



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 03:10 PM BST

PDB ID : 6Q2A
Title : Trypanosoma brucei CLK1 kinase domain in complex with a covalent aminobenzimidazole inhibitor AB1
Authors : Ma, X.; Ornelas, E.
Deposited on : 2019-08-07
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

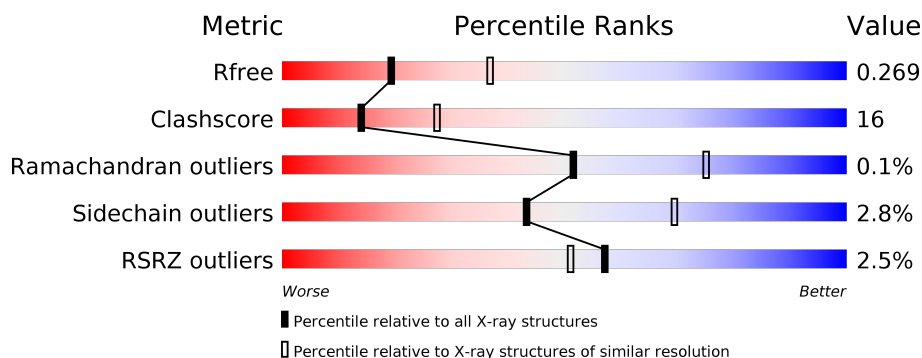
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	354	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>28%</div> <div>• •</div> </div> </div>
1	B	354	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>• • •</div> </div> </div>
1	C	354	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>26%</div> <div>• • •</div> </div> </div>
1	D	354	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• • •</div> </div> </div>
1	E	354	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• • •</div> </div> </div>
1	F	354	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>• • •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	354	
1	H	354	
1	I	354	
1	J	354	
1	K	354	
1	L	354	
1	M	354	
1	N	354	
1	O	354	
1	P	354	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	E	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 45588 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Protein kinase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	B	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	C	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	D	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	E	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	F	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	G	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	H	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	I	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	J	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	K	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	L	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	M	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	N	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	O	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			
1	P	339	Total	C	N	O	S	0	0	0
			2772	1755	508	483	26			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	GLY	-	expression tag	UNP Q382U0
A	113	PRO	-	expression tag	UNP Q382U0
A	114	SER	-	expression tag	UNP Q382U0
A	115	MET	-	expression tag	UNP Q382U0
A	116	HIS	-	expression tag	UNP Q382U0
B	112	GLY	-	expression tag	UNP Q382U0
B	113	PRO	-	expression tag	UNP Q382U0
B	114	SER	-	expression tag	UNP Q382U0
B	115	MET	-	expression tag	UNP Q382U0
B	116	HIS	-	expression tag	UNP Q382U0
C	112	GLY	-	expression tag	UNP Q382U0
C	113	PRO	-	expression tag	UNP Q382U0
C	114	SER	-	expression tag	UNP Q382U0
C	115	MET	-	expression tag	UNP Q382U0
C	116	HIS	-	expression tag	UNP Q382U0
D	112	GLY	-	expression tag	UNP Q382U0
D	113	PRO	-	expression tag	UNP Q382U0
D	114	SER	-	expression tag	UNP Q382U0
D	115	MET	-	expression tag	UNP Q382U0
D	116	HIS	-	expression tag	UNP Q382U0
E	112	GLY	-	expression tag	UNP Q382U0
E	113	PRO	-	expression tag	UNP Q382U0
E	114	SER	-	expression tag	UNP Q382U0
E	115	MET	-	expression tag	UNP Q382U0
E	116	HIS	-	expression tag	UNP Q382U0
F	112	GLY	-	expression tag	UNP Q382U0
F	113	PRO	-	expression tag	UNP Q382U0
F	114	SER	-	expression tag	UNP Q382U0
F	115	MET	-	expression tag	UNP Q382U0
F	116	HIS	-	expression tag	UNP Q382U0
G	112	GLY	-	expression tag	UNP Q382U0
G	113	PRO	-	expression tag	UNP Q382U0
G	114	SER	-	expression tag	UNP Q382U0
G	115	MET	-	expression tag	UNP Q382U0
G	116	HIS	-	expression tag	UNP Q382U0
H	112	GLY	-	expression tag	UNP Q382U0
H	113	PRO	-	expression tag	UNP Q382U0
H	114	SER	-	expression tag	UNP Q382U0
H	115	MET	-	expression tag	UNP Q382U0
H	116	HIS	-	expression tag	UNP Q382U0
I	112	GLY	-	expression tag	UNP Q382U0
I	113	PRO	-	expression tag	UNP Q382U0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	114	SER	-	expression tag	UNP Q382U0
I	115	MET	-	expression tag	UNP Q382U0
I	116	HIS	-	expression tag	UNP Q382U0
J	112	GLY	-	expression tag	UNP Q382U0
J	113	PRO	-	expression tag	UNP Q382U0
J	114	SER	-	expression tag	UNP Q382U0
J	115	MET	-	expression tag	UNP Q382U0
J	116	HIS	-	expression tag	UNP Q382U0
K	112	GLY	-	expression tag	UNP Q382U0
K	113	PRO	-	expression tag	UNP Q382U0
K	114	SER	-	expression tag	UNP Q382U0
K	115	MET	-	expression tag	UNP Q382U0
K	116	HIS	-	expression tag	UNP Q382U0
L	112	GLY	-	expression tag	UNP Q382U0
L	113	PRO	-	expression tag	UNP Q382U0
L	114	SER	-	expression tag	UNP Q382U0
L	115	MET	-	expression tag	UNP Q382U0
L	116	HIS	-	expression tag	UNP Q382U0
M	112	GLY	-	expression tag	UNP Q382U0
M	113	PRO	-	expression tag	UNP Q382U0
M	114	SER	-	expression tag	UNP Q382U0
M	115	MET	-	expression tag	UNP Q382U0
M	116	HIS	-	expression tag	UNP Q382U0
N	112	GLY	-	expression tag	UNP Q382U0
N	113	PRO	-	expression tag	UNP Q382U0
N	114	SER	-	expression tag	UNP Q382U0
N	115	MET	-	expression tag	UNP Q382U0
N	116	HIS	-	expression tag	UNP Q382U0
O	112	GLY	-	expression tag	UNP Q382U0
O	113	PRO	-	expression tag	UNP Q382U0
O	114	SER	-	expression tag	UNP Q382U0
O	115	MET	-	expression tag	UNP Q382U0
O	116	HIS	-	expression tag	UNP Q382U0
P	112	GLY	-	expression tag	UNP Q382U0
P	113	PRO	-	expression tag	UNP Q382U0
P	114	SER	-	expression tag	UNP Q382U0
P	115	MET	-	expression tag	UNP Q382U0
P	116	HIS	-	expression tag	UNP Q382U0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



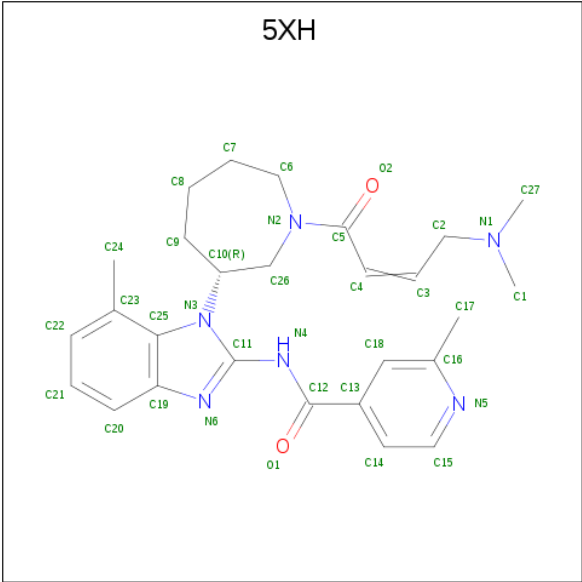
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is {N}-[1-[(3 {R})-1-[4-(dimethylamino)but-2-enoyl]azepan-3-yl]-7-methyl-benzimidazol-2-yl]-2-methyl-pyridine-4-carboxamide (three-letter code: 5XH) (formula: C₂₇H₃₄N₆O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	27	6	2		
3	B	1	Total	C	N	O	0	0
			35	27	6	2		
3	C	1	Total	C	N	O	0	0
			35	27	6	2		
3	D	1	Total	C	N	O	0	0
			35	27	6	2		
3	E	1	Total	C	N	O	0	0
			35	27	6	2		
3	F	1	Total	C	N	O	0	0
			35	27	6	2		
3	G	1	Total	C	N	O	0	0
			35	27	6	2		
3	H	1	Total	C	N	O	0	0
			35	27	6	2		
3	I	1	Total	C	N	O	0	0
			35	27	6	2		
3	J	1	Total	C	N	O	0	0
			35	27	6	2		
3	K	1	Total	C	N	O	0	0
			35	27	6	2		
3	L	1	Total	C	N	O	0	0
			35	27	6	2		
3	M	1	Total	C	N	O	0	0
			35	27	6	2		
3	N	1	Total	C	N	O	0	0
			35	27	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	O	1	Total	C	N	O	0	0
			35	27	6	2		
3	P	1	Total	C	N	O	0	0
			35	27	6	2		

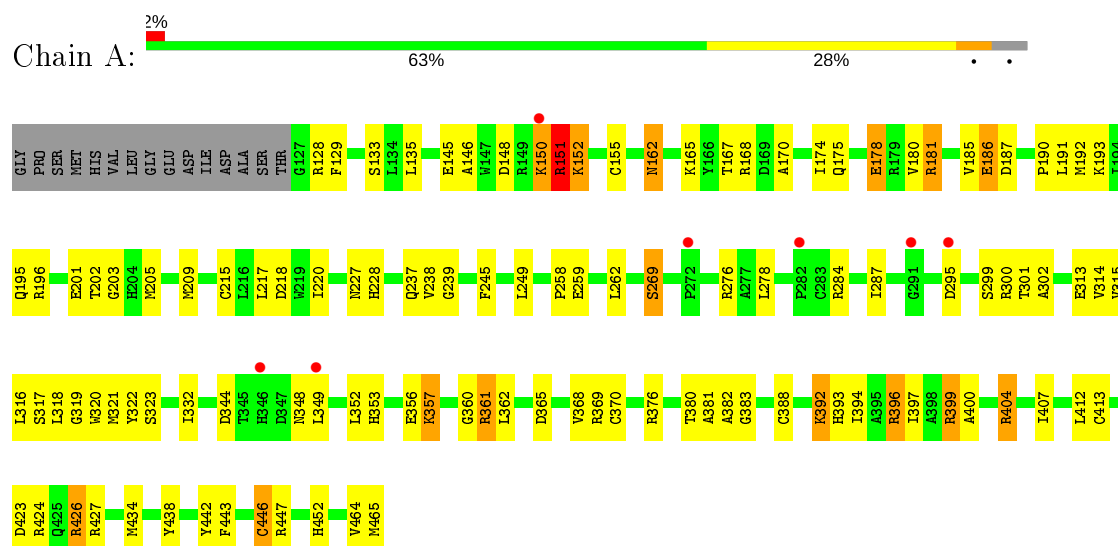
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	27	Total	O	0	0
			27	27		
4	C	37	Total	O	0	0
			37	37		
4	D	32	Total	O	0	0
			32	32		
4	E	39	Total	O	0	0
			39	39		
4	F	37	Total	O	0	0
			37	37		
4	G	31	Total	O	0	0
			31	31		
4	H	22	Total	O	0	0
			22	22		
4	I	34	Total	O	0	0
			34	34		
4	J	29	Total	O	0	0
			29	29		
4	K	29	Total	O	0	0
			29	29		
4	L	34	Total	O	0	0
			34	34		
4	M	43	Total	O	0	0
			43	43		
4	N	26	Total	O	0	0
			26	26		
4	O	28	Total	O	0	0
			28	28		
4	P	30	Total	O	0	0
			30	30		

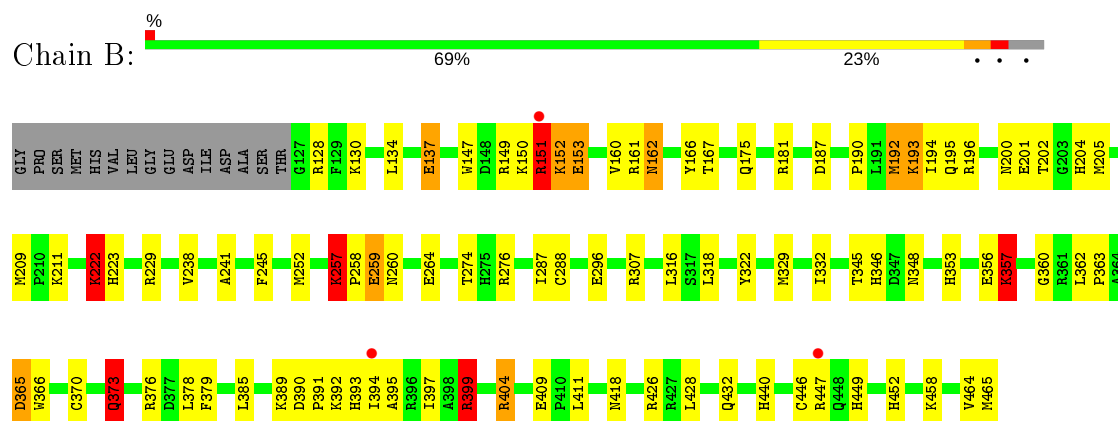
3 Residue-property plots [i](#)

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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

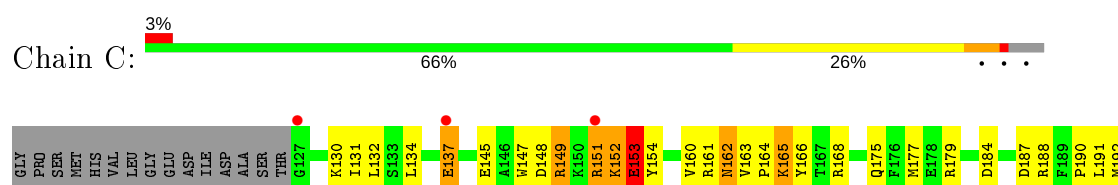
- Molecule 1: Protein kinase, putative

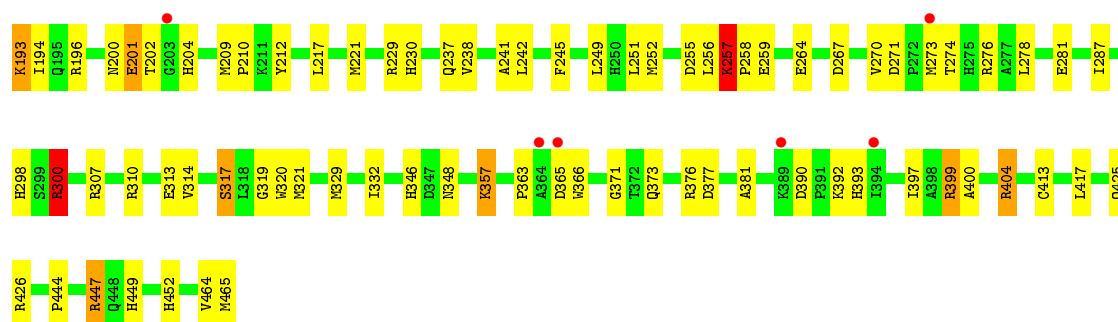


- Molecule 1: Protein kinase, putative

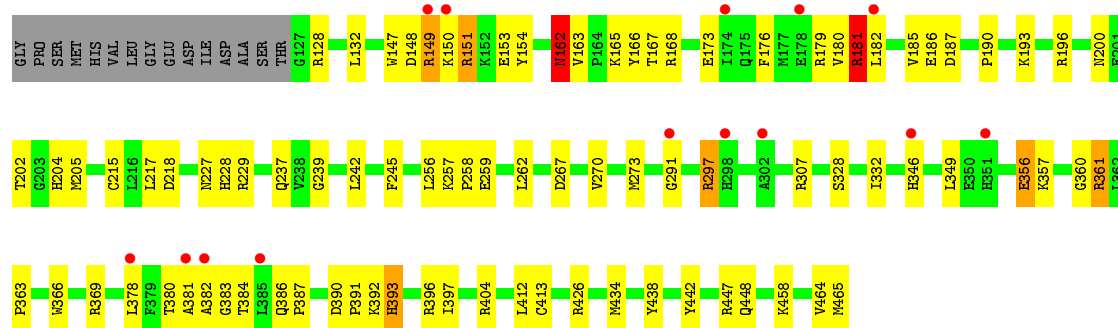


- Molecule 1: Protein kinase, putative

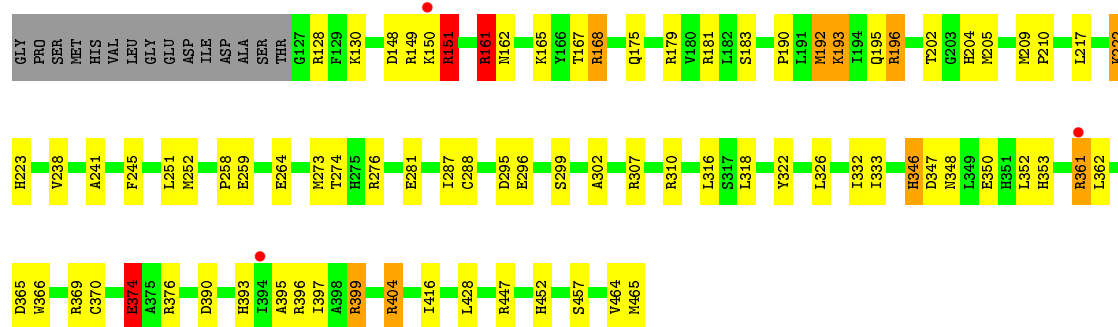




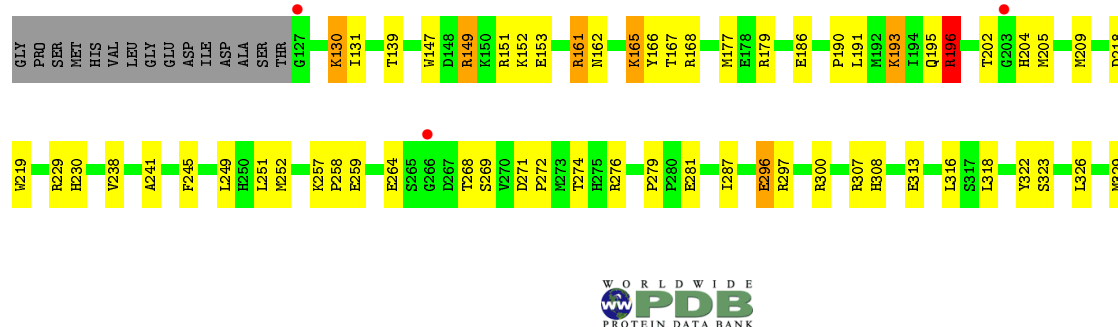
- Molecule 1: Protein kinase, putative

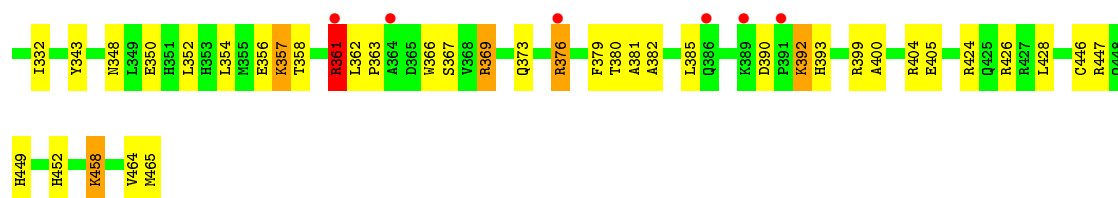


- Molecule 1: Protein kinase, putative

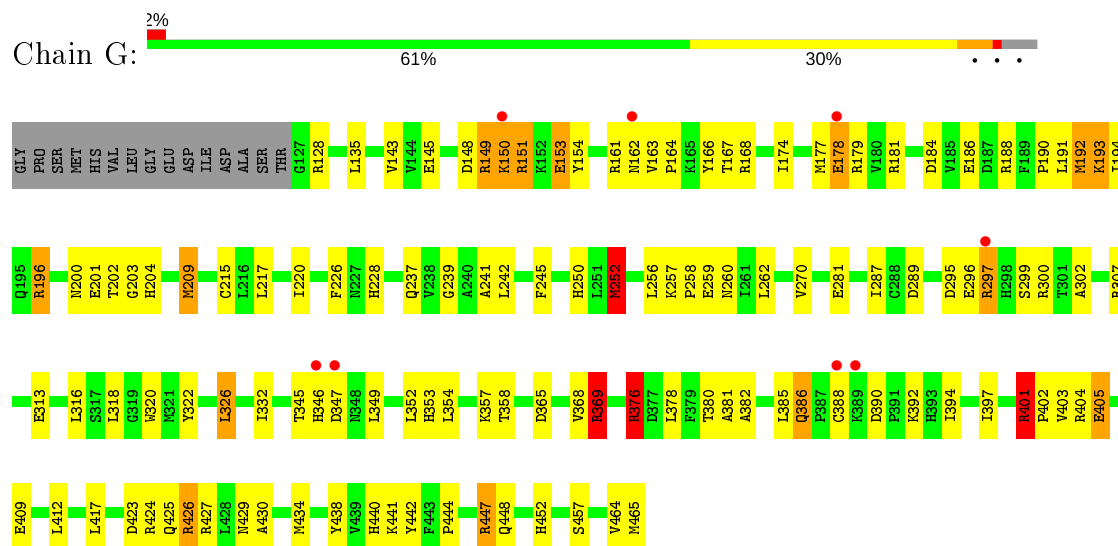


- Molecule 1: Protein kinase, putative

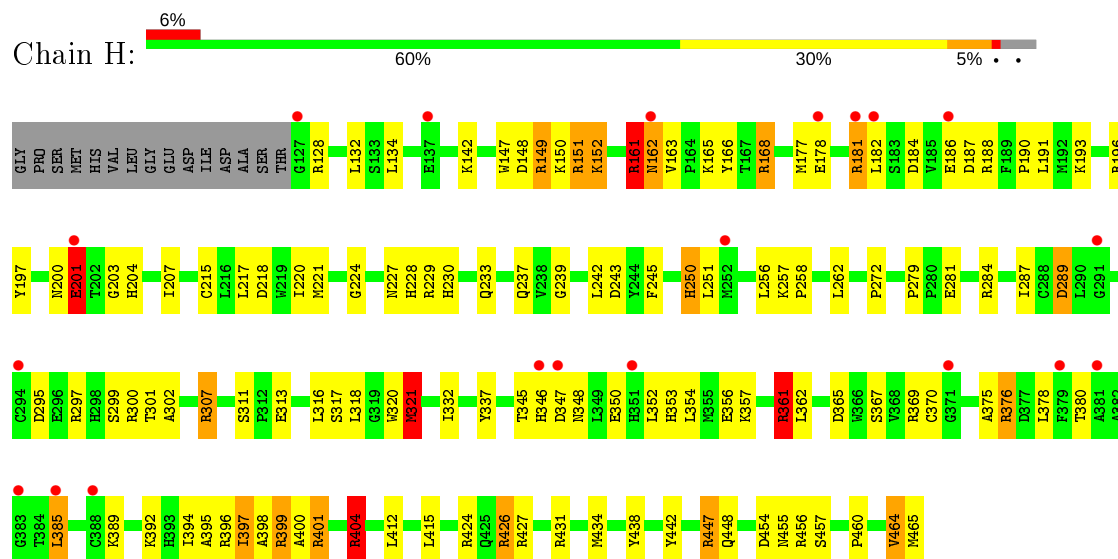




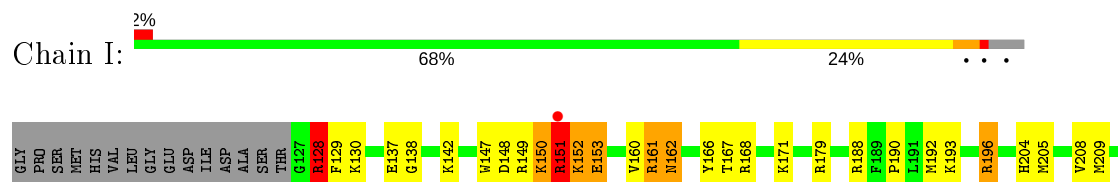
- Molecule 1: Protein kinase, putative

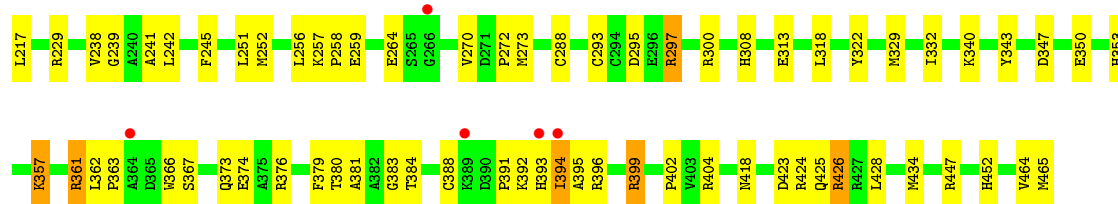


- Molecule 1: Protein kinase, putative

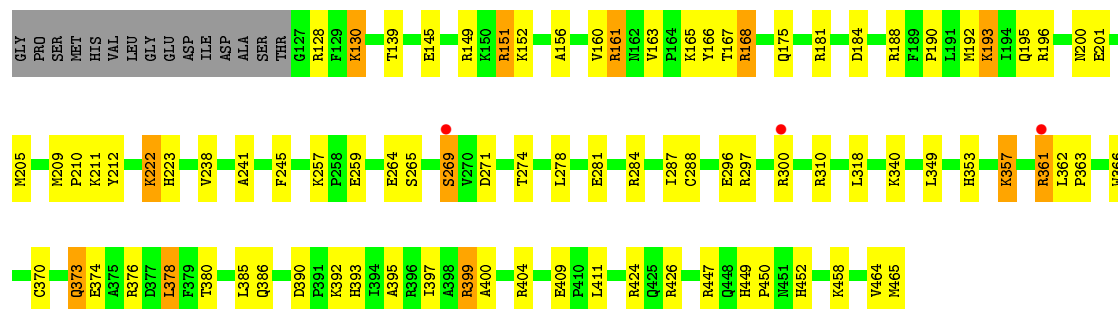


- Molecule 1: Protein kinase, putative

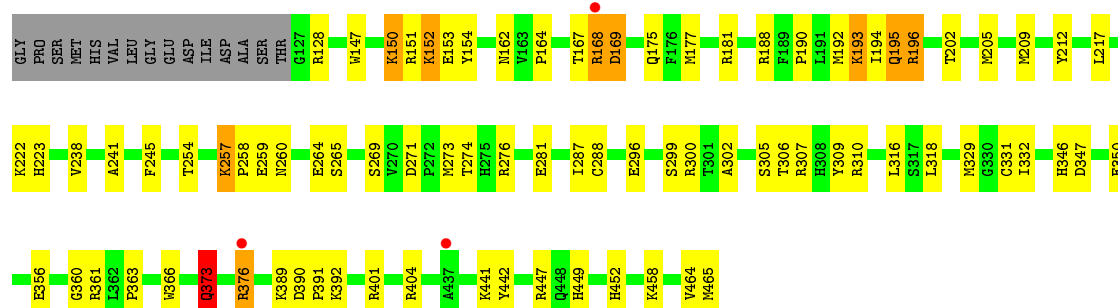




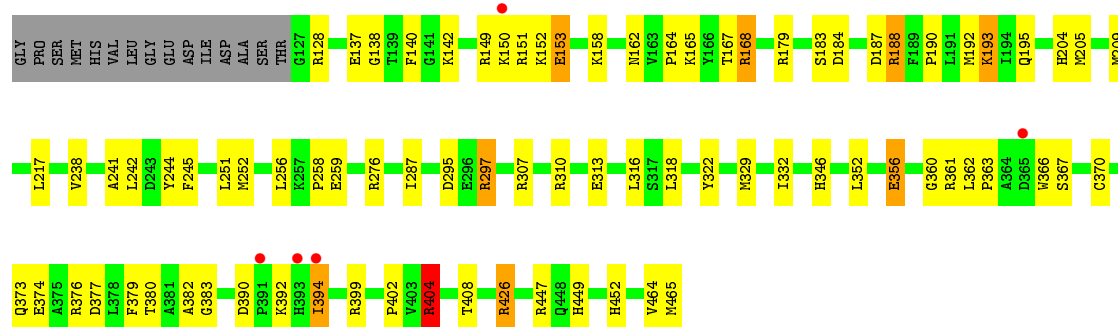
- Molecule 1: Protein kinase, putative



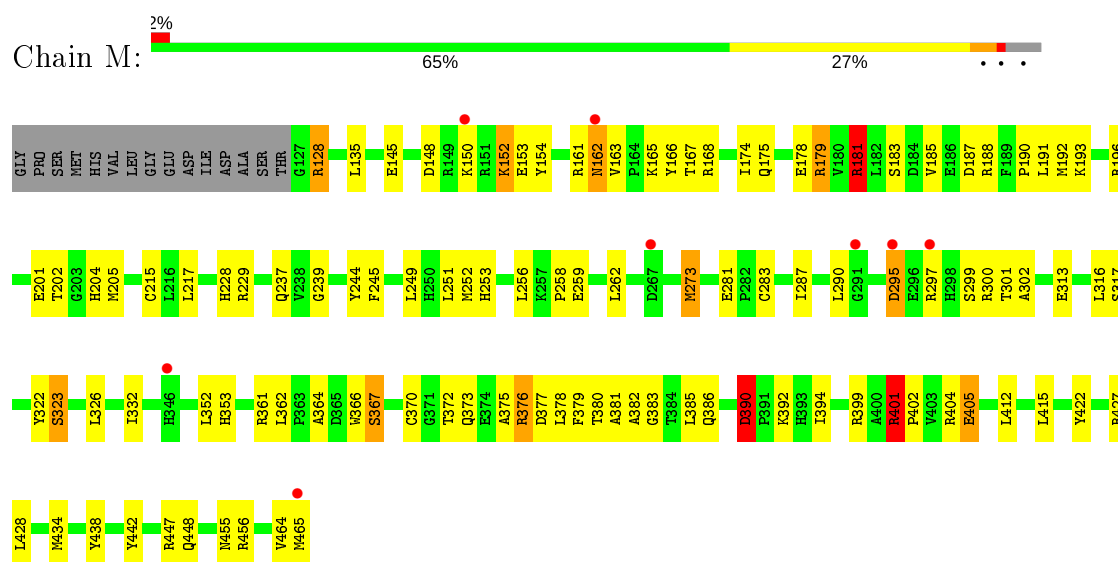
- Molecule 1: Protein kinase, putative



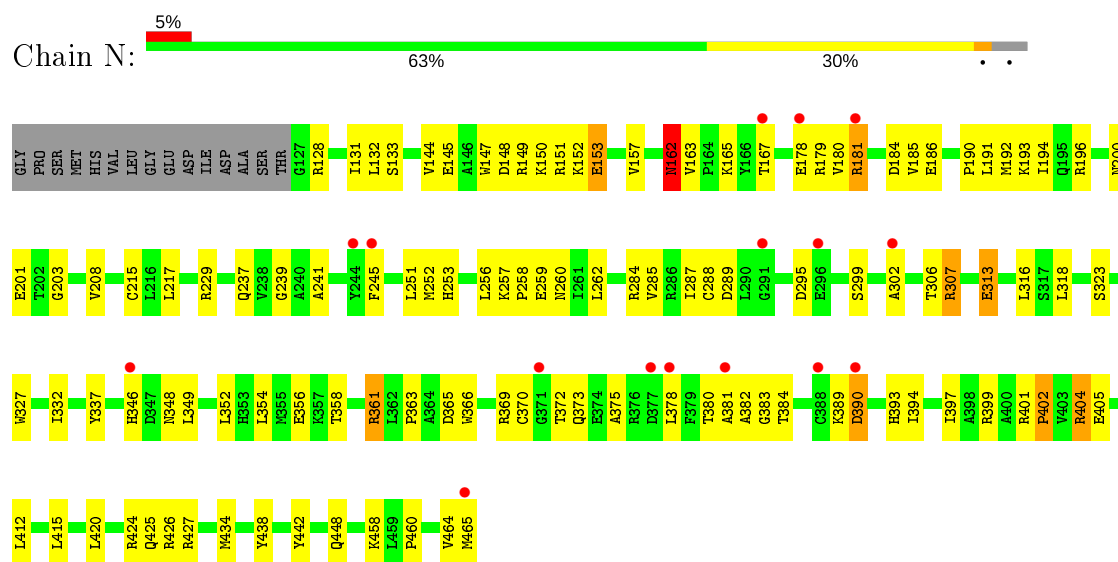
- Molecule 1: Protein kinase, putative



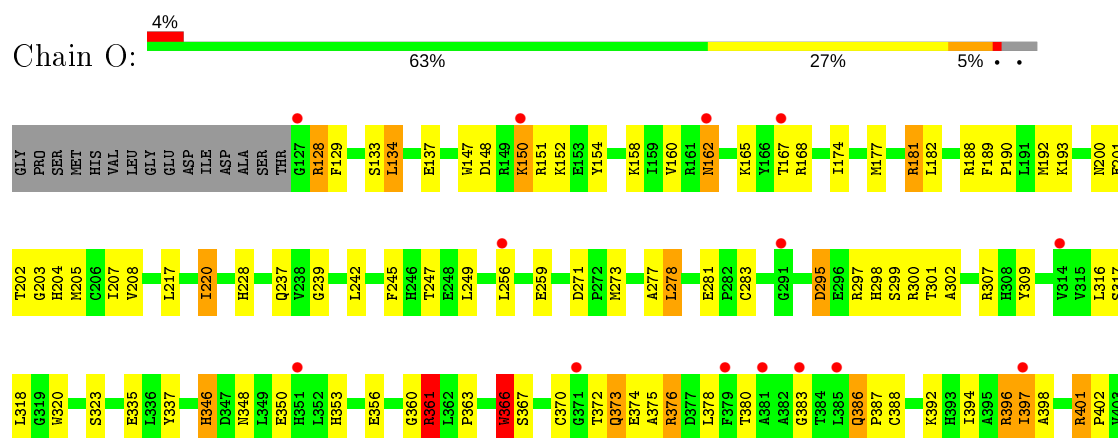
- Molecule 1: Protein kinase, putative



- Molecule 1: Protein kinase, putative

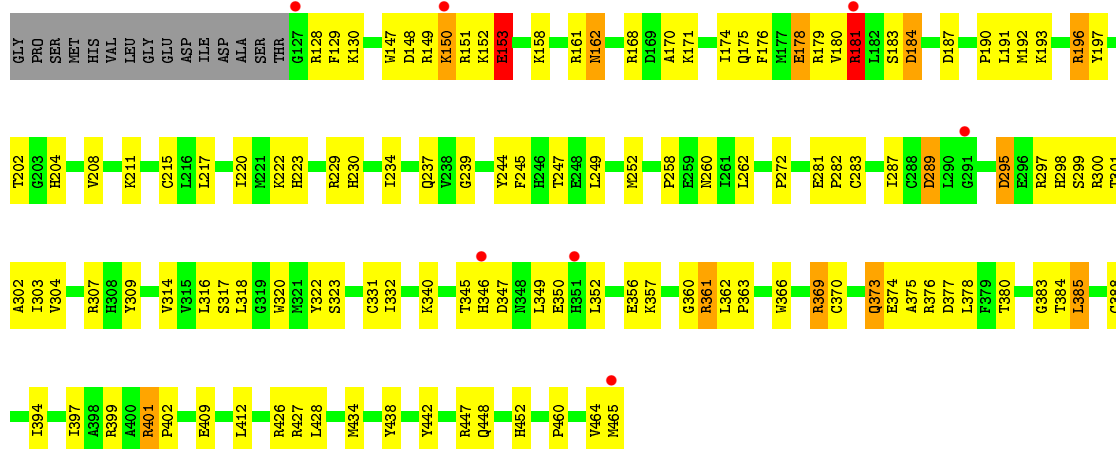


- Molecule 1: Protein kinase, putative





- Molecule 1: Protein kinase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	147.15Å 147.15Å 264.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.39 – 2.60 47.39 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.39-2.60) 98.7 (47.39-2.60)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.266 , 0.313 0.266 , 0.269	Depositor DCC
R_{free} test set	9696 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.448 for -h,-k,l 0.449 for h,-h-k,-l 0.449 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	45588	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1155e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 5XH

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	0.50	2/2844 (0.1%)	0.99	33/3847 (0.9%)
1	B	0.55	7/2844 (0.2%)	0.88	19/3847 (0.5%)
1	C	0.62	7/2844 (0.2%)	1.19	38/3847 (1.0%)
1	D	0.44	1/2844 (0.0%)	0.77	16/3847 (0.4%)
1	E	0.44	2/2844 (0.1%)	0.82	20/3847 (0.5%)
1	F	0.48	3/2844 (0.1%)	1.02	32/3847 (0.8%)
1	G	0.56	2/2844 (0.1%)	1.07	36/3847 (0.9%)
1	H	0.56	1/2844 (0.0%)	1.17	45/3847 (1.2%)
1	I	0.46	2/2844 (0.1%)	0.83	22/3847 (0.6%)
1	J	0.57	5/2844 (0.2%)	1.06	34/3847 (0.9%)
1	K	0.50	4/2844 (0.1%)	0.81	16/3847 (0.4%)
1	L	0.50	2/2844 (0.1%)	0.94	21/3847 (0.5%)
1	M	0.52	5/2844 (0.2%)	0.89	22/3847 (0.6%)
1	N	0.53	2/2844 (0.1%)	0.92	21/3847 (0.5%)
1	O	0.60	5/2844 (0.2%)	0.93	19/3847 (0.5%)
1	P	0.51	2/2844 (0.1%)	0.89	17/3847 (0.4%)
All	All	0.52	52/45504 (0.1%)	0.96	411/61552 (0.7%)

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	2
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	1
1	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	3
1	I	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	2
1	P	0	3
All	All	0	23

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	150	LYS	CD-CE	-10.51	1.25	1.51
1	J	404	ARG	CB-CG	-8.83	1.28	1.52
1	J	361	ARG	CB-CG	-8.67	1.29	1.52
1	N	402	PRO	N-CD	-8.03	1.36	1.47
1	B	259	GLU	CD-OE1	7.92	1.34	1.25
1	B	458	LYS	CD-CE	7.89	1.71	1.51
1	C	137	GLU	CD-OE2	7.81	1.34	1.25
1	C	153	GLU	CD-OE2	7.79	1.34	1.25
1	M	367	SER	CB-OG	7.79	1.52	1.42
1	L	193	LYS	CE-NZ	7.74	1.68	1.49
1	B	153	GLU	CG-CD	-7.48	1.40	1.51
1	P	181	ARG	CG-CD	7.45	1.70	1.51
1	O	128	ARG	NE-CZ	-7.31	1.23	1.33
1	F	196	ARG	CB-CG	7.14	1.71	1.52
1	E	361	ARG	NE-CZ	6.81	1.42	1.33
1	B	357	LYS	CD-CE	6.68	1.68	1.51
1	O	361	ARG	CZ-NH1	6.62	1.41	1.33
1	O	404	ARG	CB-CG	-6.58	1.34	1.52
1	L	356	GLU	CD-OE2	6.46	1.32	1.25
1	P	150	LYS	CG-CD	-6.33	1.30	1.52
1	F	196	ARG	CG-CD	6.33	1.67	1.51
1	C	196	ARG	CG-CD	6.29	1.67	1.51
1	G	297	ARG	CB-CG	6.21	1.69	1.52
1	A	178	GLU	CB-CG	-6.17	1.40	1.52
1	H	186	GLU	CB-CG	6.01	1.63	1.52
1	M	201	GLU	CD-OE2	6.00	1.32	1.25
1	M	152	LYS	CG-CD	-5.82	1.32	1.52
1	I	153	GLU	CB-CG	5.79	1.63	1.52
1	C	257	LYS	CB-CG	-5.71	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	399	ARG	CG-CD	5.68	1.66	1.51
1	M	181	ARG	CG-CD	-5.67	1.37	1.51
1	M	376	ARG	CD-NE	-5.63	1.36	1.46
1	K	193	LYS	CE-NZ	5.59	1.63	1.49
1	C	317	SER	CB-OG	5.50	1.49	1.42
1	J	376	ARG	CG-CD	5.48	1.65	1.51
1	D	153	GLU	CD-OE1	5.46	1.31	1.25
1	I	196	ARG	CG-CD	5.39	1.65	1.51
1	B	151	ARG	CZ-NH1	5.32	1.40	1.33
1	K	152	LYS	CD-CE	5.29	1.64	1.51
1	A	181	ARG	CG-CD	-5.22	1.38	1.51
1	C	300	ARG	CD-NE	-5.21	1.37	1.46
1	G	297	ARG	CG-CD	5.21	1.65	1.51
1	B	137	GLU	CD-OE2	5.16	1.31	1.25
1	K	389	LYS	C-N	-5.14	1.22	1.34
1	J	426	ARG	CG-CD	-5.13	1.39	1.51
1	O	361	ARG	CG-CD	-5.11	1.39	1.51
1	E	193	LYS	CE-NZ	5.10	1.61	1.49
1	K	150	LYS	CE-NZ	5.07	1.61	1.49
1	C	152	LYS	CB-CG	5.06	1.66	1.52
1	F	161	ARG	CG-CD	-5.03	1.39	1.51
1	B	259	GLU	CG-CD	5.02	1.59	1.51
1	J	300	ARG	CG-CD	5.00	1.64	1.51

All (411) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	404	ARG	NE-CZ-NH2	-24.96	107.82	120.30
1	C	300	ARG	NE-CZ-NH1	24.11	132.36	120.30
1	F	196	ARG	NE-CZ-NH2	-21.71	109.45	120.30
1	B	399	ARG	NE-CZ-NH2	-19.63	110.49	120.30
1	C	300	ARG	CG-CD-NE	-19.26	71.36	111.80
1	J	404	ARG	NE-CZ-NH2	-19.06	110.77	120.30
1	J	404	ARG	NE-CZ-NH1	15.47	128.03	120.30
1	P	385	LEU	CB-CG-CD2	-15.04	85.44	111.00
1	H	361	ARG	NE-CZ-NH1	-14.31	113.14	120.30
1	A	404	ARG	NE-CZ-NH1	-13.50	113.55	120.30
1	F	297	ARG	CB-CG-CD	-13.45	76.64	111.60
1	O	278	LEU	CB-CG-CD1	-13.37	88.27	111.00
1	O	392	LYS	CB-CG-CD	-13.24	77.19	111.60
1	C	399	ARG	NE-CZ-NH2	12.86	126.73	120.30
1	G	369	ARG	NE-CZ-NH2	-12.71	113.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	405	GLU	CA-CB-CG	-12.24	86.47	113.40
1	C	399	ARG	NE-CZ-NH1	-12.17	114.21	120.30
1	L	399	ARG	NE-CZ-NH1	-12.11	114.25	120.30
1	J	426	ARG	CG-CD-NE	-12.02	86.56	111.80
1	H	361	ARG	NE-CZ-NH2	11.94	126.27	120.30
1	G	326	LEU	CB-CG-CD2	-11.72	91.07	111.00
1	J	404	ARG	CG-CD-NE	-11.68	87.28	111.80
1	A	168	ARG	CG-CD-NE	-11.63	87.38	111.80
1	C	300	ARG	CA-CB-CG	-11.30	88.53	113.40
1	F	196	ARG	CD-NE-CZ	11.12	139.16	123.60
1	C	426	ARG	CG-CD-NE	-10.96	88.79	111.80
1	N	426	ARG	CG-CD-NE	-10.93	88.85	111.80
1	A	181	ARG	CA-CB-CG	-10.88	89.46	113.40
1	C	196	ARG	CG-CD-NE	10.73	134.34	111.80
1	L	399	ARG	NE-CZ-NH2	10.69	125.64	120.30
1	C	151	ARG	CG-CD-NE	-10.68	89.36	111.80
1	P	184	ASP	CB-CG-OD2	-10.59	108.77	118.30
1	C	165	LYS	CB-CG-CD	-10.53	84.21	111.60
1	C	300	ARG	CD-NE-CZ	10.53	138.34	123.60
1	I	151	ARG	NE-CZ-NH1	10.49	125.54	120.30
1	M	376	ARG	NE-CZ-NH2	-10.47	115.06	120.30
1	F	130	LYS	CA-CB-CG	-10.40	90.52	113.40
1	H	404	ARG	CB-CG-CD	10.39	138.60	111.60
1	G	376	ARG	CB-CG-CD	-10.38	84.60	111.60
1	E	151	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	F	130	LYS	CD-CE-NZ	-10.31	87.99	111.70
1	J	426	ARG	CA-CB-CG	-10.29	90.77	113.40
1	N	426	ARG	CA-CB-CG	-10.29	90.77	113.40
1	J	378	LEU	CB-CG-CD1	10.26	128.44	111.00
1	L	404	ARG	CD-NE-CZ	10.24	137.94	123.60
1	H	399	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	G	385	LEU	CB-CG-CD2	-10.21	93.64	111.00
1	H	161	ARG	CA-CB-CG	-10.00	91.41	113.40
1	G	300	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	I	196	ARG	CG-CD-NE	9.98	132.76	111.80
1	M	181	ARG	CA-CB-CG	-9.93	91.56	113.40
1	D	181	ARG	CA-CB-CG	-9.91	91.59	113.40
1	F	161	ARG	CA-CB-CG	-9.83	91.77	113.40
1	M	401	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	A	295	ASP	CB-CG-OD2	-9.79	109.49	118.30
1	B	222	LYS	CD-CE-NZ	-9.72	89.33	111.70
1	F	361	ARG	NE-CZ-NH1	-9.69	115.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	300	ARG	CG-CD-NE	9.59	131.95	111.80
1	F	399	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	N	153	GLU	CA-CB-CG	-9.54	92.41	113.40
1	J	161	ARG	CB-CG-CD	9.52	136.35	111.60
1	G	300	ARG	CG-CD-NE	-9.51	91.84	111.80
1	H	297	ARG	NE-CZ-NH1	-9.49	115.56	120.30
1	M	181	ARG	CG-CD-NE	-9.49	91.88	111.80
1	K	193	LYS	CD-CE-NZ	-9.46	89.95	111.70
1	C	152	LYS	CB-CG-CD	-9.44	87.06	111.60
1	J	168	ARG	CA-CB-CG	-9.43	92.66	113.40
1	O	386	GLN	CA-CB-CG	-9.43	92.66	113.40
1	E	151	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	H	426	ARG	CB-CG-CD	-9.39	87.17	111.60
1	A	165	LYS	CD-CE-NZ	9.39	133.30	111.70
1	F	399	ARG	CB-CG-CD	-9.33	87.33	111.60
1	H	307	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	P	184	ASP	CB-CG-OD1	9.28	126.65	118.30
1	C	426	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	O	181	ARG	CA-CB-CG	-9.20	93.15	113.40
1	K	376	ARG	CG-CD-NE	9.19	131.10	111.80
1	C	426	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	O	128	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	A	404	ARG	CB-CG-CD	-9.15	87.81	111.60
1	D	181	ARG	NE-CZ-NH1	-9.05	115.77	120.30
1	L	399	ARG	CD-NE-CZ	-8.95	111.08	123.60
1	P	181	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	H	300	ARG	CG-CD-NE	8.94	130.56	111.80
1	I	357	LYS	CD-CE-NZ	-8.92	91.19	111.70
1	C	153	GLU	CA-CB-CG	8.91	133.01	113.40
1	K	152	LYS	CD-CE-NZ	-8.91	91.21	111.70
1	M	401	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	C	300	ARG	NH1-CZ-NH2	-8.89	109.62	119.40
1	E	193	LYS	CB-CG-CD	-8.87	88.54	111.60
1	G	401	ARG	CB-CG-CD	-8.85	88.58	111.60
1	H	201	GLU	CA-CB-CG	-8.85	93.94	113.40
1	J	300	ARG	CB-CG-CD	-8.82	88.66	111.60
1	K	373	GLN	CA-CB-CG	-8.81	94.01	113.40
1	K	193	LYS	CA-CB-CG	8.79	132.74	113.40
1	L	193	LYS	CD-CE-NZ	-8.76	91.56	111.70
1	J	361	ARG	CG-CD-NE	-8.72	93.49	111.80
1	J	376	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	H	426	ARG	NE-CZ-NH2	-8.70	115.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	257	LYS	CG-CD-CE	-8.69	85.82	111.90
1	H	297	ARG	CG-CD-NE	-8.68	93.56	111.80
1	I	151	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	G	369	ARG	CD-NE-CZ	8.65	135.71	123.60
1	P	153	GLU	CB-CA-C	-8.62	93.16	110.40
1	F	161	ARG	NE-CZ-NH1	-8.62	115.99	120.30
1	H	376	ARG	CA-CB-CG	-8.59	94.50	113.40
1	C	399	ARG	CG-CD-NE	8.58	129.82	111.80
1	A	181	ARG	NE-CZ-NH1	-8.55	116.03	120.30
1	F	399	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	M	152	LYS	CD-CE-NZ	8.52	131.29	111.70
1	A	396	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	E	168	ARG	CA-CB-CG	-8.47	94.77	113.40
1	G	447	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	H	404	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	I	161	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	A	396	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	I	161	ARG	CD-NE-CZ	8.26	135.16	123.60
1	A	151	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	B	259	GLU	CA-CB-CG	8.25	131.56	113.40
1	E	193	LYS	CD-CE-NZ	-8.24	92.75	111.70
1	E	361	ARG	NE-CZ-NH1	-8.23	116.18	120.30
1	J	300	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	L	188	ARG	NE-CZ-NH1	-8.22	116.19	120.30
1	N	196	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	J	373	GLN	CA-CB-CG	-8.19	95.39	113.40
1	N	361	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	M	161	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	C	300	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	P	181	ARG	CG-CD-NE	-8.12	94.75	111.80
1	L	399	ARG	CA-CB-CG	-8.10	95.57	113.40
1	D	181	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	P	303	ILE	CG1-CB-CG2	-8.07	93.64	111.40
1	H	181	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	B	365	ASP	CB-CA-C	-8.05	94.30	110.40
1	O	396	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	P	181	ARG	CD-NE-CZ	8.03	134.84	123.60
1	G	196	ARG	CA-CB-CG	8.02	131.03	113.40
1	H	401	ARG	NE-CZ-NH1	-8.01	116.30	120.30
1	B	399	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	H	464	VAL	CG1-CB-CG2	-7.94	98.20	110.90
1	L	128	ARG	NE-CZ-NH2	-7.94	116.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	426	ARG	CA-CB-CG	-7.93	95.95	113.40
1	H	404	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	I	161	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	P	192	MET	CB-CG-SD	-7.84	88.88	112.40
1	G	196	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	F	296	GLU	C-N-CA	-7.74	102.36	121.70
1	B	193	LYS	CB-CG-CD	-7.71	91.57	111.60
1	H	321	MET	CG-SD-CE	-7.66	87.95	100.20
1	B	151	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	A	201	GLU	CA-CB-CG	-7.59	96.70	113.40
1	F	196	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	B	399	ARG	CD-NE-CZ	7.53	134.14	123.60
1	C	447	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	C	149	ARG	CA-CB-CG	-7.52	96.85	113.40
1	G	376	ARG	CG-CD-NE	7.52	127.59	111.80
1	E	161	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	J	168	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	L	193	LYS	CA-CB-CG	-7.49	96.92	113.40
1	A	180	VAL	CG1-CB-CG2	-7.45	98.98	110.90
1	H	149	ARG	CB-CG-CD	-7.45	92.23	111.60
1	G	401	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	F	149	ARG	CB-CG-CD	-7.43	92.28	111.60
1	H	300	ARG	CA-CB-CG	7.42	129.72	113.40
1	H	404	ARG	CA-CB-CG	7.42	129.72	113.40
1	N	181	ARG	CG-CD-NE	7.40	127.34	111.80
1	M	165	LYS	CB-CA-C	-7.39	95.62	110.40
1	I	394	ILE	CA-CB-CG1	-7.37	96.99	111.00
1	N	361	ARG	CG-CD-NE	7.34	127.21	111.80
1	O	404	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	M	401	ARG	CB-CG-CD	-7.30	92.62	111.60
1	H	178	GLU	CA-CB-CG	7.29	129.43	113.40
1	C	151	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	C	201	GLU	CB-CA-C	-7.28	95.85	110.40
1	I	361	ARG	CG-CD-NE	-7.21	96.65	111.80
1	H	289	ASP	CB-CG-OD2	7.19	124.77	118.30
1	G	150	LYS	CD-CE-NZ	7.18	128.21	111.70
1	J	161	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	F	193	LYS	CB-CG-CD	-7.14	93.04	111.60
1	A	426	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	H	361	ARG	CG-CD-NE	-7.11	96.86	111.80
1	E	399	ARG	NE-CZ-NH1	-7.11	116.75	120.30
1	J	168	ARG	CG-CD-NE	7.10	126.71	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	373	GLN	CA-CB-CG	-7.09	97.81	113.40
1	D	181	ARG	CD-NE-CZ	-7.08	113.69	123.60
1	L	188	ARG	CG-CD-NE	-7.07	96.95	111.80
1	A	165	LYS	CG-CD-CE	-7.05	90.74	111.90
1	H	289	ASP	CB-CG-OD1	-7.04	111.96	118.30
1	J	426	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	N	349	LEU	CB-CG-CD2	-7.02	99.06	111.00
1	N	165	LYS	CD-CE-NZ	-7.02	95.56	111.70
1	D	447	ARG	NE-CZ-NH1	-7.01	116.80	120.30
1	C	153	GLU	CG-CD-OE1	-7.00	104.29	118.30
1	A	181	ARG	CD-NE-CZ	-7.00	113.80	123.60
1	H	376	ARG	CB-CG-CD	6.98	129.75	111.60
1	E	346	HIS	CB-CA-C	-6.96	96.47	110.40
1	A	186	GLU	CA-CB-CG	-6.96	98.10	113.40
1	H	447	ARG	NE-CZ-NH1	-6.95	116.82	120.30
1	A	151	ARG	CD-NE-CZ	6.94	133.31	123.60
1	I	150	LYS	CA-CB-CG	6.92	128.62	113.40
1	N	390	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	K	376	ARG	CD-NE-CZ	6.88	133.23	123.60
1	A	151	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	C	300	ARG	CB-CG-CD	6.86	129.42	111.60
1	J	404	ARG	CD-NE-CZ	6.85	133.19	123.60
1	F	161	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	K	193	LYS	CB-CG-CD	6.82	129.34	111.60
1	P	369	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	O	220	ILE	CG1-CB-CG2	6.75	126.26	111.40
1	G	201	GLU	CA-CB-CG	-6.74	98.57	113.40
1	G	300	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	I	152	LYS	CG-CD-CE	6.73	132.09	111.90
1	I	399	ARG	CB-CG-CD	-6.71	94.16	111.60
1	A	426	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	I	361	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	F	165	LYS	CD-CE-NZ	-6.68	96.34	111.70
1	A	150	LYS	CD-CE-NZ	6.67	127.05	111.70
1	G	153	GLU	CA-CB-CG	-6.67	98.74	113.40
1	I	340	LYS	CD-CE-NZ	-6.66	96.38	111.70
1	C	193	LYS	CD-CE-NZ	-6.64	96.43	111.70
1	G	196	ARG	CB-CG-CD	-6.64	94.35	111.60
1	K	300	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	N	399	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	D	150	LYS	CD-CE-NZ	-6.62	96.48	111.70
1	H	178	GLU	CB-CA-C	-6.61	97.18	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	399	ARG	CA-CB-CG	6.58	127.88	113.40
1	M	390	ASP	N-CA-CB	-6.58	98.75	110.60
1	A	357	LYS	CD-CE-NZ	-6.57	96.60	111.70
1	E	165	LYS	CD-CE-NZ	-6.57	96.60	111.70
1	F	399	ARG	CD-NE-CZ	6.55	132.78	123.60
1	O	426	ARG	CD-NE-CZ	6.55	132.77	123.60
1	G	252	MET	CA-CB-CG	6.55	124.43	113.30
1	J	222	LYS	CA-CB-CG	6.54	127.80	113.40
1	P	289	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	N	196	ARG	CB-CG-CD	-6.51	94.67	111.60
1	P	153	GLU	N-CA-CB	6.51	122.32	110.60
1	N	426	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	399	ARG	CD-NE-CZ	-6.50	114.50	123.60
1	J	168	ARG	NE-CZ-NH2	6.43	123.51	120.30
1	G	326	LEU	CB-CG-CD1	6.39	121.87	111.00
1	A	178	GLU	CA-CB-CG	-6.39	99.34	113.40
1	E	222	LYS	CA-CB-CG	6.38	127.44	113.40
1	B	373	GLN	CA-CB-CG	-6.37	99.38	113.40
1	N	181	ARG	CD-NE-CZ	-6.37	114.68	123.60
1	H	401	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	L	394	ILE	CG1-CB-CG2	-6.35	97.44	111.40
1	K	193	LYS	N-CA-CB	6.32	121.98	110.60
1	J	357	LYS	CA-CB-CG	6.32	127.29	113.40
1	M	390	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	J	168	ARG	CD-NE-CZ	-6.29	114.80	123.60
1	N	399	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	G	401	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	J	361	ARG	CA-CB-CG	-6.27	99.61	113.40
1	G	405	GLU	N-CA-CB	-6.22	99.39	110.60
1	J	193	LYS	CD-CE-NZ	-6.22	97.39	111.70
1	L	361	ARG	CA-CB-CG	6.21	127.07	113.40
1	H	404	ARG	CD-NE-CZ	6.20	132.27	123.60
1	J	300	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	426	ARG	CD-NE-CZ	-6.19	114.94	123.60
1	G	150	LYS	CB-CA-C	-6.18	98.04	110.40
1	N	404	ARG	CA-CB-CG	6.17	126.98	113.40
1	O	392	LYS	CA-CB-CG	6.15	126.94	113.40
1	A	152	LYS	CD-CE-NZ	6.15	125.84	111.70
1	O	150	LYS	CG-CD-CE	6.14	130.32	111.90
1	F	369	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	K	361	ARG	CG-CD-NE	6.13	124.67	111.80
1	P	399	ARG	NE-CZ-NH1	-6.13	117.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	161	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	404	ARG	CG-CD-NE	-6.10	98.99	111.80
1	B	161	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	O	366	TRP	C-N-CA	-6.06	106.56	121.70
1	I	426	ARG	CA-CB-CG	6.05	126.71	113.40
1	O	397	ILE	CG1-CB-CG2	6.04	124.70	111.40
1	E	151	ARG	CD-NE-CZ	6.04	132.06	123.60
1	B	357	LYS	CG-CD-CE	6.03	130.00	111.90
1	O	134	LEU	CB-CG-CD2	-6.02	100.77	111.00
1	C	151	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	H	152	LYS	CD-CE-NZ	-6.00	97.91	111.70
1	J	376	ARG	CA-CB-CG	5.99	126.57	113.40
1	E	374	GLU	CB-CA-C	-5.99	98.43	110.40
1	H	181	ARG	CD-NE-CZ	5.97	131.96	123.60
1	J	376	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	181	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	J	300	ARG	CD-NE-CZ	5.97	131.95	123.60
1	J	458	LYS	CD-CE-NZ	5.97	125.42	111.70
1	G	426	ARG	CA-CB-CG	5.95	126.50	113.40
1	L	150	LYS	CA-CB-CG	5.95	126.49	113.40
1	I	150	LYS	CD-CE-NZ	-5.94	98.03	111.70
1	E	399	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	D	458	LYS	CD-CE-NZ	5.91	125.30	111.70
1	G	209	MET	CG-SD-CE	-5.91	90.74	100.20
1	P	369	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	F	193	LYS	CD-CE-NZ	-5.90	98.13	111.70
1	L	399	ARG	CG-CD-NE	5.89	124.18	111.80
1	O	386	GLN	CG-CD-OE1	-5.89	109.81	121.60
1	A	357	LYS	CG-CD-CE	-5.89	94.23	111.90
1	H	397	ILE	CG1-CB-CG2	5.89	124.35	111.40
1	M	376	ARG	CG-CD-NE	-5.88	99.44	111.80
1	H	168	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	D	447	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	N	196	ARG	N-CA-CB	5.85	121.13	110.60
1	A	295	ASP	CB-CG-OD1	5.83	123.55	118.30
1	I	357	LYS	CA-CB-CG	-5.82	100.60	113.40
1	J	269	SER	CB-CA-C	-5.81	99.06	110.10
1	L	399	ARG	CB-CG-CD	5.81	126.71	111.60
1	K	376	ARG	CB-CA-C	-5.80	98.80	110.40
1	G	149	ARG	CD-NE-CZ	5.79	131.71	123.60
1	H	399	ARG	CB-CG-CD	5.79	126.64	111.60
1	F	152	LYS	CG-CD-CE	-5.78	94.57	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	399	ARG	CA-CB-CG	-5.77	100.71	113.40
1	B	151	ARG	CG-CD-NE	-5.75	99.72	111.80
1	B	458	LYS	CG-CD-CE	-5.70	94.79	111.90
1	B	161	ARG	CA-CB-CG	5.70	125.94	113.40
1	F	297	ARG	N-CA-CB	5.68	120.83	110.60
1	D	181	ARG	CG-CD-NE	5.68	123.73	111.80
1	J	399	ARG	CG-CD-NE	5.68	123.73	111.80
1	H	151	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	G	178	GLU	N-CA-CB	5.67	120.80	110.60
1	L	361	ARG	CG-CD-NE	-5.67	99.90	111.80
1	E	390	ASP	N-CA-CB	-5.66	100.41	110.60
1	G	447	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	C	177	MET	CB-CG-SD	5.64	129.31	112.40
1	M	295	ASP	CB-CA-C	5.63	121.66	110.40
1	N	196	ARG	CB-CA-C	-5.61	99.18	110.40
1	F	130	LYS	CB-CG-CD	5.61	126.19	111.60
1	J	340	LYS	N-CA-CB	-5.61	100.51	110.60
1	H	385	LEU	CA-CB-CG	5.60	128.18	115.30
1	N	196	ARG	CG-CD-NE	5.60	123.55	111.80
1	O	165	LYS	CD-CE-NZ	5.59	124.56	111.70
1	M	181	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	F	369	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	O	150	LYS	CB-CG-CD	5.58	126.11	111.60
1	C	151	ARG	CB-CG-CD	-5.57	97.11	111.60
1	O	426	ARG	CA-CB-CG	-5.57	101.15	113.40
1	D	153	GLU	CB-CG-CD	-5.56	99.18	114.20
1	C	447	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	361	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	F	161	ARG	CB-CG-CD	5.55	126.03	111.60
1	B	150	LYS	CG-CD-CE	-5.54	95.28	111.90
1	P	178	GLU	CA-CB-CG	-5.54	101.21	113.40
1	A	165	LYS	CB-CG-CD	5.53	125.98	111.60
1	G	149	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	L	188	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	G	186	GLU	CG-CD-OE2	-5.51	107.28	118.30
1	C	193	LYS	CA-CB-CG	-5.50	101.30	113.40
1	D	165	LYS	CB-CA-C	-5.50	99.40	110.40
1	M	367	SER	CB-CA-C	5.50	120.55	110.10
1	K	300	ARG	CA-CB-CG	5.50	125.49	113.40
1	E	222	LYS	CD-CE-NZ	5.48	124.31	111.70
1	H	181	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	O	181	ARG	CD-NE-CZ	-5.48	115.93	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	188	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	J	399	ARG	CB-CG-CD	5.47	125.81	111.60
1	B	259	GLU	CB-CG-CD	-5.46	99.44	114.20
1	C	399	ARG	CB-CA-C	-5.46	99.48	110.40
1	D	356	GLU	OE1-CD-OE2	5.44	129.82	123.30
1	A	357	LYS	CB-CG-CD	5.43	125.71	111.60
1	L	168	ARG	CB-CG-CD	5.42	125.70	111.60
1	G	426	ARG	CG-CD-NE	5.40	123.15	111.80
1	E	404	ARG	CA-CB-CG	5.39	125.27	113.40
1	G	447	ARG	CD-NE-CZ	5.39	131.14	123.60
1	M	295	ASP	N-CA-CB	-5.38	100.92	110.60
1	P	295	ASP	CB-CA-C	-5.34	99.72	110.40
1	E	390	ASP	CB-CG-OD1	-5.34	113.50	118.30
1	I	151	ARG	CD-NE-CZ	5.33	131.07	123.60
1	B	152	LYS	CG-CD-CE	5.32	127.86	111.90
1	F	139	THR	OG1-CB-CG2	5.31	122.22	110.00
1	M	150	LYS	CD-CE-NZ	-5.29	99.54	111.70
1	J	130	LYS	CD-CE-NZ	5.28	123.84	111.70
1	F	161	ARG	CD-NE-CZ	-5.28	116.21	123.60
1	K	361	ARG	N-CA-CB	-5.27	101.12	110.60
1	N	181	ARG	CA-CB-CG	-5.26	101.83	113.40
1	H	152	LYS	CB-CG-CD	5.25	125.26	111.60
1	F	369	ARG	NH1-CZ-NH2	5.25	125.17	119.40
1	E	374	GLU	CA-CB-CG	5.22	124.89	113.40
1	A	399	ARG	N-CA-CB	-5.22	101.20	110.60
1	C	317	SER	CB-CA-C	5.22	120.02	110.10
1	C	365	ASP	CB-CG-OD2	5.17	122.96	118.30
1	H	404	ARG	CB-CA-C	-5.17	100.07	110.40
1	M	297	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	D	153	GLU	CG-CD-OE1	-5.16	107.99	118.30
1	F	297	ARG	CA-CB-CG	5.16	124.75	113.40
1	A	404	ARG	CA-CB-CG	5.16	124.74	113.40
1	N	390	ASP	CB-CG-OD2	5.15	122.94	118.30
1	L	168	ARG	CA-CB-CG	-5.15	102.06	113.40
1	H	399	ARG	CA-CB-CG	5.15	124.72	113.40
1	H	376	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	H	149	ARG	CG-CD-NE	5.14	122.59	111.80
1	G	386	GLN	CA-CB-CG	5.13	124.69	113.40
1	D	151	ARG	CG-CD-NE	-5.12	101.05	111.80
1	G	326	LEU	CD1-CG-CD2	-5.12	95.15	110.50
1	M	161	ARG	CA-CB-CG	-5.12	102.14	113.40
1	G	426	ARG	NE-CZ-NH2	-5.12	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	128	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	H	300	ARG	CB-CG-CD	-5.10	98.33	111.60
1	G	193	LYS	CD-CE-NZ	-5.09	99.99	111.70
1	B	389	LYS	CB-CA-C	-5.08	100.24	110.40
1	F	369	ARG	CG-CD-NE	5.07	122.44	111.80
1	C	399	ARG	CB-CG-CD	5.07	124.77	111.60
1	K	150	LYS	CB-CA-C	-5.06	100.28	110.40
1	B	257	LYS	CA-CB-CG	5.06	124.52	113.40
1	I	426	ARG	CG-CD-NE	5.05	122.40	111.80
1	F	376	ARG	CA-CB-CG	-5.05	102.30	113.40
1	I	161	ARG	CG-CD-NE	-5.04	101.22	111.80
1	D	396	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	E	168	ARG	CB-CG-CD	5.02	124.65	111.60
1	A	399	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	C	404	ARG	CA-CB-CG	5.01	124.43	113.40
1	K	196	ARG	N-CA-CB	5.01	119.62	110.60
1	M	376	ARG	CB-CG-CD	-5.00	98.59	111.60
1	L	297	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ARG	Peptide
1	A	162	ASN	Sidechain
1	B	373	GLN	Sidechain
1	B	399	ARG	Sidechain
1	C	300	ARG	Sidechain
1	D	162	ASN	Sidechain
1	E	150	LYS	Peptide
1	E	374	GLU	Sidechain
1	F	196	ARG	Sidechain
1	G	369	ARG	Sidechain
1	H	162	ASN	Sidechain
1	H	201	GLU	Sidechain
1	H	250	HIS	Sidechain
1	I	151	ARG	Mainchain
1	K	195	GLN	Peptide
1	L	404	ARG	Sidechain
1	M	162	ASN	Sidechain
1	N	162	ASN	Sidechain
1	O	162	ASN	Sidechain

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Mol	Chain	Res	Type	Group
1	O	346	HIS	Sidechain
1	P	153	GLU	Peptide
1	P	162	ASN	Sidechain
1	P	181	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2772	0	2765	101	4
1	B	2772	0	2767	74	0
1	C	2772	0	2767	102	4
1	D	2772	0	2767	67	0
1	E	2772	0	2767	65	0
1	F	2772	0	2767	83	0
1	G	2772	0	2767	95	0
1	H	2772	0	2767	118	0
1	I	2772	0	2767	91	0
1	J	2772	0	2766	67	3
1	K	2772	0	2767	87	1
1	L	2772	0	2767	67	0
1	M	2772	0	2767	89	1
1	N	2772	0	2765	110	0
1	O	2772	0	2767	120	3
1	P	2772	0	2767	134	0
2	A	5	0	0	0	0
2	B	15	0	0	1	0
2	C	15	0	0	1	0
2	D	5	0	0	0	0
2	E	15	0	0	3	0
2	F	15	0	0	1	0
2	G	5	0	0	1	0
2	H	10	0	0	2	0
2	I	15	0	0	0	0
2	J	15	0	0	0	0
2	K	10	0	0	1	0
2	L	10	0	0	1	0
2	M	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	5	0	0	0	0
2	O	10	0	0	1	0
2	P	10	0	0	0	0
3	A	35	0	0	2	0
3	B	35	0	0	0	0
3	C	35	0	0	0	0
3	D	35	0	0	1	0
3	E	35	0	0	0	0
3	F	35	0	0	0	0
3	G	35	0	0	0	0
3	H	35	0	0	1	0
3	I	35	0	0	0	0
3	J	35	0	0	0	0
3	K	35	0	0	0	0
3	L	35	0	0	0	0
3	M	35	0	0	0	0
3	N	35	0	0	0	0
3	O	35	0	0	0	0
3	P	35	0	0	0	0
4	A	33	0	0	7	0
4	B	27	0	0	0	0
4	C	37	0	0	7	0
4	D	32	0	0	2	0
4	E	39	0	0	5	0
4	F	37	0	0	5	0
4	G	31	0	0	2	0
4	H	22	0	0	6	0
4	I	34	0	0	6	0
4	J	29	0	0	3	0
4	K	29	0	0	3	0
4	L	34	0	0	8	0
4	M	43	0	0	8	0
4	N	26	0	0	3	0
4	O	28	0	0	4	0
4	P	30	0	0	11	0
All	All	45588	0	44267	1403	8

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 (1403) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:193:LYS:CE	1:L:193:LYS:NZ	1.68	1.52
1:N:307:ARG:NH2	1:N:346:HIS:CD2	2.08	1.22
1:B:151:ARG:HG2	1:B:153:GLU:OE1	1.40	1.21
1:K:151:ARG:HB2	1:K:153:GLU:OE2	1.43	1.18
1:N:402:PRO:HD2	1:N:405:GLU:CD	1.65	1.17
1:P:181:ARG:NH1	1:P:187:ASP:HA	1.63	1.13
1:N:356:GLU:OE2	1:N:361:ARG:HD2	1.47	1.12
1:B:357:LYS:HE2	1:D:361:ARG:HH12	1.13	1.10
1:O:402:PRO:HB2	1:O:405:GLU:HG3	1.32	1.09
1:J:373:GLN:HG2	1:J:374:GLU:N	1.56	1.09
1:O:353:HIS:HB3	1:O:397:ILE:HD13	1.35	1.08
1:N:402:PRO:HD2	1:N:405:GLU:OE1	1.55	1.06
1:I:361:ARG:HH21	1:P:361:ARG:HD2	1.15	1.06
1:H:161:ARG:HG3	1:H:162:ASN:H	0.98	1.05
1:H:307:ARG:NH2	2:H:501:SO4:O4	1.90	1.03
1:O:350:GLU:OE2	1:O:396:ARG:NH1	1.92	1.03
1:J:373:GLN:HG2	1:J:374:GLU:H	1.03	1.02
1:F:161:ARG:HG3	1:F:162:ASN:N	1.69	1.02
1:D:148:ASP:OD2	1:D:151:ARG:HB2	1.59	1.02
1:O:181:ARG:HH11	1:O:193:LYS:HB3	1.23	1.01
1:P:181:ARG:NH1	1:P:193:LYS:HE3	1.76	1.01
1:A:396:ARG:HG3	1:A:399:ARG:HH21	1.22	1.00
1:A:396:ARG:HG3	1:A:399:ARG:NH2	1.77	0.99
1:I:128:ARG:NE	1:I:150:LYS:HB3	1.75	0.99
1:A:181:ARG:NH2	1:A:185:VAL:O	1.96	0.98
1:O:128:ARG:HG3	1:O:150:LYS:HG3	1.42	0.97
1:C:298:HIS:HE1	1:C:300:ARG:NH1	1.62	0.97
1:H:161:ARG:HG3	1:H:162:ASN:N	1.56	0.96
1:H:353:HIS:HB3	1:H:397:ILE:HD13	1.46	0.96
1:C:152:LYS:O	1:C:153:GLU:HB3	1.61	0.95
1:L:193:LYS:CD	1:L:193:LYS:NZ	2.29	0.95
1:C:257:LYS:HB2	1:C:259:GLU:OE2	1.64	0.95
1:O:300:ARG:NH2	1:O:320:TRP:O	2.00	0.94
1:O:162:ASN:OD1	1:O:203:GLY:C	2.04	0.94
1:H:289:ASP:OD2	4:H:601:HOH:O	1.83	0.94
1:K:151:ARG:CB	1:K:153:GLU:OE2	2.16	0.93
1:P:380:THR:HG23	1:P:383:GLY:H	1.31	0.93
1:H:181:ARG:NE	1:H:184:ASP:O	2.01	0.92
1:M:181:ARG:HH21	1:M:185:VAL:HA	1.32	0.92
1:A:174:ILE:HG22	1:A:178:GLU:OE2	1.70	0.92
1:J:373:GLN:CG	1:J:374:GLU:N	2.32	0.92
1:H:147:TRP:HE1	1:H:149:ARG:HH11	1.07	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:307:ARG:HH22	1:N:346:HIS:HD2	1.12	0.92
1:P:373:GLN:CD	1:P:376:ARG:HD2	1.90	0.92
1:B:357:LYS:HE2	1:D:361:ARG:NH1	1.85	0.92
1:F:202:THR:HG1	1:F:204:HIS:HD1	1.17	0.91
1:P:181:ARG:HH12	1:P:187:ASP:HA	1.33	0.90
1:P:300:ARG:NH2	1:P:320:TRP:O	2.04	0.90
1:D:186:GLU:OE1	1:K:188:ARG:NH2	2.05	0.89
1:O:301:THR:HG22	1:O:317:SER:HB3	1.53	0.89
1:O:386:GLN:HG2	1:O:387:PRO:HD2	1.54	0.89
1:F:272:PRO:HB2	1:O:273:MET:HE1	1.55	0.89
1:H:404:ARG:HH21	1:K:404:ARG:CD	1.85	0.88
1:L:390:ASP:O	1:L:394:ILE:HD12	1.74	0.88
1:A:181:ARG:O	1:A:181:ARG:HG3	1.74	0.88
1:C:300:ARG:HE	1:C:319:GLY:HA2	1.39	0.87
1:E:151:ARG:NH2	1:E:196:ARG:HH12	1.71	0.87
1:C:300:ARG:NH1	1:C:320:TRP:O	2.07	0.87
1:C:298:HIS:CE1	1:C:300:ARG:NH1	2.43	0.87
1:B:187:ASP:OD1	1:B:193:LYS:HE2	1.75	0.86
1:P:148:ASP:HB3	1:P:153:GLU:HG2	1.56	0.86
1:N:356:GLU:OE2	1:N:361:ARG:CD	2.23	0.86
1:K:347:ASP:HB3	1:K:350:GLU:HG2	1.57	0.86
1:O:181:ARG:NH1	1:O:193:LYS:HB3	1.90	0.86
1:P:318:LEU:HD12	1:P:369:ARG:NH2	1.90	0.86
1:F:219:TRP:CZ3	1:F:268:THR:HG21	2.10	0.85
1:I:153:GLU:O	4:I:601:HOH:O	1.94	0.85
1:F:130:LYS:HG2	1:F:131:ILE:N	1.90	0.84
1:A:181:ARG:NH2	1:A:185:VAL:C	2.31	0.84
1:G:354:LEU:HD21	1:G:397:ILE:HA	1.58	0.84
1:C:300:ARG:NE	1:C:319:GLY:HA2	1.92	0.84
1:K:193:LYS:HG3	1:K:195:GLN:HE22	1.44	0.83
1:G:148:ASP:OD2	1:G:151:ARG:HD2	1.76	0.83
1:D:349:LEU:HG	1:D:378:LEU:HD22	1.61	0.82
1:M:249:LEU:O	4:M:601:HOH:O	1.97	0.82
1:M:380:THR:HG22	1:M:382:ALA:H	1.44	0.82
1:K:257:LYS:NZ	1:K:259:GLU:HB2	1.95	0.82
1:L:380:THR:HG22	1:L:382:ALA:H	1.44	0.82
1:G:380:THR:HG22	1:G:382:ALA:H	1.45	0.82
1:H:181:ARG:HB2	1:H:193:LYS:HD2	1.60	0.82
1:P:300:ARG:HH21	1:P:320:TRP:H	1.28	0.82
1:N:152:LYS:C	1:N:153:GLU:HG2	2.01	0.81
1:D:147:TRP:HD1	1:D:149:ARG:HD3	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:MET:HG3	1:G:209:MET:HE1	1.61	0.81
1:H:376:ARG:HG2	1:H:376:ARG:O	1.63	0.81
1:A:300:ARG:NH2	4:A:602:HOH:O	2.13	0.81
1:N:313:GLU:OE1	1:N:427:ARG:NH2	2.13	0.81
1:I:128:ARG:NH1	1:I:150:LYS:HG3	1.95	0.81
1:E:151:ARG:HH21	1:E:196:ARG:HH22	1.29	0.81
1:C:314:VAL:HG22	1:C:320:TRP:CD1	2.16	0.81
1:F:219:TRP:HZ3	1:F:268:THR:HG21	1.44	0.81
1:K:147:TRP:HZ2	1:K:152:LYS:HD3	1.45	0.81
1:H:376:ARG:NH2	1:H:380:THR:O	2.13	0.81
1:P:374:GLU:O	4:P:601:HOH:O	1.99	0.81
1:A:407:ILE:O	4:A:601:HOH:O	1.98	0.81
1:N:152:LYS:O	1:N:153:GLU:HG2	1.81	0.81
1:E:365:ASP:OD2	1:E:369:ARG:NH2	2.13	0.80
1:H:353:HIS:HB3	1:H:397:ILE:CD1	2.10	0.80
1:P:130:LYS:HD2	1:P:149:ARG:HH21	1.44	0.80
1:G:202:THR:HG23	1:G:204:HIS:HD1	1.47	0.80
1:I:361:ARG:NH2	1:P:361:ARG:HD2	1.96	0.80
1:C:165:LYS:HD2	1:C:168:ARG:HH21	1.47	0.80
1:N:148:ASP:OD2	1:N:151:ARG:HG3	1.82	0.80
1:P:181:ARG:NH1	1:P:193:LYS:CE	2.44	0.80
1:C:298:HIS:CE1	1:C:300:ARG:HH12	2.00	0.80
1:M:373:GLN:OE1	1:M:376:ARG:NH1	2.15	0.80
1:K:151:ARG:NH1	1:K:153:GLU:OE2	2.14	0.80
1:P:380:THR:CG2	1:P:383:GLY:H	1.95	0.80
1:P:174:ILE:HG22	1:P:178:GLU:OE2	1.82	0.79
1:O:299:SER:HB3	1:O:302:ALA:HB2	1.63	0.79
1:M:162:ASN:ND2	1:M:162:ASN:O	2.14	0.79
1:P:345:THR:HG22	1:P:347:ASP:H	1.48	0.79
1:H:404:ARG:NH2	1:K:404:ARG:HG2	1.98	0.79
1:F:268:THR:HG22	1:F:279:PRO:HA	1.64	0.79
1:I:388:CYS:O	1:I:394:ILE:HD11	1.83	0.78
1:P:181:ARG:NH1	1:P:187:ASP:CA	2.43	0.78
1:L:426:ARG:NH2	4:L:603:HOH:O	2.15	0.78
1:N:372:THR:HG23	1:N:375:ALA:H	1.49	0.78
1:A:181:ARG:HH22	1:A:185:VAL:C	1.87	0.78
1:F:271:ASP:OD2	1:F:274:THR:OG1	2.02	0.78
1:M:153:GLU:HG3	1:M:154:TYR:H	1.47	0.78
1:H:301:THR:HG22	1:H:317:SER:HB3	1.66	0.77
1:N:237:GLN:HE22	1:N:284:ARG:HA	1.47	0.77
1:D:346:HIS:O	1:D:346:HIS:ND1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LYS:CE	1:D:361:ARG:HH12	1.94	0.77
1:I:137:GLU:HG3	1:I:142:LYS:HG2	1.67	0.76
1:C:300:ARG:CZ	1:C:320:TRP:H	1.99	0.76
1:C:397:ILE:O	4:C:601:HOH:O	2.03	0.76
1:C:165:LYS:NZ	1:L:373:GLN:HG3	2.01	0.76
1:P:181:ARG:CZ	1:P:193:LYS:NZ	2.49	0.76
1:P:373:GLN:O	1:P:373:GLN:HG3	1.82	0.75
1:A:185:VAL:HG23	1:A:186:GLU:HG3	1.68	0.75
1:N:402:PRO:HD2	1:N:405:GLU:CG	2.17	0.75
1:C:400:ALA:N	4:C:601:HOH:O	2.19	0.74
1:M:252:MET:HG2	1:M:322:TYR:HA	1.69	0.74
1:M:181:ARG:NH2	1:M:185:VAL:HA	2.02	0.74
1:O:353:HIS:CB	1:O:397:ILE:HD13	2.14	0.74
1:P:181:ARG:HD2	1:P:193:LYS:HD3	1.68	0.74
1:F:390:ASP:OD2	1:F:392:LYS:HB2	1.88	0.74
1:P:318:LEU:HD12	1:P:369:ARG:CZ	2.18	0.74
1:M:179:ARG:HE	1:M:249:LEU:HD22	1.52	0.73
1:O:128:ARG:CG	1:O:150:LYS:HG3	2.17	0.73
1:G:162:ASN:HB2	1:G:204:HIS:HA	1.70	0.73
1:M:404:ARG:C	1:M:405:GLU:HG2	2.03	0.73
1:A:162:ASN:ND2	1:A:162:ASN:O	2.21	0.73
1:F:376:ARG:HH11	1:F:376:ARG:HG3	1.53	0.73
1:I:148:ASP:OD2	1:I:151:ARG:HB2	1.88	0.73
1:M:323:SER:HB2	4:M:603:HOH:O	1.87	0.73
1:P:181:ARG:HH11	1:P:187:ASP:HA	1.51	0.73
1:G:316:LEU:HB2	1:G:318:LEU:HD23	1.69	0.73
1:K:212:TYR:OH	4:K:601:HOH:O	2.07	0.73
1:N:285:VAL:O	4:N:601:HOH:O	2.05	0.72
1:P:299:SER:HB3	1:P:302:ALA:HB2	1.69	0.72
1:F:161:ARG:HG3	1:F:162:ASN:H	1.52	0.72
1:N:307:ARG:NH2	1:N:346:HIS:HD2	1.65	0.72
1:K:151:ARG:HD3	1:K:153:GLU:OE2	1.89	0.72
1:L:276:ARG:NH2	4:L:605:HOH:O	2.22	0.72
1:H:361:ARG:HD3	1:H:361:ARG:H	1.55	0.72
1:K:193:LYS:HG3	1:K:195:GLN:NE2	2.05	0.72
1:P:380:THR:CG2	1:P:384:THR:H	2.02	0.72
1:A:370:CYS:O	1:A:376:ARG:NH2	2.23	0.72
1:K:151:ARG:HH11	1:K:153:GLU:CD	1.92	0.72
1:K:181:ARG:NH1	1:K:193:LYS:HD2	2.05	0.72
1:P:170:ALA:O	1:P:174:ILE:HG13	1.90	0.72
1:P:181:ARG:CZ	1:P:193:LYS:HZ2	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:257:LYS:HG3	1:K:259:GLU:H	1.54	0.71
1:F:379:PHE:HA	1:F:385:LEU:HA	1.72	0.71
1:G:153:GLU:HG3	1:G:154:TYR:H	1.55	0.71
1:H:190:PRO:HG3	1:H:237:GLN:HB3	1.72	0.71
1:C:192:MET:HG2	1:C:193:LYS:H	1.55	0.71
1:N:307:ARG:NH1	1:N:346:HIS:HA	2.05	0.71
1:O:386:GLN:HG2	1:O:387:PRO:CD	2.19	0.71
1:G:346:HIS:O	1:G:346:HIS:ND1	2.22	0.71
1:G:349:LEU:HD13	1:G:378:LEU:HD22	1.73	0.71
1:H:181:ARG:HH22	1:H:193:LYS:NZ	1.89	0.71
1:D:147:TRP:CD1	1:D:149:ARG:HD3	2.24	0.70
1:J:195:GLN:HE22	1:J:210:PRO:HD3	1.56	0.70
1:A:316:LEU:HB2	1:A:318:LEU:HD21	1.70	0.70
1:G:349:LEU:HD21	1:G:386:GLN:HB2	1.71	0.70
1:J:395:ALA:O	1:J:399:ARG:HG3	1.91	0.70
1:E:151:ARG:NH2	1:E:196:ARG:NH1	2.39	0.70
1:I:167:THR:HG23	1:I:205:MET:HG2	1.73	0.70
1:J:195:GLN:OE1	1:J:209:MET:HA	1.92	0.70
1:M:181:ARG:O	1:M:181:ARG:HG3	1.85	0.70
1:H:200:ASN:OD1	1:H:201:GLU:N	2.25	0.70
1:A:396:ARG:CG	1:A:399:ARG:HH21	2.01	0.70
1:B:151:ARG:CG	1:B:153:GLU:OE1	2.30	0.70
1:K:276:ARG:NH2	4:K:602:HOH:O	2.23	0.70
1:P:181:ARG:NH2	1:P:184:ASP:O	2.25	0.70
1:I:423:ASP:HB3	1:I:426:ARG:HG3	1.73	0.70
1:G:153:GLU:HG3	1:G:154:TYR:N	2.07	0.69
1:K:257:LYS:HZ3	1:K:259:GLU:HB2	1.53	0.69
1:D:380:THR:HB	1:D:383:GLY:H	1.57	0.69
1:G:376:ARG:HD3	1:G:376:ARG:O	1.93	0.69
1:O:300:ARG:HH21	1:O:320:TRP:H	1.40	0.69
1:D:163:VAL:HB	1:D:166:TYR:HD2	1.57	0.69
1:P:181:ARG:HD2	1:P:193:LYS:CG	2.22	0.69
1:P:349:LEU:HB2	1:P:378:LEU:HD22	1.73	0.69
1:M:128:ARG:NE	1:M:148:ASP:OD1	2.19	0.69
1:O:353:HIS:NE2	1:O:386:GLN:O	2.18	0.69
1:M:364:ALA:O	4:M:602:HOH:O	2.10	0.69
1:E:310:ARG:NH1	4:E:603:HOH:O	2.26	0.69
1:H:299:SER:HB3	1:H:302:ALA:HB2	1.75	0.69
1:D:132:LEU:HD11	1:D:147:TRP:HB2	1.74	0.69
1:H:161:ARG:CG	1:H:162:ASN:N	2.47	0.69
1:A:167:THR:HG23	1:A:205:MET:HG2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:361:ARG:NH1	1:M:361:ARG:HB2	2.07	0.68
1:C:192:MET:C	1:C:193:LYS:HG2	2.13	0.68
1:F:147:TRP:HE1	1:F:149:ARG:HH11	1.42	0.68
1:C:200:ASN:OD1	4:C:602:HOH:O	2.11	0.68
1:F:380:THR:HG22	1:F:382:ALA:H	1.58	0.68
1:H:389:LYS:HA	1:H:394:ILE:HD11	1.74	0.68
1:L:252:MET:HG2	1:L:322:TYR:HA	1.76	0.68
1:I:130:LYS:HE2	1:I:149:ARG:HH21	1.59	0.68
1:P:323:SER:HB2	4:P:602:HOH:O	1.93	0.68
1:K:441:LYS:HG2	1:K:442:TYR:CE2	2.29	0.68
1:P:181:ARG:HB2	1:P:193:LYS:HG2	1.75	0.67
1:P:196:ARG:HG3	1:P:197:TYR:N	2.08	0.67
1:E:347:ASP:OD2	4:E:601:HOH:O	2.13	0.67
1:F:405:GLU:HG3	1:F:405:GLU:O	1.92	0.67
1:C:134:LEU:HD11	1:C:137:GLU:HG2	1.75	0.67
1:E:151:ARG:HH21	1:E:196:ARG:NH2	1.91	0.67
1:G:313:GLU:HA	1:G:318:LEU:HB2	1.77	0.67
1:O:128:ARG:NE	1:O:148:ASP:OD1	2.26	0.67
1:C:187:ASP:OD1	1:C:193:LYS:HE3	1.95	0.67
1:K:310:ARG:NH1	4:K:606:HOH:O	2.27	0.67
1:P:300:ARG:NH2	1:P:320:TRP:H	1.92	0.67
1:O:278:LEU:HD12	1:O:278:LEU:N	2.08	0.67
1:E:162:ASN:ND2	1:E:202:THR:O	2.28	0.67
1:M:153:GLU:HG3	1:M:154:TYR:N	2.09	0.67
1:N:307:ARG:HH22	1:N:346:HIS:CD2	1.88	0.67
1:A:185:VAL:C	1:A:186:GLU:HG3	2.11	0.67
1:L:183:SER:O	4:L:601:HOH:O	2.12	0.67
1:G:192:MET:CG	1:G:209:MET:HE1	2.24	0.67
1:N:348:ASN:HB3	1:N:378:LEU:HD21	1.77	0.67
1:C:264:GLU:HG2	1:H:448:GLN:HG2	1.78	0.66
1:F:230:HIS:HE1	1:F:281:GLU:OE2	1.78	0.66
1:M:401:ARG:HD2	1:M:402:PRO:CD	2.25	0.66
1:G:162:ASN:ND2	1:G:203:GLY:O	2.28	0.66
1:A:192:MET:CE	1:A:209:MET:SD	2.83	0.66
1:A:300:ARG:O	1:A:300:ARG:HG2	1.95	0.66
1:G:135:LEU:HD21	1:G:145:GLU:HB2	1.78	0.66
1:B:393:HIS:O	1:B:397:ILE:HG13	1.95	0.66
1:J:393:HIS:O	1:J:397:ILE:HG13	1.95	0.66
1:M:251:LEU:HG	4:M:601:HOH:O	1.95	0.66
1:E:393:HIS:O	1:E:397:ILE:HG13	1.95	0.66
1:H:454:ASP:OD2	4:H:602:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:404:ARG:NH2	1:K:404:ARG:CG	2.59	0.66
1:I:264:GLU:HG2	1:M:448:GLN:HG2	1.78	0.66
1:P:301:THR:HG22	1:P:317:SER:HB3	1.78	0.66
1:M:428:LEU:O	4:M:603:HOH:O	2.13	0.65
1:N:337:TYR:O	4:N:602:HOH:O	2.15	0.65
1:A:348:ASN:OD1	4:A:603:HOH:O	2.14	0.65
1:F:252:MET:HG2	1:F:322:TYR:HA	1.77	0.65
1:C:271:ASP:HB2	1:C:278:LEU:HD13	1.78	0.65
1:H:162:ASN:OD1	1:H:203:GLY:C	2.35	0.65
1:J:257:LYS:HD3	1:J:259:GLU:HG2	1.77	0.65
1:O:386:GLN:CG	1:O:387:PRO:HD2	2.23	0.65
1:G:226:PHE:O	4:G:601:HOH:O	2.14	0.65
1:N:316:LEU:HB2	1:N:318:LEU:HD23	1.79	0.65
1:A:276:ARG:HH21	1:B:130:LYS:NZ	1.94	0.65
1:H:257:LYS:NZ	4:H:605:HOH:O	2.29	0.65
1:M:167:THR:HG23	1:M:205:MET:HG2	1.79	0.65
1:A:181:ARG:CD	1:A:193:LYS:HD2	2.26	0.65
1:M:299:SER:OG	1:M:302:ALA:HB2	1.95	0.65
1:A:388:CYS:O	1:A:394:ILE:HD11	1.97	0.64
1:H:311:SER:HB2	1:H:313:GLU:OE1	1.96	0.64
1:K:222:LYS:HD3	1:K:223:HIS:NE2	2.11	0.64
1:E:167:THR:HG23	1:E:205:MET:HG2	1.79	0.64
1:H:361:ARG:HD3	1:H:361:ARG:N	2.11	0.64
1:D:187:ASP:OD2	1:D:193:LYS:HD2	1.98	0.64
1:J:193:LYS:O	1:J:195:GLN:NE2	2.30	0.64
1:P:181:ARG:HD2	1:P:193:LYS:HG2	1.79	0.64
1:P:181:ARG:HH22	1:P:184:ASP:CB	2.11	0.64
1:G:401:ARG:HD2	1:G:402:PRO:CD	2.27	0.64
1:I:128:ARG:CZ	1:I:150:LYS:HG3	2.27	0.64
1:N:380:THR:HB	1:N:383:GLY:H	1.63	0.64
1:H:307:ARG:HH21	1:H:346:HIS:HA	1.63	0.64
1:I:392:LYS:HE2	1:I:392:LYS:H	1.63	0.64
1:O:316:LEU:CB	1:O:318:LEU:HD13	2.28	0.64
1:C:200:ASN:OD1	1:C:201:GLU:N	2.29	0.64
1:P:158:LYS:HD2	4:P:625:HOH:O	1.96	0.64
1:A:170:ALA:O	1:A:174:ILE:HG13	1.98	0.64
1:B:151:ARG:NH1	1:B:153:GLU:OE1	2.31	0.64
1:H:161:ARG:CG	1:H:162:ASN:H	1.91	0.64
1:K:257:LYS:HG3	1:K:259:GLU:OE2	1.97	0.64
1:G:299:SER:OG	1:G:302:ALA:HB2	1.98	0.64
1:K:147:TRP:CZ2	1:K:152:LYS:HD3	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:316:LEU:HB3	1:O:318:LEU:CD1	2.27	0.64
1:M:378:LEU:C	1:M:386:GLN:HG3	2.18	0.64
1:C:147:TRP:CD1	1:C:149:ARG:HG2	2.32	0.63
1:C:258:PRO:HD3	1:C:332:ILE:HG12	1.80	0.63
1:N:147:TRP:CZ2	1:N:152:LYS:HG3	2.33	0.63
1:J:264:GLU:HG2	1:N:448:GLN:HG2	1.80	0.63
1:I:423:ASP:CB	1:I:426:ARG:HG3	2.28	0.63
1:J:139:THR:OG1	4:J:601:HOH:O	2.15	0.63
1:L:402:PRO:HB3	1:L:404:ARG:NH1	2.13	0.63
1:P:380:THR:HG22	1:P:384:THR:H	1.63	0.63
1:B:147:TRP:HZ2	1:B:152:LYS:HD3	1.62	0.63
1:O:372:THR:HB	1:O:374:GLU:OE1	1.98	0.63
1:K:257:LYS:NZ	1:K:259:GLU:CB	2.61	0.63
1:P:148:ASP:CB	1:P:153:GLU:HG2	2.29	0.63
1:A:133:SER:HB3	1:A:145:GLU:HB3	1.80	0.63
1:A:175:GLN:HA	1:A:178:GLU:OE1	1.98	0.63
1:B:162:ASN:HB2	1:B:204:HIS:CD2	2.34	0.63
1:P:181:ARG:HD2	1:P:193:LYS:CD	2.27	0.63
1:H:396:ARG:HH11	1:H:396:ARG:HG3	1.63	0.63
1:L:192:MET:C	1:L:193:LYS:HG2	2.18	0.63
1:D:297:ARG:NH1	1:N:299:SER:H	1.97	0.63
1:A:396:ARG:HA	1:A:399:ARG:HE	1.64	0.62
1:O:188:ARG:HD3	1:O:189:PHE:CZ	2.34	0.62
1:O:404:ARG:HA	1:O:413:CYS:SG	2.38	0.62
1:A:181:ARG:HD3	1:A:193:LYS:HD2	1.81	0.62
1:H:251:LEU:HD23	1:H:295:ASP:OD1	1.98	0.62
1:K:373:GLN:HG3	1:K:373:GLN:O	1.98	0.62
1:A:353:HIS:HB3	1:A:397:ILE:HD13	1.82	0.62
1:C:192:MET:HG2	1:C:193:LYS:N	2.14	0.62
1:D:390:ASP:OD2	1:D:392:LYS:HB2	1.99	0.62
1:F:165:LYS:HD2	1:F:168:ARG:HH21	1.63	0.62
1:C:165:LYS:CD	1:C:168:ARG:HH21	2.13	0.62
1:J:373:GLN:CG	1:J:374:GLU:H	1.92	0.62
1:I:313:GLU:HA	1:I:318:LEU:HD12	1.81	0.62
1:H:398:ALA:O	1:H:401:ARG:NH1	2.32	0.62
1:L:149:ARG:O	1:L:152:LYS:NZ	2.27	0.62
1:P:190:PRO:HG3	1:P:237:GLN:HB3	1.82	0.62
1:O:162:ASN:OD1	1:O:203:GLY:O	2.18	0.62
1:P:181:ARG:CZ	1:P:184:ASP:O	2.47	0.62
1:A:380:THR:HB	1:A:383:GLY:H	1.64	0.62
1:B:147:TRP:HE1	1:B:149:ARG:HD3	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:373:GLN:HA	1:O:376:ARG:NE	2.15	0.62
1:L:362:LEU:HB3	1:L:366:TRP:CE3	2.35	0.61
1:N:147:TRP:HD1	1:N:149:ARG:HD3	1.64	0.61
1:H:345:THR:HG22	1:H:347:ASP:H	1.64	0.61
1:J:181:ARG:HD2	1:J:193:LYS:HD3	1.81	0.61
1:P:196:ARG:HG3	1:P:197:TYR:H	1.63	0.61
1:E:151:ARG:HH21	1:E:196:ARG:HH12	1.48	0.61
1:J:128:ARG:O	1:J:149:ARG:HG3	2.00	0.61
1:E:222:LYS:HG3	1:E:223:HIS:NE2	2.16	0.61
1:H:181:ARG:HH22	1:H:187:ASP:HA	1.65	0.61
1:P:230:HIS:O	1:P:234:ILE:HG13	2.00	0.61
1:F:257:LYS:HE3	1:F:259:GLU:HG3	1.83	0.61
1:N:157:VAL:HG22	1:N:208:VAL:HG22	1.81	0.61
1:K:167:THR:HG23	1:K:205:MET:HG2	1.82	0.61
1:P:401:ARG:HG3	1:P:402:PRO:HD2	1.83	0.61
1:E:365:ASP:OD2	1:E:369:ARG:NE	2.34	0.61
1:H:307:ARG:NH2	1:H:346:HIS:HA	2.15	0.61
1:L:184:ASP:O	1:L:193:LYS:NZ	2.33	0.61
1:L:258:PRO:HD3	1:L:332:ILE:HG12	1.81	0.60
1:B:353:HIS:O	1:B:357:LYS:HB2	2.01	0.60
1:H:365:ASP:OD2	1:H:369:ARG:NH2	2.33	0.60
1:O:402:PRO:CB	1:O:405:GLU:HG3	2.20	0.60
1:F:274:THR:HB	1:F:276:ARG:NE	2.16	0.60
1:J:200:ASN:OD1	1:J:201:GLU:N	2.28	0.60
1:P:181:ARG:HH22	1:P:184:ASP:CG	2.05	0.60
1:E:252:MET:HG2	1:E:322:TYR:HA	1.84	0.60
1:H:163:VAL:CG2	1:H:166:TYR:HD2	2.14	0.60
1:L:167:THR:HG23	1:L:205:MET:HG2	1.84	0.60
1:M:415:LEU:HD12	1:M:438:TYR:HB3	1.83	0.60
1:C:300:ARG:NH2	1:C:320:TRP:CD1	2.69	0.60
1:M:353:HIS:HE1	1:M:386:GLN:O	1.84	0.60
1:I:128:ARG:HE	1:I:150:LYS:HB3	1.66	0.60
1:O:316:LEU:HB3	1:O:318:LEU:HD11	1.83	0.60
1:A:151:ARG:HG2	1:A:151:ARG:O	2.00	0.60
1:H:396:ARG:O	1:H:399:ARG:HB2	2.01	0.60
1:N:402:PRO:CD	1:N:405:GLU:CD	2.56	0.60
1:N:401:ARG:HB3	1:N:405:GLU:OE1	1.99	0.60
1:J:195:GLN:N	1:J:195:GLN:OE1	2.34	0.60
1:K:128:ARG:HH22	1:K:196:ARG:NH2	2.00	0.60
1:N:307:ARG:CZ	1:N:346:HIS:HA	2.31	0.60
1:P:151:ARG:NE	1:P:153:GLU:OE1	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:PRO:HG3	1:G:237:GLN:HB3	1.83	0.60
1:G:326:LEU:HD21	1:G:430:ALA:N	2.16	0.60
1:L:390:ASP:O	1:L:394:ILE:CD1	2.50	0.60
1:A:190:PRO:HG3	1:A:237:GLN:HB3	1.82	0.59
1:A:316:LEU:HB2	1:A:318:LEU:CD2	2.32	0.59
1:B:252:MET:HG2	1:B:322:TYR:HA	1.84	0.59
1:H:404:ARG:HH21	1:K:404:ARG:CG	2.14	0.59
1:N:190:PRO:HG3	1:N:237:GLN:HB3	1.84	0.59
1:H:404:ARG:HH21	1:K:404:ARG:HD3	1.67	0.59
1:I:380:THR:HG23	1:I:383:GLY:H	1.66	0.59
1:K:259:GLU:OE2	1:K:259:GLU:N	2.34	0.59
1:O:426:ARG:NH1	4:O:605:HOH:O	2.34	0.59
1:G:153:GLU:CG	1:G:154:TYR:N	2.64	0.59
1:B:222:LYS:HD2	1:B:223:HIS:NE2	2.18	0.59
1:B:257:LYS:HG2	1:B:260:ASN:CG	2.22	0.59
1:F:356:GLU:OE2	1:F:361:ARG:HB3	2.03	0.59
1:G:128:ARG:NH2	1:G:196:ARG:HD3	2.17	0.59
1:H:134:LEU:HD13	1:H:142:LYS:HE3	1.83	0.59
1:A:380:THR:HG22	1:A:382:ALA:H	1.67	0.59
1:N:402:PRO:CB	1:N:405:GLU:HG3	2.33	0.59
1:O:367:SER:HA	1:O:370:CYS:SG	2.43	0.59
1:P:357:LYS:HE3	1:P:397:ILE:O	2.03	0.59
1:A:181:ARG:CZ	1:A:185:VAL:C	2.71	0.59
1:B:202:THR:HG23	1:B:204:HIS:ND1	2.17	0.59
1:C:151:ARG:O	1:C:152:LYS:HB2	2.01	0.59
1:C:230:HIS:HE1	1:C:281:GLU:OE2	1.85	0.59
1:F:258:PRO:HD3	1:F:332:ILE:HG12	1.85	0.59
1:G:177:MET:HE2	1:G:194:ILE:HB	1.82	0.59
1:J:195:GLN:NE2	1:J:210:PRO:HD3	2.18	0.59
1:O:337:TYR:OH	4:O:601:HOH:O	2.12	0.59
1:M:362:LEU:HD22	1:M:366:TRP:CZ3	2.38	0.59
1:F:376:ARG:O	1:F:376:ARG:HG3	2.01	0.59
1:H:163:VAL:HG21	1:H:166:TYR:HD2	1.68	0.59
1:J:257:LYS:HD3	1:J:259:GLU:CG	2.32	0.59
1:H:350:GLU:OE2	1:H:396:ARG:HD2	2.02	0.58
1:N:402:PRO:HB2	1:N:405:GLU:HG3	1.84	0.58
1:B:167:THR:HG23	1:B:205:MET:HG2	1.86	0.58
1:G:297:ARG:HB3	1:P:295:ASP:OD2	2.03	0.58
1:I:245:PHE:HZ	1:I:293:CYS:HG	1.50	0.58
1:O:316:LEU:HD12	1:O:375:ALA:HB1	1.83	0.58
1:P:318:LEU:CD1	1:P:369:ARG:CZ	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:181:ARG:NH2	1:H:193:LYS:NZ	2.51	0.58
1:O:158:LYS:HD3	1:O:207:ILE:HD12	1.84	0.58
1:B:151:ARG:CZ	1:B:153:GLU:OE1	2.51	0.58
1:C:165:LYS:HZ2	1:C:168:ARG:HH21	1.51	0.58
1:F:356:GLU:HG2	1:F:361:ARG:HA	1.85	0.58
1:B:194:ILE:HA	1:B:209:MET:HG2	1.85	0.58
1:F:186:GLU:O	1:F:186:GLU:HG3	2.03	0.58
1:G:444:PRO:O	1:G:447:ARG:HD2	2.04	0.58
1:M:192:MET:CE	1:M:290:LEU:HG	2.33	0.58
1:N:299:SER:HB3	1:N:302:ALA:HB2	1.84	0.58
1:H:237:GLN:HE22	1:H:284:ARG:HA	1.68	0.58
1:I:148:ASP:CG	1:I:151:ARG:HB2	2.23	0.58
1:J:464:VAL:O	1:J:465:MET:HG2	2.03	0.58
1:O:128:ARG:HG3	1:O:150:LYS:CG	2.27	0.58
1:A:269:SER:OG	1:A:278:LEU:HB2	2.04	0.58
1:B:373:GLN:O	1:B:373:GLN:HG3	2.02	0.58
1:C:192:MET:CG	1:C:193:LYS:N	2.66	0.58
1:H:147:TRP:CD1	1:H:149:ARG:HD3	2.39	0.58
1:L:217:LEU:HD22	1:L:259:GLU:HG3	1.86	0.58
1:C:165:LYS:HZ1	1:L:373:GLN:HG3	1.67	0.58
1:A:181:ARG:HH22	1:A:186:GLU:N	2.01	0.58
1:D:167:THR:HG22	1:D:205:MET:HG2	1.85	0.58
1:L:310:ARG:NH1	4:L:610:HOH:O	2.30	0.58
1:P:181:ARG:NH2	1:P:184:ASP:CB	2.66	0.58
1:J:167:THR:HG23	1:J:205:MET:HG2	1.85	0.57
1:M:323:SER:HA	1:M:326:LEU:HD23	1.85	0.57
1:A:313:GLU:HA	1:A:318:LEU:HD23	1.86	0.57
1:F:161:ARG:HD2	1:F:162:ASN:H	1.68	0.57
1:H:313:GLU:CD	1:H:427:ARG:HH22	2.08	0.57
1:D:239:GLY:HA3	1:D:434:MET:HB3	1.86	0.57
1:O:323:SER:OG	1:O:427:ARG:HD2	2.04	0.57
1:P:183:SER:OG	1:P:244:TYR:OH	2.19	0.57
1:P:380:THR:HG22	1:P:384:THR:N	2.18	0.57
1:E:181:ARG:NH2	4:E:608:HOH:O	2.37	0.57
1:O:134:LEU:HD21	1:O:137:GLU:OE2	2.04	0.57
1:D:390:ASP:OD1	1:D:391:PRO:HD2	2.05	0.57
1:N:415:LEU:HD12	1:N:438:TYR:HB3	1.87	0.57
1:O:217:LEU:HD12	1:O:220:ILE:HD11	1.86	0.57
1:P:181:ARG:HH22	1:P:184:ASP:HB3	1.67	0.57
1:A:162:ASN:OD1	1:A:203:GLY:C	2.43	0.57
1:F:323:SER:HB2	4:F:613:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:153:GLU:N	4:I:601:HOH:O	2.23	0.57
1:N:163:VAL:O	1:N:167:THR:HG22	2.05	0.57
1:D:190:PRO:HG3	1:D:237:GLN:HB3	1.87	0.57
1:L:193:LYS:HZ3	1:L:193:LYS:CD	2.15	0.57
1:L:190:PRO:HG2	1:L:241:ALA:HB2	1.87	0.57
1:A:276:ARG:HH21	1:B:130:LYS:HZ1	1.53	0.56
1:H:181:ARG:HH22	1:H:193:LYS:HZ1	1.53	0.56
1:I:128:ARG:CZ	1:I:150:LYS:CG	2.83	0.56
1:I:147:TRP:CZ2	1:I:152:LYS:HD3	2.40	0.56
1:L:151:ARG:HB3	1:L:153:GLU:OE1	2.05	0.56
1:O:348:ASN:HB3	1:O:378:LEU:HD21	1.87	0.56
1:P:181:ARG:HH12	1:P:193:LYS:HE3	1.64	0.56
1:A:369:ARG:HH11	1:A:369:ARG:HG3	1.70	0.56
1:F:390:ASP:OD2	1:F:392:LYS:HD3	2.05	0.56
1:P:239:GLY:HA3	1:P:434:MET:HB3	1.87	0.56
1:H:337:TYR:OH	4:H:603:HOH:O	2.14	0.56
1:K:151:ARG:NH1	1:K:153:GLU:CD	2.55	0.56
1:L:383:GLY:O	4:L:604:HOH:O	2.17	0.56
1:C:175:GLN:HE22	1:F:296:GLU:CD	2.07	0.56
1:I:217:LEU:HD22	1:I:259:GLU:HG3	1.88	0.56
1:I:425:GLN:HG2	1:I:465:MET:HB3	1.86	0.56
1:D:380:THR:HG22	1:D:382:ALA:H	1.70	0.56
1:G:128:ARG:O	1:G:149:ARG:HB2	2.06	0.56
1:B:264:GLU:HG2	1:G:448:GLN:HG2	1.87	0.56
1:G:250:HIS:CD2	1:P:179:ARG:NH1	2.74	0.56
1:H:162:ASN:ND2	1:H:162:ASN:O	2.38	0.56
1:I:171:LYS:NZ	4:I:606:HOH:O	2.36	0.56
1:K:257:LYS:HZ3	1:K:259:GLU:CB	2.18	0.56
1:L:137:GLU:HG2	1:L:138:GLY:N	2.20	0.56
1:H:316:LEU:HB2	1:H:318:LEU:HD13	1.87	0.56
1:L:390:ASP:OD2	1:L:392:LYS:HB2	2.06	0.56
1:D:182:LEU:HD13	1:N:460:PRO:HA	1.87	0.56
1:I:147:TRP:HZ2	1:I:152:LYS:CD	2.18	0.56
1:O:128:ARG:HG3	1:O:150:LYS:HZ2	1.71	0.56
1:P:181:ARG:HH11	1:P:187:ASP:CA	2.16	0.56
1:P:362:LEU:CD1	1:P:385:LEU:HD11	2.36	0.56
1:P:428:LEU:O	4:P:602:HOH:O	2.18	0.56
1:H:357:LYS:NZ	1:H:397:ILE:O	2.39	0.56
1:O:174:ILE:HA	1:O:177:MET:HE2	1.88	0.56
1:P:323:SER:OG	1:P:427:ARG:NH1	2.39	0.56
1:A:299:SER:HB3	1:A:302:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:415:LEU:HD12	1:H:438:TYR:HB3	1.88	0.56
1:I:192:MET:HG2	1:I:193:LYS:N	2.21	0.56
1:B:357:LYS:HG2	1:B:397:ILE:HG22	1.88	0.55
1:C:165:LYS:NZ	1:C:168:ARG:HH21	2.03	0.55
1:P:388:CYS:O	1:P:394:ILE:HD11	2.05	0.55
1:H:313:GLU:HG2	1:H:424:ARG:HD2	1.88	0.55
1:L:187:ASP:OD1	1:L:193:LYS:HE3	2.06	0.55
1:B:390:ASP:OD2	1:B:392:LYS:HE2	2.05	0.55
1:C:310:ARG:NH1	4:C:609:HOH:O	2.36	0.55
1:C:270:VAL:HG11	1:D:154:TYR:OH	2.07	0.55
1:G:163:VAL:CG1	1:G:166:TYR:HB2	2.37	0.55
1:F:264:GLU:HG2	1:O:448:GLN:HG2	1.87	0.55
1:F:161:ARG:CG	1:F:162:ASN:N	2.55	0.55
1:H:404:ARG:NH2	1:K:404:ARG:CD	2.64	0.55
1:L:464:VAL:O	1:L:465:MET:HG2	2.06	0.55
1:N:365:ASP:OD2	1:N:369:ARG:NH2	2.39	0.55
1:O:277:ALA:C	1:O:278:LEU:HD12	2.26	0.55
1:L:187:ASP:CG	1:L:193:LYS:HE3	2.26	0.55
1:C:202:THR:HG23	1:C:204:HIS:ND1	2.21	0.55
1:D:464:VAL:HG13	1:D:464:VAL:O	2.05	0.55
1:H:162:ASN:OD1	1:H:204:HIS:N	2.39	0.55
1:K:217:LEU:HD22	1:K:259:GLU:HG3	1.88	0.55
1:P:181:ARG:NH2	1:P:184:ASP:HB3	2.20	0.55
1:G:316:LEU:CB	1:G:318:LEU:HD23	2.34	0.55
1:A:423:ASP:OD2	4:A:604:HOH:O	2.18	0.55
1:C:376:ARG:O	1:C:376:ARG:HD2	2.07	0.55
1:G:184:ASP:OD2	1:G:193:LYS:NZ	2.32	0.55
1:J:152:LYS:HG3	1:J:152:LYS:O	2.07	0.55
1:O:129:PHE:CZ	1:O:208:VAL:HG21	2.42	0.55
1:E:222:LYS:HG3	1:E:223:HIS:CD2	2.42	0.55
1:E:464:VAL:O	1:E:465:MET:HG2	2.07	0.55
1:P:373:GLN:HA	1:P:376:ARG:HD2	1.89	0.55
1:E:179:ARG:NH2	1:E:251:LEU:HD21	2.22	0.54
1:E:195:GLN:OE1	1:E:210:PRO:HD3	2.07	0.54
1:E:222:LYS:CG	1:E:223:HIS:CE1	2.89	0.54
1:E:365:ASP:OD2	1:E:369:ARG:CZ	2.54	0.54
1:A:181:ARG:HH22	1:A:186:GLU:CA	2.19	0.54
1:B:162:ASN:HB2	1:B:204:HIS:NE2	2.22	0.54
1:D:162:ASN:OD1	1:D:202:THR:O	2.25	0.54
1:F:202:THR:HG1	1:F:204:HIS:CE1	2.25	0.54
1:H:404:ARG:HH21	1:K:404:ARG:HD2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:168:ARG:NH1	1:P:171:LYS:HB2	2.22	0.54
1:F:350:GLU:HG3	1:F:393:HIS:HB3	1.90	0.54
1:I:179:ARG:NH1	1:I:251:LEU:HD21	2.23	0.54
1:C:300:ARG:O	1:C:300:ARG:HG2	2.05	0.54
1:I:128:ARG:CD	1:I:150:LYS:HB3	2.38	0.54
1:K:464:VAL:O	1:K:465:MET:HG2	2.07	0.54
1:M:183:SER:OG	1:M:244:TYR:OH	2.21	0.54
1:O:200:ASN:OD1	1:O:201:GLU:N	2.40	0.54
1:P:175:GLN:HA	1:P:178:GLU:OE1	2.07	0.54
1:I:148:ASP:O	1:I:152:LYS:N	2.36	0.54
1:J:222:LYS:HG3	1:J:223:HIS:CE1	2.42	0.54
1:M:316:LEU:HD21	1:M:352:LEU:HD21	1.90	0.54
1:B:147:TRP:NE1	1:B:149:ARG:HD3	2.22	0.54
1:C:161:ARG:HG3	1:C:162:ASN:H	1.72	0.54
1:G:349:LEU:HD21	1:G:386:GLN:CB	2.37	0.54
1:N:132:LEU:HD11	1:N:147:TRP:HB2	1.90	0.54
1:P:252:MET:HG2	1:P:322:TYR:HA	1.90	0.54
1:C:165:LYS:HD2	1:C:168:ARG:NH2	2.21	0.54
1:G:196:ARG:HH21	1:G:196:ARG:HG3	1.73	0.54
1:H:258:PRO:HD3	1:H:332:ILE:HG12	1.89	0.54
1:P:373:GLN:NE2	1:P:376:ARG:HD2	2.22	0.54
1:H:215:CYS:HA	1:H:262:LEU:HA	1.90	0.54
1:D:448:GLN:HG2	1:K:264:GLU:HG2	1.89	0.54
1:P:128:ARG:NH1	1:P:151:ARG:HD3	2.22	0.54
1:A:369:ARG:O	1:A:369:ARG:HG2	2.08	0.54
1:B:464:VAL:O	1:B:465:MET:HG2	2.08	0.54
1:C:192:MET:HG3	1:C:212:TYR:HE2	1.73	0.54
1:D:215:CYS:HA	1:D:262:LEU:HA	1.90	0.54
1:H:217:LEU:O	1:H:221:MET:HG2	2.08	0.54
1:G:148:ASP:OD2	1:G:151:ARG:CD	2.53	0.53
1:A:181:ARG:HD2	1:A:193:LYS:HD2	1.90	0.53
1:F:179:ARG:NH1	1:F:251:LEU:HD11	2.22	0.53
1:J:284:ARG:O	4:J:603:HOH:O	2.19	0.53
1:C:249:LEU:HB3	1:C:251:LEU:HD13	1.90	0.53
1:E:222:LYS:HG3	1:E:223:HIS:CE1	2.43	0.53
1:E:274:THR:HB	1:E:276:ARG:CZ	2.38	0.53
1:N:185:VAL:HG23	1:N:186:GLU:HG3	1.90	0.53
1:N:200:ASN:OD1	1:N:201:GLU:N	2.40	0.53
1:N:307:ARG:HH21	1:N:346:HIS:CD2	2.15	0.53
1:C:271:ASP:HB2	1:C:278:LEU:CD1	2.38	0.53
1:H:229:ARG:NH1	4:H:604:HOH:O	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:400:ALA:O	1:H:401:ARG:HD3	2.08	0.53
1:J:190:PRO:HG2	1:J:241:ALA:HB2	1.90	0.53
1:J:390:ASP:OD2	1:J:392:LYS:HD2	2.09	0.53
1:N:181:ARG:HG3	1:N:181:ARG:O	2.06	0.53
1:E:151:ARG:HH21	1:E:196:ARG:NH1	2.04	0.53
1:H:456:ARG:NH1	4:H:607:HOH:O	2.42	0.53
1:P:128:ARG:NH1	1:P:148:ASP:OD1	2.39	0.53
1:I:447:ARG:HA	1:I:452:HIS:CD2	2.43	0.53
1:L:187:ASP:OD1	1:L:193:LYS:CE	2.57	0.53
1:N:402:PRO:CD	1:N:405:GLU:HG3	2.39	0.53
1:O:316:LEU:CB	1:O:318:LEU:CD1	2.86	0.53
1:E:192:MET:HG2	1:E:288:CYS:HA	1.90	0.53
1:H:181:ARG:NH2	1:H:187:ASP:HA	2.23	0.53
1:H:320:TRP:O	1:H:321:MET:HG2	2.09	0.53
1:L:179:ARG:NH1	1:L:251:LEU:HD21	2.24	0.53
1:B:192:MET:HE2	1:B:288:CYS:HA	1.91	0.53
1:G:252:MET:HE3	1:G:320:TRP:HZ3	1.74	0.53
1:L:162:ASN:HB2	1:L:204:HIS:CD2	2.44	0.53
1:M:191:LEU:HD23	1:M:287:ILE:HB	1.89	0.53
1:P:222:LYS:HD3	1:P:223:HIS:NE2	2.23	0.53
1:C:242:LEU:HD21	1:C:256:LEU:HD11	1.91	0.53
1:J:160:VAL:HG12	1:J:166:TYR:HB3	1.91	0.53
1:N:442:TYR:O	4:N:604:HOH:O	2.19	0.53
1:B:307:ARG:NH1	1:B:348:ASN:OD1	2.41	0.53
1:F:165:LYS:HD2	1:F:168:ARG:NH2	2.23	0.53
1:F:202:THR:OG1	1:F:204:HIS:ND1	2.22	0.53
1:G:239:GLY:HA3	1:G:434:MET:HB3	1.89	0.53
1:I:258:PRO:HD3	1:I:332:ILE:HG12	1.90	0.53
1:J:175:GLN:NE2	1:K:296:GLU:OE2	2.37	0.53
1:O:128:ARG:HD3	1:O:129:PHE:CE2	2.44	0.53
1:J:238:VAL:HG13	1:J:287:ILE:HD11	1.91	0.52
1:L:259:GLU:N	1:L:259:GLU:OE1	2.39	0.52
1:M:316:LEU:HD12	1:M:375:ALA:HB1	1.90	0.52
1:A:464:VAL:O	1:A:465:MET:HG2	2.09	0.52
1:H:242:LEU:HD21	1:H:256:LEU:HD11	1.91	0.52
1:A:357:LYS:NZ	1:A:400:ALA:O	2.41	0.52
1:G:215:CYS:HA	1:G:262:LEU:HA	1.92	0.52
1:K:392:LYS:CD	1:K:392:LYS:H	2.22	0.52
1:N:390:ASP:O	1:N:394:ILE:HD12	2.10	0.52
1:D:307:ARG:HD2	1:D:346:HIS:HA	1.91	0.52
1:F:190:PRO:HG2	1:F:241:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:270:VAL:HG11	1:O:154:TYR:OH	2.10	0.52
1:J:161:ARG:NH1	1:J:163:VAL:HG13	2.24	0.52
1:P:129:PHE:CZ	1:P:208:VAL:HG21	2.44	0.52
1:A:185:VAL:HG23	1:A:186:GLU:CG	2.37	0.52
1:F:249:LEU:HB3	1:F:251:LEU:HD13	1.91	0.52
1:M:367:SER:HB3	1:M:379:PHE:CG	2.45	0.52
1:N:147:TRP:CD1	1:N:149:ARG:HD3	2.44	0.52
1:O:300:ARG:NH2	1:O:320:TRP:H	2.05	0.52
1:A:424:ARG:NH2	1:A:465:MET:HG3	2.24	0.52
1:H:196:ARG:HG2	1:H:197:TYR:H	1.74	0.52
1:I:147:TRP:CZ2	1:I:152:LYS:CD	2.93	0.52
1:L:183:SER:HB3	1:L:244:TYR:OH	2.09	0.52
1:C:444:PRO:O	1:C:447:ARG:HD2	2.09	0.52
1:E:238:VAL:HG13	1:E:287:ILE:HD11	1.92	0.52
1:M:163:VAL:HG23	1:M:166:TYR:HB2	1.91	0.52
1:N:215:CYS:HA	1:N:262:LEU:HA	1.91	0.52
1:D:393:HIS:O	1:D:397:ILE:HD12	2.09	0.52
1:G:135:LEU:HD12	1:G:143:VAL:HG12	1.92	0.52
1:H:147:TRP:HE1	1:H:149:ARG:NH1	1.90	0.52
1:I:130:LYS:HE2	1:I:149:ARG:NH2	2.24	0.52
1:K:151:ARG:NH1	1:K:153:GLU:OE1	2.43	0.52
1:M:404:ARG:HG3	1:M:405:GLU:HG2	1.92	0.52
1:F:464:VAL:O	1:F:465:MET:HG2	2.09	0.52
1:I:252:MET:HG2	1:I:322:TYR:HA	1.91	0.52
1:F:161:ARG:CG	1:F:162:ASN:H	2.19	0.52
1:I:257:LYS:HE3	1:I:259:GLU:HB2	1.92	0.52
1:J:188:ARG:HH22	1:N:186:GLU:CD	2.14	0.52
1:M:190:PRO:HG3	1:M:237:GLN:HB3	1.92	0.52
1:O:128:ARG:HE	1:O:150:LYS:HB2	1.75	0.52
1:B:404:ARG:HH21	1:D:404:ARG:HD3	1.75	0.51
1:O:167:THR:HG22	1:O:205:MET:HG2	1.92	0.51
1:E:395:ALA:O	1:E:399:ARG:HG3	2.10	0.51
1:G:440:HIS:HB3	1:G:447:ARG:HH21	1.75	0.51
1:H:412:LEU:HD13	1:H:438:TYR:CZ	2.46	0.51
1:I:423:ASP:HB3	1:I:426:ARG:HB2	1.92	0.51
1:J:175:GLN:HE22	1:K:296:GLU:CD	2.13	0.51
1:J:310:ARG:NH1	4:J:607:HOH:O	2.33	0.51
1:L:193:LYS:HD3	1:L:193:LYS:NZ	2.22	0.51
1:C:164:PRO:HG2	1:L:377:ASP:HB3	1.92	0.51
1:A:393:HIS:O	1:A:397:ILE:HG13	2.10	0.51
1:B:365:ASP:OD1	1:B:365:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:THR:HB	1:E:204:HIS:ND1	2.26	0.51
1:F:362:LEU:HB3	1:F:366:TRP:CE3	2.45	0.51
1:G:181:ARG:HD3	1:G:194:ILE:O	2.10	0.51
1:I:464:VAL:O	1:I:465:MET:HG2	2.10	0.51
1:J:156:ALA:O	1:J:209:MET:N	2.40	0.51
1:K:238:VAL:HG13	1:K:287:ILE:HD11	1.91	0.51
1:L:140:PHE:CD2	1:L:158:LYS:HD2	2.45	0.51
1:P:128:ARG:NE	1:P:148:ASP:OD1	2.38	0.51
1:P:237:GLN:NE2	1:P:283:CYS:O	2.37	0.51
1:A:392:LYS:N	1:A:392:LYS:HD3	2.24	0.51
1:C:179:ARG:NH1	1:C:251:LEU:HD11	2.25	0.51
1:D:412:LEU:HD13	1:D:438:TYR:CZ	2.45	0.51
1:F:161:ARG:CD	1:F:162:ASN:H	2.22	0.51
1:F:161:ARG:HB3	1:F:166:TYR:HD2	1.76	0.51
1:F:357:LYS:NZ	1:F:400:ALA:O	2.43	0.51
1:F:447:ARG:HA	1:F:452:HIS:CD2	2.45	0.51
1:I:380:THR:HG22	1:I:384:THR:O	2.10	0.51
1:O:415:LEU:HD12	1:O:438:TYR:HB3	1.93	0.51
1:P:316:LEU:CB	1:P:318:LEU:HD23	2.41	0.51
1:A:151:ARG:O	1:A:152:LYS:HG2	2.11	0.51
1:E:264:GLU:HG2	1:P:448:GLN:HG2	1.92	0.51
1:F:130:LYS:HG2	1:F:131:ILE:H	1.73	0.51
1:H:191:LEU:HD23	1:H:287:ILE:HB	1.93	0.51
1:A:258:PRO:HD3	1:A:332:ILE:HG12	1.92	0.51
1:B:258:PRO:HD3	1:B:332:ILE:HG12	1.91	0.51
1:N:358:THR:HA	1:N:402:PRO:HA	1.91	0.51
1:P:374:GLU:HA	4:P:607:HOH:O	2.11	0.51
1:A:412:LEU:HD13	1:A:438:TYR:CZ	2.45	0.51
1:B:353:HIS:HB3	1:B:397:ILE:HD13	1.92	0.51
1:D:464:VAL:O	1:D:465:MET:HG2	2.11	0.51
1:E:130:LYS:HE2	4:E:637:HOH:O	2.11	0.51
1:G:326:LEU:HD23	1:G:429:ASN:HA	1.93	0.51
1:C:273:MET:HE1	1:H:272:PRO:HB2	1.92	0.51
1:I:149:ARG:O	1:I:152:LYS:HE2	2.11	0.51
1:J:447:ARG:HA	1:J:452:HIS:CD2	2.45	0.51
1:N:148:ASP:OD2	1:N:151:ARG:CG	2.56	0.51
1:O:147:TRP:CZ2	1:O:152:LYS:HA	2.45	0.51
1:P:373:GLN:OE1	1:P:376:ARG:HD2	2.11	0.51
1:B:357:LYS:CE	1:D:361:ARG:NH1	2.65	0.51
1:G:258:PRO:HD3	1:G:332:ILE:HG12	1.92	0.51
1:G:424:ARG:NH2	1:G:465:MET:HG3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:193:LYS:HD3	1:L:193:LYS:HZ3	1.76	0.51
1:N:133:SER:OG	1:N:145:GLU:HB3	2.11	0.51
1:G:174:ILE:O	1:G:178:GLU:OE1	2.29	0.51
1:N:402:PRO:HD2	1:N:405:GLU:HG3	1.92	0.51
1:O:249:LEU:O	4:O:602:HOH:O	2.19	0.51
1:O:363:PRO:HD2	1:O:366:TRP:CD2	2.45	0.51
1:O:447:ARG:HA	1:O:452:HIS:CD2	2.46	0.51
1:F:361:ARG:HH12	1:M:361:ARG:HB2	1.75	0.50
1:H:460:PRO:HB3	1:O:182:LEU:HD13	1.93	0.50
1:P:298:HIS:CE1	1:P:300:ARG:NH2	2.79	0.50
1:G:217:LEU:HD12	1:G:220:ILE:HD11	1.92	0.50
1:M:162:ASN:ND2	1:M:162:ASN:C	2.64	0.50
1:O:190:PRO:HG3	1:O:237:GLN:HB3	1.93	0.50
1:K:151:ARG:HB2	1:K:153:GLU:CD	2.25	0.50
1:L:373:GLN:HG2	1:L:374:GLU:N	2.25	0.50
1:M:464:VAL:O	1:M:465:MET:HG2	2.12	0.50
1:N:313:GLU:CD	1:N:424:ARG:HG2	2.31	0.50
1:N:380:THR:HG22	1:N:382:ALA:H	1.75	0.50
1:P:181:ARG:CZ	1:P:193:LYS:CE	2.90	0.50
1:D:185:VAL:HG23	1:D:186:GLU:CG	2.41	0.50
1:E:183:SER:O	4:E:602:HOH:O	2.18	0.50
1:O:464:VAL:O	1:O:465:MET:HG2	2.11	0.50
1:G:257:LYS:HD2	1:G:259:GLU:OE2	2.12	0.50
1:I:395:ALA:O	1:I:399:ARG:HG3	2.12	0.50
1:K:441:LYS:HG2	1:K:442:TYR:CD2	2.46	0.50
1:M:362:LEU:HD12	1:M:385:LEU:HD11	1.93	0.50
1:N:251:LEU:HD23	1:N:295:ASP:HB3	1.94	0.50
1:P:196:ARG:CG	1:P:197:TYR:N	2.74	0.50
1:E:259:GLU:OE1	1:E:259:GLU:N	2.43	0.50
1:I:161:ARG:HG3	1:I:162:ASN:N	2.27	0.50
1:A:187:ASP:OD2	1:A:193:LYS:HG3	2.12	0.50
1:E:307:ARG:NE	2:E:501:SO4:O2	2.29	0.50
1:G:200:ASN:OD1	1:G:202:THR:HG22	2.12	0.50
1:G:357:LYS:HE2	1:G:401:ARG:HH11	1.76	0.50
1:M:187:ASP:OD1	1:M:193:LYS:NZ	2.44	0.50
1:O:412:LEU:HD13	1:O:438:TYR:CZ	2.47	0.50
1:E:217:LEU:HD22	1:E:259:GLU:HG3	1.94	0.49
1:I:350:GLU:OE2	1:I:396:ARG:HD2	2.11	0.49
1:I:362:LEU:HB3	1:I:366:TRP:CE3	2.47	0.49
1:P:377:ASP:N	4:P:601:HOH:O	2.44	0.49
1:M:187:ASP:HA	1:M:193:LYS:HZ3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:217:LEU:HD22	1:M:259:GLU:HG3	1.94	0.49
1:O:128:ARG:CZ	1:O:148:ASP:OD1	2.60	0.49
1:O:128:ARG:HG3	1:O:150:LYS:NZ	2.27	0.49
1:B:128:ARG:HH12	1:B:196:ARG:NH2	2.10	0.49
1:B:274:THR:HB	1:B:276:ARG:CZ	2.42	0.49
1:B:440:HIS:CD2	1:B:447:ARG:NE	2.80	0.49
1:E:366:TRP:CD1	1:E:369:ARG:NH2	2.80	0.49
1:I:162:ASN:HB2	1:I:204:HIS:CE1	2.47	0.49
1:I:192:MET:HG2	1:I:193:LYS:H	1.77	0.49
1:N:131:ILE:HG23	1:N:144:VAL:HG21	1.95	0.49
1:P:362:LEU:HD11	1:P:385:LEU:HD11	1.93	0.49
1:B:418:ASN:HB3	1:B:428:LEU:HG	1.93	0.49
1:E:190:PRO:HG2	1:E:241:ALA:HB2	1.94	0.49
1:I:273:MET:HG3	1:M:273:MET:HG2	1.94	0.49
1:N:327:TRP:CD2	1:N:420:LEU:HD23	2.47	0.49
1:O:316:LEU:HB2	1:O:318:LEU:HD13	1.95	0.49
1:P:464:VAL:O	1:P:465:MET:HG2	2.12	0.49
1:A:215:CYS:HA	1:A:262:LEU:HA	1.94	0.49
1:C:148:ASP:OD2	1:C:151:ARG:HB2	2.12	0.49
1:N:192:MET:HE2	1:N:288:CYS:HA	1.94	0.49
1:O:370:CYS:HB3	1:O:375:ALA:HB3	1.93	0.49
1:B:238:VAL:HG13	1:B:287:ILE:HD11	1.94	0.49
1:B:428:LEU:HD22	1:B:432:GLN:HB3	1.94	0.49
1:C:273:MET:CE	1:H:272:PRO:HB2	2.43	0.49
1:E:258:PRO:HD3	1:E:332:ILE:HG12	1.94	0.49
1:F:167:THR:HG23	1:F:205:MET:HG2	1.93	0.49
1:N:380:THR:N	1:N:384:THR:O	2.34	0.49
1:P:380:THR:HG23	1:P:383:GLY:N	2.14	0.49
1:E:151:ARG:HE	1:E:196:ARG:NH2	2.10	0.49
1:J:271:ASP:OD2	1:J:274:THR:HG23	2.12	0.49
1:J:380:THR:HG22	1:J:386:GLN:OE1	2.12	0.49
1:A:238:VAL:HG13	1:A:287:ILE:HD11	1.93	0.49
1:B:391:PRO:HD2	1:B:392:LYS:NZ	2.28	0.49
1:F:151:ARG:O	1:F:153:GLU:HG2	2.13	0.49
1:G:270:VAL:HG11	1:K:154:TYR:OH	2.12	0.49
1:H:233:GLN:O	1:H:237:GLN:HG3	2.13	0.49
1:O:148:ASP:OD2	1:O:151:ARG:HB2	2.12	0.49
1:O:177:MET:HE1	1:O:207:ILE:HD13	1.95	0.49
1:A:323:SER:OG	1:A:427:ARG:HD2	2.13	0.49
1:G:365:ASP:O	1:G:368:VAL:HG22	2.12	0.49
1:K:151:ARG:CD	1:K:153:GLU:OE2	2.57	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:217:LEU:HD22	1:O:259:GLU:HG3	1.93	0.49
1:O:323:SER:OG	1:O:427:ARG:NH1	2.46	0.49
1:D:307:ARG:CD	1:D:346:HIS:HA	2.43	0.49
1:G:388:CYS:O	1:G:394:ILE:HD11	2.12	0.49
1:B:379:PHE:CE2	1:B:385:LEU:HD13	2.48	0.48
1:C:298:HIS:HE1	1:C:300:ARG:CZ	2.22	0.48
1:G:164:PRO:HA	1:G:167:THR:OG1	2.13	0.48
1:G:464:VAL:O	1:G:465:MET:HG2	2.12	0.48
1:P:260:ASN:HB3	1:P:289:ASP:OD2	2.13	0.48
1:A:192:MET:HE2	1:A:209:MET:SD	2.53	0.48
1:D:356:GLU:HA	1:D:360:GLY:O	2.13	0.48
1:G:177:MET:HG2	1:G:192:MET:HE1	1.95	0.48
1:H:181:ARG:CZ	1:H:193:LYS:HD2	2.43	0.48
1:L:363:PRO:HD2	1:L:366:TRP:CE2	2.48	0.48
1:B:356:GLU:HA	1:B:360:GLY:O	2.13	0.48
1:C:161:ARG:HG3	1:C:162:ASN:N	2.28	0.48
1:C:194:ILE:HA	1:C:209:MET:HG2	1.94	0.48
1:C:464:VAL:O	1:C:465:MET:HG2	2.13	0.48
1:F:313:GLU:HA	1:F:318:LEU:HD12	1.95	0.48
1:H:147:TRP:HD1	1:H:149:ARG:HD3	1.78	0.48
1:M:372:THR:HG23	1:M:375:ALA:H	1.78	0.48
1:I:190:PRO:HG2	1:I:241:ALA:HB2	1.95	0.48
1:K:258:PRO:HD3	1:K:332:ILE:HG12	1.94	0.48
1:M:215:CYS:HA	1:M:262:LEU:HA	1.95	0.48
1:M:258:PRO:HD3	1:M:332:ILE:HG12	1.94	0.48
1:C:160:VAL:HG12	1:C:166:TYR:HB3	1.94	0.48
1:C:252:MET:HE1	1:C:321:MET:SD	2.53	0.48
1:E:366:TRP:HD1	1:E:369:ARG:NH2	2.11	0.48
1:I:353:HIS:O	1:I:357:LYS:HG2	2.13	0.48
1:K:162:ASN:ND2	1:K:202:THR:O	2.45	0.48
1:K:190:PRO:HG2	1:K:241:ALA:HB2	1.95	0.48
1:O:353:HIS:CB	1:O:397:ILE:CD1	2.90	0.48
1:C:357:LYS:NZ	1:C:400:ALA:O	2.47	0.48
1:G:260:ASN:HB2	1:G:289:ASP:HB2	1.95	0.48
1:M:175:GLN:HA	1:M:178:GLU:OE1	2.12	0.48
1:C:274:THR:HB	1:C:276:ARG:NE	2.29	0.48
1:C:317:SER:O	1:C:371:GLY:HA3	2.13	0.48
1:I:257:LYS:HB2	1:I:259:GLU:OE1	2.14	0.48
1:I:347:ASP:HB3	1:I:350:GLU:HB3	1.95	0.48
1:K:390:ASP:OD2	1:K:392:LYS:HD3	2.13	0.48
1:N:464:VAL:O	1:N:465:MET:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:307:ARG:HD2	1:O:346:HIS:HA	1.96	0.48
1:P:249:LEU:HA	4:P:606:HOH:O	2.13	0.48
1:N:147:TRP:HZ2	1:N:152:LYS:HG3	1.77	0.48
1:N:239:GLY:HA3	1:N:434:MET:HB3	1.95	0.48
1:C:271:ASP:OD2	1:C:274:THR:HG23	2.14	0.48
1:E:353:HIS:HB3	1:E:397:ILE:HD13	1.95	0.48
1:J:184:ASP:O	1:J:193:LYS:NZ	2.47	0.48
1:J:362:LEU:HB3	1:J:366:TRP:CE3	2.48	0.48
1:K:192:MET:HB2	1:K:288:CYS:SG	2.54	0.48
1:C:314:VAL:HG22	1:C:320:TRP:CG	2.48	0.48
1:G:402:PRO:HB2	1:G:405:GLU:HB2	1.95	0.48
1:O:380:THR:HB	1:O:383:GLY:H	1.79	0.48
1:C:161:ARG:HG2	1:C:163:VAL:HG23	1.96	0.47
1:D:162:ASN:HB2	1:D:204:HIS:CD2	2.48	0.47
1:F:179:ARG:CZ	1:F:251:LEU:HD11	2.44	0.47
1:H:181:ARG:NH2	1:H:193:LYS:CE	2.77	0.47
1:K:150:LYS:HG2	1:K:150:LYS:O	2.12	0.47
1:P:318:LEU:HD12	1:P:369:ARG:HH22	1.74	0.47
1:C:130:LYS:HE3	1:C:131:ILE:O	2.14	0.47
1:O:181:ARG:NH1	1:O:193:LYS:CB	2.71	0.47
1:P:176:PHE:O	1:P:180:VAL:HG23	2.14	0.47
1:P:307:ARG:HD2	1:P:346:HIS:HA	1.96	0.47
1:F:238:VAL:HG11	1:F:329:MET:SD	2.54	0.47
1:I:137:GLU:HG2	1:I:138:GLY:N	2.30	0.47
1:J:145:GLU:OE2	1:J:211:LYS:HE3	2.14	0.47
1:P:298:HIS:HE1	1:P:300:ARG:NH2	2.12	0.47
1:C:190:PRO:HG2	1:C:241:ALA:HB2	1.95	0.47
1:C:193:LYS:O	1:C:210:PRO:HD3	2.15	0.47
1:F:367:SER:O	1:F:376:ARG:HD2	2.14	0.47
1:I:363:PRO:HD2	1:I:366:TRP:CE2	2.50	0.47
1:I:376:ARG:HH22	1:I:381:ALA:HA	1.79	0.47
1:A:218:ASP:OD1	3:A:501:5XH:N1	2.47	0.47
1:B:362:LEU:HD22	1:B:366:TRP:CZ3	2.49	0.47
1:B:447:ARG:HA	1:B:452:HIS:CD2	2.49	0.47
1:G:326:LEU:HD23	4:G:603:HOH:O	2.15	0.47
1:I:308:HIS:ND1	1:I:343:TYR:O	2.47	0.47
1:M:323:SER:OG	1:M:427:ARG:NH1	2.47	0.47
1:N:425:GLN:OE1	1:N:464:VAL:HG13	2.14	0.47
1:O:162:ASN:OD1	1:O:204:HIS:N	2.47	0.47
1:B:175:GLN:HE22	1:E:296:GLU:CD	2.17	0.47
1:K:306:THR:HG23	1:K:309:TYR:HD2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:192:MET:HE3	1:M:290:LEU:HG	1.95	0.47
1:M:362:LEU:CD1	1:M:385:LEU:HD11	2.45	0.47
1:A:249:LEU:O	4:A:605:HOH:O	2.20	0.47
1:B:160:VAL:HG12	1:B:166:TYR:HB3	1.96	0.47
1:C:373:GLN:HG3	4:C:623:HOH:O	2.15	0.47
1:C:413:CYS:SG	1:C:417:LEU:HD12	2.55	0.47
1:E:222:LYS:HG2	1:E:223:HIS:CE1	2.48	0.47
1:E:316:LEU:HB3	1:E:370:CYS:SG	2.54	0.47
1:G:191:LEU:HD23	1:G:287:ILE:HB	1.97	0.47
1:H:353:HIS:CB	1:H:397:ILE:CD1	2.90	0.47
1:N:361:ARG:HD3	1:N:361:ARG:HA	1.30	0.47
1:O:160:VAL:CG1	1:O:205:MET:HB2	2.45	0.47
1:D:173:GLU:HG3	1:D:291:GLY:N	2.29	0.47
1:D:328:SER:O	1:D:332:ILE:HG13	2.15	0.47
1:O:298:HIS:CE1	1:O:300:ARG:NH2	2.82	0.47
1:O:350:GLU:CD	1:O:396:ARG:HH11	2.04	0.47
1:I:242:LEU:HD21	1:I:256:LEU:HD11	1.95	0.47
1:M:361:ARG:HG3	1:M:362:LEU:O	2.13	0.47
1:M:188:ARG:NH2	2:M:500:SO4:O2	2.45	0.47
1:E:151:ARG:HH21	1:E:196:ARG:CZ	2.28	0.47
1:F:376:ARG:NH1	1:F:376:ARG:HG3	2.24	0.47
1:N:180:VAL:HG12	1:N:193:LYS:HZ3	1.80	0.47
1:D:297:ARG:HH11	1:N:299:SER:HB2	1.80	0.47
1:O:181:ARG:HG3	1:O:193:LYS:HD2	1.97	0.47
1:C:217:LEU:HD22	1:C:259:GLU:HG3	1.95	0.47
1:E:316:LEU:HD21	1:E:352:LEU:HD11	1.97	0.47
1:K:257:LYS:HZ2	1:K:259:GLU:CB	2.27	0.47
1:A:353:HIS:CB	1:A:397:ILE:HD13	2.45	0.46
1:D:273:MET:HA	1:K:273:MET:SD	2.56	0.46
1:H:239:GLY:HA3	1:H:434:MET:HB3	1.97	0.46
1:I:272:PRO:HB2	1:M:273:MET:SD	2.56	0.46
1:A:191:LEU:HD23	1:A:287:ILE:HB	1.97	0.46
1:B:392:LYS:N	1:B:392:LYS:HD3	2.30	0.46
1:D:200:ASN:ND2	1:D:202:THR:HG22	2.31	0.46
1:H:243:ASP:OD2	1:H:431:ARG:HB2	2.14	0.46
1:J:385:LEU:HD23	1:J:385:LEU:HA	1.74	0.46
1:L:318:LEU:HD23	1:L:370:CYS:HA	1.96	0.46
1:M:390:ASP:O	1:M:394:ILE:HD12	2.14	0.46
1:M:412:LEU:HD13	1:M:438:TYR:CZ	2.50	0.46
1:P:202:THR:HG23	1:P:204:HIS:ND1	2.30	0.46
1:E:350:GLU:OE2	1:E:396:ARG:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:376:ARG:HD3	1:G:376:ARG:C	2.35	0.46
1:H:147:TRP:CH2	1:H:152:LYS:HG3	2.50	0.46
1:H:148:ASP:OD2	1:H:151:ARG:HG3	2.15	0.46
1:F:369:ARG:NH1	4:F:606:HOH:O	2.39	0.46
1:G:390:ASP:OD1	1:G:392:LYS:HB2	2.14	0.46
1:H:348:ASN:HB3	1:H:378:LEU:HD21	1.96	0.46
1:K:447:ARG:HA	1:K:452:HIS:CD2	2.49	0.46
1:C:191:LEU:HD23	1:C:287:ILE:HB	1.98	0.46
1:C:307:ARG:NH1	1:C:348:ASN:OD1	2.47	0.46
1:D:185:VAL:HG23	1:D:186:GLU:HG3	1.97	0.46
1:L:195:GLN:HG2	1:L:209:MET:HA	1.97	0.46
1:M:192:MET:HE2	1:M:290:LEU:HG	1.97	0.46
1:N:191:LEU:HD23	1:N:287:ILE:HB	1.97	0.46
1:P:412:LEU:HD13	1:P:438:TYR:CZ	2.51	0.46
1:C:425:GLN:HG2	1:C:465:MET:HB3	1.98	0.46
1:E:346:HIS:NE2	2:E:501:SO4:S	2.89	0.46
1:H:187:ASP:OD1	1:H:193:LYS:NZ	2.49	0.46
1:K:147:TRP:HE3	1:K:154:TYR:CD1	2.34	0.46
1:K:257:LYS:HG3	1:K:259:GLU:N	2.26	0.46
1:N:217:LEU:HD22	1:N:259:GLU:HG3	1.98	0.46
1:O:356:GLU:HA	1:O:360:GLY:O	2.15	0.46
1:P:128:ARG:HG3	1:P:150:LYS:HG2	1.98	0.46
1:A:313:GLU:OE2	1:A:427:ARG:NH1	2.46	0.46
1:C:300:ARG:NH1	1:C:320:TRP:H	2.12	0.46
1:I:238:VAL:HG11	1:I:329:MET:SD	2.56	0.46
1:L:137:GLU:HG3	1:L:142:LYS:CG	2.45	0.46
1:L:137:GLU:HG3	1:L:142:LYS:HG2	1.96	0.46
1:M:362:LEU:HD23	1:M:422:TYR:CZ	2.51	0.46
1:P:373:GLN:HA	1:P:376:ARG:CD	2.45	0.46
1:P:447:ARG:HA	1:P:452:HIS:CD2	2.50	0.46
1:A:128:ARG:HD3	1:A:129:PHE:CE2	2.51	0.46
1:A:174:ILE:CG2	1:A:178:GLU:OE2	2.52	0.46
1:A:227:ASN:HB2	4:A:624:HOH:O	2.15	0.46
1:A:369:ARG:HG2	4:A:602:HOH:O	2.15	0.46
1:E:333:ILE:HG22	1:E:416:ILE:HD11	1.98	0.46
1:A:404:ARG:HA	1:A:413:CYS:SG	2.56	0.46
1:H:132:LEU:HD11	1:H:147:TRP:HB2	1.97	0.46
1:J:409:GLU:OE2	1:J:411:LEU:N	2.49	0.46
1:L:153:GLU:OE2	1:L:153:GLU:N	2.49	0.46
1:L:464:VAL:N	4:L:616:HOH:O	2.45	0.46
1:M:456:ARG:NH1	4:M:613:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:181:ARG:CD	1:P:193:LYS:HD3	2.43	0.46
1:B:222:LYS:HD2	1:B:223:HIS:CE1	2.51	0.46
1:B:363:PRO:HB2	1:B:365:ASP:OD1	2.16	0.46
1:C:313:GLU:HG3	1:C:320:TRP:HB3	1.98	0.46
1:C:175:GLN:NE2	1:F:296:GLU:OE2	2.43	0.46
1:H:464:VAL:O	1:H:465:MET:HG2	2.16	0.46
1:J:424:ARG:NH2	1:J:465:MET:HG3	2.31	0.46
1:M:135:LEU:HD11	1:M:145:GLU:HB2	1.97	0.46
1:O:396:ARG:CZ	1:O:396:ARG:HB2	2.46	0.46
1:B:395:ALA:O	1:B:399:ARG:HG2	2.16	0.45
1:C:184:ASP:O	1:C:193:LYS:NZ	2.49	0.45
1:E:192:MET:HE1	1:E:209:MET:HG2	1.98	0.45
1:G:354:LEU:HA	1:G:354:LEU:HD23	1.47	0.45
1:I:147:TRP:HZ2	1:I:152:LYS:HD2	1.81	0.45
1:C:192:MET:HG3	1:C:212:TYR:CE2	2.51	0.45
1:G:163:VAL:HG13	1:G:166:TYR:HB2	1.98	0.45
1:I:128:ARG:CZ	1:I:150:LYS:HB3	2.44	0.45
1:K:257:LYS:HG2	1:K:260:ASN:H	1.80	0.45
1:O:239:GLY:HA3	1:O:434:MET:HB3	1.98	0.45
1:B:190:PRO:HG2	1:B:241:ALA:HB2	1.96	0.45
1:B:257:LYS:HD2	1:B:259:GLU:OE2	2.16	0.45
1:G:188:ARG:NH2	2:G:500:SO4:O4	2.44	0.45
1:J:192:MET:HB2	1:J:288:CYS:SG	2.56	0.45
1:C:192:MET:HE1	1:C:209:MET:SD	2.57	0.45
1:C:363:PRO:HD2	1:C:366:TRP:CD2	2.51	0.45
1:I:168:ARG:HG3	4:I:615:HOH:O	2.15	0.45
1:M:401:ARG:HD2	1:M:402:PRO:HD3	1.99	0.45
1:N:181:ARG:NE	1:N:193:LYS:HB3	2.32	0.45
1:N:191:LEU:HG	1:N:241:ALA:HB1	1.98	0.45
1:H:182:LEU:HD13	1:O:460:PRO:HA	1.99	0.45
1:A:228:HIS:HB3	1:A:442:TYR:CG	2.51	0.45
1:B:399:ARG:HD2	1:B:399:ARG:HA	1.45	0.45
1:C:190:PRO:HG3	1:C:237:GLN:HB3	1.99	0.45
1:C:447:ARG:HA	1:C:452:HIS:CD2	2.51	0.45
1:D:181:ARG:HD2	1:D:181:ARG:HH11	1.32	0.45
1:E:161:ARG:HG3	1:E:162:ASN:N	2.31	0.45
1:F:316:LEU:HD21	1:F:352:LEU:HD11	1.97	0.45
1:G:181:ARG:HA	1:G:193:LYS:HE2	1.97	0.45
1:H:168:ARG:HH11	1:H:168:ARG:HD3	1.47	0.45
1:L:242:LEU:HD21	1:L:256:LEU:HD11	1.99	0.45
1:O:404:ARG:HB3	1:O:404:ARG:CZ	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ARG:HE	1:A:148:ASP:CG	2.20	0.45
1:D:242:LEU:HD21	1:D:256:LEU:HD11	1.99	0.45
1:E:353:HIS:CB	1:E:397:ILE:HD13	2.47	0.45
1:G:358:THR:HB	1:G:403:VAL:HG23	1.98	0.45
1:I:367:SER:HB3	1:I:379:PHE:CD2	2.52	0.45
1:J:296:GLU:CD	1:K:175:GLN:HE22	2.20	0.45
1:O:128:ARG:NE	1:O:150:LYS:HB2	2.32	0.45
1:C:192:MET:SD	1:C:193:LYS:N	2.90	0.45
1:F:166:TYR:CD1	1:F:166:TYR:N	2.85	0.45
1:G:403:VAL:HB	1:G:417:LEU:HD21	1.99	0.45
1:G:423:ASP:OD1	1:G:425:GLN:N	2.50	0.45
1:M:152:LYS:HE3	1:M:152:LYS:HB3	1.64	0.45
1:P:181:ARG:NH1	1:P:187:ASP:N	2.65	0.45
1:A:217:LEU:HD12	1:A:220:ILE:HD11	1.98	0.45
1:B:296:GLU:OE2	1:E:175:GLN:NE2	2.48	0.45
1:B:376:ARG:HD3	1:B:376:ARG:O	2.17	0.45
1:B:390:ASP:CG	1:B:392:LYS:HE2	2.36	0.45
1:F:229:ARG:NH2	1:O:281:GLU:O	2.49	0.45
1:F:257:LYS:HB2	1:F:259:GLU:OE1	2.16	0.45
1:I:423:ASP:CG	1:I:426:ARG:HG3	2.37	0.45
1:M:273:MET:HB3	1:M:273:MET:HE3	1.87	0.45
1:N:389:LYS:HA	1:N:394:ILE:HD11	1.99	0.45
1:O:128:ARG:HD2	1:O:150:LYS:HZ3	1.81	0.45
1:O:372:THR:O	1:O:376:ARG:HD3	2.17	0.45
1:O:398:ALA:O	1:O:401:ARG:NH2	2.50	0.45
1:D:202:THR:HG23	1:D:204:HIS:ND1	2.32	0.45
1:G:178:GLU:OE1	1:G:178:GLU:N	2.47	0.45
1:H:162:ASN:HB2	1:H:204:HIS:CD2	2.51	0.45
1:H:447:ARG:O	1:H:455:ASN:ND2	2.50	0.45
1:I:464:VAL:N	4:I:610:HOH:O	2.48	0.45
1:M:316:LEU:HB3	1:M:370:CYS:SG	2.56	0.45
1:N:178:GLU:HG2	1:N:194:ILE:HG21	1.98	0.45
1:O:402:PRO:O	1:O:405:GLU:HB2	2.17	0.45
1:P:318:LEU:O	4:P:603:HOH:O	2.21	0.45
1:A:301:THR:HG22	1:A:317:SER:HB3	1.98	0.45
1:A:447:ARG:HA	1:A:452:HIS:CD2	2.52	0.45
1:L:408:THR:OG1	4:L:602:HOH:O	2.14	0.45
1:N:162:ASN:OD1	1:N:203:GLY:C	2.55	0.45
1:N:373:GLN:O	1:N:373:GLN:HG3	2.15	0.45
1:N:412:LEU:HD13	1:N:438:TYR:CZ	2.52	0.45
1:O:271:ASP:HB2	1:O:278:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:404:ARG:HH11	1:O:404:ARG:HB2	1.81	0.45
1:P:211:LYS:NZ	4:P:605:HOH:O	2.40	0.45
1:F:380:THR:HG22	1:F:381:ALA:N	2.32	0.44
1:J:362:LEU:HD22	1:J:366:TRP:CZ3	2.53	0.44
1:D:229:ARG:NH2	1:K:281:GLU:O	2.50	0.44
1:O:160:VAL:HG12	1:O:205:MET:HB2	1.99	0.44
1:O:237:GLN:NE2	1:O:283:CYS:O	2.39	0.44
1:O:297:ARG:HB2	1:O:297:ARG:HE	1.21	0.44
1:C:188:ARG:HB3	1:C:188:ARG:HE	1.34	0.44
1:D:363:PRO:HD2	1:D:366:TRP:CD2	2.52	0.44
1:G:368:VAL:HG23	1:G:369:ARG:HG3	1.98	0.44
1:H:395:ALA:O	1:H:399:ARG:HG2	2.17	0.44
1:J:353:HIS:HB3	1:J:397:ILE:HD13	1.99	0.44
1:L:390:ASP:C	1:L:394:ILE:CD1	2.85	0.44
1:M:168:ARG:HD2	1:M:168:ARG:HA	1.55	0.44
1:N:390:ASP:HB3	1:N:393:HIS:H	1.82	0.44
1:P:151:ARG:HB2	1:P:153:GLU:OE1	2.17	0.44
1:P:281:GLU:OE2	1:P:282:PRO:HA	2.16	0.44
1:A:195:GLN:O	1:A:196:ARG:HG3	2.17	0.44
1:E:346:HIS:NE2	2:E:501:SO4:O3	2.49	0.44
1:F:307:ARG:NH1	1:F:348:ASN:OD1	2.51	0.44
1:F:354:LEU:O	1:F:358:THR:HG23	2.17	0.44
1:H:181:ARG:HB2	1:H:193:LYS:CD	2.40	0.44
1:L:313:GLU:HA	1:L:318:LEU:HD12	1.99	0.44
1:B:162:ASN:OD1	1:B:202:THR:O	2.34	0.44
1:C:376:ARG:HH22	1:C:381:ALA:HA	1.83	0.44
1:H:258:PRO:HG3	1:H:332:ILE:HG23	2.00	0.44
1:I:192:MET:HB2	1:I:288:CYS:SG	2.58	0.44
1:N:316:LEU:CB	1:N:318:LEU:HD23	2.47	0.44
1:B:345:THR:O	1:B:346:HIS:HD2	2.00	0.44
1:I:179:ARG:HH12	1:I:251:LEU:HD21	1.81	0.44
1:K:147:TRP:CE3	1:K:154:TYR:CE1	3.06	0.44
1:N:258:PRO:HD3	1:N:332:ILE:HG12	1.99	0.44
1:O:456:ARG:NH1	4:O:608:HOH:O	2.51	0.44
1:G:196:ARG:HG3	1:G:196:ARG:NH2	2.33	0.44
1:G:447:ARG:HA	1:G:452:HIS:CD2	2.53	0.44
1:M:239:GLY:HA3	1:M:434:MET:HB3	1.99	0.44
1:N:162:ASN:ND2	1:N:162:ASN:C	2.71	0.44
1:N:352:LEU:CD1	1:N:378:LEU:HD23	2.48	0.44
1:P:151:ARG:O	1:P:152:LYS:HB2	2.17	0.44
1:P:357:LYS:HA	4:P:608:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:VAL:HG12	1:A:316:LEU:HD13	2.00	0.44
1:F:404:ARG:HG3	1:F:404:ARG:H	1.60	0.44
1:G:252:MET:CG	1:G:322:TYR:HA	2.48	0.44
1:G:345:THR:HG22	1:G:347:ASP:H	1.82	0.44
1:M:179:ARG:HD2	1:M:179:ARG:HH11	1.68	0.44
1:N:346:HIS:CG	1:N:346:HIS:O	2.70	0.44
1:I:239:GLY:HA3	1:I:434:MET:HB3	1.98	0.44
1:J:188:ARG:NH2	1:N:186:GLU:CD	2.70	0.44
1:K:391:PRO:HD2	1:K:392:LYS:NZ	2.33	0.44
1:L:449:HIS:NE2	2:L:501:SO4:O2	2.51	0.44
1:M:179:ARG:CZ	4:M:601:HOH:O	2.66	0.44
1:N:260:ASN:HB2	1:N:289:ASP:HB2	1.99	0.44
1:P:191:LEU:HD23	1:P:287:ILE:HB	2.00	0.44
1:P:373:GLN:O	1:P:376:ARG:HG2	2.18	0.44
1:A:192:MET:HE1	1:A:209:MET:SD	2.56	0.44
1:A:361:ARG:H	1:A:361:ARG:NE	2.16	0.44
1:F:257:LYS:HD2	1:F:259:GLU:OE1	2.17	0.44
1:H:163:VAL:CG2	1:H:166:TYR:CD2	2.99	0.44
1:I:128:ARG:HH12	1:I:196:ARG:CZ	2.31	0.44
1:I:391:PRO:HD2	1:I:392:LYS:NZ	2.33	0.44
1:J:374:GLU:O	1:J:378:LEU:HD12	2.18	0.44
1:P:181:ARG:NH2	1:P:184:ASP:C	2.70	0.44
1:A:356:GLU:HA	1:A:360:GLY:O	2.18	0.43
1:D:218:ASP:OD1	3:D:501:5XH:N1	2.51	0.43
1:E:361:ARG:HE	1:E:361:ARG:HB3	1.39	0.43
1:F:458:LYS:HD3	1:F:458:LYS:HA	1.64	0.43
1:I:192:MET:CG	1:I:193:LYS:N	2.81	0.43
1:J:151:ARG:O	1:J:152:LYS:HG2	2.17	0.43
1:L:164:PRO:O	1:L:168:ARG:HG3	2.18	0.43
1:M:404:ARG:HG3	1:M:405:GLU:CG	2.47	0.43
1:B:316:LEU:HB2	1:B:318:LEU:HG	2.00	0.43
1:C:307:ARG:HD2	1:C:346:HIS:HA	2.00	0.43
1:E:362:LEU:HD22	1:E:366:TRP:CZ3	2.53	0.43
1:F:326:LEU:HG	1:F:428:LEU:O	2.18	0.43
1:G:163:VAL:HG12	1:G:166:TYR:HB2	1.99	0.43
1:M:316:LEU:HA	1:M:375:ALA:HB1	2.00	0.43
1:N:191:LEU:O	1:N:193:LYS:HG3	2.17	0.43
1:P:345:THR:CG2	1:P:347:ASP:H	2.25	0.43
1:A:319:GLY:O	1:A:424:ARG:NH1	2.51	0.43
1:C:255:ASP:CG	1:C:257:LYS:NZ	2.71	0.43
1:G:412:LEU:HD13	1:G:438:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:307:ARG:HD2	1:L:346:HIS:HA	1.99	0.43
1:N:313:GLU:HG2	1:N:424:ARG:HD2	2.01	0.43
1:O:188:ARG:HD3	1:O:189:PHE:CE2	2.52	0.43
1:O:388:CYS:O	1:O:394:ILE:HD11	2.18	0.43
1:C:165:LYS:NZ	1:L:373:GLN:CG	2.79	0.43
1:G:128:ARG:HH22	1:G:196:ARG:NH2	2.16	0.43
1:I:423:ASP:HB3	1:I:426:ARG:CG	2.47	0.43
1:B:229:ARG:NH2	1:G:281:GLU:O	2.51	0.43
1:G:316:LEU:HD21	1:G:352:LEU:HD11	2.01	0.43
1:M:253:HIS:ND1	1:M:256:LEU:HG	2.33	0.43
1:O:188:ARG:NH2	2:O:502:SO4:O4	2.51	0.43
1:O:228:HIS:HB3	1:O:442:TYR:CG	2.53	0.43
1:P:356:GLU:HA	1:P:360:GLY:O	2.18	0.43
1:C:202:THR:HG22	4:C:602:HOH:O	2.19	0.43
1:C:300:ARG:CD	1:C:319:GLY:HA2	2.46	0.43
1:E:316:LEU:HB2	1:E:318:LEU:HG	2.01	0.43
1:G:313:GLU:CD	1:G:427:ARG:HH22	2.22	0.43
1:G:401:ARG:HD2	1:G:402:PRO:HD3	1.99	0.43
1:G:409:GLU:OE1	1:G:442:TYR:OH	2.30	0.43
1:N:257:LYS:HG2	1:N:260:ASN:ND2	2.34	0.43
1:O:202:THR:HG23	1:O:204:HIS:ND1	2.34	0.43
1:O:373:GLN:HG3	1:O:374:GLU:OE1	2.19	0.43
1:E:447:ARG:HA	1:E:452:HIS:CD2	2.52	0.43
1:K:128:ARG:HH22	1:K:196:ARG:HH21	1.66	0.43
1:K:181:ARG:HH12	1:K:193:LYS:HD2	1.79	0.43
1:C:377:ASP:HB3	1:L:164:PRO:HG2	2.00	0.43
1:O:309:TYR:OH	1:O:335:GLU:OE1	2.31	0.43
1:P:217:LEU:HD12	1:P:220:ILE:HD11	1.99	0.43
1:F:426:ARG:HA	1:F:426:ARG:HD2	1.72	0.43
1:D:179:ARG:HH22	1:N:179:ARG:NH2	2.16	0.43
1:N:252:MET:HE2	1:N:252:MET:HB2	1.85	0.43
1:O:151:ARG:O	1:O:152:LYS:HB2	2.19	0.43
1:D:228:HIS:HB3	1:D:442:TYR:CG	2.54	0.43
1:E:326:LEU:HG	1:E:428:LEU:O	2.19	0.43
1:F:191:LEU:HD23	1:F:287:ILE:HB	2.01	0.43
1:H:367:SER:HA	1:H:370:CYS:SG	2.58	0.43
1:I:380:THR:OG1	1:I:381:ALA:N	2.52	0.43
1:K:307:ARG:HD2	1:K:346:HIS:HA	2.01	0.43
1:M:401:ARG:HD2	1:M:402:PRO:HD2	1.99	0.43
1:N:370:CYS:HB3	1:N:375:ALA:HB3	2.00	0.43
1:B:147:TRP:CD1	1:B:149:ARG:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:ARG:HH22	1:D:196:ARG:NH2	2.17	0.43
1:F:424:ARG:NH2	1:F:465:MET:HG3	2.34	0.43
1:I:402:PRO:HB3	1:I:404:ARG:HE	1.83	0.43
1:K:164:PRO:O	1:K:168:ARG:HB2	2.19	0.43
1:A:174:ILE:HD13	1:A:174:ILE:HG21	1.84	0.42
1:A:217:LEU:O	1:A:220:ILE:HG13	2.18	0.42
1:A:239:GLY:HA3	1:A:434:MET:HB3	2.01	0.42
1:C:363:PRO:HD2	1:C:366:TRP:CE2	2.54	0.42
1:D:227:ASN:HB2	4:D:610:HOH:O	2.18	0.42
1:F:257:LYS:HD2	1:F:259:GLU:CD	2.40	0.42
1:M:229:ARG:NH1	4:M:606:HOH:O	2.28	0.42
1:P:184:ASP:CG	1:P:184:ASP:O	2.56	0.42
1:P:409:GLU:OE1	1:P:442:TYR:OH	2.32	0.42
1:A:316:LEU:HD21	1:A:352:LEU:HD21	2.00	0.42
1:A:356:GLU:CG	1:A:362:LEU:HG	2.49	0.42
1:D:173:GLU:HG3	1:D:291:GLY:CA	2.49	0.42
1:D:257:LYS:HD2	1:D:259:GLU:OE2	2.18	0.42
1:F:149:ARG:HA	1:F:149:ARG:HD2	1.83	0.42
1:F:195:GLN:C	1:F:196:ARG:HG3	2.39	0.42
1:L:390:ASP:N	4:L:617:HOH:O	2.51	0.42
1:M:316:LEU:HA	1:M:375:ALA:CB	2.49	0.42
1:M:367:SER:HB3	1:M:379:PHE:CD2	2.54	0.42
1:D:179:ARG:NH2	1:N:179:ARG:NH2	2.67	0.42
1:N:184:ASP:OD2	1:N:193:LYS:HE3	2.19	0.42
1:N:380:THR:OG1	1:N:384:THR:O	2.29	0.42
1:O:402:PRO:HD2	1:O:405:GLU:OE1	2.19	0.42
1:P:215:CYS:HA	1:P:262:LEU:HA	2.01	0.42
1:B:449:HIS:NE2	2:B:502:SO4:O4	2.53	0.42
1:H:362:LEU:HD11	1:H:385:LEU:HD21	2.01	0.42
1:L:238:VAL:HG13	1:L:287:ILE:HD11	2.02	0.42
1:M:237:GLN:NE2	1:M:283:CYS:O	2.37	0.42
1:N:253:HIS:ND1	1:N:256:LEU:HG	2.35	0.42
1:P:258:PRO:HD3	1:P:332:ILE:HG12	2.00	0.42
1:A:217:LEU:HD22	1:A:259:GLU:HG3	2.02	0.42
1:D:369:ARG:HG2	1:D:369:ARG:O	2.20	0.42
1:E:148:ASP:OD2	1:E:151:ARG:HG3	2.19	0.42
1:J:281:GLU:O	1:N:229:ARG:NH2	2.52	0.42
1:K:401:ARG:HA	1:K:401:ARG:HD2	1.66	0.42
1:O:380:THR:H	1:O:380:THR:HG1	1.60	0.42
1:A:365:ASP:O	1:A:368:VAL:HG22	2.20	0.42
1:D:404:ARG:HA	1:D:413:CYS:SG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:PRO:HD2	1:F:366:TRP:CE2	2.54	0.42
1:H:230:HIS:CE1	1:H:279:PRO:HG2	2.55	0.42
1:J:168:ARG:HD3	1:J:168:ARG:HH11	1.32	0.42
1:J:363:PRO:HD2	1:J:366:TRP:CD2	2.54	0.42
1:J:357:LYS:NZ	1:J:400:ALA:O	2.28	0.42
1:P:295:ASP:C	1:P:295:ASP:OD1	2.58	0.42
1:P:370:CYS:HB3	1:P:375:ALA:HB3	2.00	0.42
1:D:380:THR:HG22	1:D:381:ALA:N	2.34	0.42
1:D:386:GLN:HG3	1:D:387:PRO:HD2	2.00	0.42
1:F:177:MET:HE1	1:F:209:MET:SD	2.60	0.42
1:I:350:GLU:HG3	1:I:393:HIS:HB3	2.02	0.42
1:K:316:LEU:HB2	1:K:318:LEU:HG	2.01	0.42
1:M:313:GLU:OE2	1:M:427:ARG:NH1	2.50	0.42
1:N:402:PRO:CD	1:N:405:GLU:CG	2.91	0.42
1:P:349:LEU:HA	1:P:349:LEU:HD12	1.78	0.42
1:P:363:PRO:HD2	1:P:366:TRP:CD2	2.54	0.42
1:A:380:THR:HG22	1:A:381:ALA:N	2.35	0.42
1:B:378:LEU:O	1:B:385:LEU:HD12	2.20	0.42
1:C:154:TYR:OH	1:D:270:VAL:HG11	2.19	0.42
1:G:380:THR:HG22	1:G:381:ALA:N	2.35	0.42
1:H:177:MET:HB2	1:H:177:MET:HE3	1.84	0.42
1:H:218:ASP:OD1	3:H:503:5XH:N1	2.53	0.42
1:H:188:ARG:NH2	2:H:502:SO4:O4	2.48	0.42
1:I:208:VAL:C	1:I:209:MET:HG3	2.40	0.42
1:I:357:LYS:HD2	1:I:357:LYS:HA	1.77	0.42
1:L:356:GLU:HA	1:L:360:GLY:O	2.19	0.42
1:N:128:ARG:O	1:N:149:ARG:HG2	2.20	0.42
1:N:402:PRO:CD	1:N:405:GLU:OE1	2.45	0.42
1:N:323:SER:HB3	1:N:427:ARG:NH1	2.35	0.42
1:A:426:ARG:HD2	1:A:426:ARG:HH11	1.39	0.42
1:I:150:LYS:HD2	1:I:150:LYS:O	2.19	0.42
1:I:295:ASP:OD2	1:I:297:ARG:NH1	2.53	0.42
1:J:353:HIS:CB	1:J:397:ILE:HD13	2.49	0.42
1:K:271:ASP:OD2	1:K:274:THR:HG23	2.19	0.42
1:L:192:MET:HG2	1:L:193:LYS:N	2.34	0.42
1:O:247:THR:HB	1:O:460:PRO:HG2	2.02	0.42
1:P:345:THR:HG23	1:P:350:GLU:OE1	2.20	0.42
1:B:385:LEU:HA	1:B:385:LEU:HD12	1.74	0.42
1:K:177:MET:HE3	1:K:209:MET:SD	2.60	0.42
1:M:300:ARG:C	1:M:300:ARG:HD3	2.41	0.42
1:N:313:GLU:HA	1:N:318:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:373:GLN:HA	1:P:376:ARG:NE	2.35	0.42
1:B:195:GLN:HG2	1:B:209:MET:HA	2.02	0.42
1:D:185:VAL:N	4:D:604:HOH:O	2.34	0.42
1:G:242:LEU:HD21	1:G:256:LEU:HD11	2.01	0.42
1:G:326:LEU:CD2	1:G:429:ASN:HA	2.49	0.42
1:H:165:LYS:HE3	1:H:168:ARG:NH2	2.35	0.42
1:H:354:LEU:HA	1:H:354:LEU:HD23	1.87	0.42
1:J:160:VAL:CG1	1:J:166:TYR:HB3	2.50	0.42
1:J:193:LYS:O	1:J:210:PRO:HD3	2.20	0.42
1:J:349:LEU:HB2	1:J:378:LEU:HD23	2.02	0.42
1:L:367:SER:HB2	1:L:379:PHE:CD2	2.55	0.42
1:O:181:ARG:HD2	1:O:193:LYS:HB3	2.02	0.42
1:A:323:SER:O	1:A:427:ARG:NH1	2.47	0.41
1:D:217:LEU:HD23	1:D:259:GLU:HG3	2.03	0.41
1:E:151:ARG:NH2	1:E:196:ARG:HH22	2.07	0.41
1:H:163:VAL:HG21	1:H:166:TYR:CD2	2.50	0.41
1:H:177:MET:HE1	1:H:207:ILE:HD13	2.01	0.41
1:H:376:ARG:HG2	1:H:376:ARG:HH11	1.85	0.41
1:I:160:VAL:HG12	1:I:166:TYR:HB3	2.02	0.41
1:M:228:HIS:HB3	1:M:442:TYR:CG	2.55	0.41
1:M:380:THR:HG22	1:M:381:ALA:N	2.35	0.41
1:M:392:LYS:HA	1:M:392:LYS:HD2	1.71	0.41
1:N:162:ASN:C	1:N:162:ASN:HD22	2.22	0.41
1:O:386:GLN:HG2	1:O:387:PRO:N	2.35	0.41
1:A:146:ALA:HB3	1:A:155:CYS:SG	2.60	0.41
1:H:316:LEU:HD21	1:H:352:LEU:HD11	2.02	0.41
1:I:424:ARG:NH2	1:I:465:MET:HG3	2.34	0.41
1:M:447:ARG:O	1:M:455:ASN:ND2	2.51	0.41
1:O:148:ASP:OD2	1:O:151:ARG:CB	2.69	0.41
1:P:309:TYR:HD1	1:P:331:CYS:HB2	1.85	0.41
1:B:134:LEU:HD11	1:B:137:GLU:HG2	2.01	0.41
1:C:132:LEU:HD12	1:C:145:GLU:HG2	2.01	0.41
1:C:393:HIS:HD2	4:C:620:HOH:O	2.03	0.41
1:E:307:ARG:NH1	1:E:348:ASN:OD1	2.53	0.41
1:G:353:HIS:NE2	1:G:386:GLN:O	2.35	0.41
1:C:229:ARG:NH2	1:H:281:GLU:HB3	2.35	0.41
1:J:449:HIS:CG	1:J:450:PRO:HD2	2.55	0.41
1:K:181:ARG:NH1	1:K:193:LYS:CG	2.83	0.41
1:K:309:TYR:HD1	1:K:331:CYS:HB2	1.86	0.41
1:M:380:THR:HB	1:M:383:GLY:H	1.86	0.41
1:N:380:THR:HG22	1:N:381:ALA:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:373:GLN:HG3	1:O:374:GLU:N	2.36	0.41
1:B:151:ARG:HG2	1:B:153:GLU:CD	2.29	0.41
1:C:217:LEU:O	1:C:221:MET:HG3	2.20	0.41
1:C:238:VAL:HG11	1:C:329:MET:SD	2.60	0.41
1:F:218:ASP:OD2	4:F:601:HOH:O	2.21	0.41
1:F:449:HIS:NE2	2:F:502:SO4:O4	2.52	0.41
1:G:191:LEU:HG	1:G:241:ALA:HB1	2.02	0.41
1:H:228:HIS:HB3	1:H:442:TYR:CG	2.55	0.41
1:J:210:PRO:HG2	1:J:212:TYR:OH	2.19	0.41
1:L:238:VAL:HG11	1:L:329:MET:SD	2.60	0.41
1:M:301:THR:HB	1:M:317:SER:HB3	2.03	0.41
1:N:147:TRP:CH2	1:N:152:LYS:HG3	2.55	0.41
1:O:128:ARG:HD2	1:O:128:ARG:HH21	1.54	0.41
1:P:304:VAL:H	1:P:314:VAL:HG11	1.85	0.41
1:A:443:PHE:O	1:A:446:CYS:HB3	2.21	0.41
1:J:222:LYS:CG	1:J:223:HIS:CE1	3.03	0.41
1:N:181:ARG:HA	1:N:181:ARG:HD3	1.78	0.41
1:N:257:LYS:NZ	1:N:306:THR:OG1	2.29	0.41
1:O:181:ARG:HD2	1:O:181:ARG:HH11	1.52	0.41
1:P:181:ARG:NH1	1:P:187:ASP:H	2.19	0.41
1:P:316:LEU:HD21	1:P:352:LEU:HD21	2.01	0.41
1:P:380:THR:HG21	1:P:384:THR:H	1.84	0.41
1:A:349:LEU:O	1:A:349:LEU:HD23	2.21	0.41
1:G:441:LYS:HD3	1:G:442:TYR:CZ	2.56	0.41
1:H:128:ARG:HG3	1:H:150:LYS:HG3	2.02	0.41
1:I:128:ARG:HG2	1:I:129:PHE:CE2	2.56	0.41
1:I:152:LYS:HA	1:I:152:LYS:HD3	1.89	0.41
1:J:128:ARG:HH22	1:J:196:ARG:NH2	2.19	0.41
1:K:169:ASP:N	1:K:169:ASP:OD1	2.54	0.41
1:L:447:ARG:HA	1:L:452:HIS:CD2	2.55	0.41
1:P:147:TRP:CZ2	1:P:152:LYS:HA	2.55	0.41
1:C:217:LEU:HG	1:C:221:MET:SD	2.61	0.41
1:E:128:ARG:HA	1:E:149:ARG:HD2	2.01	0.41
1:H:376:ARG:NH1	1:H:376:ARG:O	2.54	0.41
1:I:192:MET:HE1	1:I:209:MET:SD	2.61	0.41
1:I:373:GLN:HG2	1:I:374:GLU:N	2.34	0.41
1:K:257:LYS:HG3	1:K:259:GLU:HB2	2.02	0.41
1:K:356:GLU:HA	1:K:360:GLY:O	2.21	0.41
1:K:392:LYS:N	1:K:392:LYS:CD	2.84	0.41
1:M:174:ILE:O	1:M:178:GLU:HG3	2.21	0.41
1:N:363:PRO:HD2	1:N:366:TRP:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:278:LEU:CD1	1:O:278:LEU:N	2.79	0.41
1:E:273:MET:SD	1:P:272:PRO:HB2	2.60	0.41
1:H:361:ARG:N	1:H:361:ARG:CD	2.82	0.41
1:P:316:LEU:HD12	1:P:375:ALA:HB1	2.03	0.41
1:B:318:LEU:HD23	1:B:370:CYS:HA	2.02	0.41
1:I:161:ARG:HG3	1:I:162:ASN:H	1.86	0.41
1:J:297:ARG:HB2	1:J:297:ARG:HE	1.57	0.41
1:J:349:LEU:HD11	1:J:386:GLN:O	2.20	0.41
1:K:392:LYS:H	1:K:392:LYS:HD2	1.86	0.41
1:A:314:VAL:HG22	1:A:320:TRP:CD1	2.56	0.41
1:A:192:MET:HE2	3:A:501:5XH:C15	2.51	0.41
1:G:295:ASP:OD1	1:G:296:GLU:N	2.52	0.41
1:G:401:ARG:HD2	1:G:402:PRO:HD2	2.01	0.41
1:H:356:GLU:OE2	1:H:361:ARG:HB3	2.21	0.41
1:H:396:ARG:NH1	1:H:396:ARG:HG3	2.29	0.41
1:O:316:LEU:C	1:O:318:LEU:HD13	2.41	0.41
1:P:181:ARG:CD	1:P:193:LYS:HG2	2.50	0.41
1:A:135:LEU:HD11	1:A:145:GLU:HB2	2.03	0.41
1:A:344:ASP:O	1:A:396:ARG:NH1	2.54	0.41
1:D:412:LEU:HB2	1:D:438:TYR:CE1	2.56	0.41
1:E:281:GLU:O	1:P:229:ARG:NH2	2.54	0.41
1:E:299:SER:HB3	1:E:302:ALA:HB2	2.01	0.41
1:H:220:ILE:HA	1:H:224:GLY:O	2.21	0.41
1:H:227:ASN:HD21	1:H:230:HIS:CD2	2.39	0.41
1:I:362:LEU:N	1:I:362:LEU:HD23	2.35	0.41
1:J:139:THR:HG22	1:J:166:TYR:OH	2.20	0.41
1:K:147:TRP:HE3	1:K:154:TYR:CE1	2.38	0.41
1:L:295:ASP:OD2	1:L:297:ARG:NH1	2.54	0.41
1:L:316:LEU:HD21	1:L:352:LEU:HD11	2.02	0.41
1:L:394:ILE:HD12	1:L:394:ILE:H	1.86	0.41
1:M:215:CYS:HB2	1:M:258:PRO:O	2.20	0.41
1:I:229:ARG:NH2	1:M:281:GLU:O	2.53	0.41
1:M:378:LEU:O	1:M:386:GLN:HG3	2.20	0.41
1:P:247:THR:HB	1:P:460:PRO:HG2	2.03	0.41
1:P:373:GLN:HE21	1:P:373:GLN:HB2	1.38	0.41
1:A:321:MET:HB3	1:A:322:TYR:H	1.56	0.40
1:B:200:ASN:OD1	1:B:201:GLU:N	2.54	0.40
1:B:238:VAL:HG11	1:B:329:MET:SD	2.61	0.40
1:C:134:LEU:HD21	1:C:137:GLU:CG	2.51	0.40
1:C:390:ASP:OD2	1:C:392:LYS:HB2	2.21	0.40
1:G:179:ARG:HE	1:G:179:ARG:HB2	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:195:GLN:N	1:J:195:GLN:CD	2.74	0.40
1:L:376:ARG:O	1:L:376:ARG:HD3	2.20	0.40
1:O:242:LEU:HD21	1:O:256:LEU:HD11	2.02	0.40
1:A:181:ARG:NH1	1:A:185:VAL:CA	2.84	0.40
1:A:237:GLN:OE1	1:A:284:ARG:HA	2.21	0.40
1:C:449:HIS:NE2	2:C:502:SO4:O4	2.52	0.40
1:F:313:GLU:OE2	4:F:603:HOH:O	2.22	0.40
1:F:373:GLN:OE1	4:F:602:HOH:O	2.22	0.40
1:G:192:MET:HE2	1:G:192:MET:HB3	1.89	0.40
1:I:418:ASN:HB3	1:I:428:LEU:HG	2.04	0.40
1:K:177:MET:CE	1:K:194:ILE:HB	2.52	0.40
1:K:254:THR:O	1:K:305:SER:OG	2.34	0.40
1:N:162:ASN:O	1:N:162:ASN:ND2	2.48	0.40
1:N:313:GLU:OE1	1:N:427:ARG:NH1	2.55	0.40
1:O:298:HIS:HE1	1:O:300:ARG:NH2	2.19	0.40
1:O:374:GLU:O	1:O:378:LEU:HD12	2.21	0.40
1:O:316:LEU:CD1	1:O:375:ALA:HB1	2.51	0.40
1:O:412:LEU:HB2	1:O:438:TYR:CE1	2.57	0.40
1:B:409:GLU:OE2	1:B:411:LEU:N	2.55	0.40
1:D:380:THR:OG1	1:D:384:THR:O	2.32	0.40
1:G:307:ARG:HD2	1:G:346:HIS:HA	2.04	0.40
1:K:238:VAL:HG11	1:K:329:MET:SD	2.62	0.40
1:M:202:THR:HG23	1:M:204:HIS:ND1	2.36	0.40
1:A:181:ARG:NH1	1:A:185:VAL:C	2.75	0.40
1:D:176:PHE:O	1:D:180:VAL:HG23	2.22	0.40
1:D:258:PRO:HG3	1:D:332:ILE:HG23	2.03	0.40
1:F:308:HIS:ND1	1:F:343:TYR:O	2.53	0.40
1:F:446:CYS:O	1:F:452:HIS:HB2	2.21	0.40
1:H:375:ALA:HA	1:H:378:LEU:HD13	2.02	0.40
1:K:299:SER:HB2	1:K:302:ALA:HB2	2.02	0.40
1:N:215:CYS:HB2	1:N:258:PRO:O	2.22	0.40
1:O:295:ASP:OD1	1:O:295:ASP:C	2.60	0.40
1:O:449:HIS:ND1	1:O:451:ASN:HB2	2.37	0.40
1:B:390:ASP:O	1:B:394:ILE:HG12	2.21	0.40
1:C:399:ARG:HH11	1:C:399:ARG:HD2	1.53	0.40
1:D:357:LYS:NZ	1:D:397:ILE:O	2.54	0.40
1:F:313:GLU:HA	1:F:318:LEU:HB2	2.02	0.40
1:G:228:HIS:HB3	1:G:442:TYR:CG	2.56	0.40
1:H:227:ASN:OD1	1:H:230:HIS:HD2	2.03	0.40
1:I:300:ARG:NH1	4:I:602:HOH:O	2.18	0.40
1:J:269:SER:HB2	1:J:278:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:318:LEU:HD23	1:J:370:CYS:HA	2.04	0.40
1:K:222:LYS:HD3	1:K:223:HIS:CD2	2.56	0.40
1:K:363:PRO:HD2	1:K:366:TRP:CE2	2.56	0.40
1:K:449:HIS:NE2	2:K:501:SO4:O2	2.52	0.40
1:L:404:ARG:HG3	1:L:404:ARG:HH11	1.86	0.40
1:N:313:GLU:OE1	1:N:427:ARG:CZ	2.69	0.40
1:N:354:LEU:HD21	1:N:397:ILE:HA	2.03	0.40
1:P:378:LEU:N	4:P:601:HOH:O	2.53	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:361:ARG:NH1	1:O:361:ARG:NH1[1_455]	1.32	0.88
1:A:404:ARG:NH1	1:C:404:ARG:NE[1_445]	1.80	0.40
1:A:404:ARG:NE	1:C:404:ARG:NH2[1_445]	1.98	0.22
1:A:404:ARG:NH1	1:C:404:ARG:NH2[1_445]	2.05	0.15
1:K:168:ARG:NH2	1:M:377:ASP:OD2[2_445]	2.06	0.14
1:J:361:ARG:NH1	1:O:361:ARG:CZ[1_455]	2.10	0.10
1:A:404:ARG:NH1	1:C:404:ARG:CZ[1_445]	2.15	0.05
1:J:361:ARG:CZ	1:O:361:ARG:CZ[1_455]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	337/354 (95%)	330 (98%)	7 (2%)	0	100	100
1	B	337/354 (95%)	326 (97%)	11 (3%)	0	100	100
1	C	337/354 (95%)	326 (97%)	10 (3%)	1 (0%)	41	64
1	D	337/354 (95%)	328 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	337/354 (95%)	325 (96%)	12 (4%)	0	100	100
1	F	337/354 (95%)	328 (97%)	9 (3%)	0	100	100
1	G	337/354 (95%)	324 (96%)	12 (4%)	1 (0%)	41	64
1	H	337/354 (95%)	324 (96%)	11 (3%)	2 (1%)	25	47
1	I	337/354 (95%)	328 (97%)	9 (3%)	0	100	100
1	J	337/354 (95%)	326 (97%)	11 (3%)	0	100	100
1	K	337/354 (95%)	327 (97%)	10 (3%)	0	100	100
1	L	337/354 (95%)	326 (97%)	11 (3%)	0	100	100
1	M	337/354 (95%)	328 (97%)	9 (3%)	0	100	100
1	N	337/354 (95%)	326 (97%)	11 (3%)	0	100	100
1	O	337/354 (95%)	326 (97%)	11 (3%)	0	100	100
1	P	337/354 (95%)	325 (96%)	12 (4%)	0	100	100
All	All	5392/5664 (95%)	5223 (97%)	165 (3%)	4 (0%)	51	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	457	SER
1	C	153	GLU
1	H	457	SER
1	H	321	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/317 (96%)	297 (97%)	8 (3%)	46	72
1	B	305/317 (96%)	293 (96%)	12 (4%)	32	58
1	C	305/317 (96%)	299 (98%)	6 (2%)	55	78
1	D	305/317 (96%)	296 (97%)	9 (3%)	41	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	305/317 (96%)	293 (96%)	12 (4%)	32	58
1	F	305/317 (96%)	297 (97%)	8 (3%)	46	72
1	G	305/317 (96%)	294 (96%)	11 (4%)	35	61
1	H	305/317 (96%)	298 (98%)	7 (2%)	50	75
1	I	305/317 (96%)	301 (99%)	4 (1%)	69	86
1	J	305/317 (96%)	300 (98%)	5 (2%)	62	82
1	K	305/317 (96%)	296 (97%)	9 (3%)	41	67
1	L	305/317 (96%)	300 (98%)	5 (2%)	62	82
1	M	305/317 (96%)	294 (96%)	11 (4%)	35	61
1	N	305/317 (96%)	298 (98%)	7 (2%)	50	75
1	O	305/317 (96%)	294 (96%)	11 (4%)	35	61
1	P	305/317 (96%)	295 (97%)	10 (3%)	38	64
All	All	4880/5072 (96%)	4745 (97%)	135 (3%)	43	69

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	LYS
1	A	151	ARG
1	A	202	THR
1	A	245	PHE
1	A	269	SER
1	A	361	ARG
1	A	392	LYS
1	A	446	CYS
1	B	151	ARG
1	B	162	ASN
1	B	181	ARG
1	B	192	MET
1	B	211	LYS
1	B	222	LYS
1	B	245	PHE
1	B	257	LYS
1	B	357	LYS
1	B	404	ARG
1	B	426	ARG
1	B	446	CYS
1	C	153	GLU

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Mol	Chain	Res	Type
1	C	162	ASN
1	C	245	PHE
1	C	257	LYS
1	C	267	ASP
1	C	357	LYS
1	D	149	ARG
1	D	162	ASN
1	D	168	ARG
1	D	181	ARG
1	D	245	PHE
1	D	267	ASP
1	D	297	ARG
1	D	393	HIS
1	D	426	ARG
1	E	151	ARG
1	E	161	ARG
1	E	168	ARG
1	E	192	MET
1	E	193	LYS
1	E	196	ARG
1	E	245	PHE
1	E	295	ASP
1	E	374	GLU
1	E	376	ARG
1	E	404	ARG
1	E	457	SER
1	F	193	LYS
1	F	245	PHE
1	F	269	SER
1	F	300	ARG
1	F	357	LYS
1	F	361	ARG
1	F	392	LYS
1	F	458	LYS
1	G	150	LYS
1	G	151	ARG
1	G	161	ARG
1	G	168	ARG
1	G	192	MET
1	G	245	PHE
1	G	252	MET
1	G	376	ARG

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Mol	Chain	Res	Type
1	G	401	ARG
1	G	404	ARG
1	G	426	ARG
1	H	161	ARG
1	H	245	PHE
1	H	250	HIS
1	H	361	ARG
1	H	392	LYS
1	H	404	ARG
1	H	426	ARG
1	I	128	ARG
1	I	151	ARG
1	I	162	ASN
1	I	297	ARG
1	J	130	LYS
1	J	151	ARG
1	J	165	LYS
1	J	245	PHE
1	J	265	SER
1	K	168	ARG
1	K	169	ASP
1	K	245	PHE
1	K	257	LYS
1	K	265	SER
1	K	269	SER
1	K	373	GLN
1	K	376	ARG
1	K	458	LYS
1	L	153	GLU
1	L	165	LYS
1	L	188	ARG
1	L	245	PHE
1	L	426	ARG
1	M	128	ARG
1	M	179	ARG
1	M	181	ARG
1	M	196	ARG
1	M	245	PHE
1	M	273	MET
1	M	295	ASP
1	M	323	SER
1	M	390	ASP

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Mol	Chain	Res	Type
1	M	399	ARG
1	M	401	ARG
1	N	150	LYS
1	N	162	ASN
1	N	245	PHE
1	N	307	ARG
1	N	313	GLU
1	N	404	ARG
1	N	458	LYS
1	O	133	SER
1	O	168	ARG
1	O	192	MET
1	O	245	PHE
1	O	295	ASP
1	O	361	ARG
1	O	366	TRP
1	O	373	GLN
1	O	376	ARG
1	O	401	ARG
1	O	457	SER
1	P	161	ARG
1	P	162	ASN
1	P	181	ARG
1	P	196	ARG
1	P	245	PHE
1	P	297	ARG
1	P	340	LYS
1	P	361	ARG
1	P	401	ARG
1	P	426	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	HIS
1	A	425	GLN
1	B	162	ASN
1	B	195	GLN
1	B	346	HIS
1	C	162	ASN
1	C	195	GLN
1	C	230	HIS

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Mol	Chain	Res	Type
1	C	298	HIS
1	D	175	GLN
1	F	162	ASN
1	F	230	HIS
1	F	393	HIS
1	F	418	ASN
1	G	162	ASN
1	H	195	GLN
1	H	230	HIS
1	H	237	GLN
1	I	162	ASN
1	J	393	HIS
1	K	195	GLN
1	K	230	HIS
1	K	373	GLN
1	K	393	HIS
1	K	455	ASN
1	L	162	ASN
1	L	195	GLN
1	L	393	HIS
1	L	455	ASN
1	M	195	GLN
1	M	353	HIS
1	N	230	HIS
1	N	237	GLN
1	N	346	HIS
1	O	373	GLN
1	P	373	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

49 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$
2	SO4	L	501	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	J	502	-	4,4,4	0.15	0	6,6,6	0.06	0
3	5XH	N	501	1	31,38,38	1.55	2 (6%)	35,53,53	1.38	1 (2%)
3	5XH	M	501	1	31,38,38	1.55	2 (6%)	35,53,53	1.39	1 (2%)
2	SO4	D	500	-	4,4,4	0.13	0	6,6,6	0.09	0
2	SO4	M	500	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	F	501	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.05	0
3	5XH	A	501	1	31,38,38	1.55	2 (6%)	35,53,53	1.39	1 (2%)
2	SO4	B	501	-	4,4,4	0.13	0	6,6,6	0.07	0
3	5XH	L	503	1	31,38,38	1.53	2 (6%)	35,53,53	1.36	1 (2%)
3	5XH	B	504	1	31,38,38	1.55	2 (6%)	35,53,53	1.39	1 (2%)
2	SO4	G	500	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	K	501	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	B	502	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	L	502	-	4,4,4	0.16	0	6,6,6	0.06	0
2	SO4	P	501	-	4,4,4	0.40	0	6,6,6	0.24	0
2	SO4	H	502	-	4,4,4	0.15	0	6,6,6	0.06	0
3	5XH	C	504	1	31,38,38	1.54	2 (6%)	35,53,53	1.67	1 (2%)
2	SO4	J	503	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	P	502	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	F	503	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	O	501	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	A	500	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	O	502	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	J	501	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	C	503	-	4,4,4	0.12	0	6,6,6	0.09	0
3	5XH	O	503	1	31,38,38	1.55	2 (6%)	35,53,53	1.38	1 (2%)
2	SO4	N	500	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	K	502	-	4,4,4	0.17	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	5XH	G	501	1	31,38,38	1.55	2 (6%)	35,53,53	1.42	1 (2%)
3	5XH	I	504	1	31,38,38	1.56	2 (6%)	35,53,53	1.40	1 (2%)
2	SO4	E	503	-	4,4,4	0.14	0	6,6,6	0.06	0
3	5XH	K	503	1	31,38,38	1.54	2 (6%)	35,53,53	1.41	1 (2%)
2	SO4	C	502	-	4,4,4	0.15	0	6,6,6	0.16	0
3	5XH	E	504	1	31,38,38	1.56	2 (6%)	35,53,53	1.39	1 (2%)
2	SO4	E	502	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	I	503	-	4,4,4	0.16	0	6,6,6	0.06	0
3	5XH	D	501	1	31,38,38	1.55	2 (6%)	35,53,53	1.38	1 (2%)
3	5XH	F	504	1	31,38,38	1.55	2 (6%)	35,53,53	1.40	1 (2%)
2	SO4	E	501	-	4,4,4	0.23	0	6,6,6	0.37	0
3	5XH	J	504	1	31,38,38	1.56	2 (6%)	35,53,53	1.40	1 (2%)
3	5XH	P	503	1	31,38,38	1.55	2 (6%)	35,53,53	1.41	1 (2%)
2	SO4	I	502	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	H	501	-	4,4,4	0.30	0	6,6,6	1.50	1 (16%)
2	SO4	F	502	-	4,4,4	0.15	0	6,6,6	0.17	0
3	5XH	H	503	1	31,38,38	1.54	2 (6%)	35,53,53	1.39	1 (2%)
2	SO4	I	501	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	B	503	-	4,4,4	0.15	0	6,6,6	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5XH	N	501	1	-	1/14/33/33	0/4/4/4
3	5XH	C	504	1	-	1/14/33/33	0/4/4/4
3	5XH	M	501	1	-	1/14/33/33	0/4/4/4
3	5XH	E	504	1	-	1/14/33/33	0/4/4/4
3	5XH	D	501	1	-	1/14/33/33	0/4/4/4
3	5XH	G	501	1	-	1/14/33/33	0/4/4/4
3	5XH	P	503	1	-	1/14/33/33	0/4/4/4
3	5XH	A	501	1	-	1/14/33/33	0/4/4/4
3	5XH	L	503	1	-	1/14/33/33	0/4/4/4
3	5XH	O	503	1	-	1/14/33/33	0/4/4/4
3	5XH	B	504	1	-	1/14/33/33	0/4/4/4
3	5XH	H	503	1	-	1/14/33/33	0/4/4/4
3	5XH	K	503	1	-	1/14/33/33	0/4/4/4
3	5XH	I	504	1	-	1/14/33/33	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5XH	F	504	1	-	1/14/33/33	0/4/4/4
3	5XH	J	504	1	-	1/14/33/33	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	504	5XH	C4-C3	8.01	1.52	1.32
3	J	504	5XH	C4-C3	7.99	1.52	1.32
3	P	503	5XH	C4-C3	7.97	1.52	1.32
3	I	504	5XH	C4-C3	7.96	1.52	1.32
3	A	501	5XH	C4-C3	7.96	1.52	1.32
3	F	504	5XH	C4-C3	7.96	1.52	1.32
3	G	501	5XH	C4-C3	7.95	1.52	1.32
3	O	503	5XH	C4-C3	7.95	1.52	1.32
3	M	501	5XH	C4-C3	7.94	1.52	1.32
3	N	501	5XH	C4-C3	7.94	1.52	1.32
3	D	501	5XH	C4-C3	7.92	1.52	1.32
3	B	504	5XH	C4-C3	7.91	1.52	1.32
3	H	503	5XH	C4-C3	7.91	1.52	1.32
3	C	504	5XH	C4-C3	7.89	1.52	1.32
3	K	503	5XH	C4-C3	7.88	1.52	1.32
3	L	503	5XH	C4-C3	7.82	1.52	1.32
3	N	501	5XH	C4-C5	2.17	1.51	1.48
3	I	504	5XH	C4-C5	2.16	1.51	1.48
3	O	503	5XH	C4-C5	2.15	1.51	1.48
3	J	504	5XH	C4-C5	2.13	1.51	1.48
3	E	504	5XH	C4-C5	2.12	1.51	1.48
3	A	501	5XH	C4-C5	2.12	1.51	1.48
3	L	503	5XH	C4-C5	2.11	1.51	1.48
3	F	504	5XH	C4-C5	2.11	1.51	1.48
3	B	504	5XH	C4-C5	2.10	1.51	1.48
3	C	504	5XH	C4-C5	2.10	1.51	1.48
3	D	501	5XH	C4-C5	2.10	1.51	1.48
3	P	503	5XH	C4-C5	2.09	1.51	1.48
3	K	503	5XH	C4-C5	2.08	1.51	1.48
3	H	503	5XH	C4-C5	2.08	1.51	1.48
3	G	501	5XH	C4-C5	2.07	1.51	1.48
3	M	501	5XH	C4-C5	2.06	1.51	1.48

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	504	5XH	C2-C3-C4	-9.15	109.94	124.67
3	G	501	5XH	C2-C3-C4	-7.70	112.28	124.67
3	I	504	5XH	C2-C3-C4	-7.60	112.43	124.67
3	K	503	5XH	C2-C3-C4	-7.60	112.44	124.67
3	J	504	5XH	C2-C3-C4	-7.59	112.45	124.67
3	H	503	5XH	C2-C3-C4	-7.56	112.50	124.67
3	B	504	5XH	C2-C3-C4	-7.55	112.52	124.67
3	E	504	5XH	C2-C3-C4	-7.54	112.53	124.67
3	P	503	5XH	C2-C3-C4	-7.54	112.53	124.67
3	F	504	5XH	C2-C3-C4	-7.53	112.54	124.67
3	M	501	5XH	C2-C3-C4	-7.49	112.61	124.67
3	N	501	5XH	C2-C3-C4	-7.42	112.72	124.67
3	A	501	5XH	C2-C3-C4	-7.42	112.73	124.67
3	O	503	5XH	C2-C3-C4	-7.42	112.73	124.67
3	D	501	5XH	C2-C3-C4	-7.39	112.77	124.67
3	L	503	5XH	C2-C3-C4	-7.28	112.96	124.67
2	H	501	SO4	O4-S-O1	-3.03	93.50	109.31

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	501	5XH	C2-C3-C4-C5
3	M	501	5XH	C2-C3-C4-C5
3	A	501	5XH	C2-C3-C4-C5
3	L	503	5XH	C2-C3-C4-C5
3	B	504	5XH	C2-C3-C4-C5
3	C	504	5XH	C2-C3-C4-C5
3	O	503	5XH	C2-C3-C4-C5
3	G	501	5XH	C2-C3-C4-C5
3	I	504	5XH	C2-C3-C4-C5
3	K	503	5XH	C2-C3-C4-C5
3	E	504	5XH	C2-C3-C4-C5
3	D	501	5XH	C2-C3-C4-C5
3	F	504	5XH	C2-C3-C4-C5
3	J	504	5XH	C2-C3-C4-C5
3	P	503	5XH	C2-C3-C4-C5
3	H	503	5XH	C2-C3-C4-C5

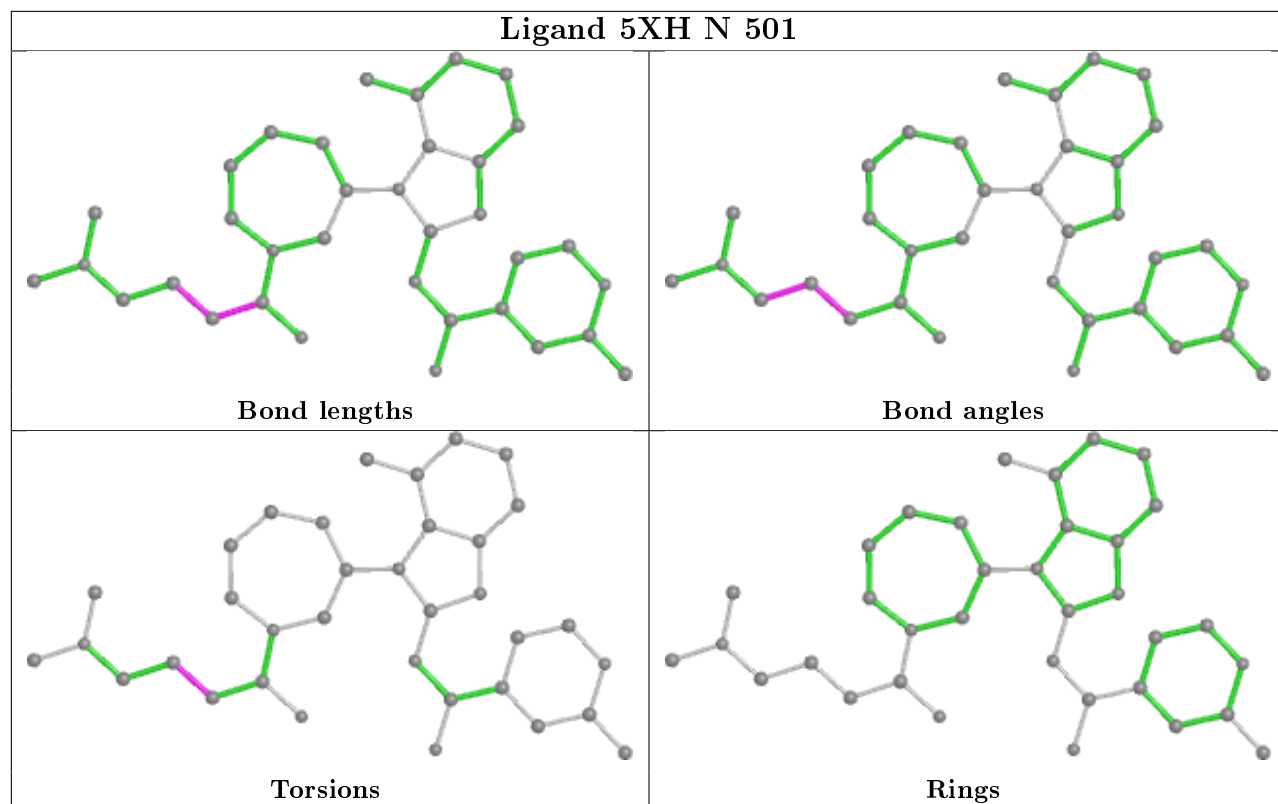
There are no ring outliers.

14 monomers are involved in 17 short contacts:

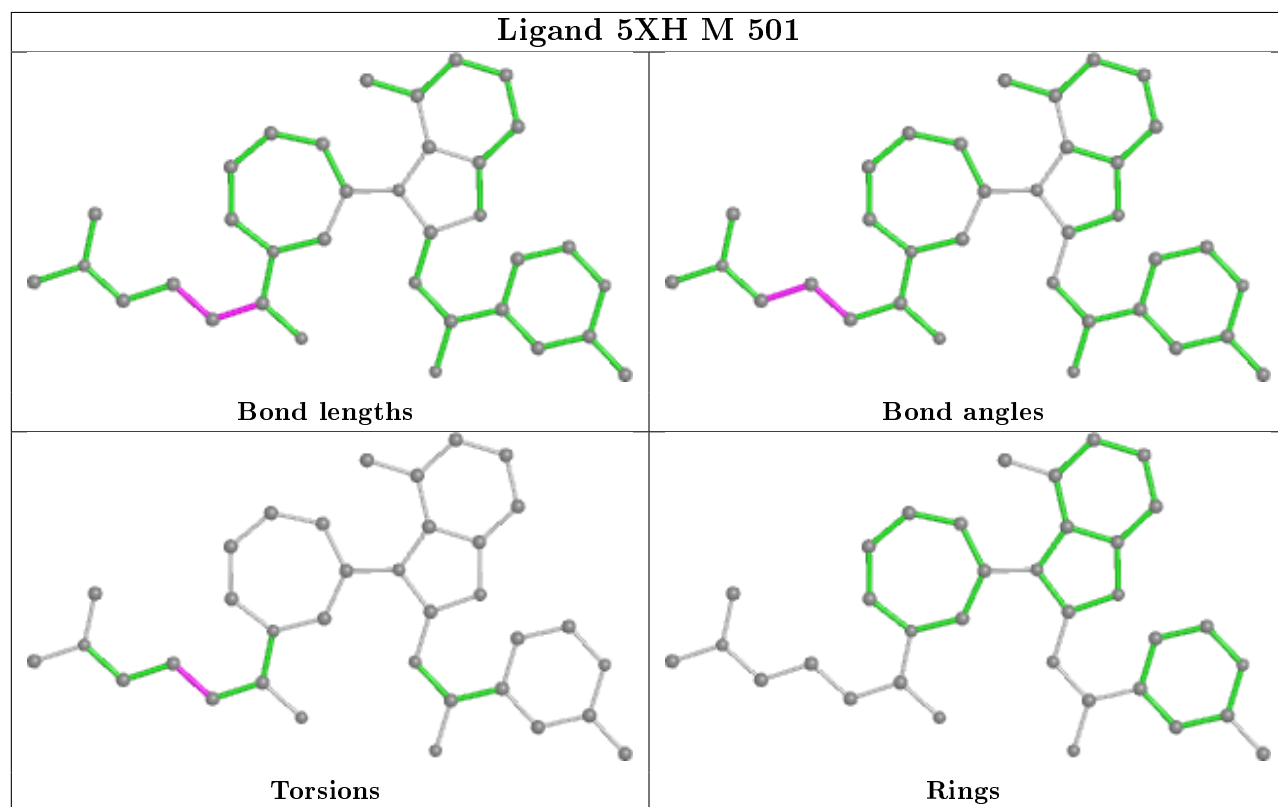
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	501	SO4	1	0
2	M	500	SO4	1	0
3	A	501	5XH	2	0
2	G	500	SO4	1	0
2	K	501	SO4	1	0
2	B	502	SO4	1	0
2	H	502	SO4	1	0
2	O	502	SO4	1	0
2	C	502	SO4	1	0
3	D	501	5XH	1	0
2	E	501	SO4	3	0
2	H	501	SO4	1	0
2	F	502	SO4	1	0
3	H	503	5XH	1	0

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

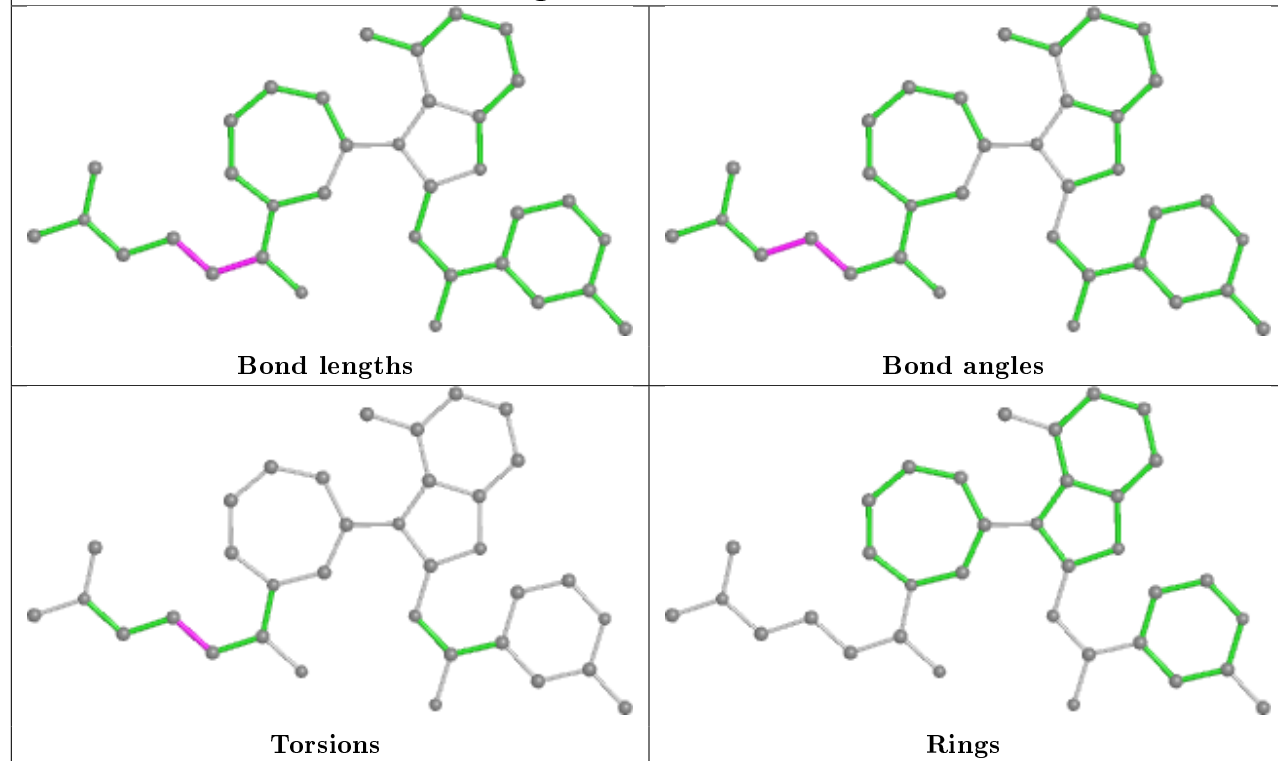
Ligand 5XH N 501



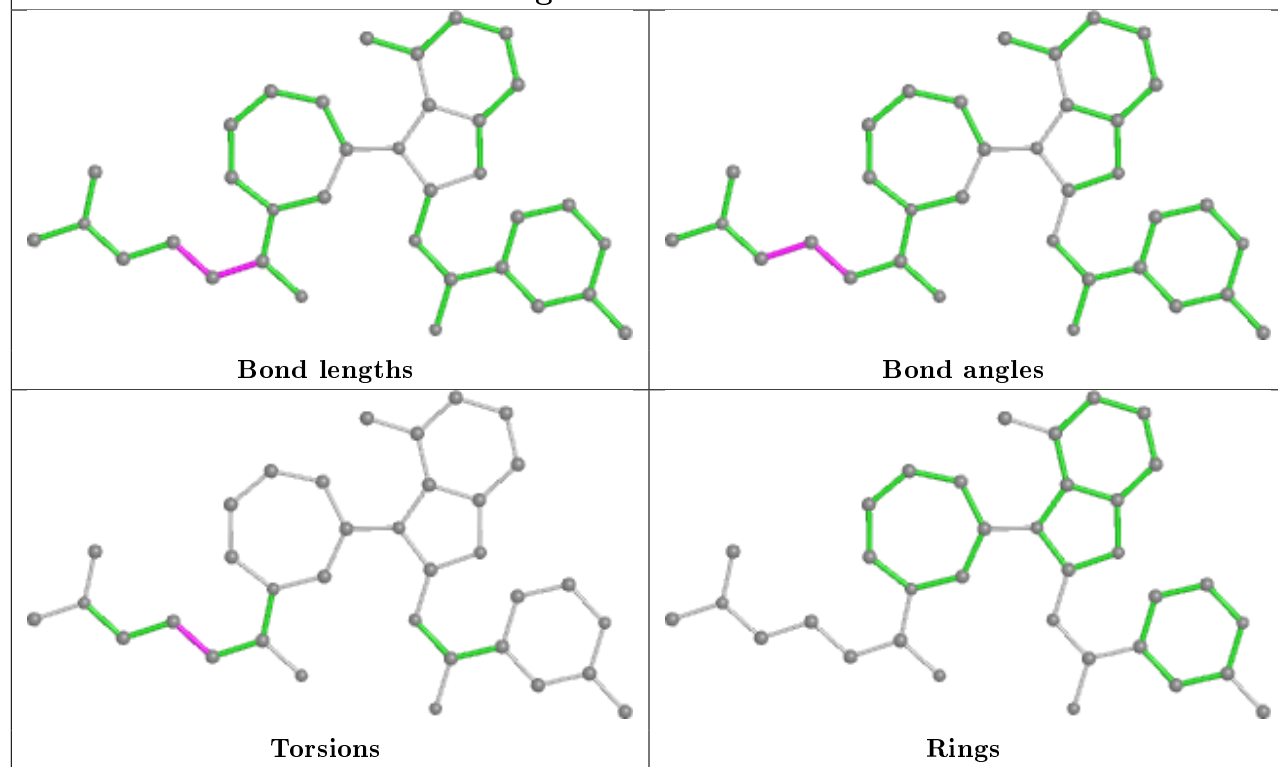
Ligand 5XH M 501



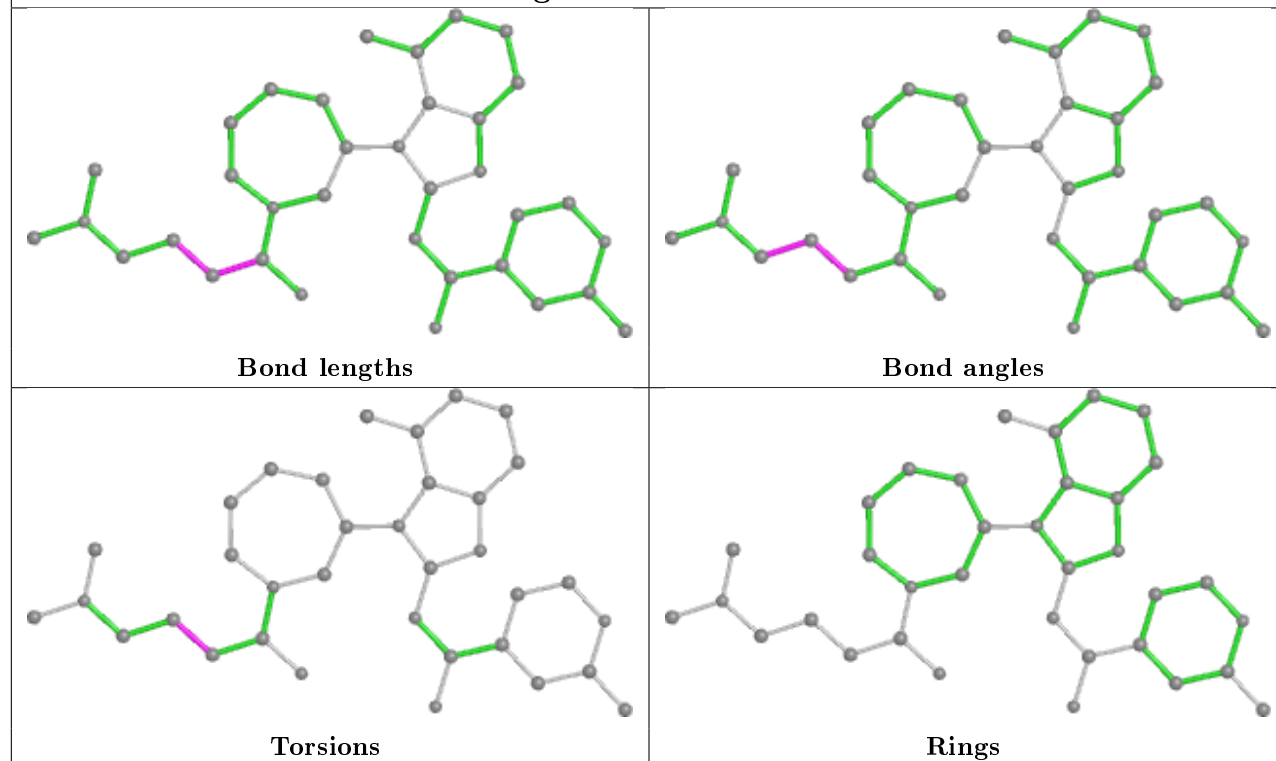
Ligand 5XH A 501



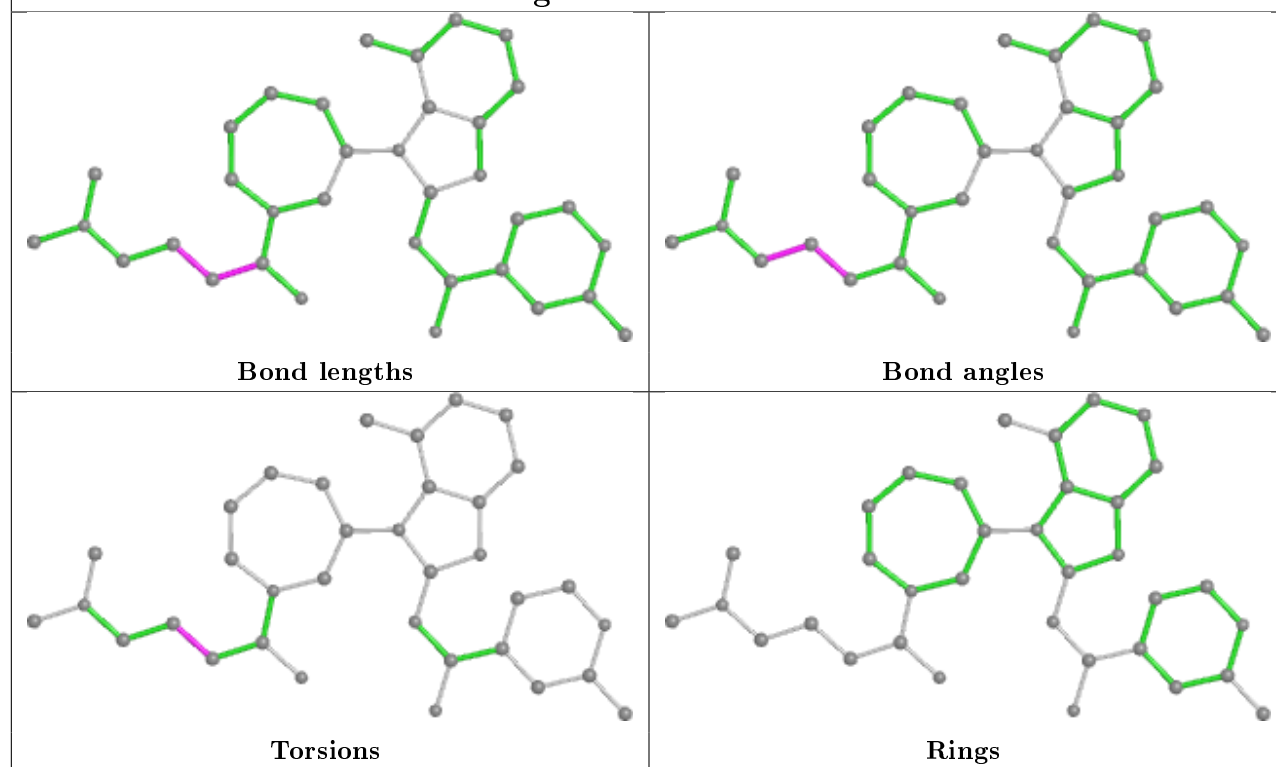
Ligand 5XH L 503



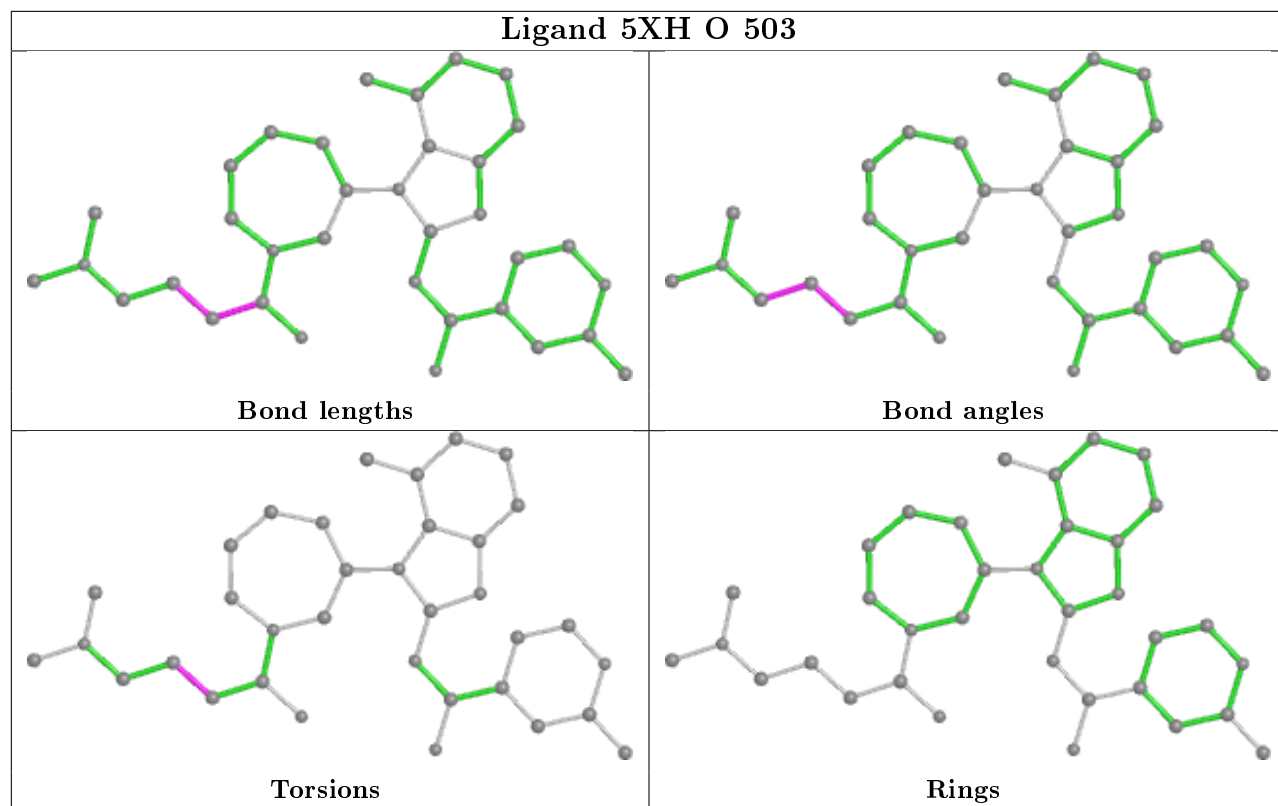
Ligand 5XH B 504



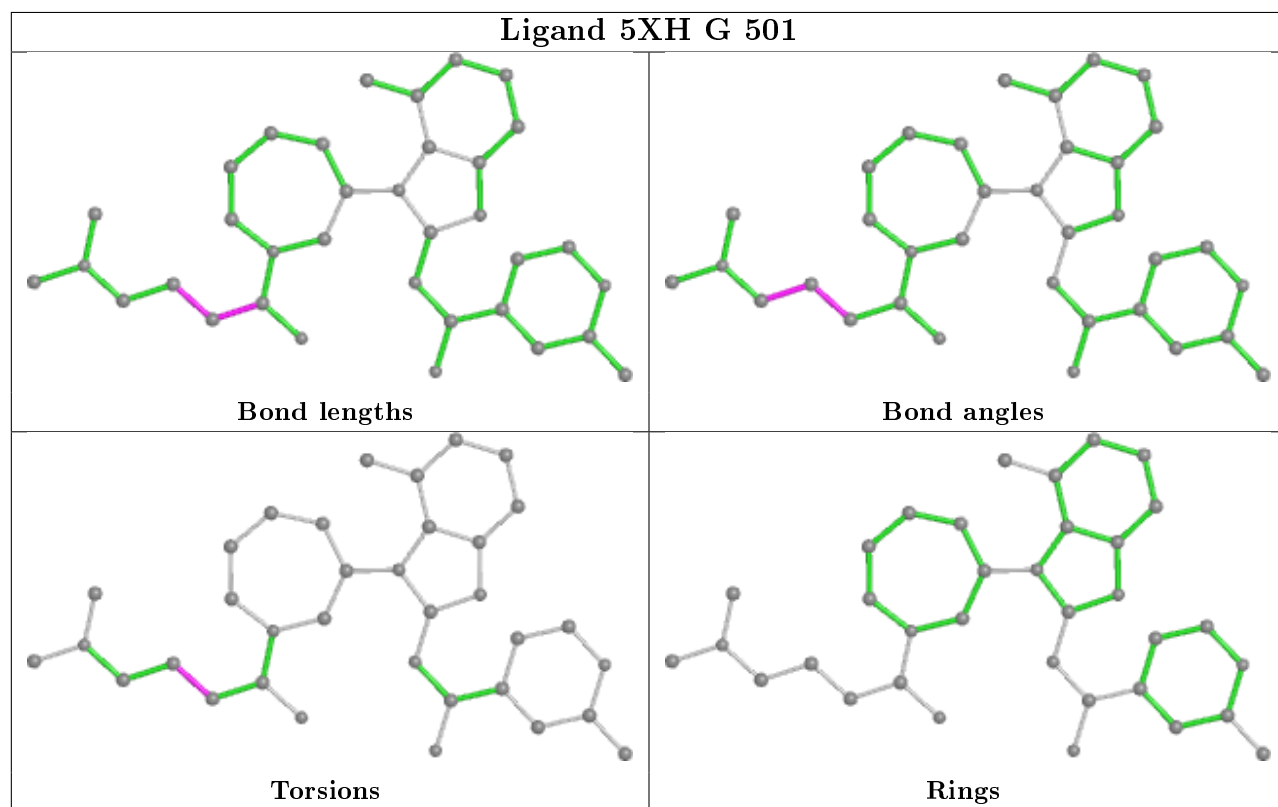
Ligand 5XH C 504



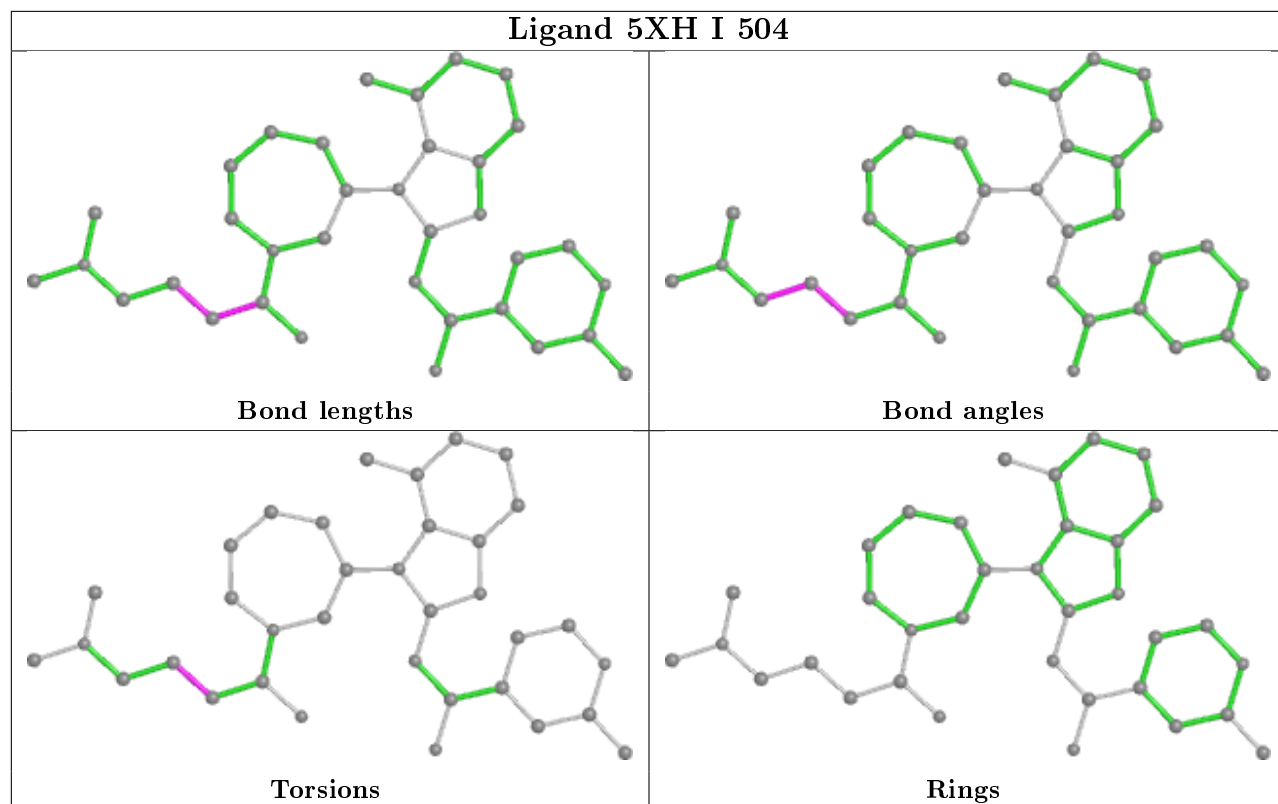
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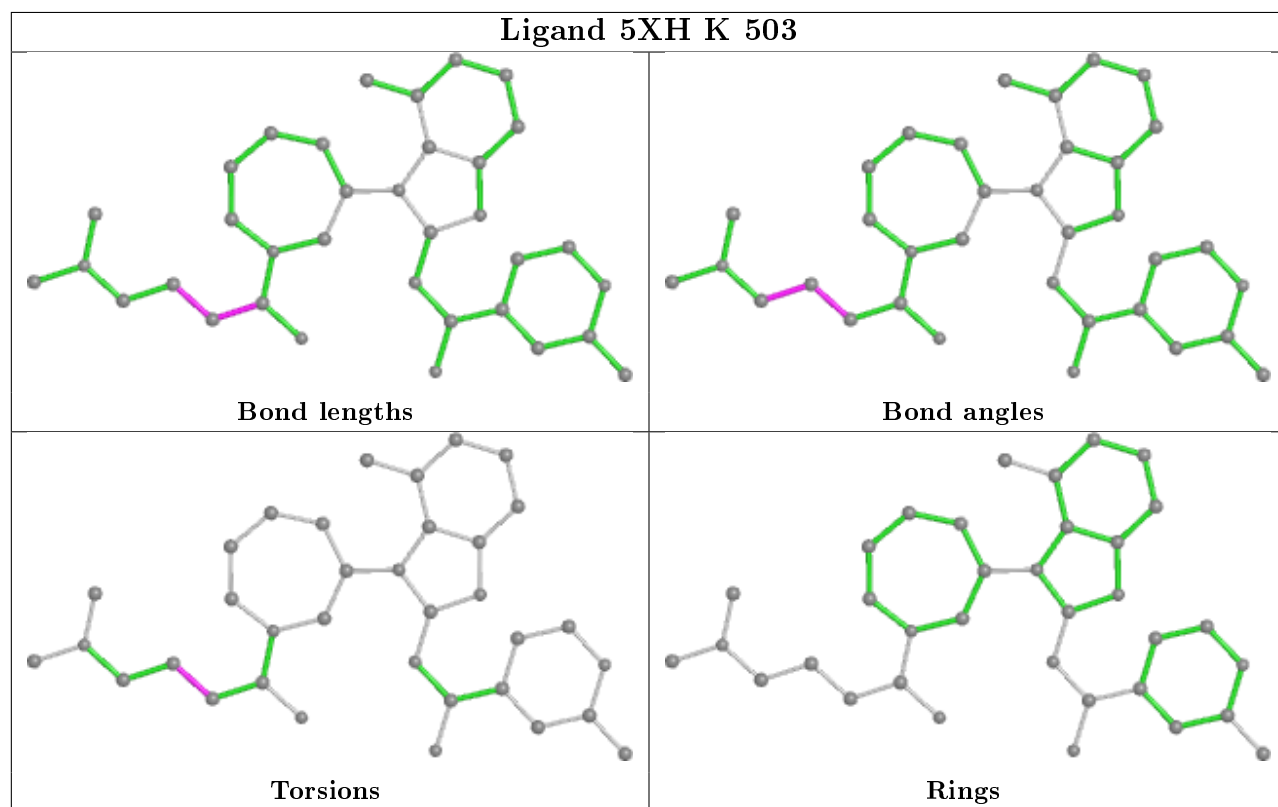
Ligand 5XH G 501



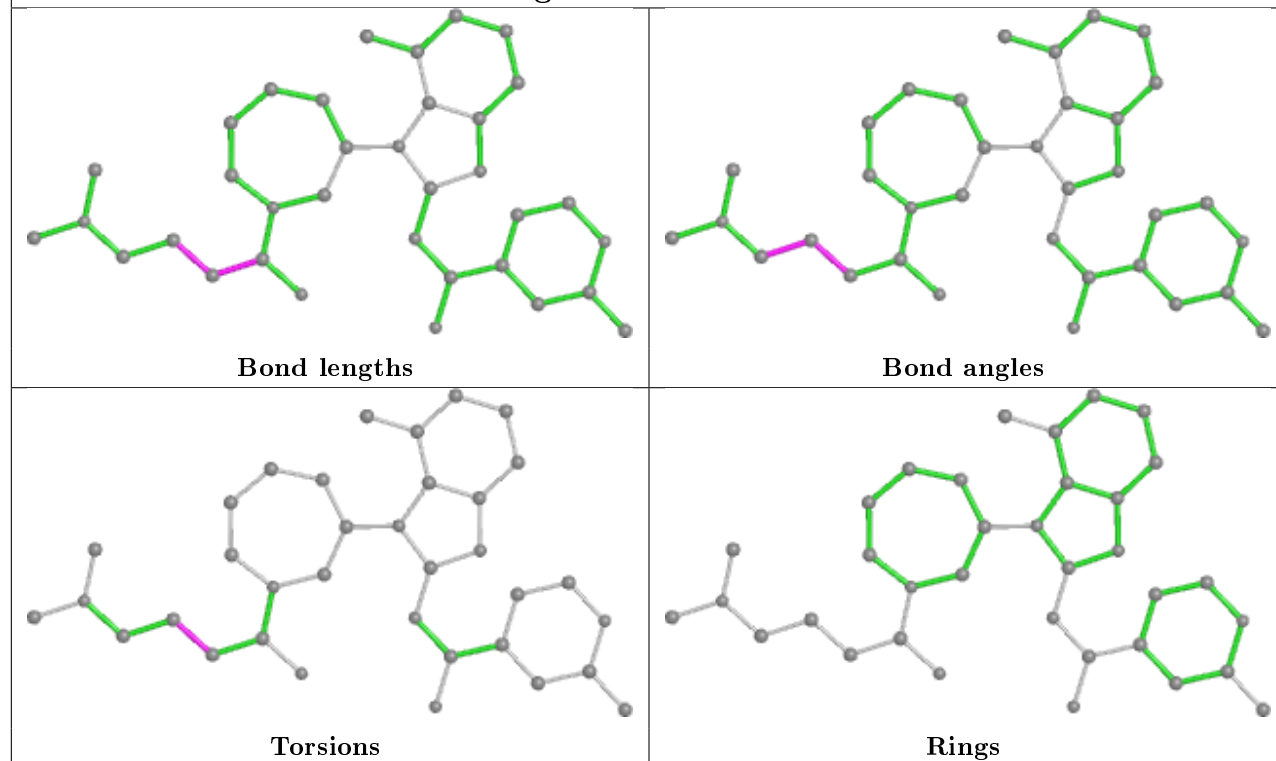
Ligand 5XH I 504



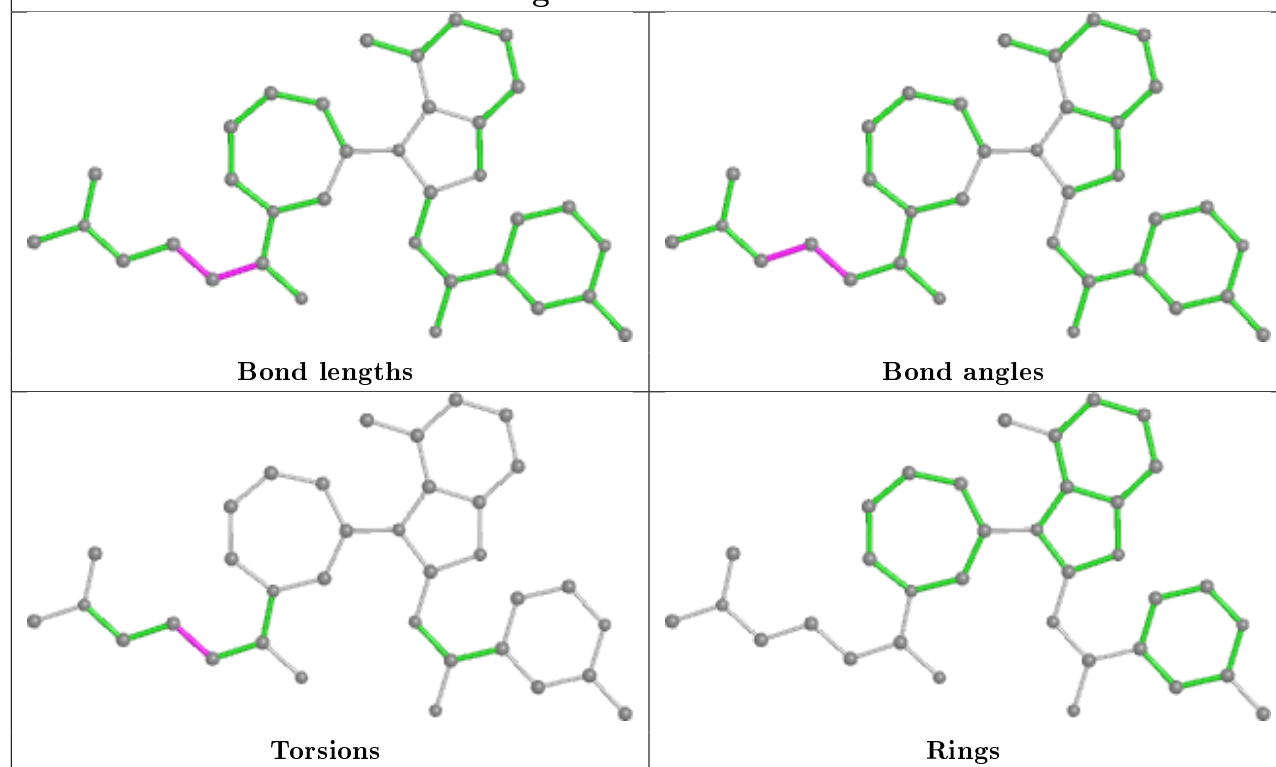
Ligand 5XH K 503



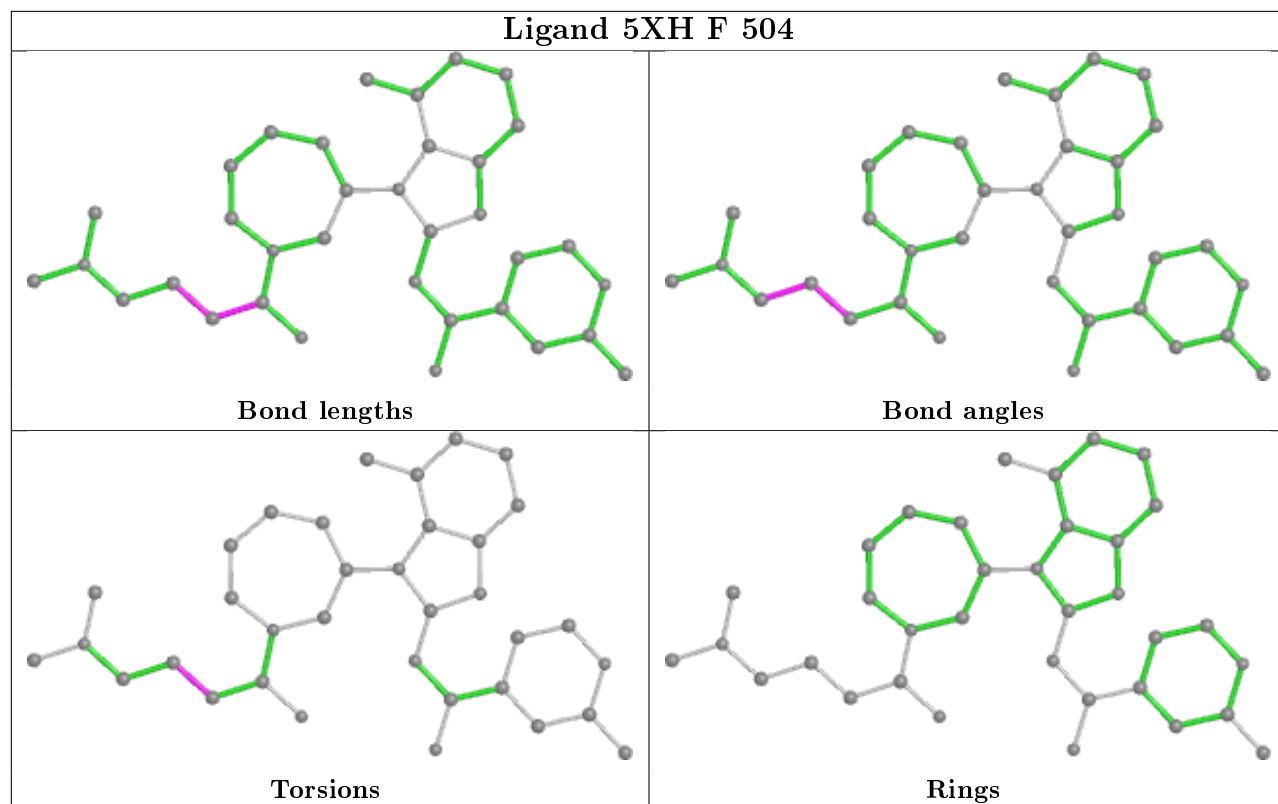
Ligand 5XH E 504



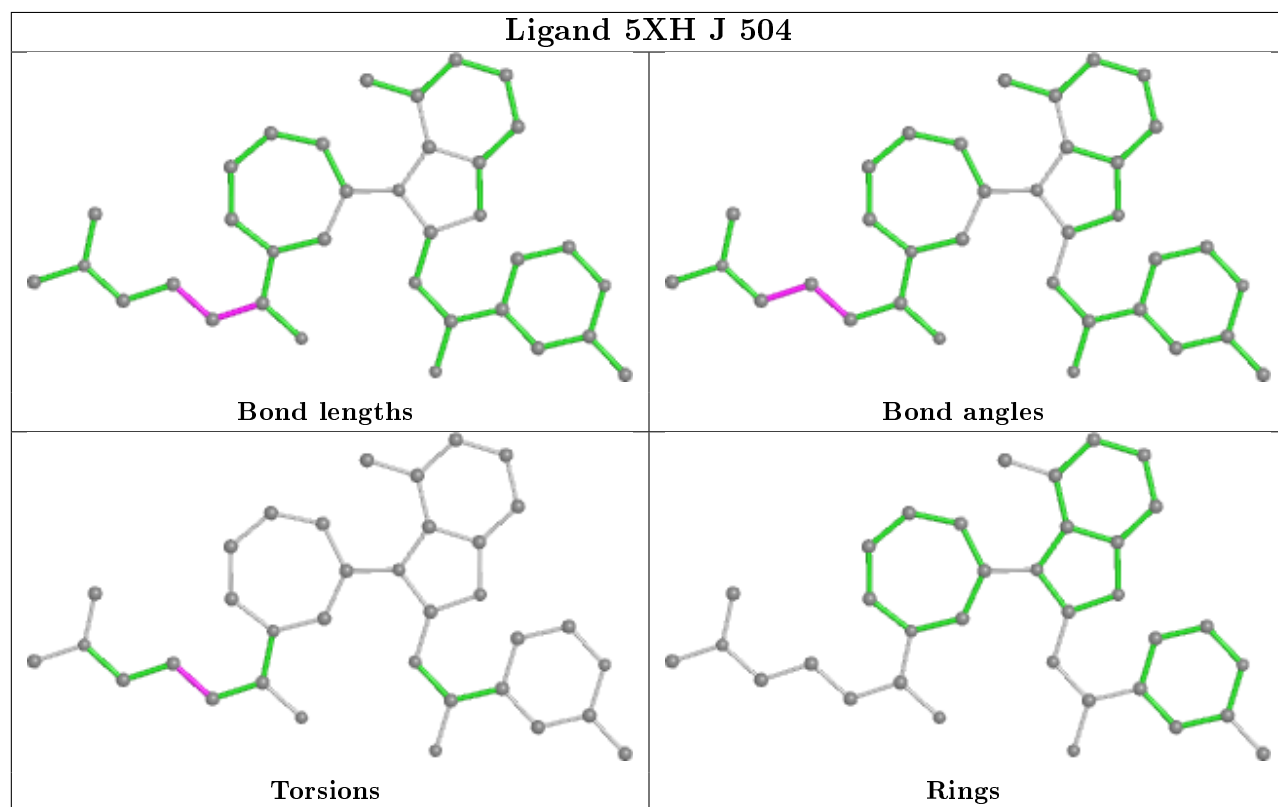
Ligand 5XH D 501

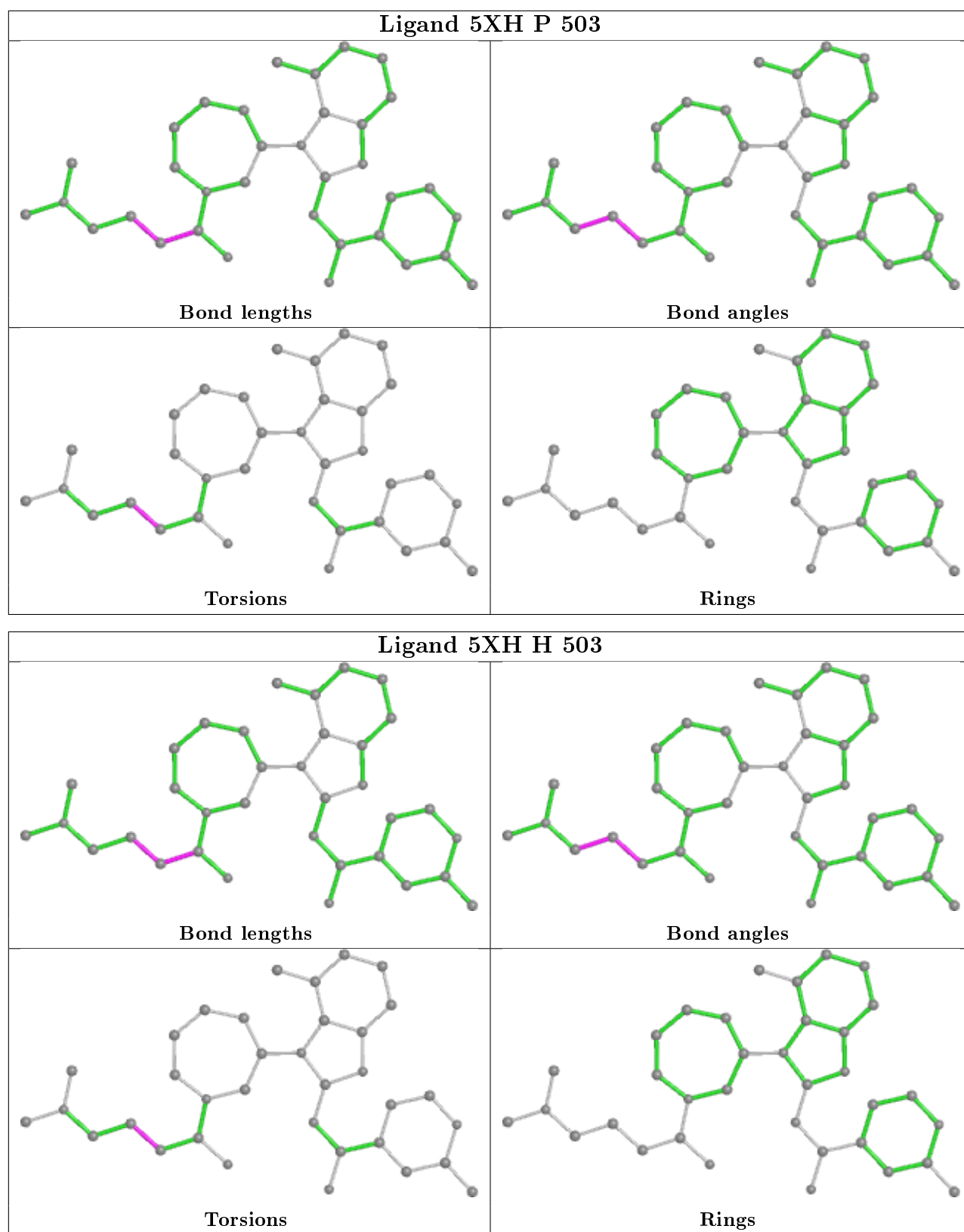


Ligand 5XH F 504



Ligand 5XH J 504





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	339/354 (95%)	0.19	7 (2%) 63 58	26, 53, 92, 116	0
1	B	339/354 (95%)	0.00	3 (0%) 84 82	26, 45, 82, 114	0
1	C	339/354 (95%)	0.14	9 (2%) 54 48	25, 46, 89, 118	0
1	D	339/354 (95%)	0.28	14 (4%) 37 30	25, 55, 97, 117	0
1	E	339/354 (95%)	0.01	3 (0%) 84 82	25, 45, 82, 106	0
1	F	339/354 (95%)	0.10	9 (2%) 54 48	25, 46, 87, 107	0
1	G	339/354 (95%)	0.20	8 (2%) 59 53	26, 52, 93, 115	0
1	H	339/354 (95%)	0.41	20 (5%) 22 17	29, 55, 102, 128	0
1	I	339/354 (95%)	0.03	6 (1%) 68 64	23, 45, 84, 111	0
1	J	339/354 (95%)	-0.00	3 (0%) 84 82	27, 46, 81, 103	0
1	K	339/354 (95%)	-0.01	3 (0%) 84 82	26, 45, 78, 101	0
1	L	339/354 (95%)	0.05	5 (1%) 73 70	23, 45, 84, 111	0
1	M	339/354 (95%)	0.21	8 (2%) 59 53	28, 53, 93, 109	0
1	N	339/354 (95%)	0.32	16 (4%) 31 25	29, 55, 96, 121	0
1	O	339/354 (95%)	0.35	14 (4%) 37 30	30, 54, 96, 142	0
1	P	339/354 (95%)	0.20	7 (2%) 63 58	27, 52, 90, 116	0
All	All	5424/5664 (95%)	0.15	135 (2%) 57 51	23, 49, 91, 142	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	127	GLY	9.2
1	O	383	GLY	5.7
1	H	181	ARG	4.4
1	D	291	GLY	4.3
1	H	346	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	291	GLY	3.9
1	G	347	ASP	3.9
1	O	291	GLY	3.8
1	C	389	LYS	3.7
1	O	127	GLY	3.7
1	G	297	ARG	3.7
1	F	266	GLY	3.7
1	C	365	ASP	3.7
1	I	151	ARG	3.6
1	C	394	ILE	3.6
1	L	150	LYS	3.5
1	F	376	ARG	3.5
1	O	371	GLY	3.5
1	A	295	ASP	3.5
1	P	150	LYS	3.4
1	H	385	LEU	3.4
1	F	203	GLY	3.4
1	H	371	GLY	3.3
1	O	150	LYS	3.3
1	M	295	ASP	3.2
1	M	297	ARG	3.2
1	P	465	MET	3.1
1	G	178	GLU	3.1
1	G	162	ASN	3.0
1	A	150	LYS	3.0
1	G	388	CYS	3.0
1	A	291	GLY	3.0
1	C	364	ALA	3.0
1	M	150	LYS	3.0
1	D	351	HIS	3.0
1	N	291	GLY	3.0
1	G	346	HIS	3.0
1	H	388	CYS	3.0
1	J	361	ARG	3.0
1	N	346	HIS	2.9
1	I	394	ILE	2.9
1	B	394	ILE	2.9
1	P	346	HIS	2.8
1	D	149	ARG	2.8
1	H	381	ALA	2.8
1	F	361	ARG	2.8
1	O	381	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	394	ILE	2.8
1	O	385	LEU	2.8
1	C	127	GLY	2.8
1	N	371	GLY	2.8
1	H	162	ASN	2.7
1	N	381	ALA	2.7
1	F	364	ALA	2.6
1	D	302	ALA	2.6
1	P	127	GLY	2.6
1	H	294	CYS	2.6
1	O	167	THR	2.5
1	M	291	GLY	2.5
1	H	347	ASP	2.5
1	H	351	HIS	2.5
1	P	351	HIS	2.5
1	N	378	LEU	2.5
1	C	203	GLY	2.5
1	P	291	GLY	2.5
1	I	266	GLY	2.5
1	D	382	ALA	2.5
1	N	178	GLU	2.5
1	K	168	ARG	2.5
1	N	388	CYS	2.4
1	H	201	GLU	2.4
1	H	383	GLY	2.4
1	D	298	HIS	2.4
1	O	351	HIS	2.4
1	G	389	LYS	2.4
1	F	386	GLN	2.4
1	M	346	HIS	2.4
1	O	379	PHE	2.4
1	M	162	ASN	2.4
1	O	397	ILE	2.4
1	L	393	HIS	2.3
1	E	361	ARG	2.3
1	D	346	HIS	2.3
1	H	178	GLU	2.3
1	N	167	THR	2.3
1	D	174	ILE	2.3
1	H	137	GLU	2.3
1	A	272	PRO	2.3
1	F	391	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	391	PRO	2.3
1	D	381	ALA	2.3
1	B	447	ARG	2.3
1	O	162	ASN	2.3
1	N	302	ALA	2.3
1	P	181	ARG	2.2
1	E	394	ILE	2.2
1	A	282	PRO	2.2
1	M	465	MET	2.2
1	N	390	ASP	2.2
1	B	151	ARG	2.2
1	D	378	LEU	2.2
1	F	127	GLY	2.2
1	O	256	LEU	2.2
1	E	150	LYS	2.2
1	K	437	ALA	2.2
1	N	465	MET	2.2
1	H	379	PHE	2.2
1	I	364	ALA	2.2
1	N	244	TYR	2.1
1	M	267	ASP	2.1
1	N	181	ARG	2.1
1	I	393	HIS	2.1
1	H	252	MET	2.1
1	I	389	LYS	2.1
1	H	186	GLU	2.1
1	D	150	LYS	2.1
1	F	389	LYS	2.1
1	G	150	LYS	2.1
1	J	300	ARG	2.1
1	D	385	LEU	2.1
1	C	137	GLU	2.1
1	L	365	ASP	2.1
1	A	346	HIS	2.1
1	D	182	LEU	2.1
1	C	151	ARG	2.1
1	K	376	ARG	2.1
1	C	273	MET	2.1
1	D	178	GLU	2.1
1	N	245	PHE	2.1
1	A	349	LEU	2.0
1	J	269	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	182	LEU	2.0
1	N	296	GLU	2.0
1	N	377	ASP	2.0
1	O	314	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	K	501	5/5	0.65	0.30	100,102,103,104	0
2	SO4	L	501	5/5	0.84	0.22	99,100,101,101	0
2	SO4	P	501	5/5	0.87	0.29	98,102,105,106	0
2	SO4	C	502	5/5	0.87	0.24	92,94,95,96	0
2	SO4	B	502	5/5	0.88	0.22	95,97,99,100	0
2	SO4	O	501	5/5	0.89	0.25	95,98,102,103	0
3	5XH	N	501	35/35	0.91	0.21	18,35,50,53	0
2	SO4	J	502	5/5	0.91	0.13	85,87,89,89	0
2	SO4	H	501	5/5	0.91	0.17	92,97,102,104	0
2	SO4	F	502	5/5	0.91	0.30	96,98,99,100	0
2	SO4	E	502	5/5	0.92	0.21	93,96,99,100	0
2	SO4	E	501	5/5	0.92	0.20	91,94,97,101	0
3	5XH	P	503	35/35	0.92	0.20	22,30,52,59	0
2	SO4	E	503	5/5	0.92	0.15	70,71,72,79	0
3	5XH	M	501	35/35	0.92	0.20	21,36,51,54	0
2	SO4	C	503	5/5	0.93	0.17	78,81,83,84	0
3	5XH	D	501	35/35	0.93	0.19	24,37,51,53	0
3	5XH	O	503	35/35	0.93	0.19	25,36,55,60	0
3	5XH	G	501	35/35	0.93	0.19	21,34,56,58	0

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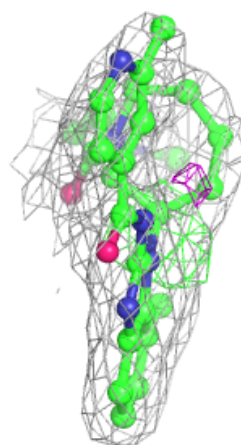
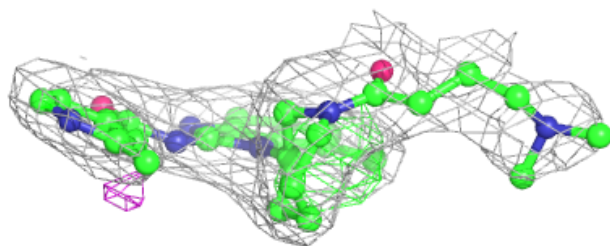
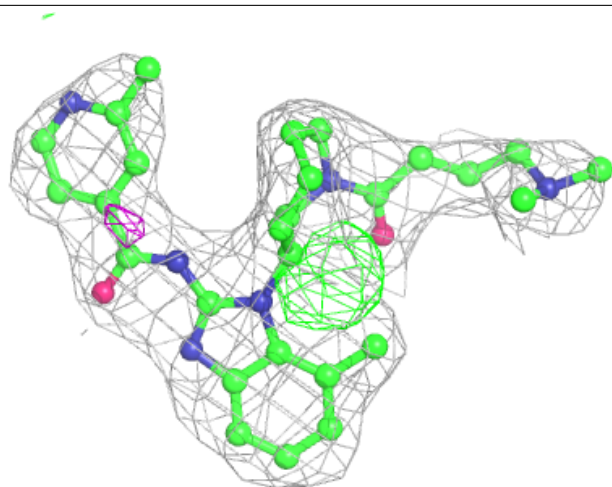
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	F	503	5/5	0.93	0.15	76,78,79,83	0
3	5XH	L	503	35/35	0.93	0.19	22,35,51,53	0
3	5XH	I	504	35/35	0.94	0.17	18,35,61,62	0
3	5XH	F	504	35/35	0.94	0.18	17,30,56,57	0
3	5XH	A	501	35/35	0.94	0.20	22,33,57,58	0
3	5XH	J	504	35/35	0.94	0.17	17,35,52,62	0
3	5XH	K	503	35/35	0.94	0.17	18,33,49,53	0
2	SO4	I	502	5/5	0.94	0.17	85,86,88,88	0
2	SO4	H	502	5/5	0.94	0.18	77,77,78,84	0
2	SO4	O	502	5/5	0.94	0.14	79,82,84,85	0
3	5XH	H	503	35/35	0.94	0.18	26,35,51,57	0
3	5XH	E	504	35/35	0.95	0.17	20,31,54,57	0
3	5XH	B	504	35/35	0.95	0.15	11,27,49,50	0
2	SO4	J	501	5/5	0.95	0.14	91,92,93,96	0
2	SO4	B	501	5/5	0.95	0.14	74,77,81,84	0
3	5XH	C	504	35/35	0.95	0.17	14,31,53,53	0
2	SO4	K	502	5/5	0.95	0.16	71,71,77,78	0
2	SO4	J	503	5/5	0.95	0.15	72,74,78,79	0
2	SO4	P	502	5/5	0.95	0.20	76,78,83,83	0
2	SO4	D	500	5/5	0.95	0.17	79,83,86,86	0
2	SO4	L	502	5/5	0.95	0.16	75,77,82,86	0
2	SO4	A	500	5/5	0.95	0.22	81,82,86,87	0
2	SO4	B	503	5/5	0.95	0.15	68,71,75,78	0
2	SO4	M	500	5/5	0.96	0.16	72,73,73,77	0
2	SO4	I	503	5/5	0.96	0.17	73,74,75,79	0
2	SO4	N	500	5/5	0.96	0.16	80,81,87,87	0
2	SO4	G	500	5/5	0.96	0.19	76,76,80,81	0
2	SO4	I	501	5/5	0.97	0.09	81,82,86,89	0
2	SO4	C	501	5/5	0.97	0.12	75,76,76,77	0
2	SO4	F	501	5/5	0.98	0.12	75,76,80,84	0

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

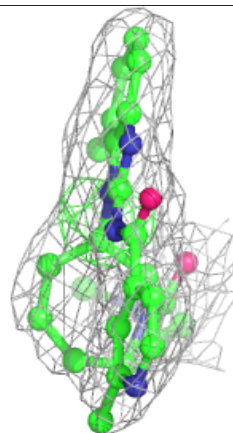
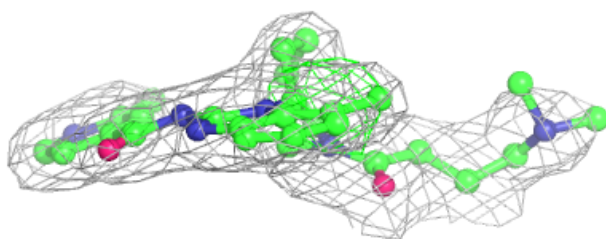
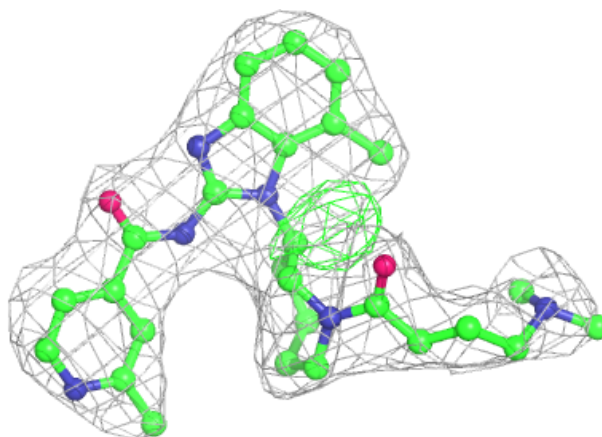
Electron density around 5XH N 501:

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



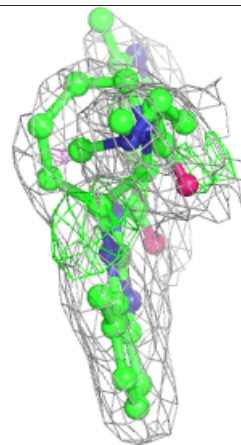
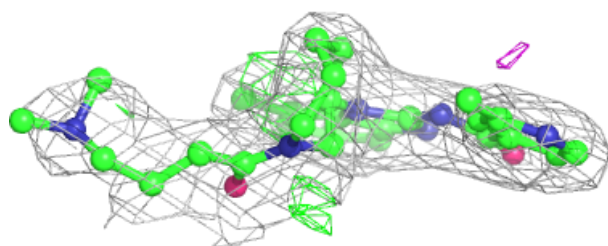
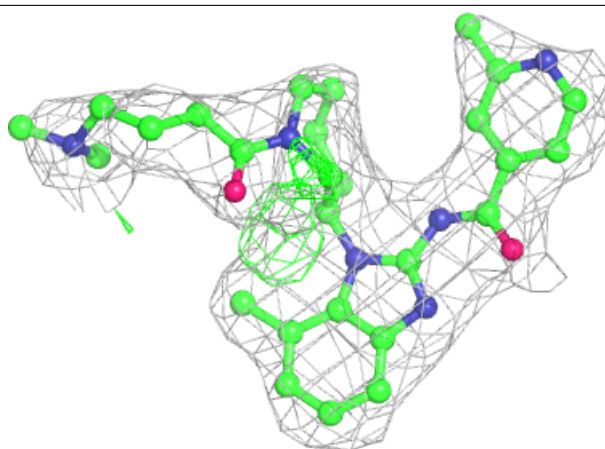
Electron density around 5XH P 503:

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



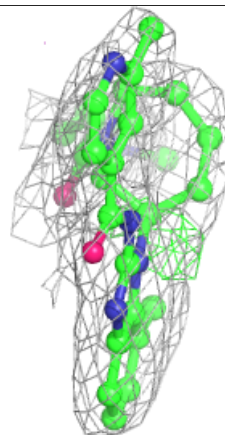
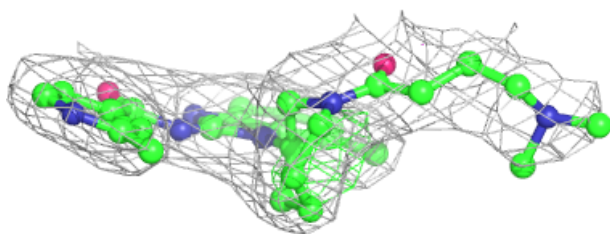
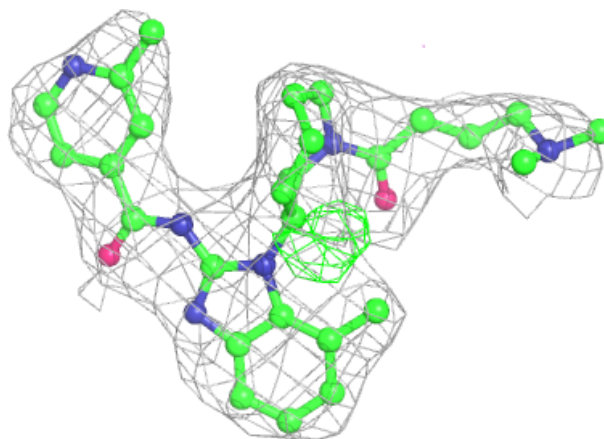
Electron density around 5XH M 501:

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



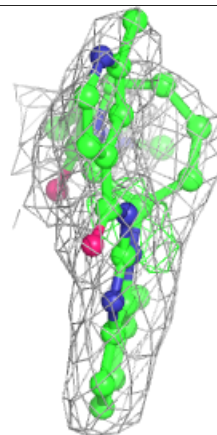
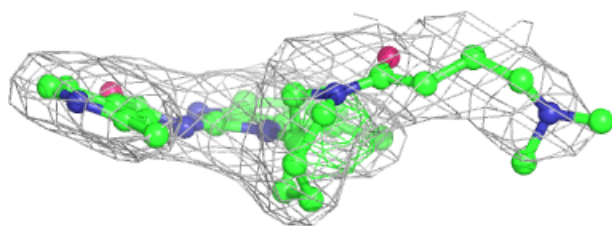
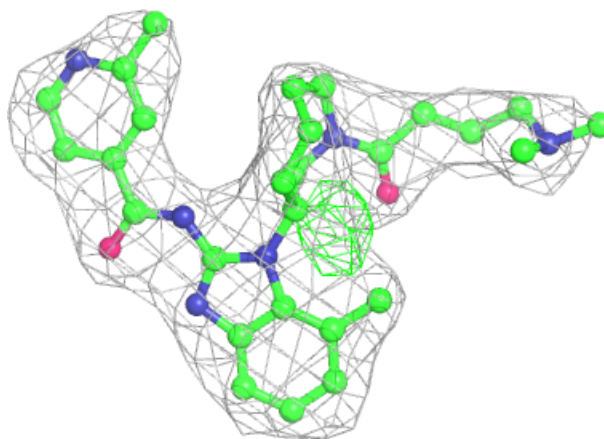
Electron density around 5XH D 501:

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



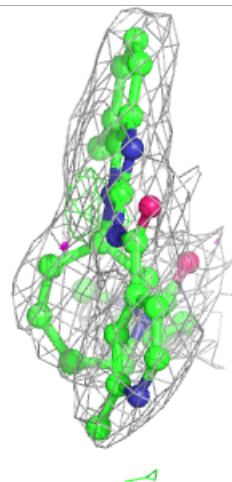
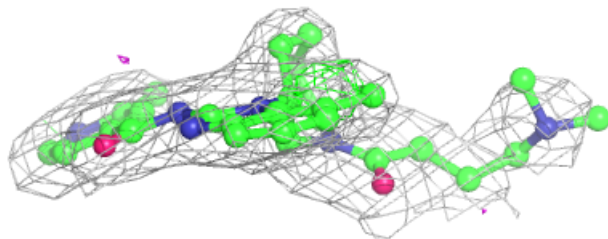
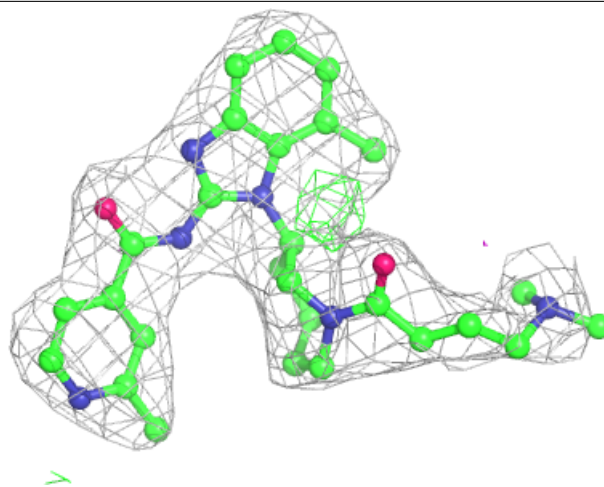
Electron density around 5XH O 503:

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



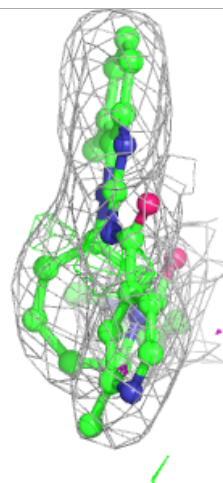
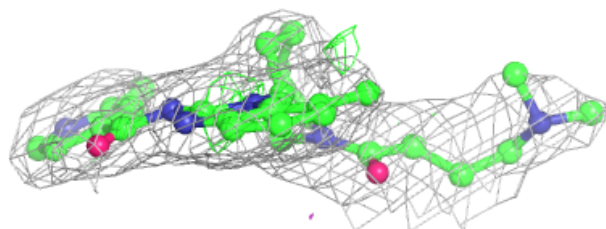
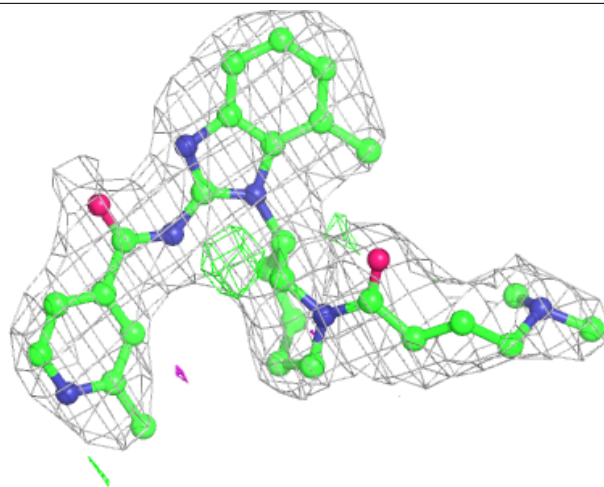
Electron density around 5XH G 501:

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



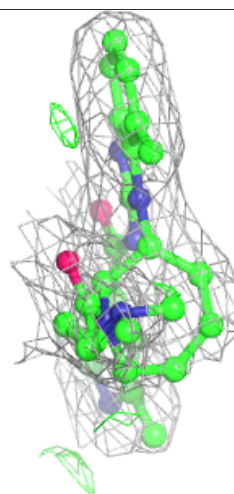
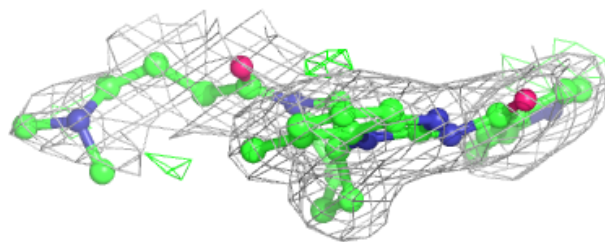
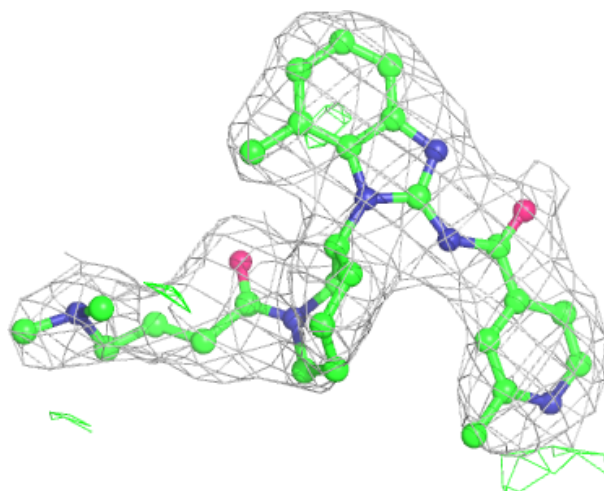
Electron density around 5XH L 503:

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



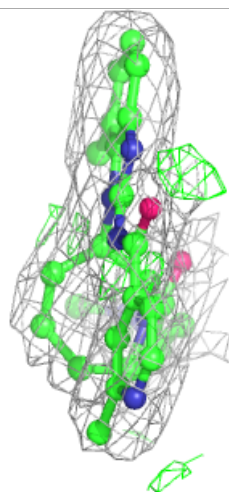
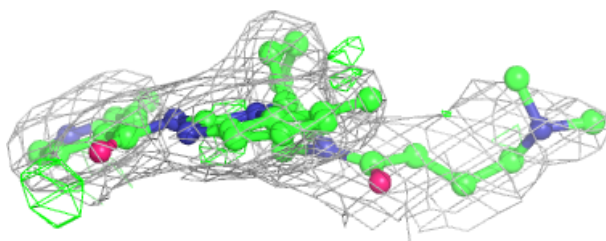
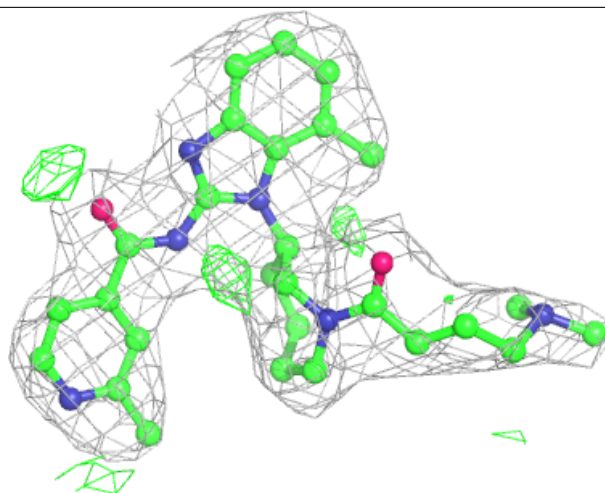
Electron density around 5XH I 504:

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



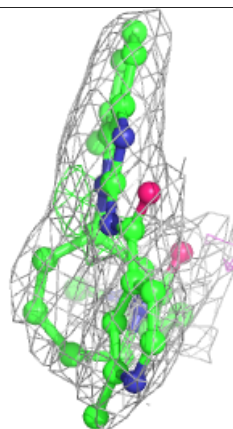
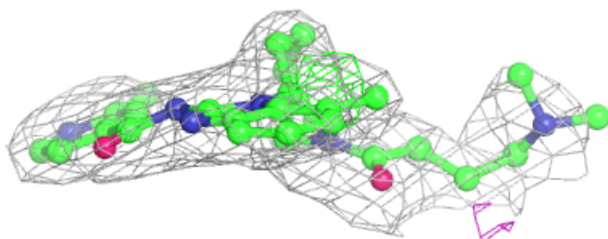
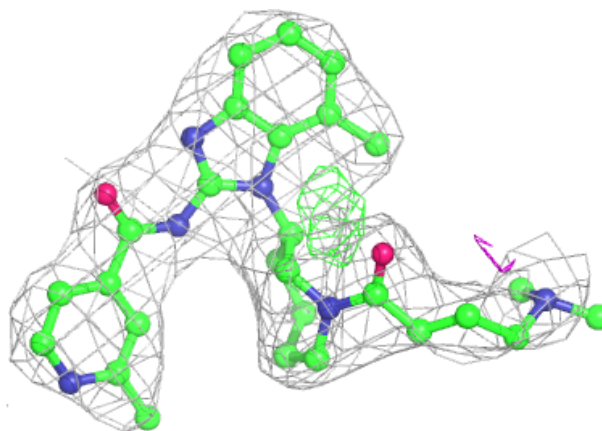
Electron density around 5XH F 504:

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and green (positive)



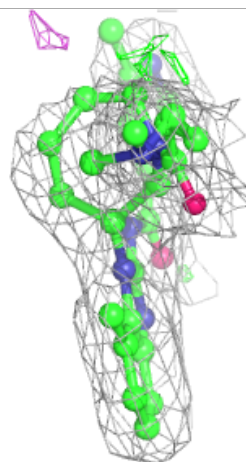
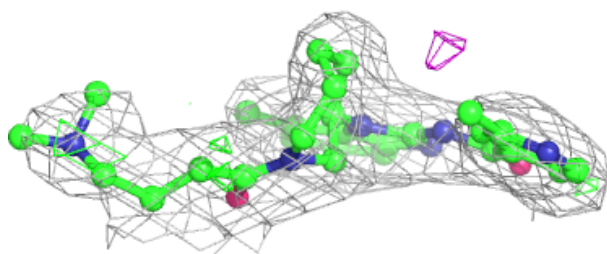
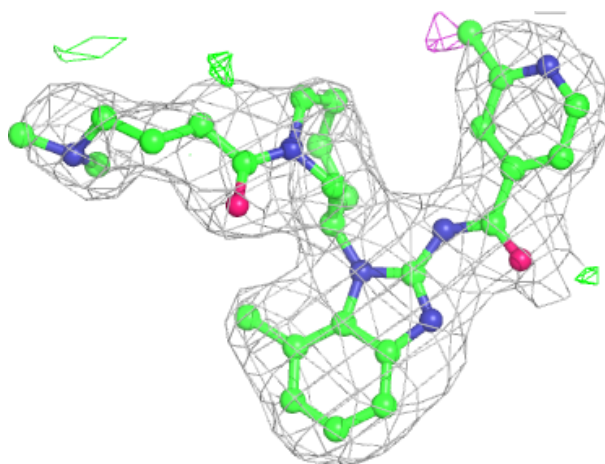
Electron density around 5XH A 501:

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



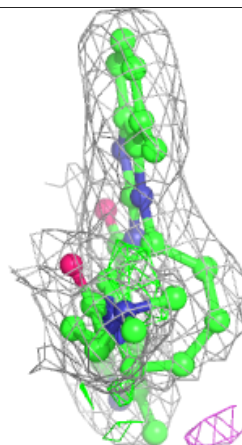
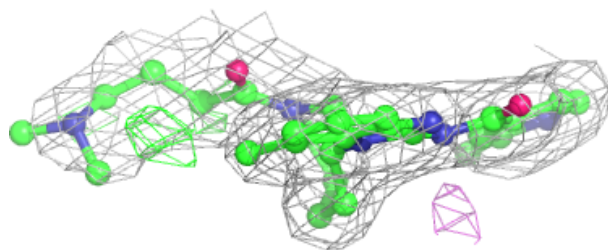
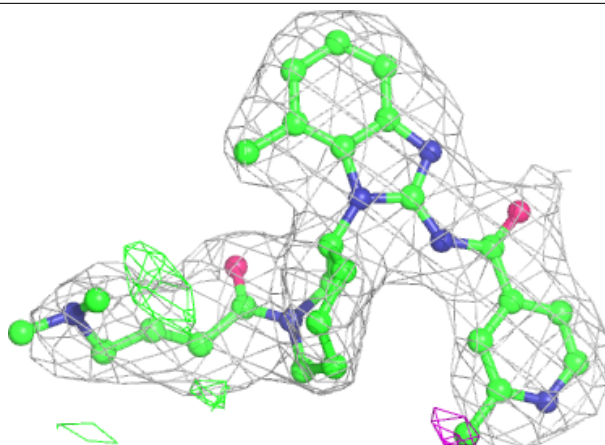
Electron density around 5XH J 504:

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



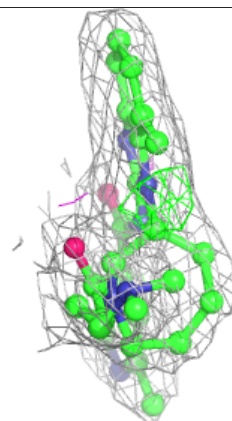
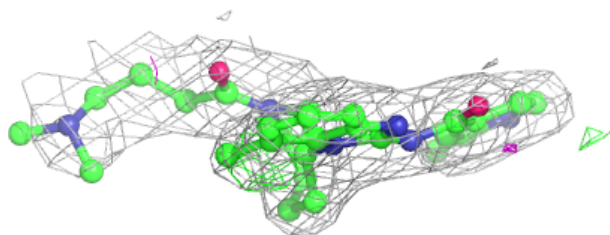
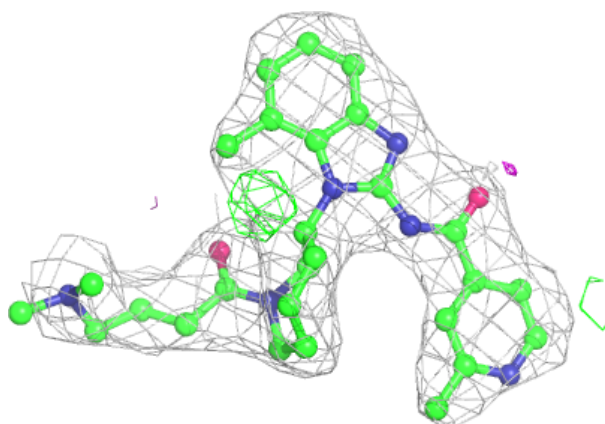
Electron density around 5XH K 503:

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



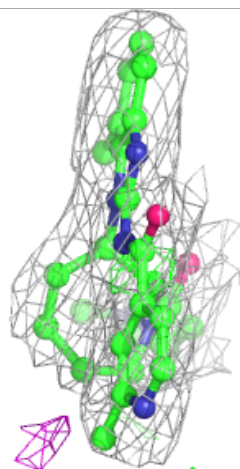
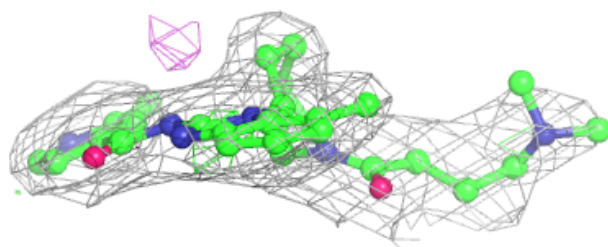
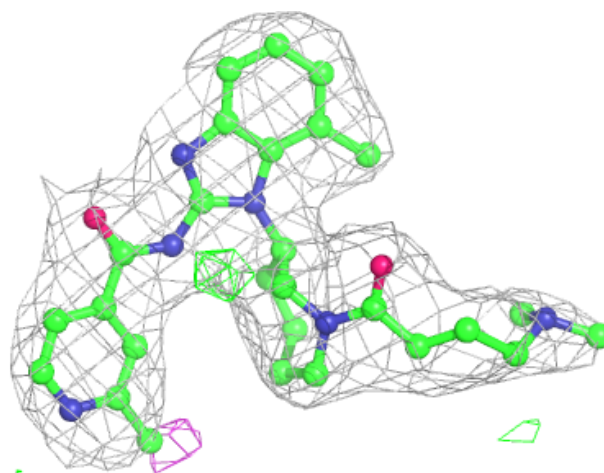
Electron density around 5XH H 503:

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and green (positive)



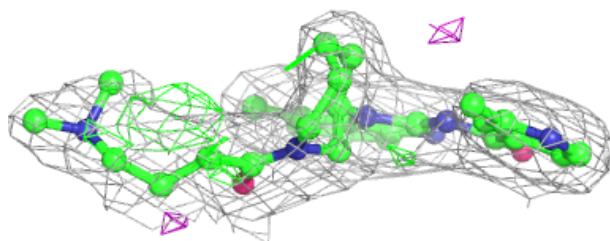
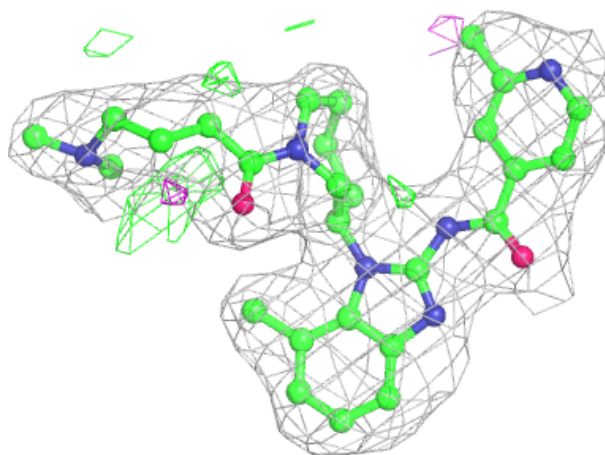
Electron density around 5XH E 504:

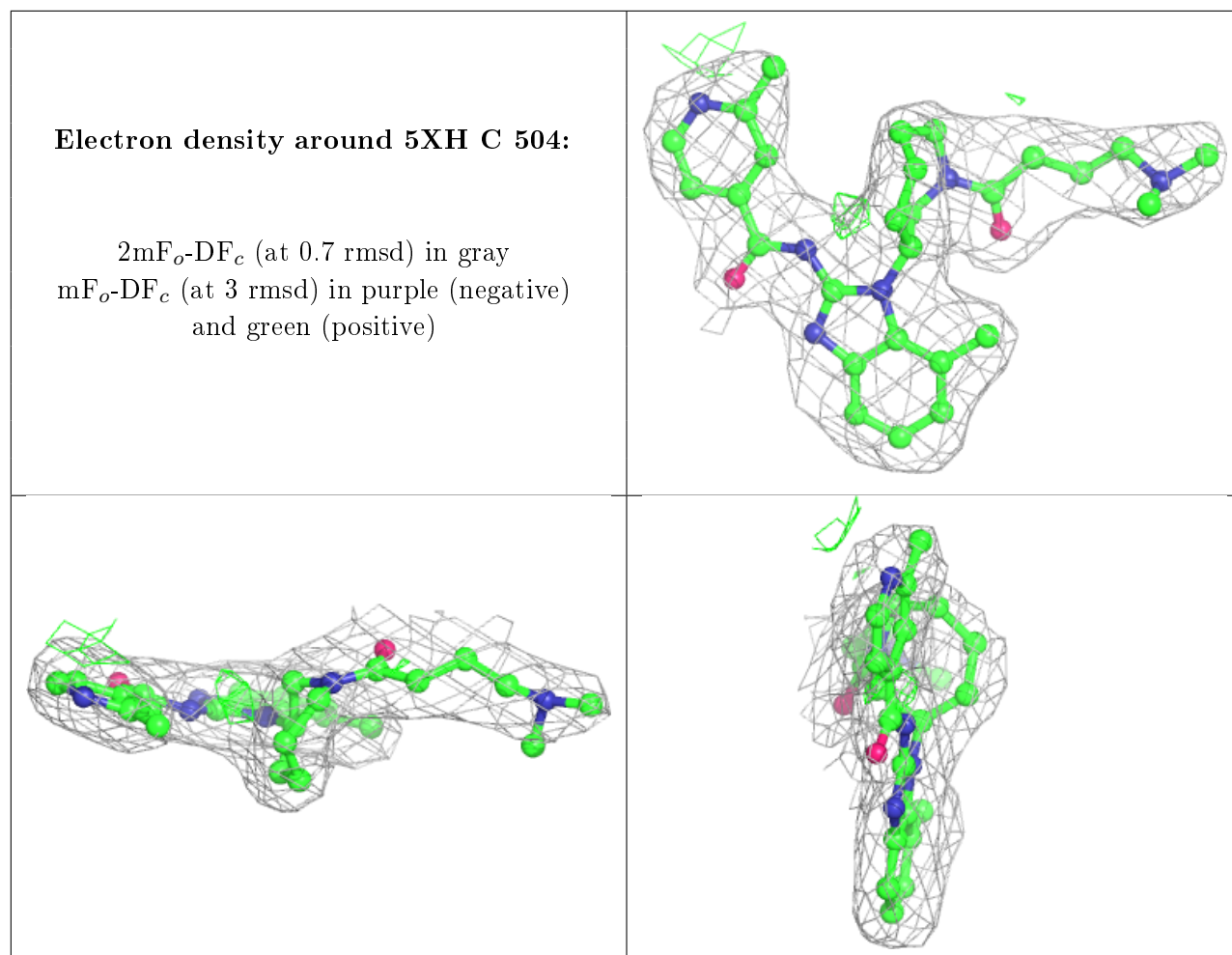
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 5XH B 504:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.