



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 04:43 PM EDT

PDB ID : 9P1X / pdb_00009p1x
EMDB ID : EMD-71144
Title : Cryo-EM structure of Nitrogenase MoFe protein from Methanosarcina acetivorans bound to the NifI inhibitor complex
Authors : Kashyap, R.; Antony, E.
Deposited on : 2025-06-11
Resolution : 3.16 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

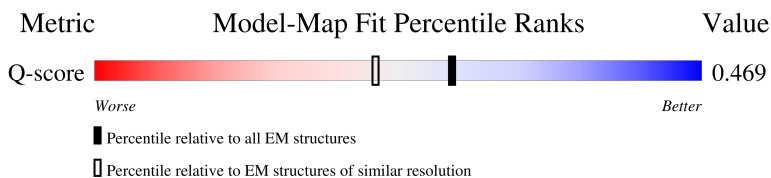
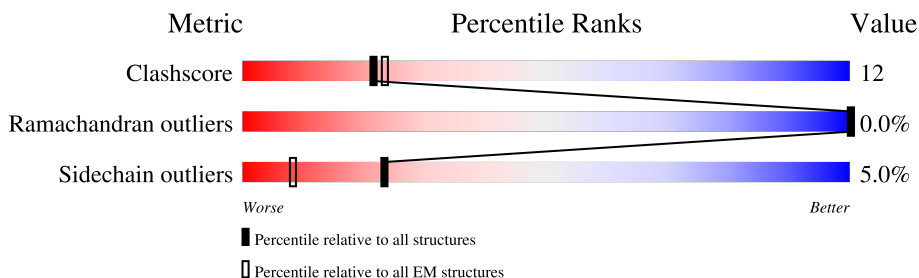
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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



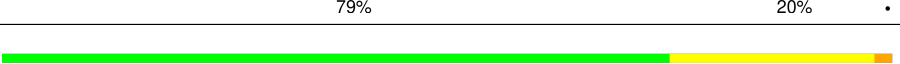
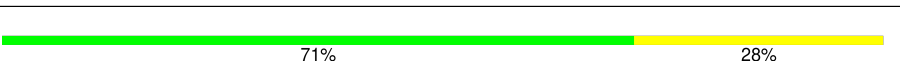
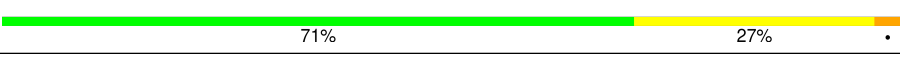
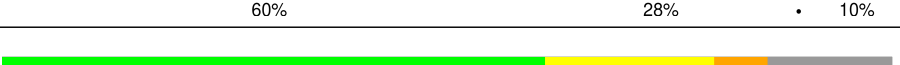
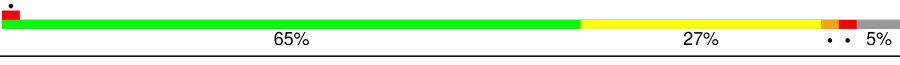
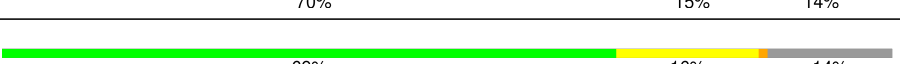
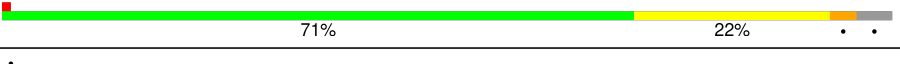
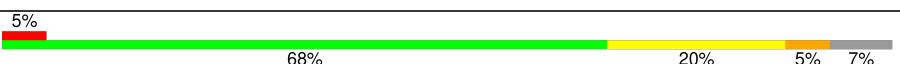
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14474 (2.66 - 3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	559	 64% 28% • 6%
1	C	559	 69% 23% • 7%
1	K	559	 65% 27% • • 6%
1	L	559	 65% 26% • 7%

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Mol	Chain	Length	Quality of chain
1	U	559	
1	V	559	
2	B	456	
2	D	456	
2	M	456	
2	N	456	
2	W	456	
2	X	456	
3	F	105	
3	H	105	
3	I	105	
3	J	105	
3	P	105	
3	R	105	
3	S	105	
3	T	105	
3	Z	105	
3	b	105	
3	c	105	
3	d	105	
4	E	125	
4	G	125	
4	O	125	
4	Q	125	
4	Y	125	

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Mol	Chain	Length	Quality of chain
4	a	125	

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
5	CLF	A	601	-	-	X	-
5	CLF	C	601	-	-	X	-
5	CLF	M	601	-	-	X	-
5	CLF	N	501	-	-	X	-
5	CLF	V	601	-	-	X	-
5	CLF	W	601	-	-	X	-
6	ICS	A	602	-	-	X	-
6	ICS	C	602	-	-	X	-
6	ICS	K	602	-	-	X	-
6	ICS	L	601	-	-	X	-
6	ICS	U	602	-	-	X	-
6	ICS	V	603	-	-	X	-
7	HCA	C	603	-	-	X	-
8	ADP	E	201	-	-	X	-
8	ADP	I	201	-	-	X	-
8	ADP	J	201	-	-	X	-
8	ADP	O	201	-	-	X	-
8	ADP	R	201	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60608 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Nitrogenase protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	525	Total	C	N	O	S	0	0
			4181	2655	720	785	21		
1	C	522	Total	C	N	O	S	0	0
			4159	2640	716	782	21		
1	K	525	Total	C	N	O	S	0	0
			4181	2655	720	785	21		
1	V	527	Total	C	N	O	S	0	0
			4190	2660	722	787	21		
1	L	519	Total	C	N	O	S	0	0
			4137	2627	713	776	21		
1	U	511	Total	C	N	O	S	0	0
			4075	2586	702	767	20		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	initiating methionine	UNP Q8TJ90
A	-29	TRP	-	expression tag	UNP Q8TJ90
A	-28	SER	-	expression tag	UNP Q8TJ90
A	-27	HIS	-	expression tag	UNP Q8TJ90
A	-26	PRO	-	expression tag	UNP Q8TJ90
A	-25	GLN	-	expression tag	UNP Q8TJ90
A	-24	PHE	-	expression tag	UNP Q8TJ90
A	-23	GLU	-	expression tag	UNP Q8TJ90
A	-22	LYS	-	expression tag	UNP Q8TJ90
A	-21	GLY	-	expression tag	UNP Q8TJ90
A	-20	GLY	-	expression tag	UNP Q8TJ90
A	-19	GLY	-	expression tag	UNP Q8TJ90
A	-18	SER	-	expression tag	UNP Q8TJ90
A	-17	GLY	-	expression tag	UNP Q8TJ90
A	-16	GLY	-	expression tag	UNP Q8TJ90
A	-15	GLY	-	expression tag	UNP Q8TJ90
A	-14	SER	-	expression tag	UNP Q8TJ90
A	-13	GLY	-	expression tag	UNP Q8TJ90

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	GLY	-	expression tag	UNP Q8TJ90
A	-11	GLY	-	expression tag	UNP Q8TJ90
A	-10	SER	-	expression tag	UNP Q8TJ90
A	-9	TRP	-	expression tag	UNP Q8TJ90
A	-8	SER	-	expression tag	UNP Q8TJ90
A	-7	HIS	-	expression tag	UNP Q8TJ90
A	-6	PRO	-	expression tag	UNP Q8TJ90
A	-5	GLN	-	expression tag	UNP Q8TJ90
A	-4	PHE	-	expression tag	UNP Q8TJ90
A	-3	GLU	-	expression tag	UNP Q8TJ90
A	-2	LYS	-	expression tag	UNP Q8TJ90
A	-1	SER	-	expression tag	UNP Q8TJ90
A	0	GLY	-	expression tag	UNP Q8TJ90
C	-30	MET	-	initiating methionine	UNP Q8TJ90
C	-29	TRP	-	expression tag	UNP Q8TJ90
C	-28	SER	-	expression tag	UNP Q8TJ90
C	-27	HIS	-	expression tag	UNP Q8TJ90
C	-26	PRO	-	expression tag	UNP Q8TJ90
C	-25	GLN	-	expression tag	UNP Q8TJ90
C	-24	PHE	-	expression tag	UNP Q8TJ90
C	-23	GLU	-	expression tag	UNP Q8TJ90
C	-22	LYS	-	expression tag	UNP Q8TJ90
C	-21	GLY	-	expression tag	UNP Q8TJ90
C	-20	GLY	-	expression tag	UNP Q8TJ90
C	-19	GLY	-	expression tag	UNP Q8TJ90
C	-18	SER	-	expression tag	UNP Q8TJ90
C	-17	GLY	-	expression tag	UNP Q8TJ90
C	-16	GLY	-	expression tag	UNP Q8TJ90
C	-15	GLY	-	expression tag	UNP Q8TJ90
C	-14	SER	-	expression tag	UNP Q8TJ90
C	-13	GLY	-	expression tag	UNP Q8TJ90
C	-12	GLY	-	expression tag	UNP Q8TJ90
C	-11	GLY	-	expression tag	UNP Q8TJ90
C	-10	SER	-	expression tag	UNP Q8TJ90
C	-9	TRP	-	expression tag	UNP Q8TJ90
C	-8	SER	-	expression tag	UNP Q8TJ90
C	-7	HIS	-	expression tag	UNP Q8TJ90
C	-6	PRO	-	expression tag	UNP Q8TJ90
C	-5	GLN	-	expression tag	UNP Q8TJ90
C	-4	PHE	-	expression tag	UNP Q8TJ90
C	-3	GLU	-	expression tag	UNP Q8TJ90
C	-2	LYS	-	expression tag	UNP Q8TJ90

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q8TJ90
C	0	GLY	-	expression tag	UNP Q8TJ90
K	-30	MET	-	initiating methionine	UNP Q8TJ90
K	-29	TRP	-	expression tag	UNP Q8TJ90
K	-28	SER	-	expression tag	UNP Q8TJ90
K	-27	HIS	-	expression tag	UNP Q8TJ90
K	-26	PRO	-	expression tag	UNP Q8TJ90
K	-25	GLN	-	expression tag	UNP Q8TJ90
K	-24	PHE	-	expression tag	UNP Q8TJ90
K	-23	GLU	-	expression tag	UNP Q8TJ90
K	-22	LYS	-	expression tag	UNP Q8TJ90
K	-21	GLY	-	expression tag	UNP Q8TJ90
K	-20	GLY	-	expression tag	UNP Q8TJ90
K	-19	GLY	-	expression tag	UNP Q8TJ90
K	-18	SER	-	expression tag	UNP Q8TJ90
K	-17	GLY	-	expression tag	UNP Q8TJ90
K	-16	GLY	-	expression tag	UNP Q8TJ90
K	-15	GLY	-	expression tag	UNP Q8TJ90
K	-14	SER	-	expression tag	UNP Q8TJ90
K	-13	GLY	-	expression tag	UNP Q8TJ90
K	-12	GLY	-	expression tag	UNP Q8TJ90
K	-11	GLY	-	expression tag	UNP Q8TJ90
K	-10	SER	-	expression tag	UNP Q8TJ90
K	-9	TRP	-	expression tag	UNP Q8TJ90
K	-8	SER	-	expression tag	UNP Q8TJ90
K	-7	HIS	-	expression tag	UNP Q8TJ90
K	-6	PRO	-	expression tag	UNP Q8TJ90
K	-5	GLN	-	expression tag	UNP Q8TJ90
K	-4	PHE	-	expression tag	UNP Q8TJ90
K	-3	GLU	-	expression tag	UNP Q8TJ90
K	-2	LYS	-	expression tag	UNP Q8TJ90
K	-1	SER	-	expression tag	UNP Q8TJ90
K	0	GLY	-	expression tag	UNP Q8TJ90
V	-30	MET	-	initiating methionine	UNP Q8TJ90
V	-29	TRP	-	expression tag	UNP Q8TJ90
V	-28	SER	-	expression tag	UNP Q8TJ90
V	-27	HIS	-	expression tag	UNP Q8TJ90
V	-26	PRO	-	expression tag	UNP Q8TJ90
V	-25	GLN	-	expression tag	UNP Q8TJ90
V	-24	PHE	-	expression tag	UNP Q8TJ90
V	-23	GLU	-	expression tag	UNP Q8TJ90
V	-22	LYS	-	expression tag	UNP Q8TJ90

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-21	GLY	-	expression tag	UNP Q8TJ90
V	-20	GLY	-	expression tag	UNP Q8TJ90
V	-19	GLY	-	expression tag	UNP Q8TJ90
V	-18	SER	-	expression tag	UNP Q8TJ90
V	-17	GLY	-	expression tag	UNP Q8TJ90
V	-16	GLY	-	expression tag	UNP Q8TJ90
V	-15	GLY	-	expression tag	UNP Q8TJ90
V	-14	SER	-	expression tag	UNP Q8TJ90
V	-13	GLY	-	expression tag	UNP Q8TJ90
V	-12	GLY	-	expression tag	UNP Q8TJ90
V	-11	GLY	-	expression tag	UNP Q8TJ90
V	-10	SER	-	expression tag	UNP Q8TJ90
V	-9	TRP	-	expression tag	UNP Q8TJ90
V	-8	SER	-	expression tag	UNP Q8TJ90
V	-7	HIS	-	expression tag	UNP Q8TJ90
V	-6	PRO	-	expression tag	UNP Q8TJ90
V	-5	GLN	-	expression tag	UNP Q8TJ90
V	-4	PHE	-	expression tag	UNP Q8TJ90
V	-3	GLU	-	expression tag	UNP Q8TJ90
V	-2	LYS	-	expression tag	UNP Q8TJ90
V	-1	SER	-	expression tag	UNP Q8TJ90
V	0	GLY	-	expression tag	UNP Q8TJ90
L	-30	MET	-	initiating methionine	UNP Q8TJ90
L	-29	TRP	-	expression tag	UNP Q8TJ90
L	-28	SER	-	expression tag	UNP Q8TJ90
L	-27	HIS	-	expression tag	UNP Q8TJ90
L	-26	PRO	-	expression tag	UNP Q8TJ90
L	-25	GLN	-	expression tag	UNP Q8TJ90
L	-24	PHE	-	expression tag	UNP Q8TJ90
L	-23	GLU	-	expression tag	UNP Q8TJ90
L	-22	LYS	-	expression tag	UNP Q8TJ90
L	-21	GLY	-	expression tag	UNP Q8TJ90
L	-20	GLY	-	expression tag	UNP Q8TJ90
L	-19	GLY	-	expression tag	UNP Q8TJ90
L	-18	SER	-	expression tag	UNP Q8TJ90
L	-17	GLY	-	expression tag	UNP Q8TJ90
L	-16	GLY	-	expression tag	UNP Q8TJ90
L	-15	GLY	-	expression tag	UNP Q8TJ90
L	-14	SER	-	expression tag	UNP Q8TJ90
L	-13	GLY	-	expression tag	UNP Q8TJ90
L	-12	GLY	-	expression tag	UNP Q8TJ90
L	-11	GLY	-	expression tag	UNP Q8TJ90

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-10	SER	-	expression tag	UNP Q8TJ90
L	-9	TRP	-	expression tag	UNP Q8TJ90
L	-8	SER	-	expression tag	UNP Q8TJ90
L	-7	HIS	-	expression tag	UNP Q8TJ90
L	-6	PRO	-	expression tag	UNP Q8TJ90
L	-5	GLN	-	expression tag	UNP Q8TJ90
L	-4	PHE	-	expression tag	UNP Q8TJ90
L	-3	GLU	-	expression tag	UNP Q8TJ90
L	-2	LYS	-	expression tag	UNP Q8TJ90
L	-1	SER	-	expression tag	UNP Q8TJ90
L	0	GLY	-	expression tag	UNP Q8TJ90
U	-30	MET	-	initiating methionine	UNP Q8TJ90
U	-29	TRP	-	expression tag	UNP Q8TJ90
U	-28	SER	-	expression tag	UNP Q8TJ90
U	-27	HIS	-	expression tag	UNP Q8TJ90
U	-26	PRO	-	expression tag	UNP Q8TJ90
U	-25	GLN	-	expression tag	UNP Q8TJ90
U	-24	PHE	-	expression tag	UNP Q8TJ90
U	-23	GLU	-	expression tag	UNP Q8TJ90
U	-22	LYS	-	expression tag	UNP Q8TJ90
U	-21	GLY	-	expression tag	UNP Q8TJ90
U	-20	GLY	-	expression tag	UNP Q8TJ90
U	-19	GLY	-	expression tag	UNP Q8TJ90
U	-18	SER	-	expression tag	UNP Q8TJ90
U	-17	GLY	-	expression tag	UNP Q8TJ90
U	-16	GLY	-	expression tag	UNP Q8TJ90
U	-15	GLY	-	expression tag	UNP Q8TJ90
U	-14	SER	-	expression tag	UNP Q8TJ90
U	-13	GLY	-	expression tag	UNP Q8TJ90
U	-12	GLY	-	expression tag	UNP Q8TJ90
U	-11	GLY	-	expression tag	UNP Q8TJ90
U	-10	SER	-	expression tag	UNP Q8TJ90
U	-9	TRP	-	expression tag	UNP Q8TJ90
U	-8	SER	-	expression tag	UNP Q8TJ90
U	-7	HIS	-	expression tag	UNP Q8TJ90
U	-6	PRO	-	expression tag	UNP Q8TJ90
U	-5	GLN	-	expression tag	UNP Q8TJ90
U	-4	PHE	-	expression tag	UNP Q8TJ90
U	-3	GLU	-	expression tag	UNP Q8TJ90
U	-2	LYS	-	expression tag	UNP Q8TJ90
U	-1	SER	-	expression tag	UNP Q8TJ90
U	0	GLY	-	expression tag	UNP Q8TJ90

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	456	Total	C	N	O	S	1	0
			3474	2202	585	665	22		
2	D	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		
2	M	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		
2	W	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		
2	X	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		
2	N	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		

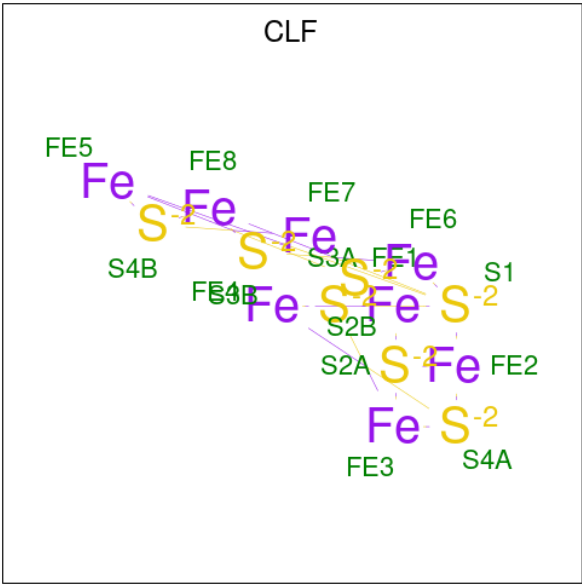
- Molecule 3 is a protein called P-II family nitrogen regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	J	95	Total	C	N	O	S	0	0
			747	469	129	140	9		
3	R	101	Total	C	N	O	S	0	0
			787	494	138	146	9		
3	T	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	b	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	d	101	Total	C	N	O	S	0	0
			795	499	138	149	9		
3	F	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	I	103	Total	C	N	O	S	0	0
			813	511	142	151	9		
3	P	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	S	100	Total	C	N	O	S	0	0
			790	496	137	148	9		
3	Z	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	c	103	Total	C	N	O	S	0	0
			813	511	142	151	9		

- Molecule 4 is a protein called P-II family nitrogen regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	120	Total	C	N	O	S	0	0
			936	588	168	174	6		
4	E	116	Total	C	N	O	S	1	0
			914	577	163	167	7		
4	Q	118	Total	C	N	O	S	0	0
			922	580	166	170	6		
4	O	116	Total	C	N	O	S	1	0
			914	577	163	167	7		
4	a	105	Total	C	N	O	S	0	0
			815	509	151	150	5		
4	Y	115	Total	C	N	O	S	1	0
			905	572	162	165	6		

- Molecule 5 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe₈S₇) (labeled as "Ligand of Interest" by depositor).



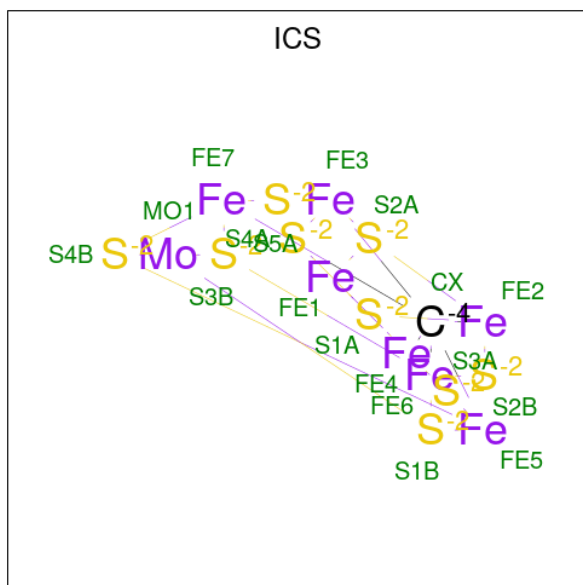
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Fe	S	0
			15	8	7	
5	C	1	Total	Fe	S	0
			15	8	7	
5	M	1	Total	Fe	S	0
			15	8	7	
5	V	1	Total	Fe	S	0
			15	8	7	
5	W	1	Total	Fe	S	0
			15	8	7	

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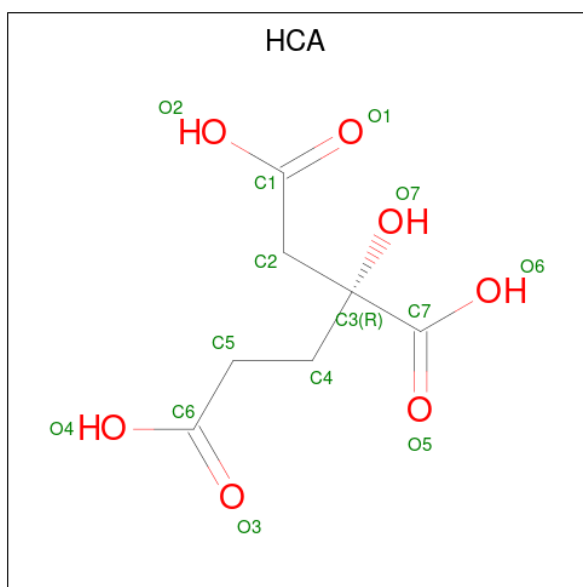
Mol	Chain	Residues	Atoms			AltConf
5	N	1	Total	Fe	S	0
			15	8	7	

- Molecule 6 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICS) (formula: CFe_7MoS_9) (labeled as "Ligand of Interest" by depositor).



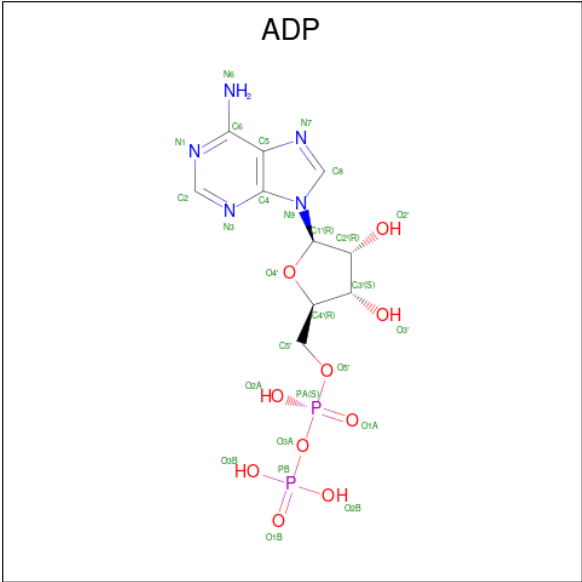
Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total 18	C 1	Fe 7	Mo 1	S 9	0	
6	C	1	Total 18	C 1	Fe 7	Mo 1	S 9	0	
6	K	1	Total 18	C 1	Fe 7	Mo 1	S 9	0	
6	V	1	Total 18	C 1	Fe 7	Mo 1	S 9	0	
6	L	1	Total 18	C 1	Fe 7	Mo 1	S 9	0	
6	U	1	Total 18	C 1	Fe 7	Mo 1	S 9	0	

- Molecule 7 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $\text{C}_7\text{H}_{10}\text{O}_7$) (labeled as "Ligand of Interest" by depositor).



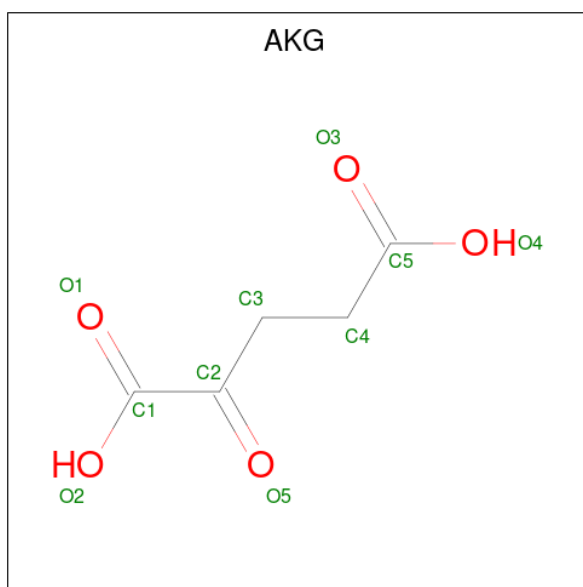
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			14	7	7	
7	C	1	Total	C	O	0
			14	7	7	
7	K	1	Total	C	O	0
			14	7	7	
7	V	1	Total	C	O	0
			14	7	7	
7	L	1	Total	C	O	0
			14	7	7	
7	U	1	Total	C	O	0
			14	7	7	

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	R	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	O	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	S	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 9 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅) (labeled as "Ligand of Interest" by depositor).

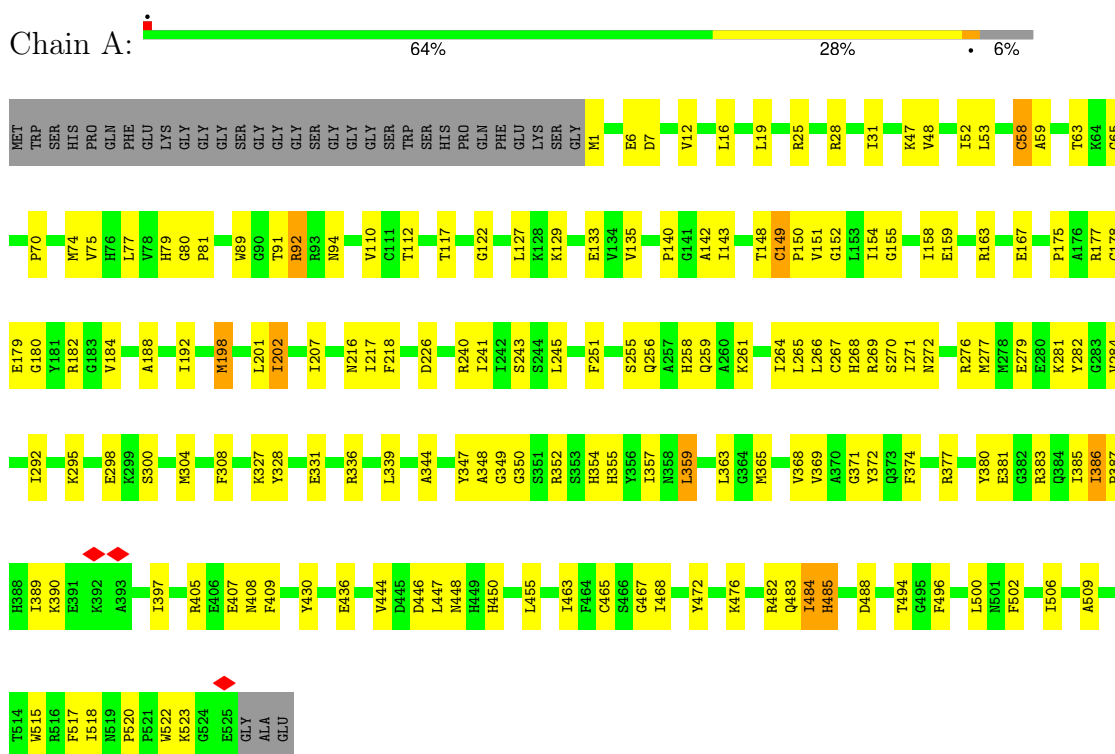


Mol	Chain	Residues	Atoms			AltConf
9	G	1	Total	C	O	0
			10	5	5	
9	a	1	Total	C	O	0
			10	5	5	
9	Y	1	Total	C	O	0
			10	5	5	

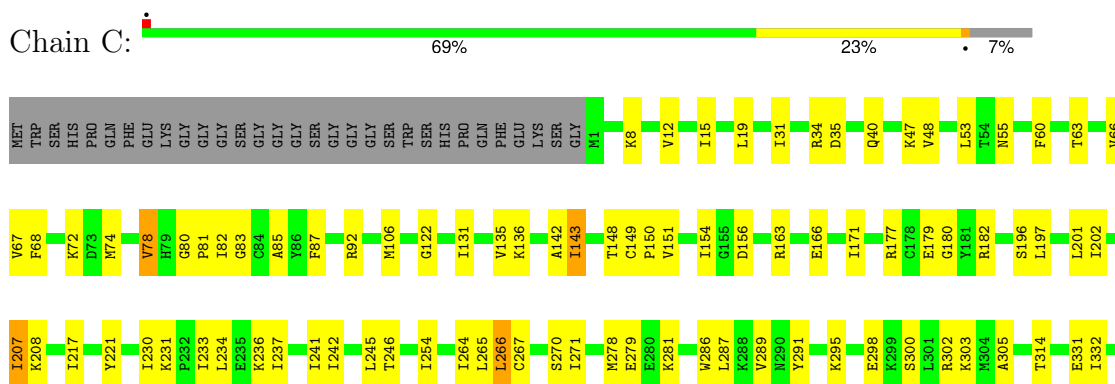
3 Residue-property plots [i](#)

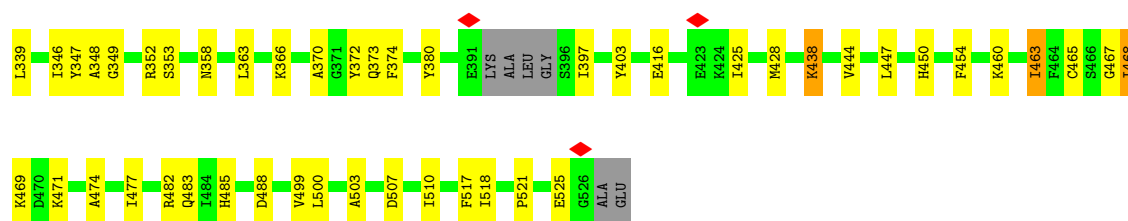
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitrogenase protein alpha chain



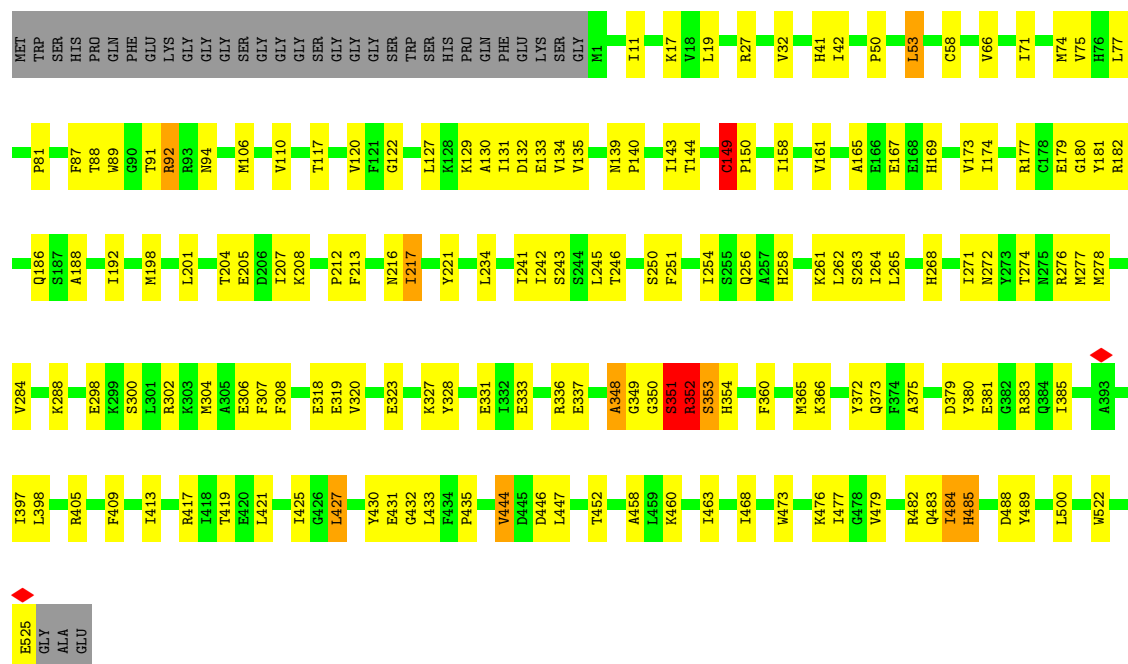
- Molecule 1: Nitrogenase protein alpha chain





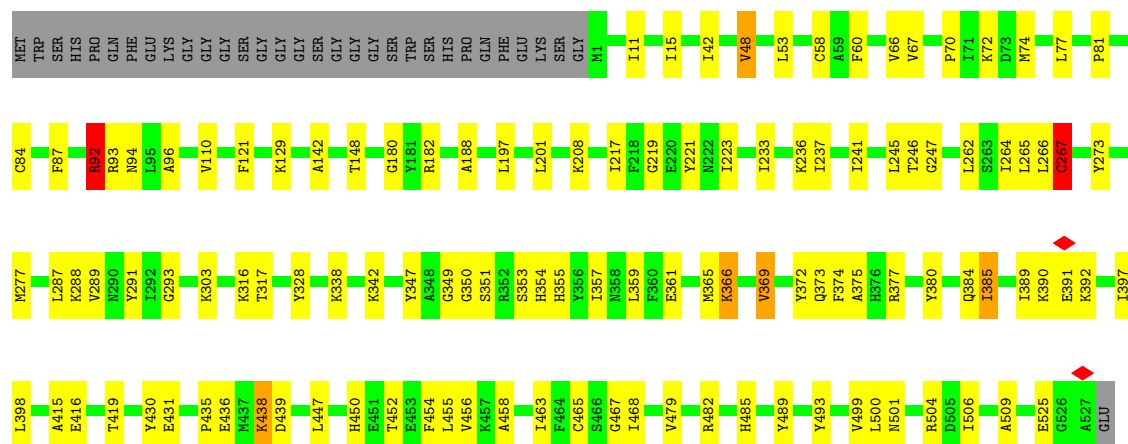
• Molecule 1: Nitrogenase protein alpha chain

Chain K: 65% 27% 6%



• Molecule 1: Nitrogenase protein alpha chain

Chain V: 73% 20% 6%



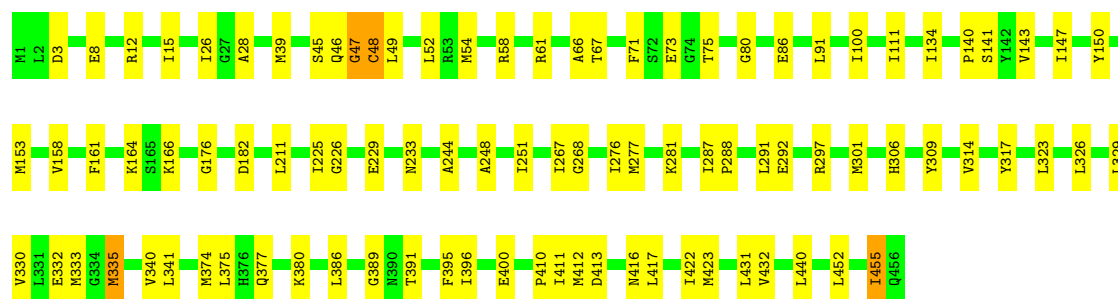
• Molecule 1: Nitrogenase protein alpha chain

Frequency	Percentage
Often	65%
Sometimes	26%
Rarely	7%

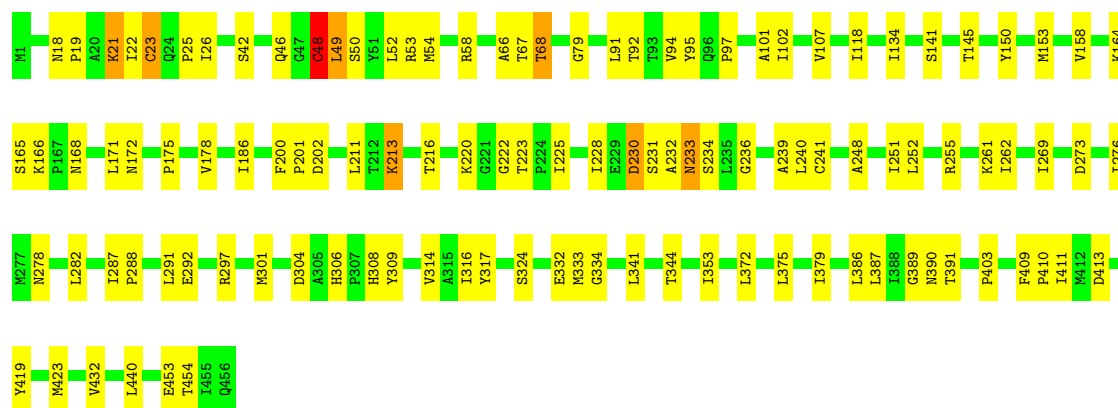


Frequency	Percentage
Often	6%
Sometimes	67%
Rarely	23%
Never	9%



Chain B:  79% 20%

• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

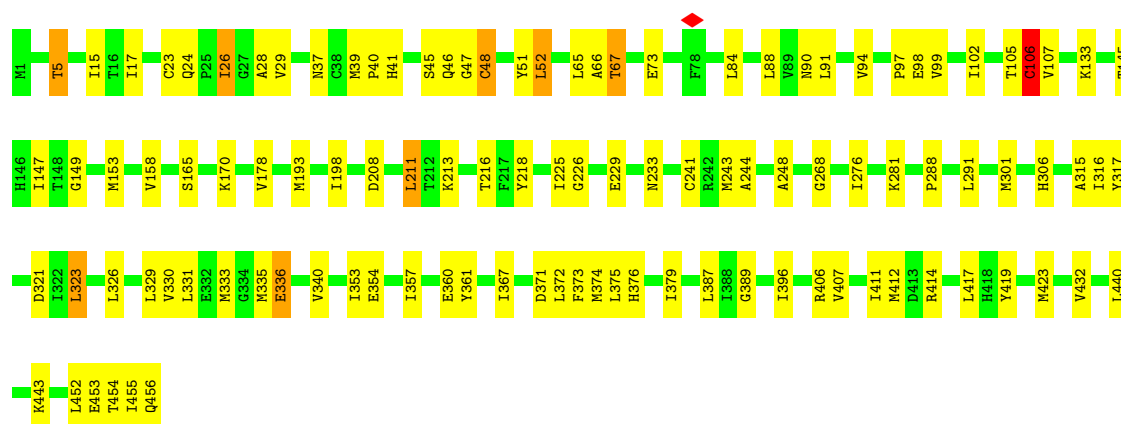
Chain D:  75% 23%

• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain M:  71% 28%

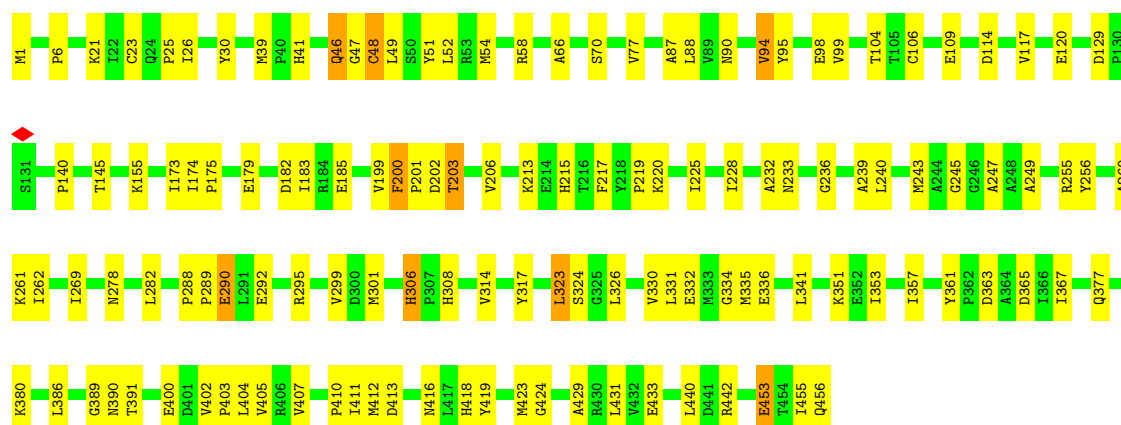
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain W:  76% 22%



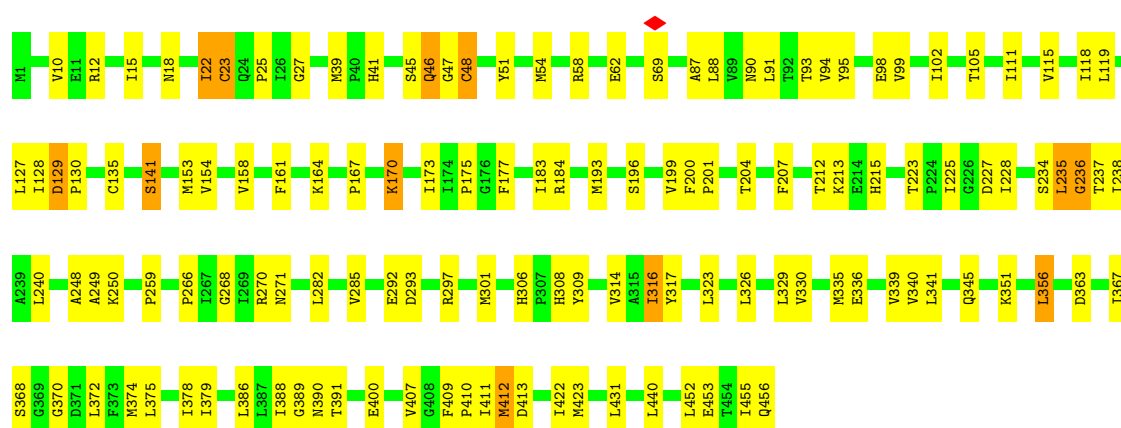
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain X: 71% 27%



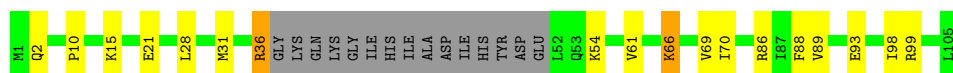
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain N: 71% 27%

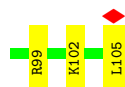


• Molecule 3: P-II family nitrogen regulatory protein

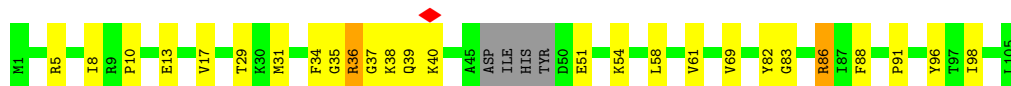
Chain H: 69% 15% 14%



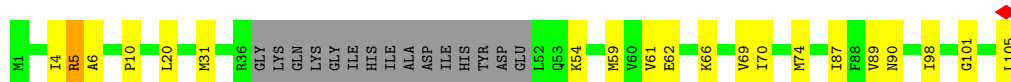
- Molecule 3: P-II family nitrogen regulatory protein



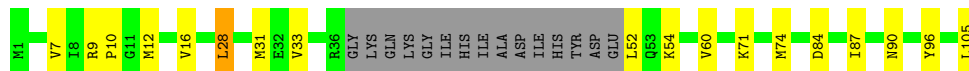
- Molecule 3: P-II family nitrogen regulatory protein



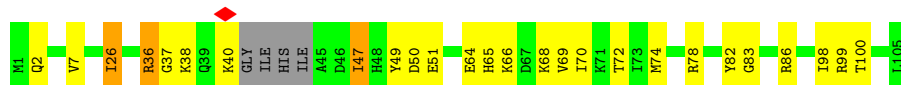
- Molecule 3: P-II family nitrogen regulatory protein



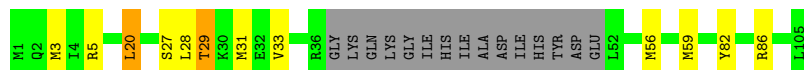
- Molecule 3: P-II family nitrogen regulatory protein



- Molecule 3: P-II family nitrogen regulatory protein

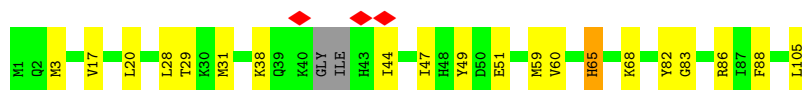


- Molecule 3: P-II family nitrogen regulatory protein



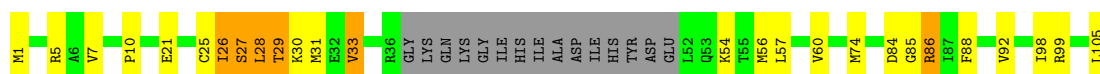
- Molecule 3: P-II family nitrogen regulatory protein

Chain I:  79% 18% ..



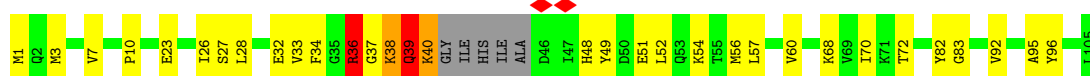
- Molecule 3: P-II family nitrogen regulatory protein

Chain P:  61% 19% 6% 14%



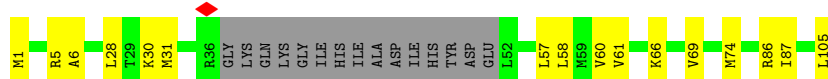
- Molecule 3: P-II family nitrogen regulatory protein

Chain S:  65% 27% .. 5%



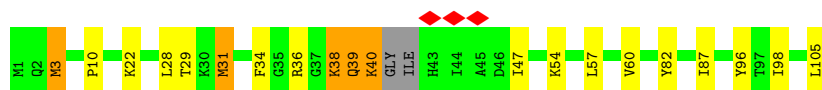
- Molecule 3: P-II family nitrogen regulatory protein

Chain Z:  70% 15% 14%



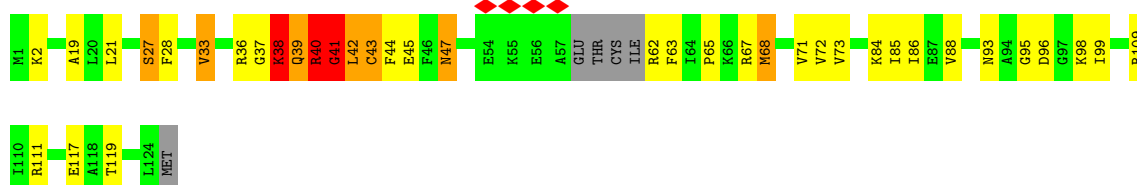
- Molecule 3: P-II family nitrogen regulatory protein

Chain c:  79% 14% 5% .



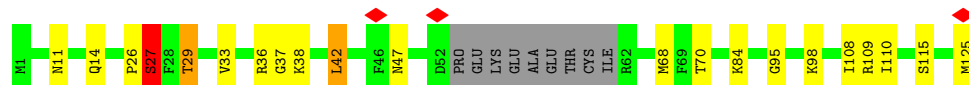
- Molecule 4: P-II family nitrogen regulatory protein

Chain G:  66% 22% 6% ..



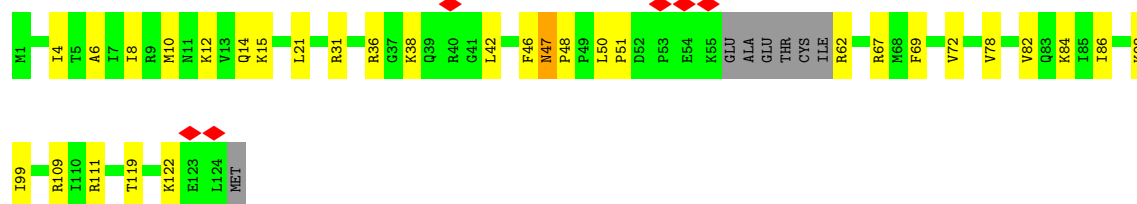
- Molecule 4: P-II family nitrogen regulatory protein

Chain E:  76% 14% 7%



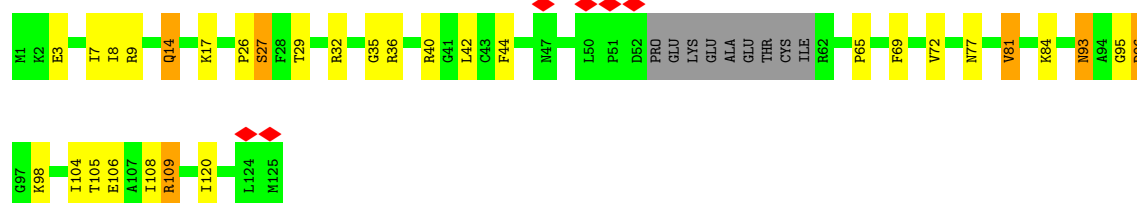
- Molecule 4: P-II family nitrogen regulatory protein

Chain Q:  5% 70% 24% 6%



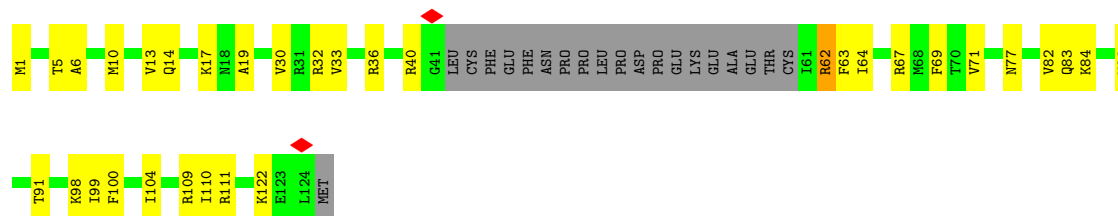
- Molecule 4: P-II family nitrogen regulatory protein

Chain O:  5% 68% 20% 5% 7%



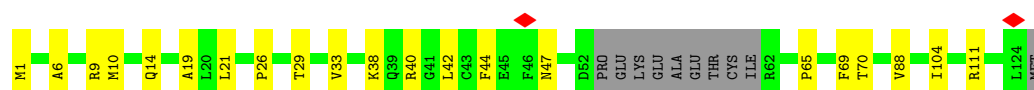
- Molecule 4: P-II family nitrogen regulatory protein

Chain a:  58% 26% 16%



- Molecule 4: P-II family nitrogen regulatory protein

Chain Y:  75% 17% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74083	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	150000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.768	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.0204	Depositor
Map size ($\text{\AA}$)	371.19998, 371.19998, 371.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.928, 0.928, 0.928	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLF, AKG, ICS, ADP, HCA

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	0.20	0/4273	0.50	7/5760 (0.1%)
1	C	0.17	0/4250	0.34	2/5728 (0.0%)
1	K	0.30	2/4273 (0.0%)	0.46	6/5760 (0.1%)
1	L	0.15	0/4227	0.32	0/5696
1	U	0.19	0/4163	0.38	5/5610 (0.1%)
1	V	0.19	0/4282	0.40	4/5772 (0.1%)
2	B	0.21	1/3548 (0.0%)	0.42	7/4819 (0.1%)
2	D	0.22	0/3537	0.51	3/4804 (0.1%)
2	M	0.17	0/3537	0.39	1/4804 (0.0%)
2	N	0.29	1/3537 (0.0%)	0.56	8/4804 (0.2%)
2	W	0.19	0/3537	0.44	10/4804 (0.2%)
2	X	0.22	0/3537	0.51	5/4804 (0.1%)
3	F	0.10	0/709	0.25	0/942
3	H	0.11	0/709	0.28	0/942
3	I	0.13	0/821	0.29	0/1092
3	J	0.12	0/754	0.32	0/1003
3	P	0.27	0/709	0.53	1/942 (0.1%)
3	R	0.19	0/793	0.38	0/1053
3	S	0.27	0/797	0.52	2/1059 (0.2%)
3	T	0.11	0/709	0.27	0/942
3	Z	0.10	0/709	0.22	0/942
3	b	0.11	0/709	0.30	0/942
3	c	0.17	0/821	0.30	0/1092
3	d	0.22	0/802	0.40	0/1066
4	E	0.23	0/928	0.64	4/1241 (0.3%)
4	G	0.38	0/947	0.69	4/1269 (0.3%)
4	O	0.26	0/928	0.55	4/1241 (0.3%)
4	Q	0.12	0/933	0.28	0/1250
4	Y	0.10	0/919	0.24	0/1231
4	a	0.12	0/820	0.28	0/1094
All	All	0.21	4/61218 (0.0%)	0.43	73/82508 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	K	0	2
1	U	0	1
1	V	0	1
2	D	0	1
3	P	0	1
3	R	0	1
3	S	0	1
3	d	0	1
4	G	0	1
4	O	0	1
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	348	ALA	C-O	-10.90	1.09	1.23
1	K	351	SER	C-O	6.42	1.32	1.24
2	N	141	SER	CA-CB	-5.70	1.44	1.53
2	B	48	CYS	CA-C	-5.56	1.45	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	CYS	CB-CA-C	-18.20	84.06	113.37
2	X	48	CYS	CB-CA-C	-14.19	87.45	110.86
1	V	267	CYS	CB-CA-C	-13.21	88.53	110.19
2	M	48	CYS	CB-CA-C	-12.73	90.89	110.88
2	B	48	CYS	CA-CB-SG	-11.47	88.02	114.40
2	D	23	CYS	CB-CA-C	-11.23	87.95	113.33
1	K	348	ALA	CA-C-O	-11.11	107.56	121.78
2	N	48	CYS	CA-CB-SG	-10.63	89.96	114.40
4	E	26	PRO	CA-C-N	-10.27	108.05	122.93
4	E	26	PRO	C-N-CA	-10.27	108.05	122.93
4	E	27	SER	N-CA-CB	-10.11	94.41	110.69
1	A	267	CYS	CA-CB-SG	-9.82	91.81	114.40
2	B	48	CYS	CA-C-N	-9.08	107.94	120.38
2	B	48	CYS	C-N-CA	-9.08	107.94	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	48	CYS	CB-CA-C	-8.92	93.24	110.11
4	E	27	SER	CB-CA-C	8.85	125.31	109.38
4	O	96	ASP	N-CA-C	-8.11	101.71	111.69
2	W	106	CYS	CA-C-N	-8.05	110.21	120.60
2	W	106	CYS	C-N-CA	-8.05	110.21	120.60
4	G	44	PHE	N-CA-C	-7.75	103.97	113.19
1	A	266	LEU	CA-C-N	-6.97	112.89	122.30
1	A	266	LEU	C-N-CA	-6.97	112.89	122.30
2	W	106	CYS	CA-CB-SG	-6.96	98.40	114.40
4	O	96	ASP	CB-CA-C	6.85	123.24	110.70
3	P	29	THR	CA-CB-OG1	-6.58	99.72	109.60
4	G	41	GLY	CA-C-N	-6.54	110.87	121.26
4	G	41	GLY	C-N-CA	-6.54	110.87	121.26
1	U	149	CYS	CA-CB-SG	-6.48	99.49	114.40
2	N	47	GLY	CA-C-N	-6.43	109.58	120.58
2	N	47	GLY	C-N-CA	-6.43	109.58	120.58
1	A	485	HIS	CA-CB-CG	6.35	120.15	113.80
2	N	23	CYS	CA-C-N	6.32	128.91	120.58
2	N	23	CYS	C-N-CA	6.32	128.91	120.58
2	N	236	GLY	CA-C-O	-6.29	115.46	121.38
2	N	23	CYS	CA-CB-SG	6.19	128.63	114.40
1	V	267	CYS	CA-C-N	-6.18	110.87	120.88
1	V	267	CYS	C-N-CA	-6.18	110.87	120.88
1	U	92	ARG	CA-C-N	-6.13	112.47	122.65
1	U	92	ARG	C-N-CA	-6.13	112.47	122.65
3	S	39	GLN	CB-CA-C	-6.07	109.56	116.54
2	W	105	THR	CA-C-N	-6.06	110.38	120.68
2	W	105	THR	C-N-CA	-6.06	110.38	120.68
2	D	48	CYS	CB-CA-C	-6.03	98.42	110.42
2	W	105	THR	O-C-N	-6.03	114.42	122.14
1	K	149	CYS	CB-CA-C	-5.89	103.43	113.04
2	X	47	GLY	CA-C-N	-5.83	111.43	120.88
2	X	47	GLY	C-N-CA	-5.83	111.43	120.88
2	X	48	CYS	CA-C-N	-5.78	112.46	120.38
2	X	48	CYS	C-N-CA	-5.78	112.46	120.38
2	B	47	GLY	O-C-N	-5.53	116.38	122.24
2	N	141	SER	CA-CB-OG	-5.50	100.10	111.10
1	V	267	CYS	CA-CB-SG	-5.47	101.81	114.40
2	W	23	CYS	CB-CA-C	5.46	119.58	109.54
1	K	485	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	K	149	CYS	N-CA-CB	5.40	116.79	110.42
1	U	149	CYS	CA-C-N	-5.40	114.05	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	149	CYS	C-N-CA	-5.40	114.05	119.56
2	W	23	CYS	CA-CB-SG	5.34	126.69	114.40
4	G	38	LYS	N-CA-C	-5.32	107.45	114.31
2	D	118	ILE	N-CA-C	-5.30	106.70	112.80
1	A	266	LEU	O-C-N	5.21	129.11	122.03
1	A	485	HIS	CB-CG-CD2	-5.16	124.49	131.20
2	W	46	GLN	CA-C-N	-5.14	113.70	120.22
2	W	46	GLN	C-N-CA	-5.14	113.70	120.22
2	B	47	GLY	CA-C-N	-5.13	110.72	121.64
2	B	47	GLY	C-N-CA	-5.13	110.72	121.64
3	S	36	ARG	N-CA-C	-5.11	102.73	110.24
4	O	26	PRO	CA-C-N	-5.10	115.97	123.00
4	O	26	PRO	C-N-CA	-5.10	115.97	123.00
1	C	266	LEU	CA-C-N	-5.05	116.06	122.77
1	C	266	LEU	C-N-CA	-5.05	116.06	122.77
1	K	149	CYS	CA-C-N	-5.02	113.65	119.47
1	K	149	CYS	C-N-CA	-5.02	113.65	119.47

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	ARG	Sidechain
2	D	233	ASN	Peptide
4	G	40	ARG	Sidechain
1	K	352	ARG	Sidechain
1	K	92	ARG	Sidechain
4	O	109	ARG	Sidechain
3	P	25	CYS	Mainchain
3	R	86	ARG	Sidechain
3	S	36	ARG	Sidechain
1	U	92	ARG	Sidechain
1	V	92	ARG	Sidechain
3	d	36	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	4181	0	4130	125	0
1	C	4159	0	4100	101	0
1	K	4181	0	4130	111	0
1	L	4137	0	4080	112	0
1	U	4075	0	4008	109	0
1	V	4190	0	4139	90	0
2	B	3474	0	3487	61	0
2	D	3467	0	3481	90	0
2	M	3467	0	3480	86	0
2	N	3467	0	3481	89	0
2	W	3467	0	3480	75	0
2	X	3467	0	3480	91	0
3	F	704	0	745	22	0
3	H	704	0	745	15	0
3	I	813	0	846	26	0
3	J	747	0	774	28	0
3	P	704	0	745	23	0
3	R	787	0	829	26	0
3	S	790	0	823	26	0
3	T	704	0	745	17	0
3	Z	704	0	745	10	0
3	b	704	0	745	14	0
3	c	813	0	846	17	0
3	d	795	0	828	24	0
4	E	914	0	952	37	0
4	G	936	0	971	32	0
4	O	914	0	952	34	0
4	Q	922	0	960	27	0
4	Y	905	0	943	13	0
4	a	815	0	863	27	0
5	A	15	0	0	7	0
5	C	15	0	0	6	0
5	M	15	0	0	5	0
5	N	15	0	0	7	0
5	V	15	0	0	7	0
5	W	15	0	0	7	0
6	A	18	0	0	12	0
6	C	18	0	0	14	0
6	K	18	0	0	6	0
6	L	18	0	0	8	0
6	U	18	0	0	12	0
6	V	18	0	0	9	0
7	A	14	0	7	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	14	0	7	6	0
7	K	14	0	7	4	0
7	L	14	0	6	1	0
7	U	14	0	7	0	0
7	V	14	0	6	4	0
8	E	27	0	12	36	0
8	I	27	0	12	19	0
8	J	27	0	12	13	0
8	O	27	0	12	15	0
8	R	27	0	12	12	0
8	S	27	0	12	3	0
8	d	27	0	12	7	0
9	G	10	0	4	3	0
9	Y	10	0	4	0	0
9	a	10	0	4	1	0
All	All	60608	0	60669	1424	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1424) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:38:LYS:HE3	8:I:201:ADP:PB	1.69	1.31
1:L:92:ARG:NH2	6:L:601:ICS:S5A	2.13	1.22
4:E:98:LYS:HD2	8:E:201:ADP:C8	1.78	1.19
3:I:38:LYS:HE3	8:I:201:ADP:O1B	1.54	1.08
5:A:601:CLF:S4A	2:B:48:CYS:SG	2.52	1.08
4:E:98:LYS:CD	8:E:201:ADP:C8	2.38	1.05
1:A:349:GLY:HA3	6:A:602:ICS:S1B	1.96	1.05
4:O:35:GLY:HA3	8:O:201:ADP:O2'	1.55	1.04
8:E:201:ADP:C2	3:F:28:LEU:CA	2.41	1.04
3:I:38:LYS:HB2	8:I:201:ADP:O3B	1.57	1.04
1:L:269:ARG:HH12	1:L:375:ALA:HA	1.26	1.01
8:O:201:ADP:N6	3:P:60:VAL:H	1.59	0.99
1:C:92:ARG:NH1	6:C:602:ICS:S3A	2.34	0.99
5:W:601:CLF:S3B	1:U:180:GLY:HA3	2.02	0.98
8:J:201:ADP:N7	4:E:27:SER:HB3	1.78	0.97
4:E:38:LYS:HG2	8:E:201:ADP:O2B	1.61	0.97
1:K:81:PRO:HB2	5:M:601:CLF:S2B	2.04	0.97
8:E:201:ADP:C2	3:F:28:LEU:C	2.46	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:98:LYS:CD	8:E:201:ADP:N7	2.32	0.93
8:E:201:ADP:C2	3:F:28:LEU:HA	2.03	0.93
1:C:221:TYR:HE2	6:C:602:ICS:S4A	1.91	0.92
1:A:374:PHE:HZ	6:A:602:ICS:S2B	1.93	0.91
3:I:86:ARG:NH1	8:I:201:ADP:C8	2.39	0.91
4:E:98:LYS:HD3	8:E:201:ADP:N7	1.87	0.90
1:C:81:PRO:HG2	5:C:601:CLF:S4B	2.12	0.90
2:X:403:PRO:HG3	2:X:442:ARG:HG3	1.53	0.90
1:A:148:THR:HG23	1:A:150:PRO:HD2	1.55	0.89
4:G:72:VAL:H	8:I:201:ADP:HN62	1.21	0.89
1:L:81:PRO:HG2	5:N:501:CLF:S3A	2.12	0.88
1:A:374:PHE:CZ	6:A:602:ICS:S2B	2.66	0.88
3:J:54:LYS:HG3	8:J:201:ADP:O3'	1.75	0.87
4:E:38:LYS:H	8:E:201:ADP:PB	1.99	0.86
1:U:66:VAL:HG13	6:U:602:ICS:S2A	2.16	0.86
2:N:23:CYS:SG	5:N:501:CLF:S2A	2.73	0.86
3:I:83:GLY:HA2	8:I:201:ADP:H5'1	1.58	0.85
1:A:350:GLY:HA3	6:A:602:ICS:S1A	2.15	0.85
8:O:201:ADP:C2	3:P:27:SER:HB3	2.11	0.84
1:K:276:ARG:HE	1:K:383:ARG:HH12	1.25	0.84
1:V:219:GLY:HA3	1:V:267:CYS:HB2	1.57	0.84
4:E:98:LYS:HD2	8:E:201:ADP:H8	1.36	0.84
2:D:200:PHE:HB2	2:D:201:PRO:HD3	1.60	0.84
1:A:81:PRO:HB2	5:A:601:CLF:S3B	2.17	0.83
1:L:352:ARG:NH1	6:L:601:ICS:S4B	2.51	0.83
4:O:35:GLY:CA	8:O:201:ADP:O2'	2.25	0.83
7:C:603:HCA:O5	2:D:54:MET:HE1	1.75	0.83
8:E:201:ADP:H2	3:F:29:THR:N	1.77	0.83
1:L:368:VAL:HG23	1:L:369:VAL:HG23	1.60	0.83
3:I:38:LYS:CE	8:I:201:ADP:PB	2.62	0.83
5:W:601:CLF:S2A	1:U:81:PRO:HB2	2.18	0.82
1:C:347:TYR:HE2	1:C:447:LEU:HB3	1.45	0.81
3:I:38:LYS:CE	8:I:201:ADP:O1B	2.29	0.81
1:A:386:ILE:HG23	1:A:387:PRO:HD3	1.62	0.81
1:C:180:GLY:HA3	5:C:601:CLF:S3A	2.21	0.81
3:P:28:LEU:HD11	3:P:57:LEU:HB3	1.62	0.81
2:X:236:GLY:HA3	2:X:282:LEU:HD23	1.64	0.80
1:A:467:GLY:HA2	1:A:485:HIS:HD2	1.46	0.80
1:A:467:GLY:HA2	1:A:485:HIS:CD2	2.16	0.80
3:H:98:ILE:HD13	4:G:86:ILE:HD13	1.63	0.79
2:M:454:THR:HB	1:L:93:ARG:HH11	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:PHE:HB3	5:C:601:CLF:S2A	2.22	0.79
2:X:23:CYS:SG	2:X:25:PRO:HD2	2.23	0.78
1:L:386:ILE:HG23	1:L:387:PRO:HD3	1.64	0.78
2:D:202:ASP:HB3	2:D:222:GLY:HA3	1.66	0.78
2:X:174:ILE:HG21	2:X:245:GLY:HA3	1.66	0.78
6:C:602:ICS:S4B	7:C:603:HCA:O7	2.42	0.78
2:D:165:SER:H	2:D:232:ALA:HB2	1.49	0.77
1:U:207:ILE:HG22	1:U:256:GLN:HB3	1.67	0.77
1:U:66:VAL:CG1	6:U:602:ICS:S2A	2.73	0.77
3:I:86:ARG:NH1	8:I:201:ADP:O4'	2.19	0.76
3:R:37:GLY:HA3	8:R:201:ADP:H3'	1.66	0.76
1:V:81:PRO:HG2	5:V:601:CLF:S4B	2.25	0.76
1:V:468:ILE:HG22	7:V:602:HCA:O3	1.84	0.76
1:C:468:ILE:HG22	7:C:603:HCA:O4	1.85	0.76
2:D:314:VAL:HG12	2:D:386:LEU:HB3	1.68	0.75
8:O:201:ADP:HN62	3:P:60:VAL:H	1.29	0.75
2:N:46:GLN:HA	2:N:69:SER:HB2	1.67	0.75
1:V:148:THR:HB	5:V:601:CLF:S4A	2.27	0.75
1:V:217:ILE:HD11	1:V:241:ILE:HD12	1.69	0.74
3:b:74:MET:HE1	3:c:98:ILE:HA	1.69	0.74
1:L:290:ASN:HD21	1:L:355:HIS:HA	1.52	0.74
1:A:182:ARG:HD3	1:A:397:ILE:HG12	1.69	0.74
1:A:202:ILE:HA	1:A:255:SER:HA	1.69	0.74
2:N:105:THR:HB	5:N:501:CLF:S4A	2.28	0.74
8:E:201:ADP:H2	3:F:28:LEU:C	1.92	0.74
1:C:286:TRP:H	1:C:428:MET:HE1	1.53	0.74
1:K:351:SER:O	1:K:353:SER:N	2.20	0.74
2:X:26:ILE:HB	2:X:52:LEU:HD22	1.70	0.74
1:A:268:HIS:O	1:A:272:ASN:HB3	1.87	0.73
1:U:149:CYS:HA	1:U:179:GLU:HG3	1.70	0.73
1:C:374:PHE:CZ	6:C:602:ICS:S5A	2.81	0.73
4:G:27:SER:HB3	8:I:201:ADP:N7	2.02	0.73
8:E:201:ADP:H2	3:F:28:LEU:CA	2.02	0.73
1:V:219:GLY:CA	1:V:267:CYS:HB2	2.19	0.73
4:Q:21:LEU:HD21	3:S:36:ARG:HH12	1.52	0.72
1:C:518:ILE:HG22	2:D:213:LYS:HD3	1.71	0.72
4:E:33:VAL:HG12	3:F:31:MET:HB3	1.70	0.72
1:U:374:PHE:HE1	6:U:602:ICS:S1A	2.12	0.72
4:E:38:LYS:N	8:E:201:ADP:O2B	2.20	0.72
2:W:99:VAL:HG11	2:W:225:ILE:HD12	1.71	0.72
3:S:37:GLY:O	3:S:49:TYR:HD1	1.73	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:331:GLU:HB3	1:K:500:LEU:HD21	1.72	0.72
4:E:37:GLY:HA3	8:E:201:ADP:O3B	1.90	0.72
4:G:27:SER:HB3	8:I:201:ADP:C8	2.25	0.72
5:A:601:CLF:S3B	2:B:141:SER:OG	2.48	0.71
4:G:37:GLY:HA3	9:G:201:AKG:H32	1.71	0.71
4:O:95:GLY:N	8:O:201:ADP:O2B	2.24	0.71
1:L:374:PHE:HE1	6:L:601:ICS:S1A	2.12	0.71
2:B:39:MET:HG2	2:B:91:LEU:HD21	1.71	0.71
1:C:148:THR:HB	5:C:601:CLF:S4A	2.31	0.71
3:I:38:LYS:CB	8:I:201:ADP:O3B	2.37	0.70
3:S:7:VAL:HG11	8:S:201:ADP:H8	1.54	0.70
1:L:287:LEU:HB3	1:L:427:LEU:HD12	1.73	0.70
2:N:41:HIS:HB2	2:N:102:ILE:HA	1.72	0.70
1:U:66:VAL:HG21	6:U:602:ICS:S2B	2.31	0.70
3:P:5:ARG:HG3	3:P:56:MET:HE3	1.73	0.70
2:M:314:VAL:HG12	2:M:386:LEU:HB3	1.73	0.70
1:L:229:GLU:HG2	1:L:492:ARG:HE	1.57	0.69
1:A:352:ARG:HB2	6:A:602:ICS:S3A	2.32	0.69
1:C:151:VAL:HG13	1:C:156:ASP:HB2	1.75	0.69
8:E:201:ADP:C2	3:F:29:THR:N	2.58	0.69
4:a:1:MET:HB2	4:a:104:ILE:HB	1.74	0.69
2:N:213:LYS:HD3	2:N:213:LYS:N	2.07	0.69
1:A:77:LEU:HD11	1:A:112:THR:HG23	1.73	0.69
1:V:349:GLY:HA2	1:V:373:GLN:HB3	1.74	0.69
1:K:351:SER:O	1:K:372:TYR:OH	2.09	0.69
2:N:391:THR:HG21	2:N:412:MET:H	1.58	0.69
1:K:351:SER:O	1:K:372:TYR:CZ	2.45	0.69
1:U:344:ALA:HB3	1:U:367:VAL:HA	1.75	0.69
1:L:349:GLY:HA2	1:L:373:GLN:HB3	1.73	0.69
4:E:36:ARG:C	8:E:201:ADP:O2'	2.35	0.69
2:D:391:THR:HG23	2:D:411:ILE:HA	1.75	0.69
2:D:236:GLY:HA3	2:D:282:LEU:HD13	1.75	0.69
1:K:351:SER:N	1:K:372:TYR:HE2	1.89	0.69
1:A:485:HIS:HA	6:A:602:ICS:S4B	2.32	0.68
1:A:331:GLU:HB3	1:A:500:LEU:HD21	1.74	0.68
2:W:443:LYS:HG2	2:W:455:ILE:HD12	1.75	0.68
2:D:102:ILE:HD11	2:D:134:ILE:HD11	1.74	0.68
6:A:602:ICS:S3B	7:A:603:HCA:H41	2.34	0.68
2:D:341:LEU:HD13	2:D:375:LEU:HB2	1.75	0.67
2:B:111:ILE:HA	4:G:65:PRO:HG3	1.76	0.67
1:U:89:TRP:H	1:U:91:THR:HG23	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:37:GLY:HA3	8:R:201:ADP:C3'	2.24	0.67
1:A:207:ILE:HG22	1:A:256:GLN:HB3	1.76	0.67
2:M:307:PRO:HA	1:L:508:MET:HE2	1.75	0.67
1:V:347:TYR:CE2	1:V:447:LEU:HB3	2.29	0.67
2:B:314:VAL:HG22	2:B:386:LEU:HB3	1.77	0.67
7:C:603:HCA:O5	2:D:54:MET:CE	2.43	0.67
2:N:45:SER:HB2	5:N:501:CLF:S4B	2.35	0.67
2:N:308:HIS:CE1	2:N:440:LEU:HD11	2.29	0.67
8:R:201:ADP:C2	4:O:29:THR:HG23	2.29	0.67
3:b:96:TYR:HB2	4:a:99:ILE:HB	1.76	0.67
3:Z:28:LEU:HD11	3:Z:57:LEU:HB3	1.76	0.67
2:X:330:VAL:HG13	2:X:335:MET:HB2	1.78	0.66
1:A:31:ILE:HB	1:A:444:VAL:HG23	1.76	0.66
1:K:351:SER:O	1:K:372:TYR:CE2	2.48	0.66
3:d:36:ARG:HG2	3:d:49:TYR:HD2	1.60	0.66
2:B:268:GLY:HA2	2:B:329:LEU:HD13	1.76	0.66
1:K:431:GLU:HB2	1:K:435:PRO:HG2	1.77	0.66
1:A:149:CYS:HA	1:A:179:GLU:HB3	1.77	0.66
4:Q:6:ALA:HB3	4:Q:69:PHE:HB2	1.78	0.66
4:Y:33:VAL:HG12	3:Z:31:MET:HB3	1.78	0.66
1:U:368:VAL:HG12	1:U:369:VAL:HG23	1.78	0.65
3:S:38:LYS:HE2	3:S:82:TYR:HB3	1.78	0.65
1:U:374:PHE:CE1	6:U:602:ICS:S1A	2.90	0.65
1:K:198:MET:HE2	1:K:277:MET:HB3	1.78	0.65
2:N:314:VAL:HG12	2:N:386:LEU:HB3	1.78	0.65
2:X:324:SER:HA	2:X:353:ILE:HD11	1.76	0.65
2:D:23:CYS:HB3	2:D:25:PRO:HD2	1.79	0.65
2:D:54:MET:HE2	2:D:58:ARG:HH22	1.60	0.65
4:a:6:ALA:HB3	4:a:69:PHE:HB2	1.78	0.65
1:A:483:GLN:HB2	1:A:488:ASP:H	1.62	0.65
1:V:374:PHE:CZ	6:V:603:ICS:S5A	2.90	0.65
2:X:261:LYS:HE3	2:X:278:ASN:HB2	1.79	0.65
3:I:86:ARG:NH1	8:I:201:ADP:H8	1.92	0.65
1:A:188:ALA:O	1:A:192:ILE:HG13	1.96	0.64
2:D:276:ILE:HD13	2:D:291:LEU:HD13	1.79	0.64
2:M:49:LEU:HD22	2:M:68:THR:HB	1.79	0.64
2:M:169:GLY:HA2	2:M:235:LEU:HD21	1.79	0.64
1:L:357:ILE:O	1:L:361:GLU:HG2	1.98	0.64
2:N:88:LEU:HB3	2:N:127:LEU:HD11	1.78	0.64
2:D:172:ASN:ND2	2:D:234:SER:HB3	2.13	0.64
1:K:71:ILE:HG21	1:K:74:MET:HE3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:261:LYS:HD3	2:D:278:ASN:HB2	1.79	0.64
2:N:175:PRO:HA	2:N:240:LEU:HD12	1.79	0.64
2:W:301:MET:HE2	2:X:419:TYR:CG	2.33	0.64
2:W:330:VAL:HG13	2:W:335:MET:HB2	1.80	0.64
8:E:201:ADP:C2	3:F:28:LEU:N	2.65	0.64
1:A:158:ILE:HG13	1:A:175:PRO:HB3	1.80	0.64
1:V:182:ARG:HD3	1:V:397:ILE:HG21	1.79	0.63
3:P:28:LEU:HD21	3:P:57:LEU:HD22	1.79	0.63
2:B:276:ILE:HD12	2:B:291:LEU:HD13	1.80	0.63
4:O:7:ILE:HD12	8:O:201:ADP:C8	2.33	0.63
2:W:211:LEU:HG	1:U:518:ILE:HD11	1.78	0.63
3:H:61:VAL:HG11	3:H:69:VAL:HG21	1.79	0.63
1:L:268:HIS:O	1:L:272:ASN:HB2	1.98	0.63
1:L:289:VAL:HG13	1:L:300:SER:HB3	1.79	0.63
8:E:201:ADP:N3	3:F:28:LEU:C	2.55	0.63
4:O:96:ASP:HB3	3:P:98:ILE:HB	1.81	0.63
1:A:75:VAL:HG13	1:A:143:ILE:HG23	1.79	0.63
1:V:66:VAL:HG11	6:V:603:ICS:S5A	2.39	0.63
3:J:54:LYS:CG	8:J:201:ADP:O3'	2.46	0.63
1:A:349:GLY:CA	6:A:602:ICS:S1B	2.80	0.63
8:J:201:ADP:N7	4:E:27:SER:CB	2.57	0.63
1:L:331:GLU:HB3	1:L:500:LEU:HD11	1.80	0.63
2:B:440:LEU:HD22	2:B:455:ILE:HG22	1.81	0.63
2:N:316:ILE:HG23	2:N:388:ILE:HB	1.79	0.63
1:C:295:LYS:HE2	1:C:358:ASN:HB2	1.81	0.63
2:D:324:SER:HA	2:D:353:ILE:HD11	1.80	0.63
1:C:83:GLY:HA3	2:D:23:CYS:SG	2.39	0.62
1:L:66:VAL:HG11	6:L:601:ICS:S2B	2.39	0.62
1:L:269:ARG:NH1	1:L:375:ALA:HA	2.07	0.62
4:O:7:ILE:CD1	8:O:201:ADP:H8	2.11	0.62
2:N:27:GLY:HA2	2:N:177:PHE:HE2	1.63	0.62
1:K:149:CYS:HA	1:K:179:GLU:HG3	1.80	0.62
1:K:298:GLU:HG2	1:K:302:ARG:HE	1.65	0.62
5:W:601:CLF:S3B	1:U:180:GLY:CA	2.84	0.62
3:H:31:MET:HE2	3:I:31:MET:HE1	1.81	0.62
3:J:35:GLY:HA3	8:J:201:ADP:O2'	1.99	0.62
2:N:23:CYS:SG	2:N:141:SER:HB3	2.39	0.62
8:E:201:ADP:C5	3:F:27:SER:HB3	2.35	0.62
4:Q:72:VAL:HG23	8:S:201:ADP:HN62	1.65	0.62
1:A:444:VAL:HG21	1:A:447:LEU:HD23	1.82	0.62
2:D:26:ILE:HB	2:D:52:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:431:GLU:HG3	1:L:435:PRO:HG2	1.81	0.62
1:A:180:GLY:HA3	5:A:601:CLF:S2A	2.40	0.61
1:C:53:LEU:HG	2:D:67:THR:HG22	1.82	0.61
1:U:211:THR:HG22	1:U:213:PHE:H	1.64	0.61
1:A:179:GLU:CD	1:A:179:GLU:H	2.09	0.61
4:E:29:THR:HG23	4:E:70:THR:HB	1.81	0.61
2:M:333:MET:SD	2:M:432:VAL:HG23	2.40	0.61
1:U:463:ILE:HB	1:U:510:ILE:HD11	1.82	0.61
4:E:38:LYS:CG	8:E:201:ADP:O2B	2.44	0.61
1:C:66:VAL:HG23	1:C:67:VAL:HG23	1.83	0.61
3:J:54:LYS:HD2	8:J:201:ADP:O3'	2.01	0.61
1:U:197:LEU:HD11	1:U:245:LEU:HD23	1.83	0.61
1:V:66:VAL:HG23	1:V:67:VAL:HG23	1.82	0.60
1:A:292:ILE:HD12	1:A:355:HIS:HB3	1.81	0.60
1:K:143:ILE:HB	1:K:173:VAL:HG12	1.83	0.60
1:U:217:ILE:HG12	1:U:264:ILE:HD11	1.82	0.60
8:E:201:ADP:H2	3:F:28:LEU:HA	1.58	0.60
1:A:300:SER:O	1:A:304:MET:HG3	2.00	0.60
1:A:74:MET:HG3	1:A:142:ALA:HB3	1.84	0.60
2:X:455:ILE:HD12	1:U:91:THR:HA	1.83	0.60
4:E:98:LYS:CE	8:E:201:ADP:C8	2.84	0.60
4:E:108:ILE:HD13	4:E:115:SER:HB2	1.84	0.60
3:S:38:LYS:CD	3:S:82:TYR:HB3	2.31	0.60
1:L:444:VAL:HG11	1:L:447:LEU:HD13	1.84	0.60
2:B:26:ILE:HB	2:B:52:LEU:HD22	1.84	0.60
2:W:147:ILE:HG23	2:W:244:ALA:HB2	1.84	0.60
1:L:301:LEU:HD12	1:L:321:ILE:HD11	1.82	0.60
1:K:89:TRP:H	1:K:91:THR:HG23	1.67	0.60
1:K:182:ARG:HD3	1:K:397:ILE:HG21	1.83	0.60
1:U:92:ARG:HH11	1:U:94:ASN:HD22	1.49	0.60
4:G:41:GLY:O	4:G:42:LEU:C	2.42	0.60
1:C:221:TYR:CE2	6:C:602:ICS:S4A	2.84	0.60
1:K:276:ARG:HE	1:K:383:ARG:NH1	1.97	0.60
1:V:328:TYR:HB3	1:V:500:LEU:HD11	1.82	0.59
4:Q:10:MET:HG3	4:Q:67:ARG:HH21	1.67	0.59
2:D:251:ILE:HG23	2:D:255:ARG:HD3	1.85	0.59
3:S:36:ARG:HE	3:S:49:TYR:HB3	1.67	0.59
2:X:182:ASP:HB3	2:X:423:MET:HE2	1.84	0.59
1:C:265:LEU:HD21	1:C:267:CYS:O	2.03	0.59
2:W:411:ILE:HG21	2:W:417:LEU:HD12	1.83	0.59
2:W:443:LYS:HE3	2:W:455:ILE:HG23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:TYR:CE2	1:C:447:LEU:HB3	2.34	0.59
2:M:45:SER:HB2	5:M:601:CLF:S2A	2.43	0.59
3:T:61:VAL:HG11	3:T:69:VAL:HG21	1.84	0.59
1:U:49:ILE:HD12	1:U:50:PRO:HD2	1.85	0.59
1:A:152:GLY:HA3	1:A:179:GLU:HG2	1.84	0.59
1:A:182:ARG:HH11	1:A:397:ILE:HG21	1.68	0.59
7:K:601:HCA:O3	7:K:601:HCA:C1	2.51	0.59
1:K:207:ILE:HD13	1:K:242:ILE:HD12	1.84	0.59
1:V:84:CYS:SG	5:V:601:CLF:S4B	3.01	0.59
2:N:341:LEU:HD23	2:N:375:LEU:HB2	1.85	0.59
8:O:201:ADP:H2	3:P:27:SER:HB3	1.68	0.59
1:K:130:ALA:HA	2:M:15:ILE:HD11	1.84	0.58
7:V:602:HCA:H51	2:X:54:MET:CE	2.33	0.58
2:W:39:MET:HG2	2:W:91:LEU:HD11	1.85	0.58
2:W:133:LYS:HD2	2:W:225:ILE:HD13	1.84	0.58
3:S:38:LYS:HD3	3:S:82:TYR:HB3	1.83	0.58
1:K:144:THR:HG22	1:K:174:ILE:HB	1.84	0.58
4:O:106:GLU:HG3	4:O:108:ILE:HD11	1.84	0.58
1:C:444:VAL:HG11	1:C:447:LEU:HD13	1.85	0.58
2:W:170:LYS:HD2	2:W:198:ILE:HG13	1.85	0.58
4:G:40:ARG:O	4:G:42:LEU:N	2.36	0.58
3:c:28:LEU:HD11	3:c:57:LEU:HB3	1.86	0.58
2:B:48:CYS:O	2:B:49:LEU:C	2.46	0.58
1:C:182:ARG:HD3	1:C:397:ILE:HG21	1.85	0.58
2:X:391:THR:HG23	2:X:411:ILE:HA	1.86	0.58
2:D:168:ASN:HD21	2:D:233:ASN:ND2	2.01	0.58
2:M:159:THR:HG23	2:M:255:ARG:HH22	1.69	0.58
2:M:333:MET:HE1	2:M:435:ILE:HD13	1.85	0.58
2:X:48:CYS:O	2:X:49:LEU:C	2.43	0.58
1:C:348:ALA:HB1	6:C:602:ICS:S2B	2.43	0.58
1:U:475:GLN:HE22	1:U:480:PRO:HA	1.69	0.58
3:T:90:ASN:HD21	3:S:92:VAL:HG22	1.69	0.58
8:O:201:ADP:HN61	3:P:60:VAL:H	1.46	0.58
1:K:350:GLY:HA2	1:K:372:TYR:CD2	2.39	0.58
2:W:106:CYS:O	2:W:107:VAL:C	2.43	0.58
3:T:101:GLY:HA2	4:Q:86:ILE:HD12	1.86	0.58
1:C:353:SER:HB2	1:C:372:TYR:HE1	1.69	0.57
1:K:27:ARG:HH12	1:K:446:ASP:HB3	1.68	0.57
3:R:96:TYR:HB3	3:P:74:MET:HE1	1.86	0.57
8:R:201:ADP:C8	4:O:27:SER:HB2	2.39	0.57
3:d:99:ARG:HE	3:d:100:THR:HG23	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:VAL:HG21	2:B:46:GLN:HE22	1.69	0.57
1:A:155:GLY:HA2	4:G:47:ASN:HD21	1.69	0.57
1:V:93:ARG:HH21	2:W:454:THR:HB	1.69	0.57
1:U:447:LEU:HD22	1:U:452:THR:HG23	1.86	0.57
1:A:129:LYS:O	1:A:133:GLU:HG3	2.05	0.57
1:L:83:GLY:HA3	2:N:23:CYS:SG	2.43	0.57
2:X:380:LYS:HG2	2:X:400:GLU:OE2	2.04	0.57
2:N:341:LEU:HD13	2:N:367:ILE:HB	1.87	0.57
1:C:483:GLN:HB2	1:C:488:ASP:H	1.68	0.57
1:K:92:ARG:HH11	1:K:94:ASN:HD22	1.52	0.57
1:V:351:SER:HB2	1:V:355:HIS:HE1	1.70	0.57
2:N:236:GLY:HA3	2:N:282:LEU:HD13	1.86	0.57
4:G:42:LEU:O	4:G:43:CYS:C	2.45	0.57
1:C:87:PHE:HE2	5:C:601:CLF:S3B	2.27	0.57
2:N:175:PRO:HD2	2:N:201:PRO:HG2	1.85	0.57
3:S:38:LYS:CE	3:S:82:TYR:HB3	2.33	0.57
2:B:100:ILE:HB	2:B:134:ILE:HG12	1.87	0.57
1:K:92:ARG:NH2	6:K:602:ICS:S3A	2.77	0.57
1:K:350:GLY:C	1:K:372:TYR:HE2	2.12	0.57
1:U:349:GLY:HA3	6:U:602:ICS:S1B	2.45	0.57
2:W:88:LEU:HD21	2:W:102:ILE:HD11	1.86	0.57
1:L:182:ARG:HD2	1:L:192:ILE:HD11	1.87	0.57
1:V:92:ARG:NH1	6:V:603:ICS:S3A	2.74	0.56
2:D:46:GLN:HA	2:D:68:THR:HG21	1.87	0.56
2:X:391:THR:HG21	2:X:412:MET:H	1.70	0.56
3:R:37:GLY:CA	8:R:201:ADP:H2'	2.36	0.56
6:L:601:ICS:S3B	7:L:602:HCA:H51	2.45	0.56
2:D:251:ILE:O	2:D:255:ARG:HG2	2.06	0.56
1:K:120:VAL:HG11	3:S:34:PHE:CG	2.39	0.56
3:b:9:ARG:HH12	3:b:84:ASP:HA	1.71	0.56
3:d:7:VAL:HG21	8:d:201:ADP:C8	2.41	0.56
3:I:28:LEU:HD13	3:I:59:MET:HE3	1.86	0.56
4:a:111:ARG:HD3	3:c:82:TYR:HA	1.88	0.56
1:A:163:ARG:O	1:A:167:GLU:HG3	2.06	0.56
1:C:366:LYS:HE2	1:C:438:LYS:HE2	1.87	0.56
1:K:131:ILE:HG21	1:K:165:ALA:HB1	1.87	0.56
2:W:360:GLU:HB3	2:W:361:TYR:CD1	2.41	0.56
3:R:36:ARG:NH1	4:O:17:LYS:HD2	2.20	0.56
3:b:90:ASN:HD21	3:c:3:MET:HE3	1.70	0.56
1:L:74:MET:HE1	1:L:174:ILE:HD12	1.88	0.56
2:N:317:TYR:CZ	2:N:389:GLY:HA3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:38:LYS:HE3	8:I:201:ADP:O3B	2.06	0.56
1:A:48:VAL:HG23	1:A:184:VAL:HG12	1.87	0.56
1:A:122:GLY:HA2	1:A:154:ILE:HD12	1.88	0.56
1:V:237:ILE:HD12	1:V:317:THR:HA	1.88	0.56
2:N:54:MET:HE2	2:N:58:ARG:HH22	1.71	0.56
1:A:344:ALA:HA	1:A:463:ILE:HG22	1.88	0.56
1:K:484:ILE:HD12	1:K:485:HIS:CD2	2.40	0.56
2:M:272:THR:O	2:M:276:ILE:HG12	2.06	0.56
2:X:331:LEU:HD11	2:X:357:ILE:HG12	1.87	0.56
4:E:36:ARG:O	8:E:201:ADP:O2'	2.23	0.56
1:A:65:GLY:O	1:A:92:ARG:HD3	2.05	0.56
1:C:231:LYS:HD2	1:C:241:ILE:HD12	1.88	0.56
1:K:75:VAL:HG13	1:K:143:ILE:HG23	1.86	0.56
1:V:60:PHE:HB3	5:V:601:CLF:S2A	2.46	0.56
2:W:178:VAL:HG11	2:W:423:MET:HE3	1.87	0.56
2:B:341:LEU:HD13	2:B:375:LEU:HB2	1.87	0.56
1:V:347:TYR:HE2	1:V:447:LEU:HB3	1.71	0.56
3:d:86:ARG:HG3	3:d:86:ARG:HH11	1.71	0.56
2:D:49:LEU:HD21	2:D:66:ALA:HB1	1.87	0.56
2:D:175:PRO:HD2	2:D:201:PRO:HD2	1.88	0.56
2:W:5:THR:HG21	2:W:376:HIS:CD2	2.40	0.56
3:H:36:ARG:HH11	3:I:17:VAL:HG13	1.70	0.56
2:M:85:LYS:HE2	2:M:118:ILE:HD11	1.88	0.55
2:W:29:VAL:HG11	2:W:52:LEU:HD21	1.88	0.55
5:W:601:CLF:S2A	1:U:81:PRO:CB	2.93	0.55
3:H:98:ILE:HG22	4:G:96:ASP:HB3	1.87	0.55
8:J:201:ADP:O1B	4:E:109:ARG:NH1	2.39	0.55
1:A:444:VAL:HG11	1:A:447:LEU:HG	1.87	0.55
2:M:329:LEU:O	2:M:333:MET:HG3	2.06	0.55
3:J:13:GLU:HG2	3:J:55:THR:HG21	1.89	0.55
1:U:483:GLN:HB2	1:U:488:ASP:H	1.71	0.55
4:G:33:VAL:HG11	4:G:68:MET:CE	2.36	0.55
4:E:95:GLY:N	8:E:201:ADP:O1A	2.34	0.55
4:O:9:ARG:HG3	4:O:95:GLY:O	2.06	0.55
3:c:10:PRO:HD3	3:c:54:LYS:HA	1.89	0.55
1:A:348:ALA:HB1	6:A:602:ICS:S3A	2.47	0.55
6:A:602:ICS:S3B	7:A:603:HCA:C4	2.95	0.55
1:V:374:PHE:HE2	6:V:603:ICS:S3B	2.28	0.55
3:b:31:MET:HG2	4:a:33:VAL:HG12	1.88	0.55
2:W:45:SER:HB3	2:W:48:CYS:SG	2.46	0.55
8:R:201:ADP:HN62	4:O:72:VAL:H	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:HG11	1:A:455:LEU:HD13	1.89	0.55
1:A:383:ARG:HG3	1:A:430:TYR:HB3	1.87	0.55
1:C:234:LEU:HA	1:C:237:ILE:HD12	1.89	0.55
3:J:8:ILE:HD11	3:J:13:GLU:HG3	1.89	0.55
2:N:391:THR:HG23	2:N:411:ILE:HA	1.88	0.55
1:A:467:GLY:CA	1:A:485:HIS:CD2	2.87	0.55
1:C:374:PHE:CZ	6:C:602:ICS:S3B	3.00	0.55
1:V:66:VAL:HA	1:V:92:ARG:CZ	2.37	0.55
1:V:287:LEU:HD21	1:V:303:LYS:HD2	1.88	0.55
2:N:323:LEU:HD12	2:N:340:VAL:HG13	1.89	0.55
1:K:188:ALA:HA	1:K:398:LEU:HD11	1.88	0.55
1:U:520:PRO:HG2	1:U:523:LYS:HG3	1.89	0.55
1:K:11:ILE:HD13	1:K:458:ALA:HB1	1.88	0.55
2:X:49:LEU:HD11	2:X:66:ALA:HB3	1.89	0.55
1:L:174:ILE:HD11	1:L:201:LEU:HG	1.89	0.55
2:N:237:THR:HG22	2:N:237:THR:O	2.07	0.55
2:N:309:TYR:HB2	2:N:335:MET:HE2	1.87	0.55
2:D:164:LYS:HG2	2:D:231:SER:HB2	1.89	0.54
2:D:223:THR:HG23	2:D:223:THR:O	2.06	0.54
2:X:39:MET:HE1	2:X:217:PHE:HE2	1.72	0.54
4:a:19:ALA:HB2	4:a:88:VAL:HG11	1.89	0.54
1:C:374:PHE:HE1	6:C:602:ICS:S2A	2.30	0.54
2:X:239:ALA:HB3	2:X:262:ILE:HG23	1.89	0.54
2:X:301:MET:HE1	2:X:429:ALA:HB1	1.87	0.54
1:C:31:ILE:HG23	1:C:444:VAL:HG12	1.89	0.54
1:V:92:ARG:HD2	1:V:223:ILE:HD11	1.90	0.54
3:J:60:VAL:HG12	3:J:105:LEU:HD11	1.89	0.54
3:d:64:GLU:HG3	3:d:65:HIS:CE1	2.42	0.54
1:L:452:THR:O	1:L:456:VAL:HG22	2.07	0.54
3:F:5:ARG:HG3	3:F:56:MET:HE3	1.89	0.54
1:A:89:TRP:H	1:A:91:THR:HG23	1.72	0.54
1:A:92:ARG:HD2	7:A:603:HCA:O4	2.07	0.54
1:K:413:ILE:HD13	1:K:417:ARG:HB3	1.90	0.54
1:V:482:ARG:HD3	1:V:509:ALA:HB2	1.88	0.54
3:J:3:MET:HE1	3:F:5:ARG:NH1	2.21	0.54
7:V:602:HCA:H51	2:X:54:MET:SD	2.48	0.54
2:W:317:TYR:CE1	2:W:389:GLY:HA3	2.42	0.54
1:K:381:GLU:HB2	1:K:385:ILE:HD13	1.88	0.54
2:M:310:HIS:HB3	1:L:508:MET:HE3	1.90	0.54
1:L:471:LYS:HD2	1:L:483:GLN:HG2	1.89	0.54
4:E:33:VAL:HG11	4:E:68:MET:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:93:ASN:O	3:P:99:ARG:HG3	2.07	0.54
1:C:148:THR:CB	5:C:601:CLF:S4A	2.96	0.54
4:G:43:CYS:C	4:G:45:GLU:H	2.15	0.54
2:X:391:THR:HG21	2:X:413:ASP:H	1.72	0.54
2:M:170:LYS:HD3	2:M:198:ILE:HG13	1.89	0.54
1:V:374:PHE:CE2	6:V:603:ICS:S3B	3.01	0.54
4:E:36:ARG:N	8:E:201:ADP:O2'	2.40	0.54
1:V:369:VAL:HG11	1:V:455:LEU:HD13	1.89	0.54
1:U:218:PHE:HB3	1:U:271:ILE:HG21	1.89	0.54
1:K:66:VAL:HG22	6:K:602:ICS:S4B	2.48	0.53
1:K:149:CYS:HB3	1:K:181:TYR:CD2	2.43	0.53
1:K:188:ALA:O	1:K:192:ILE:HG12	2.08	0.53
2:M:276:ILE:HG22	2:M:287:ILE:HD12	1.90	0.53
1:V:501:ASN:HD22	1:V:504:ARG:HH21	1.56	0.53
2:X:390:ASN:HB3	2:X:410:PRO:HD2	1.90	0.53
4:a:14:GLN:HA	4:a:17:LYS:HE3	1.90	0.53
4:Y:6:ALA:HB3	4:Y:69:PHE:HB2	1.91	0.53
2:W:268:GLY:HA2	2:W:329:LEU:HD13	1.90	0.53
2:X:179:GLU:OE1	2:X:418:HIS:HA	2.09	0.53
1:L:438:LYS:HD2	1:L:439:ASP:H	1.73	0.53
1:A:350:GLY:CA	6:A:602:ICS:S1A	2.95	0.53
1:C:465:CYS:HA	1:C:482:ARG:O	2.08	0.53
1:C:467:GLY:HA2	1:C:485:HIS:CD2	2.42	0.53
2:D:333:MET:HE3	2:D:432:VAL:HG22	1.90	0.53
2:M:173:ILE:HB	2:M:199:VAL:HG22	1.89	0.53
1:V:221:TYR:CE2	6:V:603:ICS:S4A	3.01	0.53
2:W:440:LEU:HD22	2:W:455:ILE:HG22	1.89	0.53
3:d:7:VAL:HG11	8:d:201:ADP:H1'	1.91	0.53
1:L:81:PRO:CG	5:N:501:CLF:S3A	2.92	0.53
2:N:341:LEU:HD11	2:N:370:GLY:HA3	1.90	0.53
1:U:261:LYS:HB2	1:U:308:PHE:HZ	1.73	0.53
2:M:269:ILE:HB	2:M:332:GLU:OE2	2.09	0.53
2:X:278:ASN:O	2:X:282:LEU:HD13	2.09	0.53
2:X:440:LEU:HD22	2:X:456:GLN:NE2	2.23	0.53
2:N:268:GLY:HA2	2:N:329:LEU:HD13	1.90	0.53
1:U:450:HIS:CE1	1:U:454:PHE:CD2	2.95	0.53
8:E:201:ADP:H2	3:F:29:THR:H	1.55	0.53
4:Q:111:ARG:HD3	3:S:82:TYR:HA	1.89	0.53
1:K:41:HIS:HA	1:K:381:GLU:OE2	2.09	0.53
1:V:293:GLY:HA2	1:V:359:LEU:HD13	1.90	0.53
1:A:476:LYS:HD3	2:B:211:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:TYR:OH	2:D:201:PRO:HG2	2.08	0.53
4:E:98:LYS:HE3	8:E:201:ADP:N7	2.23	0.53
1:A:63:THR:HG21	1:A:178:CYS:SG	2.48	0.53
2:B:276:ILE:HG22	2:B:287:ILE:HD12	1.91	0.53
2:B:326:LEU:HD21	2:B:422:ILE:HD11	1.90	0.53
1:K:127:LEU:HD23	1:K:161:VAL:HG11	1.90	0.53
1:V:350:GLY:HA3	6:V:603:ICS:S2A	2.49	0.53
1:U:7:ASP:O	1:U:11:ILE:HG12	2.09	0.53
1:C:197:LEU:HD23	1:C:201:LEU:HD12	1.91	0.53
2:W:333:MET:SD	2:W:432:VAL:HG22	2.49	0.53
2:N:41:HIS:CE1	2:N:91:LEU:HD21	2.44	0.53
3:J:35:GLY:CA	8:J:201:ADP:O2'	2.56	0.53
3:J:54:LYS:CD	8:J:201:ADP:O3'	2.56	0.53
3:S:39:GLN:HG2	3:S:52:LEU:HD21	1.89	0.53
1:A:359:LEU:HD21	1:A:502:PHE:CD1	2.44	0.53
1:V:66:VAL:HA	1:V:92:ARG:NH2	2.24	0.53
1:V:273:TYR:O	1:V:277:MET:HG2	2.08	0.53
2:N:115:VAL:HA	2:N:118:ILE:HG22	1.91	0.53
4:G:95:GLY:HA2	9:G:201:AKG:O5	2.09	0.53
4:E:98:LYS:CE	8:E:201:ADP:N7	2.71	0.53
3:S:10:PRO:HD3	3:S:54:LYS:HA	1.91	0.53
2:X:288:PRO:HB2	2:X:290:GLU:OE1	2.10	0.52
4:a:109:ARG:HH11	4:a:111:ARG:HH21	1.57	0.52
1:U:374:PHE:CE2	6:U:602:ICS:S1B	3.02	0.52
1:C:68:PHE:HZ	1:C:196:SER:HB2	1.74	0.52
1:C:331:GLU:HB3	1:C:500:LEU:HD11	1.91	0.52
2:X:336:GLU:HB2	2:X:361:TYR:CE1	2.44	0.52
8:d:201:ADP:N7	4:Y:29:THR:OG1	2.41	0.52
1:L:227:LEU:HG	1:L:231:LYS:HE2	1.90	0.52
2:N:23:CYS:CB	5:N:501:CLF:S2A	2.97	0.52
3:Z:60:VAL:HG12	3:Z:105:LEU:HD11	1.91	0.52
2:B:288:PRO:HD2	2:B:291:LEU:HD12	1.91	0.52
1:K:276:ARG:NE	1:K:383:ARG:HH12	2.02	0.52
3:T:20:LEU:HD13	3:T:59:MET:HE1	1.90	0.52
3:d:70:ILE:HG22	3:d:74:MET:HE2	1.90	0.52
3:d:37:GLY:O	3:d:49:TYR:HA	2.10	0.52
1:U:450:HIS:HE1	1:U:454:PHE:CD2	2.28	0.52
1:A:472:TYR:CZ	2:B:61:ARG:HG3	2.45	0.52
1:K:268:HIS:HD2	1:K:272:ASN:HB3	1.74	0.52
2:X:317:TYR:CZ	2:X:389:GLY:HA3	2.45	0.52
1:L:149:CYS:SG	5:N:501:CLF:S2B	3.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:1:MET:HE2	4:a:1:MET:H3	1.74	0.52
1:A:218:PHE:HD2	1:A:271:ILE:HG12	1.73	0.52
2:D:23:CYS:SG	2:D:141:SER:OG	2.67	0.52
2:M:440:LEU:HD22	2:M:455:ILE:HG22	1.92	0.52
1:A:261:LYS:HB2	1:A:308:PHE:HZ	1.74	0.52
1:A:276:ARG:HD3	1:A:383:ARG:HH22	1.75	0.52
2:B:182:ASP:HB3	2:B:423:MET:SD	2.50	0.52
1:K:221:TYR:CE2	6:K:602:ICS:S4A	3.03	0.52
1:V:11:ILE:HD13	1:V:458:ALA:HB1	1.92	0.52
3:d:26:ILE:HD11	1:L:21:GLU:HB2	1.92	0.52
2:X:289:PRO:HA	2:X:292:GLU:HG2	1.92	0.52
1:A:377:ARG:HE	1:A:385:ILE:HD12	1.74	0.52
1:V:180:GLY:HA3	5:V:601:CLF:S3A	2.50	0.52
2:W:29:VAL:HG22	2:W:40:PRO:HB2	1.92	0.52
1:U:245:LEU:HG	1:U:254:ILE:HG12	1.92	0.52
3:S:28:LEU:HD11	3:S:57:LEU:HB3	1.91	0.52
2:X:213:LYS:NZ	2:X:213:LYS:HB3	2.25	0.51
2:X:261:LYS:NZ	2:X:261:LYS:HB3	2.25	0.51
3:b:87:ILE:HB	3:c:96:TYR:HB2	1.92	0.51
1:L:357:ILE:HG13	1:L:437:MET:HE1	1.90	0.51
2:N:330:VAL:HG13	2:N:335:MET:HB3	1.91	0.51
4:G:43:CYS:C	4:G:45:GLU:N	2.65	0.51
2:B:158:VAL:HG21	2:B:248:ALA:HB1	1.92	0.51
1:V:354:HIS:CD2	1:V:436:GLU:HG3	2.45	0.51
4:G:38:LYS:O	4:G:39:GLN:C	2.53	0.51
1:C:467:GLY:HA2	1:C:485:HIS:HD2	1.76	0.51
1:C:485:HIS:HA	6:C:602:ICS:S1B	2.51	0.51
1:K:350:GLY:HA2	1:K:372:TYR:HD2	1.76	0.51
2:X:249:ALA:HB1	2:X:260:ALA:HB1	1.92	0.51
2:N:90:ASN:O	2:N:94:VAL:HG12	2.09	0.51
3:I:60:VAL:HG12	3:I:105:LEU:HD11	1.92	0.51
3:J:27:SER:HB2	3:F:86:ARG:HH12	1.75	0.51
3:J:37:GLY:HA2	8:J:201:ADP:O2A	2.10	0.51
1:L:374:PHE:CE1	6:L:601:ICS:S1A	2.99	0.51
2:B:317:TYR:CE1	2:B:389:GLY:HA3	2.45	0.51
7:K:601:HCA:O4	2:M:51:TYR:CE1	2.64	0.51
8:J:201:ADP:C8	4:E:27:SER:HB3	2.42	0.51
3:R:10:PRO:HD3	3:R:54:LYS:HA	1.92	0.51
2:B:61:ARG:HG2	2:D:304:ASP:HB3	1.92	0.51
1:V:467:GLY:HA2	1:V:485:HIS:HD2	1.76	0.51
2:W:24:GLN:HG2	2:W:149:GLY:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:225:ILE:O	2:W:229:GLU:HG3	2.10	0.51
3:H:66:LYS:HD3	3:H:89:VAL:HG11	1.92	0.51
3:R:88:PHE:HB3	4:O:104:ILE:HD13	1.93	0.51
1:U:124:GLU:HB2	4:a:14:GLN:HE22	1.74	0.51
1:U:217:ILE:HG21	1:U:227:LEU:HD11	1.93	0.51
4:G:111:ARG:HD3	3:I:82:TYR:HA	1.92	0.51
2:X:332:GLU:HG2	1:U:517:PHE:CE2	2.46	0.51
4:a:1:MET:HE2	4:a:1:MET:N	2.26	0.51
1:A:16:LEU:HA	1:A:19:LEU:HD12	1.93	0.51
1:A:47:LYS:HA	1:A:184:VAL:HG11	1.92	0.51
1:V:15:ILE:HG12	1:V:454:PHE:HB3	1.91	0.51
4:Q:109:ARG:HH21	4:Q:119:THR:HA	1.76	0.51
1:A:149:CYS:SG	1:A:150:PRO:HD3	2.51	0.51
1:A:217:ILE:HD11	1:A:241:ILE:HG12	1.92	0.51
2:D:200:PHE:HZ	2:D:230:ASP:HB3	1.75	0.51
2:X:225:ILE:HD12	2:X:228:ILE:HD13	1.91	0.51
1:L:202:ILE:HA	1:L:255:SER:HA	1.92	0.51
1:U:131:ILE:HD11	1:U:145:ILE:HD11	1.93	0.51
3:Z:61:VAL:HG11	3:Z:69:VAL:HG21	1.93	0.51
1:C:245:LEU:HD11	1:C:254:ILE:HG23	1.93	0.50
5:W:601:CLF:S2A	1:U:81:PRO:HG2	2.51	0.50
2:X:326:LEU:HD11	2:X:407:VAL:HG11	1.92	0.50
1:V:264:ILE:HD12	1:V:289:VAL:HG21	1.92	0.50
2:X:290:GLU:H	2:X:290:GLU:CD	2.19	0.50
2:N:223:THR:HG22	2:N:227:ASP:HB2	1.93	0.50
1:U:15:ILE:HG22	1:U:16:LEU:HD23	1.93	0.50
4:a:62:ARG:CZ	4:a:62:ARG:H	2.24	0.50
1:L:140:PRO:HG2	1:L:143:ILE:HG12	1.93	0.50
1:L:345:PHE:HB3	1:L:464:PHE:HA	1.93	0.50
1:L:353:SER:H	1:L:372:TYR:HE1	1.59	0.50
2:N:153:MET:HE3	2:N:153:MET:HA	1.93	0.50
1:C:468:ILE:HG22	7:C:603:HCA:C6	2.41	0.50
2:D:49:LEU:O	2:D:53:ARG:HG3	2.11	0.50
1:L:369:VAL:HG11	1:L:455:LEU:HD13	1.94	0.50
1:U:149:CYS:SG	1:U:150:PRO:CD	2.99	0.50
1:A:58:CYS:SG	2:B:47:GLY:HA3	2.52	0.50
2:M:273:ASP:O	2:M:277:MET:HG3	2.11	0.50
1:A:198:MET:HA	1:A:202:ILE:HG23	1.93	0.50
2:B:395:PHE:HZ	2:D:454:THR:HG23	1.77	0.50
2:M:403:PRO:HG3	2:M:442:ARG:HE	1.76	0.50
1:V:452:THR:O	1:V:456:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:287:LEU:HD21	1:U:303:LYS:HB3	1.93	0.50
1:U:292:ILE:HG22	1:U:359:LEU:HD13	1.93	0.50
2:B:140:PRO:HB2	2:B:143:VAL:HG12	1.94	0.50
1:C:266:LEU:HD22	1:C:291:TYR:CZ	2.46	0.50
1:U:216:ASN:HD21	1:U:257:ALA:HB1	1.76	0.50
8:O:201:ADP:N6	3:P:60:VAL:N	2.43	0.50
1:C:80:GLY:HA3	1:C:148:THR:OG1	2.12	0.50
2:D:297:ARG:O	2:D:301:MET:HG3	2.11	0.50
1:K:278:MET:HE3	1:K:284:VAL:HG21	1.94	0.50
2:M:268:GLY:HA2	2:M:329:LEU:HD13	1.94	0.50
8:J:201:ADP:C8	4:E:27:SER:CB	2.95	0.50
2:N:266:PRO:HA	2:N:271:ASN:HB3	1.94	0.50
4:a:13:VAL:HG21	4:a:67:ARG:HD2	1.93	0.50
1:A:515:TRP:HE3	1:A:518:ILE:HD11	1.77	0.49
2:M:326:LEU:O	2:M:330:VAL:HG23	2.12	0.49
1:L:124:GLU:HB3	4:O:14:GLN:NE2	2.26	0.49
3:I:38:LYS:CE	8:I:201:ADP:O3B	2.59	0.49
1:C:150:PRO:O	1:C:154:ILE:HG12	2.13	0.49
1:K:333:GLU:O	1:K:337:GLU:HG3	2.12	0.49
2:W:65:LEU:HB3	1:U:53:LEU:HD21	1.93	0.49
2:X:98:GLU:HG2	2:X:99:VAL:HG23	1.95	0.49
3:H:86:ARG:HD3	3:H:88:PHE:HZ	1.77	0.49
3:T:61:VAL:HA	3:T:105:LEU:HD11	1.94	0.49
2:N:173:ILE:HD13	2:N:238:ILE:HB	1.94	0.49
1:U:118:ASP:CG	1:U:126:LYS:HE3	2.37	0.49
4:Q:72:VAL:HG23	8:S:201:ADP:N6	2.27	0.49
4:O:36:ARG:HH12	4:O:40:ARG:HH22	1.60	0.49
2:D:287:ILE:HD12	2:D:287:ILE:H	1.77	0.49
2:X:54:MET:HE2	2:X:58:ARG:HH22	1.77	0.49
1:L:44:ALA:HB1	1:L:375:ALA:O	2.12	0.49
2:B:380:LYS:HG2	2:B:400:GLU:OE2	2.12	0.49
1:L:34:ARG:HG3	1:L:437:MET:HB3	1.95	0.49
1:C:202:ILE:HD13	1:C:278:MET:HE2	1.94	0.49
1:K:204:THR:HG23	1:K:205:GLU:HG2	1.94	0.49
2:M:15:ILE:HG22	2:M:17:ILE:HG13	1.94	0.49
2:X:295:ARG:O	2:X:299:VAL:HG23	2.13	0.49
3:T:5:ARG:HH12	3:S:3:MET:HE1	1.77	0.49
1:L:518:ILE:HG22	2:N:213:LYS:HE3	1.95	0.49
1:A:405:ARG:HG3	1:A:409:PHE:HE1	1.78	0.49
2:W:28:ALA:HB1	2:W:153:MET:HE2	1.95	0.49
2:X:314:VAL:HG21	2:X:330:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:66:VAL:HG12	1:V:92:ARG:HE	1.77	0.49
2:X:440:LEU:HD22	2:X:456:GLN:CD	2.38	0.49
3:R:39:GLN:HB3	3:R:82:TYR:HB3	1.95	0.49
3:d:74:MET:O	3:d:78:ARG:HG3	2.13	0.49
1:U:74:MET:HE2	1:U:144:THR:HG23	1.94	0.49
1:U:128:LYS:NZ	1:U:164:GLU:HG3	2.28	0.49
2:D:386:LEU:HD12	2:D:403:PRO:HB2	1.95	0.49
1:K:122:GLY:HA3	4:Q:14:GLN:OE1	2.13	0.49
2:M:141:SER:OG	5:M:601:CLF:S2B	2.69	0.49
1:V:72:LYS:HD3	1:V:96:ALA:HB1	1.95	0.49
1:L:8:LYS:HB3	1:L:442:ILE:HD11	1.93	0.49
1:U:198:MET:SD	1:U:277:MET:HB2	2.53	0.49
5:A:601:CLF:S4A	2:B:45:SER:HB3	2.53	0.49
1:K:360:PHE:HD1	1:K:365:MET:HE3	1.78	0.49
1:V:342:LYS:HB2	1:V:365:MET:HE3	1.95	0.49
2:X:200:PHE:CD2	2:X:201:PRO:HD3	2.48	0.49
1:L:124:GLU:H	4:O:14:GLN:HE22	1.59	0.49
1:L:229:GLU:HG3	1:L:492:ARG:HB3	1.94	0.49
1:V:77:LEU:HA	1:V:110:VAL:HG23	1.93	0.49
3:R:36:ARG:HH21	3:R:38:LYS:HZ3	1.61	0.49
1:L:312:GLU:HA	1:L:315:ARG:HG2	1.95	0.49
2:N:270:ARG:HH12	2:N:356:LEU:HD21	1.77	0.49
1:A:92:ARG:HA	7:A:603:HCA:O3	2.12	0.48
1:A:201:LEU:HD21	1:A:251:PHE:HB2	1.94	0.48
1:A:368:VAL:HG12	1:A:369:VAL:HG23	1.95	0.48
2:D:79:GLY:H	4:E:42:LEU:HD21	1.78	0.48
2:M:25:PRO:HB2	2:M:52:LEU:HD21	1.94	0.48
2:M:266:PRO:HG2	2:M:423:MET:HG2	1.95	0.48
3:d:98:ILE:HA	3:Z:74:MET:HE2	1.94	0.48
1:A:372:TYR:HD2	1:A:380:TYR:CZ	2.31	0.48
1:A:448:ASN:ND2	1:A:450:HIS:HB3	2.28	0.48
1:C:221:TYR:HD2	6:C:602:ICS:S3A	2.36	0.48
1:V:415:ALA:O	1:V:419:THR:HG23	2.13	0.48
1:A:198:MET:HE1	1:A:277:MET:HB2	1.95	0.48
2:B:416:ASN:HB3	2:D:301:MET:HE3	1.94	0.48
2:M:118:ILE:O	2:M:122:VAL:HG12	2.14	0.48
1:V:262:LEU:HD11	1:V:287:LEU:HB2	1.96	0.48
1:U:327:LYS:HG3	1:U:328:TYR:CD1	2.48	0.48
4:O:7:ILE:CD1	8:O:201:ADP:C8	2.93	0.48
1:A:347:TYR:OH	1:A:446:ASP:HA	2.14	0.48
2:B:333:MET:SD	2:B:432:VAL:HG22	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:317:TYR:CZ	2:D:389:GLY:HA3	2.48	0.48
1:K:484:ILE:HD12	1:K:485:HIS:HD2	1.79	0.48
1:V:377:ARG:HD3	1:V:390:LYS:HG2	1.94	0.48
3:R:34:PHE:CE1	1:L:120:VAL:HG21	2.48	0.48
3:R:35:GLY:HA2	4:O:29:THR:HA	1.95	0.48
3:T:98:ILE:HG23	4:Q:86:ILE:HD13	1.95	0.48
1:A:483:GLN:HB2	1:A:488:ASP:N	2.29	0.48
1:C:8:LYS:O	1:C:12:VAL:HG23	2.13	0.48
2:W:241:CYS:HB3	2:W:321:ASP:OD2	2.13	0.48
1:L:100:GLU:H	1:L:100:GLU:CD	2.21	0.48
1:L:272:ASN:HA	1:L:275:ASN:ND2	2.28	0.48
1:U:475:GLN:NE2	1:U:480:PRO:HA	2.28	0.48
1:V:288:LYS:HG2	1:V:430:TYR:CD1	2.49	0.48
3:S:23:GLU:HG3	3:S:72:THR:HG21	1.94	0.48
1:A:91:THR:HB	2:B:58:ARG:NH2	2.28	0.48
7:C:603:HCA:H52	7:C:603:HCA:H21	1.44	0.48
2:D:158:VAL:HG21	2:D:248:ALA:HB1	1.95	0.48
2:W:375:LEU:HD23	2:W:396:ILE:HD13	1.95	0.48
1:L:463:ILE:HD13	1:L:464:PHE:H	1.77	0.48
2:N:391:THR:HG21	2:N:413:ASP:H	1.78	0.48
1:C:78:VAL:HG11	1:C:85:ALA:HB2	1.96	0.48
2:W:288:PRO:HD2	2:W:291:LEU:HD12	1.94	0.48
4:E:37:GLY:HA3	8:E:201:ADP:PB	2.53	0.48
1:C:474:ALA:O	1:C:477:ILE:HG22	2.13	0.48
1:K:300:SER:O	1:K:304:MET:HG3	2.14	0.48
2:M:314:VAL:HG21	2:M:330:VAL:HG11	1.96	0.48
1:V:92:ARG:NH2	1:V:94:ASN:OD1	2.46	0.48
4:E:38:LYS:N	8:E:201:ADP:O3B	2.47	0.48
1:A:52:ILE:HG23	1:A:448:ASN:HB3	1.96	0.48
1:K:350:GLY:CA	6:K:602:ICS:S2A	3.02	0.48
2:M:145:THR:HG23	2:M:147:ILE:H	1.78	0.48
1:V:74:MET:HG2	1:V:142:ALA:HB3	1.95	0.48
1:V:129:LYS:HE2	1:V:129:LYS:HB2	1.74	0.48
2:W:276:ILE:HD12	2:W:291:LEU:HD13	1.96	0.48
2:X:341:LEU:HD13	2:X:367:ILE:HD11	1.95	0.48
1:U:65:GLY:O	1:U:92:ARG:HG3	2.13	0.48
1:U:245:LEU:HA	1:U:246:THR:HA	1.46	0.48
2:B:54:MET:O	2:B:58:ARG:HG3	2.14	0.47
1:V:392:LYS:HA	1:V:392:LYS:HD3	1.76	0.47
2:W:316:ILE:HG22	2:W:323:LEU:HD22	1.96	0.47
2:X:199:VAL:O	2:X:202:ASP:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:15:ILE:HD12	1:L:454:PHE:HD2	1.79	0.47
2:N:314:VAL:HG21	2:N:330:VAL:HG11	1.96	0.47
2:B:297:ARG:O	2:B:301:MET:HG3	2.15	0.47
2:D:391:THR:HG21	2:D:413:ASP:H	1.79	0.47
1:K:207:ILE:HG12	1:K:256:GLN:HB3	1.96	0.47
1:K:476:LYS:HD3	2:M:211:LEU:HD13	1.96	0.47
2:W:317:TYR:CE2	2:W:372:LEU:HD21	2.49	0.47
3:J:29:THR:HB	3:J:58:LEU:HB3	1.95	0.47
1:A:28:ARG:HH12	3:c:22:LYS:HA	1.78	0.47
2:D:164:LYS:HA	2:D:232:ALA:HB2	1.96	0.47
1:K:158:ILE:HD11	1:K:177:ARG:HG2	1.96	0.47
2:M:39:MET:HE2	2:M:39:MET:HB2	1.74	0.47
3:H:10:PRO:HD3	3:H:54:LYS:HA	1.96	0.47
1:A:79:HIS:CE1	1:A:127:LEU:HD13	2.50	0.47
1:C:347:TYR:HE1	1:C:373:GLN:HE21	1.60	0.47
2:D:165:SER:H	2:D:232:ALA:CB	2.22	0.47
1:K:463:ILE:HD11	1:K:482:ARG:HG2	1.97	0.47
2:W:37:ASN:HB2	2:W:98:GLU:HB2	1.96	0.47
1:U:72:LYS:HE2	1:U:96:ALA:HB1	1.95	0.47
3:I:20:LEU:HD13	3:I:59:MET:HE1	1.96	0.47
2:D:48:CYS:O	2:D:49:LEU:C	2.57	0.47
2:W:15:ILE:HD11	1:U:130:ALA:O	2.14	0.47
3:d:49:TYR:CZ	4:Y:26:PRO:HB2	2.49	0.47
1:L:202:ILE:HD13	1:L:278:MET:HE3	1.97	0.47
1:U:149:CYS:SG	1:U:150:PRO:HD3	2.54	0.47
1:U:265:LEU:HD21	1:U:275:ASN:OD1	2.15	0.47
2:D:101:ALA:HB1	2:D:153:MET:HE2	1.97	0.47
1:K:348:ALA:CB	1:K:352:ARG:HB3	2.44	0.47
2:B:226:GLY:HA2	2:B:229:GLU:OE2	2.14	0.47
2:D:239:ALA:HB3	2:D:262:ILE:HG23	1.96	0.47
1:K:50:PRO:O	2:M:87:ALA:HA	2.15	0.47
2:M:24:GLN:HE21	2:M:148:THR:HB	1.78	0.47
2:W:15:ILE:HG23	1:U:110:VAL:HG13	1.97	0.47
2:W:67:THR:HG23	1:U:51:GLY:HA2	1.95	0.47
3:J:8:ILE:HD13	3:J:57:LEU:HD11	1.96	0.47
3:T:31:MET:SD	4:Q:31:ARG:HD2	2.54	0.47
3:d:36:ARG:HA	3:d:50:ASP:O	2.15	0.47
1:L:87:PHE:CG	2:N:51:TYR:HB3	2.49	0.47
2:N:367:ILE:HD11	2:N:378:ILE:HD11	1.96	0.47
1:U:471:LYS:O	1:U:475:GLN:HG2	2.15	0.47
4:Q:78:VAL:O	4:Q:82:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:201:AKG:O2	3:c:54:LYS:HE3	2.14	0.47
4:Y:29:THR:HB	4:Y:70:THR:HB	1.97	0.47
1:C:82:ILE:HD11	2:D:19:PRO:HB3	1.95	0.47
2:W:412:MET:HE3	2:X:455:ILE:HG12	1.96	0.47
3:J:20:LEU:HD22	3:J:25:CYS:HB2	1.97	0.47
3:T:74:MET:HE1	3:S:96:TYR:HB3	1.97	0.47
3:d:38:LYS:HE2	3:d:47:ILE:HG21	1.96	0.47
2:B:422:ILE:HG13	2:B:431:LEU:HD11	1.97	0.47
1:C:363:LEU:HD21	1:C:503:ALA:HA	1.97	0.47
1:V:70:PRO:HB3	1:V:247:GLY:HA2	1.96	0.47
1:V:121:PHE:CD2	3:d:51:GLU:HB3	2.50	0.47
2:W:17:ILE:HB	2:W:373:PHE:HB2	1.96	0.47
2:B:166:LYS:HB2	2:B:166:LYS:HE2	1.75	0.47
2:X:332:GLU:HG2	1:U:517:PHE:CZ	2.50	0.47
3:R:37:GLY:HA3	8:R:201:ADP:H2'	1.97	0.47
1:A:201:LEU:HD11	1:A:251:PHE:HB2	1.98	0.46
1:C:339:LEU:HD11	1:C:507:ASP:HB2	1.97	0.46
2:D:308:HIS:CD2	2:D:440:LEU:HD21	2.49	0.46
1:V:48:VAL:HG13	2:X:70:SER:HB2	1.98	0.46
2:W:281:LYS:HB2	2:W:281:LYS:NZ	2.29	0.46
2:X:114:ASP:HB3	2:X:117:VAL:HG23	1.96	0.46
3:b:74:MET:HA	3:b:74:MET:HE3	1.98	0.46
1:L:80:GLY:HA2	1:L:114:MET:HE2	1.97	0.46
4:E:38:LYS:N	8:E:201:ADP:PB	2.80	0.46
4:E:98:LYS:CD	8:E:201:ADP:H8	2.07	0.46
4:Q:6:ALA:HA	4:Q:99:ILE:HD13	1.97	0.46
4:Q:42:LEU:HD12	4:Q:62:ARG:HD2	1.97	0.46
2:B:67:THR:HG21	2:B:91:LEU:HD13	1.96	0.46
2:D:269:ILE:HB	2:D:332:GLU:OE1	2.15	0.46
1:K:522:TRP:HZ2	2:N:292:GLU:HG2	1.81	0.46
3:S:38:LYS:HD3	3:S:83:GLY:N	2.31	0.46
1:K:261:LYS:HB2	1:K:308:PHE:HZ	1.81	0.46
1:K:264:ILE:HG21	1:K:304:MET:HE3	1.97	0.46
3:H:2:GLN:HG3	3:H:66:LYS:HE2	1.97	0.46
3:d:2:GLN:HG3	3:d:66:LYS:HD3	1.97	0.46
1:U:347:TYR:CE1	1:U:447:LEU:HB2	2.50	0.46
1:A:386:ILE:HA	1:A:389:ILE:HG12	1.97	0.46
1:C:374:PHE:HZ	6:C:602:ICS:S3B	2.37	0.46
1:K:262:LEU:HD22	1:K:307:PHE:CD1	2.50	0.46
1:L:207:ILE:HG23	1:L:242:ILE:HD13	1.97	0.46
1:U:92:ARG:NH2	6:U:602:ICS:S5A	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:386:ILE:HG22	1:U:387:PRO:HD3	1.98	0.46
4:G:109:ARG:HH21	4:G:119:THR:HA	1.79	0.46
8:E:201:ADP:C6	3:F:27:SER:HB3	2.50	0.46
1:A:407:GLU:HB3	1:A:408:ASN:H	1.50	0.46
1:K:87:PHE:CG	2:M:51:TYR:HB3	2.51	0.46
2:W:41:HIS:HB3	2:W:102:ILE:HG12	1.98	0.46
1:L:68:PHE:HD2	1:L:144:THR:HG21	1.80	0.46
1:U:66:VAL:CG2	6:U:602:ICS:S2B	3.02	0.46
2:W:301:MET:HG2	2:X:416:ASN:ND2	2.29	0.46
2:X:90:ASN:O	2:X:94:VAL:HG12	2.16	0.46
3:R:37:GLY:HA3	8:R:201:ADP:C2'	2.46	0.46
1:L:269:ARG:NH2	1:L:376:HIS:H	2.13	0.46
1:L:270:SER:C	1:L:271:ILE:HD13	2.40	0.46
1:L:413:ILE:HG13	1:L:418:ILE:HG13	1.97	0.46
3:S:40:LYS:HD2	3:S:40:LYS:HA	1.41	0.46
1:K:245:LEU:HA	1:K:246:THR:HA	1.57	0.46
1:L:137:ILE:HG12	2:N:10:VAL:HG11	1.98	0.46
1:U:15:ILE:HG12	1:U:454:PHE:HB3	1.97	0.46
1:C:289:VAL:HB	1:C:300:SER:HB3	1.97	0.46
2:M:235:LEU:HD12	2:M:283:ALA:HA	1.97	0.46
2:M:452:LEU:HD23	2:M:452:LEU:HA	1.77	0.46
2:X:173:ILE:HB	2:X:199:VAL:HG22	1.98	0.46
1:U:97:LYS:HG3	1:U:228:TRP:CZ2	2.51	0.46
1:U:485:HIS:HA	6:U:602:ICS:S4B	2.56	0.46
1:V:60:PHE:CD2	5:V:601:CLF:S2A	3.08	0.46
2:W:26:ILE:HG13	2:W:52:LEU:HG	1.97	0.46
2:X:94:VAL:HG13	2:X:95:TYR:H	1.81	0.46
1:A:79:HIS:ND1	1:A:127:LEU:HD13	2.31	0.46
1:A:339:LEU:HB3	1:A:365:MET:SD	2.56	0.46
1:A:502:PHE:O	1:A:506:ILE:HG12	2.16	0.46
2:D:225:ILE:HD12	2:D:228:ILE:HD12	1.98	0.46
1:K:88:THR:HG22	7:K:601:HCA:O4	2.15	0.46
2:M:39:MET:HE1	2:M:217:PHE:HE2	1.81	0.46
2:M:158:VAL:HG21	2:M:248:ALA:HB1	1.97	0.46
2:X:314:VAL:HG12	2:X:386:LEU:HB3	1.96	0.46
4:O:8:ILE:HD11	4:O:69:PHE:CE1	2.51	0.46
1:A:258:HIS:CE1	1:A:259:GLN:HG3	2.51	0.45
1:K:473:TRP:O	1:K:477:ILE:HG12	2.16	0.45
2:M:155:LYS:HE3	2:M:155:LYS:HB3	1.84	0.45
2:M:351:LYS:HB2	2:M:351:LYS:HE3	1.64	0.45
2:X:25:PRO:HB2	2:X:52:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:120:GLU:HA	2:X:120:GLU:OE2	2.15	0.45
1:U:219:GLY:HA3	1:U:267:CYS:H	1.80	0.45
2:W:317:TYR:C	2:W:323:LEU:HD21	2.41	0.45
2:B:323:LEU:HD23	2:B:340:VAL:HG12	1.97	0.45
1:V:465:CYS:HA	1:V:482:ARG:O	2.16	0.45
3:T:66:LYS:HB3	3:T:66:LYS:HE2	1.74	0.45
1:L:29:LYS:HB2	1:L:29:LYS:HE2	1.56	0.45
1:L:106:MET:HE3	1:L:106:MET:HB3	1.80	0.45
1:L:383:ARG:HG3	1:L:430:TYR:HB3	1.99	0.45
4:O:96:ASP:CB	3:P:98:ILE:HB	2.46	0.45
3:P:31:MET:HE2	3:P:31:MET:HB3	1.88	0.45
1:C:122:GLY:HA3	4:E:14:GLN:OE1	2.16	0.45
1:V:375:ALA:HB3	1:V:380:TYR:HE1	1.81	0.45
3:d:36:ARG:HG2	3:d:49:TYR:CD2	2.48	0.45
4:E:98:LYS:HE3	8:E:201:ADP:C8	2.51	0.45
3:F:20:LEU:HD23	3:F:59:MET:HE1	1.97	0.45
4:Q:84:LYS:HA	4:Q:84:LYS:HD3	1.71	0.45
4:Y:9:ARG:HD2	4:Y:44[A]:PHE:CE1	2.52	0.45
1:A:295:LYS:NZ	1:A:295:LYS:HB2	2.31	0.45
1:A:484:ILE:HD12	1:A:485:HIS:CD2	2.52	0.45
1:C:346:ILE:O	1:C:370:ALA:HA	2.17	0.45
2:M:331:LEU:HD21	2:M:337:PRO:HG3	1.98	0.45
1:L:239:TYR:CE1	1:L:313:LEU:HD21	2.52	0.45
4:a:110:ILE:HD11	3:c:87:ILE:HG13	1.98	0.45
2:B:301:MET:HG2	2:D:419:TYR:CE2	2.52	0.45
1:C:374:PHE:HZ	6:C:602:ICS:S5A	2.37	0.45
1:K:268:HIS:O	1:K:272:ASN:HB3	2.17	0.45
2:M:448:PRO:HG2	2:M:451:LEU:HB2	1.98	0.45
1:V:233:ILE:O	1:V:237:ILE:HG12	2.17	0.45
2:W:315:ALA:HB3	2:W:387:LEU:HD23	1.98	0.45
2:N:94:VAL:HG13	2:N:95:TYR:H	1.81	0.45
1:U:41:HIS:HA	1:U:381:GLU:OE1	2.16	0.45
3:I:65:HIS:HB3	3:I:68:LYS:HE3	1.98	0.45
1:A:77:LEU:HA	1:A:110:VAL:HG12	1.99	0.45
1:A:448:ASN:HD22	1:A:450:HIS:HB3	1.81	0.45
2:M:166:LYS:HA	2:W:226:GLY:HA3	1.98	0.45
2:M:376:HIS:HD2	2:M:396:ILE:HG12	1.82	0.45
1:V:438:LYS:HD2	1:V:439:ASP:H	1.81	0.45
2:X:109:GLU:HG3	2:X:140:PRO:HG3	1.98	0.45
1:L:219:GLY:HA3	1:L:267:CYS:H	1.81	0.45
1:L:289:VAL:HG21	1:L:304:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:203:GLY:HA2	1:U:258:HIS:CD2	2.51	0.45
3:I:38:LYS:CD	8:I:201:ADP:O3B	2.65	0.45
1:A:182:ARG:HA	2:B:73:GLU:OE2	2.17	0.45
2:D:18:ASN:HB3	2:D:372:LEU:HB2	1.99	0.45
1:K:66:VAL:HG21	6:K:602:ICS:S5A	2.56	0.45
3:J:29:THR:HG23	3:F:33:VAL:HG13	1.98	0.45
2:N:407:VAL:HG21	2:N:431:LEU:HD21	1.98	0.45
4:E:84:LYS:HA	4:E:84:LYS:HD2	1.69	0.45
3:I:86:ARG:HH11	8:I:201:ADP:C1'	2.29	0.45
4:O:9:ARG:HH11	4:O:95:GLY:HA3	1.82	0.45
3:P:86:ARG:HG3	3:P:88:PHE:CZ	2.52	0.45
2:D:166:LYS:H	2:D:232:ALA:HB1	1.82	0.45
2:D:288:PRO:HD2	2:D:291:LEU:HD12	1.99	0.45
1:V:377:ARG:HE	1:V:377:ARG:HB3	1.67	0.45
3:H:70:ILE:HD11	3:H:89:VAL:HG21	1.97	0.45
3:J:70:ILE:HG22	3:J:71:LYS:HE3	1.99	0.45
2:N:317:TYR:HA	2:N:341:LEU:O	2.17	0.45
4:Y:1:MET:HB3	4:Y:104:ILE:HB	1.99	0.45
3:Z:5:ARG:HD3	3:Z:58:LEU:HD12	1.99	0.45
2:D:200:PHE:N	2:D:200:PHE:CD1	2.84	0.45
1:K:444:VAL:HG21	1:K:447:LEU:HD12	1.99	0.45
2:M:141:SER:HB2	5:M:601:CLF:S3B	2.57	0.45
2:M:225:ILE:O	2:M:229:GLU:HG3	2.17	0.45
1:V:366:LYS:HE3	1:V:366:LYS:HB2	1.88	0.45
2:X:21:LYS:HD3	2:X:145:THR:HG22	1.99	0.45
2:X:255:ARG:HG3	2:X:256:TYR:CD2	2.52	0.45
3:R:36:ARG:HH21	3:R:38:LYS:NZ	2.13	0.45
1:L:34:ARG:HA	1:L:34:ARG:HD2	1.75	0.45
1:L:471:LYS:HG3	1:L:481:SER:OG	2.17	0.45
2:N:158:VAL:HG21	2:N:248:ALA:HB1	1.98	0.45
4:O:98:LYS:CE	8:O:201:ADP:H5'1	2.46	0.45
4:a:10:MET:HG3	4:a:67:ARG:HH21	1.82	0.45
1:A:482:ARG:HD3	1:A:509:ALA:HB2	1.99	0.44
2:B:150:TYR:CE1	2:B:176:GLY:HA2	2.52	0.44
1:C:74:MET:HG2	1:C:142:ALA:HB3	1.99	0.44
2:M:266:PRO:HA	2:M:271:ASN:HB3	1.99	0.44
2:M:302:MET:HE3	1:L:514:THR:HG22	1.99	0.44
2:W:90:ASN:O	2:W:94:VAL:HG12	2.17	0.44
2:W:326:LEU:HD11	2:W:407:VAL:HG21	1.99	0.44
2:X:175:PRO:HD3	2:X:201:PRO:HD2	1.99	0.44
1:L:122:GLY:HA3	4:O:14:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:353:SER:O	1:L:357:ILE:HG12	2.16	0.44
1:U:28:ARG:HG3	1:U:28:ARG:HH11	1.82	0.44
1:U:75:VAL:HG13	1:U:143:ILE:HG23	2.00	0.44
1:U:216:ASN:O	1:U:264:ILE:HG12	2.17	0.44
4:Q:50:LEU:HD22	4:Q:51:PRO:HD2	1.98	0.44
4:Y:38:LYS:HA	4:Y:38:LYS:HD3	1.81	0.44
1:C:477:ILE:HD12	1:C:477:ILE:HA	1.87	0.44
2:W:158:VAL:HG21	2:W:248:ALA:HB1	1.99	0.44
3:T:10:PRO:HD3	3:T:54:LYS:HA	1.99	0.44
3:d:68:LYS:O	3:d:72:THR:HG23	2.16	0.44
1:L:237:ILE:HD11	1:L:301:LEU:HD13	1.98	0.44
4:a:82:VAL:HG22	4:a:99:ILE:HG21	1.98	0.44
1:A:92:ARG:HB3	1:A:94:ASN:OD1	2.17	0.44
2:M:27:GLY:HA2	2:M:177:PHE:HE1	1.82	0.44
2:X:232:ALA:HB1	2:X:256:TYR:CG	2.52	0.44
3:d:38:LYS:HB2	3:d:82:TYR:HB3	1.97	0.44
1:U:372:TYR:HB2	1:U:380:TYR:OH	2.17	0.44
2:D:186:ILE:HG13	2:D:240:LEU:HD21	1.98	0.44
1:K:405:ARG:HG3	1:K:409:PHE:HE1	1.81	0.44
1:V:42:ILE:HD12	1:V:42:ILE:HA	1.88	0.44
4:Q:122:LYS:HB2	4:Q:122:LYS:HE3	1.75	0.44
3:S:1:MET:HE3	3:S:95:ALA:HB3	1.98	0.44
2:B:61:ARG:HH21	2:D:308:HIS:HE1	1.66	0.44
2:D:390:ASN:HB3	2:D:410:PRO:HD2	2.00	0.44
2:M:45:SER:CB	5:M:601:CLF:S2A	3.05	0.44
1:V:245:LEU:HA	1:V:246:THR:HA	1.56	0.44
1:V:338:LYS:HE2	1:V:338:LYS:HB2	1.59	0.44
1:V:347:TYR:CE1	1:V:373:GLN:HB2	2.53	0.44
1:V:450:HIS:HB2	2:X:95:TYR:CE1	2.53	0.44
2:X:453:GLU:H	2:X:453:GLU:HG3	1.55	0.44
1:L:120:VAL:HG22	4:O:32:ARG:HD3	1.99	0.44
1:L:215:ILE:HG22	1:L:262:LEU:HB3	1.99	0.44
2:N:23:CYS:HB3	2:N:25:PRO:HD2	1.99	0.44
1:U:96:ALA:HB3	1:U:106:MET:HG3	2.00	0.44
4:Q:47:ASN:CG	4:Q:48:PRO:HD3	2.42	0.44
3:P:10:PRO:HD3	3:P:54:LYS:HA	2.00	0.44
4:a:40:ARG:HH22	4:a:64:ILE:HG12	1.81	0.44
3:c:60:VAL:HG12	3:c:105:LEU:HD11	1.98	0.44
1:C:143:ILE:HD11	1:C:171:ILE:HD11	1.98	0.44
1:C:281:LYS:HD3	1:C:403:TYR:CD2	2.53	0.44
1:K:234:LEU:HD12	1:K:241:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:281:LYS:HE3	2:M:281:LYS:HB2	1.70	0.44
1:V:416:GLU:H	1:V:416:GLU:CD	2.25	0.44
3:H:98:ILE:HD11	4:G:85:ILE:HG22	2.00	0.44
3:J:15:LYS:HB3	3:J:15:LYS:HE2	1.80	0.44
1:U:325:LYS:O	1:U:329:ALA:HB2	2.18	0.44
4:Y:40:ARG:HD3	4:Y:40:ARG:HA	1.74	0.44
1:K:53:LEU:HB2	2:M:95:TYR:CE2	2.53	0.44
1:K:149:CYS:O	1:K:150:PRO:C	2.56	0.44
1:K:262:LEU:HD12	1:K:263:SER:H	1.82	0.44
1:K:288:LYS:HE3	1:K:430:TYR:CE1	2.53	0.44
1:K:327:LYS:HG3	1:K:328:TYR:CE2	2.53	0.44
2:M:46:GLN:H	2:M:46:GLN:HG2	1.65	0.44
2:M:133:LYS:HE3	2:M:229:GLU:OE2	2.17	0.44
2:M:301:MET:HE3	2:M:301:MET:HB3	1.77	0.44
1:V:482:ARG:HG3	1:V:506:ILE:HD13	2.00	0.44
3:R:61:VAL:HG11	3:R:69:VAL:HG21	1.99	0.44
3:T:70:ILE:HD12	3:T:70:ILE:H	1.83	0.44
2:N:200:PHE:CG	2:N:201:PRO:HD3	2.52	0.44
1:C:469:LYS:NZ	2:D:50:SER:HB2	2.33	0.44
1:C:471:LYS:HD2	1:C:483:GLN:HG3	2.00	0.44
2:D:261:LYS:HG3	2:D:282:LEU:HD11	1.99	0.44
1:K:354:HIS:HB2	1:K:433:LEU:HD13	1.99	0.44
2:M:106:CYS:O	2:M:107:VAL:C	2.60	0.44
1:V:288:LYS:HG2	1:V:430:TYR:HD1	1.83	0.44
3:J:10:PRO:HD3	3:J:54:LYS:HA	1.99	0.44
1:L:8:LYS:HD3	1:L:442:ILE:HD11	1.99	0.44
1:L:218:PHE:HD1	1:L:245:LEU:HB2	1.82	0.44
1:U:229:GLU:HB3	1:U:494:THR:HB	2.00	0.44
4:G:85:ILE:HG22	4:G:99:ILE:HD11	1.99	0.44
4:Q:4:ILE:HD11	4:Q:78:VAL:HG23	1.97	0.44
1:C:15:ILE:HG12	1:C:454:PHE:HB3	1.99	0.44
7:K:601:HCA:O1	7:K:601:HCA:H52	2.18	0.44
4:G:71:VAL:HG22	4:G:73:VAL:HG13	2.00	0.44
3:P:7:VAL:O	3:P:85:GLY:HA3	2.18	0.44
1:A:135:VAL:HA	1:A:140:PRO:HD2	2.00	0.43
2:D:21:LYS:HD3	2:D:145:THR:HG22	1.99	0.43
1:K:58:CYS:HB2	1:K:180:GLY:HA2	2.00	0.43
1:K:430:TYR:CE2	1:K:432:GLY:HA2	2.53	0.43
2:M:317:TYR:OH	2:M:393:GLY:HA3	2.18	0.43
2:X:404:LEU:HD12	2:X:405:VAL:N	2.33	0.43
1:L:218:PHE:HE1	1:L:245:LEU:HD13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:84:LYS:HA	4:a:84:LYS:HD3	1.75	0.43
1:A:149:CYS:HB3	5:A:601:CLF:S2A	2.59	0.43
1:A:522:TRP:HZ3	2:D:273:ASP:HB3	1.83	0.43
2:X:175:PRO:HB3	2:X:183:ILE:HG12	2.01	0.43
1:L:50:PRO:HB2	2:N:87:ALA:HB2	2.00	0.43
2:N:212:THR:C	2:N:213:LYS:HD3	2.43	0.43
2:N:266:PRO:HD2	2:N:423:MET:CE	2.48	0.43
2:N:345:GLN:HA	2:N:368:SER:OG	2.18	0.43
1:U:374:PHE:CZ	6:U:602:ICS:S1B	3.10	0.43
4:G:84:LYS:HA	4:G:84:LYS:HD3	1.74	0.43
3:I:38:LYS:CG	8:I:201:ADP:O3B	2.65	0.43
1:A:513:PRO:HG2	2:D:334:GLY:HA2	2.00	0.43
1:C:34:ARG:HD2	1:C:34:ARG:HA	1.80	0.43
1:C:148:THR:O	1:C:179:GLU:HG3	2.18	0.43
1:C:207:ILE:HD11	1:C:242:ILE:HG23	1.99	0.43
2:D:25:PRO:HB2	2:D:52:LEU:HD11	2.00	0.43
2:W:336:GLU:HB2	2:W:361:TYR:CD2	2.53	0.43
2:W:374:MET:HE2	2:W:374:MET:HB2	1.83	0.43
2:X:365:ASP:O	2:X:367:ILE:HG23	2.18	0.43
3:R:40:LYS:HG3	8:R:201:ADP:O2B	2.18	0.43
2:N:135:CYS:HB2	2:N:161:PHE:CZ	2.53	0.43
2:N:330:VAL:CG1	2:N:335:MET:HB3	2.47	0.43
2:B:49:LEU:HD11	2:B:66:ALA:HB1	2.01	0.43
2:B:267:ILE:HG21	2:B:326:LEU:HD23	2.01	0.43
2:D:23:CYS:CB	2:D:25:PRO:HD2	2.46	0.43
1:K:77:LEU:HD13	1:K:110:VAL:HG12	2.00	0.43
1:K:366:LYS:NZ	1:K:366:LYS:HB3	2.32	0.43
1:V:188:ALA:HA	1:V:398:LEU:HD11	2.00	0.43
3:R:40:LYS:HG3	8:R:201:ADP:PB	2.58	0.43
8:d:201:ADP:PB	4:Y:111:ARG:HH21	2.41	0.43
4:O:77:ASN:O	4:O:81:VAL:HG12	2.18	0.43
1:C:450:HIS:HB2	2:D:95:TYR:CE1	2.53	0.43
2:D:178:VAL:HG11	2:D:423:MET:HE3	2.00	0.43
2:D:287:ILE:HD12	2:D:287:ILE:N	2.32	0.43
1:K:132:ASP:O	1:K:135:VAL:HG12	2.19	0.43
1:K:360:PHE:CD1	1:K:365:MET:HE3	2.53	0.43
1:V:359:LEU:HD11	1:V:499:VAL:HG13	2.00	0.43
3:b:33:VAL:HB	3:c:29:THR:HG23	2.00	0.43
2:N:175:PRO:HB3	2:N:183:ILE:HG12	1.99	0.43
1:C:131:ILE:O	1:C:135:VAL:HG23	2.19	0.43
2:D:261:LYS:HE3	2:D:261:LYS:HB3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:96:GLN:H	2:M:96:GLN:HG3	1.53	0.43
1:V:374:PHE:HD1	1:V:374:PHE:O	2.01	0.43
1:V:390:LYS:HD2	1:V:390:LYS:HA	1.90	0.43
2:W:47:GLY:CA	5:W:601:CLF:S2B	3.07	0.43
2:X:317:TYR:C	2:X:323:LEU:HD21	2.43	0.43
1:L:157:ASP:O	1:L:161:VAL:HG23	2.19	0.43
1:U:166:GLU:HG2	1:U:172:LYS:HA	2.01	0.43
1:U:316:LYS:HB3	1:U:316:LYS:HE3	1.80	0.43
8:E:201:ADP:H8	8:E:201:ADP:H5'1	1.83	0.43
1:A:12:VAL:HG22	1:A:31:ILE:HD11	2.00	0.43
2:D:213:LYS:HB2	2:D:213:LYS:HE2	1.50	0.43
2:D:309:TYR:CE1	2:D:333:MET:HB3	2.53	0.43
2:D:409:PHE:HB3	2:D:410:PRO:HD3	2.00	0.43
2:M:5:THR:HG22	2:M:373:PHE:CE1	2.54	0.43
2:M:24:GLN:NE2	2:M:148:THR:HB	2.33	0.43
1:V:431:GLU:HB2	1:V:435:PRO:HG2	2.01	0.43
2:W:211:LEU:HD13	1:U:476:LYS:HD3	2.01	0.43
2:W:331:LEU:HD21	2:W:357:ILE:HA	2.01	0.43
2:X:182:ASP:CG	2:X:423:MET:HG3	2.43	0.43
2:X:261:LYS:HD3	2:X:282:LEU:HD11	2.00	0.43
3:T:6:ALA:HB2	3:T:87:ILE:HG23	2.01	0.43
3:b:33:VAL:HG12	3:c:31:MET:HG2	2.01	0.43
2:N:111:ILE:O	4:O:65:PRO:HG3	2.19	0.43
2:N:374:MET:O	2:N:378:ILE:HG13	2.18	0.43
2:N:379:ILE:HG22	2:N:400:GLU:HG3	2.00	0.43
1:U:154:ILE:HD12	4:a:10:MET:HG2	2.00	0.43
1:U:277:MET:O	1:U:281:LYS:HB2	2.19	0.43
1:U:349:GLY:CA	6:U:602:ICS:S3A	3.07	0.43
4:Q:46:PHE:HB2	4:Q:50:LEU:HG	2.00	0.43
4:Q:47:ASN:ND2	4:Q:48:PRO:HD3	2.33	0.43
1:A:58:CYS:HB3	1:A:59:ALA:H	1.41	0.43
2:D:42:SER:CB	2:D:49:LEU:HD22	2.49	0.43
1:K:133:GLU:HB2	2:M:15:ILE:CD1	2.48	0.43
1:K:372:TYR:HB2	1:K:380:TYR:OH	2.19	0.43
2:M:39:MET:HG2	2:M:91:LEU:HD11	2.00	0.43
2:W:24:GLN:HG2	2:W:149:GLY:CA	2.49	0.43
2:W:406:ARG:HD3	2:W:414:ARG:HG2	2.00	0.43
2:X:306:HIS:CE1	1:U:508:MET:HG3	2.53	0.43
3:J:99:ARG:HD3	3:F:82:TYR:HA	2.01	0.43
1:L:73:ASP:HB3	1:L:251:PHE:HD1	1.83	0.43
2:N:135:CYS:HB2	2:N:161:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:201:LEU:HD23	1:U:201:LEU:HA	1.83	0.43
3:I:38:LYS:HE2	3:I:49:TYR:CE2	2.54	0.43
1:L:118:ASP:OD2	1:L:126:LYS:HE3	2.19	0.43
1:L:208:LYS:HD3	1:L:208:LYS:HA	1.73	0.43
2:N:22:ILE:HG22	2:N:23:CYS:H	1.83	0.43
4:Y:10:MET:SD	4:Y:65:PRO:HB2	2.59	0.43
3:Z:30:LYS:HB3	3:Z:57:LEU:HD23	2.00	0.43
1:A:198:MET:HE1	1:A:277:MET:CB	2.49	0.43
2:B:330:VAL:HG13	2:B:335:MET:HB2	2.01	0.43
2:B:411:ILE:HG21	2:B:417:LEU:HD12	2.00	0.43
1:C:483:GLN:HB2	1:C:488:ASP:N	2.33	0.43
2:D:92:THR:HA	2:D:97:PRO:HD3	2.00	0.43
1:K:350:GLY:HA3	6:K:602:ICS:S2A	2.59	0.43
2:W:40:PRO:HG2	2:W:66:ALA:HB2	2.01	0.43
3:R:13:GLU:O	3:R:17:VAL:HG22	2.19	0.43
1:L:20:PRO:HD3	2:N:93:THR:HG21	2.01	0.43
1:L:119:ILE:HD11	1:L:150:PRO:HB2	2.01	0.43
1:L:346:ILE:HD11	1:L:360:PHE:CE1	2.54	0.43
2:N:237:THR:HG21	2:N:249:ALA:HA	2.01	0.43
2:B:28:ALA:HB1	2:B:153:MET:HE3	2.01	0.42
2:B:410:PRO:HB2	2:B:412:MET:HE3	2.01	0.42
1:C:34:ARG:HH11	1:C:40:GLN:HG3	1.83	0.42
2:D:200:PHE:N	2:D:200:PHE:HD1	2.16	0.42
1:K:120:VAL:HG23	4:Q:67:ARG:HH11	1.83	0.42
2:M:59:HIS:HD2	2:M:60:TYR:CE2	2.37	0.42
2:M:175:PRO:HA	2:M:240:LEU:HD12	2.01	0.42
1:V:353:SER:HB2	1:V:372:TYR:HE1	1.84	0.42
1:V:384:GLN:NE2	1:V:385:ILE:HG12	2.33	0.42
2:W:84:LEU:HD11	2:W:102:ILE:HD13	2.01	0.42
2:W:97:PRO:HA	2:W:218:TYR:HE2	1.83	0.42
2:X:41:HIS:HE1	2:X:87:ALA:HB1	1.83	0.42
3:J:70:ILE:HD12	4:E:108:ILE:HG13	2.01	0.42
3:R:51:GLU:HB3	1:L:121:PHE:CD2	2.54	0.42
1:L:266:LEU:HD12	1:L:289:VAL:O	2.19	0.42
2:N:184:ARG:NH2	2:N:204:THR:HB	2.34	0.42
1:U:482:ARG:HA	1:U:482:ARG:HD2	1.65	0.42
4:G:39:GLN:H	4:G:39:GLN:HG2	1.45	0.42
3:I:88:PHE:CE2	8:I:201:ADP:C2	3.06	0.42
1:A:177:ARG:O	1:A:192:ILE:HD13	2.20	0.42
1:A:352:ARG:CB	6:A:602:ICS:S3A	3.04	0.42
2:B:71:PHE:CE1	2:B:80:GLY:HA3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ILE:O	4:E:11:ASN:HA	2.19	0.42
1:C:230:ILE:HA	1:C:233:ILE:HD12	2.00	0.42
1:C:287:LEU:HD11	1:C:425:ILE:HD12	2.01	0.42
3:d:36:ARG:HE	4:Y:21:LEU:HD13	1.84	0.42
1:L:149:CYS:HB2	1:L:150:PRO:HD3	2.01	0.42
1:L:245:LEU:HA	1:L:246:THR:HA	1.59	0.42
2:N:390:ASN:HD22	2:N:410:PRO:HG2	1.84	0.42
3:Z:1:MET:HE2	3:Z:1:MET:HB3	1.94	0.42
1:A:159:GLU:OE1	1:A:177:ARG:HD2	2.18	0.42
1:C:287:LEU:HD22	1:C:289:VAL:HG12	2.00	0.42
1:K:135:VAL:HG11	1:K:169:HIS:ND1	2.34	0.42
1:K:375:ALA:HB1	1:K:379:ASP:HB2	2.01	0.42
3:J:9:ARG:HG2	3:J:10:PRO:HD2	2.01	0.42
1:L:351:SER:N	6:L:601:ICS:S3A	2.91	0.42
1:U:294:THR:HG23	1:U:496:PHE:HE1	1.83	0.42
4:G:19:ALA:HB2	4:G:88:VAL:HG11	2.00	0.42
4:G:38:LYS:HG3	9:G:201:AKG:H41	2.00	0.42
4:a:122:LYS:HB2	4:a:122:LYS:HE3	1.80	0.42
7:A:603:HCA:H52	7:A:603:HCA:H21	1.26	0.42
2:B:3:ASP:OD1	2:B:3:ASP:C	2.62	0.42
1:C:19:LEU:HD23	2:D:94:VAL:HG11	2.01	0.42
1:K:208:LYS:HE3	1:K:208:LYS:HB3	1.92	0.42
2:M:326:LEU:HD11	2:M:407:VAL:HG21	2.01	0.42
2:M:379:ILE:HG22	2:M:400:GLU:HG2	2.01	0.42
1:V:15:ILE:HA	1:V:454:PHE:HD2	1.83	0.42
1:V:391:GLU:OE1	1:V:392:LYS:HG2	2.19	0.42
2:W:340:VAL:HG11	2:W:353:ILE:HD12	2.00	0.42
1:L:307:PHE:CE2	1:L:421:LEU:HD13	2.55	0.42
1:L:359:LEU:HD21	1:L:499:VAL:HG13	2.02	0.42
2:N:18:ASN:HB3	2:N:372:LEU:HB2	2.01	0.42
1:A:517:PHE:CZ	2:D:332:GLU:HG2	2.55	0.42
1:V:87:PHE:CG	2:X:51:TYR:HB3	2.54	0.42
2:X:39:MET:HE2	2:X:39:MET:HB2	1.86	0.42
1:L:500:LEU:HD13	1:L:500:LEU:HA	1.88	0.42
4:G:40:ARG:O	4:G:41:GLY:C	2.62	0.42
3:F:3:MET:HE3	3:F:3:MET:HB2	1.90	0.42
4:O:7:ILE:HD13	8:O:201:ADP:H8	1.84	0.42
2:M:22:ILE:HG22	2:M:23:CYS:N	2.33	0.42
2:M:242:ARG:NH2	2:M:243:MET:HE2	2.35	0.42
2:M:416:ASN:HB3	2:N:301:MET:HE3	2.01	0.42
2:W:47:GLY:HA3	5:W:601:CLF:S2B	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:83:GLY:HA2	8:R:201:ADP:O1A	2.19	0.42
1:L:137:ILE:HD11	2:N:12:ARG:HG3	2.02	0.42
1:L:430:TYR:CE2	1:L:432:GLY:HA2	2.54	0.42
4:G:84:LYS:O	4:G:88:VAL:HG13	2.19	0.42
5:A:601:CLF:S4A	2:B:48:CYS:N	2.92	0.42
2:B:277:MET:HE1	1:C:521:PRO:HB2	2.01	0.42
1:C:372:TYR:HB2	1:C:380:TYR:OH	2.20	0.42
1:C:463:ILE:HG12	1:C:510:ILE:HD11	2.02	0.42
2:M:28:ALA:HB1	2:M:153:MET:HE3	2.01	0.42
2:M:409:PHE:HA	2:M:410:PRO:HA	1.89	0.42
2:X:308:HIS:CG	2:X:440:LEU:HD11	2.55	0.42
3:H:99:ARG:HD3	4:G:93:ASN:O	2.19	0.42
3:R:36:ARG:O	3:R:38:LYS:HG3	2.19	0.42
3:d:7:VAL:HG11	8:d:201:ADP:C8	2.55	0.42
1:L:405:ARG:HA	1:L:405:ARG:HD3	1.76	0.42
2:N:193:MET:O	2:N:285:VAL:HG11	2.19	0.42
2:N:235:LEU:O	2:N:259:PRO:HD2	2.19	0.42
2:N:409:PHE:HB3	2:N:410:PRO:HD3	2.02	0.42
4:G:98:LYS:HE3	4:G:98:LYS:HB2	1.75	0.42
2:B:374:MET:HA	2:B:377:GLN:HE21	1.84	0.42
1:C:55:ASN:HB2	1:C:373:GLN:NE2	2.35	0.42
1:C:267:CYS:HB3	1:C:270:SER:HB3	2.02	0.42
1:K:32:VAL:HG23	1:K:42:ILE:HG13	2.00	0.42
1:K:212:PRO:HG2	1:K:213:PHE:CE2	2.54	0.42
1:K:372:TYR:HE1	1:K:433:LEU:HD22	1.84	0.42
1:K:421:LEU:HD22	1:K:427:LEU:HB2	2.02	0.42
1:V:349:GLY:HA3	6:V:603:ICS:S3B	2.59	0.42
2:W:336:GLU:HB2	2:W:361:TYR:CE2	2.55	0.42
2:X:6:PRO:O	2:X:377:GLN:HG2	2.20	0.42
2:X:334:GLY:HA2	1:U:513:PRO:HG2	2.02	0.42
2:X:353:ILE:HD13	2:X:353:ILE:HA	1.84	0.42
2:X:431:LEU:HD23	2:X:431:LEU:HA	1.82	0.42
3:J:3:MET:O	3:J:89:VAL:HA	2.20	0.42
3:T:89:VAL:C	3:T:90:ASN:HD22	2.28	0.42
1:L:223:ILE:HD13	1:L:223:ILE:HA	1.86	0.42
1:C:53:LEU:HD12	2:D:95:TYR:CE2	2.54	0.42
1:V:357:ILE:O	1:V:361:GLU:HG2	2.20	0.42
2:W:452:LEU:HD12	2:W:452:LEU:HA	1.78	0.42
3:H:28:LEU:HD11	4:G:63:PHE:HE1	1.85	0.42
3:R:98:ILE:HB	3:P:84:ASP:HB3	2.01	0.42
1:L:218:PHE:CD1	1:L:245:LEU:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:170:LYS:HZ3	2:N:170:LYS:HG3	1.75	0.42
2:N:326:LEU:O	2:N:330:VAL:HG23	2.20	0.42
4:a:5:THR:HB	4:a:100:PHE:HB2	2.02	0.42
2:D:200:PHE:CZ	2:D:230:ASP:HB3	2.53	0.42
1:K:349:GLY:HA2	1:K:373:GLN:HB2	2.02	0.42
2:M:429:ALA:O	2:M:432:VAL:HG12	2.20	0.42
1:V:58:CYS:SG	5:V:601:CLF:S2A	3.18	0.42
1:V:489:TYR:CD2	2:W:456:GLN:HB2	2.55	0.42
2:X:46:GLN:H	2:X:46:GLN:HG3	1.52	0.42
3:R:5:ARG:HG2	3:R:58:LEU:HD12	2.00	0.42
1:L:218:PHE:CG	1:L:271:ILE:HG21	2.54	0.42
4:O:9:ARG:HD2	4:O:44[A]:PHE:CD1	2.55	0.42
3:S:3:MET:HB2	3:S:60:VAL:HG22	2.02	0.42
4:a:84:LYS:O	4:a:88:VAL:HG13	2.19	0.42
1:A:70:PRO:CG	1:A:92:ARG:HH12	2.33	0.41
1:A:226:ASP:HB3	1:A:494:THR:HG21	2.02	0.41
2:B:161:PHE:CD2	2:B:225:ILE:HD11	2.54	0.41
2:M:53:ARG:HH12	2:M:65:LEU:HD13	1.85	0.41
2:X:49:LEU:HD21	2:X:66:ALA:O	2.20	0.41
3:J:29:THR:HG23	3:F:33:VAL:CG1	2.50	0.41
3:b:60:VAL:HG12	3:b:105:LEU:HD11	2.02	0.41
3:d:86:ARG:HH12	8:d:201:ADP:PB	2.43	0.41
1:U:262:LEU:HD22	1:U:307:PHE:CD2	2.55	0.41
4:Q:8:ILE:HD11	4:Q:69:PHE:CE1	2.55	0.41
4:O:40:ARG:HA	4:O:40:ARG:HD3	1.68	0.41
3:P:21:GLU:HG2	3:P:26:ILE:HG23	2.01	0.41
3:S:33:VAL:HG21	3:S:56:MET:HB2	2.02	0.41
4:Y:19:ALA:HB2	4:Y:88:VAL:HG21	2.02	0.41
1:A:110:VAL:HG13	2:B:15:ILE:HG21	2.01	0.41
1:A:372:TYR:HB2	1:A:380:TYR:OH	2.20	0.41
2:B:147:ILE:HG23	2:B:244:ALA:HB2	2.02	0.41
2:B:391:THR:HG23	2:B:413:ASP:CG	2.45	0.41
1:K:306:GLU:HB3	1:K:425:ILE:HD11	2.02	0.41
1:V:92:ARG:HG2	7:V:602:HCA:O6	2.20	0.41
1:V:201:LEU:HD23	1:V:201:LEU:HA	1.90	0.41
2:W:208:ASP:HB2	2:W:419:TYR:CE1	2.55	0.41
3:J:12:MET:HE1	3:J:15:LYS:HD3	2.01	0.41
3:J:88:PHE:CE2	8:J:201:ADP:H2	2.38	0.41
3:R:91:PRO:HD3	4:O:105:THR:HG23	2.02	0.41
8:R:201:ADP:H2	4:O:29:THR:HG23	1.83	0.41
1:L:98:ALA:HB2	1:L:104:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:28:LEU:HD13	3:I:59:MET:HB3	2.01	0.41
3:S:7:VAL:HG22	3:S:56:MET:HG3	2.02	0.41
3:c:105:LEU:HD23	3:c:105:LEU:HA	1.81	0.41
1:A:269:ARG:HH12	1:A:272:ASN:HD21	1.68	0.41
1:C:163:ARG:HG3	1:C:163:ARG:HH11	1.84	0.41
1:C:281:LYS:HB3	1:C:281:LYS:HE3	1.73	0.41
1:C:469:LYS:H	1:C:469:LYS:HG2	1.59	0.41
2:D:46:GLN:H	2:D:46:GLN:HG2	1.62	0.41
1:K:271:ILE:HD13	1:K:271:ILE:HA	1.88	0.41
1:V:266:LEU:HD22	1:V:291:TYR:CZ	2.55	0.41
3:H:93:GLU:OE1	4:G:2:LYS:HE3	2.20	0.41
3:R:29:THR:HG23	3:P:33:VAL:HG13	2.02	0.41
3:R:37:GLY:HA2	4:O:27:SER:HB3	2.00	0.41
1:L:269:ARG:NH2	1:L:379:ASP:HB2	2.35	0.41
2:N:99:VAL:HG22	2:N:225:ILE:HD13	2.01	0.41
2:N:317:TYR:HE2	2:N:390:ASN:OD1	2.03	0.41
1:U:82:ILE:HD12	1:U:82:ILE:HA	1.85	0.41
4:a:36:ARG:HG3	4:a:63:PHE:CD1	2.55	0.41
3:c:39:GLN:HB3	3:c:40:LYS:H	1.59	0.41
1:A:482:ARG:HA	1:A:482:ARG:HD2	1.67	0.41
2:B:309:TYR:HB2	2:B:335:MET:HE3	2.02	0.41
1:C:352:ARG:NH1	6:C:602:ICS:S1A	2.94	0.41
2:D:453:GLU:H	2:D:453:GLU:HG3	1.64	0.41
1:K:139:ASN:N	1:K:140:PRO:HD3	2.36	0.41
3:J:17:VAL:HG22	3:J:28:LEU:HD13	2.02	0.41
3:b:28:LEU:HD21	4:a:36:ARG:HH11	1.84	0.41
1:L:264:ILE:HD13	1:L:304:MET:HE1	2.02	0.41
2:N:62:GLU:HG3	2:N:207:PHE:O	2.20	0.41
1:U:60:PHE:HA	1:U:178:CYS:HB2	2.03	0.41
4:Q:12:LYS:HA	4:Q:12:LYS:HD3	1.80	0.41
8:O:201:ADP:HN61	3:P:60:VAL:N	2.14	0.41
1:A:150:PRO:O	1:A:154:ILE:HG23	2.20	0.41
1:A:218:PHE:HB3	1:A:271:ILE:HG21	2.01	0.41
2:B:164:LYS:HA	2:B:233:ASN:OD1	2.21	0.41
2:X:206:VAL:HG13	2:X:219:PRO:HG2	2.03	0.41
3:J:74:MET:HA	4:E:110:ILE:HG23	2.02	0.41
1:L:52:ILE:HG23	1:L:448:ASN:HB3	2.03	0.41
1:L:89:TRP:HH2	2:N:372:LEU:HD12	1.85	0.41
1:U:120:VAL:HG21	3:c:34:PHE:CE1	2.56	0.41
1:U:245:LEU:HD21	1:U:254:ILE:HG23	2.03	0.41
1:A:371:GLY:HA3	1:A:444:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ILE:HG12	2:B:58:ARG:HG2	2.01	0.41
2:B:281:LYS:HE2	2:B:281:LYS:HB2	1.71	0.41
1:C:245:LEU:HA	1:C:246:THR:HA	1.54	0.41
1:K:19:LEU:HD23	2:M:94:VAL:HG21	2.01	0.41
1:K:421:LEU:HD21	1:K:425:ILE:HD12	2.03	0.41
2:W:452:LEU:O	2:W:453:GLU:HB3	2.20	0.41
3:d:68:LYS:HD3	3:d:69:VAL:N	2.36	0.41
1:L:485:HIS:HA	6:L:601:ICS:S4B	2.61	0.41
2:N:250:LYS:HD2	2:N:250:LYS:HA	1.78	0.41
1:U:121:PHE:CD1	4:a:17:LYS:HD3	2.55	0.41
1:U:482:ARG:HD3	1:U:509:ALA:HB2	2.01	0.41
3:P:1:MET:O	3:P:92:VAL:HB	2.21	0.41
1:A:63:THR:HG21	1:A:178:CYS:CB	2.51	0.41
1:A:245:LEU:HD12	1:A:245:LEU:H	1.85	0.41
1:A:354:HIS:ND1	1:A:436:GLU:HG3	2.36	0.41
1:C:217:ILE:HG12	1:C:264:ILE:HD11	2.01	0.41
1:K:318:GLU:OE2	1:K:318:GLU:HA	2.20	0.41
1:K:350:GLY:O	1:K:351:SER:C	2.62	0.41
2:X:155:LYS:HE2	2:X:247:ALA:HB1	2.02	0.41
2:X:174:ILE:O	2:X:240:LEU:HD12	2.20	0.41
3:b:10:PRO:HD3	3:b:54:LYS:HA	2.02	0.41
1:U:195:ASN:ND2	1:U:277:MET:HE1	2.35	0.41
3:Z:6:ALA:HB2	3:Z:87:ILE:HG23	2.03	0.41
3:c:38:LYS:O	3:c:39:GLN:C	2.63	0.41
1:A:272:ASN:C	1:A:272:ASN:OD1	2.63	0.41
1:A:281:LYS:HE3	1:A:282:TYR:CZ	2.56	0.41
1:C:305:ALA:HB1	1:C:314:THR:HG22	2.03	0.41
2:D:230:ASP:OD2	2:D:252:LEU:HD21	2.19	0.41
2:M:119:LEU:HD23	2:M:119:LEU:HA	1.87	0.41
2:X:30:TYR:CZ	2:X:203:THR:HG21	2.55	0.41
2:X:269:ILE:HG13	2:X:332:GLU:OE2	2.21	0.41
4:O:84:LYS:HA	4:O:84:LYS:HD3	1.56	0.41
4:a:32:ARG:HG2	4:a:67:ARG:NH1	2.35	0.41
3:c:3:MET:HB2	3:c:60:VAL:HG22	2.02	0.41
1:A:182:ARG:NH1	1:A:397:ILE:HG21	2.34	0.41
1:A:465:CYS:HB3	1:A:484:ILE:HG23	2.03	0.41
1:A:520:PRO:HG2	1:A:523:LYS:HD2	2.03	0.41
1:C:208:LYS:HD3	1:C:208:LYS:HA	1.64	0.41
1:C:236:LYS:HB3	1:C:236:LYS:HE3	1.87	0.41
1:C:270:SER:OG	1:C:271:ILE:HG12	2.20	0.41
1:C:271:ILE:HG22	1:C:271:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:GLY:HA3	6:C:602:ICS:S3B	2.61	0.41
2:D:94:VAL:HG23	2:D:95:TYR:H	1.86	0.41
1:K:351:SER:N	1:K:372:TYR:CE2	2.79	0.41
1:K:405:ARG:HG3	1:K:409:PHE:CE1	2.56	0.41
1:K:489:TYR:CG	2:N:456:GLN:HA	2.56	0.41
2:M:225:ILE:HD12	2:M:225:ILE:HA	1.91	0.41
2:M:317:TYR:HA	2:M:341:LEU:O	2.21	0.41
2:M:376:HIS:CD2	2:M:396:ILE:HG12	2.56	0.41
2:W:406:ARG:NH2	2:W:414:ARG:HH21	2.19	0.41
2:X:49:LEU:HD11	2:X:66:ALA:CB	2.50	0.41
2:X:185:GLU:CD	2:X:424:GLY:HA3	2.46	0.41
2:X:185:GLU:OE2	2:X:424:GLY:HA3	2.21	0.41
2:X:225:ILE:HD12	2:X:225:ILE:HA	1.83	0.41
3:d:83:GLY:HA2	8:d:201:ADP:PA	2.61	0.41
1:L:266:LEU:HD13	1:L:291:TYR:CE1	2.56	0.41
1:L:450:HIS:HB2	2:N:95:TYR:CE1	2.56	0.41
2:N:452:LEU:HD12	2:N:452:LEU:HA	1.89	0.41
1:U:161:VAL:O	1:U:164:GLU:HG2	2.21	0.41
4:G:86:ILE:HD13	4:G:86:ILE:HA	1.91	0.41
3:P:60:VAL:HG12	3:P:105:LEU:HD11	2.02	0.41
3:S:37:GLY:O	3:S:49:TYR:CD1	2.64	0.41
2:D:225:ILE:HD12	2:D:225:ILE:HA	1.80	0.41
1:K:217:ILE:HD13	1:K:217:ILE:HA	1.90	0.41
2:M:269:ILE:HD12	2:M:295:ARG:HG3	2.02	0.41
2:M:315:ALA:HB3	2:M:387:LEU:HD22	2.02	0.41
2:W:145:THR:HG23	2:W:147:ILE:H	1.85	0.41
3:T:66:LYS:O	3:T:70:ILE:HD12	2.20	0.41
2:N:128:ILE:HG22	2:N:130:PRO:HD2	2.02	0.41
1:U:49:ILE:HD12	1:U:50:PRO:CD	2.50	0.41
1:U:451:GLU:O	1:U:455:LEU:HD12	2.21	0.41
3:S:68:LYS:O	3:S:72:THR:HG23	2.21	0.41
1:A:476:LYS:HD3	1:A:476:LYS:HA	1.84	0.40
1:K:201:LEU:HD23	1:K:201:LEU:HA	1.86	0.40
1:K:258:HIS:HA	1:K:278:MET:HE1	2.03	0.40
1:V:197:LEU:HD23	1:V:201:LEU:HD12	2.04	0.40
1:V:482:ARG:HA	1:V:482:ARG:HD2	1.92	0.40
2:W:73:GLU:HB2	1:U:181:TYR:O	2.20	0.40
3:T:4:ILE:HD13	3:T:89:VAL:HG22	2.03	0.40
3:b:12:MET:O	3:b:16:VAL:HG23	2.21	0.40
2:N:39:MET:HE2	2:N:39:MET:HB2	1.98	0.40
2:N:129:ASP:OD1	2:N:129:ASP:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:154:VAL:HG12	2:N:248:ALA:HB2	2.03	0.40
2:N:351:LYS:HD2	2:N:351:LYS:HA	1.86	0.40
1:U:87:PHE:O	1:U:91:THR:HG21	2.20	0.40
1:U:331:GLU:HB3	1:U:500:LEU:HD11	2.03	0.40
3:I:28:LEU:HD12	3:I:29:THR:H	1.86	0.40
4:Q:15:LYS:HB3	4:Q:15:LYS:HE2	1.80	0.40
4:Q:38:LYS:HD3	4:Q:98:LYS:HE2	2.03	0.40
1:A:381:GLU:HB2	1:A:385:ILE:HD13	2.03	0.40
2:B:332:GLU:HG2	1:C:517:PHE:CZ	2.56	0.40
1:C:136:LYS:HE3	1:C:136:LYS:HB3	1.77	0.40
2:D:223:THR:O	2:D:223:THR:CG2	2.68	0.40
2:D:379:ILE:HD13	2:D:387:LEU:HD11	2.02	0.40
1:K:74:MET:SD	1:K:144:THR:HG23	2.62	0.40
1:K:320:VAL:HA	1:K:323:GLU:HG2	2.03	0.40
1:K:483:GLN:HG3	1:K:488:ASP:OD1	2.21	0.40
2:M:56:LEU:HD23	2:M:56:LEU:HA	1.93	0.40
2:M:167:PRO:HA	2:M:233:ASN:HB3	2.04	0.40
2:M:290:GLU:O	2:M:294:GLU:HG3	2.21	0.40
2:M:414:ARG:HB2	2:M:417:LEU:HD12	2.02	0.40
1:V:374:PHE:CZ	6:V:603:ICS:S2A	3.14	0.40
2:W:165:SER:HB2	2:W:233:ASN:HD21	1.85	0.40
2:W:389:GLY:O	2:W:406:ARG:HA	2.21	0.40
1:U:339:LEU:HD23	1:U:342:LYS:HE3	2.03	0.40
1:U:347:TYR:CD1	1:U:447:LEU:HD12	2.56	0.40
3:S:36:ARG:NE	3:S:49:TYR:HB3	2.36	0.40
4:a:98:LYS:HB2	4:a:98:LYS:HE2	1.76	0.40
3:Z:28:LEU:HD21	3:Z:57:LEU:HD22	2.02	0.40
1:A:80:GLY:HA3	1:A:148:THR:CG2	2.51	0.40
1:C:72:LYS:HB3	1:C:106:MET:HE3	2.03	0.40
1:C:298:GLU:HB3	1:C:302:ARG:NH1	2.37	0.40
1:C:303:LYS:HG2	1:C:425:ILE:HB	2.03	0.40
2:W:367:ILE:HD13	2:W:374:MET:SD	2.62	0.40
2:W:375:LEU:O	2:W:379:ILE:HG12	2.20	0.40
3:T:62:GLU:HG2	3:T:105:LEU:HD12	2.04	0.40
2:N:200:PHE:HB2	2:N:228:ILE:HG12	2.03	0.40
1:U:483:GLN:HB2	1:U:488:ASP:N	2.35	0.40
1:A:216:ASN:OD1	1:A:243:SER:HB2	2.21	0.40
1:A:298:GLU:HG3	1:A:496:PHE:HE1	1.86	0.40
1:A:463:ILE:HD12	1:A:463:ILE:HA	1.84	0.40
1:C:349:GLY:HA2	1:C:373:GLN:HB2	2.04	0.40
1:K:265:LEU:HD12	1:K:265:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:234:SER:C	2:D:236:GLY:N	2.78	0.40
2:D:239:ALA:C	2:D:241:CYS:H	2.28	0.40
1:K:243:SER:OG	1:K:254:ILE:HD13	2.21	0.40
2:W:51:TYR:HB3	1:U:87:PHE:CG	2.56	0.40
2:X:351:LYS:HD2	2:X:351:LYS:HA	1.92	0.40
3:H:54:LYS:HA	3:H:54:LYS:HD3	1.93	0.40
3:b:10:PRO:HD3	3:b:54:LYS:HD2	2.03	0.40
1:L:258:HIS:CE1	1:L:259:GLN:HG3	2.57	0.40
1:L:317:THR:O	1:L:321:ILE:HG12	2.22	0.40
2:N:293:ASP:HB3	2:N:297:ARG:HH21	1.86	0.40
1:U:327:LYS:HE2	1:U:327:LYS:HB2	1.82	0.40
4:Q:36:ARG:HD3	4:Q:62:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/559 (94%)	484 (92%)	39 (8%)	0	100	100
1	C	518/559 (93%)	492 (95%)	26 (5%)	0	100	100
1	K	523/559 (94%)	490 (94%)	32 (6%)	1 (0%)	43	71
1	L	513/559 (92%)	491 (96%)	22 (4%)	0	100	100
1	U	503/559 (90%)	469 (93%)	34 (7%)	0	100	100
1	V	525/559 (94%)	498 (95%)	27 (5%)	0	100	100
2	B	455/456 (100%)	433 (95%)	22 (5%)	0	100	100
2	D	454/456 (100%)	415 (91%)	39 (9%)	0	100	100
2	M	454/456 (100%)	437 (96%)	17 (4%)	0	100	100
2	N	454/456 (100%)	425 (94%)	29 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W	454/456 (100%)	436 (96%)	18 (4%)	0	100	100
2	X	454/456 (100%)	428 (94%)	26 (6%)	0	100	100
3	F	86/105 (82%)	86 (100%)	0	0	100	100
3	H	86/105 (82%)	86 (100%)	0	0	100	100
3	I	99/105 (94%)	96 (97%)	3 (3%)	0	100	100
3	J	91/105 (87%)	90 (99%)	1 (1%)	0	100	100
3	P	86/105 (82%)	84 (98%)	2 (2%)	0	100	100
3	R	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
3	S	96/105 (91%)	95 (99%)	1 (1%)	0	100	100
3	T	86/105 (82%)	85 (99%)	1 (1%)	0	100	100
3	Z	86/105 (82%)	84 (98%)	2 (2%)	0	100	100
3	b	86/105 (82%)	86 (100%)	0	0	100	100
3	c	99/105 (94%)	97 (98%)	2 (2%)	0	100	100
3	d	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
4	E	113/125 (90%)	109 (96%)	4 (4%)	0	100	100
4	G	116/125 (93%)	103 (89%)	12 (10%)	1 (1%)	14	43
4	O	113/125 (90%)	107 (95%)	6 (5%)	0	100	100
4	Q	114/125 (91%)	103 (90%)	11 (10%)	0	100	100
4	Y	112/125 (90%)	108 (96%)	4 (4%)	0	100	100
4	a	101/125 (81%)	93 (92%)	8 (8%)	0	100	100
All	All	7594/8100 (94%)	7199 (95%)	393 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	352	ARG
4	G	41	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/467 (95%)	420 (94%)	25 (6%)	19	47
1	C	443/467 (95%)	424 (96%)	19 (4%)	26	54
1	K	445/467 (95%)	417 (94%)	28 (6%)	16	44
1	L	440/467 (94%)	421 (96%)	19 (4%)	26	54
1	U	434/467 (93%)	419 (96%)	15 (4%)	32	59
1	V	445/467 (95%)	428 (96%)	17 (4%)	29	58
2	B	379/378 (100%)	368 (97%)	11 (3%)	37	63
2	D	378/378 (100%)	361 (96%)	17 (4%)	24	53
2	M	378/378 (100%)	364 (96%)	14 (4%)	30	58
2	N	378/378 (100%)	353 (93%)	25 (7%)	15	42
2	W	378/378 (100%)	362 (96%)	16 (4%)	26	55
2	X	378/378 (100%)	357 (94%)	21 (6%)	19	47
3	F	77/89 (86%)	75 (97%)	2 (3%)	40	64
3	H	77/89 (86%)	73 (95%)	4 (5%)	21	49
3	I	88/89 (99%)	83 (94%)	5 (6%)	18	47
3	J	81/89 (91%)	73 (90%)	8 (10%)	7	27
3	P	77/89 (86%)	70 (91%)	7 (9%)	9	30
3	R	85/89 (96%)	81 (95%)	4 (5%)	23	52
3	S	86/89 (97%)	76 (88%)	10 (12%)	5	21
3	T	77/89 (86%)	76 (99%)	1 (1%)	61	73
3	Z	77/89 (86%)	75 (97%)	2 (3%)	40	64
3	b	77/89 (86%)	73 (95%)	4 (5%)	21	49
3	c	88/89 (99%)	81 (92%)	7 (8%)	11	35
3	d	86/89 (97%)	83 (96%)	3 (4%)	32	59
4	E	102/109 (94%)	97 (95%)	5 (5%)	22	51
4	G	104/109 (95%)	89 (86%)	15 (14%)	3	14
4	O	102/109 (94%)	94 (92%)	8 (8%)	11	36
4	Q	103/109 (94%)	102 (99%)	1 (1%)	68	76
4	Y	101/109 (93%)	98 (97%)	3 (3%)	36	62
4	a	90/109 (83%)	84 (93%)	6 (7%)	15	42
All	All	6499/6792 (96%)	6177 (95%)	322 (5%)	23	50

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	GLU
1	A	7	ASP
1	A	25	ARG
1	A	53	LEU
1	A	117	THR
1	A	149	CYS
1	A	151	VAL
1	A	198	MET
1	A	202	ILE
1	A	240	ARG
1	A	264	ILE
1	A	265	LEU
1	A	270	SER
1	A	279	GLU
1	A	284	VAL
1	A	327	LYS
1	A	328	TYR
1	A	336	ARG
1	A	357	ILE
1	A	359	LEU
1	A	363	LEU
1	A	386	ILE
1	A	390	LYS
1	A	484	ILE
2	B	8	GLU
2	B	12	ARG
2	B	75	THR
2	B	86	GLU
2	B	251	ILE
2	B	292	GLU
2	B	306	HIS
2	B	335	MET
2	B	396	ILE
2	B	452	LEU
2	B	455	ILE
1	C	35	ASP
1	C	47	LYS
1	C	48	VAL
1	C	63	THR
1	C	78	VAL
1	C	143	ILE

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Mol	Chain	Res	Type
1	C	149	CYS
1	C	166	GLU
1	C	177	ARG
1	C	207	ILE
1	C	279	GLU
1	C	332	ILE
1	C	416	GLU
1	C	438	LYS
1	C	460	LYS
1	C	463	ILE
1	C	468	ILE
1	C	499	VAL
1	C	525	GLU
2	D	21	LYS
2	D	22	ILE
2	D	48	CYS
2	D	49	LEU
2	D	68	THR
2	D	91	LEU
2	D	107	VAL
2	D	171	LEU
2	D	211	LEU
2	D	213	LYS
2	D	216	THR
2	D	220	LYS
2	D	230	ASP
2	D	292	GLU
2	D	306	HIS
2	D	316	ILE
2	D	344	THR
1	K	17	LYS
1	K	53	LEU
1	K	106	MET
1	K	117	THR
1	K	129	LYS
1	K	134	VAL
1	K	149	CYS
1	K	167	GLU
1	K	186	GLN
1	K	216	ASN
1	K	217	ILE
1	K	250	SER

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Mol	Chain	Res	Type
1	K	251	PHE
1	K	274	THR
1	K	319	GLU
1	K	336	ARG
1	K	351	SER
1	K	352	ARG
1	K	353	SER
1	K	419	THR
1	K	427	LEU
1	K	444	VAL
1	K	452	THR
1	K	460	LYS
1	K	468	ILE
1	K	479	VAL
1	K	484	ILE
1	K	525	GLU
2	M	50	SER
2	M	73	GLU
2	M	75	THR
2	M	106	CYS
2	M	107	VAL
2	M	125	GLU
2	M	127	LEU
2	M	129	ASP
2	M	228	ILE
2	M	306	HIS
2	M	367	ILE
2	M	382	LYS
2	M	390	ASN
2	M	422	ILE
1	V	48	VAL
1	V	53	LEU
1	V	92	ARG
1	V	208	LYS
1	V	236	LYS
1	V	265	LEU
1	V	267	CYS
1	V	316	LYS
1	V	366	LYS
1	V	369	VAL
1	V	385	ILE
1	V	389	ILE

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Mol	Chain	Res	Type
1	V	438	LYS
1	V	463	ILE
1	V	479	VAL
1	V	493	TYR
1	V	525	GLU
2	W	5	THR
2	W	26	ILE
2	W	48	CYS
2	W	52	LEU
2	W	67	THR
2	W	106	CYS
2	W	193	MET
2	W	211	LEU
2	W	213	LYS
2	W	216	THR
2	W	243	MET
2	W	306	HIS
2	W	323	LEU
2	W	336	GLU
2	W	354	GLU
2	W	371	ASP
2	X	1	MET
2	X	46	GLN
2	X	77	VAL
2	X	88	LEU
2	X	94	VAL
2	X	104	THR
2	X	106	CYS
2	X	129	ASP
2	X	200	PHE
2	X	203	THR
2	X	215	HIS
2	X	220	LYS
2	X	233	ASN
2	X	243	MET
2	X	290	GLU
2	X	306	HIS
2	X	323	LEU
2	X	363	ASP
2	X	402	VAL
2	X	433	GLU
2	X	453	GLU

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Mol	Chain	Res	Type
3	H	15	LYS
3	H	21	GLU
3	H	36	ARG
3	H	66	LYS
3	J	13	GLU
3	J	21	GLU
3	J	31	MET
3	J	64	GLU
3	J	67	ASP
3	J	71	LYS
3	J	74	MET
3	J	102	LYS
3	R	8	ILE
3	R	31	MET
3	R	36	ARG
3	R	86	ARG
3	T	5	ARG
3	b	7	VAL
3	b	28	LEU
3	b	52	LEU
3	b	71	LYS
3	d	26	ILE
3	d	40	LYS
3	d	47	ILE
1	L	15	ILE
1	L	17	LYS
1	L	32	VAL
1	L	52	ILE
1	L	78	VAL
1	L	84	CYS
1	L	112	THR
1	L	121	PHE
1	L	359	LEU
1	L	362	GLU
1	L	386	ILE
1	L	398	LEU
1	L	399	GLU
1	L	409	PHE
1	L	438	LYS
1	L	452	THR
1	L	463	ILE
1	L	493	TYR

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Mol	Chain	Res	Type
1	L	500	LEU
2	N	15	ILE
2	N	22	ILE
2	N	46	GLN
2	N	48	CYS
2	N	98	GLU
2	N	119	LEU
2	N	129	ASP
2	N	164	LYS
2	N	167	PRO
2	N	170	LYS
2	N	196	SER
2	N	199	VAL
2	N	215	HIS
2	N	234	SER
2	N	235	LEU
2	N	306	HIS
2	N	316	ILE
2	N	336	GLU
2	N	339	VAL
2	N	356	LEU
2	N	363	ASP
2	N	412	MET
2	N	422	ILE
2	N	453	GLU
2	N	455	ILE
1	U	92	ARG
1	U	118	ASP
1	U	129	LYS
1	U	149	CYS
1	U	178	CYS
1	U	184	VAL
1	U	197	LEU
1	U	198	MET
1	U	200	HIS
1	U	229	GLU
1	U	310	ASP
1	U	352	ARG
1	U	353	SER
1	U	416	GLU
1	U	450	HIS
4	G	21	LEU

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Mol	Chain	Res	Type
4	G	27	SER
4	G	28	PHE
4	G	33	VAL
4	G	36	ARG
4	G	38	LYS
4	G	39	GLN
4	G	40	ARG
4	G	42	LEU
4	G	43	CYS
4	G	47	ASN
4	G	62	ARG
4	G	67	ARG
4	G	68	MET
4	G	117	GLU
4	E	27	SER
4	E	29	THR
4	E	42	LEU
4	E	47	ASN
4	E	125	MET
3	F	20	LEU
3	F	29	THR
3	I	3	MET
3	I	44	ILE
3	I	47	ILE
3	I	51	GLU
3	I	65	HIS
4	Q	47	ASN
4	O	3	GLU
4	O	14	GLN
4	O	27	SER
4	O	42	LEU
4	O	81	VAL
4	O	93	ASN
4	O	109	ARG
4	O	120	ILE
3	P	26	ILE
3	P	27	SER
3	P	28	LEU
3	P	29	THR
3	P	30	LYS
3	P	33	VAL
3	P	86	ARG

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Mol	Chain	Res	Type
3	S	26	ILE
3	S	27	SER
3	S	32	GLU
3	S	36	ARG
3	S	38	LYS
3	S	39	GLN
3	S	40	LYS
3	S	48	HIS
3	S	51	GLU
3	S	70	ILE
4	a	30	VAL
4	a	62	ARG
4	a	71	VAL
4	a	77	ASN
4	a	83	GLN
4	a	91	THR
4	Y	14	GLN
4	Y	42	LEU
4	Y	47	ASN
3	Z	66	LYS
3	Z	86	ARG
3	c	3	MET
3	c	31	MET
3	c	36	ARG
3	c	38	LYS
3	c	39	GLN
3	c	40	LYS
3	c	47	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	258	HIS
1	A	354	HIS
2	B	46	GLN
2	B	377	GLN
2	B	437	ASN
1	C	40	GLN
1	C	373	GLN
1	C	483	GLN
2	D	36	HIS

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Mol	Chain	Res	Type
2	D	172	ASN
2	D	233	ASN
2	D	308	HIS
1	K	55	ASN
1	K	94	ASN
1	K	259	GLN
1	K	449	HIS
1	K	475	GLN
1	K	485	HIS
2	M	18	ASN
2	M	24	GLN
2	M	36	HIS
2	M	37	ASN
2	M	172	ASN
2	M	377	GLN
1	V	9	GLN
1	V	272	ASN
1	V	290	ASN
1	V	449	HIS
1	V	450	HIS
2	W	90	ASN
2	W	103	HIS
2	W	152	ASN
2	W	310	HIS
2	W	346	ASN
2	W	376	HIS
2	X	416	ASN
3	H	53	GLN
3	H	65	HIS
3	J	2	GLN
3	T	90	ASN
3	d	90	ASN
1	L	40	GLN
1	L	252	HIS
1	L	290	ASN
2	N	416	ASN
1	U	94	ASN
1	U	340	GLN
1	U	373	GLN
1	U	449	HIS
1	U	475	GLN
4	G	11	ASN

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Mol	Chain	Res	Type
4	G	83	GLN
4	E	77	ASN
4	E	89	ASN
3	F	2	GLN
3	I	65	HIS
4	Q	14	GLN
4	Q	93	ASN
4	O	89	ASN
3	P	2	GLN
4	Y	11	ASN
4	Y	89	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	CLF	W	601	2,1	0,24,24	-	-	-		
6	ICS	K	602	1	6,30,30	2.18	2 (33%)	-		
5	CLF	M	601	2,1	0,24,24	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ADP	E	201	-	28,29,29	0.46	0	43,45,45	0.46	0
9	AKG	Y	201	-	9,9,9	5.24	2 (22%)	11,11,11	1.58	1 (9%)
9	AKG	G	201	-	9,9,9	5.28	2 (22%)	11,11,11	1.85	3 (27%)
6	ICS	A	602	7,1	6,30,30	1.71	1 (16%)	-		
8	ADP	d	201	-	28,29,29	0.44	0	43,45,45	0.71	1 (2%)
7	HCA	C	603	6	13,13,13	1.15	0	15,18,18	1.23	2 (13%)
8	ADP	R	201	-	28,29,29	0.47	0	43,45,45	0.44	0
9	AKG	a	201	-	9,9,9	5.62	2 (22%)	11,11,11	1.86	2 (18%)
5	CLF	N	501	2,1	0,24,24	-	-	-		
7	HCA	A	603	6	13,13,13	1.14	0	15,18,18	1.25	2 (13%)
6	ICS	L	601	7,1	6,30,30	1.79	2 (33%)	-		
5	CLF	C	601	2,1	0,24,24	-	-	-		
7	HCA	V	602	6	13,13,13	1.11	0	15,18,18	1.26	2 (13%)
8	ADP	J	201	-	28,29,29	0.44	0	43,45,45	0.45	0
8	ADP	O	201	-	28,29,29	0.47	0	43,45,45	0.48	0
8	ADP	S	201	-	28,29,29	0.48	0	43,45,45	0.77	0
5	CLF	A	601	2,1	0,24,24	-	-	-		
7	HCA	U	601	6	13,13,13	1.14	0	15,18,18	1.32	3 (20%)
5	CLF	V	601	2,1	0,24,24	-	-	-		
6	ICS	U	602	7,1	6,30,30	1.81	2 (33%)	-		
6	ICS	V	603	7,1	6,30,30	2.20	2 (33%)	-		
7	HCA	K	601	-	13,13,13	1.08	0	15,18,18	1.42	3 (20%)
8	ADP	I	201	-	28,29,29	0.49	0	43,45,45	0.47	0
7	HCA	L	602	6	13,13,13	1.14	0	15,18,18	1.22	2 (13%)
6	ICS	C	602	7,1	6,30,30	1.96	2 (33%)	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLF	W	601	2,1	-	-	0/12/10/10
5	CLF	M	601	2,1	-	-	0/12/10/10
8	ADP	E	201	-	-	6/16/32/32	0/3/3/3
9	AKG	Y	201	-	-	3/9/9/9	-
9	AKG	G	201	-	-	6/9/9/9	-
8	ADP	d	201	-	-	5/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HCA	C	603	6	-	11/17/17/17	-
8	ADP	R	201	-	-	5/16/32/32	0/3/3/3
9	AKG	a	201	-	-	4/9/9/9	-
5	CLF	N	501	2,1	-	-	0/12/10/10
7	HCA	A	603	6	-	9/17/17/17	-
5	CLF	C	601	2,1	-	-	0/12/10/10
7	HCA	V	602	6	-	7/17/17/17	-
8	ADP	J	201	-	-	5/16/32/32	0/3/3/3
8	ADP	O	201	-	-	3/16/32/32	0/3/3/3
8	ADP	S	201	-	-	4/16/32/32	0/3/3/3
5	CLF	A	601	2,1	-	-	0/12/10/10
7	HCA	U	601	6	-	10/17/17/17	-
5	CLF	V	601	2,1	-	-	0/12/10/10
7	HCA	K	601	-	-	11/17/17/17	-
8	ADP	I	201	-	-	8/16/32/32	0/3/3/3
7	HCA	L	602	6	-	9/17/17/17	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	201	AKG	C2-C1	-16.48	1.28	1.53
9	G	201	AKG	C2-C1	-15.46	1.30	1.53
9	Y	201	AKG	C2-C1	-15.32	1.30	1.53
6	V	603	ICS	S2B-FE6	-4.07	2.15	2.24
6	K	602	ICS	S2B-FE6	-4.07	2.15	2.24
6	C	602	ICS	S2B-FE6	-3.41	2.16	2.24
6	U	602	ICS	S2B-FE6	-3.12	2.17	2.24
6	A	602	ICS	S2B-FE6	-3.07	2.17	2.24
6	L	601	ICS	S2B-FE6	-2.92	2.18	2.24
9	a	201	AKG	O2-C1	-2.85	1.22	1.30
9	G	201	AKG	O2-C1	-2.81	1.22	1.30
9	Y	201	AKG	O2-C1	-2.78	1.23	1.30
6	V	603	ICS	S2B-FE2	-2.74	2.18	2.24
6	K	602	ICS	S2B-FE2	-2.65	2.18	2.24
6	C	602	ICS	S2B-FE2	-2.57	2.18	2.24
6	L	601	ICS	S2B-FE2	-2.36	2.19	2.24
6	U	602	ICS	S2B-FE2	-2.01	2.20	2.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	201	AKG	C3-C2-C1	4.28	123.13	115.86
9	a	201	AKG	C3-C2-C1	4.21	123.00	115.86
9	Y	201	AKG	C3-C2-C1	3.94	122.55	115.86
9	a	201	AKG	O1-C1-C2	-2.98	118.10	121.81
7	K	601	HCA	C2-C3-C7	-2.84	103.76	110.03
9	G	201	AKG	O1-C1-C2	-2.73	118.42	121.81
7	K	601	HCA	O5-C7-C3	-2.72	116.83	122.09
7	U	601	HCA	O7-C3-C4	-2.69	104.59	108.88
7	L	602	HCA	O5-C7-C3	-2.49	117.28	122.09
7	A	603	HCA	O5-C7-C3	-2.44	117.37	122.09
7	C	603	HCA	O5-C7-C3	-2.38	117.49	122.09
7	V	602	HCA	O5-C7-C3	-2.34	117.56	122.09
7	K	601	HCA	O6-C7-C3	2.33	117.61	113.14
7	U	601	HCA	O5-C7-C3	-2.24	117.75	122.09
7	A	603	HCA	O6-C7-C3	2.20	117.36	113.14
7	L	602	HCA	O6-C7-C3	2.19	117.34	113.14
7	V	602	HCA	O6-C7-C3	2.13	117.22	113.14
8	d	201	ADP	C3'-C2'-C1'	2.11	105.45	101.46
7	U	601	HCA	O6-C7-C3	2.09	117.15	113.14
7	C	603	HCA	O6-C7-C3	2.08	117.13	113.14
9	G	201	AKG	O2-C1-C2	2.02	119.19	113.59

There are no chirality outliers.

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	603	HCA	C2-C3-C4-C5
7	A	603	HCA	C7-C3-C4-C5
7	A	603	HCA	O7-C3-C4-C5
7	C	603	HCA	C2-C3-C4-C5
7	C	603	HCA	C2-C3-C7-O5
7	C	603	HCA	C2-C3-C7-O6
7	C	603	HCA	O7-C3-C7-O5
7	C	603	HCA	O7-C3-C7-O6
7	K	601	HCA	C1-C2-C3-C4
7	K	601	HCA	C1-C2-C3-C7
7	K	601	HCA	C4-C3-C7-O5
7	K	601	HCA	C4-C3-C7-O6
7	K	601	HCA	O7-C3-C7-O5
7	K	601	HCA	O7-C3-C7-O6
7	V	602	HCA	C2-C3-C7-O5
7	V	602	HCA	C2-C3-C7-O6
7	V	602	HCA	O7-C3-C7-O5

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Mol	Chain	Res	Type	Atoms
7	V	602	HCA	O7-C3-C7-O6
7	L	602	HCA	C2-C3-C4-C5
7	L	602	HCA	O7-C3-C4-C5
7	L	602	HCA	C2-C3-C7-O5
7	L	602	HCA	C2-C3-C7-O6
7	L	602	HCA	O7-C3-C7-O5
7	L	602	HCA	O7-C3-C7-O6
7	U	601	HCA	C7-C3-C4-C5
7	U	601	HCA	O7-C3-C4-C5
7	U	601	HCA	C2-C3-C7-O5
7	U	601	HCA	C2-C3-C7-O6
7	U	601	HCA	O7-C3-C7-O5
7	U	601	HCA	O7-C3-C7-O6
8	J	201	ADP	C5'-O5'-PA-O2A
8	J	201	ADP	C5'-O5'-PA-O3A
8	J	201	ADP	O4'-C4'-C5'-O5'
8	R	201	ADP	C5'-O5'-PA-O2A
8	R	201	ADP	C5'-O5'-PA-O3A
8	R	201	ADP	C4'-C5'-O5'-PA
8	d	201	ADP	C4'-C5'-O5'-PA
8	E	201	ADP	C5'-O5'-PA-O1A
8	E	201	ADP	C5'-O5'-PA-O2A
8	E	201	ADP	C5'-O5'-PA-O3A
8	I	201	ADP	C5'-O5'-PA-O1A
8	I	201	ADP	C5'-O5'-PA-O3A
9	G	201	AKG	O1-C1-C2-O5
9	G	201	AKG	O1-C1-C2-C3
9	G	201	AKG	O2-C1-C2-O5
9	G	201	AKG	O2-C1-C2-C3
9	a	201	AKG	O2-C1-C2-C3
9	a	201	AKG	C1-C2-C3-C4
9	Y	201	AKG	C2-C3-C4-C5
8	J	201	ADP	C3'-C4'-C5'-O5'
8	I	201	ADP	O4'-C4'-C5'-O5'
8	I	201	ADP	C3'-C4'-C5'-O5'
7	A	603	HCA	C1-C2-C3-C4
7	A	603	HCA	C1-C2-C3-C7
8	O	201	ADP	O4'-C4'-C5'-O5'
8	S	201	ADP	O4'-C4'-C5'-O5'
8	E	201	ADP	O4'-C4'-C5'-O5'
8	O	201	ADP	C3'-C4'-C5'-O5'
8	S	201	ADP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
7	C	603	HCA	C1-C2-C3-C7
7	A	603	HCA	C1-C2-C3-O7
7	K	601	HCA	C1-C2-C3-O7
7	A	603	HCA	C3-C4-C5-C6
7	C	603	HCA	C3-C4-C5-C6
7	V	602	HCA	C3-C4-C5-C6
7	U	601	HCA	C3-C4-C5-C6
7	C	603	HCA	C1-C2-C3-C4
7	U	601	HCA	C1-C2-C3-O7
8	I	201	ADP	PB-O3A-PA-O1A
8	E	201	ADP	PB-O3A-PA-O5'
7	C	603	HCA	O7-C3-C4-C5
9	a	201	AKG	O1-C1-C2-C3
8	d	201	ADP	O4'-C1'-N9-C8
7	L	602	HCA	C7-C3-C4-C5
7	U	601	HCA	C2-C3-C4-C5
7	K	601	HCA	C2-C3-C7-O5
7	K	601	HCA	C2-C3-C7-O6
7	L	602	HCA	C4-C3-C7-O5
8	E	201	ADP	C3'-C4'-C5'-O5'
7	C	603	HCA	C1-C2-C3-O7
8	J	201	ADP	C5'-O5'-PA-O1A
8	I	201	ADP	C5'-O5'-PA-O2A
8	O	201	ADP	C5'-O5'-PA-O1A
8	I	201	ADP	C4'-C5'-O5'-PA
7	L	602	HCA	C4-C3-C7-O6
7	K	601	HCA	C4-C5-C6-O4
8	d	201	ADP	O4'-C1'-N9-C4
7	K	601	HCA	C4-C5-C6-O3
7	U	601	HCA	C1-C2-C3-C4
7	V	602	HCA	C4-C5-C6-O3
9	Y	201	AKG	C3-C4-C5-O3
7	V	602	HCA	C4-C5-C6-O4
8	S	201	ADP	PB-O3A-PA-O1A
8	I	201	ADP	PB-O3A-PA-O5'
9	Y	201	AKG	C3-C4-C5-O4
9	a	201	AKG	O1-C1-C2-O5
7	C	603	HCA	C7-C3-C4-C5
7	A	603	HCA	C4-C5-C6-O4
8	R	201	ADP	C3'-C4'-C5'-O5'
8	d	201	ADP	PB-O3A-PA-O1A
7	A	603	HCA	C4-C5-C6-O3

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Mol	Chain	Res	Type	Atoms
9	G	201	AKG	C3-C4-C5-O4
8	R	201	ADP	O4'-C4'-C5'-O5'
9	G	201	AKG	C3-C4-C5-O3
8	d	201	ADP	PB-O3A-PA-O2A
8	S	201	ADP	PB-O3A-PA-O2A

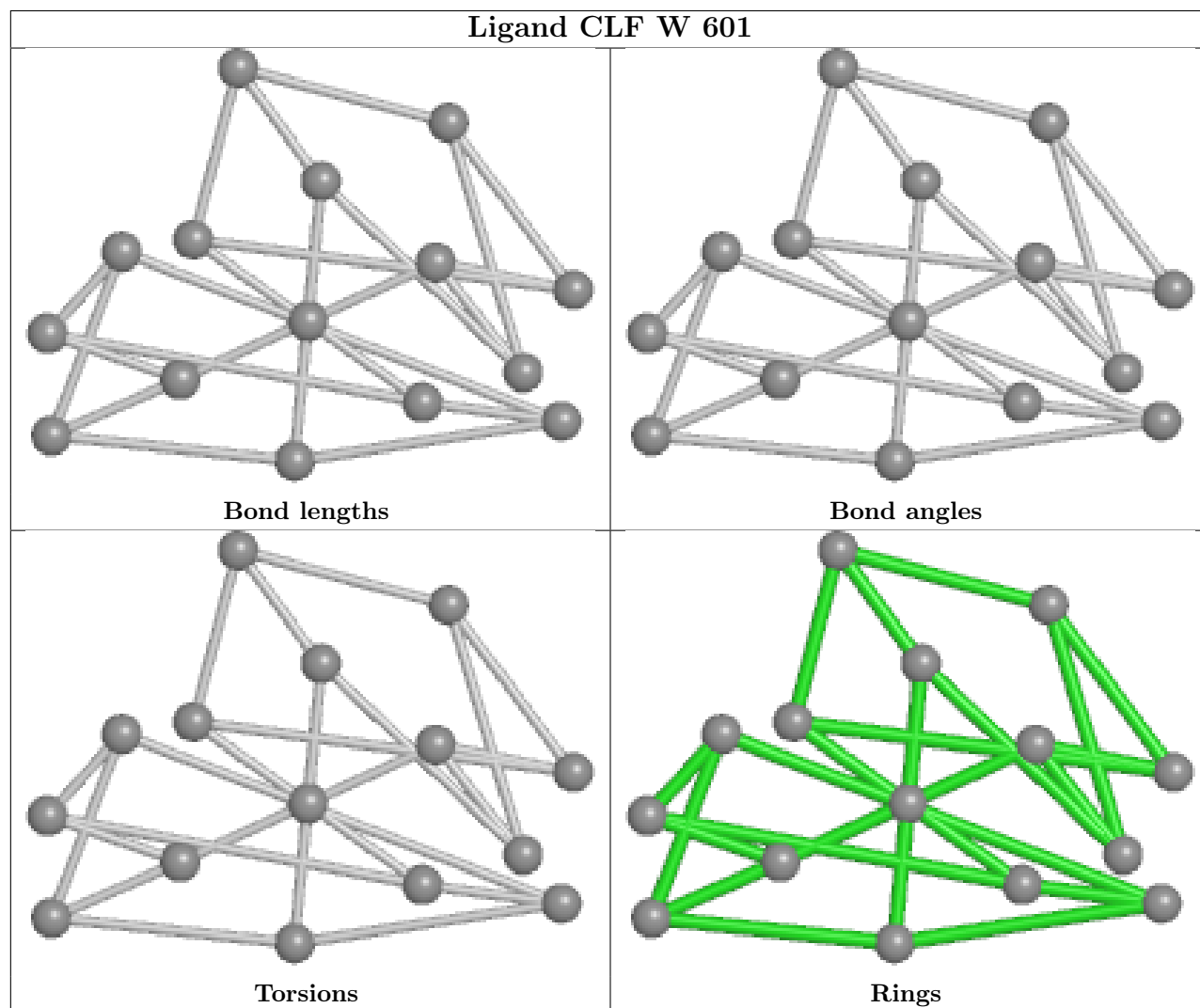
There are no ring outliers.

26 monomers are involved in 225 short contacts:

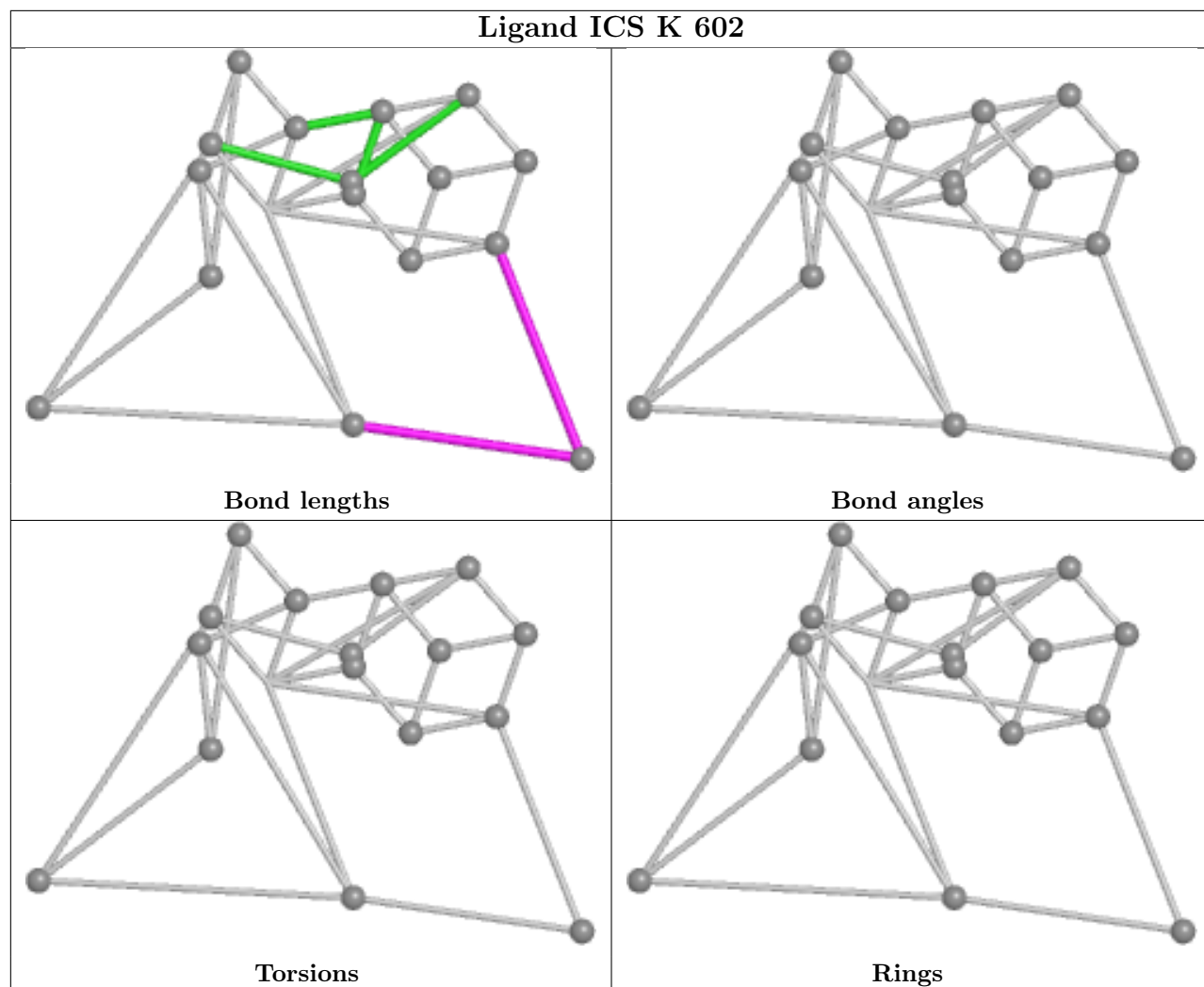
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	W	601	CLF	7	0
6	K	602	ICS	6	0
5	M	601	CLF	5	0
8	E	201	ADP	36	0
9	G	201	AKG	3	0
6	A	602	ICS	12	0
8	d	201	ADP	7	0
7	C	603	HCA	6	0
8	R	201	ADP	12	0
9	a	201	AKG	1	0
5	N	501	CLF	7	0
7	A	603	HCA	5	0
6	L	601	ICS	8	0
5	C	601	CLF	6	0
7	V	602	HCA	4	0
8	J	201	ADP	13	0
8	O	201	ADP	15	0
8	S	201	ADP	3	0
5	A	601	CLF	7	0
5	V	601	CLF	7	0
6	U	602	ICS	12	0
6	V	603	ICS	9	0
7	K	601	HCA	4	0
8	I	201	ADP	19	0
7	L	602	HCA	1	0
6	C	602	ICS	14	0

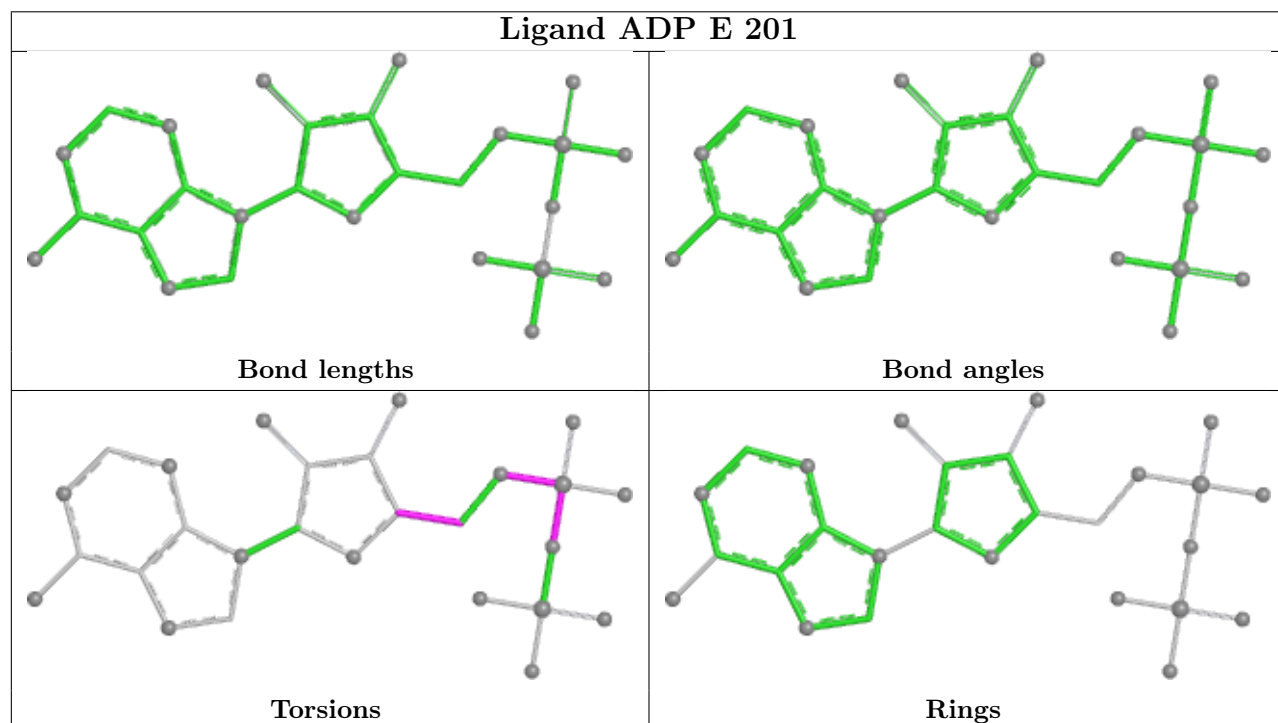
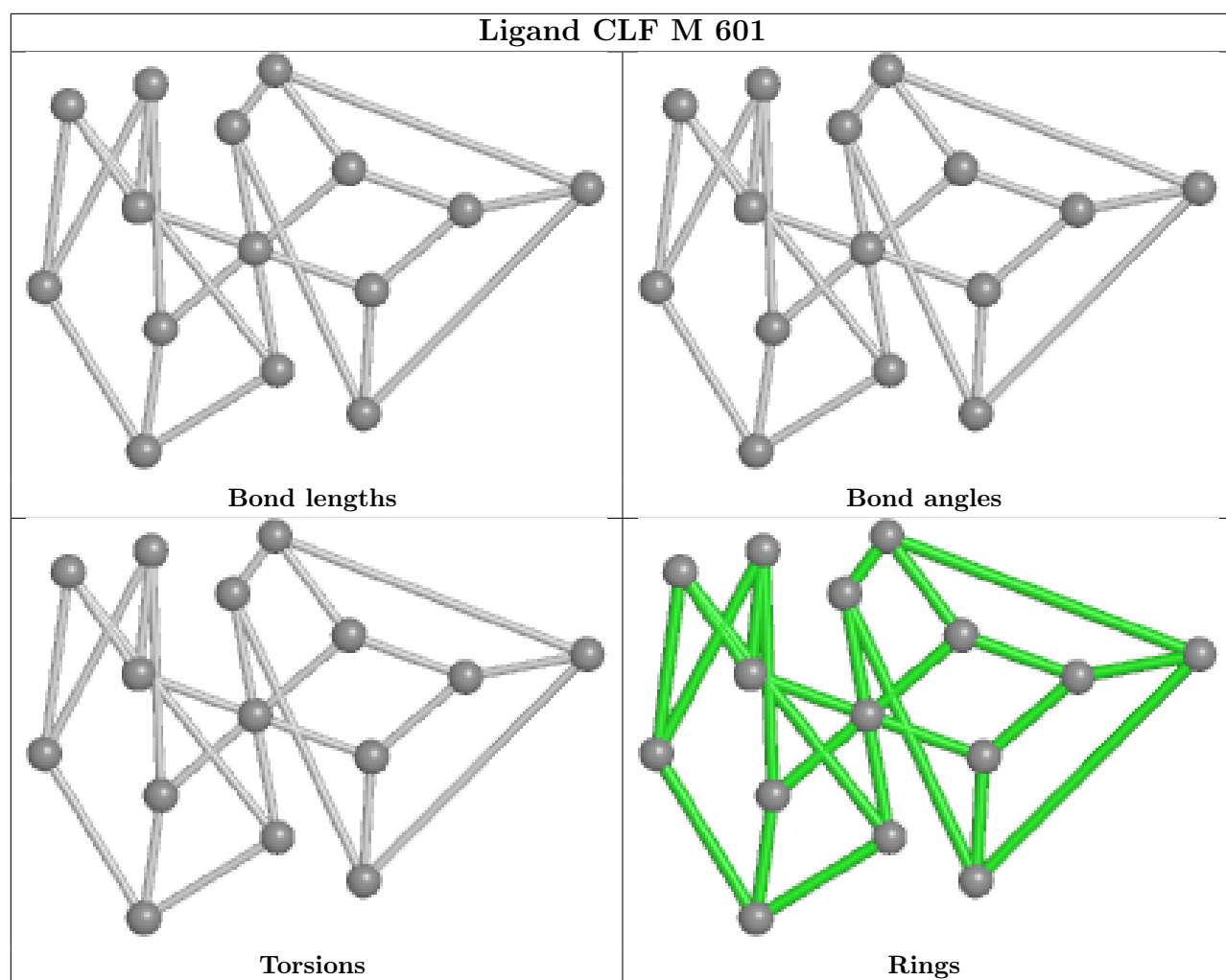
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

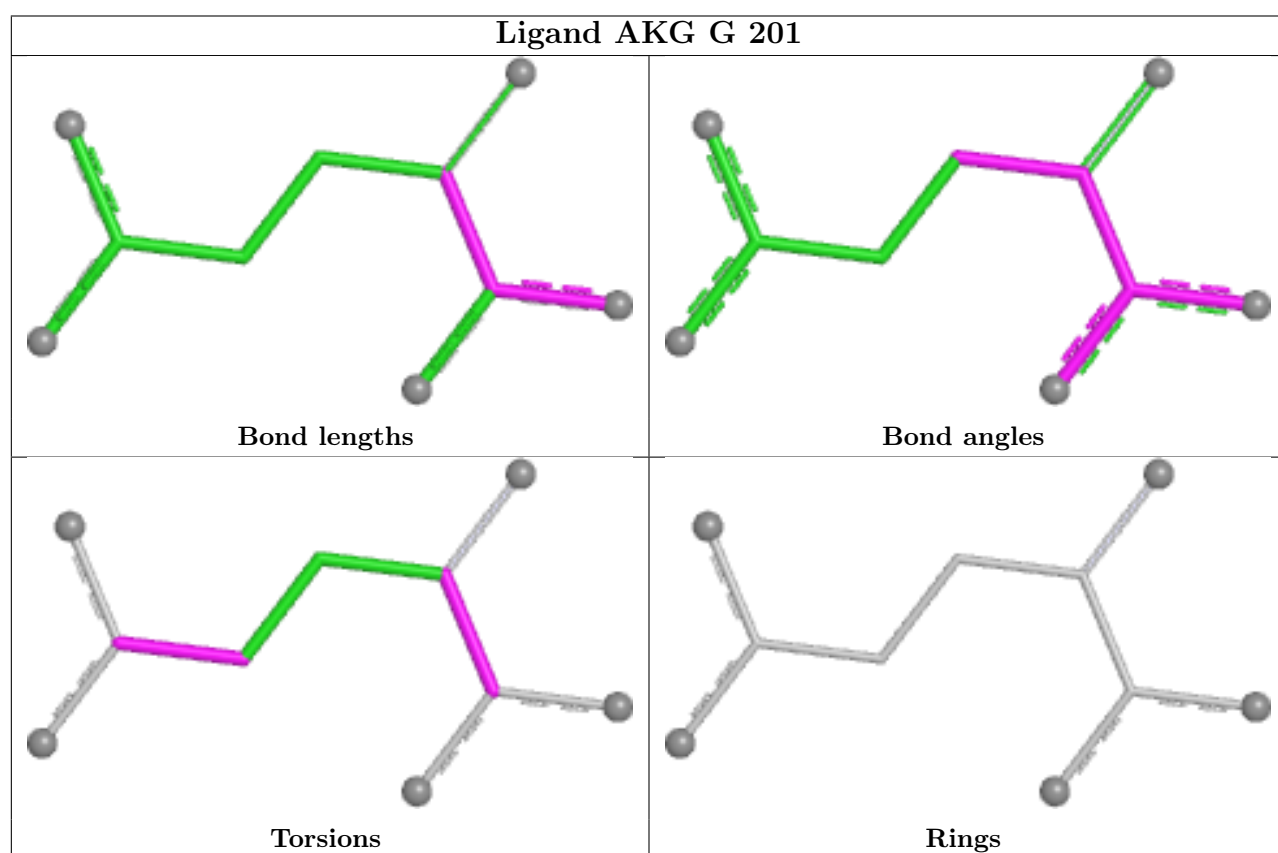
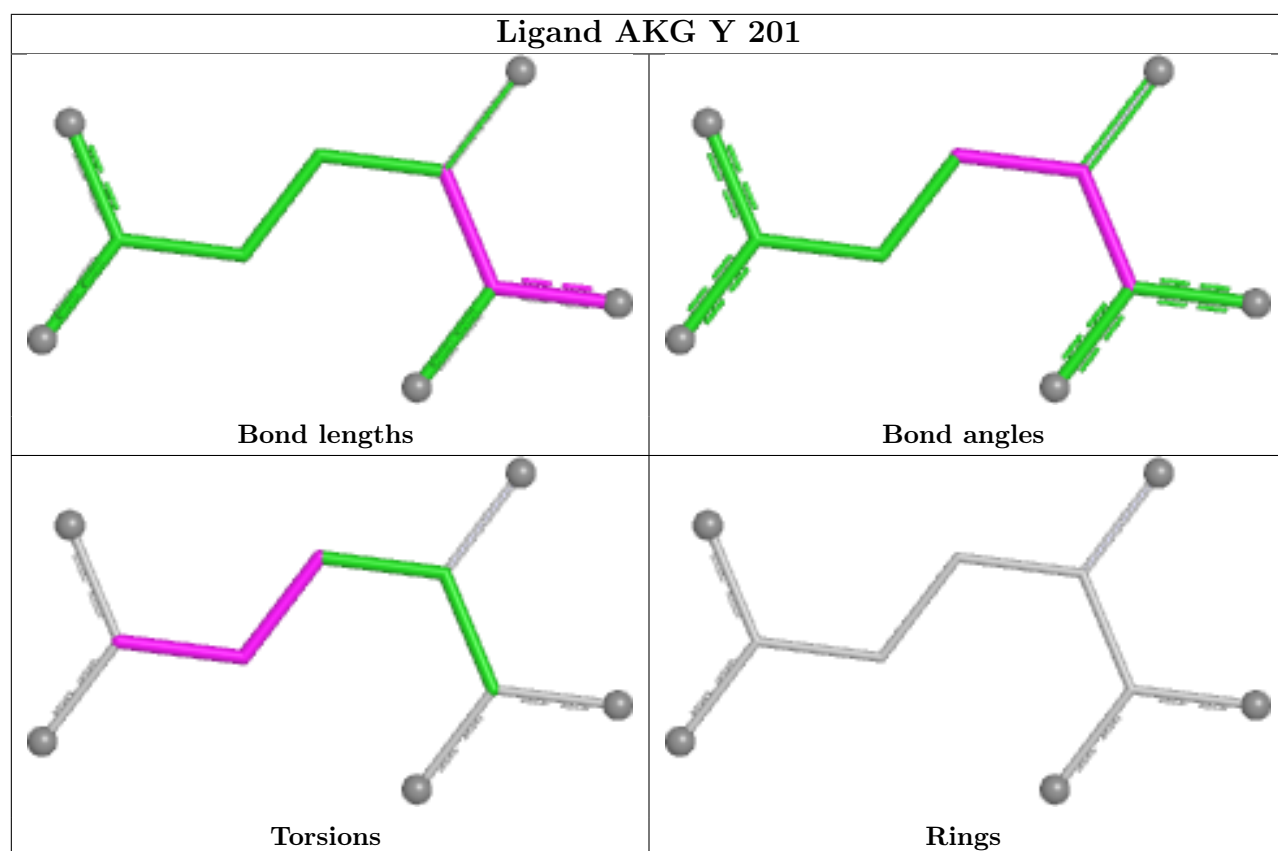
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

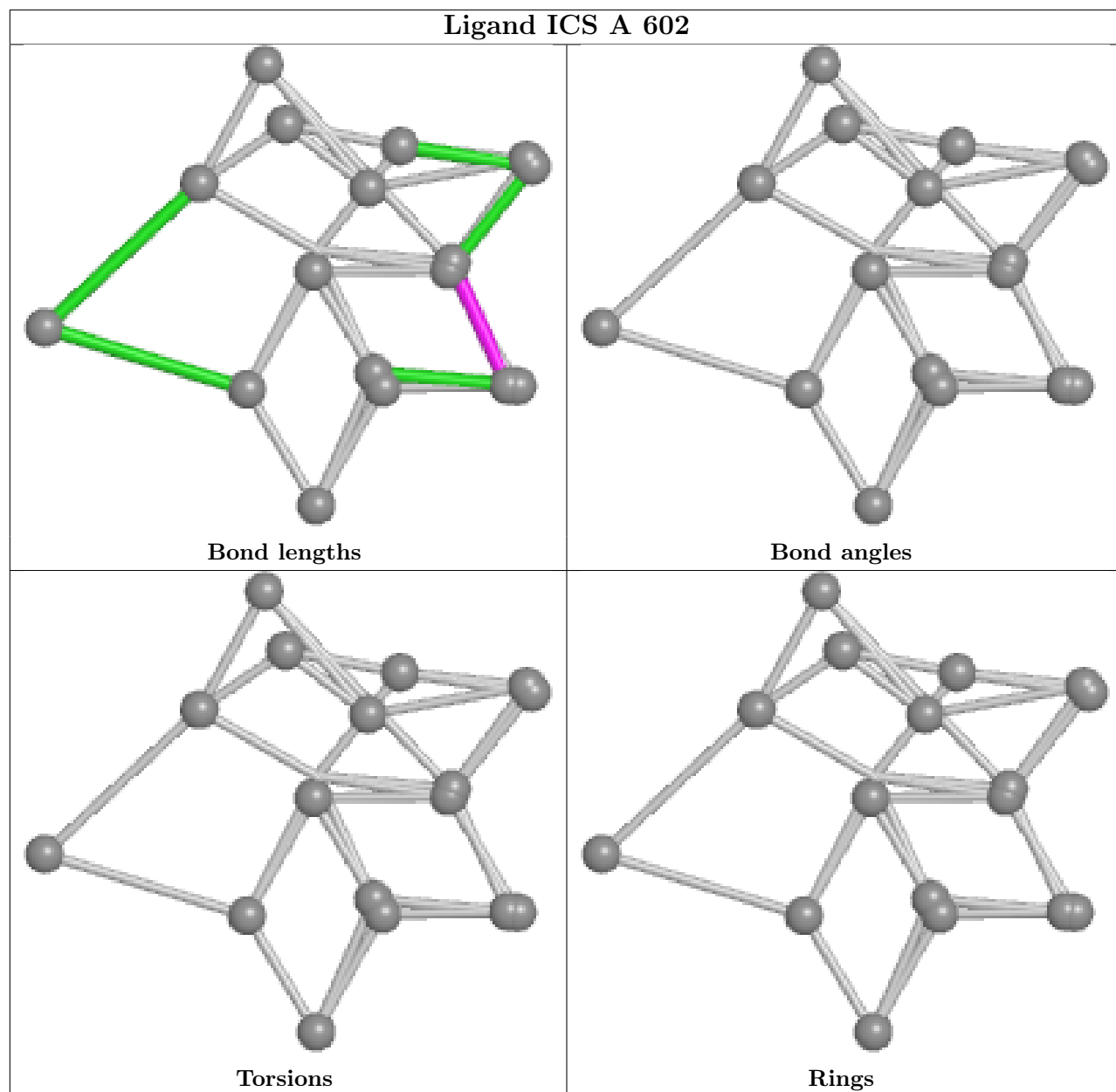


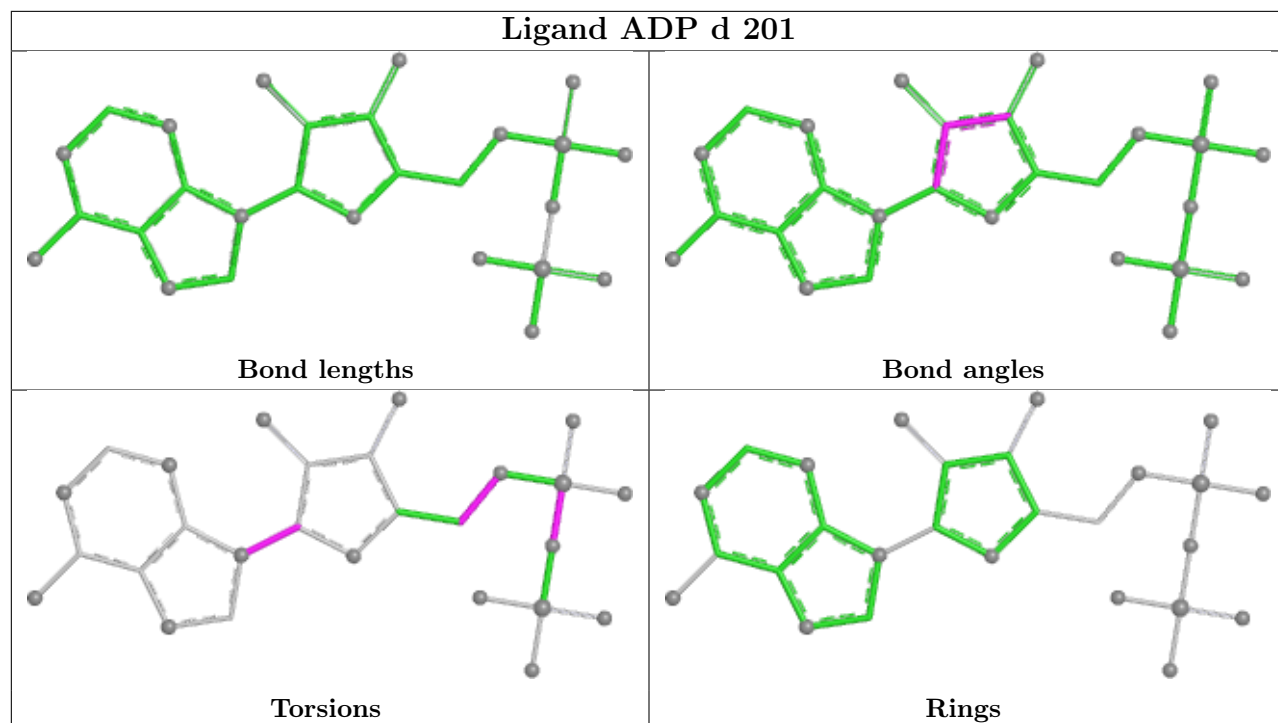
Ligand ICS K 602

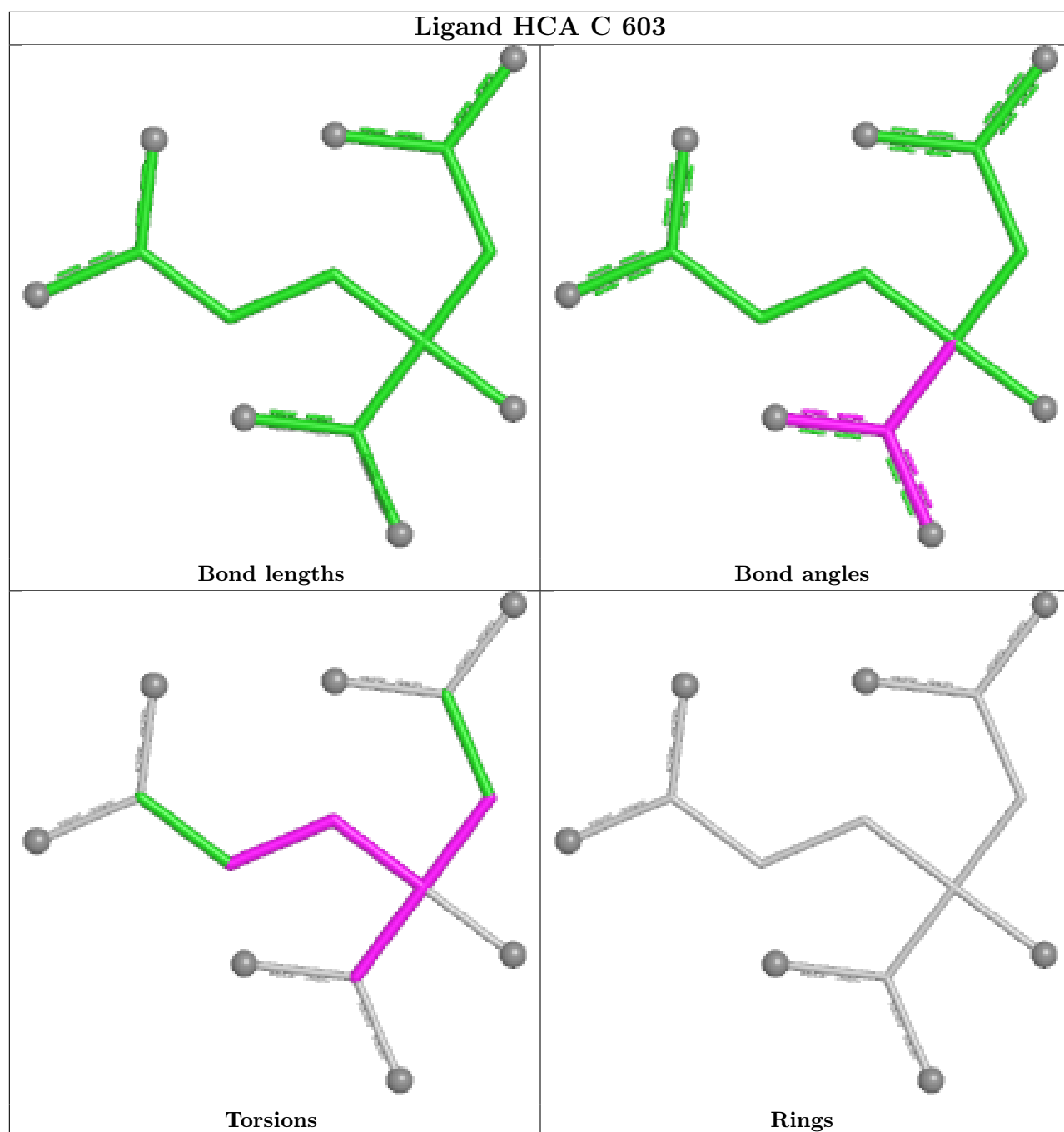


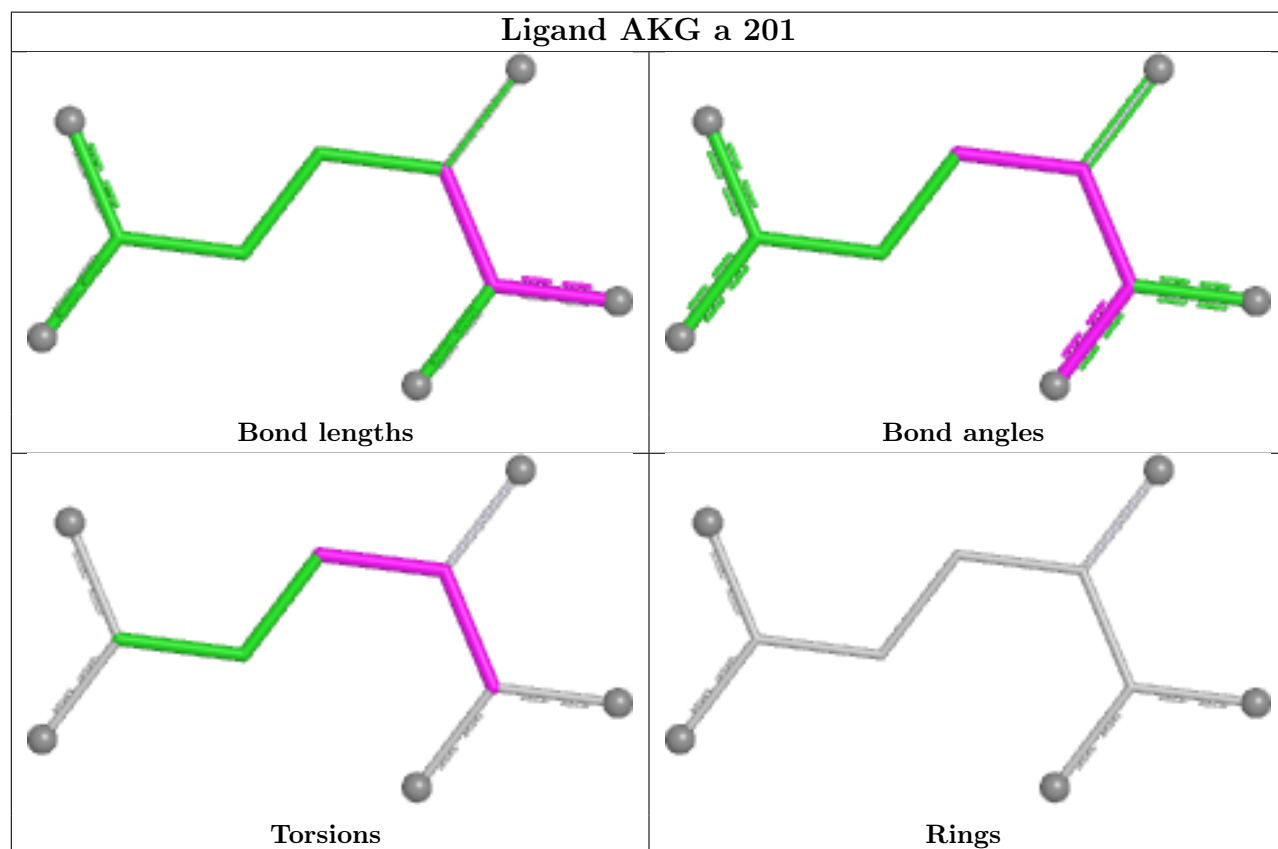
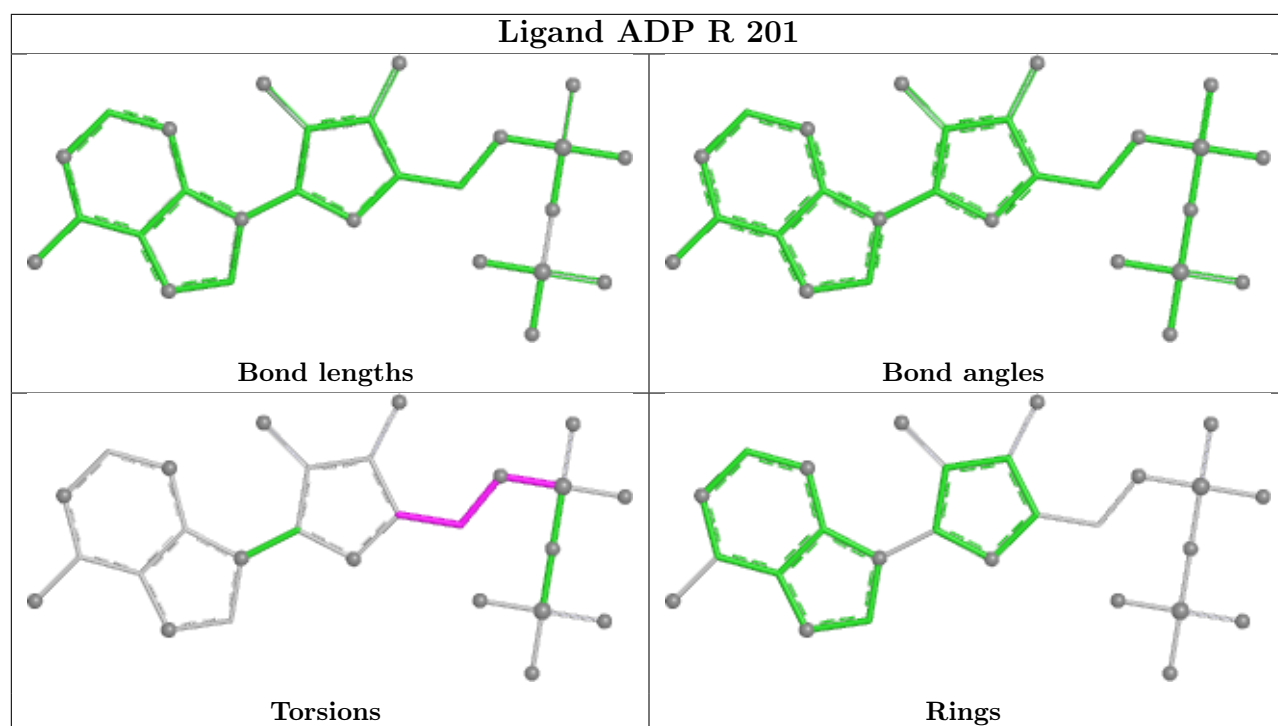


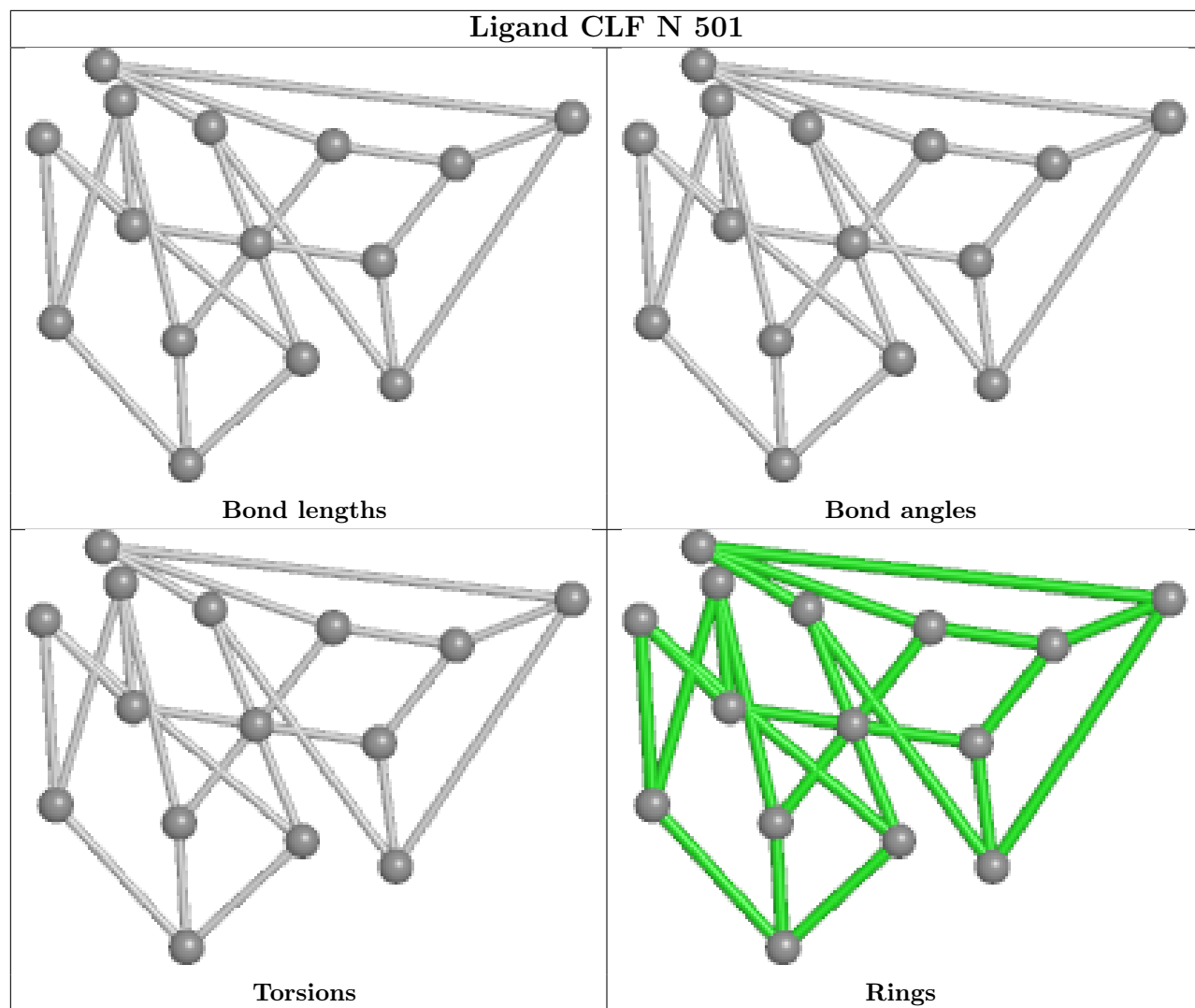


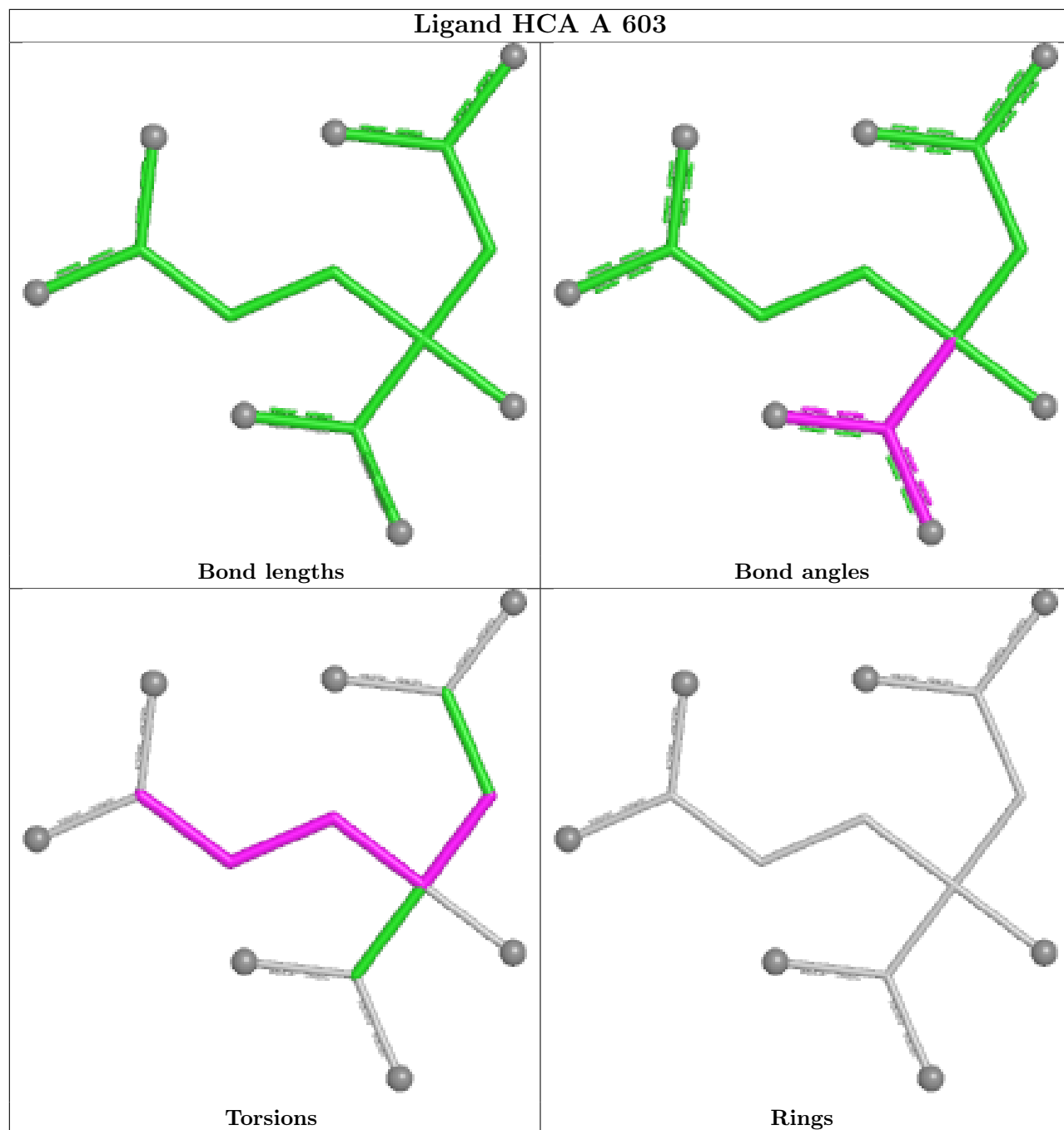


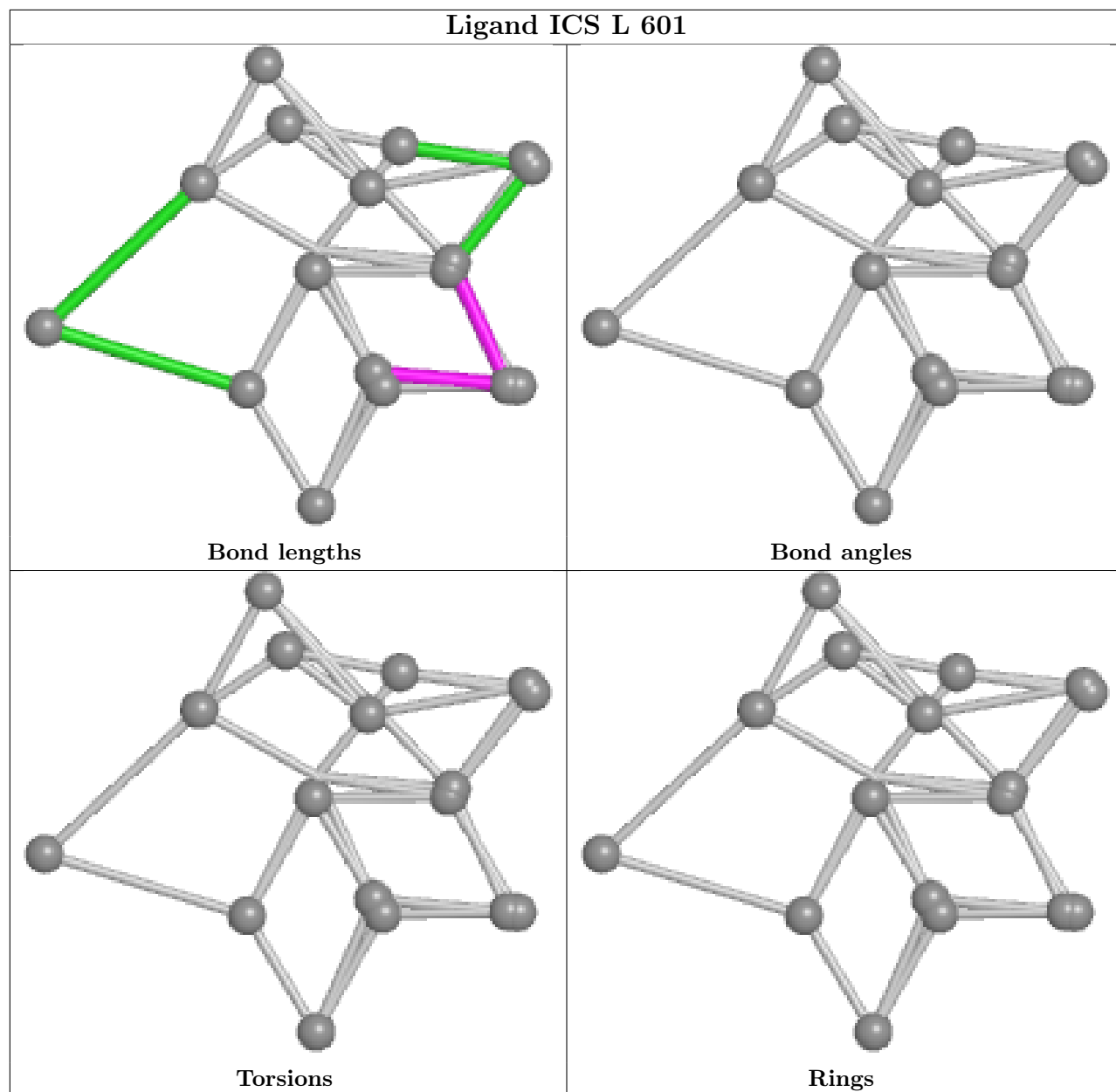


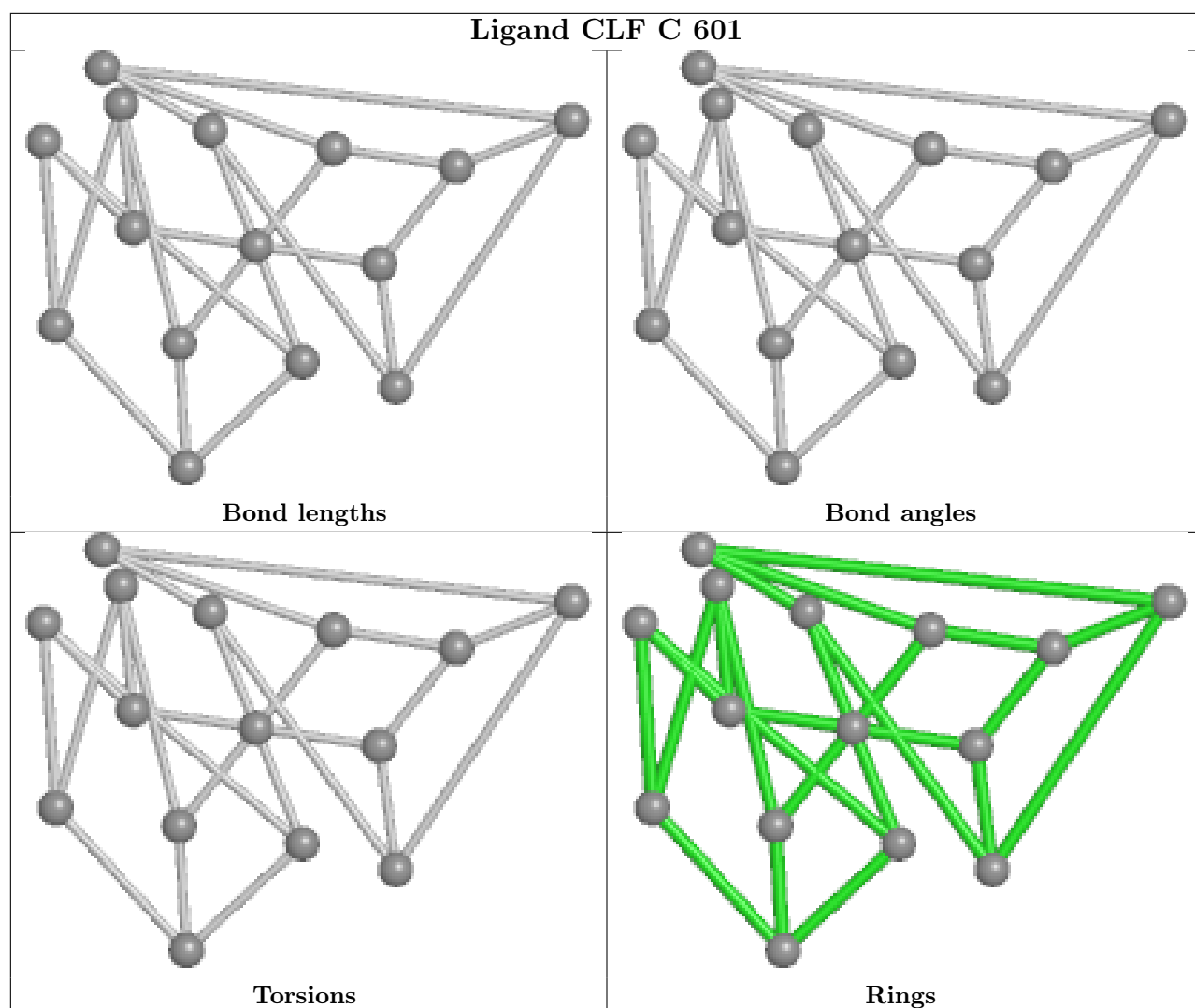


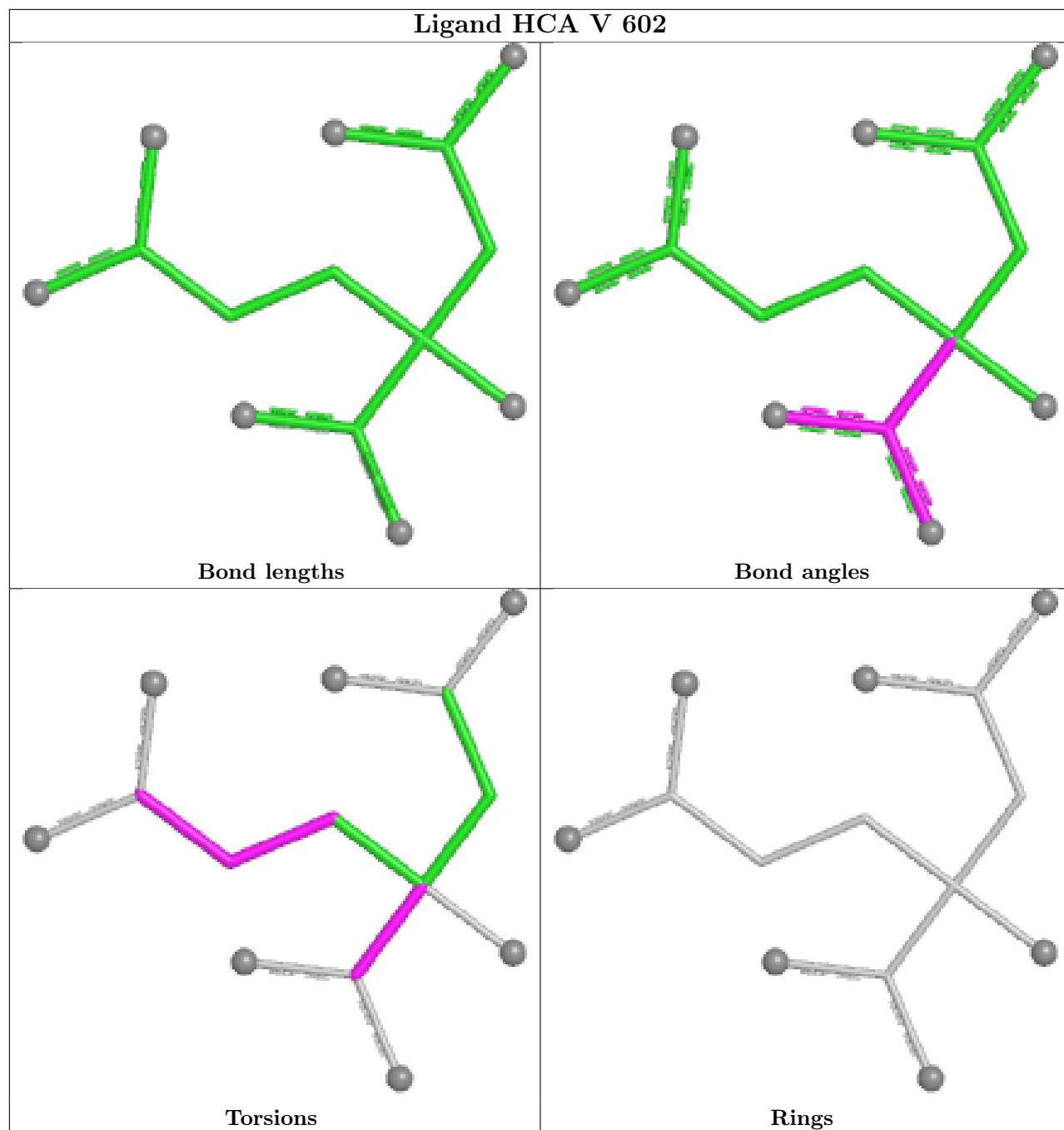


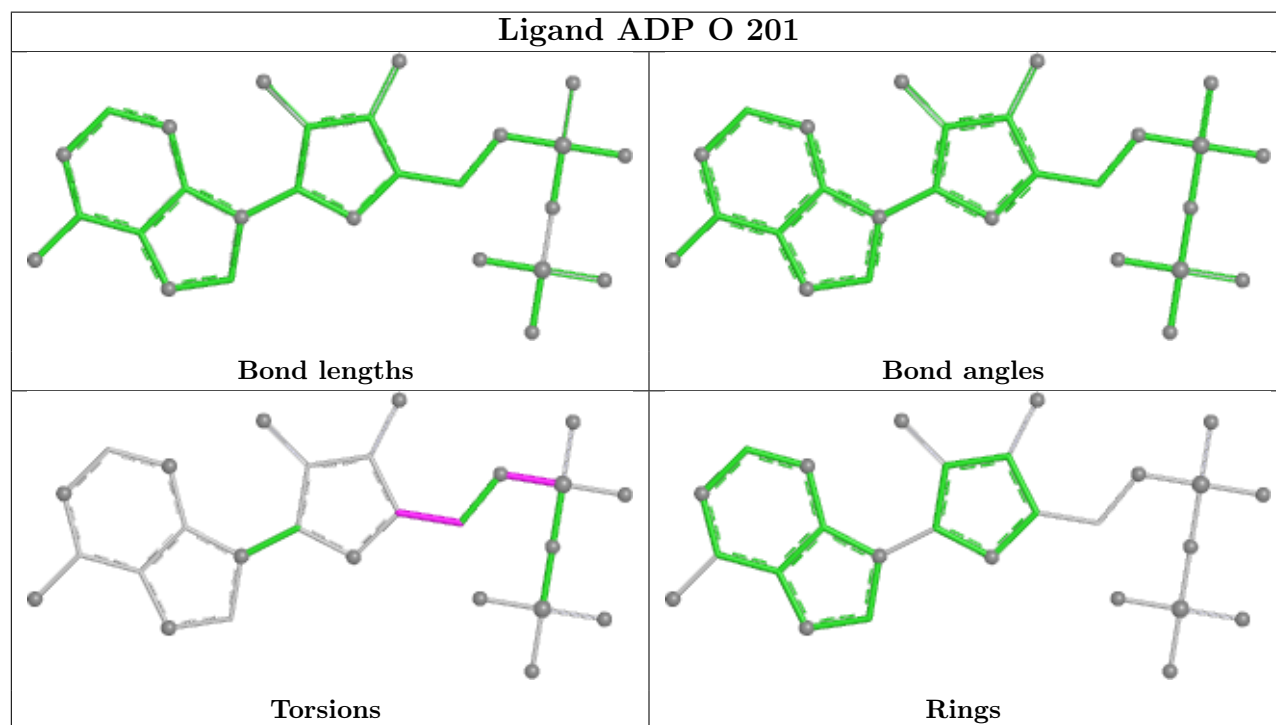
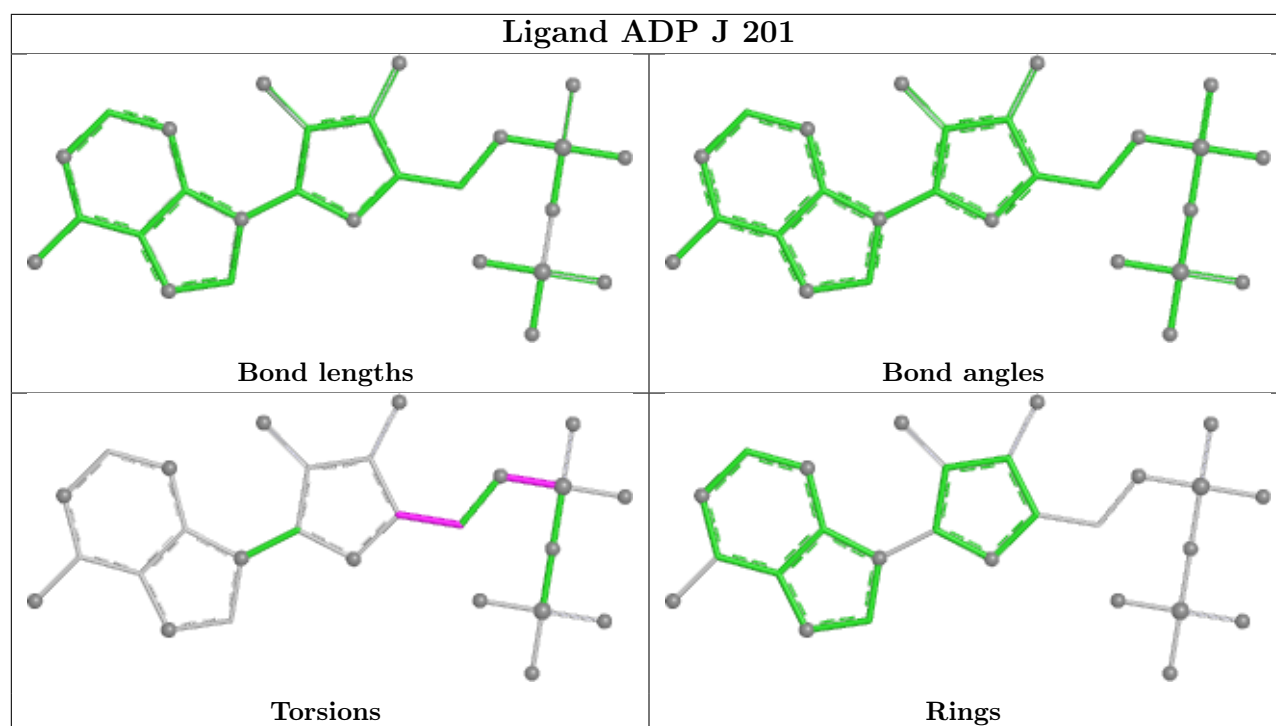


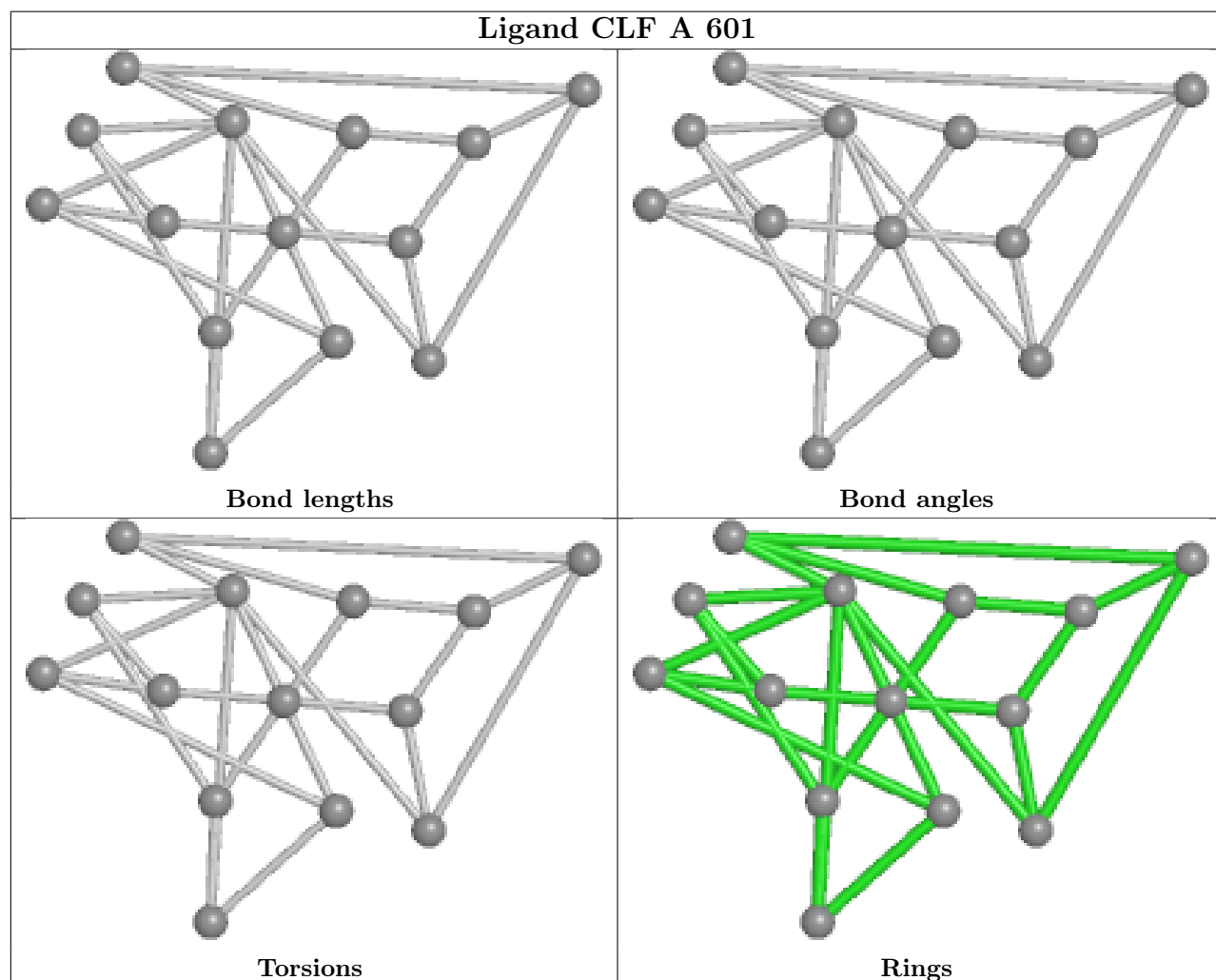
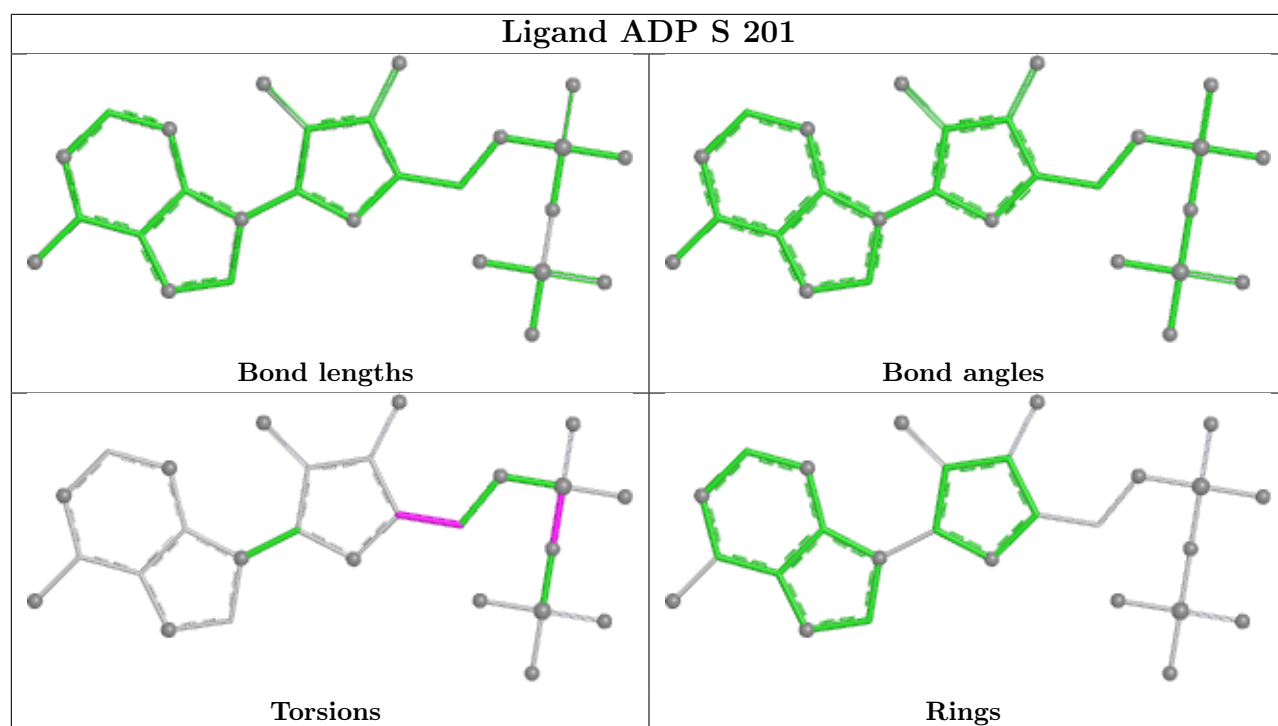


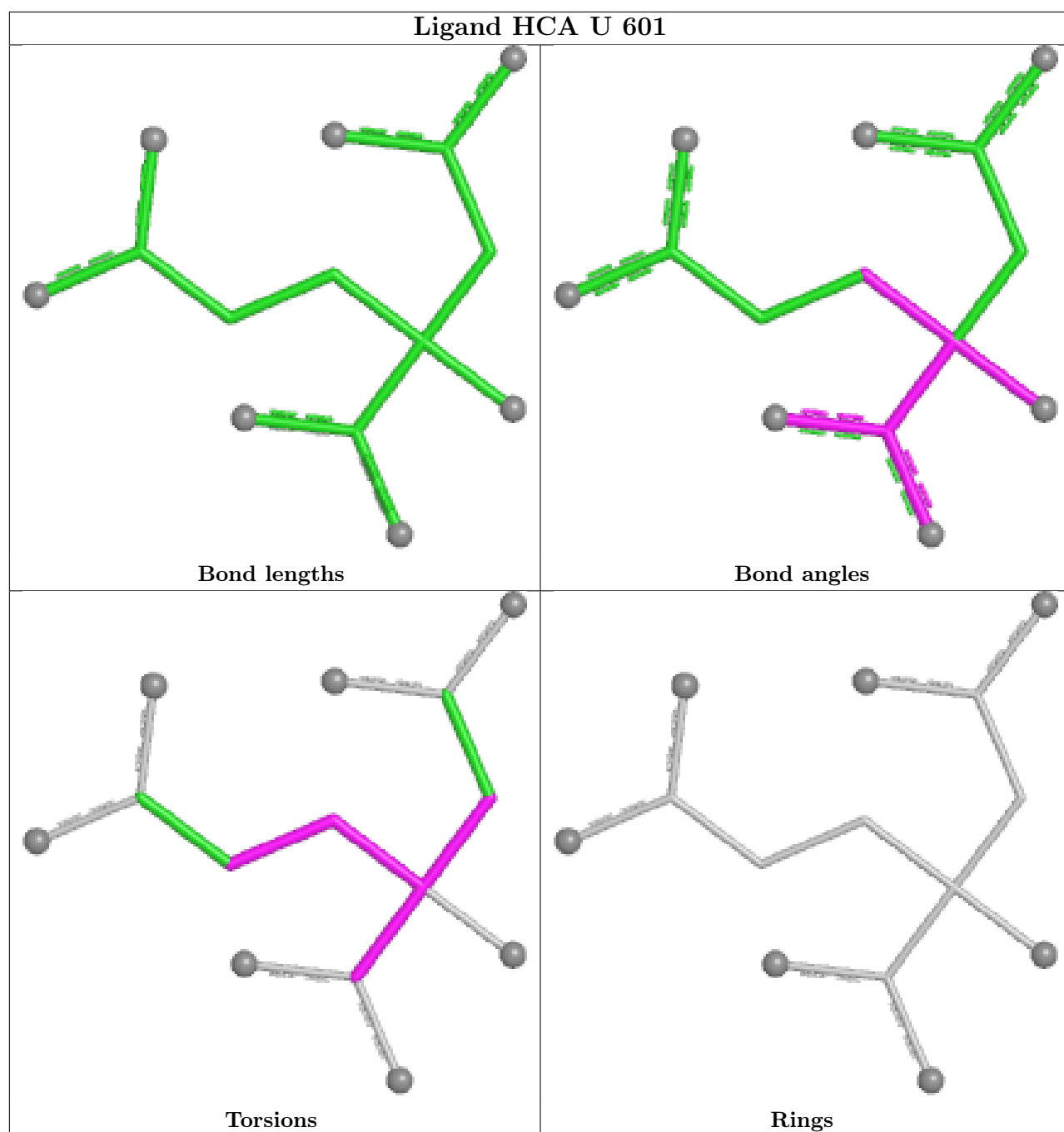


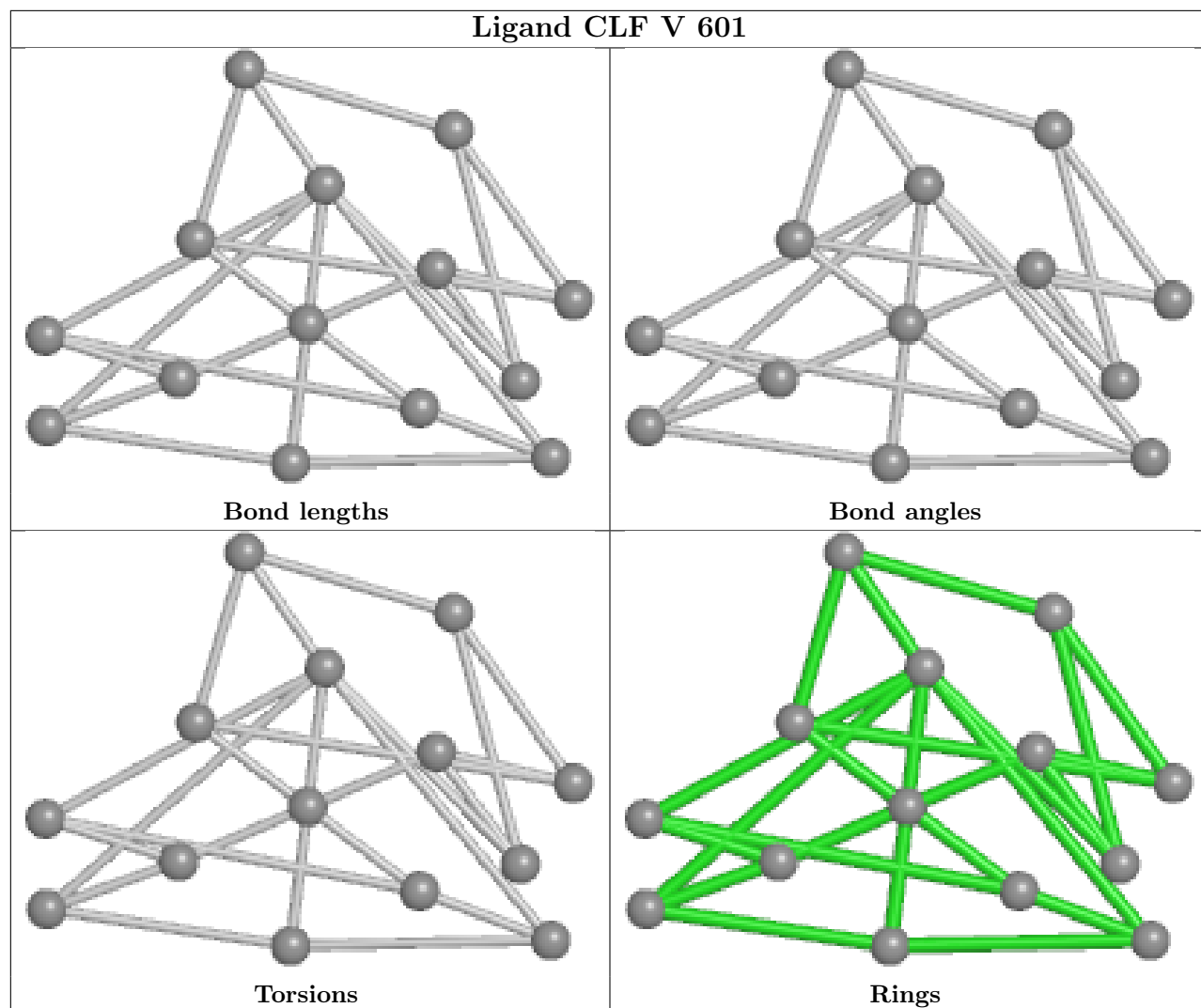




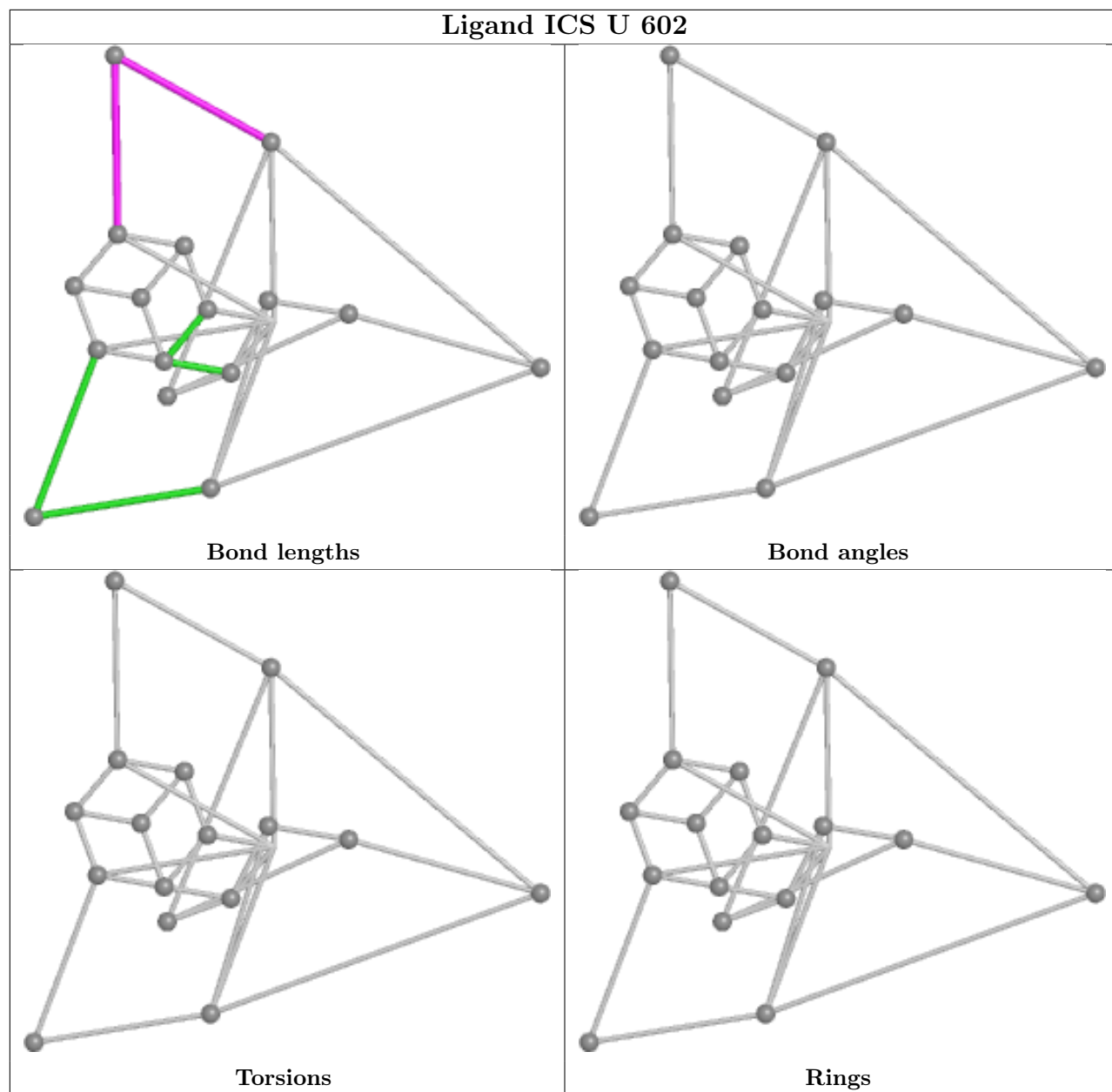


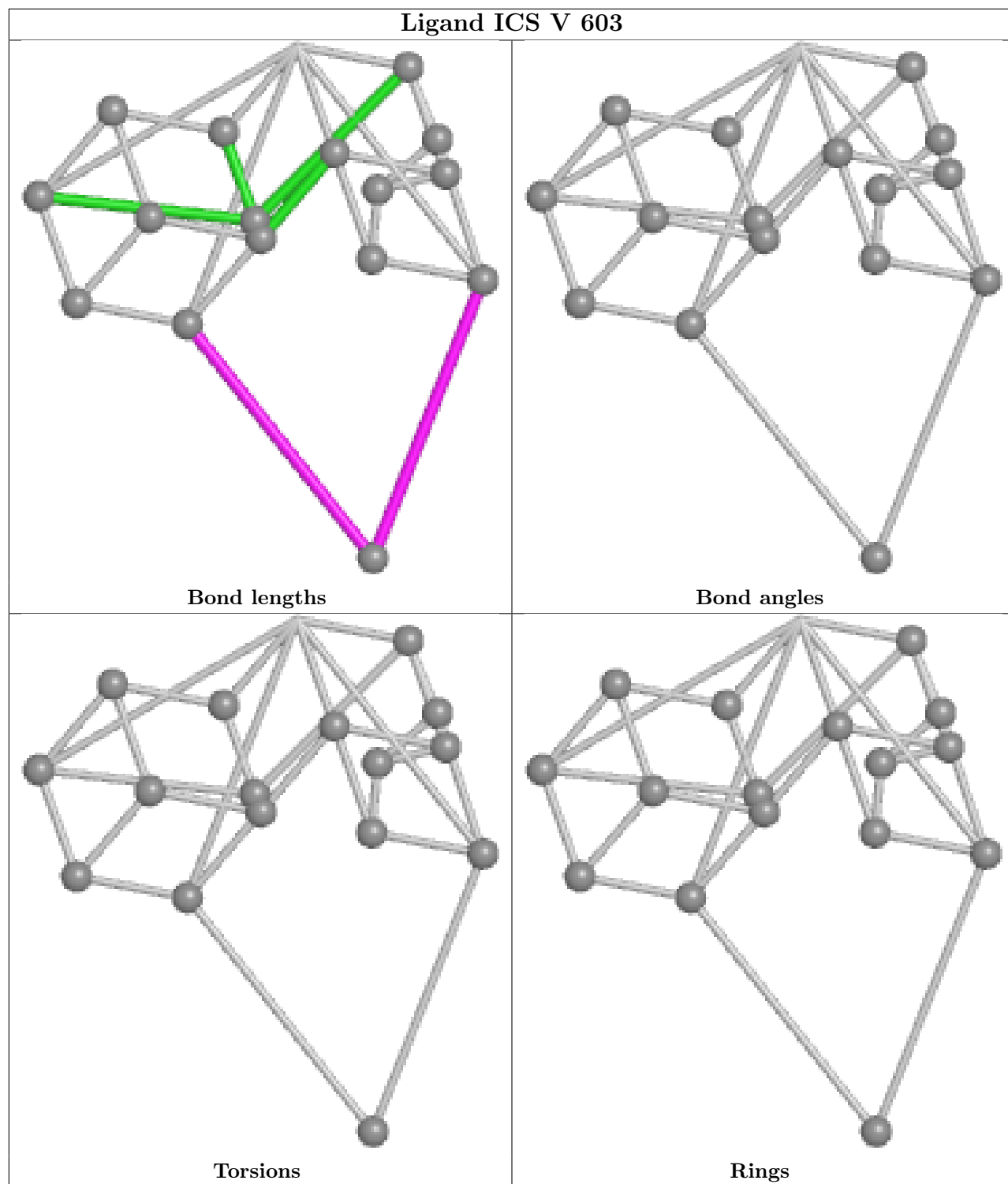


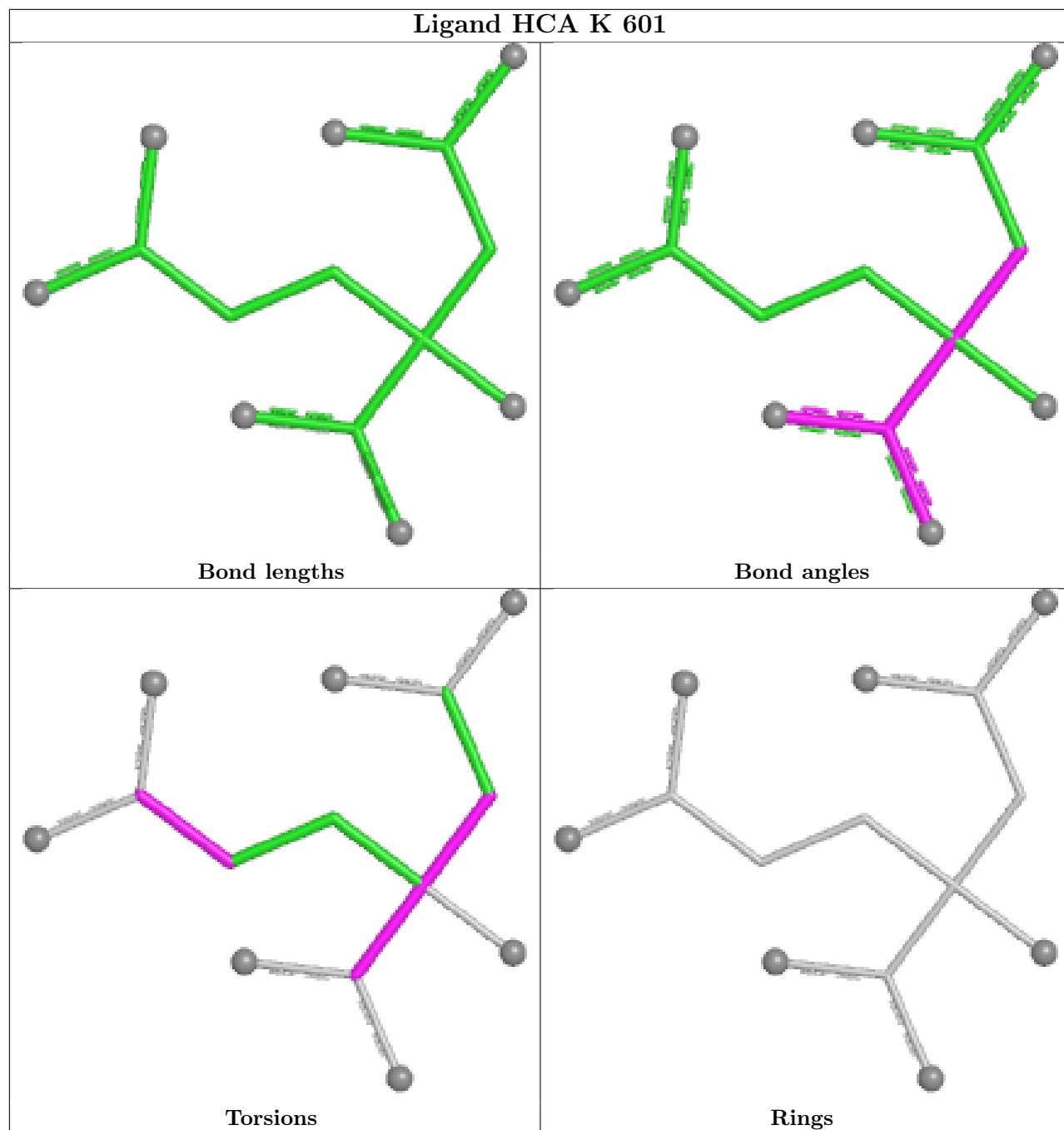


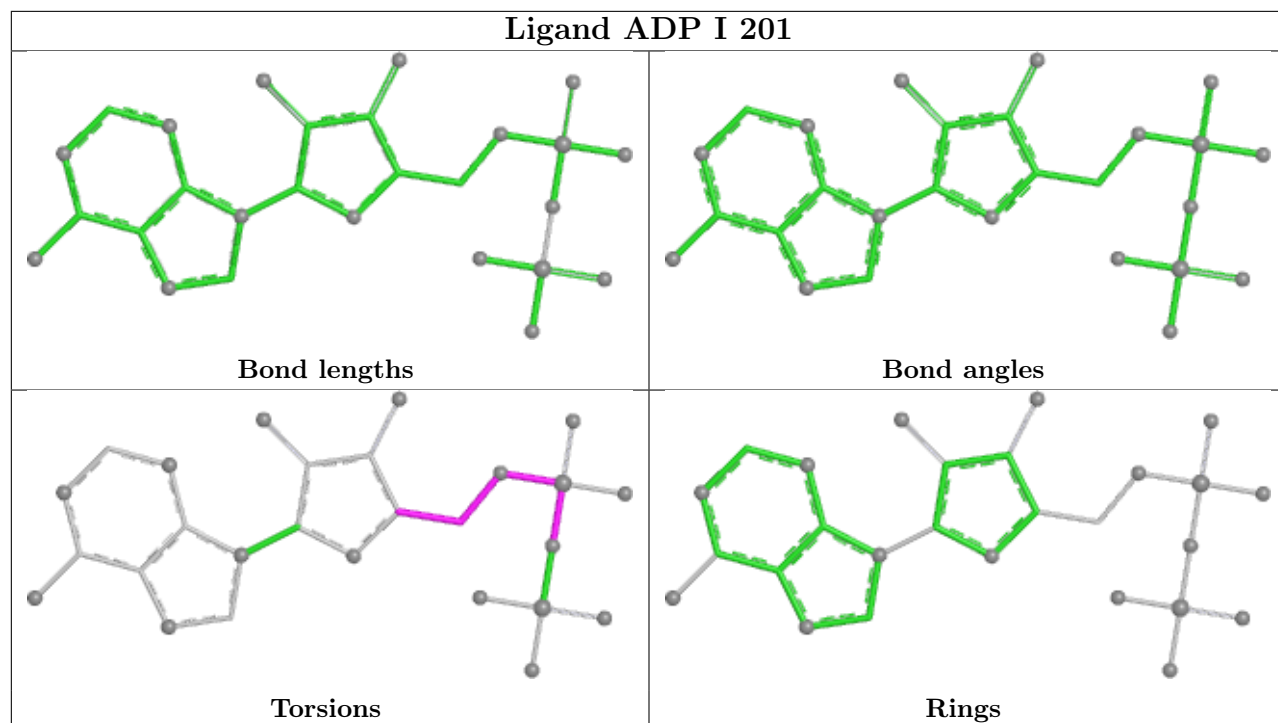


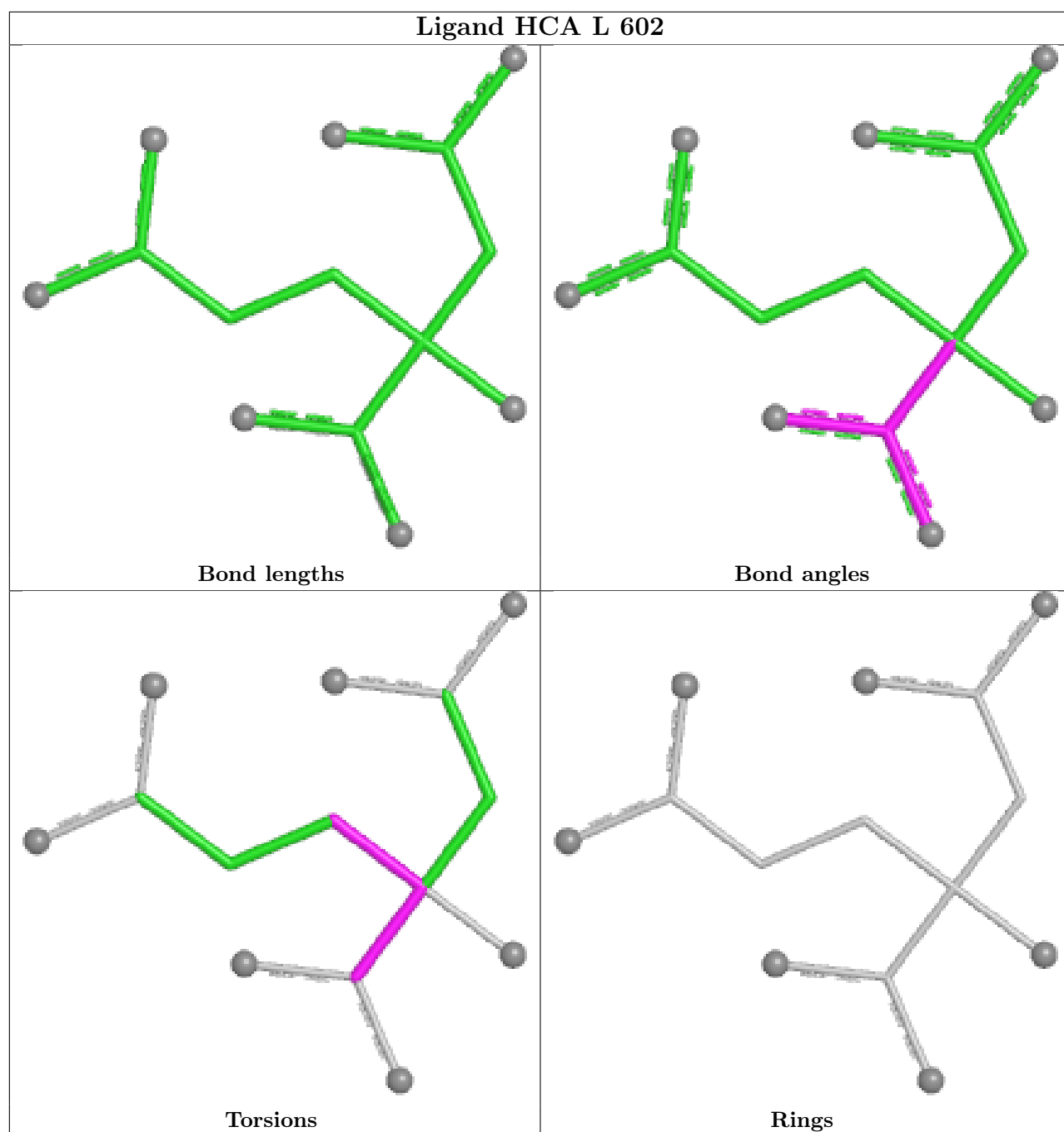
Ligand ICS U 602

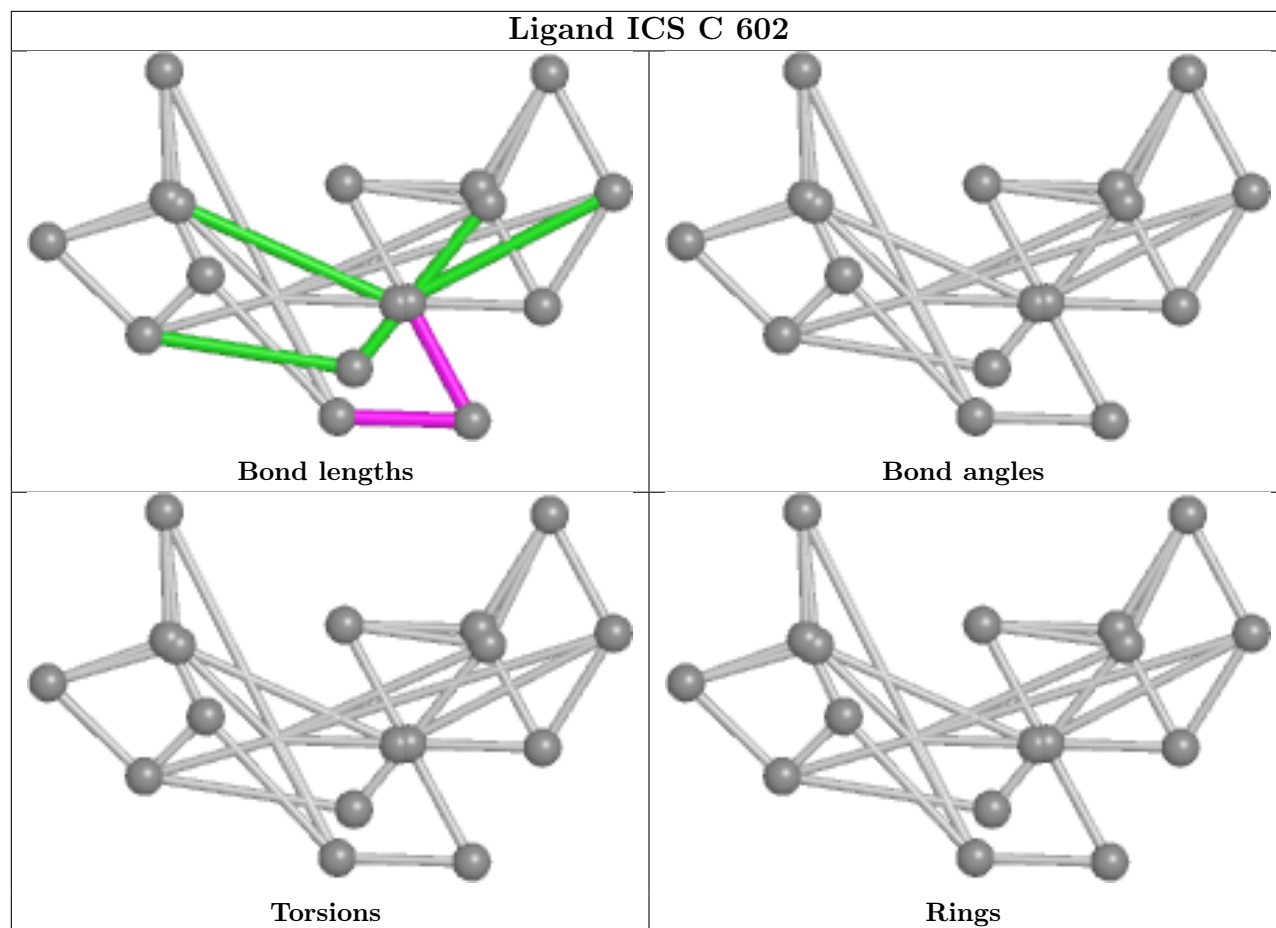












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

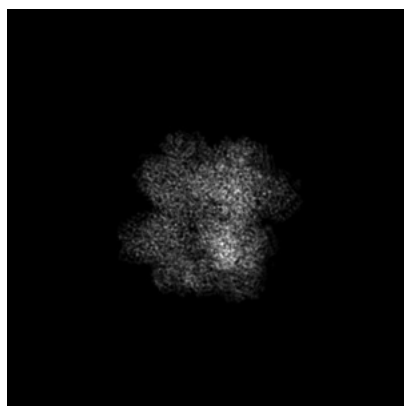
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71144. These allow visual inspection of the internal detail of the map and identification of artifacts.

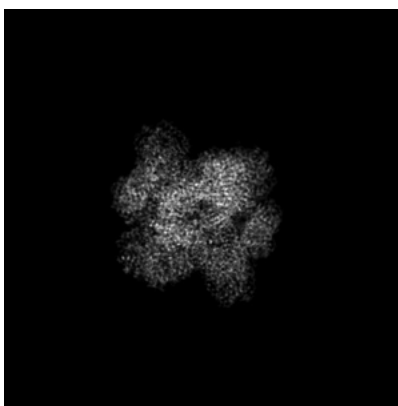
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

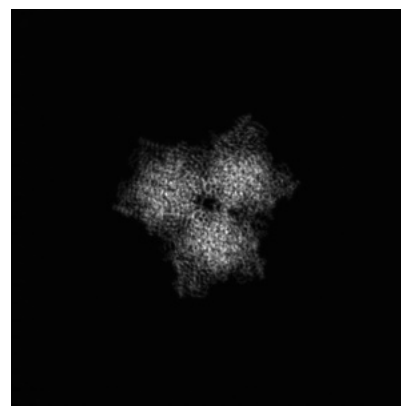
6.1.1 Primary map



X

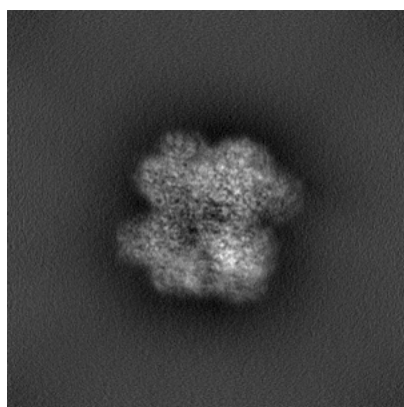


Y

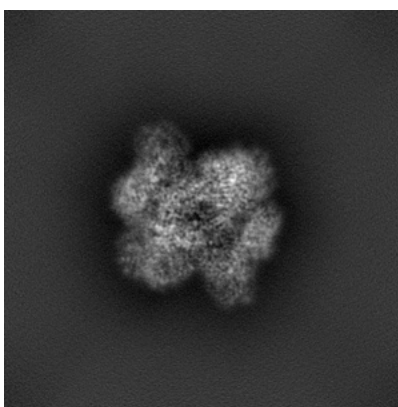


Z

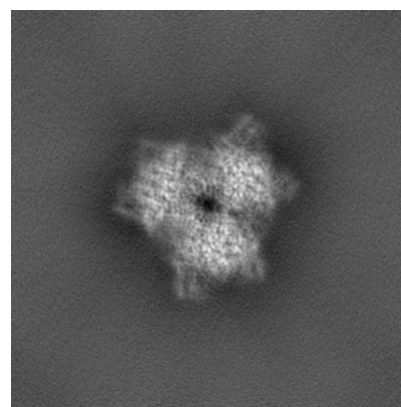
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200

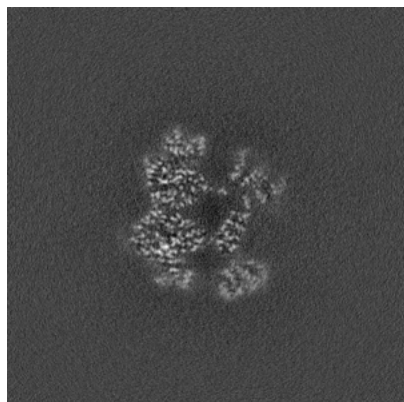


Y Index: 200

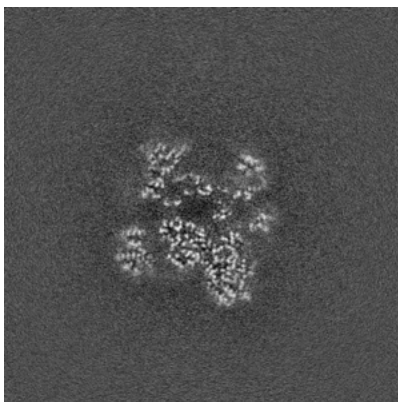


Z Index: 200

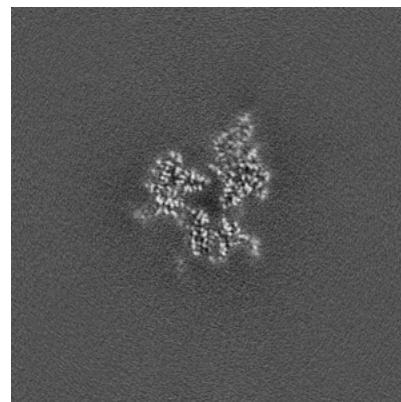
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 214

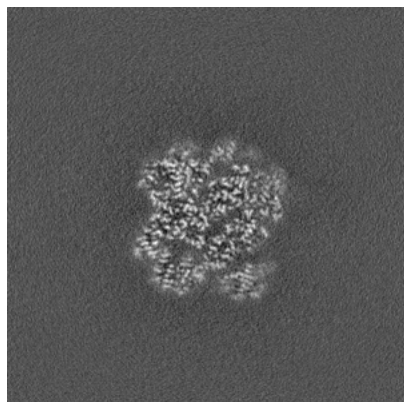


Y Index: 221

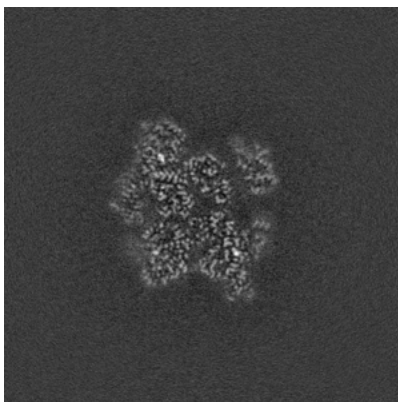


Z Index: 218

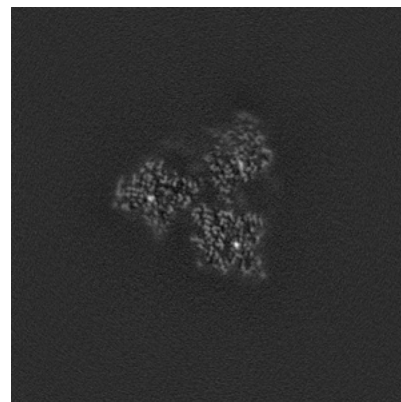
6.3.2 Raw map



X Index: 214



Y Index: 221

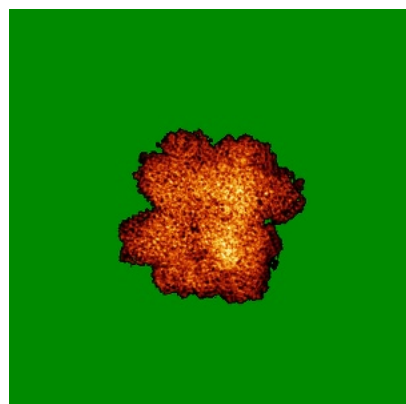


Z Index: 226

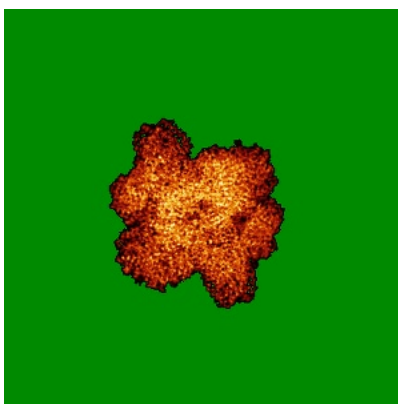
The images above show the largest variance slices of the map in three orthogonal directions.

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

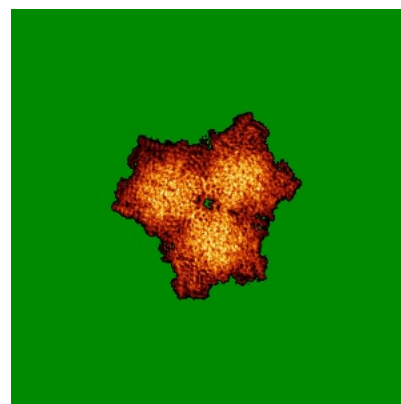
6.4.1 Primary map



X

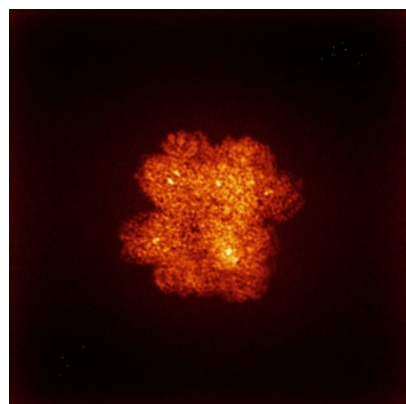


Y

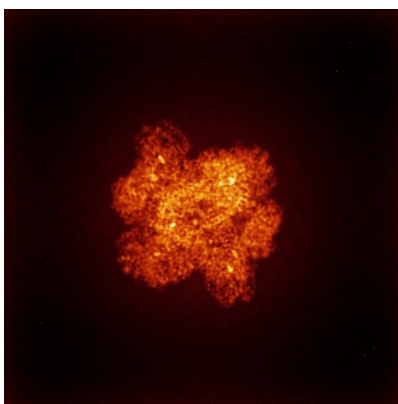


Z

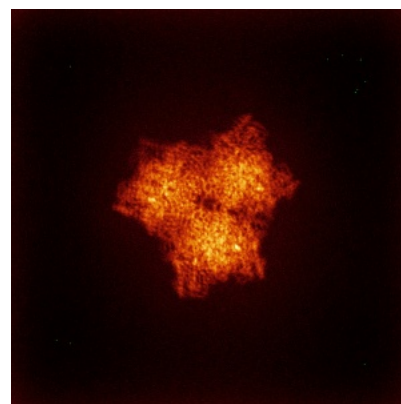
6.4.2 Raw map



X



Y

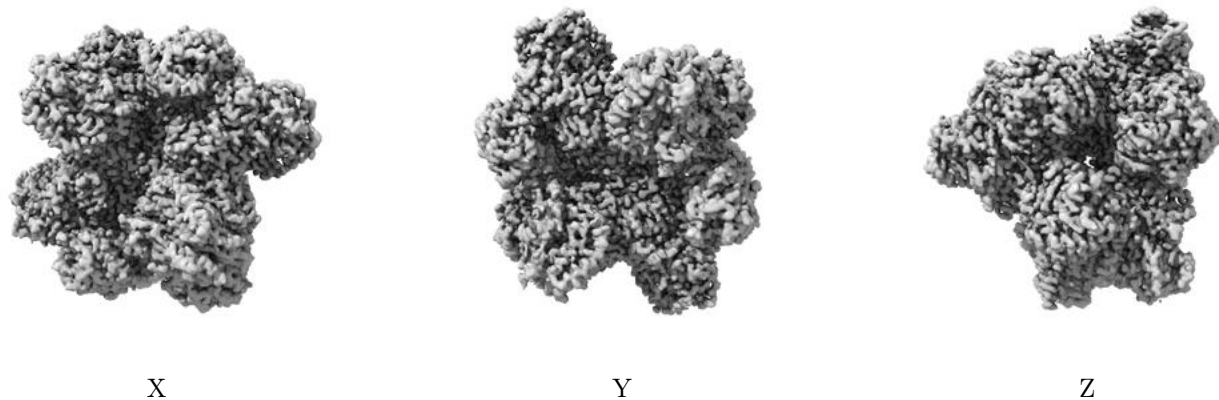


Z

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

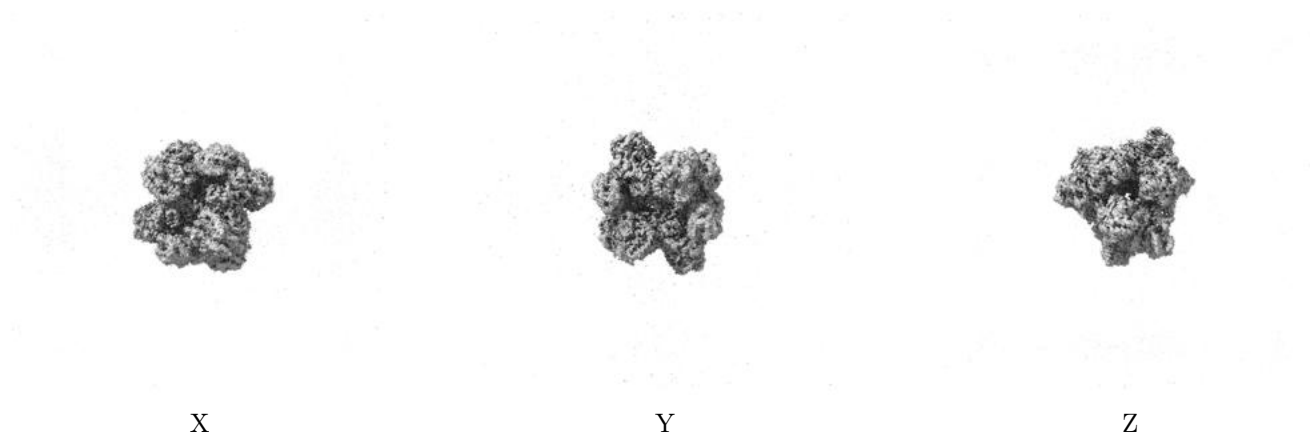
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0204. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

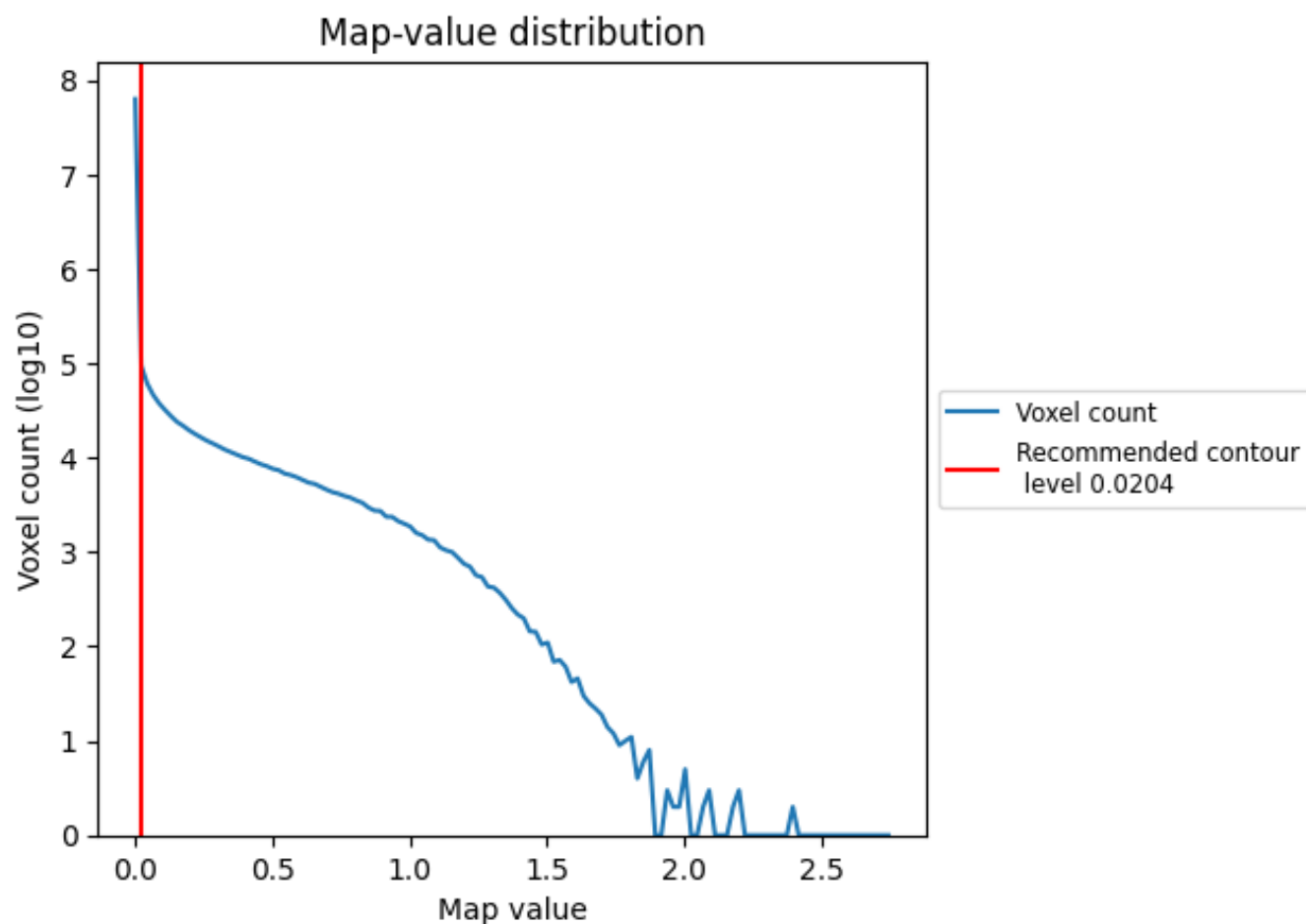
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

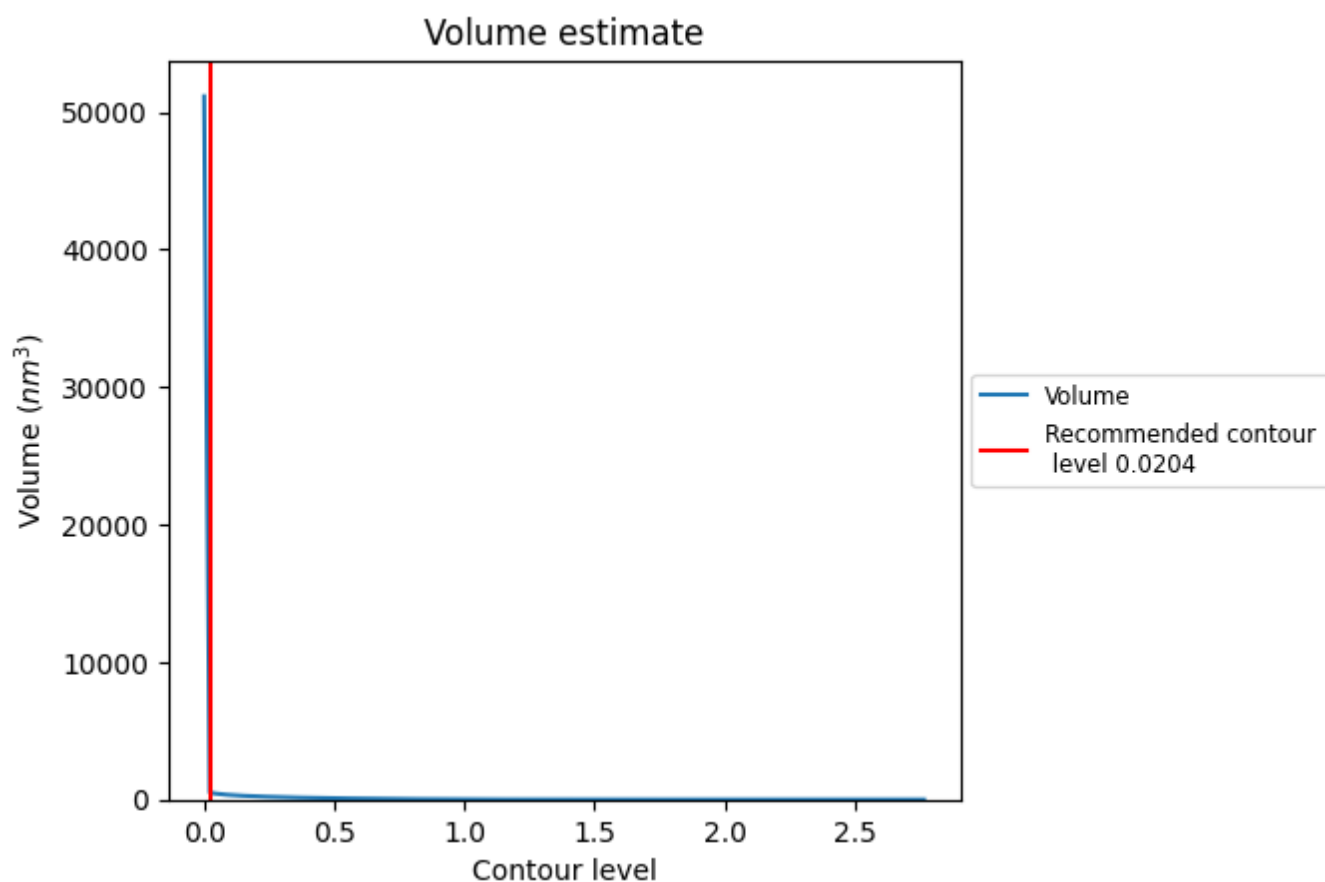
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

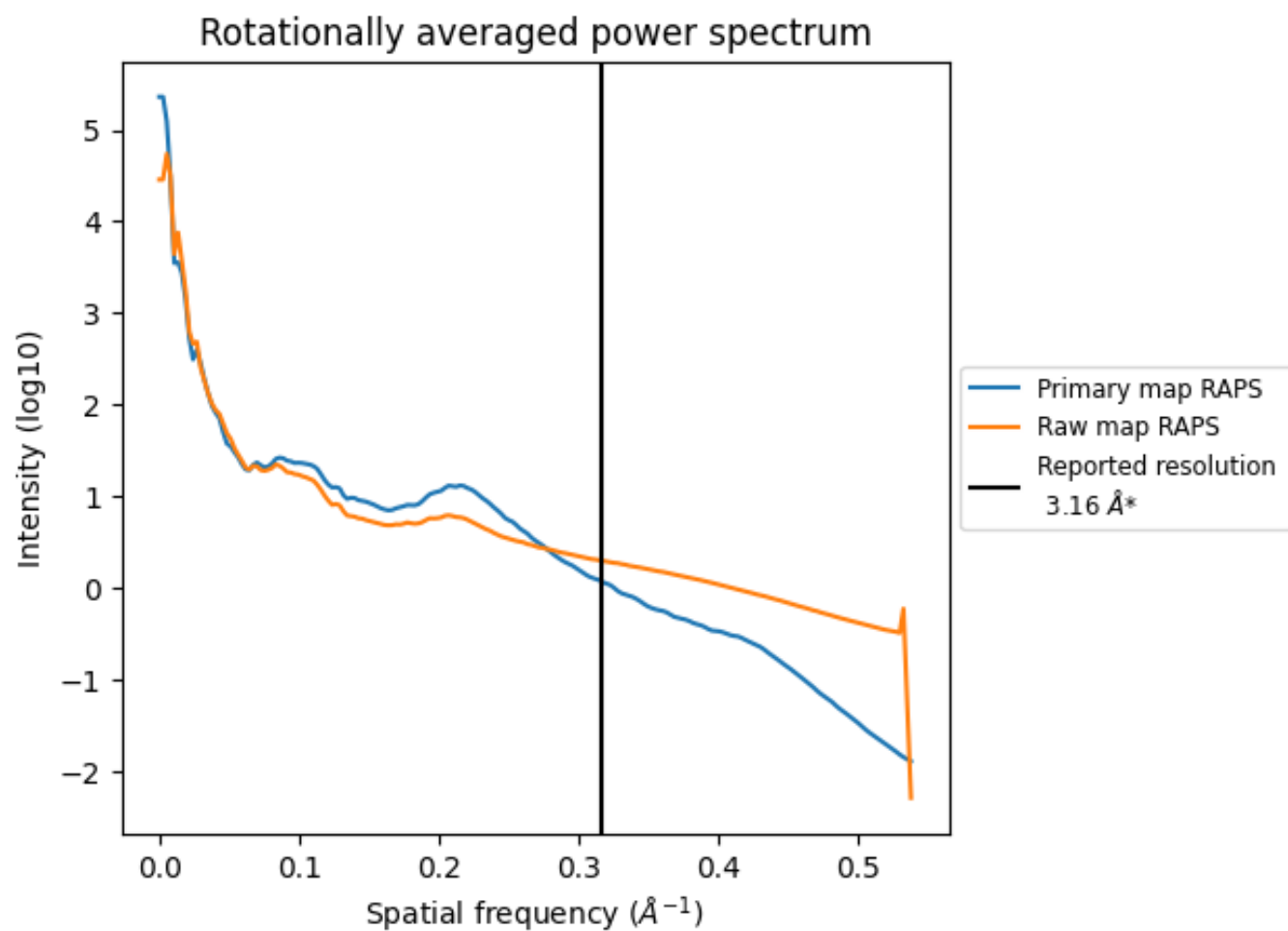
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 511 nm^3 ; this corresponds to an approximate mass of 462 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

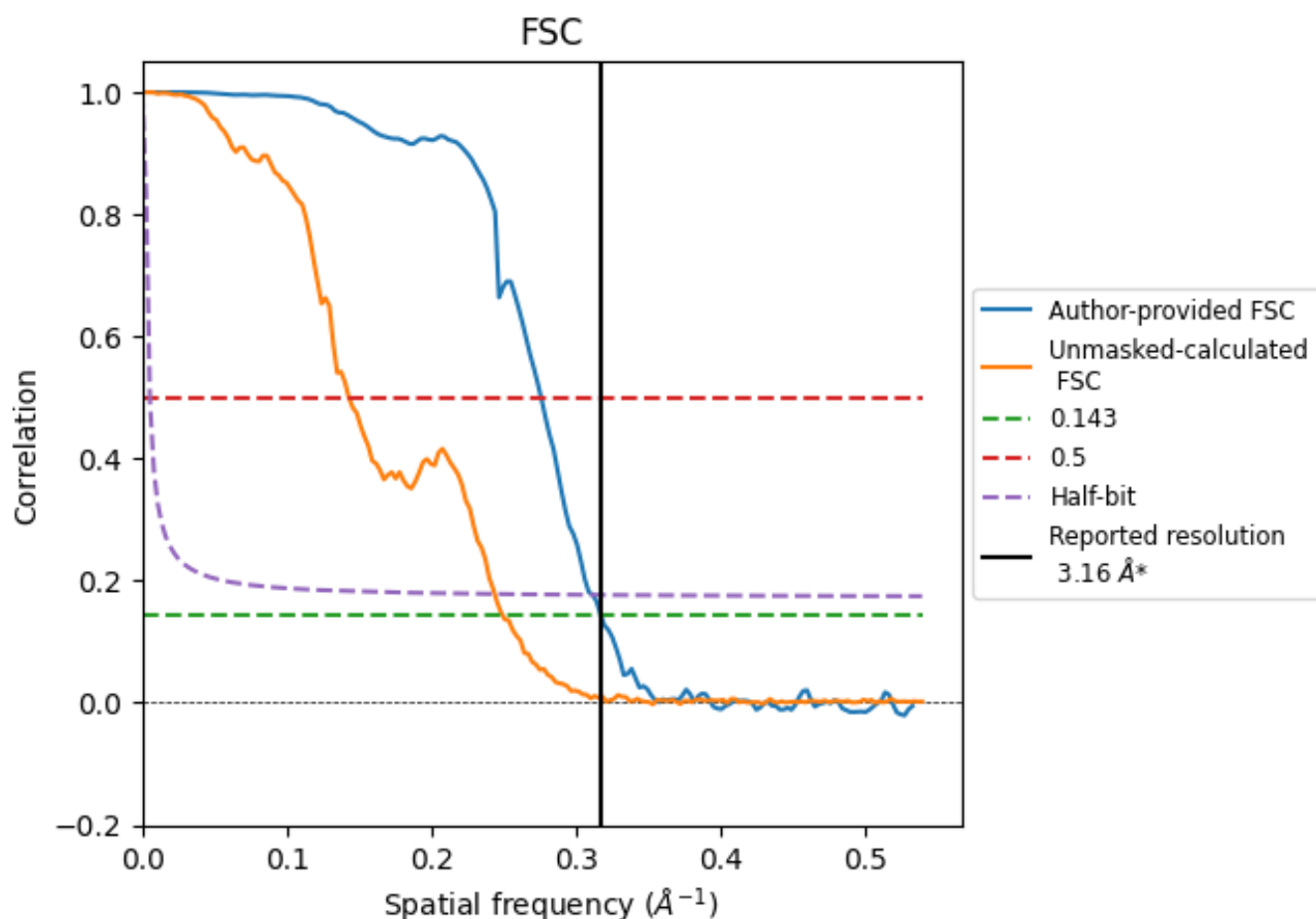


*Reported resolution corresponds to spatial frequency of $0.316 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.316 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

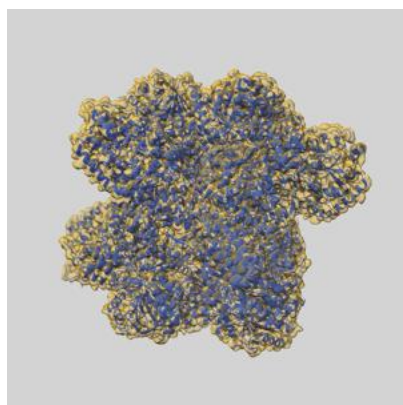
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.63	3.21
Unmasked-calculated*	4.01	7.01	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.16 by more than 10 %

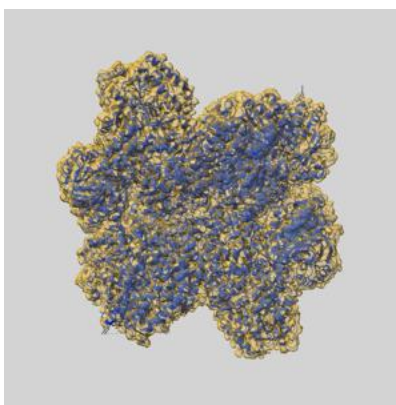
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71144 and PDB model 9P1X. Per-residue inclusion information can be found in section [3](#) on page [16](#).

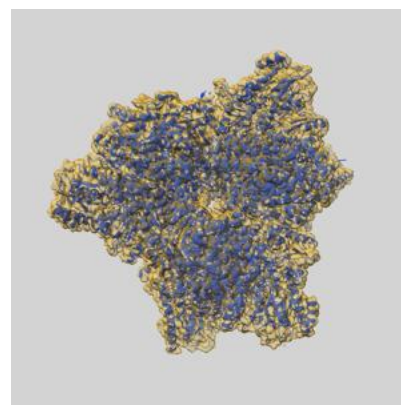
9.1 Map-model overlay [i](#)



X



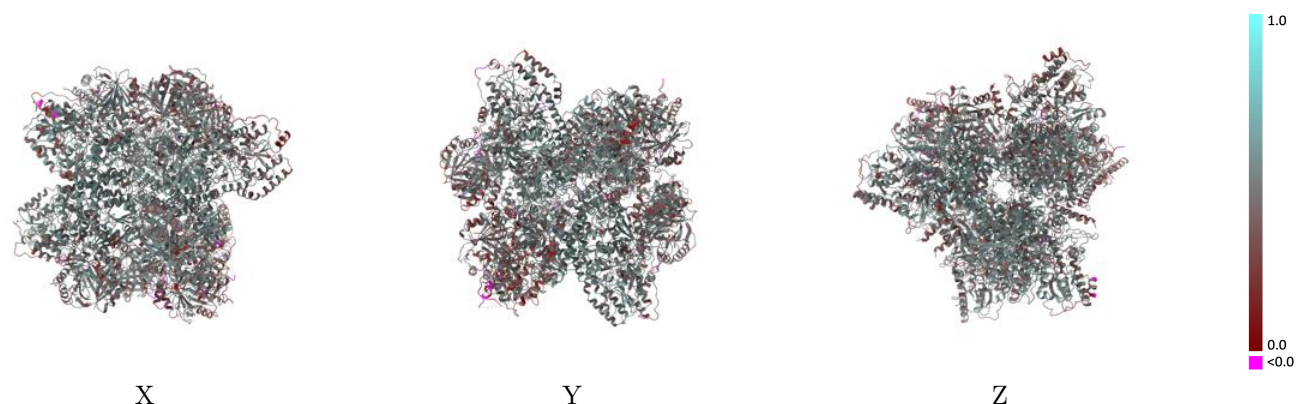
Y



Z

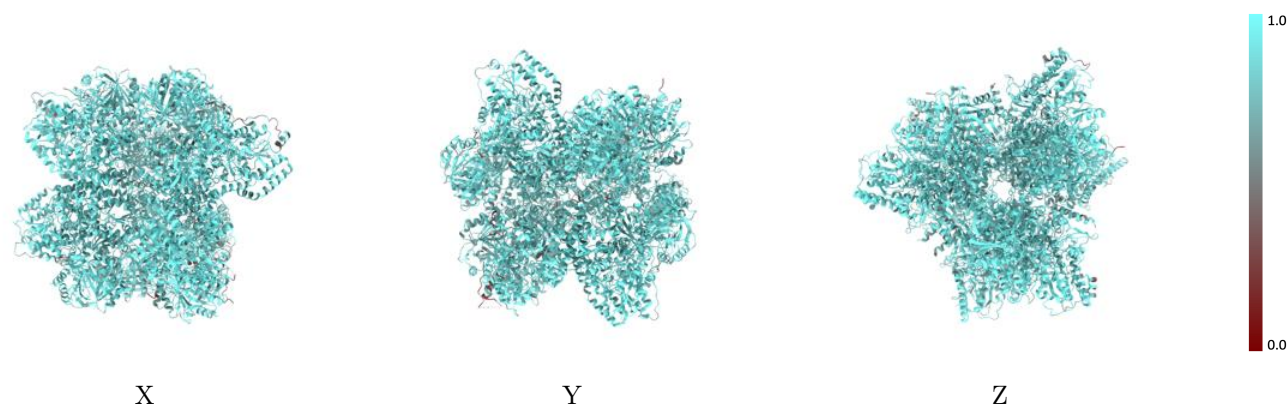
The images above show the 3D surface view of the map at the recommended contour level 0.0204 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



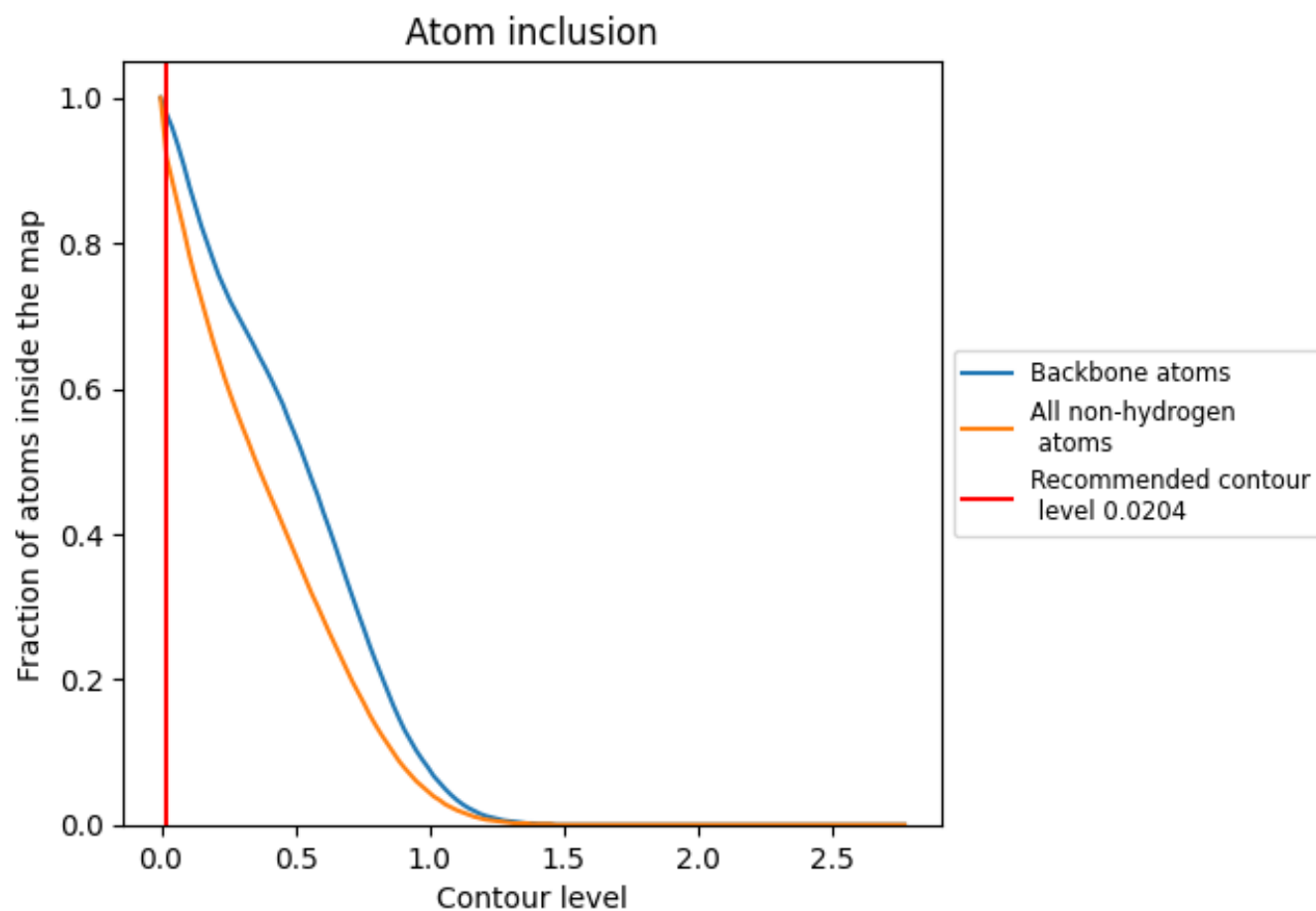
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0204).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.4690
A	 0.9340	 0.4770
B	 0.9650	 0.5350
C	 0.9320	 0.4820
D	 0.9680	 0.5280
E	 0.8980	 0.4580
F	 0.9010	 0.4670
G	 0.8950	 0.4390
H	 0.9120	 0.4550
I	 0.8720	 0.4210
J	 0.8830	 0.4440
K	 0.9300	 0.4580
L	 0.9040	 0.4410
M	 0.9630	 0.5180
N	 0.9560	 0.5090
O	 0.8450	 0.4000
P	 0.8810	 0.4350
Q	 0.8450	 0.3780
R	 0.8900	 0.4160
S	 0.8220	 0.3580
T	 0.8840	 0.4150
U	 0.8170	 0.3700
V	 0.9400	 0.4890
W	 0.9600	 0.5230
X	 0.9630	 0.5190
Y	 0.8730	 0.4210
Z	 0.8850	 0.4380
a	 0.8910	 0.4130
b	 0.8930	 0.4210
c	 0.8380	 0.3920
d	 0.8440	 0.3800

