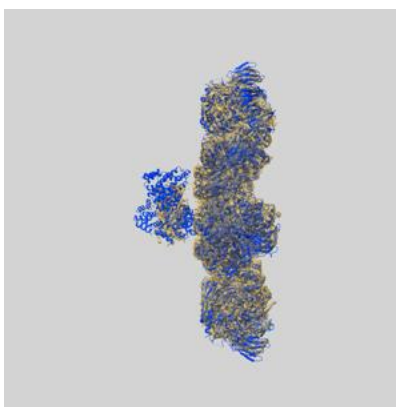
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8178 and PDB model 5JUY. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

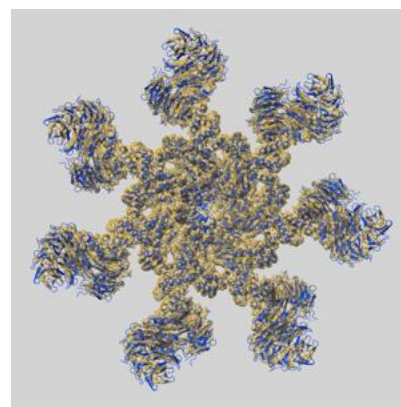
9.1 Map-model overlay [i](#)



X



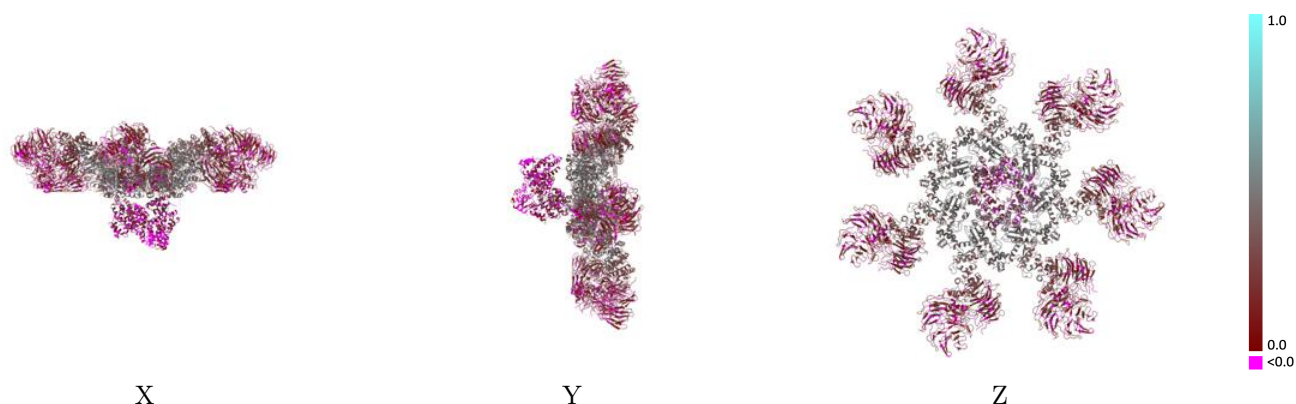
Y



Z

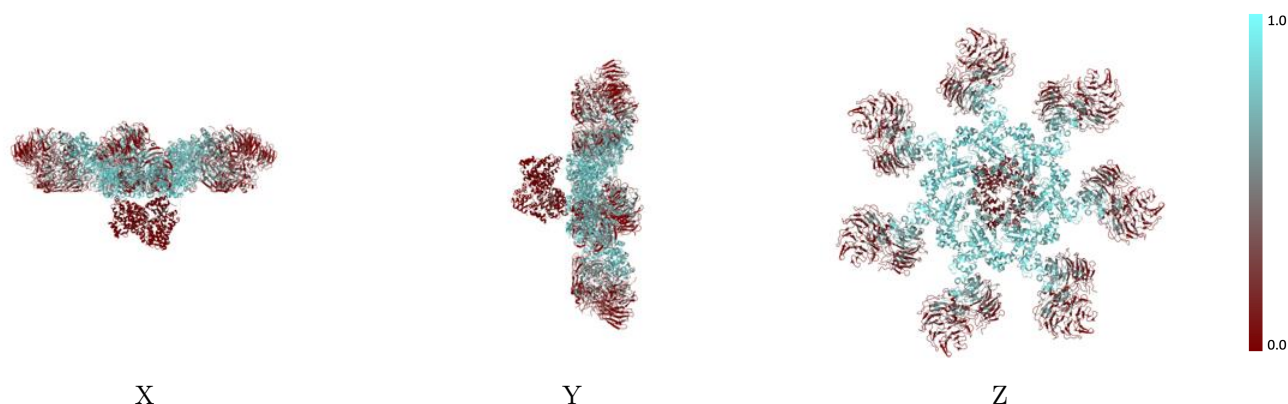
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



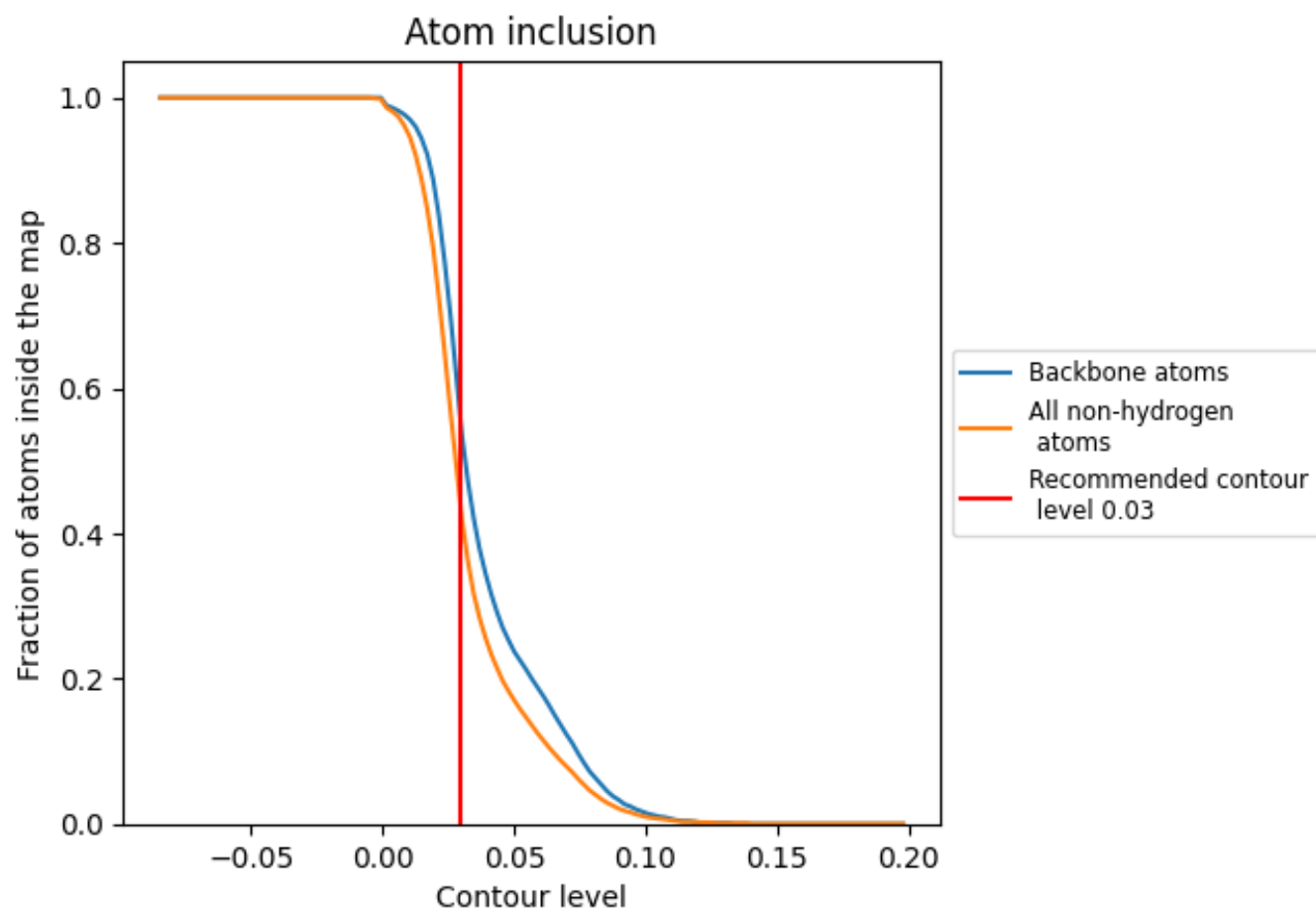
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4290	 0.2300
A	 0.4830	 0.2610
B	 0.4490	 0.2420
C	 0.4820	 0.2620
D	 0.4510	 0.2410
E	 0.4490	 0.2460
F	 0.4810	 0.2590
G	 0.4510	 0.2500
H	 0.2400	 0.1010
I	 0.2420	 0.1010
J	 0.2360	 0.1010
K	 0.2460	 0.1060
L	 0.2400	 0.1040
M	 0.2380	 0.1050
N	 0.2360	 0.1030
O	 0.1050	 0.0880
P	 0.0350	 0.0600
Q	 0.0040	 -0.0130
R	 0.0040	 -0.0470

