



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 12:06 PM UTC

PDB ID : 8FYW / pdb_00008fyw
EMDB ID : EMD-29598
Title : Cryo-EM Structure of genome containing AAV2
Authors : Bennett, A.D.; Mckenna, R.
Deposited on : 2023-01-26
Resolution : 2.84 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.dev132
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) : 2.49

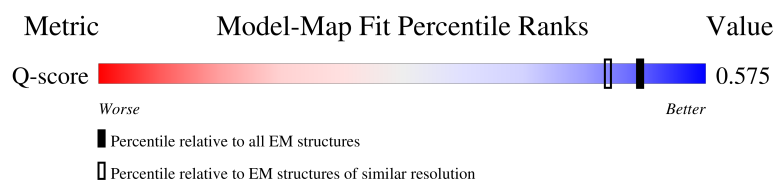
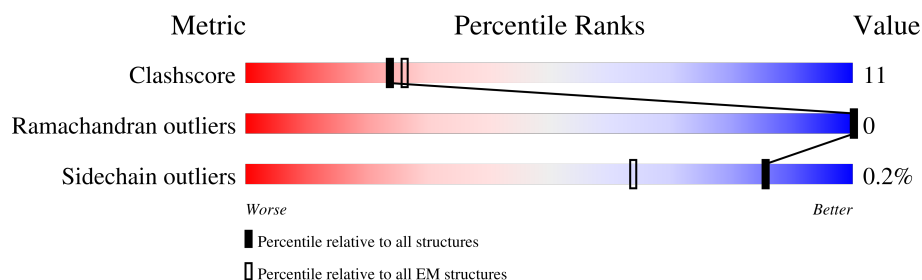
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 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.



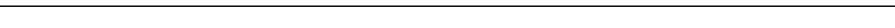
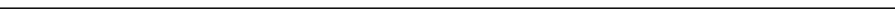
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11884 (2.34 - 3.34)

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	1	735	
1	2	735	
1	3	735	
1	4	735	

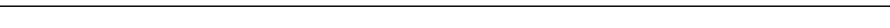
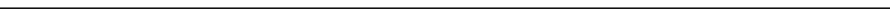
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Mol	Chain	Length	Quality of chain
1	5	735	
1	6	735	
1	7	735	
1	8	735	
1	A	735	
1	B	735	
1	C	735	
1	D	735	
1	E	735	
1	F	735	
1	G	735	
1	H	735	
1	I	735	
1	J	735	
1	K	735	
1	L	735	
1	M	735	
1	N	735	
1	O	735	
1	P	735	
1	Q	735	
1	R	735	
1	S	735	
1	T	735	
1	U	735	

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Mol	Chain	Length	Quality of chain
1	V	735	
1	W	735	
1	X	735	
1	Y	735	
1	Z	735	
1	a	735	
1	b	735	
1	c	735	
1	d	735	
1	e	735	
1	f	735	
1	g	735	
1	h	735	
1	i	735	
1	j	735	
1	k	735	
1	l	735	
1	m	735	
1	n	735	
1	o	735	
1	p	735	
1	q	735	
1	r	735	
1	s	735	
1	t	735	

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Mol	Chain	Length	Quality of chain
1	u	735	 52% 18% 29%
1	v	735	 53% 17% 29%
1	w	735	 53% 18% 29%
1	x	735	 53% 17% 29%
1	y	735	 53% 17% 29%
1	z	735	 54% 17% 29%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 251220 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	B	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	C	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	D	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	E	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	F	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	G	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	H	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	I	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	J	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	K	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	L	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	M	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	N	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	O	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	P	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	Q	519	Total 4166	C 2620	N 731	O 802	S 13	2	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	S	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	T	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	U	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	V	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	W	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	X	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	Y	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	Z	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	a	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	b	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	c	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	d	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	e	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	f	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	g	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	h	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	i	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	j	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	k	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	l	519	Total 4166	C 2620	N 731	O 802	S 13	2	0

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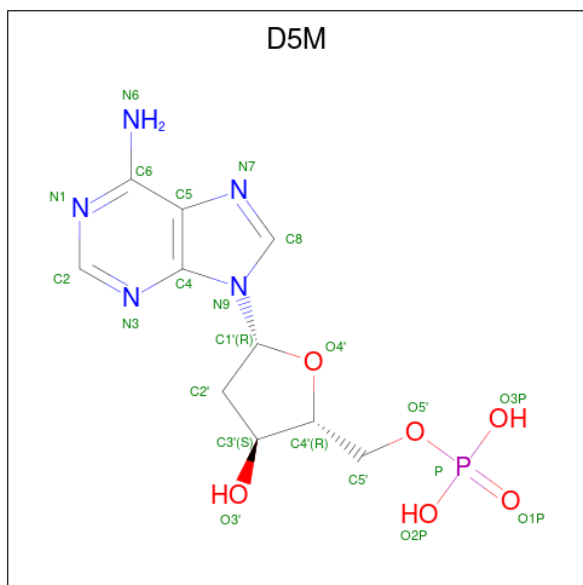
Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	n	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	o	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	p	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	q	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	r	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	s	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	t	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	u	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	v	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	w	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	x	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	y	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	z	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	1	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	2	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	3	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	4	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	5	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	6	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	7	519	Total 4166	C 2620	N 731	O 802	S 13	2	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	519	Total	C	N	O	S	2	0
			4166	2620	731	802	13		

- Molecule 2 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (CCD ID: D5M) (formula: $C_{10}H_{14}N_5O_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	B	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	C	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	D	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	E	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	F	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	G	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	H	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	I	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	J	1	Total	C	N	O	P	0
			21	10	5	5	1	

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Mol	Chain	Residues	Atoms					AltConf
2	K	1	Total 21	C 10	N 5	O 5	P 1	0
2	L	1	Total 21	C 10	N 5	O 5	P 1	0
2	M	1	Total 21	C 10	N 5	O 5	P 1	0
2	N	1	Total 21	C 10	N 5	O 5	P 1	0
2	O	1	Total 21	C 10	N 5	O 5	P 1	0
2	P	1	Total 21	C 10	N 5	O 5	P 1	0
2	Q	1	Total 21	C 10	N 5	O 5	P 1	0
2	R	1	Total 21	C 10	N 5	O 5	P 1	0
2	S	1	Total 21	C 10	N 5	O 5	P 1	0
2	T	1	Total 21	C 10	N 5	O 5	P 1	0
2	U	1	Total 21	C 10	N 5	O 5	P 1	0
2	V	1	Total 21	C 10	N 5	O 5	P 1	0
2	W	1	Total 21	C 10	N 5	O 5	P 1	0
2	X	1	Total 21	C 10	N 5	O 5	P 1	0
2	Y	1	Total 21	C 10	N 5	O 5	P 1	0
2	Z	1	Total 21	C 10	N 5	O 5	P 1	0
2	a	1	Total 21	C 10	N 5	O 5	P 1	0
2	b	1	Total 21	C 10	N 5	O 5	P 1	0
2	c	1	Total 21	C 10	N 5	O 5	P 1	0
2	d	1	Total 21	C 10	N 5	O 5	P 1	0
2	e	1	Total 21	C 10	N 5	O 5	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
2	f	1	Total 21	C 10	N 5	O 5	P 1	0
2	g	1	Total 21	C 10	N 5	O 5	P 1	0
2	h	1	Total 21	C 10	N 5	O 5	P 1	0
2	i	1	Total 21	C 10	N 5	O 5	P 1	0
2	j	1	Total 21	C 10	N 5	O 5	P 1	0
2	k	1	Total 21	C 10	N 5	O 5	P 1	0
2	l	1	Total 21	C 10	N 5	O 5	P 1	0
2	m	1	Total 21	C 10	N 5	O 5	P 1	0
2	n	1	Total 21	C 10	N 5	O 5	P 1	0
2	o	1	Total 21	C 10	N 5	O 5	P 1	0
2	p	1	Total 21	C 10	N 5	O 5	P 1	0
2	q	1	Total 21	C 10	N 5	O 5	P 1	0
2	r	1	Total 21	C 10	N 5	O 5	P 1	0
2	s	1	Total 21	C 10	N 5	O 5	P 1	0
2	t	1	Total 21	C 10	N 5	O 5	P 1	0
2	u	1	Total 21	C 10	N 5	O 5	P 1	0
2	v	1	Total 21	C 10	N 5	O 5	P 1	0
2	w	1	Total 21	C 10	N 5	O 5	P 1	0
2	x	1	Total 21	C 10	N 5	O 5	P 1	0
2	y	1	Total 21	C 10	N 5	O 5	P 1	0
2	z	1	Total 21	C 10	N 5	O 5	P 1	0

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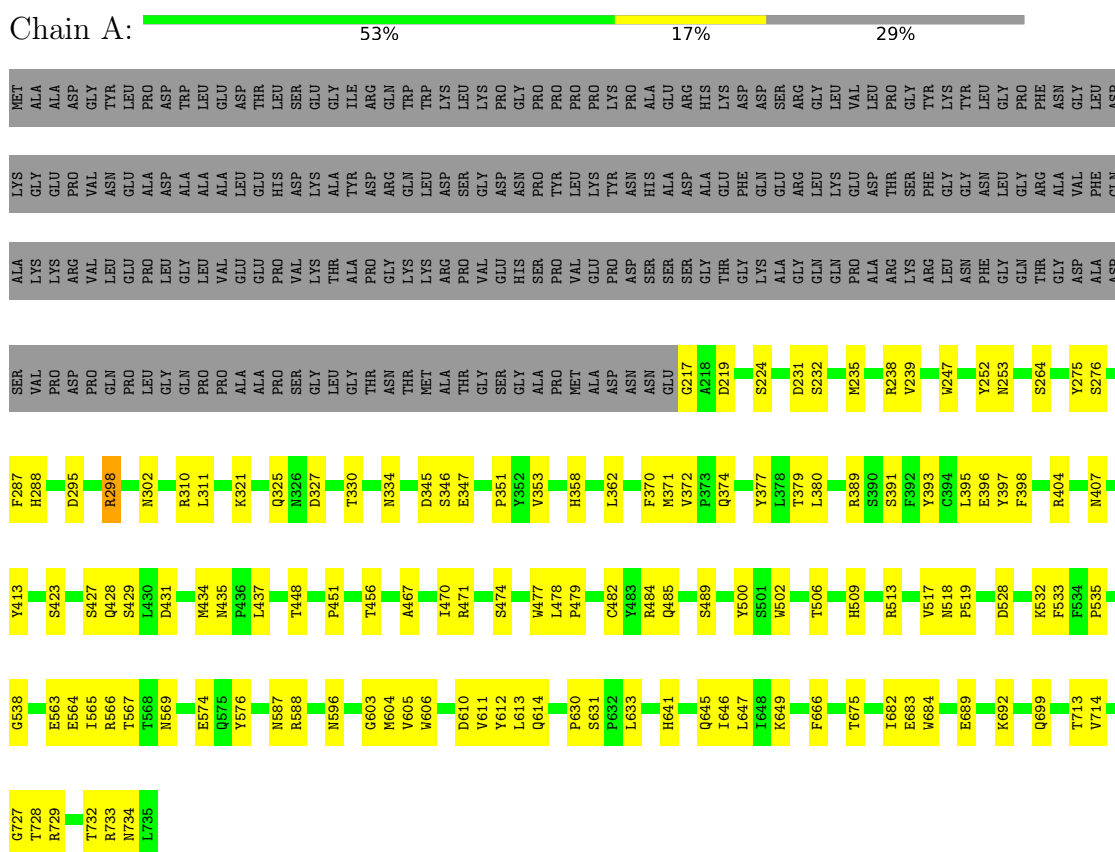
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Mol	Chain	Residues	Atoms					AltConf
2	1	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	2	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	3	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	4	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	5	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	6	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	7	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	8	1	Total	C	N	O	P	0
			21	10	5	5	1	

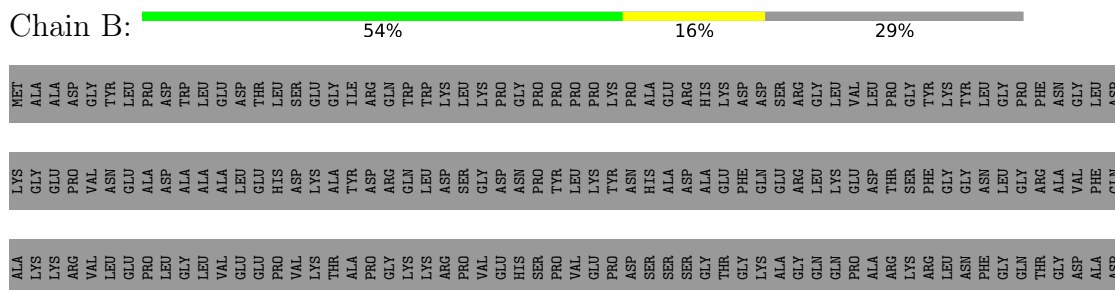
3 Residue-property plots

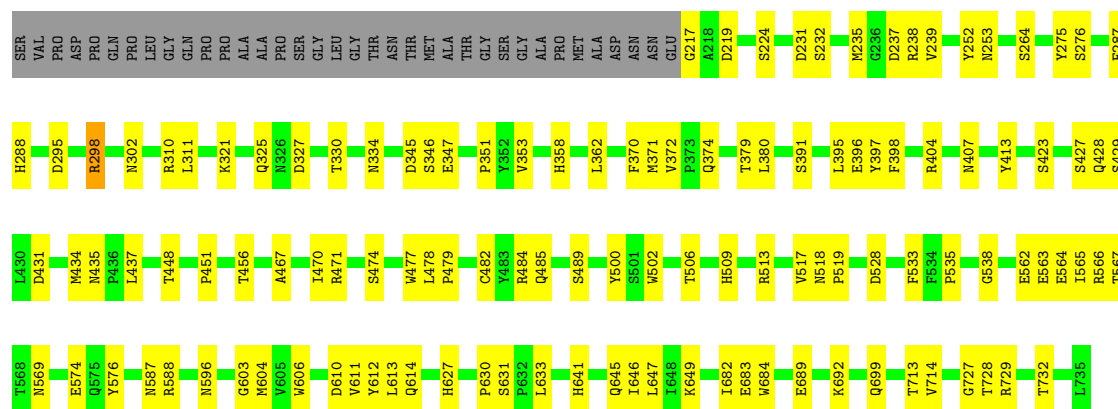
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Capsid protein VP1



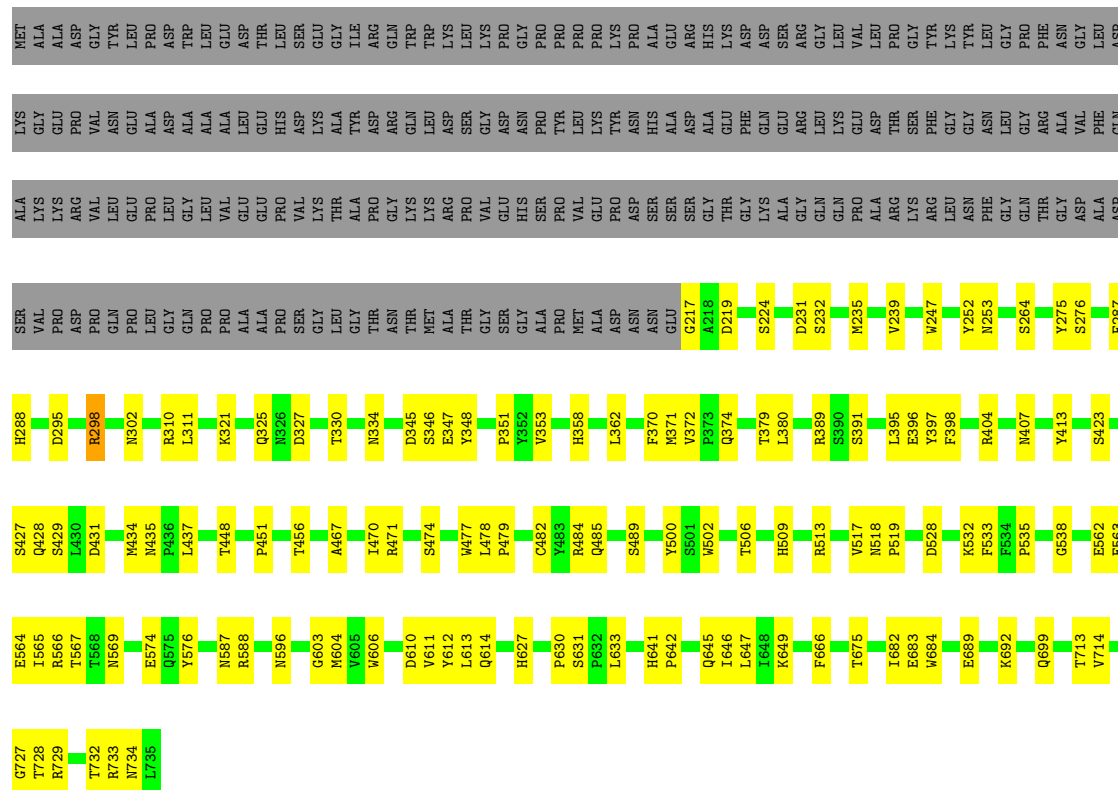
• Molecule 1: Capsid protein VP1





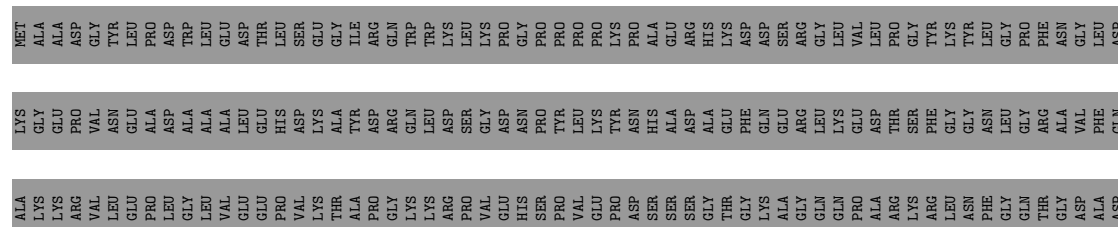
• Molecule 1: Capsid protein VP1

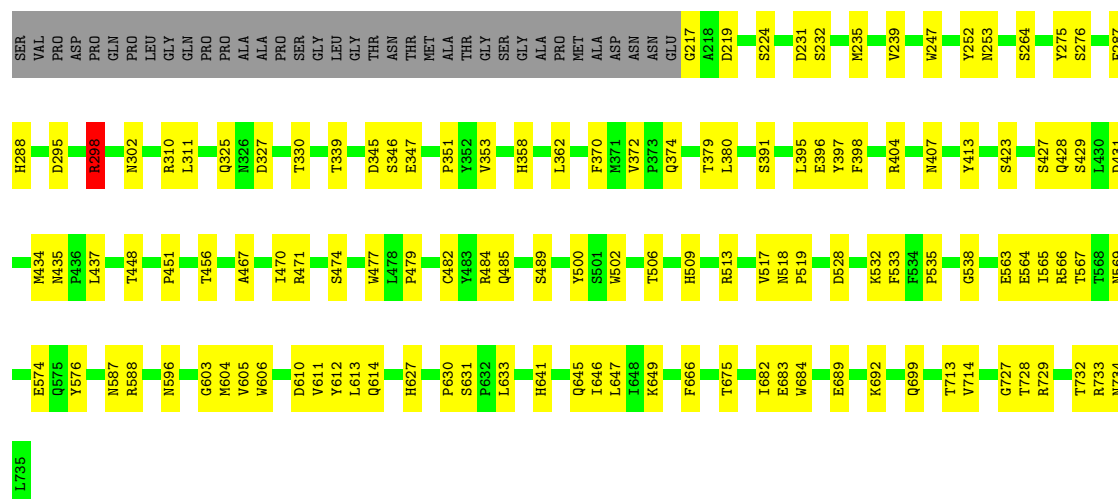
Chain C: 53% 17% 29%



• Molecule 1: Capsid protein VP1

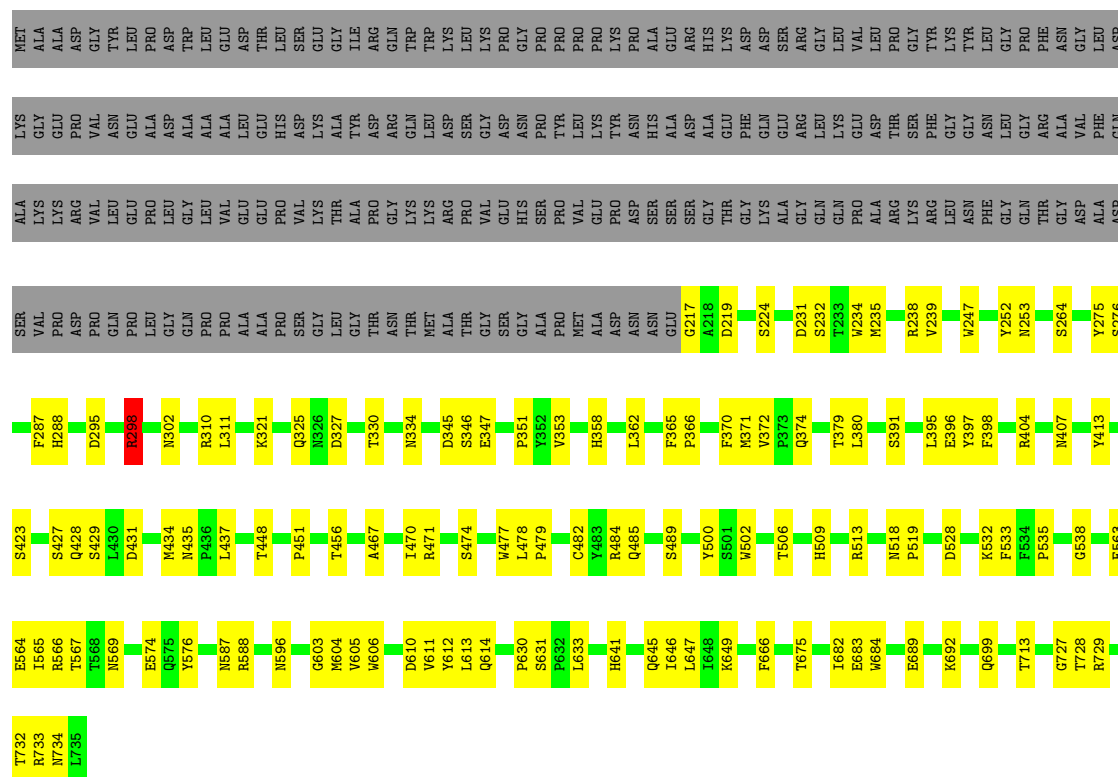
Chain D: 54% 17% 29%





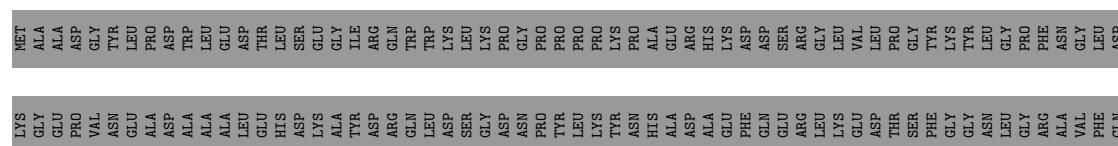
• Molecule 1: Capsid protein VP1

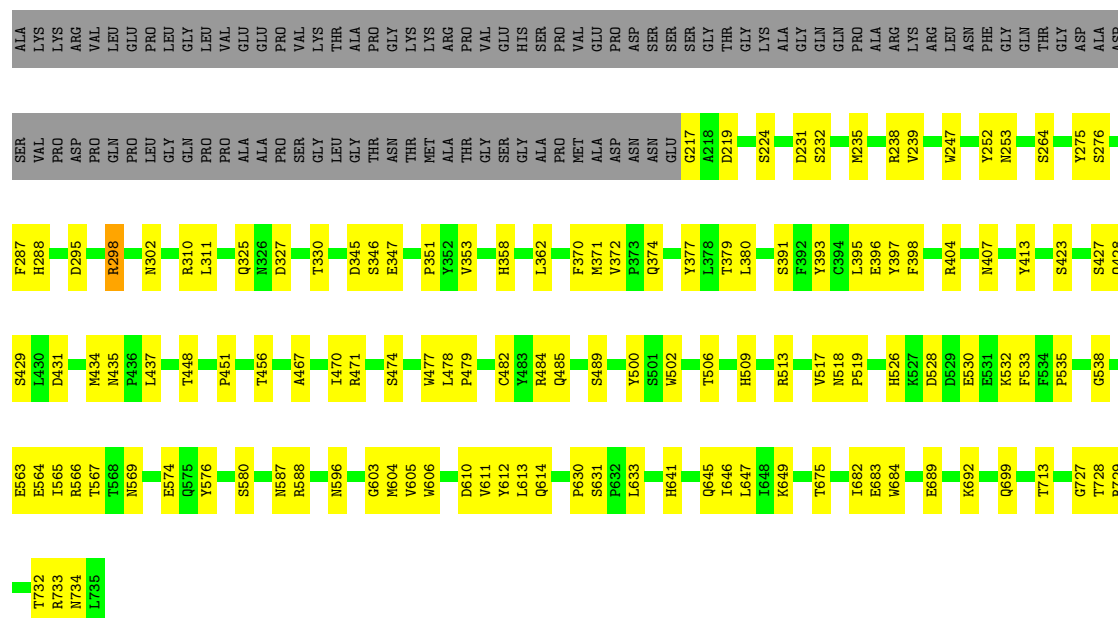
Chain E: 53% 17% 29%



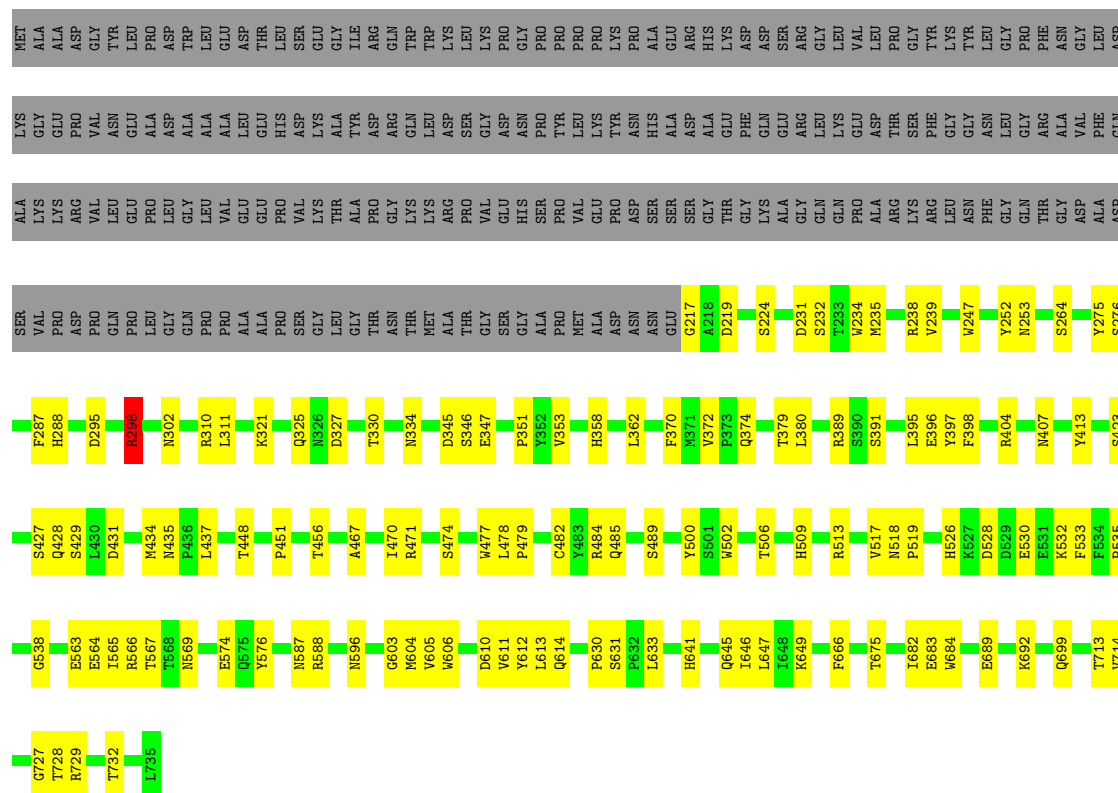
• Molecule 1: Capsid protein VP1

Chain F: 53% 17% 29%





- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



MET	ALA	LYS	VAL	SER	ALA	LYS	VAL	SER	R294	S429	G727	
ALA	LYS	GLY	PRO	VAL	LYS	GLY	PRO	VAL	D295	L430	T728	
ASP	ARG	GLU	ASP	ASP	ASP	D431	ASP	ASP	R298	D431	R729	
GLY	VAL	ASN	PRO	GLN	LEU	M434	GLN	PRO	N302	M434	T732	
LEU	LEU	GLU	LEU	LEU	PRO	N435	LEU	PRO	R310	N435	R733	
PRO	ALA	ALA	PRO	LEU	GLY	L437	ALA	LEU	L311	L437	N734	
ASP	ASP	ASP	GLN	GLY	ASP	T448	ASP	GLY	R310	T448	L735	
TRP	ALA	LEU	ALA	PRO	ALA	P451	ALA	PRO	K321	P451		
LEU	LEU	LEU	LEU	ALA	GLU	Q325	LEU	LEU	Q325	Q325		
ASP	ASP	GLU	GLU	ALA	GLU	N326	ASP	GLU	N326	N326		
THR	THR	HIS	VAL	PRO	THR	D327	THR	THR	D327	T456		
LEU	LEU	ASP	ASP	ASP	ASP	A467	LEU	ASP	T330	A467		
SER	GLY	LYS	GLY	SER	GLY	N587	SER	GLY	T330	N587		
GLY	GLY	LYS	LEU	LEU	LEU	R588	GLY	LEU	T330	R588		
ILE	TYR	ALA	THR	THR	ALA	I470	ILE	THR	N334	I470		
ARG	ASP	TYR	THR	THR	ALA	R471	ARG	THR	N334	R471		
GLN	ASP	ASP	ASN	GLY	PRO	S474	GLN	ASN	T339	S474		
TRP	GLN	GLY	THR	THR	GLY	W477	TRP	THR	D345	W477		
TRP	LEU	LEU	LEU	ALA	LEU	L478	TRP	LEU	S346	L478		
LYS	LEU	LEU	LEU	VAL	LEU	P479	LYS	LEU	E347	P479		
LEU	LEU	LYS	LEU	VAL	LEU	C482	LEU	LEU	P351	C482		
LYS	LYS	ASP	PRO	GLY	PRO	Y483	LYS	PRO	Y352	Y483		
PRO	PRO	GLY	ASP	GLY	PRO	R484	PRO	ASP	V353	R484		
PRO	PRO	PRO	PRO	GLY	PRO	Q485	PRO	PRO	H358	Q485		
PRO	PRO	PRO	PRO	GLY	PRO	S489	PRO	PRO	P351	S489		
PRO	PRO	LYS	PRO	GLY	PRO	Y500	PRO	PRO	L362	Y500		
LYS	LYS	TYR	ASN	ASP	ASN	W502	LYS	ASN	F370	W502		
ALA	ALA	ASP	ALA	GLY	ALA	T506	ALA	ASP	M371	T506		
ARG	ARG	ALA	ASP	ALA	ASP	Q645	ARG	ALA	V372	Q645		
HIS	HIS	GLY	ALA	GLY	GLY	I646	HIS	GLY	P373	I646		
LYS	LYS	THR	GLY	THR	THR	L647	LYS	THR	Q374	L647		
ASP	ASP	PHE	GLY	ASP	ASP	K649	ASP	PHE	T379	K649		
GLY	GLY	GLY	GLY	GLY	GLY	F666	GLY	GLY	L380	F666		
ASP	ASP	LEU	LEU	LEU	LEU	T675	ASP	LEU	S391	T675		
ARG	ARG	LYS	VAL	GLY	VAL	I682	ARG	VAL	L395	I682		
LEU	LEU	LEU	LEU	LEU	LEU	E683	LEU	LEU	E396	E683		
LYS	LYS	TYR	GLY	TYR	TYR	W684	LYS	TYR	Y397	W684		
TYR	TYR	PHE	GLY	PHE	PHE	E689	TYR	PHE	F398	E689		
GLY	GLY	GLY	GLY	GLY	GLY	K692	GLY	GLY	R404	K692		
LYS	LYS	GLY	GLY	GLY	GLY	T701	LYS	GLY	N253	T701		
TYR	TYR	GLY	GLY	GLY	GLY	T713	TYR	GLY	S264	T713		
LEU	LEU	GLY	GLY	GLY	GLY	V714	LEU	GLY	Y275	V714		
ASN	ASN	ASN	ASN	ASN	ASN		ASN	ASN	S276			
PHE	PHE	GLY	GLY	GLY	GLY		PHE	GLY	Y276			
PRO	PRO	GLY	GLY	GLY	GLY		PRO	GLY	F287			
GLY	GLY	GLY	GLY	GLY	GLY		GLY	GLY	H288			
ASN	ASN	GLY	GLY	GLY	GLY		ASN	GLY				
GLY	GLY	GLY	GLY	GLY	GLY		GLY	GLY				
ASP	ASP	GLY	GLY	GLY	GLY		ASP	GLY				

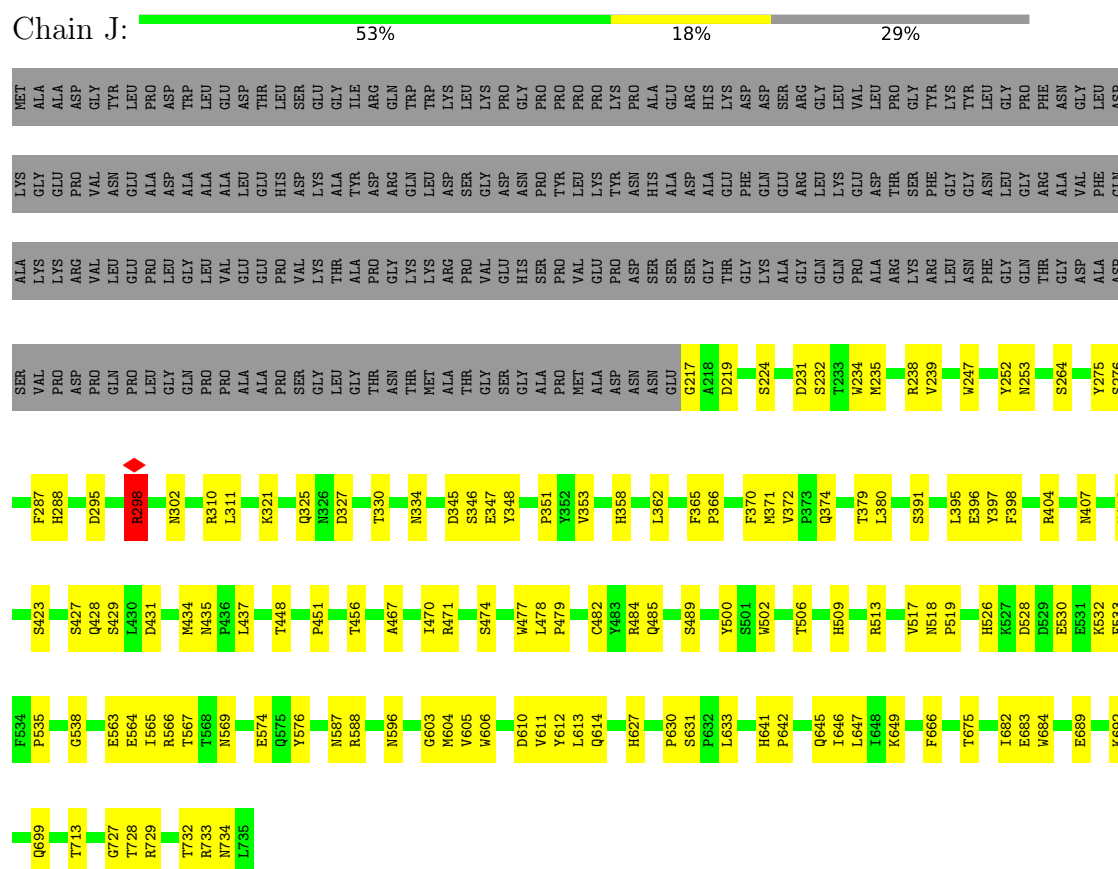
● Molecule 1: Capsid protein VP1



MET	ALA	LYS	VAL	SER	ALA	LYS	VAL	SER	F287	S429	F542	T713
ALA	LYS	GLY	PRO	VAL	LYS	GLY	PRO	VAL	H288	L430	M558	V714
ASP	ARG	GLU	ASP	ASP	ASP	D431	ASP	ASP	D295	D431	G727	T728
GLY	VAL	ASN	PRO	GLN	LEU	M434	GLN	PRO	R298	M434	R729	
LEU	LEU	GLU	LEU	LEU	PRO	N435	LEU	PRO	N302	N435	T732	
PRO	ALA	ALA	PRO	LEU	GLY	L437	ALA	LEU	R310	L437	R733	
ASP	ASP	ASP	GLN	GLY	ASP	T448	ASP	GLY	L311	T448	N734	
TRP	ALA	LEU	ALA	PRO	ALA	P451	ALA	PRO	Q325	P451	L735	
LEU	LEU	LEU	LEU	ALA	GLU	Q325	LEU	LEU	N326	Q325		
ASP	ASP	GLU	GLU	ALA	GLU	D327	ASP	GLU	T330	D327		
THR	THR	HIS	VAL	PRO	THR	A467	THR	THR	T330	A467		
LEU	LEU	ASP	ASP	ASP	ASP	I470	LEU	ASP	T330	I470		
SER	GLY	LYS	GLY	SER	GLY	R471	SER	GLY	T330	R471		
GLY	GLY	LYS	LEU	LEU	LEU	S474	GLY	LEU	D345	S474		
ILE	TYR	ALA	THR	THR	ALA	W477	ILE	THR	E347	W477		
ARG	ASP	TYR	THR	THR	ALA	L478	ARG	THR	P351	L478		
GLN	ASP	ASP	ASN	GLY	PRO	P479	GLN	ASN	Y352	P479		
TRP	GLN	GLY	THR	THR	GLY	C482	TRP	THR	V353	C482		
TRP	LEU	LEU	LEU	VAL	LEU	Y483	TRP	LEU	H358	Y483		
LYS	LYS	ASP	PRO	GLY	PRO	R484	LYS	PRO	L362	R484		
PRO	PRO	GLY	ASP	GLY	PRO	Q485	PRO	ASP	P365	Q485		
PRO	PRO	PRO	PRO	GLY	PRO	S489	PRO	PRO	P366	S489		
PRO	PRO	LYS	PRO	GLY	PRO	Y500	PRO	PRO	F370	Y500		
LYS	LYS	TYR	ASN	ASP	ASN	W502	LYS	ASN	M371	W502		
ALA	ALA	ASP	ALA	GLY	ALA	T506	ALA	ASP	V372	T506		
ARG	ARG	ALA	ASP	ALA	ASP	Q645	ARG	ALA	P373	Q645		
HIS	HIS	GLY	ALA	GLY	GLY	I646	HIS	GLY	Q374	I646		
LYS	LYS	THR	GLY	THR	THR	L647	LYS	THR	T379	L647		
ASP	ASP	PHE	GLY	ASP	ASP	K649	ASP	PHE	L380	K649		
GLY	GLY	GLY	GLY	GLY	GLY	F666	GLY	GLY	S391	F666		
ASP	ASP	LEU	LEU	LEU	LEU	T675	ASP	LEU	L395	T675		
ARG	ARG	LYS	VAL	GLY	VAL	I682	ARG	VAL	E396	I682		
LEU	LEU	LEU	LEU	LEU	LEU	E683	LEU	LEU	Y397	E683		
LYS	LYS	TYR	GLY	TYR	TYR	W684	LYS	TYR	F398	W684		
TYR	TYR	PHE	GLY	PHE	PHE	E689	TYR	PHE	R404	E689		
GLY	GLY	GLY	GLY	GLY	GLY	K692	GLY	GLY	N253	K692		
LYS	LYS	GLY	GLY	GLY	GLY	T701	LYS	GLY	S264	T701		
TYR	TYR	GLY	GLY	GLY	GLY	T713	TYR	GLY	Y275	T713		
LEU	LEU	GLY	GLY	GLY	GLY	V714	LEU	GLY	S276	V714		
ASN	ASN	ASN	ASN	ASN	ASN		ASN	ASN				
PHE	PHE	GLY	GLY	GLY	GLY		PHE	GLY				
PRO	PRO	GLY	GLY	GLY	GLY		PRO	GLY				
GLY	GLY	GLY	GLY	GLY	GLY		GLY	GLY				
ASN	ASN	GLY	GLY	GLY	GLY		ASN	GLY				
GLY	GLY	GLY	GLY	GLY	GLY		GLY	GLY				
ASP	ASP	GLY	GLY	GLY	GLY		ASP	GLY				

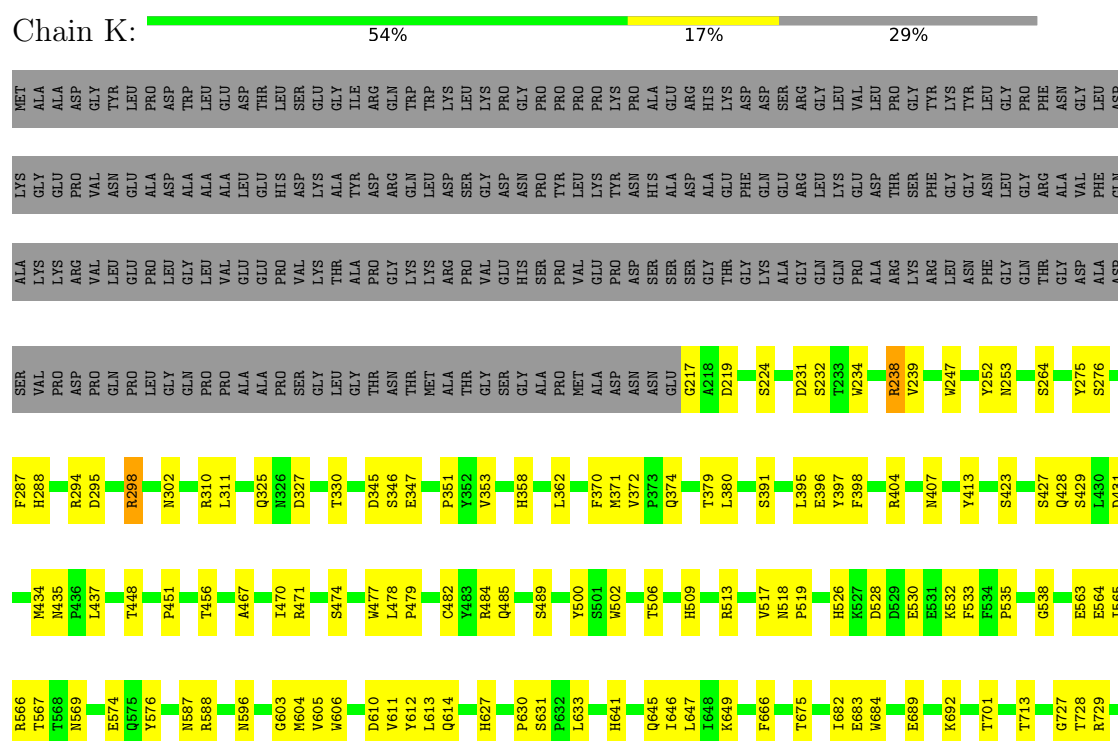
- Molecule 1: Capsid protein VP1

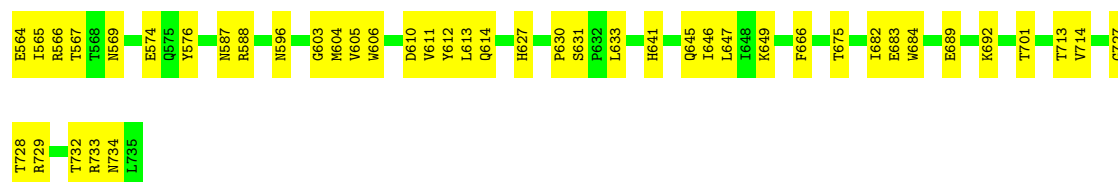
Chain J:



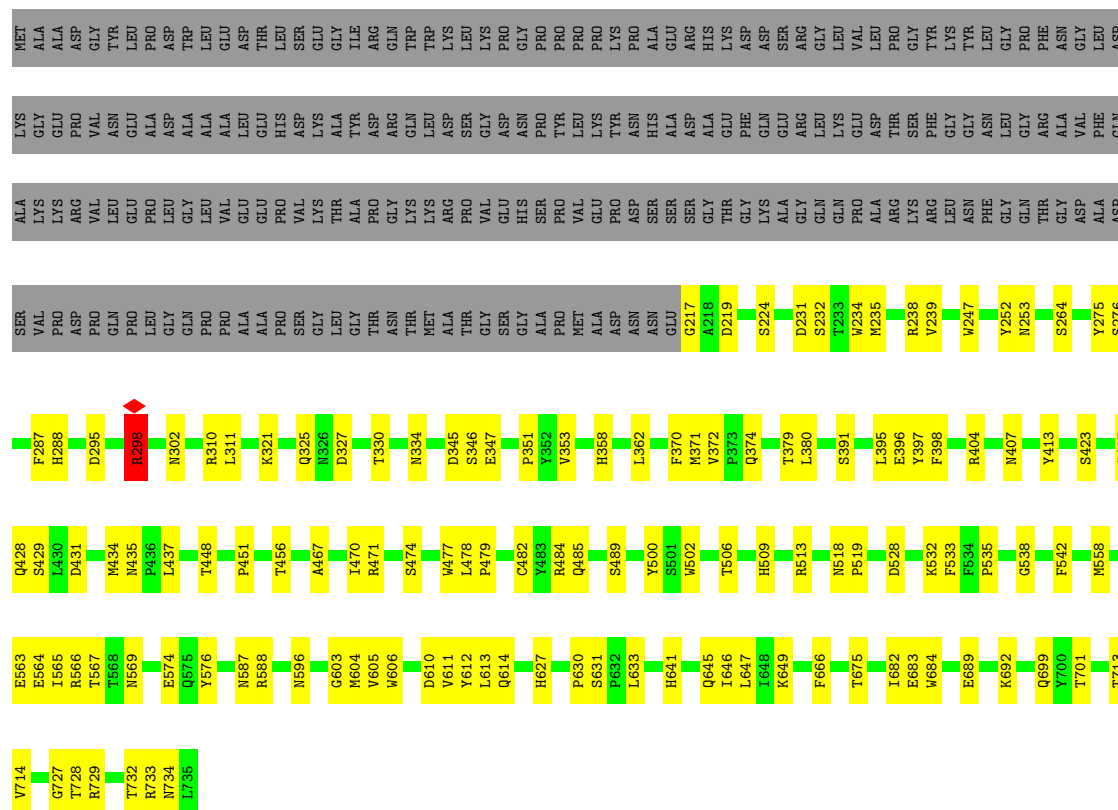
- Molecule 1: Capsid protein VP1

Chain K:

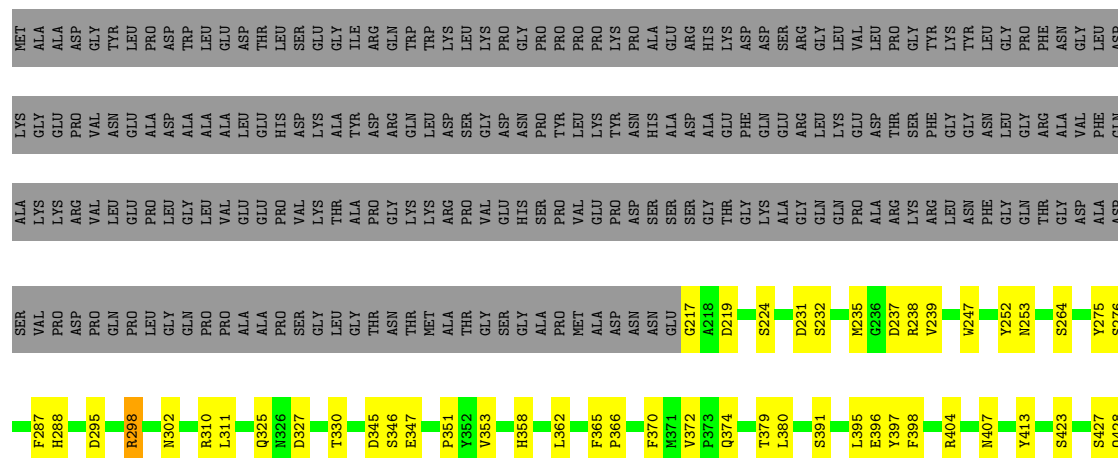


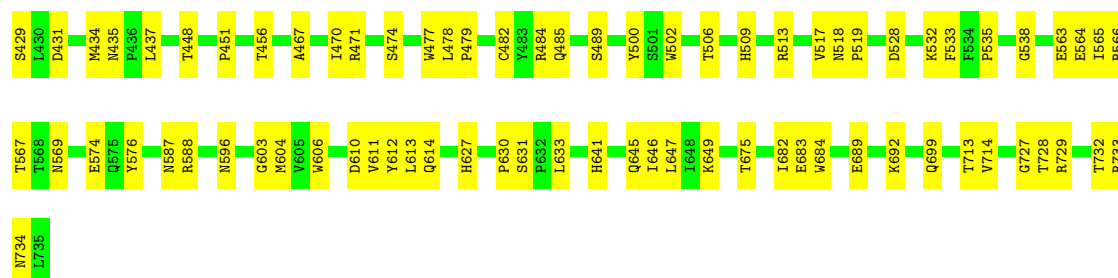


● Molecule 1: Capsid protein VP1

Chain N:  53% 18% 29%

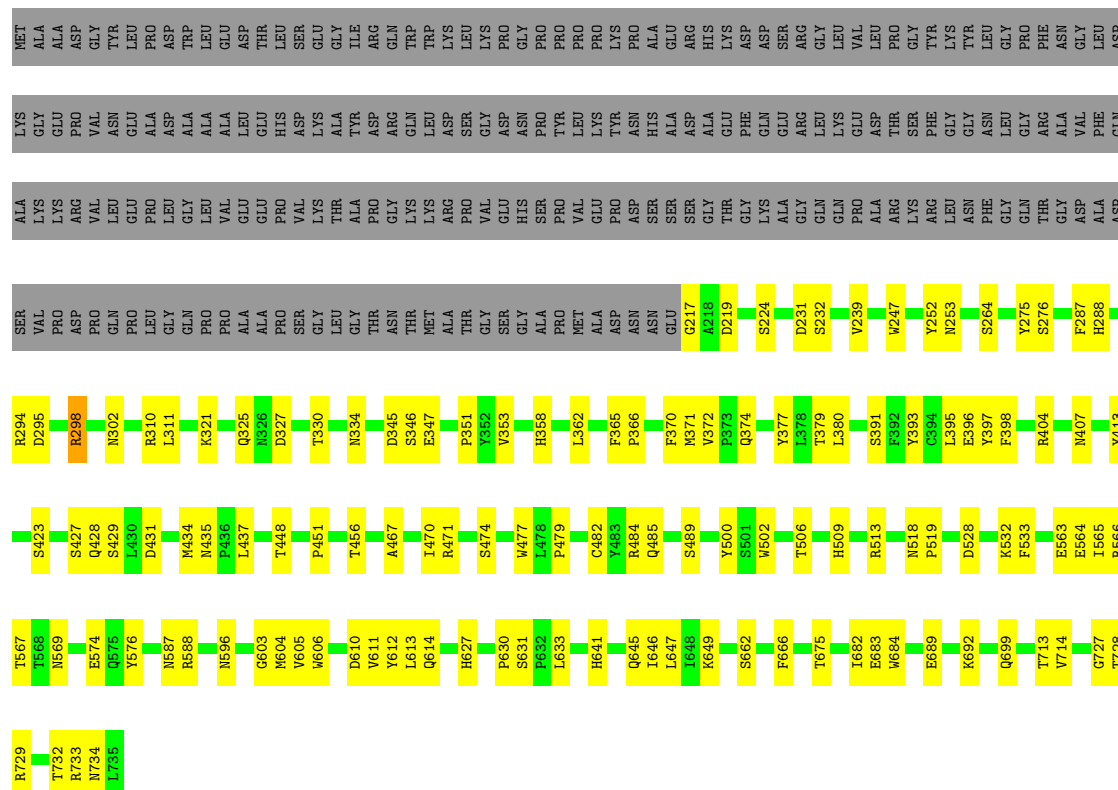
● Molecule 1: Capsid protein VP1

Chain O:  54% 17% 29%



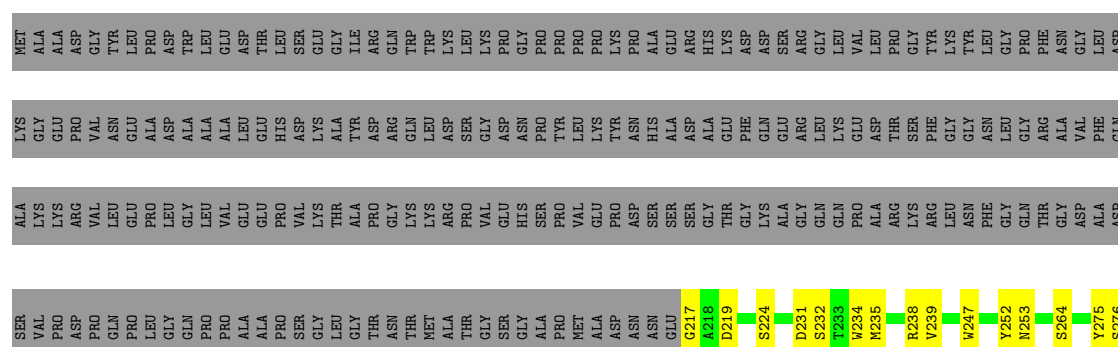
• Molecule 1: Capsid protein VP1

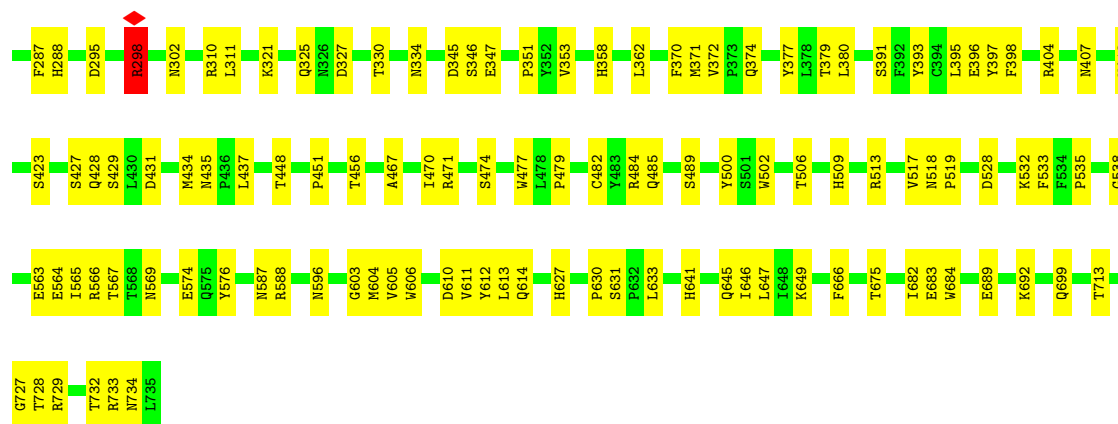
Chain P: 53% 17% 29%



• Molecule 1: Capsid protein VP1

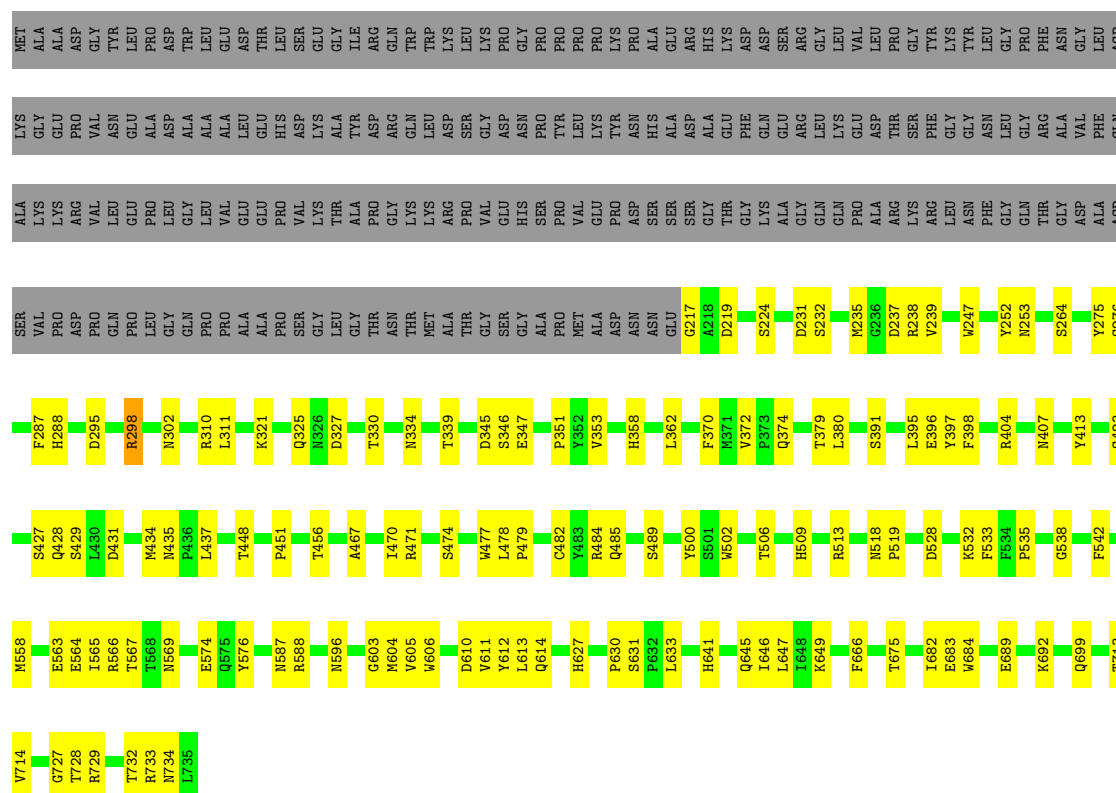
Chain Q: 53% 17% 29%





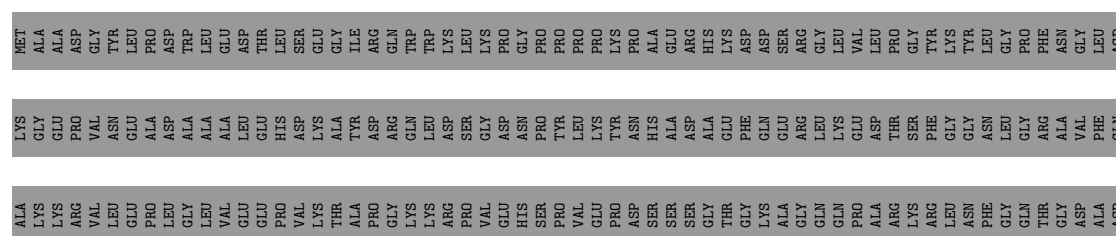
• Molecule 1: Capsid protein VP1

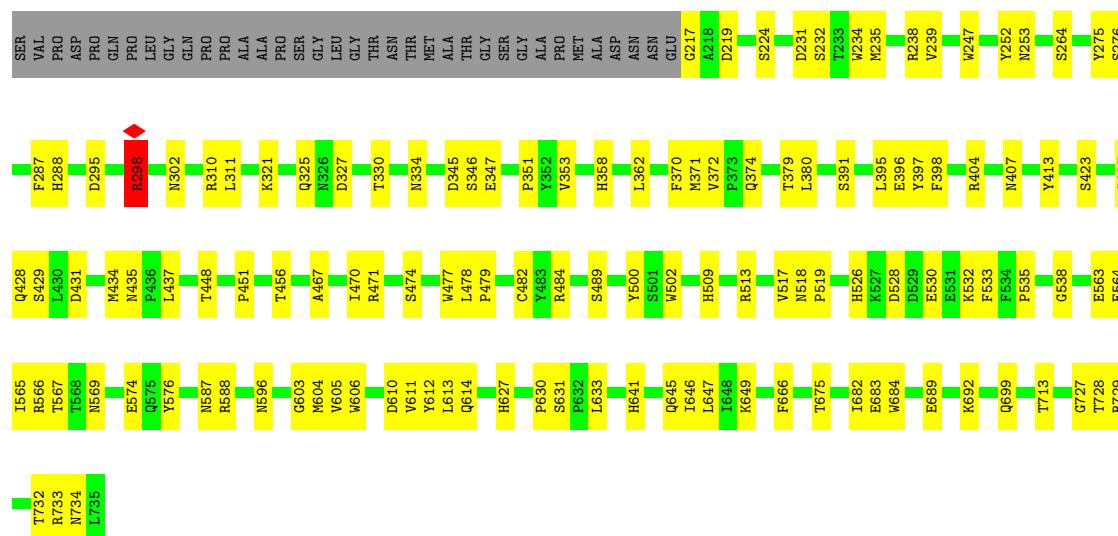
Chain R: 53% 17% 29%



• Molecule 1: Capsid protein VP1

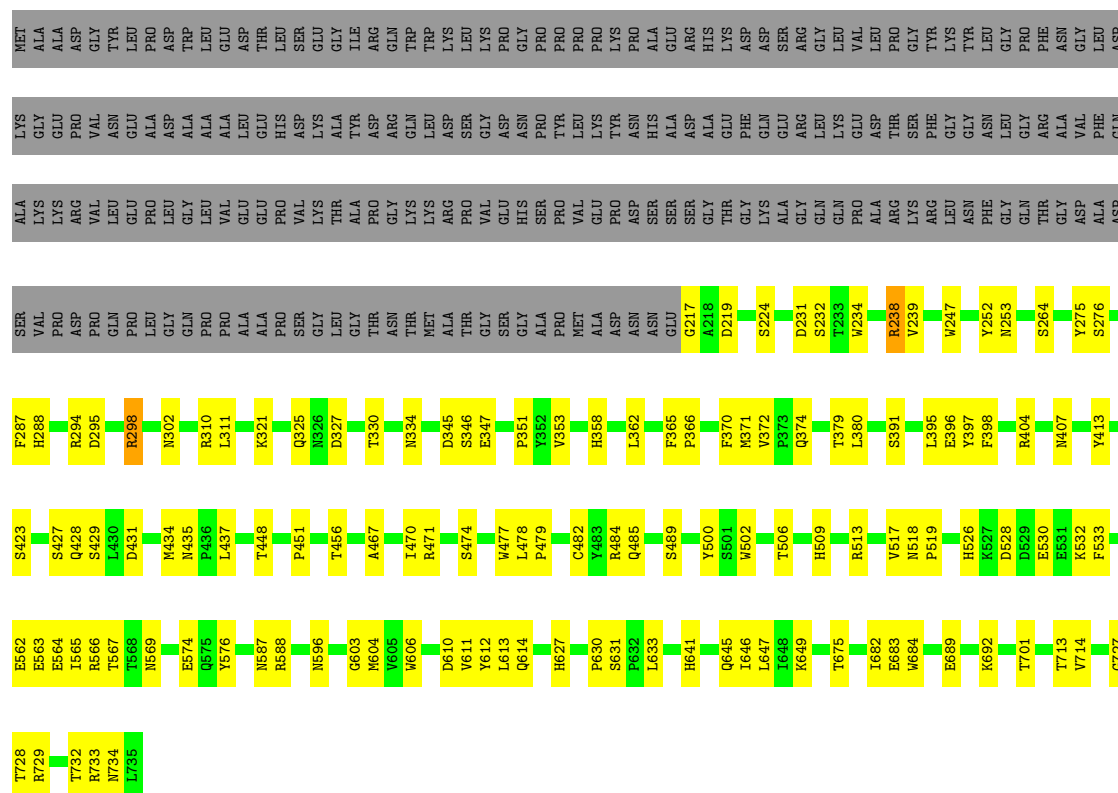
Chain S: 53% 17% 29%





• Molecule 1: Capsid protein VP1

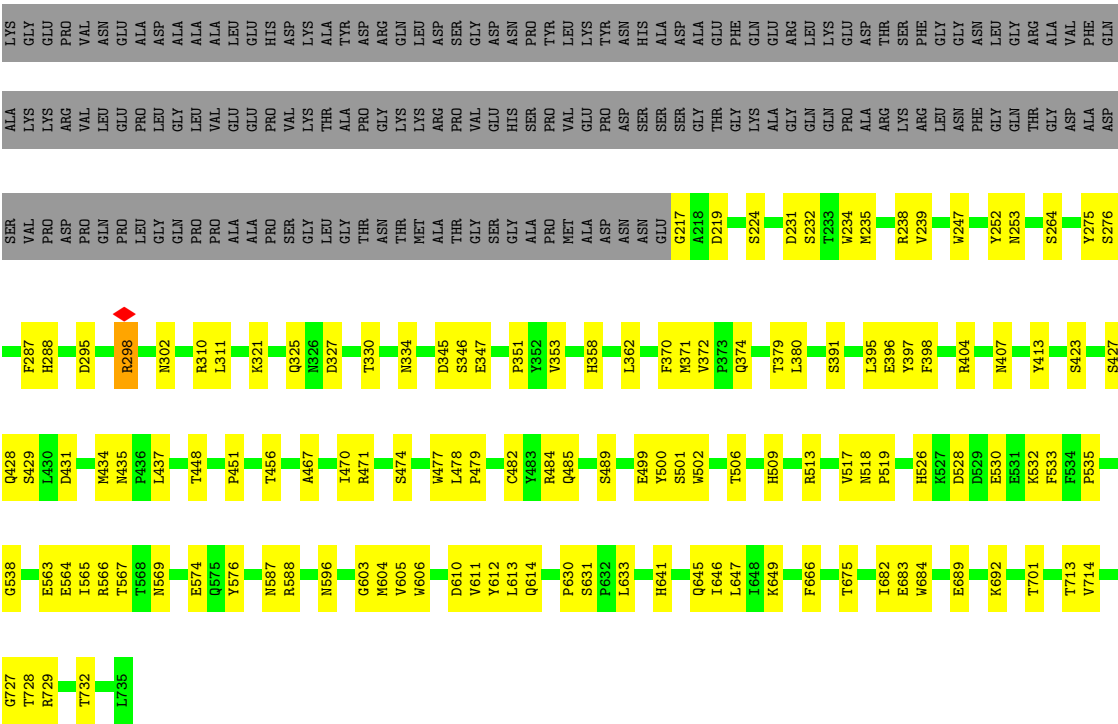
Chain T: 53% 17% 29%



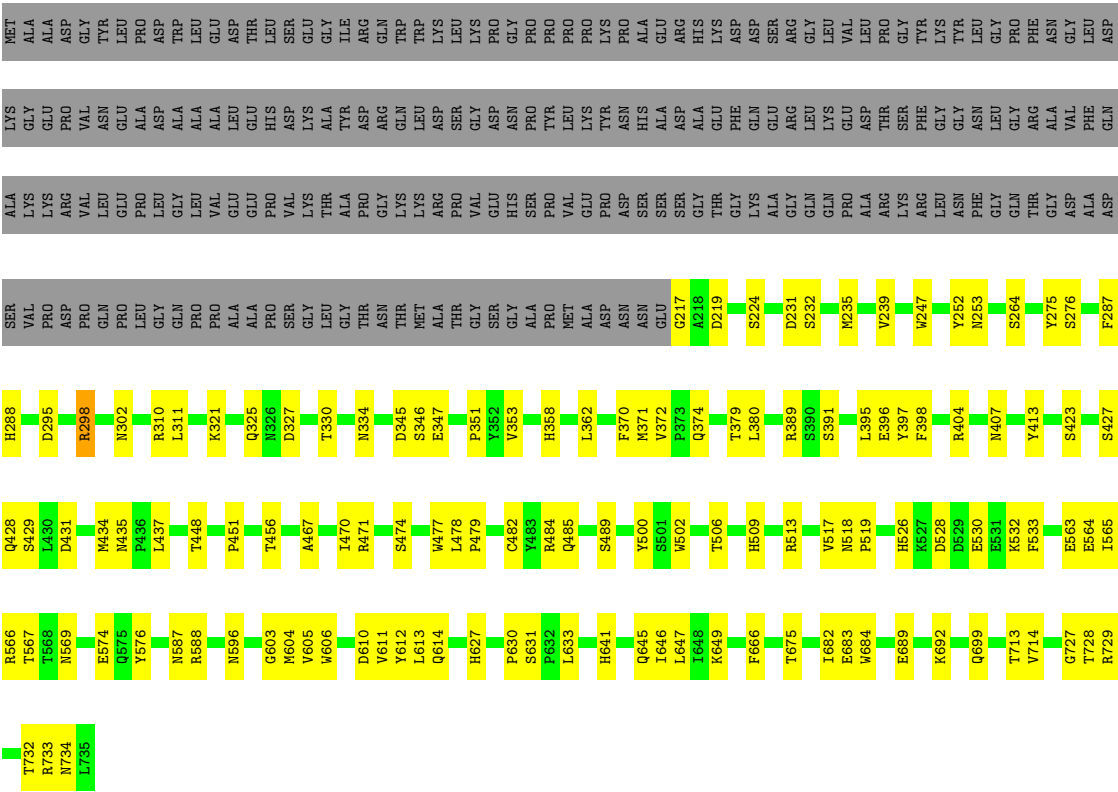
• Molecule 1: Capsid protein VP1

Chain U: 53% 17% 29%





● Molecule 1: Capsid protein VP1



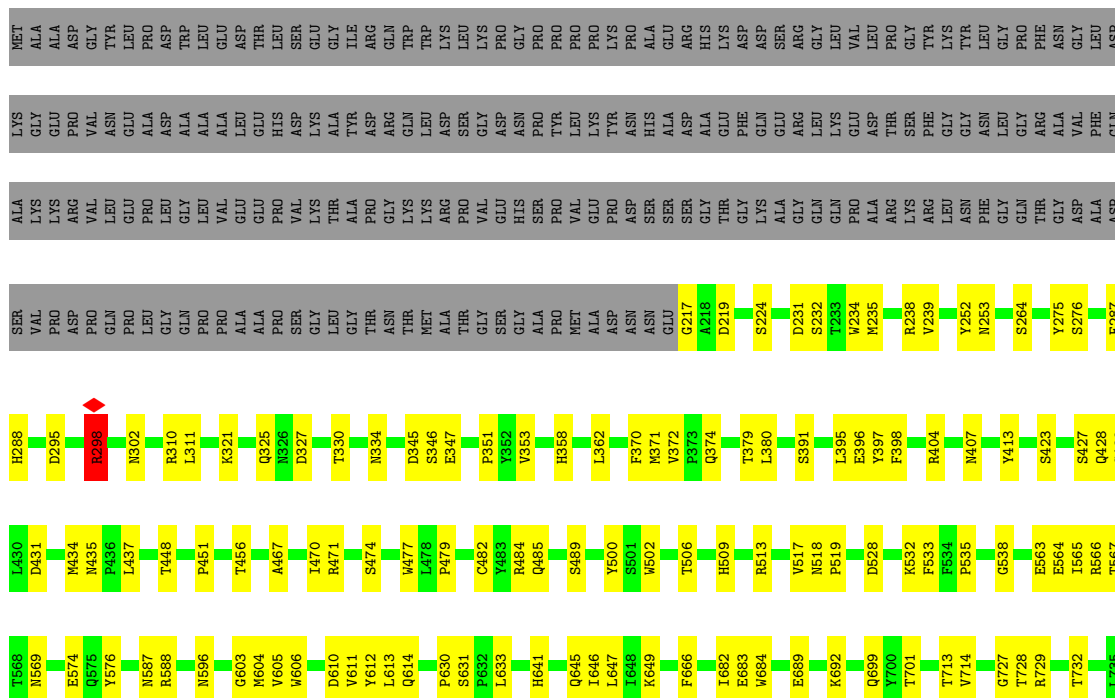
● Molecule 1: Capsid protein VP1

Response	Percentage
Yes	53%
No	17%
Don't know	29%

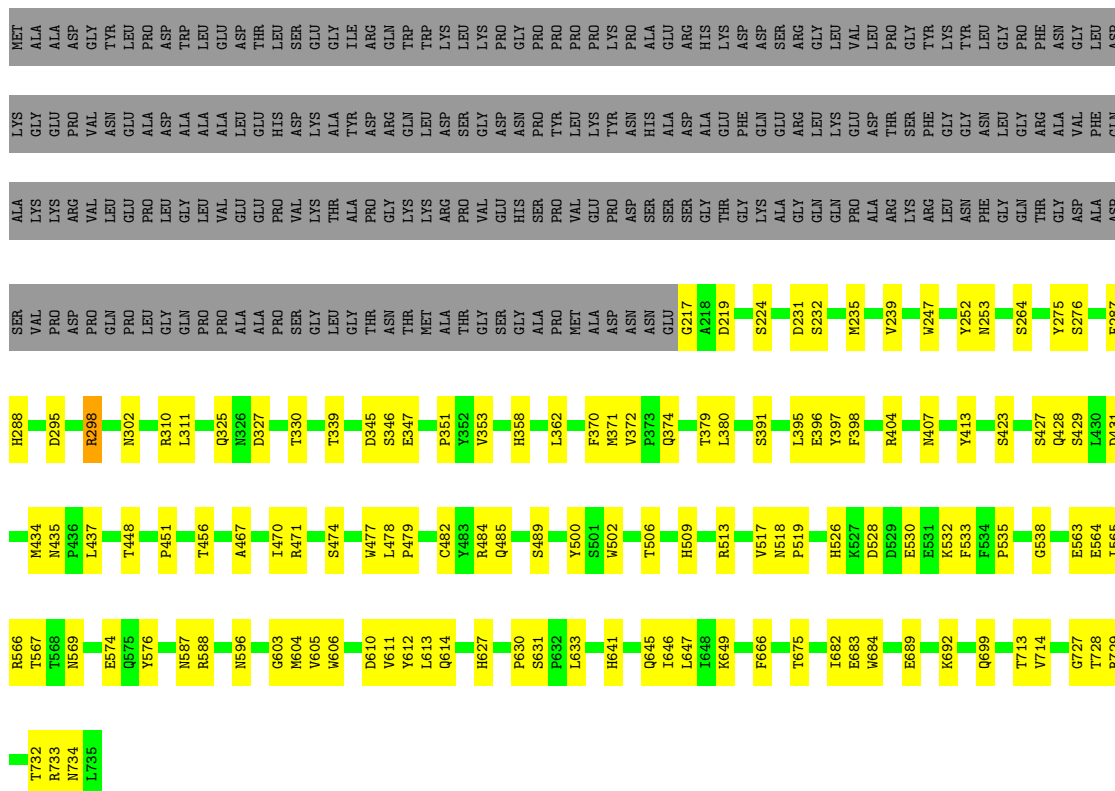


Device Type	Percentage
Smartphone	54%
Tablet	17%
Feature phone	29%



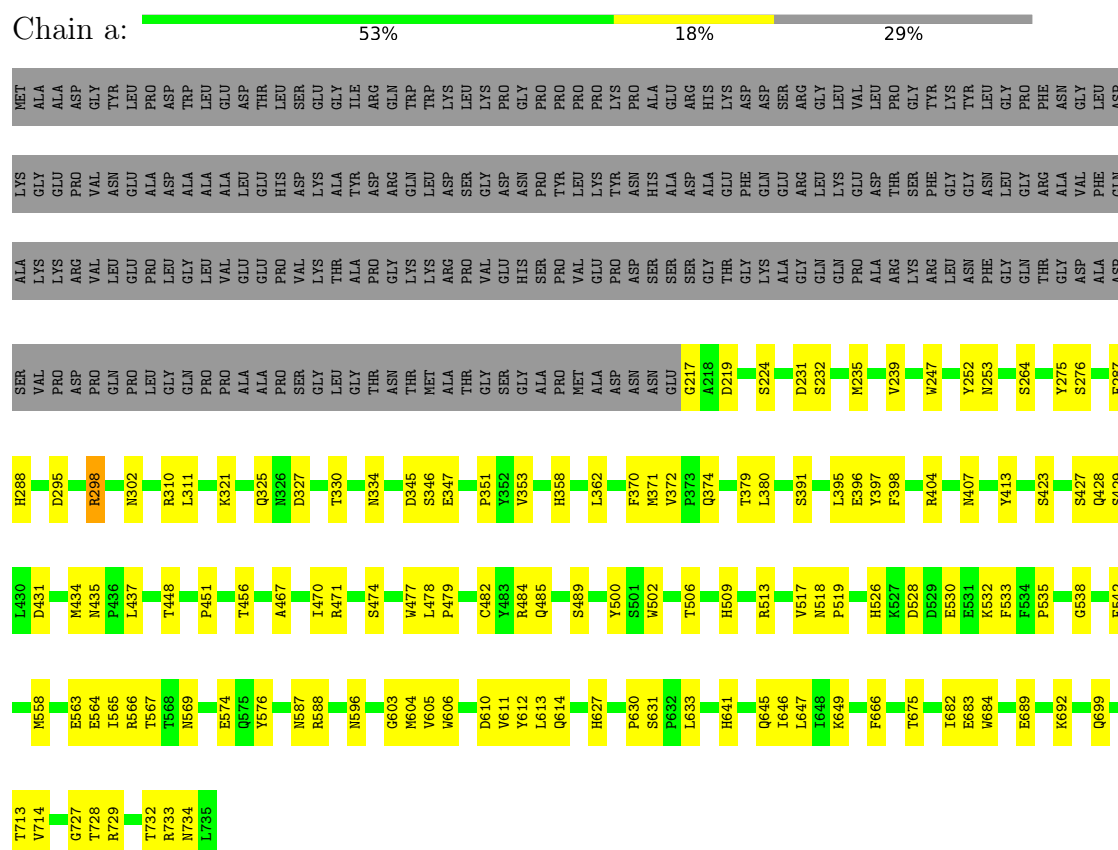


- Molecule 1: Capsid protein VP1



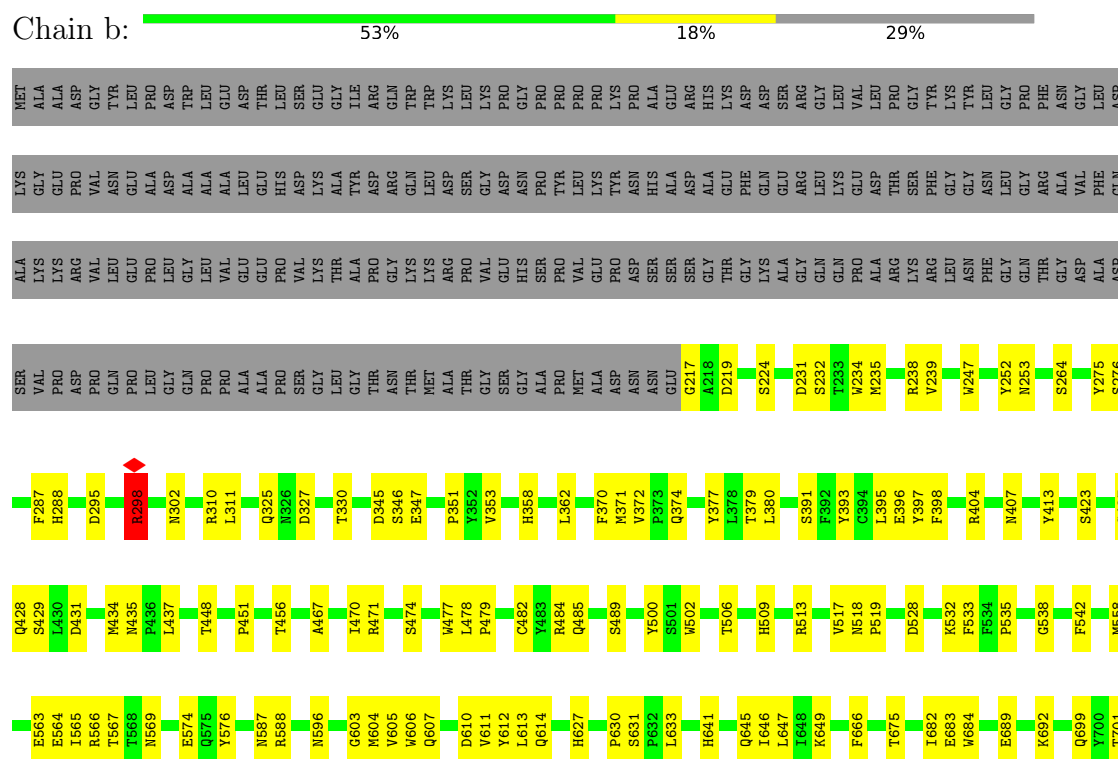
- Molecule 1: Capsid protein VP1

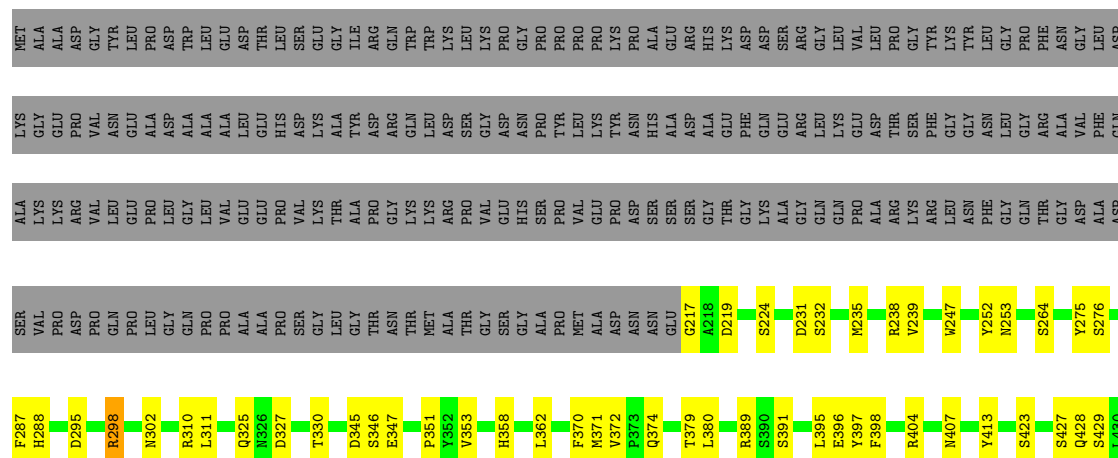
Chain a:

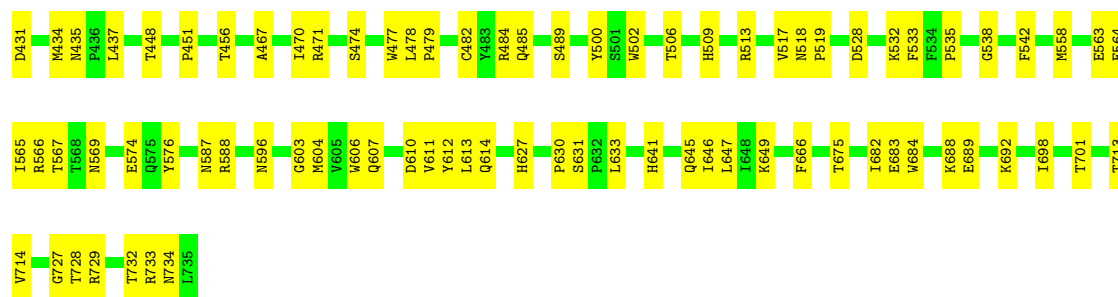


- Molecule 1: Capsid protein VP1

Chain b:

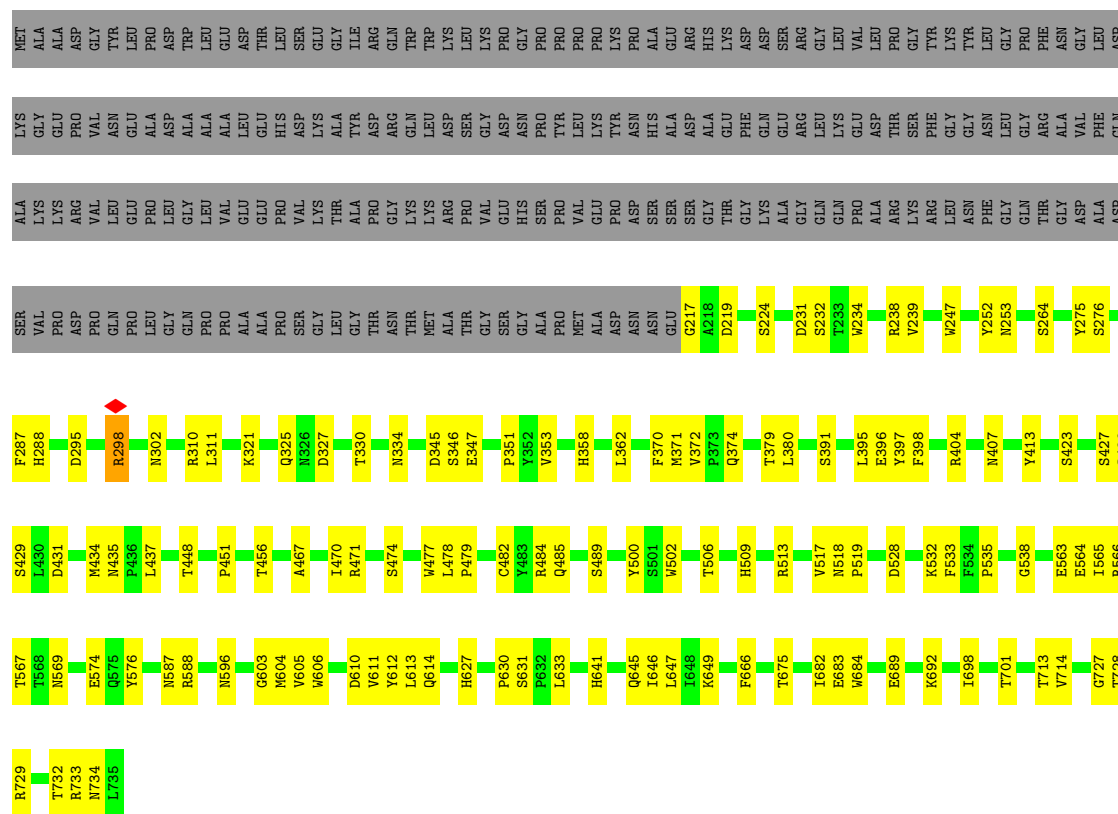






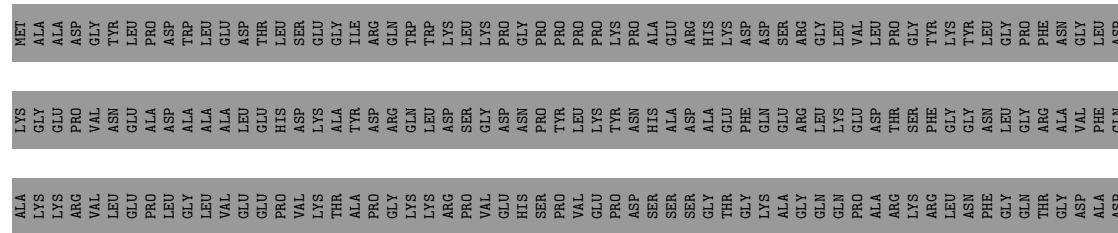
• Molecule 1: Capsid protein VP1

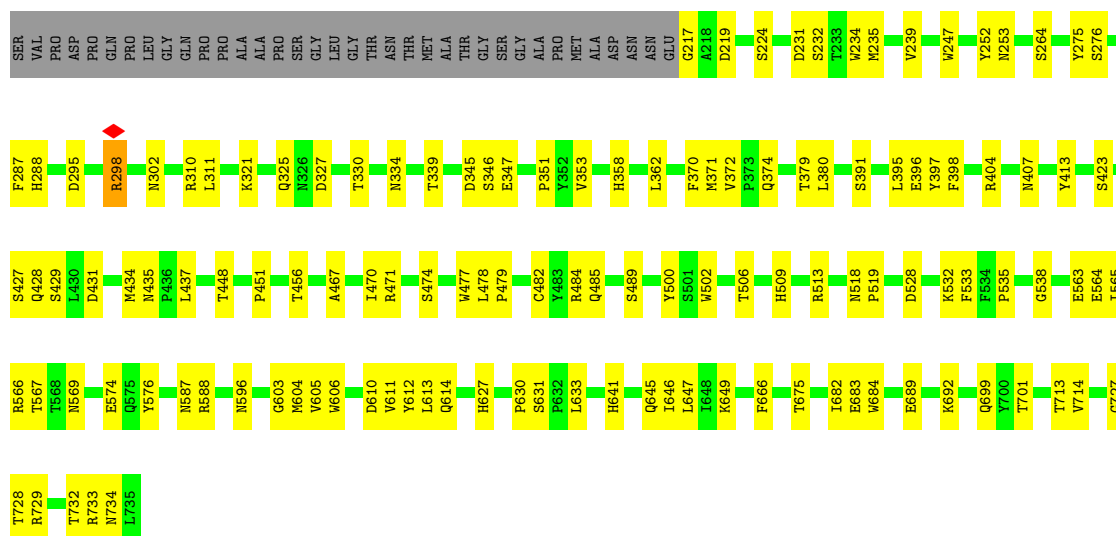
Chain g: 53% 17% 29%



• Molecule 1: Capsid protein VP1

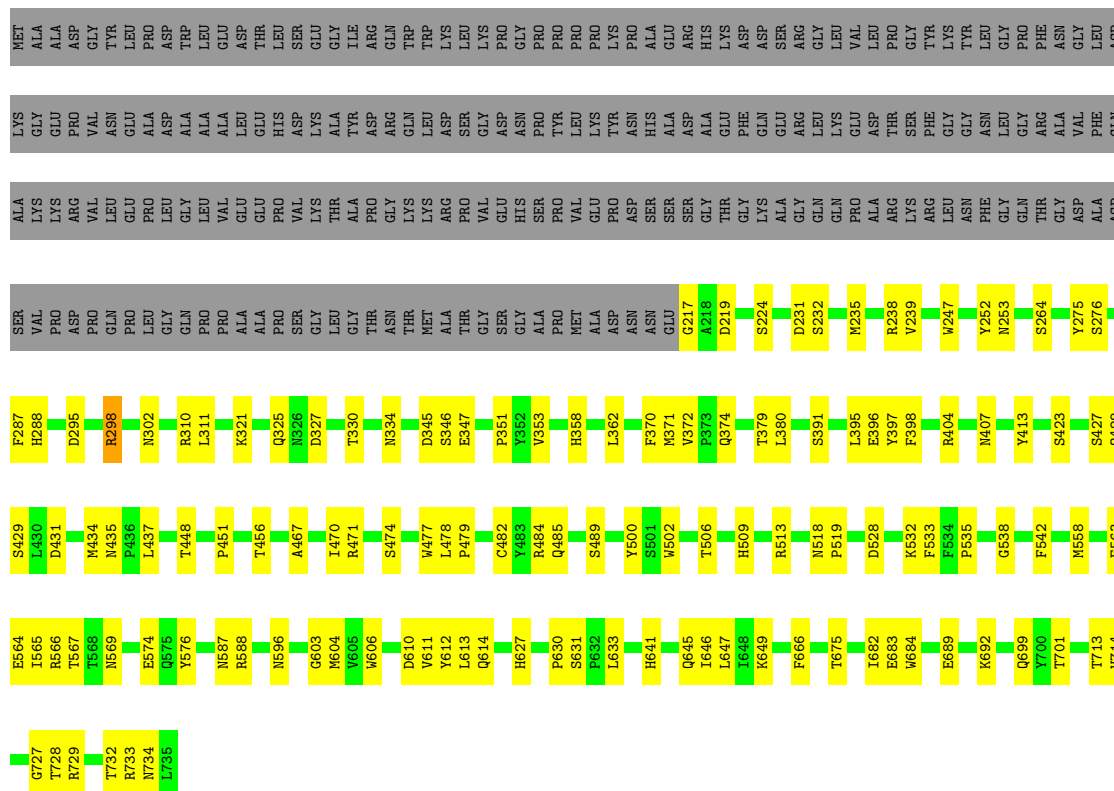
Chain h: 53% 17% 29%





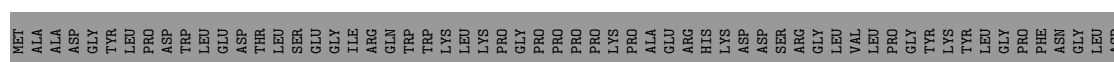
• Molecule 1: Capsid protein VP1

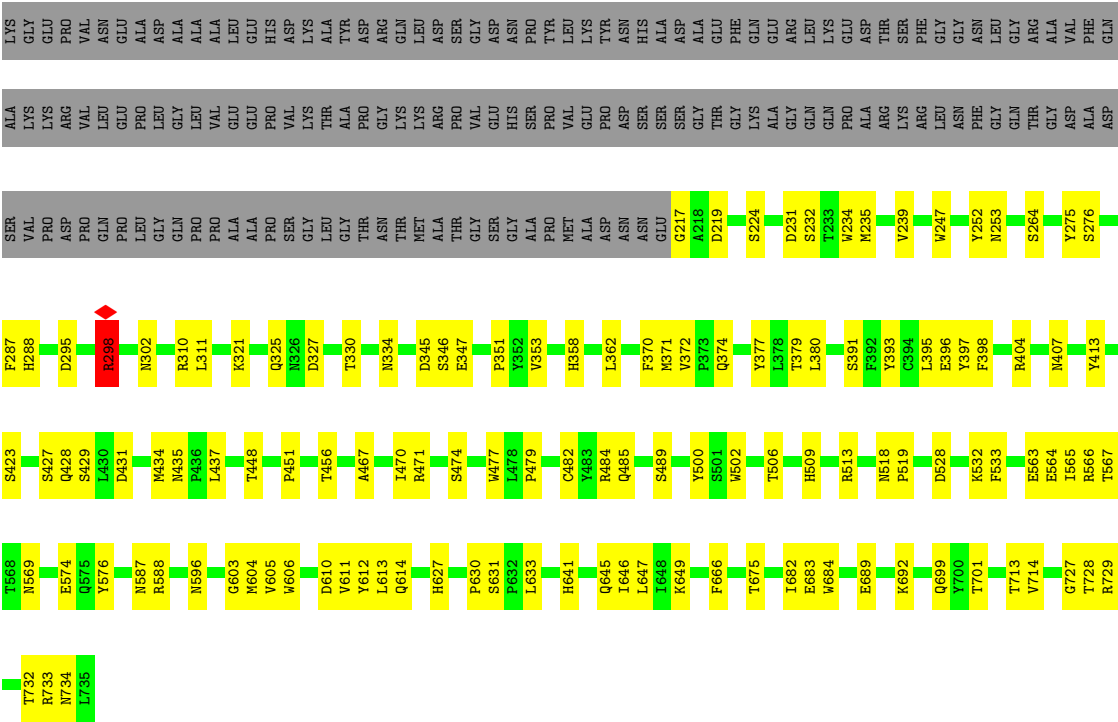
Chain i: 53% 17% 29%



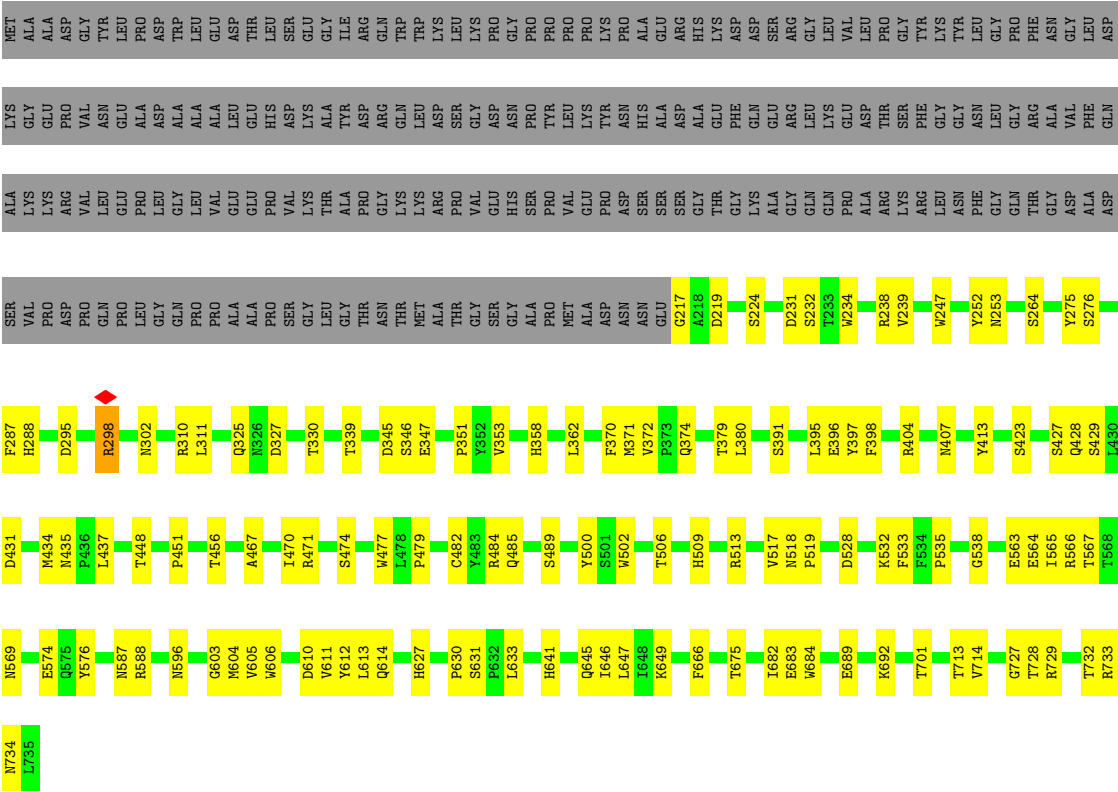
• Molecule 1: Capsid protein VP1

Chain j: 53% 17% 29%





• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

App Type	Percentage
Shopping app	53%
Social media app	18%
Productivity app	29%



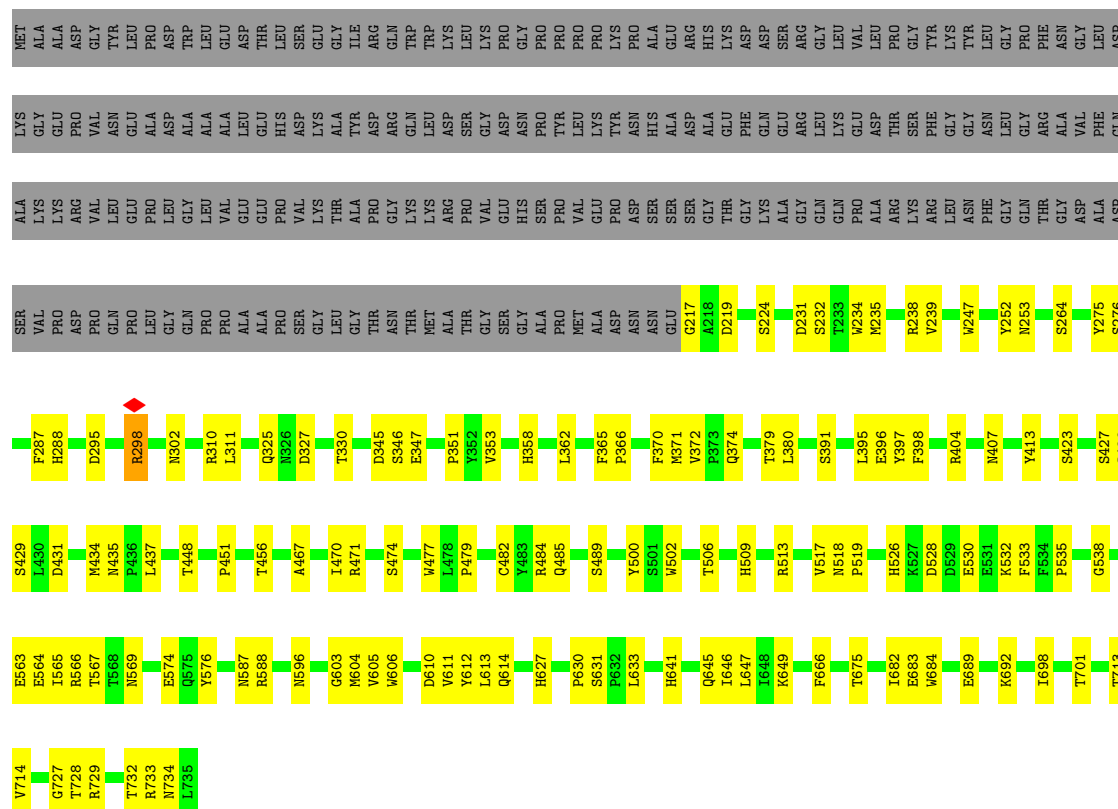
Response	Percentage
Yes	53%
No	18%
Don't know	29%





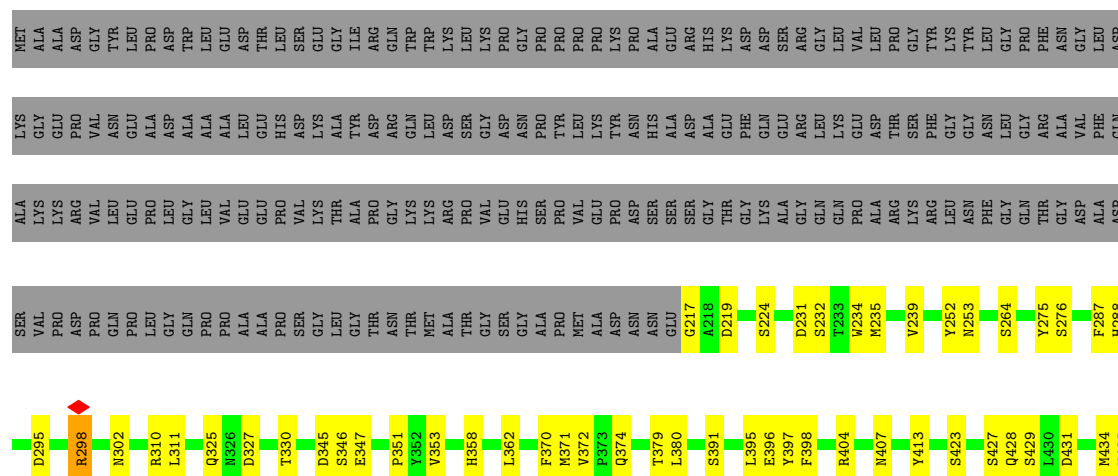
● Molecule 1: Capsid protein VP1

Chain n: 53% 18% 29%



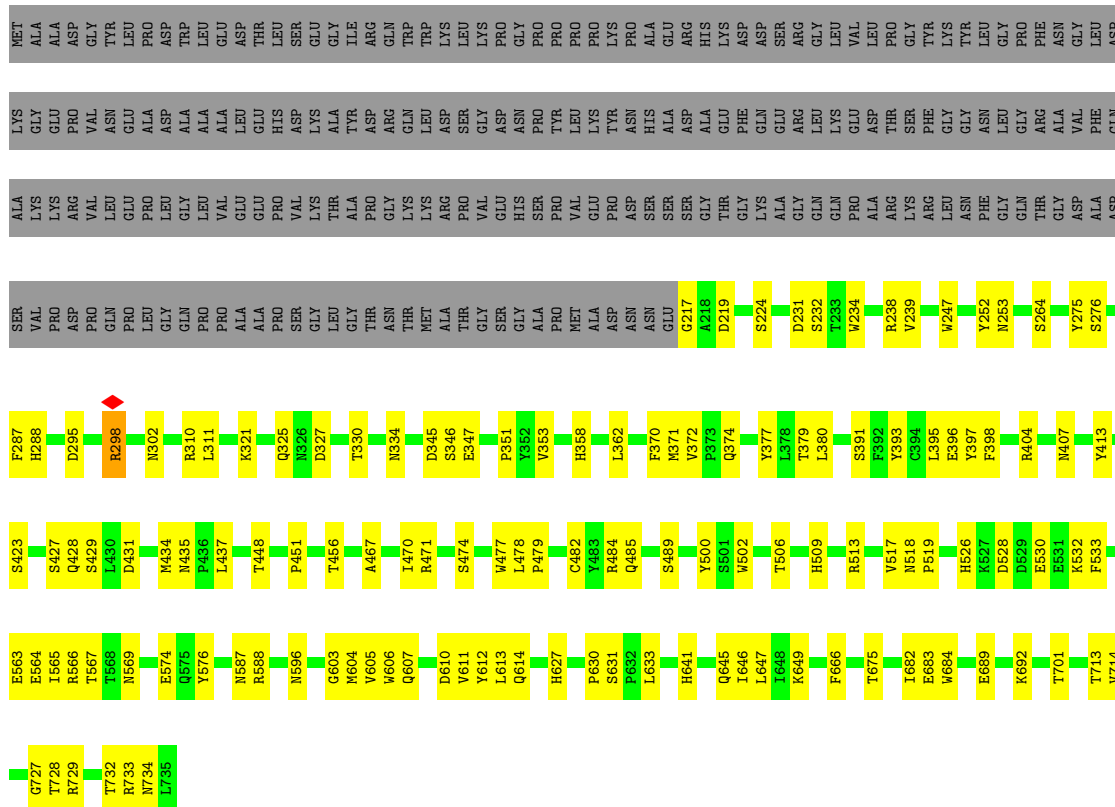
● Molecule 1: Capsid protein VP1

Chain o: 54% 16% 29%

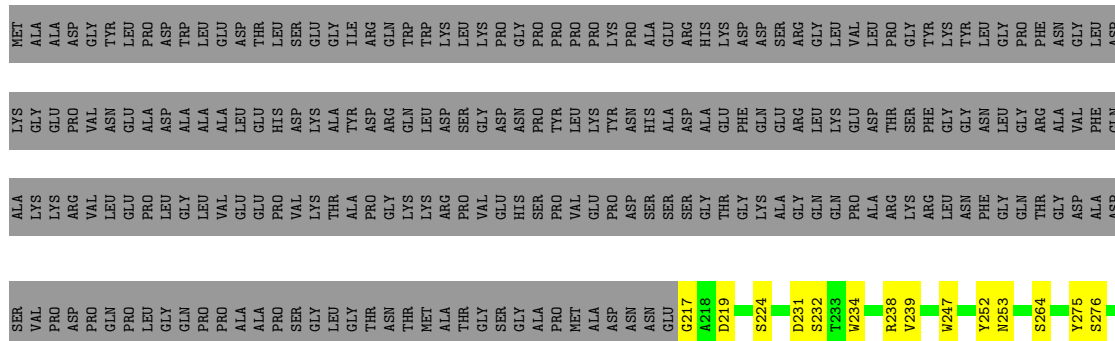


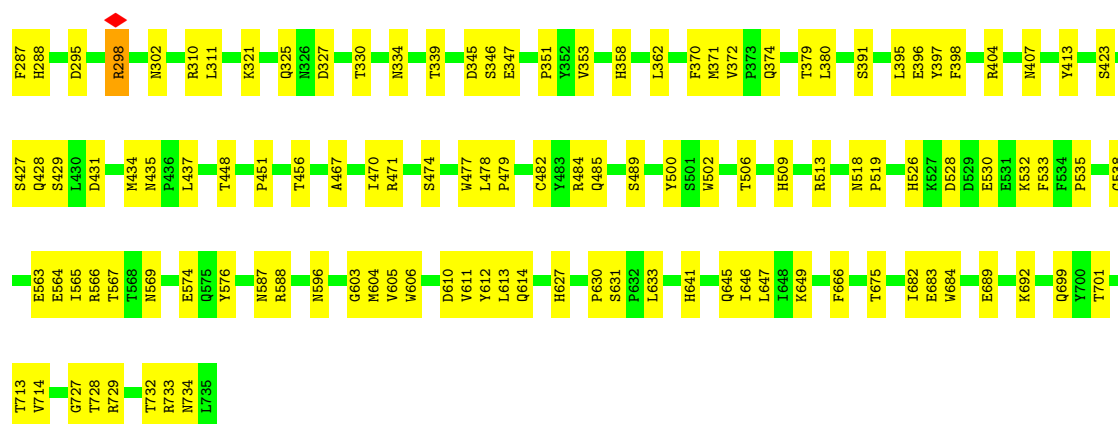


Chain p:

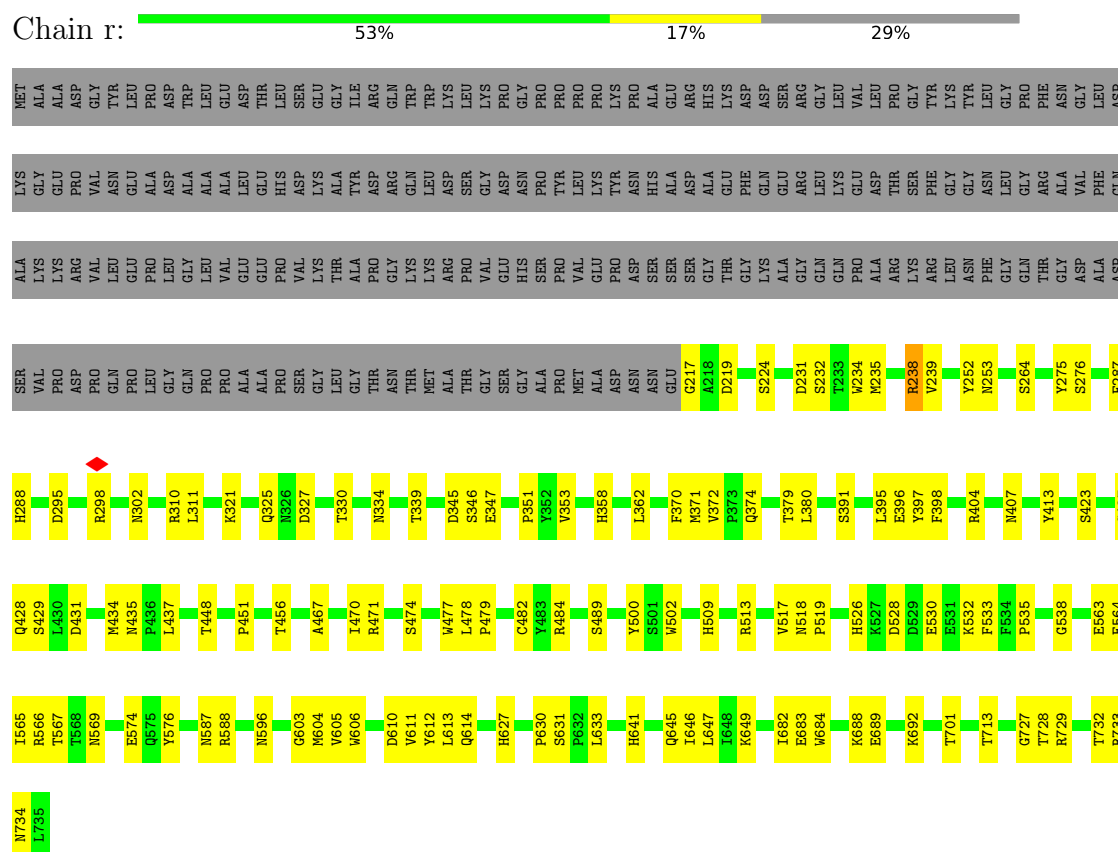


Chain q: 53% 18% 29%

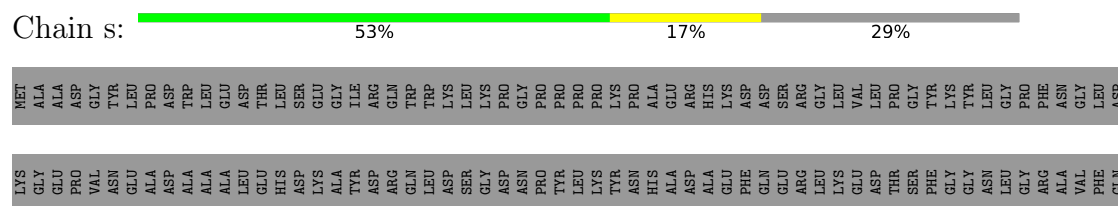


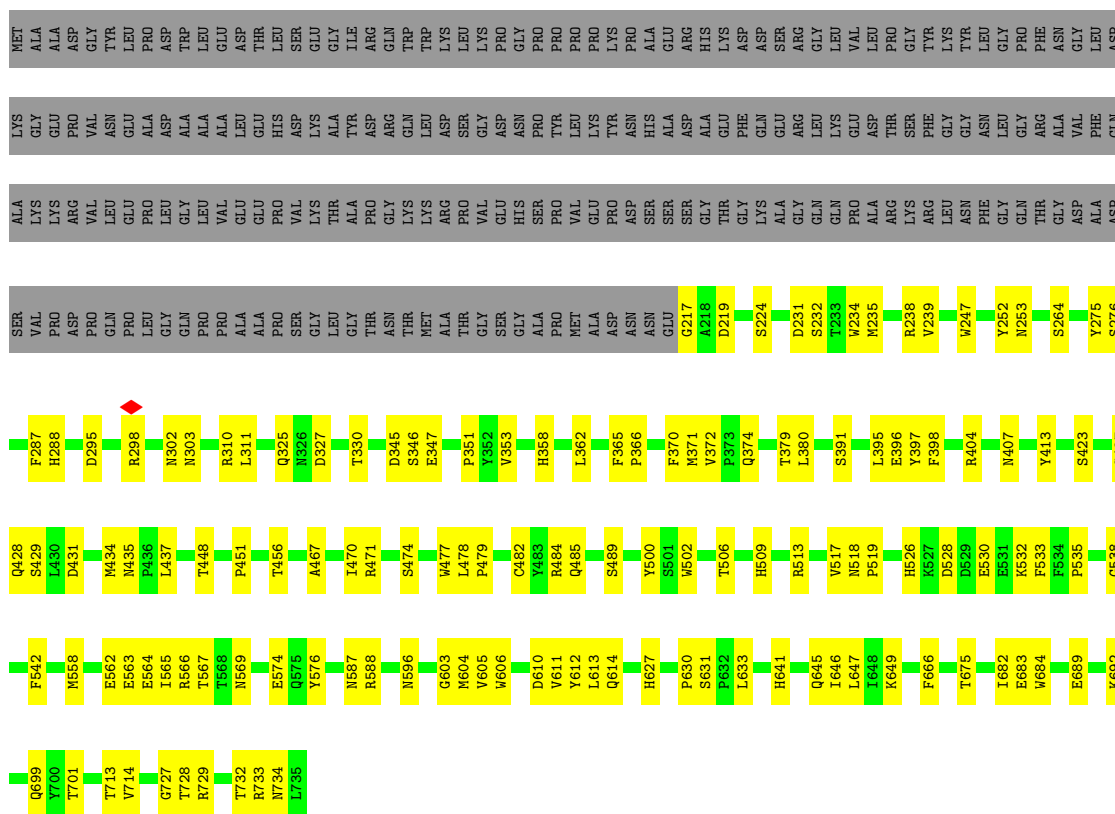


• Molecule 1: Capsid protein VP1

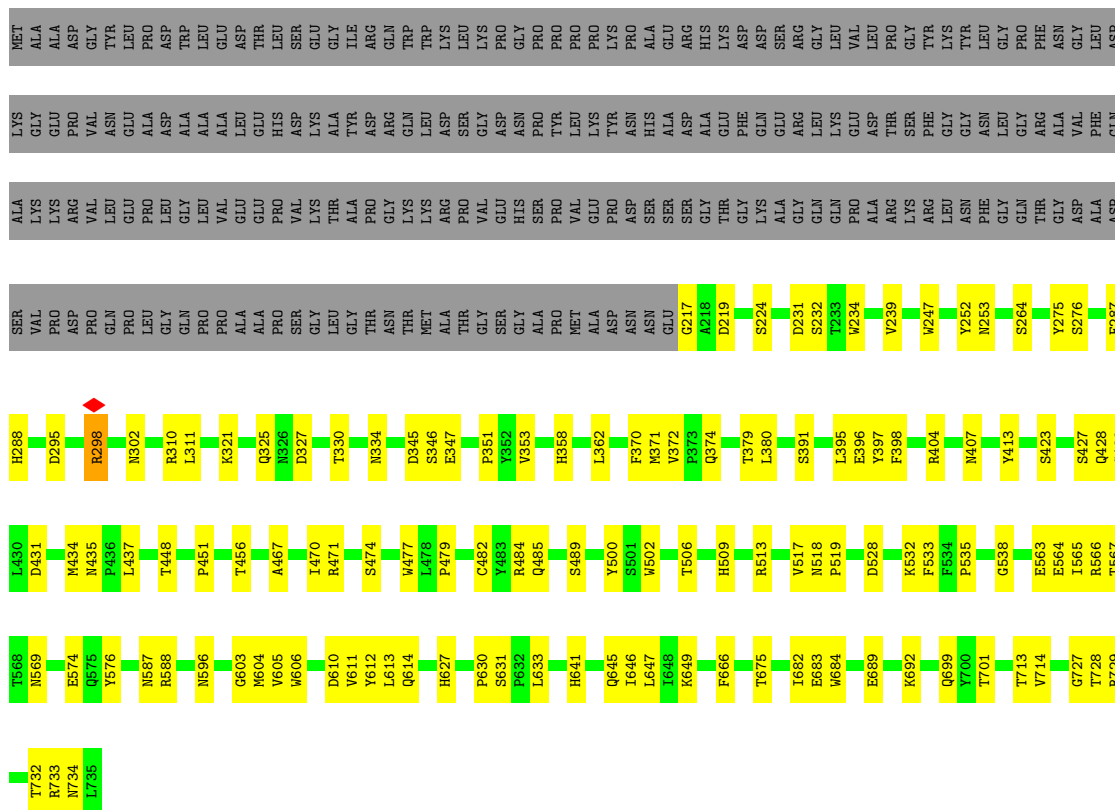


• Molecule 1: Capsid protein VP1

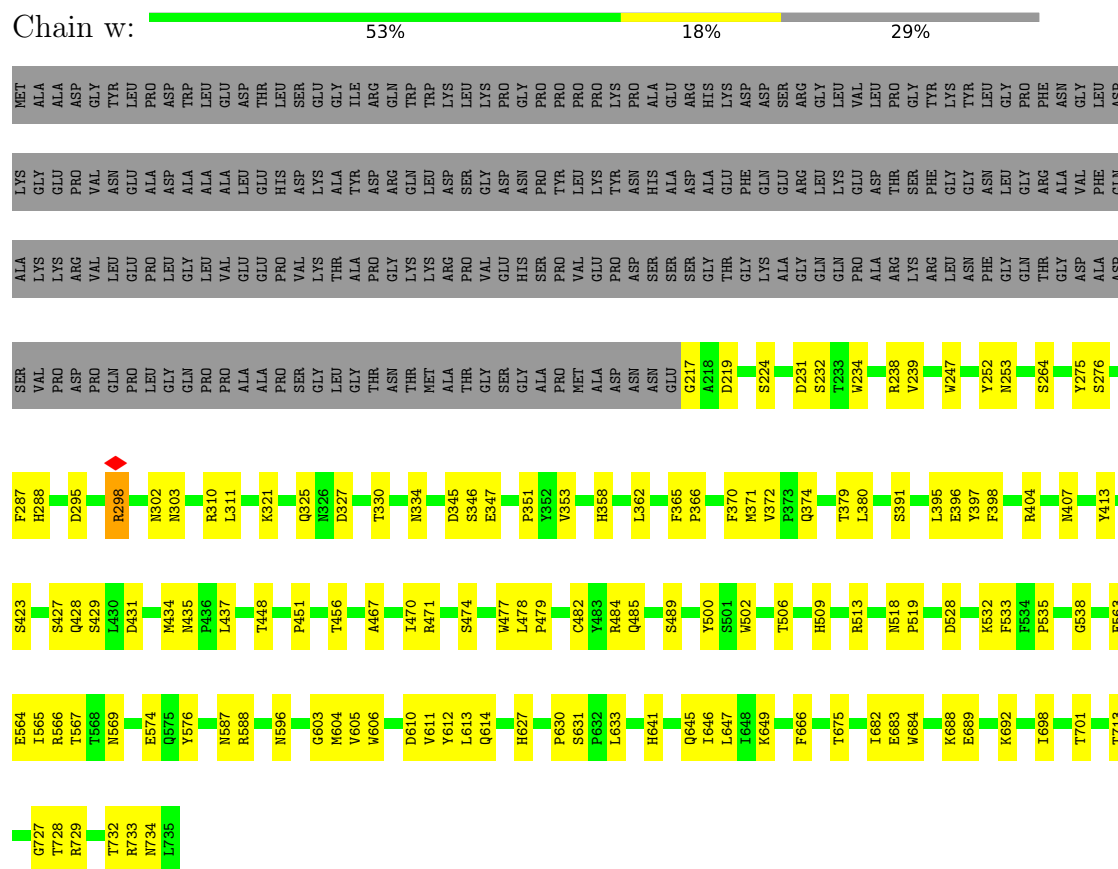




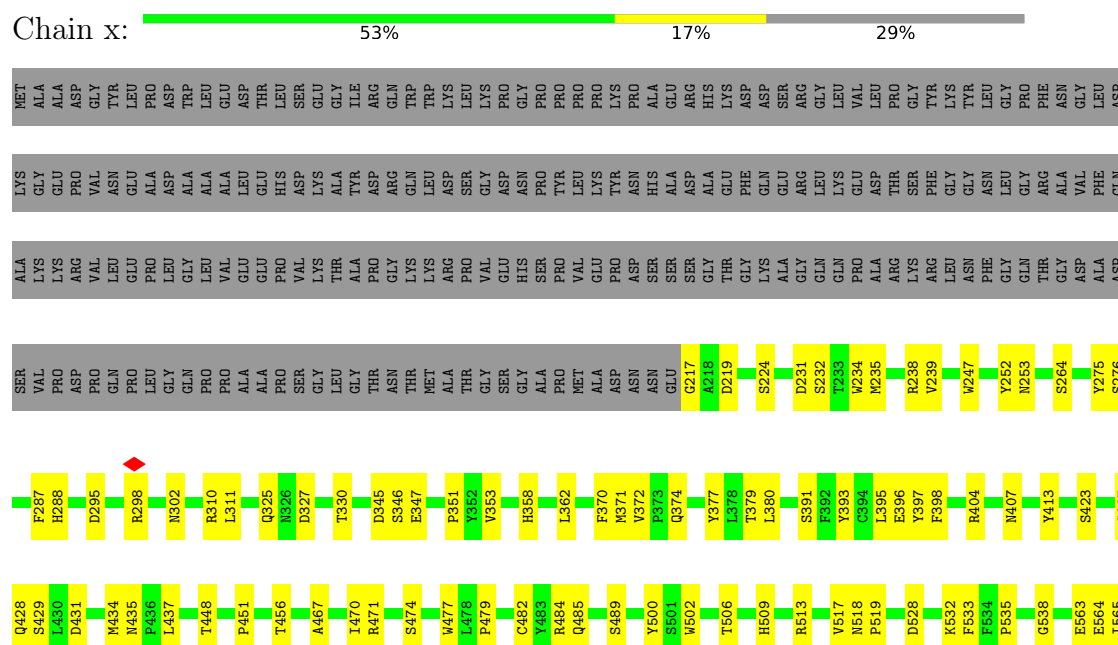
- Molecule 1: Capsid protein VP1

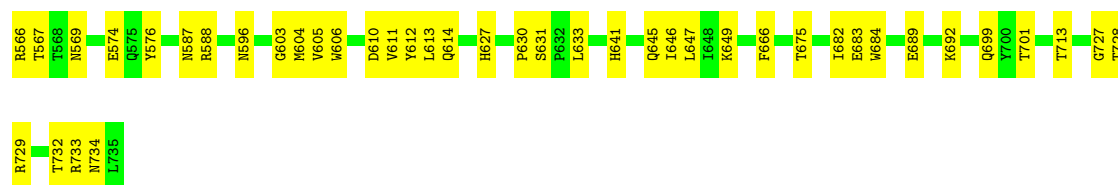


● Molecule 1: Capsid protein VP1

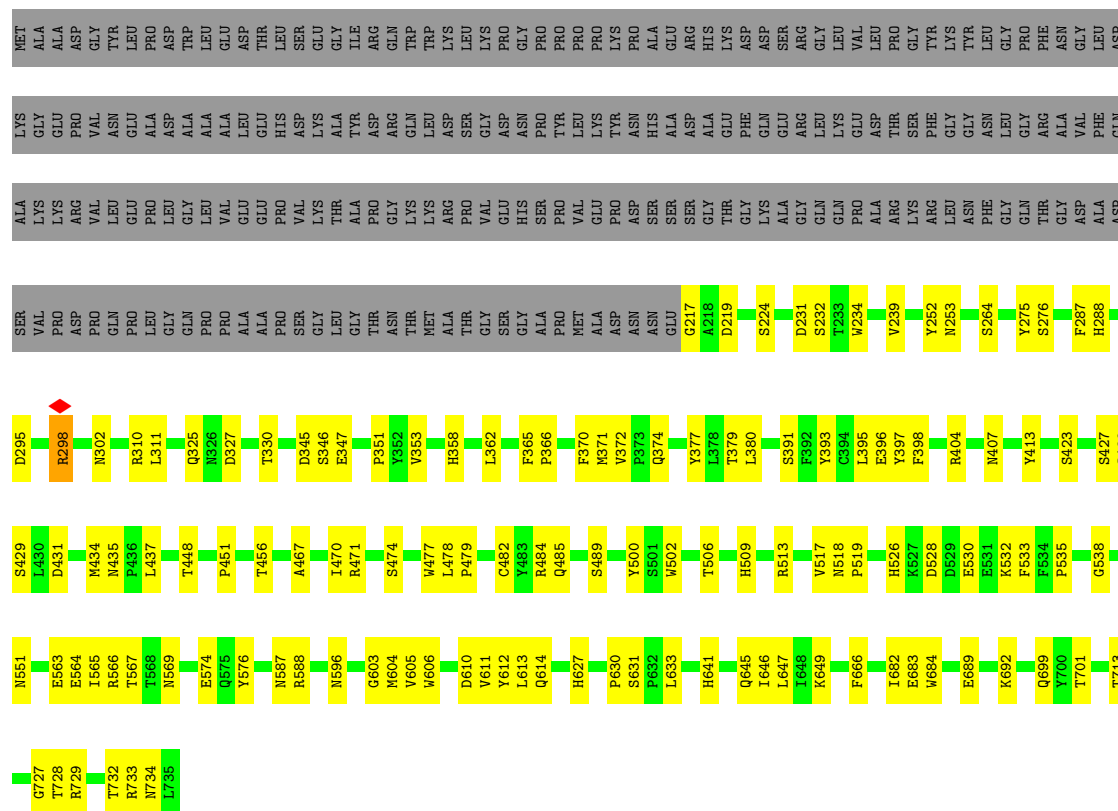


● Molecule 1: Capsid protein VP1

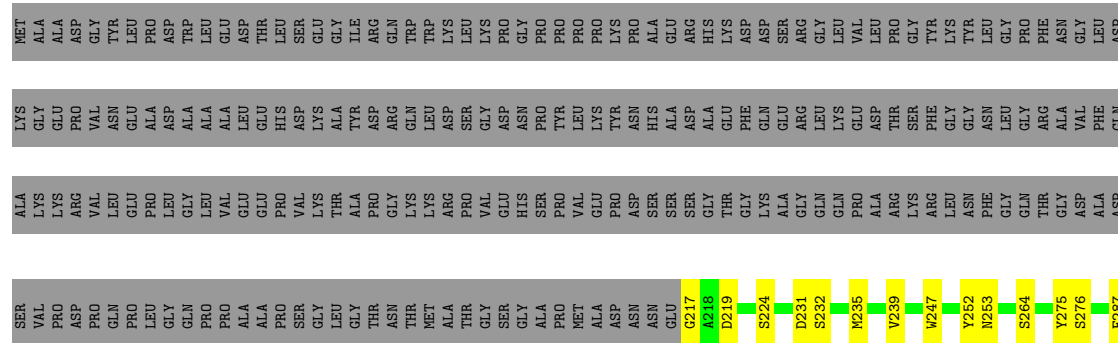


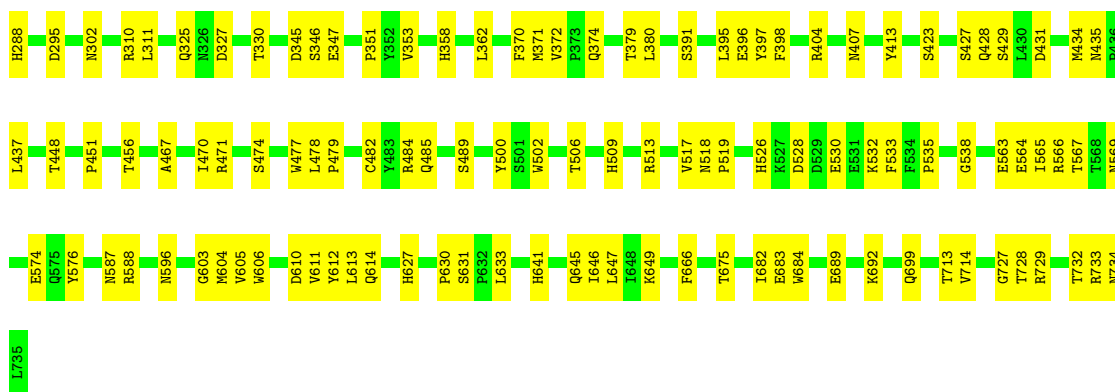


• Molecule 1: Capsid protein VP1



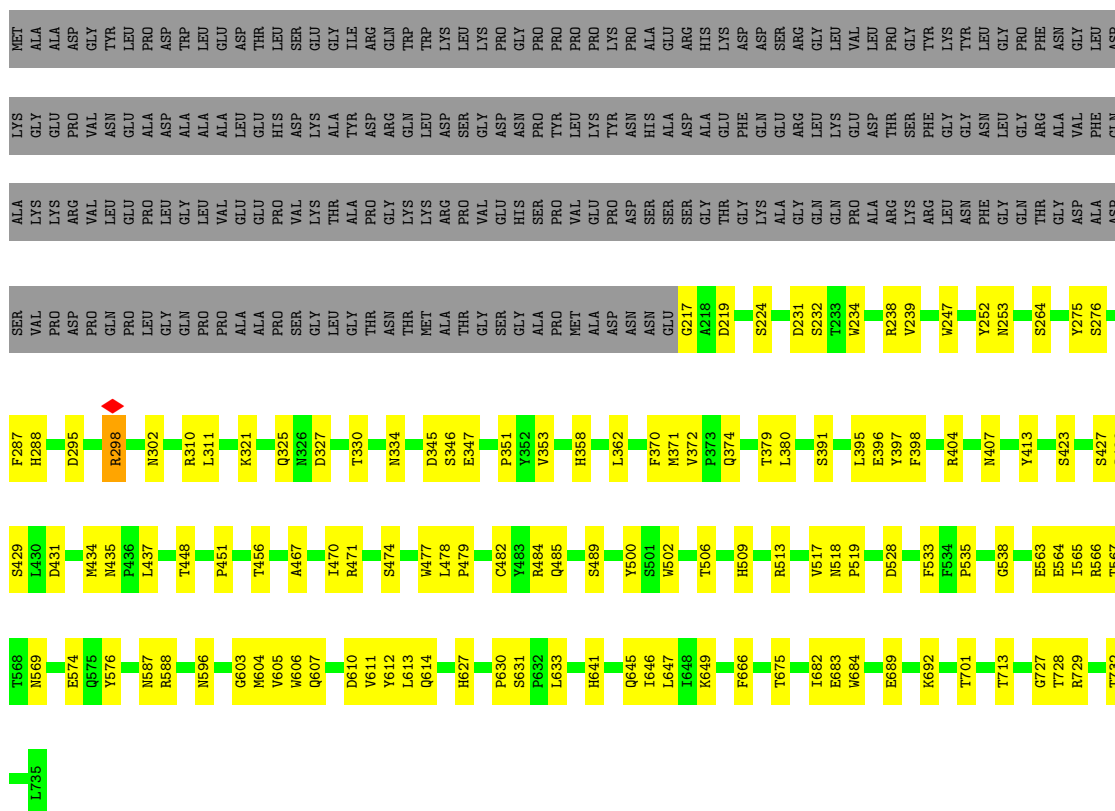
• Molecule 1: Capsid protein VP1





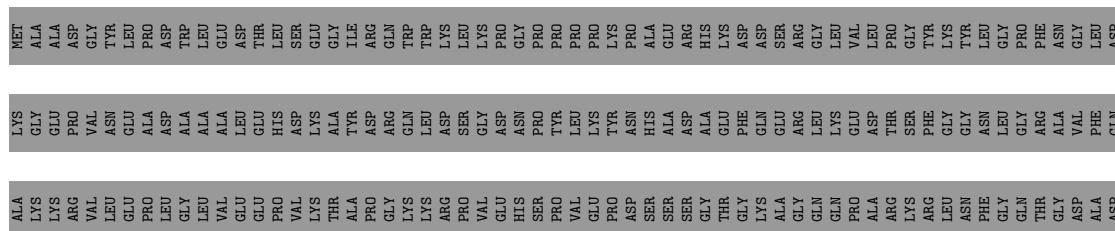
- Molecule 1: Capsid protein VP1

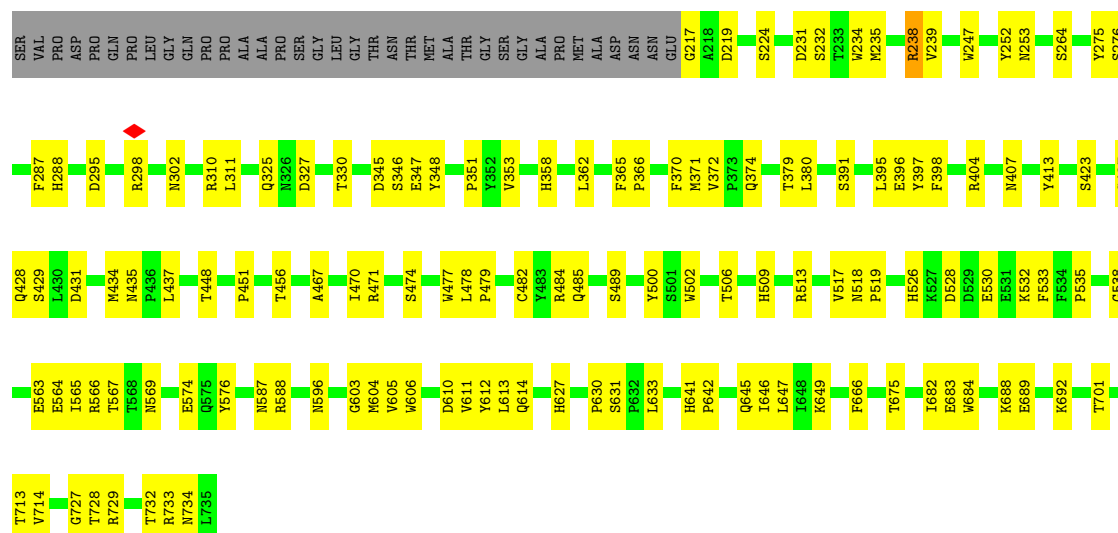
Chain 1: 54% 17% 29%



- Molecule 1: Capsid protein VP1

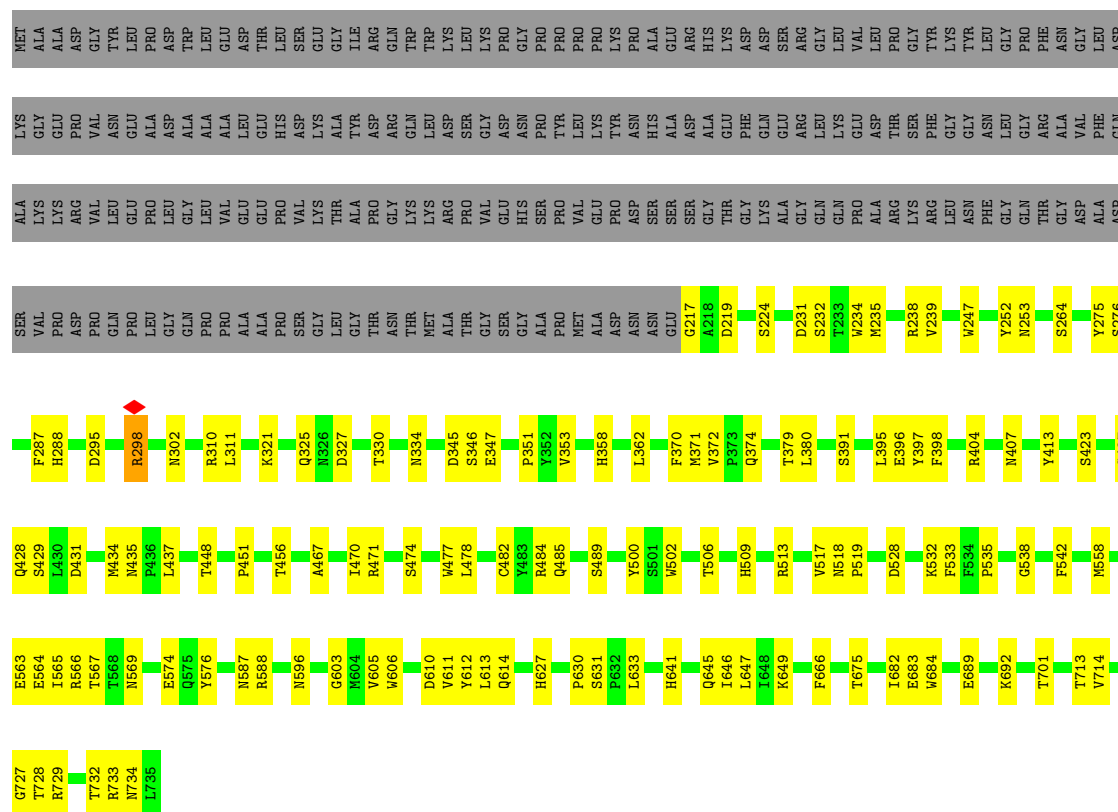
Chain 2: 53% 18% 29%





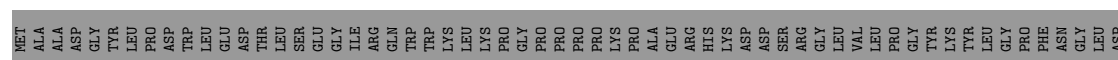
• Molecule 1: Capsid protein VP1

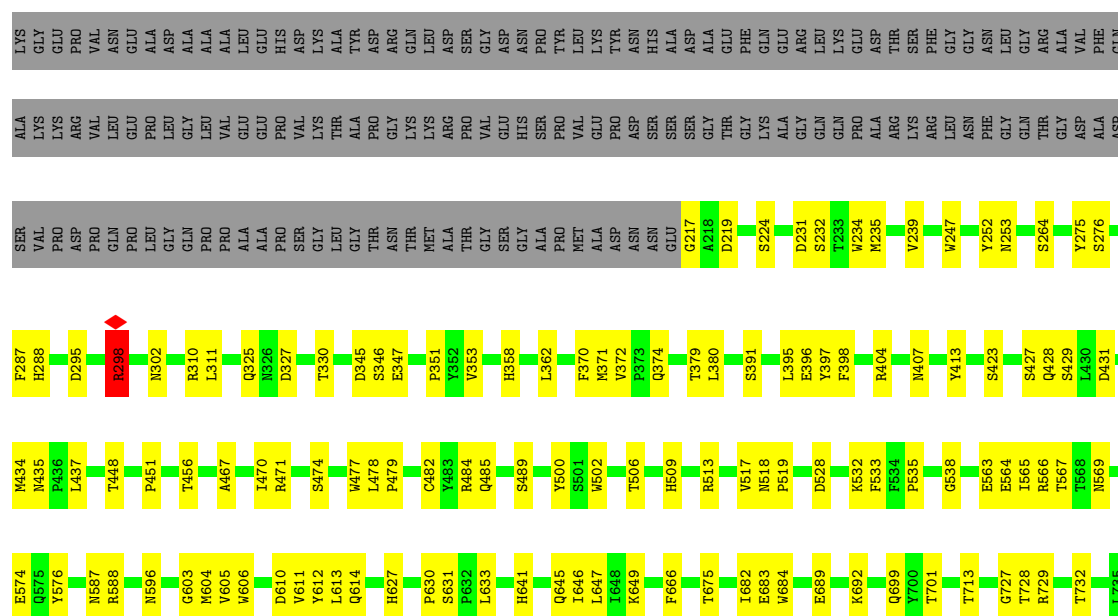
Chain 3: 53% 17% 29%



• Molecule 1: Capsid protein VP1

Chain 4: 54% 17% 29%





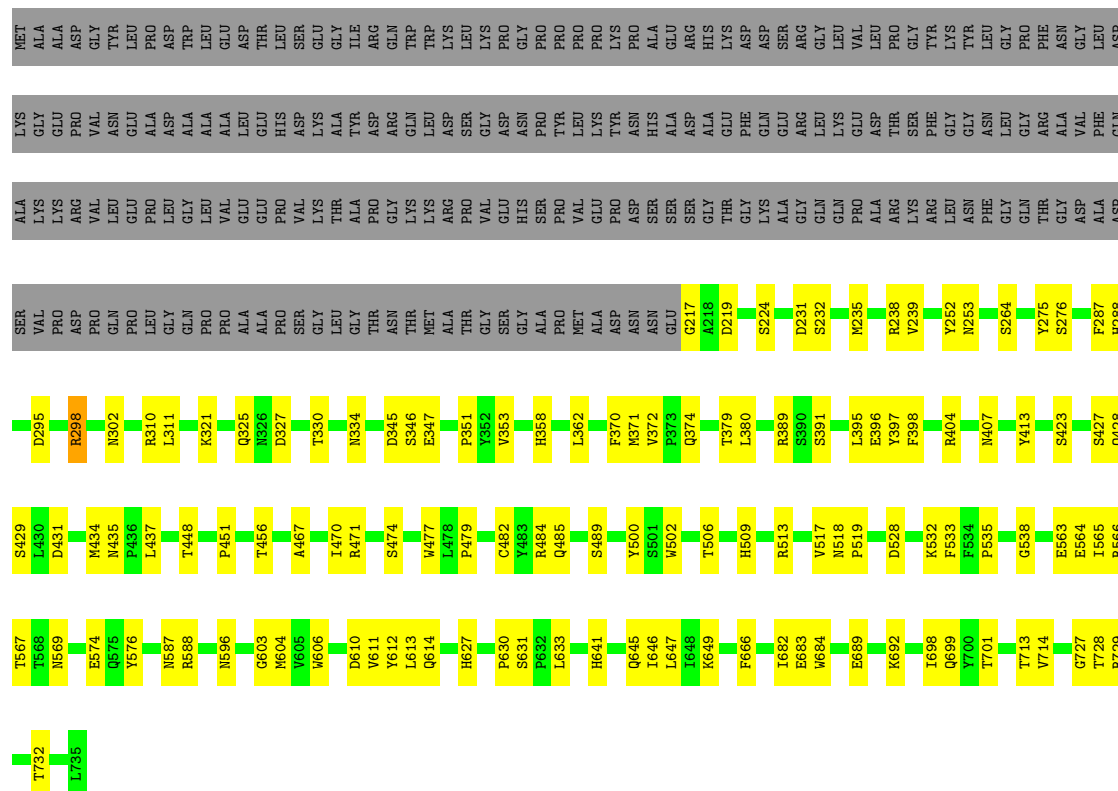
• Molecule 1: Capsid protein VP1

Chain 5: 53% 18% 29%



• Molecule 1: Capsid protein VP1

Chain 6: 53% 17% 29%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3838	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-64 (8k x 8k)	Depositor
Maximum map value	13.476	Depositor
Minimum map value	-8.449	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	373.66, 373.66, 373.66	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.099, 1.099, 1.099	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: D5M

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	1	0.42	0/4297	0.60	3/5855 (0.1%)
1	2	0.38	0/4297	0.60	3/5855 (0.1%)
1	3	0.37	0/4297	0.59	3/5855 (0.1%)
1	4	0.43	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	5	0.43	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	6	0.38	0/4297	0.60	3/5855 (0.1%)
1	7	0.38	0/4297	0.59	3/5855 (0.1%)
1	8	0.40	0/4297	0.60	3/5855 (0.1%)
1	A	0.38	0/4297	0.59	3/5855 (0.1%)
1	B	0.38	0/4297	0.60	3/5855 (0.1%)
1	C	0.38	0/4297	0.59	3/5855 (0.1%)
1	D	0.40	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	E	0.39	0/4297	0.60	7/5855 (0.1%)
1	F	0.38	0/4297	0.59	3/5855 (0.1%)
1	G	0.39	0/4297	0.60	7/5855 (0.1%)
1	H	0.38	0/4297	0.60	3/5855 (0.1%)
1	I	0.37	0/4297	0.60	7/5855 (0.1%)
1	J	0.42	2/4297 (0.0%)	0.61	3/5855 (0.1%)
1	K	0.38	0/4297	0.60	3/5855 (0.1%)
1	L	0.36	0/4297	0.59	3/5855 (0.1%)
1	M	0.37	0/4297	0.59	3/5855 (0.1%)
1	N	0.38	0/4297	0.59	7/5855 (0.1%)
1	O	0.37	0/4297	0.59	3/5855 (0.1%)
1	P	0.38	0/4297	0.60	3/5855 (0.1%)
1	Q	0.37	0/4297	0.60	7/5855 (0.1%)
1	R	0.38	0/4297	0.59	3/5855 (0.1%)
1	S	0.42	2/4297 (0.0%)	0.61	3/5855 (0.1%)
1	T	0.38	0/4297	0.60	3/5855 (0.1%)
1	U	0.36	0/4297	0.60	3/5855 (0.1%)
1	V	0.37	0/4297	0.59	3/5855 (0.1%)
1	W	0.40	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	X	0.37	0/4297	0.59	3/5855 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.37	0/4297	0.59	7/5855 (0.1%)
1	Z	0.37	0/4297	0.59	3/5855 (0.1%)
1	a	0.39	2/4297 (0.0%)	0.59	3/5855 (0.1%)
1	b	0.41	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	c	0.38	0/4297	0.59	3/5855 (0.1%)
1	d	0.39	2/4297 (0.0%)	0.59	3/5855 (0.1%)
1	e	0.41	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	f	0.38	0/4297	0.60	3/5855 (0.1%)
1	g	0.38	0/4297	0.59	3/5855 (0.1%)
1	h	0.42	2/4297 (0.0%)	0.59	3/5855 (0.1%)
1	i	0.38	0/4297	0.59	3/5855 (0.1%)
1	j	0.43	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	k	0.38	0/4297	0.60	3/5855 (0.1%)
1	l	0.40	0/4297	0.60	3/5855 (0.1%)
1	m	0.43	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	n	0.37	0/4297	0.58	3/5855 (0.1%)
1	o	0.42	2/4297 (0.0%)	0.59	3/5855 (0.1%)
1	p	0.38	0/4297	0.59	3/5855 (0.1%)
1	q	0.42	0/4297	0.60	3/5855 (0.1%)
1	r	0.38	0/4297	0.60	3/5855 (0.1%)
1	s	0.39	0/4297	0.59	3/5855 (0.1%)
1	t	0.40	0/4297	0.60	3/5855 (0.1%)
1	u	0.40	0/4297	0.59	3/5855 (0.1%)
1	v	0.42	0/4297	0.60	3/5855 (0.1%)
1	w	0.40	0/4297	0.60	3/5855 (0.1%)
1	x	0.40	0/4297	0.60	3/5855 (0.1%)
1	y	0.42	0/4297	0.60	3/5855 (0.1%)
1	z	0.39	0/4297	0.59	3/5855 (0.1%)
All	All	0.39	28/257820 (0.0%)	0.60	204/351300 (0.1%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	m	298[A]	ARG	CA-CB	6.99	1.65	1.53
1	m	298[B]	ARG	CA-CB	6.99	1.65	1.53
1	4	298[A]	ARG	CA-CB	6.99	1.65	1.53
1	4	298[B]	ARG	CA-CB	6.99	1.65	1.53
1	S	298[A]	ARG	CA-CB	6.28	1.64	1.53
1	S	298[B]	ARG	CA-CB	6.28	1.64	1.53
1	J	298[A]	ARG	CA-CB	6.25	1.64	1.53
1	J	298[B]	ARG	CA-CB	6.25	1.64	1.53
1	h	298[A]	ARG	CA-CB	6.17	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	h	298[B]	ARG	CA-CB	6.17	1.64	1.53
1	o	298[A]	ARG	CA-CB	6.17	1.64	1.53
1	o	298[B]	ARG	CA-CB	6.17	1.64	1.53
1	j	298[A]	ARG	CA-CB	5.69	1.63	1.53
1	j	298[B]	ARG	CA-CB	5.69	1.63	1.53
1	5	298[A]	ARG	CA-CB	5.69	1.63	1.53
1	5	298[B]	ARG	CA-CB	5.69	1.63	1.53
1	b	298[A]	ARG	CA-CB	5.58	1.62	1.53
1	b	298[B]	ARG	CA-CB	5.58	1.62	1.53
1	e	298[A]	ARG	CA-CB	5.53	1.62	1.53
1	e	298[B]	ARG	CA-CB	5.53	1.62	1.53
1	W	298[A]	ARG	CA-CB	5.34	1.62	1.53
1	W	298[B]	ARG	CA-CB	5.34	1.62	1.53
1	D	298[A]	ARG	CA-CB	5.30	1.62	1.53
1	D	298[B]	ARG	CA-CB	5.30	1.62	1.53
1	d	298[A]	ARG	CA-CB	5.08	1.62	1.53
1	d	298[B]	ARG	CA-CB	5.08	1.62	1.53
1	a	298[A]	ARG	CA-CB	5.03	1.62	1.53
1	a	298[B]	ARG	CA-CB	5.03	1.62	1.53

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	264	SER	CB-CA-C	-6.12	109.50	116.54
1	1	264	SER	CB-CA-C	-6.12	109.51	116.54
1	j	264	SER	CB-CA-C	-6.11	109.52	116.54
1	5	264	SER	CB-CA-C	-6.11	109.52	116.54
1	c	264	SER	CB-CA-C	-6.10	109.52	116.54
1	x	264	SER	CB-CA-C	-6.10	109.53	116.54
1	p	264	SER	CB-CA-C	-6.10	109.53	116.54
1	f	264	SER	CB-CA-C	-6.09	109.54	116.54
1	V	264	SER	CB-CA-C	-6.09	109.54	116.54
1	s	264	SER	CB-CA-C	-6.09	109.54	116.54
1	z	264	SER	CB-CA-C	-6.09	109.54	116.54
1	B	264	SER	CB-CA-C	-6.09	109.54	116.54
1	a	264	SER	CB-CA-C	-6.09	109.54	116.54
1	r	264	SER	CB-CA-C	-6.09	109.54	116.54
1	2	264	SER	CB-CA-C	-6.09	109.54	116.54
1	b	264	SER	CB-CA-C	-6.08	109.54	116.54
1	e	264	SER	CB-CA-C	-6.08	109.54	116.54
1	7	264	SER	CB-CA-C	-6.08	109.54	116.54
1	W	264	SER	CB-CA-C	-6.08	109.55	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	m	264	SER	CB-CA-C	-6.08	109.55	116.54
1	4	264	SER	CB-CA-C	-6.08	109.55	116.54
1	y	264	SER	CB-CA-C	-6.08	109.55	116.54
1	8	264	SER	CB-CA-C	-6.08	109.55	116.54
1	d	264	SER	CB-CA-C	-6.08	109.55	116.54
1	J	264	SER	CB-CA-C	-6.07	109.56	116.54
1	M	264	SER	CB-CA-C	-6.07	109.56	116.54
1	O	264	SER	CB-CA-C	-6.07	109.56	116.54
1	T	264	SER	CB-CA-C	-6.07	109.56	116.54
1	U	264	SER	CB-CA-C	-6.07	109.56	116.54
1	Z	264	SER	CB-CA-C	-6.07	109.56	116.54
1	g	264	SER	CB-CA-C	-6.07	109.56	116.54
1	t	264	SER	CB-CA-C	-6.07	109.56	116.54
1	w	264	SER	CB-CA-C	-6.07	109.56	116.54
1	q	264	SER	CB-CA-C	-6.07	109.56	116.54
1	A	264	SER	CB-CA-C	-6.06	109.57	116.54
1	X	264	SER	CB-CA-C	-6.06	109.57	116.54
1	i	264	SER	CB-CA-C	-6.06	109.57	116.54
1	k	264	SER	CB-CA-C	-6.06	109.57	116.54
1	6	264	SER	CB-CA-C	-6.06	109.57	116.54
1	C	264	SER	CB-CA-C	-6.06	109.57	116.54
1	F	264	SER	CB-CA-C	-6.06	109.58	116.54
1	n	264	SER	CB-CA-C	-6.05	109.58	116.54
1	u	264	SER	CB-CA-C	-6.05	109.58	116.54
1	D	264	SER	CB-CA-C	-6.05	109.58	116.54
1	H	264	SER	CB-CA-C	-6.05	109.58	116.54
1	K	264	SER	CB-CA-C	-6.05	109.58	116.54
1	E	264	SER	CB-CA-C	-6.05	109.59	116.54
1	G	264	SER	CB-CA-C	-6.05	109.59	116.54
1	h	264	SER	CB-CA-C	-6.05	109.59	116.54
1	l	264	SER	CB-CA-C	-6.05	109.59	116.54
1	o	264	SER	CB-CA-C	-6.05	109.59	116.54
1	L	264	SER	CB-CA-C	-6.04	109.59	116.54
1	S	264	SER	CB-CA-C	-6.04	109.59	116.54
1	N	264	SER	CB-CA-C	-6.04	109.59	116.54
1	P	264	SER	CB-CA-C	-6.04	109.59	116.54
1	Q	264	SER	CB-CA-C	-6.04	109.59	116.54
1	v	264	SER	CB-CA-C	-6.04	109.59	116.54
1	R	264	SER	CB-CA-C	-6.04	109.59	116.54
1	Y	264	SER	CB-CA-C	-6.03	109.60	116.54
1	I	264	SER	CB-CA-C	-6.03	109.60	116.54
1	H	327	ASP	CB-CA-C	-5.97	109.71	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	327	ASP	CB-CA-C	-5.97	109.71	116.63
1	R	327	ASP	CB-CA-C	-5.96	109.71	116.63
1	f	327	ASP	CB-CA-C	-5.96	109.72	116.63
1	Q	327	ASP	CB-CA-C	-5.96	109.72	116.63
1	N	327	ASP	CB-CA-C	-5.95	109.72	116.63
1	O	327	ASP	CB-CA-C	-5.95	109.72	116.63
1	h	327	ASP	CB-CA-C	-5.95	109.72	116.63
1	o	327	ASP	CB-CA-C	-5.95	109.72	116.63
1	T	327	ASP	CB-CA-C	-5.95	109.73	116.63
1	8	327	ASP	CB-CA-C	-5.95	109.73	116.63
1	S	327	ASP	CB-CA-C	-5.95	109.73	116.63
1	q	327	ASP	CB-CA-C	-5.95	109.73	116.63
1	l	327	ASP	CB-CA-C	-5.95	109.73	116.63
1	t	327	ASP	CB-CA-C	-5.94	109.73	116.63
1	b	327	ASP	CB-CA-C	-5.94	109.74	116.63
1	d	327	ASP	CB-CA-C	-5.94	109.74	116.63
1	e	327	ASP	CB-CA-C	-5.94	109.74	116.63
1	3	327	ASP	CB-CA-C	-5.94	109.74	116.63
1	C	327	ASP	CB-CA-C	-5.94	109.74	116.63
1	Z	327	ASP	CB-CA-C	-5.94	109.74	116.63
1	g	327	ASP	CB-CA-C	-5.94	109.74	116.63
1	Y	327	ASP	CB-CA-C	-5.93	109.75	116.63
1	y	327	ASP	CB-CA-C	-5.93	109.75	116.63
1	D	327	ASP	CB-CA-C	-5.93	109.75	116.63
1	W	327	ASP	CB-CA-C	-5.93	109.75	116.63
1	I	327	ASP	CB-CA-C	-5.93	109.76	116.63
1	a	327	ASP	CB-CA-C	-5.93	109.76	116.63
1	l	327	ASP	CB-CA-C	-5.93	109.75	116.63
1	4	327	ASP	CB-CA-C	-5.93	109.75	116.63
1	c	327	ASP	CB-CA-C	-5.92	109.76	116.63
1	v	327	ASP	CB-CA-C	-5.92	109.76	116.63
1	j	327	ASP	CB-CA-C	-5.92	109.76	116.63
1	5	327	ASP	CB-CA-C	-5.92	109.76	116.63
1	U	327	ASP	CB-CA-C	-5.92	109.76	116.63
1	i	327	ASP	CB-CA-C	-5.92	109.76	116.63
1	7	327	ASP	CB-CA-C	-5.92	109.76	116.63
1	K	327	ASP	CB-CA-C	-5.92	109.77	116.63
1	w	327	ASP	CB-CA-C	-5.92	109.77	116.63
1	E	327	ASP	CB-CA-C	-5.92	109.77	116.63
1	F	327	ASP	CB-CA-C	-5.92	109.77	116.63
1	V	327	ASP	CB-CA-C	-5.91	109.77	116.63
1	n	327	ASP	CB-CA-C	-5.91	109.77	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	r	327	ASP	CB-CA-C	-5.91	109.77	116.63
1	s	327	ASP	CB-CA-C	-5.91	109.77	116.63
1	z	327	ASP	CB-CA-C	-5.91	109.77	116.63
1	2	327	ASP	CB-CA-C	-5.91	109.77	116.63
1	m	327	ASP	CB-CA-C	-5.91	109.78	116.63
1	p	327	ASP	CB-CA-C	-5.91	109.78	116.63
1	P	327	ASP	CB-CA-C	-5.91	109.78	116.63
1	M	327	ASP	CB-CA-C	-5.90	109.79	116.63
1	B	327	ASP	CB-CA-C	-5.90	109.79	116.63
1	G	327	ASP	CB-CA-C	-5.90	109.79	116.63
1	L	327	ASP	CB-CA-C	-5.89	109.79	116.63
1	k	327	ASP	CB-CA-C	-5.89	109.80	116.63
1	6	327	ASP	CB-CA-C	-5.89	109.80	116.63
1	A	327	ASP	CB-CA-C	-5.89	109.80	116.63
1	u	327	ASP	CB-CA-C	-5.88	109.81	116.63
1	x	327	ASP	CB-CA-C	-5.88	109.81	116.63
1	J	327	ASP	CB-CA-C	-5.86	109.83	116.63
1	I	298[A]	ARG	CA-C-N	5.64	129.01	121.90
1	I	298[A]	ARG	C-N-CA	5.64	129.01	121.90
1	I	298[B]	ARG	CA-C-N	5.64	129.01	121.90
1	I	298[B]	ARG	C-N-CA	5.64	129.01	121.90
1	Q	298[A]	ARG	CA-C-N	5.60	128.95	121.90
1	Q	298[A]	ARG	C-N-CA	5.60	128.95	121.90
1	Q	298[B]	ARG	CA-C-N	5.60	128.95	121.90
1	Q	298[B]	ARG	C-N-CA	5.60	128.95	121.90
1	G	298[A]	ARG	CA-C-N	5.49	128.97	122.44
1	G	298[A]	ARG	C-N-CA	5.49	128.97	122.44
1	G	298[B]	ARG	CA-C-N	5.49	128.97	122.44
1	G	298[B]	ARG	C-N-CA	5.49	128.97	122.44
1	E	298[A]	ARG	CA-C-N	5.47	128.96	122.44
1	E	298[A]	ARG	C-N-CA	5.47	128.96	122.44
1	E	298[B]	ARG	CA-C-N	5.47	128.96	122.44
1	E	298[B]	ARG	C-N-CA	5.47	128.96	122.44
1	N	219	ASP	N-CA-C	5.42	116.02	108.00
1	l	219	ASP	N-CA-C	5.42	116.01	108.00
1	t	219	ASP	N-CA-C	5.41	116.01	108.00
1	Q	219	ASP	N-CA-C	5.41	116.01	108.00
1	f	219	ASP	N-CA-C	5.41	116.01	108.00
1	S	219	ASP	N-CA-C	5.41	116.00	108.00
1	w	219	ASP	N-CA-C	5.41	116.00	108.00
1	K	219	ASP	N-CA-C	5.40	116.00	108.00
1	i	219	ASP	N-CA-C	5.40	116.00	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ASP	N-CA-C	5.40	116.00	108.00
1	V	219	ASP	N-CA-C	5.40	116.00	108.00
1	B	219	ASP	N-CA-C	5.40	115.99	108.00
1	k	219	ASP	N-CA-C	5.40	115.99	108.00
1	s	219	ASP	N-CA-C	5.40	115.99	108.00
1	z	219	ASP	N-CA-C	5.40	115.99	108.00
1	P	219	ASP	N-CA-C	5.40	115.99	108.00
1	C	219	ASP	N-CA-C	5.40	115.99	108.00
1	M	219	ASP	N-CA-C	5.40	115.99	108.00
1	O	219	ASP	N-CA-C	5.40	115.99	108.00
1	Z	219	ASP	N-CA-C	5.40	115.99	108.00
1	6	219	ASP	N-CA-C	5.40	115.99	108.00
1	D	219	ASP	N-CA-C	5.39	115.98	108.00
1	W	219	ASP	N-CA-C	5.39	115.98	108.00
1	m	219	ASP	N-CA-C	5.39	115.98	108.00
1	v	219	ASP	N-CA-C	5.39	115.98	108.00
1	y	219	ASP	N-CA-C	5.39	115.98	108.00
1	4	219	ASP	N-CA-C	5.39	115.98	108.00
1	7	219	ASP	N-CA-C	5.39	115.98	108.00
1	X	219	ASP	N-CA-C	5.39	115.98	108.00
1	a	219	ASP	N-CA-C	5.39	115.98	108.00
1	b	219	ASP	N-CA-C	5.39	115.98	108.00
1	3	219	ASP	N-CA-C	5.39	115.98	108.00
1	g	219	ASP	N-CA-C	5.39	115.98	108.00
1	h	219	ASP	N-CA-C	5.39	115.98	108.00
1	p	219	ASP	N-CA-C	5.39	115.98	108.00
1	I	219	ASP	N-CA-C	5.39	115.97	108.00
1	o	219	ASP	N-CA-C	5.39	115.97	108.00
1	c	219	ASP	N-CA-C	5.38	115.97	108.00
1	r	219	ASP	N-CA-C	5.38	115.97	108.00
1	u	219	ASP	N-CA-C	5.38	115.97	108.00
1	x	219	ASP	N-CA-C	5.38	115.97	108.00
1	2	219	ASP	N-CA-C	5.38	115.97	108.00
1	T	219	ASP	N-CA-C	5.38	115.96	108.00
1	q	219	ASP	N-CA-C	5.38	115.96	108.00
1	E	219	ASP	N-CA-C	5.38	115.96	108.00
1	d	219	ASP	N-CA-C	5.38	115.96	108.00
1	n	219	ASP	N-CA-C	5.38	115.96	108.00
1	H	219	ASP	N-CA-C	5.38	115.96	108.00
1	1	219	ASP	N-CA-C	5.38	115.96	108.00
1	8	219	ASP	N-CA-C	5.38	115.96	108.00
1	L	219	ASP	N-CA-C	5.37	115.95	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	219	ASP	N-CA-C	5.37	115.95	108.00
1	J	219	ASP	N-CA-C	5.37	115.95	108.00
1	R	219	ASP	N-CA-C	5.37	115.95	108.00
1	e	219	ASP	N-CA-C	5.37	115.94	108.00
1	G	219	ASP	N-CA-C	5.37	115.94	108.00
1	F	219	ASP	N-CA-C	5.36	115.94	108.00
1	Y	219	ASP	N-CA-C	5.35	115.92	108.00
1	j	219	ASP	N-CA-C	5.35	115.92	108.00
1	5	219	ASP	N-CA-C	5.35	115.92	108.00
1	Y	298[A]	ARG	CA-C-N	5.30	128.57	121.90
1	Y	298[A]	ARG	C-N-CA	5.30	128.57	121.90
1	Y	298[B]	ARG	CA-C-N	5.30	128.57	121.90
1	Y	298[B]	ARG	C-N-CA	5.30	128.57	121.90
1	N	298[A]	ARG	CA-C-N	5.23	128.50	121.90
1	N	298[A]	ARG	C-N-CA	5.23	128.50	121.90
1	N	298[B]	ARG	CA-C-N	5.23	128.50	121.90
1	N	298[B]	ARG	C-N-CA	5.23	128.50	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4166	0	3926	109	0
1	2	4166	0	3926	116	0
1	3	4166	0	3926	108	0
1	4	4166	0	3926	108	0
1	5	4166	0	3926	115	0
1	6	4166	0	3926	111	0
1	7	4166	0	3926	106	0
1	8	4166	0	3926	118	0
1	A	4166	0	3926	108	0
1	B	4166	0	3926	104	0
1	C	4166	0	3926	112	0
1	D	4166	0	3926	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4166	0	3926	110	0
1	F	4166	0	3926	108	0
1	G	4166	0	3926	108	0
1	H	4166	0	3926	108	0
1	I	4166	0	3926	115	0
1	J	4166	0	3926	112	0
1	K	4166	0	3926	107	0
1	L	4166	0	3926	118	0
1	M	4166	0	3926	110	0
1	N	4166	0	3926	115	0
1	O	4166	0	3926	106	0
1	P	4166	0	3926	104	0
1	Q	4166	0	3926	113	0
1	R	4166	0	3926	107	0
1	S	4166	0	3926	108	0
1	T	4166	0	3926	111	0
1	U	4166	0	3926	115	0
1	V	4166	0	3926	107	0
1	W	4166	0	3926	108	0
1	X	4166	0	3926	107	0
1	Y	4166	0	3926	112	0
1	Z	4166	0	3926	108	0
1	a	4166	0	3926	105	0
1	b	4166	0	3926	116	0
1	c	4166	0	3926	103	0
1	d	4166	0	3926	104	0
1	e	4166	0	3926	114	0
1	f	4166	0	3926	111	0
1	g	4166	0	3926	113	0
1	h	4166	0	3926	108	0
1	i	4166	0	3926	108	0
1	j	4166	0	3926	108	0
1	k	4166	0	3926	107	0
1	l	4166	0	3926	118	0
1	m	4166	0	3926	115	0
1	n	4166	0	3926	112	0
1	o	4166	0	3926	104	0
1	p	4166	0	3926	111	0
1	q	4166	0	3926	114	0
1	r	4166	0	3926	111	0
1	s	4166	0	3926	105	0
1	t	4166	0	3926	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	u	4166	0	3926	114	0
1	v	4166	0	3926	109	0
1	w	4166	0	3926	115	0
1	x	4166	0	3926	108	0
1	y	4166	0	3926	112	0
1	z	4166	0	3926	106	0
2	1	21	0	12	1	0
2	2	21	0	12	1	0
2	3	21	0	12	1	0
2	4	21	0	12	1	0
2	5	21	0	12	1	0
2	6	21	0	12	1	0
2	7	21	0	12	1	0
2	8	21	0	12	1	0
2	A	21	0	12	1	0
2	B	21	0	12	1	0
2	C	21	0	12	1	0
2	D	21	0	12	1	0
2	E	21	0	12	1	0
2	F	21	0	12	1	0
2	G	21	0	12	1	0
2	H	21	0	12	1	0
2	I	21	0	12	1	0
2	J	21	0	12	1	0
2	K	21	0	12	1	0
2	L	21	0	12	1	0
2	M	21	0	12	1	0
2	N	21	0	12	1	0
2	O	21	0	12	1	0
2	P	21	0	12	1	0
2	Q	21	0	12	1	0
2	R	21	0	12	1	0
2	S	21	0	12	1	0
2	T	21	0	12	1	0
2	U	21	0	12	1	0
2	V	21	0	12	1	0
2	W	21	0	12	1	0
2	X	21	0	12	1	0
2	Y	21	0	12	1	0
2	Z	21	0	12	1	0
2	a	21	0	12	1	0
2	b	21	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	c	21	0	12	1	0
2	d	21	0	12	1	0
2	e	21	0	12	1	0
2	f	21	0	12	1	0
2	g	21	0	12	1	0
2	h	21	0	12	1	0
2	i	21	0	12	1	0
2	j	21	0	12	1	0
2	k	21	0	12	1	0
2	l	21	0	12	1	0
2	m	21	0	12	1	0
2	n	21	0	12	1	0
2	o	21	0	12	1	0
2	p	21	0	12	1	0
2	q	21	0	12	1	0
2	r	21	0	12	1	0
2	s	21	0	12	1	0
2	t	21	0	12	1	0
2	u	21	0	12	1	0
2	v	21	0	12	1	0
2	w	21	0	12	1	0
2	x	21	0	12	1	0
2	y	21	0	12	1	0
2	z	21	0	12	1	0
All	All	251220	0	236280	5297	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 11.

All (5297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:298[A]:ARG:HH21	1:U:298[A]:ARG:HG2	1.31	0.94
1:L:298[A]:ARG:HG2	1:L:298[A]:ARG:HH21	1.31	0.93
1:3:298[A]:ARG:HG2	1:3:298[A]:ARG:HH21	1.38	0.87
1:n:298[A]:ARG:HG2	1:n:298[A]:ARG:HH21	1.38	0.87
1:C:431:ASP:OD2	1:Y:513:ARG:NH1	2.14	0.81
1:b:513:ARG:NH1	1:d:431:ASP:OD2	2.15	0.80
1:J:431:ASP:OD2	1:1:513:ARG:NH1	2.15	0.80
1:Y:298[A]:ARG:HG2	1:Y:298[A]:ARG:HH21	1.45	0.80
1:L:513:ARG:NH1	1:R:431:ASP:OD2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:431:ASP:OD2	1:k:513:ARG:NH1	2.15	0.80
1:H:513:ARG:NH1	1:T:431:ASP:OD2	2.15	0.80
1:P:431:ASP:OD2	1:X:513:ARG:NH1	2.15	0.80
1:B:431:ASP:OD2	1:U:513:ARG:NH1	2.14	0.80
1:I:513:ARG:NH1	1:O:431:ASP:OD2	2.15	0.80
1:W:431:ASP:OD2	1:l:513:ARG:NH1	2.14	0.80
1:j:513:ARG:NH1	1:4:431:ASP:OD2	2.15	0.80
1:I:431:ASP:OD2	1:6:513:ARG:NH1	2.15	0.79
1:K:431:ASP:OD2	1:P:513:ARG:NH1	2.15	0.79
1:N:513:ARG:NH1	1:V:431:ASP:OD2	2.14	0.79
1:S:431:ASP:OD2	1:q:513:ARG:NH1	2.15	0.79
1:A:513:ARG:NH1	1:f:431:ASP:OD2	2.16	0.79
1:E:513:ARG:NH1	1:i:431:ASP:OD2	2.15	0.79
1:F:431:ASP:OD2	1:3:513:ARG:NH1	2.15	0.79
1:m:431:ASP:OD2	1:5:513:ARG:NH1	2.15	0.79
1:D:431:ASP:OD2	1:8:513:ARG:NH1	2.14	0.79
1:D:513:ARG:NH1	1:x:431:ASP:OD2	2.15	0.79
1:G:431:ASP:OD2	1:g:513:ARG:NH1	2.15	0.79
1:Y:431:ASP:OD2	1:t:513:ARG:NH1	2.15	0.79
1:e:431:ASP:OD2	1:y:513:ARG:NH1	2.15	0.79
1:f:513:ARG:NH1	1:n:431:ASP:OD2	2.16	0.79
1:A:431:ASP:OD2	1:n:513:ARG:NH1	2.15	0.79
1:G:513:ARG:NH1	1:7:431:ASP:OD2	2.15	0.79
1:S:513:ARG:NH1	1:z:431:ASP:OD2	2.15	0.79
1:b:431:ASP:OD2	1:v:513:ARG:NH1	2.15	0.79
1:o:431:ASP:OD2	1:4:513:ARG:NH1	2.15	0.79
1:F:513:ARG:NH1	1:c:431:ASP:OD2	2.15	0.79
1:L:431:ASP:OD2	1:r:513:ARG:NH1	2.15	0.79
1:N:298[A]:ARG:HG2	1:N:298[A]:ARG:HH21	1.45	0.79
1:N:431:ASP:OD2	1:w:513:ARG:NH1	2.15	0.79
1:a:431:ASP:OD2	1:e:513:ARG:NH1	2.15	0.79
1:E:431:ASP:OD2	1:p:513:ARG:NH1	2.15	0.79
1:K:513:ARG:NH1	1:X:431:ASP:OD2	2.15	0.79
1:W:513:ARG:NH1	1:u:431:ASP:OD2	2.15	0.79
1:h:431:ASP:OD2	1:m:513:ARG:NH1	2.15	0.79
1:B:513:ARG:NH1	1:2:431:ASP:OD2	2.16	0.79
1:Q:238[B]:ARG:HD3	1:Q:683:GLU:OE2	1.83	0.79
1:M:431:ASP:OD2	1:T:513:ARG:NH1	2.15	0.79
1:a:513:ARG:NH1	1:y:431:ASP:OD2	2.16	0.79
1:g:431:ASP:OD2	1:7:513:ARG:NH1	2.16	0.79
1:j:431:ASP:OD2	1:o:513:ARG:NH1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:238[B]:ARG:HD3	1:I:683:GLU:OE2	1.83	0.79
1:Q:513:ARG:NH1	1:Z:431:ASP:OD2	2.15	0.79
1:c:513:ARG:NH1	1:3:431:ASP:OD2	2.16	0.79
1:q:431:ASP:OD2	1:z:513:ARG:NH1	2.16	0.79
1:H:431:ASP:OD2	1:M:513:ARG:NH1	2.15	0.78
1:J:513:ARG:NH1	1:s:431:ASP:OD2	2.15	0.78
1:O:513:ARG:NH1	1:6:431:ASP:OD2	2.16	0.78
1:U:431:ASP:OD2	1:2:513:ARG:NH1	2.15	0.78
1:l:431:ASP:OD2	1:u:513:ARG:NH1	2.16	0.78
1:C:513:ARG:NH1	1:t:431:ASP:OD2	2.16	0.78
1:Z:513:ARG:NH1	1:k:431:ASP:OD2	2.16	0.78
1:R:513:ARG:NH1	1:r:431:ASP:OD2	2.16	0.78
1:d:513:ARG:NH1	1:v:431:ASP:OD2	2.16	0.78
1:s:513:ARG:NH1	1:l:431:ASP:OD2	2.16	0.78
1:i:513:ARG:NH1	1:p:431:ASP:OD2	2.16	0.78
1:h:513:ARG:NH1	1:5:431:ASP:OD2	2.16	0.77
1:V:513:ARG:NH1	1:w:431:ASP:OD2	2.16	0.77
1:x:513:ARG:NH1	1:8:431:ASP:OD2	2.16	0.77
1:Y:238[B]:ARG:HD3	1:Y:683:GLU:OE2	1.84	0.76
1:N:238[B]:ARG:HD3	1:N:683:GLU:OE2	1.84	0.76
1:R:298[A]:ARG:HH21	1:R:298[A]:ARG:HG2	1.50	0.76
1:m:528:ASP:OD1	1:m:566:ARG:NH1	2.19	0.76
1:S:528:ASP:OD1	1:S:566:ARG:NH1	2.19	0.76
1:T:528:ASP:OD1	1:T:566:ARG:NH1	2.19	0.76
1:X:528:ASP:OD1	1:X:566:ARG:NH1	2.19	0.76
1:o:528:ASP:OD1	1:o:566:ARG:NH1	2.19	0.76
1:r:528:ASP:OD1	1:r:566:ARG:NH1	2.19	0.76
1:P:528:ASP:OD1	1:P:566:ARG:NH1	2.19	0.76
1:Q:528:ASP:OD1	1:Q:566:ARG:NH1	2.19	0.76
1:j:528:ASP:OD1	1:j:566:ARG:NH1	2.19	0.76
1:x:528:ASP:OD1	1:x:566:ARG:NH1	2.19	0.76
1:Y:528:ASP:OD1	1:Y:566:ARG:NH1	2.19	0.76
1:l:528:ASP:OD1	1:l:566:ARG:NH1	2.19	0.76
1:G:528:ASP:OD1	1:G:566:ARG:NH1	2.19	0.75
1:I:528:ASP:OD1	1:I:566:ARG:NH1	2.19	0.75
1:K:528:ASP:OD1	1:K:566:ARG:NH1	2.19	0.75
1:M:298[A]:ARG:HH21	1:M:298[A]:ARG:HG2	1.50	0.75
1:O:528:ASP:OD1	1:O:566:ARG:NH1	2.19	0.75
1:S:295:ASP:OD2	1:V:397:TYR:OH	2.05	0.75
1:4:528:ASP:OD1	1:4:566:ARG:NH1	2.19	0.75
1:7:528:ASP:OD1	1:7:566:ARG:NH1	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:528:ASP:OD1	1:g:566:ARG:NH1	2.19	0.75
1:n:528:ASP:OD1	1:n:566:ARG:NH1	2.19	0.75
1:t:528:ASP:OD1	1:t:566:ARG:NH1	2.19	0.75
1:u:528:ASP:OD1	1:u:566:ARG:NH1	2.19	0.75
1:2:528:ASP:OD1	1:2:566:ARG:NH1	2.19	0.75
1:C:528:ASP:OD1	1:C:566:ARG:NH1	2.19	0.75
1:H:528:ASP:OD1	1:H:566:ARG:NH1	2.19	0.75
1:d:528:ASP:OD1	1:d:566:ARG:NH1	2.19	0.75
1:l:528:ASP:OD1	1:l:566:ARG:NH1	2.19	0.75
1:5:528:ASP:OD1	1:5:566:ARG:NH1	2.19	0.75
1:B:528:ASP:OD1	1:B:566:ARG:NH1	2.19	0.75
1:J:528:ASP:OD1	1:J:566:ARG:NH1	2.19	0.75
1:L:528:ASP:OD1	1:L:566:ARG:NH1	2.19	0.75
1:b:528:ASP:OD1	1:b:566:ARG:NH1	2.19	0.75
1:t:379:THR:HG21	1:t:391:SER:H	1.52	0.75
1:A:528:ASP:OD1	1:A:566:ARG:NH1	2.19	0.75
1:B:298[A]:ARG:HH21	1:B:298[A]:ARG:HG2	1.51	0.75
1:F:528:ASP:OD1	1:F:566:ARG:NH1	2.19	0.75
1:G:379:THR:HG21	1:G:391:SER:H	1.52	0.75
1:M:528:ASP:OD1	1:M:566:ARG:NH1	2.19	0.75
1:f:528:ASP:OD1	1:f:566:ARG:NH1	2.19	0.75
1:h:528:ASP:OD1	1:h:566:ARG:NH1	2.19	0.75
1:y:528:ASP:OD1	1:y:566:ARG:NH1	2.19	0.75
1:z:528:ASP:OD1	1:z:566:ARG:NH1	2.19	0.75
1:D:528:ASP:OD1	1:D:566:ARG:NH1	2.19	0.75
1:Z:528:ASP:OD1	1:Z:566:ARG:NH1	2.19	0.75
1:v:528:ASP:OD1	1:v:566:ARG:NH1	2.19	0.75
1:E:528:ASP:OD1	1:E:566:ARG:NH1	2.19	0.75
1:c:528:ASP:OD1	1:c:566:ARG:NH1	2.19	0.75
1:e:379:THR:HG21	1:e:391:SER:H	1.52	0.75
1:e:528:ASP:OD1	1:e:566:ARG:NH1	2.19	0.75
1:k:528:ASP:OD1	1:k:566:ARG:NH1	2.19	0.75
1:q:528:ASP:OD1	1:q:566:ARG:NH1	2.19	0.75
1:w:528:ASP:OD1	1:w:566:ARG:NH1	2.19	0.75
1:8:528:ASP:OD1	1:8:566:ARG:NH1	2.19	0.75
1:E:379:THR:HG21	1:E:391:SER:H	1.52	0.75
1:R:528:ASP:OD1	1:R:566:ARG:NH1	2.19	0.75
1:U:379:THR:HG21	1:U:391:SER:H	1.52	0.75
1:X:298[A]:ARG:HH21	1:X:298[A]:ARG:HG2	1.51	0.75
1:i:528:ASP:OD1	1:i:566:ARG:NH1	2.19	0.75
1:U:528:ASP:OD1	1:U:566:ARG:NH1	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:528:ASP:OD1	1:W:566:ARG:NH1	2.19	0.75
1:X:379:THR:HG21	1:X:391:SER:H	1.52	0.75
1:c:379:THR:HG21	1:c:391:SER:H	1.52	0.75
1:i:379:THR:HG21	1:i:391:SER:H	1.52	0.75
1:o:379:THR:HG21	1:o:391:SER:H	1.52	0.75
1:s:379:THR:HG21	1:s:391:SER:H	1.52	0.75
1:v:379:THR:HG21	1:v:391:SER:H	1.52	0.75
1:w:379:THR:HG21	1:w:391:SER:H	1.52	0.75
1:6:528:ASP:OD1	1:6:566:ARG:NH1	2.19	0.75
1:D:397:TYR:OH	1:b:295:ASP:OD2	2.05	0.74
1:N:379:THR:HG21	1:N:391:SER:H	1.52	0.74
1:N:528:ASP:OD1	1:N:566:ARG:NH1	2.19	0.74
1:s:528:ASP:OD1	1:s:566:ARG:NH1	2.19	0.74
1:A:379:THR:HG21	1:A:391:SER:H	1.52	0.74
1:f:379:THR:HG21	1:f:391:SER:H	1.52	0.74
1:q:379:THR:HG21	1:q:391:SER:H	1.52	0.74
1:B:379:THR:HG21	1:B:391:SER:H	1.52	0.74
1:J:397:TYR:OH	1:8:295:ASP:OD2	2.06	0.74
1:S:397:TYR:OH	1:l:295:ASP:OD2	2.06	0.74
1:l:379:THR:HG21	1:l:391:SER:H	1.52	0.74
1:C:397:TYR:OH	1:J:295:ASP:OD2	2.05	0.74
1:R:379:THR:HG21	1:R:391:SER:H	1.52	0.74
1:V:528:ASP:OD1	1:V:566:ARG:NH1	2.19	0.74
1:W:295:ASP:OD2	1:Z:397:TYR:OH	2.06	0.74
1:a:295:ASP:OD2	1:7:397:TYR:OH	2.06	0.74
1:b:379:THR:HG21	1:b:391:SER:H	1.52	0.74
1:m:379:THR:HG21	1:m:391:SER:H	1.52	0.74
1:n:379:THR:HG21	1:n:391:SER:H	1.52	0.74
1:p:379:THR:HG21	1:p:391:SER:H	1.52	0.74
1:p:528:ASP:OD1	1:p:566:ARG:NH1	2.19	0.74
1:5:379:THR:HG21	1:5:391:SER:H	1.52	0.74
1:E:397:TYR:OH	1:N:295:ASP:OD2	2.06	0.74
1:H:379:THR:HG21	1:H:391:SER:H	1.52	0.74
1:T:379:THR:HG21	1:T:391:SER:H	1.52	0.74
1:V:379:THR:HG21	1:V:391:SER:H	1.52	0.74
1:a:379:THR:HG21	1:a:391:SER:H	1.52	0.74
1:a:528:ASP:OD1	1:a:566:ARG:NH1	2.19	0.74
1:h:397:TYR:OH	1:j:295:ASP:OD2	2.06	0.74
1:3:379:THR:HG21	1:3:391:SER:H	1.52	0.74
1:3:528:ASP:OD1	1:3:566:ARG:NH1	2.19	0.74
1:7:379:THR:HG21	1:7:391:SER:H	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:THR:HG21	1:C:391:SER:H	1.52	0.74
1:D:345:ASP:OD1	1:D:346:SER:N	2.21	0.74
1:W:379:THR:HG21	1:W:391:SER:H	1.52	0.74
1:Y:397:TYR:OH	1:3:295:ASP:OD2	2.06	0.74
1:g:379:THR:HG21	1:g:391:SER:H	1.52	0.74
1:I:379:THR:HG21	1:I:391:SER:H	1.52	0.74
1:Y:379:THR:HG21	1:Y:391:SER:H	1.52	0.74
1:d:379:THR:HG21	1:d:391:SER:H	1.52	0.74
1:k:345:ASP:OD1	1:k:346:SER:N	2.21	0.74
1:A:345:ASP:OD1	1:A:346:SER:N	2.21	0.74
1:B:397:TYR:OH	1:G:295:ASP:OD2	2.06	0.74
1:J:345:ASP:OD1	1:J:346:SER:N	2.21	0.74
1:M:345:ASP:OD1	1:M:346:SER:N	2.21	0.74
1:Q:379:THR:HG21	1:Q:391:SER:H	1.52	0.74
1:Z:379:THR:HG21	1:Z:391:SER:H	1.52	0.74
1:h:345:ASP:OD1	1:h:346:SER:N	2.21	0.74
1:l:379:THR:HG21	1:l:391:SER:H	1.52	0.74
1:v:345:ASP:OD1	1:v:346:SER:N	2.21	0.74
1:x:379:THR:HG21	1:x:391:SER:H	1.52	0.74
1:2:345:ASP:OD1	1:2:346:SER:N	2.21	0.74
1:D:295:ASP:OD2	1:O:397:TYR:OH	2.06	0.74
1:K:379:THR:HG21	1:K:391:SER:H	1.52	0.74
1:O:379:THR:HG21	1:O:391:SER:H	1.52	0.74
1:R:345:ASP:OD1	1:R:346:SER:N	2.21	0.74
1:o:295:ASP:OD2	1:s:397:TYR:OH	2.06	0.74
1:u:379:THR:HG21	1:u:391:SER:H	1.52	0.74
1:1:295:ASP:OD2	1:4:397:TYR:OH	2.06	0.74
1:6:379:THR:HG21	1:6:391:SER:H	1.52	0.74
1:8:379:THR:HG21	1:8:391:SER:H	1.52	0.74
1:F:295:ASP:OD2	1:P:397:TYR:OH	2.06	0.73
1:F:397:TYR:OH	1:I:295:ASP:OD2	2.06	0.73
1:J:379:THR:HG21	1:J:391:SER:H	1.52	0.73
1:W:397:TYR:OH	1:e:295:ASP:OD2	2.05	0.73
1:j:397:TYR:OH	1:y:295:ASP:OD2	2.06	0.73
1:p:397:TYR:OH	1:r:295:ASP:OD2	2.07	0.73
1:r:379:THR:HG21	1:r:391:SER:H	1.52	0.73
1:u:295:ASP:OD2	1:y:397:TYR:OH	2.06	0.73
1:4:379:THR:HG21	1:4:391:SER:H	1.52	0.73
1:A:295:ASP:OD2	1:H:397:TYR:OH	2.06	0.73
1:D:379:THR:HG21	1:D:391:SER:H	1.52	0.73
1:M:397:TYR:OH	1:P:295:ASP:OD2	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:345:ASP:OD1	1:N:346:SER:N	2.21	0.73
1:O:295:ASP:OD2	1:r:397:TYR:OH	2.06	0.73
1:S:379:THR:HG21	1:S:391:SER:H	1.52	0.73
1:X:345:ASP:OD1	1:X:346:SER:N	2.21	0.73
1:Z:295:ASP:OD2	1:2:397:TYR:OH	2.06	0.73
1:d:397:TYR:OH	1:m:295:ASP:OD2	2.05	0.73
1:q:345:ASP:OD1	1:q:346:SER:N	2.21	0.73
1:2:379:THR:HG21	1:2:391:SER:H	1.52	0.73
1:6:295:ASP:OD2	1:8:397:TYR:OH	2.06	0.73
1:I:397:TYR:OH	1:L:295:ASP:OD2	2.06	0.73
1:K:345:ASP:OD1	1:K:346:SER:N	2.21	0.73
1:Y:345:ASP:OD1	1:Y:346:SER:N	2.21	0.73
1:i:345:ASP:OD1	1:i:346:SER:N	2.21	0.73
1:k:295:ASP:OD2	1:l:397:TYR:OH	2.06	0.73
1:o:345:ASP:OD1	1:o:346:SER:N	2.21	0.73
1:y:379:THR:HG21	1:y:391:SER:H	1.52	0.73
1:4:345:ASP:OD1	1:4:346:SER:N	2.21	0.73
1:F:379:THR:HG21	1:F:391:SER:H	1.52	0.73
1:L:379:THR:HG21	1:L:391:SER:H	1.52	0.73
1:V:345:ASP:OD1	1:V:346:SER:N	2.21	0.73
1:a:397:TYR:OH	1:4:295:ASP:OD2	2.05	0.73
1:h:295:ASP:OD2	1:z:397:TYR:OH	2.06	0.73
1:k:379:THR:HG21	1:k:391:SER:H	1.52	0.73
1:d:295:ASP:OD2	1:i:397:TYR:OH	2.06	0.73
1:f:295:ASP:OD2	1:k:397:TYR:OH	2.07	0.73
1:j:379:THR:HG21	1:j:391:SER:H	1.52	0.73
1:m:397:TYR:OH	1:q:295:ASP:OD2	2.06	0.73
1:z:379:THR:HG21	1:z:391:SER:H	1.52	0.73
1:7:345:ASP:OD1	1:7:346:SER:N	2.21	0.73
1:L:397:TYR:OH	1:M:295:ASP:OD2	2.06	0.73
1:p:345:ASP:OD1	1:p:346:SER:N	2.21	0.73
1:I:345:ASP:OD1	1:I:346:SER:N	2.21	0.73
1:N:397:TYR:OH	1:n:295:ASP:OD2	2.06	0.73
1:P:379:THR:HG21	1:P:391:SER:H	1.52	0.73
1:Q:397:TYR:OH	1:U:295:ASP:OD2	2.06	0.73
1:V:295:ASP:OD2	1:f:397:TYR:OH	2.06	0.73
1:e:345:ASP:OD1	1:e:346:SER:N	2.21	0.73
1:u:397:TYR:OH	1:z:295:ASP:OD2	2.06	0.73
1:v:295:ASP:OD2	1:5:397:TYR:OH	2.06	0.73
1:8:345:ASP:OD1	1:8:346:SER:N	2.21	0.73
1:H:295:ASP:OD2	1:X:397:TYR:OH	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:345:ASP:OD1	1:U:346:SER:N	2.21	0.73
1:U:397:TYR:OH	1:X:295:ASP:OD2	2.06	0.73
1:c:345:ASP:OD1	1:c:346:SER:N	2.21	0.73
1:e:397:TYR:OH	1:g:295:ASP:OD2	2.06	0.73
1:i:295:ASP:OD2	1:w:397:TYR:OH	2.07	0.73
1:s:295:ASP:OD2	1:x:397:TYR:OH	2.06	0.73
1:t:295:ASP:OD2	1:l:397:TYR:OH	2.06	0.73
1:u:345:ASP:OD1	1:u:346:SER:N	2.21	0.73
1:v:397:TYR:OH	1:x:295:ASP:OD2	2.06	0.73
1:G:397:TYR:OH	1:Y:295:ASP:OD2	2.06	0.73
1:T:295:ASP:OD2	1:n:397:TYR:OH	2.07	0.73
1:Z:345:ASP:OD1	1:Z:346:SER:N	2.21	0.73
1:b:397:TYR:OH	1:p:295:ASP:OD2	2.06	0.73
1:C:295:ASP:OD2	1:c:397:TYR:OH	2.07	0.72
1:R:295:ASP:OD2	1:T:397:TYR:OH	2.06	0.72
1:T:345:ASP:OD1	1:T:346:SER:N	2.21	0.72
1:s:345:ASP:OD1	1:s:346:SER:N	2.21	0.72
1:H:345:ASP:OD1	1:H:346:SER:N	2.21	0.72
1:K:295:ASP:OD2	1:3:397:TYR:OH	2.07	0.72
1:o:397:TYR:OH	1:5:295:ASP:OD2	2.06	0.72
1:G:345:ASP:OD1	1:G:346:SER:N	2.21	0.72
1:b:345:ASP:OD1	1:b:346:SER:N	2.21	0.72
1:t:397:TYR:OH	1:7:295:ASP:OD2	2.07	0.72
1:5:345:ASP:OD1	1:5:346:SER:N	2.21	0.72
1:g:345:ASP:OD1	1:g:346:SER:N	2.21	0.72
1:C:345:ASP:OD1	1:C:346:SER:N	2.21	0.72
1:M:379:THR:HG21	1:M:391:SER:H	1.52	0.72
1:m:345:ASP:OD1	1:m:346:SER:N	2.21	0.72
1:W:345:ASP:OD1	1:W:346:SER:N	2.21	0.72
1:g:397:TYR:OH	1:2:295:ASP:OD2	2.06	0.72
1:h:379:THR:HG21	1:h:391:SER:H	1.52	0.72
1:q:397:TYR:OH	1:w:295:ASP:OD2	2.06	0.72
1:t:345:ASP:OD1	1:t:346:SER:N	2.21	0.72
1:6:345:ASP:OD1	1:6:346:SER:N	2.21	0.72
1:B:295:ASP:OD2	1:K:397:TYR:OH	2.07	0.72
1:c:295:ASP:OD2	1:6:397:TYR:OH	2.07	0.72
1:f:345:ASP:OD1	1:f:346:SER:N	2.21	0.72
1:3:238[A]:ARG:HD2	1:3:683:GLU:OE2	1.90	0.72
1:E:295:ASP:OD2	1:R:397:TYR:OH	2.06	0.72
1:Q:345:ASP:OD1	1:Q:346:SER:N	2.21	0.72
1:O:345:ASP:OD1	1:O:346:SER:N	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:345:ASP:OD1	1:l:346:SER:N	2.21	0.72
1:A:397:TYR:OH	1:Q:295:ASP:OD2	2.07	0.71
1:x:345:ASP:OD1	1:x:346:SER:N	2.21	0.71
1:F:345:ASP:OD1	1:F:346:SER:N	2.21	0.71
1:y:345:ASP:OD1	1:y:346:SER:N	2.21	0.71
1:Q:298[A]:ARG:HG2	1:Q:298[A]:ARG:HH21	1.54	0.71
1:3:345:ASP:OD1	1:3:346:SER:N	2.21	0.71
1:a:345:ASP:OD1	1:a:346:SER:N	2.21	0.71
1:S:345:ASP:OD1	1:S:346:SER:N	2.21	0.71
1:n:238[A]:ARG:HD2	1:n:683:GLU:OE2	1.90	0.71
1:I:298[A]:ARG:HG2	1:I:298[A]:ARG:HH21	1.55	0.71
1:r:345:ASP:OD1	1:r:346:SER:N	2.21	0.71
1:E:345:ASP:OD1	1:E:346:SER:N	2.21	0.70
1:d:345:ASP:OD1	1:d:346:SER:N	2.21	0.70
1:8:234:TRP:HB3	1:8:298[A]:ARG:CZ	2.21	0.70
1:L:345:ASP:OD1	1:L:346:SER:N	2.21	0.70
1:j:345:ASP:OD1	1:j:346:SER:N	2.21	0.70
1:w:345:ASP:OD1	1:w:346:SER:N	2.21	0.70
1:n:345:ASP:OD1	1:n:346:SER:N	2.21	0.70
1:P:345:ASP:OD1	1:P:346:SER:N	2.21	0.70
1:z:345:ASP:OD1	1:z:346:SER:N	2.21	0.70
1:Z:518:ASN:HB3	1:Z:519:PRO:HD3	1.74	0.70
1:l:234:TRP:HB3	1:l:298[A]:ARG:CZ	2.22	0.70
1:3:518:ASN:HB3	1:3:519:PRO:HD3	1.74	0.70
1:S:518:ASN:HB3	1:S:519:PRO:HD3	1.74	0.69
1:a:518:ASN:HB3	1:a:519:PRO:HD3	1.74	0.69
1:8:518:ASN:HB3	1:8:519:PRO:HD3	1.74	0.69
1:A:298[A]:ARG:HG2	1:A:298[A]:ARG:HH21	1.58	0.69
1:H:518:ASN:HB3	1:H:519:PRO:HD3	1.74	0.69
1:r:518:ASN:HB3	1:r:519:PRO:HD3	1.74	0.69
1:5:518:ASN:HB3	1:5:519:PRO:HD3	1.74	0.69
1:J:518:ASN:HB3	1:J:519:PRO:HD3	1.74	0.69
1:V:518:ASN:HB3	1:V:519:PRO:HD3	1.74	0.69
1:d:518:ASN:HB3	1:d:519:PRO:HD3	1.74	0.69
1:n:518:ASN:HB3	1:n:519:PRO:HD3	1.74	0.69
1:2:518:ASN:HB3	1:2:519:PRO:HD3	1.74	0.69
1:u:518:ASN:HB3	1:u:519:PRO:HD3	1.74	0.69
1:I:518:ASN:HB3	1:I:519:PRO:HD3	1.75	0.69
1:O:518:ASN:HB3	1:O:519:PRO:HD3	1.74	0.69
1:Q:518:ASN:HB3	1:Q:519:PRO:HD3	1.75	0.69
1:W:518:ASN:HB3	1:W:519:PRO:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:518:ASN:HB3	1:l:519:PRO:HD3	1.74	0.69
1:p:518:ASN:HB3	1:p:519:PRO:HD3	1.74	0.69
1:x:518:ASN:HB3	1:x:519:PRO:HD3	1.74	0.69
1:1:345:ASP:OD1	1:1:346:SER:N	2.21	0.69
1:6:518:ASN:HB3	1:6:519:PRO:HD3	1.74	0.69
1:F:298[A]:ARG:HG2	1:F:298[A]:ARG:HH21	1.57	0.69
1:m:518:ASN:HB3	1:m:519:PRO:HD3	1.74	0.69
1:B:345:ASP:OD1	1:B:346:SER:N	2.21	0.69
1:P:518:ASN:HB3	1:P:519:PRO:HD3	1.74	0.69
1:T:518:ASN:HB3	1:T:519:PRO:HD3	1.74	0.69
1:j:518:ASN:HB3	1:j:519:PRO:HD3	1.74	0.69
1:K:633:LEU:HD11	1:X:603:GLY:HA3	1.75	0.68
1:Z:633:LEU:HD11	1:k:603:GLY:HA3	1.75	0.68
1:X:518:ASN:HB3	1:X:519:PRO:HD3	1.75	0.68
1:Y:518:ASN:HB3	1:Y:519:PRO:HD3	1.74	0.68
1:c:518:ASN:HB3	1:c:519:PRO:HD3	1.74	0.68
1:e:518:ASN:HB3	1:e:519:PRO:HD3	1.74	0.68
1:k:298[A]:ARG:HH21	1:k:298[A]:ARG:HG2	1.57	0.68
1:o:518:ASN:HB3	1:o:519:PRO:HD3	1.74	0.68
1:q:569:ASN:HD21	1:q:606:TRP:HB2	1.59	0.68
1:7:518:ASN:HB3	1:7:519:PRO:HD3	1.74	0.68
1:K:298[A]:ARG:HG2	1:K:298[A]:ARG:HH21	1.57	0.68
1:K:518:ASN:HB3	1:K:519:PRO:HD3	1.74	0.68
1:O:633:LEU:HD11	1:6:603:GLY:HA3	1.75	0.68
1:a:633:LEU:HD11	1:y:603:GLY:HA3	1.76	0.68
1:p:298[A]:ARG:HH21	1:p:298[A]:ARG:HG2	1.58	0.68
1:v:518:ASN:HB3	1:v:519:PRO:HD3	1.74	0.68
1:A:518:ASN:HB3	1:A:519:PRO:HD3	1.74	0.68
1:A:633:LEU:HD11	1:f:603:GLY:HA3	1.76	0.68
1:R:569:ASN:HD21	1:R:606:TRP:HB2	1.59	0.68
1:R:633:LEU:HD11	1:r:603:GLY:HA3	1.76	0.68
1:a:569:ASN:HD21	1:a:606:TRP:HB2	1.59	0.68
1:b:569:ASN:HD21	1:b:606:TRP:HB2	1.59	0.68
1:h:569:ASN:HD21	1:h:606:TRP:HB2	1.59	0.68
1:o:603:GLY:HA3	1:4:633:LEU:HD11	1.76	0.68
1:3:569:ASN:HD21	1:3:606:TRP:HB2	1.59	0.68
1:D:603:GLY:HA3	1:8:633:LEU:HD11	1.76	0.68
1:D:633:LEU:HD11	1:x:603:GLY:HA3	1.76	0.68
1:X:569:ASN:HD21	1:X:606:TRP:HB2	1.59	0.68
1:d:633:LEU:HD11	1:v:603:GLY:HA3	1.76	0.68
1:o:569:ASN:HD21	1:o:606:TRP:HB2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:518:ASN:HB3	1:s:519:PRO:HD3	1.74	0.68
1:x:569:ASN:HD21	1:x:606:TRP:HB2	1.59	0.68
1:4:518:ASN:HB3	1:4:519:PRO:HD3	1.74	0.68
1:E:298[A]:ARG:HH21	1:E:298[A]:ARG:HG2	1.59	0.68
1:F:603:GLY:HA3	1:3:633:LEU:HD11	1.76	0.68
1:M:569:ASN:HD21	1:M:606:TRP:HB2	1.59	0.68
1:f:518:ASN:HB3	1:f:519:PRO:HD3	1.74	0.68
1:f:569:ASN:HD21	1:f:606:TRP:HB2	1.59	0.68
1:y:518:ASN:HB3	1:y:519:PRO:HD3	1.74	0.68
1:y:569:ASN:HD21	1:y:606:TRP:HB2	1.59	0.68
1:I:569:ASN:HD21	1:I:606:TRP:HB2	1.59	0.68
1:I:633:LEU:HD11	1:O:603:GLY:HA3	1.76	0.68
1:Q:569:ASN:HD21	1:Q:606:TRP:HB2	1.59	0.68
1:W:603:GLY:HA3	1:l:633:LEU:HD11	1.76	0.68
1:b:518:ASN:HB3	1:b:519:PRO:HD3	1.74	0.68
1:n:569:ASN:HD21	1:n:606:TRP:HB2	1.59	0.68
1:t:518:ASN:HB3	1:t:519:PRO:HD3	1.74	0.68
1:u:569:ASN:HD21	1:u:606:TRP:HB2	1.59	0.68
1:C:518:ASN:HB3	1:C:519:PRO:HD3	1.74	0.68
1:E:633:LEU:HD11	1:i:603:GLY:HA3	1.76	0.68
1:N:603:GLY:HA3	1:w:633:LEU:HD11	1.76	0.68
1:N:633:LEU:HD11	1:V:603:GLY:HA3	1.76	0.68
1:Q:603:GLY:HA3	1:k:633:LEU:HD11	1.76	0.68
1:R:518:ASN:HB3	1:R:519:PRO:HD3	1.74	0.68
1:i:633:LEU:HD11	1:p:603:GLY:HA3	1.76	0.68
1:k:518:ASN:HB3	1:k:519:PRO:HD3	1.74	0.68
1:C:569:ASN:HD21	1:C:606:TRP:HB2	1.59	0.68
1:C:603:GLY:HA3	1:Y:633:LEU:HD11	1.76	0.68
1:F:569:ASN:HD21	1:F:606:TRP:HB2	1.59	0.68
1:G:518:ASN:HB3	1:G:519:PRO:HD3	1.74	0.68
1:L:518:ASN:HB3	1:L:519:PRO:HD3	1.74	0.68
1:N:569:ASN:HD21	1:N:606:TRP:HB2	1.59	0.68
1:U:518:ASN:HB3	1:U:519:PRO:HD3	1.74	0.68
1:Z:569:ASN:HD21	1:Z:606:TRP:HB2	1.59	0.68
1:d:569:ASN:HD21	1:d:606:TRP:HB2	1.59	0.68
1:i:569:ASN:HD21	1:i:606:TRP:HB2	1.59	0.68
1:r:569:ASN:HD21	1:r:606:TRP:HB2	1.59	0.68
1:D:518:ASN:HB3	1:D:519:PRO:HD3	1.75	0.67
1:F:518:ASN:HB3	1:F:519:PRO:HD3	1.74	0.67
1:G:298[A]:ARG:HG2	1:G:298[A]:ARG:HH21	1.59	0.67
1:M:518:ASN:HB3	1:M:519:PRO:HD3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:569:ASN:HD21	1:S:606:TRP:HB2	1.59	0.67
1:S:603:GLY:HA3	1:q:633:LEU:HD11	1.76	0.67
1:f:633:LEU:HD11	1:n:603:GLY:HA3	1.76	0.67
1:k:569:ASN:HD21	1:k:606:TRP:HB2	1.59	0.67
1:l:603:GLY:HA3	1:u:633:LEU:HD11	1.76	0.67
1:m:569:ASN:HD21	1:m:606:TRP:HB2	1.59	0.67
1:z:518:ASN:HB3	1:z:519:PRO:HD3	1.74	0.67
1:8:569:ASN:HD21	1:8:606:TRP:HB2	1.59	0.67
1:A:603:GLY:HA3	1:n:633:LEU:HD11	1.76	0.67
1:D:569:ASN:HD21	1:D:606:TRP:HB2	1.59	0.67
1:K:603:GLY:HA3	1:P:633:LEU:HD11	1.76	0.67
1:L:633:LEU:HD11	1:R:603:GLY:HA3	1.76	0.67
1:T:569:ASN:HD21	1:T:606:TRP:HB2	1.59	0.67
1:V:633:LEU:HD11	1:w:603:GLY:HA3	1.76	0.67
1:g:569:ASN:HD21	1:g:606:TRP:HB2	1.59	0.67
1:g:603:GLY:HA3	1:7:633:LEU:HD11	1.76	0.67
1:q:518:ASN:HB3	1:q:519:PRO:HD3	1.74	0.67
1:6:298[A]:ARG:HG2	1:6:298[A]:ARG:HH21	1.57	0.67
1:T:298[A]:ARG:HG2	1:T:298[A]:ARG:HH21	1.57	0.67
1:b:633:LEU:HD11	1:d:603:GLY:HA3	1.76	0.67
1:g:518:ASN:HB3	1:g:519:PRO:HD3	1.74	0.67
1:h:518:ASN:HB3	1:h:519:PRO:HD3	1.74	0.67
1:s:633:LEU:HD11	1:1:603:GLY:HA3	1.76	0.67
1:5:569:ASN:HD21	1:5:606:TRP:HB2	1.59	0.67
1:B:569:ASN:HD21	1:B:606:TRP:HB2	1.59	0.67
1:C:633:LEU:HD11	1:t:603:GLY:HA3	1.76	0.67
1:H:633:LEU:HD11	1:T:603:GLY:HA3	1.76	0.67
1:M:603:GLY:HA3	1:T:633:LEU:HD11	1.75	0.67
1:i:518:ASN:HB3	1:i:519:PRO:HD3	1.74	0.67
1:z:569:ASN:HD21	1:z:606:TRP:HB2	1.59	0.67
1:1:518:ASN:HB3	1:1:519:PRO:HD3	1.74	0.67
1:B:603:GLY:HA3	1:U:633:LEU:HD11	1.76	0.67
1:N:518:ASN:HB3	1:N:519:PRO:HD3	1.74	0.67
1:W:569:ASN:HD21	1:W:606:TRP:HB2	1.59	0.67
1:g:238[A]:ARG:HD2	1:g:683:GLU:OE2	1.95	0.67
1:t:569:ASN:HD21	1:t:606:TRP:HB2	1.59	0.67
1:1:569:ASN:HD21	1:1:606:TRP:HB2	1.59	0.67
1:2:569:ASN:HD21	1:2:606:TRP:HB2	1.59	0.67
1:6:569:ASN:HD21	1:6:606:TRP:HB2	1.59	0.67
1:E:603:GLY:HA3	1:p:633:LEU:HD11	1.76	0.67
1:H:603:GLY:HA3	1:M:633:LEU:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:603:GLY:HA3	1:v:633:LEU:HD11	1.76	0.67
1:h:633:LEU:HD11	1:5:603:GLY:HA3	1.76	0.67
1:p:238[A]:ARG:HD2	1:p:683:GLU:OE2	1.95	0.67
1:q:603:GLY:HA3	1:z:633:LEU:HD11	1.76	0.67
1:B:518:ASN:HB3	1:B:519:PRO:HD3	1.74	0.67
1:G:569:ASN:HD21	1:G:606:TRP:HB2	1.59	0.67
1:H:569:ASN:HD21	1:H:606:TRP:HB2	1.59	0.67
1:L:569:ASN:HD21	1:L:606:TRP:HB2	1.59	0.67
1:g:298[A]:ARG:HG2	1:g:298[A]:ARG:HH21	1.58	0.67
1:J:569:ASN:HD21	1:J:606:TRP:HB2	1.59	0.67
1:J:633:LEU:HD11	1:s:603:GLY:HA3	1.76	0.67
1:L:603:GLY:HA3	1:r:633:LEU:HD11	1.76	0.67
1:P:603:GLY:HA3	1:X:633:LEU:HD11	1.76	0.67
1:S:633:LEU:HD11	1:z:603:GLY:HA3	1.76	0.67
1:h:603:GLY:HA3	1:m:633:LEU:HD11	1.76	0.67
1:j:569:ASN:HD21	1:j:606:TRP:HB2	1.59	0.67
1:j:603:GLY:HA3	1:o:633:LEU:HD11	1.76	0.67
1:w:518:ASN:HB3	1:w:519:PRO:HD3	1.74	0.67
1:B:633:LEU:HD11	1:2:603:GLY:HA3	1.76	0.67
1:E:518:ASN:HB3	1:E:519:PRO:HD3	1.74	0.67
1:G:633:LEU:HD11	1:7:603:GLY:HA3	1.76	0.67
1:W:633:LEU:HD11	1:u:603:GLY:HA3	1.76	0.67
1:j:633:LEU:HD11	1:4:603:GLY:HA3	1.76	0.67
1:Q:633:LEU:HD11	1:Z:603:GLY:HA3	1.76	0.67
1:U:569:ASN:HD21	1:U:606:TRP:HB2	1.59	0.67
1:Z:298[A]:ARG:HG2	1:Z:298[A]:ARG:HH21	1.61	0.67
1:c:484:ARG:NH1	1:c:596:ASN:OD1	2.27	0.67
1:m:603:GLY:HA3	1:5:633:LEU:HD11	1.76	0.67
1:x:633:LEU:HD11	1:8:603:GLY:HA3	1.76	0.67
1:P:569:ASN:HD21	1:P:606:TRP:HB2	1.59	0.66
1:e:484:ARG:NH1	1:e:596:ASN:OD1	2.27	0.66
1:h:484:ARG:NH1	1:h:596:ASN:OD1	2.27	0.66
1:s:569:ASN:HD21	1:s:606:TRP:HB2	1.59	0.66
1:w:569:ASN:HD21	1:w:606:TRP:HB2	1.59	0.66
1:U:603:GLY:HA3	1:2:633:LEU:HD11	1.76	0.66
1:Y:569:ASN:HD21	1:Y:606:TRP:HB2	1.59	0.66
1:E:569:ASN:HD21	1:E:606:TRP:HB2	1.59	0.66
1:G:603:GLY:HA3	1:g:633:LEU:HD11	1.76	0.66
1:M:484:ARG:NH1	1:M:596:ASN:OD1	2.28	0.66
1:c:569:ASN:HD21	1:c:606:TRP:HB2	1.59	0.66
1:v:569:ASN:HD21	1:v:606:TRP:HB2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:569:ASN:HD21	1:7:606:TRP:HB2	1.59	0.66
1:H:298[A]:ARG:HH21	1:H:298[A]:ARG:HG2	1.60	0.66
1:j:484:ARG:NH1	1:j:596:ASN:OD1	2.27	0.66
1:4:569:ASN:HD21	1:4:606:TRP:HB2	1.59	0.66
1:K:569:ASN:HD21	1:K:606:TRP:HB2	1.59	0.66
1:e:569:ASN:HD21	1:e:606:TRP:HB2	1.59	0.66
1:x:612:TYR:HA	1:x:727:GLY:HA2	1.78	0.66
1:E:484:ARG:NH1	1:E:596:ASN:OD1	2.27	0.66
1:F:612:TYR:HA	1:F:727:GLY:HA2	1.78	0.66
1:c:633:LEU:HD11	1:3:603:GLY:HA3	1.76	0.66
1:y:612:TYR:HA	1:y:727:GLY:HA2	1.78	0.66
1:A:569:ASN:HD21	1:A:606:TRP:HB2	1.59	0.66
1:P:484:ARG:NH1	1:P:596:ASN:OD1	2.27	0.66
1:Y:603:GLY:HA3	1:t:633:LEU:HD11	1.76	0.66
1:w:484:ARG:NH1	1:w:596:ASN:OD1	2.28	0.66
1:G:612:TYR:HA	1:G:727:GLY:HA2	1.78	0.66
1:Q:612:TYR:HA	1:Q:727:GLY:HA2	1.78	0.66
1:a:603:GLY:HA3	1:e:633:LEU:HD11	1.76	0.66
1:E:238[B]:ARG:HD3	1:E:683:GLU:OE2	1.96	0.66
1:I:603:GLY:HA3	1:6:633:LEU:HD11	1.76	0.66
1:N:612:TYR:HA	1:N:727:GLY:HA2	1.78	0.66
1:Q:484:ARG:NH1	1:Q:596:ASN:OD1	2.27	0.66
1:h:612:TYR:HA	1:h:727:GLY:HA2	1.78	0.66
1:t:612:TYR:HA	1:t:727:GLY:HA2	1.78	0.66
1:M:612:TYR:HA	1:M:727:GLY:HA2	1.78	0.66
1:Y:484:ARG:NH1	1:Y:596:ASN:OD1	2.27	0.66
1:a:612:TYR:HA	1:a:727:GLY:HA2	1.78	0.66
1:i:612:TYR:HA	1:i:727:GLY:HA2	1.78	0.66
1:o:612:TYR:HA	1:o:727:GLY:HA2	1.78	0.66
1:3:612:TYR:HA	1:3:727:GLY:HA2	1.78	0.66
1:4:484:ARG:NH1	1:4:596:ASN:OD1	2.28	0.66
1:7:484:ARG:NH1	1:7:596:ASN:OD1	2.28	0.66
1:F:633:LEU:HD11	1:c:603:GLY:HA3	1.75	0.65
1:H:612:TYR:HA	1:H:727:GLY:HA2	1.78	0.65
1:R:612:TYR:HA	1:R:727:GLY:HA2	1.78	0.65
1:Y:612:TYR:HA	1:Y:727:GLY:HA2	1.78	0.65
1:Z:612:TYR:HA	1:Z:727:GLY:HA2	1.78	0.65
1:J:603:GLY:HA3	1:1:633:LEU:HD11	1.76	0.65
1:K:484:ARG:NH1	1:K:596:ASN:OD1	2.27	0.65
1:7:612:TYR:HA	1:7:727:GLY:HA2	1.78	0.65
1:A:612:TYR:HA	1:A:727:GLY:HA2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:238[B]:ARG:HD3	1:G:683:GLU:OE2	1.96	0.65
1:X:612:TYR:HA	1:X:727:GLY:HA2	1.78	0.65
1:e:603:GLY:HA3	1:y:633:LEU:HD11	1.76	0.65
1:q:612:TYR:HA	1:q:727:GLY:HA2	1.78	0.65
1:u:484:ARG:NH1	1:u:596:ASN:OD1	2.28	0.65
1:u:612:TYR:HA	1:u:727:GLY:HA2	1.78	0.65
1:1:612:TYR:HA	1:1:727:GLY:HA2	1.78	0.65
1:5:612:TYR:HA	1:5:727:GLY:HA2	1.78	0.65
1:8:612:TYR:HA	1:8:727:GLY:HA2	1.78	0.65
1:I:484:ARG:NH1	1:I:596:ASN:OD1	2.27	0.65
1:p:569:ASN:HD21	1:p:606:TRP:HB2	1.59	0.65
1:B:612:TYR:HA	1:B:727:GLY:HA2	1.78	0.65
1:I:612:TYR:HA	1:I:727:GLY:HA2	1.78	0.65
1:P:612:TYR:HA	1:P:727:GLY:HA2	1.78	0.65
1:X:234:TRP:CD2	1:X:298[A]:ARG:HD3	2.32	0.65
1:v:612:TYR:HA	1:v:727:GLY:HA2	1.78	0.65
1:y:234:TRP:CD2	1:y:298[A]:ARG:HD3	2.32	0.65
1:2:612:TYR:HA	1:2:727:GLY:HA2	1.78	0.65
1:4:612:TYR:HA	1:4:727:GLY:HA2	1.78	0.65
1:D:484:ARG:NH1	1:D:596:ASN:OD1	2.27	0.65
1:L:298[A]:ARG:HG2	1:L:298[A]:ARG:NH2	2.06	0.65
1:V:569:ASN:HD21	1:V:606:TRP:HB2	1.59	0.65
1:p:612:TYR:HA	1:p:727:GLY:HA2	1.78	0.65
1:V:612:TYR:HA	1:V:727:GLY:HA2	1.78	0.65
1:j:612:TYR:HA	1:j:727:GLY:HA2	1.78	0.65
1:J:612:TYR:HA	1:J:727:GLY:HA2	1.78	0.65
1:K:612:TYR:HA	1:K:727:GLY:HA2	1.78	0.65
1:O:569:ASN:HD21	1:O:606:TRP:HB2	1.59	0.65
1:l:569:ASN:HD21	1:l:606:TRP:HB2	1.59	0.65
1:O:298[A]:ARG:HG2	1:O:298[A]:ARG:HH21	1.60	0.65
1:S:612:TYR:HA	1:S:727:GLY:HA2	1.78	0.65
1:U:612:TYR:HA	1:U:727:GLY:HA2	1.78	0.65
1:k:612:TYR:HA	1:k:727:GLY:HA2	1.78	0.65
1:s:612:TYR:HA	1:s:727:GLY:HA2	1.78	0.65
1:D:612:TYR:HA	1:D:727:GLY:HA2	1.78	0.65
1:k:484:ARG:NH1	1:k:596:ASN:OD1	2.28	0.65
1:M:234:TRP:CD2	1:M:298[A]:ARG:HD3	2.32	0.64
1:b:612:TYR:HA	1:b:727:GLY:HA2	1.78	0.64
1:r:612:TYR:HA	1:r:727:GLY:HA2	1.78	0.64
1:5:484:ARG:NH1	1:5:596:ASN:OD1	2.27	0.64
1:P:298[A]:ARG:HH21	1:P:298[A]:ARG:HG2	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:234:TRP:CD2	1:5:298[A]:ARG:HD3	2.32	0.64
1:f:612:TYR:HA	1:f:727:GLY:HA2	1.78	0.64
1:2:298[A]:ARG:HH22	1:2:688:LYS:NZ	1.95	0.64
1:O:612:TYR:HA	1:O:727:GLY:HA2	1.78	0.64
1:W:612:TYR:HA	1:W:727:GLY:HA2	1.78	0.64
1:a:484:ARG:NH1	1:a:596:ASN:OD1	2.28	0.64
1:n:612:TYR:HA	1:n:727:GLY:HA2	1.78	0.64
1:H:484:ARG:NH1	1:H:596:ASN:OD1	2.27	0.64
1:d:612:TYR:HA	1:d:727:GLY:HA2	1.78	0.64
1:g:612:TYR:HA	1:g:727:GLY:HA2	1.78	0.64
1:l:238[A]:ARG:HD2	1:l:683:GLU:OE2	1.98	0.64
1:l:612:TYR:HA	1:l:727:GLY:HA2	1.78	0.64
1:3:484:ARG:NH1	1:3:596:ASN:OD1	2.27	0.64
1:L:612:TYR:HA	1:L:727:GLY:HA2	1.78	0.64
1:r:298[A]:ARG:HH22	1:r:688:LYS:NZ	1.95	0.64
1:C:612:TYR:HA	1:C:727:GLY:HA2	1.78	0.64
1:E:612:TYR:HA	1:E:727:GLY:HA2	1.78	0.64
1:6:612:TYR:HA	1:6:727:GLY:HA2	1.78	0.64
1:c:612:TYR:HA	1:c:727:GLY:HA2	1.78	0.64
1:m:612:TYR:HA	1:m:727:GLY:HA2	1.78	0.64
1:v:234:TRP:CD2	1:v:298[A]:ARG:HD3	2.32	0.64
1:w:612:TYR:HA	1:w:727:GLY:HA2	1.78	0.64
1:c:298[A]:ARG:HH21	1:c:298[A]:ARG:HG2	1.63	0.64
1:e:612:TYR:HA	1:e:727:GLY:HA2	1.78	0.64
1:f:298[A]:ARG:HG2	1:f:298[A]:ARG:HH21	1.62	0.64
1:T:612:TYR:HA	1:T:727:GLY:HA2	1.78	0.64
1:W:484:ARG:NH1	1:W:596:ASN:OD1	2.27	0.64
1:z:612:TYR:HA	1:z:727:GLY:HA2	1.78	0.64
1:8:238[A]:ARG:HD2	1:8:683:GLU:OE2	1.97	0.64
1:Z:484:ARG:NH1	1:Z:596:ASN:OD1	2.27	0.63
1:B:484:ARG:NH1	1:B:596:ASN:OD1	2.28	0.63
1:6:484:ARG:NH1	1:6:596:ASN:OD1	2.28	0.63
1:r:298[A]:ARG:HG2	1:r:298[A]:ARG:HH21	1.63	0.63
1:1:484:ARG:NH1	1:1:596:ASN:OD1	2.28	0.63
1:j:234:TRP:CD2	1:j:298[A]:ARG:HD3	2.32	0.63
1:T:484:ARG:NH1	1:T:596:ASN:OD1	2.27	0.63
1:m:484:ARG:NH1	1:m:596:ASN:OD1	2.28	0.63
1:8:484:ARG:NH1	1:8:596:ASN:OD1	2.28	0.63
1:U:238[A]:ARG:HD2	1:U:683:GLU:OE2	1.99	0.63
1:Y:234:TRP:CZ2	1:Y:298[A]:ARG:HB3	2.34	0.63
1:N:234:TRP:CZ2	1:N:298[A]:ARG:HB3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:298[A]:ARG:HH21	1:2:298[A]:ARG:HG2	1.63	0.62
1:h:234:TRP:CD2	1:h:298[A]:ARG:HD3	2.34	0.62
1:o:484:ARG:NH1	1:o:596:ASN:OD1	2.27	0.62
1:V:298[A]:ARG:HG2	1:V:298[A]:ARG:HH21	1.64	0.62
1:X:484:ARG:NH1	1:X:596:ASN:OD1	2.28	0.62
1:y:484:ARG:NH1	1:y:596:ASN:OD1	2.27	0.62
1:L:238[A]:ARG:HD2	1:L:683:GLU:OE2	1.99	0.62
1:d:484:ARG:NH1	1:d:596:ASN:OD1	2.27	0.62
1:4:234:TRP:CG	1:4:298[A]:ARG:HD3	2.35	0.62
1:R:484:ARG:NH1	1:R:596:ASN:OD1	2.28	0.62
1:e:234:TRP:HB3	1:e:298[A]:ARG:CZ	2.30	0.62
1:8:298[A]:ARG:HH21	1:8:298[A]:ARG:HG2	1.65	0.62
1:F:484:ARG:NH1	1:F:596:ASN:OD1	2.28	0.62
1:G:484:ARG:NH1	1:G:596:ASN:OD1	2.27	0.61
1:V:484:ARG:NH1	1:V:596:ASN:OD1	2.28	0.61
1:k:238[A]:ARG:HD2	1:k:683:GLU:OE2	2.00	0.61
1:t:484:ARG:NH1	1:t:596:ASN:OD1	2.28	0.61
1:b:234:TRP:HB3	1:b:298[A]:ARG:CZ	2.30	0.61
1:n:484:ARG:NH1	1:n:596:ASN:OD1	2.28	0.61
1:F:302:ASN:HD21	1:K:302:ASN:HD21	1.48	0.61
1:m:234:TRP:CG	1:m:298[A]:ARG:HD3	2.35	0.61
1:6:238[A]:ARG:HD2	1:6:683:GLU:OE2	2.00	0.61
1:f:484:ARG:NH1	1:f:596:ASN:OD1	2.28	0.61
1:q:484:ARG:NH1	1:q:596:ASN:OD1	2.28	0.61
1:r:298[A]:ARG:HH22	1:r:688:LYS:HZ1	1.48	0.61
1:U:302:ASN:HD21	1:Z:302:ASN:HD21	1.49	0.61
1:b:484:ARG:NH1	1:b:596:ASN:OD1	2.27	0.61
1:o:234:TRP:CD2	1:o:298[A]:ARG:HD3	2.34	0.61
1:p:484:ARG:NH1	1:p:596:ASN:OD1	2.28	0.61
1:N:217:GLY:HA3	1:N:407:ASN:HA	1.83	0.61
1:R:217:GLY:HA3	1:R:407:ASN:HA	1.83	0.61
1:c:217:GLY:HA3	1:c:407:ASN:HA	1.83	0.61
1:i:217:GLY:HA3	1:i:407:ASN:HA	1.83	0.61
1:q:217:GLY:HA3	1:q:407:ASN:HA	1.83	0.61
1:8:217:GLY:HA3	1:8:407:ASN:HA	1.83	0.61
1:P:217:GLY:HA3	1:P:407:ASN:HA	1.83	0.61
1:S:302:ASN:HD21	1:w:302:ASN:HD21	1.49	0.61
1:Y:234:TRP:NE1	1:Y:298[B]:ARG:HD2	2.15	0.61
1:Z:217:GLY:HA3	1:Z:407:ASN:HA	1.83	0.61
1:e:217:GLY:HA3	1:e:407:ASN:HA	1.83	0.61
1:i:484:ARG:NH1	1:i:596:ASN:OD1	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:217:GLY:HA3	1:j:407:ASN:HA	1.83	0.61
1:3:234:TRP:CE2	1:3:298[B]:ARG:HD2	2.36	0.61
1:A:302:ASN:HD21	1:T:302:ASN:HD21	1.48	0.61
1:L:302:ASN:HD21	1:O:302:ASN:HD21	1.49	0.61
1:M:238[A]:ARG:HD2	1:M:683:GLU:OE2	2.01	0.61
1:M:298[A]:ARG:HG2	1:M:298[A]:ARG:NH2	2.15	0.61
1:O:217:GLY:HA3	1:O:407:ASN:HA	1.83	0.61
1:Y:217:GLY:HA3	1:Y:407:ASN:HA	1.83	0.61
1:v:217:GLY:HA3	1:v:407:ASN:HA	1.83	0.61
1:x:217:GLY:HA3	1:x:407:ASN:HA	1.83	0.61
1:D:302:ASN:HD21	1:6:302:ASN:HD21	1.49	0.61
1:E:302:ASN:HD21	1:r:302:ASN:HD21	1.49	0.61
1:M:217:GLY:HA3	1:M:407:ASN:HA	1.83	0.61
1:Q:217:GLY:HA3	1:Q:407:ASN:HA	1.83	0.61
1:X:217:GLY:HA3	1:X:407:ASN:HA	1.83	0.61
1:X:238[A]:ARG:HD2	1:X:683:GLU:OE2	2.01	0.61
1:e:238[B]:ARG:HD3	1:e:683:GLU:OE2	2.01	0.61
1:h:217:GLY:HA3	1:h:407:ASN:HA	1.83	0.61
1:o:217:GLY:HA3	1:o:407:ASN:HA	1.83	0.61
1:B:217:GLY:HA3	1:B:407:ASN:HA	1.83	0.60
1:N:484:ARG:NH1	1:N:596:ASN:OD1	2.27	0.60
1:O:484:ARG:NH1	1:O:596:ASN:OD1	2.27	0.60
1:l:217:GLY:HA3	1:l:407:ASN:HA	1.83	0.60
1:7:217:GLY:HA3	1:7:407:ASN:HA	1.83	0.60
1:A:217:GLY:HA3	1:A:407:ASN:HA	1.83	0.60
1:Y:238[A]:ARG:HD2	1:Y:683:GLU:OE2	2.01	0.60
1:s:484:ARG:NH1	1:s:596:ASN:OD1	2.27	0.60
1:1:217:GLY:HA3	1:1:407:ASN:HA	1.83	0.60
1:W:302:ASN:HD21	1:k:302:ASN:HD21	1.49	0.60
1:l:298[A]:ARG:HG2	1:l:298[A]:ARG:HH21	1.65	0.60
1:v:484:ARG:NH1	1:v:596:ASN:OD1	2.27	0.60
1:J:484:ARG:NH1	1:J:596:ASN:OD1	2.28	0.60
1:K:217:GLY:HA3	1:K:407:ASN:HA	1.83	0.60
1:N:302:ASN:HD21	1:i:302:ASN:HD21	1.49	0.60
1:V:217:GLY:HA3	1:V:407:ASN:HA	1.83	0.60
1:d:302:ASN:HD21	1:p:302:ASN:HD21	1.49	0.60
1:f:217:GLY:HA3	1:f:407:ASN:HA	1.83	0.60
1:u:217:GLY:HA3	1:u:407:ASN:HA	1.83	0.60
1:I:217:GLY:HA3	1:I:407:ASN:HA	1.83	0.60
1:I:302:ASN:HD21	1:c:302:ASN:HD21	1.48	0.60
1:N:234:TRP:NE1	1:N:298[B]:ARG:HD2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:302:ASN:HD21	1:n:302:ASN:HD21	1.49	0.60
1:b:217:GLY:HA3	1:b:407:ASN:HA	1.83	0.60
1:l:484:ARG:NH1	1:l:596:ASN:OD1	2.27	0.60
1:p:217:GLY:HA3	1:p:407:ASN:HA	1.83	0.60
1:2:484:ARG:NH1	1:2:596:ASN:OD1	2.28	0.60
1:4:217:GLY:HA3	1:4:407:ASN:HA	1.83	0.60
1:5:217:GLY:HA3	1:5:407:ASN:HA	1.83	0.60
1:A:484:ARG:NH1	1:A:596:ASN:OD1	2.27	0.60
1:A:500:TYR:CE2	1:f:448:THR:HG21	2.37	0.60
1:B:448:THR:HG21	1:U:500:TYR:CE2	2.37	0.60
1:C:298[A]:ARG:HG2	1:C:298[A]:ARG:HH21	1.64	0.60
1:C:500:TYR:CE2	1:t:448:THR:HG21	2.36	0.60
1:F:500:TYR:CE2	1:c:448:THR:HG21	2.36	0.60
1:H:217:GLY:HA3	1:H:407:ASN:HA	1.83	0.60
1:K:448:THR:HG21	1:P:500:TYR:CE2	2.37	0.60
1:L:217:GLY:HA3	1:L:407:ASN:HA	1.83	0.60
1:Q:500:TYR:CE2	1:Z:448:THR:HG21	2.37	0.60
1:T:217:GLY:HA3	1:T:407:ASN:HA	1.83	0.60
1:U:484:ARG:NH1	1:U:596:ASN:OD1	2.28	0.60
1:m:217:GLY:HA3	1:m:407:ASN:HA	1.83	0.60
1:n:234:TRP:CE2	1:n:298[B]:ARG:HD2	2.36	0.60
1:P:252:TYR:OH	1:P:372:VAL:O	2.20	0.60
1:a:217:GLY:HA3	1:a:407:ASN:HA	1.83	0.60
1:j:252:TYR:OH	1:j:372:VAL:O	2.20	0.60
1:m:252:TYR:OH	1:m:372:VAL:O	2.20	0.60
1:y:252:TYR:OH	1:y:372:VAL:O	2.20	0.60
1:z:484:ARG:NH1	1:z:596:ASN:OD1	2.27	0.60
1:B:302:ASN:HD21	1:X:302:ASN:HD21	1.48	0.60
1:F:252:TYR:OH	1:F:372:VAL:O	2.20	0.60
1:G:302:ASN:HD21	1:2:302:ASN:HD21	1.49	0.60
1:O:252:TYR:OH	1:O:372:VAL:O	2.20	0.60
1:S:217:GLY:HA3	1:S:407:ASN:HA	1.83	0.60
1:T:252:TYR:OH	1:T:372:VAL:O	2.20	0.60
1:r:217:GLY:HA3	1:r:407:ASN:HA	1.83	0.60
1:s:302:ASN:HD21	1:8:302:ASN:HD21	1.50	0.60
1:z:217:GLY:HA3	1:z:407:ASN:HA	1.83	0.60
1:z:252:TYR:OH	1:z:372:VAL:O	2.20	0.60
1:F:448:THR:HG21	1:3:500:TYR:CE2	2.37	0.60
1:F:610:ASP:OD1	1:F:611:VAL:N	2.35	0.60
1:G:500:TYR:CE2	1:7:448:THR:HG21	2.37	0.60
1:L:252:TYR:OH	1:L:372:VAL:O	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:500:TYR:CE2	1:r:448:THR:HG21	2.36	0.60
1:b:238[B]:ARG:HD3	1:b:683:GLU:OE2	2.01	0.60
1:e:252:TYR:OH	1:e:372:VAL:O	2.20	0.60
1:h:610:ASP:OD1	1:h:611:VAL:N	2.35	0.60
1:i:610:ASP:OD1	1:i:611:VAL:N	2.35	0.60
1:l:252:TYR:OH	1:l:372:VAL:O	2.20	0.60
1:m:302:ASN:HD21	1:v:302:ASN:HD21	1.50	0.60
1:2:298[A]:ARG:HH22	1:2:688:LYS:HZ1	1.48	0.60
1:3:217:GLY:HA3	1:3:407:ASN:HA	1.83	0.60
1:3:610:ASP:OD1	1:3:611:VAL:N	2.35	0.60
1:C:484:ARG:NH1	1:C:596:ASN:OD1	2.27	0.60
1:K:500:TYR:CE2	1:X:448:THR:HG21	2.37	0.60
1:M:610:ASP:OD1	1:M:611:VAL:N	2.35	0.60
1:Q:252:TYR:OH	1:Q:372:VAL:O	2.20	0.60
1:Z:500:TYR:CE2	1:k:448:THR:HG21	2.37	0.60
1:a:610:ASP:OD1	1:a:611:VAL:N	2.35	0.60
1:c:252:TYR:OH	1:c:372:VAL:O	2.20	0.60
1:j:610:ASP:OD1	1:j:611:VAL:N	2.35	0.60
1:y:610:ASP:OD1	1:y:611:VAL:N	2.35	0.60
1:z:610:ASP:OD1	1:z:611:VAL:N	2.35	0.60
1:B:500:TYR:CE2	1:2:448:THR:HG21	2.36	0.59
1:G:610:ASP:OD1	1:G:611:VAL:N	2.35	0.59
1:H:302:ASN:HD21	1:P:302:ASN:HD21	1.48	0.59
1:H:500:TYR:CE2	1:T:448:THR:HG21	2.37	0.59
1:L:484:ARG:NH1	1:L:596:ASN:OD1	2.27	0.59
1:N:610:ASP:OD1	1:N:611:VAL:N	2.35	0.59
1:P:610:ASP:OD1	1:P:611:VAL:N	2.35	0.59
1:S:484:ARG:NH1	1:S:596:ASN:OD1	2.27	0.59
1:W:217:GLY:HA3	1:W:407:ASN:HA	1.83	0.59
1:l:302:ASN:HD21	1:z:302:ASN:HD21	1.50	0.59
1:s:610:ASP:OD1	1:s:611:VAL:N	2.35	0.59
1:t:610:ASP:OD1	1:t:611:VAL:N	2.35	0.59
1:x:252:TYR:OH	1:x:372:VAL:O	2.20	0.59
1:y:302:ASN:HD21	1:4:302:ASN:HD21	1.50	0.59
1:2:610:ASP:OD1	1:2:611:VAL:N	2.35	0.59
1:D:217:GLY:HA3	1:D:407:ASN:HA	1.83	0.59
1:J:610:ASP:OD1	1:J:611:VAL:N	2.35	0.59
1:L:610:ASP:OD1	1:L:611:VAL:N	2.35	0.59
1:O:610:ASP:OD1	1:O:611:VAL:N	2.35	0.59
1:T:610:ASP:OD1	1:T:611:VAL:N	2.35	0.59
1:V:500:TYR:CE2	1:w:448:THR:HG21	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r:484:ARG:NH1	1:r:596:ASN:OD1	2.28	0.59
1:r:610:ASP:OD1	1:r:611:VAL:N	2.35	0.59
1:1:610:ASP:OD1	1:1:611:VAL:N	2.35	0.59
1:7:610:ASP:OD1	1:7:611:VAL:N	2.35	0.59
1:A:610:ASP:OD1	1:A:611:VAL:N	2.35	0.59
1:B:252:TYR:OH	1:B:372:VAL:O	2.20	0.59
1:B:610:ASP:OD1	1:B:611:VAL:N	2.35	0.59
1:C:217:GLY:HA3	1:C:407:ASN:HA	1.83	0.59
1:C:302:ASN:HD21	1:3:302:ASN:HD21	1.49	0.59
1:H:448:THR:HG21	1:M:500:TYR:CE2	2.37	0.59
1:I:234:TRP:CZ2	1:I:298[B]:ARG:HB2	2.37	0.59
1:J:217:GLY:HA3	1:J:407:ASN:HA	1.83	0.59
1:M:448:THR:HG21	1:T:500:TYR:CE2	2.37	0.59
1:Q:234:TRP:CZ2	1:Q:298[B]:ARG:HB2	2.37	0.59
1:S:252:TYR:OH	1:S:372:VAL:O	2.20	0.59
1:S:610:ASP:OD1	1:S:611:VAL:N	2.35	0.59
1:U:610:ASP:OD1	1:U:611:VAL:N	2.35	0.59
1:V:252:TYR:OH	1:V:372:VAL:O	2.20	0.59
1:W:610:ASP:OD1	1:W:611:VAL:N	2.35	0.59
1:Z:610:ASP:OD1	1:Z:611:VAL:N	2.35	0.59
1:d:610:ASP:OD1	1:d:611:VAL:N	2.35	0.59
1:k:252:TYR:OH	1:k:372:VAL:O	2.20	0.59
1:l:610:ASP:OD1	1:l:611:VAL:N	2.35	0.59
1:v:610:ASP:OD1	1:v:611:VAL:N	2.35	0.59
1:1:252:TYR:OH	1:1:372:VAL:O	2.20	0.59
1:6:610:ASP:OD1	1:6:611:VAL:N	2.35	0.59
1:I:610:ASP:OD1	1:I:611:VAL:N	2.35	0.59
1:Y:610:ASP:OD1	1:Y:611:VAL:N	2.35	0.59
1:a:302:ASN:HD21	1:g:302:ASN:HD21	1.49	0.59
1:g:217:GLY:HA3	1:g:407:ASN:HA	1.83	0.59
1:g:484:ARG:NH1	1:g:596:ASN:OD1	2.28	0.59
1:k:610:ASP:OD1	1:k:611:VAL:N	2.35	0.59
1:m:610:ASP:OD1	1:m:611:VAL:N	2.35	0.59
1:u:610:ASP:OD1	1:u:611:VAL:N	2.35	0.59
1:2:217:GLY:HA3	1:2:407:ASN:HA	1.83	0.59
1:8:610:ASP:OD1	1:8:611:VAL:N	2.35	0.59
1:A:448:THR:HG21	1:n:500:TYR:CE2	2.36	0.59
1:D:610:ASP:OD1	1:D:611:VAL:N	2.35	0.59
1:E:500:TYR:CE2	1:i:448:THR:HG21	2.37	0.59
1:L:500:TYR:CE2	1:R:448:THR:HG21	2.37	0.59
1:P:448:THR:HG21	1:X:500:TYR:CE2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:448:THR:HG21	1:2:500:TYR:CE2	2.38	0.59
1:d:217:GLY:HA3	1:d:407:ASN:HA	1.83	0.59
1:f:500:TYR:CE2	1:n:448:THR:HG21	2.37	0.59
1:o:610:ASP:OD1	1:o:611:VAL:N	2.35	0.59
1:p:252:TYR:OH	1:p:372:VAL:O	2.20	0.59
1:6:217:GLY:HA3	1:6:407:ASN:HA	1.83	0.59
1:C:448:THR:HG21	1:Y:500:TYR:CE2	2.38	0.59
1:E:217:GLY:HA3	1:E:407:ASN:HA	1.83	0.59
1:K:610:ASP:OD1	1:K:611:VAL:N	2.35	0.59
1:R:610:ASP:OD1	1:R:611:VAL:N	2.35	0.59
1:X:610:ASP:OD1	1:X:611:VAL:N	2.35	0.59
1:g:448:THR:HG21	1:7:500:TYR:CE2	2.38	0.59
1:k:217:GLY:HA3	1:k:407:ASN:HA	1.83	0.59
1:n:217:GLY:HA3	1:n:407:ASN:HA	1.83	0.59
1:n:610:ASP:OD1	1:n:611:VAL:N	2.35	0.59
1:s:217:GLY:HA3	1:s:407:ASN:HA	1.83	0.59
1:G:252:TYR:OH	1:G:372:VAL:O	2.20	0.59
1:I:252:TYR:OH	1:I:372:VAL:O	2.20	0.59
1:J:500:TYR:CE2	1:s:448:THR:HG21	2.38	0.59
1:Q:302:ASN:HD21	1:f:302:ASN:HD21	1.48	0.59
1:U:217:GLY:HA3	1:U:407:ASN:HA	1.83	0.59
1:V:610:ASP:OD1	1:V:611:VAL:N	2.35	0.59
1:a:500:TYR:CE2	1:y:448:THR:HG21	2.38	0.59
1:b:610:ASP:OD1	1:b:611:VAL:N	2.35	0.59
1:e:610:ASP:OD1	1:e:611:VAL:N	2.35	0.59
1:q:610:ASP:OD1	1:q:611:VAL:N	2.35	0.59
1:t:252:TYR:OH	1:t:372:VAL:O	2.20	0.59
1:4:610:ASP:OD1	1:4:611:VAL:N	2.35	0.59
1:X:298[A]:ARG:HG2	1:X:298[A]:ARG:NH2	2.15	0.59
1:a:252:TYR:OH	1:a:372:VAL:O	2.20	0.59
1:c:610:ASP:OD1	1:c:611:VAL:N	2.35	0.59
1:f:610:ASP:OD1	1:f:611:VAL:N	2.35	0.59
1:w:217:GLY:HA3	1:w:407:ASN:HA	1.83	0.59
1:D:500:TYR:CE2	1:x:448:THR:HG21	2.37	0.59
1:N:238[A]:ARG:HD2	1:N:683:GLU:OE2	2.01	0.59
1:c:500:TYR:CE2	1:3:448:THR:HG21	2.38	0.59
1:e:302:ASN:HD21	1:u:302:ASN:HD21	1.49	0.59
1:p:610:ASP:OD1	1:p:611:VAL:N	2.35	0.59
1:s:500:TYR:CE2	1:1:448:THR:HG21	2.38	0.59
1:u:252:TYR:OH	1:u:372:VAL:O	2.20	0.59
1:x:484:ARG:NH1	1:x:596:ASN:OD1	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:234:TRP:CD2	1:I:298[A]:ARG:HD3	2.38	0.59
1:O:500:TYR:CE2	1:6:448:THR:HG21	2.37	0.59
1:W:500:TYR:CE2	1:u:448:THR:HG21	2.37	0.59
1:m:428:GLN:NE2	1:5:351:PRO:HB3	2.18	0.59
1:5:610:ASP:OD1	1:5:611:VAL:N	2.35	0.59
1:H:610:ASP:OD1	1:H:611:VAL:N	2.35	0.58
1:I:500:TYR:CE2	1:O:448:THR:HG21	2.37	0.58
1:P:310:ARG:NE	1:P:683:GLU:OE1	2.36	0.58
1:Q:234:TRP:CD2	1:Q:298[A]:ARG:HD3	2.38	0.58
1:Q:310:ARG:NE	1:Q:683:GLU:OE1	2.37	0.58
1:S:234:TRP:CG	1:S:298[A]:ARG:HD3	2.38	0.58
1:Y:302:ASN:HD21	1:7:302:ASN:HD21	1.49	0.58
1:t:217:GLY:HA3	1:t:407:ASN:HA	1.83	0.58
1:t:234:TRP:CE2	1:t:298[B]:ARG:HD2	2.38	0.58
1:5:252:TYR:OH	1:5:372:VAL:O	2.20	0.58
1:E:252:TYR:OH	1:E:372:VAL:O	2.20	0.58
1:E:610:ASP:OD1	1:E:611:VAL:N	2.35	0.58
1:G:217:GLY:HA3	1:G:407:ASN:HA	1.83	0.58
1:G:448:THR:HG21	1:g:500:TYR:CE2	2.38	0.58
1:J:302:ASN:HD21	1:t:302:ASN:HD21	1.49	0.58
1:J:310:ARG:NE	1:J:683:GLU:OE1	2.37	0.58
1:K:252:TYR:OH	1:K:372:VAL:O	2.20	0.58
1:M:252:TYR:OH	1:M:372:VAL:O	2.20	0.58
1:f:310:ARG:NE	1:f:683:GLU:OE1	2.36	0.58
1:h:351:PRO:HB3	1:5:428:GLN:NE2	2.19	0.58
1:j:310:ARG:NE	1:j:683:GLU:OE1	2.37	0.58
1:o:252:TYR:OH	1:o:372:VAL:O	2.20	0.58
1:w:610:ASP:OD1	1:w:611:VAL:N	2.35	0.58
1:x:310:ARG:NE	1:x:683:GLU:OE1	2.37	0.58
1:2:310:ARG:NE	1:2:683:GLU:OE1	2.37	0.58
1:4:252:TYR:OH	1:4:372:VAL:O	2.20	0.58
1:B:310:ARG:NE	1:B:683:GLU:OE1	2.37	0.58
1:H:252:TYR:OH	1:H:372:VAL:O	2.20	0.58
1:M:302:ASN:HD21	1:R:302:ASN:HD21	1.48	0.58
1:Q:610:ASP:OD1	1:Q:611:VAL:N	2.35	0.58
1:S:310:ARG:NE	1:S:683:GLU:OE1	2.37	0.58
1:U:234:TRP:CZ2	1:U:298[A]:ARG:HB3	2.39	0.58
1:W:252:TYR:OH	1:W:372:VAL:O	2.20	0.58
1:Y:234:TRP:HB3	1:Y:298[A]:ARG:CZ	2.33	0.58
1:Y:448:THR:HG21	1:t:500:TYR:CE2	2.39	0.58
1:b:252:TYR:OH	1:b:372:VAL:O	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:310:ARG:NE	1:b:683:GLU:OE1	2.37	0.58
1:e:234:TRP:CZ2	1:e:298[A]:ARG:HB3	2.38	0.58
1:t:234:TRP:CD2	1:t:298[A]:ARG:HD3	2.39	0.58
1:6:252:TYR:OH	1:6:372:VAL:O	2.20	0.58
1:8:252:TYR:OH	1:8:372:VAL:O	2.20	0.58
1:H:310:ARG:NE	1:H:683:GLU:OE1	2.37	0.58
1:N:234:TRP:HB3	1:N:298[A]:ARG:CZ	2.33	0.58
1:W:310:ARG:NE	1:W:683:GLU:OE1	2.37	0.58
1:X:252:TYR:OH	1:X:372:VAL:O	2.20	0.58
1:Z:252:TYR:OH	1:Z:372:VAL:O	2.20	0.58
1:h:500:TYR:CE2	1:5:448:THR:HG21	2.39	0.58
1:o:302:ASN:HD21	1:1:302:ASN:HD21	1.50	0.58
1:r:310:ARG:NE	1:r:683:GLU:OE1	2.37	0.58
1:w:252:TYR:OH	1:w:372:VAL:O	2.20	0.58
1:x:500:TYR:CE2	1:8:448:THR:HG21	2.39	0.58
1:1:310:ARG:NE	1:1:683:GLU:OE1	2.37	0.58
1:6:310:ARG:NE	1:6:683:GLU:OE1	2.37	0.58
1:E:310:ARG:NE	1:E:683:GLU:OE1	2.37	0.58
1:I:310:ARG:NE	1:I:683:GLU:OE1	2.37	0.58
1:M:310:ARG:NE	1:M:683:GLU:OE1	2.36	0.58
1:T:310:ARG:NE	1:T:683:GLU:OE1	2.37	0.58
1:b:234:TRP:CZ2	1:b:298[A]:ARG:HB3	2.38	0.58
1:o:448:THR:HG21	1:4:500:TYR:CE2	2.38	0.58
1:u:310:ARG:NE	1:u:683:GLU:OE1	2.37	0.58
1:w:310:ARG:NE	1:w:683:GLU:OE1	2.37	0.58
1:x:610:ASP:OD1	1:x:611:VAL:N	2.35	0.58
1:3:310:ARG:NE	1:3:683:GLU:OE1	2.37	0.58
1:5:310:ARG:NE	1:5:683:GLU:OE1	2.36	0.58
1:D:448:THR:HG21	1:8:500:TYR:CE2	2.39	0.58
1:L:310:ARG:NE	1:L:683:GLU:OE1	2.37	0.58
1:a:310:ARG:NE	1:a:683:GLU:OE1	2.37	0.58
1:b:302:ASN:HD21	1:x:302:ASN:HD21	1.49	0.58
1:b:500:TYR:CE2	1:d:448:THR:HG21	2.38	0.58
1:e:310:ARG:NE	1:e:683:GLU:OE1	2.37	0.58
1:e:428:GLN:NE2	1:y:351:PRO:HB3	2.18	0.58
1:f:252:TYR:OH	1:f:372:VAL:O	2.20	0.58
1:g:252:TYR:OH	1:g:372:VAL:O	2.20	0.58
1:h:310:ARG:NE	1:h:683:GLU:OE1	2.37	0.58
1:j:500:TYR:CE2	1:4:448:THR:HG21	2.39	0.58
1:m:310:ARG:NE	1:m:683:GLU:OE1	2.36	0.58
1:s:351:PRO:HB3	1:1:428:GLN:NE2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:252:TYR:OH	1:v:372:VAL:O	2.20	0.58
1:y:217:GLY:HA3	1:y:407:ASN:HA	1.83	0.58
1:z:310:ARG:NE	1:z:683:GLU:OE1	2.37	0.58
1:3:252:TYR:OH	1:3:372:VAL:O	2.20	0.58
1:C:252:TYR:OH	1:C:372:VAL:O	2.20	0.58
1:F:217:GLY:HA3	1:F:407:ASN:HA	1.83	0.58
1:J:252:TYR:OH	1:J:372:VAL:O	2.20	0.58
1:h:448:THR:HG21	1:m:500:TYR:CE2	2.38	0.58
1:k:234:TRP:CE2	1:k:298[B]:ARG:HD2	2.39	0.58
1:q:428:GLN:NE2	1:z:351:PRO:HB3	2.19	0.58
1:s:252:TYR:OH	1:s:372:VAL:O	2.20	0.58
1:t:310:ARG:NE	1:t:683:GLU:OE1	2.37	0.58
1:2:252:TYR:OH	1:2:372:VAL:O	2.20	0.58
1:G:310:ARG:NE	1:G:683:GLU:OE1	2.37	0.58
1:N:428:GLN:NE2	1:w:351:PRO:HB3	2.19	0.58
1:R:310:ARG:NE	1:R:683:GLU:OE1	2.37	0.58
1:U:252:TYR:OH	1:U:372:VAL:O	2.20	0.58
1:c:310:ARG:NE	1:c:683:GLU:OE1	2.37	0.58
1:d:500:TYR:CE2	1:v:448:THR:HG21	2.38	0.58
1:h:428:GLN:NE2	1:m:351:PRO:HB3	2.19	0.58
1:q:310:ARG:NE	1:q:683:GLU:OE1	2.37	0.58
1:x:351:PRO:HB3	1:8:428:GLN:NE2	2.18	0.58
1:A:252:TYR:OH	1:A:372:VAL:O	2.20	0.58
1:N:252:TYR:OH	1:N:372:VAL:O	2.20	0.58
1:X:310:ARG:NE	1:X:683:GLU:OE1	2.36	0.58
1:g:610:ASP:OD1	1:g:611:VAL:N	2.35	0.58
1:i:500:TYR:CE2	1:p:448:THR:HG21	2.38	0.58
1:n:310:ARG:NE	1:n:683:GLU:OE1	2.36	0.58
1:q:448:THR:HG21	1:z:500:TYR:CE2	2.38	0.58
1:s:310:ARG:NE	1:s:683:GLU:OE1	2.37	0.58
1:w:234:TRP:CE2	1:w:298[B]:ARG:HD2	2.38	0.58
1:6:234:TRP:CE2	1:6:298[B]:ARG:HD2	2.39	0.58
1:C:610:ASP:OD1	1:C:611:VAL:N	2.35	0.58
1:E:428:GLN:NE2	1:p:351:PRO:HB3	2.19	0.58
1:I:448:THR:HG21	1:6:500:TYR:CE2	2.38	0.58
1:K:310:ARG:NE	1:K:683:GLU:OE1	2.37	0.58
1:L:448:THR:HG21	1:r:500:TYR:CE2	2.38	0.58
1:N:500:TYR:CE2	1:V:448:THR:HG21	2.38	0.58
1:O:310:ARG:NE	1:O:683:GLU:OE1	2.37	0.58
1:Q:448:THR:HG21	1:k:500:TYR:CE2	2.38	0.58
1:S:448:THR:HG21	1:q:500:TYR:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:500:TYR:CE2	1:z:448:THR:HG21	2.38	0.58
1:U:310:ARG:NE	1:U:683:GLU:OE1	2.37	0.58
1:Y:310:ARG:NE	1:Y:683:GLU:OE1	2.37	0.58
1:a:448:THR:HG21	1:e:500:TYR:CE2	2.38	0.58
1:b:448:THR:HG21	1:v:500:TYR:CE2	2.39	0.58
1:d:310:ARG:NE	1:d:683:GLU:OE1	2.37	0.58
1:g:310:ARG:NE	1:g:683:GLU:OE1	2.36	0.58
1:j:448:THR:HG21	1:o:500:TYR:CE2	2.39	0.58
1:o:310:ARG:NE	1:o:683:GLU:OE1	2.37	0.58
1:4:310:ARG:NE	1:4:683:GLU:OE1	2.36	0.58
1:7:310:ARG:NE	1:7:683:GLU:OE1	2.37	0.58
1:C:429:SER:HA	1:C:567:THR:HB	1.87	0.57
1:F:429:SER:HA	1:F:567:THR:HB	1.86	0.57
1:I:234:TRP:CZ2	1:I:298[A]:ARG:HB3	2.39	0.57
1:N:448:THR:HG21	1:w:500:TYR:CE2	2.39	0.57
1:Q:429:SER:HA	1:Q:567:THR:HB	1.86	0.57
1:g:429:SER:HA	1:g:567:THR:HB	1.86	0.57
1:h:302:ASN:HD21	1:q:302:ASN:HD21	1.50	0.57
1:i:252:TYR:OH	1:i:372:VAL:O	2.20	0.57
1:l:310:ARG:NE	1:l:683:GLU:OE1	2.37	0.57
1:l:428:GLN:NE2	1:u:351:PRO:HB3	2.18	0.57
1:m:448:THR:HG21	1:5:500:TYR:CE2	2.39	0.57
1:V:310:ARG:NE	1:V:683:GLU:OE1	2.37	0.57
1:b:428:GLN:NE2	1:v:351:PRO:HB3	2.18	0.57
1:d:252:TYR:OH	1:d:372:VAL:O	2.20	0.57
1:j:302:ASN:HD21	1:5:302:ASN:HD21	1.50	0.57
1:n:252:TYR:OH	1:n:372:VAL:O	2.20	0.57
1:A:310:ARG:NE	1:A:683:GLU:OE1	2.36	0.57
1:C:310:ARG:NE	1:C:683:GLU:OE1	2.37	0.57
1:D:429:SER:HA	1:D:567:THR:HB	1.86	0.57
1:E:429:SER:HA	1:E:567:THR:HB	1.86	0.57
1:E:448:THR:HG21	1:p:500:TYR:CE2	2.38	0.57
1:Q:428:GLN:NE2	1:k:351:PRO:HB3	2.19	0.57
1:Z:310:ARG:NE	1:Z:683:GLU:OE1	2.37	0.57
1:d:351:PRO:HB3	1:v:428:GLN:NE2	2.20	0.57
1:j:428:GLN:NE2	1:o:351:PRO:HB3	2.19	0.57
1:p:310:ARG:NE	1:p:683:GLU:OE1	2.37	0.57
1:r:429:SER:HA	1:r:567:THR:HB	1.86	0.57
1:x:429:SER:HA	1:x:567:THR:HB	1.86	0.57
1:y:310:ARG:NE	1:y:683:GLU:OE1	2.36	0.57
1:y:429:SER:HA	1:y:567:THR:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:SER:HA	1:B:567:THR:HB	1.86	0.57
1:D:252:TYR:OH	1:D:372:VAL:O	2.20	0.57
1:D:428:GLN:NE2	1:8:351:PRO:HB3	2.19	0.57
1:F:310:ARG:NE	1:F:683:GLU:OE1	2.37	0.57
1:I:428:GLN:NE2	1:6:351:PRO:HB3	2.19	0.57
1:L:429:SER:HA	1:L:567:THR:HB	1.86	0.57
1:W:429:SER:HA	1:W:567:THR:HB	1.86	0.57
1:a:428:GLN:NE2	1:e:351:PRO:HB3	2.20	0.57
1:e:448:THR:HG21	1:y:500:TYR:CE2	2.39	0.57
1:k:310:ARG:NE	1:k:683:GLU:OE1	2.37	0.57
1:k:429:SER:HA	1:k:567:THR:HB	1.86	0.57
1:v:310:ARG:NE	1:v:683:GLU:OE1	2.36	0.57
1:w:429:SER:HA	1:w:567:THR:HB	1.86	0.57
1:4:429:SER:HA	1:4:567:THR:HB	1.86	0.57
1:8:310:ARG:NE	1:8:683:GLU:OE1	2.37	0.57
1:D:310:ARG:NE	1:D:683:GLU:OE1	2.37	0.57
1:I:429:SER:HA	1:I:567:THR:HB	1.86	0.57
1:K:429:SER:HA	1:K:567:THR:HB	1.86	0.57
1:S:428:GLN:NE2	1:q:351:PRO:HB3	2.19	0.57
1:S:429:SER:HA	1:S:567:THR:HB	1.87	0.57
1:Y:428:GLN:NE2	1:t:351:PRO:HB3	2.19	0.57
1:b:429:SER:HA	1:b:567:THR:HB	1.86	0.57
1:i:351:PRO:HB3	1:p:428:GLN:NE2	2.20	0.57
1:j:351:PRO:HB3	1:4:428:GLN:NE2	2.18	0.57
1:r:252:TYR:OH	1:r:372:VAL:O	2.20	0.57
1:u:429:SER:HA	1:u:567:THR:HB	1.86	0.57
1:z:429:SER:HA	1:z:567:THR:HB	1.86	0.57
1:G:429:SER:HA	1:G:567:THR:HB	1.86	0.57
1:J:234:TRP:CG	1:J:298[A]:ARG:HD3	2.38	0.57
1:N:310:ARG:NE	1:N:683:GLU:OE1	2.37	0.57
1:V:351:PRO:HB3	1:w:428:GLN:NE2	2.20	0.57
1:Y:252:TYR:OH	1:Y:372:VAL:O	2.20	0.57
1:f:429:SER:HA	1:f:567:THR:HB	1.87	0.57
1:o:429:SER:HA	1:o:567:THR:HB	1.86	0.57
1:u:234:TRP:CE3	1:u:298[A]:ARG:HD3	2.39	0.57
1:1:429:SER:HA	1:1:567:THR:HB	1.87	0.57
1:6:429:SER:HA	1:6:567:THR:HB	1.86	0.57
1:A:429:SER:HA	1:A:567:THR:HB	1.87	0.57
1:J:428:GLN:NE2	1:1:351:PRO:HB3	2.19	0.57
1:L:234:TRP:CZ2	1:L:298[A]:ARG:HB3	2.39	0.57
1:L:428:GLN:NE2	1:r:351:PRO:HB3	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:448:THR:HG21	1:l:500:TYR:CE2	2.39	0.57
1:X:429:SER:HA	1:X:567:THR:HB	1.87	0.57
1:i:310:ARG:NE	1:i:683:GLU:OE1	2.37	0.57
1:t:429:SER:HA	1:t:567:THR:HB	1.86	0.57
1:v:429:SER:HA	1:v:567:THR:HB	1.87	0.57
1:w:234:TRP:CD2	1:w:298[A]:ARG:HD3	2.39	0.57
1:x:234:TRP:CE3	1:x:298[A]:ARG:HD3	2.39	0.57
1:h:252:TYR:OH	1:h:372:VAL:O	2.20	0.57
1:l:448:THR:HG21	1:u:500:TYR:CE2	2.39	0.57
1:J:448:THR:HG21	1:1:500:TYR:CE2	2.39	0.57
1:Q:234:TRP:CZ2	1:Q:298[A]:ARG:HB3	2.39	0.57
1:S:351:PRO:HB3	1:z:428:GLN:NE2	2.20	0.57
1:7:252:TYR:OH	1:7:372:VAL:O	2.20	0.57
1:D:351:PRO:HB3	1:x:428:GLN:NE2	2.20	0.57
1:R:252:TYR:OH	1:R:372:VAL:O	2.20	0.57
1:V:429:SER:HA	1:V:567:THR:HB	1.86	0.57
1:a:429:SER:HA	1:a:567:THR:HB	1.87	0.57
1:p:429:SER:HA	1:p:567:THR:HB	1.87	0.57
1:q:252:TYR:OH	1:q:372:VAL:O	2.20	0.57
1:3:429:SER:HA	1:3:567:THR:HB	1.86	0.57
1:G:428:GLN:NE2	1:g:351:PRO:HB3	2.19	0.56
1:b:351:PRO:HB3	1:d:428:GLN:NE2	2.20	0.56
1:g:428:GLN:NE2	1:7:351:PRO:HB3	2.20	0.56
1:j:247:TRP:O	1:j:675:THR:OG1	2.17	0.56
1:W:351:PRO:HB3	1:u:428:GLN:NE2	2.20	0.56
1:Y:429:SER:HA	1:Y:567:THR:HB	1.86	0.56
1:d:429:SER:HA	1:d:567:THR:HB	1.87	0.56
1:n:429:SER:HA	1:n:567:THR:HB	1.86	0.56
1:P:247:TRP:O	1:P:675:THR:OG1	2.17	0.56
1:Y:234:TRP:CZ2	1:Y:298[B]:ARG:HB2	2.40	0.56
1:a:351:PRO:HB3	1:y:428:GLN:NE2	2.19	0.56
1:c:351:PRO:HB3	1:3:428:GLN:NE2	2.21	0.56
1:o:428:GLN:NE2	1:4:351:PRO:HB3	2.19	0.56
1:4:234:TRP:CD2	1:4:298[A]:ARG:HD3	2.41	0.56
1:5:234:TRP:CG	1:5:298[A]:ARG:HD3	2.40	0.56
1:7:429:SER:HA	1:7:567:THR:HB	1.86	0.56
1:W:428:GLN:NE2	1:l:351:PRO:HB3	2.19	0.56
1:Z:351:PRO:HB3	1:k:428:GLN:NE2	2.20	0.56
1:j:429:SER:HA	1:j:567:THR:HB	1.86	0.56
1:x:353:VAL:HG11	1:8:435:ASN:HB2	1.88	0.56
1:N:351:PRO:HB3	1:V:428:GLN:NE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:429:SER:HA	1:P:567:THR:HB	1.86	0.56
1:U:298[A]:ARG:HG2	1:U:298[A]:ARG:NH2	2.06	0.56
1:b:298[A]:ARG:HG2	1:b:298[A]:ARG:HH21	1.71	0.56
1:h:569:ASN:ND2	1:h:606:TRP:HB2	2.21	0.56
1:2:429:SER:HA	1:2:567:THR:HB	1.86	0.56
1:C:351:PRO:HB3	1:t:428:GLN:NE2	2.20	0.56
1:H:428:GLN:NE2	1:M:351:PRO:HB3	2.21	0.56
1:J:429:SER:HA	1:J:567:THR:HB	1.86	0.56
1:O:429:SER:HA	1:O:567:THR:HB	1.86	0.56
1:C:428:GLN:NE2	1:Y:351:PRO:HB3	2.20	0.56
1:E:247:TRP:O	1:E:675:THR:OG1	2.17	0.56
1:J:351:PRO:HB3	1:s:428:GLN:NE2	2.20	0.56
1:O:569:ASN:ND2	1:O:606:TRP:HB2	2.21	0.56
1:T:429:SER:HA	1:T:567:THR:HB	1.86	0.56
1:h:429:SER:HA	1:h:567:THR:HB	1.87	0.56
1:l:429:SER:HA	1:l:567:THR:HB	1.87	0.56
1:w:298[A]:ARG:HH22	1:w:688:LYS:NZ	2.04	0.56
1:L:351:PRO:HB3	1:R:428:GLN:NE2	2.21	0.56
1:M:428:GLN:NE2	1:T:351:PRO:HB3	2.21	0.56
1:M:429:SER:HA	1:M:567:THR:HB	1.87	0.56
1:M:569:ASN:ND2	1:M:606:TRP:HB2	2.21	0.56
1:R:429:SER:HA	1:R:567:THR:HB	1.86	0.56
1:U:428:GLN:NE2	1:2:351:PRO:HB3	2.20	0.56
1:l:569:ASN:ND2	1:l:606:TRP:HB2	2.21	0.56
1:q:234:TRP:CD2	1:q:298[A]:ARG:HD3	2.41	0.56
1:q:429:SER:HA	1:q:567:THR:HB	1.87	0.56
1:s:429:SER:HA	1:s:567:THR:HB	1.86	0.56
1:Q:298[A]:ARG:HG2	1:Q:298[A]:ARG:NH2	2.21	0.56
1:U:429:SER:HA	1:U:567:THR:HB	1.86	0.56
1:U:569:ASN:ND2	1:U:606:TRP:HB2	2.21	0.56
1:f:351:PRO:HB3	1:n:428:GLN:NE2	2.20	0.56
1:h:353:VAL:HG11	1:5:435:ASN:HB2	1.88	0.56
1:j:234:TRP:CG	1:j:298[A]:ARG:HD3	2.40	0.56
1:m:429:SER:HA	1:m:567:THR:HB	1.86	0.56
1:S:569:ASN:ND2	1:S:606:TRP:HB2	2.21	0.56
1:T:569:ASN:ND2	1:T:606:TRP:HB2	2.21	0.56
1:Z:429:SER:HA	1:Z:567:THR:HB	1.86	0.56
1:b:569:ASN:ND2	1:b:606:TRP:HB2	2.21	0.56
1:e:429:SER:HA	1:e:567:THR:HB	1.86	0.56
1:f:569:ASN:ND2	1:f:606:TRP:HB2	2.21	0.56
1:r:569:ASN:ND2	1:r:606:TRP:HB2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:234:TRP:CD2	1:1:298[A]:ARG:HD3	2.41	0.56
1:5:569:ASN:ND2	1:5:606:TRP:HB2	2.21	0.56
1:6:569:ASN:ND2	1:6:606:TRP:HB2	2.21	0.56
1:A:428:GLN:NE2	1:n:351:PRO:HB3	2.21	0.55
1:H:569:ASN:ND2	1:H:606:TRP:HB2	2.21	0.55
1:c:569:ASN:ND2	1:c:606:TRP:HB2	2.21	0.55
1:m:569:ASN:ND2	1:m:606:TRP:HB2	2.21	0.55
1:s:569:ASN:ND2	1:s:606:TRP:HB2	2.21	0.55
1:2:234:TRP:CE2	1:2:298[B]:ARG:HD2	2.41	0.55
1:B:428:GLN:NE2	1:U:351:PRO:HB3	2.21	0.55
1:D:298[A]:ARG:HG2	1:D:298[A]:ARG:HH21	1.71	0.55
1:E:351:PRO:HB3	1:i:428:GLN:NE2	2.21	0.55
1:H:351:PRO:HB3	1:T:428:GLN:NE2	2.21	0.55
1:K:569:ASN:ND2	1:K:606:TRP:HB2	2.21	0.55
1:N:234:TRP:CZ2	1:N:298[B]:ARG:HB2	2.40	0.55
1:N:429:SER:HA	1:N:567:THR:HB	1.86	0.55
1:O:351:PRO:HB3	1:6:428:GLN:NE2	2.20	0.55
1:P:428:GLN:NE2	1:X:351:PRO:HB3	2.21	0.55
1:W:569:ASN:ND2	1:W:606:TRP:HB2	2.21	0.55
1:e:569:ASN:ND2	1:e:606:TRP:HB2	2.21	0.55
1:i:429:SER:HA	1:i:567:THR:HB	1.86	0.55
1:j:435:ASN:HB2	1:o:353:VAL:HG11	1.88	0.55
1:8:429:SER:HA	1:8:567:THR:HB	1.87	0.55
1:P:294:ARG:HG3	1:P:298[B]:ARG:HH11	1.72	0.55
1:W:298[A]:ARG:HG2	1:W:298[A]:ARG:HH21	1.71	0.55
1:Z:569:ASN:ND2	1:Z:606:TRP:HB2	2.21	0.55
1:b:428:GLN:HE22	1:v:351:PRO:HB3	1.72	0.55
1:c:429:SER:HA	1:c:567:THR:HB	1.87	0.55
1:d:353:VAL:HG11	1:v:435:ASN:HB2	1.89	0.55
1:e:428:GLN:HE22	1:y:351:PRO:HB3	1.72	0.55
1:n:287:PHE:HB2	1:n:613:LEU:O	2.07	0.55
1:s:287:PHE:HB2	1:s:613:LEU:O	2.07	0.55
1:4:569:ASN:ND2	1:4:606:TRP:HB2	2.21	0.55
1:5:429:SER:HA	1:5:567:THR:HB	1.86	0.55
1:F:428:GLN:NE2	1:3:351:PRO:HB3	2.21	0.55
1:G:351:PRO:HB3	1:7:428:GLN:NE2	2.21	0.55
1:L:234:TRP:NE1	1:L:298[B]:ARG:HD2	2.22	0.55
1:Q:351:PRO:HB3	1:Z:428:GLN:NE2	2.21	0.55
1:Q:569:ASN:ND2	1:Q:606:TRP:HB2	2.21	0.55
1:X:287:PHE:HB2	1:X:613:LEU:O	2.07	0.55
1:a:287:PHE:HB2	1:a:613:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:435:ASN:HB2	1:v:353:VAL:HG11	1.88	0.55
1:d:287:PHE:HB2	1:d:613:LEU:O	2.07	0.55
1:j:353:VAL:HG11	1:4:435:ASN:HB2	1.89	0.55
1:l:435:ASN:HB2	1:u:353:VAL:HG11	1.88	0.55
1:m:435:ASN:HB2	1:5:353:VAL:HG11	1.89	0.55
1:u:287:PHE:HB2	1:u:613:LEU:O	2.07	0.55
1:3:287:PHE:HB2	1:3:613:LEU:O	2.07	0.55
1:8:569:ASN:ND2	1:8:606:TRP:HB2	2.21	0.55
1:H:429:SER:HA	1:H:567:THR:HB	1.87	0.55
1:I:287:PHE:HB2	1:I:613:LEU:O	2.07	0.55
1:P:287:PHE:HB2	1:P:613:LEU:O	2.07	0.55
1:U:287:PHE:HB2	1:U:613:LEU:O	2.07	0.55
1:V:569:ASN:ND2	1:V:606:TRP:HB2	2.21	0.55
1:l:287:PHE:HB2	1:l:613:LEU:O	2.07	0.55
1:o:287:PHE:HB2	1:o:613:LEU:O	2.07	0.55
1:s:353:VAL:HG11	1:1:435:ASN:HB2	1.88	0.55
1:w:569:ASN:ND2	1:w:606:TRP:HB2	2.21	0.55
1:x:569:ASN:ND2	1:x:606:TRP:HB2	2.21	0.55
1:7:287:PHE:HB2	1:7:613:LEU:O	2.07	0.55
1:E:569:ASN:ND2	1:E:606:TRP:HB2	2.21	0.55
1:O:287:PHE:HB2	1:O:613:LEU:O	2.07	0.55
1:R:351:PRO:HB3	1:r:428:GLN:NE2	2.21	0.55
1:Y:287:PHE:HB2	1:Y:613:LEU:O	2.07	0.55
1:j:287:PHE:HB2	1:j:613:LEU:O	2.07	0.55
1:j:569:ASN:ND2	1:j:606:TRP:HB2	2.21	0.55
1:m:234:TRP:CD2	1:m:298[A]:ARG:HD3	2.41	0.55
1:q:287:PHE:HB2	1:q:613:LEU:O	2.07	0.55
1:t:298[A]:ARG:HH22	1:t:688:LYS:NZ	2.04	0.55
1:x:351:PRO:HB3	1:8:428:GLN:HE22	1.72	0.55
1:Q:287:PHE:HB2	1:Q:613:LEU:O	2.07	0.55
1:R:287:PHE:HB2	1:R:613:LEU:O	2.07	0.55
1:p:569:ASN:ND2	1:p:606:TRP:HB2	2.21	0.55
1:x:287:PHE:HB2	1:x:613:LEU:O	2.07	0.55
1:A:287:PHE:HB2	1:A:613:LEU:O	2.07	0.55
1:I:569:ASN:ND2	1:I:606:TRP:HB2	2.21	0.55
1:P:569:ASN:ND2	1:P:606:TRP:HB2	2.21	0.55
1:a:353:VAL:HG11	1:y:435:ASN:HB2	1.89	0.55
1:e:435:ASN:HB2	1:y:353:VAL:HG11	1.88	0.55
1:C:287:PHE:HB2	1:C:613:LEU:O	2.07	0.55
1:I:351:PRO:HB3	1:O:428:GLN:NE2	2.21	0.55
1:J:569:ASN:ND2	1:J:606:TRP:HB2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:287:PHE:HB2	1:T:613:LEU:O	2.07	0.55
1:g:287:PHE:HB2	1:g:613:LEU:O	2.07	0.55
1:m:287:PHE:HB2	1:m:613:LEU:O	2.07	0.55
1:u:569:ASN:ND2	1:u:606:TRP:HB2	2.21	0.55
1:v:287:PHE:HB2	1:v:613:LEU:O	2.07	0.55
1:w:287:PHE:HB2	1:w:613:LEU:O	2.07	0.55
1:4:287:PHE:HB2	1:4:613:LEU:O	2.07	0.55
1:D:428:GLN:HE22	1:8:351:PRO:HB3	1.72	0.55
1:F:287:PHE:HB2	1:F:613:LEU:O	2.07	0.55
1:I:428:GLN:HE22	1:6:351:PRO:HB3	1.72	0.55
1:J:428:GLN:HE22	1:1:351:PRO:HB3	1.72	0.55
1:K:287:PHE:HB2	1:K:613:LEU:O	2.07	0.55
1:M:287:PHE:HB2	1:M:613:LEU:O	2.07	0.55
1:W:287:PHE:HB2	1:W:613:LEU:O	2.07	0.55
1:h:287:PHE:HB2	1:h:613:LEU:O	2.07	0.55
1:y:287:PHE:HB2	1:y:613:LEU:O	2.07	0.55
1:2:569:ASN:ND2	1:2:606:TRP:HB2	2.21	0.55
1:6:287:PHE:HB2	1:6:613:LEU:O	2.07	0.55
1:E:287:PHE:HB2	1:E:613:LEU:O	2.07	0.54
1:H:294:ARG:HG3	1:H:298[B]:ARG:HH11	1.72	0.54
1:K:428:GLN:NE2	1:P:351:PRO:HB3	2.21	0.54
1:U:234:TRP:NE1	1:U:298[B]:ARG:HD2	2.22	0.54
1:a:569:ASN:ND2	1:a:606:TRP:HB2	2.21	0.54
1:f:287:PHE:HB2	1:f:613:LEU:O	2.07	0.54
1:o:569:ASN:ND2	1:o:606:TRP:HB2	2.21	0.54
1:r:234:TRP:CE2	1:r:298[B]:ARG:HD2	2.41	0.54
1:8:287:PHE:HB2	1:8:613:LEU:O	2.07	0.54
1:B:351:PRO:HB3	1:2:428:GLN:NE2	2.21	0.54
1:Y:569:ASN:ND2	1:Y:606:TRP:HB2	2.21	0.54
1:b:287:PHE:HB2	1:b:613:LEU:O	2.07	0.54
1:i:287:PHE:HB2	1:i:613:LEU:O	2.07	0.54
1:i:353:VAL:HG11	1:p:435:ASN:HB2	1.89	0.54
1:j:351:PRO:HB3	1:4:428:GLN:HE22	1.72	0.54
1:k:287:PHE:HB2	1:k:613:LEU:O	2.07	0.54
1:t:287:PHE:HB2	1:t:613:LEU:O	2.07	0.54
1:3:569:ASN:ND2	1:3:606:TRP:HB2	2.21	0.54
1:B:287:PHE:HB2	1:B:613:LEU:O	2.07	0.54
1:D:287:PHE:HB2	1:D:613:LEU:O	2.07	0.54
1:D:569:ASN:ND2	1:D:606:TRP:HB2	2.21	0.54
1:G:287:PHE:HB2	1:G:613:LEU:O	2.07	0.54
1:N:569:ASN:ND2	1:N:606:TRP:HB2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:231:ASP:OD1	1:V:232:SER:N	2.41	0.54
1:W:231:ASP:OD1	1:W:232:SER:N	2.41	0.54
1:X:569:ASN:ND2	1:X:606:TRP:HB2	2.21	0.54
1:Z:287:PHE:HB2	1:Z:613:LEU:O	2.07	0.54
1:b:234:TRP:CZ2	1:b:298[B]:ARG:HB2	2.43	0.54
1:h:428:GLN:HE22	1:m:351:PRO:HB3	1.73	0.54
1:n:569:ASN:ND2	1:n:606:TRP:HB2	2.21	0.54
1:p:231:ASP:OD1	1:p:232:SER:N	2.41	0.54
1:6:231:ASP:OD1	1:6:232:SER:N	2.41	0.54
1:7:569:ASN:ND2	1:7:606:TRP:HB2	2.21	0.54
1:K:351:PRO:HB3	1:X:428:GLN:NE2	2.21	0.54
1:N:287:PHE:HB2	1:N:613:LEU:O	2.07	0.54
1:P:231:ASP:OD1	1:P:232:SER:N	2.41	0.54
1:S:231:ASP:OD1	1:S:232:SER:N	2.41	0.54
1:T:231:ASP:OD1	1:T:232:SER:N	2.41	0.54
1:U:231:ASP:OD1	1:U:232:SER:N	2.41	0.54
1:Y:435:ASN:HB2	1:t:353:VAL:HG11	1.89	0.54
1:e:298[A]:ARG:HH21	1:e:298[A]:ARG:HG2	1.71	0.54
1:k:569:ASN:ND2	1:k:606:TRP:HB2	2.21	0.54
1:l:428:GLN:HE22	1:u:351:PRO:HB3	1.72	0.54
1:m:231:ASP:OD1	1:m:232:SER:N	2.41	0.54
1:o:231:ASP:OD1	1:o:232:SER:N	2.41	0.54
1:o:428:GLN:HE22	1:4:351:PRO:HB3	1.73	0.54
1:r:231:ASP:OD1	1:r:232:SER:N	2.41	0.54
1:r:287:PHE:HB2	1:r:613:LEU:O	2.07	0.54
1:1:287:PHE:HB2	1:1:613:LEU:O	2.07	0.54
1:C:353:VAL:HG11	1:t:435:ASN:HB2	1.90	0.54
1:N:435:ASN:HB2	1:w:353:VAL:HG11	1.89	0.54
1:Q:231:ASP:OD1	1:Q:232:SER:N	2.41	0.54
1:W:428:GLN:HE22	1:l:351:PRO:HB3	1.72	0.54
1:X:231:ASP:OD1	1:X:232:SER:N	2.41	0.54
1:d:569:ASN:ND2	1:d:606:TRP:HB2	2.21	0.54
1:i:569:ASN:ND2	1:i:606:TRP:HB2	2.21	0.54
1:j:231:ASP:OD1	1:j:232:SER:N	2.41	0.54
1:q:569:ASN:ND2	1:q:606:TRP:HB2	2.21	0.54
1:s:231:ASP:OD1	1:s:232:SER:N	2.41	0.54
1:x:231:ASP:OD1	1:x:232:SER:N	2.41	0.54
1:J:287:PHE:HB2	1:J:613:LEU:O	2.07	0.54
1:L:569:ASN:ND2	1:L:606:TRP:HB2	2.21	0.54
1:N:351:PRO:HB3	1:V:428:GLN:HE22	1.73	0.54
1:O:353:VAL:HG11	1:6:435:ASN:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:287:PHE:HB2	1:S:613:LEU:O	2.07	0.54
1:i:231:ASP:OD1	1:i:232:SER:N	2.41	0.54
1:o:435:ASN:HB2	1:4:353:VAL:HG11	1.89	0.54
1:p:287:PHE:HB2	1:p:613:LEU:O	2.07	0.54
1:G:231:ASP:OD1	1:G:232:SER:N	2.41	0.54
1:N:231:ASP:OD1	1:N:232:SER:N	2.41	0.54
1:Q:428:GLN:HE22	1:k:351:PRO:HB3	1.72	0.54
1:S:428:GLN:HE22	1:q:351:PRO:HB3	1.72	0.54
1:V:287:PHE:HB2	1:V:613:LEU:O	2.07	0.54
1:d:247:TRP:O	1:d:675:THR:OG1	2.17	0.54
1:g:435:ASN:HB2	1:7:353:VAL:HG11	1.89	0.54
1:s:351:PRO:HB3	1:1:428:GLN:HE22	1.73	0.54
1:t:231:ASP:OD1	1:t:232:SER:N	2.41	0.54
1:z:569:ASN:ND2	1:z:606:TRP:HB2	2.21	0.54
1:2:287:PHE:HB2	1:2:613:LEU:O	2.07	0.54
1:C:231:ASP:OD1	1:C:232:SER:N	2.41	0.54
1:R:569:ASN:ND2	1:R:606:TRP:HB2	2.21	0.54
1:a:435:ASN:HB2	1:e:353:VAL:HG11	1.90	0.54
1:h:435:ASN:HB2	1:m:353:VAL:HG11	1.89	0.54
1:i:351:PRO:HB3	1:p:428:GLN:HE22	1.73	0.54
1:n:247:TRP:O	1:n:675:THR:OG1	2.17	0.54
1:q:231:ASP:OD1	1:q:232:SER:N	2.41	0.54
1:y:569:ASN:ND2	1:y:606:TRP:HB2	2.21	0.54
1:z:287:PHE:HB2	1:z:613:LEU:O	2.07	0.54
1:L:287:PHE:HB2	1:L:613:LEU:O	2.07	0.54
1:R:231:ASP:OD1	1:R:232:SER:N	2.41	0.54
1:S:234:TRP:CD2	1:S:298[A]:ARG:HD3	2.43	0.54
1:g:231:ASP:OD1	1:g:232:SER:N	2.41	0.54
1:w:231:ASP:OD1	1:w:232:SER:N	2.41	0.54
1:A:231:ASP:OD1	1:A:232:SER:N	2.41	0.54
1:E:231:ASP:OD1	1:E:232:SER:N	2.41	0.54
1:F:569:ASN:ND2	1:F:606:TRP:HB2	2.21	0.54
1:Y:428:GLN:HE22	1:t:351:PRO:HB3	1.72	0.54
1:a:428:GLN:HE22	1:e:351:PRO:HB3	1.73	0.54
1:c:287:PHE:HB2	1:c:613:LEU:O	2.07	0.54
1:e:234:TRP:CZ2	1:e:298[B]:ARG:HB2	2.43	0.54
1:e:287:PHE:HB2	1:e:613:LEU:O	2.07	0.54
1:k:563:GLU:O	1:k:566:ARG:HG3	2.08	0.54
1:l:231:ASP:OD1	1:l:232:SER:N	2.41	0.54
1:m:428:GLN:HE22	1:5:351:PRO:HB3	1.72	0.54
1:1:563:GLU:O	1:1:566:ARG:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:563:GLU:O	1:2:566:ARG:HG3	2.08	0.54
1:A:569:ASN:ND2	1:A:606:TRP:HB2	2.21	0.53
1:D:563:GLU:O	1:D:566:ARG:HG3	2.09	0.53
1:F:351:PRO:HB3	1:c:428:GLN:NE2	2.22	0.53
1:G:428:GLN:HE22	1:g:351:PRO:HB3	1.72	0.53
1:G:569:ASN:ND2	1:G:606:TRP:HB2	2.21	0.53
1:H:287:PHE:HB2	1:H:613:LEU:O	2.07	0.53
1:J:234:TRP:CD2	1:J:298[A]:ARG:HD3	2.43	0.53
1:J:563:GLU:O	1:J:566:ARG:HG3	2.08	0.53
1:K:563:GLU:O	1:K:566:ARG:HG3	2.08	0.53
1:L:563:GLU:O	1:L:566:ARG:HG3	2.08	0.53
1:N:563:GLU:O	1:N:566:ARG:HG3	2.08	0.53
1:S:234:TRP:CZ2	1:S:298[A]:ARG:HB3	2.44	0.53
1:W:353:VAL:HG11	1:u:435:ASN:HB2	1.90	0.53
1:g:428:GLN:HE22	1:7:351:PRO:HB3	1.73	0.53
1:i:563:GLU:O	1:i:566:ARG:HG3	2.08	0.53
1:v:231:ASP:OD1	1:v:232:SER:N	2.41	0.53
1:y:563:GLU:O	1:y:566:ARG:HG3	2.08	0.53
1:B:563:GLU:O	1:B:566:ARG:HG3	2.09	0.53
1:B:569:ASN:ND2	1:B:606:TRP:HB2	2.21	0.53
1:C:428:GLN:HE22	1:Y:351:PRO:HB3	1.73	0.53
1:C:569:ASN:ND2	1:C:606:TRP:HB2	2.21	0.53
1:F:563:GLU:O	1:F:566:ARG:HG3	2.08	0.53
1:U:428:GLN:HE22	1:2:351:PRO:HB3	1.73	0.53
1:W:435:ASN:HB2	1:l:353:VAL:HG11	1.91	0.53
1:d:231:ASP:OD1	1:d:232:SER:N	2.41	0.53
1:f:563:GLU:O	1:f:566:ARG:HG3	2.08	0.53
1:n:231:ASP:OD1	1:n:232:SER:N	2.41	0.53
1:o:563:GLU:O	1:o:566:ARG:HG3	2.08	0.53
1:q:428:GLN:HE22	1:z:351:PRO:HB3	1.73	0.53
1:q:435:ASN:HB2	1:z:353:VAL:HG11	1.88	0.53
1:t:569:ASN:ND2	1:t:606:TRP:HB2	2.21	0.53
1:u:231:ASP:OD1	1:u:232:SER:N	2.41	0.53
1:v:569:ASN:ND2	1:v:606:TRP:HB2	2.21	0.53
1:z:563:GLU:O	1:z:566:ARG:HG3	2.09	0.53
1:4:563:GLU:O	1:4:566:ARG:HG3	2.08	0.53
1:5:287:PHE:HB2	1:5:613:LEU:O	2.07	0.53
1:5:563:GLU:O	1:5:566:ARG:HG3	2.08	0.53
1:8:563:GLU:O	1:8:566:ARG:HG3	2.09	0.53
1:A:563:GLU:O	1:A:566:ARG:HG3	2.08	0.53
1:G:563:GLU:O	1:G:566:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:563:GLU:O	1:H:566:ARG:HG3	2.09	0.53
1:I:231:ASP:OD1	1:I:232:SER:N	2.41	0.53
1:J:231:ASP:OD1	1:J:232:SER:N	2.41	0.53
1:O:231:ASP:OD1	1:O:232:SER:N	2.41	0.53
1:O:563:GLU:O	1:O:566:ARG:HG3	2.08	0.53
1:Y:231:ASP:OD1	1:Y:232:SER:N	2.41	0.53
1:Z:353:VAL:HG11	1:k:435:ASN:HB2	1.90	0.53
1:Z:563:GLU:O	1:Z:566:ARG:HG3	2.09	0.53
1:a:351:PRO:HB3	1:y:428:GLN:HE22	1.73	0.53
1:a:563:GLU:O	1:a:566:ARG:HG3	2.08	0.53
1:g:569:ASN:ND2	1:g:606:TRP:HB2	2.21	0.53
1:t:563:GLU:O	1:t:566:ARG:HG3	2.08	0.53
1:y:231:ASP:OD1	1:y:232:SER:N	2.41	0.53
1:2:231:ASP:OD1	1:2:232:SER:N	2.41	0.53
1:7:231:ASP:OD1	1:7:232:SER:N	2.41	0.53
1:A:351:PRO:HB3	1:f:428:GLN:NE2	2.22	0.53
1:F:231:ASP:OD1	1:F:232:SER:N	2.41	0.53
1:F:428:GLN:HE22	1:3:351:PRO:HB3	1.74	0.53
1:J:351:PRO:HB3	1:s:428:GLN:HE22	1.74	0.53
1:P:563:GLU:O	1:P:566:ARG:HG3	2.09	0.53
1:X:563:GLU:O	1:X:566:ARG:HG3	2.09	0.53
1:b:563:GLU:O	1:b:566:ARG:HG3	2.09	0.53
1:c:353:VAL:HG11	1:3:435:ASN:HB2	1.91	0.53
1:d:413:TYR:OH	1:d:641:HIS:O	2.26	0.53
1:j:563:GLU:O	1:j:566:ARG:HG3	2.08	0.53
1:l:563:GLU:O	1:l:566:ARG:HG3	2.09	0.53
1:n:413:TYR:OH	1:n:641:HIS:O	2.26	0.53
1:1:569:ASN:ND2	1:1:606:TRP:HB2	2.21	0.53
1:D:435:ASN:HB2	1:8:353:VAL:HG11	1.90	0.53
1:J:413:TYR:OH	1:J:641:HIS:O	2.26	0.53
1:S:234:TRP:CZ2	1:S:298[B]:ARG:HB2	2.44	0.53
1:S:435:ASN:HB2	1:q:353:VAL:HG11	1.90	0.53
1:V:353:VAL:HG11	1:w:435:ASN:HB2	1.90	0.53
1:b:353:VAL:HG11	1:d:435:ASN:HB2	1.90	0.53
1:d:351:PRO:HB3	1:v:428:GLN:HE22	1.74	0.53
1:v:234:TRP:CD2	1:v:298[B]:ARG:HD2	2.44	0.53
1:v:563:GLU:O	1:v:566:ARG:HG3	2.08	0.53
1:3:563:GLU:O	1:3:566:ARG:HG3	2.08	0.53
1:C:563:GLU:O	1:C:566:ARG:HG3	2.08	0.53
1:L:428:GLN:HE22	1:r:351:PRO:HB3	1.73	0.53
1:M:428:GLN:HE22	1:T:351:PRO:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:563:GLU:O	1:S:566:ARG:HG3	2.08	0.53
1:T:563:GLU:O	1:T:566:ARG:HG3	2.08	0.53
1:g:563:GLU:O	1:g:566:ARG:HG3	2.09	0.53
1:r:563:GLU:O	1:r:566:ARG:HG3	2.09	0.53
1:u:413:TYR:OH	1:u:641:HIS:O	2.26	0.53
1:N:428:GLN:HE22	1:w:351:PRO:HB3	1.72	0.53
1:Q:351:PRO:HB3	1:Z:428:GLN:HE22	1.74	0.53
1:S:353:VAL:H	1:S:645:GLN:NE2	2.07	0.53
1:Y:563:GLU:O	1:Y:566:ARG:HG3	2.08	0.53
1:c:353:VAL:H	1:c:645:GLN:NE2	2.07	0.53
1:h:351:PRO:HB3	1:5:428:GLN:HE22	1.73	0.53
1:h:353:VAL:H	1:h:645:GLN:NE2	2.07	0.53
1:x:563:GLU:O	1:x:566:ARG:HG3	2.08	0.53
1:y:234:TRP:CD2	1:y:298[B]:ARG:HD2	2.44	0.53
1:z:231:ASP:OD1	1:z:232:SER:N	2.41	0.53
1:2:413:TYR:OH	1:2:641:HIS:O	2.26	0.53
1:B:428:GLN:HE22	1:U:351:PRO:HB3	1.74	0.53
1:D:353:VAL:H	1:D:645:GLN:NE2	2.07	0.53
1:E:428:GLN:HE22	1:p:351:PRO:HB3	1.72	0.53
1:G:435:ASN:HB2	1:g:353:VAL:HG11	1.91	0.53
1:I:413:TYR:OH	1:I:641:HIS:O	2.26	0.53
1:I:563:GLU:O	1:I:566:ARG:HG3	2.08	0.53
1:K:231:ASP:OD1	1:K:232:SER:N	2.41	0.53
1:L:231:ASP:OD1	1:L:232:SER:N	2.41	0.53
1:L:351:PRO:HB3	1:R:428:GLN:HE22	1.74	0.53
1:M:353:VAL:H	1:M:645:GLN:NE2	2.07	0.53
1:R:563:GLU:O	1:R:566:ARG:HG3	2.09	0.53
1:S:351:PRO:HB3	1:z:428:GLN:HE22	1.74	0.53
1:W:351:PRO:HB3	1:u:428:GLN:HE22	1.74	0.53
1:b:351:PRO:HB3	1:d:428:GLN:HE22	1.73	0.53
1:c:231:ASP:OD1	1:c:232:SER:N	2.41	0.53
1:f:353:VAL:HG11	1:n:435:ASN:HB2	1.90	0.53
1:k:353:VAL:H	1:k:645:GLN:NE2	2.07	0.53
1:m:563:GLU:O	1:m:566:ARG:HG3	2.08	0.53
1:q:563:GLU:O	1:q:566:ARG:HG3	2.08	0.53
1:r:353:VAL:H	1:r:645:GLN:NE2	2.07	0.53
1:u:563:GLU:O	1:u:566:ARG:HG3	2.08	0.53
1:z:353:VAL:H	1:z:645:GLN:NE2	2.07	0.53
1:4:231:ASP:OD1	1:4:232:SER:N	2.41	0.53
1:I:351:PRO:HB3	1:O:428:GLN:HE22	1.74	0.53
1:P:298[A]:ARG:HG2	1:P:298[A]:ARG:NH2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:563:GLU:O	1:Q:566:ARG:HG3	2.08	0.53
1:U:563:GLU:O	1:U:566:ARG:HG3	2.08	0.53
1:V:353:VAL:H	1:V:645:GLN:NE2	2.07	0.53
1:Z:351:PRO:HB3	1:k:428:GLN:HE22	1.74	0.53
1:c:351:PRO:HB3	1:3:428:GLN:HE22	1.74	0.53
1:e:353:VAL:H	1:e:645:GLN:NE2	2.07	0.53
1:j:428:GLN:HE22	1:o:351:PRO:HB3	1.73	0.53
1:o:239:VAL:HG13	1:o:684:TRP:HB2	1.91	0.53
1:p:353:VAL:H	1:p:645:GLN:NE2	2.07	0.53
1:q:353:VAL:H	1:q:645:GLN:NE2	2.07	0.53
1:s:247:TRP:O	1:s:675:THR:OG1	2.17	0.53
1:s:563:GLU:O	1:s:566:ARG:HG3	2.08	0.53
1:5:231:ASP:OD1	1:5:232:SER:N	2.41	0.53
1:7:563:GLU:O	1:7:566:ARG:HG3	2.08	0.53
1:H:231:ASP:OD1	1:H:232:SER:N	2.41	0.53
1:J:435:ASN:HB2	1:1:353:VAL:HG11	1.90	0.53
1:L:353:VAL:H	1:L:645:GLN:NE2	2.07	0.53
1:M:563:GLU:O	1:M:566:ARG:HG3	2.08	0.53
1:O:353:VAL:H	1:O:645:GLN:NE2	2.07	0.53
1:R:353:VAL:H	1:R:645:GLN:NE2	2.07	0.53
1:S:298[A]:ARG:HG2	1:S:298[A]:ARG:HH21	1.74	0.53
1:T:353:VAL:H	1:T:645:GLN:NE2	2.07	0.53
1:V:563:GLU:O	1:V:566:ARG:HG3	2.09	0.53
1:X:239:VAL:HG13	1:X:684:TRP:HB2	1.91	0.53
1:d:353:VAL:H	1:d:645:GLN:NE2	2.07	0.53
1:d:563:GLU:O	1:d:566:ARG:HG3	2.08	0.53
1:e:231:ASP:OD1	1:e:232:SER:N	2.41	0.53
1:h:563:GLU:O	1:h:566:ARG:HG3	2.08	0.53
1:l:353:VAL:H	1:l:645:GLN:NE2	2.07	0.53
1:m:353:VAL:H	1:m:645:GLN:NE2	2.07	0.53
1:n:563:GLU:O	1:n:566:ARG:HG3	2.08	0.53
1:y:239:VAL:HG13	1:y:684:TRP:HB2	1.91	0.53
1:z:239:VAL:HG13	1:z:684:TRP:HB2	1.91	0.53
1:K:351:PRO:HB3	1:X:428:GLN:HE22	1.74	0.52
1:L:239:VAL:HG13	1:L:684:TRP:HB2	1.92	0.52
1:Q:234:TRP:CE2	1:Q:298[A]:ARG:HD3	2.45	0.52
1:e:239:VAL:HG13	1:e:684:TRP:HB2	1.91	0.52
1:f:353:VAL:H	1:f:645:GLN:NE2	2.07	0.52
1:p:563:GLU:O	1:p:566:ARG:HG3	2.09	0.52
1:u:239:VAL:HG13	1:u:684:TRP:HB2	1.91	0.52
1:F:239:VAL:HG13	1:F:684:TRP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:353:VAL:H	1:H:645:GLN:NE2	2.07	0.52
1:I:435:ASN:HB2	1:6:353:VAL:HG11	1.91	0.52
1:J:234:TRP:CZ2	1:J:298[A]:ARG:HB3	2.44	0.52
1:M:231:ASP:OD1	1:M:232:SER:N	2.41	0.52
1:P:428:GLN:HE22	1:X:351:PRO:HB3	1.74	0.52
1:S:353:VAL:HG11	1:z:435:ASN:HB2	1.90	0.52
1:U:247:TRP:O	1:U:675:THR:OG1	2.17	0.52
1:a:231:ASP:OD1	1:a:232:SER:N	2.41	0.52
1:h:231:ASP:OD1	1:h:232:SER:N	2.41	0.52
1:n:239:VAL:HG13	1:n:684:TRP:HB2	1.91	0.52
1:n:353:VAL:H	1:n:645:GLN:NE2	2.07	0.52
1:C:353:VAL:H	1:C:645:GLN:NE2	2.07	0.52
1:D:351:PRO:HB3	1:x:428:GLN:HE22	1.74	0.52
1:I:239:VAL:HG13	1:I:684:TRP:HB2	1.91	0.52
1:O:351:PRO:HB3	1:6:428:GLN:HE22	1.74	0.52
1:Q:239:VAL:HG13	1:Q:684:TRP:HB2	1.91	0.52
1:U:353:VAL:H	1:U:645:GLN:NE2	2.07	0.52
1:Y:353:VAL:H	1:Y:645:GLN:NE2	2.07	0.52
1:a:353:VAL:H	1:a:645:GLN:NE2	2.07	0.52
1:b:353:VAL:H	1:b:645:GLN:NE2	2.07	0.52
1:d:239:VAL:HG13	1:d:684:TRP:HB2	1.92	0.52
1:g:234:TRP:HB3	1:g:298[A]:ARG:CZ	2.40	0.52
1:g:353:VAL:H	1:g:645:GLN:NE2	2.07	0.52
1:h:234:TRP:CG	1:h:298[A]:ARG:HD3	2.44	0.52
1:s:353:VAL:H	1:s:645:GLN:NE2	2.07	0.52
1:x:239:VAL:HG13	1:x:684:TRP:HB2	1.92	0.52
1:x:353:VAL:H	1:x:645:GLN:NE2	2.07	0.52
1:3:231:ASP:OD1	1:3:232:SER:N	2.41	0.52
1:4:353:VAL:H	1:4:645:GLN:NE2	2.07	0.52
1:5:353:VAL:H	1:5:645:GLN:NE2	2.07	0.52
1:A:428:GLN:HE22	1:n:351:PRO:HB3	1.74	0.52
1:D:353:VAL:HG11	1:x:435:ASN:HB2	1.90	0.52
1:E:239:VAL:HG13	1:E:684:TRP:HB2	1.91	0.52
1:G:353:VAL:HG11	1:7:435:ASN:HB2	1.91	0.52
1:J:353:VAL:HG11	1:s:435:ASN:HB2	1.90	0.52
1:N:239:VAL:HG13	1:N:684:TRP:HB2	1.92	0.52
1:Q:353:VAL:H	1:Q:645:GLN:NE2	2.07	0.52
1:U:239:VAL:HG13	1:U:684:TRP:HB2	1.92	0.52
1:V:247:TRP:O	1:V:675:THR:OG1	2.17	0.52
1:b:234:TRP:NE1	1:b:298[B]:ARG:HD2	2.24	0.52
1:c:239:VAL:HG13	1:c:684:TRP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:413:TYR:OH	1:c:641:HIS:O	2.26	0.52
1:i:239:VAL:HG13	1:i:684:TRP:HB2	1.91	0.52
1:q:239:VAL:HG13	1:q:684:TRP:HB2	1.92	0.52
1:s:239:VAL:HG13	1:s:684:TRP:HB2	1.91	0.52
1:t:239:VAL:HG13	1:t:684:TRP:HB2	1.91	0.52
1:w:239:VAL:HG13	1:w:684:TRP:HB2	1.91	0.52
1:w:563:GLU:O	1:w:566:ARG:HG3	2.08	0.52
1:1:353:VAL:H	1:1:645:GLN:NE2	2.07	0.52
1:3:353:VAL:H	1:3:645:GLN:NE2	2.07	0.52
1:7:353:VAL:H	1:7:645:GLN:NE2	2.07	0.52
1:8:239:VAL:HG13	1:8:684:TRP:HB2	1.91	0.52
1:B:353:VAL:H	1:B:645:GLN:NE2	2.07	0.52
1:C:239:VAL:HG13	1:C:684:TRP:HB2	1.92	0.52
1:C:247:TRP:O	1:C:675:THR:OG1	2.17	0.52
1:C:351:PRO:HB3	1:t:428:GLN:HE22	1.74	0.52
1:E:563:GLU:O	1:E:566:ARG:HG3	2.08	0.52
1:G:351:PRO:HB3	1:7:428:GLN:HE22	1.74	0.52
1:I:353:VAL:H	1:I:645:GLN:NE2	2.07	0.52
1:K:353:VAL:H	1:K:645:GLN:NE2	2.07	0.52
1:K:428:GLN:HE22	1:P:351:PRO:HB3	1.74	0.52
1:R:239:VAL:HG13	1:R:684:TRP:HB2	1.92	0.52
1:R:353:VAL:HG11	1:r:435:ASN:HB2	1.91	0.52
1:Z:239:VAL:HG13	1:Z:684:TRP:HB2	1.91	0.52
1:e:234:TRP:NE1	1:e:298[B]:ARG:HD2	2.24	0.52
1:g:247:TRP:O	1:g:675:THR:OG1	2.17	0.52
1:u:353:VAL:H	1:u:645:GLN:NE2	2.07	0.52
1:z:247:TRP:O	1:z:675:THR:OG1	2.17	0.52
1:1:234:TRP:HB3	1:1:298[A]:ARG:CZ	2.40	0.52
1:C:358:HIS:NE2	1:t:434:MET:HB2	2.25	0.52
1:E:353:VAL:HG11	1:i:435:ASN:HB2	1.91	0.52
1:E:435:ASN:HB2	1:p:353:VAL:HG11	1.91	0.52
1:G:239:VAL:HG13	1:G:684:TRP:HB2	1.91	0.52
1:H:428:GLN:HE22	1:M:351:PRO:HB3	1.74	0.52
1:M:239:VAL:HG13	1:M:684:TRP:HB2	1.92	0.52
1:h:239:VAL:HG13	1:h:684:TRP:HB2	1.91	0.52
1:j:239:VAL:HG13	1:j:684:TRP:HB2	1.91	0.52
1:r:234:TRP:CE3	1:r:298[A]:ARG:HD3	2.45	0.52
1:2:239:VAL:HG13	1:2:684:TRP:HB2	1.91	0.52
1:B:351:PRO:HB3	1:2:428:GLN:HE22	1.75	0.52
1:D:231:ASP:OD1	1:D:232:SER:N	2.41	0.52
1:E:353:VAL:H	1:E:645:GLN:NE2	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:298[A]:ARG:HG2	1:I:298[A]:ARG:NH2	2.21	0.52
1:Q:353:VAL:HG11	1:Z:435:ASN:HB2	1.92	0.52
1:Q:435:ASN:HB2	1:k:353:VAL:HG11	1.91	0.52
1:W:239:VAL:HG13	1:W:684:TRP:HB2	1.91	0.52
1:X:353:VAL:H	1:X:645:GLN:NE2	2.07	0.52
1:Z:231:ASP:OD1	1:Z:232:SER:N	2.41	0.52
1:d:358:HIS:NE2	1:v:434:MET:HB2	2.25	0.52
1:f:351:PRO:HB3	1:n:428:GLN:HE22	1.74	0.52
1:g:239:VAL:HG13	1:g:684:TRP:HB2	1.91	0.52
1:k:231:ASP:OD1	1:k:232:SER:N	2.41	0.52
1:o:234:TRP:CG	1:o:298[A]:ARG:HD3	2.44	0.52
1:o:353:VAL:H	1:o:645:GLN:NE2	2.07	0.52
1:p:247:TRP:O	1:p:675:THR:OG1	2.17	0.52
1:2:234:TRP:CD2	1:2:298[A]:ARG:HD3	2.45	0.52
1:8:231:ASP:OD1	1:8:232:SER:N	2.41	0.52
1:8:353:VAL:H	1:8:645:GLN:HE22	1.58	0.52
1:F:353:VAL:H	1:F:645:GLN:HE22	1.58	0.52
1:I:353:VAL:H	1:I:645:GLN:HE22	1.58	0.52
1:J:239:VAL:HG13	1:J:684:TRP:HB2	1.92	0.52
1:N:353:VAL:H	1:N:645:GLN:NE2	2.07	0.52
1:P:239:VAL:HG13	1:P:684:TRP:HB2	1.92	0.52
1:U:234:TRP:CD2	1:U:298[A]:ARG:HD3	2.45	0.52
1:Z:353:VAL:H	1:Z:645:GLN:HE22	1.58	0.52
1:c:353:VAL:H	1:c:645:GLN:HE22	1.58	0.52
1:i:353:VAL:H	1:i:645:GLN:NE2	2.07	0.52
1:p:413:TYR:OH	1:p:641:HIS:O	2.26	0.52
1:s:353:VAL:H	1:s:645:GLN:HE22	1.58	0.52
1:u:247:TRP:O	1:u:675:THR:OG1	2.17	0.52
1:w:353:VAL:H	1:w:645:GLN:NE2	2.07	0.52
1:2:234:TRP:CE3	1:2:298[A]:ARG:HD3	2.44	0.52
1:6:239:VAL:HG13	1:6:684:TRP:HB2	1.92	0.52
1:6:353:VAL:H	1:6:645:GLN:NE2	2.07	0.52
1:A:353:VAL:H	1:A:645:GLN:NE2	2.07	0.52
1:F:351:PRO:HB3	1:c:428:GLN:HE22	1.75	0.52
1:G:353:VAL:H	1:G:645:GLN:NE2	2.07	0.52
1:L:247:TRP:O	1:L:675:THR:OG1	2.17	0.52
1:L:435:ASN:HB2	1:r:353:VAL:HG11	1.91	0.52
1:U:353:VAL:H	1:U:645:GLN:HE22	1.58	0.52
1:W:353:VAL:H	1:W:645:GLN:NE2	2.07	0.52
1:Z:247:TRP:O	1:Z:675:THR:OG1	2.17	0.52
1:b:239:VAL:HG13	1:b:684:TRP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:563:GLU:O	1:c:566:ARG:HG3	2.09	0.52
1:i:247:TRP:O	1:i:675:THR:OG1	2.17	0.52
1:i:413:TYR:OH	1:i:641:HIS:O	2.26	0.52
1:p:239:VAL:HG13	1:p:684:TRP:HB2	1.91	0.52
1:r:234:TRP:CD2	1:r:298[A]:ARG:HD3	2.45	0.52
1:u:353:VAL:H	1:u:645:GLN:HE22	1.58	0.52
1:y:353:VAL:H	1:y:645:GLN:HE22	1.58	0.52
1:A:298[A]:ARG:HG2	1:A:298[A]:ARG:NH2	2.24	0.52
1:F:435:ASN:HB2	1:3:353:VAL:HG11	1.92	0.52
1:G:353:VAL:H	1:G:645:GLN:HE22	1.58	0.52
1:N:353:VAL:HG11	1:V:435:ASN:HB2	1.92	0.52
1:V:351:PRO:HB3	1:w:428:GLN:HE22	1.74	0.52
1:V:413:TYR:OH	1:V:641:HIS:O	2.26	0.52
1:b:247:TRP:O	1:b:675:THR:OG1	2.17	0.52
1:d:482:CYS:SG	1:d:576:TYR:HB2	2.50	0.52
1:e:353:VAL:H	1:e:645:GLN:HE22	1.58	0.52
1:f:239:VAL:HG13	1:f:684:TRP:HB2	1.91	0.52
1:h:482:CYS:SG	1:h:576:TYR:HB2	2.50	0.52
1:n:482:CYS:SG	1:n:576:TYR:HB2	2.50	0.52
1:q:234:TRP:HB3	1:q:298[A]:ARG:CZ	2.40	0.52
1:t:353:VAL:H	1:t:645:GLN:NE2	2.07	0.52
1:x:482:CYS:SG	1:x:576:TYR:HB2	2.50	0.52
1:5:239:VAL:HG13	1:5:684:TRP:HB2	1.91	0.52
1:E:358:HIS:NE2	1:i:434:MET:HB2	2.26	0.51
1:H:435:ASN:HB2	1:M:353:VAL:HG11	1.92	0.51
1:J:353:VAL:H	1:J:645:GLN:NE2	2.07	0.51
1:M:482:CYS:SG	1:M:576:TYR:HB2	2.50	0.51
1:N:413:TYR:OH	1:N:641:HIS:O	2.26	0.51
1:O:239:VAL:HG13	1:O:684:TRP:HB2	1.92	0.51
1:a:565:ILE:HD11	1:a:729:ARG:NH1	2.26	0.51
1:e:563:GLU:O	1:e:566:ARG:HG3	2.09	0.51
1:f:247:TRP:O	1:f:675:THR:OG1	2.17	0.51
1:f:353:VAL:H	1:f:645:GLN:HE22	1.58	0.51
1:j:434:MET:HB2	1:o:358:HIS:NE2	2.25	0.51
1:l:239:VAL:HG13	1:l:684:TRP:HB2	1.91	0.51
1:r:482:CYS:SG	1:r:576:TYR:HB2	2.50	0.51
1:t:353:VAL:H	1:t:645:GLN:HE22	1.58	0.51
1:v:353:VAL:H	1:v:645:GLN:NE2	2.07	0.51
1:1:353:VAL:H	1:1:645:GLN:HE22	1.58	0.51
1:6:563:GLU:O	1:6:566:ARG:HG3	2.09	0.51
1:8:353:VAL:H	1:8:645:GLN:NE2	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PRO:HB3	1:f:428:GLN:HE22	1.75	0.51
1:B:231:ASP:OD1	1:B:232:SER:N	2.41	0.51
1:B:353:VAL:H	1:B:645:GLN:HE22	1.58	0.51
1:F:353:VAL:H	1:F:645:GLN:NE2	2.07	0.51
1:G:565:ILE:HD11	1:G:729:ARG:NH1	2.25	0.51
1:H:353:VAL:HG11	1:T:435:ASN:HB2	1.92	0.51
1:J:234:TRP:CZ2	1:J:298[B]:ARG:HB2	2.44	0.51
1:K:435:ASN:HB2	1:P:353:VAL:HG11	1.92	0.51
1:Q:482:CYS:SG	1:Q:576:TYR:HB2	2.51	0.51
1:S:353:VAL:H	1:S:645:GLN:HE22	1.58	0.51
1:S:482:CYS:SG	1:S:576:TYR:HB2	2.50	0.51
1:V:239:VAL:HG13	1:V:684:TRP:HB2	1.92	0.51
1:Z:353:VAL:H	1:Z:645:GLN:NE2	2.07	0.51
1:a:358:HIS:NE2	1:y:434:MET:HB2	2.25	0.51
1:b:353:VAL:H	1:b:645:GLN:HE22	1.58	0.51
1:c:565:ILE:HD11	1:c:729:ARG:NH1	2.26	0.51
1:e:565:ILE:HD11	1:e:729:ARG:NH1	2.25	0.51
1:j:565:ILE:HD11	1:j:729:ARG:NH1	2.25	0.51
1:m:413:TYR:OH	1:m:641:HIS:O	2.26	0.51
1:r:353:VAL:H	1:r:645:GLN:HE22	1.58	0.51
1:s:398:PHE:CE1	1:l:692:LYS:HG3	2.46	0.51
1:y:353:VAL:H	1:y:645:GLN:NE2	2.07	0.51
1:z:353:VAL:H	1:z:645:GLN:HE22	1.58	0.51
1:l:413:TYR:OH	1:l:641:HIS:O	2.26	0.51
1:2:353:VAL:H	1:2:645:GLN:NE2	2.07	0.51
1:3:565:ILE:HD11	1:3:729:ARG:NH1	2.26	0.51
1:A:353:VAL:H	1:A:645:GLN:HE22	1.58	0.51
1:A:435:ASN:HB2	1:n:353:VAL:HG11	1.93	0.51
1:B:482:CYS:SG	1:B:576:TYR:HB2	2.50	0.51
1:F:482:CYS:SG	1:F:576:TYR:HB2	2.50	0.51
1:H:239:VAL:HG13	1:H:684:TRP:HB2	1.92	0.51
1:I:247:TRP:O	1:I:675:THR:OG1	2.17	0.51
1:L:353:VAL:H	1:L:645:GLN:HE22	1.58	0.51
1:N:247:TRP:O	1:N:675:THR:OG1	2.17	0.51
1:P:353:VAL:H	1:P:645:GLN:NE2	2.07	0.51
1:P:565:ILE:HD11	1:P:729:ARG:NH1	2.26	0.51
1:R:358:HIS:NE2	1:r:434:MET:HB2	2.25	0.51
1:V:358:HIS:NE2	1:w:434:MET:HB2	2.25	0.51
1:V:565:ILE:HD11	1:V:729:ARG:NH1	2.25	0.51
1:W:563:GLU:O	1:W:566:ARG:HG3	2.09	0.51
1:a:239:VAL:HG13	1:a:684:TRP:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:692:LYS:HG3	1:o:398:PHE:CE1	2.46	0.51
1:k:353:VAL:H	1:k:645:GLN:HE22	1.58	0.51
1:n:565:ILE:HD11	1:n:729:ARG:NH1	2.25	0.51
1:t:565:ILE:HD11	1:t:729:ARG:NH1	2.25	0.51
1:v:353:VAL:H	1:v:645:GLN:HE22	1.58	0.51
1:x:358:HIS:NE2	1:8:434:MET:HB2	2.26	0.51
1:4:565:ILE:HD11	1:4:729:ARG:NH1	2.25	0.51
1:8:234:TRP:CZ2	1:8:298[A]:ARG:HB3	2.45	0.51
1:A:353:VAL:HG11	1:f:435:ASN:HB2	1.92	0.51
1:C:435:ASN:HB2	1:Y:353:VAL:HG11	1.92	0.51
1:I:234:TRP:CE2	1:I:298[A]:ARG:HD3	2.44	0.51
1:J:247:TRP:O	1:J:675:THR:OG1	2.17	0.51
1:O:353:VAL:H	1:O:645:GLN:HE22	1.58	0.51
1:O:482:CYS:SG	1:O:576:TYR:HB2	2.50	0.51
1:P:353:VAL:H	1:P:645:GLN:HE22	1.58	0.51
1:R:351:PRO:HB3	1:r:428:GLN:HE22	1.75	0.51
1:T:413:TYR:OH	1:T:641:HIS:O	2.26	0.51
1:U:435:ASN:HB2	1:2:353:VAL:HG11	1.91	0.51
1:X:482:CYS:SG	1:X:576:TYR:HB2	2.50	0.51
1:d:565:ILE:HD11	1:d:729:ARG:NH1	2.26	0.51
1:g:482:CYS:SG	1:g:576:TYR:HB2	2.50	0.51
1:j:353:VAL:H	1:j:645:GLN:NE2	2.07	0.51
1:l:353:VAL:H	1:l:645:GLN:HE22	1.58	0.51
1:l:434:MET:HB2	1:u:358:HIS:NE2	2.26	0.51
1:o:482:CYS:SG	1:o:576:TYR:HB2	2.50	0.51
1:p:234:TRP:HB3	1:p:298[A]:ARG:CZ	2.40	0.51
1:y:482:CYS:SG	1:y:576:TYR:HB2	2.50	0.51
1:1:231:ASP:OD1	1:1:232:SER:N	2.41	0.51
1:1:482:CYS:SG	1:1:576:TYR:HB2	2.50	0.51
1:B:353:VAL:HG11	1:2:435:ASN:HB2	1.91	0.51
1:B:413:TYR:OH	1:B:641:HIS:O	2.26	0.51
1:C:482:CYS:SG	1:C:576:TYR:HB2	2.50	0.51
1:C:565:ILE:HD11	1:C:729:ARG:NH1	2.25	0.51
1:D:353:VAL:H	1:D:645:GLN:HE22	1.58	0.51
1:H:358:HIS:NE2	1:T:434:MET:HB2	2.26	0.51
1:I:353:VAL:HG11	1:O:435:ASN:HB2	1.92	0.51
1:K:565:ILE:HD11	1:K:729:ARG:NH1	2.25	0.51
1:N:482:CYS:SG	1:N:576:TYR:HB2	2.50	0.51
1:W:358:HIS:NE2	1:u:434:MET:HB2	2.25	0.51
1:Y:239:VAL:HG13	1:Y:684:TRP:HB2	1.92	0.51
1:a:353:VAL:H	1:a:645:GLN:HE22	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:482:CYS:SG	1:f:576:TYR:HB2	2.50	0.51
1:h:358:HIS:NE2	1:5:434:MET:HB2	2.25	0.51
1:h:434:MET:HB2	1:m:358:HIS:NE2	2.26	0.51
1:j:353:VAL:H	1:j:645:GLN:HE22	1.58	0.51
1:l:482:CYS:SG	1:l:576:TYR:HB2	2.50	0.51
1:m:239:VAL:HG13	1:m:684:TRP:HB2	1.91	0.51
1:m:353:VAL:H	1:m:645:GLN:HE22	1.58	0.51
1:p:565:ILE:HD11	1:p:729:ARG:NH1	2.26	0.51
1:q:565:ILE:HD11	1:q:729:ARG:NH1	2.25	0.51
1:s:358:HIS:NE2	1:1:434:MET:HB2	2.25	0.51
1:s:413:TYR:OH	1:s:641:HIS:O	2.26	0.51
1:t:234:TRP:CE3	1:t:298[A]:ARG:HD3	2.46	0.51
1:w:482:CYS:SG	1:w:576:TYR:HB2	2.50	0.51
1:1:247:TRP:O	1:1:675:THR:OG1	2.17	0.51
1:2:353:VAL:H	1:2:645:GLN:HE22	1.58	0.51
1:3:239:VAL:HG13	1:3:684:TRP:HB2	1.91	0.51
1:3:353:VAL:H	1:3:645:GLN:HE22	1.58	0.51
1:5:565:ILE:HD11	1:5:729:ARG:NH1	2.25	0.51
1:C:353:VAL:H	1:C:645:GLN:HE22	1.58	0.51
1:H:482:CYS:SG	1:H:576:TYR:HB2	2.50	0.51
1:H:565:ILE:HD11	1:H:729:ARG:NH1	2.26	0.51
1:J:353:VAL:H	1:J:645:GLN:HE22	1.58	0.51
1:P:434:MET:HB2	1:X:358:HIS:NE2	2.26	0.51
1:P:435:ASN:HB2	1:X:353:VAL:HG11	1.93	0.51
1:P:482:CYS:SG	1:P:576:TYR:HB2	2.50	0.51
1:Q:358:HIS:NE2	1:Z:434:MET:HB2	2.26	0.51
1:Q:565:ILE:HD11	1:Q:729:ARG:NH1	2.25	0.51
1:R:565:ILE:HD11	1:R:729:ARG:NH1	2.25	0.51
1:T:239:VAL:HG13	1:T:684:TRP:HB2	1.91	0.51
1:T:353:VAL:H	1:T:645:GLN:HE22	1.58	0.51
1:Y:565:ILE:HD11	1:Y:729:ARG:NH1	2.25	0.51
1:Z:482:CYS:SG	1:Z:576:TYR:HB2	2.50	0.51
1:b:482:CYS:SG	1:b:576:TYR:HB2	2.50	0.51
1:c:482:CYS:SG	1:c:576:TYR:HB2	2.50	0.51
1:e:482:CYS:SG	1:e:576:TYR:HB2	2.50	0.51
1:g:565:ILE:HD11	1:g:729:ARG:NH1	2.25	0.51
1:j:482:CYS:SG	1:j:576:TYR:HB2	2.50	0.51
1:m:434:MET:HB2	1:5:358:HIS:NE2	2.26	0.51
1:s:482:CYS:SG	1:s:576:TYR:HB2	2.50	0.51
1:u:482:CYS:SG	1:u:576:TYR:HB2	2.50	0.51
1:x:565:ILE:HD11	1:x:729:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:239:VAL:HG13	1:1:684:TRP:HB2	1.92	0.51
1:2:565:ILE:HD11	1:2:729:ARG:NH1	2.25	0.51
1:7:239:VAL:HG13	1:7:684:TRP:HB2	1.92	0.51
1:7:565:ILE:HD11	1:7:729:ARG:NH1	2.25	0.51
1:8:565:ILE:HD11	1:8:729:ARG:NH1	2.25	0.51
1:A:253:ASN:OD1	1:A:374:GLN:NE2	2.44	0.51
1:B:239:VAL:HG13	1:B:684:TRP:HB2	1.91	0.51
1:E:482:CYS:SG	1:E:576:TYR:HB2	2.51	0.51
1:M:435:ASN:HB2	1:T:353:VAL:HG11	1.92	0.51
1:N:253:ASN:OD1	1:N:374:GLN:NE2	2.44	0.51
1:N:434:MET:HB2	1:w:358:HIS:NE2	2.26	0.51
1:O:358:HIS:NE2	1:6:434:MET:HB2	2.25	0.51
1:R:253:ASN:OD1	1:R:374:GLN:NE2	2.44	0.51
1:T:253:ASN:OD1	1:T:374:GLN:NE2	2.44	0.51
1:U:482:CYS:SG	1:U:576:TYR:HB2	2.50	0.51
1:W:565:ILE:HD11	1:W:729:ARG:NH1	2.25	0.51
1:Z:565:ILE:HD11	1:Z:729:ARG:NH1	2.25	0.51
1:a:413:TYR:OH	1:a:641:HIS:O	2.26	0.51
1:b:253:ASN:OD1	1:b:374:GLN:NE2	2.44	0.51
1:e:434:MET:HB2	1:y:358:HIS:NE2	2.26	0.51
1:g:353:VAL:H	1:g:645:GLN:HE22	1.58	0.51
1:i:253:ASN:OD1	1:i:374:GLN:NE2	2.44	0.51
1:i:482:CYS:SG	1:i:576:TYR:HB2	2.50	0.51
1:o:565:ILE:HD11	1:o:729:ARG:NH1	2.25	0.51
1:o:692:LYS:HG3	1:4:398:PHE:CE1	2.46	0.51
1:p:234:TRP:CE2	1:p:298[B]:ARG:HD2	2.46	0.51
1:q:253:ASN:OD1	1:q:374:GLN:NE2	2.44	0.51
1:v:239:VAL:HG13	1:v:684:TRP:HB2	1.91	0.51
1:v:253:ASN:OD1	1:v:374:GLN:NE2	2.44	0.51
1:2:482:CYS:SG	1:2:576:TYR:HB2	2.50	0.51
1:4:482:CYS:SG	1:4:576:TYR:HB2	2.50	0.51
1:5:482:CYS:SG	1:5:576:TYR:HB2	2.50	0.51
1:6:482:CYS:SG	1:6:576:TYR:HB2	2.51	0.51
1:7:353:VAL:H	1:7:645:GLN:HE22	1.58	0.51
1:8:253:ASN:OD1	1:8:374:GLN:NE2	2.44	0.51
1:8:482:CYS:SG	1:8:576:TYR:HB2	2.51	0.51
1:A:482:CYS:SG	1:A:576:TYR:HB2	2.50	0.51
1:E:234:TRP:CZ2	1:E:298[B]:ARG:HB2	2.46	0.51
1:E:413:TYR:OH	1:E:641:HIS:O	2.26	0.51
1:F:358:HIS:NE2	1:c:434:MET:HB2	2.26	0.51
1:H:253:ASN:OD1	1:H:374:GLN:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:253:ASN:OD1	1:I:374:GLN:NE2	2.44	0.51
1:I:482:CYS:SG	1:I:576:TYR:HB2	2.51	0.51
1:J:253:ASN:OD1	1:J:374:GLN:NE2	2.44	0.51
1:J:358:HIS:NE2	1:s:434:MET:HB2	2.26	0.51
1:J:565:ILE:HD11	1:J:729:ARG:NH1	2.25	0.51
1:K:482:CYS:SG	1:K:576:TYR:HB2	2.51	0.51
1:L:234:TRP:CD2	1:L:298[A]:ARG:HD3	2.45	0.51
1:S:247:TRP:O	1:S:675:THR:OG1	2.17	0.51
1:U:253:ASN:OD1	1:U:374:GLN:NE2	2.44	0.51
1:U:565:ILE:HD11	1:U:729:ARG:NH1	2.25	0.51
1:W:482:CYS:SG	1:W:576:TYR:HB2	2.51	0.51
1:X:565:ILE:HD11	1:X:729:ARG:NH1	2.25	0.51
1:Y:353:VAL:H	1:Y:645:GLN:HE22	1.58	0.51
1:Z:253:ASN:OD1	1:Z:374:GLN:NE2	2.44	0.51
1:a:398:PHE:CE1	1:y:692:LYS:HG3	2.46	0.51
1:e:234:TRP:CG	1:e:298[A]:ARG:HD3	2.46	0.51
1:f:253:ASN:OD1	1:f:374:GLN:NE2	2.44	0.51
1:f:358:HIS:NE2	1:n:434:MET:HB2	2.26	0.51
1:g:434:MET:HB2	1:7:358:HIS:NE2	2.26	0.51
1:h:253:ASN:OD1	1:h:374:GLN:NE2	2.44	0.51
1:m:253:ASN:OD1	1:m:374:GLN:NE2	2.44	0.51
1:q:434:MET:HB2	1:z:358:HIS:NE2	2.25	0.51
1:u:253:ASN:OD1	1:u:374:GLN:NE2	2.44	0.51
1:w:253:ASN:OD1	1:w:374:GLN:NE2	2.44	0.51
1:x:253:ASN:OD1	1:x:374:GLN:NE2	2.44	0.51
1:3:413:TYR:OH	1:3:641:HIS:O	2.26	0.51
1:6:253:ASN:OD1	1:6:374:GLN:NE2	2.44	0.51
1:6:565:ILE:HD11	1:6:729:ARG:NH1	2.26	0.51
1:D:358:HIS:NE2	1:x:434:MET:HB2	2.25	0.51
1:E:253:ASN:OD1	1:E:374:GLN:NE2	2.44	0.51
1:G:358:HIS:NE2	1:7:434:MET:HB2	2.26	0.51
1:G:434:MET:HB2	1:g:358:HIS:NE2	2.26	0.51
1:J:298[A]:ARG:HH21	1:J:298[A]:ARG:HG2	1.74	0.51
1:J:482:CYS:SG	1:J:576:TYR:HB2	2.51	0.51
1:L:565:ILE:HD11	1:L:729:ARG:NH1	2.25	0.51
1:M:253:ASN:OD1	1:M:374:GLN:NE2	2.44	0.51
1:Q:253:ASN:OD1	1:Q:374:GLN:NE2	2.44	0.51
1:U:413:TYR:OH	1:U:641:HIS:O	2.26	0.51
1:W:253:ASN:OD1	1:W:374:GLN:NE2	2.44	0.51
1:Y:482:CYS:SG	1:Y:576:TYR:HB2	2.50	0.51
1:f:231:ASP:OD1	1:f:232:SER:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:398:PHE:CE1	1:4:692:LYS:HG3	2.46	0.51
1:m:692:LYS:HG3	1:5:398:PHE:CE1	2.46	0.51
1:o:434:MET:HB2	1:4:358:HIS:NE2	2.26	0.51
1:s:253:ASN:OD1	1:s:374:GLN:NE2	2.44	0.51
1:w:413:TYR:OH	1:w:641:HIS:O	2.26	0.51
1:w:565:ILE:HD11	1:w:729:ARG:NH1	2.25	0.51
1:2:247:TRP:O	1:2:675:THR:OG1	2.17	0.51
1:2:253:ASN:OD1	1:2:374:GLN:NE2	2.44	0.51
1:5:253:ASN:OD1	1:5:374:GLN:NE2	2.44	0.51
1:A:239:VAL:HG13	1:A:684:TRP:HB2	1.92	0.51
1:B:253:ASN:OD1	1:B:374:GLN:NE2	2.44	0.51
1:C:253:ASN:OD1	1:C:374:GLN:NE2	2.44	0.51
1:D:239:VAL:HG13	1:D:684:TRP:HB2	1.91	0.51
1:F:565:ILE:HD11	1:F:729:ARG:NH1	2.25	0.51
1:G:234:TRP:CD2	1:G:298[A]:ARG:HD3	2.46	0.51
1:G:482:CYS:SG	1:G:576:TYR:HB2	2.51	0.51
1:K:353:VAL:HG11	1:X:435:ASN:HB2	1.92	0.51
1:L:253:ASN:OD1	1:L:374:GLN:NE2	2.44	0.51
1:M:434:MET:HB2	1:T:358:HIS:NE2	2.26	0.51
1:N:565:ILE:HD11	1:N:729:ARG:NH1	2.25	0.51
1:P:253:ASN:OD1	1:P:374:GLN:NE2	2.44	0.51
1:V:398:PHE:CE1	1:w:692:LYS:HG3	2.46	0.51
1:Z:358:HIS:NE2	1:k:434:MET:HB2	2.25	0.51
1:a:253:ASN:OD1	1:a:374:GLN:NE2	2.44	0.51
1:c:253:ASN:OD1	1:c:374:GLN:NE2	2.44	0.51
1:c:358:HIS:NE2	1:3:434:MET:HB2	2.26	0.51
1:d:398:PHE:CE1	1:v:692:LYS:HG3	2.46	0.51
1:f:565:ILE:HD11	1:f:729:ARG:NH1	2.25	0.51
1:i:358:HIS:NE2	1:p:434:MET:HB2	2.26	0.51
1:j:253:ASN:OD1	1:j:374:GLN:NE2	2.44	0.51
1:l:565:ILE:HD11	1:l:729:ARG:NH1	2.25	0.51
1:o:353:VAL:H	1:o:645:GLN:HE22	1.58	0.51
1:q:482:CYS:SG	1:q:576:TYR:HB2	2.50	0.51
1:s:565:ILE:HD11	1:s:729:ARG:NH1	2.25	0.51
1:t:253:ASN:OD1	1:t:374:GLN:NE2	2.44	0.51
1:t:482:CYS:SG	1:t:576:TYR:HB2	2.50	0.51
1:v:482:CYS:SG	1:v:576:TYR:HB2	2.50	0.51
1:z:253:ASN:OD1	1:z:374:GLN:NE2	2.44	0.51
1:1:253:ASN:OD1	1:1:374:GLN:NE2	2.44	0.51
1:3:253:ASN:OD1	1:3:374:GLN:NE2	2.44	0.51
1:B:434:MET:HB2	1:U:358:HIS:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:351:PRO:HB3	1:i:428:GLN:HE22	1.74	0.50
1:E:565:ILE:HD11	1:E:729:ARG:NH1	2.25	0.50
1:G:253:ASN:OD1	1:G:374:GLN:NE2	2.44	0.50
1:H:351:PRO:HB3	1:T:428:GLN:HE22	1.74	0.50
1:I:358:HIS:NE2	1:O:434:MET:HB2	2.26	0.50
1:J:423:SER:O	1:J:729:ARG:HA	2.11	0.50
1:R:482:CYS:SG	1:R:576:TYR:HB2	2.51	0.50
1:V:253:ASN:OD1	1:V:374:GLN:NE2	2.44	0.50
1:X:353:VAL:H	1:X:645:GLN:HE22	1.58	0.50
1:a:423:SER:O	1:a:729:ARG:HA	2.11	0.50
1:b:358:HIS:NE2	1:d:434:MET:HB2	2.26	0.50
1:g:253:ASN:OD1	1:g:374:GLN:NE2	2.44	0.50
1:h:565:ILE:HD11	1:h:729:ARG:NH1	2.25	0.50
1:i:423:SER:O	1:i:729:ARG:HA	2.11	0.50
1:l:692:LYS:HG3	1:u:398:PHE:CE1	2.46	0.50
1:p:253:ASN:OD1	1:p:374:GLN:NE2	2.44	0.50
1:y:565:ILE:HD11	1:y:729:ARG:NH1	2.25	0.50
1:z:423:SER:O	1:z:729:ARG:HA	2.12	0.50
1:z:565:ILE:HD11	1:z:729:ARG:NH1	2.25	0.50
1:1:565:ILE:HD11	1:1:729:ARG:NH1	2.25	0.50
1:2:423:SER:O	1:2:729:ARG:HA	2.11	0.50
1:7:482:CYS:SG	1:7:576:TYR:HB2	2.50	0.50
1:A:434:MET:HB2	1:n:358:HIS:NE2	2.27	0.50
1:B:358:HIS:NE2	1:2:434:MET:HB2	2.26	0.50
1:C:398:PHE:CE1	1:t:692:LYS:HG3	2.46	0.50
1:H:423:SER:O	1:H:729:ARG:HA	2.12	0.50
1:I:565:ILE:HD11	1:I:729:ARG:NH1	2.25	0.50
1:K:358:HIS:NE2	1:X:434:MET:HB2	2.26	0.50
1:K:434:MET:HB2	1:P:358:HIS:NE2	2.26	0.50
1:L:482:CYS:SG	1:L:576:TYR:HB2	2.50	0.50
1:M:565:ILE:HD11	1:M:729:ARG:NH1	2.25	0.50
1:S:358:HIS:NE2	1:z:434:MET:HB2	2.26	0.50
1:U:434:MET:HB2	1:2:358:HIS:NE2	2.26	0.50
1:Y:434:MET:HB2	1:t:358:HIS:NE2	2.26	0.50
1:a:434:MET:HB2	1:e:358:HIS:NE2	2.26	0.50
1:b:565:ILE:HD11	1:b:729:ARG:NH1	2.26	0.50
1:d:253:ASN:OD1	1:d:374:GLN:NE2	2.44	0.50
1:e:253:ASN:OD1	1:e:374:GLN:NE2	2.44	0.50
1:h:398:PHE:CE1	1:5:692:LYS:HG3	2.46	0.50
1:k:239:VAL:HG13	1:k:684:TRP:HB2	1.92	0.50
1:l:234:TRP:CZ2	1:l:298[A]:ARG:HB3	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:253:ASN:OD1	1:n:374:GLN:NE2	2.44	0.50
1:n:423:SER:O	1:n:729:ARG:HA	2.12	0.50
1:p:353:VAL:H	1:p:645:GLN:HE22	1.58	0.50
1:r:565:ILE:HD11	1:r:729:ARG:NH1	2.25	0.50
1:z:482:CYS:SG	1:z:576:TYR:HB2	2.50	0.50
1:3:423:SER:O	1:3:729:ARG:HA	2.12	0.50
1:5:423:SER:O	1:5:729:ARG:HA	2.12	0.50
1:B:435:ASN:HB2	1:U:353:VAL:HG11	1.93	0.50
1:C:429:SER:OG	1:C:431:ASP:OD1	2.28	0.50
1:F:434:MET:HB2	1:3:358:HIS:NE2	2.26	0.50
1:H:353:VAL:H	1:H:645:GLN:HE22	1.58	0.50
1:H:429:SER:OG	1:H:431:ASP:OD1	2.28	0.50
1:I:434:MET:HB2	1:6:358:HIS:NE2	2.26	0.50
1:L:423:SER:O	1:L:729:ARG:HA	2.12	0.50
1:N:423:SER:O	1:N:729:ARG:HA	2.12	0.50
1:O:565:ILE:HD11	1:O:729:ARG:NH1	2.25	0.50
1:S:434:MET:HB2	1:q:358:HIS:NE2	2.26	0.50
1:S:565:ILE:HD11	1:S:729:ARG:NH1	2.25	0.50
1:V:353:VAL:H	1:V:645:GLN:HE22	1.58	0.50
1:W:398:PHE:CE1	1:u:692:LYS:HG3	2.47	0.50
1:W:434:MET:HB2	1:l:358:HIS:NE2	2.26	0.50
1:b:231:ASP:OD1	1:b:232:SER:N	2.41	0.50
1:d:423:SER:O	1:d:729:ARG:HA	2.12	0.50
1:i:565:ILE:HD11	1:i:729:ARG:NH1	2.25	0.50
1:j:358:HIS:NE2	1:4:434:MET:HB2	2.26	0.50
1:k:482:CYS:SG	1:k:576:TYR:HB2	2.51	0.50
1:u:565:ILE:HD11	1:u:729:ARG:NH1	2.25	0.50
1:v:565:ILE:HD11	1:v:729:ARG:NH1	2.25	0.50
1:w:234:TRP:CE3	1:w:298[A]:ARG:HD3	2.46	0.50
1:x:353:VAL:H	1:x:645:GLN:HE22	1.58	0.50
1:5:353:VAL:H	1:5:645:GLN:HE22	1.58	0.50
1:7:423:SER:O	1:7:729:ARG:HA	2.11	0.50
1:A:565:ILE:HD11	1:A:729:ARG:NH1	2.25	0.50
1:B:565:ILE:HD11	1:B:729:ARG:NH1	2.25	0.50
1:H:434:MET:HB2	1:M:358:HIS:NE2	2.26	0.50
1:Q:353:VAL:H	1:Q:645:GLN:HE22	1.58	0.50
1:V:423:SER:O	1:V:729:ARG:HA	2.11	0.50
1:V:482:CYS:SG	1:V:576:TYR:HB2	2.50	0.50
1:X:253:ASN:OD1	1:X:374:GLN:NE2	2.44	0.50
1:Y:423:SER:O	1:Y:729:ARG:HA	2.12	0.50
1:Z:413:TYR:OH	1:Z:641:HIS:O	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:413:TYR:OH	1:b:641:HIS:O	2.26	0.50
1:b:423:SER:O	1:b:729:ARG:HA	2.11	0.50
1:h:692:LYS:HG3	1:m:398:PHE:CE1	2.46	0.50
1:l:610:ASP:OD1	1:l:728:THR:HG22	2.12	0.50
1:q:692:LYS:HG3	1:z:398:PHE:CE1	2.46	0.50
1:x:234:TRP:CD2	1:x:298[A]:ARG:HD3	2.47	0.50
1:x:398:PHE:CE1	1:8:692:LYS:HG3	2.46	0.50
1:8:413:TYR:OH	1:8:641:HIS:O	2.26	0.50
1:B:423:SER:O	1:B:729:ARG:HA	2.12	0.50
1:B:610:ASP:OD1	1:B:728:THR:HG22	2.12	0.50
1:D:482:CYS:SG	1:D:576:TYR:HB2	2.51	0.50
1:L:234:TRP:CE2	1:L:298[B]:ARG:HD2	2.47	0.50
1:L:434:MET:HB2	1:r:358:HIS:NE2	2.26	0.50
1:M:423:SER:O	1:M:729:ARG:HA	2.12	0.50
1:N:353:VAL:H	1:N:645:GLN:HE22	1.58	0.50
1:O:610:ASP:OD1	1:O:728:THR:HG22	2.12	0.50
1:T:565:ILE:HD11	1:T:729:ARG:NH1	2.25	0.50
1:W:353:VAL:H	1:W:645:GLN:HE22	1.58	0.50
1:b:234:TRP:CG	1:b:298[A]:ARG:HD3	2.46	0.50
1:f:413:TYR:OH	1:f:641:HIS:O	2.26	0.50
1:h:423:SER:O	1:h:729:ARG:HA	2.12	0.50
1:i:353:VAL:H	1:i:645:GLN:HE22	1.58	0.50
1:k:253:ASN:OD1	1:k:374:GLN:NE2	2.44	0.50
1:l:238[B]:ARG:HD3	1:l:683:GLU:OE2	2.12	0.50
1:p:423:SER:O	1:p:729:ARG:HA	2.12	0.50
1:p:482:CYS:SG	1:p:576:TYR:HB2	2.50	0.50
1:q:610:ASP:OD1	1:q:728:THR:HG22	2.12	0.50
1:1:423:SER:O	1:1:729:ARG:HA	2.12	0.50
1:1:610:ASP:OD1	1:1:728:THR:HG22	2.12	0.50
1:6:353:VAL:H	1:6:645:GLN:HE22	1.58	0.50
1:8:423:SER:O	1:8:729:ARG:HA	2.11	0.50
1:D:253:ASN:OD1	1:D:374:GLN:NE2	2.44	0.50
1:F:353:VAL:HG11	1:c:435:ASN:HB2	1.93	0.50
1:F:423:SER:O	1:F:729:ARG:HA	2.12	0.50
1:N:610:ASP:OD1	1:N:728:THR:HG22	2.12	0.50
1:R:610:ASP:OD1	1:R:728:THR:HG22	2.12	0.50
1:S:239:VAL:HG13	1:S:684:TRP:HB2	1.91	0.50
1:T:610:ASP:OD1	1:T:728:THR:HG22	2.12	0.50
1:Y:253:ASN:OD1	1:Y:374:GLN:NE2	2.44	0.50
1:f:423:SER:O	1:f:729:ARG:HA	2.12	0.50
1:g:234:TRP:CE2	1:g:298[B]:ARG:HD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:423:SER:O	1:k:729:ARG:HA	2.12	0.50
1:m:610:ASP:OD1	1:m:728:THR:HG22	2.12	0.50
1:o:253:ASN:OD1	1:o:374:GLN:NE2	2.44	0.50
1:o:413:TYR:OH	1:o:641:HIS:O	2.26	0.50
1:s:423:SER:O	1:s:729:ARG:HA	2.12	0.50
1:y:423:SER:O	1:y:729:ARG:HA	2.12	0.50
1:4:239:VAL:HG13	1:4:684:TRP:HB2	1.91	0.50
1:7:253:ASN:OD1	1:7:374:GLN:NE2	2.44	0.50
1:D:423:SER:O	1:D:729:ARG:HA	2.12	0.50
1:G:234:TRP:CZ2	1:G:298[B]:ARG:HB2	2.46	0.50
1:G:423:SER:O	1:G:729:ARG:HA	2.11	0.50
1:K:239:VAL:HG13	1:K:684:TRP:HB2	1.91	0.50
1:S:610:ASP:OD1	1:S:728:THR:HG22	2.12	0.50
1:U:423:SER:O	1:U:729:ARG:HA	2.12	0.50
1:U:610:ASP:OD1	1:U:728:THR:HG22	2.12	0.50
1:V:610:ASP:OD1	1:V:728:THR:HG22	2.12	0.50
1:Z:423:SER:O	1:Z:729:ARG:HA	2.12	0.50
1:Z:429:SER:OG	1:Z:431:ASP:OD1	2.28	0.50
1:a:482:CYS:SG	1:a:576:TYR:HB2	2.51	0.50
1:g:610:ASP:OD1	1:g:728:THR:HG22	2.12	0.50
1:i:610:ASP:OD1	1:i:728:THR:HG22	2.12	0.50
1:k:565:ILE:HD11	1:k:729:ARG:NH1	2.26	0.50
1:m:565:ILE:HD11	1:m:729:ARG:NH1	2.25	0.50
1:p:610:ASP:OD1	1:p:728:THR:HG22	2.12	0.50
1:q:413:TYR:OH	1:q:641:HIS:O	2.26	0.50
1:r:239:VAL:HG13	1:r:684:TRP:HB2	1.91	0.50
1:r:610:ASP:OD1	1:r:728:THR:HG22	2.12	0.50
1:s:610:ASP:OD1	1:s:728:THR:HG22	2.12	0.50
1:u:610:ASP:OD1	1:u:728:THR:HG22	2.12	0.50
1:A:423:SER:O	1:A:729:ARG:HA	2.12	0.50
1:C:610:ASP:OD1	1:C:728:THR:HG22	2.12	0.50
1:D:565:ILE:HD11	1:D:729:ARG:NH1	2.25	0.50
1:E:353:VAL:H	1:E:645:GLN:HE22	1.58	0.50
1:E:429:SER:OG	1:E:431:ASP:OD1	2.28	0.50
1:F:413:TYR:OH	1:F:641:HIS:O	2.26	0.50
1:G:610:ASP:OD1	1:G:728:THR:HG22	2.12	0.50
1:I:610:ASP:OD1	1:I:728:THR:HG22	2.12	0.50
1:L:234:TRP:CZ2	1:L:298[B]:ARG:HB2	2.47	0.50
1:Q:423:SER:O	1:Q:729:ARG:HA	2.12	0.50
1:R:413:TYR:OH	1:R:641:HIS:O	2.26	0.50
1:R:423:SER:O	1:R:729:ARG:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:482:CYS:SG	1:T:576:TYR:HB2	2.50	0.50
1:c:610:ASP:OD1	1:c:728:THR:HG22	2.12	0.50
1:h:610:ASP:OD1	1:h:728:THR:HG22	2.12	0.50
1:i:398:PHE:CE1	1:p:692:LYS:HG3	2.47	0.50
1:m:482:CYS:SG	1:m:576:TYR:HB2	2.50	0.50
1:t:610:ASP:OD1	1:t:728:THR:HG22	2.12	0.50
1:x:423:SER:O	1:x:729:ARG:HA	2.12	0.50
1:y:413:TYR:OH	1:y:641:HIS:O	2.26	0.50
1:4:234:TRP:CZ2	1:4:298[A]:ARG:HB3	2.46	0.50
1:D:434:MET:HB2	1:8:358:HIS:NE2	2.26	0.50
1:J:434:MET:HB2	1:1:358:HIS:NE2	2.26	0.50
1:L:358:HIS:NE2	1:R:434:MET:HB2	2.26	0.50
1:L:413:TYR:OH	1:L:641:HIS:O	2.26	0.50
1:M:610:ASP:OD1	1:M:728:THR:HG22	2.12	0.50
1:N:358:HIS:NE2	1:V:434:MET:HB2	2.26	0.50
1:T:423:SER:O	1:T:729:ARG:HA	2.11	0.50
1:Y:692:LYS:HG3	1:t:398:PHE:CE1	2.47	0.50
1:q:353:VAL:H	1:q:645:GLN:HE22	1.58	0.50
1:q:423:SER:O	1:q:729:ARG:HA	2.12	0.50
1:t:423:SER:O	1:t:729:ARG:HA	2.12	0.50
1:v:423:SER:O	1:v:729:ARG:HA	2.12	0.50
1:w:353:VAL:H	1:w:645:GLN:HE22	1.58	0.50
1:w:423:SER:O	1:w:729:ARG:HA	2.12	0.50
1:w:429:SER:OG	1:w:431:ASP:OD1	2.28	0.50
1:z:413:TYR:OH	1:z:641:HIS:O	2.26	0.50
1:3:482:CYS:SG	1:3:576:TYR:HB2	2.50	0.50
1:6:423:SER:O	1:6:729:ARG:HA	2.12	0.50
1:8:238[B]:ARG:HD3	1:8:683:GLU:OE2	2.11	0.50
1:E:234:TRP:CD2	1:E:298[A]:ARG:HD3	2.47	0.49
1:E:423:SER:O	1:E:729:ARG:HA	2.12	0.49
1:E:434:MET:HB2	1:p:358:HIS:NE2	2.26	0.49
1:F:247:TRP:O	1:F:675:THR:OG1	2.17	0.49
1:F:610:ASP:OD1	1:F:728:THR:HG22	2.12	0.49
1:J:692:LYS:HG3	1:1:398:PHE:CE1	2.47	0.49
1:R:353:VAL:H	1:R:645:GLN:HE22	1.58	0.49
1:T:238[A]:ARG:HD2	1:T:683:GLU:OE2	2.11	0.49
1:T:298[A]:ARG:HG2	1:T:298[A]:ARG:NH2	2.27	0.49
1:W:423:SER:O	1:W:729:ARG:HA	2.12	0.49
1:X:413:TYR:OH	1:X:641:HIS:O	2.26	0.49
1:g:692:LYS:HG3	1:7:398:PHE:CE1	2.47	0.49
1:k:610:ASP:OD1	1:k:728:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:423:SER:O	1:m:729:ARG:HA	2.12	0.49
1:o:423:SER:O	1:o:729:ARG:HA	2.12	0.49
1:x:610:ASP:OD1	1:x:728:THR:HG22	2.12	0.49
1:y:610:ASP:OD1	1:y:728:THR:HG22	2.12	0.49
1:8:429:SER:OG	1:8:431:ASP:OD1	2.28	0.49
1:A:610:ASP:OD1	1:A:728:THR:HG22	2.12	0.49
1:C:434:MET:HB2	1:Y:358:HIS:NE2	2.26	0.49
1:D:610:ASP:OD1	1:D:728:THR:HG22	2.12	0.49
1:K:253:ASN:OD1	1:K:374:GLN:NE2	2.44	0.49
1:K:423:SER:O	1:K:729:ARG:HA	2.12	0.49
1:P:610:ASP:OD1	1:P:728:THR:HG22	2.12	0.49
1:S:253:ASN:OD1	1:S:374:GLN:NE2	2.44	0.49
1:X:423:SER:O	1:X:729:ARG:HA	2.12	0.49
1:a:610:ASP:OD1	1:a:728:THR:HG22	2.12	0.49
1:e:610:ASP:OD1	1:e:728:THR:HG22	2.12	0.49
1:h:353:VAL:H	1:h:645:GLN:HE22	1.58	0.49
1:h:413:TYR:OH	1:h:641:HIS:O	2.26	0.49
1:m:234:TRP:CZ2	1:m:298[A]:ARG:HB3	2.46	0.49
1:r:253:ASN:OD1	1:r:374:GLN:NE2	2.44	0.49
1:y:234:TRP:CE2	1:y:298[B]:ARG:HD2	2.47	0.49
1:4:253:ASN:OD1	1:4:374:GLN:NE2	2.44	0.49
1:I:423:SER:O	1:I:729:ARG:HA	2.11	0.49
1:N:692:LYS:HG3	1:w:398:PHE:CE1	2.47	0.49
1:Q:434:MET:HB2	1:k:358:HIS:NE2	2.26	0.49
1:Q:610:ASP:OD1	1:Q:728:THR:HG22	2.12	0.49
1:U:234:TRP:CE2	1:U:298[B]:ARG:HD2	2.47	0.49
1:b:434:MET:HB2	1:v:358:HIS:NE2	2.26	0.49
1:b:610:ASP:OD1	1:b:728:THR:HG22	2.12	0.49
1:e:692:LYS:HG3	1:y:398:PHE:CE1	2.47	0.49
1:f:610:ASP:OD1	1:f:728:THR:HG22	2.12	0.49
1:j:610:ASP:OD1	1:j:728:THR:HG22	2.12	0.49
1:t:247:TRP:O	1:t:675:THR:OG1	2.17	0.49
1:u:423:SER:O	1:u:729:ARG:HA	2.12	0.49
1:v:610:ASP:OD1	1:v:728:THR:HG22	2.12	0.49
1:3:610:ASP:OD1	1:3:728:THR:HG22	2.12	0.49
1:4:423:SER:O	1:4:729:ARG:HA	2.12	0.49
1:6:234:TRP:CD2	1:6:298[A]:ARG:HD3	2.47	0.49
1:A:358:HIS:NE2	1:f:434:MET:HB2	2.26	0.49
1:D:398:PHE:CE1	1:x:692:LYS:HG3	2.47	0.49
1:M:353:VAL:H	1:M:645:GLN:HE22	1.58	0.49
1:O:423:SER:O	1:O:729:ARG:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:398:PHE:CE1	1:k:692:LYS:HG3	2.47	0.49
1:b:692:LYS:HG3	1:v:398:PHE:CE1	2.47	0.49
1:k:234:TRP:CD2	1:k:298[A]:ARG:HD3	2.47	0.49
1:m:234:TRP:CD1	1:m:298[B]:ARG:HD2	2.48	0.49
1:u:234:TRP:CD2	1:u:298[A]:ARG:HD3	2.47	0.49
1:C:423:SER:O	1:C:729:ARG:HA	2.12	0.49
1:G:247:TRP:O	1:G:675:THR:OG1	2.17	0.49
1:H:298[A]:ARG:HG2	1:H:298[A]:ARG:NH2	2.22	0.49
1:M:413:TYR:OH	1:M:641:HIS:O	2.26	0.49
1:O:398:PHE:CE1	1:6:692:LYS:HG3	2.47	0.49
1:l:423:SER:O	1:l:729:ARG:HA	2.12	0.49
1:v:234:TRP:CE2	1:v:298[B]:ARG:HD2	2.48	0.49
1:y:253:ASN:OD1	1:y:374:GLN:NE2	2.44	0.49
1:4:234:TRP:CD1	1:4:298[B]:ARG:HD2	2.48	0.49
1:A:395:LEU:HD13	1:A:647:LEU:HD23	1.95	0.49
1:D:395:LEU:HD13	1:D:647:LEU:HD23	1.95	0.49
1:E:395:LEU:HD13	1:E:647:LEU:HD23	1.95	0.49
1:G:398:PHE:CE1	1:7:692:LYS:HG3	2.48	0.49
1:L:238[B]:ARG:HD3	1:L:683:GLU:OE2	2.13	0.49
1:L:610:ASP:OD1	1:L:728:THR:HG22	2.12	0.49
1:O:395:LEU:HD13	1:O:647:LEU:HD23	1.95	0.49
1:O:429:SER:OG	1:O:431:ASP:OD1	2.28	0.49
1:Q:395:LEU:HD13	1:Q:647:LEU:HD23	1.95	0.49
1:U:234:TRP:CZ2	1:U:298[B]:ARG:HB2	2.47	0.49
1:V:395:LEU:HD13	1:V:647:LEU:HD23	1.95	0.49
1:Z:427:SER:HB3	1:Z:732:THR:CG2	2.43	0.49
1:a:395:LEU:HD13	1:a:647:LEU:HD23	1.95	0.49
1:c:423:SER:O	1:c:729:ARG:HA	2.12	0.49
1:e:423:SER:O	1:e:729:ARG:HA	2.12	0.49
1:g:423:SER:O	1:g:729:ARG:HA	2.12	0.49
1:p:395:LEU:HD13	1:p:647:LEU:HD23	1.95	0.49
1:w:395:LEU:HD13	1:w:647:LEU:HD23	1.95	0.49
1:2:427:SER:HB3	1:2:732:THR:CG2	2.43	0.49
1:D:692:LYS:HG3	1:8:398:PHE:CE1	2.47	0.49
1:F:253:ASN:OD1	1:F:374:GLN:NE2	2.44	0.49
1:U:427:SER:HB3	1:U:732:THR:CG2	2.43	0.49
1:c:224:SER:H	1:6:407:ASN:HD21	1.61	0.49
1:g:587:ASN:OD1	1:g:588:ARG:NH2	2.46	0.49
1:j:423:SER:O	1:j:729:ARG:HA	2.12	0.49
1:l:253:ASN:OD1	1:l:374:GLN:NE2	2.44	0.49
1:l:395:LEU:HD13	1:l:647:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:413:TYR:OH	1:t:641:HIS:O	2.26	0.49
1:v:395:LEU:HD13	1:v:647:LEU:HD23	1.95	0.49
1:w:427:SER:HB3	1:w:732:THR:CG2	2.43	0.49
1:x:395:LEU:HD13	1:x:647:LEU:HD23	1.95	0.49
1:2:395:LEU:HD13	1:2:647:LEU:HD23	1.95	0.49
1:2:610:ASP:OD1	1:2:728:THR:HG22	2.12	0.49
1:3:395:LEU:HD13	1:3:647:LEU:HD23	1.95	0.49
1:4:353:VAL:H	1:4:645:GLN:HE22	1.58	0.49
1:5:610:ASP:OD1	1:5:728:THR:HG22	2.12	0.49
1:8:247:TRP:O	1:8:675:THR:OG1	2.17	0.49
1:8:427:SER:HB3	1:8:732:THR:CG2	2.43	0.49
1:A:587:ASN:OD1	1:A:588:ARG:NH2	2.46	0.49
1:C:427:SER:HB3	1:C:732:THR:CG2	2.43	0.49
1:C:587:ASN:OD1	1:C:588:ARG:NH2	2.46	0.49
1:E:427:SER:HB3	1:E:732:THR:CG2	2.43	0.49
1:H:610:ASP:OD1	1:H:728:THR:HG22	2.12	0.49
1:I:427:SER:HB3	1:I:732:THR:CG2	2.43	0.49
1:J:395:LEU:HD13	1:J:647:LEU:HD23	1.95	0.49
1:J:427:SER:HB3	1:J:732:THR:CG2	2.43	0.49
1:O:253:ASN:OD1	1:O:374:GLN:NE2	2.44	0.49
1:P:423:SER:O	1:P:729:ARG:HA	2.12	0.49
1:T:395:LEU:HD13	1:T:647:LEU:HD23	1.95	0.49
1:U:238[B]:ARG:HD3	1:U:683:GLU:OE2	2.13	0.49
1:W:395:LEU:HD13	1:W:647:LEU:HD23	1.95	0.49
1:Y:427:SER:HB3	1:Y:732:THR:CG2	2.43	0.49
1:Y:587:ASN:OD1	1:Y:588:ARG:NH2	2.46	0.49
1:b:398:PHE:CE1	1:d:692:LYS:HG3	2.48	0.49
1:b:587:ASN:OD1	1:b:588:ARG:NH2	2.46	0.49
1:d:353:VAL:H	1:d:645:GLN:HE22	1.58	0.49
1:f:587:ASN:OD1	1:f:588:ARG:NH2	2.46	0.49
1:g:427:SER:HB3	1:g:732:THR:CG2	2.43	0.49
1:j:587:ASN:OD1	1:j:588:ARG:NH2	2.46	0.49
1:k:395:LEU:HD13	1:k:647:LEU:HD23	1.95	0.49
1:n:298[A]:ARG:HG2	1:n:298[A]:ARG:NH2	2.16	0.49
1:n:353:VAL:H	1:n:645:GLN:HE22	1.58	0.49
1:o:610:ASP:OD1	1:o:728:THR:HG22	2.12	0.49
1:s:427:SER:HB3	1:s:732:THR:CG2	2.43	0.49
1:v:587:ASN:OD1	1:v:588:ARG:NH2	2.46	0.49
1:3:427:SER:HB3	1:3:732:THR:CG2	2.43	0.49
1:4:610:ASP:OD1	1:4:728:THR:HG22	2.12	0.49
1:6:395:LEU:HD13	1:6:647:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:427:SER:HB3	1:7:732:THR:CG2	2.43	0.49
1:B:237:ASP:OD2	1:B:238[B]:ARG:NH2	2.46	0.49
1:B:398:PHE:CE1	1:2:692:LYS:HG3	2.48	0.49
1:G:413:TYR:OH	1:G:641:HIS:O	2.26	0.49
1:I:692:LYS:HG3	1:6:398:PHE:CE1	2.48	0.49
1:J:610:ASP:OD1	1:J:728:THR:HG22	2.12	0.49
1:K:238[A]:ARG:HD2	1:K:683:GLU:OE2	2.12	0.49
1:P:587:ASN:OD1	1:P:588:ARG:NH2	2.46	0.49
1:W:692:LYS:HG3	1:l:398:PHE:CE1	2.47	0.49
1:a:427:SER:HB3	1:a:732:THR:CG2	2.43	0.49
1:c:427:SER:HB3	1:c:732:THR:CG2	2.43	0.49
1:e:427:SER:HB3	1:e:732:THR:CG2	2.43	0.49
1:k:427:SER:HB3	1:k:732:THR:CG2	2.43	0.49
1:l:429:SER:OG	1:l:431:ASP:OD1	2.28	0.49
1:n:610:ASP:OD1	1:n:728:THR:HG22	2.12	0.49
1:r:587:ASN:OD1	1:r:588:ARG:NH2	2.46	0.49
1:u:395:LEU:HD13	1:u:647:LEU:HD23	1.95	0.49
1:x:427:SER:HB3	1:x:732:THR:CG2	2.43	0.49
1:z:610:ASP:OD1	1:z:728:THR:HG22	2.12	0.49
1:6:610:ASP:OD1	1:6:728:THR:HG22	2.12	0.49
1:7:587:ASN:OD1	1:7:588:ARG:NH2	2.46	0.49
1:D:427:SER:HB3	1:D:732:THR:CG2	2.43	0.49
1:F:587:ASN:OD1	1:F:588:ARG:NH2	2.46	0.49
1:H:427:SER:HB3	1:H:732:THR:CG2	2.43	0.49
1:I:395:LEU:HD13	1:I:647:LEU:HD23	1.95	0.49
1:K:353:VAL:H	1:K:645:GLN:HE22	1.58	0.49
1:K:610:ASP:OD1	1:K:728:THR:HG22	2.12	0.49
1:L:353:VAL:HG11	1:R:435:ASN:HB2	1.93	0.49
1:M:427:SER:HB3	1:M:732:THR:CG2	2.43	0.49
1:Q:427:SER:HB3	1:Q:732:THR:CG2	2.43	0.49
1:R:427:SER:HB3	1:R:732:THR:CG2	2.43	0.49
1:S:587:ASN:OD1	1:S:588:ARG:NH2	2.46	0.49
1:U:587:ASN:OD1	1:U:588:ARG:NH2	2.46	0.49
1:X:587:ASN:OD1	1:X:588:ARG:NH2	2.46	0.49
1:d:610:ASP:OD1	1:d:728:THR:HG22	2.12	0.49
1:h:587:ASN:OD1	1:h:588:ARG:NH2	2.46	0.49
1:m:395:LEU:HD13	1:m:647:LEU:HD23	1.95	0.49
1:s:587:ASN:OD1	1:s:588:ARG:NH2	2.46	0.49
1:u:427:SER:HB3	1:u:732:THR:CG2	2.43	0.49
1:y:429:SER:OG	1:y:431:ASP:OD1	2.28	0.49
1:y:587:ASN:OD1	1:y:588:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:429:SER:OG	1:1:431:ASP:OD1	2.28	0.49
1:5:427:SER:HB3	1:5:732:THR:CG2	2.43	0.49
1:6:587:ASN:OD1	1:6:588:ARG:NH2	2.46	0.49
1:C:395:LEU:HD13	1:C:647:LEU:HD23	1.95	0.48
1:E:398:PHE:CE1	1:i:692:LYS:HG3	2.48	0.48
1:F:509:HIS:NE2	1:c:574:GLU:OE1	2.46	0.48
1:M:587:ASN:OD1	1:M:588:ARG:NH2	2.46	0.48
1:S:692:LYS:HG3	1:q:398:PHE:CE1	2.47	0.48
1:V:427:SER:HB3	1:V:732:THR:CG2	2.43	0.48
1:W:587:ASN:OD1	1:W:588:ARG:NH2	2.46	0.48
1:W:610:ASP:OD1	1:W:728:THR:HG22	2.12	0.48
1:X:610:ASP:OD1	1:X:728:THR:HG22	2.12	0.48
1:Y:413:TYR:OH	1:Y:641:HIS:O	2.26	0.48
1:Y:610:ASP:OD1	1:Y:728:THR:HG22	2.12	0.48
1:Z:395:LEU:HD13	1:Z:647:LEU:HD23	1.95	0.48
1:d:587:ASN:OD1	1:d:588:ARG:NH2	2.46	0.48
1:g:395:LEU:HD13	1:g:647:LEU:HD23	1.95	0.48
1:h:427:SER:HB3	1:h:732:THR:CG2	2.43	0.48
1:n:587:ASN:OD1	1:n:588:ARG:NH2	2.46	0.48
1:o:587:ASN:OD1	1:o:588:ARG:NH2	2.46	0.48
1:q:427:SER:HB3	1:q:732:THR:CG2	2.43	0.48
1:A:224:SER:H	1:H:407:ASN:HD21	1.61	0.48
1:E:587:ASN:OD1	1:E:588:ARG:NH2	2.46	0.48
1:E:692:LYS:HG3	1:p:398:PHE:CE1	2.48	0.48
1:F:429:SER:OG	1:F:431:ASP:OD1	2.28	0.48
1:K:395:LEU:HD13	1:K:647:LEU:HD23	1.95	0.48
1:T:587:ASN:OD1	1:T:588:ARG:NH2	2.46	0.48
1:f:398:PHE:CE1	1:n:692:LYS:HG3	2.48	0.48
1:m:587:ASN:OD1	1:m:588:ARG:NH2	2.46	0.48
1:p:427:SER:HB3	1:p:732:THR:CG2	2.43	0.48
1:w:587:ASN:OD1	1:w:588:ARG:NH2	2.46	0.48
1:w:610:ASP:OD1	1:w:728:THR:HG22	2.12	0.48
1:8:395:LEU:HD13	1:8:647:LEU:HD23	1.95	0.48
1:A:275:TYR:OH	1:Q:713:THR:HG21	2.13	0.48
1:A:427:SER:HB3	1:A:732:THR:CG2	2.43	0.48
1:E:610:ASP:OD1	1:E:728:THR:HG22	2.12	0.48
1:G:395:LEU:HD13	1:G:647:LEU:HD23	1.95	0.48
1:J:398:PHE:CE1	1:s:692:LYS:HG3	2.47	0.48
1:K:467:ALA:HA	1:K:470:ILE:HD11	1.96	0.48
1:N:398:PHE:CE1	1:V:692:LYS:HG3	2.48	0.48
1:S:398:PHE:CE1	1:z:692:LYS:HG3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:423:SER:O	1:S:729:ARG:HA	2.12	0.48
1:a:587:ASN:OD1	1:a:588:ARG:NH2	2.46	0.48
1:b:234:TRP:CD1	1:b:298[B]:ARG:HD2	2.48	0.48
1:r:423:SER:O	1:r:729:ARG:HA	2.11	0.48
1:t:395:LEU:HD13	1:t:647:LEU:HD23	1.95	0.48
1:7:610:ASP:OD1	1:7:728:THR:HG22	2.12	0.48
1:E:288:HIS:HD2	1:E:614:GLN:HB2	1.79	0.48
1:G:692:LYS:HG3	1:g:398:PHE:CE1	2.48	0.48
1:J:467:ALA:HA	1:J:470:ILE:HD11	1.96	0.48
1:K:398:PHE:CE1	1:X:692:LYS:HG3	2.49	0.48
1:R:398:PHE:CE1	1:r:692:LYS:HG3	2.48	0.48
1:W:467:ALA:HA	1:W:470:ILE:HD11	1.96	0.48
1:a:692:LYS:HG3	1:e:398:PHE:CE1	2.48	0.48
1:b:427:SER:HB3	1:b:732:THR:CG2	2.43	0.48
1:e:413:TYR:OH	1:e:641:HIS:O	2.26	0.48
1:f:427:SER:HB3	1:f:732:THR:CG2	2.43	0.48
1:r:395:LEU:HD13	1:r:647:LEU:HD23	1.95	0.48
1:v:427:SER:HB3	1:v:732:THR:CG2	2.43	0.48
1:w:247:TRP:O	1:w:675:THR:OG1	2.17	0.48
1:w:288:HIS:HD2	1:w:614:GLN:HB2	1.79	0.48
1:w:298[A]:ARG:HH22	1:w:688:LYS:HZ1	1.60	0.48
1:2:467:ALA:HA	1:2:470:ILE:HD11	1.96	0.48
1:3:587:ASN:OD1	1:3:588:ARG:NH2	2.46	0.48
1:7:467:ALA:HA	1:7:470:ILE:HD11	1.96	0.48
1:8:610:ASP:OD1	1:8:728:THR:HG22	2.12	0.48
1:G:427:SER:HB3	1:G:732:THR:CG2	2.43	0.48
1:G:429:SER:OG	1:G:431:ASP:OD1	2.28	0.48
1:G:467:ALA:HA	1:G:470:ILE:HD11	1.96	0.48
1:G:587:ASN:OD1	1:G:588:ARG:NH2	2.46	0.48
1:I:398:PHE:CE1	1:O:692:LYS:HG3	2.49	0.48
1:I:587:ASN:OD1	1:I:588:ARG:NH2	2.46	0.48
1:K:587:ASN:OD1	1:K:588:ARG:NH2	2.46	0.48
1:L:429:SER:OG	1:L:431:ASP:OD1	2.28	0.48
1:O:427:SER:HB3	1:O:732:THR:CG2	2.43	0.48
1:P:427:SER:HB3	1:P:732:THR:CG2	2.43	0.48
1:R:288:HIS:HD2	1:R:614:GLN:HB2	1.79	0.48
1:R:587:ASN:OD1	1:R:588:ARG:NH2	2.46	0.48
1:Y:395:LEU:HD13	1:Y:647:LEU:HD23	1.95	0.48
1:Y:467:ALA:HA	1:Y:470:ILE:HD11	1.96	0.48
1:Z:610:ASP:OD1	1:Z:728:THR:HG22	2.12	0.48
1:g:413:TYR:OH	1:g:641:HIS:O	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:467:ALA:HA	1:i:470:ILE:HD11	1.96	0.48
1:j:427:SER:HB3	1:j:732:THR:CG2	2.43	0.48
1:q:288:HIS:HD2	1:q:614:GLN:HB2	1.79	0.48
1:q:587:ASN:OD1	1:q:588:ARG:NH2	2.46	0.48
1:t:429:SER:OG	1:t:431:ASP:OD1	2.28	0.48
1:u:587:ASN:OD1	1:u:588:ARG:NH2	2.46	0.48
1:z:395:LEU:HD13	1:z:647:LEU:HD23	1.95	0.48
1:z:429:SER:OG	1:z:431:ASP:OD1	2.28	0.48
1:1:427:SER:HB3	1:1:732:THR:CG2	2.43	0.48
1:4:395:LEU:HD13	1:4:647:LEU:HD23	1.95	0.48
1:4:467:ALA:HA	1:4:470:ILE:HD11	1.96	0.48
1:4:587:ASN:OD1	1:4:588:ARG:NH2	2.46	0.48
1:6:467:ALA:HA	1:6:470:ILE:HD11	1.96	0.48
1:7:413:TYR:OH	1:7:641:HIS:O	2.26	0.48
1:8:234:TRP:NE1	1:8:298[B]:ARG:HD2	2.28	0.48
1:B:427:SER:HB3	1:B:732:THR:CG2	2.43	0.48
1:B:467:ALA:HA	1:B:470:ILE:HD11	1.96	0.48
1:D:247:TRP:O	1:D:675:THR:OG1	2.17	0.48
1:E:234:TRP:CZ2	1:E:298[A]:ARG:HB3	2.49	0.48
1:I:288:HIS:HD2	1:I:614:GLN:HB2	1.79	0.48
1:L:395:LEU:HD13	1:L:647:LEU:HD23	1.95	0.48
1:N:395:LEU:HD13	1:N:647:LEU:HD23	1.95	0.48
1:R:237:ASP:OD2	1:R:238[B]:ARG:NH2	2.47	0.48
1:S:395:LEU:HD13	1:S:647:LEU:HD23	1.95	0.48
1:a:288:HIS:HD2	1:a:614:GLN:HB2	1.79	0.48
1:c:587:ASN:OD1	1:c:588:ARG:NH2	2.46	0.48
1:e:587:ASN:OD1	1:e:588:ARG:NH2	2.46	0.48
1:f:224:SER:H	1:k:407:ASN:HD21	1.62	0.48
1:f:298[A]:ARG:HH22	1:f:688:LYS:HZ1	1.62	0.48
1:i:288:HIS:HD2	1:i:614:GLN:HB2	1.79	0.48
1:m:234:TRP:CZ2	1:m:298[B]:ARG:HB2	2.49	0.48
1:p:587:ASN:OD1	1:p:588:ARG:NH2	2.46	0.48
1:t:427:SER:HB3	1:t:732:THR:CG2	2.43	0.48
1:t:587:ASN:OD1	1:t:588:ARG:NH2	2.46	0.48
1:u:288:HIS:HD2	1:u:614:GLN:HB2	1.79	0.48
1:3:288:HIS:HD2	1:3:614:GLN:HB2	1.79	0.48
1:5:413:TYR:OH	1:5:641:HIS:O	2.26	0.48
1:5:587:ASN:OD1	1:5:588:ARG:NH2	2.46	0.48
1:7:395:LEU:HD13	1:7:647:LEU:HD23	1.95	0.48
1:8:587:ASN:OD1	1:8:588:ARG:NH2	2.46	0.48
1:H:398:PHE:CE1	1:T:692:LYS:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:427:SER:HB3	1:L:732:THR:CG2	2.43	0.48
1:N:288:HIS:HD2	1:N:614:GLN:HB2	1.79	0.48
1:N:467:ALA:HA	1:N:470:ILE:HD11	1.96	0.48
1:O:587:ASN:OD1	1:O:588:ARG:NH2	2.46	0.48
1:Q:288:HIS:HD2	1:Q:614:GLN:HB2	1.79	0.48
1:Q:692:LYS:HG3	1:k:398:PHE:CE1	2.48	0.48
1:V:587:ASN:OD1	1:V:588:ARG:NH2	2.46	0.48
1:W:413:TYR:OH	1:W:641:HIS:O	2.26	0.48
1:c:395:LEU:HD13	1:c:647:LEU:HD23	1.95	0.48
1:i:395:LEU:HD13	1:i:647:LEU:HD23	1.95	0.48
1:l:427:SER:HB3	1:l:732:THR:CG2	2.43	0.48
1:t:467:ALA:HA	1:t:470:ILE:HD11	1.96	0.48
1:x:288:HIS:HD2	1:x:614:GLN:HB2	1.79	0.48
1:z:427:SER:HB3	1:z:732:THR:CG2	2.43	0.48
1:1:467:ALA:HA	1:1:470:ILE:HD11	1.96	0.48
1:2:288:HIS:HD2	1:2:614:GLN:HB2	1.79	0.48
1:2:587:ASN:OD1	1:2:588:ARG:NH2	2.46	0.48
1:6:413:TYR:OH	1:6:641:HIS:O	2.26	0.48
1:6:427:SER:HB3	1:6:732:THR:CG2	2.43	0.48
1:A:509:HIS:NE2	1:f:574:GLU:OE1	2.46	0.48
1:B:692:LYS:HG3	1:U:398:PHE:CE1	2.49	0.48
1:C:413:TYR:OH	1:C:641:HIS:O	2.26	0.48
1:D:587:ASN:OD1	1:D:588:ARG:NH2	2.46	0.48
1:F:427:SER:HB3	1:F:732:THR:CG2	2.43	0.48
1:H:587:ASN:OD1	1:H:588:ARG:NH2	2.46	0.48
1:J:288:HIS:HD2	1:J:614:GLN:HB2	1.79	0.48
1:K:574:GLU:OE1	1:P:509:HIS:NE2	2.47	0.48
1:L:407:ASN:HD21	1:M:224:SER:H	1.62	0.48
1:L:587:ASN:OD1	1:L:588:ARG:NH2	2.46	0.48
1:M:395:LEU:HD13	1:M:647:LEU:HD23	1.95	0.48
1:O:288:HIS:HD2	1:O:614:GLN:HB2	1.79	0.48
1:R:224:SER:H	1:T:407:ASN:HD21	1.62	0.48
1:R:518:ASN:HB3	1:r:474:SER:HA	1.96	0.48
1:T:427:SER:HB3	1:T:732:THR:CG2	2.43	0.48
1:W:427:SER:HB3	1:W:732:THR:CG2	2.43	0.48
1:X:395:LEU:HD13	1:X:647:LEU:HD23	1.95	0.48
1:Z:587:ASN:OD1	1:Z:588:ARG:NH2	2.46	0.48
1:a:467:ALA:HA	1:a:470:ILE:HD11	1.96	0.48
1:d:395:LEU:HD13	1:d:647:LEU:HD23	1.95	0.48
1:e:395:LEU:HD13	1:e:647:LEU:HD23	1.95	0.48
1:h:395:LEU:HD13	1:h:647:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:288:HIS:HD2	1:l:614:GLN:HB2	1.79	0.48
1:u:429:SER:OG	1:u:431:ASP:OD1	2.28	0.48
1:x:467:ALA:HA	1:x:470:ILE:HD11	1.96	0.48
1:y:467:ALA:HA	1:y:470:ILE:HD11	1.96	0.48
1:1:587:ASN:OD1	1:1:588:ARG:NH2	2.46	0.48
1:B:587:ASN:OD1	1:B:588:ARG:NH2	2.46	0.48
1:C:692:LYS:HG3	1:Y:398:PHE:CE1	2.48	0.48
1:D:467:ALA:HA	1:D:470:ILE:HD11	1.96	0.48
1:F:467:ALA:HA	1:F:470:ILE:HD11	1.96	0.48
1:H:413:TYR:OH	1:H:641:HIS:O	2.26	0.48
1:I:396:GLU:OE2	1:I:649:LYS:HE2	2.14	0.48
1:J:587:ASN:OD1	1:J:588:ARG:NH2	2.46	0.48
1:K:298[A]:ARG:HG2	1:K:298[A]:ARG:NH2	2.27	0.48
1:K:692:LYS:HG3	1:P:398:PHE:CE1	2.49	0.48
1:M:692:LYS:HG3	1:T:398:PHE:CE1	2.49	0.48
1:N:427:SER:HB3	1:N:732:THR:CG2	2.43	0.48
1:N:587:ASN:OD1	1:N:588:ARG:NH2	2.46	0.48
1:P:467:ALA:HA	1:P:470:ILE:HD11	1.96	0.48
1:Q:467:ALA:HA	1:Q:470:ILE:HD11	1.96	0.48
1:R:396:GLU:OE2	1:R:649:LYS:HE2	2.14	0.48
1:S:288:HIS:HD2	1:S:614:GLN:HB2	1.79	0.48
1:W:429:SER:OG	1:W:431:ASP:OD1	2.28	0.48
1:Z:288:HIS:HD2	1:Z:614:GLN:HB2	1.79	0.48
1:Z:467:ALA:HA	1:Z:470:ILE:HD11	1.96	0.48
1:d:288:HIS:HD2	1:d:614:GLN:HB2	1.79	0.48
1:f:288:HIS:HD2	1:f:614:GLN:HB2	1.79	0.48
1:h:288:HIS:HD2	1:h:614:GLN:HB2	1.79	0.48
1:i:427:SER:HB3	1:i:732:THR:CG2	2.43	0.48
1:k:467:ALA:HA	1:k:470:ILE:HD11	1.96	0.48
1:k:587:ASN:OD1	1:k:588:ARG:NH2	2.46	0.48
1:n:288:HIS:HD2	1:n:614:GLN:HB2	1.79	0.48
1:q:395:LEU:HD13	1:q:647:LEU:HD23	1.95	0.48
1:q:396:GLU:OE2	1:q:649:LYS:HE2	2.14	0.48
1:v:288:HIS:HD2	1:v:614:GLN:HB2	1.79	0.48
1:z:587:ASN:OD1	1:z:588:ARG:NH2	2.46	0.48
1:5:288:HIS:HD2	1:5:614:GLN:HB2	1.79	0.48
1:6:396:GLU:OE2	1:6:649:LYS:HE2	2.14	0.48
1:8:467:ALA:HA	1:8:470:ILE:HD11	1.96	0.48
1:D:713:THR:HG21	1:O:275:TYR:OH	2.14	0.48
1:E:509:HIS:NE2	1:i:574:GLU:OE1	2.47	0.48
1:E:713:THR:HG21	1:R:275:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:TYR:OH	1:I:713:THR:HG21	2.14	0.48
1:F:692:LYS:HG3	1:3:398:PHE:CE1	2.49	0.48
1:H:288:HIS:HD2	1:H:614:GLN:HB2	1.79	0.48
1:I:429:SER:OG	1:I:431:ASP:OD1	2.28	0.48
1:L:692:LYS:HG3	1:r:398:PHE:CE1	2.48	0.48
1:M:288:HIS:HD2	1:M:614:GLN:HB2	1.79	0.48
1:P:395:LEU:HD13	1:P:647:LEU:HD23	1.95	0.48
1:Q:398:PHE:CE1	1:Z:692:LYS:HG3	2.49	0.48
1:R:395:LEU:HD13	1:R:647:LEU:HD23	1.95	0.48
1:R:509:HIS:NE2	1:r:574:GLU:OE1	2.47	0.48
1:T:396:GLU:OE2	1:T:649:LYS:HE2	2.14	0.48
1:W:396:GLU:OE2	1:W:649:LYS:HE2	2.14	0.48
1:X:247:TRP:O	1:X:675:THR:OG1	2.17	0.48
1:d:396:GLU:OE2	1:d:649:LYS:HE2	2.14	0.48
1:i:587:ASN:OD1	1:i:588:ARG:NH2	2.46	0.48
1:l:587:ASN:OD1	1:l:588:ARG:NH2	2.46	0.48
1:m:396:GLU:OE2	1:m:649:LYS:HE2	2.14	0.48
1:m:427:SER:HB3	1:m:732:THR:CG2	2.43	0.48
1:n:395:LEU:HD13	1:n:647:LEU:HD23	1.95	0.48
1:o:395:LEU:HD13	1:o:647:LEU:HD23	1.95	0.48
1:r:467:ALA:HA	1:r:470:ILE:HD11	1.96	0.48
1:u:396:GLU:OE2	1:u:649:LYS:HE2	2.14	0.48
1:y:427:SER:HB3	1:y:732:THR:CG2	2.43	0.48
1:3:467:ALA:HA	1:3:470:ILE:HD11	1.96	0.48
1:B:509:HIS:NE2	1:2:574:GLU:OE1	2.47	0.47
1:H:395:LEU:HD13	1:H:647:LEU:HD23	1.95	0.47
1:J:275:TYR:OH	1:8:713:THR:HG21	2.14	0.47
1:Q:429:SER:OG	1:Q:431:ASP:OD1	2.28	0.47
1:R:298[A]:ARG:HG2	1:R:298[A]:ARG:NH2	2.24	0.47
1:S:467:ALA:HA	1:S:470:ILE:HD11	1.96	0.47
1:U:396:GLU:OE2	1:U:649:LYS:HE2	2.14	0.47
1:U:692:LYS:HG3	1:2:398:PHE:CE1	2.48	0.47
1:b:288:HIS:HD2	1:b:614:GLN:HB2	1.79	0.47
1:d:713:THR:HG21	1:i:275:TYR:OH	2.14	0.47
1:f:395:LEU:HD13	1:f:647:LEU:HD23	1.95	0.47
1:g:429:SER:OG	1:g:431:ASP:OD1	2.28	0.47
1:j:395:LEU:HD13	1:j:647:LEU:HD23	1.95	0.47
1:j:467:ALA:HA	1:j:470:ILE:HD11	1.96	0.47
1:p:396:GLU:OE2	1:p:649:LYS:HE2	2.14	0.47
1:s:396:GLU:OE2	1:s:649:LYS:HE2	2.14	0.47
1:y:395:LEU:HD13	1:y:647:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:288:HIS:HD2	1:8:614:GLN:HB2	1.79	0.47
1:A:288:HIS:HD2	1:A:614:GLN:HB2	1.79	0.47
1:D:275:TYR:OH	1:b:713:THR:HG21	2.14	0.47
1:F:224:SER:H	1:P:407:ASN:HD21	1.61	0.47
1:F:395:LEU:HD13	1:F:647:LEU:HD23	1.95	0.47
1:F:396:GLU:OE2	1:F:649:LYS:HE2	2.14	0.47
1:F:713:THR:HG21	1:P:275:TYR:OH	2.15	0.47
1:H:467:ALA:HA	1:H:470:ILE:HD11	1.96	0.47
1:K:427:SER:HB3	1:K:732:THR:CG2	2.43	0.47
1:L:398:PHE:CE1	1:R:692:LYS:HG3	2.49	0.47
1:S:427:SER:HB3	1:S:732:THR:CG2	2.43	0.47
1:U:395:LEU:HD13	1:U:647:LEU:HD23	1.95	0.47
1:V:396:GLU:OE2	1:V:649:LYS:HE2	2.14	0.47
1:X:429:SER:OG	1:X:431:ASP:OD1	2.28	0.47
1:Y:234:TRP:CH2	1:Y:298[B]:ARG:HB2	2.49	0.47
1:c:467:ALA:HA	1:c:470:ILE:HD11	1.96	0.47
1:d:518:ASN:HB3	1:v:474:SER:HA	1.96	0.47
1:k:247:TRP:O	1:k:675:THR:OG1	2.17	0.47
1:k:288:HIS:HD2	1:k:614:GLN:HB2	1.79	0.47
1:n:396:GLU:OE2	1:n:649:LYS:HE2	2.14	0.47
1:r:288:HIS:HD2	1:r:614:GLN:HB2	1.79	0.47
1:s:395:LEU:HD13	1:s:647:LEU:HD23	1.95	0.47
1:s:467:ALA:HA	1:s:470:ILE:HD11	1.96	0.47
1:t:345:ASP:O	1:t:346:SER:OG	2.32	0.47
1:y:396:GLU:OE2	1:y:649:LYS:HE2	2.14	0.47
1:1:395:LEU:HD13	1:1:647:LEU:HD23	1.95	0.47
1:4:427:SER:HB3	1:4:732:THR:CG2	2.43	0.47
1:5:247:TRP:O	1:5:675:THR:OG1	2.17	0.47
1:5:467:ALA:HA	1:5:470:ILE:HD11	1.96	0.47
1:B:275:TYR:OH	1:G:713:THR:HG21	2.14	0.47
1:B:288:HIS:HD2	1:B:614:GLN:HB2	1.79	0.47
1:B:562:GLU:OE2	1:B:612:TYR:OH	2.31	0.47
1:H:247:TRP:O	1:H:675:THR:OG1	2.17	0.47
1:H:574:GLU:OE1	1:M:509:HIS:NE2	2.48	0.47
1:I:509:HIS:NE2	1:O:574:GLU:OE1	2.48	0.47
1:N:407:ASN:HD21	1:n:224:SER:H	1.63	0.47
1:P:692:LYS:HG3	1:X:398:PHE:CE1	2.49	0.47
1:S:413:TYR:OH	1:S:641:HIS:O	2.26	0.47
1:S:713:THR:HG21	1:V:275:TYR:OH	2.14	0.47
1:V:518:ASN:HB3	1:w:474:SER:HA	1.96	0.47
1:X:427:SER:HB3	1:X:732:THR:CG2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:377:TYR:HH	1:b:393:TYR:H	1.62	0.47
1:b:395:LEU:HD13	1:b:647:LEU:HD23	1.95	0.47
1:d:275:TYR:OH	1:m:713:THR:HG21	2.14	0.47
1:e:234:TRP:CD1	1:e:298[B]:ARG:HD2	2.48	0.47
1:h:713:THR:HG21	1:z:275:TYR:OH	2.14	0.47
1:n:427:SER:HB3	1:n:732:THR:CG2	2.43	0.47
1:o:427:SER:HB3	1:o:732:THR:CG2	2.43	0.47
1:o:429:SER:OG	1:o:431:ASP:OD1	2.28	0.47
1:r:413:TYR:OH	1:r:641:HIS:O	2.26	0.47
1:1:288:HIS:HD2	1:1:614:GLN:HB2	1.79	0.47
1:1:713:THR:HG21	1:4:275:TYR:OH	2.15	0.47
1:6:429:SER:OG	1:6:431:ASP:OD1	2.28	0.47
1:A:396:GLU:OE2	1:A:649:LYS:HE2	2.14	0.47
1:B:395:LEU:HD13	1:B:647:LEU:HD23	1.95	0.47
1:G:288:HIS:HD2	1:G:614:GLN:HB2	1.79	0.47
1:H:692:LYS:HG3	1:M:398:PHE:CE1	2.49	0.47
1:M:396:GLU:OE2	1:M:649:LYS:HE2	2.14	0.47
1:O:509:HIS:NE2	1:6:574:GLU:OE1	2.47	0.47
1:P:396:GLU:OE2	1:P:649:LYS:HE2	2.14	0.47
1:Q:509:HIS:NE2	1:Z:574:GLU:OE1	2.48	0.47
1:T:467:ALA:HA	1:T:470:ILE:HD11	1.96	0.47
1:U:467:ALA:HA	1:U:470:ILE:HD11	1.96	0.47
1:V:713:THR:HG21	1:f:275:TYR:OH	2.14	0.47
1:W:288:HIS:HD2	1:W:614:GLN:HB2	1.79	0.47
1:W:713:THR:HG21	1:Z:275:TYR:OH	2.14	0.47
1:Y:396:GLU:OE2	1:Y:649:LYS:HE2	2.14	0.47
1:c:398:PHE:CE1	1:3:692:LYS:HG3	2.49	0.47
1:i:224:SER:H	1:w:407:ASN:HD21	1.62	0.47
1:l:467:ALA:HA	1:l:470:ILE:HD11	1.96	0.47
1:r:427:SER:HB3	1:r:732:THR:CG2	2.43	0.47
1:s:713:THR:HG21	1:x:275:TYR:OH	2.14	0.47
1:3:298[A]:ARG:HG2	1:3:298[A]:ARG:NH2	2.16	0.47
1:5:395:LEU:HD13	1:5:647:LEU:HD23	1.95	0.47
1:B:713:THR:HG21	1:K:275:TYR:OH	2.15	0.47
1:C:288:HIS:HD2	1:C:614:GLN:HB2	1.79	0.47
1:C:396:GLU:OE2	1:C:649:LYS:HE2	2.14	0.47
1:C:509:HIS:NE2	1:t:574:GLU:OE1	2.48	0.47
1:D:288:HIS:HD2	1:D:614:GLN:HB2	1.79	0.47
1:G:234:TRP:CZ2	1:G:298[A]:ARG:HB3	2.49	0.47
1:H:509:HIS:NE2	1:T:574:GLU:OE1	2.47	0.47
1:O:467:ALA:HA	1:O:470:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:587:ASN:OD1	1:Q:588:ARG:NH2	2.46	0.47
1:R:713:THR:HG21	1:T:275:TYR:OH	2.15	0.47
1:S:275:TYR:OH	1:l:713:THR:HG21	2.14	0.47
1:V:509:HIS:NE2	1:w:574:GLU:OE1	2.48	0.47
1:Z:713:THR:HG21	1:2:275:TYR:OH	2.15	0.47
1:a:275:TYR:OH	1:4:713:THR:HG21	2.14	0.47
1:a:518:ASN:HB3	1:y:474:SER:HA	1.97	0.47
1:b:467:ALA:HA	1:b:470:ILE:HD11	1.96	0.47
1:c:396:GLU:OE2	1:c:649:LYS:HE2	2.14	0.47
1:c:429:SER:OG	1:c:431:ASP:OD1	2.28	0.47
1:d:427:SER:HB3	1:d:732:THR:CG2	2.43	0.47
1:e:467:ALA:HA	1:e:470:ILE:HD11	1.96	0.47
1:f:467:ALA:HA	1:f:470:ILE:HD11	1.96	0.47
1:g:467:ALA:HA	1:g:470:ILE:HD11	1.96	0.47
1:h:396:GLU:OE2	1:h:649:LYS:HE2	2.14	0.47
1:j:396:GLU:OE2	1:j:649:LYS:HE2	2.14	0.47
1:v:396:GLU:OE2	1:v:649:LYS:HE2	2.14	0.47
1:v:467:ALA:HA	1:v:470:ILE:HD11	1.96	0.47
1:w:234:TRP:CD2	1:w:298[B]:ARG:HD2	2.49	0.47
1:x:587:ASN:OD1	1:x:588:ARG:NH2	2.46	0.47
1:6:288:HIS:HD2	1:6:614:GLN:HB2	1.79	0.47
1:7:396:GLU:OE2	1:7:649:LYS:HE2	2.14	0.47
1:C:467:ALA:HA	1:C:470:ILE:HD11	1.96	0.47
1:D:518:ASN:HB3	1:x:474:SER:HA	1.96	0.47
1:E:518:ASN:HB3	1:i:474:SER:HA	1.96	0.47
1:L:396:GLU:OE2	1:L:649:LYS:HE2	2.14	0.47
1:M:574:GLU:OE1	1:T:509:HIS:NE2	2.48	0.47
1:O:396:GLU:OE2	1:O:649:LYS:HE2	2.14	0.47
1:T:288:HIS:HD2	1:T:614:GLN:HB2	1.79	0.47
1:Y:407:ASN:HD21	1:3:224:SER:H	1.63	0.47
1:g:288:HIS:HD2	1:g:614:GLN:HB2	1.79	0.47
1:g:396:GLU:OE2	1:g:649:LYS:HE2	2.14	0.47
1:i:396:GLU:OE2	1:i:649:LYS:HE2	2.14	0.47
1:j:275:TYR:OH	1:y:713:THR:HG21	2.15	0.47
1:m:467:ALA:HA	1:m:470:ILE:HD11	1.96	0.47
1:t:288:HIS:HD2	1:t:614:GLN:HB2	1.79	0.47
1:t:713:THR:HG21	1:1:275:TYR:OH	2.15	0.47
1:v:407:ASN:HD21	1:x:224:SER:H	1.63	0.47
1:z:396:GLU:OE2	1:z:649:LYS:HE2	2.14	0.47
1:6:713:THR:HG21	1:8:275:TYR:OH	2.15	0.47
1:A:467:ALA:HA	1:A:470:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:GLU:OE2	1:B:649:LYS:HE2	2.14	0.47
1:C:518:ASN:HB3	1:t:474:SER:HA	1.96	0.47
1:D:509:HIS:NE2	1:x:574:GLU:OE1	2.48	0.47
1:E:275:TYR:OH	1:N:713:THR:HG21	2.14	0.47
1:I:467:ALA:HA	1:I:470:ILE:HD11	1.96	0.47
1:J:396:GLU:OE2	1:J:649:LYS:HE2	2.14	0.47
1:L:275:TYR:OH	1:M:713:THR:HG21	2.15	0.47
1:N:275:TYR:OH	1:n:713:THR:HG21	2.15	0.47
1:N:396:GLU:OE2	1:N:649:LYS:HE2	2.14	0.47
1:P:574:GLU:OE1	1:X:509:HIS:NE2	2.47	0.47
1:Q:275:TYR:OH	1:U:713:THR:HG21	2.15	0.47
1:S:396:GLU:OE2	1:S:649:LYS:HE2	2.14	0.47
1:V:467:ALA:HA	1:V:470:ILE:HD11	1.96	0.47
1:a:396:GLU:OE2	1:a:649:LYS:HE2	2.14	0.47
1:a:713:THR:HG21	1:7:275:TYR:OH	2.14	0.47
1:b:396:GLU:OE2	1:b:649:LYS:HE2	2.14	0.47
1:c:509:HIS:NE2	1:3:574:GLU:OE1	2.47	0.47
1:d:224:SER:H	1:i:407:ASN:HD21	1.63	0.47
1:d:467:ALA:HA	1:d:470:ILE:HD11	1.96	0.47
1:e:396:GLU:OE2	1:e:649:LYS:HE2	2.14	0.47
1:e:429:SER:OG	1:e:431:ASP:OD1	2.28	0.47
1:f:713:THR:HG21	1:k:275:TYR:OH	2.15	0.47
1:j:377:TYR:HH	1:j:393:TYR:H	1.63	0.47
1:l:234:TRP:NE1	1:l:298[B]:ARG:HD2	2.29	0.47
1:l:396:GLU:OE2	1:l:649:LYS:HE2	2.14	0.47
1:m:275:TYR:OH	1:q:713:THR:HG21	2.15	0.47
1:m:288:HIS:HD2	1:m:614:GLN:HB2	1.79	0.47
1:n:467:ALA:HA	1:n:470:ILE:HD11	1.96	0.47
1:o:288:HIS:HD2	1:o:614:GLN:HB2	1.79	0.47
1:p:467:ALA:HA	1:p:470:ILE:HD11	1.96	0.47
1:r:396:GLU:OE2	1:r:649:LYS:HE2	2.14	0.47
1:t:234:TRP:CD2	1:t:298[B]:ARG:HD2	2.49	0.47
1:t:396:GLU:OE2	1:t:649:LYS:HE2	2.14	0.47
1:u:224:SER:H	1:y:407:ASN:HD21	1.63	0.47
1:u:467:ALA:HA	1:u:470:ILE:HD11	1.96	0.47
1:u:713:THR:HG21	1:y:275:TYR:OH	2.15	0.47
1:w:298[A]:ARG:HG2	1:w:298[A]:ARG:HH21	1.80	0.47
1:w:396:GLU:OE2	1:w:649:LYS:HE2	2.14	0.47
1:6:224:SER:H	1:8:407:ASN:HD21	1.62	0.47
1:E:396:GLU:OE2	1:E:649:LYS:HE2	2.14	0.47
1:G:396:GLU:OE2	1:G:649:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:518:ASN:HB3	1:7:474:SER:HA	1.96	0.47
1:M:275:TYR:OH	1:P:713:THR:HG21	2.15	0.47
1:O:713:THR:HG21	1:r:275:TYR:OH	2.15	0.47
1:P:288:HIS:HD2	1:P:614:GLN:HB2	1.79	0.47
1:Q:396:GLU:OE2	1:Q:649:LYS:HE2	2.14	0.47
1:X:288:HIS:HD2	1:X:614:GLN:HB2	1.79	0.47
1:Y:288:HIS:HD2	1:Y:614:GLN:HB2	1.79	0.47
1:Z:396:GLU:OE2	1:Z:649:LYS:HE2	2.14	0.47
1:a:224:SER:H	1:7:407:ASN:HD21	1.63	0.47
1:c:288:HIS:HD2	1:c:614:GLN:HB2	1.79	0.47
1:f:509:HIS:NE2	1:n:574:GLU:OE1	2.48	0.47
1:i:713:THR:HG21	1:w:275:TYR:OH	2.15	0.47
1:k:713:THR:HG21	1:l:275:TYR:OH	2.15	0.47
1:t:224:SER:H	1:1:407:ASN:HD21	1.63	0.47
1:v:275:TYR:OH	1:x:713:THR:HG21	2.15	0.47
1:1:396:GLU:OE2	1:1:649:LYS:HE2	2.14	0.47
1:3:396:GLU:OE2	1:3:649:LYS:HE2	2.14	0.47
1:4:234:TRP:CZ2	1:4:298[B]:ARG:HB2	2.49	0.47
1:E:467:ALA:HA	1:E:470:ILE:HD11	1.96	0.47
1:K:288:HIS:HD2	1:K:614:GLN:HB2	1.79	0.47
1:X:467:ALA:HA	1:X:470:ILE:HD11	1.96	0.47
1:Z:518:ASN:HB3	1:k:474:SER:HA	1.96	0.47
1:f:396:GLU:OE2	1:f:649:LYS:HE2	2.14	0.47
1:k:396:GLU:OE2	1:k:649:LYS:HE2	2.14	0.47
1:l:413:TYR:OH	1:l:641:HIS:O	2.26	0.47
1:o:467:ALA:HA	1:o:470:ILE:HD11	1.96	0.47
1:q:275:TYR:OH	1:w:713:THR:HG21	2.15	0.47
1:2:396:GLU:OE2	1:2:649:LYS:HE2	2.14	0.47
1:4:288:HIS:HD2	1:4:614:GLN:HB2	1.79	0.47
1:4:413:TYR:OH	1:4:641:HIS:O	2.26	0.47
1:7:288:HIS:HD2	1:7:614:GLN:HB2	1.79	0.47
1:A:713:THR:HG21	1:H:275:TYR:OH	2.15	0.47
1:B:474:SER:HA	1:U:518:ASN:HB3	1.97	0.47
1:G:275:TYR:OH	1:Y:713:THR:HG21	2.14	0.47
1:N:234:TRP:CH2	1:N:298[B]:ARG:HB2	2.49	0.47
1:W:275:TYR:OH	1:e:713:THR:HG21	2.14	0.47
1:c:518:ASN:HB3	1:3:474:SER:HA	1.97	0.47
1:e:407:ASN:HD21	1:g:224:SER:H	1.63	0.47
1:j:288:HIS:HD2	1:j:614:GLN:HB2	1.79	0.47
1:o:396:GLU:OE2	1:o:649:LYS:HE2	2.14	0.47
1:s:518:ASN:HB3	1:1:474:SER:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:467:ALA:HA	1:w:470:ILE:HD11	1.96	0.47
1:x:396:GLU:OE2	1:x:649:LYS:HE2	2.14	0.47
1:x:413:TYR:OH	1:x:641:HIS:O	2.26	0.47
1:8:396:GLU:OE2	1:8:649:LYS:HE2	2.14	0.47
1:A:518:ASN:HB3	1:f:474:SER:HA	1.96	0.46
1:C:275:TYR:OH	1:J:713:THR:HG21	2.14	0.46
1:D:396:GLU:OE2	1:D:649:LYS:HE2	2.14	0.46
1:F:288:HIS:HD2	1:F:614:GLN:HB2	1.79	0.46
1:F:518:ASN:HB3	1:c:474:SER:HA	1.96	0.46
1:J:509:HIS:NE2	1:s:574:GLU:OE1	2.48	0.46
1:K:224:SER:H	1:3:407:ASN:HD21	1.62	0.46
1:K:509:HIS:NE2	1:X:574:GLU:OE1	2.48	0.46
1:Z:509:HIS:NE2	1:k:574:GLU:OE1	2.47	0.46
1:b:275:TYR:OH	1:p:713:THR:HG21	2.15	0.46
1:g:407:ASN:HD21	1:2:224:SER:H	1.62	0.46
1:k:298[A]:ARG:HH21	1:k:298[A]:ARG:CG	2.28	0.46
1:x:377:TYR:HH	1:x:393:TYR:H	1.61	0.46
1:y:288:HIS:HD2	1:y:614:GLN:HB2	1.79	0.46
1:1:565:ILE:HG22	1:1:569:ASN:HB2	1.98	0.46
1:A:345:ASP:O	1:A:346:SER:OG	2.32	0.46
1:A:692:LYS:HG3	1:n:398:PHE:CE1	2.50	0.46
1:F:513:ARG:HD2	1:c:431:ASP:OD2	2.15	0.46
1:G:509:HIS:NE2	1:7:574:GLU:OE1	2.47	0.46
1:H:713:THR:HG21	1:X:275:TYR:OH	2.15	0.46
1:J:238[B]:ARG:HD3	1:J:683:GLU:OE2	2.16	0.46
1:L:288:HIS:HD2	1:L:614:GLN:HB2	1.79	0.46
1:M:467:ALA:HA	1:M:470:ILE:HD11	1.96	0.46
1:Q:518:ASN:HB3	1:Z:474:SER:HA	1.97	0.46
1:T:713:THR:HG21	1:n:275:TYR:OH	2.15	0.46
1:X:396:GLU:OE2	1:X:649:LYS:HE2	2.14	0.46
1:Y:275:TYR:OH	1:3:713:THR:HG21	2.15	0.46
1:c:565:ILE:HG22	1:c:569:ASN:HB2	1.98	0.46
1:e:288:HIS:HD2	1:e:614:GLN:HB2	1.79	0.46
1:h:275:TYR:OH	1:j:713:THR:HG21	2.14	0.46
1:o:713:THR:HG21	1:s:275:TYR:OH	2.14	0.46
1:q:474:SER:HA	1:z:518:ASN:HB3	1.97	0.46
1:v:713:THR:HG21	1:5:275:TYR:OH	2.15	0.46
1:z:467:ALA:HA	1:z:470:ILE:HD11	1.96	0.46
1:A:398:PHE:CE1	1:f:692:LYS:HG3	2.50	0.46
1:B:565:ILE:HG22	1:B:569:ASN:HB2	1.98	0.46
1:C:713:THR:HG21	1:c:275:TYR:OH	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:396:GLU:OE2	1:H:649:LYS:HE2	2.14	0.46
1:I:565:ILE:HG22	1:I:569:ASN:HB2	1.98	0.46
1:K:413:TYR:OH	1:K:641:HIS:O	2.26	0.46
1:O:413:TYR:OH	1:O:641:HIS:O	2.26	0.46
1:V:288:HIS:HD2	1:V:614:GLN:HB2	1.79	0.46
1:W:224:SER:H	1:Z:407:ASN:HD21	1.63	0.46
1:W:518:ASN:HB3	1:u:474:SER:HA	1.96	0.46
1:b:565:ILE:HG22	1:b:569:ASN:HB2	1.98	0.46
1:e:565:ILE:HG22	1:e:569:ASN:HB2	1.98	0.46
1:f:565:ILE:HG22	1:f:569:ASN:HB2	1.98	0.46
1:g:574:GLU:OE1	1:7:509:HIS:NE2	2.49	0.46
1:h:224:SER:H	1:z:407:ASN:HD21	1.64	0.46
1:h:630:PRO:O	1:5:477:TRP:HH2	1.99	0.46
1:p:275:TYR:OH	1:r:713:THR:HG21	2.15	0.46
1:s:288:HIS:HD2	1:s:614:GLN:HB2	1.79	0.46
1:t:565:ILE:HG22	1:t:569:ASN:HB2	1.98	0.46
1:v:345:ASP:O	1:v:346:SER:OG	2.32	0.46
1:z:288:HIS:HD2	1:z:614:GLN:HB2	1.79	0.46
1:3:565:ILE:HG22	1:3:569:ASN:HB2	1.98	0.46
1:5:396:GLU:OE2	1:5:649:LYS:HE2	2.14	0.46
1:A:474:SER:HA	1:n:518:ASN:HB3	1.98	0.46
1:A:513:ARG:HD2	1:f:431:ASP:OD2	2.15	0.46
1:E:565:ILE:HG22	1:E:569:ASN:HB2	1.98	0.46
1:F:448:THR:HG21	1:3:500:TYR:CZ	2.51	0.46
1:G:565:ILE:HG22	1:G:569:ASN:HB2	1.98	0.46
1:K:396:GLU:OE2	1:K:649:LYS:HE2	2.14	0.46
1:L:467:ALA:HA	1:L:470:ILE:HD11	1.96	0.46
1:L:518:ASN:HB3	1:R:474:SER:HA	1.97	0.46
1:Q:413:TYR:OH	1:Q:641:HIS:O	2.26	0.46
1:R:467:ALA:HA	1:R:470:ILE:HD11	1.96	0.46
1:T:224:SER:H	1:n:407:ASN:HD21	1.62	0.46
1:T:565:ILE:HG22	1:T:569:ASN:HB2	1.98	0.46
1:U:288:HIS:HD2	1:U:614:GLN:HB2	1.79	0.46
1:V:224:SER:H	1:f:407:ASN:HD21	1.63	0.46
1:a:509:HIS:NE2	1:y:574:GLU:OE1	2.48	0.46
1:a:565:ILE:HG22	1:a:569:ASN:HB2	1.98	0.46
1:b:407:ASN:HD21	1:p:224:SER:H	1.63	0.46
1:d:509:HIS:NE2	1:v:574:GLU:OE1	2.48	0.46
1:g:474:SER:HA	1:7:518:ASN:HB3	1.97	0.46
1:h:467:ALA:HA	1:h:470:ILE:HD11	1.96	0.46
1:p:288:HIS:HD2	1:p:614:GLN:HB2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:467:ALA:HA	1:q:470:ILE:HD11	1.96	0.46
1:r:238[A]:ARG:HD2	1:r:683:GLU:OE2	2.16	0.46
1:t:275:TYR:OH	1:7:713:THR:HG21	2.15	0.46
1:2:345:ASP:O	1:2:346:SER:OG	2.32	0.46
1:4:396:GLU:OE2	1:4:649:LYS:HE2	2.14	0.46
1:A:429:SER:OG	1:A:431:ASP:OD1	2.28	0.46
1:A:489:SER:HB3	1:A:533:PHE:CE1	2.51	0.46
1:B:298[A]:ARG:HG2	1:B:298[A]:ARG:NH2	2.24	0.46
1:B:407:ASN:HD21	1:G:224:SER:H	1.63	0.46
1:B:574:GLU:OE1	1:U:509:HIS:NE2	2.48	0.46
1:I:437:LEU:HD11	1:6:276:SER:HB2	1.98	0.46
1:J:345:ASP:O	1:J:346:SER:OG	2.32	0.46
1:L:509:HIS:NE2	1:R:574:GLU:OE1	2.48	0.46
1:O:224:SER:H	1:r:407:ASN:HD21	1.62	0.46
1:U:407:ASN:HD21	1:X:224:SER:H	1.62	0.46
1:Y:451:PRO:HA	1:Y:456:THR:HA	1.98	0.46
1:e:275:TYR:OH	1:g:713:THR:HG21	2.15	0.46
1:g:275:TYR:OH	1:2:713:THR:HG21	2.15	0.46
1:h:247:TRP:O	1:h:675:THR:OG1	2.17	0.46
1:l:234:TRP:CE2	1:l:298[B]:ARG:HD2	2.51	0.46
1:m:565:ILE:HG22	1:m:569:ASN:HB2	1.98	0.46
1:o:275:TYR:OH	1:5:713:THR:HG21	2.14	0.46
1:r:429:SER:OG	1:r:431:ASP:OD1	2.28	0.46
1:u:565:ILE:HG22	1:u:569:ASN:HB2	1.98	0.46
1:x:630:PRO:O	1:8:477:TRP:HH2	1.99	0.46
1:3:234:TRP:CD2	1:3:298[A]:ARG:HD3	2.51	0.46
1:8:234:TRP:CE2	1:8:298[B]:ARG:HD2	2.50	0.46
1:A:500:TYR:CZ	1:f:448:THR:HG21	2.51	0.46
1:A:574:GLU:OE1	1:n:509:HIS:NE2	2.49	0.46
1:B:518:ASN:HB3	1:2:474:SER:HA	1.96	0.46
1:D:565:ILE:HD12	1:D:565:ILE:HG23	1.77	0.46
1:F:474:SER:HA	1:3:518:ASN:HB3	1.98	0.46
1:F:574:GLU:OE1	1:3:509:HIS:NE2	2.48	0.46
1:K:448:THR:HG21	1:P:500:TYR:CZ	2.51	0.46
1:K:474:SER:HA	1:P:518:ASN:HB3	1.97	0.46
1:K:500:TYR:CZ	1:X:448:THR:HG21	2.51	0.46
1:S:238[B]:ARG:HD3	1:S:683:GLU:OE2	2.16	0.46
1:S:509:HIS:NE2	1:z:574:GLU:OE1	2.48	0.46
1:U:565:ILE:HG22	1:U:569:ASN:HB2	1.98	0.46
1:W:509:HIS:NE2	1:u:574:GLU:OE1	2.48	0.46
1:k:565:ILE:HG22	1:k:569:ASN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:489:SER:HB3	1:n:533:PHE:CE1	2.51	0.46
1:s:630:PRO:O	1:1:477:TRP:HH2	1.99	0.46
1:t:298[A]:ARG:HG2	1:t:298[A]:ARG:HH21	1.80	0.46
1:u:275:TYR:OH	1:z:713:THR:HG21	2.14	0.46
1:v:489:SER:HB3	1:v:533:PHE:CE1	2.51	0.46
1:w:565:ILE:HG22	1:w:569:ASN:HB2	1.98	0.46
1:y:451:PRO:HA	1:y:456:THR:HA	1.98	0.46
1:7:451:PRO:HA	1:7:456:THR:HA	1.98	0.46
1:7:489:SER:HB3	1:7:533:PHE:CE1	2.51	0.46
1:B:429:SER:OG	1:B:431:ASP:OD1	2.28	0.46
1:C:404:ARG:H	1:C:407:ASN:HD22	1.64	0.46
1:C:489:SER:HB3	1:C:533:PHE:CE1	2.51	0.46
1:C:574:GLU:OE1	1:Y:509:HIS:NE2	2.49	0.46
1:D:565:ILE:HG22	1:D:569:ASN:HB2	1.98	0.46
1:F:451:PRO:HA	1:F:456:THR:HA	1.98	0.46
1:H:518:ASN:HB3	1:T:474:SER:HA	1.97	0.46
1:I:451:PRO:HA	1:I:456:THR:HA	1.98	0.46
1:I:518:ASN:HB3	1:O:474:SER:HA	1.97	0.46
1:K:713:THR:HG21	1:3:275:TYR:OH	2.15	0.46
1:M:407:ASN:HD21	1:P:224:SER:H	1.62	0.46
1:O:489:SER:HB3	1:O:533:PHE:CE1	2.51	0.46
1:O:518:ASN:HB3	1:6:474:SER:HA	1.96	0.46
1:P:451:PRO:HA	1:P:456:THR:HA	1.98	0.46
1:Q:407:ASN:HD21	1:U:224:SER:H	1.63	0.46
1:Q:437:LEU:HD11	1:k:276:SER:HB2	1.98	0.46
1:Q:565:ILE:HG22	1:Q:569:ASN:HB2	1.98	0.46
1:S:518:ASN:HB3	1:z:474:SER:HA	1.97	0.46
1:Y:404:ARG:H	1:Y:407:ASN:HD22	1.64	0.46
1:Y:565:ILE:HG22	1:Y:569:ASN:HB2	1.98	0.46
1:c:489:SER:HB3	1:c:533:PHE:CE1	2.51	0.46
1:e:489:SER:HB3	1:e:533:PHE:CE1	2.51	0.46
1:g:404:ARG:H	1:g:407:ASN:HD22	1.64	0.46
1:g:489:SER:HB3	1:g:533:PHE:CE1	2.51	0.46
1:i:509:HIS:NE2	1:p:574:GLU:OE1	2.49	0.46
1:j:451:PRO:HA	1:j:456:THR:HA	1.98	0.46
1:l:489:SER:HB3	1:l:533:PHE:CE1	2.51	0.46
1:p:565:ILE:HG22	1:p:569:ASN:HB2	1.98	0.46
1:q:489:SER:HB3	1:q:533:PHE:CE1	2.51	0.46
1:s:224:SER:H	1:x:407:ASN:HD21	1.63	0.46
1:s:565:ILE:HG22	1:s:569:ASN:HB2	1.98	0.46
1:t:489:SER:HB3	1:t:533:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:451:PRO:HA	1:u:456:THR:HA	1.98	0.46
1:v:429:SER:OG	1:v:431:ASP:OD1	2.28	0.46
1:7:404:ARG:H	1:7:407:ASN:HD22	1.64	0.46
1:8:565:ILE:HG22	1:8:569:ASN:HB2	1.97	0.46
1:B:224:SER:H	1:K:407:ASN:HD21	1.62	0.46
1:C:500:TYR:CZ	1:t:448:THR:HG21	2.51	0.46
1:D:407:ASN:HD21	1:b:224:SER:H	1.64	0.46
1:F:489:SER:HB3	1:F:533:PHE:CE1	2.51	0.46
1:F:565:ILE:HG22	1:F:569:ASN:HB2	1.98	0.46
1:G:437:LEU:HD11	1:g:276:SER:HB2	1.98	0.46
1:G:451:PRO:HA	1:G:456:THR:HA	1.98	0.46
1:H:565:ILE:HG22	1:H:569:ASN:HB2	1.97	0.46
1:I:275:TYR:OH	1:L:713:THR:HG21	2.15	0.46
1:J:489:SER:HB3	1:J:533:PHE:CE1	2.51	0.46
1:Q:377:TYR:HH	1:Q:393:TYR:H	1.62	0.46
1:R:247:TRP:O	1:R:675:THR:OG1	2.17	0.46
1:S:429:SER:OG	1:S:431:ASP:OD1	2.28	0.46
1:S:437:LEU:HD11	1:q:276:SER:HB2	1.98	0.46
1:U:489:SER:HB3	1:U:533:PHE:CE1	2.51	0.46
1:U:574:GLU:OE1	1:2:509:HIS:NE2	2.49	0.46
1:X:489:SER:HB3	1:X:533:PHE:CE1	2.51	0.46
1:X:565:ILE:HG22	1:X:569:ASN:HB2	1.98	0.46
1:Y:489:SER:HB3	1:Y:533:PHE:CE1	2.51	0.46
1:a:630:PRO:O	1:y:477:TRP:HH2	1.99	0.46
1:b:234:TRP:CH2	1:b:298[B]:ARG:HB2	2.51	0.46
1:d:489:SER:HB3	1:d:533:PHE:CE1	2.51	0.46
1:o:489:SER:HB3	1:o:533:PHE:CE1	2.51	0.46
1:o:565:ILE:HG22	1:o:569:ASN:HB2	1.98	0.46
1:p:407:ASN:HD21	1:r:224:SER:H	1.62	0.46
1:q:407:ASN:HD21	1:w:224:SER:H	1.63	0.46
1:t:407:ASN:HD21	1:7:224:SER:H	1.62	0.46
1:t:565:ILE:HD12	1:t:565:ILE:HG23	1.77	0.46
1:v:234:TRP:CE3	1:v:298[A]:ARG:HD3	2.51	0.46
1:v:413:TYR:OH	1:v:641:HIS:O	2.26	0.46
1:A:404:ARG:H	1:A:407:ASN:HD22	1.64	0.46
1:C:224:SER:H	1:c:407:ASN:HD21	1.64	0.46
1:F:398:PHE:CE1	1:c:692:LYS:HG3	2.50	0.46
1:F:407:ASN:HD21	1:I:224:SER:H	1.64	0.46
1:G:489:SER:HB3	1:G:533:PHE:CE1	2.51	0.46
1:P:448:THR:HG21	1:X:500:TYR:CZ	2.51	0.46
1:P:565:ILE:HG22	1:P:569:ASN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:451:PRO:HA	1:Q:456:THR:HA	1.98	0.46
1:Q:489:SER:HB3	1:Q:533:PHE:CE1	2.51	0.46
1:R:451:PRO:HA	1:R:456:THR:HA	1.98	0.46
1:R:489:SER:HB3	1:R:533:PHE:CE1	2.51	0.46
1:U:404:ARG:H	1:U:407:ASN:HD22	1.64	0.46
1:V:565:ILE:HG22	1:V:569:ASN:HB2	1.98	0.46
1:Z:565:ILE:HG22	1:Z:569:ASN:HB2	1.98	0.46
1:c:713:THR:HG21	1:6:275:TYR:OH	2.15	0.46
1:e:234:TRP:CH2	1:e:298[B]:ARG:HB2	2.51	0.46
1:e:404:ARG:H	1:e:407:ASN:HD22	1.64	0.46
1:j:489:SER:HB3	1:j:533:PHE:CE1	2.51	0.46
1:l:477:TRP:HH2	1:u:630:PRO:O	1.99	0.46
1:o:404:ARG:H	1:o:407:ASN:HD22	1.64	0.46
1:q:247:TRP:O	1:q:675:THR:OG1	2.17	0.46
1:q:477:TRP:HH2	1:z:630:PRO:O	1.99	0.46
1:s:489:SER:HB3	1:s:533:PHE:CE1	2.51	0.46
1:t:451:PRO:HA	1:t:456:THR:HA	1.98	0.46
1:x:451:PRO:HA	1:x:456:THR:HA	1.98	0.46
1:x:489:SER:HB3	1:x:533:PHE:CE1	2.51	0.46
1:x:565:ILE:HG22	1:x:569:ASN:HB2	1.98	0.46
1:5:565:ILE:HG22	1:5:569:ASN:HB2	1.98	0.46
1:7:565:ILE:HG22	1:7:569:ASN:HB2	1.98	0.46
1:A:451:PRO:HA	1:A:456:THR:HA	1.98	0.46
1:D:437:LEU:HD11	1:8:276:SER:HB2	1.98	0.46
1:F:298[A]:ARG:HG2	1:F:298[A]:ARG:NH2	2.23	0.46
1:J:565:ILE:HG22	1:J:569:ASN:HB2	1.98	0.46
1:N:565:ILE:HG22	1:N:569:ASN:HB2	1.98	0.46
1:O:247:TRP:O	1:O:675:THR:OG1	2.17	0.46
1:P:489:SER:HB3	1:P:533:PHE:CE1	2.51	0.46
1:Q:404:ARG:H	1:Q:407:ASN:HD22	1.64	0.46
1:R:565:ILE:HG22	1:R:569:ASN:HB2	1.98	0.46
1:S:565:ILE:HG22	1:S:569:ASN:HB2	1.98	0.46
1:W:407:ASN:HD21	1:e:224:SER:H	1.64	0.46
1:X:404:ARG:H	1:X:407:ASN:HD22	1.64	0.46
1:a:474:SER:HA	1:e:518:ASN:HB3	1.98	0.46
1:c:404:ARG:H	1:c:407:ASN:HD22	1.64	0.46
1:c:500:TYR:CZ	1:3:448:THR:HG21	2.51	0.46
1:g:477:TRP:HH2	1:7:630:PRO:O	1.99	0.46
1:i:404:ARG:H	1:i:407:ASN:HD22	1.64	0.46
1:j:407:ASN:HD21	1:y:224:SER:H	1.64	0.46
1:j:477:TRP:HH2	1:o:630:PRO:O	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:565:ILE:HG22	1:j:569:ASN:HB2	1.98	0.46
1:k:451:PRO:HA	1:k:456:THR:HA	1.98	0.46
1:m:407:ASN:HD21	1:q:224:SER:H	1.64	0.46
1:m:489:SER:HB3	1:m:533:PHE:CE1	2.51	0.46
1:o:451:PRO:HA	1:o:456:THR:HA	1.98	0.46
1:v:404:ARG:H	1:v:407:ASN:HD22	1.64	0.46
1:v:451:PRO:HA	1:v:456:THR:HA	1.98	0.46
1:y:489:SER:HB3	1:y:533:PHE:CE1	2.51	0.46
1:y:565:ILE:HG22	1:y:569:ASN:HB2	1.98	0.46
1:2:489:SER:HB3	1:2:533:PHE:CE1	2.51	0.46
1:2:565:ILE:HG22	1:2:569:ASN:HB2	1.98	0.46
1:6:404:ARG:H	1:6:407:ASN:HD22	1.64	0.46
1:A:238[B]:ARG:HD3	1:A:683:GLU:OE2	2.16	0.45
1:A:448:THR:HG21	1:n:500:TYR:CZ	2.50	0.45
1:B:437:LEU:HD11	1:U:276:SER:HB2	1.98	0.45
1:B:500:TYR:CZ	1:2:448:THR:HG21	2.51	0.45
1:C:407:ASN:HD21	1:J:224:SER:H	1.63	0.45
1:D:451:PRO:HA	1:D:456:THR:HA	1.98	0.45
1:G:574:GLU:OE1	1:g:509:HIS:NE2	2.50	0.45
1:H:224:SER:H	1:X:407:ASN:HD21	1.62	0.45
1:I:404:ARG:H	1:I:407:ASN:HD22	1.64	0.45
1:K:518:ASN:HB3	1:X:474:SER:HA	1.97	0.45
1:M:247:TRP:O	1:M:675:THR:OG1	2.17	0.45
1:M:474:SER:HA	1:T:518:ASN:HB3	1.97	0.45
1:N:404:ARG:H	1:N:407:ASN:HD22	1.64	0.45
1:T:489:SER:HB3	1:T:533:PHE:CE1	2.51	0.45
1:V:630:PRO:O	1:w:477:TRP:HH2	1.99	0.45
1:W:404:ARG:H	1:W:407:ASN:HD22	1.64	0.45
1:Z:224:SER:H	1:2:407:ASN:HD21	1.62	0.45
1:Z:451:PRO:HA	1:Z:456:THR:HA	1.98	0.45
1:b:509:HIS:NE2	1:d:574:GLU:OE1	2.49	0.45
1:d:451:PRO:HA	1:d:456:THR:HA	1.98	0.45
1:f:500:TYR:CZ	1:n:448:THR:HG21	2.51	0.45
1:g:565:ILE:HG22	1:g:569:ASN:HB2	1.97	0.45
1:h:509:HIS:NE2	1:5:574:GLU:OE1	2.50	0.45
1:h:565:ILE:HG22	1:h:569:ASN:HB2	1.98	0.45
1:i:518:ASN:HB3	1:p:474:SER:HA	1.97	0.45
1:i:565:ILE:HG22	1:i:569:ASN:HB2	1.98	0.45
1:l:565:ILE:HG22	1:l:569:ASN:HB2	1.98	0.45
1:m:451:PRO:HA	1:m:456:THR:HA	1.98	0.45
1:n:234:TRP:CD2	1:n:298[A]:ARG:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:451:PRO:HA	1:n:456:THR:HA	1.98	0.45
1:q:451:PRO:HA	1:q:456:THR:HA	1.98	0.45
1:q:565:ILE:HG22	1:q:569:ASN:HB2	1.98	0.45
1:r:565:ILE:HG22	1:r:569:ASN:HB2	1.98	0.45
1:s:404:ARG:H	1:s:407:ASN:HD22	1.64	0.45
1:u:404:ARG:H	1:u:407:ASN:HD22	1.64	0.45
1:x:404:ARG:H	1:x:407:ASN:HD22	1.64	0.45
1:6:451:PRO:HA	1:6:456:THR:HA	1.98	0.45
1:8:451:PRO:HA	1:8:456:THR:HA	1.98	0.45
1:A:413:TYR:OH	1:A:641:HIS:O	2.26	0.45
1:C:437:LEU:HD11	1:Y:276:SER:HB2	1.98	0.45
1:C:565:ILE:HG22	1:C:569:ASN:HB2	1.98	0.45
1:E:574:GLU:OE1	1:p:509:HIS:NE2	2.50	0.45
1:F:502:TRP:CZ2	1:c:471:ARG:HD2	2.52	0.45
1:H:437:LEU:HD11	1:M:276:SER:HB2	1.99	0.45
1:M:565:ILE:HG22	1:M:569:ASN:HB2	1.98	0.45
1:O:565:ILE:HG22	1:O:569:ASN:HB2	1.98	0.45
1:O:630:PRO:O	1:6:477:TRP:HH2	2.00	0.45
1:Q:574:GLU:OE1	1:k:509:HIS:NE2	2.50	0.45
1:R:513:ARG:HD2	1:r:431:ASP:OD2	2.17	0.45
1:W:451:PRO:HA	1:W:456:THR:HA	1.98	0.45
1:X:451:PRO:HA	1:X:456:THR:HA	1.98	0.45
1:m:477:TRP:HH2	1:5:630:PRO:O	2.00	0.45
1:q:565:ILE:HD12	1:q:565:ILE:HG23	1.77	0.45
1:3:489:SER:HB3	1:3:533:PHE:CE1	2.51	0.45
1:4:451:PRO:HA	1:4:456:THR:HA	1.98	0.45
1:4:489:SER:HB3	1:4:533:PHE:CE1	2.51	0.45
1:5:489:SER:HB3	1:5:533:PHE:CE1	2.51	0.45
1:A:437:LEU:HD11	1:n:276:SER:HB2	1.98	0.45
1:D:224:SER:H	1:O:407:ASN:HD21	1.63	0.45
1:E:407:ASN:HD21	1:N:224:SER:H	1.64	0.45
1:J:404:ARG:H	1:J:407:ASN:HD22	1.64	0.45
1:J:518:ASN:HB3	1:s:474:SER:HA	1.97	0.45
1:L:234:TRP:CE2	1:L:298[A]:ARG:HD3	2.51	0.45
1:M:489:SER:HB3	1:M:533:PHE:CE1	2.51	0.45
1:N:509:HIS:NE2	1:V:574:GLU:OE1	2.49	0.45
1:P:377:TYR:HH	1:P:393:TYR:H	1.64	0.45
1:Q:500:TYR:CZ	1:Z:448:THR:HG21	2.51	0.45
1:S:489:SER:HB3	1:S:533:PHE:CE1	2.51	0.45
1:T:451:PRO:HA	1:T:456:THR:HA	1.98	0.45
1:U:234:TRP:CH2	1:U:298[B]:ARG:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:489:SER:HB3	1:a:533:PHE:CE1	2.51	0.45
1:b:437:LEU:HD11	1:v:276:SER:HB2	1.99	0.45
1:b:489:SER:HB3	1:b:533:PHE:CE1	2.51	0.45
1:g:234:TRP:CD2	1:g:298[A]:ARG:HD3	2.52	0.45
1:h:574:GLU:OE1	1:m:509:HIS:NE2	2.50	0.45
1:l:574:GLU:OE1	1:u:509:HIS:NE2	2.50	0.45
1:r:489:SER:HB3	1:r:533:PHE:CE1	2.51	0.45
1:x:518:ASN:HB3	1:8:474:SER:HA	1.98	0.45
1:2:238[A]:ARG:HD2	1:2:683:GLU:OE2	2.15	0.45
1:2:404:ARG:H	1:2:407:ASN:HD22	1.64	0.45
1:3:234:TRP:NE1	1:3:298[B]:ARG:HD2	2.31	0.45
1:6:565:ILE:HG22	1:6:569:ASN:HB2	1.98	0.45
1:A:407:ASN:HD21	1:Q:224:SER:H	1.64	0.45
1:A:565:ILE:HG22	1:A:569:ASN:HB2	1.98	0.45
1:B:451:PRO:HA	1:B:456:THR:HA	1.98	0.45
1:F:500:TYR:CZ	1:c:448:THR:HG21	2.51	0.45
1:H:513:ARG:HD2	1:T:431:ASP:OD2	2.17	0.45
1:J:437:LEU:HD11	1:1:276:SER:HB2	1.98	0.45
1:K:489:SER:HB3	1:K:533:PHE:CE1	2.51	0.45
1:P:437:LEU:HD11	1:X:276:SER:HB2	1.99	0.45
1:R:429:SER:OG	1:R:431:ASP:OD1	2.28	0.45
1:S:224:SER:H	1:V:407:ASN:HD21	1.63	0.45
1:U:234:TRP:CE2	1:U:298[A]:ARG:HD3	2.51	0.45
1:U:275:TYR:OH	1:X:713:THR:HG21	2.15	0.45
1:W:565:ILE:HG22	1:W:569:ASN:HB2	1.98	0.45
1:Y:311:LEU:HB3	1:Y:682:ILE:HG12	1.99	0.45
1:a:404:ARG:H	1:a:407:ASN:HD22	1.64	0.45
1:a:451:PRO:HA	1:a:456:THR:HA	1.98	0.45
1:c:451:PRO:HA	1:c:456:THR:HA	1.98	0.45
1:d:630:PRO:O	1:v:477:TRP:HH2	1.99	0.45
1:e:451:PRO:HA	1:e:456:THR:HA	1.98	0.45
1:f:518:ASN:HB3	1:n:474:SER:HA	1.97	0.45
1:h:451:PRO:HA	1:h:456:THR:HA	1.98	0.45
1:h:489:SER:HB3	1:h:533:PHE:CE1	2.51	0.45
1:i:630:PRO:O	1:p:477:TRP:HH2	1.99	0.45
1:l:247:TRP:O	1:l:675:THR:OG1	2.17	0.45
1:p:404:ARG:H	1:p:407:ASN:HD22	1.64	0.45
1:q:234:TRP:CG	1:q:298[A]:ARG:HD3	2.52	0.45
1:r:404:ARG:H	1:r:407:ASN:HD22	1.64	0.45
1:3:404:ARG:H	1:3:407:ASN:HD22	1.64	0.45
1:3:451:PRO:HA	1:3:456:THR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:SER:HB3	1:B:533:PHE:CE1	2.51	0.45
1:B:513:ARG:HD2	1:2:431:ASP:OD2	2.17	0.45
1:E:500:TYR:CZ	1:i:448:THR:HG21	2.52	0.45
1:E:513:ARG:HD2	1:i:431:ASP:OD2	2.17	0.45
1:G:500:TYR:CZ	1:7:448:THR:HG21	2.52	0.45
1:G:513:ARG:HD2	1:7:431:ASP:OD2	2.17	0.45
1:H:451:PRO:HA	1:H:456:THR:HA	1.98	0.45
1:H:489:SER:HB3	1:H:533:PHE:CE1	2.51	0.45
1:L:574:GLU:OE1	1:r:509:HIS:NE2	2.49	0.45
1:N:477:TRP:HH2	1:w:630:PRO:O	2.00	0.45
1:N:574:GLU:OE1	1:w:509:HIS:NE2	2.50	0.45
1:S:404:ARG:H	1:S:407:ASN:HD22	1.64	0.45
1:T:234:TRP:CD2	1:T:298[A]:ARG:HD3	2.52	0.45
1:T:429:SER:OG	1:T:431:ASP:OD1	2.28	0.45
1:V:489:SER:HB3	1:V:533:PHE:CE1	2.51	0.45
1:X:345:ASP:O	1:X:346:SER:OG	2.32	0.45
1:Z:565:ILE:HD12	1:Z:565:ILE:HG23	1.77	0.45
1:a:574:GLU:OE1	1:e:509:HIS:NE2	2.49	0.45
1:e:234:TRP:CD2	1:e:298[A]:ARG:HD3	2.52	0.45
1:e:477:TRP:HH2	1:y:630:PRO:O	2.00	0.45
1:f:429:SER:OG	1:f:431:ASP:OD1	2.28	0.45
1:f:489:SER:HB3	1:f:533:PHE:CE1	2.51	0.45
1:i:451:PRO:HA	1:i:456:THR:HA	1.98	0.45
1:k:224:SER:H	1:l:407:ASN:HD21	1.63	0.45
1:k:565:ILE:HD12	1:k:565:ILE:HG23	1.77	0.45
1:l:404:ARG:H	1:l:407:ASN:HD22	1.64	0.45
1:m:429:SER:OG	1:m:431:ASP:OD1	2.28	0.45
1:o:477:TRP:HH2	1:4:630:PRO:O	2.00	0.45
1:p:489:SER:HB3	1:p:533:PHE:CE1	2.51	0.45
1:u:489:SER:HB3	1:u:533:PHE:CE1	2.51	0.45
1:v:565:ILE:HG22	1:v:569:ASN:HB2	1.98	0.45
1:z:311:LEU:HB3	1:z:682:ILE:HG12	1.99	0.45
1:6:489:SER:HB3	1:6:533:PHE:CE1	2.51	0.45
1:7:311:LEU:HB3	1:7:682:ILE:HG12	1.99	0.45
1:C:474:SER:HA	1:Y:518:ASN:HB3	1.98	0.45
1:E:489:SER:HB3	1:E:533:PHE:CE1	2.51	0.45
1:F:404:ARG:H	1:F:407:ASN:HD22	1.64	0.45
1:H:431:ASP:OD2	1:M:513:ARG:HD2	2.17	0.45
1:I:489:SER:HB3	1:I:533:PHE:CE1	2.51	0.45
1:K:451:PRO:HA	1:K:456:THR:HA	1.98	0.45
1:K:565:ILE:HG22	1:K:569:ASN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:311:LEU:HB3	1:L:682:ILE:HG12	1.99	0.45
1:L:404:ARG:H	1:L:407:ASN:HD22	1.64	0.45
1:L:448:THR:HG21	1:r:500:TYR:CZ	2.52	0.45
1:L:500:TYR:CZ	1:R:448:THR:HG21	2.51	0.45
1:M:451:PRO:HA	1:M:456:THR:HA	1.98	0.45
1:N:451:PRO:HA	1:N:456:THR:HA	1.98	0.45
1:O:500:TYR:CZ	1:6:448:THR:HG21	2.52	0.45
1:Q:513:ARG:HD2	1:Z:431:ASP:OD2	2.17	0.45
1:R:311:LEU:HB3	1:R:682:ILE:HG12	1.99	0.45
1:S:451:PRO:HA	1:S:456:THR:HA	1.98	0.45
1:V:404:ARG:H	1:V:407:ASN:HD22	1.64	0.45
1:b:234:TRP:CD2	1:b:298[A]:ARG:HD3	2.52	0.45
1:c:311:LEU:HB3	1:c:682:ILE:HG12	1.99	0.45
1:h:518:ASN:HB3	1:5:474:SER:HA	1.97	0.45
1:j:474:SER:HA	1:o:518:ASN:HB3	1.97	0.45
1:l:234:TRP:CD2	1:l:298[A]:ARG:HD3	2.52	0.45
1:q:311:LEU:HB3	1:q:682:ILE:HG12	1.99	0.45
1:s:509:HIS:NE2	1:1:574:GLU:OE1	2.50	0.45
1:w:489:SER:HB3	1:w:533:PHE:CE1	2.51	0.45
1:x:311:LEU:HB3	1:x:682:ILE:HG12	1.99	0.45
1:1:451:PRO:HA	1:1:456:THR:HA	1.98	0.45
1:1:489:SER:HB3	1:1:533:PHE:CE1	2.51	0.45
1:4:565:ILE:HG22	1:4:569:ASN:HB2	1.98	0.45
1:5:451:PRO:HA	1:5:456:THR:HA	1.98	0.45
1:A:311:LEU:HB3	1:A:682:ILE:HG12	1.99	0.45
1:D:630:PRO:O	1:x:477:TRP:HH2	2.00	0.45
1:H:448:THR:HG21	1:M:500:TYR:CZ	2.51	0.45
1:J:451:PRO:HA	1:J:456:THR:HA	1.98	0.45
1:K:431:ASP:OD2	1:P:513:ARG:HD2	2.16	0.45
1:L:234:TRP:CH2	1:L:298[B]:ARG:HB2	2.51	0.45
1:L:451:PRO:HA	1:L:456:THR:HA	1.98	0.45
1:L:474:SER:HA	1:r:518:ASN:HB3	1.98	0.45
1:L:565:ILE:HG22	1:L:569:ASN:HB2	1.98	0.45
1:N:234:TRP:CE2	1:N:298[B]:ARG:HD2	2.51	0.45
1:O:311:LEU:HB3	1:O:682:ILE:HG12	1.99	0.45
1:O:404:ARG:H	1:O:407:ASN:HD22	1.64	0.45
1:T:311:LEU:HB3	1:T:682:ILE:HG12	1.99	0.45
1:U:437:LEU:HD11	1:2:276:SER:HB2	1.99	0.45
1:W:489:SER:HB3	1:W:533:PHE:CE1	2.51	0.45
1:W:574:GLU:OE1	1:l:509:HIS:NE2	2.50	0.45
1:Y:234:TRP:CE2	1:Y:298[B]:ARG:HD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:311:LEU:HB3	1:Z:682:ILE:HG12	1.99	0.45
1:Z:489:SER:HB3	1:Z:533:PHE:CE1	2.51	0.45
1:e:311:LEU:HB3	1:e:682:ILE:HG12	1.99	0.45
1:i:311:LEU:HB3	1:i:682:ILE:HG12	1.99	0.45
1:l:311:LEU:HB3	1:l:682:ILE:HG12	1.99	0.45
1:q:574:GLU:OE1	1:z:509:HIS:NE2	2.50	0.45
1:r:311:LEU:HB3	1:r:682:ILE:HG12	1.99	0.45
1:r:451:PRO:HA	1:r:456:THR:HA	1.98	0.45
1:u:311:LEU:HB3	1:u:682:ILE:HG12	1.99	0.45
1:x:509:HIS:NE2	1:8:574:GLU:OE1	2.50	0.45
1:y:404:ARG:H	1:y:407:ASN:HD22	1.64	0.45
1:z:404:ARG:H	1:z:407:ASN:HD22	1.64	0.45
1:z:565:ILE:HG22	1:z:569:ASN:HB2	1.98	0.45
1:8:311:LEU:HB3	1:8:682:ILE:HG12	1.99	0.45
1:E:437:LEU:HD11	1:p:276:SER:HB2	1.98	0.45
1:F:311:LEU:HB3	1:F:682:ILE:HG12	1.99	0.45
1:H:474:SER:HA	1:M:518:ASN:HB3	1.98	0.45
1:H:500:TYR:CZ	1:T:448:THR:HG21	2.51	0.45
1:I:311:LEU:HB3	1:I:682:ILE:HG12	1.99	0.45
1:K:234:TRP:CD2	1:K:298[A]:ARG:HD3	2.52	0.45
1:K:311:LEU:HB3	1:K:682:ILE:HG12	1.99	0.45
1:L:489:SER:HB3	1:L:533:PHE:CE1	2.51	0.45
1:N:276:SER:HB2	1:V:437:LEU:HD11	1.98	0.45
1:N:311:LEU:HB3	1:N:682:ILE:HG12	1.99	0.45
1:P:474:SER:HA	1:X:518:ASN:HB3	1.98	0.45
1:Q:311:LEU:HB3	1:Q:682:ILE:HG12	1.99	0.45
1:S:630:PRO:O	1:z:477:TRP:HH2	2.00	0.45
1:W:311:LEU:HB3	1:W:682:ILE:HG12	1.99	0.45
1:W:500:TYR:CZ	1:u:448:THR:HG21	2.52	0.45
1:Y:437:LEU:HD11	1:t:276:SER:HB2	1.99	0.45
1:j:574:GLU:OE1	1:o:509:HIS:NE2	2.50	0.45
1:k:489:SER:HB3	1:k:533:PHE:CE1	2.51	0.45
1:m:311:LEU:HB3	1:m:682:ILE:HG12	1.99	0.45
1:o:345:ASP:O	1:o:346:SER:OG	2.32	0.45
1:q:429:SER:OG	1:q:431:ASP:OD1	2.28	0.45
1:s:451:PRO:HA	1:s:456:THR:HA	1.98	0.45
1:v:311:LEU:HB3	1:v:682:ILE:HG12	1.99	0.45
1:y:234:TRP:CE3	1:y:298[A]:ARG:HD3	2.51	0.45
1:z:451:PRO:HA	1:z:456:THR:HA	1.98	0.45
1:2:311:LEU:HB3	1:2:682:ILE:HG12	1.99	0.45
1:2:451:PRO:HA	1:2:456:THR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:489:SER:HB3	1:8:533:PHE:CE1	2.51	0.45
1:A:471:ARG:HD2	1:n:502:TRP:CZ2	2.52	0.45
1:C:311:LEU:HB3	1:C:682:ILE:HG12	1.99	0.45
1:D:489:SER:HB3	1:D:533:PHE:CE1	2.51	0.45
1:E:224:SER:H	1:R:407:ASN:HD21	1.63	0.45
1:F:437:LEU:HD11	1:3:276:SER:HB2	1.99	0.45
1:I:407:ASN:HD21	1:L:224:SER:H	1.63	0.45
1:J:311:LEU:HB3	1:J:682:ILE:HG12	1.99	0.45
1:M:448:THR:HG21	1:T:500:TYR:CZ	2.51	0.45
1:P:431:ASP:OD2	1:X:513:ARG:HD2	2.17	0.45
1:b:429:SER:OG	1:b:431:ASP:OD1	2.28	0.45
1:e:437:LEU:HD11	1:y:276:SER:HB2	1.99	0.45
1:g:311:LEU:HB3	1:g:682:ILE:HG12	1.99	0.45
1:h:407:ASN:HD21	1:j:224:SER:H	1.64	0.45
1:h:474:SER:HA	1:m:518:ASN:HB3	1.98	0.45
1:o:224:SER:H	1:s:407:ASN:HD21	1.64	0.45
1:o:474:SER:HA	1:4:518:ASN:HB3	1.98	0.45
1:p:234:TRP:CD2	1:p:298[A]:ARG:HD3	2.52	0.45
1:u:407:ASN:HD21	1:z:224:SER:H	1.63	0.45
1:y:311:LEU:HB3	1:y:682:ILE:HG12	1.99	0.45
1:z:489:SER:HB3	1:z:533:PHE:CE1	2.51	0.45
1:4:311:LEU:HB3	1:4:682:ILE:HG12	1.99	0.45
1:6:311:LEU:HB3	1:6:682:ILE:HG12	1.99	0.45
1:C:451:PRO:HA	1:C:456:THR:HA	1.98	0.45
1:E:451:PRO:HA	1:E:456:THR:HA	1.98	0.45
1:I:513:ARG:HD2	1:O:431:ASP:OD2	2.17	0.45
1:I:574:GLU:OE1	1:6:509:HIS:NE2	2.49	0.45
1:L:437:LEU:HD11	1:r:276:SER:HB2	1.99	0.45
1:N:474:SER:HA	1:w:518:ASN:HB3	1.99	0.45
1:Q:474:SER:HA	1:k:518:ASN:HB3	1.99	0.45
1:S:311:LEU:HB3	1:S:682:ILE:HG12	1.99	0.45
1:U:451:PRO:HA	1:U:456:THR:HA	1.98	0.45
1:V:500:TYR:CZ	1:w:448:THR:HG21	2.51	0.45
1:d:345:ASP:O	1:d:346:SER:OG	2.32	0.45
1:e:574:GLU:OE1	1:y:509:HIS:NE2	2.50	0.45
1:i:489:SER:HB3	1:i:533:PHE:CE1	2.51	0.45
1:i:500:TYR:CZ	1:p:448:THR:HG21	2.52	0.45
1:j:413:TYR:OH	1:j:641:HIS:O	2.26	0.45
1:j:630:PRO:O	1:4:477:TRP:HH2	2.00	0.45
1:o:574:GLU:OE1	1:4:509:HIS:NE2	2.50	0.45
1:v:247:TRP:O	1:v:675:THR:OG1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:325:GLN:HA	1:v:330:THR:HG22	1.99	0.45
1:1:224:SER:H	1:4:407:ASN:HD21	1.64	0.45
1:4:247:TRP:O	1:4:675:THR:OG1	2.17	0.45
1:5:429:SER:OG	1:5:431:ASP:OD1	2.28	0.45
1:A:502:TRP:CZ2	1:f:471:ARG:HD2	2.52	0.44
1:A:565:ILE:HD12	1:A:565:ILE:HG23	1.77	0.44
1:D:311:LEU:HB3	1:D:682:ILE:HG12	1.99	0.44
1:D:413:TYR:OH	1:D:641:HIS:O	2.26	0.44
1:E:474:SER:HA	1:p:518:ASN:HB3	1.99	0.44
1:F:377:TYR:HH	1:F:393:TYR:H	1.63	0.44
1:G:448:THR:HG21	1:g:500:TYR:CZ	2.53	0.44
1:H:502:TRP:CZ2	1:T:471:ARG:HD2	2.53	0.44
1:K:502:TRP:CZ2	1:X:471:ARG:HD2	2.52	0.44
1:L:513:ARG:HD2	1:R:431:ASP:OD2	2.17	0.44
1:N:489:SER:HB3	1:N:533:PHE:CE1	2.51	0.44
1:N:518:ASN:HB3	1:V:474:SER:HA	1.98	0.44
1:O:451:PRO:HA	1:O:456:THR:HA	1.98	0.44
1:R:500:TYR:CZ	1:r:448:THR:HG21	2.51	0.44
1:a:437:LEU:HD11	1:e:276:SER:HB2	1.99	0.44
1:d:407:ASN:HD21	1:m:224:SER:H	1.64	0.44
1:j:509:HIS:NE2	1:4:574:GLU:OE1	2.51	0.44
1:k:311:LEU:HB3	1:k:682:ILE:HG12	1.99	0.44
1:k:413:TYR:OH	1:k:641:HIS:O	2.26	0.44
1:l:451:PRO:HA	1:l:456:THR:HA	1.98	0.44
1:n:234:TRP:NE1	1:n:298[B]:ARG:HD2	2.31	0.44
1:w:451:PRO:HA	1:w:456:THR:HA	1.98	0.44
1:A:325:GLN:HA	1:A:330:THR:HG22	2.00	0.44
1:B:431:ASP:OD2	1:U:513:ARG:HD2	2.17	0.44
1:B:448:THR:HG21	1:U:500:TYR:CZ	2.52	0.44
1:E:325:GLN:HA	1:E:330:THR:HG22	1.99	0.44
1:F:345:ASP:O	1:F:346:SER:OG	2.32	0.44
1:L:477:TRP:HH2	1:r:630:PRO:O	2.01	0.44
1:M:471:ARG:HD2	1:T:502:TRP:CZ2	2.53	0.44
1:S:500:TYR:CZ	1:z:448:THR:HG21	2.53	0.44
1:U:448:THR:HG21	1:2:500:TYR:CZ	2.52	0.44
1:b:451:PRO:HA	1:b:456:THR:HA	1.98	0.44
1:d:404:ARG:H	1:d:407:ASN:HD22	1.64	0.44
1:f:451:PRO:HA	1:f:456:THR:HA	1.98	0.44
1:g:451:PRO:HA	1:g:456:THR:HA	1.98	0.44
1:n:345:ASP:O	1:n:346:SER:OG	2.32	0.44
1:t:404:ARG:H	1:t:407:ASN:HD22	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:325:GLN:HA	1:w:330:THR:HG22	1.99	0.44
1:4:404:ARG:H	1:4:407:ASN:HD22	1.64	0.44
1:8:404:ARG:H	1:8:407:ASN:HD22	1.64	0.44
1:A:247:TRP:O	1:A:675:THR:OG1	2.17	0.44
1:B:471:ARG:HD2	1:U:502:TRP:CZ2	2.53	0.44
1:B:502:TRP:CZ2	1:2:471:ARG:HD2	2.52	0.44
1:B:630:PRO:O	1:2:477:TRP:HH2	2.01	0.44
1:D:500:TYR:CZ	1:x:448:THR:HG21	2.52	0.44
1:G:325:GLN:HA	1:G:330:THR:HG22	1.99	0.44
1:G:404:ARG:H	1:G:407:ASN:HD22	1.64	0.44
1:H:471:ARG:HD2	1:M:502:TRP:CZ2	2.53	0.44
1:I:325:GLN:HA	1:I:330:THR:HG22	1.99	0.44
1:M:325:GLN:HA	1:M:330:THR:HG22	1.99	0.44
1:M:437:LEU:HD11	1:T:276:SER:HB2	1.99	0.44
1:N:513:ARG:HD2	1:V:431:ASP:OD2	2.18	0.44
1:R:630:PRO:O	1:r:477:TRP:HH2	2.01	0.44
1:S:474:SER:HA	1:q:518:ASN:HB3	1.99	0.44
1:S:477:TRP:HH2	1:q:630:PRO:O	2.01	0.44
1:U:325:GLN:HA	1:U:330:THR:HG22	1.99	0.44
1:Y:474:SER:HA	1:t:518:ASN:HB3	1.99	0.44
1:Y:477:TRP:HH2	1:t:630:PRO:O	2.00	0.44
1:Y:574:GLU:OE1	1:t:509:HIS:NE2	2.50	0.44
1:Z:404:ARG:H	1:Z:407:ASN:HD22	1.64	0.44
1:b:477:TRP:HH2	1:v:630:PRO:O	2.00	0.44
1:d:325:GLN:HA	1:d:330:THR:HG22	1.99	0.44
1:h:325:GLN:HA	1:h:330:THR:HG22	1.99	0.44
1:j:325:GLN:HA	1:j:330:THR:HG22	1.99	0.44
1:m:437:LEU:HD11	1:5:276:SER:HB2	1.99	0.44
1:q:325:GLN:HA	1:q:330:THR:HG22	1.99	0.44
1:s:325:GLN:HA	1:s:330:THR:HG22	1.99	0.44
1:t:325:GLN:HA	1:t:330:THR:HG22	1.99	0.44
1:u:325:GLN:HA	1:u:330:THR:HG22	1.99	0.44
1:8:565:ILE:HD12	1:8:565:ILE:HG23	1.77	0.44
1:B:404:ARG:H	1:B:407:ASN:HD22	1.64	0.44
1:K:404:ARG:H	1:K:407:ASN:HD22	1.64	0.44
1:K:471:ARG:HD2	1:P:502:TRP:CZ2	2.52	0.44
1:M:431:ASP:OD2	1:T:513:ARG:HD2	2.17	0.44
1:P:325:GLN:HA	1:P:330:THR:HG22	2.00	0.44
1:P:413:TYR:OH	1:P:641:HIS:O	2.26	0.44
1:R:325:GLN:HA	1:R:330:THR:HG22	1.99	0.44
1:R:404:ARG:H	1:R:407:ASN:HD22	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:404:ARG:H	1:T:407:ASN:HD22	1.64	0.44
1:U:474:SER:HA	1:2:518:ASN:HB3	1.98	0.44
1:X:311:LEU:HB3	1:X:682:ILE:HG12	1.99	0.44
1:a:500:TYR:CZ	1:y:448:THR:HG21	2.53	0.44
1:c:689:GLU:OE1	1:c:689:GLU:N	2.51	0.44
1:d:311:LEU:HB3	1:d:682:ILE:HG12	1.99	0.44
1:e:689:GLU:N	1:e:689:GLU:OE1	2.51	0.44
1:h:477:TRP:HH2	1:m:630:PRO:O	2.00	0.44
1:j:404:ARG:H	1:j:407:ASN:HD22	1.64	0.44
1:l:474:SER:HA	1:u:518:ASN:HB3	1.98	0.44
1:m:325:GLN:HA	1:m:330:THR:HG22	1.99	0.44
1:m:404:ARG:H	1:m:407:ASN:HD22	1.64	0.44
1:n:311:LEU:HB3	1:n:682:ILE:HG12	1.99	0.44
1:n:325:GLN:HA	1:n:330:THR:HG22	1.99	0.44
1:n:404:ARG:H	1:n:407:ASN:HD22	1.64	0.44
1:n:564:GLU:H	1:n:564:GLU:CD	2.26	0.44
1:o:407:ASN:HD21	1:5:224:SER:H	1.64	0.44
1:p:451:PRO:HA	1:p:456:THR:HA	1.98	0.44
1:q:404:ARG:H	1:q:407:ASN:HD22	1.64	0.44
1:t:689:GLU:OE1	1:t:689:GLU:N	2.51	0.44
1:v:224:SER:H	1:5:407:ASN:HD21	1.64	0.44
1:x:247:TRP:O	1:x:675:THR:OG1	2.17	0.44
1:y:345:ASP:O	1:y:346:SER:OG	2.32	0.44
1:5:404:ARG:H	1:5:407:ASN:HD22	1.64	0.44
1:D:404:ARG:H	1:D:407:ASN:HD22	1.64	0.44
1:D:574:GLU:OE1	1:8:509:HIS:NE2	2.50	0.44
1:E:630:PRO:O	1:i:477:TRP:HH2	2.01	0.44
1:G:689:GLU:OE1	1:G:689:GLU:N	2.51	0.44
1:I:448:THR:HG21	1:6:500:TYR:CZ	2.53	0.44
1:L:325:GLN:HA	1:L:330:THR:HG22	1.99	0.44
1:L:689:GLU:OE1	1:L:689:GLU:N	2.51	0.44
1:N:325:GLN:HA	1:N:330:THR:HG22	1.99	0.44
1:N:437:LEU:HD11	1:w:276:SER:HB2	1.99	0.44
1:P:404:ARG:H	1:P:407:ASN:HD22	1.64	0.44
1:Q:448:THR:HG21	1:k:500:TYR:CZ	2.53	0.44
1:Q:689:GLU:OE1	1:Q:689:GLU:N	2.51	0.44
1:T:325:GLN:HA	1:T:330:THR:HG22	2.00	0.44
1:W:477:TRP:HH2	1:l:630:PRO:O	2.01	0.44
1:W:513:ARG:HD2	1:u:431:ASP:OD2	2.18	0.44
1:W:564:GLU:H	1:W:564:GLU:CD	2.26	0.44
1:Z:500:TYR:CZ	1:k:448:THR:HG21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:630:PRO:O	1:k:477:TRP:HH2	2.00	0.44
1:c:513:ARG:HD2	1:3:431:ASP:OD2	2.18	0.44
1:i:325:GLN:HA	1:i:330:THR:HG22	1.99	0.44
1:k:404:ARG:H	1:k:407:ASN:HD22	1.64	0.44
1:m:574:GLU:OE1	1:5:509:HIS:NE2	2.51	0.44
1:m:689:GLU:N	1:m:689:GLU:OE1	2.51	0.44
1:o:311:LEU:HB3	1:o:682:ILE:HG12	1.99	0.44
1:o:325:GLN:HA	1:o:330:THR:HG22	1.99	0.44
1:x:345:ASP:O	1:x:346:SER:OG	2.32	0.44
1:y:377:TYR:HH	1:y:393:TYR:H	1.63	0.44
1:z:325:GLN:HA	1:z:330:THR:HG22	1.99	0.44
1:1:234:TRP:CG	1:1:298[A]:ARG:HD3	2.52	0.44
1:1:404:ARG:H	1:1:407:ASN:HD22	1.64	0.44
1:5:564:GLU:H	1:5:564:GLU:CD	2.26	0.44
1:E:404:ARG:H	1:E:407:ASN:HD22	1.64	0.44
1:F:431:ASP:OD2	1:3:513:ARG:HD2	2.18	0.44
1:G:474:SER:HA	1:g:518:ASN:HB3	1.99	0.44
1:G:502:TRP:CZ2	1:7:471:ARG:HD2	2.53	0.44
1:H:564:GLU:H	1:H:564:GLU:CD	2.26	0.44
1:J:325:GLN:HA	1:J:330:THR:HG22	1.99	0.44
1:J:477:TRP:HH2	1:1:630:PRO:O	2.01	0.44
1:K:247:TRP:O	1:K:675:THR:OG1	2.17	0.44
1:L:502:TRP:CZ2	1:R:471:ARG:HD2	2.53	0.44
1:S:407:ASN:HD21	1:l:224:SER:H	1.65	0.44
1:S:689:GLU:OE1	1:S:689:GLU:N	2.51	0.44
1:T:294:ARG:HG3	1:T:298[B]:ARG:HH11	1.82	0.44
1:T:689:GLU:OE1	1:T:689:GLU:N	2.51	0.44
1:V:451:PRO:HA	1:V:456:THR:HA	1.98	0.44
1:X:325:GLN:HA	1:X:330:THR:HG22	2.00	0.44
1:Z:564:GLU:H	1:Z:564:GLU:CD	2.26	0.44
1:a:247:TRP:O	1:a:675:THR:OG1	2.17	0.44
1:a:477:TRP:HH2	1:e:630:PRO:O	2.01	0.44
1:b:404:ARG:H	1:b:407:ASN:HD22	1.64	0.44
1:b:500:TYR:CZ	1:d:448:THR:HG21	2.53	0.44
1:c:247:TRP:O	1:c:675:THR:OG1	2.17	0.44
1:c:276:SER:HB2	1:3:437:LEU:HD11	2.00	0.44
1:d:564:GLU:H	1:d:564:GLU:CD	2.26	0.44
1:e:325:GLN:HA	1:e:330:THR:HG22	1.99	0.44
1:j:518:ASN:HB3	1:4:474:SER:HA	1.99	0.44
1:r:689:GLU:OE1	1:r:689:GLU:N	2.51	0.44
1:u:564:GLU:CD	1:u:564:GLU:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:404:ARG:H	1:w:407:ASN:HD22	1.64	0.44
1:x:689:GLU:N	1:x:689:GLU:OE1	2.51	0.44
1:z:689:GLU:OE1	1:z:689:GLU:N	2.51	0.44
1:5:311:LEU:HB3	1:5:682:ILE:HG12	1.99	0.44
1:5:325:GLN:HA	1:5:330:THR:HG22	1.99	0.44
1:6:564:GLU:H	1:6:564:GLU:CD	2.26	0.44
1:8:564:GLU:H	1:8:564:GLU:CD	2.26	0.44
1:C:325:GLN:HA	1:C:330:THR:HG22	1.99	0.44
1:C:630:PRO:O	1:t:477:TRP:HH2	1.99	0.44
1:D:474:SER:HA	1:8:518:ASN:HB3	1.99	0.44
1:D:564:GLU:H	1:D:564:GLU:CD	2.26	0.44
1:D:689:GLU:OE1	1:D:689:GLU:N	2.51	0.44
1:E:311:LEU:HB3	1:E:682:ILE:HG12	1.99	0.44
1:H:404:ARG:H	1:H:407:ASN:HD22	1.64	0.44
1:I:564:GLU:H	1:I:564:GLU:CD	2.26	0.44
1:J:574:GLU:OE1	1:1:509:HIS:NE2	2.51	0.44
1:K:437:LEU:HD11	1:P:276:SER:HB2	1.99	0.44
1:P:471:ARG:HD2	1:X:502:TRP:CZ2	2.53	0.44
1:P:564:GLU:CD	1:P:564:GLU:H	2.26	0.44
1:Q:234:TRP:CH2	1:Q:298[A]:ARG:HB3	2.52	0.44
1:R:564:GLU:H	1:R:564:GLU:CD	2.26	0.44
1:V:502:TRP:CZ2	1:w:471:ARG:HD2	2.53	0.44
1:Y:448:THR:HG21	1:t:500:TYR:CZ	2.53	0.44
1:a:448:THR:HG21	1:e:500:TYR:CZ	2.53	0.44
1:e:247:TRP:O	1:e:675:THR:OG1	2.17	0.44
1:g:448:THR:HG21	1:7:500:TYR:CZ	2.52	0.44
1:h:689:GLU:N	1:h:689:GLU:OE1	2.51	0.44
1:j:564:GLU:H	1:j:564:GLU:CD	2.26	0.44
1:k:689:GLU:OE1	1:k:689:GLU:N	2.51	0.44
1:m:474:SER:HA	1:5:518:ASN:HB3	1.99	0.44
1:n:565:ILE:HG22	1:n:569:ASN:HB2	1.98	0.44
1:o:448:THR:HG21	1:4:500:TYR:CZ	2.53	0.44
1:q:564:GLU:H	1:q:564:GLU:CD	2.26	0.44
1:v:565:ILE:HD12	1:v:565:ILE:HG23	1.77	0.44
1:w:311:LEU:HB3	1:w:682:ILE:HG12	1.99	0.44
1:x:500:TYR:CZ	1:8:448:THR:HG21	2.53	0.44
1:2:325:GLN:HA	1:2:330:THR:HG22	1.99	0.44
1:A:431:ASP:OD2	1:n:513:ARG:HD2	2.18	0.44
1:B:689:GLU:N	1:B:689:GLU:OE1	2.51	0.44
1:G:407:ASN:HD21	1:Y:224:SER:H	1.64	0.44
1:G:564:GLU:H	1:G:564:GLU:CD	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:311:LEU:HB3	1:H:682:ILE:HG12	1.99	0.44
1:J:699:GLN:H	1:t:701:THR:HG23	1.83	0.44
1:K:564:GLU:H	1:K:564:GLU:CD	2.26	0.44
1:L:276:SER:HB2	1:R:437:LEU:HD11	1.98	0.44
1:M:689:GLU:N	1:M:689:GLU:OE1	2.51	0.44
1:N:448:THR:HG21	1:w:500:TYR:CZ	2.53	0.44
1:O:502:TRP:CZ2	1:6:471:ARG:HD2	2.53	0.44
1:R:502:TRP:CZ2	1:r:471:ARG:HD2	2.52	0.44
1:S:699:GLN:H	1:w:701:THR:HG23	1.83	0.44
1:U:689:GLU:N	1:U:689:GLU:OE1	2.51	0.44
1:W:325:GLN:HA	1:W:330:THR:HG22	1.99	0.44
1:a:407:ASN:HD21	1:4:224:SER:H	1.64	0.44
1:b:518:ASN:HB3	1:d:474:SER:HA	1.98	0.44
1:c:325:GLN:HA	1:c:330:THR:HG22	1.99	0.44
1:c:630:PRO:O	1:3:477:TRP:HH2	2.01	0.44
1:d:565:ILE:HG22	1:d:569:ASN:HB2	1.98	0.44
1:d:699:GLN:H	1:p:701:THR:HG23	1.83	0.44
1:f:311:LEU:HB3	1:f:682:ILE:HG12	1.99	0.44
1:g:325:GLN:HA	1:g:330:THR:HG22	1.99	0.44
1:h:311:LEU:HB3	1:h:682:ILE:HG12	1.99	0.44
1:j:429:SER:OG	1:j:431:ASP:OD1	2.28	0.44
1:k:564:GLU:H	1:k:564:GLU:CD	2.26	0.44
1:t:564:GLU:H	1:t:564:GLU:CD	2.26	0.44
1:u:345:ASP:O	1:u:346:SER:OG	2.32	0.44
1:1:311:LEU:HB3	1:1:682:ILE:HG12	1.99	0.44
1:1:689:GLU:OE1	1:1:689:GLU:N	2.51	0.44
1:4:564:GLU:H	1:4:564:GLU:CD	2.26	0.44
1:6:689:GLU:OE1	1:6:689:GLU:N	2.51	0.44
1:8:689:GLU:OE1	1:8:689:GLU:N	2.51	0.44
1:A:276:SER:HB2	1:f:437:LEU:HD11	2.00	0.44
1:A:377:TYR:HH	1:A:393:TYR:H	1.65	0.44
1:D:513:ARG:HD2	1:x:431:ASP:OD2	2.18	0.44
1:G:630:PRO:O	1:7:477:TRP:HH2	2.01	0.44
1:H:325:GLN:HA	1:H:330:THR:HG22	2.00	0.44
1:J:500:TYR:CZ	1:s:448:THR:HG21	2.53	0.44
1:J:564:GLU:H	1:J:564:GLU:CD	2.26	0.44
1:K:276:SER:HB2	1:X:437:LEU:HD11	1.99	0.44
1:N:500:TYR:CZ	1:V:448:THR:HG21	2.53	0.44
1:P:429:SER:OG	1:P:431:ASP:OD1	2.28	0.44
1:R:689:GLU:N	1:R:689:GLU:OE1	2.51	0.44
1:S:574:GLU:OE1	1:q:509:HIS:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:311:LEU:HB3	1:V:682:ILE:HG12	1.99	0.44
1:V:513:ARG:HD2	1:w:431:ASP:OD2	2.18	0.44
1:W:689:GLU:OE1	1:W:689:GLU:N	2.51	0.44
1:Z:689:GLU:OE1	1:Z:689:GLU:N	2.51	0.44
1:b:311:LEU:HB3	1:b:682:ILE:HG12	1.99	0.44
1:b:574:GLU:OE1	1:v:509:HIS:NE2	2.50	0.44
1:d:353:VAL:CG1	1:v:435:ASN:HB2	2.48	0.44
1:f:298[A]:ARG:HH22	1:f:688:LYS:NZ	2.16	0.44
1:f:345:ASP:O	1:f:346:SER:OG	2.32	0.44
1:f:404:ARG:H	1:f:407:ASN:HD22	1.64	0.44
1:h:564:GLU:H	1:h:564:GLU:CD	2.26	0.44
1:p:311:LEU:HB3	1:p:682:ILE:HG12	1.99	0.44
1:p:429:SER:OG	1:p:431:ASP:OD1	2.28	0.44
1:s:689:GLU:N	1:s:689:GLU:OE1	2.51	0.44
1:l:325:GLN:HA	1:l:330:THR:HG22	1.99	0.44
1:2:564:GLU:H	1:2:564:GLU:CD	2.26	0.44
1:B:311:LEU:HB3	1:B:682:ILE:HG12	1.99	0.43
1:E:448:THR:HG21	1:p:500:TYR:CZ	2.53	0.43
1:E:477:TRP:HH2	1:p:630:PRO:O	2.01	0.43
1:H:689:GLU:OE1	1:H:689:GLU:N	2.51	0.43
1:I:276:SER:HB2	1:O:437:LEU:HD11	2.00	0.43
1:I:500:TYR:CZ	1:O:448:THR:HG21	2.51	0.43
1:K:513:ARG:HD2	1:X:431:ASP:OD2	2.17	0.43
1:P:565:ILE:HG23	1:P:565:ILE:HD12	1.77	0.43
1:Q:247:TRP:O	1:Q:675:THR:OG1	2.17	0.43
1:U:234:TRP:HB3	1:U:298[A]:ARG:CZ	2.48	0.43
1:V:689:GLU:OE1	1:V:689:GLU:N	2.51	0.43
1:W:630:PRO:O	1:u:477:TRP:HH2	2.00	0.43
1:b:276:SER:HB2	1:d:437:LEU:HD11	1.99	0.43
1:h:404:ARG:H	1:h:407:ASN:HD22	1.64	0.43
1:j:276:SER:HB2	1:4:437:LEU:HD11	1.99	0.43
1:j:689:GLU:OE1	1:j:689:GLU:N	2.51	0.43
1:p:377:TYR:HH	1:p:393:TYR:H	1.64	0.43
1:p:689:GLU:N	1:p:689:GLU:OE1	2.51	0.43
1:q:689:GLU:OE1	1:q:689:GLU:N	2.51	0.43
1:3:247:TRP:O	1:3:675:THR:OG1	2.17	0.43
1:5:689:GLU:N	1:5:689:GLU:OE1	2.51	0.43
1:6:325:GLN:HA	1:6:330:THR:HG22	1.99	0.43
1:8:325:GLN:HA	1:8:330:THR:HG22	1.99	0.43
1:A:564:GLU:H	1:A:564:GLU:CD	2.26	0.43
1:B:325:GLN:HA	1:B:330:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:ASP:OD2	1:Y:513:ARG:HD2	2.18	0.43
1:F:477:TRP:HH2	1:3:630:PRO:O	2.02	0.43
1:I:345:ASP:O	1:I:346:SER:OG	2.32	0.43
1:I:474:SER:HA	1:6:518:ASN:HB3	1.99	0.43
1:K:294:ARG:HG3	1:K:298[B]:ARG:HH11	1.82	0.43
1:K:325:GLN:HA	1:K:330:THR:HG22	1.99	0.43
1:M:311:LEU:HB3	1:M:682:ILE:HG12	1.99	0.43
1:M:404:ARG:H	1:M:407:ASN:HD22	1.64	0.43
1:M:564:GLU:H	1:M:564:GLU:CD	2.26	0.43
1:N:234:TRP:CD2	1:N:298[A]:ARG:HD3	2.53	0.43
1:Q:325:GLN:HA	1:Q:330:THR:HG22	1.99	0.43
1:Q:477:TRP:HH2	1:k:630:PRO:O	2.01	0.43
1:Q:630:PRO:O	1:Z:477:TRP:HH2	2.02	0.43
1:b:345:ASP:O	1:b:346:SER:OG	2.32	0.43
1:e:474:SER:HA	1:y:518:ASN:HB3	1.99	0.43
1:j:311:LEU:HB3	1:j:682:ILE:HG12	1.99	0.43
1:j:448:THR:HG21	1:o:500:TYR:CZ	2.53	0.43
1:t:298[A]:ARG:HH22	1:t:688:LYS:HZ1	1.66	0.43
1:x:353:VAL:CG1	1:8:435:ASN:HB2	2.48	0.43
1:y:325:GLN:HA	1:y:330:THR:HG22	1.99	0.43
1:2:689:GLU:N	1:2:689:GLU:OE1	2.51	0.43
1:4:234:TRP:CH2	1:4:298[B]:ARG:HB2	2.54	0.43
1:F:238[B]:ARG:HD3	1:F:683:GLU:OE2	2.17	0.43
1:F:325:GLN:HA	1:F:330:THR:HG22	1.99	0.43
1:G:311:LEU:HB3	1:G:682:ILE:HG12	1.99	0.43
1:I:234:TRP:CH2	1:I:298[A]:ARG:HB3	2.52	0.43
1:J:513:ARG:HD2	1:s:431:ASP:OD2	2.18	0.43
1:L:564:GLU:H	1:L:564:GLU:CD	2.26	0.43
1:P:311:LEU:HB3	1:P:682:ILE:HG12	1.99	0.43
1:P:689:GLU:N	1:P:689:GLU:OE1	2.51	0.43
1:S:513:ARG:HD2	1:z:431:ASP:OD2	2.18	0.43
1:Z:325:GLN:HA	1:Z:330:THR:HG22	2.00	0.43
1:c:502:TRP:CZ2	1:3:471:ARG:HD2	2.53	0.43
1:q:448:THR:HG21	1:z:500:TYR:CZ	2.53	0.43
1:v:564:GLU:H	1:v:564:GLU:CD	2.26	0.43
1:x:325:GLN:HA	1:x:330:THR:HG22	1.99	0.43
1:4:325:GLN:HA	1:4:330:THR:HG22	1.99	0.43
1:D:699:GLN:H	1:6:701:THR:HG23	1.83	0.43
1:E:564:GLU:H	1:E:564:GLU:CD	2.26	0.43
1:H:276:SER:HB2	1:T:437:LEU:HD11	2.00	0.43
1:J:448:THR:HG21	1:1:500:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:689:GLU:OE1	1:K:689:GLU:N	2.51	0.43
1:O:689:GLU:OE1	1:O:689:GLU:N	2.51	0.43
1:U:471:ARG:HD2	1:2:502:TRP:CZ2	2.53	0.43
1:W:437:LEU:HD11	1:l:276:SER:HB2	1.98	0.43
1:W:448:THR:HG21	1:l:500:TYR:CZ	2.53	0.43
1:a:325:GLN:HA	1:a:330:THR:HG22	1.99	0.43
1:a:689:GLU:OE1	1:a:689:GLU:N	2.51	0.43
1:f:502:TRP:CZ2	1:n:471:ARG:HD2	2.53	0.43
1:l:689:GLU:OE1	1:l:689:GLU:N	2.51	0.43
1:o:437:LEU:HD11	1:4:276:SER:HB2	2.00	0.43
1:p:564:GLU:H	1:p:564:GLU:CD	2.26	0.43
1:s:311:LEU:HB3	1:s:682:ILE:HG12	1.99	0.43
1:s:699:GLN:H	1:8:701:THR:HG23	1.84	0.43
1:t:311:LEU:HB3	1:t:682:ILE:HG12	1.99	0.43
1:w:564:GLU:H	1:w:564:GLU:CD	2.26	0.43
1:w:689:GLU:OE1	1:w:689:GLU:N	2.51	0.43
1:x:276:SER:HB2	1:8:437:LEU:HD11	2.00	0.43
1:x:627:HIS:HB3	1:8:605:VAL:HG12	2.01	0.43
1:z:564:GLU:H	1:z:564:GLU:CD	2.26	0.43
1:5:234:TRP:CH2	1:5:298[B]:ARG:HB2	2.53	0.43
1:7:689:GLU:OE1	1:7:689:GLU:N	2.51	0.43
1:C:502:TRP:CZ2	1:t:471:ARG:HD2	2.53	0.43
1:E:379:THR:HG22	1:E:380:LEU:N	2.34	0.43
1:E:689:GLU:N	1:E:689:GLU:OE1	2.51	0.43
1:H:630:PRO:O	1:T:477:TRP:HH2	2.02	0.43
1:I:502:TRP:CZ2	1:O:471:ARG:HD2	2.53	0.43
1:J:276:SER:HB2	1:s:437:LEU:HD11	2.01	0.43
1:J:689:GLU:N	1:J:689:GLU:OE1	2.51	0.43
1:K:630:PRO:O	1:X:477:TRP:HH2	2.02	0.43
1:Q:276:SER:HB2	1:Z:437:LEU:HD11	2.00	0.43
1:T:345:ASP:O	1:T:346:SER:OG	2.32	0.43
1:U:311:LEU:HB3	1:U:682:ILE:HG12	1.99	0.43
1:V:325:GLN:HA	1:V:330:THR:HG22	1.99	0.43
1:V:564:GLU:H	1:V:564:GLU:CD	2.26	0.43
1:Z:502:TRP:CZ2	1:k:471:ARG:HD2	2.53	0.43
1:b:325:GLN:HA	1:b:330:THR:HG22	1.99	0.43
1:g:379:THR:HG22	1:g:380:LEU:N	2.34	0.43
1:g:689:GLU:OE1	1:g:689:GLU:N	2.51	0.43
1:h:276:SER:HB2	1:5:437:LEU:HD11	2.01	0.43
1:h:353:VAL:CG1	1:5:435:ASN:HB2	2.48	0.43
1:h:699:GLN:H	1:q:701:THR:HG23	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:353:VAL:CG1	1:4:435:ASN:HB2	2.49	0.43
1:j:500:TYR:CZ	1:4:448:THR:HG21	2.54	0.43
1:j:627:HIS:HB3	1:4:605:VAL:HG12	2.01	0.43
1:l:437:LEU:HD11	1:u:276:SER:HB2	2.00	0.43
1:p:325:GLN:HA	1:p:330:THR:HG22	1.99	0.43
1:s:565:ILE:HD12	1:s:565:ILE:HG23	1.77	0.43
1:y:701:THR:HG23	1:4:699:GLN:H	1.84	0.43
1:3:325:GLN:HA	1:3:330:THR:HG22	1.99	0.43
1:8:234:TRP:CD2	1:8:298[A]:ARG:HD3	2.53	0.43
1:C:379:THR:HG22	1:C:380:LEU:N	2.34	0.43
1:C:477:TRP:HH2	1:Y:630:PRO:O	2.02	0.43
1:C:565:ILE:HD12	1:C:565:ILE:HG23	1.77	0.43
1:C:689:GLU:OE1	1:C:689:GLU:N	2.51	0.43
1:D:477:TRP:HH2	1:8:630:PRO:O	2.01	0.43
1:H:477:TRP:HH2	1:M:630:PRO:O	2.02	0.43
1:I:630:PRO:O	1:O:477:TRP:HH2	2.02	0.43
1:I:689:GLU:OE1	1:I:689:GLU:N	2.51	0.43
1:Q:502:TRP:CZ2	1:Z:471:ARG:HD2	2.53	0.43
1:U:564:GLU:H	1:U:564:GLU:CD	2.26	0.43
1:W:474:SER:HA	1:l:518:ASN:HB3	1.99	0.43
1:X:294:ARG:HG3	1:X:298[B]:ARG:HH11	1.83	0.43
1:Y:234:TRP:CD2	1:Y:298[A]:ARG:HD3	2.53	0.43
1:Y:689:GLU:OE1	1:Y:689:GLU:N	2.51	0.43
1:a:311:LEU:HB3	1:a:682:ILE:HG12	1.99	0.43
1:b:666:PHE:HZ	1:p:371:MET:HG3	1.84	0.43
1:d:500:TYR:CZ	1:v:448:THR:HG21	2.53	0.43
1:d:689:GLU:OE1	1:d:689:GLU:N	2.51	0.43
1:f:325:GLN:HA	1:f:330:THR:HG22	2.00	0.43
1:f:630:PRO:O	1:n:477:TRP:HH2	2.00	0.43
1:g:435:ASN:HB2	1:7:353:VAL:CG1	2.49	0.43
1:g:471:ARG:HD2	1:7:502:TRP:CZ2	2.54	0.43
1:j:437:LEU:HD11	1:o:276:SER:HB2	2.01	0.43
1:l:325:GLN:HA	1:l:330:THR:HG22	1.99	0.43
1:q:238[A]:ARG:HD2	1:q:683:GLU:OE2	2.18	0.43
1:r:379:THR:HG22	1:r:380:LEU:N	2.34	0.43
1:3:311:LEU:HB3	1:3:682:ILE:HG12	1.99	0.43
1:3:689:GLU:OE1	1:3:689:GLU:N	2.51	0.43
1:4:689:GLU:OE1	1:4:689:GLU:N	2.51	0.43
1:C:448:THR:HG21	1:Y:500:TYR:CZ	2.53	0.43
1:C:513:ARG:HD2	1:t:431:ASP:OD2	2.18	0.43
1:D:502:TRP:CZ2	1:x:471:ARG:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:SER:HB2	1:c:437:LEU:HD11	2.00	0.43
1:F:379:THR:HG22	1:F:380:LEU:N	2.34	0.43
1:F:471:ARG:HD2	1:3:502:TRP:CZ2	2.53	0.43
1:I:234:TRP:CH2	1:I:298[B]:ARG:HB2	2.53	0.43
1:L:234:TRP:CH2	1:L:298[A]:ARG:HB3	2.54	0.43
1:O:325:GLN:HA	1:O:330:THR:HG22	2.00	0.43
1:Q:234:TRP:CH2	1:Q:298[B]:ARG:HB2	2.53	0.43
1:R:379:THR:HG22	1:R:380:LEU:N	2.34	0.43
1:S:379:THR:HG22	1:S:380:LEU:N	2.34	0.43
1:U:477:TRP:HH2	1:2:630:PRO:O	2.01	0.43
1:U:565:ILE:HD12	1:U:565:ILE:HG23	1.77	0.43
1:Y:325:GLN:HA	1:Y:330:THR:HG22	1.99	0.43
1:Z:513:ARG:HD2	1:k:431:ASP:OD2	2.18	0.43
1:a:353:VAL:CG1	1:y:435:ASN:HB2	2.48	0.43
1:a:513:ARG:HD2	1:y:431:ASP:OD2	2.19	0.43
1:f:276:SER:HB2	1:n:437:LEU:HD11	2.00	0.43
1:i:502:TRP:CZ2	1:p:471:ARG:HD2	2.54	0.43
1:j:565:ILE:HG23	1:j:565:ILE:HD12	1.77	0.43
1:l:379:THR:HG22	1:l:380:LEU:N	2.34	0.43
1:l:564:GLU:H	1:l:564:GLU:CD	2.26	0.43
1:n:689:GLU:OE1	1:n:689:GLU:N	2.51	0.43
1:q:666:PHE:HZ	1:w:371:MET:HG3	1.84	0.43
1:s:353:VAL:CG1	1:1:435:ASN:HB2	2.48	0.43
1:s:564:GLU:H	1:s:564:GLU:CD	2.26	0.43
1:u:689:GLU:OE1	1:u:689:GLU:N	2.51	0.43
1:v:371:MET:HG3	1:5:666:PHE:HZ	1.84	0.43
1:w:379:THR:HG22	1:w:380:LEU:N	2.34	0.43
1:7:325:GLN:HA	1:7:330:THR:HG22	2.00	0.43
1:7:631:SER:HB2	2:7:901:D5M:N7	2.34	0.43
1:C:353:VAL:CG1	1:t:435:ASN:HB2	2.49	0.43
1:F:630:PRO:O	1:c:477:TRP:HH2	2.02	0.43
1:G:276:SER:HB2	1:7:437:LEU:HD11	2.01	0.43
1:J:605:VAL:HG12	1:1:627:HIS:HB3	2.01	0.43
1:J:630:PRO:O	1:s:477:TRP:HH2	2.00	0.43
1:L:234:TRP:HB3	1:L:298[A]:ARG:CZ	2.48	0.43
1:L:471:ARG:HD2	1:r:502:TRP:CZ2	2.53	0.43
1:N:502:TRP:CZ2	1:V:471:ARG:HD2	2.54	0.43
1:O:379:THR:HG22	1:O:380:LEU:N	2.34	0.43
1:R:345:ASP:O	1:R:346:SER:OG	2.32	0.43
1:S:276:SER:HB2	1:z:437:LEU:HD11	2.01	0.43
1:X:689:GLU:N	1:X:689:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:631:SER:HB2	2:Y:901:D5M:N7	2.34	0.43
1:b:379:THR:HG22	1:b:380:LEU:N	2.34	0.43
1:b:474:SER:HA	1:v:518:ASN:HB3	1.99	0.43
1:b:689:GLU:OE1	1:b:689:GLU:N	2.51	0.43
1:f:564:GLU:H	1:f:564:GLU:CD	2.26	0.43
1:i:631:SER:HB2	2:i:901:D5M:N7	2.34	0.43
1:j:234:TRP:CH2	1:j:298[B]:ARG:HB2	2.53	0.43
1:j:435:ASN:HB2	1:o:353:VAL:CG1	2.48	0.43
1:m:345:ASP:O	1:m:346:SER:OG	2.32	0.43
1:m:699:GLN:H	1:v:701:THR:HG23	1.84	0.43
1:n:298[A]:ARG:HH21	1:n:298[A]:ARG:CG	2.19	0.43
1:o:379:THR:HG22	1:o:380:LEU:N	2.34	0.43
1:o:631:SER:HB2	2:o:901:D5M:N7	2.34	0.43
1:p:379:THR:HG22	1:p:380:LEU:N	2.34	0.43
1:q:605:VAL:HG12	1:z:627:HIS:HB3	2.01	0.43
1:s:500:TYR:CZ	1:1:448:THR:HG21	2.53	0.43
1:1:238[A]:ARG:HD2	1:1:683:GLU:OE2	2.18	0.43
1:1:565:ILE:HG23	1:1:565:ILE:HD12	1.77	0.43
1:2:365:PHE:HA	1:2:366:PRO:HD3	1.92	0.43
1:A:689:GLU:OE1	1:A:689:GLU:N	2.51	0.43
1:A:699:GLN:H	1:T:701:THR:HG23	1.84	0.43
1:C:471:ARG:HD2	1:Y:502:TRP:CZ2	2.54	0.43
1:E:471:ARG:HD2	1:p:502:TRP:CZ2	2.54	0.43
1:E:502:TRP:CZ2	1:i:471:ARG:HD2	2.53	0.43
1:J:407:ASN:HD21	1:8:224:SER:H	1.65	0.43
1:J:502:TRP:CZ2	1:s:471:ARG:HD2	2.54	0.43
1:K:631:SER:HB2	2:K:901:D5M:N7	2.34	0.43
1:N:631:SER:HB2	2:N:901:D5M:N7	2.34	0.43
1:V:379:THR:HG22	1:V:380:LEU:N	2.34	0.43
1:X:234:TRP:CE2	1:X:298[A]:ARG:HD3	2.53	0.43
1:X:379:THR:HG22	1:X:380:LEU:N	2.34	0.43
1:X:564:GLU:H	1:X:564:GLU:CD	2.26	0.43
1:X:631:SER:HB2	2:X:901:D5M:N7	2.34	0.43
1:Z:379:THR:HG22	1:Z:380:LEU:N	2.34	0.43
1:b:564:GLU:H	1:b:564:GLU:CD	2.26	0.43
1:b:605:VAL:HG12	1:v:627:HIS:HB3	2.00	0.43
1:c:298[A]:ARG:HH22	1:c:688:LYS:NZ	2.16	0.43
1:f:379:THR:HG22	1:f:380:LEU:N	2.34	0.43
1:f:513:ARG:HD2	1:n:431:ASP:OD2	2.18	0.43
1:f:689:GLU:OE1	1:f:689:GLU:N	2.51	0.43
1:g:437:LEU:HD11	1:7:276:SER:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:666:PHE:HZ	1:j:371:MET:HG3	1.84	0.43
1:m:234:TRP:CH2	1:m:298[B]:ARG:HB2	2.54	0.43
1:m:565:ILE:HG23	1:m:565:ILE:HD12	1.77	0.43
1:o:689:GLU:OE1	1:o:689:GLU:N	2.51	0.43
1:q:379:THR:HG22	1:q:380:LEU:N	2.34	0.43
1:q:435:ASN:HB2	1:z:353:VAL:CG1	2.48	0.43
1:u:379:THR:HG22	1:u:380:LEU:N	2.34	0.43
1:x:565:ILE:HD12	1:x:565:ILE:HG23	1.77	0.43
1:y:379:THR:HG22	1:y:380:LEU:N	2.34	0.43
1:z:631:SER:HB2	2:z:901:D5M:N7	2.34	0.43
1:1:234:TRP:CE2	1:1:298[B]:ARG:HD2	2.54	0.43
1:4:631:SER:HB2	2:4:901:D5M:N7	2.34	0.43
1:A:631:SER:HB2	2:A:901:D5M:N7	2.34	0.43
1:B:345:ASP:O	1:B:346:SER:OG	2.32	0.43
1:B:477:TRP:HH2	1:U:630:PRO:O	2.02	0.43
1:F:689:GLU:OE1	1:F:689:GLU:N	2.51	0.43
1:I:379:THR:HG22	1:I:380:LEU:N	2.34	0.43
1:J:379:THR:HG22	1:J:380:LEU:N	2.34	0.43
1:K:345:ASP:O	1:K:346:SER:OG	2.32	0.43
1:L:379:THR:HG22	1:L:380:LEU:N	2.34	0.43
1:L:631:SER:HB2	2:L:901:D5M:N7	2.34	0.43
1:M:294:ARG:HG3	1:M:298[B]:ARG:HH11	1.83	0.43
1:M:379:THR:HG22	1:M:380:LEU:N	2.34	0.43
1:O:564:GLU:H	1:O:564:GLU:CD	2.26	0.43
1:P:631:SER:HB2	2:P:901:D5M:N7	2.34	0.43
1:Q:471:ARG:HD2	1:k:502:TRP:CZ2	2.54	0.43
1:Q:564:GLU:H	1:Q:564:GLU:CD	2.26	0.43
1:S:325:GLN:HA	1:S:330:THR:HG22	1.99	0.43
1:U:431:ASP:OD2	1:2:513:ARG:HD2	2.19	0.43
1:W:276:SER:HB2	1:u:437:LEU:HD11	2.01	0.43
1:e:435:ASN:HB2	1:y:353:VAL:CG1	2.48	0.43
1:e:448:THR:HG21	1:y:500:TYR:CZ	2.54	0.43
1:g:631:SER:HB2	2:g:901:D5M:N7	2.34	0.43
1:h:379:THR:HG22	1:h:380:LEU:N	2.34	0.43
1:h:437:LEU:HD11	1:m:276:SER:HB2	2.00	0.43
1:h:500:TYR:CZ	1:5:448:THR:HG21	2.53	0.43
1:j:631:SER:HB2	2:j:901:D5M:N7	2.34	0.43
1:m:379:THR:HG22	1:m:380:LEU:N	2.34	0.43
1:q:234:TRP:CE2	1:q:298[B]:ARG:HD2	2.54	0.43
1:r:325:GLN:HA	1:r:330:THR:HG22	1.99	0.43
1:s:429:SER:OG	1:s:431:ASP:OD1	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:666:PHE:HZ	1:x:371:MET:HG3	1.84	0.43
1:v:689:GLU:OE1	1:v:689:GLU:N	2.51	0.43
1:x:564:GLU:H	1:x:564:GLU:CD	2.26	0.43
1:y:689:GLU:OE1	1:y:689:GLU:N	2.51	0.43
1:z:379:THR:HG22	1:z:380:LEU:N	2.34	0.43
1:1:371:MET:HG3	1:4:666:PHE:HZ	1.84	0.43
1:6:247:TRP:O	1:6:675:THR:OG1	2.17	0.43
1:8:379:THR:HG22	1:8:380:LEU:N	2.34	0.43
1:8:631:SER:HB2	2:8:901:D5M:N7	2.34	0.43
1:C:631:SER:HB2	2:C:901:D5M:N7	2.34	0.42
1:D:379:THR:HG22	1:D:380:LEU:N	2.34	0.42
1:H:345:ASP:O	1:H:346:SER:OG	2.32	0.42
1:I:477:TRP:HH2	1:6:630:PRO:O	2.01	0.42
1:J:474:SER:HA	1:1:518:ASN:HB3	1.99	0.42
1:O:513:ARG:HD2	1:6:431:ASP:OD2	2.18	0.42
1:P:477:TRP:HH2	1:X:630:PRO:O	2.02	0.42
1:S:605:VAL:HG12	1:q:627:HIS:HB3	2.01	0.42
1:S:631:SER:HB2	2:S:901:D5M:N7	2.34	0.42
1:T:379:THR:HG22	1:T:380:LEU:N	2.34	0.42
1:T:631:SER:HB2	2:T:901:D5M:N7	2.34	0.42
1:V:565:ILE:HD12	1:V:565:ILE:HG23	1.77	0.42
1:W:247:TRP:O	1:W:675:THR:OG1	2.17	0.42
1:W:502:TRP:CZ2	1:u:471:ARG:HD2	2.54	0.42
1:Y:379:THR:HG22	1:Y:380:LEU:N	2.34	0.42
1:Z:631:SER:HB2	2:Z:901:D5M:N7	2.34	0.42
1:b:448:THR:HG21	1:v:500:TYR:CZ	2.54	0.42
1:e:605:VAL:HG12	1:y:627:HIS:HB3	2.00	0.42
1:h:448:THR:HG21	1:m:500:TYR:CZ	2.53	0.42
1:h:631:SER:HB2	2:h:901:D5M:N7	2.34	0.42
1:o:564:GLU:H	1:o:564:GLU:CD	2.26	0.42
1:r:564:GLU:H	1:r:564:GLU:CD	2.26	0.42
1:r:631:SER:HB2	2:r:901:D5M:N7	2.34	0.42
1:s:276:SER:HB2	1:1:437:LEU:HD11	2.01	0.42
1:v:631:SER:HB2	2:v:901:D5M:N7	2.34	0.42
1:5:234:TRP:CE2	1:5:298[B]:ARG:HD2	2.54	0.42
1:7:379:THR:HG22	1:7:380:LEU:N	2.34	0.42
1:B:565:ILE:HG23	1:B:565:ILE:HD12	1.77	0.42
1:C:562:GLU:OE2	1:C:612:TYR:OH	2.31	0.42
1:D:276:SER:HB2	1:x:437:LEU:HD11	2.01	0.42
1:E:631:SER:HB2	2:E:901:D5M:N7	2.34	0.42
1:I:631:SER:HB2	2:I:901:D5M:N7	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:477:TRP:HH2	1:P:630:PRO:O	2.02	0.42
1:L:431:ASP:OD2	1:r:513:ARG:HD2	2.19	0.42
1:M:477:TRP:HH2	1:T:630:PRO:O	2.01	0.42
1:M:631:SER:HB2	2:M:901:D5M:N7	2.34	0.42
1:R:631:SER:HB2	2:R:901:D5M:N7	2.34	0.42
1:S:502:TRP:CZ2	1:z:471:ARG:HD2	2.54	0.42
1:S:564:GLU:H	1:S:564:GLU:CD	2.26	0.42
1:a:431:ASP:OD2	1:e:513:ARG:HD2	2.19	0.42
1:b:630:PRO:O	1:d:477:TRP:HH2	2.01	0.42
1:b:631:SER:HB2	2:b:901:D5M:N7	2.34	0.42
1:i:379:THR:HG22	1:i:380:LEU:N	2.34	0.42
1:i:429:SER:OG	1:i:431:ASP:OD1	2.28	0.42
1:i:564:GLU:H	1:i:564:GLU:CD	2.26	0.42
1:i:689:GLU:OE1	1:i:689:GLU:N	2.51	0.42
1:l:448:THR:HG21	1:u:500:TYR:CZ	2.53	0.42
1:m:435:ASN:HB2	1:5:353:VAL:CG1	2.49	0.42
1:m:631:SER:HB2	2:m:901:D5M:N7	2.34	0.42
1:o:666:PHE:HZ	1:5:371:MET:HG3	1.84	0.42
1:q:345:ASP:O	1:q:346:SER:OG	2.32	0.42
1:q:631:SER:HB2	2:q:901:D5M:N7	2.34	0.42
1:q:646:ILE:C	1:q:647:LEU:HD12	2.44	0.42
1:u:631:SER:HB2	2:u:901:D5M:N7	2.34	0.42
1:y:564:GLU:H	1:y:564:GLU:CD	2.26	0.42
1:2:379:THR:HG22	1:2:380:LEU:N	2.34	0.42
1:6:371:MET:HG3	1:8:666:PHE:HZ	1.84	0.42
1:D:325:GLN:HA	1:D:330:THR:HG22	1.99	0.42
1:F:564:GLU:H	1:F:564:GLU:CD	2.26	0.42
1:F:646:ILE:C	1:F:647:LEU:HD12	2.45	0.42
1:G:477:TRP:HH2	1:g:630:PRO:O	2.01	0.42
1:G:646:ILE:C	1:G:647:LEU:HD12	2.45	0.42
1:I:605:VAL:HG12	1:6:627:HIS:HB3	2.02	0.42
1:J:565:ILE:HD12	1:J:565:ILE:HG23	1.77	0.42
1:N:379:THR:HG22	1:N:380:LEU:N	2.34	0.42
1:N:689:GLU:OE1	1:N:689:GLU:N	2.51	0.42
1:O:353:VAL:CG1	1:6:435:ASN:HB2	2.50	0.42
1:Q:565:ILE:HD12	1:Q:565:ILE:HG23	1.77	0.42
1:Q:646:ILE:C	1:Q:647:LEU:HD12	2.45	0.42
1:R:276:SER:HB2	1:r:437:LEU:HD11	2.01	0.42
1:R:646:ILE:C	1:R:647:LEU:HD12	2.45	0.42
1:U:429:SER:OG	1:U:431:ASP:OD1	2.28	0.42
1:V:646:ILE:C	1:V:647:LEU:HD12	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:699:GLN:H	1:k:701:THR:HG23	1.83	0.42
1:d:365:PHE:HA	1:d:366:PRO:HD3	1.92	0.42
1:d:631:SER:HB2	2:d:901:D5M:N7	2.34	0.42
1:f:631:SER:HB2	2:f:901:D5M:N7	2.34	0.42
1:h:646:ILE:C	1:h:647:LEU:HD12	2.45	0.42
1:i:513:ARG:HD2	1:p:431:ASP:OD2	2.20	0.42
1:j:666:PHE:HZ	1:y:371:MET:HG3	1.84	0.42
1:k:325:GLN:HA	1:k:330:THR:HG22	1.99	0.42
1:m:234:TRP:HB3	1:m:298[A]:ARG:CZ	2.49	0.42
1:m:605:VAL:HG12	1:5:627:HIS:HB3	2.01	0.42
1:n:379:THR:HG22	1:n:380:LEU:N	2.34	0.42
1:n:631:SER:HB2	2:n:901:D5M:N7	2.34	0.42
1:o:371:MET:HG3	1:s:666:PHE:HZ	1.85	0.42
1:t:371:MET:HG3	1:1:666:PHE:HZ	1.84	0.42
1:x:646:ILE:C	1:x:647:LEU:HD12	2.45	0.42
1:y:646:ILE:C	1:y:647:LEU:HD12	2.45	0.42
1:8:234:TRP:CD1	1:8:298[B]:ARG:HD2	2.54	0.42
1:A:646:ILE:C	1:A:647:LEU:HD12	2.45	0.42
1:B:564:GLU:H	1:B:564:GLU:CD	2.26	0.42
1:E:605:VAL:HG12	1:p:627:HIS:HB3	2.02	0.42
1:J:631:SER:HB2	2:J:901:D5M:N7	2.34	0.42
1:K:646:ILE:C	1:K:647:LEU:HD12	2.45	0.42
1:L:630:PRO:O	1:R:477:TRP:HH2	2.02	0.42
1:M:646:ILE:C	1:M:647:LEU:HD12	2.45	0.42
1:N:467:ALA:O	1:N:470:ILE:HG12	2.20	0.42
1:N:564:GLU:H	1:N:564:GLU:CD	2.26	0.42
1:N:630:PRO:O	1:V:477:TRP:HH2	2.02	0.42
1:O:565:ILE:HD12	1:O:565:ILE:HG23	1.77	0.42
1:S:448:THR:HG21	1:q:500:TYR:CZ	2.53	0.42
1:T:564:GLU:H	1:T:564:GLU:CD	2.26	0.42
1:X:467:ALA:O	1:X:470:ILE:HG12	2.20	0.42
1:Y:471:ARG:HD2	1:t:502:TRP:CZ2	2.55	0.42
1:Z:646:ILE:C	1:Z:647:LEU:HD12	2.45	0.42
1:d:379:THR:HG22	1:d:380:LEU:N	2.34	0.42
1:d:502:TRP:CZ2	1:v:471:ARG:HD2	2.54	0.42
1:e:467:ALA:O	1:e:470:ILE:HG12	2.20	0.42
1:i:467:ALA:O	1:i:470:ILE:HG12	2.20	0.42
1:j:379:THR:HG22	1:j:380:LEU:N	2.34	0.42
1:j:699:GLN:H	1:5:701:THR:HG23	1.85	0.42
1:k:379:THR:HG22	1:k:380:LEU:N	2.34	0.42
1:m:448:THR:HG21	1:5:500:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:467:ALA:O	1:o:470:ILE:HG12	2.20	0.42
1:o:699:GLN:H	1:1:701:THR:HG23	1.83	0.42
1:s:502:TRP:CZ2	1:1:471:ARG:HD2	2.55	0.42
1:t:646:ILE:C	1:t:647:LEU:HD12	2.45	0.42
1:w:631:SER:HB2	2:w:901:D5M:N7	2.34	0.42
1:4:646:ILE:C	1:4:647:LEU:HD12	2.45	0.42
1:5:345:ASP:O	1:5:346:SER:OG	2.32	0.42
1:8:646:ILE:C	1:8:647:LEU:HD12	2.45	0.42
1:D:631:SER:HB2	2:D:901:D5M:N7	2.34	0.42
1:E:365:PHE:HA	1:E:366:PRO:HD3	1.92	0.42
1:H:631:SER:HB2	2:H:901:D5M:N7	2.34	0.42
1:I:431:ASP:OD2	1:6:513:ARG:HD2	2.20	0.42
1:I:542:PHE:O	1:I:558:MET:N	2.29	0.42
1:M:234:TRP:CE2	1:M:298[A]:ARG:HD3	2.53	0.42
1:N:666:PHE:HZ	1:n:371:MET:HG3	1.85	0.42
1:O:365:PHE:HA	1:O:366:PRO:HD3	1.92	0.42
1:W:353:VAL:CG1	1:u:435:ASN:HB2	2.50	0.42
1:Z:276:SER:HB2	1:k:437:LEU:HD11	2.01	0.42
1:a:379:THR:HG22	1:a:380:LEU:N	2.34	0.42
1:c:467:ALA:O	1:c:470:ILE:HG12	2.20	0.42
1:d:666:PHE:HZ	1:m:371:MET:HG3	1.85	0.42
1:g:565:ILE:HG23	1:g:565:ILE:HD12	1.77	0.42
1:h:471:ARG:HD2	1:m:502:TRP:CZ2	2.55	0.42
1:i:298[A]:ARG:HG2	1:i:298[A]:ARG:HH21	1.84	0.42
1:j:234:TRP:CE2	1:j:298[B]:ARG:HD2	2.54	0.42
1:j:605:VAL:HG12	1:o:627:HIS:HB3	2.01	0.42
1:m:564:GLU:H	1:m:564:GLU:CD	2.26	0.42
1:o:471:ARG:HD2	1:4:502:TRP:CZ2	2.55	0.42
1:p:646:ILE:C	1:p:647:LEU:HD12	2.45	0.42
1:q:467:ALA:O	1:q:470:ILE:HG12	2.20	0.42
1:s:631:SER:HB2	2:s:901:D5M:N7	2.34	0.42
1:v:646:ILE:C	1:v:647:LEU:HD12	2.45	0.42
1:1:345:ASP:O	1:1:346:SER:OG	2.32	0.42
1:1:646:ILE:C	1:1:647:LEU:HD12	2.45	0.42
1:3:298[A]:ARG:HH21	1:3:298[A]:ARG:CG	2.19	0.42
1:3:379:THR:HG22	1:3:380:LEU:N	2.34	0.42
1:6:467:ALA:O	1:6:470:ILE:HG12	2.20	0.42
1:6:631:SER:HB2	2:6:901:D5M:N7	2.34	0.42
1:A:467:ALA:O	1:A:470:ILE:HG12	2.20	0.42
1:B:276:SER:HB2	1:2:437:LEU:HD11	2.01	0.42
1:B:646:ILE:C	1:B:647:LEU:HD12	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:ILE:C	1:C:647:LEU:HD12	2.45	0.42
1:D:448:THR:HG21	1:8:500:TYR:CZ	2.53	0.42
1:I:701:THR:HG23	1:c:699:GLN:H	1.85	0.42
1:J:666:PHE:HZ	1:8:371:MET:HG3	1.84	0.42
1:N:429:SER:OG	1:N:431:ASP:OD1	2.28	0.42
1:N:435:ASN:HB2	1:w:353:VAL:CG1	2.49	0.42
1:P:379:THR:HG22	1:P:380:LEU:N	2.34	0.42
1:R:467:ALA:O	1:R:470:ILE:HG12	2.20	0.42
1:T:467:ALA:O	1:T:470:ILE:HG12	2.20	0.42
1:U:234:TRP:CH2	1:U:298[A]:ARG:HB3	2.54	0.42
1:U:631:SER:HB2	2:U:901:D5M:N7	2.34	0.42
1:W:467:ALA:O	1:W:470:ILE:HG12	2.20	0.42
1:W:631:SER:HB2	2:W:901:D5M:N7	2.34	0.42
1:Y:701:THR:HG23	1:7:699:GLN:H	1.85	0.42
1:c:379:THR:HG22	1:c:380:LEU:N	2.34	0.42
1:c:646:ILE:C	1:c:647:LEU:HD12	2.45	0.42
1:e:379:THR:HG22	1:e:380:LEU:N	2.34	0.42
1:e:646:ILE:C	1:e:647:LEU:HD12	2.45	0.42
1:e:666:PHE:HZ	1:g:371:MET:HG3	1.84	0.42
1:g:646:ILE:C	1:g:647:LEU:HD12	2.45	0.42
1:k:631:SER:HB2	2:k:901:D5M:N7	2.34	0.42
1:l:365:PHE:HA	1:l:366:PRO:HD3	1.92	0.42
1:p:631:SER:HB2	2:p:901:D5M:N7	2.34	0.42
1:q:471:ARG:HD2	1:z:502:TRP:CZ2	2.55	0.42
1:t:467:ALA:O	1:t:470:ILE:HG12	2.20	0.42
1:v:467:ALA:O	1:v:470:ILE:HG12	2.20	0.42
1:w:646:ILE:C	1:w:647:LEU:HD12	2.45	0.42
1:1:564:GLU:H	1:1:564:GLU:CD	2.26	0.42
1:2:565:ILE:HD12	1:2:565:ILE:HG23	1.77	0.42
1:2:631:SER:HB2	2:2:901:D5M:N7	2.34	0.42
1:5:631:SER:HB2	2:5:901:D5M:N7	2.34	0.42
1:6:646:ILE:C	1:6:647:LEU:HD12	2.45	0.42
1:7:467:ALA:O	1:7:470:ILE:HG12	2.20	0.42
1:A:630:PRO:O	1:f:477:TRP:HH2	2.01	0.42
1:C:564:GLU:H	1:C:564:GLU:CD	2.26	0.42
1:E:431:ASP:OD2	1:p:513:ARG:HD2	2.20	0.42
1:E:646:ILE:C	1:E:647:LEU:HD12	2.45	0.42
1:F:489:SER:HB2	1:F:532:LYS:HG2	2.02	0.42
1:G:467:ALA:O	1:G:470:ILE:HG12	2.20	0.42
1:G:471:ARG:HD2	1:g:502:TRP:CZ2	2.54	0.42
1:H:379:THR:HG22	1:H:380:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:467:ALA:O	1:I:470:ILE:HG12	2.20	0.42
1:I:489:SER:HB2	1:I:532:LYS:HG2	2.02	0.42
1:O:345:ASP:O	1:O:346:SER:OG	2.32	0.42
1:Q:431:ASP:OD2	1:k:513:ARG:HD2	2.20	0.42
1:S:646:ILE:C	1:S:647:LEU:HD12	2.45	0.42
1:T:565:ILE:HG23	1:T:565:ILE:HD12	1.77	0.42
1:U:467:ALA:O	1:U:470:ILE:HG12	2.20	0.42
1:U:563:GLU:O	1:U:565:ILE:N	2.53	0.42
1:V:353:VAL:CG1	1:w:435:ASN:HB2	2.49	0.42
1:W:471:ARG:HD2	1:l:502:TRP:CZ2	2.55	0.42
1:W:646:ILE:C	1:W:647:LEU:HD12	2.45	0.42
1:Y:467:ALA:O	1:Y:470:ILE:HG12	2.20	0.42
1:d:513:ARG:HD2	1:v:431:ASP:OD2	2.19	0.42
1:g:431:ASP:OD2	1:7:513:ARG:HD2	2.20	0.42
1:g:467:ALA:O	1:g:470:ILE:HG12	2.20	0.42
1:h:502:TRP:CZ2	1:5:471:ARG:HD2	2.55	0.42
1:h:605:VAL:HG12	1:m:627:HIS:HB3	2.02	0.42
1:h:627:HIS:HB3	1:5:605:VAL:HG12	2.01	0.42
1:i:276:SER:HB2	1:p:437:LEU:HD11	2.01	0.42
1:l:631:SER:HB2	2:l:901:D5M:N7	2.34	0.42
1:m:247:TRP:O	1:m:675:THR:OG1	2.17	0.42
1:m:467:ALA:O	1:m:470:ILE:HG12	2.20	0.42
1:n:365:PHE:HA	1:n:366:PRO:HD3	1.92	0.42
1:o:489:SER:HB2	1:o:532:LYS:HG2	2.02	0.42
1:r:646:ILE:C	1:r:647:LEU:HD12	2.45	0.42
1:u:467:ALA:O	1:u:470:ILE:HG12	2.20	0.42
1:u:535:PRO:HB2	1:u:538:GLY:HA3	2.02	0.42
1:w:565:ILE:HG23	1:w:565:ILE:HD12	1.77	0.42
1:y:489:SER:HB2	1:y:532:LYS:HG2	2.02	0.42
1:z:646:ILE:C	1:z:647:LEU:HD12	2.45	0.42
1:4:234:TRP:HB3	1:4:298[A]:ARG:CZ	2.49	0.42
1:5:379:THR:HG22	1:5:380:LEU:N	2.34	0.42
1:5:467:ALA:O	1:5:470:ILE:HG12	2.20	0.42
1:A:477:TRP:HH2	1:n:630:PRO:O	2.02	0.42
1:C:467:ALA:O	1:C:470:ILE:HG12	2.20	0.42
1:E:565:ILE:HG23	1:E:565:ILE:HD12	1.77	0.42
1:F:535:PRO:HB2	1:F:538:GLY:HA3	2.02	0.42
1:H:467:ALA:O	1:H:470:ILE:HG12	2.20	0.42
1:I:471:ARG:HD2	1:6:502:TRP:CZ2	2.54	0.42
1:I:535:PRO:HB2	1:I:538:GLY:HA3	2.02	0.42
1:L:605:VAL:HG12	1:r:627:HIS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:646:ILE:C	1:L:647:LEU:HD12	2.45	0.42
1:M:467:ALA:O	1:M:470:ILE:HG12	2.20	0.42
1:N:646:ILE:C	1:N:647:LEU:HD12	2.45	0.42
1:N:701:THR:HG23	1:i:699:GLN:H	1.85	0.42
1:O:563:GLU:O	1:O:565:ILE:N	2.53	0.42
1:O:631:SER:HB2	2:O:901:D5M:N7	2.34	0.42
1:R:479:PRO:O	1:R:604:MET:HG3	2.20	0.42
1:S:353:VAL:CG1	1:z:435:ASN:HB2	2.50	0.42
1:T:563:GLU:O	1:T:565:ILE:N	2.53	0.42
1:V:631:SER:HB2	2:V:901:D5M:N7	2.34	0.42
1:a:471:ARG:HD2	1:e:502:TRP:CZ2	2.54	0.42
1:c:564:GLU:H	1:c:564:GLU:CD	2.26	0.42
1:e:564:GLU:H	1:e:564:GLU:CD	2.26	0.42
1:g:564:GLU:H	1:g:564:GLU:CD	2.26	0.42
1:h:467:ALA:O	1:h:470:ILE:HG12	2.20	0.42
1:l:563:GLU:O	1:l:565:ILE:N	2.53	0.42
1:l:701:THR:HG23	1:z:699:GLN:H	1.84	0.42
1:m:666:PHE:HZ	1:q:371:MET:HG3	1.84	0.42
1:q:479:PRO:O	1:q:604:MET:HG3	2.20	0.42
1:r:479:PRO:O	1:r:604:MET:HG3	2.20	0.42
1:s:467:ALA:O	1:s:470:ILE:HG12	2.20	0.42
1:s:563:GLU:O	1:s:565:ILE:N	2.53	0.42
1:u:479:PRO:O	1:u:604:MET:HG3	2.20	0.42
1:u:489:SER:HB2	1:u:532:LYS:HG2	2.02	0.42
1:v:379:THR:HG22	1:v:380:LEU:N	2.34	0.42
1:w:535:PRO:HB2	1:w:538:GLY:HA3	2.02	0.42
1:x:479:PRO:O	1:x:604:MET:HG3	2.20	0.42
1:y:535:PRO:HB2	1:y:538:GLY:HA3	2.02	0.42
1:y:563:GLU:O	1:y:565:ILE:N	2.53	0.42
1:1:379:THR:HG22	1:1:380:LEU:N	2.34	0.42
1:1:631:SER:HB2	2:1:901:D5M:N7	2.34	0.42
1:3:564:GLU:H	1:3:564:GLU:CD	2.26	0.42
1:8:479:PRO:O	1:8:604:MET:HG3	2.20	0.42
1:A:379:THR:HG22	1:A:380:LEU:N	2.34	0.42
1:B:379:THR:HG22	1:B:380:LEU:N	2.34	0.42
1:D:563:GLU:O	1:D:565:ILE:N	2.53	0.42
1:D:666:PHE:HZ	1:b:371:MET:HG3	1.85	0.42
1:E:276:SER:HB2	1:i:437:LEU:HD11	2.01	0.42
1:E:535:PRO:HB2	1:E:538:GLY:HA3	2.02	0.42
1:E:699:GLN:H	1:r:701:THR:HG23	1.85	0.42
1:F:563:GLU:O	1:F:565:ILE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:631:SER:HB2	2:F:901:D5M:N7	2.34	0.42
1:J:365:PHE:HA	1:J:366:PRO:HD3	1.92	0.42
1:J:435:ASN:HB2	1:1:353:VAL:CG1	2.50	0.42
1:L:489:SER:HB2	1:L:532:LYS:HG2	2.02	0.42
1:M:701:THR:HG23	1:R:699:GLN:H	1.85	0.42
1:Q:479:PRO:O	1:Q:604:MET:HG3	2.20	0.42
1:S:479:PRO:O	1:S:604:MET:HG3	2.20	0.42
1:T:479:PRO:O	1:T:604:MET:HG3	2.20	0.42
1:U:379:THR:HG22	1:U:380:LEU:N	2.34	0.42
1:W:379:THR:HG22	1:W:380:LEU:N	2.34	0.42
1:X:479:PRO:O	1:X:604:MET:HG3	2.20	0.42
1:Y:435:ASN:HB2	1:t:353:VAL:CG1	2.49	0.42
1:Y:666:PHE:HZ	1:3:371:MET:HG3	1.85	0.42
1:Z:563:GLU:O	1:Z:565:ILE:N	2.53	0.42
1:a:276:SER:HB2	1:y:437:LEU:HD11	2.02	0.42
1:a:502:TRP:CZ2	1:y:471:ARG:HD2	2.54	0.42
1:a:564:GLU:H	1:a:564:GLU:CD	2.26	0.42
1:a:699:GLN:H	1:g:701:THR:HG23	1.83	0.42
1:b:502:TRP:CZ2	1:d:471:ARG:HD2	2.55	0.42
1:c:479:PRO:O	1:c:604:MET:HG3	2.20	0.42
1:e:479:PRO:O	1:e:604:MET:HG3	2.20	0.42
1:g:666:PHE:HZ	1:2:371:MET:HG3	1.85	0.42
1:h:563:GLU:O	1:h:565:ILE:N	2.53	0.42
1:i:627:HIS:HB3	1:p:605:VAL:HG12	2.02	0.42
1:k:563:GLU:O	1:k:565:ILE:N	2.53	0.42
1:l:345:ASP:O	1:l:346:SER:OG	2.32	0.42
1:l:479:PRO:O	1:l:604:MET:HG3	2.20	0.42
1:l:605:VAL:HG12	1:u:627:HIS:HB3	2.01	0.42
1:m:471:ARG:HD2	1:5:502:TRP:CZ2	2.55	0.42
1:m:563:GLU:O	1:m:565:ILE:N	2.53	0.42
1:m:646:ILE:C	1:m:647:LEU:HD12	2.45	0.42
1:p:565:ILE:HD12	1:p:565:ILE:HG23	1.77	0.42
1:u:371:MET:HG3	1:y:666:PHE:HZ	1.84	0.42
1:w:479:PRO:O	1:w:604:MET:HG3	2.20	0.42
1:8:467:ALA:O	1:8:470:ILE:HG12	2.20	0.42
1:8:563:GLU:O	1:8:565:ILE:N	2.53	0.42
1:A:362:LEU:HD23	1:A:370:PHE:CZ	2.55	0.42
1:B:467:ALA:O	1:B:470:ILE:HG12	2.20	0.42
1:B:631:SER:HB2	2:B:901:D5M:N7	2.34	0.42
1:D:431:ASP:OD2	1:8:513:ARG:HD2	2.20	0.42
1:E:345:ASP:C	1:E:347:GLU:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:PRO:O	1:E:604:MET:HG3	2.20	0.42
1:G:379:THR:HG22	1:G:380:LEU:N	2.34	0.42
1:G:431:ASP:OD2	1:g:513:ARG:HD2	2.20	0.42
1:G:699:GLN:H	1:2:701:THR:HG23	1.85	0.42
1:I:362:LEU:HD23	1:I:370:PHE:CZ	2.55	0.42
1:I:479:PRO:O	1:I:604:MET:HG3	2.20	0.42
1:K:345:ASP:C	1:K:347:GLU:H	2.28	0.42
1:K:479:PRO:O	1:K:604:MET:HG3	2.20	0.42
1:M:563:GLU:O	1:M:565:ILE:N	2.53	0.42
1:O:479:PRO:O	1:O:604:MET:HG3	2.20	0.42
1:P:467:ALA:O	1:P:470:ILE:HG12	2.20	0.42
1:P:563:GLU:O	1:P:565:ILE:N	2.53	0.42
1:Q:489:SER:HB2	1:Q:532:LYS:HG2	2.02	0.42
1:S:435:ASN:HB2	1:q:353:VAL:CG1	2.50	0.42
1:T:646:ILE:C	1:T:647:LEU:HD12	2.45	0.42
1:U:362:LEU:HD23	1:U:370:PHE:CZ	2.55	0.42
1:V:362:LEU:HD23	1:V:370:PHE:CZ	2.55	0.42
1:V:699:GLN:H	1:n:701:THR:HG23	1.85	0.42
1:W:605:VAL:HG12	1:l:627:HIS:HB3	2.02	0.42
1:X:489:SER:HB2	1:X:532:LYS:HG2	2.02	0.42
1:Y:345:ASP:C	1:Y:347:GLU:H	2.28	0.42
1:Y:563:GLU:O	1:Y:565:ILE:N	2.53	0.42
1:Z:353:VAL:CG1	1:k:435:ASN:HB2	2.50	0.42
1:Z:467:ALA:O	1:Z:470:ILE:HG12	2.20	0.42
1:Z:479:PRO:O	1:Z:604:MET:HG3	2.20	0.42
1:a:605:VAL:HG12	1:e:627:HIS:HB3	2.02	0.42
1:a:627:HIS:HB3	1:y:605:VAL:HG12	2.02	0.42
1:a:666:PHE:HZ	1:4:371:MET:HG3	1.85	0.42
1:b:513:ARG:HD2	1:d:431:ASP:OD2	2.19	0.42
1:b:646:ILE:C	1:b:647:LEU:HD12	2.45	0.42
1:b:701:THR:HG23	1:x:699:GLN:H	1.85	0.42
1:f:563:GLU:O	1:f:565:ILE:N	2.53	0.42
1:f:646:ILE:C	1:f:647:LEU:HD12	2.45	0.42
1:i:646:ILE:C	1:i:647:LEU:HD12	2.45	0.42
1:j:563:GLU:O	1:j:565:ILE:N	2.53	0.42
1:k:371:MET:HG3	1:l:666:PHE:HZ	1.84	0.42
1:l:435:ASN:HB2	1:u:353:VAL:CG1	2.48	0.42
1:m:479:PRO:O	1:m:604:MET:HG3	2.20	0.42
1:o:479:PRO:O	1:o:604:MET:HG3	2.20	0.42
1:p:362:LEU:HD23	1:p:370:PHE:CZ	2.55	0.42
1:q:437:LEU:HD11	1:z:276:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:345:ASP:C	1:s:347:GLU:H	2.28	0.42
1:s:362:LEU:HD23	1:s:370:PHE:CZ	2.55	0.42
1:s:379:THR:HG22	1:s:380:LEU:N	2.34	0.42
1:t:479:PRO:O	1:t:604:MET:HG3	2.20	0.42
1:u:362:LEU:HD23	1:u:370:PHE:CZ	2.55	0.42
1:u:542:PHE:O	1:u:558:MET:N	2.29	0.42
1:v:362:LEU:HD23	1:v:370:PHE:CZ	2.55	0.42
1:w:365:PHE:HA	1:w:366:PRO:HD3	1.92	0.42
1:x:362:LEU:HD23	1:x:370:PHE:CZ	2.55	0.42
1:x:467:ALA:O	1:x:470:ILE:HG12	2.20	0.42
1:x:489:SER:HB2	1:x:532:LYS:HG2	2.02	0.42
1:1:298[A]:ARG:HH21	1:1:298[A]:ARG:HG2	1.85	0.42
1:1:467:ALA:O	1:1:470:ILE:HG12	2.20	0.42
1:3:646:ILE:C	1:3:647:LEU:HD12	2.45	0.42
1:5:362:LEU:HD23	1:5:370:PHE:CZ	2.55	0.42
1:6:379:THR:HG22	1:6:380:LEU:N	2.34	0.42
1:6:535:PRO:HB2	1:6:538:GLY:HA3	2.02	0.42
1:7:563:GLU:O	1:7:565:ILE:N	2.53	0.42
1:8:362:LEU:HD23	1:8:370:PHE:CZ	2.55	0.42
1:C:276:SER:HB2	1:t:437:LEU:HD11	2.02	0.41
1:C:563:GLU:O	1:C:565:ILE:N	2.53	0.41
1:D:471:ARG:HD2	1:8:502:TRP:CZ2	2.55	0.41
1:F:467:ALA:O	1:F:470:ILE:HG12	2.20	0.41
1:G:362:LEU:HD23	1:G:370:PHE:CZ	2.55	0.41
1:G:479:PRO:O	1:G:604:MET:HG3	2.20	0.41
1:H:362:LEU:HD23	1:H:370:PHE:CZ	2.55	0.41
1:H:646:ILE:C	1:H:647:LEU:HD12	2.45	0.41
1:K:362:LEU:HD23	1:K:370:PHE:CZ	2.55	0.41
1:K:379:THR:HG22	1:K:380:LEU:N	2.34	0.41
1:L:467:ALA:O	1:L:470:ILE:HG12	2.20	0.41
1:M:362:LEU:HD23	1:M:370:PHE:CZ	2.55	0.41
1:N:471:ARG:HD2	1:w:502:TRP:CZ2	2.55	0.41
1:N:605:VAL:HG12	1:w:627:HIS:HB3	2.01	0.41
1:P:646:ILE:C	1:P:647:LEU:HD12	2.45	0.41
1:Q:362:LEU:HD23	1:Q:370:PHE:CZ	2.55	0.41
1:Q:467:ALA:O	1:Q:470:ILE:HG12	2.20	0.41
1:Q:605:VAL:HG12	1:k:627:HIS:HB3	2.02	0.41
1:Q:631:SER:HB2	2:Q:901:D5M:N7	2.34	0.41
1:U:345:ASP:C	1:U:347:GLU:H	2.28	0.41
1:W:489:SER:HB2	1:W:532:LYS:HG2	2.02	0.41
1:W:535:PRO:HB2	1:W:538:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:646:ILE:C	1:X:647:LEU:HD12	2.45	0.41
1:Z:362:LEU:HD23	1:Z:370:PHE:CZ	2.55	0.41
1:a:646:ILE:C	1:a:647:LEU:HD12	2.45	0.41
1:b:362:LEU:HD23	1:b:370:PHE:CZ	2.55	0.41
1:b:542:PHE:O	1:b:558:MET:N	2.29	0.41
1:e:471:ARG:HD2	1:y:502:TRP:CZ2	2.55	0.41
1:f:362:LEU:HD23	1:f:370:PHE:CZ	2.55	0.41
1:g:563:GLU:O	1:g:565:ILE:N	2.53	0.41
1:h:362:LEU:HD23	1:h:370:PHE:CZ	2.55	0.41
1:i:563:GLU:O	1:i:565:ILE:N	2.53	0.41
1:j:471:ARG:HD2	1:o:502:TRP:CZ2	2.55	0.41
1:j:646:ILE:C	1:j:647:LEU:HD12	2.45	0.41
1:l:234:TRP:CD1	1:l:298[B]:ARG:HD2	2.55	0.41
1:l:565:ILE:HD12	1:l:565:ILE:HG23	1.77	0.41
1:p:563:GLU:O	1:p:565:ILE:N	2.53	0.41
1:q:362:LEU:HD23	1:q:370:PHE:CZ	2.55	0.41
1:s:646:ILE:C	1:s:647:LEU:HD12	2.45	0.41
1:t:489:SER:HB2	1:t:532:LYS:HG2	2.02	0.41
1:w:345:ASP:C	1:w:347:GLU:H	2.28	0.41
1:y:631:SER:HB2	2:y:901:D5M:N7	2.34	0.41
1:z:489:SER:HB2	1:z:532:LYS:HG2	2.02	0.41
1:z:563:GLU:O	1:z:565:ILE:N	2.53	0.41
1:3:467:ALA:O	1:3:470:ILE:HG12	2.20	0.41
1:4:345:ASP:C	1:4:347:GLU:H	2.28	0.41
1:4:479:PRO:O	1:4:604:MET:HG3	2.20	0.41
1:4:535:PRO:HB2	1:4:538:GLY:HA3	2.02	0.41
1:5:646:ILE:C	1:5:647:LEU:HD12	2.45	0.41
1:6:298[A]:ARG:HH21	1:6:298[A]:ARG:CG	2.28	0.41
1:7:345:ASP:C	1:7:347:GLU:H	2.28	0.41
1:7:489:SER:HB2	1:7:532:LYS:HG2	2.02	0.41
1:7:564:GLU:H	1:7:564:GLU:CD	2.26	0.41
1:A:479:PRO:O	1:A:604:MET:HG3	2.20	0.41
1:A:535:PRO:HB2	1:A:538:GLY:HA3	2.02	0.41
1:A:563:GLU:O	1:A:565:ILE:N	2.53	0.41
1:C:666:PHE:HZ	1:J:371:MET:HG3	1.85	0.41
1:C:699:GLN:H	1:3:701:THR:HG23	1.84	0.41
1:D:345:ASP:C	1:D:347:GLU:H	2.28	0.41
1:G:435:ASN:HB2	1:g:353:VAL:CG1	2.51	0.41
1:G:563:GLU:O	1:G:565:ILE:N	2.53	0.41
1:G:631:SER:HB2	2:G:901:D5M:N7	2.34	0.41
1:I:365:PHE:HA	1:I:366:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:471:ARG:HD2	1:I:502:TRP:CZ2	2.55	0.41
1:L:345:ASP:C	1:L:347:GLU:H	2.28	0.41
1:L:563:GLU:O	1:L:565:ILE:N	2.53	0.41
1:M:489:SER:HB2	1:M:532:LYS:HG2	2.02	0.41
1:N:479:PRO:O	1:N:604:MET:HG3	2.20	0.41
1:N:563:GLU:O	1:N:565:ILE:N	2.53	0.41
1:Q:379:THR:HG22	1:Q:380:LEU:N	2.34	0.41
1:R:362:LEU:HD23	1:R:370:PHE:CZ	2.55	0.41
1:S:489:SER:HB2	1:S:532:LYS:HG2	2.02	0.41
1:T:345:ASP:C	1:T:347:GLU:H	2.28	0.41
1:U:646:ILE:C	1:U:647:LEU:HD12	2.45	0.41
1:V:563:GLU:O	1:V:565:ILE:N	2.53	0.41
1:W:435:ASN:HB2	1:I:353:VAL:CG1	2.51	0.41
1:W:485:GLN:NE2	1:W:506:THR:HG21	2.36	0.41
1:Y:485:GLN:NE2	1:Y:506:THR:HG21	2.36	0.41
1:Y:489:SER:HB2	1:Y:532:LYS:HG2	2.02	0.41
1:a:467:ALA:O	1:a:470:ILE:HG12	2.20	0.41
1:a:563:GLU:O	1:a:565:ILE:N	2.53	0.41
1:b:435:ASN:HB2	1:v:353:VAL:CG1	2.48	0.41
1:b:563:GLU:O	1:b:565:ILE:N	2.53	0.41
1:d:627:HIS:HB3	1:v:605:VAL:HG12	2.02	0.41
1:e:699:GLN:H	1:u:701:THR:HG23	1.85	0.41
1:e:701:THR:HG23	1:u:699:GLN:H	1.85	0.41
1:h:431:ASP:OD2	1:m:513:ARG:HD2	2.20	0.41
1:h:489:SER:HB2	1:h:532:LYS:HG2	2.02	0.41
1:i:489:SER:HB2	1:i:532:LYS:HG2	2.02	0.41
1:i:535:PRO:HB2	1:i:538:GLY:HA3	2.02	0.41
1:j:362:LEU:HD23	1:j:370:PHE:CZ	2.55	0.41
1:j:467:ALA:O	1:j:470:ILE:HG12	2.20	0.41
1:k:345:ASP:C	1:k:347:GLU:H	2.28	0.41
1:l:471:ARG:HD2	1:u:502:TRP:CZ2	2.55	0.41
1:n:489:SER:HB2	1:n:532:LYS:HG2	2.02	0.41
1:o:605:VAL:HG12	1:4:627:HIS:HB3	2.02	0.41
1:o:646:ILE:C	1:o:647:LEU:HD12	2.45	0.41
1:r:467:ALA:O	1:r:470:ILE:HG12	2.20	0.41
1:t:379:THR:HG22	1:t:380:LEU:N	2.34	0.41
1:t:563:GLU:O	1:t:565:ILE:N	2.53	0.41
1:u:563:GLU:O	1:u:565:ILE:N	2.53	0.41
1:v:479:PRO:O	1:v:604:MET:HG3	2.20	0.41
1:v:563:GLU:O	1:v:565:ILE:N	2.53	0.41
1:w:489:SER:HB2	1:w:532:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:467:ALA:O	1:y:470:ILE:HG12	2.20	0.41
1:z:345:ASP:C	1:z:347:GLU:H	2.28	0.41
1:z:467:ALA:O	1:z:470:ILE:HG12	2.20	0.41
1:2:467:ALA:O	1:2:470:ILE:HG12	2.20	0.41
1:3:362:LEU:HD23	1:3:370:PHE:CZ	2.55	0.41
1:3:563:GLU:O	1:3:565:ILE:N	2.53	0.41
1:3:631:SER:HB2	2:3:901:D5M:N7	2.34	0.41
1:4:362:LEU:HD23	1:4:370:PHE:CZ	2.55	0.41
1:4:379:THR:HG22	1:4:380:LEU:N	2.34	0.41
1:5:565:ILE:HG23	1:5:565:ILE:HD12	1.77	0.41
1:7:565:ILE:HD12	1:7:565:ILE:HG23	1.77	0.41
1:7:646:ILE:C	1:7:647:LEU:HD12	2.45	0.41
1:8:489:SER:HB2	1:8:532:LYS:HG2	2.02	0.41
1:B:563:GLU:O	1:B:565:ILE:N	2.53	0.41
1:C:345:ASP:C	1:C:347:GLU:H	2.28	0.41
1:C:489:SER:HB2	1:C:532:LYS:HG2	2.02	0.41
1:D:479:PRO:O	1:D:604:MET:HG3	2.20	0.41
1:E:489:SER:HB2	1:E:532:LYS:HG2	2.02	0.41
1:F:362:LEU:HD23	1:F:370:PHE:CZ	2.55	0.41
1:F:477:TRP:O	1:F:478:LEU:HD12	2.21	0.41
1:I:563:GLU:O	1:I:565:ILE:N	2.53	0.41
1:J:467:ALA:O	1:J:470:ILE:HG12	2.20	0.41
1:J:489:SER:HB2	1:J:532:LYS:HG2	2.02	0.41
1:J:563:GLU:O	1:J:565:ILE:N	2.53	0.41
1:L:701:THR:HG23	1:O:699:GLN:H	1.85	0.41
1:M:479:PRO:O	1:M:604:MET:HG3	2.20	0.41
1:M:535:PRO:HB2	1:M:538:GLY:HA3	2.02	0.41
1:N:485:GLN:NE2	1:N:506:THR:HG21	2.36	0.41
1:N:535:PRO:HB2	1:N:538:GLY:HA3	2.02	0.41
1:P:362:LEU:HD23	1:P:370:PHE:CZ	2.55	0.41
1:T:247:TRP:O	1:T:675:THR:OG1	2.17	0.41
1:T:362:LEU:HD23	1:T:370:PHE:CZ	2.55	0.41
1:U:666:PHE:HZ	1:X:371:MET:HG3	1.86	0.41
1:V:627:HIS:HB3	1:w:605:VAL:HG12	2.02	0.41
1:W:362:LEU:HD23	1:W:370:PHE:CZ	2.55	0.41
1:Y:298[A]:ARG:HG2	1:Y:298[A]:ARG:NH2	2.24	0.41
1:Y:564:GLU:H	1:Y:564:GLU:CD	2.26	0.41
1:Y:646:ILE:C	1:Y:647:LEU:HD12	2.45	0.41
1:Z:489:SER:HB2	1:Z:532:LYS:HG2	2.02	0.41
1:a:362:LEU:HD23	1:a:370:PHE:CZ	2.55	0.41
1:a:535:PRO:HB2	1:a:538:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:631:SER:HB2	2:a:901:D5M:N7	2.34	0.41
1:b:467:ALA:O	1:b:470:ILE:HG12	2.20	0.41
1:b:489:SER:HB2	1:b:532:LYS:HG2	2.02	0.41
1:c:563:GLU:O	1:c:565:ILE:N	2.53	0.41
1:d:489:SER:HB2	1:d:532:LYS:HG2	2.02	0.41
1:e:631:SER:HB2	2:e:901:D5M:N7	2.34	0.41
1:g:345:ASP:C	1:g:347:GLU:H	2.28	0.41
1:g:489:SER:HB2	1:g:532:LYS:HG2	2.02	0.41
1:g:605:VAL:HG12	1:7:627:HIS:HB3	2.02	0.41
1:i:479:PRO:O	1:i:604:MET:HG3	2.20	0.41
1:i:485:GLN:NE2	1:i:506:THR:HG21	2.36	0.41
1:k:479:PRO:O	1:k:604:MET:HG3	2.20	0.41
1:m:345:ASP:C	1:m:347:GLU:H	2.28	0.41
1:n:467:ALA:O	1:n:470:ILE:HG12	2.20	0.41
1:r:489:SER:HB2	1:r:532:LYS:HG2	2.02	0.41
1:t:362:LEU:HD23	1:t:370:PHE:CZ	2.55	0.41
1:t:631:SER:HB2	2:t:901:D5M:N7	2.34	0.41
1:u:646:ILE:C	1:u:647:LEU:HD12	2.45	0.41
1:v:535:PRO:HB2	1:v:538:GLY:HA3	2.02	0.41
1:x:379:THR:HG22	1:x:380:LEU:N	2.34	0.41
1:x:631:SER:HB2	2:x:901:D5M:N7	2.34	0.41
1:y:477:TRP:O	1:y:478:LEU:HD12	2.21	0.41
1:1:345:ASP:C	1:1:347:GLU:H	2.28	0.41
1:1:563:GLU:O	1:1:565:ILE:N	2.53	0.41
1:2:362:LEU:HD23	1:2:370:PHE:CZ	2.55	0.41
1:2:477:TRP:O	1:2:478:LEU:HD12	2.21	0.41
1:2:489:SER:HB2	1:2:532:LYS:HG2	2.02	0.41
1:2:563:GLU:O	1:2:565:ILE:N	2.53	0.41
1:3:535:PRO:HB2	1:3:538:GLY:HA3	2.02	0.41
1:3:542:PHE:O	1:3:558:MET:N	2.29	0.41
1:4:467:ALA:O	1:4:470:ILE:HG12	2.20	0.41
1:5:345:ASP:C	1:5:347:GLU:H	2.28	0.41
1:5:563:GLU:O	1:5:565:ILE:N	2.53	0.41
1:6:485:GLN:NE2	1:6:506:THR:HG21	2.36	0.41
1:6:489:SER:HB2	1:6:532:LYS:HG2	2.02	0.41
1:7:479:PRO:O	1:7:604:MET:HG3	2.20	0.41
1:7:485:GLN:NE2	1:7:506:THR:HG21	2.36	0.41
1:A:345:ASP:C	1:A:347:GLU:H	2.28	0.41
1:B:345:ASP:C	1:B:347:GLU:H	2.28	0.41
1:F:605:VAL:HG12	1:3:627:HIS:HB3	2.03	0.41
1:G:234:TRP:CG	1:G:298[A]:ARG:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:477:TRP:O	1:G:478:LEU:HD12	2.21	0.41
1:G:485:GLN:NE2	1:G:506:THR:HG21	2.36	0.41
1:G:489:SER:HB2	1:G:532:LYS:HG2	2.02	0.41
1:H:345:ASP:C	1:H:347:GLU:H	2.28	0.41
1:H:479:PRO:O	1:H:604:MET:HG3	2.20	0.41
1:H:565:ILE:HG23	1:H:565:ILE:HD12	1.77	0.41
1:I:435:ASN:HB2	1:6:353:VAL:CG1	2.51	0.41
1:I:646:ILE:C	1:I:647:LEU:HD12	2.45	0.41
1:J:362:LEU:HD23	1:J:370:PHE:CZ	2.55	0.41
1:J:477:TRP:O	1:J:478:LEU:HD12	2.21	0.41
1:K:535:PRO:HB2	1:K:538:GLY:HA3	2.02	0.41
1:K:563:GLU:O	1:K:565:ILE:N	2.53	0.41
1:M:345:ASP:O	1:M:346:SER:OG	2.32	0.41
1:N:362:LEU:HD23	1:N:370:PHE:CZ	2.55	0.41
1:N:489:SER:HB2	1:N:532:LYS:HG2	2.02	0.41
1:O:345:ASP:C	1:O:347:GLU:H	2.28	0.41
1:O:362:LEU:HD23	1:O:370:PHE:CZ	2.55	0.41
1:R:563:GLU:O	1:R:565:ILE:N	2.53	0.41
1:S:467:ALA:O	1:S:470:ILE:HG12	2.20	0.41
1:S:471:ARG:HD2	1:q:502:TRP:CZ2	2.55	0.41
1:U:499:GLU:OE2	1:U:501:SER:OG	2.34	0.41
1:U:605:VAL:HG12	1:2:627:HIS:HB3	2.02	0.41
1:W:345:ASP:C	1:W:347:GLU:H	2.28	0.41
1:W:365:PHE:HA	1:W:366:PRO:HD3	1.92	0.41
1:Y:479:PRO:O	1:Y:604:MET:HG3	2.20	0.41
1:Y:565:ILE:HD12	1:Y:565:ILE:HG23	1.77	0.41
1:Y:605:VAL:HG12	1:t:627:HIS:HB3	2.01	0.41
1:Z:477:TRP:O	1:Z:478:LEU:HD12	2.21	0.41
1:b:471:ARG:HD2	1:v:502:TRP:CZ2	2.55	0.41
1:d:276:SER:HB2	1:v:437:LEU:HD11	2.02	0.41
1:d:345:ASP:C	1:d:347:GLU:H	2.28	0.41
1:d:467:ALA:O	1:d:470:ILE:HG12	2.20	0.41
1:d:479:PRO:O	1:d:604:MET:HG3	2.20	0.41
1:d:563:GLU:O	1:d:565:ILE:N	2.53	0.41
1:f:467:ALA:O	1:f:470:ILE:HG12	2.20	0.41
1:h:479:PRO:O	1:h:604:MET:HG3	2.20	0.41
1:h:513:ARG:HD2	1:5:431:ASP:OD2	2.21	0.41
1:h:535:PRO:HB2	1:h:538:GLY:HA3	2.02	0.41
1:k:362:LEU:HD23	1:k:370:PHE:CZ	2.55	0.41
1:l:345:ASP:C	1:l:347:GLU:H	2.28	0.41
1:l:362:LEU:HD23	1:l:370:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:646:ILE:C	1:l:647:LEU:HD12	2.45	0.41
1:m:362:LEU:HD23	1:m:370:PHE:CZ	2.55	0.41
1:n:563:GLU:O	1:n:565:ILE:N	2.53	0.41
1:p:345:ASP:O	1:p:346:SER:OG	2.32	0.41
1:q:298[A]:ARG:HH21	1:q:298[A]:ARG:HG2	1.85	0.41
1:q:563:GLU:O	1:q:565:ILE:N	2.53	0.41
1:t:477:TRP:O	1:t:478:LEU:HD12	2.21	0.41
1:u:365:PHE:HA	1:u:366:PRO:HD3	1.92	0.41
1:1:477:TRP:O	1:1:478:LEU:HD12	2.21	0.41
1:5:479:PRO:O	1:5:604:MET:HG3	2.20	0.41
1:5:535:PRO:HB2	1:5:538:GLY:HA3	2.02	0.41
1:6:362:LEU:HD23	1:6:370:PHE:CZ	2.55	0.41
1:A:605:VAL:HG12	1:n:627:HIS:HB3	2.03	0.41
1:B:477:TRP:O	1:B:478:LEU:HD12	2.21	0.41
1:B:613:LEU:HB3	1:B:614:GLN:OE1	2.21	0.41
1:C:348:TYR:OH	1:C:642:PRO:O	2.32	0.41
1:D:362:LEU:HD23	1:D:370:PHE:CZ	2.55	0.41
1:D:646:ILE:C	1:D:647:LEU:HD12	2.45	0.41
1:E:563:GLU:O	1:E:565:ILE:N	2.53	0.41
1:F:699:GLN:H	1:K:701:THR:HG23	1.85	0.41
1:G:605:VAL:HG12	1:g:627:HIS:HB3	2.02	0.41
1:H:563:GLU:O	1:H:565:ILE:N	2.53	0.41
1:J:646:ILE:C	1:J:647:LEU:HD12	2.45	0.41
1:K:467:ALA:O	1:K:470:ILE:HG12	2.20	0.41
1:K:613:LEU:HB3	1:K:614:GLN:OE1	2.21	0.41
1:M:429:SER:OG	1:M:431:ASP:OD1	2.28	0.41
1:N:477:TRP:O	1:N:478:LEU:HD12	2.21	0.41
1:O:646:ILE:C	1:O:647:LEU:HD12	2.45	0.41
1:O:733:ARG:HG2	1:O:734:ASN:N	2.36	0.41
1:R:613:LEU:HB3	1:R:614:GLN:OE1	2.21	0.41
1:S:733:ARG:HG2	1:S:734:ASN:N	2.36	0.41
1:T:371:MET:HG3	1:n:666:PHE:HZ	1.86	0.41
1:T:562:GLU:OE2	1:T:612:TYR:OH	2.31	0.41
1:V:345:ASP:O	1:V:346:SER:OG	2.32	0.41
1:V:467:ALA:O	1:V:470:ILE:HG12	2.20	0.41
1:V:477:TRP:O	1:V:478:LEU:HD12	2.21	0.41
1:W:627:HIS:HB3	1:u:605:VAL:HG12	2.03	0.41
1:Z:485:GLN:NE2	1:Z:506:THR:HG21	2.36	0.41
1:b:353:VAL:CG1	1:d:435:ASN:HB2	2.50	0.41
1:b:479:PRO:O	1:b:604:MET:HG3	2.20	0.41
1:b:733:ARG:HG2	1:b:734:ASN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:631:SER:HB2	2:c:901:D5M:N7	2.34	0.41
1:e:563:GLU:O	1:e:565:ILE:N	2.53	0.41
1:f:371:MET:HG3	1:k:666:PHE:HZ	1.86	0.41
1:f:489:SER:HB2	1:f:532:LYS:HG2	2.02	0.41
1:h:485:GLN:NE2	1:h:506:THR:HG21	2.36	0.41
1:i:613:LEU:HB3	1:i:614:GLN:OE1	2.21	0.41
1:k:646:ILE:C	1:k:647:LEU:HD12	2.45	0.41
1:l:733:ARG:HG2	1:l:734:ASN:N	2.36	0.41
1:n:345:ASP:C	1:n:347:GLU:H	2.28	0.41
1:n:479:PRO:O	1:n:604:MET:HG3	2.20	0.41
1:o:345:ASP:C	1:o:347:GLU:H	2.28	0.41
1:o:733:ARG:HG2	1:o:734:ASN:N	2.36	0.41
1:p:666:PHE:HZ	1:r:371:MET:HG3	1.85	0.41
1:q:613:LEU:HB3	1:q:614:GLN:OE1	2.21	0.41
1:r:733:ARG:HG2	1:r:734:ASN:N	2.36	0.41
1:s:535:PRO:HB2	1:s:538:GLY:HA3	2.02	0.41
1:t:485:GLN:NE2	1:t:506:THR:HG21	2.36	0.41
1:w:563:GLU:O	1:w:565:ILE:N	2.53	0.41
1:y:362:LEU:HD23	1:y:370:PHE:CZ	2.55	0.41
1:z:535:PRO:HB2	1:z:538:GLY:HA3	2.02	0.41
1:1:234:TRP:CD1	1:1:298[B]:ARG:NH2	2.89	0.41
1:1:613:LEU:HB3	1:1:614:GLN:OE1	2.21	0.41
1:2:646:ILE:C	1:2:647:LEU:HD12	2.45	0.41
1:4:563:GLU:O	1:4:565:ILE:N	2.53	0.41
1:8:477:TRP:O	1:8:478:LEU:HD12	2.21	0.41
1:B:699:GLN:H	1:X:701:THR:HG23	1.85	0.41
1:C:362:LEU:HD23	1:C:370:PHE:CZ	2.55	0.41
1:E:234:TRP:CG	1:E:298[A]:ARG:HD3	2.55	0.41
1:H:733:ARG:HG2	1:H:734:ASN:N	2.36	0.41
1:I:562:GLU:OE2	1:I:612:TYR:OH	2.31	0.41
1:J:431:ASP:OD2	1:1:513:ARG:HD2	2.21	0.41
1:K:489:SER:HB2	1:K:532:LYS:HG2	2.02	0.41
1:L:435:ASN:HB2	1:r:353:VAL:CG1	2.51	0.41
1:L:517:VAL:HG23	1:L:517:VAL:O	2.21	0.41
1:M:485:GLN:NE2	1:M:506:THR:HG21	2.36	0.41
1:M:733:ARG:HG2	1:M:734:ASN:N	2.36	0.41
1:N:345:ASP:C	1:N:347:GLU:H	2.28	0.41
1:N:431:ASP:OD2	1:w:513:ARG:HD2	2.21	0.41
1:N:613:LEU:HB3	1:N:614:GLN:OE1	2.21	0.41
1:Q:485:GLN:NE2	1:Q:506:THR:HG21	2.36	0.41
1:R:485:GLN:NE2	1:R:506:THR:HG21	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:713:THR:HG22	1:T:714:VAL:N	2.36	0.41
1:U:535:PRO:HB2	1:U:538:GLY:HA3	2.02	0.41
1:U:713:THR:HG22	1:U:714:VAL:N	2.36	0.41
1:V:345:ASP:C	1:V:347:GLU:H	2.28	0.41
1:W:371:MET:HG3	1:Z:666:PHE:HZ	1.86	0.41
1:W:431:ASP:OD2	1:l:513:ARG:HD2	2.20	0.41
1:X:733:ARG:HG2	1:X:734:ASN:N	2.36	0.41
1:Y:431:ASP:OD2	1:t:513:ARG:HD2	2.21	0.41
1:Y:613:LEU:HB3	1:Y:614:GLN:OE1	2.21	0.41
1:Z:345:ASP:C	1:Z:347:GLU:H	2.28	0.41
1:a:613:LEU:HB3	1:a:614:GLN:OE1	2.21	0.41
1:c:362:LEU:HD23	1:c:370:PHE:CZ	2.55	0.41
1:d:517:VAL:HG23	1:d:517:VAL:O	2.21	0.41
1:e:535:PRO:HB2	1:e:538:GLY:HA3	2.02	0.41
1:f:345:ASP:C	1:f:347:GLU:H	2.28	0.41
1:f:353:VAL:CG1	1:n:435:ASN:HB2	2.50	0.41
1:g:362:LEU:HD23	1:g:370:PHE:CZ	2.55	0.41
1:h:371:MET:HG3	1:z:666:PHE:HZ	1.85	0.41
1:h:435:ASN:HB2	1:m:353:VAL:CG1	2.49	0.41
1:h:733:ARG:HG2	1:h:734:ASN:N	2.36	0.41
1:i:362:LEU:HD23	1:i:370:PHE:CZ	2.55	0.41
1:i:477:TRP:O	1:i:478:LEU:HD12	2.21	0.41
1:j:701:THR:HG23	1:5:699:GLN:H	1.85	0.41
1:l:234:TRP:CG	1:l:298[A]:ARG:HD3	2.55	0.41
1:m:365:PHE:HA	1:m:366:PRO:HD3	1.92	0.41
1:m:701:THR:HG23	1:v:699:GLN:H	1.86	0.41
1:m:713:THR:HG22	1:m:714:VAL:N	2.36	0.41
1:n:485:GLN:NE2	1:n:506:THR:HG21	2.36	0.41
1:n:517:VAL:HG23	1:n:517:VAL:O	2.21	0.41
1:n:646:ILE:C	1:n:647:LEU:HD12	2.45	0.41
1:p:345:ASP:C	1:p:347:GLU:H	2.28	0.41
1:p:467:ALA:O	1:p:470:ILE:HG12	2.20	0.41
1:p:477:TRP:O	1:p:478:LEU:HD12	2.21	0.41
1:q:431:ASP:OD2	1:z:513:ARG:HD2	2.21	0.41
1:s:627:HIS:HB3	1:l:605:VAL:HG12	2.01	0.41
1:t:345:ASP:C	1:t:347:GLU:H	2.28	0.41
1:u:562:GLU:OE2	1:u:612:TYR:OH	2.31	0.41
1:u:666:PHE:HZ	1:z:371:MET:HG3	1.85	0.41
1:u:733:ARG:HG2	1:u:734:ASN:N	2.36	0.41
1:w:362:LEU:HD23	1:w:370:PHE:CZ	2.55	0.41
1:x:485:GLN:NE2	1:x:506:THR:HG21	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:535:PRO:HB2	1:x:538:GLY:HA3	2.02	0.41
1:y:345:ASP:C	1:y:347:GLU:H	2.29	0.41
1:y:365:PHE:HA	1:y:366:PRO:HD3	1.92	0.41
1:2:348:TYR:OH	1:2:642:PRO:O	2.32	0.41
1:2:485:GLN:NE2	1:2:506:THR:HG21	2.36	0.41
1:2:517:VAL:O	1:2:517:VAL:HG23	2.21	0.41
1:3:613:LEU:HB3	1:3:614:GLN:OE1	2.21	0.41
1:4:489:SER:HB2	1:4:532:LYS:HG2	2.02	0.41
1:4:613:LEU:HB3	1:4:614:GLN:OE1	2.21	0.41
1:7:298[A]:ARG:HG2	1:7:298[A]:ARG:HH21	1.84	0.41
1:7:613:LEU:HB3	1:7:614:GLN:OE1	2.21	0.41
1:8:345:ASP:C	1:8:347:GLU:H	2.28	0.41
1:8:485:GLN:NE2	1:8:506:THR:HG21	2.36	0.41
1:A:517:VAL:O	1:A:517:VAL:HG23	2.21	0.41
1:C:398:PHE:CZ	1:t:692:LYS:HG3	2.56	0.41
1:C:733:ARG:HG2	1:C:734:ASN:N	2.36	0.41
1:D:435:ASN:HB2	1:8:353:VAL:CG1	2.51	0.41
1:D:713:THR:HG22	1:D:714:VAL:N	2.36	0.41
1:D:733:ARG:HG2	1:D:734:ASN:N	2.36	0.41
1:E:467:ALA:O	1:E:470:ILE:HG12	2.20	0.41
1:G:345:ASP:C	1:G:347:GLU:H	2.28	0.41
1:H:485:GLN:NE2	1:H:506:THR:HG21	2.36	0.41
1:H:542:PHE:O	1:H:558:MET:N	2.29	0.41
1:I:345:ASP:C	1:I:347:GLU:H	2.28	0.41
1:I:517:VAL:HG23	1:I:517:VAL:O	2.21	0.41
1:I:733:ARG:HG2	1:I:734:ASN:N	2.36	0.41
1:J:348:TYR:OH	1:J:642:PRO:O	2.32	0.41
1:J:485:GLN:NE2	1:J:506:THR:HG21	2.36	0.41
1:J:517:VAL:O	1:J:517:VAL:HG23	2.21	0.41
1:K:477:TRP:O	1:K:478:LEU:HD12	2.21	0.41
1:K:565:ILE:HD12	1:K:565:ILE:HG23	1.77	0.41
1:L:535:PRO:HB2	1:L:538:GLY:HA3	2.02	0.41
1:M:345:ASP:C	1:M:347:GLU:H	2.28	0.41
1:O:517:VAL:HG23	1:O:517:VAL:O	2.21	0.41
1:P:713:THR:HG22	1:P:714:VAL:N	2.36	0.41
1:Q:535:PRO:HB2	1:Q:538:GLY:HA3	2.02	0.41
1:Q:563:GLU:O	1:Q:565:ILE:N	2.53	0.41
1:R:353:VAL:CG1	1:r:435:ASN:HB2	2.51	0.41
1:S:345:ASP:C	1:S:347:GLU:H	2.29	0.41
1:S:371:MET:HG3	1:V:666:PHE:HZ	1.85	0.41
1:S:431:ASP:OD2	1:q:513:ARG:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:627:HIS:HB3	1:z:605:VAL:HG12	2.03	0.41
1:T:733:ARG:HG2	1:T:734:ASN:N	2.36	0.41
1:V:429:SER:OG	1:V:431:ASP:OD1	2.28	0.41
1:W:666:PHE:HZ	1:e:371:MET:HG3	1.85	0.41
1:X:345:ASP:C	1:X:347:GLU:H	2.28	0.41
1:Y:362:LEU:HD23	1:Y:370:PHE:CZ	2.55	0.41
1:Y:713:THR:HG22	1:Y:714:VAL:N	2.36	0.41
1:a:542:PHE:O	1:a:558:MET:N	2.29	0.41
1:b:345:ASP:C	1:b:347:GLU:H	2.28	0.41
1:b:613:LEU:HB3	1:b:614:GLN:OE1	2.21	0.41
1:c:489:SER:HB2	1:c:532:LYS:HG2	2.02	0.41
1:c:535:PRO:HB2	1:c:538:GLY:HA3	2.02	0.41
1:d:371:MET:HG3	1:i:666:PHE:HZ	1.86	0.41
1:d:646:ILE:C	1:d:647:LEU:HD12	2.45	0.41
1:e:489:SER:HB2	1:e:532:LYS:HG2	2.02	0.41
1:e:713:THR:HG22	1:e:714:VAL:N	2.36	0.41
1:f:479:PRO:O	1:f:604:MET:HG3	2.20	0.41
1:f:542:PHE:O	1:f:558:MET:N	2.29	0.41
1:f:733:ARG:HG2	1:f:734:ASN:N	2.36	0.41
1:g:613:LEU:HB3	1:g:614:GLN:OE1	2.21	0.41
1:h:345:ASP:C	1:h:347:GLU:H	2.28	0.41
1:h:429:SER:OG	1:h:431:ASP:OD1	2.28	0.41
1:i:345:ASP:C	1:i:347:GLU:H	2.28	0.41
1:j:502:TRP:CZ2	1:4:471:ARG:HD2	2.55	0.41
1:j:713:THR:HG22	1:j:714:VAL:N	2.36	0.41
1:k:733:ARG:HG2	1:k:734:ASN:N	2.36	0.41
1:l:234:TRP:CH2	1:l:298[B]:ARG:HB2	2.56	0.41
1:o:435:ASN:HB2	1:4:353:VAL:CG1	2.49	0.41
1:o:517:VAL:HG23	1:o:517:VAL:O	2.21	0.41
1:o:563:GLU:O	1:o:565:ILE:N	2.53	0.41
1:q:485:GLN:NE2	1:q:506:THR:HG21	2.36	0.41
1:q:733:ARG:HG2	1:q:734:ASN:N	2.36	0.41
1:r:345:ASP:C	1:r:347:GLU:H	2.28	0.41
1:s:499:GLU:OE2	1:s:501:SER:OG	2.34	0.41
1:u:345:ASP:C	1:u:347:GLU:H	2.28	0.41
1:w:467:ALA:O	1:w:470:ILE:HG12	2.20	0.41
1:z:517:VAL:HG23	1:z:517:VAL:O	2.21	0.41
1:2:733:ARG:HG2	1:2:734:ASN:N	2.36	0.41
1:3:489:SER:HB2	1:3:532:LYS:HG2	2.02	0.41
1:4:485:GLN:NE2	1:4:506:THR:HG21	2.36	0.41
1:5:485:GLN:NE2	1:5:506:THR:HG21	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:733:ARG:HG2	1:5:734:ASN:N	2.36	0.41
1:6:345:ASP:C	1:6:347:GLU:H	2.28	0.41
1:7:362:LEU:HD23	1:7:370:PHE:CZ	2.55	0.41
1:7:535:PRO:HB2	1:7:538:GLY:HA3	2.02	0.41
1:7:713:THR:HG22	1:7:714:VAL:N	2.36	0.41
1:8:234:TRP:CH2	1:8:298[B]:ARG:HB2	2.56	0.41
1:A:733:ARG:HG2	1:A:734:ASN:N	2.36	0.41
1:C:517:VAL:O	1:C:517:VAL:HG23	2.21	0.41
1:D:489:SER:HB2	1:D:532:LYS:HG2	2.02	0.41
1:E:435:ASN:HB2	1:p:353:VAL:CG1	2.51	0.41
1:E:666:PHE:HZ	1:N:371:MET:HG3	1.85	0.41
1:F:345:ASP:C	1:F:347:GLU:H	2.28	0.41
1:H:535:PRO:HB2	1:H:538:GLY:HA3	2.02	0.41
1:I:666:PHE:HZ	1:L:371:MET:HG3	1.85	0.41
1:J:613:LEU:HB3	1:J:614:GLN:OE1	2.21	0.41
1:O:489:SER:HB2	1:O:532:LYS:HG2	2.02	0.41
1:P:485:GLN:NE2	1:P:506:THR:HG21	2.36	0.41
1:R:733:ARG:HG2	1:R:734:ASN:N	2.36	0.41
1:S:563:GLU:O	1:S:565:ILE:N	2.53	0.41
1:U:477:TRP:O	1:U:478:LEU:HD12	2.21	0.41
1:V:485:GLN:NE2	1:V:506:THR:HG21	2.36	0.41
1:W:713:THR:HG22	1:W:714:VAL:N	2.36	0.41
1:X:362:LEU:HD23	1:X:370:PHE:CZ	2.55	0.41
1:X:517:VAL:HG23	1:X:517:VAL:O	2.21	0.41
1:X:563:GLU:O	1:X:565:ILE:N	2.53	0.41
1:Z:345:ASP:O	1:Z:346:SER:OG	2.32	0.41
1:a:489:SER:HB2	1:a:532:LYS:HG2	2.02	0.41
1:c:627:HIS:HB3	1:3:605:VAL:HG12	2.03	0.41
1:c:713:THR:HG22	1:c:714:VAL:N	2.36	0.41
1:d:485:GLN:NE2	1:d:506:THR:HG21	2.36	0.41
1:f:613:LEU:HB3	1:f:614:GLN:OE1	2.21	0.41
1:g:517:VAL:O	1:g:517:VAL:HG23	2.21	0.41
1:g:733:ARG:HG2	1:g:734:ASN:N	2.36	0.41
1:h:345:ASP:O	1:h:346:SER:OG	2.32	0.41
1:j:431:ASP:OD2	1:o:513:ARG:HD2	2.21	0.41
1:j:485:GLN:NE2	1:j:506:THR:HG21	2.36	0.41
1:j:489:SER:HB2	1:j:532:LYS:HG2	2.02	0.41
1:k:713:THR:HG22	1:k:714:VAL:N	2.36	0.41
1:l:517:VAL:HG23	1:l:517:VAL:O	2.21	0.41
1:m:733:ARG:HG2	1:m:734:ASN:N	2.36	0.41
1:o:362:LEU:HD23	1:o:370:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:431:ASP:OD2	1:4:513:ARG:HD2	2.20	0.41
1:r:517:VAL:HG23	1:r:517:VAL:O	2.21	0.41
1:r:563:GLU:O	1:r:565:ILE:N	2.53	0.41
1:s:371:MET:HG3	1:x:666:PHE:HZ	1.85	0.41
1:s:479:PRO:O	1:s:604:MET:HG3	2.20	0.41
1:s:513:ARG:HD2	1:1:431:ASP:OD2	2.21	0.41
1:s:713:THR:HG22	1:s:714:VAL:N	2.36	0.41
1:t:535:PRO:HB2	1:t:538:GLY:HA3	2.02	0.41
1:t:666:PHE:HZ	1:7:371:MET:HG3	1.85	0.41
1:u:517:VAL:HG23	1:u:517:VAL:O	2.21	0.41
1:v:345:ASP:C	1:v:347:GLU:H	2.29	0.41
1:v:485:GLN:NE2	1:v:506:THR:HG21	2.36	0.41
1:v:517:VAL:O	1:v:517:VAL:HG23	2.21	0.41
1:v:733:ARG:HG2	1:v:734:ASN:N	2.36	0.41
1:x:502:TRP:CZ2	1:8:471:ARG:HD2	2.55	0.41
1:x:563:GLU:O	1:x:565:ILE:N	2.53	0.41
1:x:613:LEU:HB3	1:x:614:GLN:OE1	2.21	0.41
1:y:479:PRO:O	1:y:604:MET:HG3	2.20	0.41
1:z:362:LEU:HD23	1:z:370:PHE:CZ	2.55	0.41
1:2:535:PRO:HB2	1:2:538:GLY:HA3	2.02	0.41
1:6:365:PHE:HA	1:6:366:PRO:HD3	1.92	0.41
1:6:713:THR:HG22	1:6:714:VAL:N	2.36	0.41
1:8:535:PRO:HB2	1:8:538:GLY:HA3	2.02	0.41
1:A:485:GLN:NE2	1:A:506:THR:HG21	2.36	0.41
1:A:613:LEU:HB3	1:A:614:GLN:OE1	2.21	0.41
1:B:353:VAL:CG1	1:2:435:ASN:HB2	2.51	0.41
1:B:485:GLN:NE2	1:B:506:THR:HG21	2.36	0.41
1:B:535:PRO:HB2	1:B:538:GLY:HA3	2.02	0.41
1:C:371:MET:CE	1:c:662:SER:H	2.34	0.41
1:C:389:ARG:HG2	1:t:698:ILE:HD12	2.03	0.41
1:C:477:TRP:O	1:C:478:LEU:HD12	2.21	0.41
1:C:479:PRO:O	1:C:604:MET:HG3	2.20	0.41
1:C:613:LEU:HB3	1:C:614:GLN:OE1	2.21	0.41
1:C:713:THR:HG22	1:C:714:VAL:N	2.36	0.41
1:D:605:VAL:HG12	1:8:627:HIS:HB3	2.02	0.41
1:E:353:VAL:CG1	1:i:435:ASN:HB2	2.51	0.41
1:E:362:LEU:HD23	1:E:370:PHE:CZ	2.55	0.41
1:E:485:GLN:NE2	1:E:506:THR:HG21	2.36	0.41
1:E:733:ARG:HG2	1:E:734:ASN:N	2.36	0.41
1:F:479:PRO:O	1:F:604:MET:HG3	2.20	0.41
1:F:565:ILE:HG23	1:F:565:ILE:HD12	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:517:VAL:HG23	1:G:517:VAL:O	2.21	0.41
1:G:535:PRO:HB2	1:G:538:GLY:HA3	2.02	0.41
1:H:517:VAL:HG23	1:H:517:VAL:O	2.21	0.41
1:H:613:LEU:HB3	1:H:614:GLN:OE1	2.21	0.41
1:H:701:THR:HG23	1:P:699:GLN:H	1.86	0.41
1:H:713:THR:HG22	1:H:714:VAL:N	2.36	0.41
1:I:485:GLN:NE2	1:I:506:THR:HG21	2.36	0.41
1:J:345:ASP:C	1:J:347:GLU:H	2.28	0.41
1:J:479:PRO:O	1:J:604:MET:HG3	2.20	0.41
1:J:535:PRO:HB2	1:J:538:GLY:HA3	2.02	0.41
1:J:733:ARG:HG2	1:J:734:ASN:N	2.36	0.41
1:K:371:MET:HG3	1:3:666:PHE:HZ	1.86	0.41
1:K:485:GLN:NE2	1:K:506:THR:HG21	2.36	0.41
1:K:517:VAL:O	1:K:517:VAL:HG23	2.21	0.41
1:L:362:LEU:HD23	1:L:370:PHE:CZ	2.55	0.41
1:L:613:LEU:HB3	1:L:614:GLN:OE1	2.21	0.41
1:L:713:THR:HG22	1:L:714:VAL:N	2.36	0.41
1:M:613:LEU:HB3	1:M:614:GLN:OE1	2.21	0.41
1:M:666:PHE:HZ	1:P:371:MET:HG3	1.86	0.41
1:N:542:PHE:O	1:N:558:MET:N	2.29	0.41
1:N:713:THR:HG22	1:N:714:VAL:N	2.36	0.41
1:O:237:ASP:OD2	1:O:238[B]:ARG:NH2	2.54	0.41
1:O:485:GLN:NE2	1:O:506:THR:HG21	2.36	0.41
1:O:627:HIS:HB3	1:6:605:VAL:HG12	2.03	0.41
1:P:479:PRO:O	1:P:604:MET:HG3	2.20	0.41
1:P:489:SER:HB2	1:P:532:LYS:HG2	2.02	0.41
1:Q:517:VAL:O	1:Q:517:VAL:HG23	2.21	0.41
1:Q:613:LEU:HB3	1:Q:614:GLN:OE1	2.21	0.41
1:Q:666:PHE:HZ	1:U:371:MET:HG3	1.85	0.41
1:R:477:TRP:O	1:R:478:LEU:HD12	2.21	0.41
1:R:535:PRO:HB2	1:R:538:GLY:HA3	2.02	0.41
1:R:713:THR:HG22	1:R:714:VAL:N	2.36	0.41
1:S:517:VAL:HG23	1:S:517:VAL:O	2.21	0.41
1:T:365:PHE:HA	1:T:366:PRO:HD3	1.92	0.41
1:T:517:VAL:HG23	1:T:517:VAL:O	2.21	0.41
1:U:321:LYS:HE2	1:U:334:ASN:OD1	2.21	0.41
1:U:479:PRO:O	1:U:604:MET:HG3	2.20	0.41
1:U:489:SER:HB2	1:U:532:LYS:HG2	2.02	0.41
1:U:517:VAL:O	1:U:517:VAL:HG23	2.21	0.41
1:V:517:VAL:HG23	1:V:517:VAL:O	2.21	0.41
1:V:713:THR:HG22	1:V:714:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:733:ARG:HG2	1:V:734:ASN:N	2.36	0.41
1:W:479:PRO:O	1:W:604:MET:HG3	2.20	0.41
1:W:563:GLU:O	1:W:565:ILE:N	2.53	0.41
1:W:613:LEU:HB3	1:W:614:GLN:OE1	2.21	0.41
1:W:733:ARG:HG2	1:W:734:ASN:N	2.36	0.41
1:X:234:TRP:CE2	1:X:298[B]:ARG:HD2	2.56	0.41
1:Y:535:PRO:HB2	1:Y:538:GLY:HA3	2.02	0.41
1:Z:535:PRO:HB2	1:Z:538:GLY:HA3	2.02	0.41
1:Z:613:LEU:HB3	1:Z:614:GLN:OE1	2.21	0.41
1:Z:733:ARG:HG2	1:Z:734:ASN:N	2.36	0.41
1:a:371:MET:HG3	1:7:666:PHE:HZ	1.86	0.41
1:a:733:ARG:HG2	1:a:734:ASN:N	2.36	0.41
1:b:517:VAL:HG23	1:b:517:VAL:O	2.21	0.41
1:b:627:HIS:HB3	1:d:605:VAL:HG12	2.02	0.41
1:c:477:TRP:O	1:c:478:LEU:HD12	2.21	0.41
1:d:362:LEU:HD23	1:d:370:PHE:CZ	2.55	0.41
1:d:565:ILE:HG22	1:d:565:ILE:O	2.21	0.41
1:e:362:LEU:HD23	1:e:370:PHE:CZ	2.55	0.41
1:e:477:TRP:O	1:e:478:LEU:HD12	2.21	0.41
1:e:565:ILE:HG22	1:e:565:ILE:O	2.21	0.41
1:f:517:VAL:O	1:f:517:VAL:HG23	2.21	0.41
1:g:479:PRO:O	1:g:604:MET:HG3	2.20	0.41
1:g:713:THR:HG22	1:g:714:VAL:N	2.36	0.41
1:h:613:LEU:HB3	1:h:614:GLN:OE1	2.21	0.41
1:i:371:MET:HG3	1:w:666:PHE:HZ	1.85	0.41
1:i:565:ILE:HG22	1:i:565:ILE:O	2.21	0.41
1:i:713:THR:HG22	1:i:714:VAL:N	2.36	0.41
1:j:234:TRP:CD2	1:j:298[B]:ARG:HD2	2.55	0.41
1:l:485:GLN:NE2	1:l:506:THR:HG21	2.36	0.41
1:l:489:SER:HB2	1:l:532:LYS:HG2	2.02	0.41
1:m:517:VAL:HG23	1:m:517:VAL:O	2.21	0.41
1:n:565:ILE:HG22	1:n:565:ILE:O	2.21	0.41
1:n:733:ARG:HG2	1:n:734:ASN:N	2.36	0.41
1:p:485:GLN:NE2	1:p:506:THR:HG21	2.36	0.41
1:p:517:VAL:HG23	1:p:517:VAL:O	2.21	0.41
1:p:713:THR:HG22	1:p:714:VAL:N	2.36	0.41
1:p:733:ARG:HG2	1:p:734:ASN:N	2.36	0.41
1:q:234:TRP:CD1	1:q:298[B]:ARG:NH2	2.89	0.41
1:s:321:LYS:HE2	1:s:334:ASN:OD1	2.21	0.41
1:s:477:TRP:O	1:s:478:LEU:HD12	2.21	0.41
1:s:517:VAL:HG23	1:s:517:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:517:VAL:HG23	1:t:517:VAL:O	2.21	0.41
1:u:485:GLN:NE2	1:u:506:THR:HG21	2.36	0.41
1:v:613:LEU:HB3	1:v:614:GLN:OE1	2.21	0.41
1:w:485:GLN:NE2	1:w:506:THR:HG21	2.36	0.41
1:w:613:LEU:HB3	1:w:614:GLN:OE1	2.21	0.41
1:w:733:ARG:HG2	1:w:734:ASN:N	2.36	0.41
1:x:517:VAL:O	1:x:517:VAL:HG23	2.21	0.41
1:y:565:ILE:HG23	1:y:565:ILE:HD12	1.77	0.41
1:y:699:GLN:H	1:4:701:THR:HG23	1.86	0.41
1:1:362:LEU:HD23	1:1:370:PHE:CZ	2.55	0.41
1:2:345:ASP:C	1:2:347:GLU:H	2.28	0.41
1:2:613:LEU:HB3	1:2:614:GLN:OE1	2.21	0.41
1:3:485:GLN:NE2	1:3:506:THR:HG21	2.36	0.41
1:3:733:ARG:HG2	1:3:734:ASN:N	2.36	0.41
1:4:477:TRP:O	1:4:478:LEU:HD12	2.21	0.41
1:4:517:VAL:O	1:4:517:VAL:HG23	2.21	0.41
1:5:613:LEU:HB3	1:5:614:GLN:OE1	2.21	0.41
1:5:713:THR:HG22	1:5:714:VAL:N	2.36	0.41
1:6:479:PRO:O	1:6:604:MET:HG3	2.20	0.41
1:6:613:LEU:HB3	1:6:614:GLN:OE1	2.21	0.41
1:6:733:ARG:HG2	1:6:734:ASN:N	2.36	0.41
1:8:234:TRP:CG	1:8:298[A]:ARG:HD3	2.55	0.41
1:8:613:LEU:HB3	1:8:614:GLN:OE1	2.21	0.41
1:A:389:ARG:HG2	1:f:698:ILE:HD12	2.03	0.41
1:A:489:SER:HB2	1:A:532:LYS:HG2	2.02	0.41
1:B:362:LEU:HD23	1:B:370:PHE:CZ	2.55	0.41
1:C:485:GLN:NE2	1:C:506:THR:HG21	2.36	0.41
1:D:429:SER:OG	1:D:431:ASP:OD1	2.28	0.41
1:D:467:ALA:O	1:D:470:ILE:HG12	2.20	0.41
1:D:535:PRO:HB2	1:D:538:GLY:HA3	2.02	0.41
1:E:613:LEU:HB3	1:E:614:GLN:OE1	2.21	0.41
1:G:666:PHE:HZ	1:Y:371:MET:HG3	1.85	0.41
1:J:353:VAL:CG1	1:s:435:ASN:HB2	2.50	0.41
1:K:565:ILE:HG22	1:K:565:ILE:O	2.21	0.41
1:L:479:PRO:O	1:L:604:MET:HG3	2.20	0.41
1:L:627:HIS:HB3	1:R:605:VAL:HG12	2.03	0.41
1:M:321:LYS:HE2	1:M:334:ASN:OD1	2.21	0.41
1:M:605:VAL:HG12	1:T:627:HIS:HB3	2.03	0.41
1:M:713:THR:HG22	1:M:714:VAL:N	2.36	0.41
1:N:565:ILE:HG22	1:N:565:ILE:O	2.21	0.41
1:Q:345:ASP:C	1:Q:347:GLU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:362:LEU:HD23	1:S:370:PHE:CZ	2.55	0.41
1:U:701:THR:HG23	1:Z:699:GLN:H	1.85	0.41
1:V:565:ILE:HG22	1:V:565:ILE:O	2.21	0.41
1:W:565:ILE:HG22	1:W:565:ILE:O	2.21	0.41
1:Y:321:LYS:HE2	1:Y:334:ASN:OD1	2.21	0.41
1:Z:371:MET:HG3	1:2:666:PHE:HZ	1.86	0.41
1:Z:517:VAL:HG23	1:Z:517:VAL:O	2.21	0.41
1:a:485:GLN:NE2	1:a:506:THR:HG21	2.36	0.41
1:b:535:PRO:HB2	1:b:538:GLY:HA3	2.02	0.41
1:c:345:ASP:C	1:c:347:GLU:H	2.28	0.41
1:c:565:ILE:HG22	1:c:565:ILE:O	2.21	0.41
1:c:613:LEU:HB3	1:c:614:GLN:OE1	2.21	0.41
1:d:613:LEU:HB3	1:d:614:GLN:OE1	2.21	0.41
1:d:733:ARG:HG2	1:d:734:ASN:N	2.36	0.41
1:e:613:LEU:HB3	1:e:614:GLN:OE1	2.21	0.41
1:h:321:LYS:HE2	1:h:334:ASN:OD1	2.21	0.41
1:j:345:ASP:C	1:j:347:GLU:H	2.28	0.41
1:k:489:SER:HB2	1:k:532:LYS:HG2	2.02	0.41
1:k:535:PRO:HB2	1:k:538:GLY:HA3	2.02	0.41
1:l:713:THR:HG22	1:l:714:VAL:N	2.36	0.41
1:m:477:TRP:O	1:m:478:LEU:HD12	2.21	0.41
1:n:362:LEU:HD23	1:n:370:PHE:CZ	2.55	0.41
1:p:479:PRO:O	1:p:604:MET:HG3	2.20	0.41
1:p:565:ILE:HG22	1:p:565:ILE:O	2.21	0.41
1:q:477:TRP:O	1:q:478:LEU:HD12	2.21	0.41
1:q:489:SER:HB2	1:q:532:LYS:HG2	2.02	0.41
1:x:513:ARG:HD2	1:8:431:ASP:OD2	2.21	0.41
1:z:479:PRO:O	1:z:604:MET:HG3	2.20	0.41
1:z:713:THR:HG22	1:z:714:VAL:N	2.36	0.41
1:1:485:GLN:NE2	1:1:506:THR:HG21	2.36	0.41
1:2:479:PRO:O	1:2:604:MET:HG3	2.20	0.41
1:3:477:TRP:O	1:3:478:LEU:HD12	2.21	0.41
1:3:713:THR:HG22	1:3:714:VAL:N	2.36	0.41
1:4:565:ILE:HD12	1:4:565:ILE:HG23	1.77	0.41
1:5:234:TRP:CD2	1:5:298[B]:ARG:HD2	2.55	0.41
1:5:321:LYS:HE2	1:5:334:ASN:OD1	2.21	0.41
1:5:517:VAL:HG23	1:5:517:VAL:O	2.21	0.41
1:5:565:ILE:HG22	1:5:565:ILE:O	2.21	0.41
1:6:563:GLU:O	1:6:565:ILE:N	2.53	0.41
1:6:565:ILE:HG22	1:6:565:ILE:O	2.21	0.41
1:7:321:LYS:HE2	1:7:334:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:345:ASP:O	1:8:346:SER:OG	2.32	0.41
1:8:733:ARG:HG2	1:8:734:ASN:N	2.36	0.41
1:A:321:LYS:HE2	1:A:334:ASN:OD1	2.21	0.40
1:A:565:ILE:HG22	1:A:565:ILE:O	2.21	0.40
1:B:398:PHE:CZ	1:2:692:LYS:HG3	2.57	0.40
1:B:479:PRO:O	1:B:604:MET:HG3	2.20	0.40
1:D:353:VAL:CG1	1:x:435:ASN:HB2	2.50	0.40
1:D:485:GLN:NE2	1:D:506:THR:HG21	2.36	0.40
1:F:517:VAL:HG23	1:F:517:VAL:O	2.21	0.40
1:G:526:HIS:CD2	1:G:530:GLU:O	2.75	0.40
1:H:321:LYS:HE2	1:H:334:ASN:OD1	2.21	0.40
1:H:371:MET:HG3	1:X:666:PHE:HZ	1.86	0.40
1:H:565:ILE:HG22	1:H:565:ILE:O	2.21	0.40
1:I:477:TRP:O	1:I:478:LEU:HD12	2.21	0.40
1:I:613:LEU:HB3	1:I:614:GLN:OE1	2.21	0.40
1:L:485:GLN:NE2	1:L:506:THR:HG21	2.36	0.40
1:L:614:GLN:OE1	1:L:614:GLN:N	2.55	0.40
1:M:477:TRP:O	1:M:478:LEU:HD12	2.21	0.40
1:N:321:LYS:HE2	1:N:334:ASN:OD1	2.21	0.40
1:Q:699:GLN:H	1:f:701:THR:HG23	1.86	0.40
1:R:321:LYS:HE2	1:R:334:ASN:OD1	2.21	0.40
1:R:489:SER:HB2	1:R:532:LYS:HG2	2.02	0.40
1:T:477:TRP:O	1:T:478:LEU:HD12	2.21	0.40
1:T:526:HIS:CD2	1:T:530:GLU:O	2.75	0.40
1:V:371:MET:HG3	1:f:666:PHE:HZ	1.86	0.40
1:V:389:ARG:HG2	1:w:698:ILE:HD12	2.03	0.40
1:V:479:PRO:O	1:V:604:MET:HG3	2.20	0.40
1:V:526:HIS:CD2	1:V:530:GLU:O	2.75	0.40
1:W:398:PHE:CZ	1:u:692:LYS:HG3	2.57	0.40
1:a:321:LYS:HE2	1:a:334:ASN:OD1	2.21	0.40
1:a:517:VAL:HG23	1:a:517:VAL:O	2.21	0.40
1:a:713:THR:HG22	1:a:714:VAL:N	2.36	0.40
1:b:485:GLN:NE2	1:b:506:THR:HG21	2.36	0.40
1:b:713:THR:HG22	1:b:714:VAL:N	2.36	0.40
1:e:345:ASP:C	1:e:347:GLU:H	2.28	0.40
1:e:526:HIS:CD2	1:e:530:GLU:O	2.75	0.40
1:f:485:GLN:NE2	1:f:506:THR:HG21	2.36	0.40
1:g:477:TRP:O	1:g:478:LEU:HD12	2.21	0.40
1:g:485:GLN:NE2	1:g:506:THR:HG21	2.36	0.40
1:h:477:TRP:O	1:h:478:LEU:HD12	2.21	0.40
1:h:701:THR:HG23	1:q:699:GLN:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:713:THR:HG22	1:h:714:VAL:N	2.36	0.40
1:i:353:VAL:CG1	1:p:435:ASN:HB2	2.49	0.40
1:j:479:PRO:O	1:j:604:MET:HG3	2.20	0.40
1:k:485:GLN:NE2	1:k:506:THR:HG21	2.36	0.40
1:k:517:VAL:O	1:k:517:VAL:HG23	2.21	0.40
1:l:467:ALA:O	1:l:470:ILE:HG12	2.20	0.40
1:m:431:ASP:OD2	1:5:513:ARG:HD2	2.21	0.40
1:n:613:LEU:HB3	1:n:614:GLN:OE1	2.21	0.40
1:p:526:HIS:CD2	1:p:530:GLU:O	2.75	0.40
1:q:713:THR:HG22	1:q:714:VAL:N	2.36	0.40
1:r:362:LEU:HD23	1:r:370:PHE:CZ	2.55	0.40
1:r:535:PRO:HB2	1:r:538:GLY:HA3	2.02	0.40
1:s:489:SER:HB2	1:s:532:LYS:HG2	2.02	0.40
1:t:613:LEU:HB3	1:t:614:GLN:OE1	2.21	0.40
1:u:613:LEU:HB3	1:u:614:GLN:OE1	2.21	0.40
1:v:489:SER:HB2	1:v:532:LYS:HG2	2.02	0.40
1:v:565:ILE:HG22	1:v:565:ILE:O	2.21	0.40
1:v:713:THR:HG22	1:v:714:VAL:N	2.36	0.40
1:w:321:LYS:HE2	1:w:334:ASN:OD1	2.21	0.40
1:x:345:ASP:C	1:x:347:GLU:H	2.28	0.40
1:z:613:LEU:HB3	1:z:614:GLN:OE1	2.21	0.40
1:1:517:VAL:HG23	1:1:517:VAL:O	2.21	0.40
1:1:535:PRO:HB2	1:1:538:GLY:HA3	2.02	0.40
1:5:234:TRP:CZ2	1:5:298[A]:ARG:HB3	2.56	0.40
1:5:542:PHE:O	1:5:558:MET:N	2.29	0.40
1:A:713:THR:HG22	1:A:714:VAL:N	2.36	0.40
1:B:321:LYS:HE2	1:B:334:ASN:OD1	2.21	0.40
1:B:517:VAL:HG23	1:B:517:VAL:O	2.21	0.40
1:B:713:THR:HG22	1:B:714:VAL:N	2.36	0.40
1:E:321:LYS:HE2	1:E:334:ASN:OD1	2.21	0.40
1:E:371:MET:HG3	1:R:666:PHE:HZ	1.86	0.40
1:E:477:TRP:O	1:E:478:LEU:HD12	2.21	0.40
1:F:526:HIS:CD2	1:F:530:GLU:O	2.75	0.40
1:F:614:GLN:OE1	1:F:614:GLN:N	2.55	0.40
1:G:321:LYS:HE2	1:G:334:ASN:OD1	2.21	0.40
1:G:353:VAL:CG1	1:7:435:ASN:HB2	2.51	0.40
1:G:613:LEU:HB3	1:G:614:GLN:OE1	2.21	0.40
1:I:526:HIS:CD2	1:I:530:GLU:O	2.75	0.40
1:J:627:HIS:HB3	1:s:605:VAL:HG12	2.03	0.40
1:K:605:VAL:HG12	1:P:627:HIS:HB3	2.04	0.40
1:L:565:ILE:HG22	1:L:565:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:666:PHE:HZ	1:M:371:MET:HG3	1.85	0.40
1:L:733:ARG:HG2	1:L:734:ASN:N	2.36	0.40
1:M:238[A]:ARG:CD	1:M:683:GLU:OE2	2.68	0.40
1:N:733:ARG:HG2	1:N:734:ASN:N	2.36	0.40
1:O:467:ALA:O	1:O:470:ILE:HG12	2.20	0.40
1:O:477:TRP:O	1:O:478:LEU:HD12	2.21	0.40
1:O:713:THR:HG22	1:O:714:VAL:N	2.36	0.40
1:P:345:ASP:C	1:P:347:GLU:H	2.28	0.40
1:P:613:LEU:HB3	1:P:614:GLN:OE1	2.21	0.40
1:Q:614:GLN:OE1	1:Q:614:GLN:N	2.55	0.40
1:R:542:PHE:O	1:R:558:MET:N	2.29	0.40
1:S:321:LYS:HE2	1:S:334:ASN:OD1	2.21	0.40
1:S:535:PRO:HB2	1:S:538:GLY:HA3	2.02	0.40
1:S:613:LEU:HB3	1:S:614:GLN:OE1	2.21	0.40
1:U:565:ILE:HG22	1:U:565:ILE:O	2.21	0.40
1:V:489:SER:HB2	1:V:532:LYS:HG2	2.02	0.40
1:W:477:TRP:O	1:W:478:LEU:HD12	2.21	0.40
1:X:238[A]:ARG:CD	1:X:683:GLU:OE2	2.67	0.40
1:X:477:TRP:O	1:X:478:LEU:HD12	2.21	0.40
1:Z:526:HIS:CD2	1:Z:530:GLU:O	2.75	0.40
1:a:345:ASP:C	1:a:347:GLU:H	2.28	0.40
1:c:526:HIS:CD2	1:c:530:GLU:O	2.75	0.40
1:d:398:PHE:CE1	1:v:692:LYS:HE2	2.57	0.40
1:d:535:PRO:HB2	1:d:538:GLY:HA3	2.02	0.40
1:f:477:TRP:O	1:f:478:LEU:HD12	2.21	0.40
1:f:535:PRO:HB2	1:f:538:GLY:HA3	2.02	0.40
1:f:627:HIS:HB3	1:n:605:VAL:HG12	2.03	0.40
1:g:234:TRP:CD1	1:g:298[B]:ARG:NH2	2.90	0.40
1:i:321:LYS:HE2	1:i:334:ASN:OD1	2.21	0.40
1:i:733:ARG:HG2	1:i:734:ASN:N	2.36	0.40
1:j:234:TRP:CZ2	1:j:298[A]:ARG:HB3	2.56	0.40
1:k:467:ALA:O	1:k:470:ILE:HG12	2.20	0.40
1:l:535:PRO:HB2	1:l:538:GLY:HA3	2.02	0.40
1:m:526:HIS:CD2	1:m:530:GLU:O	2.75	0.40
1:m:613:LEU:HB3	1:m:614:GLN:OE1	2.21	0.40
1:p:489:SER:HB2	1:p:532:LYS:HG2	2.02	0.40
1:q:321:LYS:HE2	1:q:334:ASN:OD1	2.21	0.40
1:q:345:ASP:C	1:q:347:GLU:H	2.28	0.40
1:q:535:PRO:HB2	1:q:538:GLY:HA3	2.02	0.40
1:s:565:ILE:HG22	1:s:565:ILE:O	2.21	0.40
1:t:321:LYS:HE2	1:t:334:ASN:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:526:HIS:CD2	1:t:530:GLU:O	2.75	0.40
1:u:526:HIS:CD2	1:u:530:GLU:O	2.75	0.40
1:u:713:THR:HG22	1:u:714:VAL:N	2.36	0.40
1:v:321:LYS:HE2	1:v:334:ASN:OD1	2.21	0.40
1:x:565:ILE:HG22	1:x:565:ILE:O	2.21	0.40
1:x:614:GLN:OE1	1:x:614:GLN:N	2.55	0.40
1:y:565:ILE:HG22	1:y:565:ILE:O	2.21	0.40
1:y:614:GLN:OE1	1:y:614:GLN:N	2.55	0.40
1:z:614:GLN:OE1	1:z:614:GLN:N	2.55	0.40
1:z:733:ARG:HG2	1:z:734:ASN:N	2.36	0.40
1:1:321:LYS:HE2	1:1:334:ASN:OD1	2.21	0.40
1:3:321:LYS:HE2	1:3:334:ASN:OD1	2.21	0.40
1:5:477:TRP:O	1:5:478:LEU:HD12	2.21	0.40
1:8:517:VAL:HG23	1:8:517:VAL:O	2.21	0.40
1:B:371:MET:HG3	1:K:666:PHE:HZ	1.86	0.40
1:B:627:HIS:HB3	1:2:605:VAL:HG12	2.04	0.40
1:C:614:GLN:OE1	1:C:614:GLN:N	2.55	0.40
1:D:379:THR:HG22	1:D:380:LEU:H	1.87	0.40
1:D:517:VAL:O	1:D:517:VAL:HG23	2.21	0.40
1:D:614:GLN:OE1	1:D:614:GLN:N	2.55	0.40
1:D:627:HIS:HB3	1:x:605:VAL:HG12	2.03	0.40
1:E:614:GLN:OE1	1:E:614:GLN:N	2.55	0.40
1:F:565:ILE:HG22	1:F:565:ILE:O	2.21	0.40
1:G:389:ARG:HG2	1:7:698:ILE:HD12	2.04	0.40
1:G:713:THR:HG22	1:G:714:VAL:N	2.36	0.40
1:H:477:TRP:O	1:H:478:LEU:HD12	2.21	0.40
1:H:605:VAL:HG12	1:M:627:HIS:HB3	2.03	0.40
1:I:713:THR:HG22	1:I:714:VAL:N	2.36	0.40
1:L:379:THR:HG22	1:L:380:LEU:H	1.87	0.40
1:L:477:TRP:O	1:L:478:LEU:HD12	2.21	0.40
1:L:526:HIS:CD2	1:L:530:GLU:O	2.75	0.40
1:M:339:THR:HG22	1:M:404:ARG:HG3	2.04	0.40
1:O:276:SER:HB2	1:6:437:LEU:HD11	2.01	0.40
1:O:535:PRO:HB2	1:O:538:GLY:HA3	2.02	0.40
1:Q:627:HIS:HB3	1:Z:605:VAL:HG12	2.04	0.40
1:R:339:THR:HG22	1:R:404:ARG:HG3	2.04	0.40
1:R:345:ASP:C	1:R:347:GLU:H	2.28	0.40
1:R:379:THR:HG22	1:R:380:LEU:H	1.87	0.40
1:S:477:TRP:O	1:S:478:LEU:HD12	2.21	0.40
1:S:666:PHE:HZ	1:l:371:MET:HG3	1.84	0.40
1:T:613:LEU:HB3	1:T:614:GLN:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:485:GLN:NE2	1:U:506:THR:HG21	2.36	0.40
1:V:276:SER:HB2	1:w:437:LEU:HD11	2.02	0.40
1:X:565:ILE:HG23	1:X:607:GLN:HB2	2.04	0.40
1:Z:627:HIS:HB3	1:k:605:VAL:HG12	2.03	0.40
1:a:477:TRP:O	1:a:478:LEU:HD12	2.21	0.40
1:b:699:GLN:H	1:x:701:THR:HG23	1.85	0.40
1:d:526:HIS:CD2	1:d:530:GLU:O	2.75	0.40
1:e:485:GLN:NE2	1:e:506:THR:HG21	2.36	0.40
1:f:713:THR:HG22	1:f:714:VAL:N	2.36	0.40
1:g:565:ILE:HG22	1:g:565:ILE:O	2.21	0.40
1:j:613:LEU:HB3	1:j:614:GLN:OE1	2.21	0.40
1:k:613:LEU:HB3	1:k:614:GLN:OE1	2.21	0.40
1:k:614:GLN:OE1	1:k:614:GLN:N	2.55	0.40
1:l:613:LEU:HB3	1:l:614:GLN:OE1	2.21	0.40
1:m:489:SER:HB2	1:m:532:LYS:HG2	2.02	0.40
1:n:526:HIS:CD2	1:n:530:GLU:O	2.75	0.40
1:o:477:TRP:O	1:o:478:LEU:HD12	2.21	0.40
1:q:339:THR:HG22	1:q:404:ARG:HG3	2.04	0.40
1:r:321:LYS:HE2	1:r:334:ASN:OD1	2.21	0.40
1:r:477:TRP:O	1:r:478:LEU:HD12	2.21	0.40
1:r:613:LEU:HB3	1:r:614:GLN:OE1	2.21	0.40
1:s:485:GLN:NE2	1:s:506:THR:HG21	2.36	0.40
1:u:477:TRP:O	1:u:478:LEU:HD12	2.21	0.40
1:w:477:TRP:O	1:w:478:LEU:HD12	2.21	0.40
1:w:614:GLN:OE1	1:w:614:GLN:N	2.55	0.40
1:x:733:ARG:HG2	1:x:734:ASN:N	2.36	0.40
1:y:517:VAL:HG23	1:y:517:VAL:O	2.21	0.40
1:y:526:HIS:CD2	1:y:530:GLU:O	2.75	0.40
1:z:379:THR:HG22	1:z:380:LEU:H	1.87	0.40
1:z:485:GLN:NE2	1:z:506:THR:HG21	2.36	0.40
1:z:565:ILE:HG22	1:z:565:ILE:O	2.21	0.40
1:1:479:PRO:O	1:1:604:MET:HG3	2.20	0.40
1:3:345:ASP:C	1:3:347:GLU:H	2.28	0.40
1:4:565:ILE:HG22	1:4:565:ILE:O	2.21	0.40
1:6:477:TRP:O	1:6:478:LEU:HD12	2.21	0.40
1:7:517:VAL:HG23	1:7:517:VAL:O	2.21	0.40
1:8:526:HIS:CD2	1:8:530:GLU:O	2.75	0.40
1:C:435:ASN:HB2	1:Y:353:VAL:CG1	2.52	0.40
1:C:535:PRO:HB2	1:C:538:GLY:HA3	2.02	0.40
1:C:565:ILE:HG22	1:C:565:ILE:O	2.21	0.40
1:D:339:THR:HG22	1:D:404:ARG:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:371:MET:CE	1:P:662:SER:H	2.35	0.40
1:F:371:MET:HG3	1:P:666:PHE:HZ	1.87	0.40
1:H:339:THR:HG22	1:H:404:ARG:HG3	2.04	0.40
1:H:379:THR:HG22	1:H:380:LEU:H	1.87	0.40
1:I:614:GLN:OE1	1:I:614:GLN:N	2.55	0.40
1:J:321:LYS:HE2	1:J:334:ASN:OD1	2.21	0.40
1:J:526:HIS:CD2	1:J:530:GLU:O	2.75	0.40
1:N:379:THR:HG22	1:N:380:LEU:H	1.87	0.40
1:N:699:GLN:H	1:i:701:THR:HG23	1.87	0.40
1:O:614:GLN:OE1	1:O:614:GLN:N	2.55	0.40
1:P:605:VAL:HG12	1:X:627:HIS:HB3	2.03	0.40
1:P:733:ARG:HG2	1:P:734:ASN:N	2.36	0.40
1:Q:565:ILE:HG22	1:Q:565:ILE:O	2.21	0.40
1:S:526:HIS:CD2	1:S:530:GLU:O	2.75	0.40
1:T:321:LYS:HE2	1:T:334:ASN:OD1	2.21	0.40
1:U:526:HIS:CD2	1:U:530:GLU:O	2.75	0.40
1:V:321:LYS:HE2	1:V:334:ASN:OD1	2.21	0.40
1:V:398:PHE:CZ	1:w:692:LYS:HG3	2.56	0.40
1:W:339:THR:HG22	1:W:404:ARG:HG3	2.04	0.40
1:W:526:HIS:CD2	1:W:530:GLU:O	2.75	0.40
1:W:614:GLN:OE1	1:W:614:GLN:N	2.55	0.40
1:X:535:PRO:HB2	1:X:538:GLY:HA3	2.02	0.40
1:Y:517:VAL:O	1:Y:517:VAL:HG23	2.21	0.40
1:Y:699:GLN:H	1:7:701:THR:HG23	1.87	0.40
1:Z:713:THR:HG22	1:Z:714:VAL:N	2.36	0.40
1:a:565:ILE:HG22	1:a:565:ILE:O	2.21	0.40
1:b:477:TRP:O	1:b:478:LEU:HD12	2.21	0.40
1:e:379:THR:HG22	1:e:380:LEU:H	1.87	0.40
1:e:517:VAL:O	1:e:517:VAL:HG23	2.21	0.40
1:g:321:LYS:HE2	1:g:334:ASN:OD1	2.21	0.40
1:g:698:ILE:HD12	1:7:389:ARG:HG2	2.04	0.40
1:h:339:THR:HG22	1:h:404:ARG:HG3	2.04	0.40
1:i:379:THR:HG22	1:i:380:LEU:H	1.87	0.40
1:i:542:PHE:O	1:i:558:MET:N	2.29	0.40
1:j:733:ARG:HG2	1:j:734:ASN:N	2.36	0.40
1:k:339:THR:HG22	1:k:404:ARG:HG3	2.04	0.40
1:k:379:THR:HG22	1:k:380:LEU:H	1.87	0.40
1:l:614:GLN:OE1	1:l:614:GLN:N	2.55	0.40
1:m:321:LYS:HE2	1:m:334:ASN:OD1	2.21	0.40
1:n:535:PRO:HB2	1:n:538:GLY:HA3	2.02	0.40
1:n:713:THR:HG22	1:n:714:VAL:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:535:PRO:HB2	1:o:538:GLY:HA3	2.02	0.40
1:o:713:THR:HG22	1:o:714:VAL:N	2.36	0.40
1:q:379:THR:HG22	1:q:380:LEU:H	1.87	0.40
1:s:526:HIS:CD2	1:s:530:GLU:O	2.75	0.40
1:t:565:ILE:HG22	1:t:565:ILE:O	2.21	0.40
1:u:395:LEU:HA	1:u:395:LEU:HD23	1.93	0.40
1:u:614:GLN:OE1	1:u:614:GLN:N	2.55	0.40
1:y:485:GLN:NE2	1:y:506:THR:HG21	2.36	0.40
1:z:477:TRP:O	1:z:478:LEU:HD12	2.21	0.40
1:z:526:HIS:CD2	1:z:530:GLU:O	2.75	0.40
1:1:565:ILE:HG23	1:1:607:GLN:HB2	2.04	0.40
1:2:526:HIS:CD2	1:2:530:GLU:O	2.75	0.40
1:6:526:HIS:CD2	1:6:530:GLU:O	2.75	0.40
1:6:614:GLN:OE1	1:6:614:GLN:N	2.55	0.40
1:7:565:ILE:HG22	1:7:565:ILE:O	2.21	0.40
1:A:371:MET:HG3	1:H:666:PHE:HZ	1.87	0.40
1:A:477:TRP:O	1:A:478:LEU:HD12	2.21	0.40
1:A:666:PHE:HZ	1:Q:371:MET:HG3	1.86	0.40
1:C:321:LYS:HE2	1:C:334:ASN:OD1	2.21	0.40
1:C:379:THR:HG22	1:C:380:LEU:H	1.87	0.40
1:C:398:PHE:CE1	1:t:692:LYS:HE2	2.57	0.40
1:C:627:HIS:HB3	1:t:605:VAL:HG12	2.03	0.40
1:D:613:LEU:HB3	1:D:614:GLN:OE1	2.21	0.40
1:E:379:THR:HG22	1:E:380:LEU:H	1.87	0.40
1:F:485:GLN:NE2	1:F:506:THR:HG21	2.36	0.40
1:F:580:SER:O	1:3:484:ARG:HD3	2.22	0.40
1:F:613:LEU:HB3	1:F:614:GLN:OE1	2.21	0.40
1:F:733:ARG:HG2	1:F:734:ASN:N	2.36	0.40
1:H:526:HIS:CD2	1:H:530:GLU:O	2.75	0.40
1:I:234:TRP:CG	1:I:298[A]:ARG:HD3	2.57	0.40
1:K:526:HIS:CD2	1:K:530:GLU:O	2.75	0.40
1:K:627:HIS:HB3	1:X:605:VAL:HG12	2.03	0.40
1:N:627:HIS:HB3	1:V:605:VAL:HG12	2.03	0.40
1:O:613:LEU:HB3	1:O:614:GLN:OE1	2.21	0.40
1:P:321:LYS:HE2	1:P:334:ASN:OD1	2.21	0.40
1:P:365:PHE:HA	1:P:366:PRO:HD3	1.92	0.40
1:Q:321:LYS:HE2	1:Q:334:ASN:OD1	2.21	0.40
1:Q:379:THR:HG22	1:Q:380:LEU:H	1.87	0.40
1:Q:733:ARG:HG2	1:Q:734:ASN:N	2.36	0.40
1:R:627:HIS:HB3	1:r:605:VAL:HG12	2.04	0.40
1:T:485:GLN:NE2	1:T:506:THR:HG21	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:489:SER:HB2	1:T:532:LYS:HG2	2.02	0.40
1:T:565:ILE:HG22	1:T:565:ILE:O	2.21	0.40
1:T:614:GLN:OE1	1:T:614:GLN:N	2.55	0.40
1:Y:565:ILE:HG22	1:Y:565:ILE:O	2.21	0.40
1:Z:339:THR:HG22	1:Z:404:ARG:HG3	2.04	0.40
1:a:398:PHE:CZ	1:y:692:LYS:HG3	2.57	0.40
1:a:479:PRO:O	1:a:604:MET:HG3	2.20	0.40
1:a:526:HIS:CD2	1:a:530:GLU:O	2.75	0.40
1:b:565:ILE:HG23	1:b:607:GLN:HB2	2.04	0.40
1:c:371:MET:HG3	1:6:666:PHE:HZ	1.86	0.40
1:c:379:THR:HG22	1:c:380:LEU:H	1.87	0.40
1:c:485:GLN:NE2	1:c:506:THR:HG21	2.36	0.40
1:e:461:GLN:HB3	1:y:551:ASN:HA	2.04	0.40
1:f:379:THR:HG22	1:f:380:LEU:H	1.87	0.40
1:f:389:ARG:HG2	1:n:698:ILE:HD12	2.04	0.40
1:f:565:ILE:HG23	1:f:607:GLN:HB2	2.04	0.40
1:g:234:TRP:HB3	1:g:298[A]:ARG:NE	2.37	0.40
1:g:535:PRO:HB2	1:g:538:GLY:HA3	2.02	0.40
1:g:614:GLN:OE1	1:g:614:GLN:N	2.55	0.40
1:j:321:LYS:HE2	1:j:334:ASN:OD1	2.21	0.40
1:l:431:ASP:OD2	1:u:513:ARG:HD2	2.21	0.40
1:l:477:TRP:O	1:l:478:LEU:HD12	2.21	0.40
1:l:542:PHE:O	1:l:558:MET:N	2.30	0.40
1:m:485:GLN:NE2	1:m:506:THR:HG21	2.36	0.40
1:m:614:GLN:OE1	1:m:614:GLN:N	2.55	0.40
1:n:395:LEU:HD23	1:n:395:LEU:HA	1.93	0.40
1:o:565:ILE:HG23	1:o:607:GLN:HB2	2.04	0.40
1:p:321:LYS:HE2	1:p:334:ASN:OD1	2.21	0.40
1:p:565:ILE:HG23	1:p:607:GLN:HB2	2.04	0.40
1:q:526:HIS:CD2	1:q:530:GLU:O	2.75	0.40
1:r:339:THR:HG22	1:r:404:ARG:HG3	2.04	0.40
1:r:526:HIS:CD2	1:r:530:GLU:O	2.75	0.40
1:t:713:THR:HG22	1:t:714:VAL:N	2.36	0.40
1:x:379:THR:HG22	1:x:380:LEU:H	1.87	0.40
1:y:613:LEU:HB3	1:y:614:GLN:OE1	2.21	0.40
1:y:733:ARG:HG2	1:y:734:ASN:N	2.36	0.40
1:2:614:GLN:OE1	1:2:614:GLN:N	2.55	0.40
1:2:713:THR:HG22	1:2:714:VAL:N	2.36	0.40
1:3:517:VAL:HG23	1:3:517:VAL:O	2.21	0.40
1:5:339:THR:HG22	1:5:404:ARG:HG3	2.04	0.40
1:5:379:THR:HG22	1:5:380:LEU:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:339:THR:HG22	1:6:404:ARG:HG3	2.04	0.40
1:6:345:ASP:O	1:6:346:SER:OG	2.32	0.40
1:8:339:THR:HG22	1:8:404:ARG:HG3	2.04	0.40
1:8:565:ILE:HG22	1:8:565:ILE:O	2.21	0.40
1:8:713:THR:HG22	1:8:714:VAL:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	2	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	3	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	4	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	5	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	6	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	7	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	8	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	A	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	B	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	C	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	D	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	E	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	F	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	G	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	H	519/735 (71%)	499 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	J	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	K	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	L	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	M	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	N	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	O	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	P	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	Q	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	R	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	S	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	T	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	U	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	V	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	W	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	X	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	Y	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	Z	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	a	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	b	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	c	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	d	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	e	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	f	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	g	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	h	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	i	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	j	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	k	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	l	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	m	519/735 (71%)	500 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	n	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	o	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	p	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	q	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	r	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	s	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	t	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	u	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	v	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	w	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	x	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	y	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	z	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
All	All	31140/44100 (71%)	29964 (96%)	1176 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	2	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	3	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	4	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	5	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	6	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	7	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	8	461/630 (73%)	459 (100%)	2 (0%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	B	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	C	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	D	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	E	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	F	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	G	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	H	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	I	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	J	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	K	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	L	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	M	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	N	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	O	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	P	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	Q	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	R	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	S	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	T	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	U	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	V	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	W	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	X	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	Y	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	Z	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	a	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	b	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	c	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	d	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	e	461/630 (73%)	459 (100%)	2 (0%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	f	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	g	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	h	461/630 (73%)	461 (100%)	0	100	100
1	i	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	j	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	k	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	l	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	m	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	n	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	o	461/630 (73%)	461 (100%)	0	100	100
1	p	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	q	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	r	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	s	461/630 (73%)	461 (100%)	0	100	100
1	t	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	u	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	v	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	w	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	x	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	y	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	z	461/630 (73%)	461 (100%)	0	100	100
All	All	27660/37800 (73%)	27532 (100%)	128 (0%)	85	90

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298[A]	ARG
1	A	298[B]	ARG
1	B	298[A]	ARG
1	B	298[B]	ARG
1	C	298[A]	ARG
1	C	298[B]	ARG
1	D	298[A]	ARG
1	D	298[B]	ARG
1	E	298[A]	ARG

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Mol	Chain	Res	Type
1	E	298[B]	ARG
1	F	298[A]	ARG
1	F	298[B]	ARG
1	G	298[A]	ARG
1	G	298[B]	ARG
1	H	298[A]	ARG
1	H	298[B]	ARG
1	I	298[A]	ARG
1	I	298[B]	ARG
1	J	298[A]	ARG
1	J	298[B]	ARG
1	K	238[A]	ARG
1	K	238[B]	ARG
1	K	298[A]	ARG
1	K	298[B]	ARG
1	L	298[A]	ARG
1	L	298[B]	ARG
1	M	298[A]	ARG
1	M	298[B]	ARG
1	N	298[A]	ARG
1	N	298[B]	ARG
1	O	298[A]	ARG
1	O	298[B]	ARG
1	P	298[A]	ARG
1	P	298[B]	ARG
1	Q	298[A]	ARG
1	Q	298[B]	ARG
1	R	298[A]	ARG
1	R	298[B]	ARG
1	S	298[A]	ARG
1	S	298[B]	ARG
1	T	238[A]	ARG
1	T	238[B]	ARG
1	T	298[A]	ARG
1	T	298[B]	ARG
1	U	298[A]	ARG
1	U	298[B]	ARG
1	V	298[A]	ARG
1	V	298[B]	ARG
1	W	298[A]	ARG
1	W	298[B]	ARG
1	X	298[A]	ARG

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Mol	Chain	Res	Type
1	X	298[B]	ARG
1	Y	298[A]	ARG
1	Y	298[B]	ARG
1	Z	298[A]	ARG
1	Z	298[B]	ARG
1	a	298[A]	ARG
1	a	298[B]	ARG
1	b	298[A]	ARG
1	b	298[B]	ARG
1	c	238[A]	ARG
1	c	238[B]	ARG
1	c	298[A]	ARG
1	c	298[B]	ARG
1	d	298[A]	ARG
1	d	298[B]	ARG
1	e	298[A]	ARG
1	e	298[B]	ARG
1	f	238[A]	ARG
1	f	238[B]	ARG
1	f	298[A]	ARG
1	f	298[B]	ARG
1	g	298[A]	ARG
1	g	298[B]	ARG
1	i	238[A]	ARG
1	i	238[B]	ARG
1	i	298[A]	ARG
1	i	298[B]	ARG
1	j	298[A]	ARG
1	j	298[B]	ARG
1	k	298[A]	ARG
1	k	298[B]	ARG
1	l	298[A]	ARG
1	l	298[B]	ARG
1	m	298[A]	ARG
1	m	298[B]	ARG
1	n	298[A]	ARG
1	n	298[B]	ARG
1	p	298[A]	ARG
1	p	298[B]	ARG
1	q	298[A]	ARG
1	q	298[B]	ARG
1	r	238[A]	ARG

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Mol	Chain	Res	Type
1	r	238[B]	ARG
1	t	238[A]	ARG
1	t	238[B]	ARG
1	t	298[A]	ARG
1	t	298[B]	ARG
1	u	238[A]	ARG
1	u	238[B]	ARG
1	v	298[A]	ARG
1	v	298[B]	ARG
1	w	238[A]	ARG
1	w	238[B]	ARG
1	w	298[A]	ARG
1	w	298[B]	ARG
1	x	238[A]	ARG
1	x	238[B]	ARG
1	y	298[A]	ARG
1	y	298[B]	ARG
1	1	298[A]	ARG
1	1	298[B]	ARG
1	2	238[A]	ARG
1	2	238[B]	ARG
1	3	298[A]	ARG
1	3	298[B]	ARG
1	4	298[A]	ARG
1	4	298[B]	ARG
1	5	298[A]	ARG
1	5	298[B]	ARG
1	6	298[A]	ARG
1	6	298[B]	ARG
1	7	238[A]	ARG
1	7	238[B]	ARG
1	7	298[A]	ARG
1	7	298[B]	ARG
1	8	298[A]	ARG
1	8	298[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (861) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	A	271	HIS
1	A	312	ASN

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Mol	Chain	Res	Type
1	A	326	ASN
1	A	407	ASN
1	A	421	HIS
1	A	426	HIS
1	A	428	GLN
1	A	485	GLN
1	A	518	ASN
1	A	629	HIS
1	A	645	GLN
1	B	229	HIS
1	B	271	HIS
1	B	302	ASN
1	B	312	ASN
1	B	326	ASN
1	B	407	ASN
1	B	421	HIS
1	B	426	HIS
1	B	428	GLN
1	B	485	GLN
1	B	518	ASN
1	B	584	GLN
1	B	629	HIS
1	B	645	GLN
1	C	229	HIS
1	C	271	HIS
1	C	302	ASN
1	C	312	ASN
1	C	326	ASN
1	C	407	ASN
1	C	421	HIS
1	C	426	HIS
1	C	428	GLN
1	C	485	GLN
1	C	518	ASN
1	C	584	GLN
1	C	629	HIS
1	C	641	HIS
1	C	645	GLN
1	C	717	ASN
1	D	229	HIS
1	D	271	HIS
1	D	312	ASN

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Mol	Chain	Res	Type
1	D	326	ASN
1	D	407	ASN
1	D	421	HIS
1	D	426	HIS
1	D	428	GLN
1	D	485	GLN
1	D	518	ASN
1	D	584	GLN
1	D	629	HIS
1	D	641	HIS
1	D	645	GLN
1	E	229	HIS
1	E	271	HIS
1	E	302	ASN
1	E	312	ASN
1	E	326	ASN
1	E	407	ASN
1	E	421	HIS
1	E	426	HIS
1	E	428	GLN
1	E	485	GLN
1	E	518	ASN
1	E	584	GLN
1	E	629	HIS
1	E	641	HIS
1	E	645	GLN
1	F	229	HIS
1	F	271	HIS
1	F	312	ASN
1	F	326	ASN
1	F	407	ASN
1	F	421	HIS
1	F	426	HIS
1	F	428	GLN
1	F	485	GLN
1	F	518	ASN
1	F	584	GLN
1	F	629	HIS
1	F	645	GLN
1	F	717	ASN
1	G	229	HIS
1	G	271	HIS

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Mol	Chain	Res	Type
1	G	302	ASN
1	G	312	ASN
1	G	326	ASN
1	G	407	ASN
1	G	421	HIS
1	G	426	HIS
1	G	428	GLN
1	G	485	GLN
1	G	518	ASN
1	G	584	GLN
1	G	629	HIS
1	G	641	HIS
1	G	645	GLN
1	G	717	ASN
1	H	229	HIS
1	H	271	HIS
1	H	302	ASN
1	H	312	ASN
1	H	326	ASN
1	H	407	ASN
1	H	421	HIS
1	H	426	HIS
1	H	428	GLN
1	H	485	GLN
1	H	518	ASN
1	H	584	GLN
1	H	629	HIS
1	H	645	GLN
1	H	717	ASN
1	I	229	HIS
1	I	271	HIS
1	I	302	ASN
1	I	326	ASN
1	I	407	ASN
1	I	421	HIS
1	I	426	HIS
1	I	428	GLN
1	I	485	GLN
1	I	518	ASN
1	I	584	GLN
1	I	629	HIS
1	I	641	HIS

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Mol	Chain	Res	Type
1	I	645	GLN
1	I	717	ASN
1	J	229	HIS
1	J	271	HIS
1	J	312	ASN
1	J	326	ASN
1	J	407	ASN
1	J	421	HIS
1	J	426	HIS
1	J	428	GLN
1	J	485	GLN
1	J	518	ASN
1	J	584	GLN
1	J	629	HIS
1	J	641	HIS
1	J	645	GLN
1	J	717	ASN
1	K	229	HIS
1	K	271	HIS
1	K	302	ASN
1	K	326	ASN
1	K	407	ASN
1	K	421	HIS
1	K	426	HIS
1	K	428	GLN
1	K	485	GLN
1	K	518	ASN
1	K	584	GLN
1	K	629	HIS
1	K	641	HIS
1	K	645	GLN
1	K	717	ASN
1	L	229	HIS
1	L	271	HIS
1	L	302	ASN
1	L	326	ASN
1	L	407	ASN
1	L	421	HIS
1	L	426	HIS
1	L	428	GLN
1	L	485	GLN
1	L	518	ASN

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Mol	Chain	Res	Type
1	L	584	GLN
1	L	629	HIS
1	L	641	HIS
1	L	645	GLN
1	L	717	ASN
1	M	229	HIS
1	M	271	HIS
1	M	312	ASN
1	M	326	ASN
1	M	407	ASN
1	M	421	HIS
1	M	426	HIS
1	M	428	GLN
1	M	485	GLN
1	M	518	ASN
1	M	584	GLN
1	M	629	HIS
1	M	645	GLN
1	N	229	HIS
1	N	271	HIS
1	N	302	ASN
1	N	312	ASN
1	N	326	ASN
1	N	407	ASN
1	N	421	HIS
1	N	426	HIS
1	N	428	GLN
1	N	485	GLN
1	N	518	ASN
1	N	584	GLN
1	N	629	HIS
1	N	645	GLN
1	N	717	ASN
1	O	229	HIS
1	O	271	HIS
1	O	312	ASN
1	O	326	ASN
1	O	407	ASN
1	O	421	HIS
1	O	426	HIS
1	O	428	GLN
1	O	485	GLN

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Mol	Chain	Res	Type
1	O	518	ASN
1	O	584	GLN
1	O	629	HIS
1	O	645	GLN
1	O	717	ASN
1	P	229	HIS
1	P	271	HIS
1	P	312	ASN
1	P	326	ASN
1	P	407	ASN
1	P	421	HIS
1	P	426	HIS
1	P	428	GLN
1	P	485	GLN
1	P	518	ASN
1	P	584	GLN
1	P	629	HIS
1	P	645	GLN
1	Q	229	HIS
1	Q	271	HIS
1	Q	302	ASN
1	Q	312	ASN
1	Q	326	ASN
1	Q	407	ASN
1	Q	421	HIS
1	Q	426	HIS
1	Q	428	GLN
1	Q	485	GLN
1	Q	518	ASN
1	Q	584	GLN
1	Q	629	HIS
1	Q	641	HIS
1	Q	645	GLN
1	R	229	HIS
1	R	271	HIS
1	R	302	ASN
1	R	326	ASN
1	R	407	ASN
1	R	421	HIS
1	R	426	HIS
1	R	428	GLN
1	R	485	GLN

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Mol	Chain	Res	Type
1	R	518	ASN
1	R	584	GLN
1	R	629	HIS
1	R	645	GLN
1	S	229	HIS
1	S	271	HIS
1	S	312	ASN
1	S	326	ASN
1	S	407	ASN
1	S	421	HIS
1	S	426	HIS
1	S	428	GLN
1	S	485	GLN
1	S	518	ASN
1	S	584	GLN
1	S	629	HIS
1	S	641	HIS
1	S	645	GLN
1	T	229	HIS
1	T	271	HIS
1	T	302	ASN
1	T	312	ASN
1	T	326	ASN
1	T	407	ASN
1	T	421	HIS
1	T	426	HIS
1	T	428	GLN
1	T	485	GLN
1	T	518	ASN
1	T	584	GLN
1	T	629	HIS
1	T	645	GLN
1	U	229	HIS
1	U	271	HIS
1	U	302	ASN
1	U	312	ASN
1	U	326	ASN
1	U	407	ASN
1	U	421	HIS
1	U	426	HIS
1	U	428	GLN
1	U	485	GLN

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Mol	Chain	Res	Type
1	U	518	ASN
1	U	584	GLN
1	U	629	HIS
1	U	641	HIS
1	U	645	GLN
1	V	229	HIS
1	V	271	HIS
1	V	302	ASN
1	V	312	ASN
1	V	326	ASN
1	V	407	ASN
1	V	421	HIS
1	V	426	HIS
1	V	428	GLN
1	V	485	GLN
1	V	518	ASN
1	V	584	GLN
1	V	629	HIS
1	V	645	GLN
1	V	717	ASN
1	W	229	HIS
1	W	271	HIS
1	W	312	ASN
1	W	326	ASN
1	W	407	ASN
1	W	421	HIS
1	W	426	HIS
1	W	428	GLN
1	W	485	GLN
1	W	518	ASN
1	W	584	GLN
1	W	629	HIS
1	W	645	GLN
1	W	717	ASN
1	X	229	HIS
1	X	271	HIS
1	X	312	ASN
1	X	326	ASN
1	X	407	ASN
1	X	421	HIS
1	X	426	HIS
1	X	428	GLN

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Mol	Chain	Res	Type
1	X	485	GLN
1	X	518	ASN
1	X	584	GLN
1	X	629	HIS
1	X	641	HIS
1	X	645	GLN
1	Y	229	HIS
1	Y	271	HIS
1	Y	302	ASN
1	Y	326	ASN
1	Y	407	ASN
1	Y	421	HIS
1	Y	426	HIS
1	Y	428	GLN
1	Y	485	GLN
1	Y	518	ASN
1	Y	584	GLN
1	Y	629	HIS
1	Y	645	GLN
1	Y	717	ASN
1	Z	229	HIS
1	Z	271	HIS
1	Z	326	ASN
1	Z	407	ASN
1	Z	421	HIS
1	Z	426	HIS
1	Z	428	GLN
1	Z	485	GLN
1	Z	518	ASN
1	Z	584	GLN
1	Z	629	HIS
1	Z	645	GLN
1	Z	717	ASN
1	a	229	HIS
1	a	271	HIS
1	a	302	ASN
1	a	312	ASN
1	a	326	ASN
1	a	407	ASN
1	a	421	HIS
1	a	426	HIS
1	a	428	GLN

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Mol	Chain	Res	Type
1	a	485	GLN
1	a	518	ASN
1	a	584	GLN
1	a	629	HIS
1	a	645	GLN
1	a	717	ASN
1	b	229	HIS
1	b	271	HIS
1	b	302	ASN
1	b	312	ASN
1	b	326	ASN
1	b	407	ASN
1	b	421	HIS
1	b	426	HIS
1	b	428	GLN
1	b	485	GLN
1	b	518	ASN
1	b	584	GLN
1	b	629	HIS
1	b	641	HIS
1	b	645	GLN
1	b	717	ASN
1	c	229	HIS
1	c	271	HIS
1	c	312	ASN
1	c	326	ASN
1	c	407	ASN
1	c	421	HIS
1	c	426	HIS
1	c	428	GLN
1	c	485	GLN
1	c	518	ASN
1	c	584	GLN
1	c	629	HIS
1	c	645	GLN
1	c	717	ASN
1	d	229	HIS
1	d	271	HIS
1	d	302	ASN
1	d	312	ASN
1	d	326	ASN
1	d	407	ASN

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Mol	Chain	Res	Type
1	d	421	HIS
1	d	426	HIS
1	d	428	GLN
1	d	485	GLN
1	d	518	ASN
1	d	584	GLN
1	d	629	HIS
1	d	641	HIS
1	d	645	GLN
1	d	717	ASN
1	e	229	HIS
1	e	271	HIS
1	e	302	ASN
1	e	312	ASN
1	e	326	ASN
1	e	407	ASN
1	e	421	HIS
1	e	426	HIS
1	e	428	GLN
1	e	485	GLN
1	e	518	ASN
1	e	584	GLN
1	e	629	HIS
1	e	645	GLN
1	e	717	ASN
1	f	229	HIS
1	f	271	HIS
1	f	312	ASN
1	f	326	ASN
1	f	407	ASN
1	f	421	HIS
1	f	426	HIS
1	f	428	GLN
1	f	485	GLN
1	f	518	ASN
1	f	584	GLN
1	f	629	HIS
1	f	641	HIS
1	f	645	GLN
1	f	717	ASN
1	g	229	HIS
1	g	271	HIS

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Mol	Chain	Res	Type
1	g	312	ASN
1	g	326	ASN
1	g	407	ASN
1	g	421	HIS
1	g	426	HIS
1	g	428	GLN
1	g	485	GLN
1	g	518	ASN
1	g	584	GLN
1	g	629	HIS
1	g	641	HIS
1	g	645	GLN
1	g	717	ASN
1	h	229	HIS
1	h	271	HIS
1	h	302	ASN
1	h	312	ASN
1	h	326	ASN
1	h	407	ASN
1	h	421	HIS
1	h	426	HIS
1	h	428	GLN
1	h	485	GLN
1	h	518	ASN
1	h	584	GLN
1	h	629	HIS
1	h	645	GLN
1	i	229	HIS
1	i	271	HIS
1	i	312	ASN
1	i	326	ASN
1	i	407	ASN
1	i	421	HIS
1	i	426	HIS
1	i	428	GLN
1	i	485	GLN
1	i	518	ASN
1	i	584	GLN
1	i	629	HIS
1	i	645	GLN
1	i	717	ASN
1	j	229	HIS

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Mol	Chain	Res	Type
1	j	271	HIS
1	j	302	ASN
1	j	312	ASN
1	j	326	ASN
1	j	407	ASN
1	j	421	HIS
1	j	426	HIS
1	j	428	GLN
1	j	485	GLN
1	j	518	ASN
1	j	584	GLN
1	j	629	HIS
1	j	645	GLN
1	k	229	HIS
1	k	271	HIS
1	k	302	ASN
1	k	312	ASN
1	k	326	ASN
1	k	407	ASN
1	k	421	HIS
1	k	426	HIS
1	k	428	GLN
1	k	485	GLN
1	k	518	ASN
1	k	584	GLN
1	k	629	HIS
1	k	641	HIS
1	k	645	GLN
1	l	229	HIS
1	l	271	HIS
1	l	302	ASN
1	l	312	ASN
1	l	326	ASN
1	l	407	ASN
1	l	421	HIS
1	l	426	HIS
1	l	428	GLN
1	l	485	GLN
1	l	518	ASN
1	l	584	GLN
1	l	629	HIS
1	l	645	GLN

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Mol	Chain	Res	Type
1	l	717	ASN
1	m	229	HIS
1	m	271	HIS
1	m	302	ASN
1	m	312	ASN
1	m	326	ASN
1	m	407	ASN
1	m	421	HIS
1	m	426	HIS
1	m	428	GLN
1	m	485	GLN
1	m	518	ASN
1	m	584	GLN
1	m	629	HIS
1	m	645	GLN
1	n	229	HIS
1	n	271	HIS
1	n	312	ASN
1	n	326	ASN
1	n	407	ASN
1	n	421	HIS
1	n	426	HIS
1	n	428	GLN
1	n	485	GLN
1	n	518	ASN
1	n	584	GLN
1	n	629	HIS
1	n	641	HIS
1	n	645	GLN
1	o	229	HIS
1	o	271	HIS
1	o	312	ASN
1	o	326	ASN
1	o	407	ASN
1	o	421	HIS
1	o	426	HIS
1	o	428	GLN
1	o	485	GLN
1	o	518	ASN
1	o	584	GLN
1	o	629	HIS
1	o	641	HIS

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Mol	Chain	Res	Type
1	o	645	GLN
1	o	717	ASN
1	p	229	HIS
1	p	271	HIS
1	p	312	ASN
1	p	326	ASN
1	p	407	ASN
1	p	421	HIS
1	p	426	HIS
1	p	428	GLN
1	p	485	GLN
1	p	518	ASN
1	p	584	GLN
1	p	629	HIS
1	p	645	GLN
1	p	717	ASN
1	q	229	HIS
1	q	271	HIS
1	q	326	ASN
1	q	407	ASN
1	q	421	HIS
1	q	426	HIS
1	q	428	GLN
1	q	485	GLN
1	q	518	ASN
1	q	584	GLN
1	q	629	HIS
1	q	645	GLN
1	r	229	HIS
1	r	271	HIS
1	r	312	ASN
1	r	326	ASN
1	r	407	ASN
1	r	421	HIS
1	r	426	HIS
1	r	428	GLN
1	r	485	GLN
1	r	518	ASN
1	r	584	GLN
1	r	629	HIS
1	r	641	HIS
1	r	645	GLN

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Mol	Chain	Res	Type
1	s	229	HIS
1	s	271	HIS
1	s	312	ASN
1	s	326	ASN
1	s	407	ASN
1	s	421	HIS
1	s	426	HIS
1	s	428	GLN
1	s	485	GLN
1	s	518	ASN
1	s	584	GLN
1	s	629	HIS
1	s	641	HIS
1	s	645	GLN
1	t	229	HIS
1	t	271	HIS
1	t	302	ASN
1	t	312	ASN
1	t	326	ASN
1	t	407	ASN
1	t	421	HIS
1	t	426	HIS
1	t	428	GLN
1	t	485	GLN
1	t	518	ASN
1	t	584	GLN
1	t	629	HIS
1	t	645	GLN
1	t	717	ASN
1	u	229	HIS
1	u	271	HIS
1	u	326	ASN
1	u	407	ASN
1	u	421	HIS
1	u	426	HIS
1	u	428	GLN
1	u	485	GLN
1	u	518	ASN
1	u	584	GLN
1	u	629	HIS
1	u	641	HIS
1	u	645	GLN

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Mol	Chain	Res	Type
1	u	717	ASN
1	v	229	HIS
1	v	271	HIS
1	v	312	ASN
1	v	326	ASN
1	v	407	ASN
1	v	421	HIS
1	v	426	HIS
1	v	428	GLN
1	v	485	GLN
1	v	518	ASN
1	v	584	GLN
1	v	629	HIS
1	v	645	GLN
1	w	229	HIS
1	w	271	HIS
1	w	302	ASN
1	w	326	ASN
1	w	407	ASN
1	w	421	HIS
1	w	426	HIS
1	w	428	GLN
1	w	485	GLN
1	w	518	ASN
1	w	584	GLN
1	w	629	HIS
1	w	641	HIS
1	w	645	GLN
1	x	229	HIS
1	x	271	HIS
1	x	312	ASN
1	x	326	ASN
1	x	407	ASN
1	x	421	HIS
1	x	426	HIS
1	x	428	GLN
1	x	485	GLN
1	x	518	ASN
1	x	584	GLN
1	x	629	HIS
1	x	641	HIS
1	x	645	GLN

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Mol	Chain	Res	Type
1	x	717	ASN
1	y	229	HIS
1	y	271	HIS
1	y	312	ASN
1	y	326	ASN
1	y	407	ASN
1	y	421	HIS
1	y	426	HIS
1	y	428	GLN
1	y	485	GLN
1	y	518	ASN
1	y	584	GLN
1	y	629	HIS
1	y	645	GLN
1	y	717	ASN
1	z	229	HIS
1	z	271	HIS
1	z	326	ASN
1	z	407	ASN
1	z	421	HIS
1	z	426	HIS
1	z	428	GLN
1	z	485	GLN
1	z	518	ASN
1	z	584	GLN
1	z	629	HIS
1	z	641	HIS
1	z	645	GLN
1	z	717	ASN
1	1	229	HIS
1	1	271	HIS
1	1	302	ASN
1	1	312	ASN
1	1	326	ASN
1	1	407	ASN
1	1	421	HIS
1	1	426	HIS
1	1	428	GLN
1	1	485	GLN
1	1	518	ASN
1	1	584	GLN
1	1	629	HIS

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Mol	Chain	Res	Type
1	1	645	GLN
1	2	229	HIS
1	2	271	HIS
1	2	312	ASN
1	2	326	ASN
1	2	407	ASN
1	2	421	HIS
1	2	426	HIS
1	2	428	GLN
1	2	485	GLN
1	2	518	ASN
1	2	584	GLN
1	2	629	HIS
1	2	641	HIS
1	2	645	GLN
1	2	717	ASN
1	3	229	HIS
1	3	271	HIS
1	3	312	ASN
1	3	326	ASN
1	3	407	ASN
1	3	421	HIS
1	3	426	HIS
1	3	428	GLN
1	3	485	GLN
1	3	518	ASN
1	3	584	GLN
1	3	629	HIS
1	3	645	GLN
1	3	717	ASN
1	4	229	HIS
1	4	271	HIS
1	4	302	ASN
1	4	326	ASN
1	4	407	ASN
1	4	421	HIS
1	4	426	HIS
1	4	428	GLN
1	4	485	GLN
1	4	518	ASN
1	4	584	GLN
1	4	629	HIS

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Mol	Chain	Res	Type
1	4	645	GLN
1	4	717	ASN
1	5	229	HIS
1	5	271	HIS
1	5	312	ASN
1	5	326	ASN
1	5	407	ASN
1	5	421	HIS
1	5	426	HIS
1	5	428	GLN
1	5	485	GLN
1	5	518	ASN
1	5	584	GLN
1	5	629	HIS
1	5	645	GLN
1	5	717	ASN
1	6	229	HIS
1	6	271	HIS
1	6	302	ASN
1	6	312	ASN
1	6	326	ASN
1	6	407	ASN
1	6	421	HIS
1	6	426	HIS
1	6	428	GLN
1	6	485	GLN
1	6	518	ASN
1	6	584	GLN
1	6	629	HIS
1	6	645	GLN
1	6	717	ASN
1	7	229	HIS
1	7	271	HIS
1	7	326	ASN
1	7	407	ASN
1	7	421	HIS
1	7	426	HIS
1	7	428	GLN
1	7	485	GLN
1	7	518	ASN
1	7	584	GLN
1	7	629	HIS

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Mol	Chain	Res	Type
1	7	645	GLN
1	7	717	ASN
1	8	229	HIS
1	8	271	HIS
1	8	302	ASN
1	8	312	ASN
1	8	326	ASN
1	8	407	ASN
1	8	421	HIS
1	8	426	HIS
1	8	428	GLN
1	8	485	GLN
1	8	518	ASN
1	8	584	GLN
1	8	629	HIS
1	8	641	HIS
1	8	645	GLN
1	8	717	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](#)

60 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	D5M	e	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	2	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	x	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	W	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	P	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	K	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	L	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	q	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	z	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	M	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	v	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	F	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	4	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	D	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	J	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	p	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	f	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	H	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	m	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	Z	901	-	20,23,24	0.38	0	28,33,36	0.28	0
2	D5M	7	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	a	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	1	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	X	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	i	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	E	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	k	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	t	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	u	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	3	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	T	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	S	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	A	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	R	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	I	901	-	20,23,24	0.38	0	28,33,36	0.28	0
2	D5M	O	901	-	20,23,24	0.37	0	28,33,36	0.28	0
2	D5M	V	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	b	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	G	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	Y	901	-	20,23,24	0.38	0	28,33,36	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	D5M	B	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	C	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	N	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	y	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	c	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	5	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	l	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	j	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	g	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	Q	901	-	20,23,24	0.37	0	28,33,36	0.28	0
2	D5M	d	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	6	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	h	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	U	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	s	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	r	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	n	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	8	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	o	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	w	901	-	20,23,24	0.37	0	28,33,36	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D5M	e	901	-	-	5/7/21/22	0/3/3/3
2	D5M	2	901	-	-	5/7/21/22	0/3/3/3
2	D5M	x	901	-	-	5/7/21/22	0/3/3/3
2	D5M	W	901	-	-	5/7/21/22	0/3/3/3
2	D5M	P	901	-	-	5/7/21/22	0/3/3/3
2	D5M	K	901	-	-	5/7/21/22	0/3/3/3
2	D5M	L	901	-	-	5/7/21/22	0/3/3/3
2	D5M	q	901	-	-	5/7/21/22	0/3/3/3
2	D5M	z	901	-	-	5/7/21/22	0/3/3/3
2	D5M	M	901	-	-	5/7/21/22	0/3/3/3
2	D5M	v	901	-	-	5/7/21/22	0/3/3/3
2	D5M	F	901	-	-	5/7/21/22	0/3/3/3
2	D5M	4	901	-	-	5/7/21/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D5M	D	901	-	-	5/7/21/22	0/3/3/3
2	D5M	J	901	-	-	5/7/21/22	0/3/3/3
2	D5M	p	901	-	-	5/7/21/22	0/3/3/3
2	D5M	f	901	-	-	5/7/21/22	0/3/3/3
2	D5M	H	901	-	-	5/7/21/22	0/3/3/3
2	D5M	m	901	-	-	5/7/21/22	0/3/3/3
2	D5M	Z	901	-	-	5/7/21/22	0/3/3/3
2	D5M	7	901	-	-	5/7/21/22	0/3/3/3
2	D5M	a	901	-	-	5/7/21/22	0/3/3/3
2	D5M	l	901	-	-	5/7/21/22	0/3/3/3
2	D5M	X	901	-	-	5/7/21/22	0/3/3/3
2	D5M	i	901	-	-	5/7/21/22	0/3/3/3
2	D5M	E	901	-	-	5/7/21/22	0/3/3/3
2	D5M	k	901	-	-	5/7/21/22	0/3/3/3
2	D5M	t	901	-	-	5/7/21/22	0/3/3/3
2	D5M	u	901	-	-	5/7/21/22	0/3/3/3
2	D5M	3	901	-	-	5/7/21/22	0/3/3/3
2	D5M	T	901	-	-	5/7/21/22	0/3/3/3
2	D5M	S	901	-	-	5/7/21/22	0/3/3/3
2	D5M	A	901	-	-	5/7/21/22	0/3/3/3
2	D5M	R	901	-	-	5/7/21/22	0/3/3/3
2	D5M	I	901	-	-	5/7/21/22	0/3/3/3
2	D5M	O	901	-	-	5/7/21/22	0/3/3/3
2	D5M	V	901	-	-	5/7/21/22	0/3/3/3
2	D5M	b	901	-	-	5/7/21/22	0/3/3/3
2	D5M	G	901	-	-	5/7/21/22	0/3/3/3
2	D5M	Y	901	-	-	5/7/21/22	0/3/3/3
2	D5M	B	901	-	-	5/7/21/22	0/3/3/3
2	D5M	C	901	-	-	5/7/21/22	0/3/3/3
2	D5M	N	901	-	-	5/7/21/22	0/3/3/3
2	D5M	y	901	-	-	5/7/21/22	0/3/3/3
2	D5M	c	901	-	-	5/7/21/22	0/3/3/3
2	D5M	5	901	-	-	5/7/21/22	0/3/3/3
2	D5M	l	901	-	-	5/7/21/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D5M	j	901	-	-	5/7/21/22	0/3/3/3
2	D5M	g	901	-	-	5/7/21/22	0/3/3/3
2	D5M	Q	901	-	-	5/7/21/22	0/3/3/3
2	D5M	d	901	-	-	5/7/21/22	0/3/3/3
2	D5M	6	901	-	-	5/7/21/22	0/3/3/3
2	D5M	h	901	-	-	5/7/21/22	0/3/3/3
2	D5M	U	901	-	-	5/7/21/22	0/3/3/3
2	D5M	s	901	-	-	5/7/21/22	0/3/3/3
2	D5M	r	901	-	-	5/7/21/22	0/3/3/3
2	D5M	n	901	-	-	5/7/21/22	0/3/3/3
2	D5M	8	901	-	-	5/7/21/22	0/3/3/3
2	D5M	o	901	-	-	5/7/21/22	0/3/3/3
2	D5M	w	901	-	-	5/7/21/22	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (300) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	D5M	O4'-C1'-N9-C4
2	B	901	D5M	O4'-C1'-N9-C4
2	C	901	D5M	O4'-C1'-N9-C4
2	D	901	D5M	O4'-C1'-N9-C4
2	E	901	D5M	O4'-C1'-N9-C4
2	F	901	D5M	O4'-C1'-N9-C4
2	G	901	D5M	O4'-C1'-N9-C4
2	H	901	D5M	O4'-C1'-N9-C4
2	I	901	D5M	O4'-C1'-N9-C4
2	J	901	D5M	O4'-C1'-N9-C4
2	K	901	D5M	O4'-C1'-N9-C4
2	L	901	D5M	O4'-C1'-N9-C4
2	M	901	D5M	O4'-C1'-N9-C4
2	N	901	D5M	O4'-C1'-N9-C4
2	O	901	D5M	O4'-C1'-N9-C4
2	P	901	D5M	O4'-C1'-N9-C4
2	Q	901	D5M	O4'-C1'-N9-C4
2	R	901	D5M	O4'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
2	S	901	D5M	O4'-C1'-N9-C4
2	T	901	D5M	O4'-C1'-N9-C4
2	U	901	D5M	O4'-C1'-N9-C4
2	V	901	D5M	O4'-C1'-N9-C4
2	W	901	D5M	O4'-C1'-N9-C4
2	X	901	D5M	O4'-C1'-N9-C4
2	Y	901	D5M	O4'-C1'-N9-C4
2	Z	901	D5M	O4'-C1'-N9-C4
2	a	901	D5M	O4'-C1'-N9-C4
2	b	901	D5M	O4'-C1'-N9-C4
2	c	901	D5M	O4'-C1'-N9-C4
2	d	901	D5M	O4'-C1'-N9-C4
2	e	901	D5M	O4'-C1'-N9-C4
2	f	901	D5M	O4'-C1'-N9-C4
2	g	901	D5M	O4'-C1'-N9-C4
2	h	901	D5M	O4'-C1'-N9-C4
2	i	901	D5M	O4'-C1'-N9-C4
2	j	901	D5M	O4'-C1'-N9-C4
2	k	901	D5M	O4'-C1'-N9-C4
2	l	901	D5M	O4'-C1'-N9-C4
2	m	901	D5M	O4'-C1'-N9-C4
2	n	901	D5M	O4'-C1'-N9-C4
2	o	901	D5M	O4'-C1'-N9-C4
2	p	901	D5M	O4'-C1'-N9-C4
2	q	901	D5M	O4'-C1'-N9-C4
2	r	901	D5M	O4'-C1'-N9-C4
2	s	901	D5M	O4'-C1'-N9-C4
2	t	901	D5M	O4'-C1'-N9-C4
2	u	901	D5M	O4'-C1'-N9-C4
2	v	901	D5M	O4'-C1'-N9-C4
2	w	901	D5M	O4'-C1'-N9-C4
2	x	901	D5M	O4'-C1'-N9-C4
2	y	901	D5M	O4'-C1'-N9-C4
2	z	901	D5M	O4'-C1'-N9-C4
2	1	901	D5M	O4'-C1'-N9-C4
2	2	901	D5M	O4'-C1'-N9-C4
2	3	901	D5M	O4'-C1'-N9-C4
2	4	901	D5M	O4'-C1'-N9-C4
2	5	901	D5M	O4'-C1'-N9-C4
2	6	901	D5M	O4'-C1'-N9-C4
2	7	901	D5M	O4'-C1'-N9-C4
2	8	901	D5M	O4'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
2	A	901	D5M	O4'-C1'-N9-C8
2	B	901	D5M	O4'-C1'-N9-C8
2	C	901	D5M	O4'-C1'-N9-C8
2	D	901	D5M	O4'-C1'-N9-C8
2	E	901	D5M	O4'-C1'-N9-C8
2	F	901	D5M	O4'-C1'-N9-C8
2	G	901	D5M	O4'-C1'-N9-C8
2	H	901	D5M	O4'-C1'-N9-C8
2	I	901	D5M	O4'-C1'-N9-C8
2	J	901	D5M	O4'-C1'-N9-C8
2	K	901	D5M	O4'-C1'-N9-C8
2	L	901	D5M	O4'-C1'-N9-C8
2	M	901	D5M	O4'-C1'-N9-C8
2	N	901	D5M	O4'-C1'-N9-C8
2	O	901	D5M	O4'-C1'-N9-C8
2	P	901	D5M	O4'-C1'-N9-C8
2	Q	901	D5M	O4'-C1'-N9-C8
2	R	901	D5M	O4'-C1'-N9-C8
2	S	901	D5M	O4'-C1'-N9-C8
2	T	901	D5M	O4'-C1'-N9-C8
2	U	901	D5M	O4'-C1'-N9-C8
2	V	901	D5M	O4'-C1'-N9-C8
2	W	901	D5M	O4'-C1'-N9-C8
2	X	901	D5M	O4'-C1'-N9-C8
2	Y	901	D5M	O4'-C1'-N9-C8
2	Z	901	D5M	O4'-C1'-N9-C8
2	a	901	D5M	O4'-C1'-N9-C8
2	b	901	D5M	O4'-C1'-N9-C8
2	c	901	D5M	O4'-C1'-N9-C8
2	d	901	D5M	O4'-C1'-N9-C8
2	e	901	D5M	O4'-C1'-N9-C8
2	f	901	D5M	O4'-C1'-N9-C8
2	g	901	D5M	O4'-C1'-N9-C8
2	h	901	D5M	O4'-C1'-N9-C8
2	i	901	D5M	O4'-C1'-N9-C8
2	j	901	D5M	O4'-C1'-N9-C8
2	k	901	D5M	O4'-C1'-N9-C8
2	l	901	D5M	O4'-C1'-N9-C8
2	m	901	D5M	O4'-C1'-N9-C8
2	n	901	D5M	O4'-C1'-N9-C8
2	o	901	D5M	O4'-C1'-N9-C8
2	p	901	D5M	O4'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
2	q	901	D5M	O4'-C1'-N9-C8
2	r	901	D5M	O4'-C1'-N9-C8
2	s	901	D5M	O4'-C1'-N9-C8
2	t	901	D5M	O4'-C1'-N9-C8
2	u	901	D5M	O4'-C1'-N9-C8
2	v	901	D5M	O4'-C1'-N9-C8
2	w	901	D5M	O4'-C1'-N9-C8
2	x	901	D5M	O4'-C1'-N9-C8
2	y	901	D5M	O4'-C1'-N9-C8
2	z	901	D5M	O4'-C1'-N9-C8
2	1	901	D5M	O4'-C1'-N9-C8
2	2	901	D5M	O4'-C1'-N9-C8
2	3	901	D5M	O4'-C1'-N9-C8
2	4	901	D5M	O4'-C1'-N9-C8
2	5	901	D5M	O4'-C1'-N9-C8
2	6	901	D5M	O4'-C1'-N9-C8
2	7	901	D5M	O4'-C1'-N9-C8
2	8	901	D5M	O4'-C1'-N9-C8
2	A	901	D5M	C3'-C4'-C5'-O5'
2	B	901	D5M	C3'-C4'-C5'-O5'
2	C	901	D5M	C3'-C4'-C5'-O5'
2	D	901	D5M	C3'-C4'-C5'-O5'
2	E	901	D5M	C3'-C4'-C5'-O5'
2	F	901	D5M	C3'-C4'-C5'-O5'
2	G	901	D5M	C3'-C4'-C5'-O5'
2	H	901	D5M	C3'-C4'-C5'-O5'
2	I	901	D5M	C3'-C4'-C5'-O5'
2	J	901	D5M	C3'-C4'-C5'-O5'
2	K	901	D5M	C3'-C4'-C5'-O5'
2	L	901	D5M	C3'-C4'-C5'-O5'
2	M	901	D5M	C3'-C4'-C5'-O5'
2	N	901	D5M	C3'-C4'-C5'-O5'
2	O	901	D5M	C3'-C4'-C5'-O5'
2	P	901	D5M	C3'-C4'-C5'-O5'
2	Q	901	D5M	C3'-C4'-C5'-O5'
2	R	901	D5M	C3'-C4'-C5'-O5'
2	S	901	D5M	C3'-C4'-C5'-O5'
2	T	901	D5M	C3'-C4'-C5'-O5'
2	U	901	D5M	C3'-C4'-C5'-O5'
2	V	901	D5M	C3'-C4'-C5'-O5'
2	W	901	D5M	C3'-C4'-C5'-O5'
2	X	901	D5M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	Y	901	D5M	C3'-C4'-C5'-O5'
2	Z	901	D5M	C3'-C4'-C5'-O5'
2	a	901	D5M	C3'-C4'-C5'-O5'
2	b	901	D5M	C3'-C4'-C5'-O5'
2	c	901	D5M	C3'-C4'-C5'-O5'
2	d	901	D5M	C3'-C4'-C5'-O5'
2	e	901	D5M	C3'-C4'-C5'-O5'
2	f	901	D5M	C3'-C4'-C5'-O5'
2	g	901	D5M	C3'-C4'-C5'-O5'
2	h	901	D5M	C3'-C4'-C5'-O5'
2	i	901	D5M	C3'-C4'-C5'-O5'
2	j	901	D5M	C3'-C4'-C5'-O5'
2	k	901	D5M	C3'-C4'-C5'-O5'
2	l	901	D5M	C3'-C4'-C5'-O5'
2	m	901	D5M	C3'-C4'-C5'-O5'
2	n	901	D5M	C3'-C4'-C5'-O5'
2	o	901	D5M	C3'-C4'-C5'-O5'
2	p	901	D5M	C3'-C4'-C5'-O5'
2	q	901	D5M	C3'-C4'-C5'-O5'
2	r	901	D5M	C3'-C4'-C5'-O5'
2	s	901	D5M	C3'-C4'-C5'-O5'
2	t	901	D5M	C3'-C4'-C5'-O5'
2	u	901	D5M	C3'-C4'-C5'-O5'
2	v	901	D5M	C3'-C4'-C5'-O5'
2	w	901	D5M	C3'-C4'-C5'-O5'
2	x	901	D5M	C3'-C4'-C5'-O5'
2	y	901	D5M	C3'-C4'-C5'-O5'
2	z	901	D5M	C3'-C4'-C5'-O5'
2	1	901	D5M	C3'-C4'-C5'-O5'
2	2	901	D5M	C3'-C4'-C5'-O5'
2	3	901	D5M	C3'-C4'-C5'-O5'
2	4	901	D5M	C3'-C4'-C5'-O5'
2	5	901	D5M	C3'-C4'-C5'-O5'
2	6	901	D5M	C3'-C4'-C5'-O5'
2	7	901	D5M	C3'-C4'-C5'-O5'
2	8	901	D5M	C3'-C4'-C5'-O5'
2	A	901	D5M	C2'-C1'-N9-C4
2	B	901	D5M	C2'-C1'-N9-C4
2	C	901	D5M	C2'-C1'-N9-C4
2	D	901	D5M	C2'-C1'-N9-C4
2	E	901	D5M	C2'-C1'-N9-C4
2	F	901	D5M	C2'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
2	G	901	D5M	C2'-C1'-N9-C4
2	H	901	D5M	C2'-C1'-N9-C4
2	I	901	D5M	C2'-C1'-N9-C4
2	J	901	D5M	C2'-C1'-N9-C4
2	K	901	D5M	C2'-C1'-N9-C4
2	L	901	D5M	C2'-C1'-N9-C4
2	M	901	D5M	C2'-C1'-N9-C4
2	N	901	D5M	C2'-C1'-N9-C4
2	O	901	D5M	C2'-C1'-N9-C4
2	P	901	D5M	C2'-C1'-N9-C4
2	Q	901	D5M	C2'-C1'-N9-C4
2	R	901	D5M	C2'-C1'-N9-C4
2	S	901	D5M	C2'-C1'-N9-C4
2	T	901	D5M	C2'-C1'-N9-C4
2	U	901	D5M	C2'-C1'-N9-C4
2	V	901	D5M	C2'-C1'-N9-C4
2	W	901	D5M	C2'-C1'-N9-C4
2	X	901	D5M	C2'-C1'-N9-C4
2	Y	901	D5M	C2'-C1'-N9-C4
2	Z	901	D5M	C2'-C1'-N9-C4
2	a	901	D5M	C2'-C1'-N9-C4
2	b	901	D5M	C2'-C1'-N9-C4
2	c	901	D5M	C2'-C1'-N9-C4
2	d	901	D5M	C2'-C1'-N9-C4
2	e	901	D5M	C2'-C1'-N9-C4
2	f	901	D5M	C2'-C1'-N9-C4
2	g	901	D5M	C2'-C1'-N9-C4
2	h	901	D5M	C2'-C1'-N9-C4
2	i	901	D5M	C2'-C1'-N9-C4
2	j	901	D5M	C2'-C1'-N9-C4
2	k	901	D5M	C2'-C1'-N9-C4
2	l	901	D5M	C2'-C1'-N9-C4
2	m	901	D5M	C2'-C1'-N9-C4
2	n	901	D5M	C2'-C1'-N9-C4
2	o	901	D5M	C2'-C1'-N9-C4
2	p	901	D5M	C2'-C1'-N9-C4
2	q	901	D5M	C2'-C1'-N9-C4
2	r	901	D5M	C2'-C1'-N9-C4
2	s	901	D5M	C2'-C1'-N9-C4
2	t	901	D5M	C2'-C1'-N9-C4
2	u	901	D5M	C2'-C1'-N9-C4
2	v	901	D5M	C2'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
2	w	901	D5M	C2'-C1'-N9-C4
2	x	901	D5M	C2'-C1'-N9-C4
2	y	901	D5M	C2'-C1'-N9-C4
2	z	901	D5M	C2'-C1'-N9-C4
2	1	901	D5M	C2'-C1'-N9-C4
2	2	901	D5M	C2'-C1'-N9-C4
2	3	901	D5M	C2'-C1'-N9-C4
2	4	901	D5M	C2'-C1'-N9-C4
2	5	901	D5M	C2'-C1'-N9-C4
2	6	901	D5M	C2'-C1'-N9-C4
2	7	901	D5M	C2'-C1'-N9-C4
2	8	901	D5M	C2'-C1'-N9-C4
2	A	901	D5M	O4'-C4'-C5'-O5'
2	B	901	D5M	O4'-C4'-C5'-O5'
2	C	901	D5M	O4'-C4'-C5'-O5'
2	D	901	D5M	O4'-C4'-C5'-O5'
2	E	901	D5M	O4'-C4'-C5'-O5'
2	F	901	D5M	O4'-C4'-C5'-O5'
2	G	901	D5M	O4'-C4'-C5'-O5'
2	I	901	D5M	O4'-C4'-C5'-O5'
2	O	901	D5M	O4'-C4'-C5'-O5'
2	P	901	D5M	O4'-C4'-C5'-O5'
2	T	901	D5M	O4'-C4'-C5'-O5'
2	V	901	D5M	O4'-C4'-C5'-O5'
2	W	901	D5M	O4'-C4'-C5'-O5'
2	Y	901	D5M	O4'-C4'-C5'-O5'
2	Z	901	D5M	O4'-C4'-C5'-O5'
2	b	901	D5M	O4'-C4'-C5'-O5'
2	e	901	D5M	O4'-C4'-C5'-O5'
2	f	901	D5M	O4'-C4'-C5'-O5'
2	g	901	D5M	O4'-C4'-C5'-O5'
2	h	901	D5M	O4'-C4'-C5'-O5'
2	j	901	D5M	O4'-C4'-C5'-O5'
2	l	901	D5M	O4'-C4'-C5'-O5'
2	m	901	D5M	O4'-C4'-C5'-O5'
2	o	901	D5M	O4'-C4'-C5'-O5'
2	q	901	D5M	O4'-C4'-C5'-O5'
2	t	901	D5M	O4'-C4'-C5'-O5'
2	u	901	D5M	O4'-C4'-C5'-O5'
2	v	901	D5M	O4'-C4'-C5'-O5'
2	w	901	D5M	O4'-C4'-C5'-O5'
2	x	901	D5M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	y	901	D5M	O4'-C4'-C5'-O5'
2	1	901	D5M	O4'-C4'-C5'-O5'
2	2	901	D5M	O4'-C4'-C5'-O5'
2	3	901	D5M	O4'-C4'-C5'-O5'
2	4	901	D5M	O4'-C4'-C5'-O5'
2	5	901	D5M	O4'-C4'-C5'-O5'
2	6	901	D5M	O4'-C4'-C5'-O5'
2	8	901	D5M	O4'-C4'-C5'-O5'
2	H	901	D5M	O4'-C4'-C5'-O5'
2	J	901	D5M	O4'-C4'-C5'-O5'
2	K	901	D5M	O4'-C4'-C5'-O5'
2	L	901	D5M	O4'-C4'-C5'-O5'
2	M	901	D5M	O4'-C4'-C5'-O5'
2	N	901	D5M	O4'-C4'-C5'-O5'
2	Q	901	D5M	O4'-C4'-C5'-O5'
2	R	901	D5M	O4'-C4'-C5'-O5'
2	S	901	D5M	O4'-C4'-C5'-O5'
2	U	901	D5M	O4'-C4'-C5'-O5'
2	X	901	D5M	O4'-C4'-C5'-O5'
2	a	901	D5M	O4'-C4'-C5'-O5'
2	c	901	D5M	O4'-C4'-C5'-O5'
2	d	901	D5M	O4'-C4'-C5'-O5'
2	i	901	D5M	O4'-C4'-C5'-O5'
2	k	901	D5M	O4'-C4'-C5'-O5'
2	n	901	D5M	O4'-C4'-C5'-O5'
2	p	901	D5M	O4'-C4'-C5'-O5'
2	r	901	D5M	O4'-C4'-C5'-O5'
2	s	901	D5M	O4'-C4'-C5'-O5'
2	z	901	D5M	O4'-C4'-C5'-O5'
2	7	901	D5M	O4'-C4'-C5'-O5'

There are no ring outliers.

60 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	e	901	D5M	1	0
2	2	901	D5M	1	0
2	x	901	D5M	1	0
2	W	901	D5M	1	0
2	P	901	D5M	1	0
2	K	901	D5M	1	0
2	L	901	D5M	1	0

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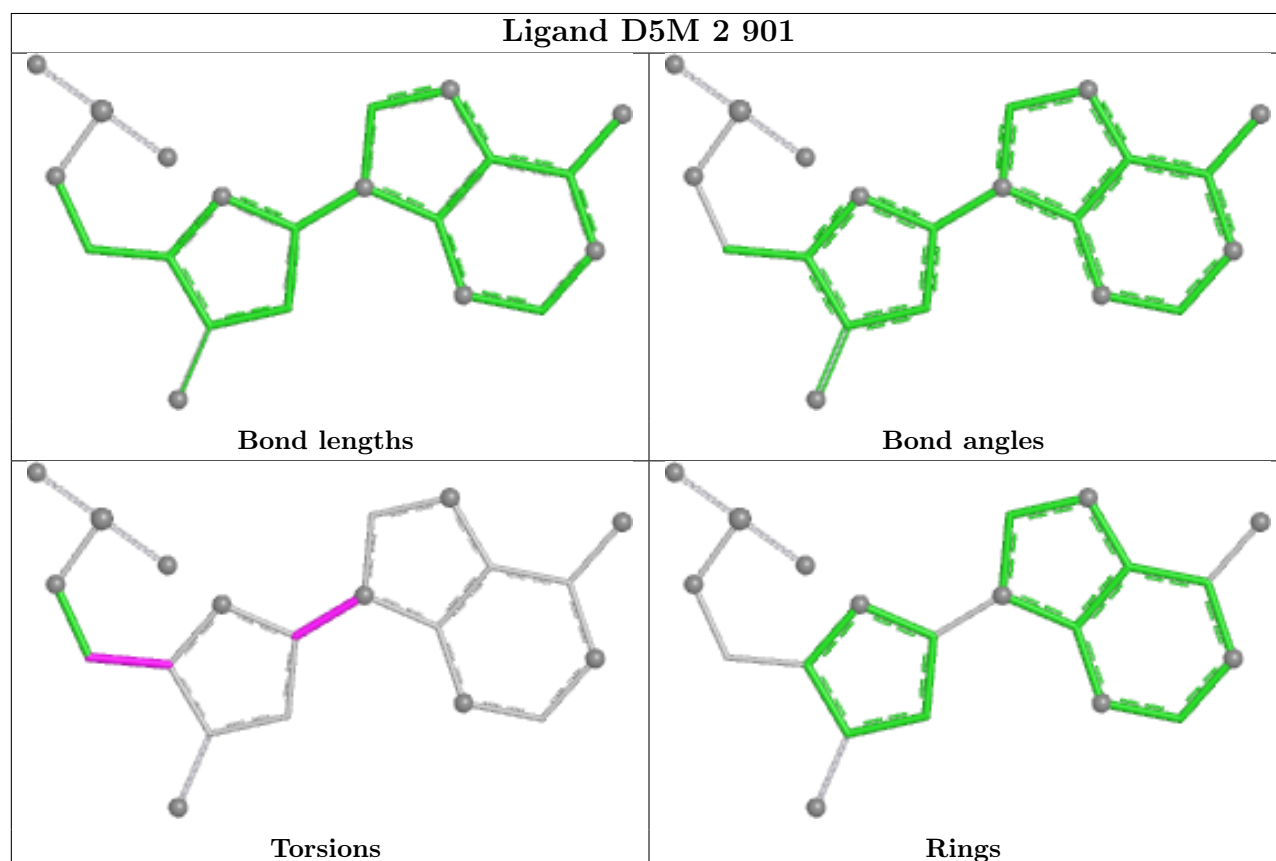
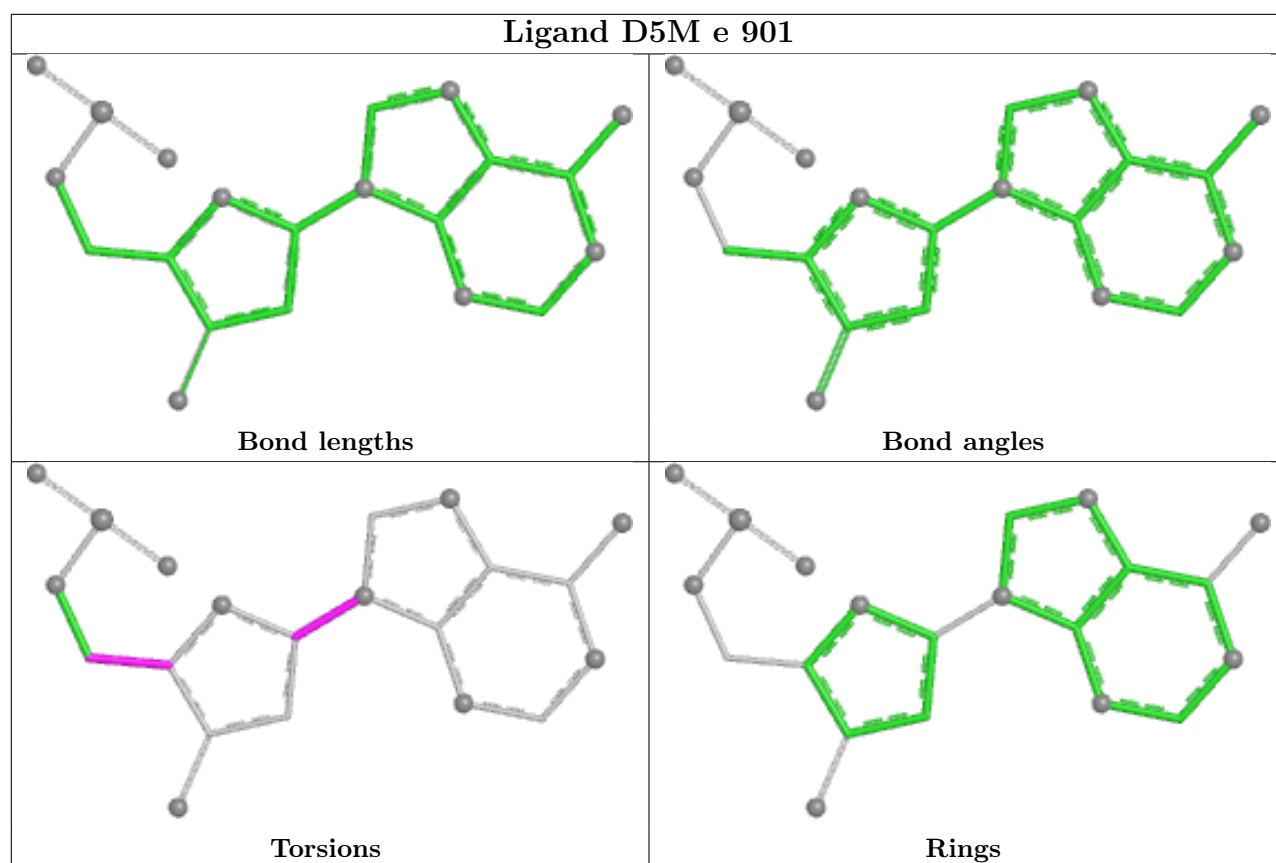
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	q	901	D5M	1	0
2	z	901	D5M	1	0
2	M	901	D5M	1	0
2	v	901	D5M	1	0
2	F	901	D5M	1	0
2	4	901	D5M	1	0
2	D	901	D5M	1	0
2	J	901	D5M	1	0
2	p	901	D5M	1	0
2	f	901	D5M	1	0
2	H	901	D5M	1	0
2	m	901	D5M	1	0
2	Z	901	D5M	1	0
2	7	901	D5M	1	0
2	a	901	D5M	1	0
2	1	901	D5M	1	0
2	X	901	D5M	1	0
2	i	901	D5M	1	0
2	E	901	D5M	1	0
2	k	901	D5M	1	0
2	t	901	D5M	1	0
2	u	901	D5M	1	0
2	3	901	D5M	1	0
2	T	901	D5M	1	0
2	S	901	D5M	1	0
2	A	901	D5M	1	0
2	R	901	D5M	1	0
2	I	901	D5M	1	0
2	O	901	D5M	1	0
2	V	901	D5M	1	0
2	b	901	D5M	1	0
2	G	901	D5M	1	0
2	Y	901	D5M	1	0
2	B	901	D5M	1	0
2	C	901	D5M	1	0
2	N	901	D5M	1	0
2	y	901	D5M	1	0
2	c	901	D5M	1	0
2	5	901	D5M	1	0
2	l	901	D5M	1	0
2	j	901	D5M	1	0
2	g	901	D5M	1	0

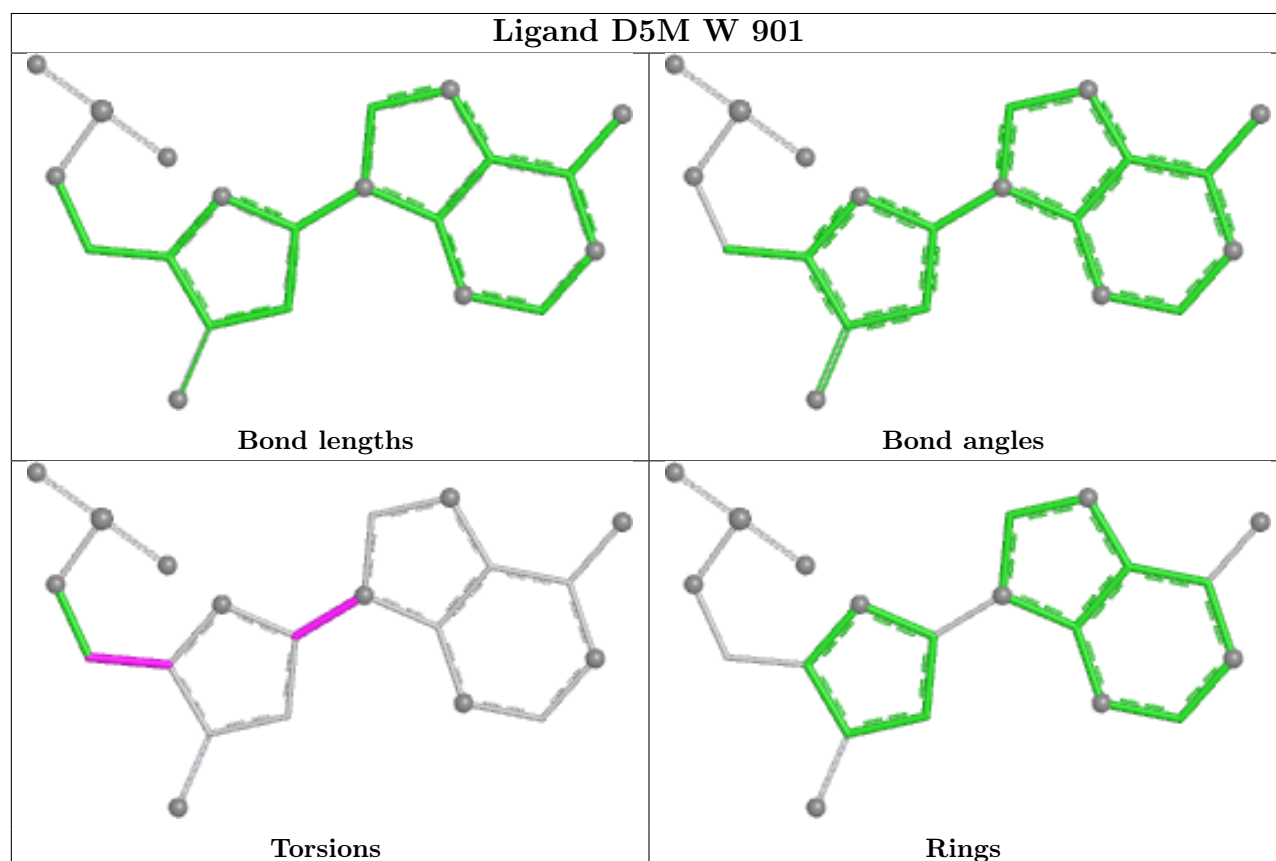
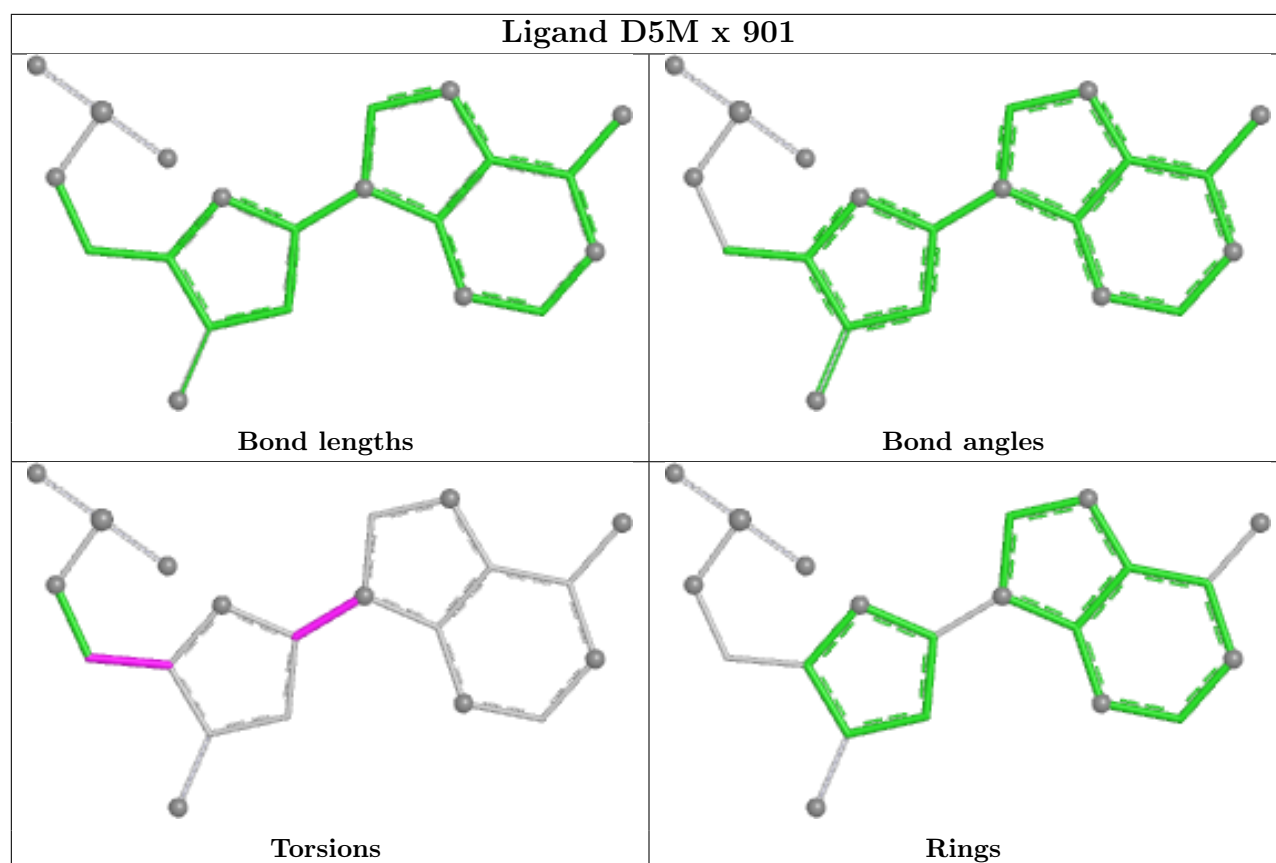
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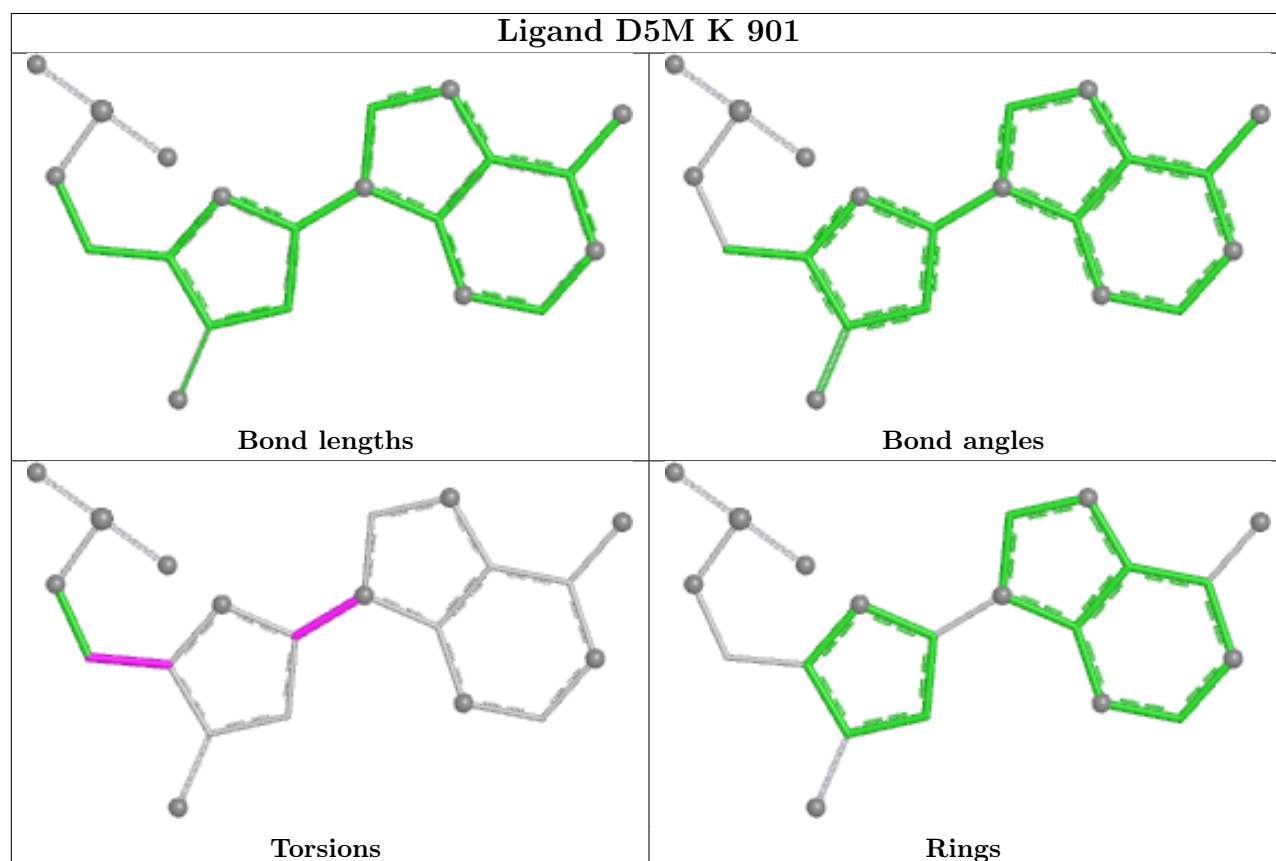
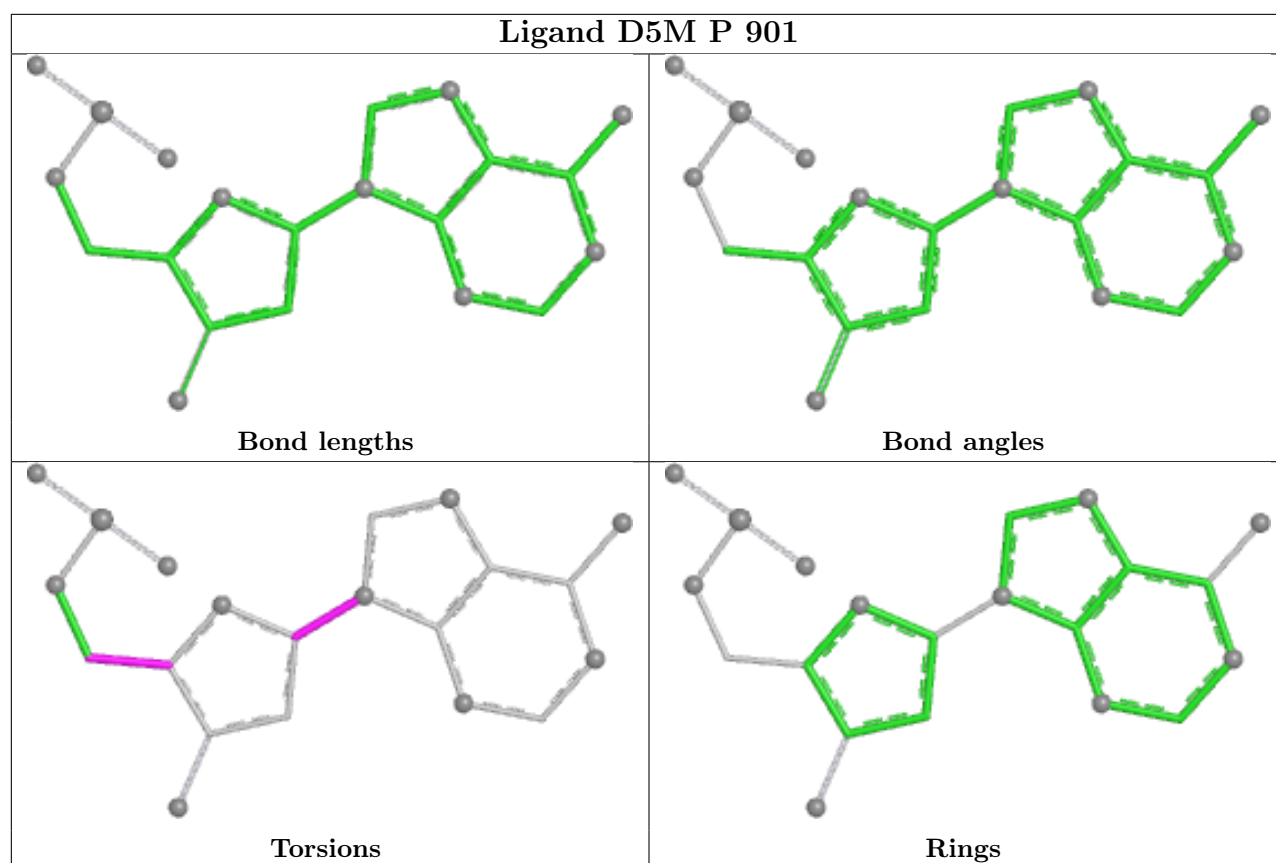
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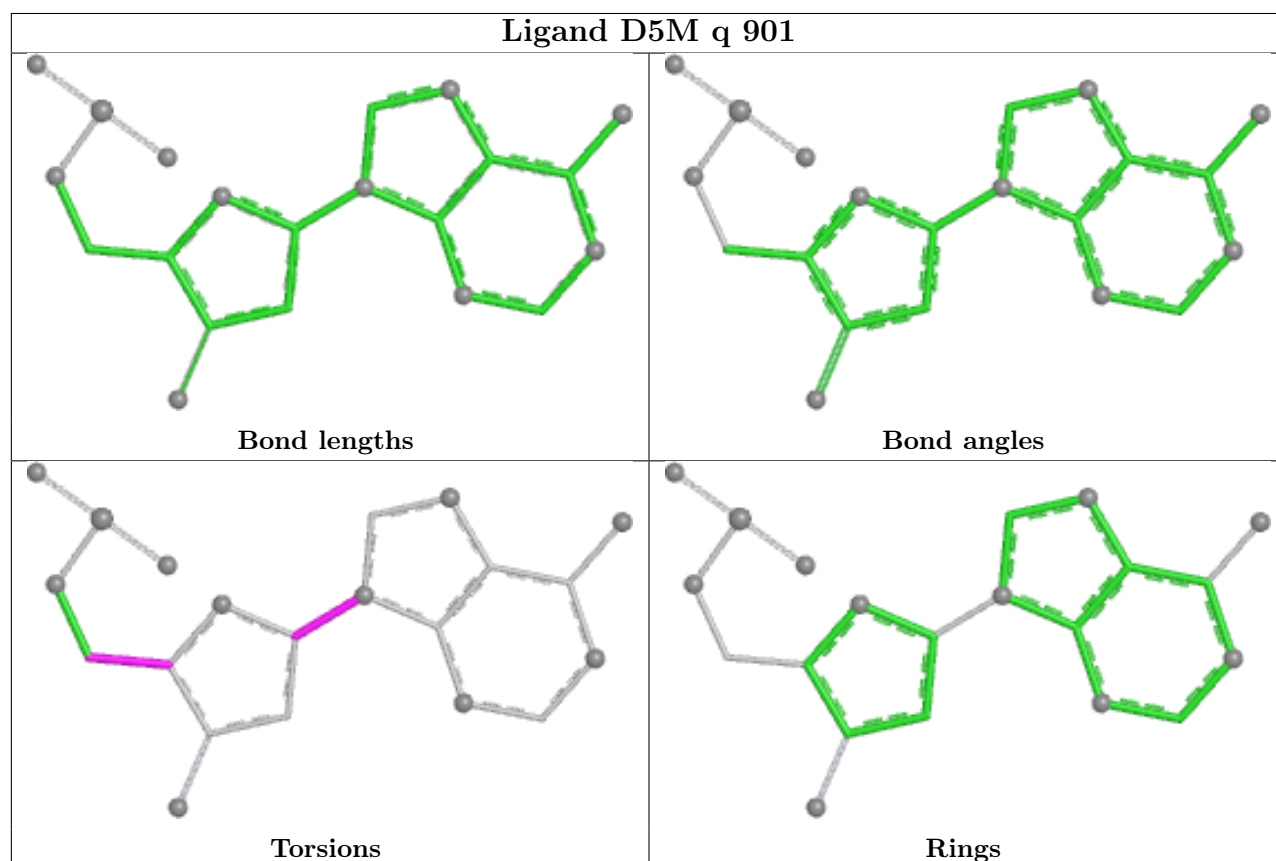
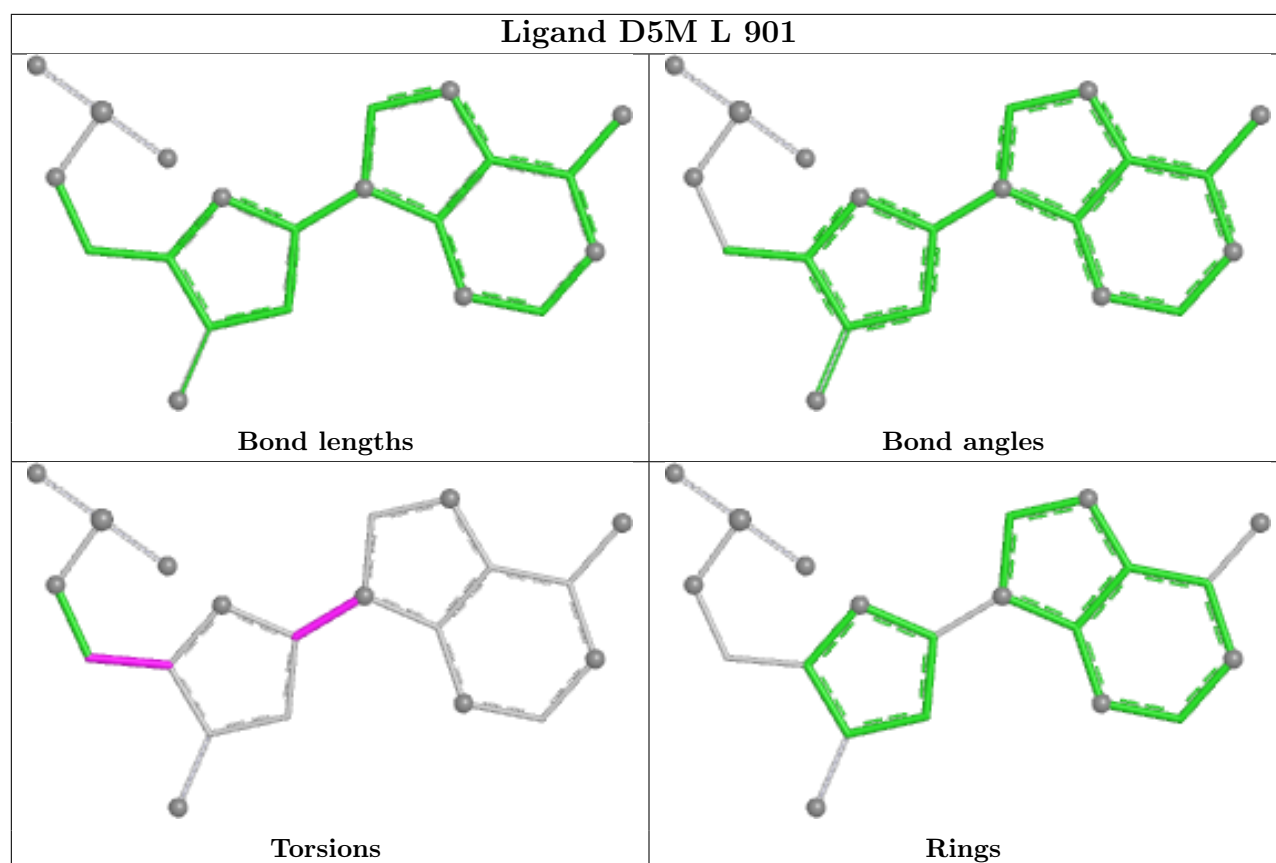
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	901	D5M	1	0
2	d	901	D5M	1	0
2	6	901	D5M	1	0
2	h	901	D5M	1	0
2	U	901	D5M	1	0
2	s	901	D5M	1	0
2	r	901	D5M	1	0
2	n	901	D5M	1	0
2	8	901	D5M	1	0
2	o	901	D5M	1	0
2	w	901	D5M	1	0

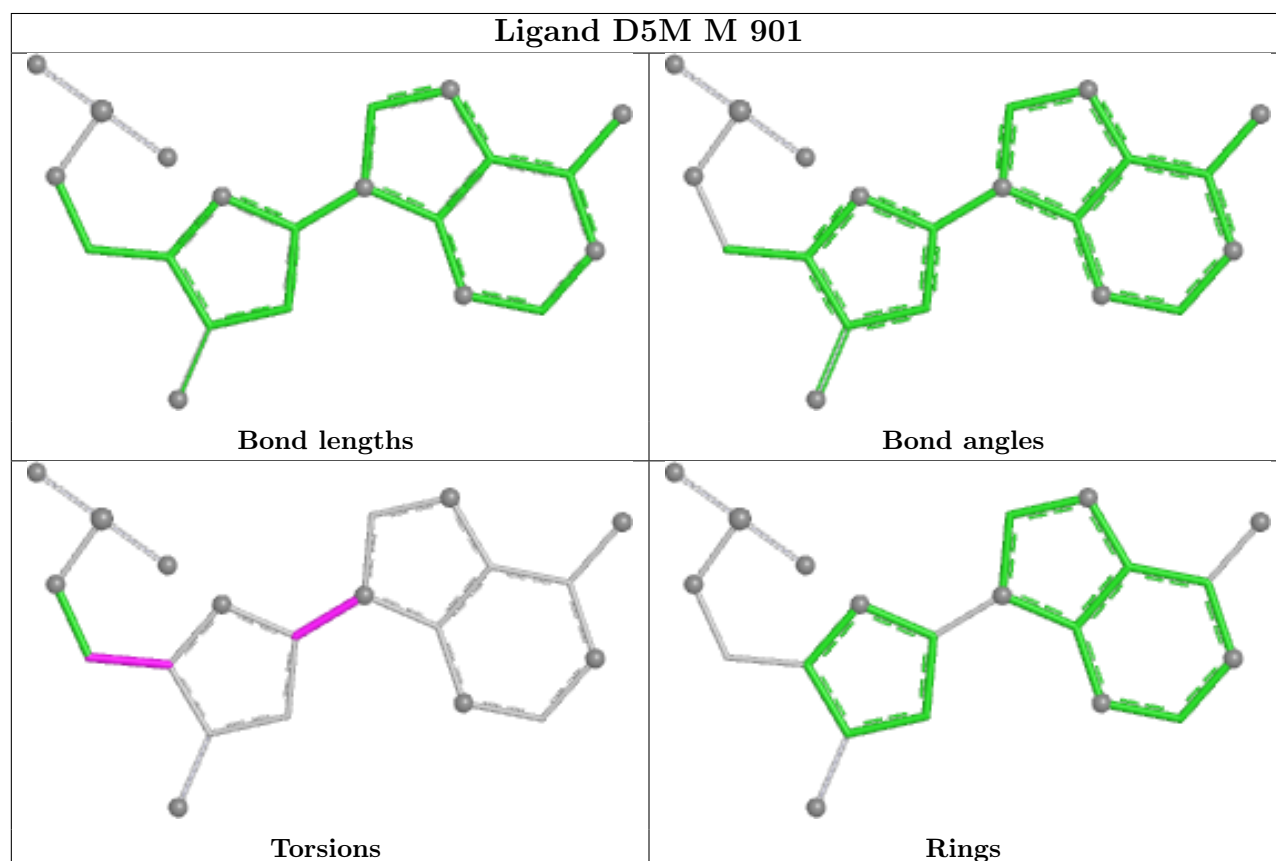
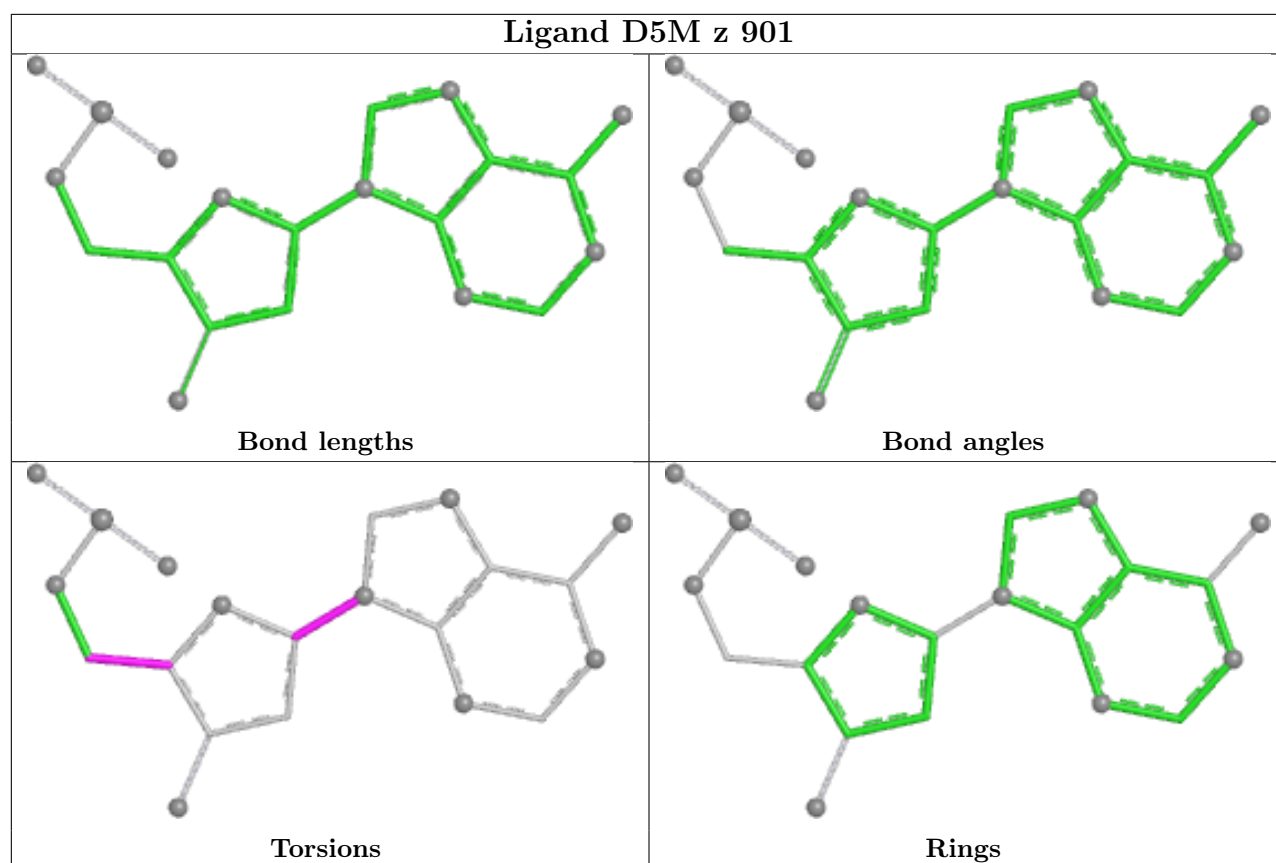
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

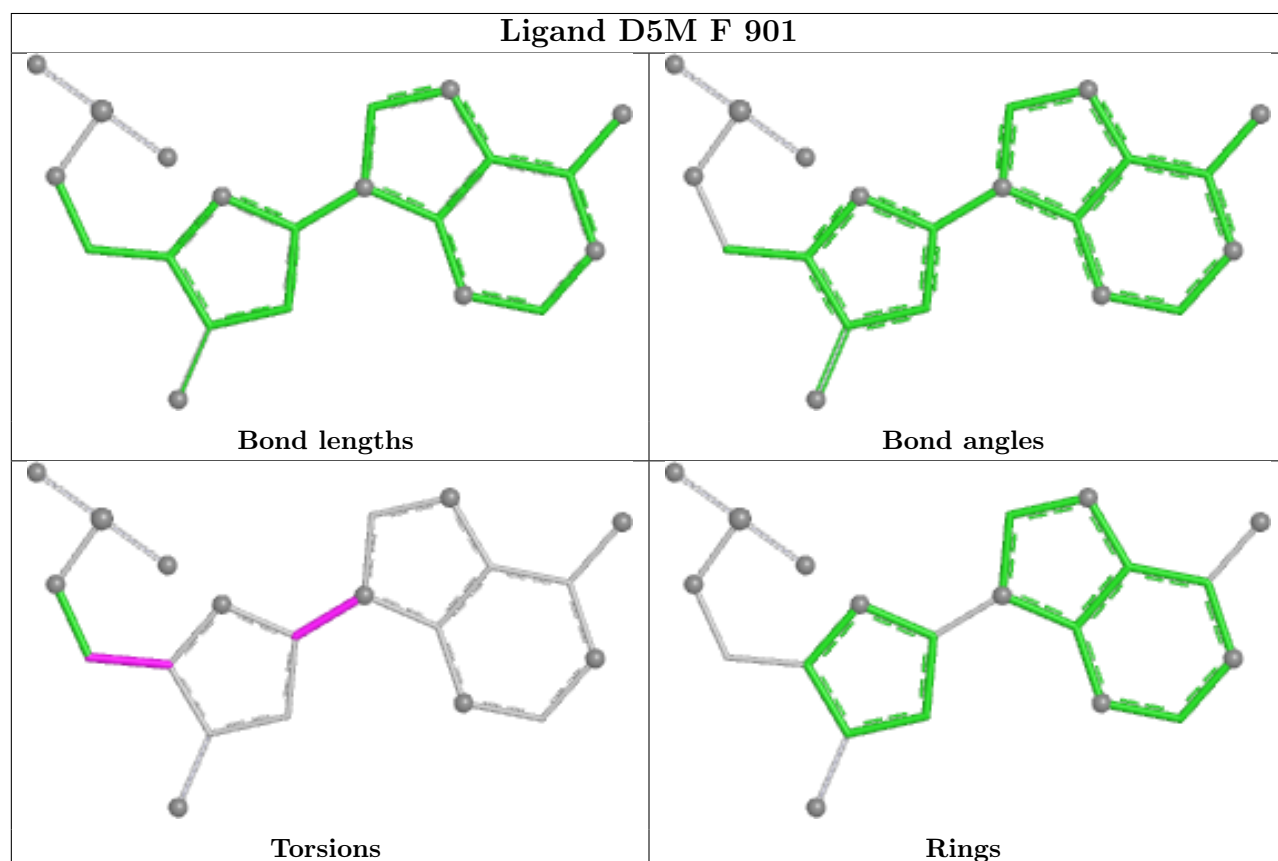
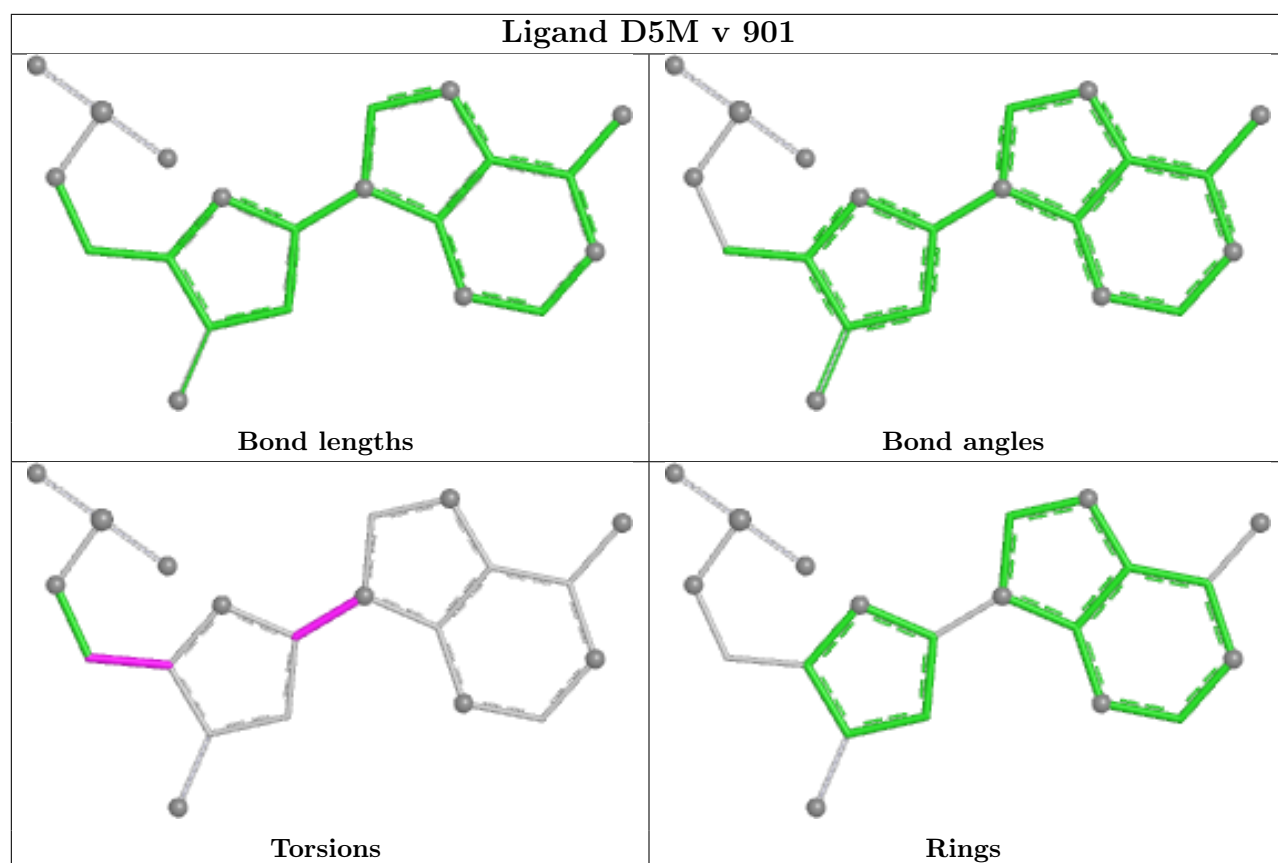


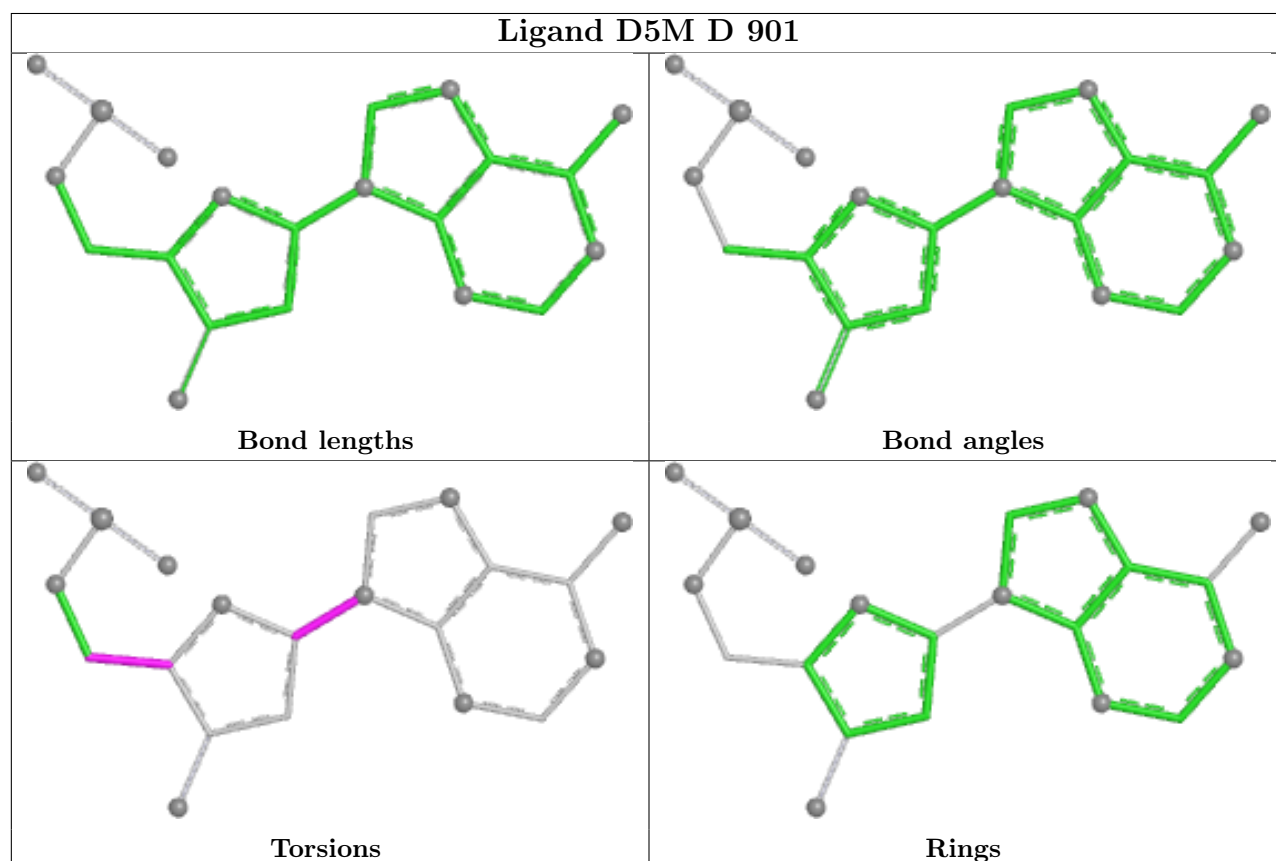
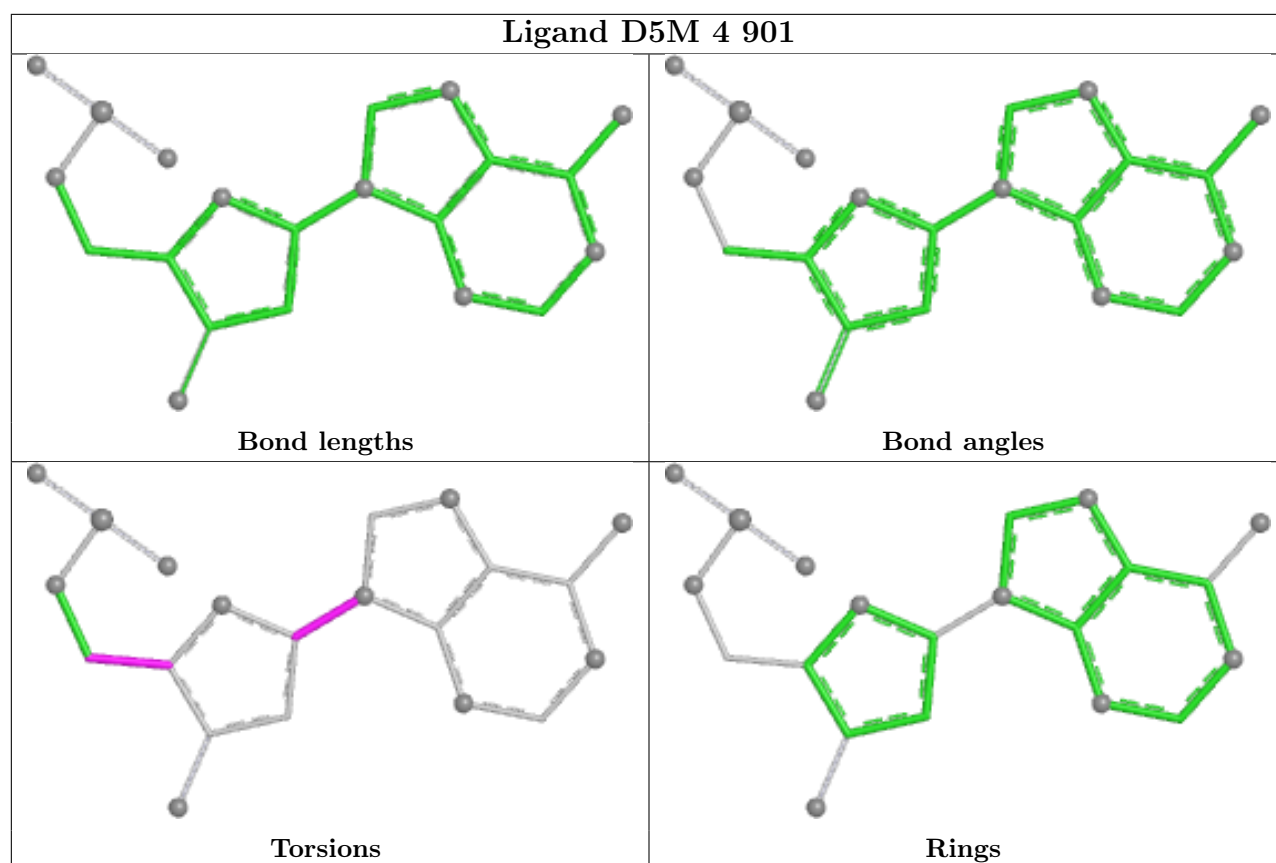


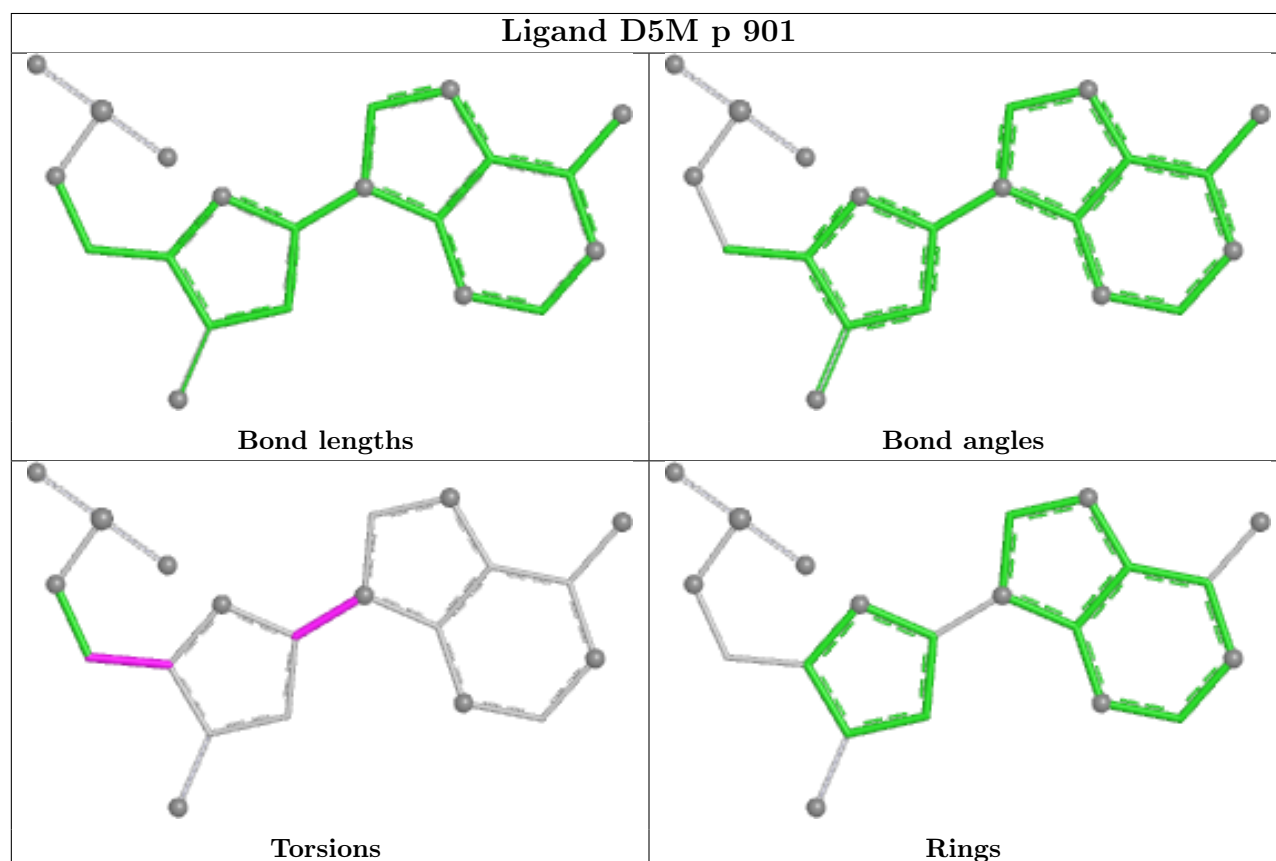
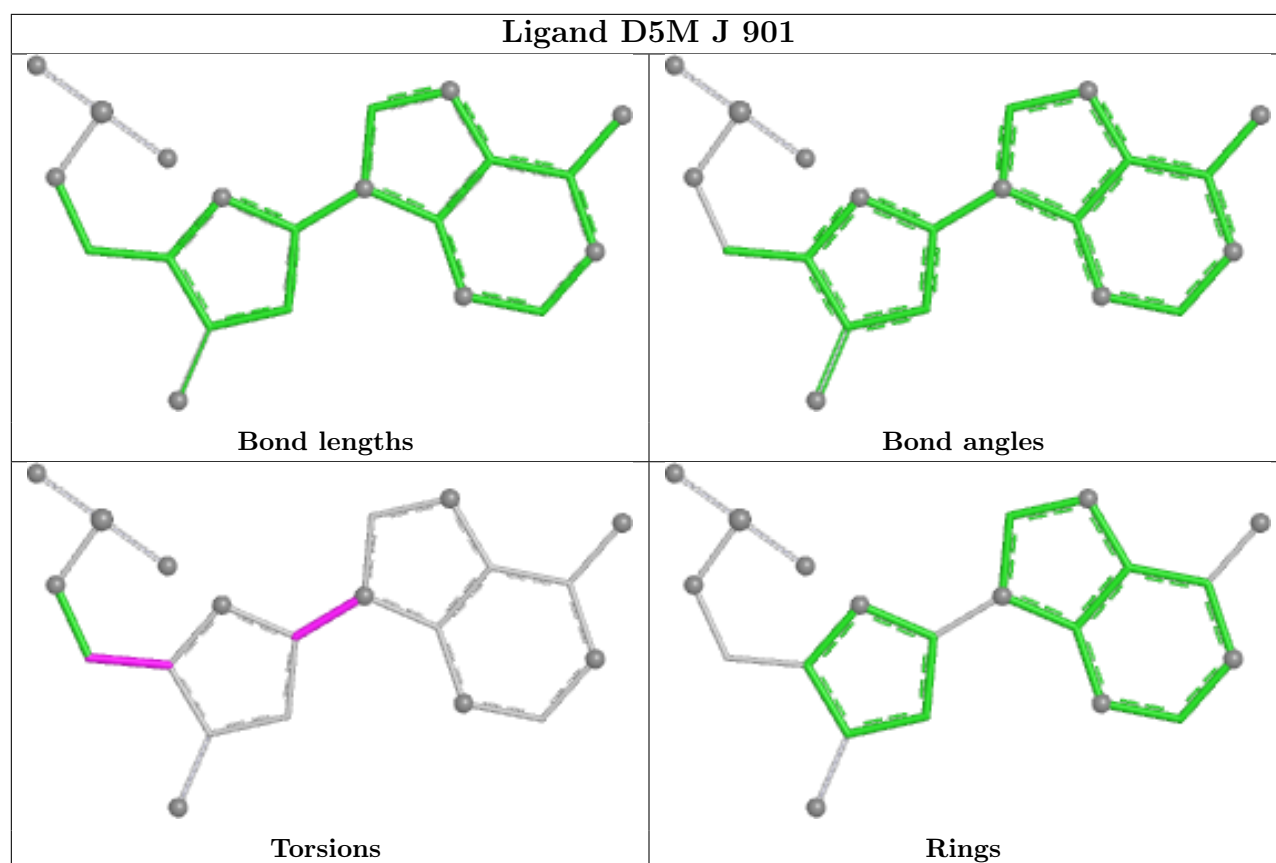


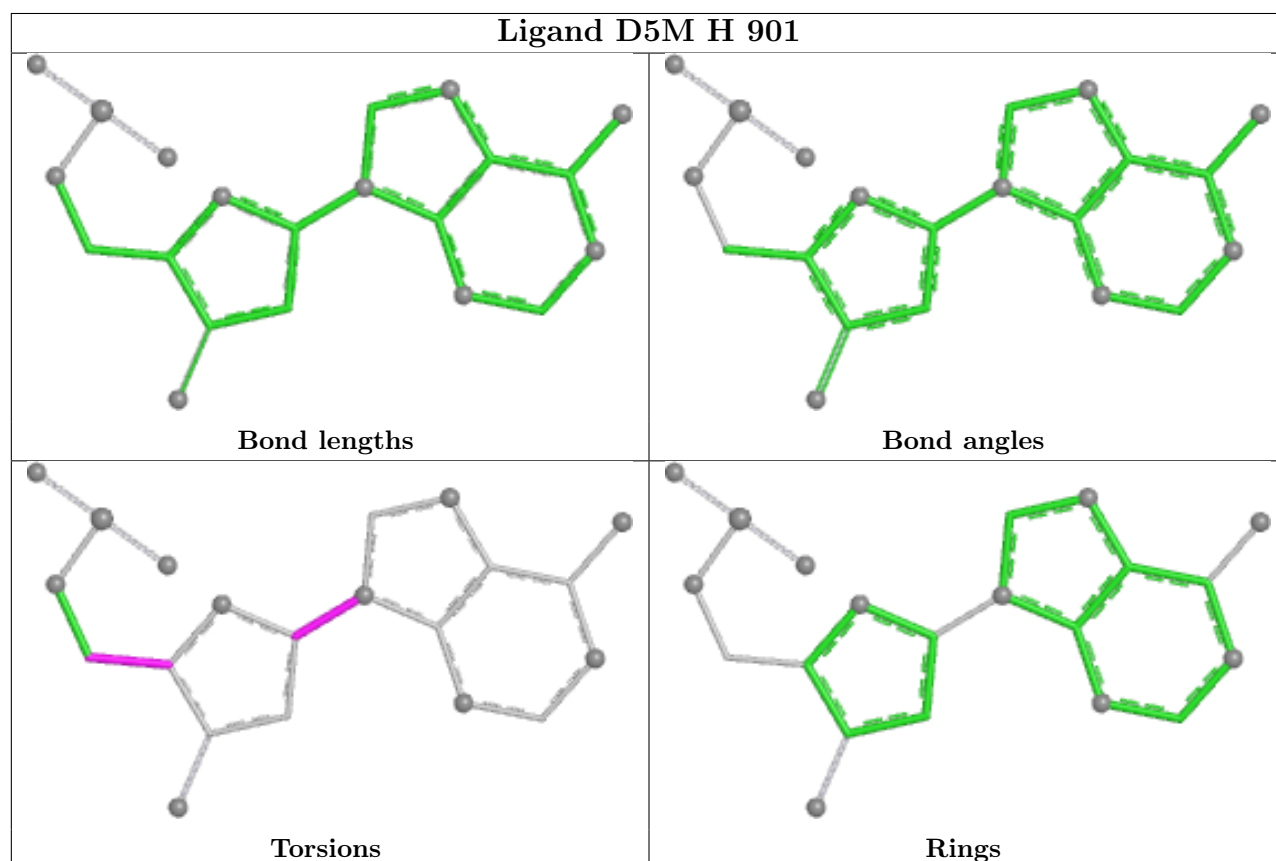
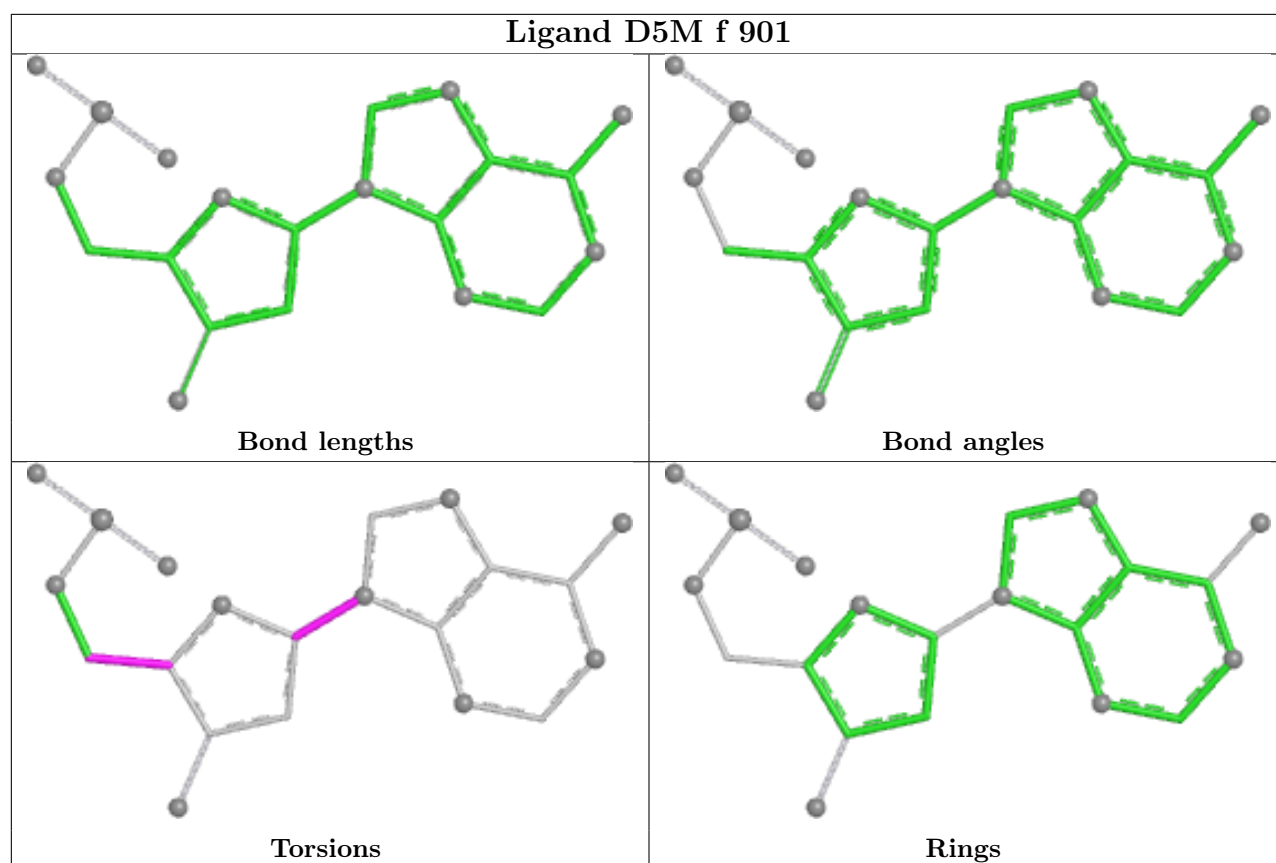


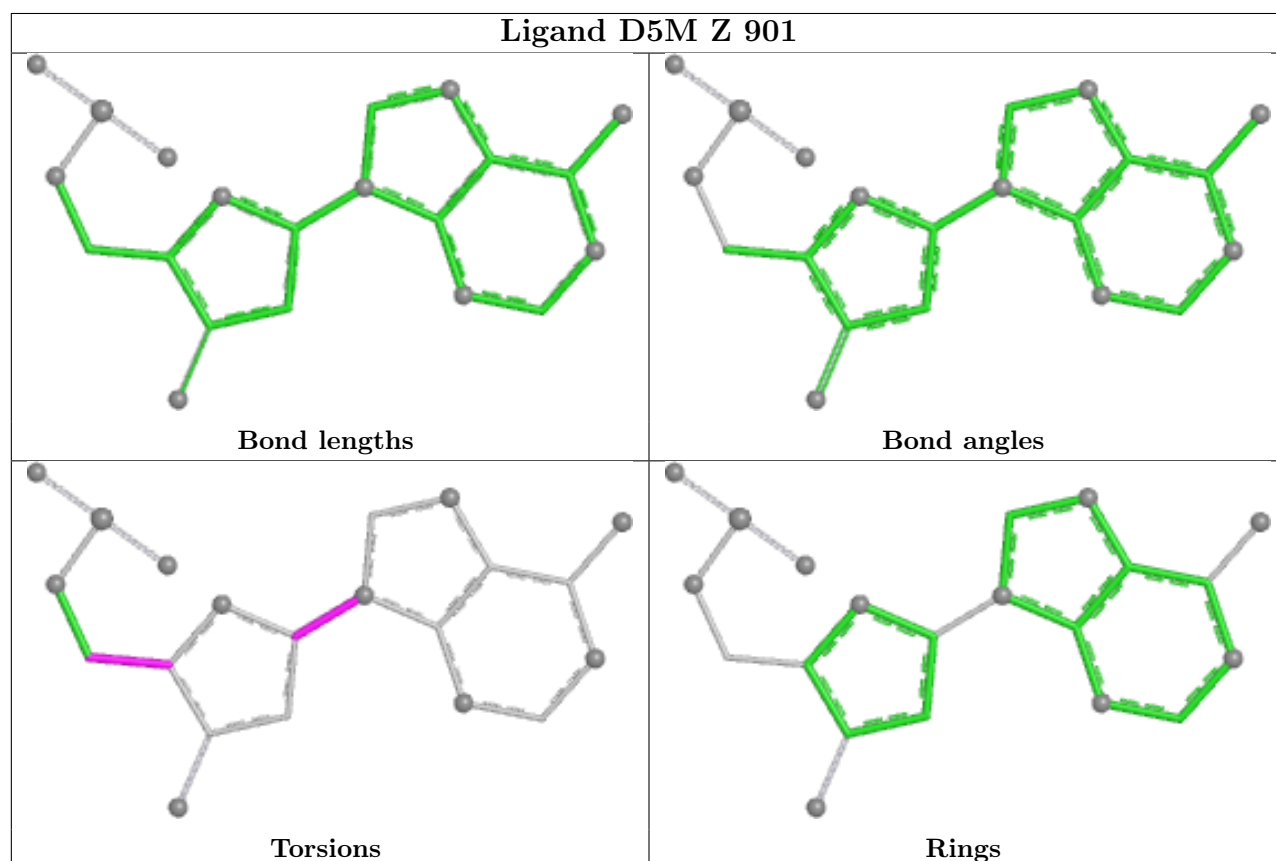
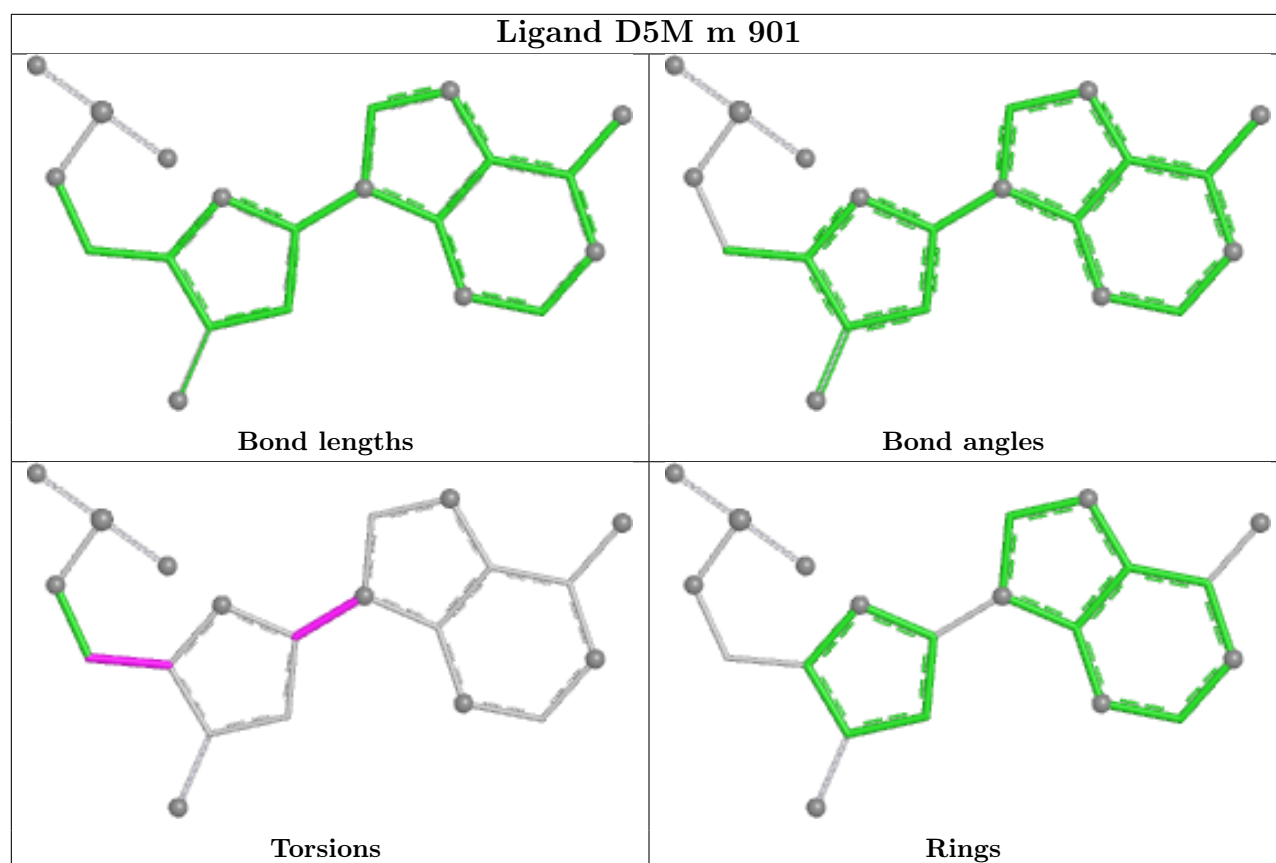




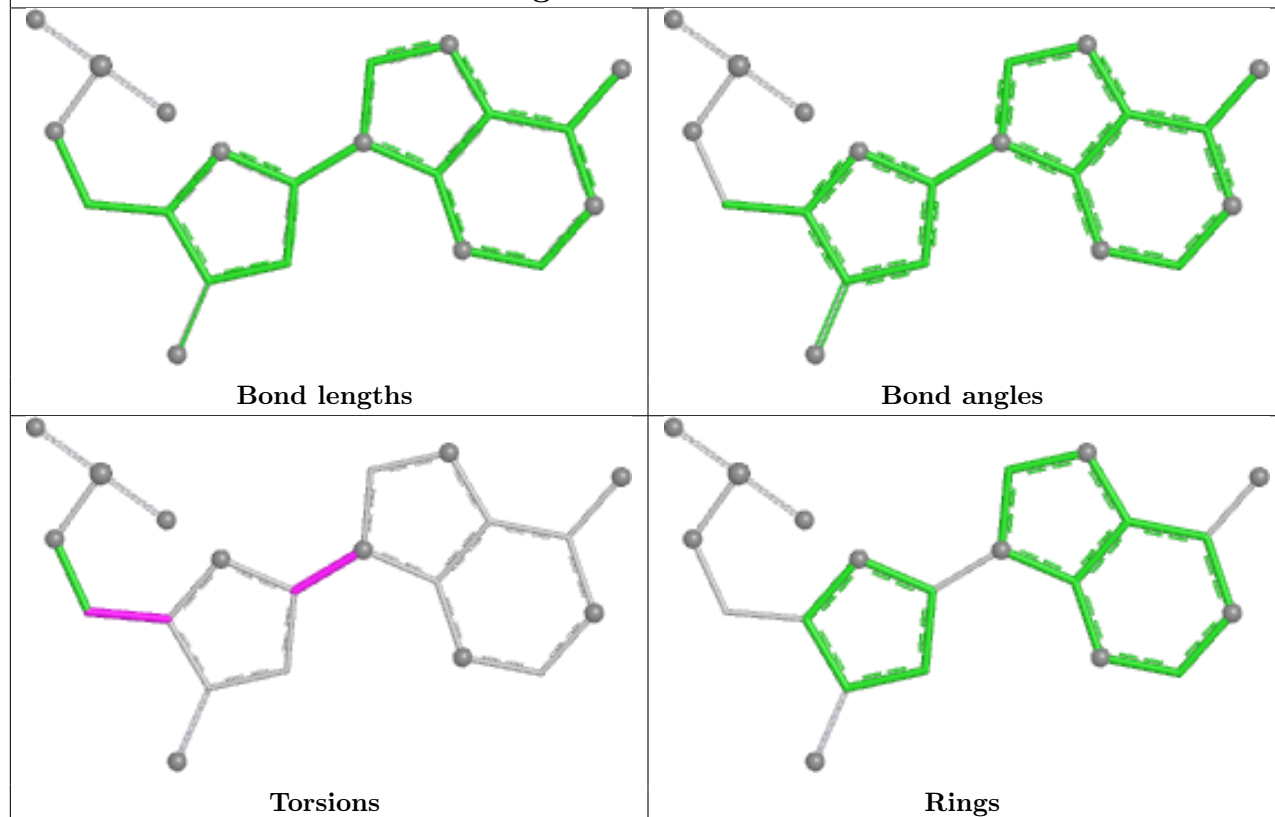




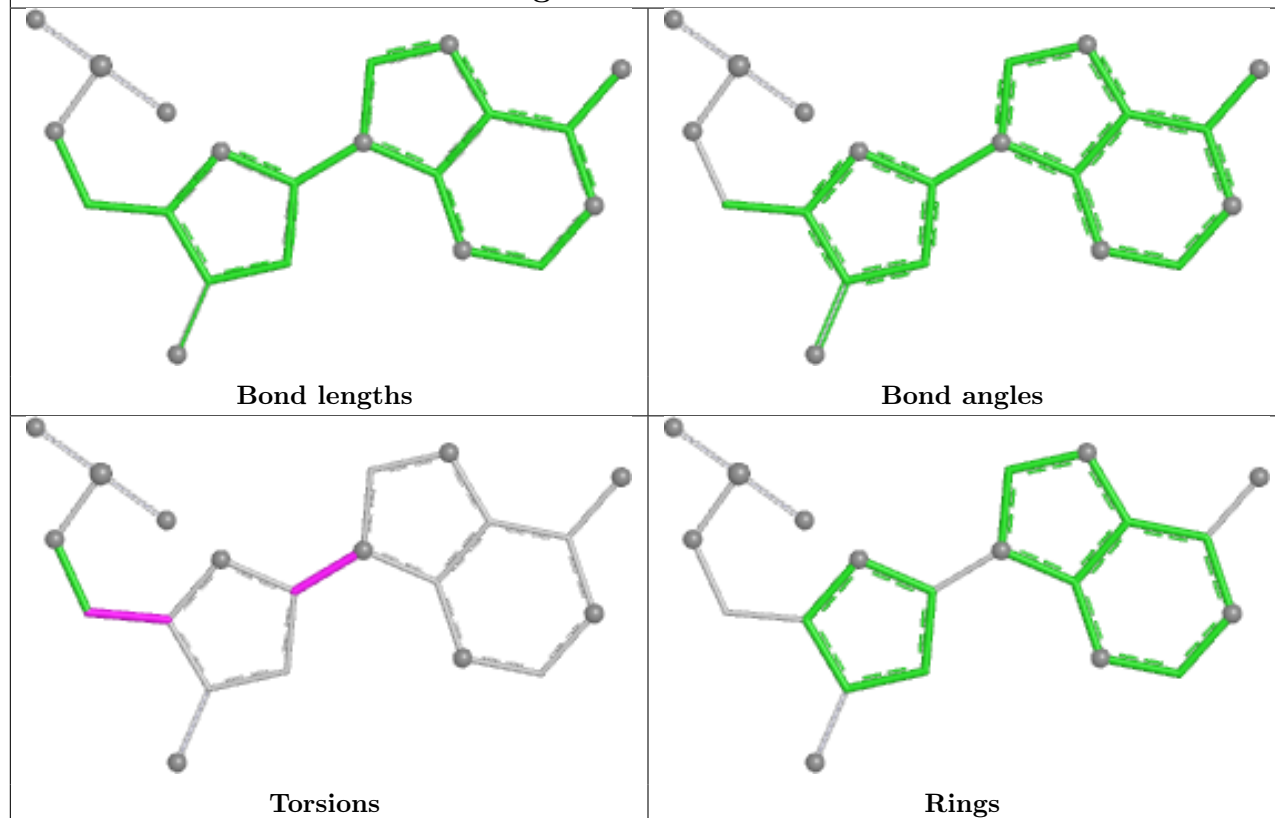


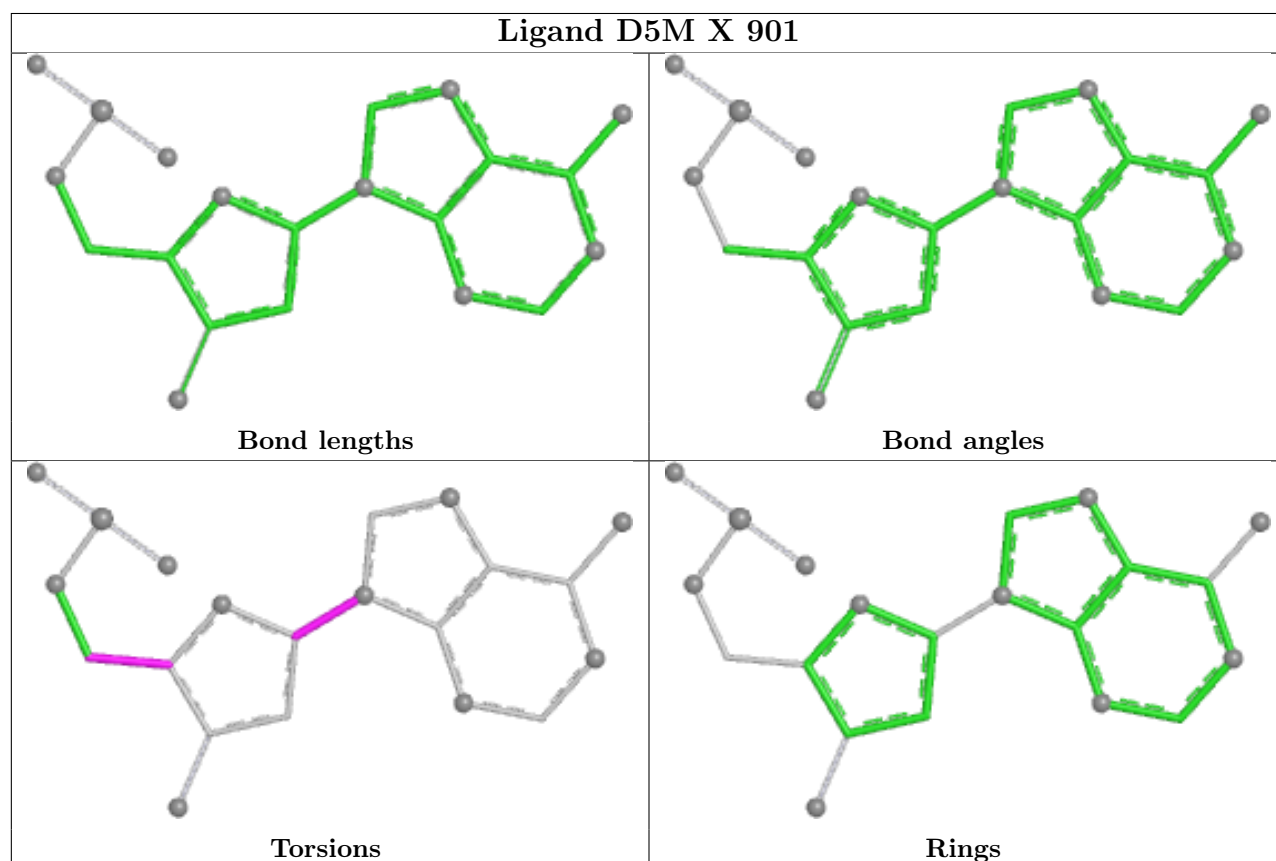
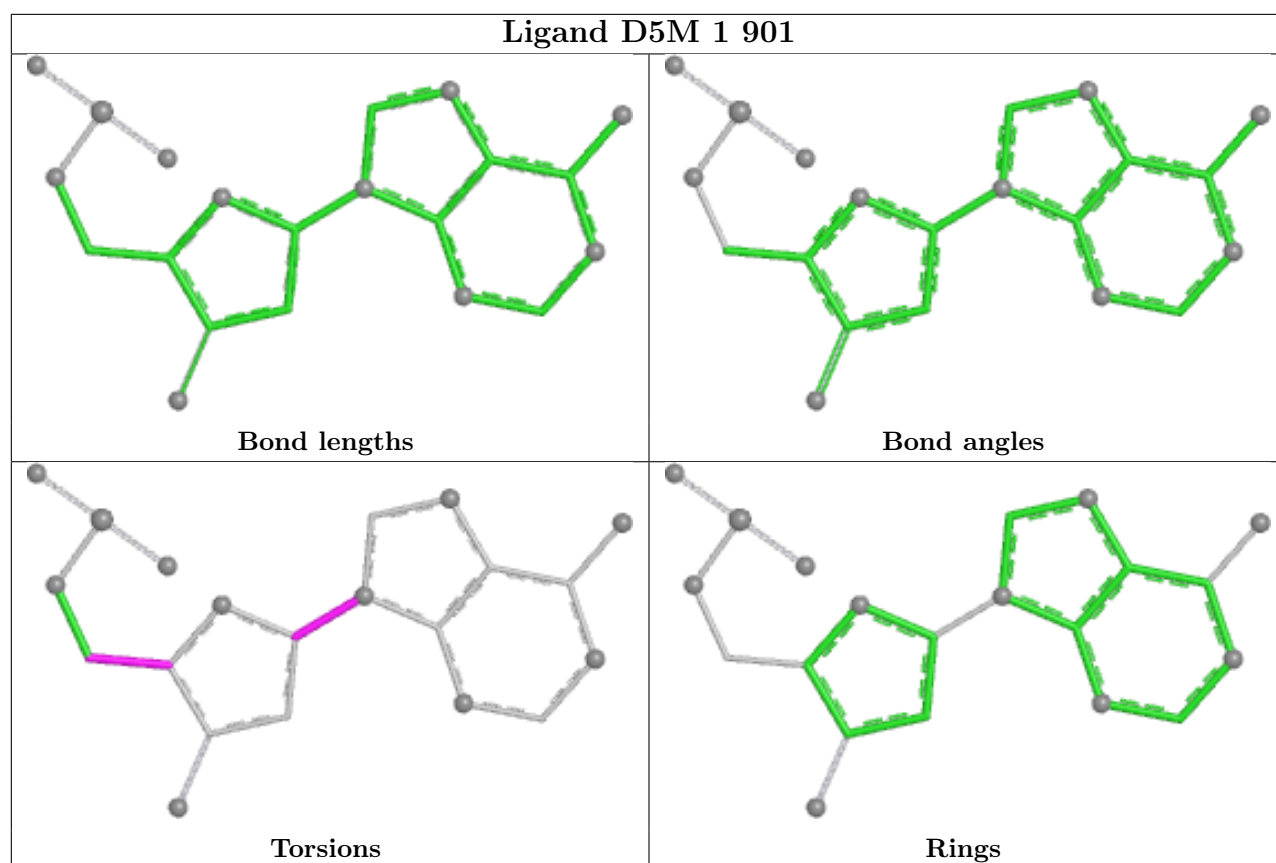


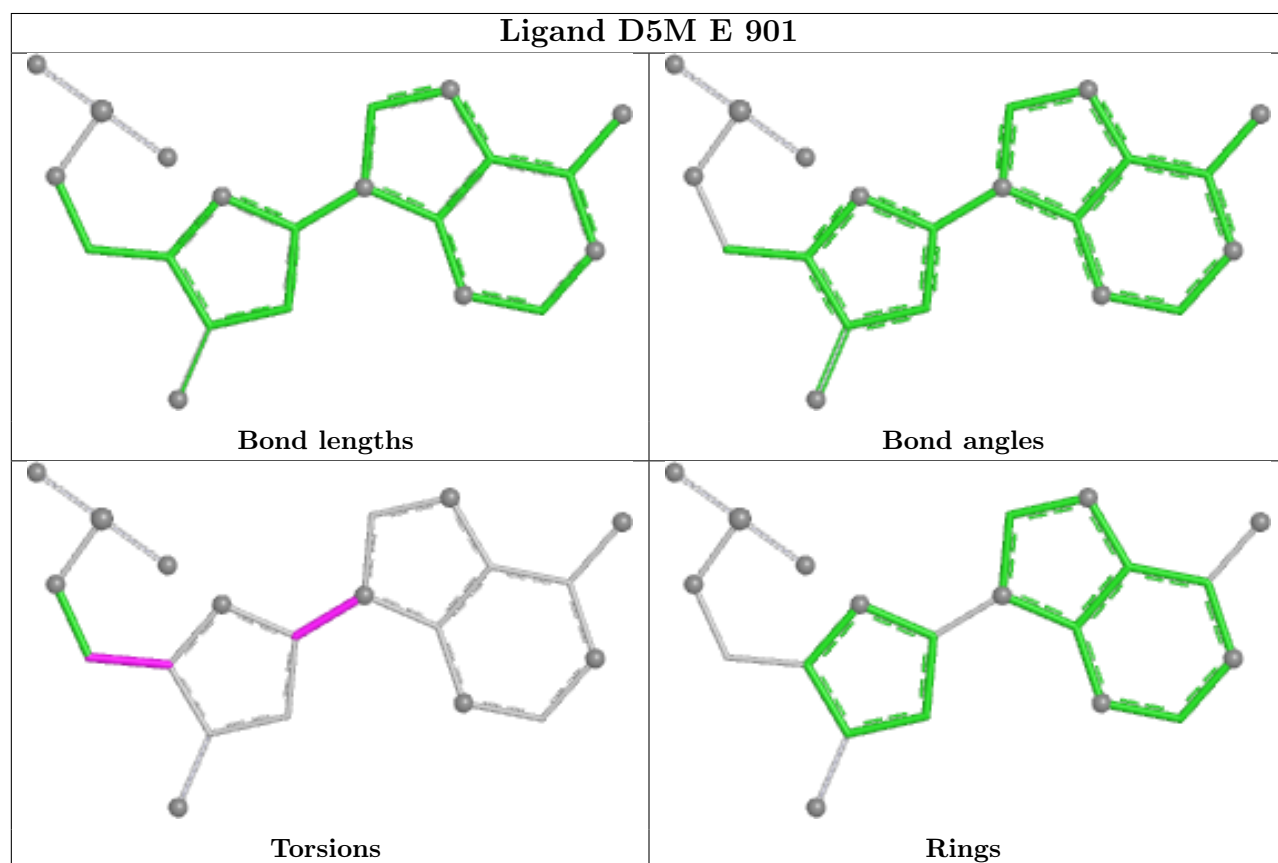
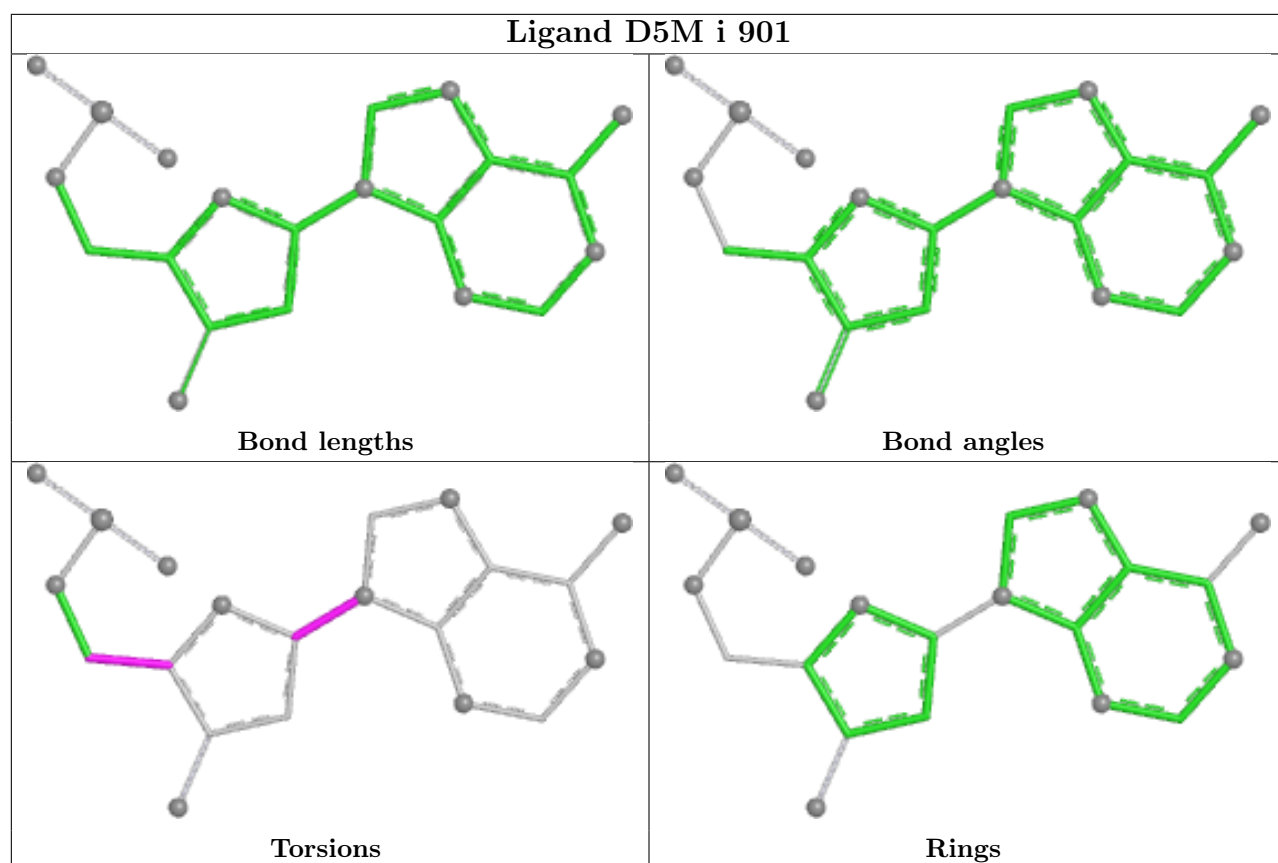
Ligand D5M 7 901

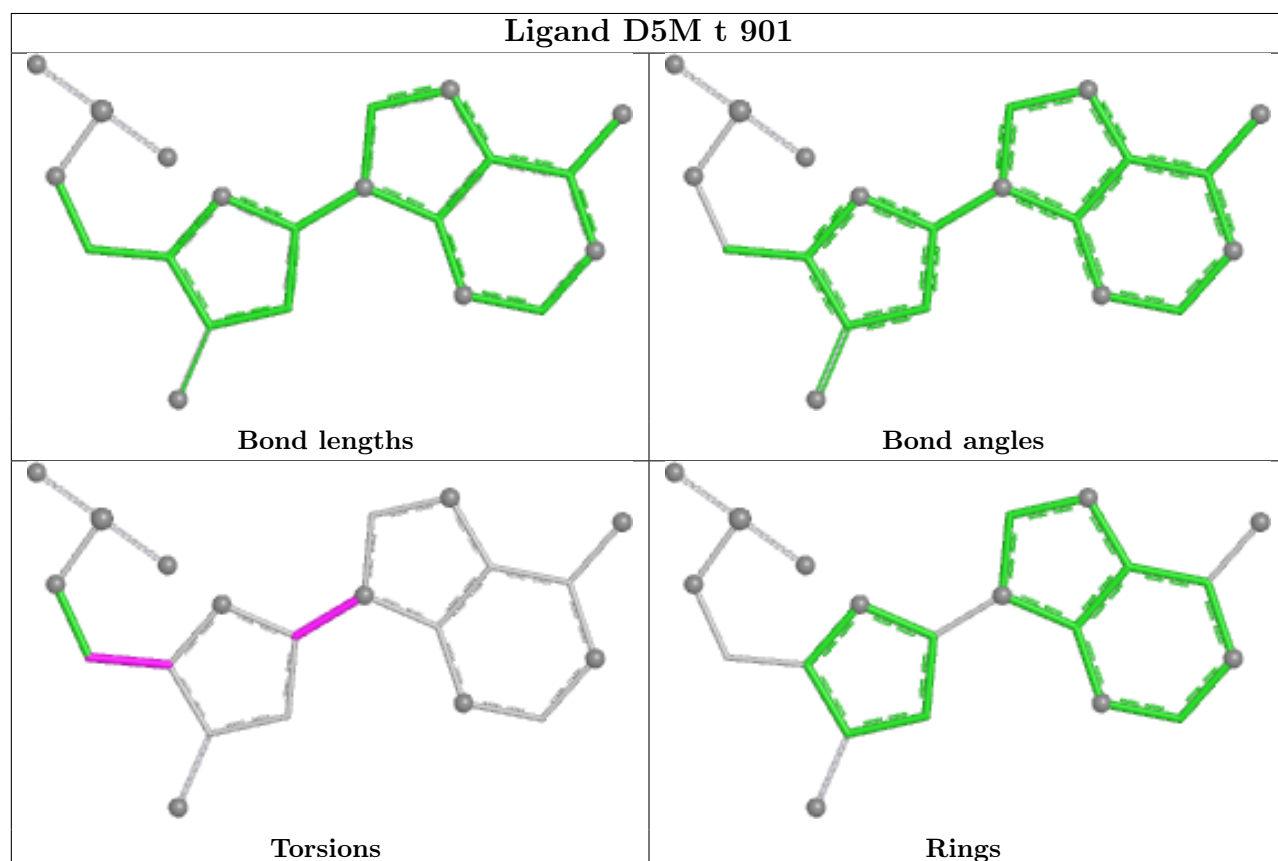
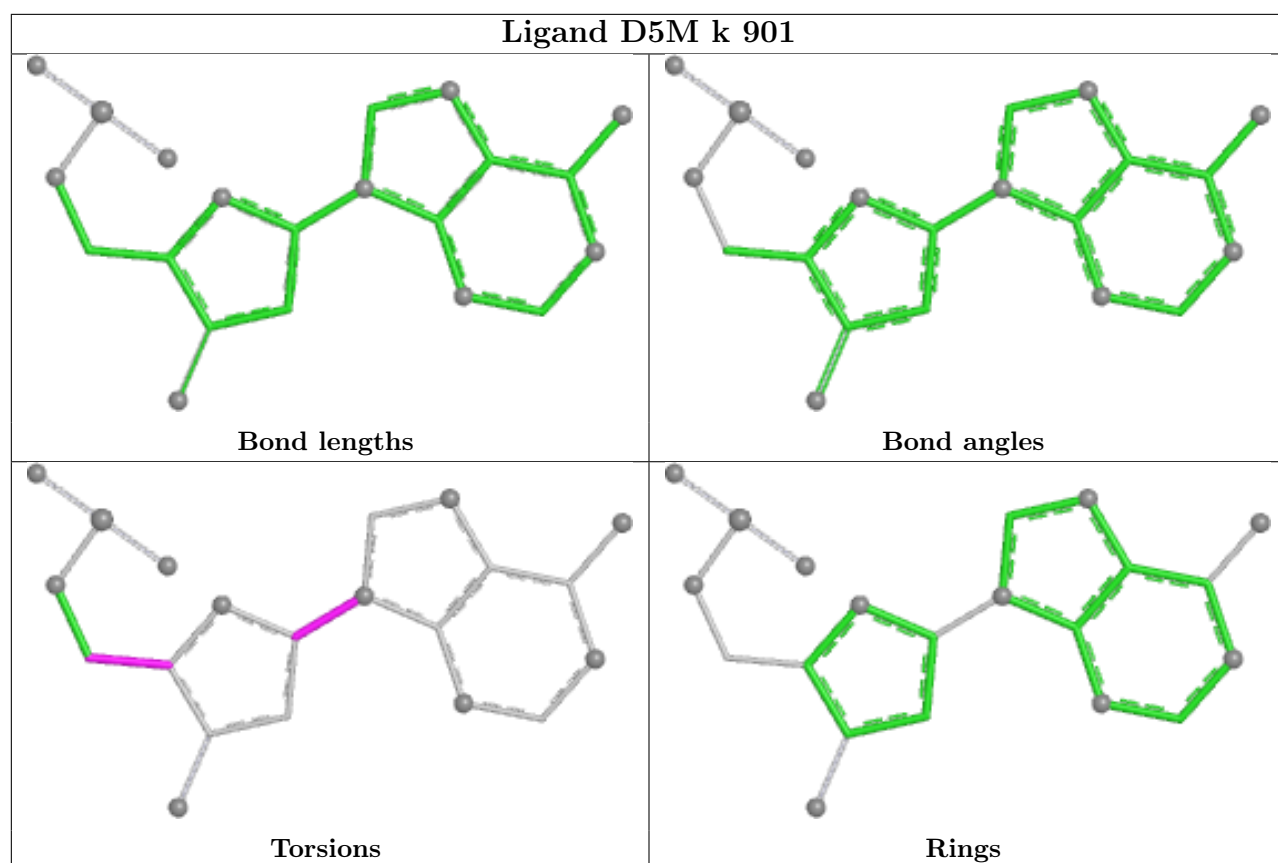


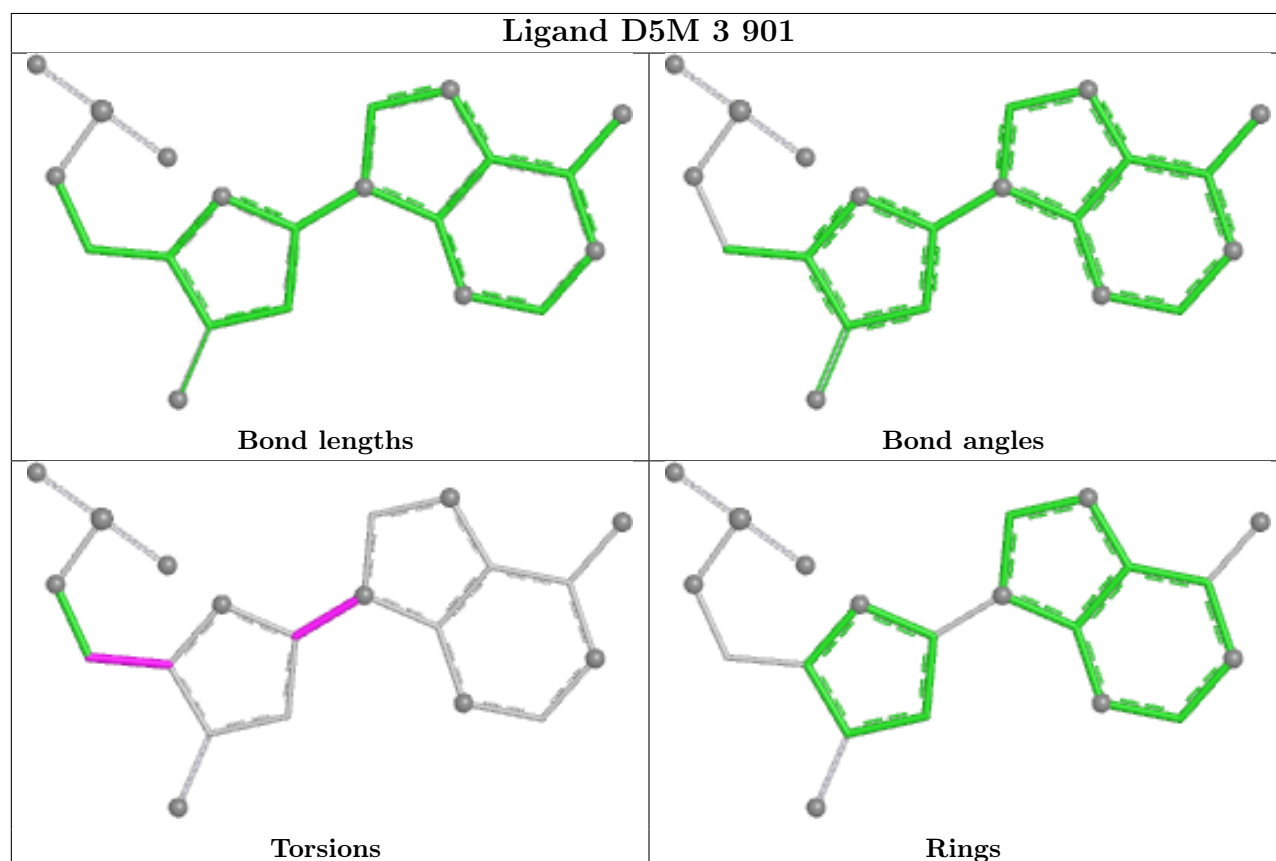
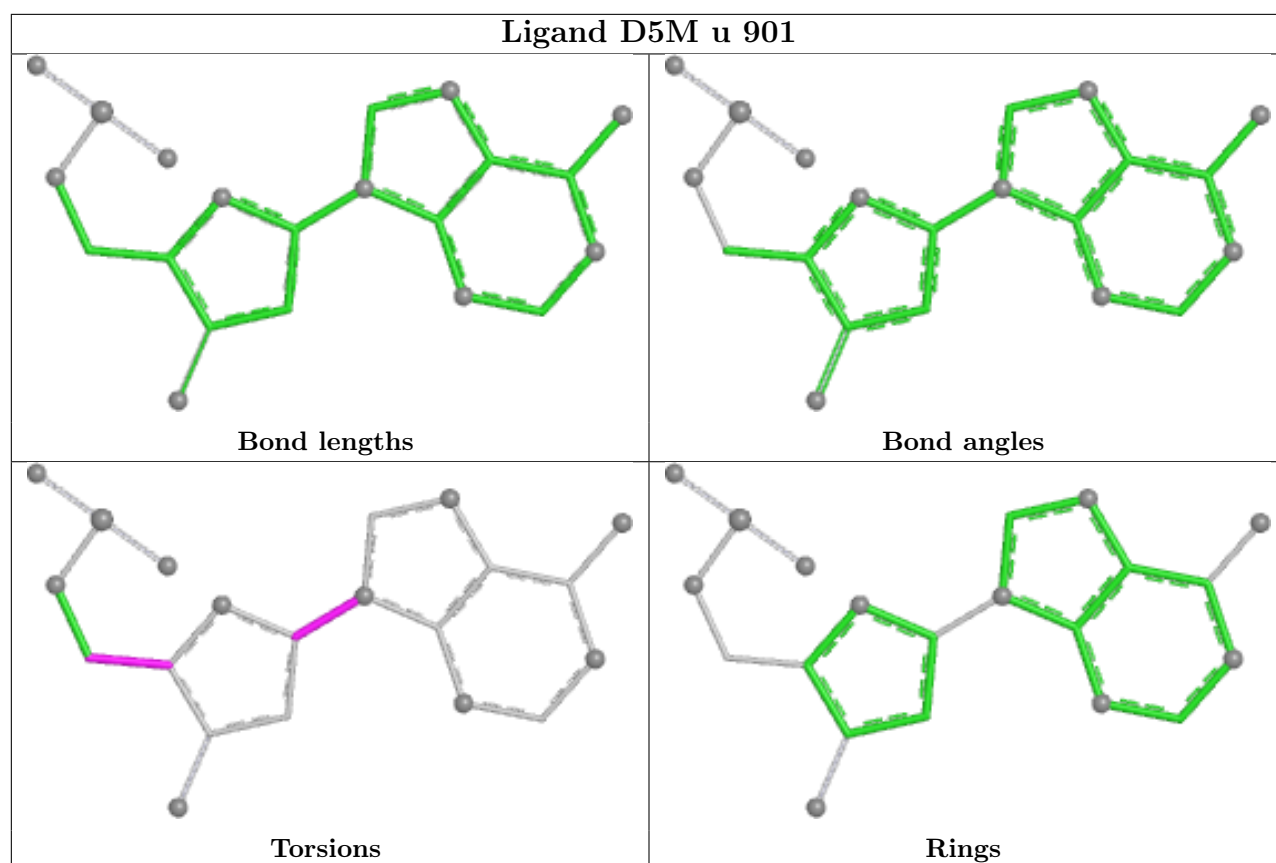
Ligand D5M a 901

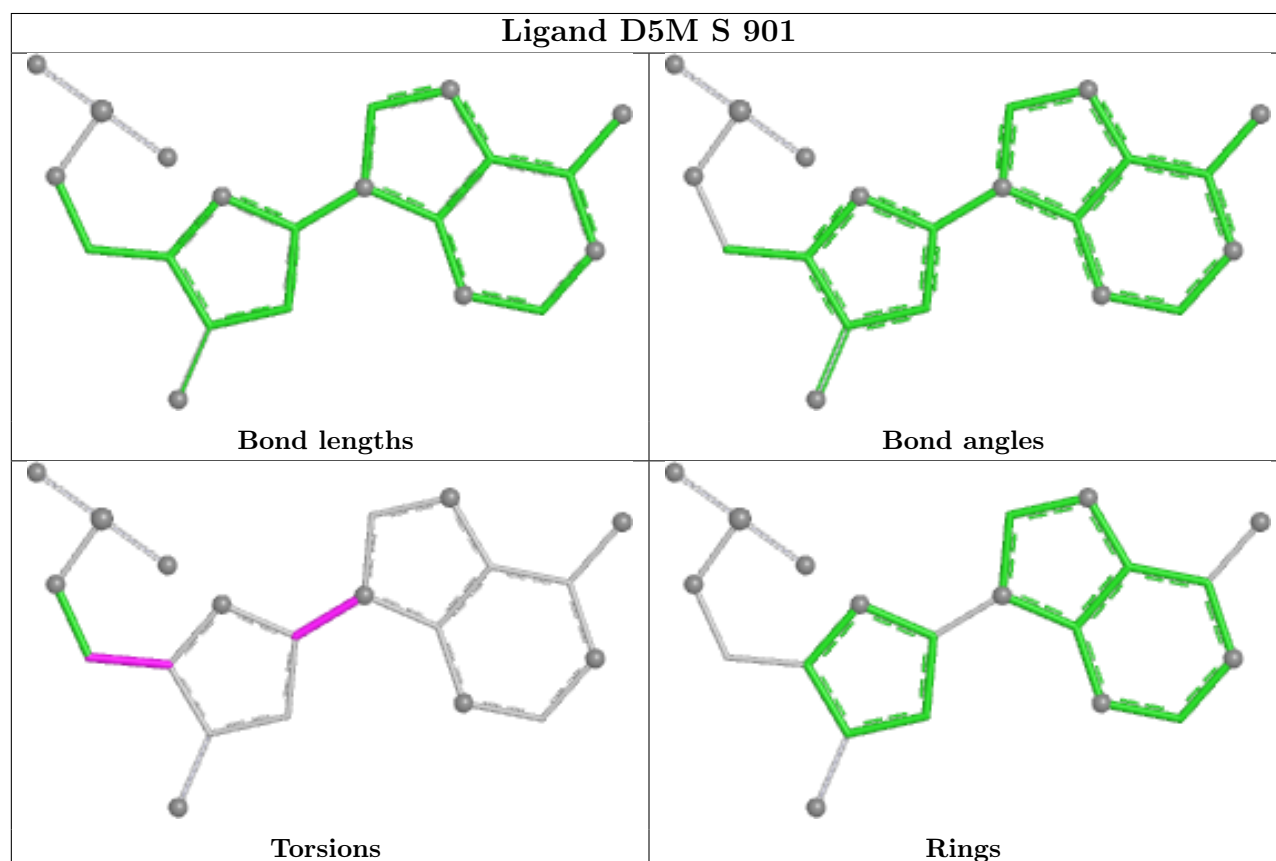
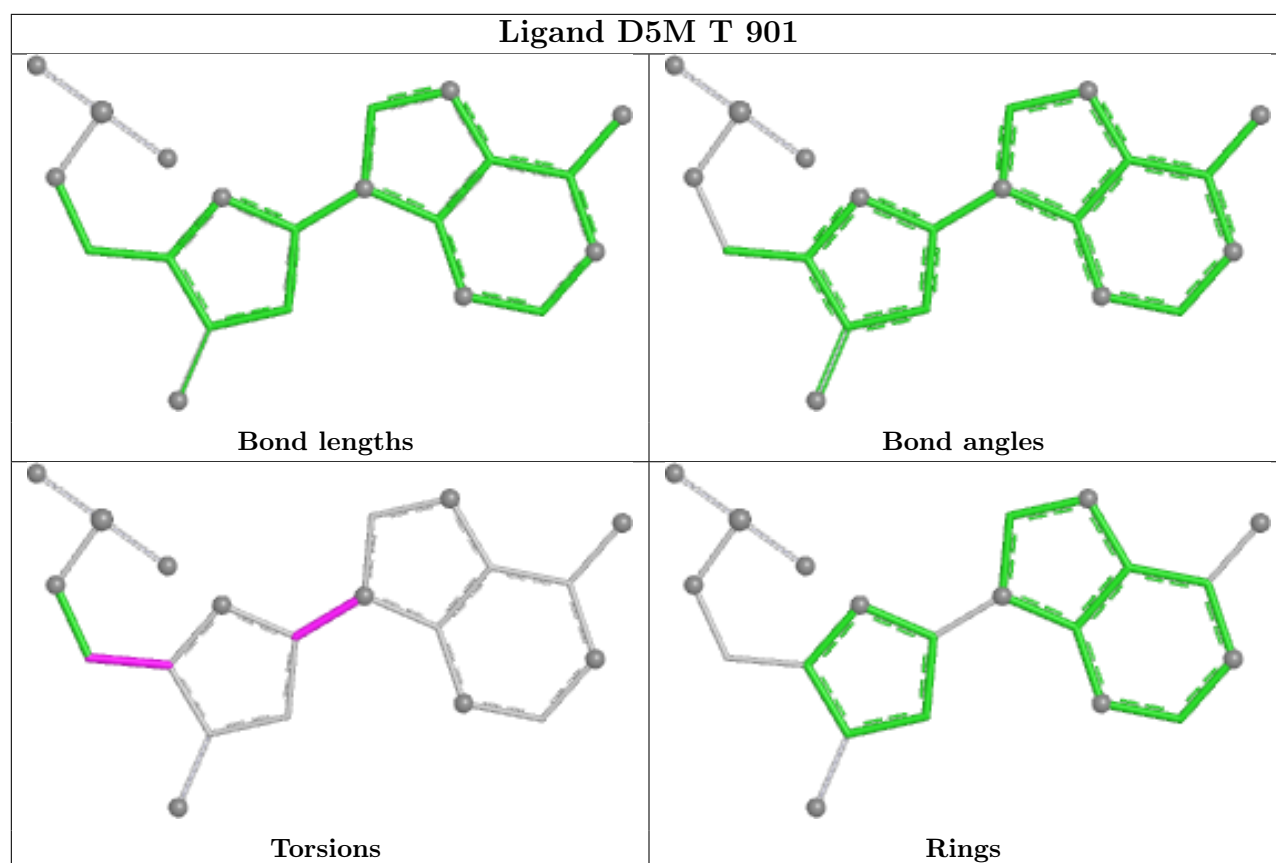


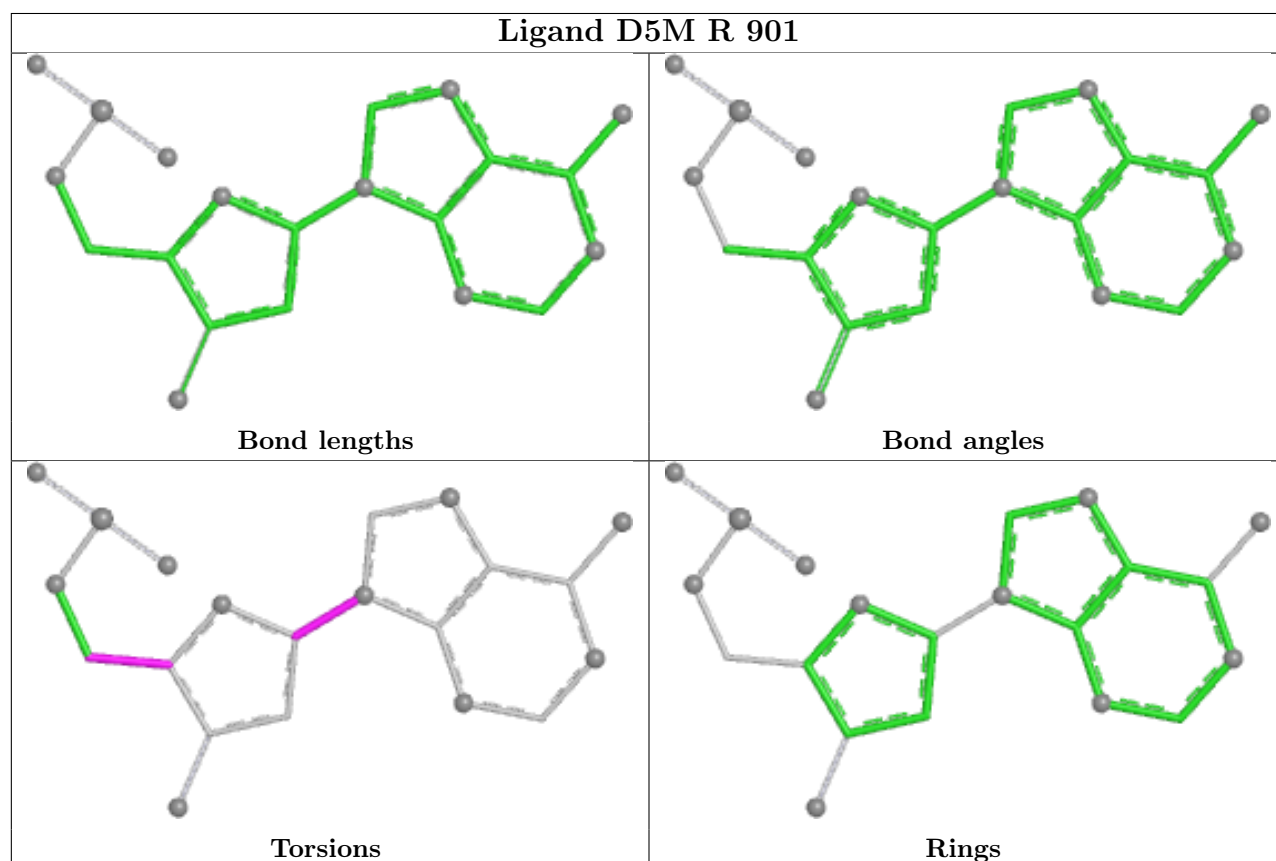
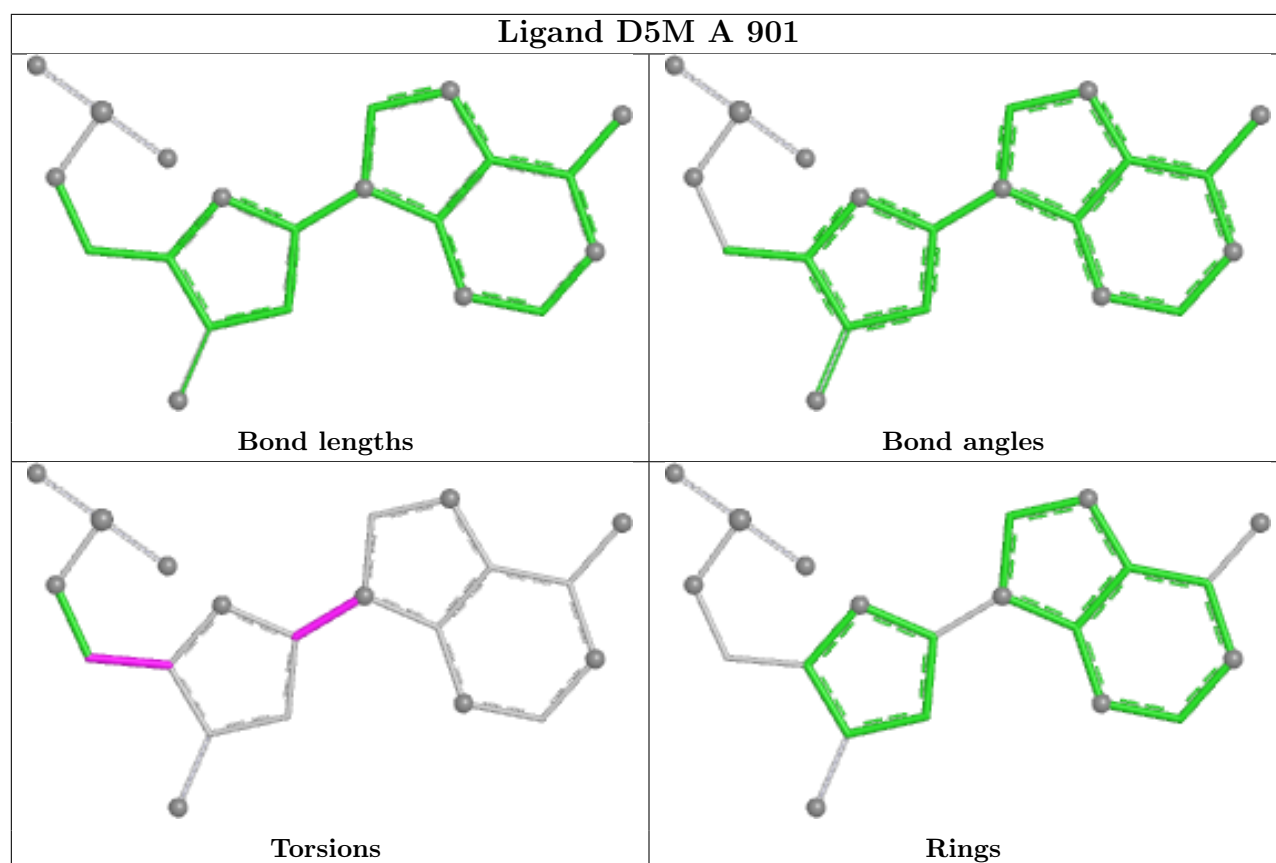


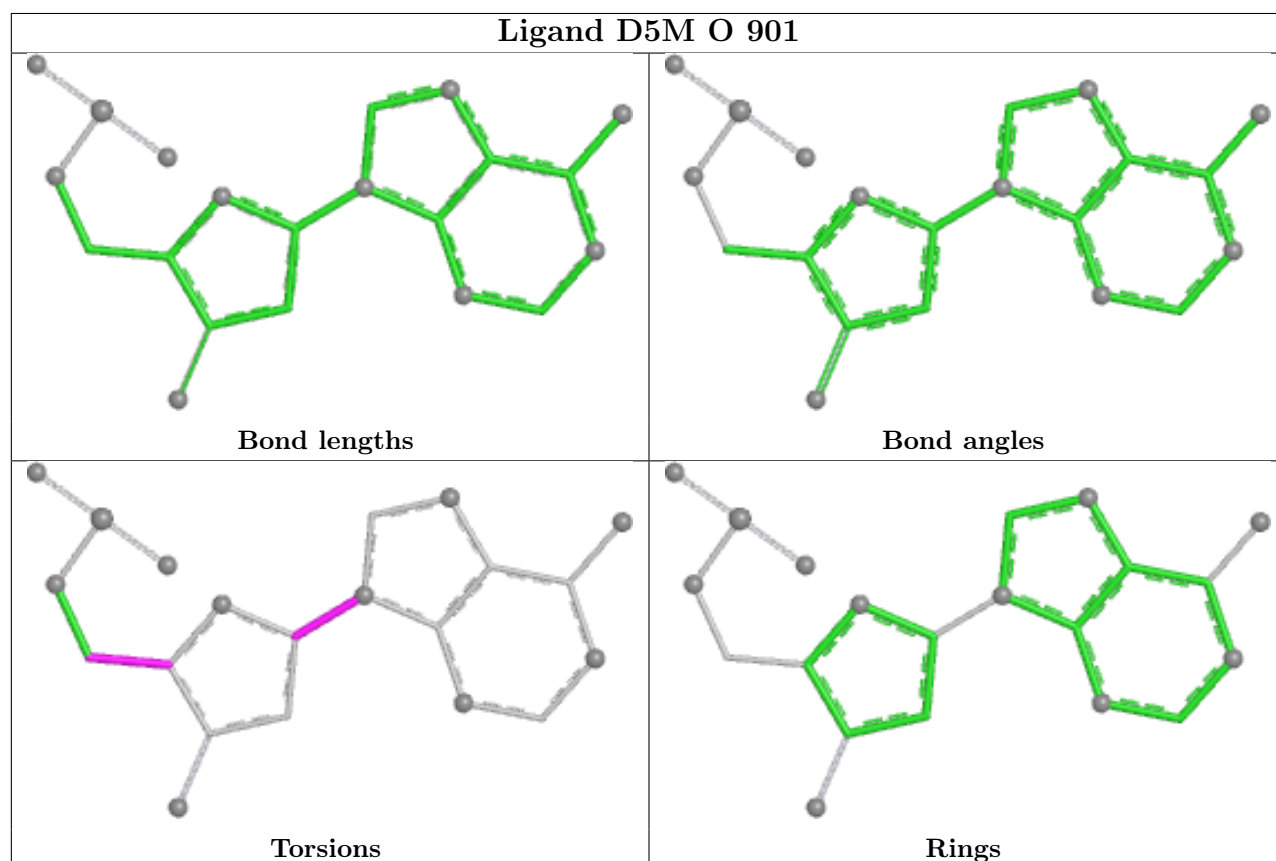
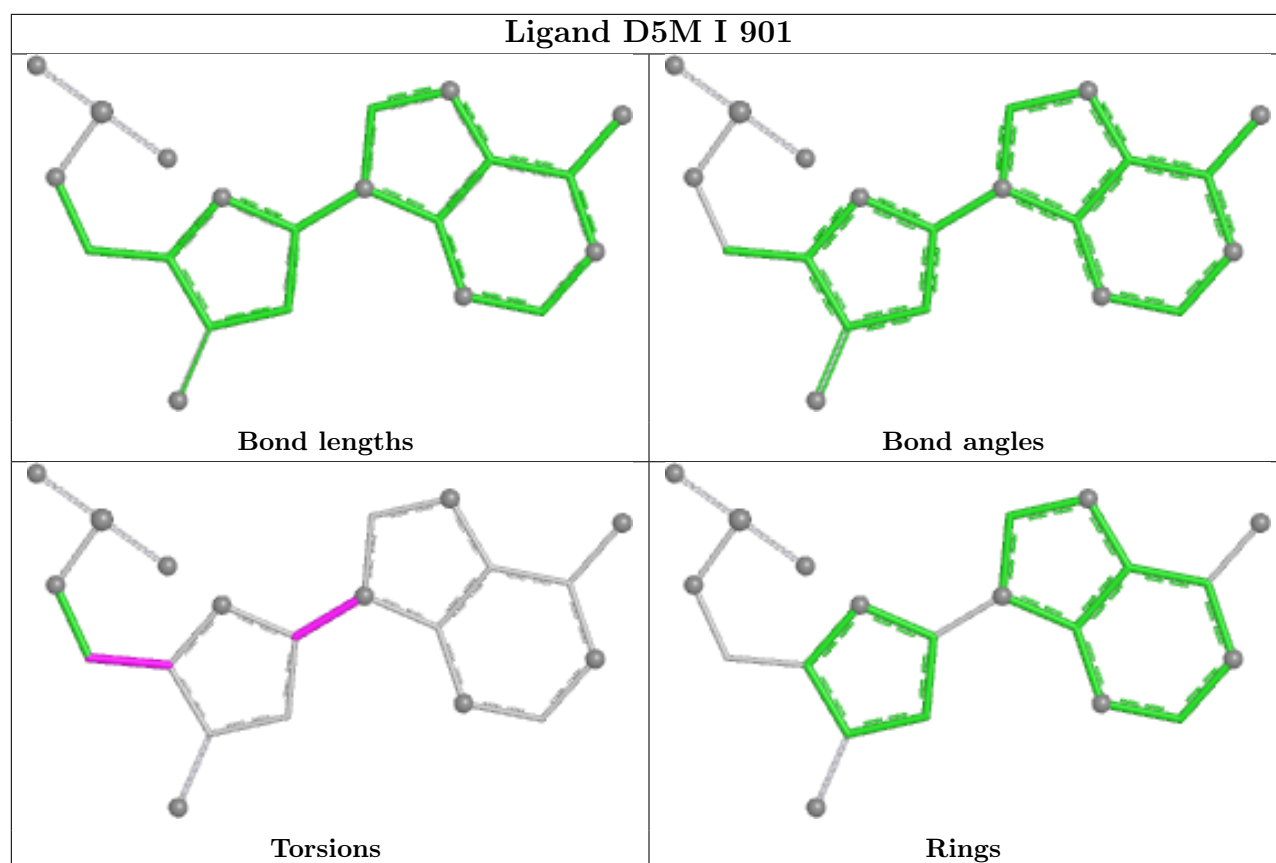


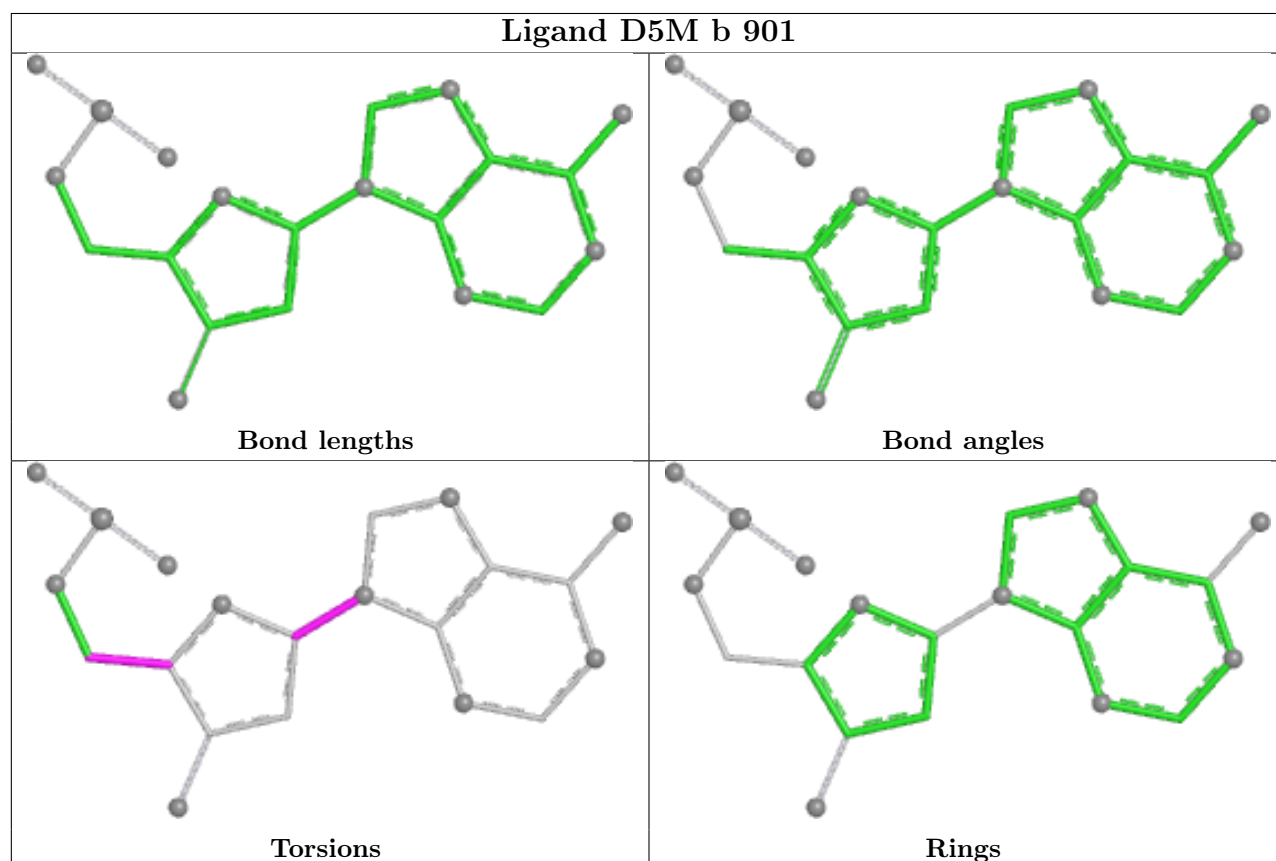
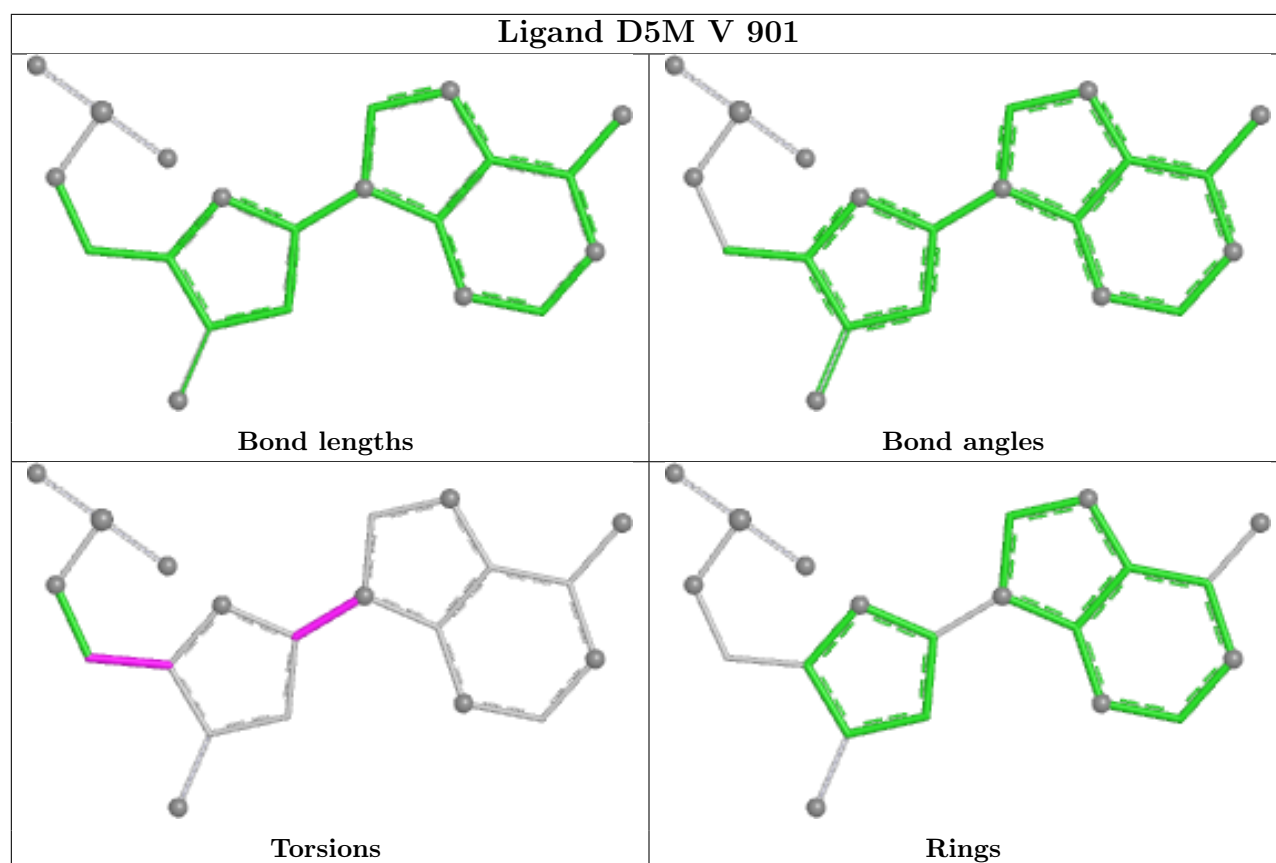


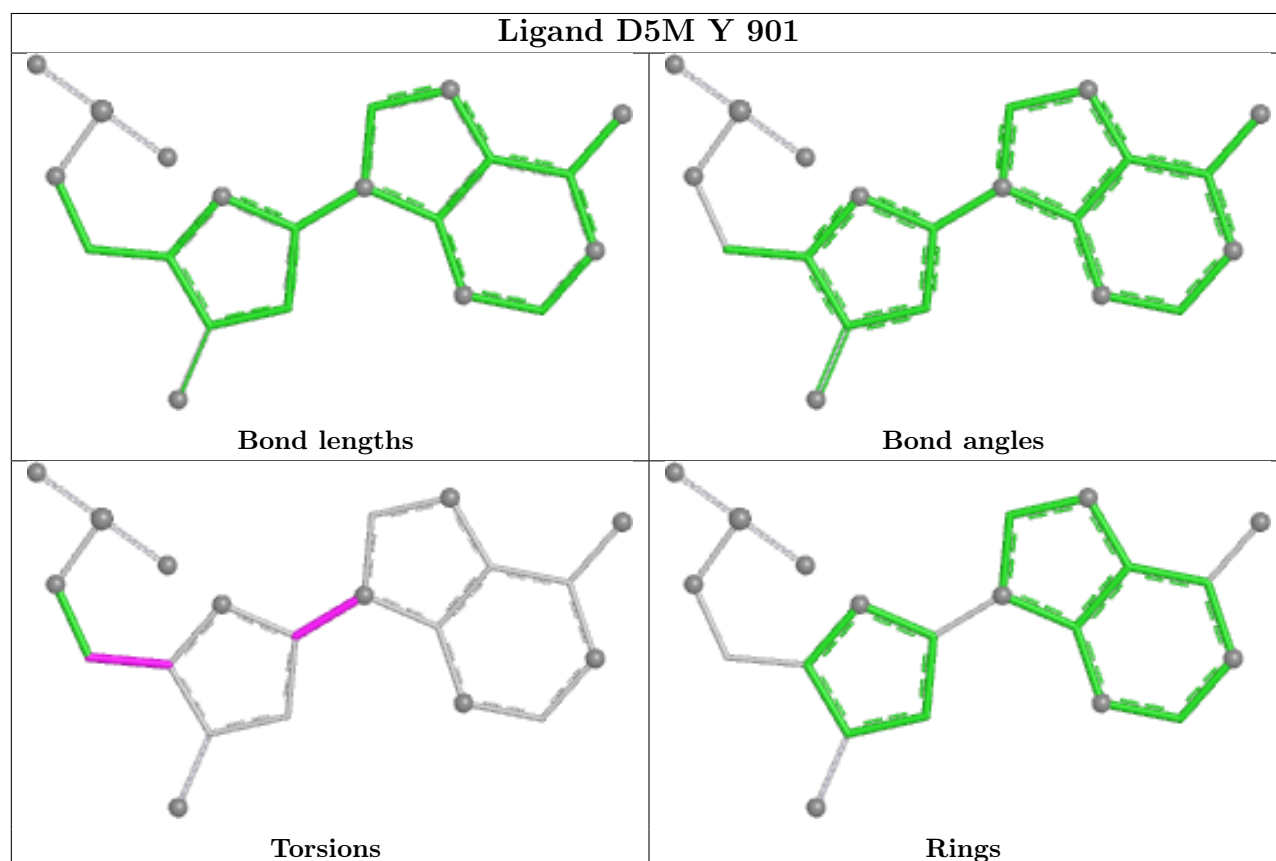
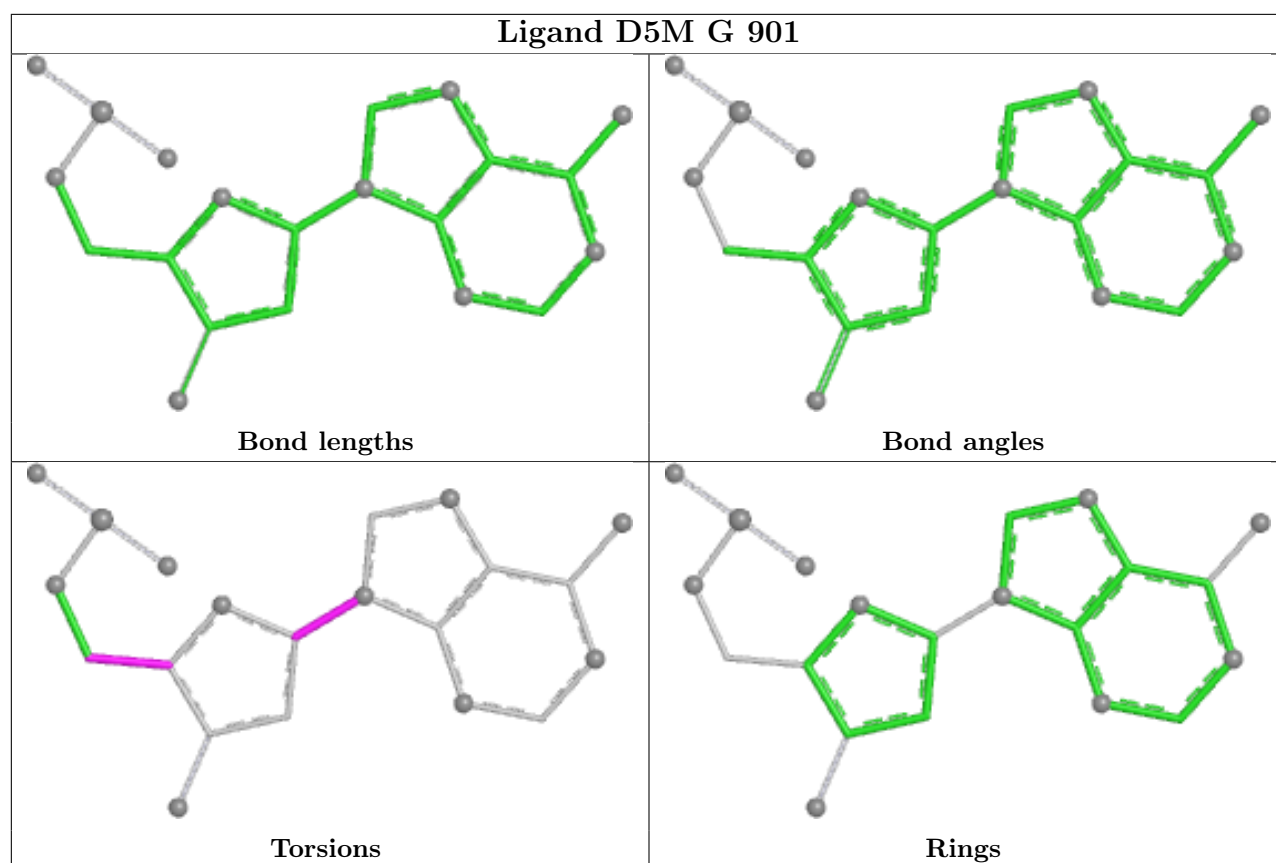


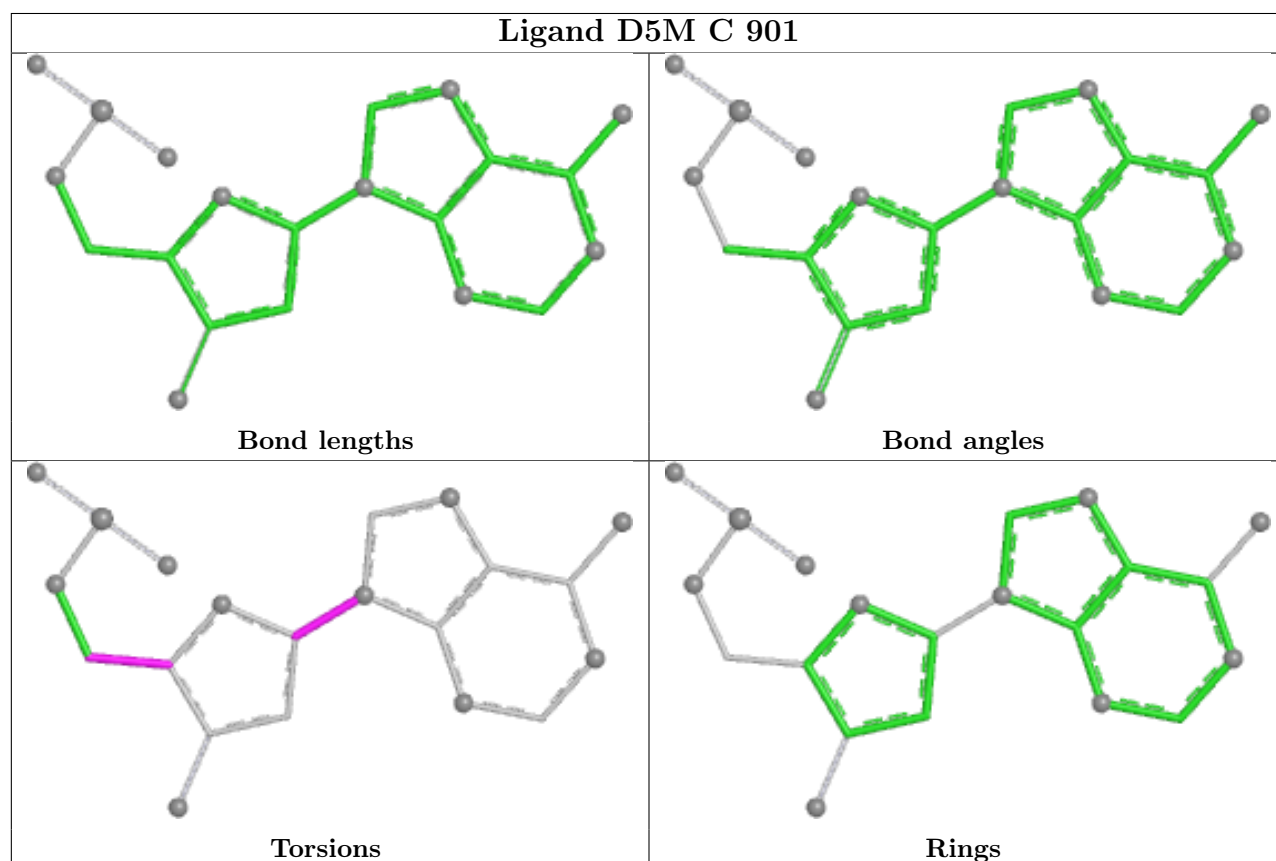
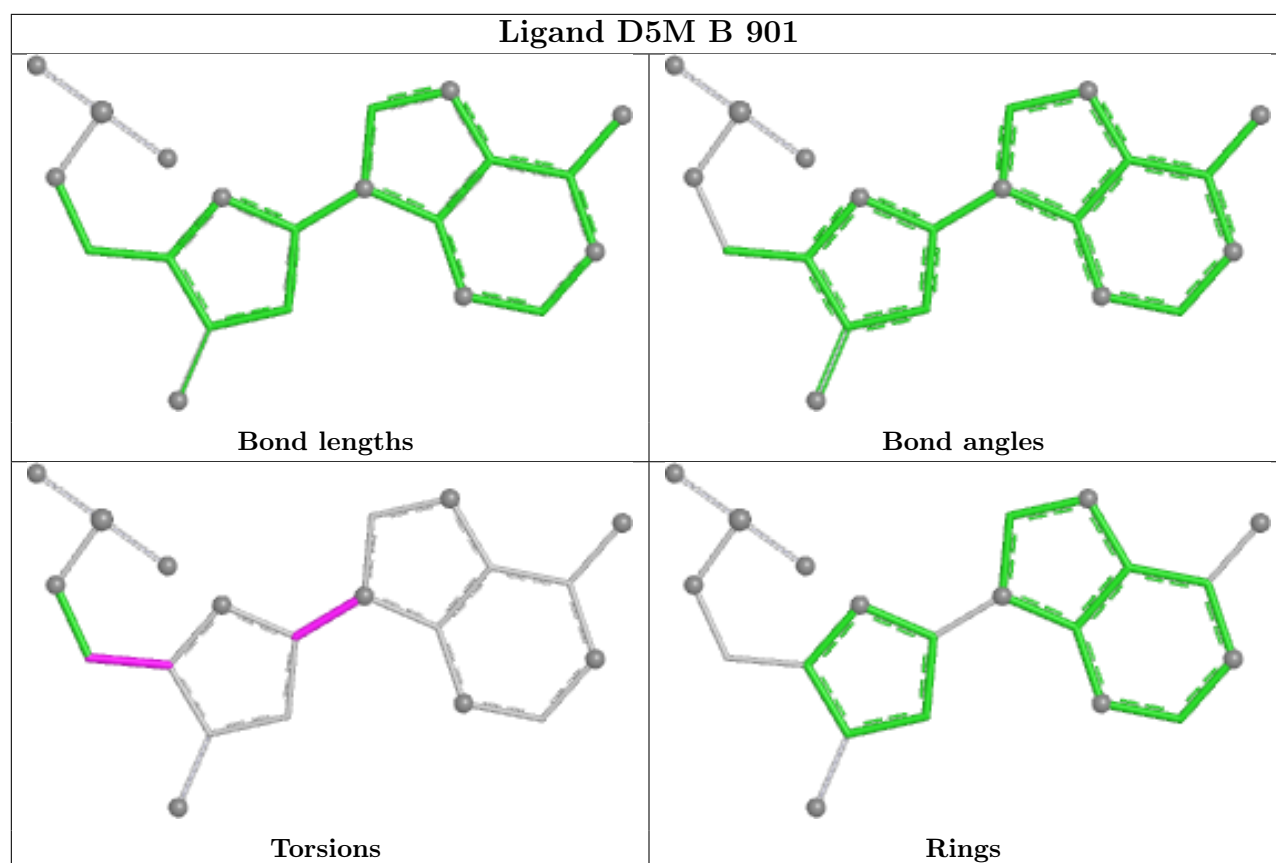


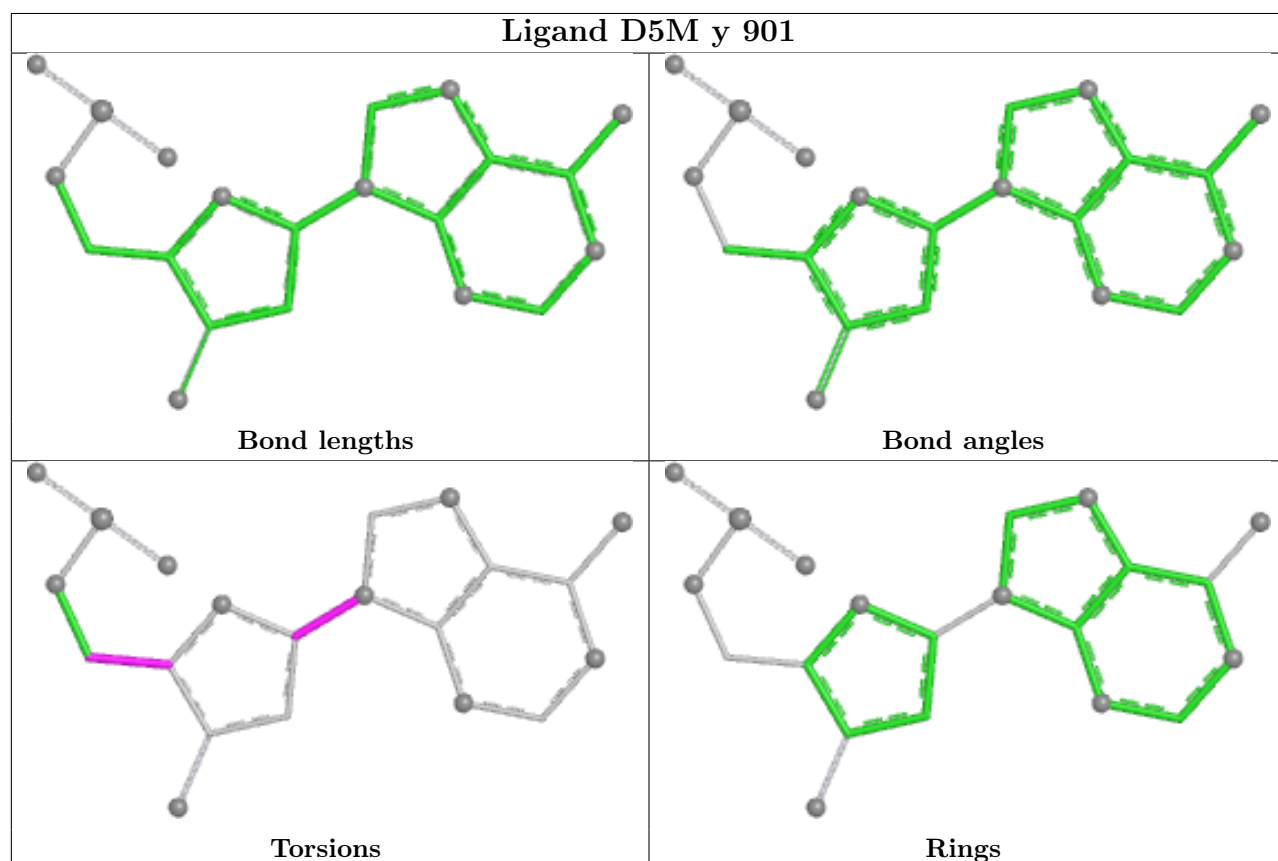
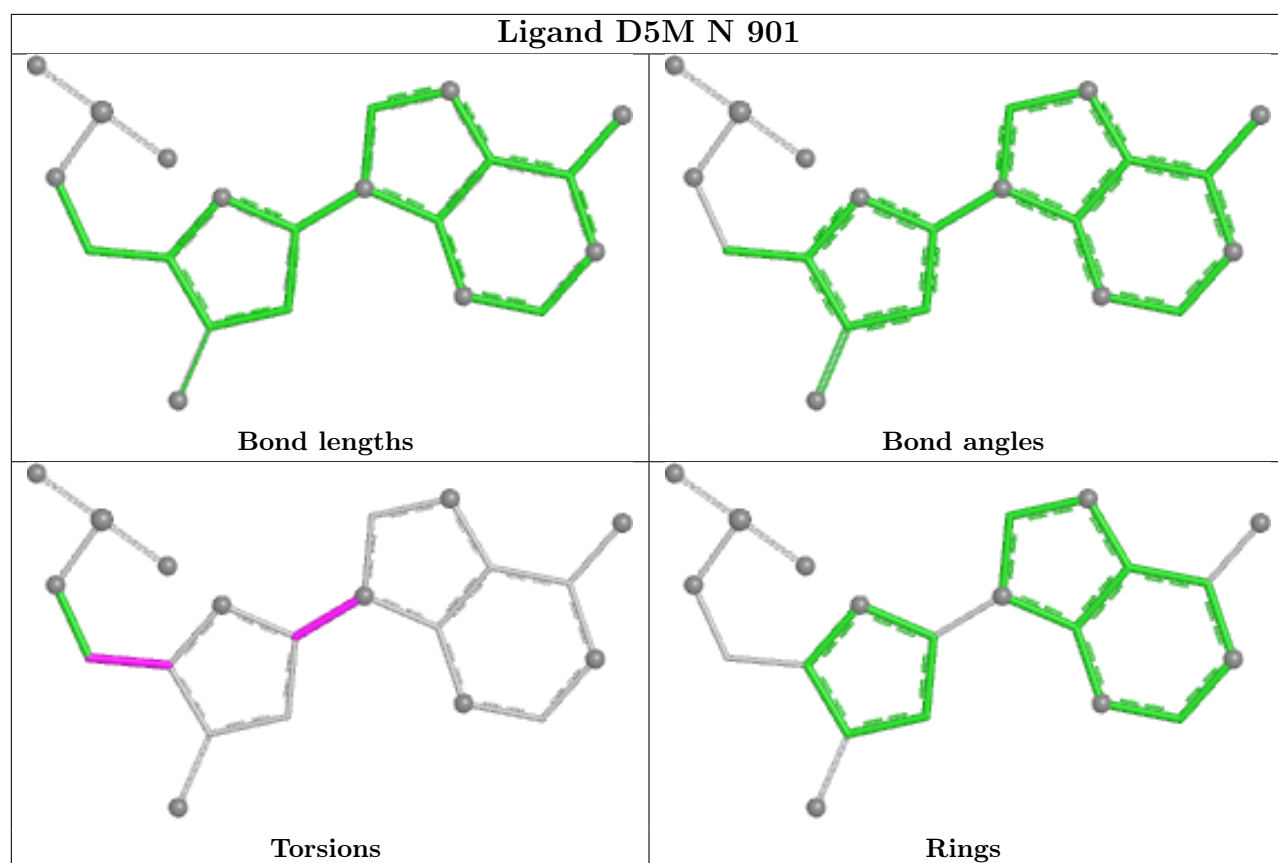


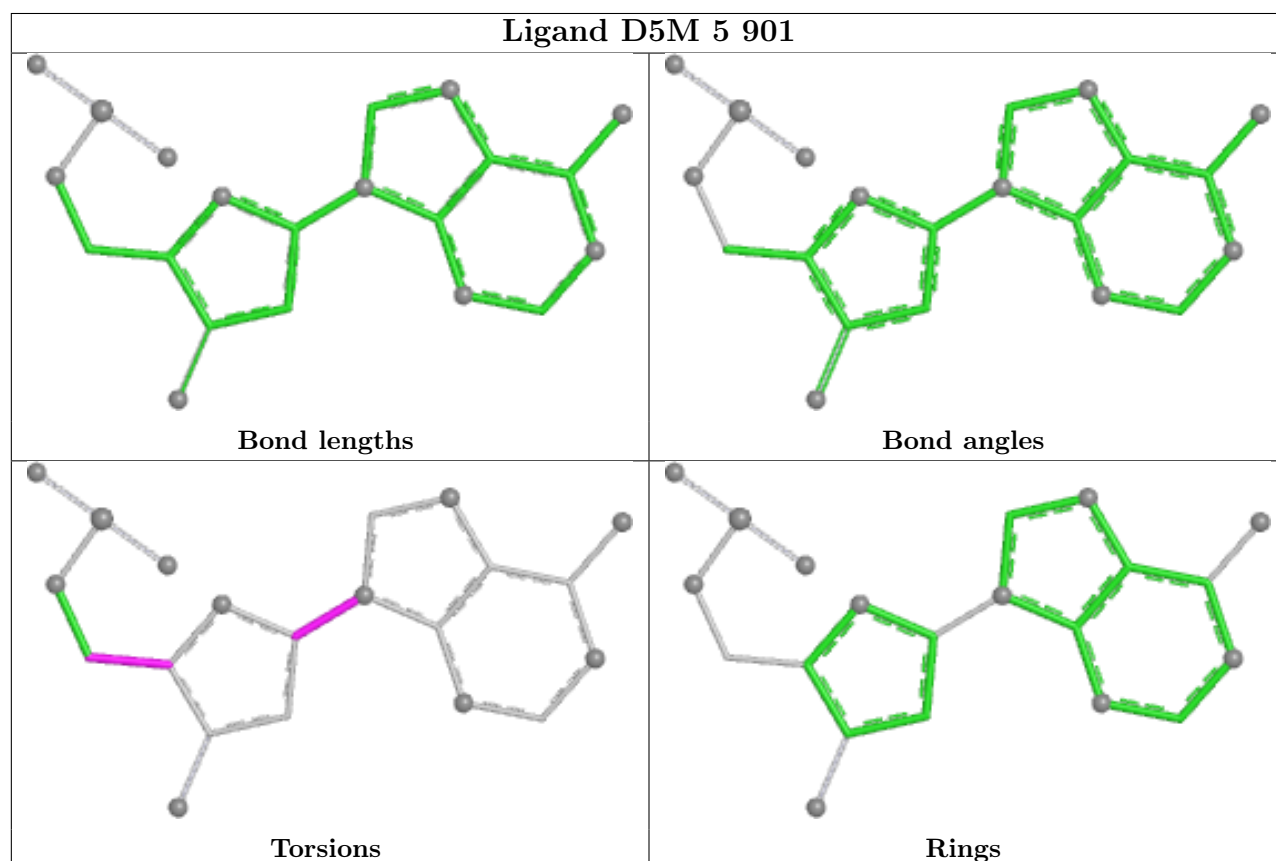
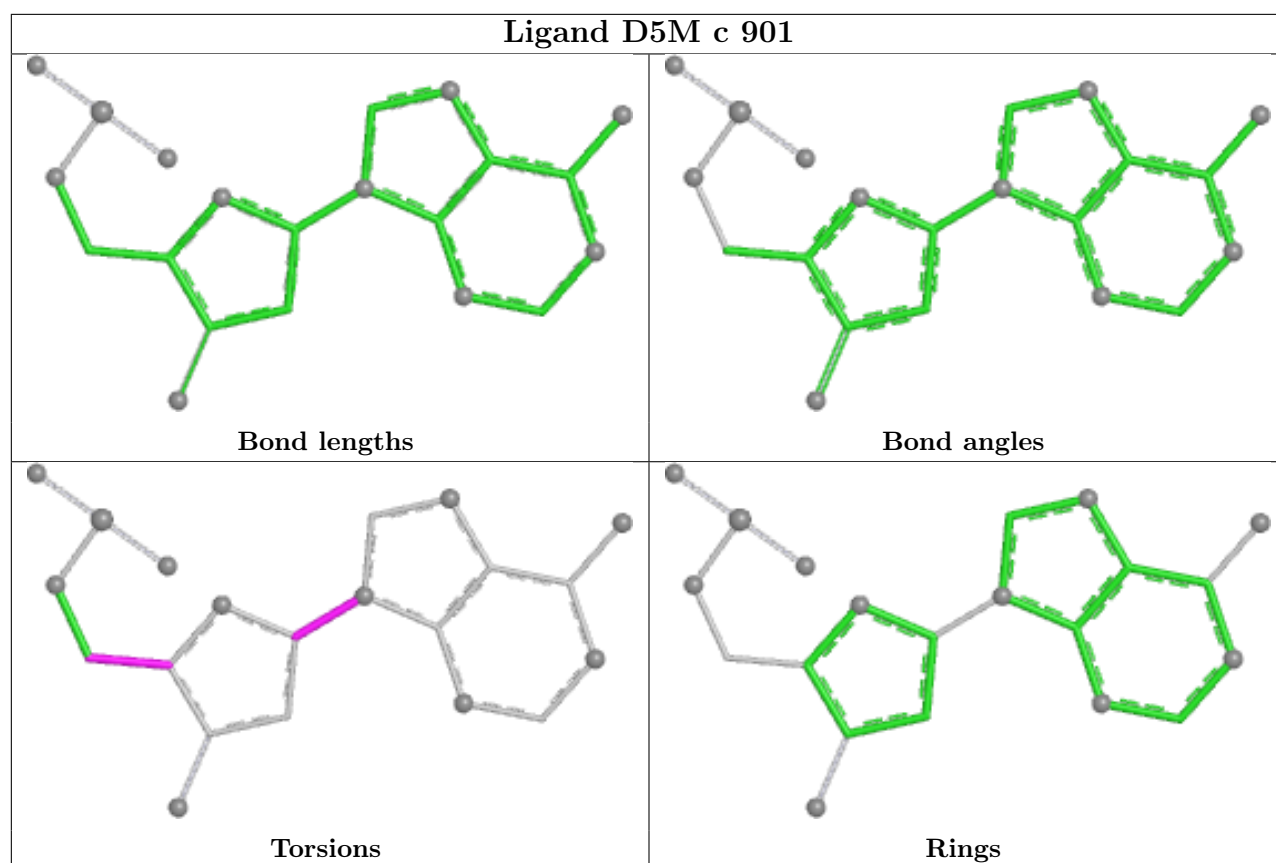


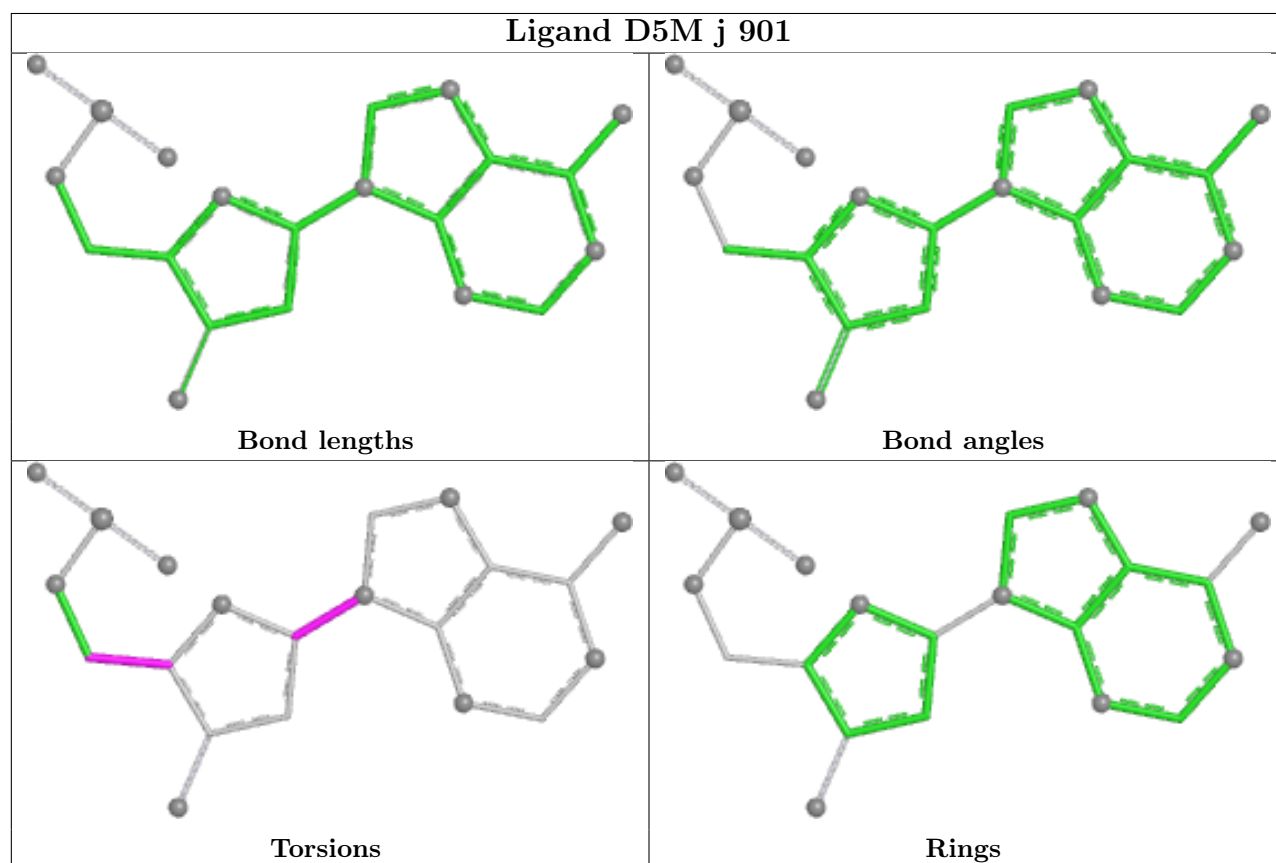
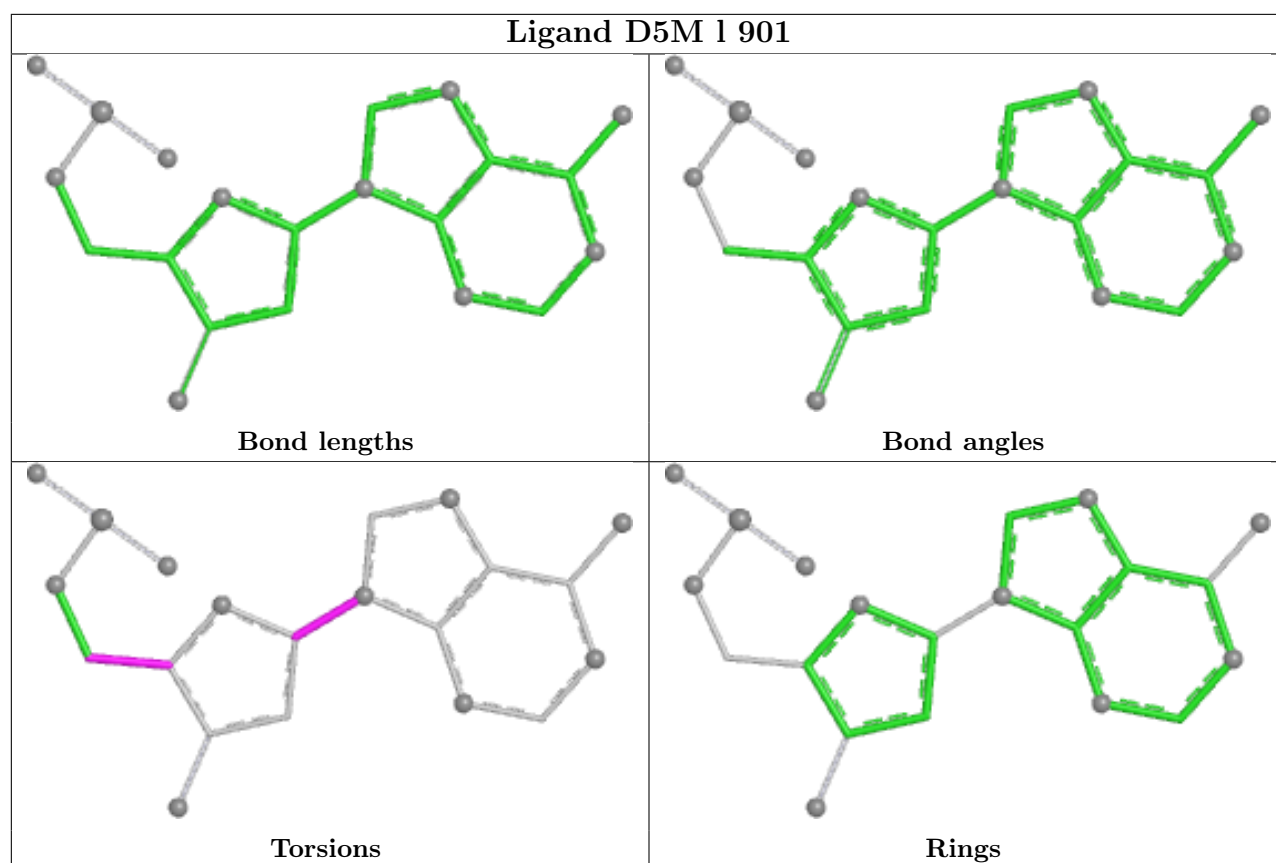


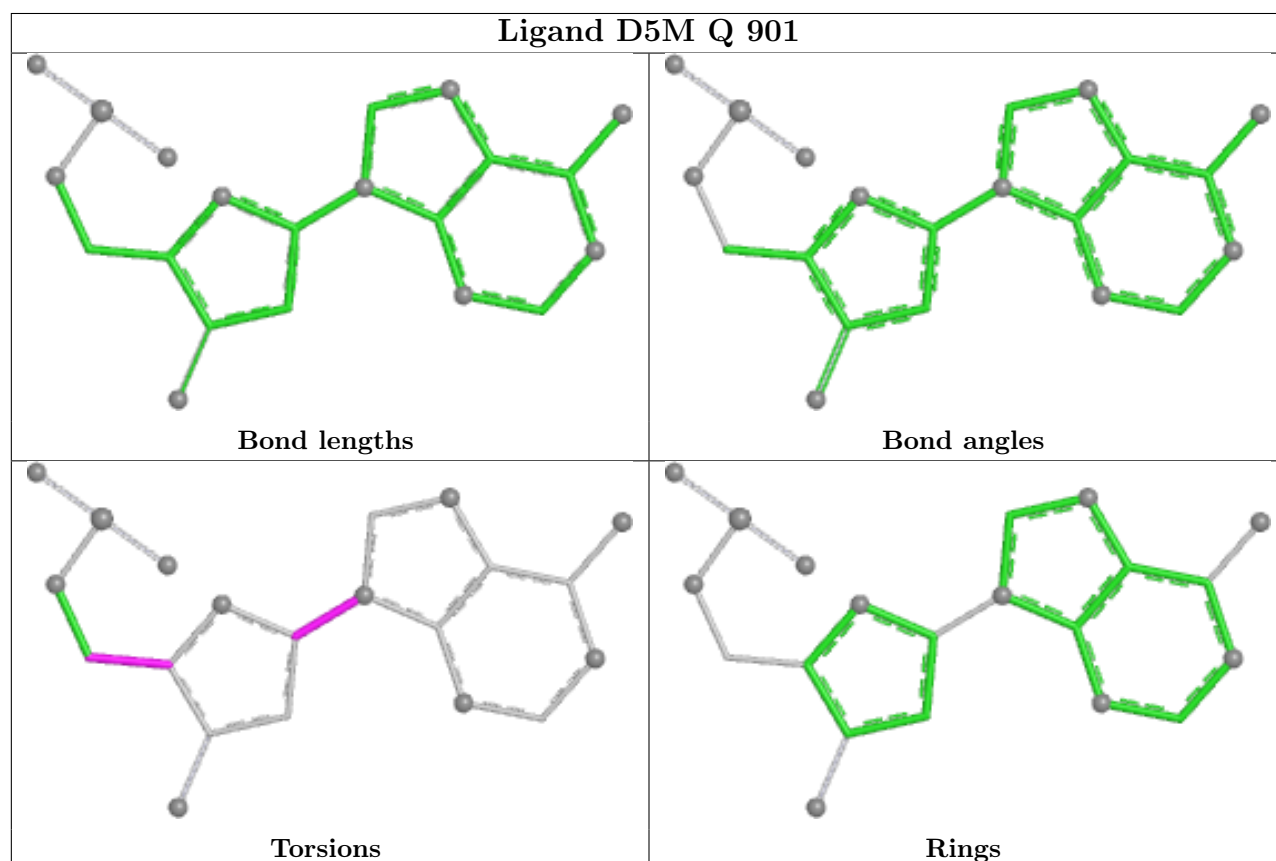
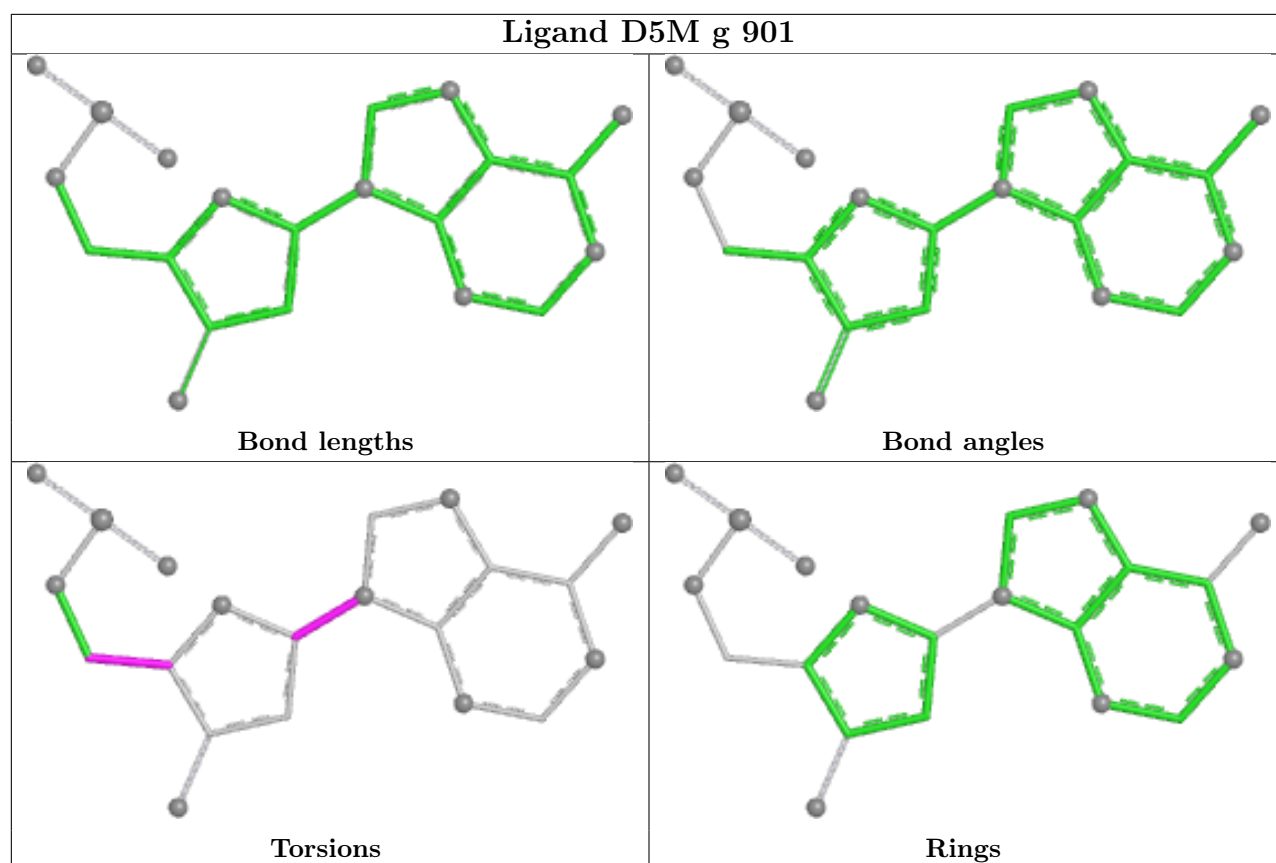


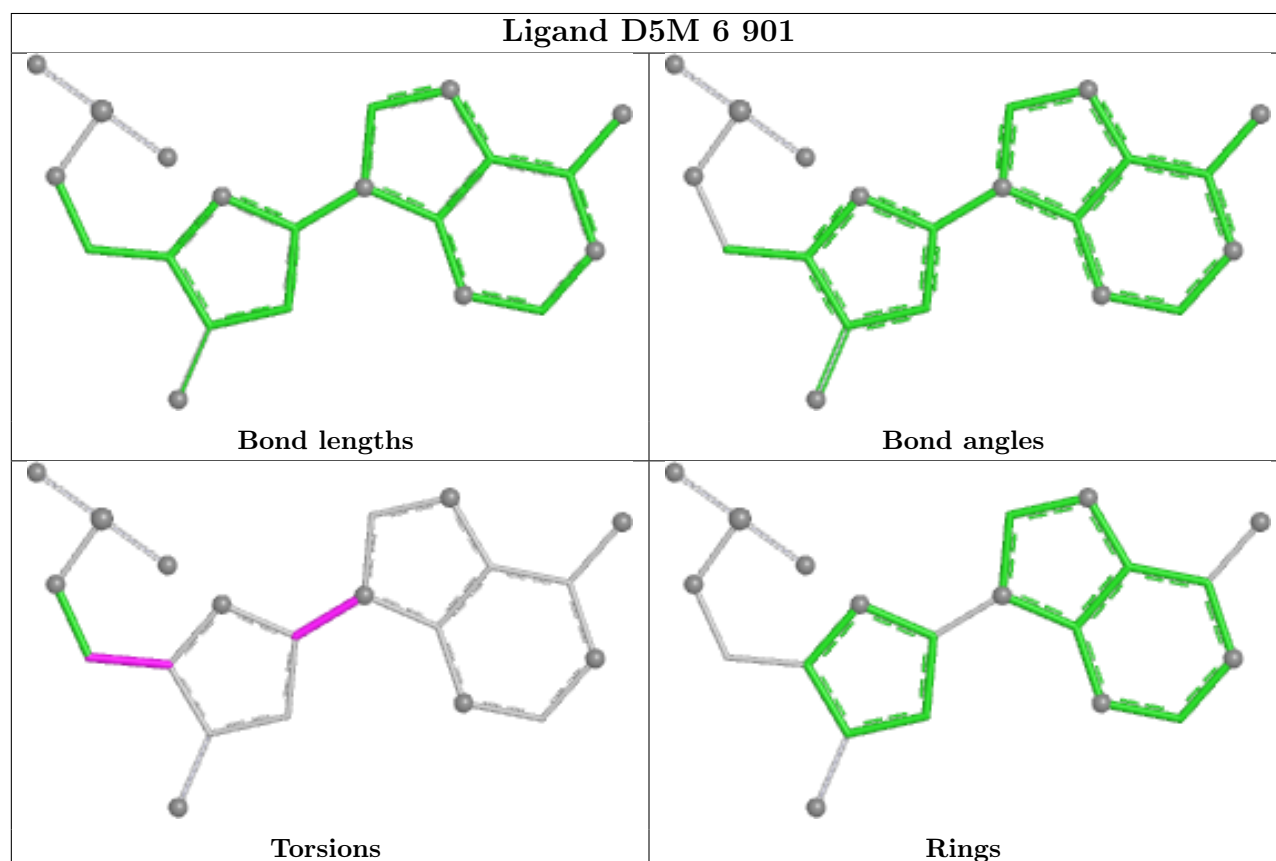
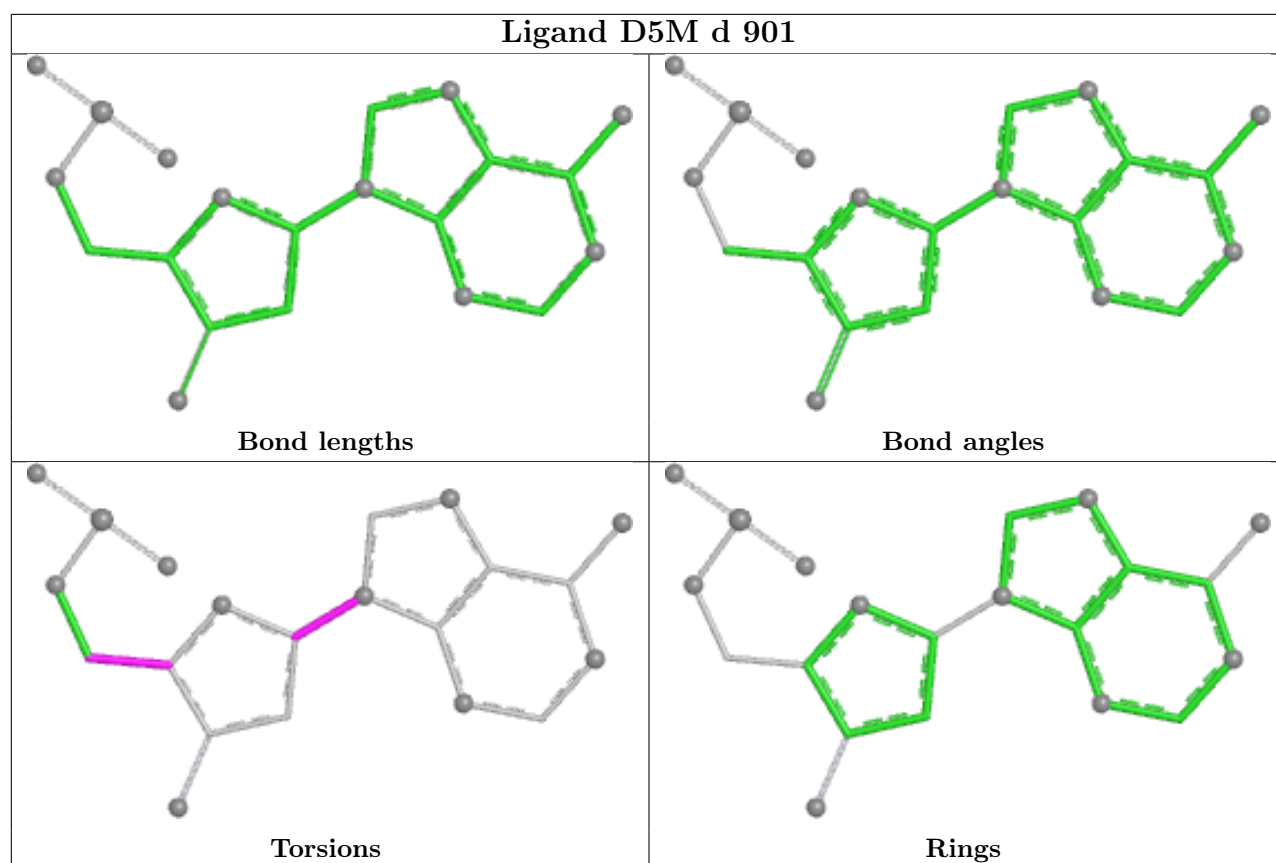


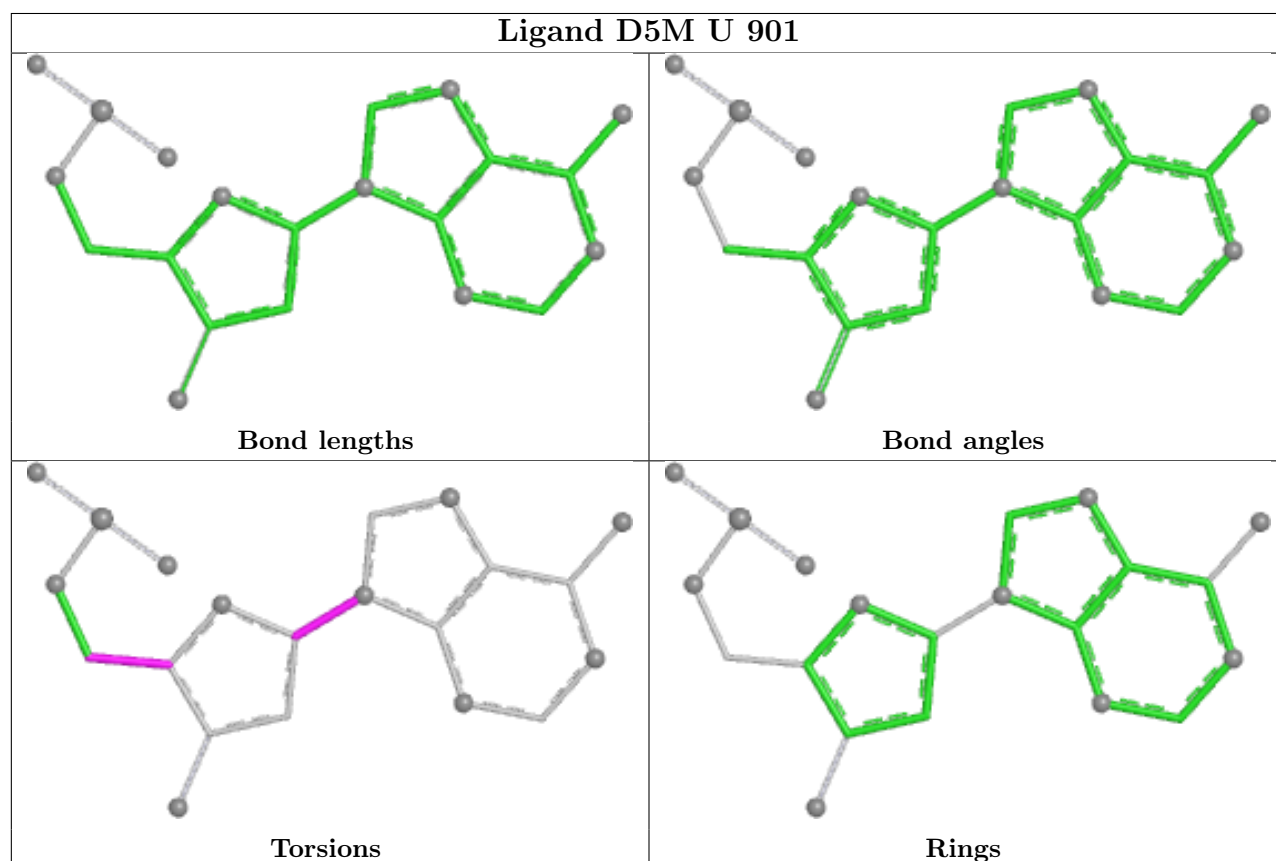
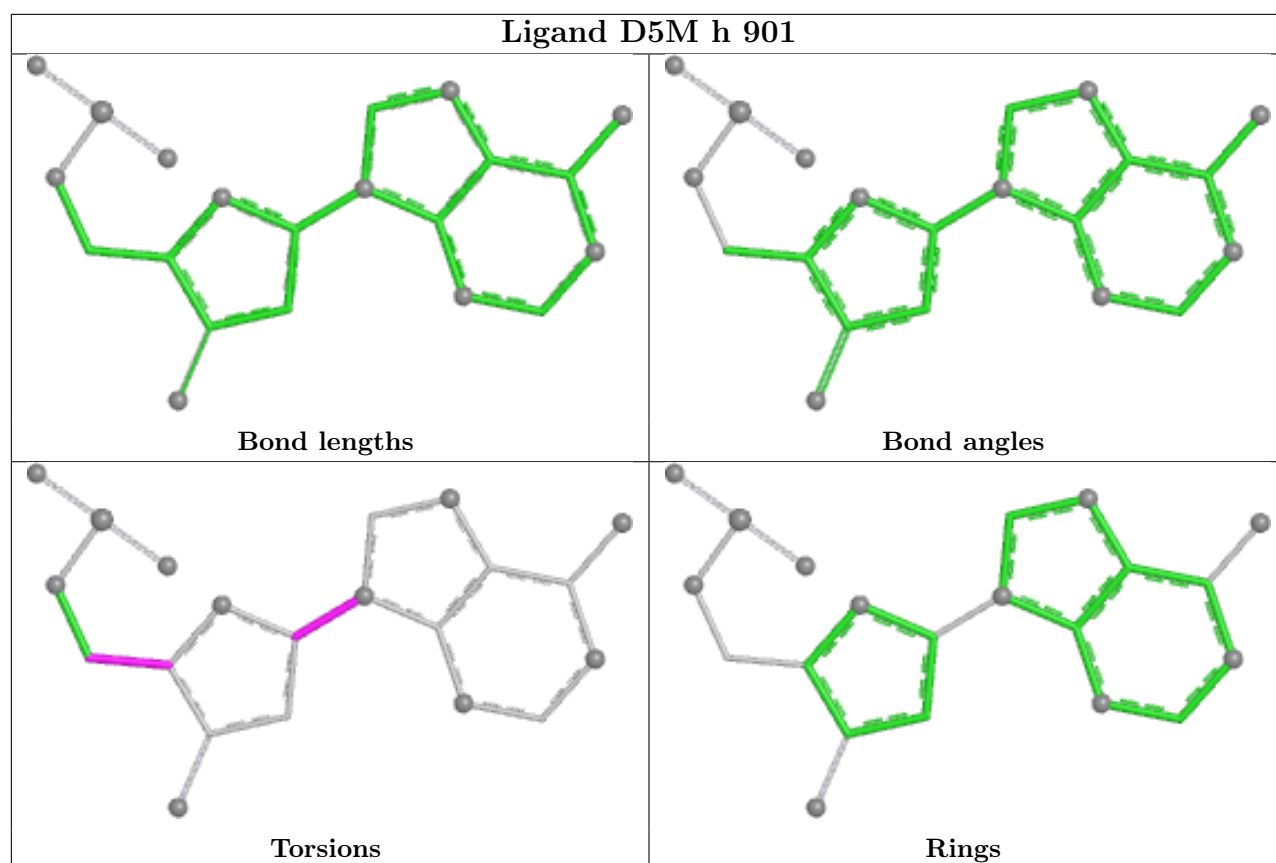


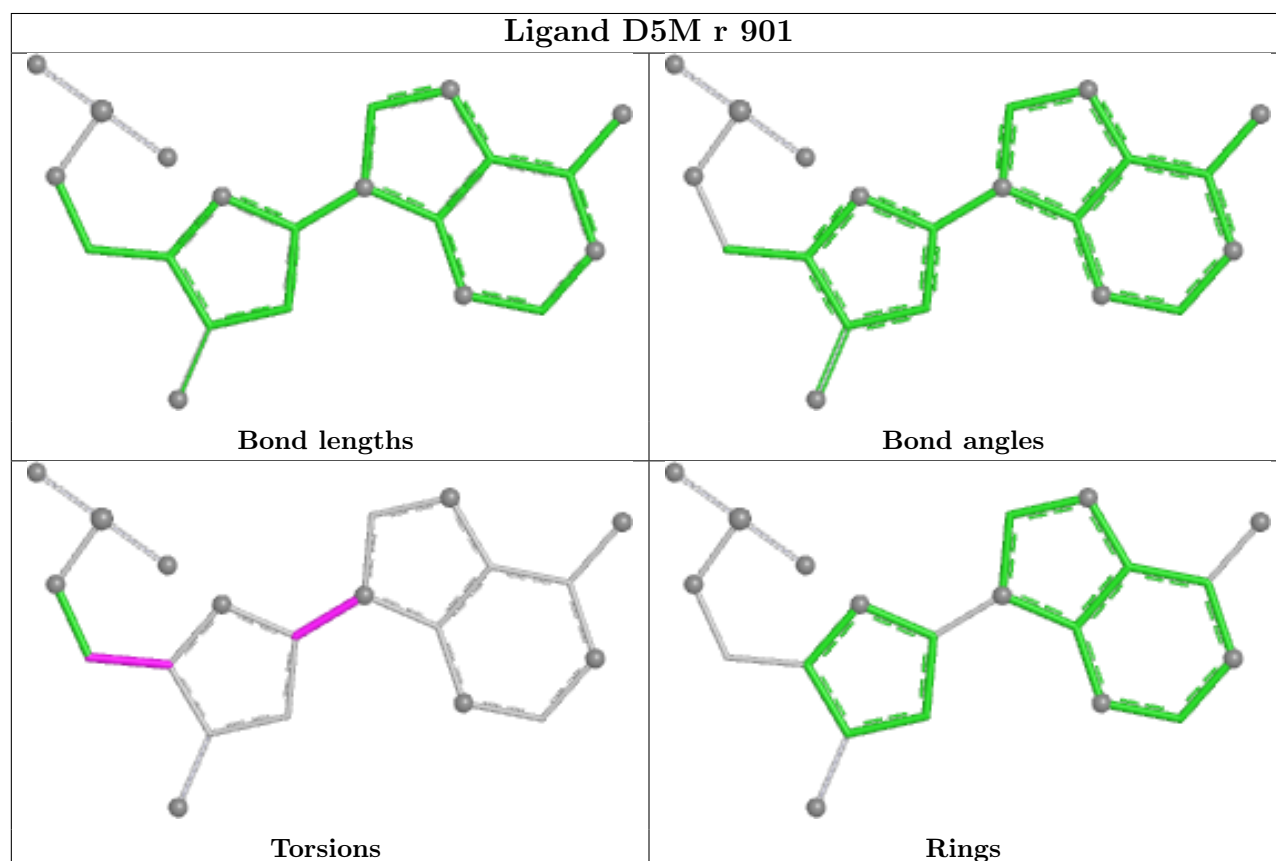
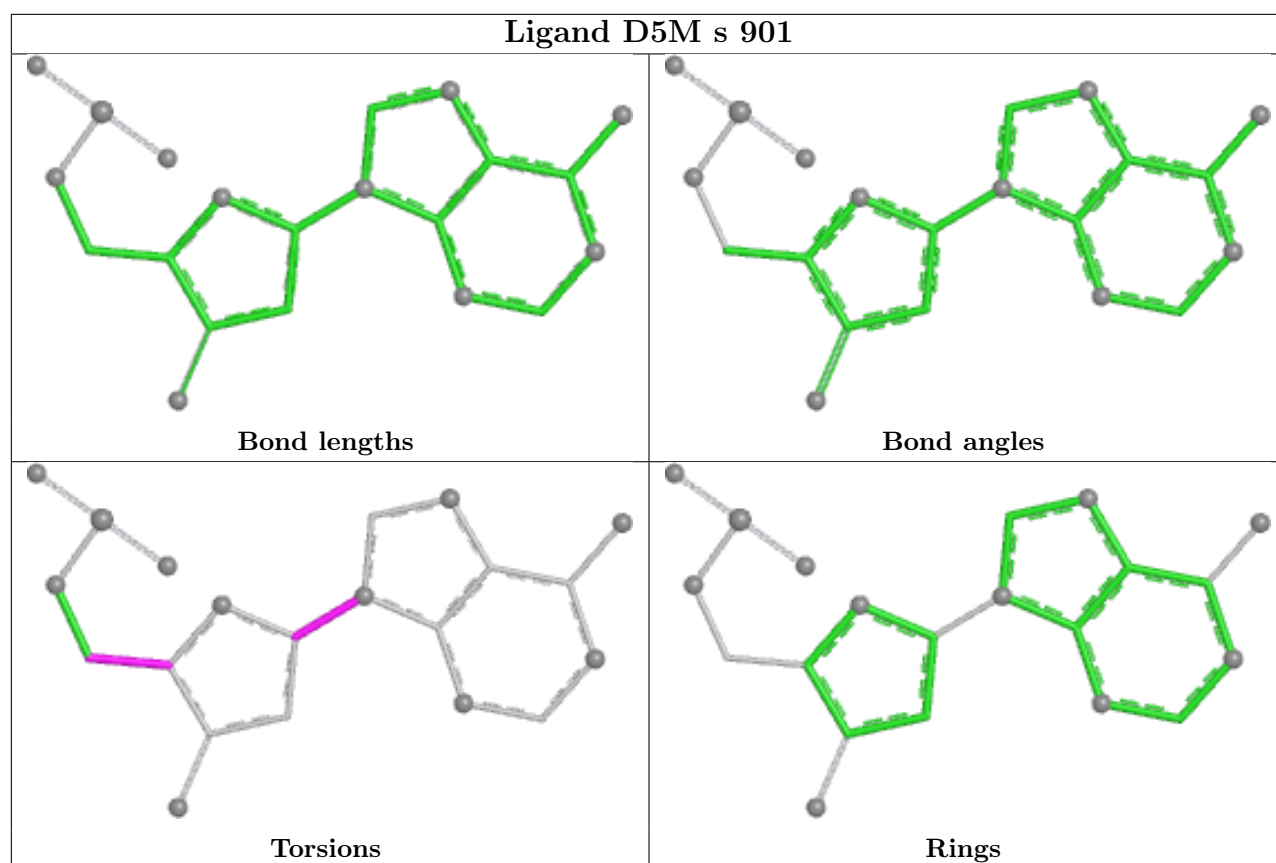


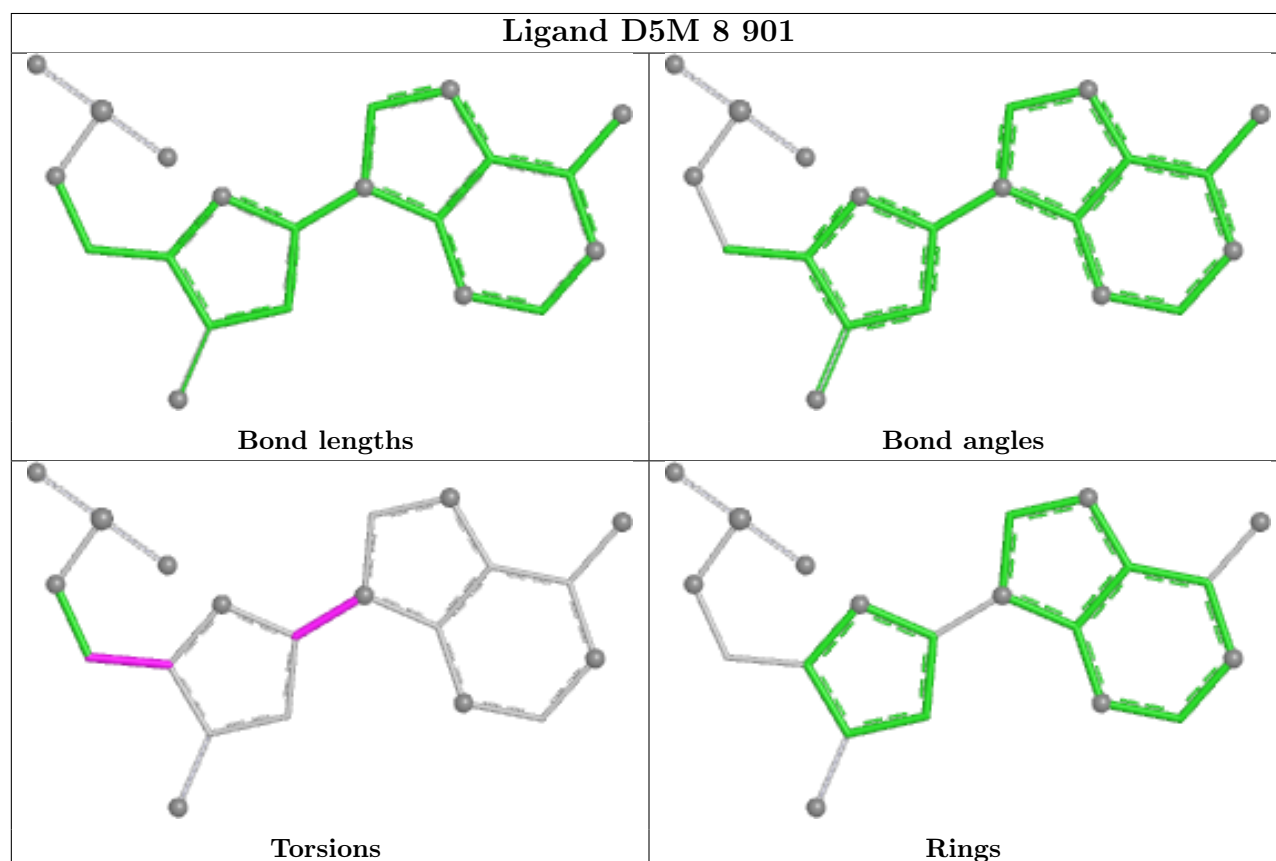
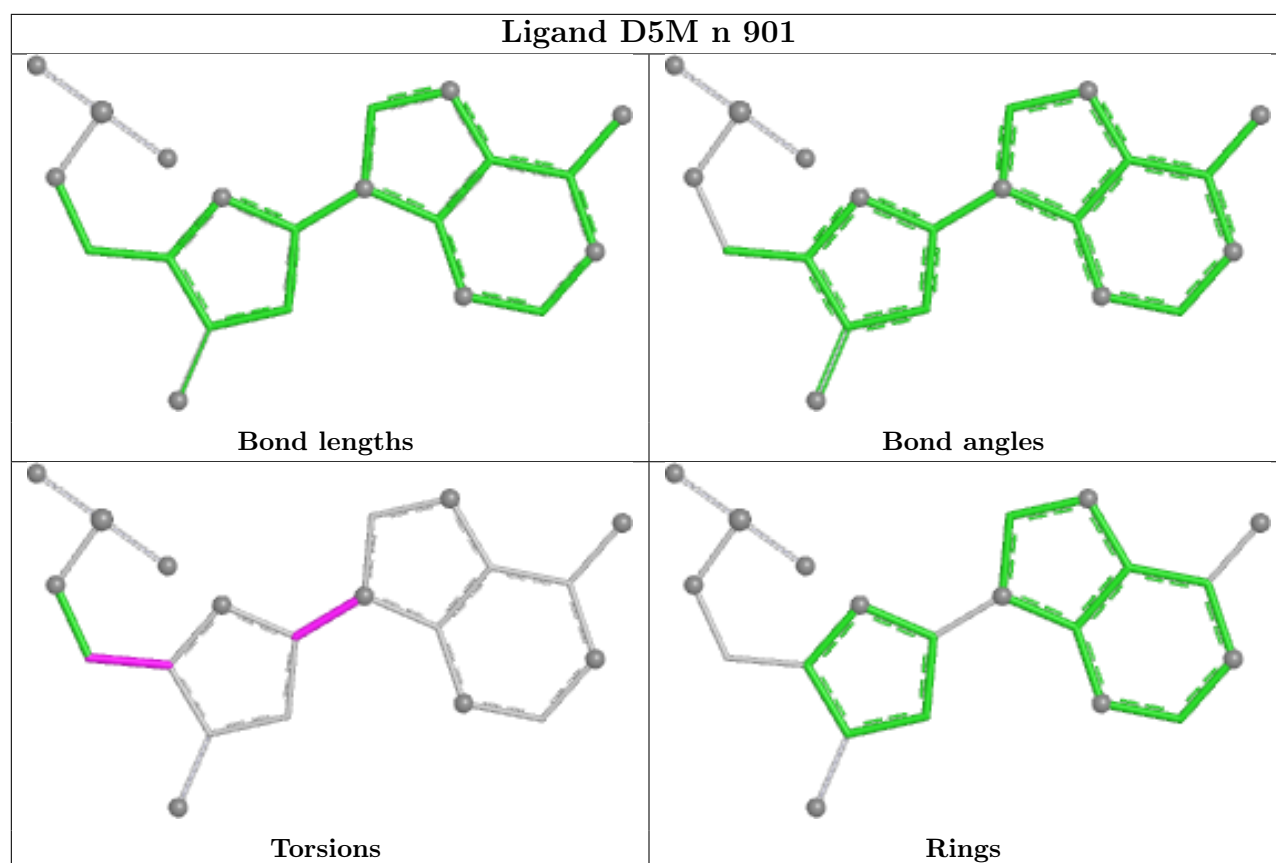


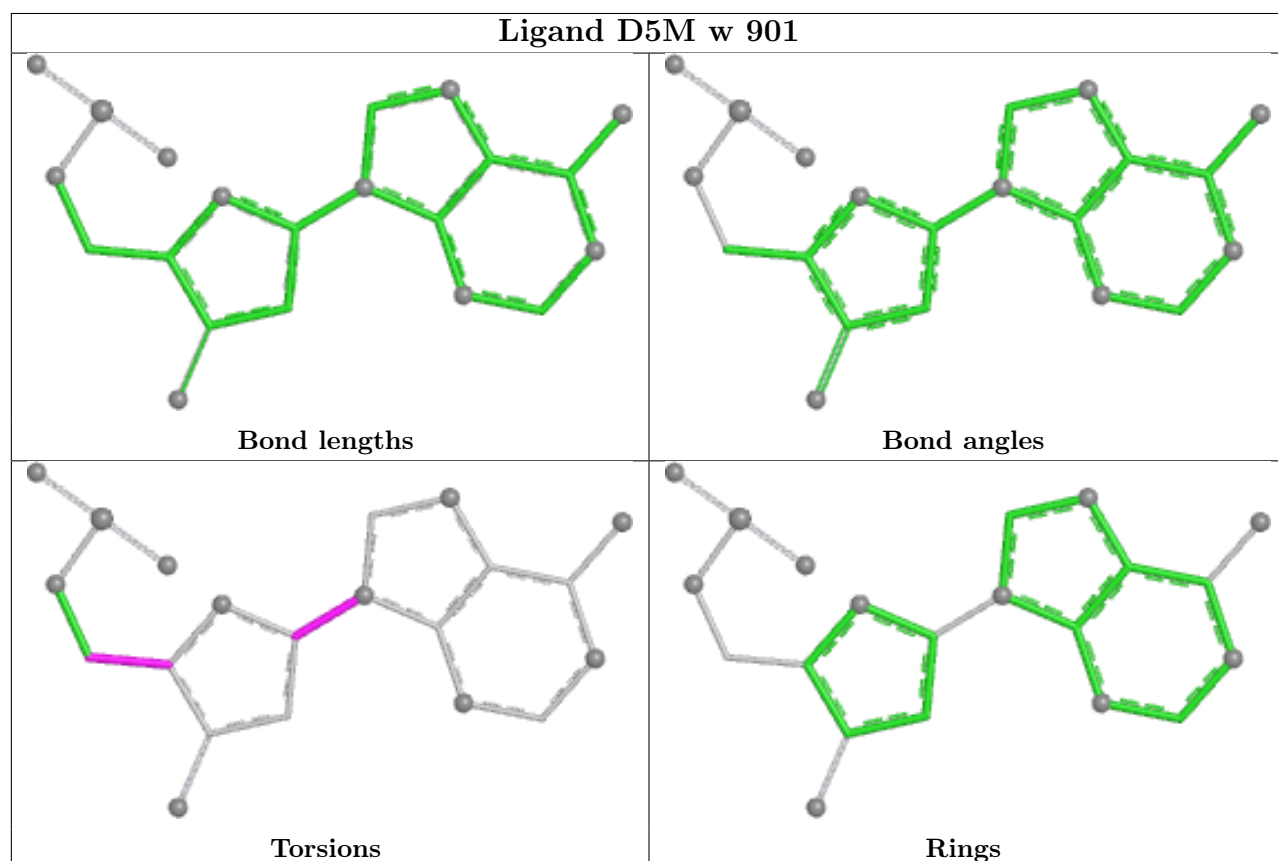
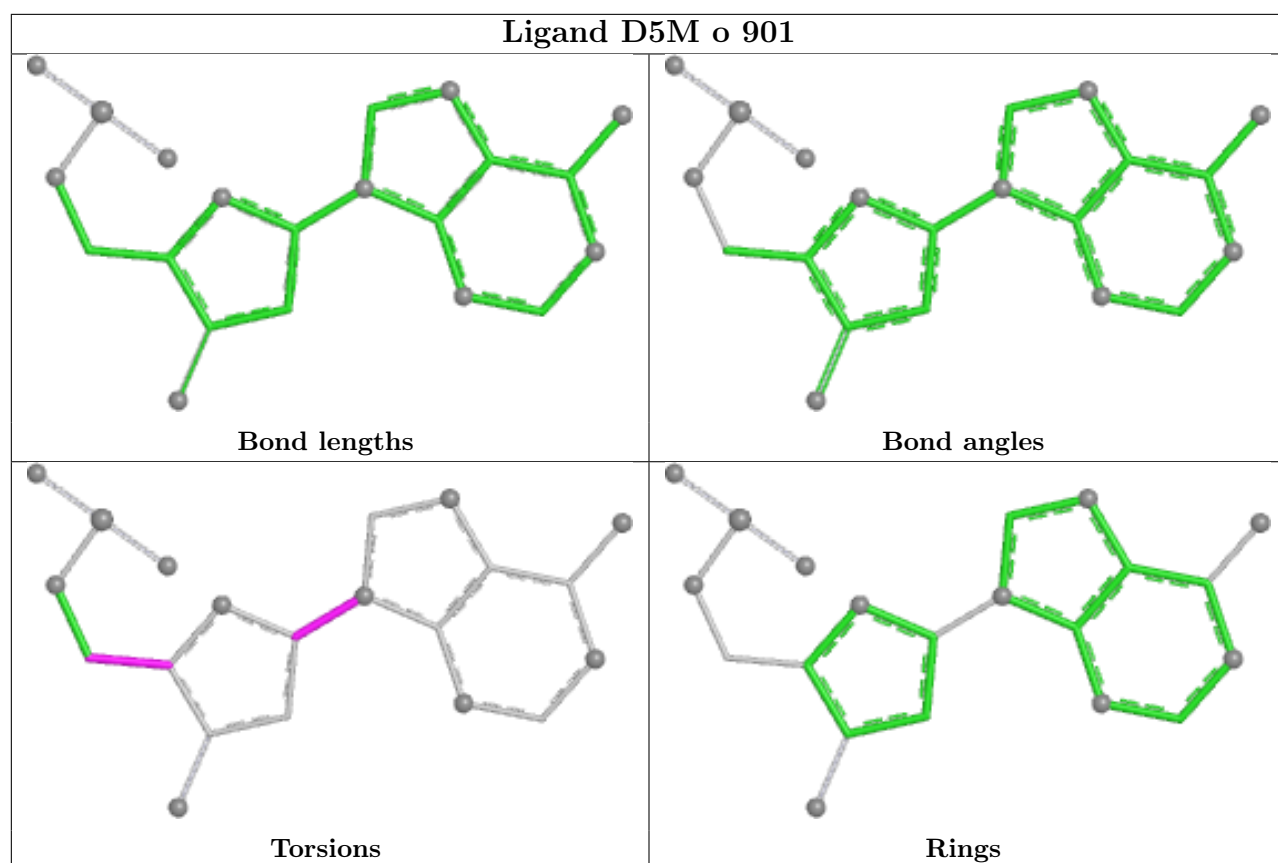












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

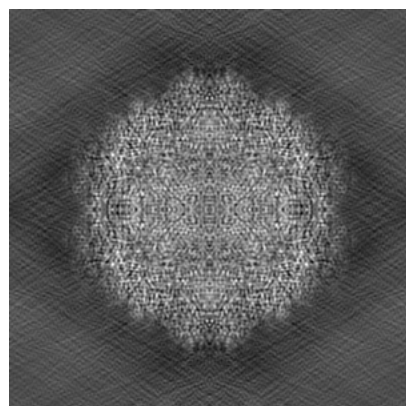
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29598. These allow visual inspection of the internal detail of the map and identification of artifacts.

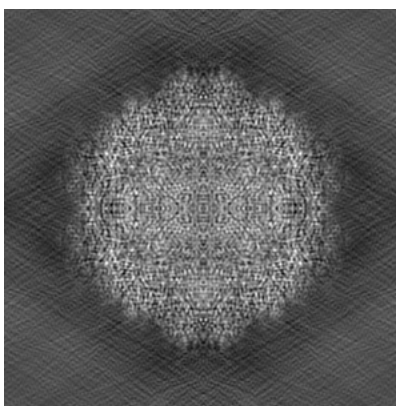
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

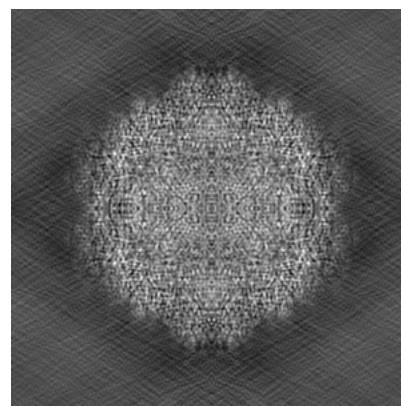
6.1.1 Primary map



X

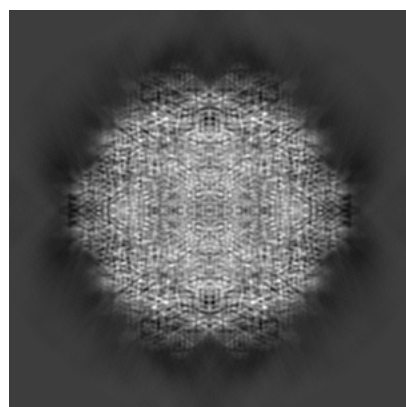


Y

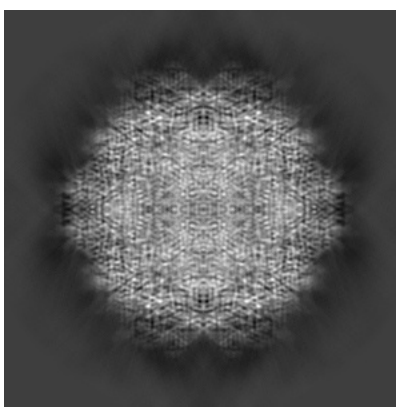


Z

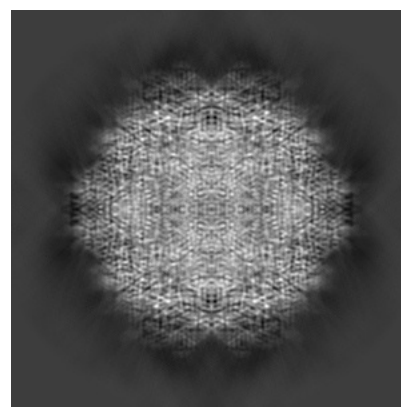
6.1.2 Raw map



X



Y

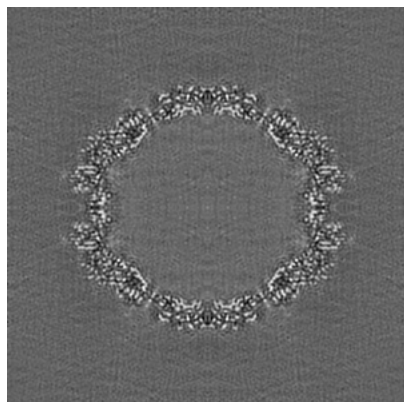


Z

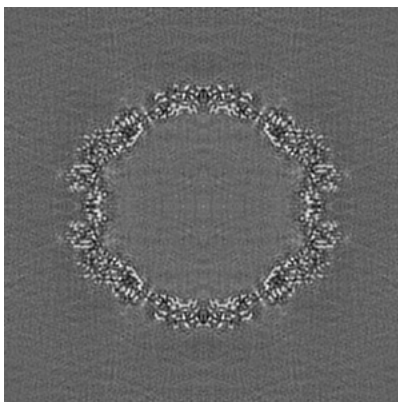
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

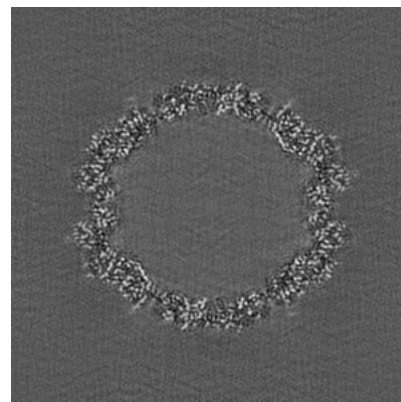
6.2.1 Primary map



X Index: 170

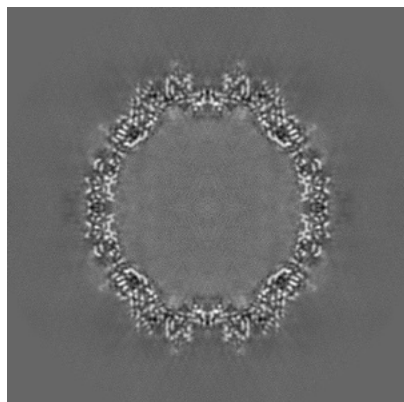


Y Index: 170

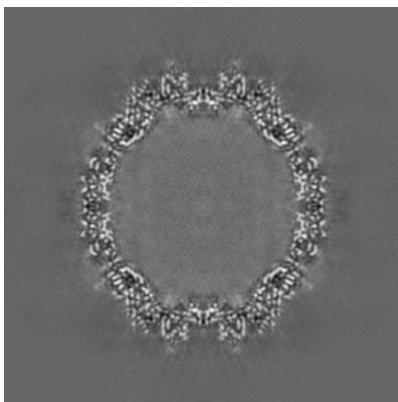


Z Index: 170

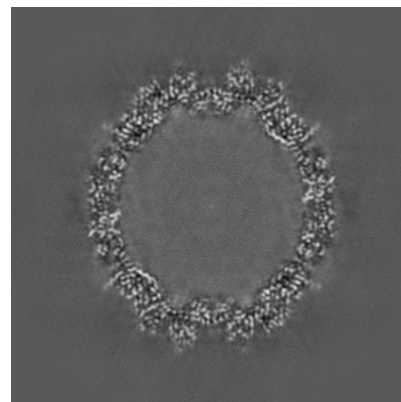
6.2.2 Raw map



X Index: 170



Y Index: 170

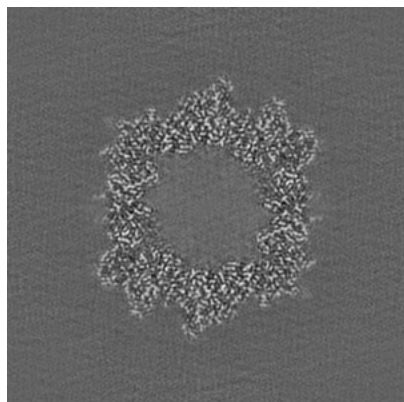


Z Index: 170

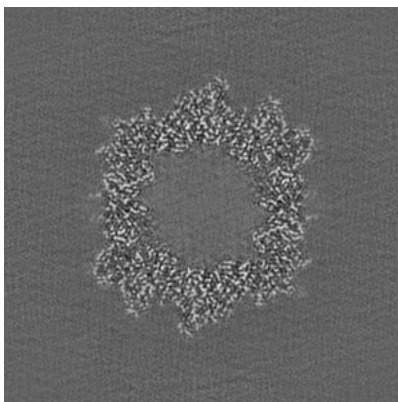
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

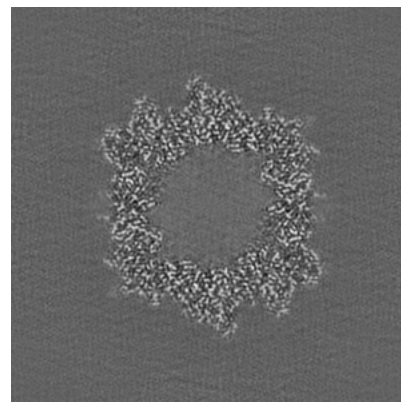
6.3.1 Primary map



X Index: 231

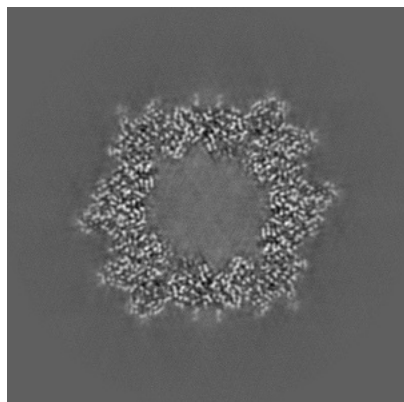


Y Index: 231

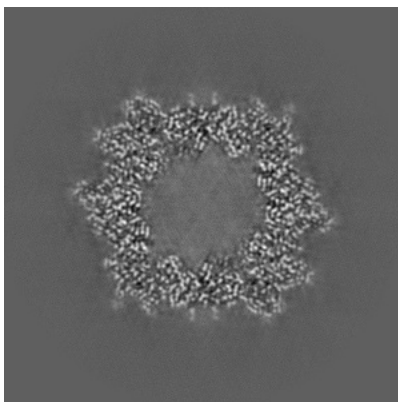


Z Index: 108

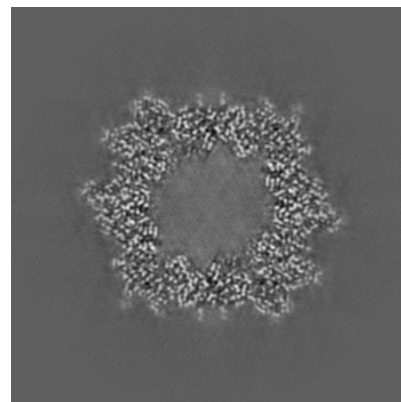
6.3.2 Raw map



X Index: 231



Y Index: 109

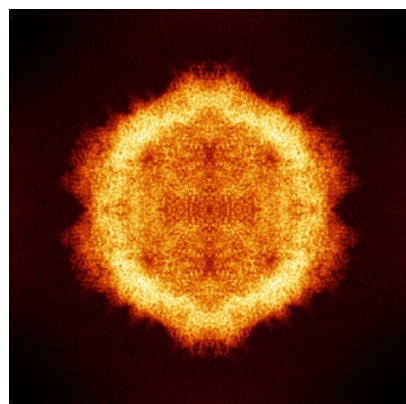


Z Index: 108

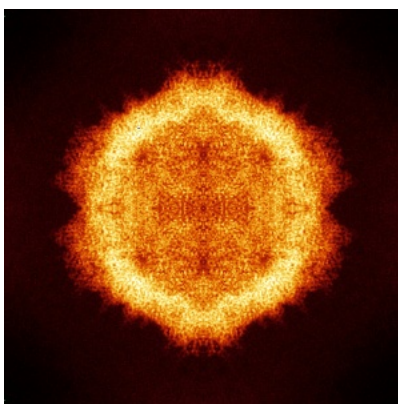
The images above show the largest variance slices of the map in three orthogonal directions.

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

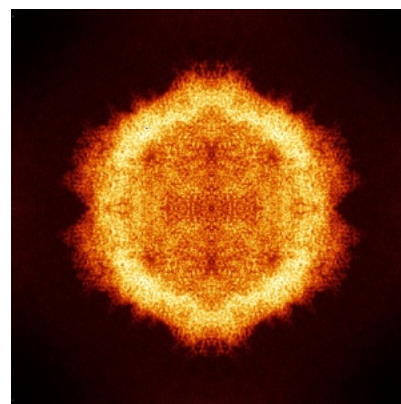
6.4.1 Primary map



X

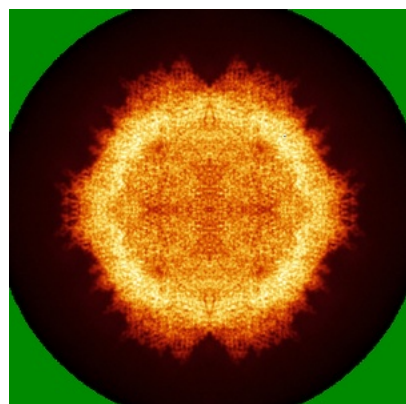


Y

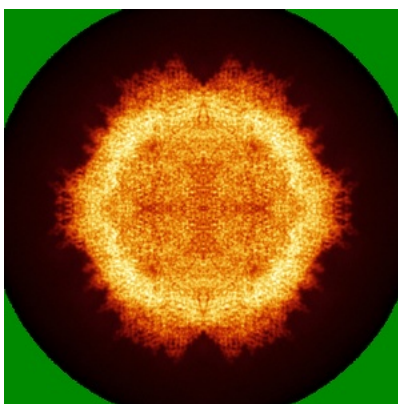


Z

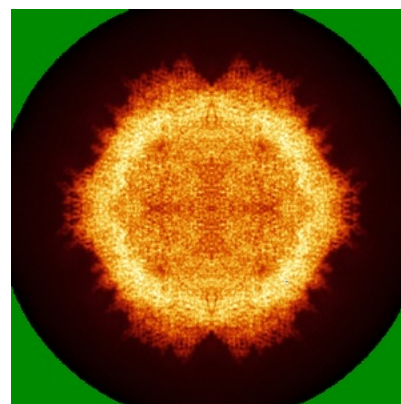
6.4.2 Raw map



X



Y

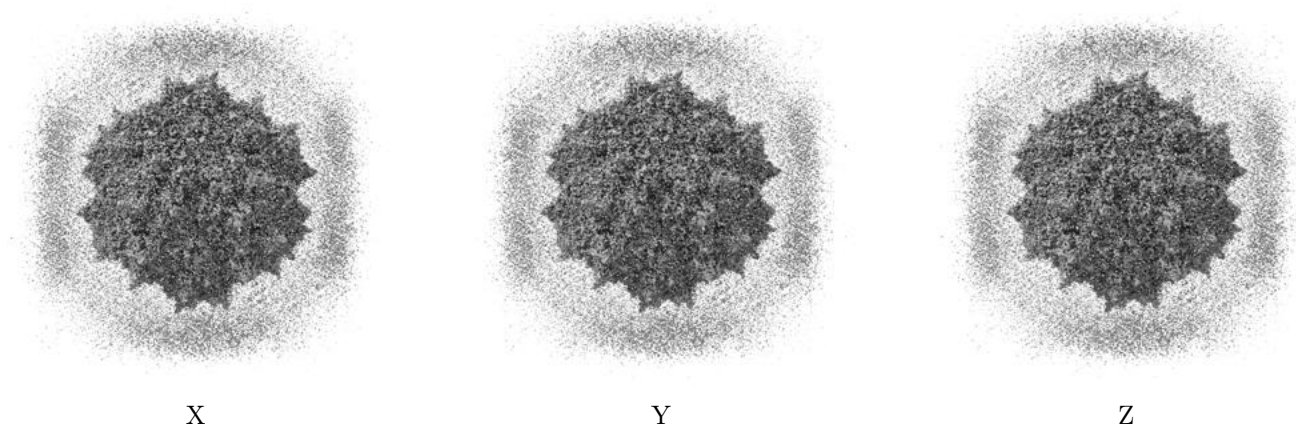


Z

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.

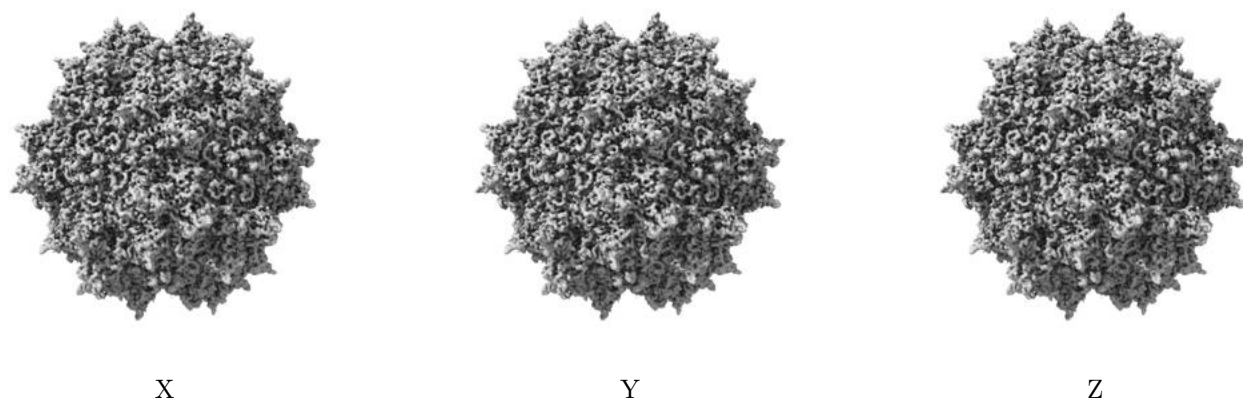
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. 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.

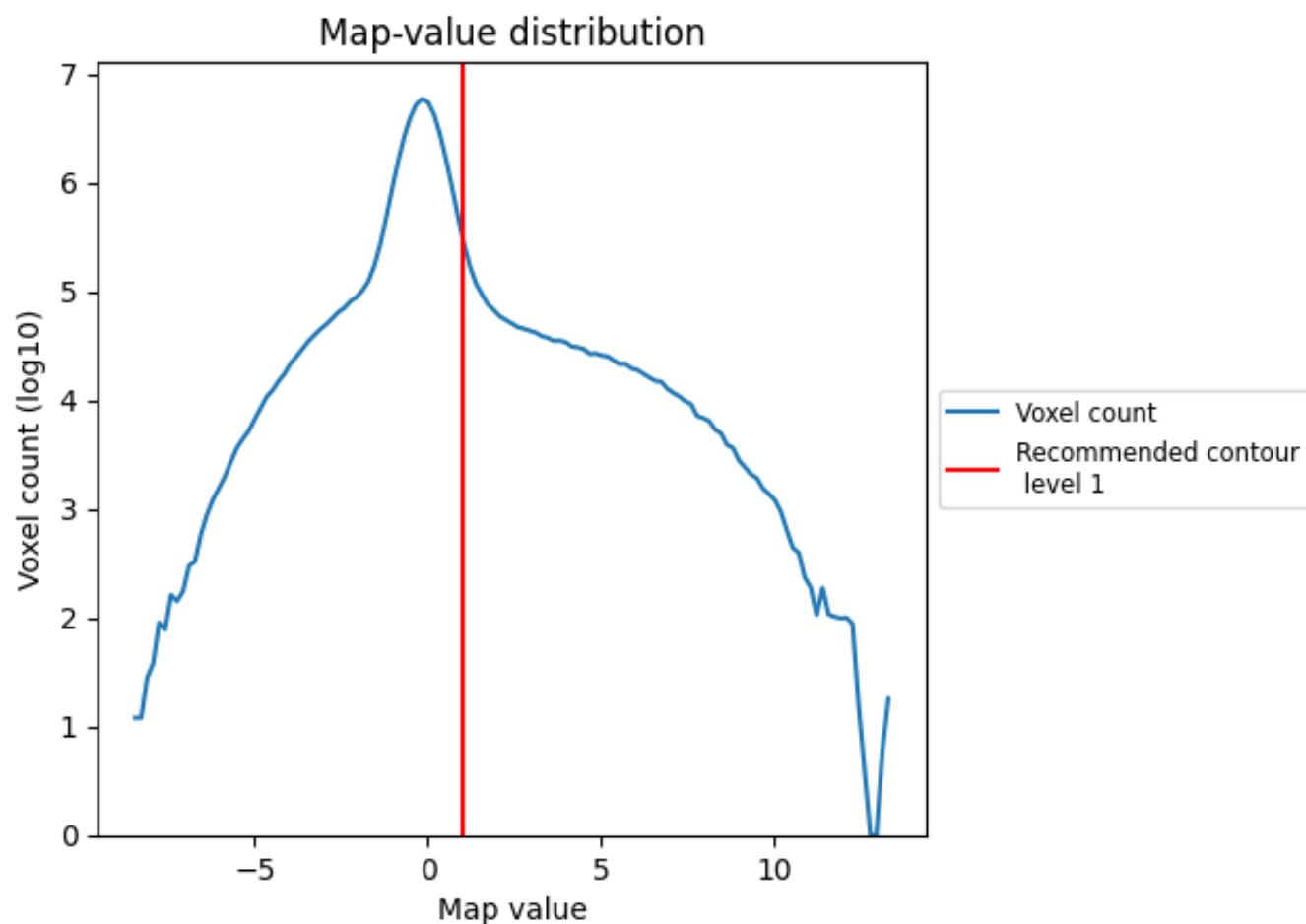
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

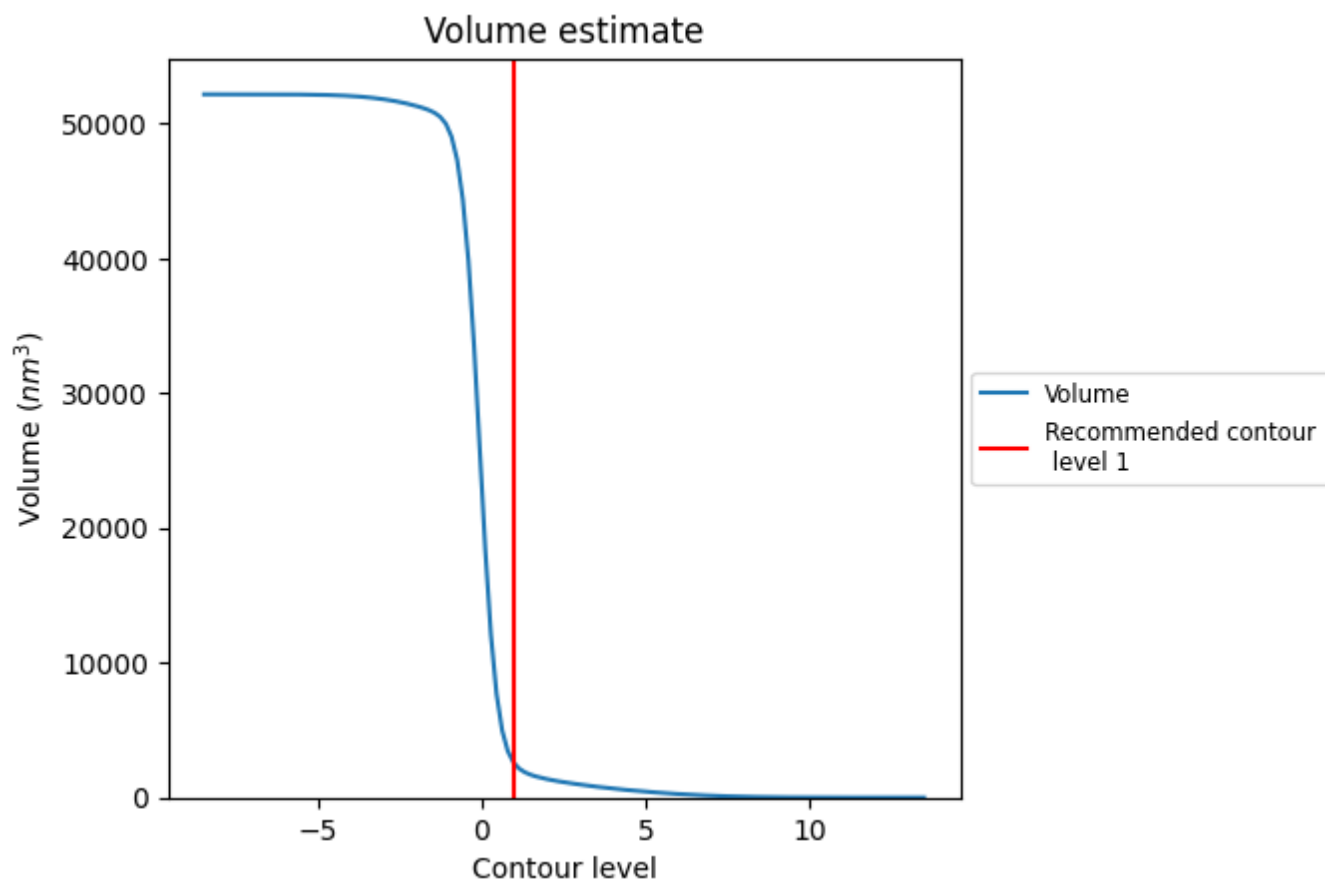
This section contains the results of statistical analysis of the map.

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.

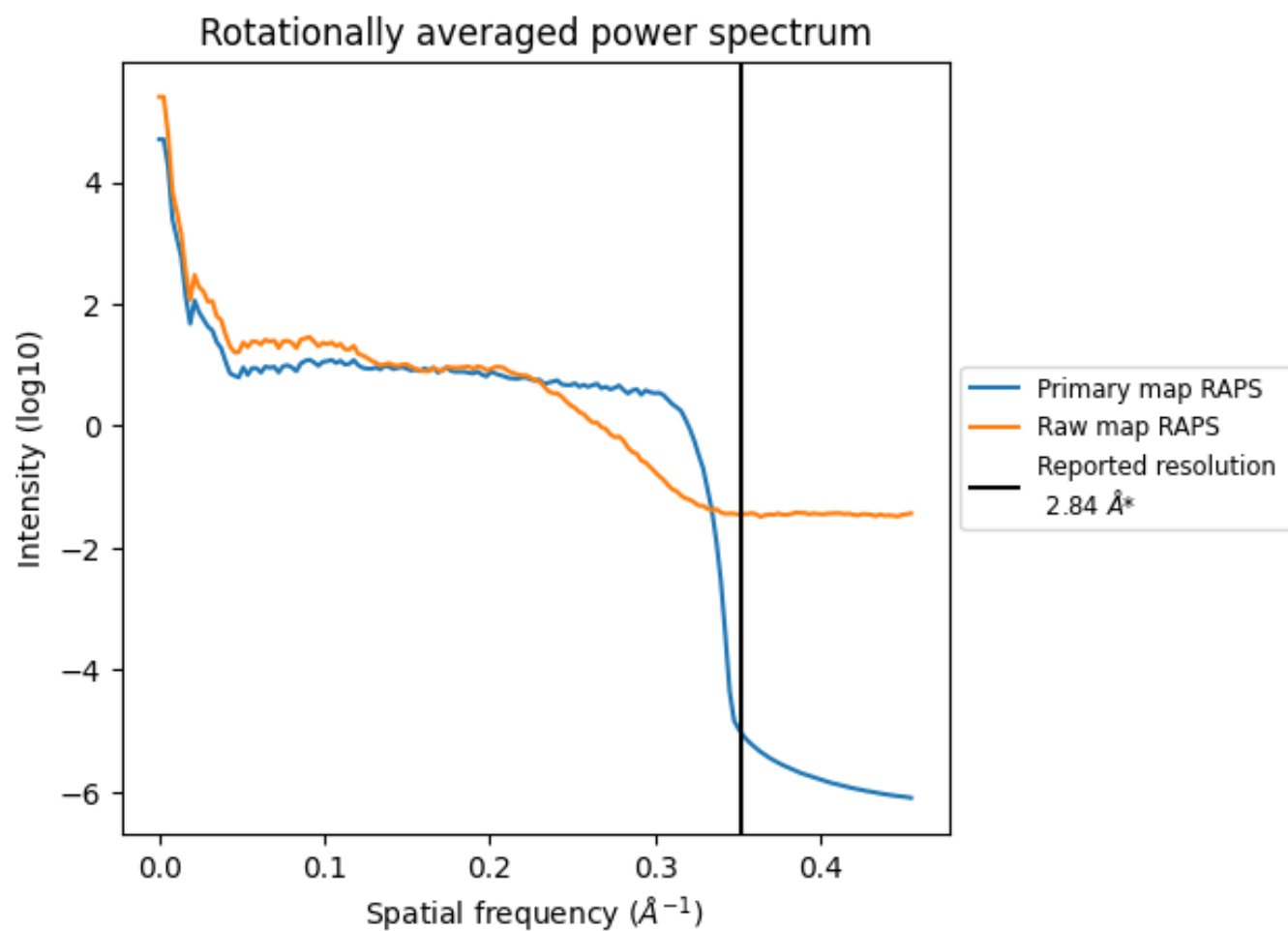
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2536 nm³; this corresponds to an approximate mass of 2291 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 ⓘ

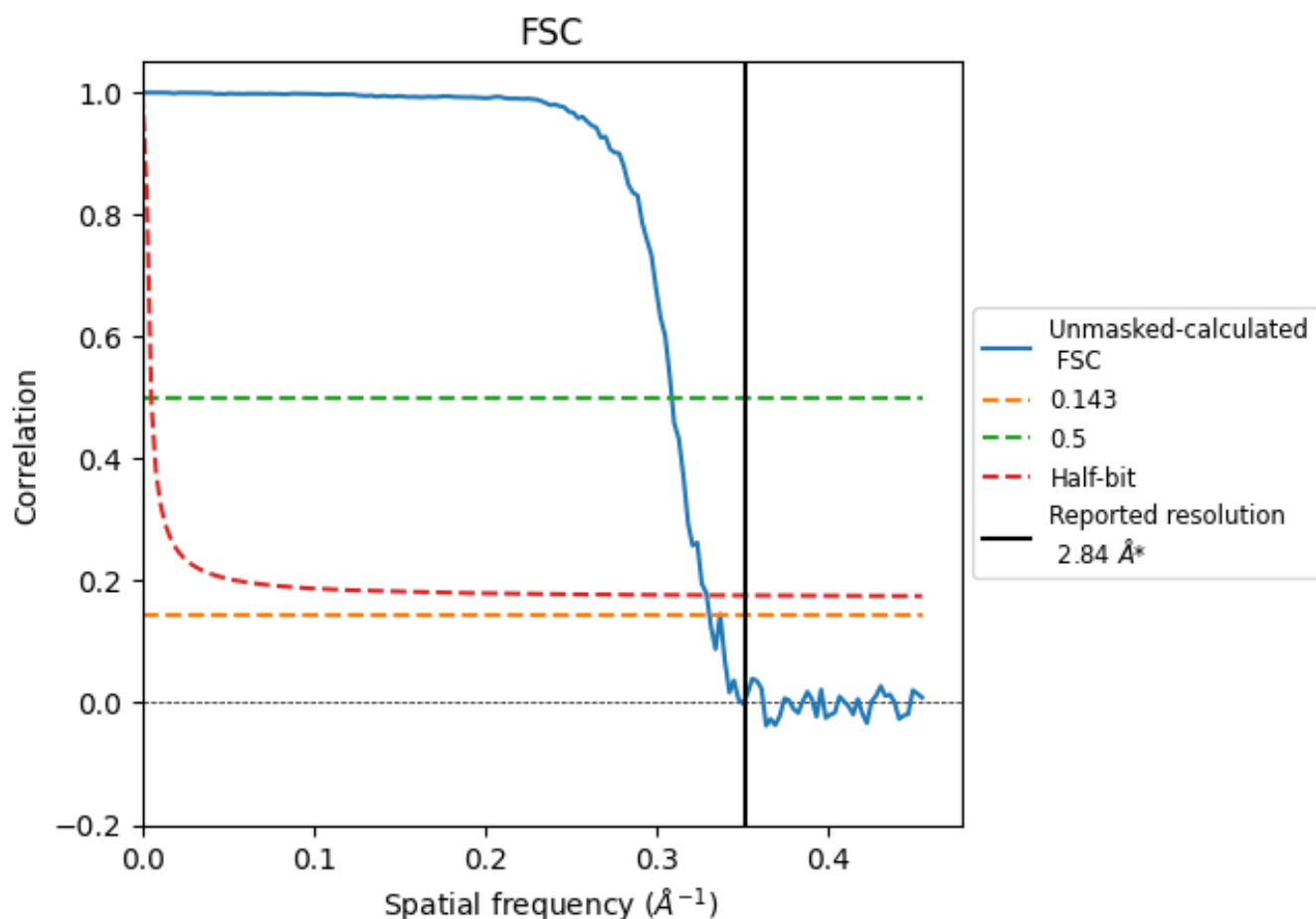


*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

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 $0.352 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

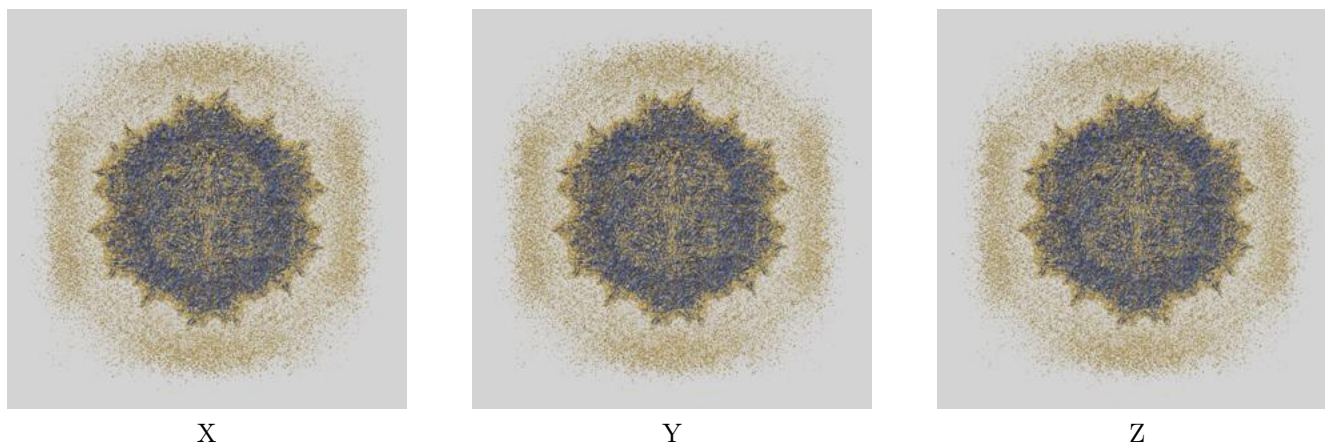
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.02	3.24	3.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

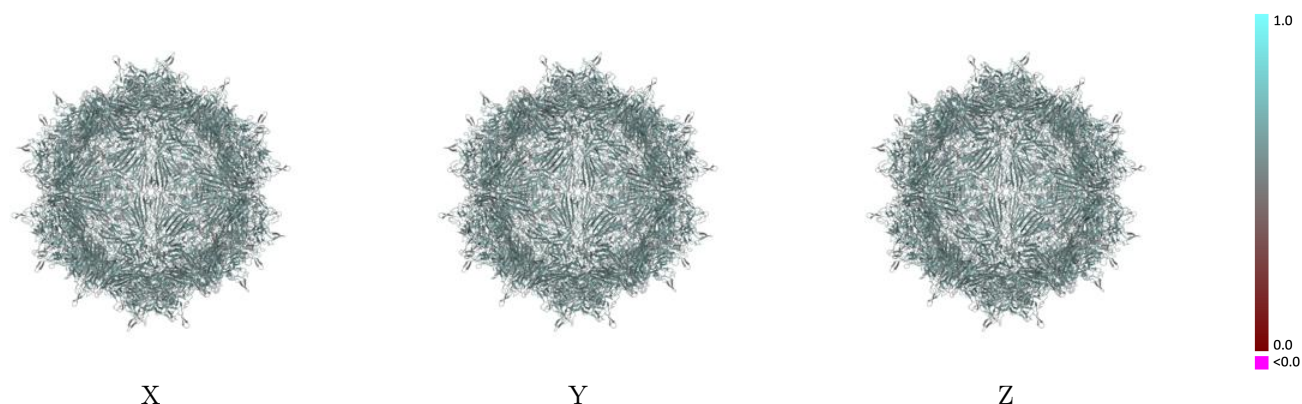
This section contains information regarding the fit between EMDB map EMD-29598 and PDB model 8FYW. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



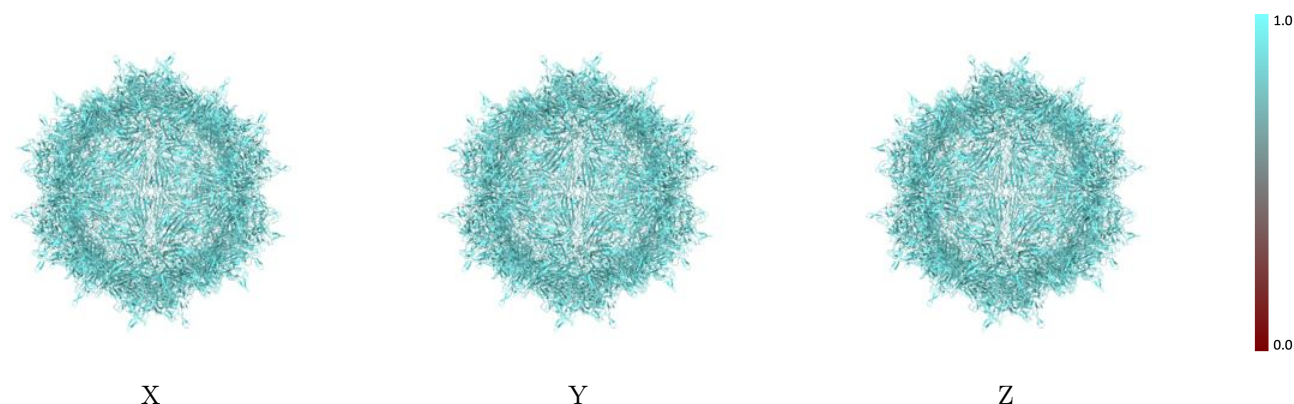
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



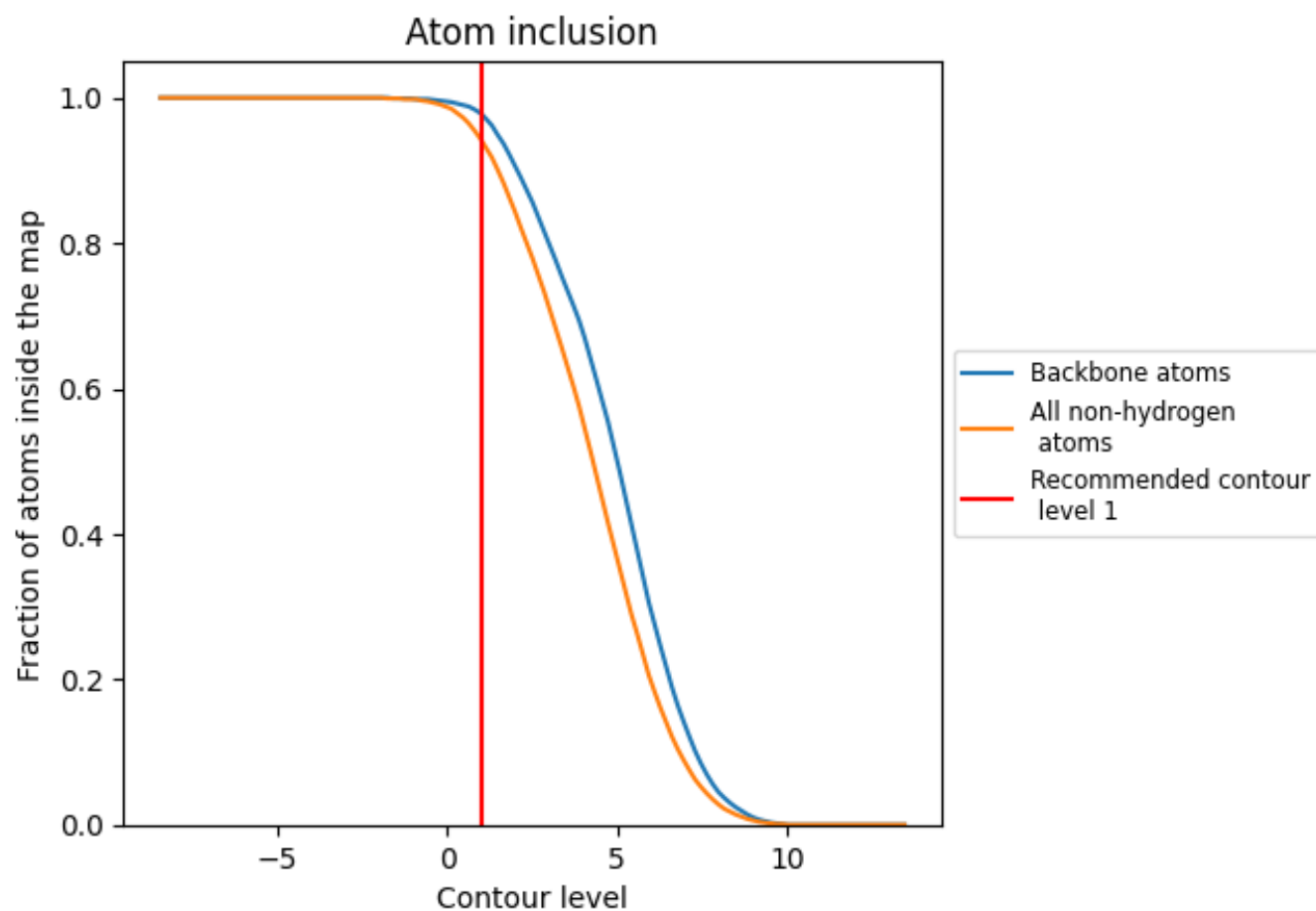
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9420	 0.5750
1	 0.9420	 0.5730
2	 0.9430	 0.5750
3	 0.9430	 0.5760
4	 0.9410	 0.5740
5	 0.9420	 0.5750
6	 0.9420	 0.5760
7	 0.9420	 0.5750
8	 0.9410	 0.5730
A	 0.9430	 0.5760
B	 0.9430	 0.5750
C	 0.9410	 0.5760
D	 0.9420	 0.5760
E	 0.9420	 0.5750
F	 0.9430	 0.5760
G	 0.9420	 0.5750
H	 0.9420	 0.5760
I	 0.9400	 0.5750
J	 0.9430	 0.5740
K	 0.9400	 0.5750
L	 0.9420	 0.5740
M	 0.9410	 0.5750
N	 0.9410	 0.5760
O	 0.9410	 0.5750
P	 0.9420	 0.5760
Q	 0.9400	 0.5750
R	 0.9430	 0.5740
S	 0.9430	 0.5740
T	 0.9400	 0.5750
U	 0.9420	 0.5740
V	 0.9410	 0.5760
W	 0.9420	 0.5760
X	 0.9410	 0.5740
Y	 0.9410	 0.5750
Z	 0.9410	 0.5750



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Chain	Atom inclusion	Q-score
a	 0.9440	 0.5760
b	 0.9430	 0.5750
c	 0.9430	 0.5770
d	 0.9440	 0.5760
e	 0.9430	 0.5750
f	 0.9420	 0.5770
g	 0.9400	 0.5750
h	 0.9410	 0.5740
i	 0.9420	 0.5770
j	 0.9420	 0.5740
k	 0.9420	 0.5750
l	 0.9410	 0.5740
m	 0.9410	 0.5740
n	 0.9430	 0.5750
o	 0.9410	 0.5750
p	 0.9400	 0.5740
q	 0.9420	 0.5740
r	 0.9430	 0.5740
s	 0.9430	 0.5750
t	 0.9410	 0.5750
u	 0.9410	 0.5750
v	 0.9440	 0.5740
w	 0.9410	 0.5740
x	 0.9410	 0.5750
y	 0.9440	 0.5760
z	 0.9420	 0.5740