



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:59 PM UTC

PDB ID : 2FHH / pdb_00002fhh
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome in complex with a peptidyl boronate inhibitor MLN-273
Authors : Li, H.
Deposited on : 2005-12-23
Resolution : 2.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

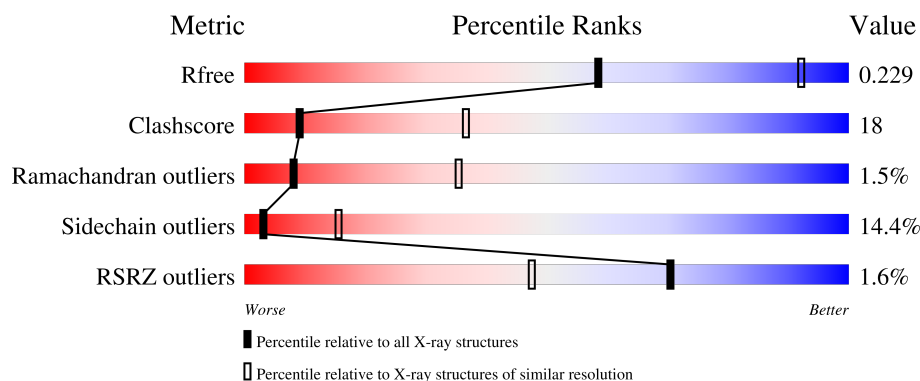
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	1	251	2% 51% 31% 5% 12%
1	A	251	2% 53% 29% 6% 12%
1	B	251	% 54% 29% 5% 12%
1	D	251	% 52% 31% • 12%
1	F	251	2% 51% 31% 6% 12%

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Mol	Chain	Length	Quality of chain
1	I	251	
1	K	251	
1	M	251	
1	O	251	
1	Q	251	
1	S	251	
1	U	251	
1	W	251	
1	Y	251	
2	2	240	
2	C	240	
2	E	240	
2	G	240	
2	H	240	
2	J	240	
2	L	240	
2	N	240	
2	P	240	
2	R	240	
2	T	240	
2	V	240	
2	X	240	
2	Z	240	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47389 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 20S proteasome, alpha and beta subunits.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	B	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	D	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	F	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	I	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	K	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	M	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	O	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	Q	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	S	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	U	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	W	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	Y	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	1	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	GB 76783992

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	cloning artifact	GB 76783992
A	0	SER	-	cloning artifact	GB 76783992
A	1	SER	-	cloning artifact	GB 76783992
B	-2	MET	-	initiating methionine	GB 76783992
B	-1	ASN	-	cloning artifact	GB 76783992
B	0	SER	-	cloning artifact	GB 76783992
B	1	SER	-	cloning artifact	GB 76783992
D	-2	MET	-	initiating methionine	GB 76783992
D	-1	ASN	-	cloning artifact	GB 76783992
D	0	SER	-	cloning artifact	GB 76783992
D	1	SER	-	cloning artifact	GB 76783992
F	-2	MET	-	initiating methionine	GB 76783992
F	-1	ASN	-	cloning artifact	GB 76783992
F	0	SER	-	cloning artifact	GB 76783992
F	1	SER	-	cloning artifact	GB 76783992
I	-2	MET	-	initiating methionine	GB 76783992
I	-1	ASN	-	cloning artifact	GB 76783992
I	0	SER	-	cloning artifact	GB 76783992
I	1	SER	-	cloning artifact	GB 76783992
K	-2	MET	-	initiating methionine	GB 76783992
K	-1	ASN	-	cloning artifact	GB 76783992
K	0	SER	-	cloning artifact	GB 76783992
K	1	SER	-	cloning artifact	GB 76783992
M	-2	MET	-	initiating methionine	GB 76783992
M	-1	ASN	-	cloning artifact	GB 76783992
M	0	SER	-	cloning artifact	GB 76783992
M	1	SER	-	cloning artifact	GB 76783992
O	-2	MET	-	initiating methionine	GB 76783992
O	-1	ASN	-	cloning artifact	GB 76783992
O	0	SER	-	cloning artifact	GB 76783992
O	1	SER	-	cloning artifact	GB 76783992
Q	-2	MET	-	initiating methionine	GB 76783992
Q	-1	ASN	-	cloning artifact	GB 76783992
Q	0	SER	-	cloning artifact	GB 76783992
Q	1	SER	-	cloning artifact	GB 76783992
S	-2	MET	-	initiating methionine	GB 76783992
S	-1	ASN	-	cloning artifact	GB 76783992
S	0	SER	-	cloning artifact	GB 76783992
S	1	SER	-	cloning artifact	GB 76783992
U	-2	MET	-	initiating methionine	GB 76783992
U	-1	ASN	-	cloning artifact	GB 76783992
U	0	SER	-	cloning artifact	GB 76783992

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Chain	Residue	Modelled	Actual	Comment	Reference
U	1	SER	-	cloning artifact	GB 76783992
W	-2	MET	-	initiating methionine	GB 76783992
W	-1	ASN	-	cloning artifact	GB 76783992
W	0	SER	-	cloning artifact	GB 76783992
W	1	SER	-	cloning artifact	GB 76783992
Y	-2	MET	-	initiating methionine	GB 76783992
Y	-1	ASN	-	cloning artifact	GB 76783992
Y	0	SER	-	cloning artifact	GB 76783992
Y	1	SER	-	cloning artifact	GB 76783992
1	-2	MET	-	initiating methionine	GB 76783992
1	-1	ASN	-	cloning artifact	GB 76783992
1	0	SER	-	cloning artifact	GB 76783992
1	1	SER	-	cloning artifact	GB 76783992

- Molecule 2 is a protein called proteasome, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	C	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	E	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	G	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	J	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	L	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	N	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	P	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	R	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	T	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	V	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	X	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	Z	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	535	HIS	-	expression tag	GB 13881852
H	536	HIS	-	expression tag	GB 13881852
H	537	HIS	-	expression tag	GB 13881852
H	538	HIS	-	expression tag	GB 13881852
H	539	HIS	-	expression tag	GB 13881852
H	540	HIS	-	expression tag	GB 13881852
C	535	HIS	-	expression tag	GB 13881852
C	536	HIS	-	expression tag	GB 13881852
C	537	HIS	-	expression tag	GB 13881852
C	538	HIS	-	expression tag	GB 13881852
C	539	HIS	-	expression tag	GB 13881852
C	540	HIS	-	expression tag	GB 13881852
E	535	HIS	-	expression tag	GB 13881852
E	536	HIS	-	expression tag	GB 13881852
E	537	HIS	-	expression tag	GB 13881852
E	538	HIS	-	expression tag	GB 13881852
E	539	HIS	-	expression tag	GB 13881852
E	540	HIS	-	expression tag	GB 13881852
G	535	HIS	-	expression tag	GB 13881852
G	536	HIS	-	expression tag	GB 13881852
G	537	HIS	-	expression tag	GB 13881852
G	538	HIS	-	expression tag	GB 13881852
G	539	HIS	-	expression tag	GB 13881852
G	540	HIS	-	expression tag	GB 13881852
J	535	HIS	-	expression tag	GB 13881852
J	536	HIS	-	expression tag	GB 13881852
J	537	HIS	-	expression tag	GB 13881852
J	538	HIS	-	expression tag	GB 13881852
J	539	HIS	-	expression tag	GB 13881852
J	540	HIS	-	expression tag	GB 13881852
L	535	HIS	-	expression tag	GB 13881852
L	536	HIS	-	expression tag	GB 13881852
L	537	HIS	-	expression tag	GB 13881852
L	538	HIS	-	expression tag	GB 13881852
L	539	HIS	-	expression tag	GB 13881852
L	540	HIS	-	expression tag	GB 13881852

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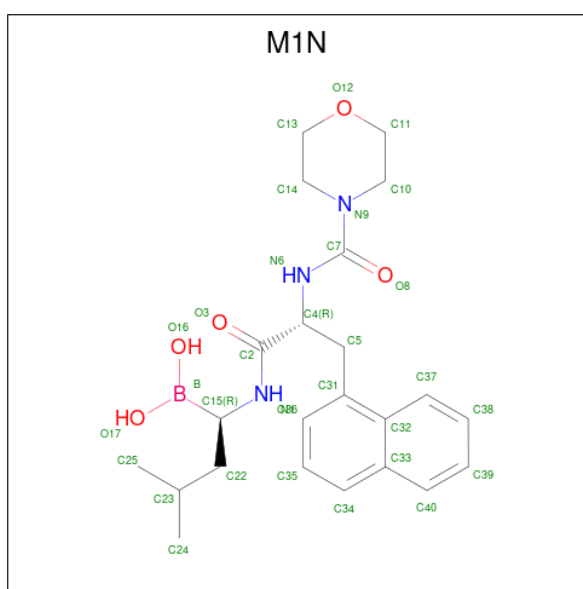
Chain	Residue	Modelled	Actual	Comment	Reference
N	535	HIS	-	expression tag	GB 13881852
N	536	HIS	-	expression tag	GB 13881852
N	537	HIS	-	expression tag	GB 13881852
N	538	HIS	-	expression tag	GB 13881852
N	539	HIS	-	expression tag	GB 13881852
N	540	HIS	-	expression tag	GB 13881852
P	535	HIS	-	expression tag	GB 13881852
P	536	HIS	-	expression tag	GB 13881852
P	537	HIS	-	expression tag	GB 13881852
P	538	HIS	-	expression tag	GB 13881852
P	539	HIS	-	expression tag	GB 13881852
P	540	HIS	-	expression tag	GB 13881852
R	535	HIS	-	expression tag	GB 13881852
R	536	HIS	-	expression tag	GB 13881852
R	537	HIS	-	expression tag	GB 13881852
R	538	HIS	-	expression tag	GB 13881852
R	539	HIS	-	expression tag	GB 13881852
R	540	HIS	-	expression tag	GB 13881852
T	535	HIS	-	expression tag	GB 13881852
T	536	HIS	-	expression tag	GB 13881852
T	537	HIS	-	expression tag	GB 13881852
T	538	HIS	-	expression tag	GB 13881852
T	539	HIS	-	expression tag	GB 13881852
T	540	HIS	-	expression tag	GB 13881852
V	535	HIS	-	expression tag	GB 13881852
V	536	HIS	-	expression tag	GB 13881852
V	537	HIS	-	expression tag	GB 13881852
V	538	HIS	-	expression tag	GB 13881852
V	539	HIS	-	expression tag	GB 13881852
V	540	HIS	-	expression tag	GB 13881852
X	535	HIS	-	expression tag	GB 13881852
X	536	HIS	-	expression tag	GB 13881852
X	537	HIS	-	expression tag	GB 13881852
X	538	HIS	-	expression tag	GB 13881852
X	539	HIS	-	expression tag	GB 13881852
X	540	HIS	-	expression tag	GB 13881852
Z	535	HIS	-	expression tag	GB 13881852
Z	536	HIS	-	expression tag	GB 13881852
Z	537	HIS	-	expression tag	GB 13881852
Z	538	HIS	-	expression tag	GB 13881852
Z	539	HIS	-	expression tag	GB 13881852
Z	540	HIS	-	expression tag	GB 13881852

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Chain	Residue	Modelled	Actual	Comment	Reference
2	535	HIS	-	expression tag	GB 13881852
2	536	HIS	-	expression tag	GB 13881852
2	537	HIS	-	expression tag	GB 13881852
2	538	HIS	-	expression tag	GB 13881852
2	539	HIS	-	expression tag	GB 13881852
2	540	HIS	-	expression tag	GB 13881852

- Molecule 3 is (1R)-3-METHYL-1- {[N-(MORPHOLIN-4-YLCARBONYL)-3-(1-NAPHTHYL)-D-ALANYL]AMINO}BUTYLBORONIC ACID (CCD ID: M1N) (formula: $C_{23}H_{32}BN_3O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	C	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	E	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	G	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	J	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	L	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	N	1	Total	B	C	N	O	0	0
			32	1	23	3	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	P	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	R	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	T	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	V	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	X	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	Z	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	2	1	Total	B	C	N	O	0	0
			32	1	23	3	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	H	16	Total	O	0	0
			16	16		
4	B	10	Total	O	0	0
			10	10		
4	C	20	Total	O	0	0
			20	20		
4	D	4	Total	O	0	0
			4	4		
4	E	10	Total	O	0	0
			10	10		
4	F	7	Total	O	0	0
			7	7		
4	G	16	Total	O	0	0
			16	16		
4	I	11	Total	O	0	0
			11	11		
4	J	13	Total	O	0	0
			13	13		
4	K	9	Total	O	0	0
			9	9		
4	L	14	Total	O	0	0
			14	14		

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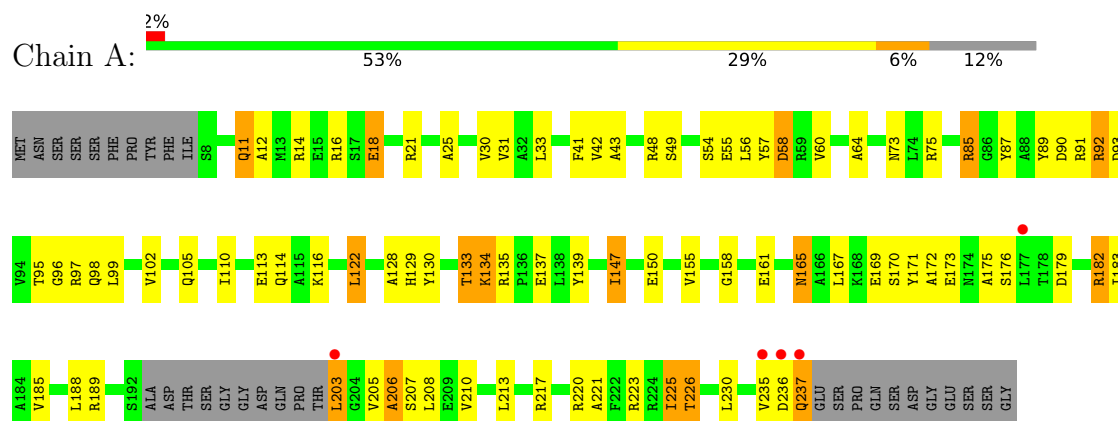
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	13	Total 13	O 13	0	0
4	N	12	Total 12	O 12	0	0
4	O	15	Total 15	O 15	0	0
4	P	15	Total 15	O 15	0	0
4	Q	6	Total 6	O 6	0	0
4	R	12	Total 12	O 12	0	0
4	S	5	Total 5	O 5	0	0
4	T	8	Total 8	O 8	0	0
4	U	2	Total 2	O 2	0	0
4	V	20	Total 20	O 20	0	0
4	W	7	Total 7	O 7	0	0
4	X	20	Total 20	O 20	0	0
4	Y	11	Total 11	O 11	0	0
4	Z	8	Total 8	O 8	0	0
4	1	6	Total 6	O 6	0	0
4	2	21	Total 21	O 21	0	0

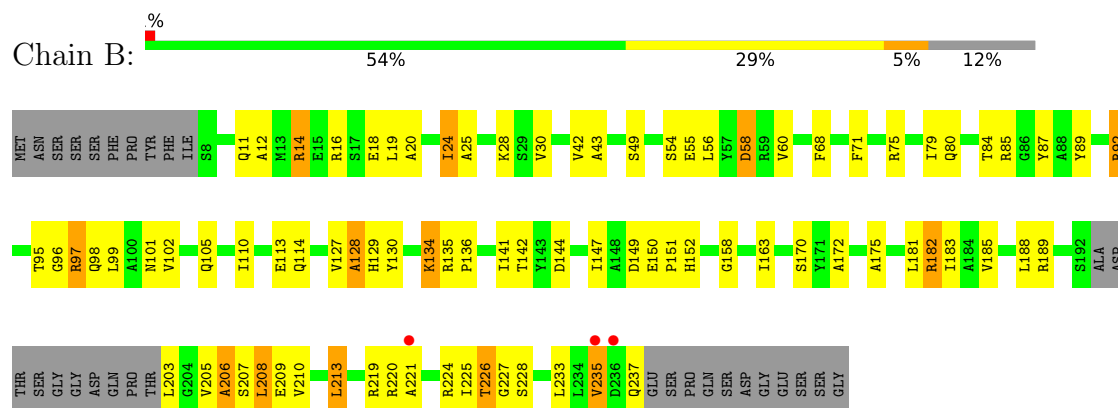
3 Residue-property plots

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

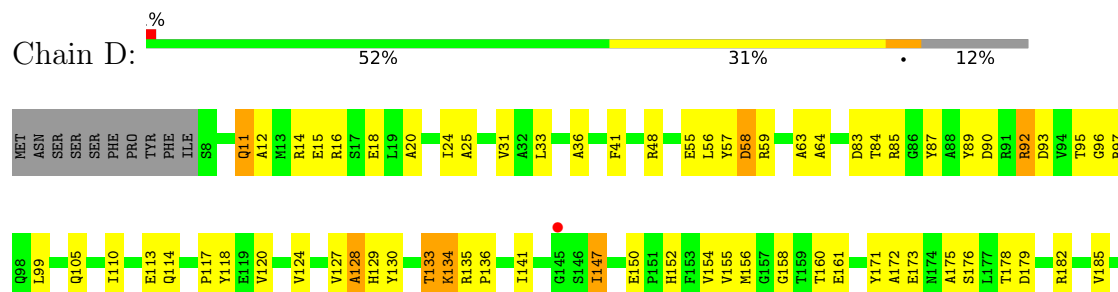
- Molecule 1: 20S proteasome, alpha and beta subunits

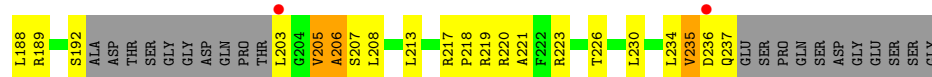


- Molecule 1: 20S proteasome, alpha and beta subunits

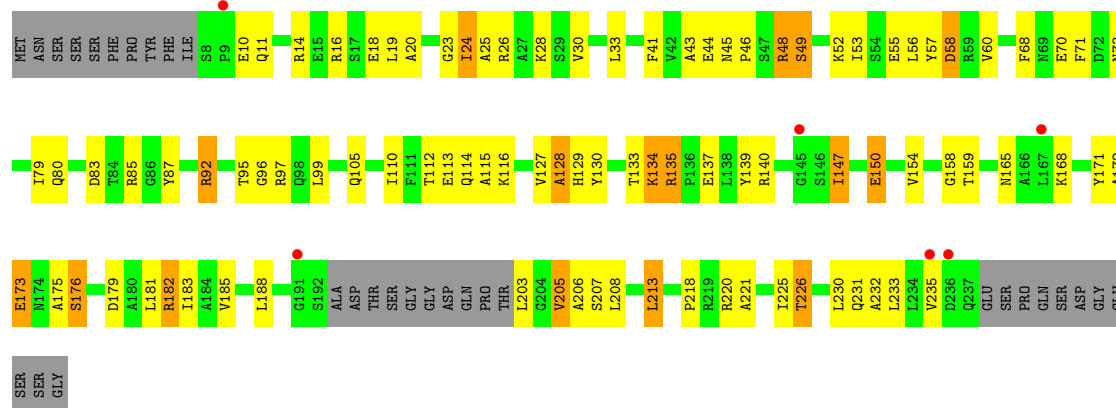


- Molecule 1: 20S proteasome, alpha and beta subunits

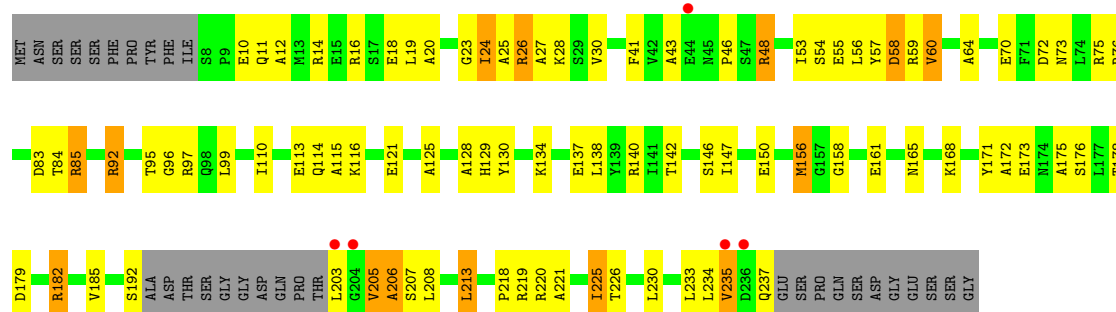




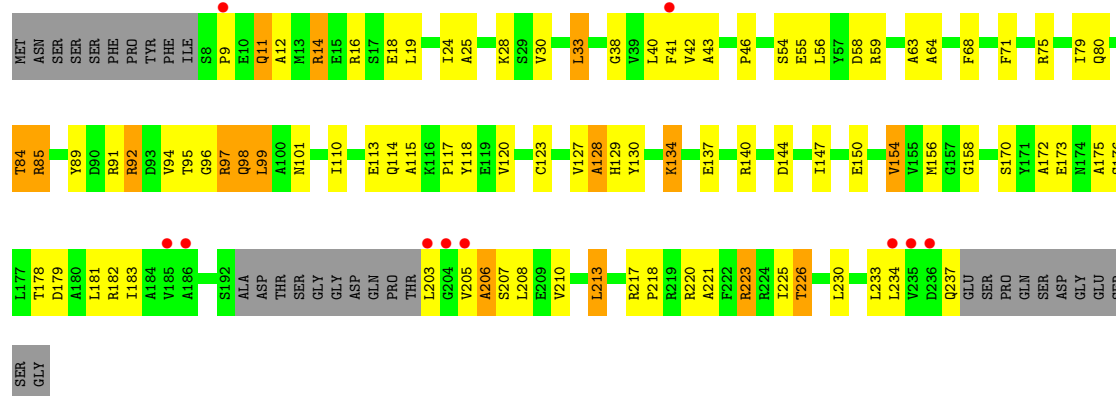
- Molecule 1: 20S proteasome, alpha and beta subunits



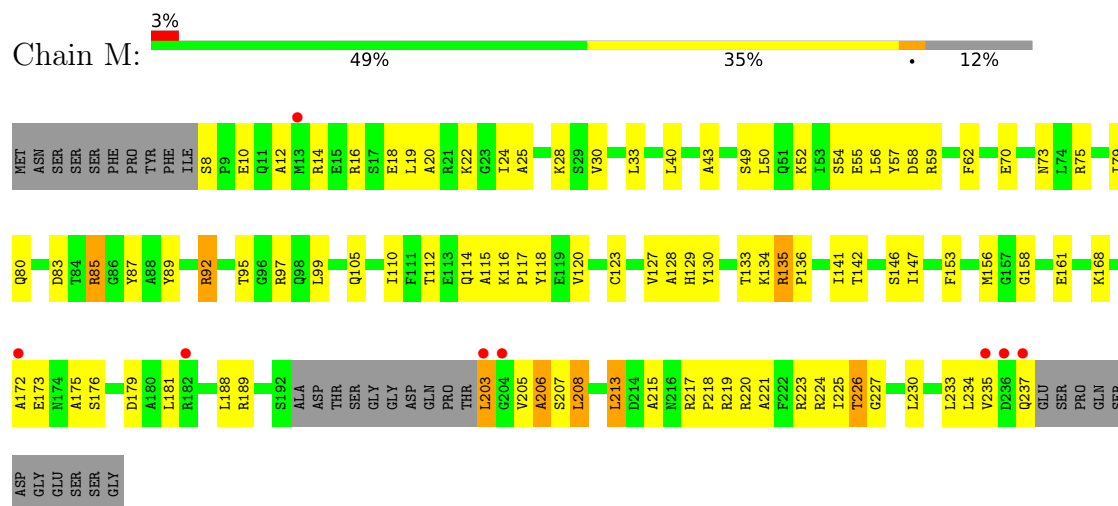
- Molecule 1: 20S proteasome, alpha and beta subunits



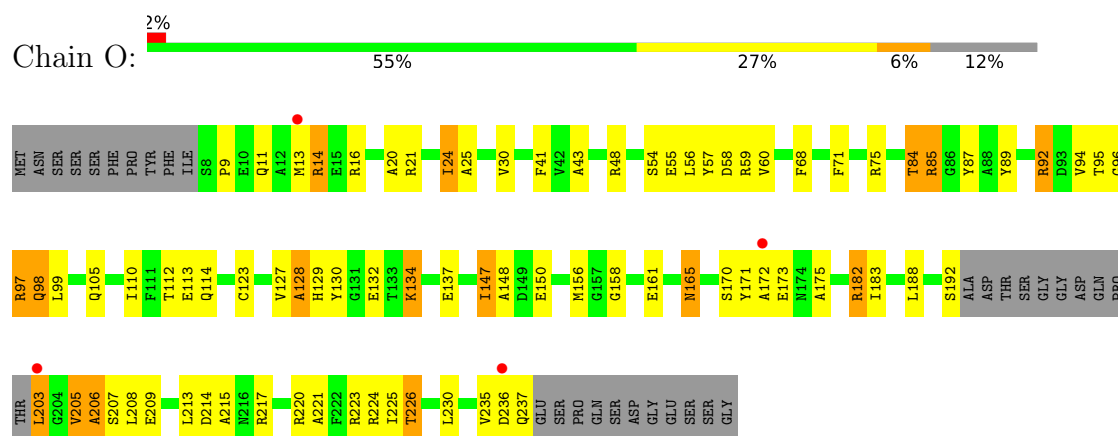
- Molecule 1: 20S proteasome, alpha and beta subunits



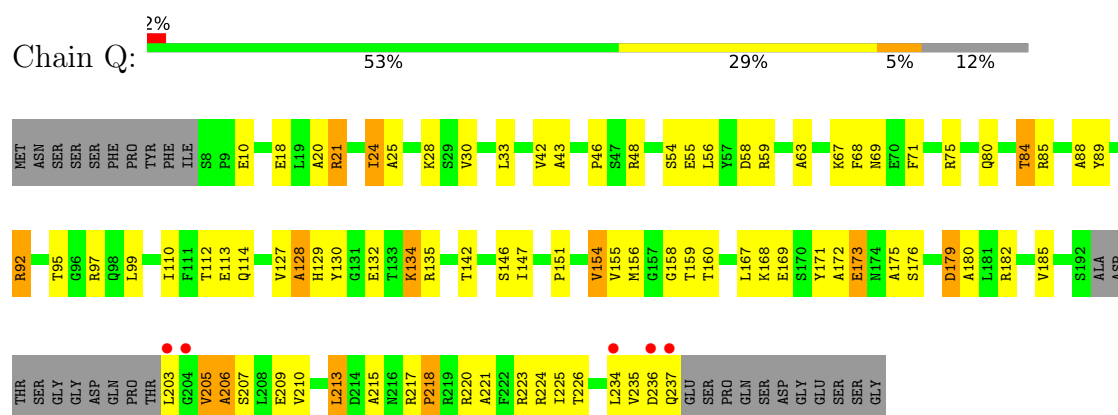
- Molecule 1: 20S proteasome, alpha and beta subunits



- Molecule 1: 20S proteasome, alpha and beta subunits

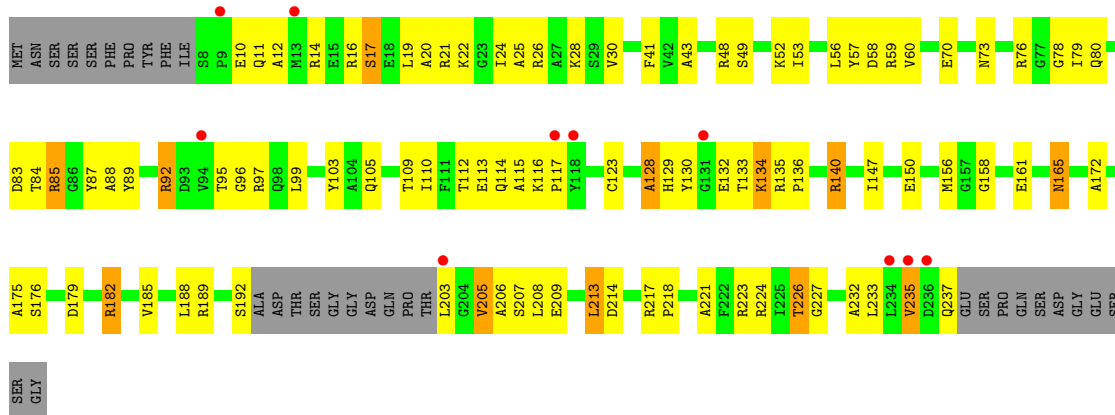


- Molecule 1: 20S proteasome, alpha and beta subunits

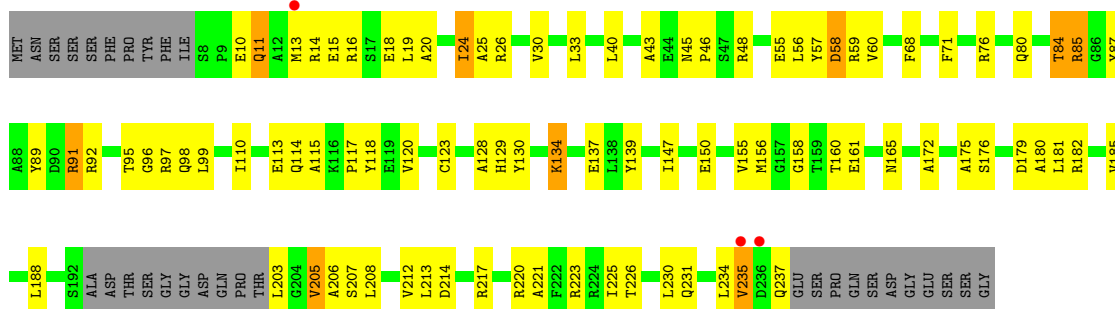


- Molecule 1: 20S proteasome, alpha and beta subunits

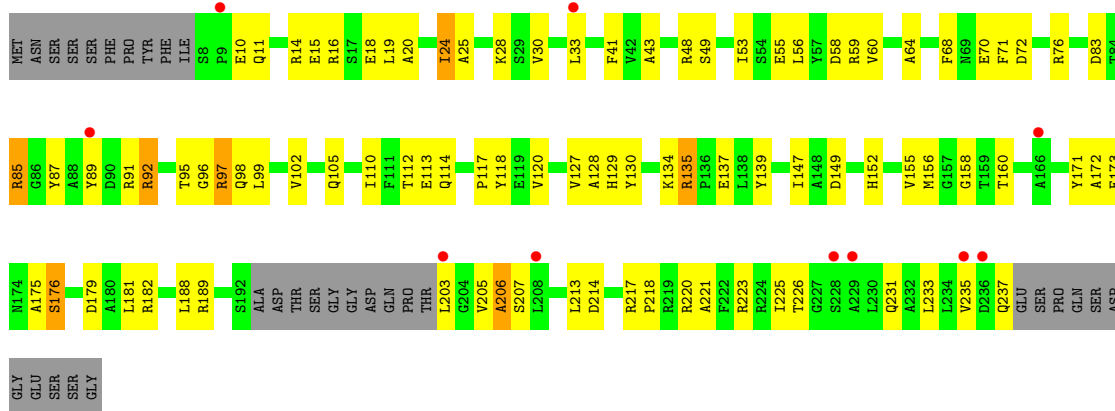




- Molecule 1: 20S proteasome, alpha and beta subunits

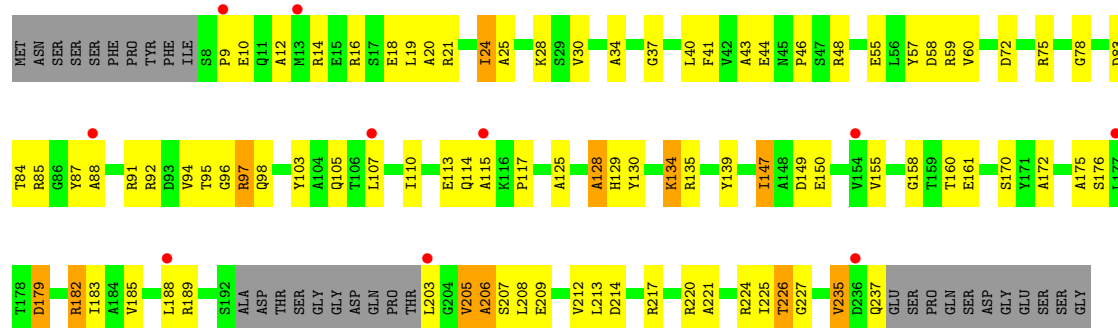


- Molecule 1: 20S proteasome, alpha and beta subunits

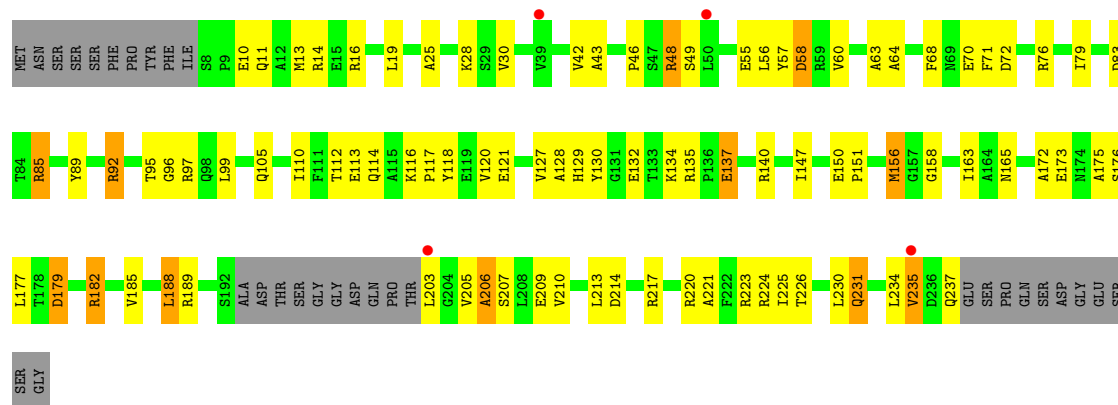


- Molecule 1: 20S proteasome, alpha and beta subunits

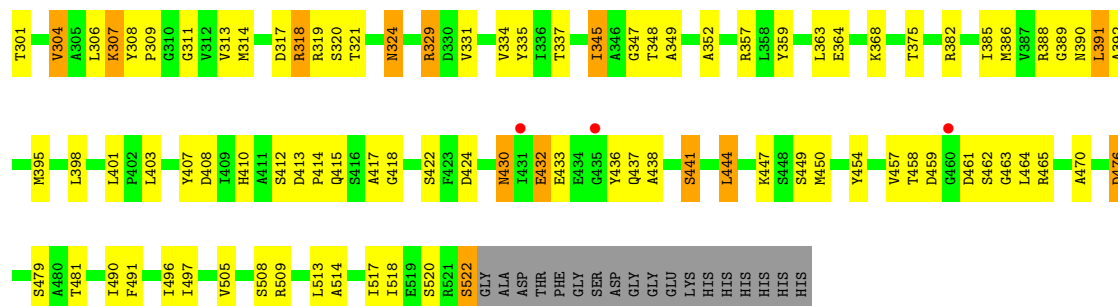




- Molecule 1: 20S proteasome, alpha and beta subunits

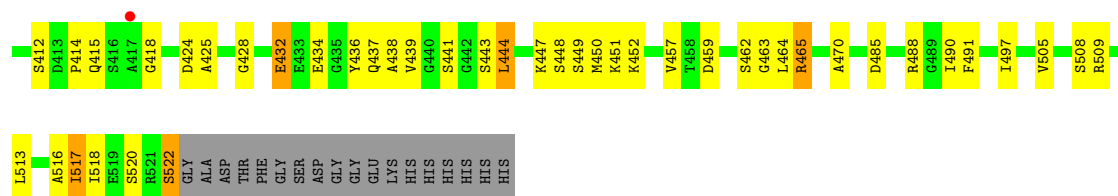


- Molecule 2: proteasome, beta subunit



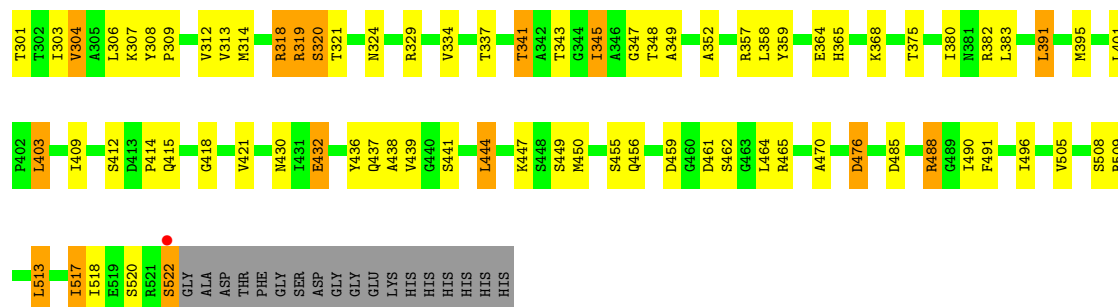
- Molecule 2: proteasome, beta subunit





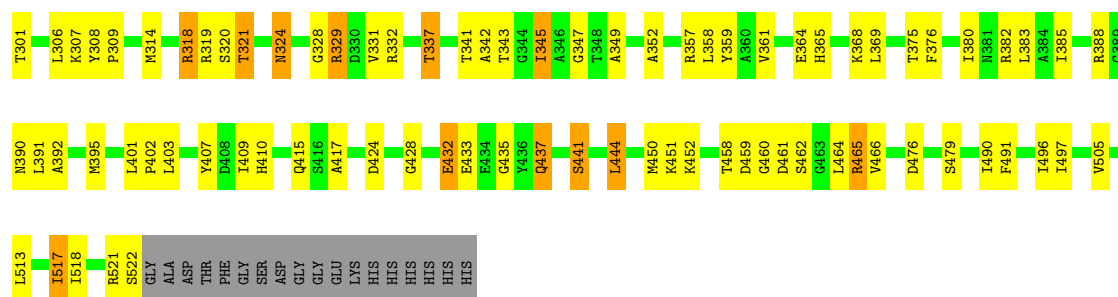
- Molecule 2: proteasome, beta subunit

Chain E: 60% 26% 6% 8%



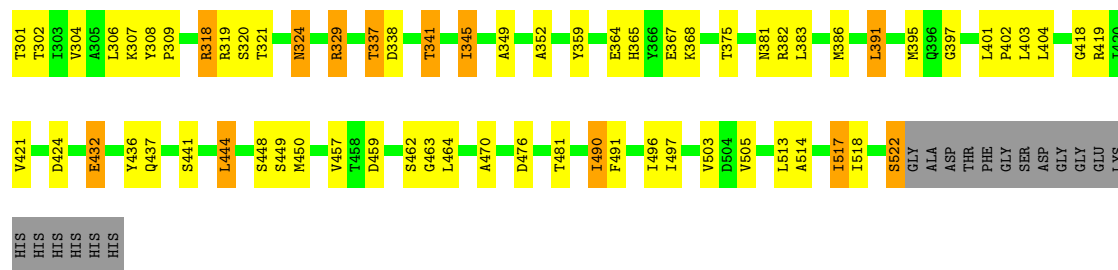
- Molecule 2: proteasome, beta subunit

Chain G: 59% 29% 5% 8%



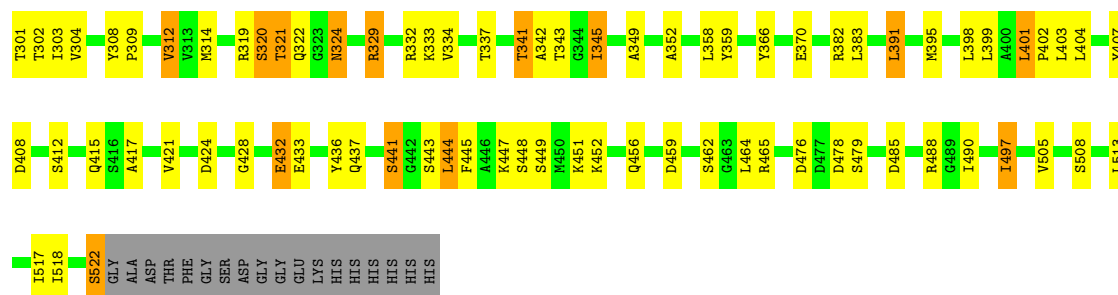
- Molecule 2: proteasome, beta subunit

Chain J: 65% 23% 5% 8%



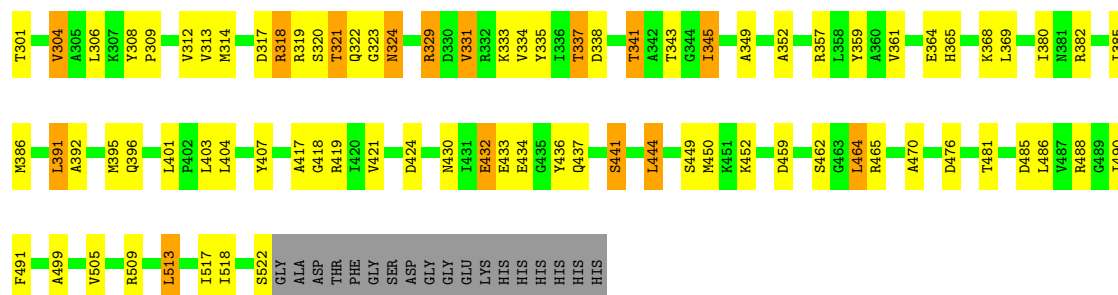
- Molecule 2: proteasome, beta subunit

Chain L: 60% 26% 6% 8%



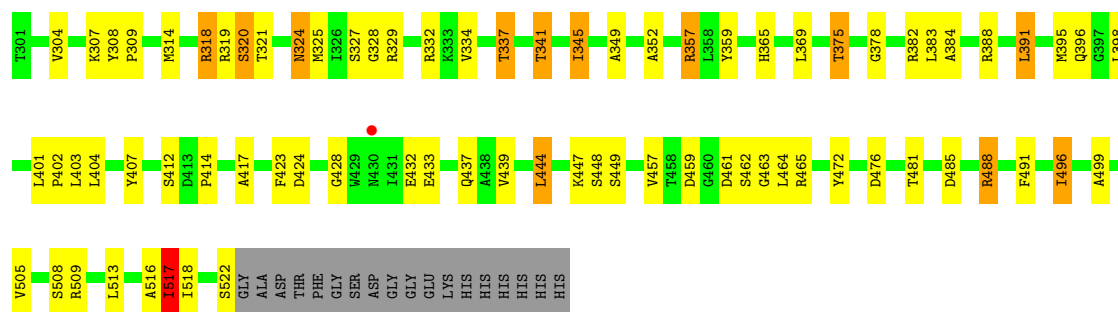
- Molecule 2: proteasome, beta subunit

Chain N: 58% 28% 6% 8%



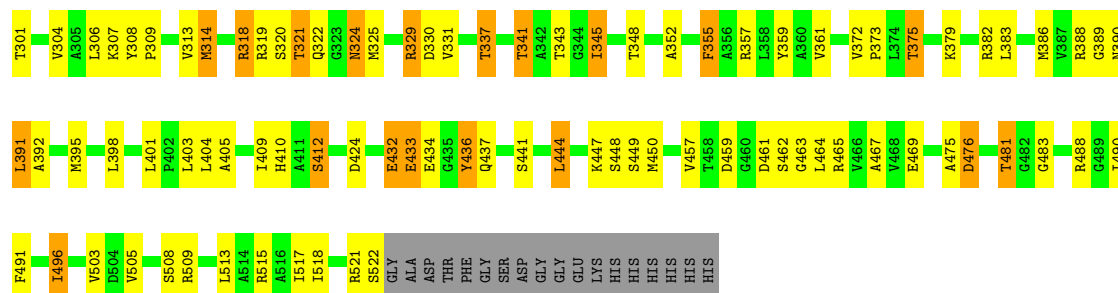
- Molecule 2: proteasome, beta subunit

Chain P: 60% 27% 5% 8%



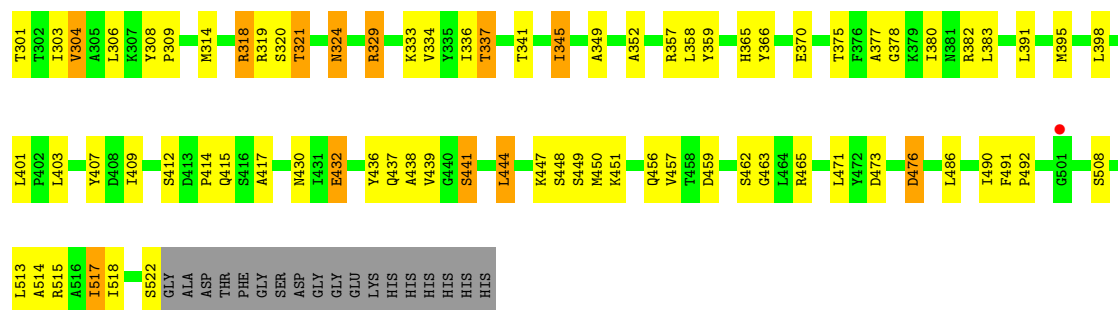
- Molecule 2: proteasome, beta subunit

Chain R: 56% 29% 8% 8%



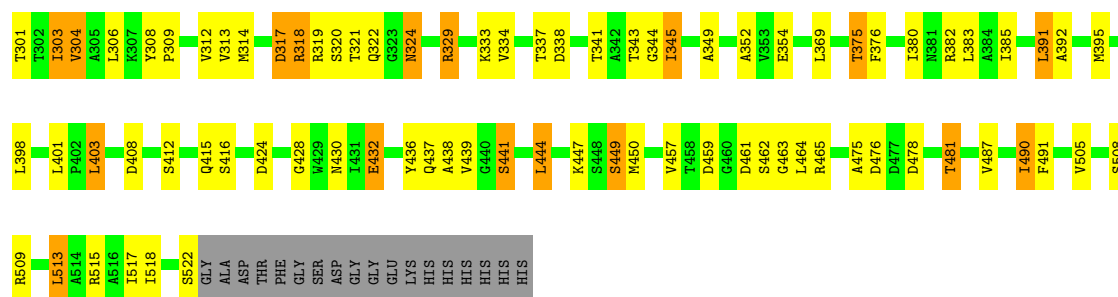
- Molecule 2: proteasome, beta subunit

Chain T: 



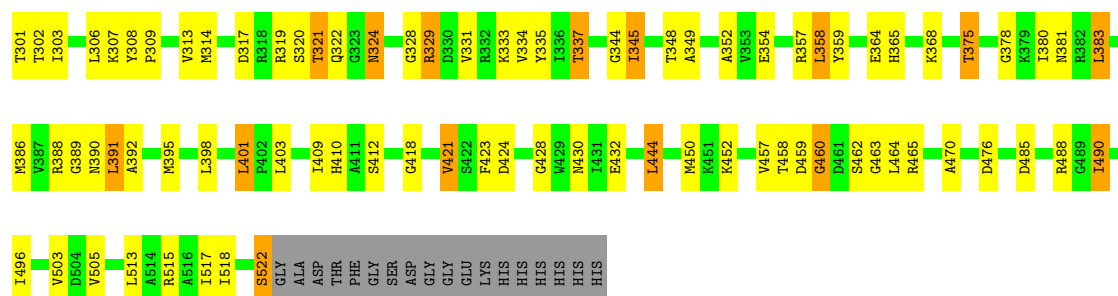
- Molecule 2: proteasome, beta subunit

Chain V: 



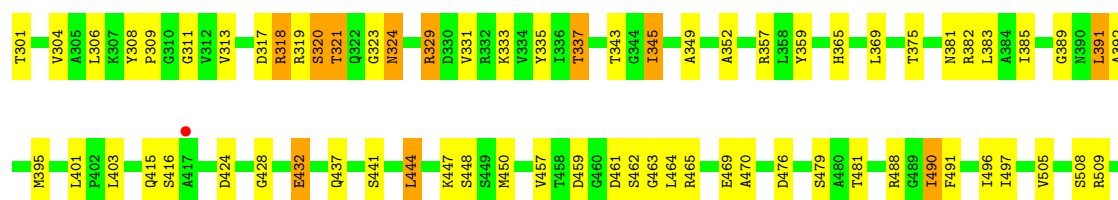
- Molecule 2: proteasome, beta subunit

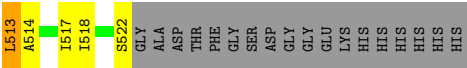
Chain X: 



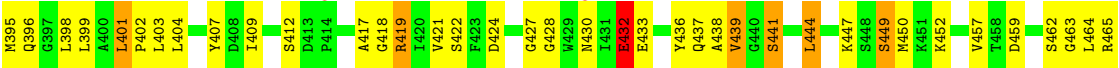
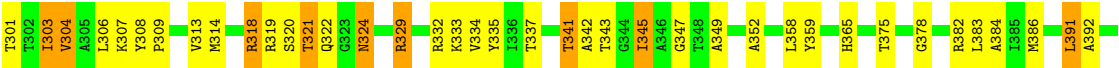
- Molecule 2: proteasome, beta subunit

Chain Z: 





● Molecule 2: proteasome, beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	173.96Å 116.17Å 200.20Å 90.00° 112.71° 90.00°	Depositor
Resolution (Å)	50.00 – 2.99 50.00 – 2.99	Depositor EDS
% Data completeness (in resolution range)	94.1 (50.00-2.99) 94.1 (50.00-2.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.226 , 0.262 0.227 , 0.229	Depositor DCC
R_{free} test set	4257 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 91.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	47389	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: M1N

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	0.58	0/1717	0.89	0/2320
1	A	0.59	0/1717	0.90	0/2320
1	B	0.57	0/1717	0.92	1/2320 (0.0%)
1	D	0.58	0/1717	0.92	0/2320
1	F	0.57	0/1717	0.92	0/2320
1	I	0.58	0/1717	0.90	0/2320
1	K	0.57	0/1717	0.89	1/2320 (0.0%)
1	M	0.56	0/1717	0.92	0/2320
1	O	0.56	0/1717	0.89	2/2320 (0.1%)
1	Q	0.60	0/1717	0.90	0/2320
1	S	0.58	0/1717	0.91	0/2320
1	U	0.58	0/1717	0.92	0/2320
1	W	0.62	2/1717 (0.1%)	0.93	1/2320 (0.0%)
1	Y	0.57	0/1717	0.90	1/2320 (0.0%)
2	2	0.69	0/1662	0.97	1/2254 (0.0%)
2	C	0.73	0/1662	0.96	1/2254 (0.0%)
2	E	0.70	0/1662	0.97	0/2254
2	G	0.68	0/1662	0.97	2/2254 (0.1%)
2	H	0.76	0/1662	0.98	1/2254 (0.0%)
2	J	0.68	0/1662	0.98	1/2254 (0.0%)
2	L	0.70	0/1662	0.97	1/2254 (0.0%)
2	N	0.66	0/1662	0.98	3/2254 (0.1%)
2	P	0.70	0/1662	0.98	2/2254 (0.1%)
2	R	0.69	1/1662 (0.1%)	0.96	1/2254 (0.0%)
2	T	0.69	2/1662 (0.1%)	0.97	1/2254 (0.0%)
2	V	0.65	0/1662	0.94	1/2254 (0.0%)
2	X	0.67	0/1662	0.95	1/2254 (0.0%)
2	Z	0.66	0/1662	0.97	2/2254 (0.1%)
All	All	0.64	5/47306 (0.0%)	0.94	24/64036 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	412	SER	CB-OG	8.17	1.58	1.42
1	W	173	GLU	CD-OE1	7.81	1.40	1.25
1	W	173	GLU	CD-OE2	6.69	1.38	1.25
2	T	456	GLN	CD-NE2	6.35	1.46	1.33
2	T	336	ILE	CA-CB	5.29	1.59	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	432	GLU	N-CA-C	6.52	118.05	111.07
2	V	432	GLU	N-CA-C	6.44	118.30	111.28
2	L	432	GLU	N-CA-C	6.40	118.26	111.28
2	N	434	GLU	N-CA-C	-6.33	104.79	114.16
2	J	432	GLU	N-CA-C	6.12	117.95	111.28
2	C	432	GLU	N-CA-C	6.08	117.91	111.28
2	X	432	GLU	N-CA-C	5.99	117.89	111.36
2	Z	432	GLU	N-CA-C	5.94	117.76	111.28
2	P	432	GLU	N-CA-C	5.93	117.82	111.36
2	N	432	GLU	N-CA-C	5.77	117.57	111.28
2	R	432	GLU	N-CA-C	5.77	117.56	111.28
2	T	432	GLU	N-CA-C	5.61	117.07	111.07
1	K	97	ARG	N-CA-C	-5.48	105.39	111.36
1	B	97	ARG	N-CA-C	-5.41	105.47	111.36
2	P	517	ILE	CB-CA-C	-5.38	104.99	111.88
1	Y	97	ARG	N-CA-C	-5.19	105.70	111.36
2	H	432	GLU	N-CA-C	5.16	116.90	111.28
2	G	347	GLY	N-CA-C	5.08	117.70	111.45
2	Z	323	GLY	N-CA-C	-5.08	102.32	110.95
1	W	97	ARG	N-CA-C	-5.06	105.77	111.28
1	O	84	THR	N-CA-CB	5.05	117.39	110.07
1	O	97	ARG	N-CA-C	-5.04	105.78	111.28
2	G	432	GLU	N-CA-C	5.01	116.75	111.28
2	N	323	GLY	N-CA-C	-5.01	101.31	113.18

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	1692	0	1688	75	0
1	A	1692	0	1688	56	1
1	B	1692	0	1688	55	0
1	D	1692	0	1688	58	1
1	F	1692	0	1688	66	0
1	I	1692	0	1688	57	0
1	K	1692	0	1688	66	0
1	M	1692	0	1688	69	0
1	O	1692	0	1688	62	0
1	Q	1692	0	1688	48	0
1	S	1692	0	1688	71	0
1	U	1692	0	1688	59	0
1	W	1692	0	1688	64	0
1	Y	1692	0	1688	56	0
2	2	1638	0	1629	79	0
2	C	1638	0	1629	72	0
2	E	1638	0	1629	59	0
2	G	1638	0	1629	72	0
2	H	1638	0	1629	69	0
2	J	1638	0	1629	58	0
2	L	1638	0	1629	68	0
2	N	1638	0	1629	81	0
2	P	1638	0	1629	60	0
2	R	1638	0	1629	59	0
2	T	1638	0	1629	56	0
2	V	1638	0	1629	71	0
2	X	1638	0	1629	75	0
2	Z	1638	0	1629	64	0
3	2	32	0	32	10	0
3	C	32	0	32	12	0
3	E	32	0	32	15	0
3	G	32	0	32	10	0
3	H	32	0	32	12	0
3	J	32	0	32	17	0
3	L	32	0	32	16	0
3	N	32	0	32	16	0
3	P	32	0	32	14	0
3	R	32	0	32	9	0
3	T	32	0	32	11	0
3	V	32	0	32	17	0
3	X	32	0	32	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Z	32	0	32	16	0
4	1	6	0	0	4	0
4	2	21	0	0	4	0
4	A	10	0	0	0	0
4	B	10	0	0	2	0
4	C	20	0	0	6	0
4	D	4	0	0	2	0
4	E	10	0	0	1	0
4	F	7	0	0	4	0
4	G	16	0	0	2	0
4	H	16	0	0	4	0
4	I	11	0	0	2	0
4	J	13	0	0	1	0
4	K	9	0	0	0	0
4	L	14	0	0	2	0
4	M	13	0	0	5	0
4	N	12	0	0	3	0
4	O	15	0	0	1	0
4	P	15	0	0	5	0
4	Q	6	0	0	3	0
4	R	12	0	0	4	0
4	S	5	0	0	0	0
4	T	8	0	0	2	0
4	U	2	0	0	0	0
4	V	20	0	0	5	0
4	W	7	0	0	2	0
4	X	20	0	0	14	0
4	Y	11	0	0	5	0
4	Z	8	0	0	0	0
All	All	47389	0	46886	1718	1

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 18.

All (1718) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:424:ASP:HA	4:C:542:HOH:O	1.37	1.22
2:X:303:ILE:HG13	4:X:58:HOH:O	1.35	1.22
2:N:304:VAL:CG2	2:N:450:MET:HE1	1.76	1.14
2:L:314:MET:HE3	2:L:334:VAL:HG13	1.30	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:444:LEU:HD12	2:Z:444:LEU:HD12	1.31	1.08
2:L:444:LEU:HD12	2:P:444:LEU:HD12	1.35	1.07
3:N:273:M1N:H221	3:N:273:M1N:O16	1.55	1.06
2:H:444:LEU:CD1	2:E:444:LEU:HD12	1.85	1.05
2:N:444:LEU:HD12	2:V:444:LEU:HD12	1.37	1.05
2:H:444:LEU:HD12	2:E:444:LEU:HD12	1.08	1.04
2:H:444:LEU:HD12	2:E:444:LEU:CD1	1.86	1.04
2:N:304:VAL:HG21	2:N:450:MET:HE1	1.03	1.02
1:D:11:GLN:HG2	1:D:14:ARG:HH12	1.23	1.01
1:K:85:ARG:HG2	1:K:85:ARG:HH11	1.24	0.98
2:E:430:ASN:HB3	4:E:87:HOH:O	1.63	0.98
1:D:59:ARG:HG3	1:D:129:HIS:HD2	1.29	0.96
2:N:304:VAL:HG21	2:N:450:MET:CE	1.96	0.96
1:F:231:GLN:HG3	4:F:252:HOH:O	1.65	0.95
1:U:11:GLN:HG2	1:U:14:ARG:HH12	1.29	0.95
2:C:465:ARG:HG3	2:C:465:ARG:HH11	1.31	0.94
2:V:349:ALA:H	3:V:273:M1N:C35	1.80	0.94
2:N:349:ALA:H	3:N:273:M1N:C35	1.81	0.93
2:N:324:ASN:H	2:N:324:ASN:HD22	1.13	0.92
2:N:337:THR:OG1	2:N:343:THR:HG22	1.70	0.91
1:O:85:ARG:CG	1:O:85:ARG:HH11	1.83	0.90
1:S:92:ARG:HD2	1:S:129:HIS:CE1	2.05	0.90
2:N:349:ALA:H	3:N:273:M1N:H35	1.34	0.90
2:C:301:THR:HG21	3:C:273:M1N:O16	1.72	0.90
2:R:321:THR:O	3:R:273:M1N:H51	1.72	0.89
2:V:349:ALA:H	3:V:273:M1N:H35	1.36	0.89
1:M:85:ARG:HG2	1:M:85:ARG:HH11	1.35	0.88
2:2:314:MET:HE3	2:2:334:VAL:HG13	1.53	0.88
1:O:85:ARG:HH11	1:O:85:ARG:HG2	1.37	0.88
3:Z:273:M1N:H221	3:Z:273:M1N:O16	1.74	0.88
2:C:304:VAL:HG21	2:C:450:MET:HE1	1.54	0.88
2:L:337:THR:OG1	2:L:343:THR:HG22	1.74	0.88
2:H:395:MET:HE2	2:H:395:MET:HA	1.54	0.88
2:2:403:LEU:HD12	2:2:439:VAL:HG22	1.54	0.87
1:Q:88:ALA:O	2:Z:381:ASN:ND2	2.07	0.87
2:H:314:MET:HE3	2:H:334:VAL:HG13	1.56	0.87
2:G:444:LEU:HD12	2:2:444:LEU:HD12	1.54	0.87
1:W:83:ASP:OD2	2:X:365:HIS:HD2	1.57	0.87
1:Q:59:ARG:HG3	1:Q:129:HIS:HD2	1.39	0.86
2:X:395:MET:HE2	2:X:395:MET:HA	1.55	0.86
2:Z:437:GLN:OE1	2:Z:447:LYS:HD3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:444:LEU:HD12	2:R:444:LEU:HD12	1.59	0.85
2:N:349:ALA:N	3:N:273:M1N:H35	1.91	0.85
2:V:349:ALA:N	3:V:273:M1N:H35	1.89	0.85
3:X:273:M1N:H221	3:X:273:M1N:O16	1.76	0.85
3:G:273:M1N:H40	2:N:424:ASP:OD1	1.77	0.85
3:R:273:M1N:HN1	3:R:273:M1N:H252	1.42	0.84
1:S:11:GLN:HG2	1:S:14:ARG:NH1	1.92	0.84
1:M:85:ARG:HH11	1:M:85:ARG:CG	1.90	0.84
2:J:324:ASN:HD22	2:J:324:ASN:H	1.25	0.84
2:P:314:MET:HE3	2:P:334:VAL:HG13	1.60	0.84
1:1:110:ILE:HG23	1:1:114:GLN:HG3	1.60	0.82
2:X:317:ASP:OD1	2:X:333:LYS:NZ	2.11	0.82
2:X:391:LEU:O	2:X:395:MET:HG2	1.78	0.82
1:D:92:ARG:HD2	1:D:129:HIS:CE1	2.15	0.82
2:N:314:MET:HE3	2:N:334:VAL:HG13	1.61	0.82
1:Y:37:GLY:HA3	4:Y:256:HOH:O	1.77	0.82
1:A:56:LEU:HD13	1:A:99:LEU:HD23	1.59	0.82
4:Q:254:HOH:O	2:Z:375:THR:HG21	1.78	0.82
2:V:462:SER:O	2:V:465:ARG:HG2	1.78	0.82
2:T:476:ASP:HB2	4:X:20:HOH:O	1.79	0.82
2:2:321:THR:O	3:2:273:M1N:H51	1.80	0.81
2:G:321:THR:O	3:G:273:M1N:H37	1.80	0.81
1:S:83:ASP:OD2	2:T:365:HIS:HD2	1.63	0.81
2:H:465:ARG:HH11	2:H:465:ARG:HG3	1.46	0.81
1:K:85:ARG:HH11	1:K:85:ARG:CG	1.94	0.81
2:N:321:THR:O	3:N:273:M1N:H37	1.81	0.81
3:2:273:M1N:H221	3:2:273:M1N:O16	1.81	0.81
2:2:465:ARG:HD3	4:2:544:HOH:O	1.80	0.81
2:V:319:ARG:HG3	4:V:552:HOH:O	1.81	0.80
2:J:321:THR:O	3:J:273:M1N:H51	1.81	0.80
1:1:92:ARG:HD2	1:1:129:HIS:CE1	2.15	0.80
2:H:465:ARG:HD3	4:H:547:HOH:O	1.82	0.79
1:S:56:LEU:HD13	1:S:99:LEU:HD22	1.63	0.79
2:C:465:ARG:HH11	2:C:465:ARG:CG	1.95	0.79
1:Y:87:TYR:O	2:Z:357:ARG:NH2	2.16	0.78
2:G:464:LEU:HD12	2:G:496:ILE:HD11	1.63	0.78
2:J:329:ARG:NH2	2:R:476:ASP:O	2.16	0.78
2:N:395:MET:HA	2:N:395:MET:HE2	1.66	0.78
2:H:430:ASN:HB3	4:H:551:HOH:O	1.82	0.78
2:X:345:ILE:N	4:X:58:HOH:O	2.16	0.78
2:T:314:MET:HE3	2:T:334:VAL:HG13	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:230:LEU:HD21	1:K:234:LEU:HD13	1.65	0.77
2:R:483:GLY:HA2	4:R:46:HOH:O	1.84	0.77
2:X:321:THR:O	3:X:273:M1N:H51	1.82	0.77
1:F:92:ARG:HG3	1:F:129:HIS:HE1	1.50	0.77
2:X:314:MET:HE3	2:X:334:VAL:HG13	1.65	0.77
2:X:485:ASP:OD2	2:X:488:ARG:HB2	1.84	0.77
2:E:395:MET:HE2	2:E:395:MET:HA	1.66	0.77
1:B:110:ILE:HG23	1:B:114:GLN:HG3	1.66	0.77
1:I:60:VAL:HG21	1:I:96:GLY:HA3	1.65	0.77
2:X:345:ILE:HD13	2:X:352:ALA:HB1	1.67	0.77
2:G:349:ALA:H	3:G:273:M1N:C35	1.97	0.77
2:J:345:ILE:HD13	2:J:352:ALA:HB1	1.65	0.77
2:Z:465:ARG:HB2	2:Z:513:LEU:HD21	1.66	0.77
2:H:349:ALA:HA	3:H:273:M1N:H243	1.67	0.77
2:L:444:LEU:CD1	2:P:444:LEU:HD12	2.14	0.77
2:T:382:ARG:HD3	1:I:89:TYR:CD1	2.20	0.77
2:Z:349:ALA:HB2	3:Z:273:M1N:H252	1.67	0.76
3:E:273:M1N:HN1	3:E:273:M1N:C25	1.98	0.76
1:Q:110:ILE:HG23	1:Q:114:GLN:HG3	1.66	0.76
2:X:424:ASP:OD1	3:Z:273:M1N:H40	1.86	0.76
2:J:444:LEU:HD12	2:Z:444:LEU:CD1	2.14	0.75
2:T:476:ASP:HA	4:T:88:HOH:O	1.85	0.75
2:2:395:MET:HE2	2:2:395:MET:HA	1.66	0.75
2:H:324:ASN:ND2	2:H:324:ASN:H	1.84	0.75
3:C:273:M1N:O16	3:C:273:M1N:H221	1.85	0.75
1:I:83:ASP:OD2	2:J:365:HIS:HD2	1.70	0.75
2:P:321:THR:O	3:P:273:M1N:H37	1.84	0.75
1:I:14:ARG:HB3	1:I:14:ARG:HH11	1.49	0.75
2:V:321:THR:O	3:V:273:M1N:H37	1.86	0.75
2:L:437:GLN:OE1	2:L:447:LYS:HD3	1.87	0.75
2:Z:321:THR:O	3:Z:273:M1N:H37	1.86	0.74
3:H:273:M1N:H221	3:H:273:M1N:O16	1.87	0.74
2:N:337:THR:HG21	2:N:359:TYR:CD2	2.22	0.74
1:O:14:ARG:HB3	1:O:14:ARG:HH11	1.52	0.74
2:X:452:LYS:HA	4:X:4:HOH:O	1.88	0.74
2:H:324:ASN:H	2:H:324:ASN:HD22	1.35	0.74
1:D:11:GLN:HG2	1:D:14:ARG:NH1	2.01	0.74
2:N:324:ASN:HD22	2:N:324:ASN:N	1.84	0.74
2:V:301:THR:HG21	3:V:273:M1N:O16	1.88	0.74
1:D:59:ARG:HG3	1:D:129:HIS:CD2	2.19	0.74
2:E:382:ARG:HD3	1:K:89:TYR:CD1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:214:ASP:OD2	1:O:217:ARG:HG2	1.87	0.73
1:A:182:ARG:HG3	1:A:235:VAL:HB	1.69	0.73
2:E:308:TYR:HB2	2:E:309:PRO:HD2	1.70	0.73
1:B:42:VAL:HG22	1:B:210:VAL:HG22	1.70	0.73
1:B:208:LEU:HB3	4:B:251:HOH:O	1.89	0.73
1:I:176:SER:HB3	1:I:179:ASP:OD1	1.88	0.73
2:R:337:THR:HG21	2:R:359:TYR:CD2	2.24	0.73
1:I:92:ARG:HD2	1:I:129:HIS:CE1	2.24	0.73
2:Z:301:THR:HG21	3:Z:273:M1N:O16	1.87	0.73
1:M:224:ARG:HD2	4:M:255:HOH:O	1.88	0.73
1:O:56:LEU:HD13	1:O:99:LEU:HD22	1.71	0.73
1:O:59:ARG:HG3	1:O:129:HIS:HD2	1.53	0.73
3:E:273:M1N:HN1	3:E:273:M1N:H252	1.53	0.72
2:J:349:ALA:H	3:J:273:M1N:C35	2.03	0.72
2:T:321:THR:O	3:T:273:M1N:C5	2.38	0.72
2:T:321:THR:O	3:T:273:M1N:H51	1.87	0.72
2:T:345:ILE:HD13	2:T:352:ALA:HB1	1.70	0.72
2:Z:459:ASP:H	2:Z:462:SER:HB3	1.53	0.72
2:P:308:TYR:HB2	2:P:309:PRO:HD2	1.71	0.72
2:C:450:MET:HE3	2:C:470:ALA:CB	2.18	0.72
1:I:72:ASP:O	1:I:76:ARG:HG3	1.89	0.72
1:K:59:ARG:HG3	1:K:129:HIS:HD2	1.55	0.72
2:R:436:TYR:CD2	2:R:450:MET:HG2	2.24	0.72
1:W:68:PHE:HA	1:W:71:PHE:CE2	2.25	0.72
2:N:364:GLU:HG2	2:N:368:LYS:HE2	1.71	0.72
1:O:94:VAL:HA	1:O:98:GLN:HE22	1.55	0.72
2:R:509:ARG:HG3	4:R:254:HOH:O	1.87	0.72
2:L:444:LEU:HD12	2:P:444:LEU:CD1	2.18	0.72
1:S:85:ARG:HG2	1:S:85:ARG:HH11	1.54	0.72
2:L:464:LEU:HD11	2:L:505:VAL:HG11	1.70	0.71
2:L:456:GLN:HE22	2:L:465:ARG:HH12	1.38	0.71
2:R:462:SER:O	2:R:465:ARG:HG2	1.90	0.71
2:C:465:ARG:HG3	2:C:465:ARG:NH1	2.00	0.71
1:D:92:ARG:HG3	1:D:129:HIS:HE1	1.54	0.71
1:K:217:ARG:NH2	1:K:223:ARG:HG3	2.06	0.71
2:E:462:SER:O	2:E:465:ARG:HG2	1.91	0.71
2:X:337:THR:HG21	2:X:359:TYR:CD2	2.25	0.71
1:B:30:VAL:HG13	1:B:43:ALA:HB2	1.73	0.71
2:L:345:ILE:HD13	2:L:352:ALA:HB1	1.70	0.71
2:2:464:LEU:HD12	2:2:496:ILE:HD11	1.73	0.71
2:G:321:THR:O	3:G:273:M1N:H51	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:337:THR:HG21	2:T:359:TYR:CD2	2.24	0.71
3:V:273:M1N:O16	3:V:273:M1N:H221	1.89	0.71
2:C:304:VAL:CG2	2:C:450:MET:HE1	2.21	0.71
2:G:364:GLU:HG2	2:G:368:LYS:HE2	1.73	0.71
2:L:349:ALA:H	3:L:273:M1N:C35	2.03	0.71
2:T:301:THR:N	2:T:441:SER:HG	1.89	0.71
2:V:301:THR:N	2:V:441:SER:HG	1.88	0.71
1:1:217:ARG:HH21	1:1:223:ARG:HG3	1.56	0.70
2:C:301:THR:HG21	3:C:273:M1N:H16	1.57	0.70
1:D:128:ALA:HB2	1:D:134:LYS:HB3	1.72	0.70
2:T:459:ASP:H	2:T:462:SER:HB3	1.56	0.70
2:V:395:MET:HA	2:V:395:MET:HE2	1.74	0.70
2:J:301:THR:HG21	3:J:273:M1N:O16	1.91	0.70
2:J:395:MET:HE2	2:J:395:MET:HA	1.74	0.70
1:S:92:ARG:HD2	1:S:129:HIS:ND1	2.05	0.70
1:D:56:LEU:HD13	1:D:99:LEU:HD23	1.74	0.70
2:V:349:ALA:HA	3:V:273:M1N:H243	1.73	0.70
2:V:391:LEU:O	2:V:395:MET:HG2	1.92	0.70
1:D:55:GLU:OE2	1:D:220:ARG:HD2	1.91	0.70
1:O:59:ARG:HG3	1:O:129:HIS:CD2	2.27	0.70
1:W:85:ARG:HG2	1:W:85:ARG:HH11	1.57	0.70
2:C:318:ARG:HG2	4:C:551:HOH:O	1.90	0.69
2:2:485:ASP:OD2	2:2:488:ARG:HB2	1.92	0.69
1:Y:72:ASP:OD2	4:Y:258:HOH:O	2.10	0.69
1:A:217:ARG:HH21	1:A:223:ARG:HG3	1.57	0.69
2:C:509:ARG:HG2	4:C:541:HOH:O	1.92	0.69
1:K:56:LEU:HD13	1:K:99:LEU:HD22	1.73	0.69
1:M:56:LEU:HD13	1:M:99:LEU:HD22	1.74	0.69
2:T:382:ARG:HD3	1:1:89:TYR:HD1	1.56	0.69
1:W:56:LEU:HD13	1:W:99:LEU:HD22	1.73	0.69
2:E:485:ASP:OD2	2:E:488:ARG:HB2	1.93	0.69
2:R:308:TYR:HB2	2:R:309:PRO:HD2	1.75	0.69
2:R:437:GLN:OE1	2:R:447:LYS:HD3	1.92	0.69
1:B:151:PRO:HD2	4:B:255:HOH:O	1.91	0.69
2:T:321:THR:O	3:T:273:M1N:H37	1.93	0.69
2:J:337:THR:HG21	2:J:359:TYR:CD2	2.27	0.69
2:P:341:THR:CG2	2:P:404:LEU:HD11	2.23	0.69
2:G:459:ASP:H	2:G:462:SER:HB3	1.57	0.69
1:B:205:VAL:HG12	1:B:206:ALA:H	1.58	0.69
2:C:301:THR:N	2:C:441:SER:HG	1.90	0.69
2:T:476:ASP:CB	4:X:20:HOH:O	2.37	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:465:ARG:HB2	2:Z:513:LEU:CD2	2.22	0.69
2:C:509:ARG:CG	4:C:541:HOH:O	2.40	0.69
2:T:349:ALA:H	3:T:273:M1N:C35	2.06	0.69
2:Z:345:ILE:HD13	2:Z:352:ALA:HB1	1.75	0.69
1:U:10:GLU:HA	1:1:19:LEU:HD12	1.75	0.68
2:G:337:THR:OG1	2:G:343:THR:HG22	1.93	0.68
2:V:321:THR:O	3:V:273:M1N:H52	1.92	0.68
2:V:459:ASP:H	2:V:462:SER:HB3	1.57	0.68
1:F:165:ASN:HD22	1:F:168:LYS:HZ3	1.39	0.68
1:M:92:ARG:HH11	1:M:92:ARG:HB2	1.59	0.68
2:L:518:ILE:O	2:L:522:SER:HB2	1.93	0.68
1:I:56:LEU:HD13	1:I:99:LEU:HD22	1.74	0.68
2:Z:513:LEU:O	2:Z:517:ILE:HG12	1.94	0.68
1:1:14:ARG:HB3	1:1:14:ARG:NH1	2.07	0.68
2:H:321:THR:O	3:H:273:M1N:H37	1.94	0.68
1:B:92:ARG:HD2	1:B:129:HIS:ND1	2.10	0.68
2:C:518:ILE:O	2:C:522:SER:HB2	1.94	0.68
2:Z:349:ALA:H	3:Z:273:M1N:C35	2.07	0.68
2:G:308:TYR:HB2	2:G:309:PRO:HD2	1.75	0.67
1:B:189:ARG:CZ	1:B:237:GLN:HB3	2.24	0.67
1:Q:68:PHE:HA	1:Q:71:PHE:CE2	2.30	0.67
2:X:518:ILE:O	2:X:522:SER:HB2	1.94	0.67
2:E:464:LEU:HD11	2:E:505:VAL:HG11	1.76	0.67
2:G:321:THR:O	3:G:273:M1N:C5	2.43	0.67
2:J:318:ARG:HD3	2:J:491:PHE:O	1.95	0.67
1:W:83:ASP:OD2	2:X:365:HIS:CD2	2.45	0.67
1:W:49:SER:HB2	1:Y:97:ARG:NH1	2.09	0.67
1:O:9:PRO:HD2	1:U:15:GLU:OE1	1.95	0.67
2:T:318:ARG:HD3	2:T:491:PHE:O	1.93	0.67
2:C:308:TYR:HB2	2:C:309:PRO:HD2	1.76	0.67
1:O:123:CYS:HB3	1:O:156:MET:HE1	1.76	0.67
2:V:314:MET:HE3	2:V:334:VAL:HG13	1.77	0.67
2:X:515:ARG:HA	2:X:518:ILE:HD12	1.76	0.67
2:P:464:LEU:HD11	2:P:505:VAL:HG11	1.77	0.67
1:I:23:GLY:HA2	1:I:26:ARG:NH1	2.10	0.66
1:S:217:ARG:NH2	1:S:223:ARG:HG3	2.10	0.66
2:C:329:ARG:NH2	2:E:476:ASP:O	2.28	0.66
1:1:16:ARG:HE	1:1:117:PRO:HD3	1.60	0.66
2:J:391:LEU:O	2:J:395:MET:HG2	1.95	0.66
1:O:205:VAL:C	1:O:207:SER:H	2.03	0.66
2:P:375:THR:HB	2:P:378:GLY:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:75:ARG:NH2	4:Y:254:HOH:O	2.28	0.66
3:R:273:M1N:H252	3:R:273:M1N:N1	2.09	0.66
2:G:437:GLN:OE1	2:G:437:GLN:HA	1.94	0.66
2:J:324:ASN:H	2:J:324:ASN:ND2	1.93	0.66
2:L:424:ASP:OD1	3:N:273:M1N:H40	1.94	0.66
1:U:11:GLN:HG2	1:U:14:ARG:NH1	2.06	0.66
2:2:324:ASN:HD22	2:2:324:ASN:C	2.04	0.66
2:2:375:THR:HB	2:2:378:GLY:H	1.60	0.66
2:C:459:ASP:H	2:C:462:SER:HB3	1.61	0.66
2:R:395:MET:HE2	2:R:395:MET:HA	1.78	0.66
1:U:59:ARG:HG3	1:U:129:HIS:HD2	1.60	0.66
2:P:509:ARG:HG3	4:P:547:HOH:O	1.96	0.66
1:B:92:ARG:HD2	1:B:129:HIS:CE1	2.31	0.66
2:G:382:ARG:HD3	1:W:89:TYR:HD1	1.62	0.66
2:T:314:MET:CE	2:T:334:VAL:HG13	2.24	0.66
2:2:301:THR:N	2:2:441:SER:HG	1.94	0.66
2:C:301:THR:CG2	3:C:273:M1N:O16	2.45	0.65
1:I:70:GLU:OE2	1:I:116:LYS:NZ	2.30	0.65
2:L:391:LEU:O	2:L:395:MET:HG2	1.95	0.65
2:P:459:ASP:H	2:P:462:SER:HB3	1.60	0.65
2:X:450:MET:HE3	2:X:470:ALA:CB	2.26	0.65
3:P:273:M1N:HN1	3:P:273:M1N:H253	1.61	0.65
2:2:459:ASP:H	2:2:462:SER:HB3	1.59	0.65
2:H:459:ASP:H	2:H:462:SER:HB3	1.62	0.65
2:G:337:THR:HG21	2:G:359:TYR:CD2	2.31	0.65
1:U:59:ARG:HG3	1:U:129:HIS:CD2	2.31	0.65
1:A:161:GLU:O	1:A:165:ASN:HB2	1.95	0.65
2:E:348:THR:HG23	3:E:273:M1N:H35	1.77	0.65
2:J:349:ALA:HB2	3:J:273:M1N:H252	1.78	0.65
2:L:456:GLN:HE22	2:L:465:ARG:NH1	1.94	0.65
2:J:341:THR:HG22	2:J:404:LEU:HD11	1.76	0.65
1:I:205:VAL:HG12	1:I:206:ALA:H	1.62	0.65
2:V:375:THR:HG22	4:V:548:HOH:O	1.97	0.65
1:K:128:ALA:HB2	1:K:134:LYS:HB3	1.77	0.65
2:E:459:ASP:H	2:E:462:SER:HB3	1.61	0.65
3:J:273:M1N:O16	3:J:273:M1N:H221	1.97	0.65
2:L:452:LYS:HD3	4:L:549:HOH:O	1.96	0.65
1:I:121:GLU:OE2	1:I:156:MET:HB3	1.96	0.65
1:F:135:ARG:HB2	4:F:253:HOH:O	1.96	0.65
1:I:205:VAL:C	1:I:207:SER:H	2.05	0.65
2:L:459:ASP:H	2:L:462:SER:HB3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:217:ARG:HH21	1:O:223:ARG:HG3	1.62	0.65
2:C:485:ASP:OD2	2:C:488:ARG:HB2	1.98	0.64
1:I:172:ALA:HB3	1:I:175:ALA:HB2	1.80	0.64
2:V:518:ILE:O	2:V:522:SER:HB2	1.96	0.64
1:S:140:ARG:HB3	1:S:140:ARG:HH11	1.61	0.64
2:G:318:ARG:HD3	2:G:491:PHE:O	1.97	0.64
1:D:25:ALA:O	1:D:158:GLY:HA2	1.98	0.64
2:R:324:ASN:C	2:R:324:ASN:HD22	2.06	0.64
1:F:56:LEU:HD13	1:F:99:LEU:HD22	1.79	0.64
1:Y:205:VAL:C	1:Y:207:SER:H	2.05	0.64
3:L:273:M1N:HN1	3:L:273:M1N:C25	2.10	0.64
1:O:14:ARG:HB3	1:O:14:ARG:NH1	2.12	0.64
2:R:357:ARG:O	2:R:361:VAL:HG23	1.98	0.64
1:1:151:PRO:HD2	4:1:253:HOH:O	1.97	0.64
1:1:172:ALA:HB3	1:1:175:ALA:HB2	1.80	0.64
2:E:465:ARG:HH11	2:E:465:ARG:HG3	1.63	0.64
1:A:93:ASP:OD1	2:P:375:THR:OG1	2.15	0.64
1:Q:92:ARG:HG3	1:Q:129:HIS:CE1	2.32	0.64
1:W:20:ALA:O	1:W:24:ILE:HG12	1.98	0.64
2:G:382:ARG:HD3	1:W:89:TYR:CD1	2.33	0.63
1:M:55:GLU:OE2	1:M:220:ARG:HD2	1.98	0.63
1:M:226:THR:HA	4:M:252:HOH:O	1.97	0.63
2:N:349:ALA:HB2	3:N:273:M1N:H252	1.80	0.63
1:D:90:ASP:HB3	1:D:93:ASP:OD1	1.98	0.63
2:E:314:MET:HE3	2:E:334:VAL:HG13	1.79	0.63
2:L:301:THR:N	2:L:441:SER:HG	1.96	0.63
2:X:464:LEU:HD12	2:X:496:ILE:HD11	1.80	0.63
1:1:30:VAL:HG13	1:1:43:ALA:HB2	1.80	0.63
1:M:189:ARG:HH22	1:M:235:VAL:HG13	1.63	0.63
2:R:301:THR:N	2:R:441:SER:HG	1.96	0.63
2:X:424:ASP:HB3	2:X:428:GLY:H	1.62	0.63
2:H:314:MET:HE3	2:H:334:VAL:CG1	2.28	0.63
1:S:48:ARG:HD2	1:1:137:GLU:OE2	1.99	0.63
1:Y:55:GLU:OE2	1:Y:220:ARG:HD2	1.98	0.63
2:N:321:THR:O	3:N:273:M1N:H52	1.99	0.63
1:1:217:ARG:NH2	1:1:223:ARG:HG3	2.14	0.63
1:A:87:TYR:O	2:H:357:ARG:NH2	2.32	0.63
1:A:170:SER:HB2	1:A:183:ILE:HD12	1.80	0.63
2:C:391:LEU:O	2:C:395:MET:HG2	1.99	0.63
1:D:48:ARG:HD2	1:K:137:GLU:OE2	1.99	0.63
2:J:459:ASP:H	2:J:462:SER:HB3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:324:ASN:H	2:N:324:ASN:ND2	1.92	0.63
2:N:444:LEU:CD1	2:V:444:LEU:HD12	2.22	0.63
1:U:95:THR:OG1	1:U:98:GLN:HG3	1.98	0.63
2:2:518:ILE:O	2:2:522:SER:HB2	1.98	0.63
1:S:14:ARG:NH1	1:S:14:ARG:HB2	2.13	0.63
2:X:349:ALA:HA	3:X:273:M1N:H243	1.80	0.63
1:F:11:GLN:HG3	1:F:14:ARG:HH12	1.64	0.63
1:Q:10:GLU:HA	1:Y:19:LEU:HD12	1.79	0.63
1:U:60:VAL:HG21	1:U:96:GLY:HA3	1.81	0.63
1:W:14:ARG:HB3	1:W:14:ARG:NH1	2.14	0.63
1:W:110:ILE:HG23	1:W:114:GLN:HG3	1.80	0.63
1:W:189:ARG:NH2	1:W:237:GLN:HB3	2.14	0.63
2:Z:324:ASN:HD22	2:Z:324:ASN:H	1.47	0.63
1:F:165:ASN:HD22	1:F:168:LYS:NZ	1.95	0.63
1:K:205:VAL:C	1:K:207:SER:H	2.07	0.63
1:Y:34:ALA:HB3	4:Y:249:HOH:O	1.99	0.63
1:M:59:ARG:HG3	1:M:129:HIS:CD2	2.34	0.62
1:W:205:VAL:HG12	1:W:206:ALA:H	1.64	0.62
2:G:349:ALA:H	3:G:273:M1N:H35	1.64	0.62
1:O:85:ARG:CG	1:O:85:ARG:NH1	2.52	0.62
2:T:436:TYR:HB2	2:T:450:MET:SD	2.39	0.62
2:Z:392:ALA:O	2:Z:395:MET:HB2	1.99	0.62
2:G:452:LYS:NZ	2:2:449:SER:HB2	2.13	0.62
1:S:110:ILE:HG23	1:S:114:GLN:HG3	1.81	0.62
1:A:217:ARG:NH2	1:A:223:ARG:HG3	2.14	0.62
2:P:345:ILE:HD13	2:P:352:ALA:HB1	1.81	0.62
1:M:205:VAL:C	1:M:207:SER:H	2.07	0.62
2:R:457:VAL:HG22	2:R:463:GLY:HA2	1.80	0.62
2:H:476:ASP:O	2:L:329:ARG:NH2	2.30	0.62
2:E:382:ARG:HD3	1:K:89:TYR:HD1	1.62	0.62
2:R:459:ASP:H	2:R:462:SER:HB3	1.63	0.62
3:R:273:M1N:N1	3:R:273:M1N:C25	2.63	0.62
1:U:89:TYR:CD1	2:2:382:ARG:HD3	2.34	0.62
2:Z:318:ARG:HD3	2:Z:491:PHE:O	1.99	0.62
1:F:92:ARG:HG3	1:F:129:HIS:CE1	2.34	0.62
2:G:345:ILE:HD13	2:G:352:ALA:HB1	1.82	0.62
1:K:85:ARG:HG2	1:K:85:ARG:NH1	2.04	0.62
2:P:462:SER:O	2:P:465:ARG:HG2	2.00	0.62
1:D:176:SER:HB3	1:D:179:ASP:OD1	2.00	0.62
2:L:349:ALA:N	3:L:273:M1N:H35	2.15	0.62
1:S:205:VAL:C	1:S:207:SER:H	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:60:VAL:HG21	1:1:96:GLY:HA3	1.82	0.62
2:E:321:THR:O	3:E:273:M1N:H51	2.00	0.62
3:R:273:M1N:HN1	3:R:273:M1N:C25	2.13	0.62
1:U:205:VAL:C	1:U:207:SER:H	2.08	0.62
1:F:73:ASN:HD22	1:W:105:GLN:NE2	1.98	0.61
2:G:518:ILE:O	2:G:522:SER:HB2	1.99	0.61
1:Q:205:VAL:C	1:Q:207:SER:H	2.08	0.61
2:2:308:TYR:HB2	2:2:309:PRO:HD2	1.80	0.61
2:N:444:LEU:HD12	2:V:444:LEU:CD1	2.22	0.61
2:P:513:LEU:O	2:P:517:ILE:HG12	2.00	0.61
2:T:444:LEU:HD12	2:X:444:LEU:HD12	1.82	0.61
1:1:25:ALA:O	1:1:158:GLY:HA2	2.01	0.61
1:1:56:LEU:HD13	1:1:99:LEU:HD22	1.82	0.61
1:B:172:ALA:HB3	1:B:175:ALA:HB2	1.81	0.61
1:W:14:ARG:HB3	1:W:14:ARG:HH11	1.64	0.61
1:1:230:LEU:HD21	1:1:234:LEU:HD13	1.81	0.61
3:P:273:M1N:H40	2:V:424:ASP:OD1	2.00	0.61
1:A:185:VAL:HB	1:A:235:VAL:HG11	1.83	0.61
2:C:349:ALA:HB2	3:C:273:M1N:H252	1.81	0.61
1:I:20:ALA:O	1:I:24:ILE:HG12	2.01	0.61
2:C:424:ASP:OD1	3:J:273:M1N:H40	2.00	0.61
1:Q:56:LEU:HD13	1:Q:99:LEU:HD22	1.81	0.61
2:H:324:ASN:HD22	2:H:324:ASN:N	1.95	0.61
2:C:321:THR:O	3:C:273:M1N:H51	2.01	0.61
1:D:83:ASP:OD2	2:E:365:HIS:CD2	2.53	0.61
1:F:92:ARG:HD2	1:F:129:HIS:CE1	2.36	0.61
2:X:307:LYS:HD2	2:X:418:GLY:O	2.01	0.61
2:2:441:SER:HB2	2:2:478:ASP:OD2	2.00	0.61
1:A:205:VAL:C	1:A:207:SER:H	2.08	0.61
1:D:92:ARG:HG3	1:D:129:HIS:CE1	2.35	0.61
2:J:306:LEU:HD23	2:J:436:TYR:HB3	1.83	0.61
2:X:462:SER:O	2:X:465:ARG:HG2	2.01	0.61
2:Z:349:ALA:CB	3:Z:273:M1N:H252	2.31	0.61
1:F:205:VAL:C	1:F:207:SER:H	2.09	0.61
3:J:273:M1N:HN1	3:J:273:M1N:C25	2.14	0.61
1:Y:25:ALA:O	1:Y:158:GLY:HA2	2.00	0.61
1:F:110:ILE:HG12	1:F:114:GLN:HG3	1.83	0.60
1:I:12:ALA:O	1:I:16:ARG:HG2	2.02	0.60
2:2:345:ILE:HD13	2:2:352:ALA:HB1	1.83	0.60
2:L:456:GLN:NE2	2:L:465:ARG:NH1	2.49	0.60
3:L:273:M1N:HN1	3:L:273:M1N:H252	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:395:MET:HA	2:C:395:MET:HE2	1.83	0.60
2:N:318:ARG:HD3	2:N:491:PHE:O	2.01	0.60
2:N:380:ILE:HD11	2:N:421:VAL:HG21	1.81	0.60
2:N:459:ASP:H	2:N:462:SER:HB3	1.65	0.60
2:R:518:ILE:O	2:R:522:SER:HB2	2.00	0.60
2:V:513:LEU:O	2:V:517:ILE:HG12	2.00	0.60
2:X:329:ARG:NH2	2:2:476:ASP:O	2.34	0.60
1:F:87:TYR:O	2:G:357:ARG:NH2	2.34	0.60
2:J:321:THR:O	3:J:273:M1N:C5	2.49	0.60
1:B:19:LEU:HD12	1:I:10:GLU:HA	1.83	0.60
1:D:161:GLU:H	1:D:161:GLU:CD	2.10	0.60
1:F:20:ALA:O	1:F:24:ILE:HG12	2.01	0.60
1:O:14:ARG:HH11	1:O:14:ARG:CB	2.14	0.60
2:2:419:ARG:HH11	2:2:419:ARG:HG3	1.66	0.60
2:E:318:ARG:HD3	2:E:491:PHE:O	2.01	0.60
2:T:395:MET:HE2	2:T:395:MET:HA	1.83	0.60
1:U:11:GLN:CG	1:U:14:ARG:HH12	2.11	0.60
2:E:314:MET:CE	2:E:334:VAL:HG13	2.31	0.60
2:E:391:LEU:O	2:E:395:MET:HG2	2.02	0.60
2:G:444:LEU:HD12	2:2:444:LEU:CD1	2.31	0.60
1:I:182:ARG:HD3	1:I:235:VAL:HB	1.83	0.60
1:K:25:ALA:O	1:K:158:GLY:HA2	2.02	0.60
2:N:301:THR:N	2:N:441:SER:HG	2.00	0.60
2:2:515:ARG:HA	2:2:518:ILE:HD12	1.84	0.60
1:D:110:ILE:HG23	1:D:114:GLN:HG3	1.81	0.60
1:Q:89:TYR:CD1	2:Z:382:ARG:HD3	2.37	0.60
2:T:473:ASP:HA	4:X:20:HOH:O	2.01	0.60
1:1:205:VAL:C	1:1:207:SER:H	2.10	0.60
3:H:273:M1N:H40	2:P:424:ASP:OD1	2.02	0.60
2:G:395:MET:HE2	2:G:395:MET:HA	1.84	0.60
1:S:25:ALA:O	1:S:158:GLY:HA2	2.02	0.60
2:J:321:THR:O	3:J:273:M1N:H37	2.02	0.59
1:O:25:ALA:O	1:O:158:GLY:HA2	2.02	0.59
1:O:217:ARG:NH2	1:O:223:ARG:HG3	2.15	0.59
1:W:205:VAL:C	1:W:207:SER:H	2.10	0.59
1:A:85:ARG:HH11	1:A:85:ARG:HG2	1.67	0.59
1:B:205:VAL:HG12	1:B:206:ALA:N	2.17	0.59
2:G:320:SER:HB2	2:G:331:VAL:HG21	1.84	0.59
3:L:273:M1N:C22	3:L:273:M1N:O16	2.50	0.59
1:S:85:ARG:HG2	1:S:85:ARG:NH1	2.18	0.59
1:U:55:GLU:OE2	1:U:220:ARG:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:345:ILE:HD13	2:H:352:ALA:HB1	1.85	0.59
2:T:518:ILE:O	2:T:522:SER:HB2	2.02	0.59
1:F:25:ALA:O	1:F:158:GLY:HA2	2.03	0.59
2:J:450:MET:HE3	2:J:470:ALA:CB	2.32	0.59
2:L:308:TYR:HB2	2:L:309:PRO:HD2	1.84	0.59
1:M:205:VAL:HG12	1:M:206:ALA:N	2.17	0.59
1:S:217:ARG:HH21	1:S:223:ARG:HG3	1.68	0.59
2:C:425:ALA:N	4:C:542:HOH:O	2.34	0.59
1:K:230:LEU:CD2	1:K:234:LEU:HD13	2.33	0.59
2:L:349:ALA:HB2	3:L:273:M1N:H252	1.85	0.59
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.84	0.59
1:Q:217:ARG:HH21	1:Q:223:ARG:HG3	1.68	0.59
1:U:25:ALA:O	1:U:158:GLY:HA2	2.02	0.59
2:V:437:GLN:OE1	2:V:447:LYS:HD3	2.03	0.59
1:D:172:ALA:HB3	1:D:175:ALA:HB2	1.85	0.59
1:O:205:VAL:HG12	1:O:206:ALA:H	1.66	0.59
1:S:20:ALA:O	1:S:24:ILE:HG12	2.02	0.59
2:V:318:ARG:HD3	2:V:491:PHE:O	2.03	0.59
1:Y:172:ALA:HB3	1:Y:175:ALA:HB2	1.85	0.59
1:D:205:VAL:C	1:D:207:SER:H	2.09	0.59
2:G:301:THR:N	2:G:441:SER:OG	2.36	0.59
2:L:337:THR:HG1	2:L:343:THR:HG22	1.66	0.59
2:2:349:ALA:HB2	3:2:273:M1N:H252	1.84	0.59
2:P:349:ALA:HB2	3:P:273:M1N:H252	1.83	0.59
1:B:25:ALA:O	1:B:158:GLY:HA2	2.02	0.58
2:X:430:ASN:ND2	4:X:16:HOH:O	2.31	0.58
2:X:450:MET:HE3	2:X:470:ALA:HB2	1.84	0.58
2:H:407:TYR:CE1	2:H:417:ALA:HB3	2.38	0.58
2:C:301:THR:N	2:C:441:SER:OG	2.36	0.58
1:S:19:LEU:HD12	1:1:10:GLU:HA	1.84	0.58
2:V:424:ASP:HB3	2:V:428:GLY:H	1.67	0.58
2:G:513:LEU:O	2:G:517:ILE:HG12	2.03	0.58
2:P:349:ALA:HA	3:P:273:M1N:H243	1.85	0.58
2:V:337:THR:OG1	2:V:343:THR:HG22	2.03	0.58
1:1:11:GLN:HG2	1:1:14:ARG:HH12	1.68	0.58
2:2:419:ARG:HH11	2:2:419:ARG:CG	2.16	0.58
2:E:518:ILE:O	2:E:522:SER:HB2	2.03	0.58
1:M:25:ALA:O	1:M:158:GLY:HA2	2.03	0.58
2:T:462:SER:O	2:T:465:ARG:HG2	2.03	0.58
1:W:98:GLN:O	1:W:102:VAL:HG23	2.03	0.58
2:L:321:THR:O	3:L:273:M1N:H37	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:314:MET:HE3	2:E:334:VAL:HG22	1.85	0.58
2:2:419:ARG:HG3	2:2:419:ARG:NH1	2.17	0.58
1:M:224:ARG:NH1	4:M:255:HOH:O	2.36	0.58
1:Q:25:ALA:O	1:Q:158:GLY:HA2	2.03	0.58
1:1:14:ARG:HH11	1:1:14:ARG:CB	2.16	0.58
2:G:345:ILE:HD12	2:G:345:ILE:O	2.03	0.58
2:T:451:LYS:HB3	4:T:12:HOH:O	2.03	0.58
2:H:349:ALA:H	3:H:273:M1N:C35	2.16	0.58
2:L:345:ILE:HD12	2:L:345:ILE:O	2.04	0.58
3:P:273:M1N:HN1	3:P:273:M1N:C25	2.16	0.58
1:U:96:GLY:HA2	1:U:99:LEU:HD13	1.85	0.58
1:B:205:VAL:C	1:B:207:SER:H	2.11	0.58
2:C:345:ILE:HD13	2:C:352:ALA:HB1	1.86	0.58
2:G:464:LEU:HD11	2:G:505:VAL:HG11	1.86	0.58
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.86	0.58
2:H:465:ARG:HG3	2:H:465:ARG:NH1	2.18	0.57
2:E:450:MET:HE3	2:E:470:ALA:CB	2.34	0.57
2:L:349:ALA:H	3:L:273:M1N:C36	2.17	0.57
2:N:321:THR:O	3:N:273:M1N:C5	2.52	0.57
2:Z:518:ILE:O	2:Z:522:SER:HB2	2.04	0.57
2:R:409:ILE:HG13	2:R:410:HIS:HD2	1.69	0.57
1:1:92:ARG:HD2	1:1:129:HIS:ND1	2.18	0.57
2:C:304:VAL:HG21	2:C:450:MET:CE	2.28	0.57
1:O:60:VAL:HG21	1:O:96:GLY:HA3	1.84	0.57
1:W:25:ALA:O	1:W:158:GLY:HA2	2.03	0.57
2:H:349:ALA:H	3:H:273:M1N:C36	2.17	0.57
1:M:87:TYR:O	2:N:357:ARG:NH2	2.37	0.57
1:U:30:VAL:HG13	1:U:43:ALA:HB2	1.86	0.57
1:W:30:VAL:HG13	1:W:43:ALA:HB2	1.85	0.57
2:C:513:LEU:O	2:C:517:ILE:HG12	2.04	0.57
1:F:19:LEU:HD12	1:W:10:GLU:HA	1.85	0.57
1:F:30:VAL:HG13	1:F:43:ALA:HB2	1.87	0.57
1:O:213:LEU:HA	1:O:221:ALA:O	2.05	0.57
1:Q:172:ALA:HB3	1:Q:175:ALA:HB2	1.86	0.57
2:2:391:LEU:O	2:2:395:MET:HG2	2.04	0.57
1:A:189:ARG:HH22	1:A:235:VAL:HG13	1.69	0.57
2:C:349:ALA:H	3:C:273:M1N:C35	2.17	0.57
2:G:465:ARG:HB2	2:G:513:LEU:HD21	1.85	0.57
2:V:349:ALA:H	3:V:273:M1N:C36	2.18	0.57
2:Z:395:MET:HE2	2:Z:395:MET:HA	1.86	0.57
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:383:LEU:HD21	2:G:402:PRO:CG	2.35	0.57
2:T:308:TYR:HB2	2:T:309:PRO:HD2	1.87	0.57
1:B:135:ARG:HH22	1:B:152:HIS:HD2	1.53	0.57
2:E:321:THR:O	3:E:273:M1N:C5	2.53	0.57
1:I:25:ALA:O	1:I:158:GLY:HA2	2.05	0.57
2:J:382:ARG:HD3	1:S:89:TYR:CD1	2.40	0.57
1:S:11:GLN:HG2	1:S:14:ARG:HH12	1.66	0.57
1:A:92:ARG:HD2	1:A:129:HIS:ND1	2.20	0.57
2:C:452:LYS:HE2	2:R:521:ARG:NH2	2.19	0.57
1:I:110:ILE:HG23	1:I:114:GLN:HG3	1.87	0.57
1:Q:151:PRO:HD2	4:Q:249:HOH:O	2.04	0.57
2:E:321:THR:O	3:E:273:M1N:H37	2.05	0.56
1:I:11:GLN:HG3	1:I:14:ARG:HH12	1.69	0.56
2:P:318:ARG:HD3	2:P:491:PHE:O	2.05	0.56
2:X:344:GLY:C	4:X:58:HOH:O	2.48	0.56
1:Y:40:LEU:HD12	1:Y:212:VAL:HG12	1.87	0.56
2:H:318:ARG:HD3	2:H:491:PHE:O	2.05	0.56
2:V:376:PHE:CE2	2:V:380:ILE:HD11	2.39	0.56
2:H:391:LEU:O	2:H:395:MET:HG2	2.05	0.56
1:F:110:ILE:HG23	1:F:114:GLN:HG3	1.87	0.56
1:I:73:ASN:HB2	1:S:105:GLN:HE22	1.70	0.56
2:J:383:LEU:HD21	2:J:402:PRO:HG2	1.86	0.56
1:K:19:LEU:HD12	1:M:10:GLU:HA	1.86	0.56
1:M:230:LEU:HD21	1:M:234:LEU:HD13	1.85	0.56
2:R:321:THR:O	3:R:273:M1N:C5	2.48	0.56
1:W:41:PHE:HB3	1:W:53:ILE:HD13	1.87	0.56
2:X:359:TYR:HA	2:X:386:MET:HE1	1.87	0.56
2:P:388:ARG:NH1	4:P:551:HOH:O	2.39	0.56
2:Z:317:ASP:OD1	2:Z:333:LYS:NZ	2.37	0.56
2:Z:335:TYR:HE1	2:Z:345:ILE:HD11	1.71	0.56
3:E:273:M1N:C22	3:E:273:M1N:O16	2.53	0.56
2:G:444:LEU:CD1	2:2:444:LEU:HD12	2.31	0.56
2:L:513:LEU:O	2:L:517:ILE:HG12	2.06	0.56
1:W:15:GLU:OE1	1:Y:9:PRO:HD2	2.06	0.56
1:1:182:ARG:HH11	1:1:182:ARG:HB2	1.69	0.56
1:A:25:ALA:O	1:A:158:GLY:HA2	2.04	0.56
2:H:395:MET:HA	2:H:395:MET:CE	2.31	0.56
2:H:518:ILE:O	2:H:522:SER:HB2	2.06	0.56
1:M:110:ILE:HG23	1:M:114:GLN:HG3	1.87	0.56
2:N:314:MET:HE3	2:N:334:VAL:CG1	2.31	0.56
2:N:349:ALA:H	3:N:273:M1N:C36	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:321:THR:O	3:V:273:M1N:C5	2.53	0.56
2:X:324:ASN:HD22	2:X:324:ASN:C	2.14	0.56
1:1:121:GLU:OE2	1:1:156:MET:HB3	2.06	0.56
2:2:329:ARG:O	2:2:490:ILE:HG21	2.06	0.56
2:H:461:ASP:OD1	2:H:509:ARG:HD2	2.06	0.56
2:G:306:LEU:HD11	2:G:450:MET:HE2	1.86	0.56
2:J:349:ALA:H	3:J:273:M1N:H35	1.70	0.56
2:N:465:ARG:HB2	2:N:513:LEU:CD2	2.35	0.56
1:Q:127:VAL:HG22	1:Q:215:ALA:HB2	1.87	0.56
1:Y:59:ARG:HG3	1:Y:129:HIS:HD2	1.71	0.56
1:Y:213:LEU:HA	1:Y:221:ALA:O	2.05	0.56
1:1:213:LEU:HA	1:1:221:ALA:O	2.06	0.56
2:2:341:THR:HG22	2:2:404:LEU:HD11	1.88	0.56
2:E:461:ASP:OD1	2:E:509:ARG:HD2	2.06	0.56
2:J:518:ILE:O	2:J:522:SER:HB2	2.06	0.56
1:K:205:VAL:HG12	1:K:206:ALA:N	2.21	0.56
2:N:518:ILE:O	2:N:522:SER:HB2	2.06	0.56
1:O:20:ALA:O	1:O:24:ILE:HG12	2.05	0.56
1:B:12:ALA:O	1:B:16:ARG:HG2	2.06	0.56
1:B:20:ALA:O	1:B:24:ILE:HG12	2.06	0.56
1:B:30:VAL:HG22	1:B:43:ALA:HB1	1.87	0.56
1:B:182:ARG:NH1	1:B:182:ARG:HB2	2.21	0.56
2:C:317:ASP:OD1	2:C:333:LYS:NZ	2.39	0.56
1:S:172:ALA:HB3	1:S:175:ALA:HB2	1.86	0.56
1:Y:94:VAL:HA	1:Y:98:GLN:HE22	1.71	0.56
2:G:452:LYS:HZ3	2:2:449:SER:HB2	1.71	0.56
1:M:83:ASP:OD2	2:N:365:HIS:HD2	1.89	0.56
2:N:318:ARG:O	2:N:331:VAL:HG23	2.06	0.56
2:T:345:ILE:HD12	2:T:345:ILE:O	2.06	0.56
2:T:513:LEU:O	2:T:517:ILE:HG12	2.06	0.56
1:W:155:VAL:HG12	1:W:160:THR:HG22	1.88	0.56
2:2:462:SER:O	2:2:465:ARG:HG2	2.06	0.56
2:J:444:LEU:CD1	2:Z:444:LEU:HD12	2.21	0.55
1:K:56:LEU:HD23	1:K:79:ILE:HG13	1.88	0.55
2:P:341:THR:HG22	2:P:404:LEU:HD11	1.88	0.55
2:T:514:ALA:O	2:T:518:ILE:HG13	2.06	0.55
1:Y:214:ASP:OD2	1:Y:217:ARG:HG2	2.05	0.55
2:E:513:LEU:O	2:E:517:ILE:HG12	2.06	0.55
2:L:321:THR:O	3:L:273:M1N:C5	2.54	0.55
1:M:20:ALA:O	1:M:24:ILE:HG12	2.05	0.55
1:B:98:GLN:O	1:B:102:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:337:THR:OG1	2:L:343:THR:CG2	2.51	0.55
1:D:87:TYR:O	2:E:357:ARG:NH2	2.39	0.55
2:G:307:LYS:NZ	2:G:433:GLU:HA	2.21	0.55
2:P:365:HIS:CE1	2:P:369:LEU:HD11	2.41	0.55
1:Q:171:TYR:CE2	1:Q:173:GLU:HA	2.40	0.55
2:T:321:THR:O	3:T:273:M1N:H52	2.05	0.55
1:U:134:LYS:HA	1:U:134:LYS:HE2	1.89	0.55
1:A:110:ILE:HG23	1:A:114:GLN:HG3	1.89	0.55
1:Q:127:VAL:CG2	1:Q:215:ALA:HB2	2.36	0.55
1:Y:128:ALA:HB2	1:Y:134:LYS:HB3	1.89	0.55
1:F:128:ALA:HB2	1:F:134:LYS:HB3	1.88	0.55
2:L:349:ALA:H	3:L:273:M1N:H35	1.71	0.55
1:O:123:CYS:CB	1:O:156:MET:HE1	2.37	0.55
1:S:161:GLU:O	1:S:165:ASN:HB2	2.06	0.55
2:J:324:ASN:HD22	2:J:324:ASN:N	1.91	0.55
1:K:115:ALA:HB3	1:M:112:THR:HG23	1.88	0.55
2:N:486:LEU:HD11	2:N:518:ILE:HD13	1.89	0.55
2:P:407:TYR:CE1	2:P:417:ALA:HB3	2.42	0.55
1:I:110:ILE:HA	1:I:114:GLN:HG2	1.88	0.55
2:2:341:THR:CG2	2:2:404:LEU:HD11	2.37	0.55
1:B:55:GLU:OE2	1:B:220:ARG:HD2	2.06	0.55
1:S:83:ASP:OD2	2:T:365:HIS:CD2	2.53	0.55
2:T:486:LEU:HD11	2:T:518:ILE:HD13	1.89	0.55
2:2:459:ASP:HB2	4:2:552:HOH:O	2.07	0.55
1:F:23:GLY:HA2	1:F:26:ARG:HE	1.72	0.55
2:G:349:ALA:N	3:G:273:M1N:H35	2.21	0.55
1:K:11:GLN:HG2	1:K:14:ARG:HH12	1.72	0.55
2:L:462:SER:O	2:L:465:ARG:HG2	2.07	0.55
1:O:182:ARG:HD3	1:O:235:VAL:HG23	1.89	0.55
1:U:172:ALA:HB3	1:U:175:ALA:HB2	1.87	0.55
1:I:205:VAL:HG12	1:I:206:ALA:N	2.21	0.55
1:O:92:ARG:HB2	1:O:92:ARG:HH11	1.72	0.54
2:V:392:ALA:O	2:V:395:MET:HB2	2.07	0.54
1:Y:170:SER:HB2	1:Y:183:ILE:HD12	1.89	0.54
2:Z:349:ALA:H	3:Z:273:M1N:C36	2.20	0.54
2:2:432:GLU:HG3	2:2:437:GLN:HB2	1.87	0.54
1:F:10:GLU:HA	1:M:19:LEU:HD12	1.88	0.54
2:G:332:ARG:HD3	4:G:223:HOH:O	2.08	0.54
1:Q:20:ALA:O	1:Q:24:ILE:HG12	2.07	0.54
2:R:355:PHE:CE1	2:R:386:MET:HG2	2.42	0.54
2:T:324:ASN:C	2:T:324:ASN:HD22	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:33:LEU:HD11	1:U:180:ALA:HB1	1.88	0.54
1:U:213:LEU:HA	1:U:221:ALA:O	2.07	0.54
1:W:205:VAL:HG12	1:W:206:ALA:N	2.22	0.54
1:Y:139:TYR:CD2	1:Y:149:ASP:HB3	2.42	0.54
2:H:308:TYR:HB2	2:H:309:PRO:HD2	1.90	0.54
1:K:16:ARG:HE	1:K:117:PRO:HD3	1.71	0.54
2:R:318:ARG:HB3	2:R:331:VAL:O	2.07	0.54
1:S:116:LYS:HB2	1:I:13:MET:HE3	1.89	0.54
2:Z:457:VAL:HG22	2:Z:463:GLY:HA2	1.88	0.54
1:F:182:ARG:NH1	1:F:182:ARG:HB2	2.23	0.54
2:J:308:TYR:HB2	2:J:309:PRO:HD2	1.90	0.54
1:K:110:ILE:HA	1:K:114:GLN:HG2	1.89	0.54
2:R:307:LYS:NZ	2:R:433:GLU:HA	2.23	0.54
2:V:301:THR:HG21	3:V:273:M1N:H16	1.72	0.54
2:H:307:LYS:HD2	2:H:418:GLY:O	2.06	0.54
3:E:273:M1N:C25	3:E:273:M1N:N1	2.71	0.54
1:O:9:PRO:HD3	4:O:249:HOH:O	2.07	0.54
1:Q:59:ARG:HG3	1:Q:129:HIS:CD2	2.30	0.54
1:U:161:GLU:O	1:U:165:ASN:HB2	2.07	0.54
2:2:337:THR:HG21	2:2:359:TYR:CD2	2.43	0.54
2:G:329:ARG:O	2:G:490:ILE:HG21	2.07	0.54
1:K:115:ALA:HB3	1:M:112:THR:CG2	2.38	0.54
2:V:303:ILE:HG21	4:V:553:HOH:O	2.08	0.54
2:X:459:ASP:H	2:X:462:SER:HB3	1.73	0.54
2:E:319:ARG:HG3	2:E:320:SER:N	2.22	0.54
2:E:437:GLN:OE1	2:E:447:LYS:HD3	2.08	0.54
2:Z:464:LEU:HD11	2:Z:505:VAL:HG11	1.89	0.54
2:J:514:ALA:O	2:J:518:ILE:HG13	2.07	0.54
2:H:301:THR:N	2:H:441:SER:OG	2.41	0.54
1:D:36:ALA:HA	4:D:250:HOH:O	2.07	0.54
1:M:30:VAL:HG22	1:M:43:ALA:HB1	1.89	0.54
2:R:306:LEU:HD12	2:R:467:ALA:HB2	1.89	0.54
1:U:185:VAL:HB	1:U:235:VAL:CG1	2.38	0.54
1:Y:209:GLU:OE2	1:Y:224:ARG:NH2	2.41	0.54
2:C:324:ASN:HD22	2:C:324:ASN:C	2.15	0.54
2:L:303:ILE:HD11	2:L:333:LYS:HB3	1.88	0.54
1:O:128:ALA:HB2	1:O:134:LYS:HB3	1.90	0.54
2:P:412:SER:O	2:P:414:PRO:HD3	2.08	0.54
2:Z:329:ARG:O	2:Z:490:ILE:HG21	2.07	0.54
1:F:185:VAL:HB	1:F:235:VAL:HG11	1.90	0.53
1:I:220:ARG:NH2	2:J:367:GLU:OE2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:432:GLU:HG3	2:N:437:GLN:HB2	1.90	0.53
2:R:341:THR:HG22	2:R:404:LEU:HD11	1.89	0.53
2:T:349:ALA:H	3:T:273:M1N:H35	1.72	0.53
2:T:377:ALA:HA	2:T:380:ILE:HD12	1.90	0.53
1:Y:176:SER:H	1:Y:179:ASP:HB2	1.71	0.53
1:F:68:PHE:HA	1:F:71:PHE:CE2	2.44	0.53
2:G:349:ALA:HB2	3:G:273:M1N:H252	1.90	0.53
2:G:521:ARG:HH22	2:2:452:LYS:NZ	2.06	0.53
2:L:445:PHE:CE1	2:P:444:LEU:HD11	2.43	0.53
1:Q:92:ARG:HG3	1:Q:129:HIS:HE1	1.71	0.53
2:R:464:LEU:HD11	2:R:505:VAL:HG11	1.89	0.53
2:N:335:TYR:HE1	2:N:345:ILE:HD11	1.72	0.53
2:R:345:ILE:HD13	2:R:352:ALA:HB1	1.89	0.53
2:R:475:ALA:HB2	2:R:481:THR:HG22	1.89	0.53
1:S:14:ARG:HB2	1:S:14:ARG:HH11	1.71	0.53
1:S:213:LEU:HA	1:S:221:ALA:O	2.08	0.53
1:U:14:ARG:HB3	1:U:14:ARG:CZ	2.38	0.53
2:V:432:GLU:HG3	2:V:437:GLN:HB2	1.90	0.53
2:G:424:ASP:OD2	3:X:273:M1N:H34	2.07	0.53
1:W:55:GLU:OE2	1:W:220:ARG:HD2	2.08	0.53
2:C:462:SER:O	2:C:465:ARG:HG2	2.08	0.53
1:I:60:VAL:HG21	1:I:96:GLY:CA	2.37	0.53
1:M:213:LEU:HA	1:M:221:ALA:O	2.09	0.53
1:W:85:ARG:HH11	1:W:85:ARG:CG	2.20	0.53
1:Y:16:ARG:HE	1:Y:117:PRO:HD3	1.74	0.53
2:C:437:GLN:OE1	2:C:447:LYS:HD3	2.08	0.53
1:D:135:ARG:HD3	1:D:136:PRO:HD2	1.91	0.53
2:E:380:ILE:HD11	2:E:421:VAL:HG21	1.89	0.53
1:F:185:VAL:HB	1:F:235:VAL:CG1	2.38	0.53
1:F:226:THR:O	1:F:230:LEU:HB2	2.08	0.53
2:G:465:ARG:HG3	2:G:466:VAL:N	2.24	0.53
1:K:182:ARG:HB2	1:K:182:ARG:NH1	2.23	0.53
2:P:457:VAL:HG22	2:P:463:GLY:HA2	1.91	0.53
2:T:457:VAL:HG22	2:T:463:GLY:HA2	1.91	0.53
2:2:345:ILE:HB	2:2:352:ALA:HB1	1.91	0.53
1:A:55:GLU:OE2	1:A:220:ARG:HD2	2.08	0.53
2:P:391:LEU:O	2:P:395:MET:HG2	2.09	0.53
2:X:457:VAL:HG22	2:X:463:GLY:HA2	1.90	0.53
2:X:464:LEU:HD11	2:X:505:VAL:HG21	1.90	0.53
1:Y:28:LYS:HE3	1:Y:44:GLU:HG3	1.90	0.53
1:A:176:SER:HB3	1:A:179:ASP:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:457:VAL:HG22	2:H:463:GLY:HA2	1.91	0.53
2:C:457:VAL:HG22	2:C:463:GLY:HA2	1.90	0.53
1:D:89:TYR:CE1	2:R:382:ARG:HD3	2.44	0.53
1:D:219:ARG:HG2	1:D:219:ARG:HH11	1.73	0.53
2:G:451:LYS:NZ	2:2:473:ASP:OD1	2.38	0.53
1:O:13:MET:HG3	1:U:19:LEU:HD11	1.90	0.53
2:P:383:LEU:HD21	2:P:402:PRO:CG	2.38	0.53
1:Y:41:PHE:HE2	1:Y:213:LEU:HD13	1.73	0.53
1:B:54:SER:CB	1:B:75:ARG:HD2	2.39	0.53
1:I:19:LEU:HD12	1:S:10:GLU:HA	1.90	0.53
2:P:349:ALA:H	3:P:273:M1N:C36	2.21	0.53
1:Q:142:THR:OG1	1:Q:146:SER:HB2	2.09	0.53
2:X:321:THR:O	3:X:273:M1N:C5	2.53	0.53
1:1:72:ASP:O	1:1:76:ARG:HG3	2.09	0.53
1:1:140:ARG:HB3	1:1:140:ARG:NH1	2.24	0.53
2:L:312:VAL:HG23	2:L:497:ILE:HD12	1.90	0.53
2:L:382:ARG:HD3	1:M:89:TYR:CD1	2.44	0.53
2:V:349:ALA:N	3:V:273:M1N:C35	2.54	0.53
1:B:185:VAL:HB	1:B:235:VAL:CG1	2.39	0.52
1:M:12:ALA:O	1:M:16:ARG:HG2	2.09	0.52
3:P:273:M1N:H221	3:P:273:M1N:O16	2.10	0.52
2:R:345:ILE:HD12	2:R:345:ILE:O	2.09	0.52
1:W:16:ARG:HE	1:W:117:PRO:HD3	1.73	0.52
2:X:457:VAL:HB	4:X:115:HOH:O	2.09	0.52
2:N:513:LEU:O	2:N:517:ILE:HG12	2.08	0.52
2:P:337:THR:HG21	2:P:359:TYR:CD2	2.44	0.52
2:X:349:ALA:H	3:X:273:M1N:C35	2.23	0.52
2:L:321:THR:O	3:L:273:M1N:H52	2.09	0.52
2:N:317:ASP:OD1	2:N:333:LYS:NZ	2.42	0.52
2:N:395:MET:HE2	2:N:395:MET:CA	2.39	0.52
1:O:203:LEU:HG	1:O:237:GLN:HE22	1.74	0.52
1:U:20:ALA:O	1:U:24:ILE:HG12	2.09	0.52
1:D:176:SER:H	1:D:179:ASP:HB2	1.74	0.52
2:J:301:THR:HG22	2:J:302:THR:N	2.25	0.52
2:J:338:ASP:OD1	2:J:341:THR:OG1	2.14	0.52
2:Z:321:THR:O	3:Z:273:M1N:H51	2.08	0.52
2:2:314:MET:HE2	2:2:342:ALA:HB1	1.92	0.52
1:A:12:ALA:O	1:A:16:ARG:HG2	2.09	0.52
2:C:314:MET:HE3	2:C:334:VAL:HG13	1.90	0.52
1:K:92:ARG:HH11	1:K:92:ARG:HB2	1.73	0.52
1:K:176:SER:HB3	1:K:179:ASP:OD1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:349:ALA:N	3:L:273:M1N:C35	2.69	0.52
1:M:33:LEU:HD11	1:M:40:LEU:HD23	1.90	0.52
2:P:349:ALA:H	3:P:273:M1N:C35	2.22	0.52
1:Q:213:LEU:HA	1:Q:221:ALA:O	2.09	0.52
2:T:349:ALA:N	3:T:273:M1N:H35	2.25	0.52
2:V:465:ARG:HB2	2:V:513:LEU:HD21	1.91	0.52
1:Y:185:VAL:HB	1:Y:235:VAL:CG1	2.40	0.52
1:F:127:VAL:HG11	1:F:213:LEU:HB3	1.92	0.52
2:G:424:ASP:CG	3:X:273:M1N:H40	2.34	0.52
1:I:178:THR:HB	1:I:233:LEU:HD23	1.91	0.52
2:X:490:ILE:HA	4:X:74:HOH:O	2.10	0.52
1:A:54:SER:CB	1:A:75:ARG:HD2	2.40	0.52
1:A:64:ALA:CB	1:A:122:LEU:HD12	2.40	0.52
1:M:118:TYR:HB3	1:M:120:VAL:HG22	1.92	0.52
2:N:395:MET:HA	2:N:395:MET:CE	2.34	0.52
2:P:424:ASP:HB3	2:P:428:GLY:N	2.24	0.52
2:T:303:ILE:HD11	2:T:333:LYS:HB3	1.90	0.52
1:U:176:SER:H	1:U:179:ASP:HB2	1.74	0.52
1:F:16:ARG:NH2	1:F:114:GLN:O	2.43	0.52
1:F:165:ASN:ND2	1:F:168:LYS:NZ	2.57	0.52
2:P:461:ASP:OD1	2:P:509:ARG:HD2	2.10	0.52
1:S:185:VAL:HB	1:S:235:VAL:CG1	2.40	0.52
1:D:185:VAL:HB	1:D:235:VAL:CG1	2.40	0.52
1:Q:205:VAL:HG12	1:Q:206:ALA:H	1.74	0.52
3:T:273:M1N:C25	3:T:273:M1N:HN1	2.23	0.52
1:F:48:ARG:NH2	1:W:135:ARG:HD2	2.25	0.52
1:M:123:CYS:HB3	1:M:156:MET:HE1	1.91	0.52
2:P:439:VAL:HG11	4:P:548:HOH:O	2.09	0.52
1:W:60:VAL:HG21	1:W:96:GLY:HA3	1.92	0.52
1:F:182:ARG:HB2	1:F:182:ARG:HH11	1.75	0.51
1:I:55:GLU:OE1	1:I:220:ARG:NH1	2.43	0.51
2:N:321:THR:HG22	4:N:543:HOH:O	2.09	0.51
2:P:327:SER:OG	3:P:273:M1N:H38	2.08	0.51
2:X:320:SER:HB3	2:X:328:GLY:HA3	1.92	0.51
1:I:55:GLU:OE2	1:I:220:ARG:HD2	2.10	0.51
1:A:90:ASP:HB3	1:A:93:ASP:OD1	2.10	0.51
1:F:213:LEU:HA	1:F:221:ALA:O	2.10	0.51
1:I:213:LEU:HA	1:I:221:ALA:O	2.10	0.51
1:K:181:LEU:HD23	1:K:233:LEU:HB3	1.92	0.51
1:W:87:TYR:HA	2:X:357:ARG:HH21	1.75	0.51
1:W:223:ARG:HA	4:W:253:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:382:ARG:NH1	2:C:385:ILE:HD13	2.26	0.51
2:N:509:ARG:HG3	4:N:541:HOH:O	2.10	0.51
1:W:213:LEU:HA	1:W:221:ALA:O	2.10	0.51
2:X:380:ILE:HD11	2:X:421:VAL:HG21	1.92	0.51
1:A:64:ALA:HB2	1:A:122:LEU:HD12	1.92	0.51
1:A:185:VAL:HB	1:A:235:VAL:CG1	2.40	0.51
1:K:176:SER:H	1:K:179:ASP:HB2	1.75	0.51
1:O:85:ARG:HH11	1:O:85:ARG:HG3	1.70	0.51
1:Q:63:ALA:O	1:Q:156:MET:HE1	2.10	0.51
2:C:432:GLU:HG3	2:C:437:GLN:HB2	1.92	0.51
1:D:96:GLY:HA2	1:D:99:LEU:HB2	1.92	0.51
1:M:181:LEU:HD23	1:M:233:LEU:HB3	1.90	0.51
1:W:92:ARG:HB2	1:W:92:ARG:HH11	1.75	0.51
1:I:209:GLU:OE2	1:I:224:ARG:NH2	2.43	0.51
2:J:345:ILE:HD12	2:J:345:ILE:O	2.09	0.51
1:M:203:LEU:HA	4:M:260:HOH:O	2.09	0.51
1:M:85:ARG:CG	1:M:85:ARG:NH1	2.59	0.51
1:Y:226:THR:HG23	1:Y:227:GLY:N	2.26	0.51
2:2:513:LEU:O	2:2:517:ILE:HG12	2.10	0.51
2:E:337:THR:HG21	2:E:359:TYR:CE2	2.46	0.51
2:L:329:ARG:O	2:L:490:ILE:HG21	2.11	0.51
2:N:450:MET:HE3	2:N:470:ALA:CB	2.40	0.51
2:V:345:ILE:HD13	2:V:352:ALA:HB1	1.91	0.51
1:I:132:GLU:HA	4:I:252:HOH:O	2.11	0.51
1:D:59:ARG:CG	1:D:129:HIS:HD2	2.11	0.51
2:G:382:ARG:NH1	2:G:385:ILE:HD13	2.26	0.51
1:K:213:LEU:HA	1:K:221:ALA:O	2.11	0.51
2:P:324:ASN:HD22	2:P:324:ASN:C	2.18	0.51
1:A:213:LEU:HA	1:A:221:ALA:O	2.11	0.51
2:C:424:ASP:HB3	2:C:428:GLY:N	2.26	0.51
2:N:345:ILE:HD13	2:N:352:ALA:HB1	1.93	0.51
2:R:322:GLN:O	2:R:322:GLN:HG2	2.11	0.51
1:I:64:ALA:HA	1:I:156:MET:HE3	1.92	0.51
2:E:382:ARG:HD3	1:K:89:TYR:CE1	2.46	0.50
1:I:59:ARG:HG3	1:I:129:HIS:CD2	2.47	0.50
2:L:407:TYR:CE1	2:L:417:ALA:HB3	2.46	0.50
2:R:337:THR:OG1	2:R:343:THR:HG22	2.12	0.50
1:S:182:ARG:HB2	1:S:182:ARG:NH1	2.26	0.50
2:T:306:LEU:HD23	2:T:436:TYR:HB3	1.92	0.50
1:B:213:LEU:HA	1:B:221:ALA:O	2.11	0.50
1:D:20:ALA:O	1:D:24:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:345:ILE:HD13	2:E:352:ALA:HB1	1.93	0.50
1:I:230:LEU:HD21	1:I:234:LEU:HD13	1.92	0.50
1:K:59:ARG:CZ	1:K:221:ALA:HB2	2.42	0.50
1:W:176:SER:H	1:W:179:ASP:HB2	1.76	0.50
1:D:15:GLU:OE1	1:K:9:PRO:HD2	2.11	0.50
1:O:112:THR:HG22	1:U:115:ALA:HB3	1.92	0.50
1:Q:30:VAL:HG22	1:Q:43:ALA:HB1	1.93	0.50
2:R:513:LEU:O	2:R:517:ILE:HG12	2.11	0.50
2:Z:319:ARG:HG3	2:Z:320:SER:N	2.27	0.50
2:C:314:MET:HE1	2:C:342:ALA:C	2.36	0.50
2:C:337:THR:OG1	2:C:343:THR:HG22	2.12	0.50
1:D:213:LEU:HA	1:D:221:ALA:O	2.12	0.50
1:K:123:CYS:HB3	1:K:156:MET:HE1	1.92	0.50
1:K:205:VAL:CG1	1:K:206:ALA:N	2.75	0.50
2:L:456:GLN:NE2	2:L:465:ARG:HH12	2.06	0.50
2:N:452:LYS:NZ	2:V:449:SER:HB2	2.25	0.50
2:Z:324:ASN:H	2:Z:324:ASN:ND2	2.08	0.50
1:K:24:ILE:HD11	1:K:120:VAL:C	2.37	0.50
1:M:142:THR:OG1	1:M:146:SER:HB2	2.12	0.50
2:N:341:THR:HG22	2:N:404:LEU:HD11	1.92	0.50
1:U:185:VAL:HB	1:U:235:VAL:HG11	1.92	0.50
2:V:349:ALA:HB2	3:V:273:M1N:H252	1.92	0.50
2:X:383:LEU:HD13	2:X:423:PHE:CE1	2.46	0.50
2:N:349:ALA:HB3	3:N:273:M1N:C34	2.42	0.50
1:Y:20:ALA:O	1:Y:24:ILE:HG12	2.11	0.50
1:D:127:VAL:HG12	1:D:213:LEU:HD23	1.94	0.50
1:F:115:ALA:HB3	1:W:112:THR:HG23	1.94	0.50
1:Y:185:VAL:HB	1:Y:235:VAL:HG11	1.94	0.50
2:Z:301:THR:HG21	3:Z:273:M1N:H16	1.73	0.50
2:G:465:ARG:HB2	2:G:513:LEU:CD2	2.42	0.50
2:L:324:ASN:ND2	2:L:324:ASN:H	2.09	0.50
2:N:382:ARG:CZ	2:N:385:ILE:HD12	2.42	0.50
1:Q:80:GLN:O	1:Q:84:THR:OG1	2.30	0.50
1:U:40:LEU:HA	1:U:212:VAL:HG12	1.94	0.50
1:W:214:ASP:OD2	1:W:217:ARG:HG2	2.11	0.50
2:H:513:LEU:O	2:H:517:ILE:HG12	2.11	0.50
2:C:318:ARG:HD3	2:C:491:PHE:O	2.12	0.50
2:C:448:SER:OG	2:R:448:SER:HB3	2.12	0.50
2:J:464:LEU:HD23	2:J:513:LEU:HD12	1.94	0.50
1:O:87:TYR:HA	2:P:357:ARG:HH21	1.77	0.50
2:P:383:LEU:HD21	2:P:402:PRO:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:462:SER:O	2:H:465:ARG:HG2	2.12	0.49
1:D:92:ARG:CD	1:D:129:HIS:CE1	2.92	0.49
1:I:225:ILE:HG22	1:I:230:LEU:HB2	1.93	0.49
2:J:457:VAL:HG22	2:J:463:GLY:HA2	1.94	0.49
1:K:80:GLN:O	1:K:84:THR:OG1	2.30	0.49
1:M:225:ILE:HG22	1:M:230:LEU:HB2	1.93	0.49
2:N:349:ALA:N	3:N:273:M1N:C35	2.57	0.49
4:W:254:HOH:O	2:X:354:GLU:HG3	2.12	0.49
2:C:452:LYS:HE2	2:R:521:ARG:HH22	1.78	0.49
2:N:465:ARG:HB2	2:N:513:LEU:HD22	1.94	0.49
1:O:85:ARG:HG2	1:O:85:ARG:NH1	2.16	0.49
1:S:60:VAL:HG21	1:S:96:GLY:HA3	1.94	0.49
2:T:432:GLU:HG3	2:T:437:GLN:HB2	1.95	0.49
1:U:155:VAL:HG12	1:U:160:THR:HG22	1.94	0.49
1:Y:155:VAL:HG12	1:Y:160:THR:HG22	1.94	0.49
2:Z:308:TYR:HB2	2:Z:309:PRO:HD2	1.94	0.49
2:2:437:GLN:OE1	2:2:447:LYS:HD3	2.12	0.49
2:E:301:THR:N	2:E:441:SER:OG	2.46	0.49
1:B:181:LEU:HD23	1:B:233:LEU:HB3	1.95	0.49
1:M:83:ASP:OD2	2:N:365:HIS:CD2	2.65	0.49
2:N:322:GLN:HG2	2:N:322:GLN:O	2.13	0.49
2:V:436:TYR:HB2	2:V:450:MET:SD	2.52	0.49
2:X:381:ASN:ND2	1:Y:88:ALA:O	2.45	0.49
1:B:14:ARG:HB3	1:B:14:ARG:HH11	1.77	0.49
1:F:55:GLU:OE2	1:F:220:ARG:HD2	2.12	0.49
1:I:30:VAL:HG22	1:I:43:ALA:HB1	1.94	0.49
1:M:189:ARG:NH2	1:M:235:VAL:HG13	2.26	0.49
2:N:349:ALA:HB3	3:N:273:M1N:C35	2.42	0.49
2:N:464:LEU:HD11	2:N:505:VAL:HG11	1.94	0.49
2:R:318:ARG:HD3	2:R:491:PHE:O	2.11	0.49
2:X:321:THR:O	3:X:273:M1N:H37	2.12	0.49
2:X:322:GLN:HE21	3:X:273:M1N:C38	2.26	0.49
2:X:358:LEU:HD23	4:X:141:HOH:O	2.12	0.49
1:A:172:ALA:HB3	1:A:175:ALA:HB2	1.95	0.49
2:H:382:ARG:HD3	1:B:89:TYR:CD1	2.48	0.49
1:F:176:SER:H	1:F:179:ASP:HB2	1.78	0.49
2:G:409:ILE:HG13	2:G:410:HIS:CD2	2.47	0.49
1:M:217:ARG:HH21	1:M:223:ARG:HG3	1.77	0.49
2:R:391:LEU:O	2:R:395:MET:HG2	2.11	0.49
2:Z:301:THR:N	2:Z:441:SER:OG	2.46	0.49
2:2:392:ALA:O	2:2:395:MET:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLN:HG2	1:A:14:ARG:HH12	1.77	0.49
2:C:301:THR:CG2	3:C:273:M1N:H16	2.22	0.49
2:E:450:MET:HE3	2:E:470:ALA:HB2	1.94	0.49
1:1:56:LEU:HB2	1:1:60:VAL:HG13	1.95	0.49
1:I:161:GLU:O	1:I:165:ASN:HB2	2.13	0.49
1:K:42:VAL:HG22	1:K:210:VAL:HG22	1.93	0.49
1:K:59:ARG:CG	1:K:129:HIS:HD2	2.25	0.49
1:K:226:THR:O	1:K:230:LEU:HB2	2.13	0.49
2:L:465:ARG:HB3	2:L:513:LEU:CD2	2.43	0.49
1:O:30:VAL:HG13	1:O:43:ALA:HB2	1.95	0.49
2:V:424:ASP:HB2	2:V:428:GLY:O	2.13	0.49
2:Z:301:THR:N	2:Z:441:SER:HG	2.10	0.49
1:U:76:ARG:HG2	2:V:369:LEU:HD22	1.95	0.49
1:Y:83:ASP:OD2	2:Z:365:HIS:HD2	1.96	0.49
1:1:83:ASP:OD2	2:2:365:HIS:HD2	1.95	0.49
1:1:182:ARG:HB2	1:1:182:ARG:NH1	2.28	0.49
2:2:304:VAL:HG23	2:2:438:ALA:HB2	1.95	0.49
2:G:357:ARG:O	2:G:361:VAL:HG23	2.12	0.49
1:K:85:ARG:CG	1:K:85:ARG:NH1	2.61	0.49
2:L:399:LEU:HD11	2:L:401:LEU:HD13	1.94	0.49
2:N:391:LEU:O	2:N:395:MET:HG2	2.13	0.49
1:S:56:LEU:HB2	1:S:60:VAL:HG13	1.93	0.49
2:T:304:VAL:HG22	2:T:450:MET:HE1	1.95	0.49
1:U:223:ARG:HH11	1:U:225:ILE:HD11	1.78	0.49
1:W:189:ARG:CZ	1:W:237:GLN:HB3	2.43	0.49
2:Z:321:THR:O	3:Z:273:M1N:C5	2.61	0.49
1:1:30:VAL:HG22	1:1:43:ALA:HB1	1.94	0.49
2:G:307:LYS:HE2	2:G:435:GLY:HA2	1.95	0.48
2:J:381:ASN:ND2	1:S:88:ALA:O	2.46	0.48
2:L:399:LEU:CD1	2:L:401:LEU:HD13	2.43	0.48
2:R:469:GLU:HG3	2:R:517:ILE:HD12	1.94	0.48
2:Z:337:THR:HG21	2:Z:359:TYR:CD2	2.47	0.48
1:1:85:ARG:HH11	1:1:85:ARG:HG2	1.76	0.48
2:H:364:GLU:HG2	2:H:368:LYS:HE2	1.95	0.48
2:E:465:ARG:HG3	2:E:465:ARG:NH1	2.25	0.48
1:I:115:ALA:HB3	1:S:112:THR:HG22	1.94	0.48
1:1:110:ILE:HG21	1:1:118:TYR:CD1	2.47	0.48
2:H:331:VAL:HG11	3:H:273:M1N:H251	1.93	0.48
2:C:450:MET:HE3	2:C:470:ALA:HB2	1.92	0.48
2:J:349:ALA:N	3:J:273:M1N:H35	2.28	0.48
2:N:338:ASP:C	2:N:338:ASP:OD1	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:424:ASP:HB3	2:P:428:GLY:H	1.76	0.48
2:H:450:MET:HE3	2:H:470:ALA:CB	2.43	0.48
1:B:185:VAL:HB	1:B:235:VAL:HG11	1.94	0.48
1:I:92:ARG:HB2	1:I:92:ARG:HH11	1.77	0.48
1:U:85:ARG:NH1	1:U:89:TYR:HE2	2.11	0.48
2:V:322:GLN:O	2:V:322:GLN:HG2	2.12	0.48
1:B:209:GLU:OE2	1:B:224:ARG:NH2	2.46	0.48
1:F:48:ARG:HH22	1:W:135:ARG:HD2	1.78	0.48
1:I:48:ARG:HH22	1:S:135:ARG:HB3	1.79	0.48
1:K:172:ALA:HB3	1:K:175:ALA:HB2	1.94	0.48
1:W:56:LEU:HB2	1:W:60:VAL:HG13	1.96	0.48
1:I:177:LEU:CB	4:I:251:HOH:O	2.60	0.48
2:E:304:VAL:HG23	2:E:438:ALA:HB2	1.95	0.48
2:E:337:THR:HG21	2:E:359:TYR:CD2	2.49	0.48
1:K:41:PHE:HE2	1:K:213:LEU:HD22	1.79	0.48
1:U:16:ARG:HE	1:U:117:PRO:HD3	1.78	0.48
1:U:137:GLU:OE2	1:I:48:ARG:HD2	2.14	0.48
2:X:348:THR:HG23	3:X:273:M1N:H35	1.95	0.48
2:X:364:GLU:HG2	2:X:368:LYS:HE2	1.94	0.48
2:2:321:THR:O	3:2:273:M1N:C5	2.56	0.48
1:A:182:ARG:HG3	1:A:235:VAL:CB	2.39	0.48
2:C:319:ARG:HG3	2:C:320:SER:N	2.29	0.48
2:G:321:THR:O	3:G:273:M1N:H52	2.11	0.48
3:P:273:M1N:O16	3:P:273:M1N:C22	2.61	0.48
1:S:56:LEU:HD23	1:S:79:ILE:HG13	1.96	0.48
1:A:89:TYR:CD1	2:P:382:ARG:HD3	2.48	0.48
2:E:337:THR:HB	2:E:341:THR:HB	1.95	0.48
1:I:64:ALA:HA	1:I:156:MET:HE1	1.96	0.48
1:I:42:VAL:HG22	1:I:210:VAL:HG22	1.95	0.48
2:C:365:HIS:CE1	2:C:369:LEU:HD11	2.49	0.48
2:J:349:ALA:H	3:J:273:M1N:C36	2.27	0.48
1:M:205:VAL:CG1	1:M:206:ALA:N	2.77	0.48
1:Q:127:VAL:HG11	1:Q:213:LEU:HB3	1.96	0.48
1:Q:176:SER:H	1:Q:179:ASP:HB2	1.77	0.48
2:R:341:THR:CG2	2:R:404:LEU:HD11	2.44	0.48
1:U:95:THR:C	1:U:97:ARG:H	2.22	0.48
1:I:118:TYR:HB3	1:I:120:VAL:HG22	1.94	0.48
1:I:214:ASP:OD2	1:I:217:ARG:HG2	2.13	0.48
2:L:301:THR:HG22	2:L:302:THR:N	2.29	0.48
1:M:58:ASP:OD1	1:M:219:ARG:NH1	2.47	0.48
1:U:80:GLN:O	1:U:84:THR:OG1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:308:TYR:HB2	2:X:309:PRO:HD2	1.96	0.48
2:2:457:VAL:HG22	2:2:463:GLY:HA2	1.94	0.48
2:E:496:ILE:HG13	2:E:505:VAL:CG2	2.44	0.47
1:F:110:ILE:HA	1:F:114:GLN:HG2	1.96	0.47
1:Q:112:THR:HG22	1:Y:115:ALA:HB3	1.96	0.47
1:1:189:ARG:NH2	1:1:237:GLN:HB3	2.29	0.47
1:D:185:VAL:HB	1:D:235:VAL:HG11	1.96	0.47
2:E:349:ALA:H	3:E:273:M1N:C35	2.27	0.47
1:O:170:SER:HB2	1:O:183:ILE:HD12	1.95	0.47
1:Q:155:VAL:HG12	1:Q:160:THR:HG22	1.95	0.47
1:S:12:ALA:O	1:S:16:ARG:HG2	2.13	0.47
1:S:176:SER:H	1:S:179:ASP:HB2	1.79	0.47
1:1:140:ARG:HB3	1:1:140:ARG:HH11	1.79	0.47
1:1:205:VAL:CG1	1:1:206:ALA:H	2.25	0.47
1:Q:68:PHE:HD1	1:Q:71:PHE:CZ	2.32	0.47
2:X:444:LEU:HD22	2:X:444:LEU:HA	1.72	0.47
1:Y:60:VAL:HG21	1:Y:96:GLY:HA3	1.95	0.47
2:2:349:ALA:H	3:2:273:M1N:C36	2.27	0.47
2:2:403:LEU:HB2	2:2:439:VAL:HG21	1.96	0.47
1:B:135:ARG:HH22	1:B:152:HIS:CD2	2.32	0.47
1:O:85:ARG:NH1	1:O:85:ARG:HG3	2.28	0.47
1:O:161:GLU:O	1:O:165:ASN:HB2	2.14	0.47
1:S:226:THR:HG23	1:S:227:GLY:N	2.29	0.47
2:H:514:ALA:O	2:H:518:ILE:HG13	2.14	0.47
2:C:424:ASP:HB3	2:C:428:GLY:H	1.80	0.47
2:J:324:ASN:ND2	2:J:324:ASN:N	2.58	0.47
2:X:308:TYR:CE2	2:X:460:GLY:HA2	2.48	0.47
2:X:452:LYS:HD3	4:X:4:HOH:O	2.14	0.47
1:A:11:GLN:HG2	1:A:14:ARG:NH1	2.28	0.47
2:G:324:ASN:C	2:G:324:ASN:HD22	2.21	0.47
1:I:176:SER:H	1:I:179:ASP:HB2	1.80	0.47
2:P:485:ASP:OD2	2:P:488:ARG:HB2	2.14	0.47
2:V:317:ASP:OD1	2:V:333:LYS:NZ	2.47	0.47
2:H:335:TYR:HE1	2:H:345:ILE:HD11	1.79	0.47
2:V:301:THR:CG2	3:V:273:M1N:O16	2.60	0.47
1:W:172:ALA:HB3	1:W:175:ALA:HB2	1.96	0.47
2:H:337:THR:HG22	2:H:363:LEU:HD12	1.96	0.47
1:F:105:GLN:NE2	1:M:73:ASN:HD22	2.13	0.47
1:F:171:TYR:CE2	1:F:173:GLU:HA	2.49	0.47
2:G:320:SER:HB3	2:G:328:GLY:HA3	1.97	0.47
1:I:142:THR:OG1	1:I:146:SER:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:68:PHE:HA	1:K:71:PHE:CE2	2.50	0.47
2:R:375:THR:O	2:R:379:LYS:HG3	2.15	0.47
2:V:321:THR:HG22	3:V:273:M1N:O3	2.14	0.47
1:W:118:TYR:HB3	1:W:120:VAL:HG22	1.96	0.47
1:Y:110:ILE:HG23	1:Y:114:GLN:HG3	1.97	0.47
1:1:97:ARG:HH11	1:1:97:ARG:HG3	1.80	0.47
2:2:335:TYR:HE1	2:2:345:ILE:HD11	1.80	0.47
2:H:382:ARG:NH1	2:H:385:ILE:HD13	2.30	0.47
2:L:349:ALA:HB3	3:L:273:M1N:C35	2.45	0.47
2:L:432:GLU:HG3	2:L:437:GLN:HB2	1.97	0.47
2:N:306:LEU:HD23	2:N:436:TYR:HB3	1.95	0.47
2:P:314:MET:HE3	2:P:334:VAL:CG1	2.40	0.47
2:R:321:THR:O	3:R:273:M1N:H37	2.15	0.47
1:S:176:SER:HB3	1:S:179:ASP:OD1	2.15	0.47
1:D:141:ILE:HG13	1:D:147:ILE:HG12	1.97	0.47
2:G:314:MET:HE1	2:G:342:ALA:C	2.40	0.47
2:L:337:THR:HG21	2:L:359:TYR:CE2	2.50	0.47
1:M:205:VAL:CG1	1:M:206:ALA:H	2.28	0.47
1:Q:55:GLU:OE2	1:Q:220:ARG:HD2	2.14	0.47
1:S:59:ARG:HG3	1:S:129:HIS:CD2	2.50	0.47
1:1:185:VAL:HB	1:1:235:VAL:CG1	2.45	0.47
2:2:318:ARG:HD3	2:2:491:PHE:O	2.15	0.47
2:2:349:ALA:CB	3:2:273:M1N:H252	2.45	0.47
2:C:337:THR:OG1	2:C:343:THR:CG2	2.63	0.46
1:D:56:LEU:HD13	1:D:99:LEU:CD2	2.43	0.46
1:D:95:THR:C	1:D:97:ARG:H	2.23	0.46
2:G:407:TYR:CE1	2:G:417:ALA:HB3	2.49	0.46
2:L:321:THR:O	3:L:273:M1N:H51	2.15	0.46
2:R:348:THR:HG23	3:R:273:M1N:H35	1.97	0.46
2:T:304:VAL:CG2	2:T:450:MET:HE1	2.45	0.46
1:W:19:LEU:HD12	1:Y:10:GLU:HA	1.97	0.46
1:W:72:ASP:O	1:W:76:ARG:HG3	2.15	0.46
2:H:329:ARG:O	2:H:490:ILE:HG21	2.15	0.46
2:J:301:THR:HG21	3:J:273:M1N:H16	1.79	0.46
1:K:59:ARG:HG3	1:K:129:HIS:CD2	2.43	0.46
2:N:452:LYS:HZ1	2:V:449:SER:HB2	1.80	0.46
1:Q:154:VAL:HG21	4:Q:253:HOH:O	2.14	0.46
1:S:16:ARG:HE	1:S:117:PRO:HD3	1.80	0.46
1:1:231:GLN:HA	1:1:231:GLN:HE21	1.80	0.46
2:2:436:TYR:HB2	2:2:450:MET:SD	2.55	0.46
2:H:432:GLU:HG3	2:H:437:GLN:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:436:TYR:OH	2:L:451:LYS:HG3	2.15	0.46
1:M:205:VAL:HG12	1:M:206:ALA:H	1.79	0.46
2:C:318:ARG:HB3	2:C:331:VAL:O	2.15	0.46
2:C:320:SER:HB3	2:C:328:GLY:HA3	1.98	0.46
1:F:28:LYS:HE3	1:F:44:GLU:HG3	1.97	0.46
1:M:127:VAL:CG2	1:M:215:ALA:HB2	2.46	0.46
2:N:318:ARG:HE	2:N:318:ARG:HB3	1.53	0.46
2:N:392:ALA:O	2:N:395:MET:HB2	2.14	0.46
1:Q:33:LEU:HD11	1:Q:180:ALA:HB1	1.97	0.46
1:S:92:ARG:HD2	1:S:129:HIS:HE1	1.70	0.46
2:Z:349:ALA:H	3:Z:273:M1N:H35	1.79	0.46
3:P:273:M1N:C25	3:P:273:M1N:N1	2.78	0.46
2:X:464:LEU:HD11	2:X:505:VAL:HG11	1.98	0.46
2:Z:450:MET:HE3	2:Z:470:ALA:CB	2.46	0.46
1:A:137:GLU:HG2	1:A:139:TYR:CE2	2.51	0.46
1:D:63:ALA:O	1:D:156:MET:HE1	2.15	0.46
1:K:114:GLN:OE1	1:K:114:GLN:HA	2.16	0.46
2:L:441:SER:HB2	2:L:478:ASP:OD2	2.15	0.46
1:O:172:ALA:HB3	1:O:175:ALA:HB2	1.98	0.46
1:O:205:VAL:C	1:O:207:SER:N	2.73	0.46
2:R:515:ARG:NH1	4:R:263:HOH:O	2.45	0.46
1:S:30:VAL:HG13	1:S:43:ALA:HB2	1.96	0.46
2:2:303:ILE:HD11	2:2:333:LYS:HB3	1.97	0.46
2:2:321:THR:O	3:2:273:M1N:H37	2.16	0.46
1:A:42:VAL:HG22	1:A:210:VAL:HG22	1.98	0.46
1:F:41:PHE:HB3	1:F:53:ILE:HD13	1.97	0.46
1:S:73:ASN:HD22	1:1:105:GLN:NE2	2.13	0.46
1:W:95:THR:C	1:W:97:ARG:H	2.24	0.46
2:X:301:THR:HG21	3:X:273:M1N:O16	2.15	0.46
2:X:375:THR:HB	2:X:378:GLY:H	1.81	0.46
2:Z:395:MET:HA	2:Z:395:MET:CE	2.45	0.46
2:H:392:ALA:O	2:H:395:MET:HB2	2.16	0.46
1:B:110:ILE:HA	1:B:114:GLN:HG2	1.98	0.46
2:C:307:LYS:HD2	2:C:418:GLY:O	2.15	0.46
2:C:349:ALA:H	3:C:273:M1N:C36	2.29	0.46
2:C:452:LYS:HA	2:C:452:LYS:HD3	1.76	0.46
1:D:217:ARG:HH21	1:D:223:ARG:HG3	1.80	0.46
2:J:301:THR:CG2	2:J:302:THR:N	2.79	0.46
1:M:28:LYS:HB2	1:M:52:LYS:NZ	2.30	0.46
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.51	0.46
1:U:118:TYR:HB3	1:U:120:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:VAL:HG22	1:A:43:ALA:HB1	1.97	0.46
1:B:68:PHE:HA	1:B:71:PHE:CE2	2.51	0.46
2:C:412:SER:O	2:C:414:PRO:HD3	2.15	0.46
1:F:56:LEU:HD23	1:F:79:ILE:HG13	1.98	0.46
2:G:388:ARG:HE	2:G:388:ARG:HB2	1.54	0.46
2:X:409:ILE:HG13	2:X:410:HIS:CD2	2.50	0.46
1:Y:139:TYR:CE2	1:Y:149:ASP:HB3	2.51	0.46
1:Y:182:ARG:NH1	1:Y:182:ARG:HB2	2.30	0.46
2:H:301:THR:N	2:H:441:SER:HG	2.14	0.46
1:F:60:VAL:HG21	1:F:96:GLY:HA3	1.98	0.46
2:G:424:ASP:HB3	2:G:428:GLY:H	1.80	0.46
1:I:55:GLU:OE2	1:I:220:ARG:HD2	2.16	0.46
1:K:64:ALA:HA	1:K:156:MET:HE3	1.98	0.46
2:L:319:ARG:HG3	2:L:320:SER:N	2.31	0.46
2:V:345:ILE:HB	2:V:352:ALA:HB1	1.97	0.46
2:V:349:ALA:HB3	3:V:273:M1N:C34	2.46	0.46
1:I:96:GLY:HA2	1:I:99:LEU:HB2	1.97	0.46
2:2:314:MET:CE	2:2:334:VAL:HG13	2.36	0.46
1:B:226:THR:OG1	1:B:227:GLY:N	2.49	0.45
1:I:56:LEU:HB2	1:I:60:VAL:HG13	1.97	0.45
2:P:437:GLN:OE1	2:P:447:LYS:HD3	2.17	0.45
1:S:110:ILE:HA	1:S:114:GLN:HG3	1.97	0.45
2:T:349:ALA:HB2	3:T:273:M1N:H252	1.98	0.45
3:T:273:M1N:H36	3:T:273:M1N:H4	1.86	0.45
1:W:217:ARG:HH21	1:W:223:ARG:HG3	1.81	0.45
2:Z:365:HIS:CE1	2:Z:369:LEU:HD11	2.50	0.45
1:A:49:SER:HB2	1:B:97:ARG:HH11	1.82	0.45
2:H:307:LYS:NZ	2:H:433:GLU:HA	2.31	0.45
1:F:115:ALA:HB3	1:W:112:THR:CG2	2.46	0.45
2:G:437:GLN:OE1	2:G:437:GLN:CA	2.63	0.45
1:I:85:ARG:HG2	4:I:250:HOH:O	2.15	0.45
2:J:397:GLY:HA2	4:J:541:HOH:O	2.16	0.45
1:O:16:ARG:NH2	1:O:114:GLN:O	2.48	0.45
2:P:345:ILE:HD12	2:P:345:ILE:O	2.16	0.45
2:X:485:ASP:OD2	2:X:488:ARG:CB	2.59	0.45
1:A:226:THR:O	1:A:230:LEU:HB2	2.16	0.45
1:K:55:GLU:OE2	1:K:220:ARG:HD2	2.15	0.45
1:O:137:GLU:OE2	1:U:48:ARG:HD2	2.15	0.45
1:S:87:TYR:O	2:T:357:ARG:NH2	2.49	0.45
1:S:135:ARG:HA	1:S:136:PRO:HD2	1.87	0.45
3:T:273:M1N:C22	3:T:273:M1N:O16	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:214:ASP:OD2	1:U:217:ARG:HG2	2.17	0.45
1:D:230:LEU:HD21	1:D:234:LEU:HD13	1.97	0.45
2:E:347:GLY:H	3:E:273:M1N:H16	1.63	0.45
2:G:301:THR:N	2:G:441:SER:HG	2.14	0.45
2:G:521:ARG:NH2	2:2:452:LYS:NZ	2.65	0.45
1:K:11:GLN:CG	1:K:14:ARG:HH12	2.29	0.45
2:L:408:ASP:HA	4:L:548:HOH:O	2.17	0.45
2:N:349:ALA:CB	3:N:273:M1N:H252	2.45	0.45
1:O:59:ARG:CG	1:O:129:HIS:HD2	2.27	0.45
1:O:95:THR:C	1:O:97:ARG:H	2.24	0.45
1:U:182:ARG:NH1	1:U:182:ARG:HB2	2.32	0.45
2:V:344:GLY:C	4:V:553:HOH:O	2.59	0.45
1:A:48:ARG:HH22	1:B:135:ARG:HB3	1.80	0.45
2:G:309:PRO:HG3	2:G:458:THR:O	2.16	0.45
2:L:424:ASP:HB3	2:L:428:GLY:N	2.32	0.45
2:L:465:ARG:HB3	2:L:513:LEU:HD21	1.98	0.45
2:T:437:GLN:OE1	2:T:447:LYS:HD3	2.17	0.45
1:Y:30:VAL:HG22	1:Y:43:ALA:HB1	1.98	0.45
1:Y:185:VAL:HG12	1:Y:189:ARG:NH1	2.31	0.45
1:1:76:ARG:HA	1:1:79:ILE:HD12	1.98	0.45
2:2:424:ASP:HB3	2:2:428:GLY:N	2.31	0.45
1:B:56:LEU:HD23	1:B:79:ILE:HG13	1.98	0.45
1:B:56:LEU:HD13	1:B:99:LEU:HD22	1.98	0.45
1:B:95:THR:C	1:B:97:ARG:H	2.25	0.45
2:G:392:ALA:O	2:G:395:MET:HB2	2.17	0.45
1:I:185:VAL:HB	1:I:235:VAL:CG1	2.46	0.45
2:N:324:ASN:N	2:N:324:ASN:ND2	2.55	0.45
1:Q:128:ALA:HB2	1:Q:134:LYS:HB3	1.98	0.45
2:X:395:MET:HE2	2:X:395:MET:CA	2.36	0.45
1:Y:41:PHE:HZ	1:Y:125:ALA:HB3	1.82	0.45
2:2:424:ASP:HB2	4:2:545:HOH:O	2.16	0.45
1:A:182:ARG:HA	1:A:235:VAL:HB	1.99	0.45
1:D:135:ARG:HH22	1:D:152:HIS:HD2	1.63	0.45
1:I:58:ASP:OD1	1:I:219:ARG:NH1	2.50	0.45
2:R:388:ARG:C	2:R:390:ASN:H	2.24	0.45
1:A:95:THR:C	1:A:97:ARG:H	2.25	0.45
1:B:60:VAL:HG21	1:B:96:GLY:HA3	1.99	0.45
1:B:170:SER:HB2	1:B:183:ILE:HD12	1.99	0.45
2:E:349:ALA:HA	3:E:273:M1N:H243	1.99	0.45
2:L:301:THR:CG2	2:L:302:THR:N	2.79	0.45
1:M:161:GLU:CD	1:M:161:GLU:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:9:PRO:O	1:O:13:MET:HG2	2.17	0.45
1:S:123:CYS:HB2	1:S:156:MET:CE	2.47	0.45
2:T:383:LEU:O	2:T:383:LEU:HD23	2.17	0.45
2:T:444:LEU:HD12	2:X:444:LEU:CD1	2.47	0.45
2:H:496:ILE:HG12	2:H:505:VAL:CG2	2.47	0.45
1:D:118:TYR:HB3	1:D:120:VAL:HG22	1.98	0.45
2:E:432:GLU:HG3	2:E:437:GLN:HB2	1.97	0.45
1:I:83:ASP:OD2	2:J:365:HIS:CD2	2.60	0.45
2:J:307:LYS:HD2	2:J:418:GLY:O	2.17	0.45
2:L:465:ARG:CB	2:L:513:LEU:HD22	2.47	0.45
2:N:465:ARG:HB2	2:N:513:LEU:HD21	1.98	0.45
2:R:436:TYR:N	2:R:436:TYR:CD1	2.85	0.45
1:Y:12:ALA:HA	4:Y:251:HOH:O	2.16	0.45
3:L:273:M1N:O16	3:L:273:M1N:H221	2.16	0.45
2:P:407:TYR:CE2	2:P:499:ALA:HA	2.51	0.45
1:Q:209:GLU:OE2	1:Q:224:ARG:NH2	2.49	0.45
2:V:304:VAL:CG2	2:V:450:MET:HE1	2.47	0.45
1:W:41:PHE:HE2	1:W:213:LEU:HD13	1.81	0.45
2:2:322:GLN:O	2:2:322:GLN:HG2	2.16	0.45
2:H:388:ARG:C	2:H:390:ASN:H	2.25	0.44
1:B:98:GLN:O	1:B:101:ASN:HB2	2.17	0.44
2:G:376:PHE:CE2	2:G:380:ILE:HD11	2.52	0.44
2:P:321:THR:O	3:P:273:M1N:H51	2.18	0.44
1:S:115:ALA:HB3	1:1:112:THR:HG23	1.99	0.44
2:2:319:ARG:O	2:2:333:LYS:NZ	2.45	0.44
1:B:135:ARG:HA	1:B:136:PRO:HD2	1.90	0.44
1:F:137:GLU:HG2	1:F:139:TYR:CE1	2.51	0.44
1:K:95:THR:C	1:K:97:ARG:H	2.25	0.44
2:N:308:TYR:HB2	2:N:309:PRO:HD2	1.98	0.44
1:U:13:MET:HE3	1:1:116:LYS:HB2	1.99	0.44
1:U:230:LEU:HD21	1:U:234:LEU:HD13	1.98	0.44
2:V:461:ASP:OD1	2:V:509:ARG:NH1	2.50	0.44
2:Z:459:ASP:O	2:Z:462:SER:HB3	2.17	0.44
1:1:63:ALA:O	1:1:156:MET:HE1	2.18	0.44
2:H:436:TYR:HB2	2:H:450:MET:SD	2.57	0.44
1:D:16:ARG:HE	1:D:117:PRO:HD3	1.83	0.44
1:I:56:LEU:HD13	1:I:99:LEU:CD2	2.47	0.44
1:K:205:VAL:C	1:K:207:SER:N	2.75	0.44
2:L:349:ALA:HB3	3:L:273:M1N:C34	2.47	0.44
1:M:176:SER:H	1:M:179:ASP:HB2	1.82	0.44
2:P:384:ALA:HB2	2:P:423:PHE:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:110:ILE:HG23	1:U:114:GLN:HG3	1.98	0.44
2:X:306:LEU:HB2	2:X:313:VAL:CG1	2.47	0.44
1:Y:28:LYS:HE2	1:Y:46:PRO:HD3	1.98	0.44
2:Z:349:ALA:N	3:Z:273:M1N:H35	2.31	0.44
1:1:70:GLU:OE2	1:1:116:LYS:NZ	2.50	0.44
1:1:163:ILE:HG23	1:1:188:LEU:HA	1.98	0.44
2:H:318:ARG:HB3	2:H:331:VAL:O	2.17	0.44
2:J:450:MET:HE3	2:J:470:ALA:HB2	1.98	0.44
2:L:341:THR:HG22	2:L:404:LEU:HD11	1.99	0.44
1:S:123:CYS:HB2	1:S:156:MET:HE1	1.98	0.44
1:W:70:GLU:OE1	1:W:118:TYR:HA	2.16	0.44
1:Y:139:TYR:HD2	1:Y:147:ILE:HD11	1.81	0.44
2:Z:391:LEU:O	2:Z:395:MET:HG2	2.18	0.44
2:2:464:LEU:HD11	2:2:505:VAL:HG11	1.99	0.44
1:D:12:ALA:O	1:D:16:ARG:HG2	2.17	0.44
2:J:301:THR:CG2	3:J:273:M1N:O16	2.62	0.44
2:P:472:TYR:HE2	4:P:553:HOH:O	2.00	0.44
1:S:189:ARG:CZ	1:S:237:GLN:HB3	2.47	0.44
1:S:209:GLU:OE2	1:S:224:ARG:NH2	2.49	0.44
1:U:123:CYS:HB2	1:U:156:MET:HE1	2.00	0.44
1:A:133:THR:O	1:A:134:LYS:HE2	2.17	0.44
2:C:321:THR:O	3:C:273:M1N:C5	2.66	0.44
1:M:54:SER:CB	1:M:75:ARG:HD2	2.47	0.44
1:W:64:ALA:HA	1:W:156:MET:HE3	2.00	0.44
1:Y:95:THR:C	1:Y:97:ARG:H	2.25	0.44
2:Z:304:VAL:CG2	2:Z:450:MET:SD	3.06	0.44
2:2:337:THR:OG1	2:2:343:THR:HG22	2.18	0.44
2:2:433:GLU:HB3	4:2:554:HOH:O	2.17	0.44
1:F:70:GLU:OE2	1:F:116:LYS:NZ	2.48	0.44
1:F:172:ALA:HB3	1:F:175:ALA:HB2	1.99	0.44
2:G:307:LYS:HZ1	2:G:433:GLU:HA	1.83	0.44
2:G:518:ILE:HG23	2:V:487:VAL:CG2	2.48	0.44
2:J:364:GLU:HG2	2:J:368:LYS:HE2	2.00	0.44
2:N:365:HIS:CE1	2:N:369:LEU:HD11	2.53	0.44
2:N:436:TYR:HB2	2:N:450:MET:SD	2.57	0.44
1:O:226:THR:O	1:O:230:LEU:HB2	2.18	0.44
2:T:366:TYR:CZ	2:T:370:GLU:HG3	2.52	0.44
1:W:127:VAL:HG13	1:W:127:VAL:O	2.16	0.44
2:H:395:MET:HE2	2:H:395:MET:CA	2.38	0.44
1:B:96:GLY:HA2	1:B:99:LEU:HB2	2.00	0.44
2:C:348:THR:HG23	3:C:273:M1N:H35	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:92:ARG:HD2	1:I:129:HIS:NE2	2.31	0.44
1:I:205:VAL:C	1:I:207:SER:N	2.73	0.44
1:K:140:ARG:HH11	1:K:154:VAL:HG22	1.83	0.44
1:U:137:GLU:HG2	1:U:139:TYR:CE1	2.53	0.44
2:V:308:TYR:HB2	2:V:309:PRO:HD2	1.99	0.44
1:W:110:ILE:HA	1:W:114:GLN:HG2	2.00	0.44
1:F:45:ASN:HA	1:F:46:PRO:HD2	1.91	0.44
1:F:179:ASP:O	1:F:183:ILE:HG12	2.18	0.44
1:O:127:VAL:CG2	1:O:215:ALA:HB2	2.48	0.44
2:P:345:ILE:HB	2:P:352:ALA:HB1	2.00	0.44
2:T:412:SER:O	2:T:414:PRO:HD3	2.18	0.44
1:U:56:LEU:HD13	1:U:99:LEU:HD22	1.99	0.44
1:W:30:VAL:HG22	1:W:43:ALA:HB1	1.99	0.44
2:Z:306:LEU:HB2	2:Z:313:VAL:HG12	2.00	0.44
1:A:98:GLN:O	1:A:102:VAL:HG23	2.18	0.43
1:B:141:ILE:HD12	1:B:141:ILE:N	2.33	0.43
2:J:349:ALA:N	3:J:273:M1N:C35	2.78	0.43
1:M:70:GLU:OE2	1:M:116:LYS:NZ	2.50	0.43
2:T:407:TYR:CE1	2:T:417:ALA:HB3	2.53	0.43
1:W:182:ARG:HA	1:W:235:VAL:HB	2.00	0.43
1:W:205:VAL:CG1	1:W:206:ALA:H	2.29	0.43
1:A:92:ARG:HB2	1:A:92:ARG:HH11	1.83	0.43
1:A:147:ILE:C	1:A:147:ILE:HD13	2.43	0.43
2:H:309:PRO:HG2	2:H:458:THR:O	2.17	0.43
1:D:96:GLY:O	1:D:124:VAL:HG11	2.18	0.43
1:F:110:ILE:HG12	1:F:114:GLN:CG	2.46	0.43
2:N:485:ASP:OD2	2:N:488:ARG:HB2	2.17	0.43
1:O:54:SER:CB	1:O:75:ARG:HD2	2.48	0.43
1:W:181:LEU:HD23	1:W:233:LEU:HB3	2.00	0.43
2:Z:337:THR:OG1	2:Z:343:THR:HG22	2.17	0.43
3:H:273:M1N:O16	3:H:273:M1N:C22	2.54	0.43
1:B:142:THR:OG1	1:B:144:ASP:OD1	2.28	0.43
1:D:161:GLU:CD	1:D:161:GLU:N	2.76	0.43
1:Q:67:LYS:HG2	1:Q:69:ASN:OD1	2.18	0.43
1:Y:59:ARG:HG3	1:Y:129:HIS:CD2	2.52	0.43
1:Y:83:ASP:CG	2:Z:365:HIS:HD2	2.27	0.43
2:Z:488:ARG:HB3	2:Z:490:ILE:HG12	2.00	0.43
1:I:189:ARG:CZ	1:I:237:GLN:HB3	2.47	0.43
2:2:349:ALA:H	3:2:273:M1N:C35	2.31	0.43
2:2:424:ASP:HB3	2:2:428:GLY:H	1.83	0.43
1:D:97:ARG:HB2	4:D:249:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:364:GLU:HG2	2:E:368:LYS:HE2	2.00	0.43
2:E:439:VAL:O	2:E:439:VAL:HG23	2.18	0.43
1:F:57:TYR:O	1:F:58:ASP:C	2.61	0.43
1:K:24:ILE:HD11	1:K:120:VAL:CA	2.49	0.43
1:O:110:ILE:HA	1:O:114:GLN:HG2	2.00	0.43
2:T:515:ARG:HA	2:T:518:ILE:HD12	2.01	0.43
1:W:48:ARG:HH22	1:Y:135:ARG:HD2	1.81	0.43
1:W:139:TYR:CD2	1:W:149:ASP:HB3	2.53	0.43
1:Y:205:VAL:HG12	1:Y:206:ALA:H	1.83	0.43
1:A:73:ASN:HD22	1:B:105:GLN:NE2	2.16	0.43
1:A:92:ARG:HD2	1:A:129:HIS:CE1	2.53	0.43
2:C:465:ARG:HH11	2:C:465:ARG:CB	2.31	0.43
2:E:314:MET:HE1	2:E:343:THR:C	2.43	0.43
2:E:456:GLN:HE22	2:E:465:ARG:NH1	2.16	0.43
2:J:513:LEU:O	2:J:517:ILE:HG12	2.18	0.43
1:K:38:GLY:HA2	1:K:127:VAL:HG21	1.99	0.43
1:M:189:ARG:CZ	1:M:237:GLN:HB3	2.48	0.43
1:Q:95:THR:C	1:Q:97:ARG:H	2.26	0.43
1:Q:182:ARG:HA	1:Q:235:VAL:HB	2.00	0.43
1:A:225:ILE:HG22	1:A:230:LEU:HB2	1.99	0.43
2:E:403:LEU:HG	2:E:439:VAL:HG13	2.01	0.43
3:J:273:M1N:H252	3:J:273:M1N:HN1	1.83	0.43
1:M:30:VAL:HG22	1:M:43:ALA:CB	2.49	0.43
2:R:386:MET:HE3	2:R:386:MET:HB2	1.88	0.43
1:Y:91:ARG:HE	1:Y:91:ARG:HB3	1.68	0.43
2:Z:391:LEU:CD2	2:Z:395:MET:HE3	2.49	0.43
2:G:365:HIS:CE1	2:G:369:LEU:HD11	2.53	0.43
2:G:432:GLU:HG3	2:G:437:GLN:HB2	2.00	0.43
2:L:464:LEU:O	2:L:464:LEU:HD23	2.19	0.43
3:N:273:M1N:H36	3:N:273:M1N:H4	1.89	0.43
2:P:321:THR:O	3:P:273:M1N:C5	2.67	0.43
1:Q:30:VAL:HG22	1:Q:43:ALA:CB	2.48	0.43
2:R:464:LEU:HD12	2:R:496:ILE:HD11	1.99	0.43
2:V:337:THR:OG1	2:V:343:THR:CG2	2.65	0.43
2:Z:432:GLU:HG3	2:Z:437:GLN:HB2	2.00	0.43
2:2:347:GLY:C	3:2:273:M1N:H142	2.44	0.43
2:2:401:LEU:HA	2:2:402:PRO:HD3	1.88	0.43
1:B:30:VAL:HG22	1:B:43:ALA:CB	2.47	0.43
2:E:349:ALA:HB2	3:E:273:M1N:H252	2.00	0.43
1:K:94:VAL:HA	1:K:98:GLN:HE22	1.84	0.43
1:M:135:ARG:HA	1:M:136:PRO:HD2	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:386:MET:HE3	2:N:386:MET:HB2	1.87	0.43
1:Q:205:VAL:C	1:Q:207:SER:N	2.76	0.43
1:U:30:VAL:HG22	1:U:43:ALA:HB1	2.00	0.43
1:B:58:ASP:OD1	1:B:219:ARG:NH1	2.52	0.43
1:B:92:ARG:HH11	1:B:92:ARG:HB2	1.84	0.43
1:K:12:ALA:O	1:K:16:ARG:HG2	2.18	0.43
2:L:485:ASP:CG	2:L:488:ARG:HB2	2.43	0.43
1:M:56:LEU:HD23	1:M:79:ILE:HG13	2.01	0.43
1:O:205:VAL:O	1:O:207:SER:N	2.51	0.43
1:S:28:LYS:HB2	1:S:52:LYS:NZ	2.33	0.43
1:S:182:ARG:HB2	1:S:182:ARG:HH11	1.84	0.43
2:X:302:THR:O	2:X:303:ILE:HD13	2.18	0.43
2:Z:304:VAL:HG21	2:Z:450:MET:HE1	2.00	0.43
2:2:307:LYS:HD2	2:2:418:GLY:O	2.18	0.43
2:2:449:SER:OG	2:2:450:MET:N	2.52	0.43
1:A:171:TYR:CE2	1:A:173:GLU:HA	2.54	0.43
2:H:306:LEU:CD2	2:H:454:TYR:HE1	2.31	0.43
2:H:359:TYR:HA	2:H:386:MET:HE1	2.01	0.43
2:H:437:GLN:OE1	2:H:447:LYS:HD3	2.19	0.43
1:D:155:VAL:HG12	1:D:160:THR:HG22	2.01	0.43
1:M:172:ALA:HB3	1:M:175:ALA:HB2	2.01	0.43
2:P:496:ILE:HG13	2:P:505:VAL:HG22	2.01	0.43
1:U:85:ARG:NH1	1:U:89:TYR:CE2	2.87	0.43
2:H:465:ARG:HA	2:H:513:LEU:HD13	2.00	0.42
2:E:306:LEU:HB2	2:E:313:VAL:CG1	2.49	0.42
1:F:95:THR:C	1:F:97:ARG:H	2.26	0.42
2:J:337:THR:HG21	2:J:359:TYR:CE2	2.53	0.42
2:J:341:THR:CG2	2:J:404:LEU:HD11	2.45	0.42
1:M:16:ARG:HE	1:M:117:PRO:HD3	1.84	0.42
2:N:304:VAL:CG2	2:N:450:MET:CE	2.70	0.42
2:N:349:ALA:CB	3:N:273:M1N:C35	2.97	0.42
1:O:147:ILE:HD13	1:O:148:ALA:N	2.33	0.42
2:P:320:SER:HB3	2:P:328:GLY:HA3	2.00	0.42
1:U:85:ARG:HG2	1:U:85:ARG:HH11	1.84	0.42
1:1:176:SER:H	1:1:179:ASP:HB2	1.83	0.42
2:2:359:TYR:HA	2:2:386:MET:HE1	2.00	0.42
1:A:176:SER:H	1:A:179:ASP:HB2	1.83	0.42
1:K:16:ARG:NH2	1:K:114:GLN:O	2.52	0.42
2:R:337:THR:HG21	2:R:359:TYR:HD2	1.80	0.42
1:U:123:CYS:CB	1:U:156:MET:HE1	2.48	0.42
2:V:475:ALA:HB2	2:V:481:THR:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:388:ARG:C	2:X:390:ASN:H	2.26	0.42
2:Z:461:ASP:OD1	2:Z:509:ARG:HD2	2.19	0.42
2:2:513:LEU:O	2:2:516:ALA:HB3	2.19	0.42
1:A:183:ILE:HD13	1:A:183:ILE:HA	1.84	0.42
1:I:57:TYR:O	1:I:58:ASP:C	2.62	0.42
2:L:383:LEU:HD21	2:L:402:PRO:CG	2.50	0.42
2:L:432:GLU:O	2:L:433:GLU:C	2.63	0.42
2:N:418:GLY:C	2:N:419:ARG:HD2	2.45	0.42
1:O:89:TYR:CD1	2:V:382:ARG:HD3	2.54	0.42
2:P:496:ILE:HG13	2:P:505:VAL:CG2	2.49	0.42
1:S:214:ASP:OD2	1:S:217:ARG:HG2	2.20	0.42
2:T:382:ARG:HD3	1:I:89:TYR:CE1	2.53	0.42
2:V:324:ASN:C	2:V:324:ASN:HD22	2.28	0.42
2:X:335:TYR:HE1	2:X:345:ILE:HD11	1.83	0.42
2:X:424:ASP:OD2	3:Z:273:M1N:H34	2.19	0.42
2:Z:349:ALA:N	3:Z:273:M1N:C35	2.79	0.42
1:B:127:VAL:HG13	1:B:127:VAL:O	2.20	0.42
1:D:41:PHE:HE2	1:D:213:LEU:HD13	1.83	0.42
1:D:64:ALA:HA	1:D:156:MET:HE3	2.01	0.42
1:K:33:LEU:HD11	1:K:40:LEU:HD23	2.02	0.42
2:R:301:THR:N	2:R:441:SER:OG	2.51	0.42
1:U:181:LEU:O	1:U:185:VAL:HG23	2.20	0.42
1:W:71:PHE:CD1	1:W:71:PHE:C	2.98	0.42
2:X:401:LEU:HD12	2:X:401:LEU:HA	1.77	0.42
1:Y:139:TYR:CD2	1:Y:147:ILE:HD11	2.53	0.42
1:F:154:VAL:HG13	4:F:254:HOH:O	2.19	0.42
1:K:54:SER:OG	1:K:55:GLU:N	2.52	0.42
1:O:127:VAL:HG22	1:O:215:ALA:HB2	2.01	0.42
1:Q:54:SER:CB	1:Q:75:ARG:HD2	2.49	0.42
1:S:179:ASP:O	1:S:182:ARG:HB3	2.19	0.42
1:S:232:ALA:C	1:S:233:LEU:HD12	2.44	0.42
2:T:304:VAL:HG23	2:T:438:ALA:HB2	2.01	0.42
2:X:424:ASP:HB3	2:X:428:GLY:N	2.30	0.42
2:X:513:LEU:O	2:X:517:ILE:HG12	2.19	0.42
2:H:464:LEU:HD23	2:H:513:LEU:HD12	2.01	0.42
3:E:273:M1N:O16	3:E:273:M1N:H221	2.18	0.42
1:F:83:ASP:OD2	2:G:365:HIS:HD2	2.02	0.42
2:G:329:ARG:HE	2:G:329:ARG:HB3	1.64	0.42
3:G:273:M1N:HN1	3:G:273:M1N:C25	2.31	0.42
1:M:56:LEU:HG	1:M:62:PHE:HB2	2.02	0.42
2:N:306:LEU:CD2	2:N:436:TYR:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:19:LEU:HD23	1:U:19:LEU:C	2.44	0.42
2:X:392:ALA:O	2:X:395:MET:HB2	2.20	0.42
1:1:97:ARG:HG3	1:1:97:ARG:NH1	2.34	0.42
2:E:303:ILE:HB	2:E:439:VAL:HG22	2.01	0.42
1:K:118:TYR:HB3	1:K:120:VAL:HG22	2.01	0.42
2:N:407:TYR:CE2	2:N:499:ALA:HA	2.55	0.42
1:O:94:VAL:HA	1:O:98:GLN:NE2	2.28	0.42
1:Q:42:VAL:HG22	1:Q:210:VAL:HG22	2.01	0.42
2:R:306:LEU:HB2	2:R:313:VAL:HG13	2.02	0.42
2:R:372:VAL:HG12	2:R:373:PRO:O	2.19	0.42
1:W:59:ARG:HG3	1:W:129:HIS:CD2	2.54	0.42
2:X:452:LYS:CA	4:X:4:HOH:O	2.59	0.42
1:1:28:LYS:HE2	1:1:46:PRO:HD3	2.02	0.42
3:H:273:M1N:HN1	3:H:273:M1N:C25	2.32	0.42
2:C:444:LEU:HD22	2:C:444:LEU:HA	1.88	0.42
2:C:513:LEU:O	2:C:516:ALA:HB3	2.20	0.42
2:E:412:SER:O	2:E:414:PRO:HD3	2.19	0.42
2:G:521:ARG:HH22	2:2:452:LYS:HZ1	1.66	0.42
1:I:171:TYR:CE2	1:I:173:GLU:HA	2.54	0.42
1:K:54:SER:HB3	1:K:75:ARG:HD2	2.01	0.42
1:K:170:SER:HB2	1:K:183:ILE:HD12	2.01	0.42
1:O:87:TYR:O	2:P:357:ARG:NH2	2.52	0.42
1:Q:217:ARG:HA	1:Q:218:PRO:HD3	1.93	0.42
2:T:375:THR:HB	2:T:378:GLY:H	1.84	0.42
2:C:382:ARG:HA	2:C:382:ARG:HD2	1.78	0.42
2:C:436:TYR:OH	2:C:451:LYS:HG3	2.20	0.42
1:F:49:SER:HB2	1:W:97:ARG:HH11	1.85	0.42
1:I:41:PHE:HB3	1:I:53:ILE:HD13	2.01	0.42
2:J:318:ARG:HH11	2:J:490:ILE:HG22	1.85	0.42
1:S:17:SER:O	1:S:21:ARG:HB2	2.19	0.42
2:V:304:VAL:HG23	2:V:438:ALA:HB2	2.02	0.42
2:X:424:ASP:HB2	2:X:428:GLY:O	2.20	0.42
1:Y:78:GLY:HA3	1:Y:103:TYR:OH	2.20	0.42
1:1:177:LEU:HB2	4:1:251:HOH:O	2.18	0.42
2:H:321:THR:O	3:H:273:M1N:H51	2.20	0.42
1:D:57:TYR:O	1:D:58:ASP:C	2.63	0.42
1:K:63:ALA:O	1:K:156:MET:HE1	2.20	0.42
1:M:217:ARG:NH2	1:M:223:ARG:HG3	2.34	0.42
2:P:395:MET:HE2	2:P:395:MET:HA	2.01	0.42
1:U:68:PHE:HA	1:U:71:PHE:CE2	2.55	0.42
1:U:205:VAL:C	1:U:207:SER:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:TYR:O	2:C:357:ARG:NH2	2.53	0.41
2:E:436:TYR:HB2	2:E:450:MET:SD	2.60	0.41
1:F:181:LEU:HD23	1:F:233:LEU:HB3	2.01	0.41
1:F:182:ARG:HA	1:F:235:VAL:HB	2.01	0.41
1:F:231:GLN:CG	4:F:252:HOH:O	2.45	0.41
1:I:30:VAL:HG13	1:I:43:ALA:HB2	2.01	0.41
2:R:324:ASN:C	2:R:324:ASN:ND2	2.77	0.41
2:R:329:ARG:HE	2:R:329:ARG:HB3	1.65	0.41
1:S:11:GLN:HA	1:S:14:ARG:HH11	1.84	0.41
1:S:41:PHE:HB3	1:S:53:ILE:HD13	2.02	0.41
1:S:70:GLU:OE2	1:S:116:LYS:NZ	2.51	0.41
2:V:306:LEU:HB2	2:V:313:VAL:HG13	2.00	0.41
2:V:349:ALA:HB3	3:V:273:M1N:C35	2.49	0.41
1:W:110:ILE:HG21	1:W:118:TYR:CD1	2.54	0.41
1:I:95:THR:C	1:I:97:ARG:H	2.28	0.41
1:D:205:VAL:C	1:D:207:SER:N	2.77	0.41
1:F:10:GLU:OE2	1:M:22:LYS:HD2	2.19	0.41
1:F:140:ARG:NH1	1:F:150:GLU:OE2	2.52	0.41
1:K:28:LYS:HE2	1:K:46:PRO:HD3	2.01	0.41
1:U:91:ARG:HE	1:U:91:ARG:HB3	1.66	0.41
2:V:317:ASP:O	2:V:333:LYS:HD2	2.20	0.41
2:V:464:LEU:HD11	2:V:505:VAL:HG21	2.01	0.41
1:I:92:ARG:HB2	1:I:92:ARG:HH11	1.85	0.41
2:J:301:THR:N	2:J:441:SER:OG	2.53	0.41
1:K:30:VAL:HG13	1:K:43:ALA:HB2	2.02	0.41
1:M:57:TYR:O	1:M:58:ASP:C	2.63	0.41
1:S:76:ARG:HA	1:S:79:ILE:HD12	2.02	0.41
2:V:457:VAL:HG22	2:V:463:GLY:HA2	2.03	0.41
1:W:214:ASP:CG	1:W:223:ARG:NH2	2.78	0.41
2:X:349:ALA:H	3:X:273:M1N:C36	2.34	0.41
1:I:205:VAL:C	1:I:207:SER:N	2.77	0.41
1:A:41:PHE:HE2	1:A:213:LEU:HD13	1.85	0.41
2:C:345:ILE:HD12	2:C:345:ILE:O	2.20	0.41
2:E:345:ILE:HD12	2:E:345:ILE:O	2.20	0.41
1:F:112:THR:HG22	1:M:115:ALA:HB3	2.01	0.41
1:F:147:ILE:HD13	1:M:50:LEU:HD11	2.03	0.41
2:G:383:LEU:HD21	2:G:402:PRO:HG2	2.03	0.41
2:J:359:TYR:HA	2:J:386:MET:HE1	2.02	0.41
3:J:273:M1N:H36	3:J:273:M1N:H4	1.76	0.41
1:M:85:ARG:HG2	1:M:85:ARG:NH1	2.15	0.41
1:Q:28:LYS:HE2	1:Q:46:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:182:ARG:HA	1:S:235:VAL:HB	2.02	0.41
1:Y:110:ILE:HA	1:Y:114:GLN:HG2	2.02	0.41
2:Z:424:ASP:HB3	2:Z:428:GLY:N	2.36	0.41
1:1:127:VAL:HG11	1:1:213:LEU:HB3	2.01	0.41
1:A:203:LEU:HG	1:A:237:GLN:OE1	2.19	0.41
2:H:304:VAL:HG23	2:H:438:ALA:HB2	2.02	0.41
2:C:436:TYR:HB2	2:C:450:MET:SD	2.60	0.41
1:D:189:ARG:CZ	1:D:237:GLN:HB3	2.50	0.41
2:E:307:LYS:HD2	2:E:418:GLY:O	2.20	0.41
1:F:92:ARG:HB2	1:F:92:ARG:HH11	1.85	0.41
2:G:424:ASP:HB3	2:G:428:GLY:N	2.35	0.41
2:L:314:MET:HE2	2:L:342:ALA:HB1	2.02	0.41
2:N:329:ARG:O	2:N:490:ILE:HG21	2.21	0.41
1:O:55:GLU:OE2	1:O:220:ARG:HD2	2.20	0.41
1:Q:234:LEU:HG	1:Q:235:VAL:N	2.35	0.41
2:Z:469:GLU:HG3	2:Z:517:ILE:HD12	2.02	0.41
1:I:41:PHE:HZ	1:I:125:ALA:HB3	1.85	0.41
1:M:141:ILE:N	1:M:141:ILE:HD12	2.35	0.41
1:O:171:TYR:CE2	1:O:173:GLU:HA	2.55	0.41
1:Q:21:ARG:HB3	1:Q:21:ARG:NH1	2.35	0.41
1:Q:167:LEU:C	1:Q:169:GLU:N	2.77	0.41
2:R:306:LEU:HB2	2:R:313:VAL:CG1	2.50	0.41
2:R:330:ASP:N	2:R:330:ASP:OD1	2.54	0.41
1:S:95:THR:C	1:S:97:ARG:H	2.28	0.41
1:U:85:ARG:HH11	1:U:89:TYR:HE2	1.69	0.41
2:H:311:GLY:HA3	2:H:497:ILE:O	2.21	0.41
1:I:27:ALA:HB1	4:I:252:HOH:O	2.21	0.41
2:J:383:LEU:HD21	2:J:402:PRO:CG	2.50	0.41
2:N:341:THR:CG2	2:N:404:LEU:HD11	2.50	0.41
1:O:30:VAL:HG22	1:O:43:ALA:HB1	2.02	0.41
2:P:518:ILE:O	2:P:522:SER:HB2	2.20	0.41
1:S:78:GLY:HA3	1:S:103:TYR:OH	2.21	0.41
2:V:424:ASP:HB2	2:V:428:GLY:C	2.46	0.41
1:A:31:VAL:HG22	1:A:155:VAL:HG13	2.03	0.41
2:H:306:LEU:CD2	2:H:454:TYR:CE1	3.04	0.41
2:H:408:ASP:C	2:H:410:HIS:H	2.29	0.41
1:B:128:ALA:HB2	1:B:134:LYS:HB3	2.01	0.41
1:B:163:ILE:HG23	1:B:188:LEU:HA	2.02	0.41
2:C:321:THR:O	3:C:273:M1N:H37	2.21	0.41
1:D:205:VAL:HG12	1:D:206:ALA:H	1.85	0.41
3:E:273:M1N:H36	3:E:273:M1N:H4	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:127:VAL:HG22	1:M:215:ALA:HB2	2.02	0.41
2:N:345:ILE:O	2:N:345:ILE:HD12	2.19	0.41
1:O:41:PHE:HE2	1:O:213:LEU:HD13	1.86	0.41
2:R:432:GLU:HG3	2:R:437:GLN:HB2	2.03	0.41
1:S:22:LYS:HB3	1:S:26:ARG:NH2	2.36	0.41
1:S:57:TYR:O	1:S:58:ASP:C	2.64	0.41
2:T:471:LEU:HD13	2:T:492:PRO:HB3	2.02	0.41
2:X:345:ILE:HB	2:X:352:ALA:HB1	2.03	0.41
1:I:57:TYR:O	1:I:58:ASP:C	2.64	0.41
2:H:324:ASN:ND2	2:H:324:ASN:N	2.49	0.41
2:H:348:THR:HA	3:H:273:M1N:H36	2.03	0.41
1:B:205:VAL:CG1	1:B:206:ALA:H	2.31	0.41
1:D:89:TYR:CD1	2:R:382:ARG:HD3	2.56	0.41
1:D:171:TYR:CE2	1:D:173:GLU:HA	2.56	0.41
2:E:321:THR:O	3:E:273:M1N:H52	2.21	0.41
1:F:28:LYS:HB2	1:F:52:LYS:NZ	2.36	0.41
1:I:28:LYS:HE2	1:I:46:PRO:HD3	2.01	0.41
1:I:30:VAL:HG22	1:I:43:ALA:CB	2.51	0.41
1:I:95:THR:C	1:I:97:ARG:H	2.29	0.41
1:K:91:ARG:HE	1:K:91:ARG:HB3	1.65	0.41
2:L:424:ASP:HB3	2:L:428:GLY:H	1.86	0.41
1:M:95:THR:C	1:M:97:ARG:H	2.28	0.41
1:M:127:VAL:O	1:M:127:VAL:HG13	2.20	0.41
1:M:153:PHE:HZ	1:M:168:LYS:HG2	1.86	0.41
1:M:208:LEU:HB3	4:M:254:HOH:O	2.19	0.41
1:M:226:THR:OG1	1:M:227:GLY:N	2.53	0.41
2:N:407:TYR:CE1	2:N:417:ALA:HB3	2.55	0.41
1:O:24:ILE:HG12	1:O:24:ILE:H	1.77	0.41
2:P:513:LEU:O	2:P:516:ALA:HB3	2.21	0.41
2:R:314:MET:HE2	2:R:405:ALA:HB3	2.03	0.41
1:S:128:ALA:HB2	1:S:134:LYS:HB3	2.02	0.41
2:T:329:ARG:O	2:T:490:ILE:HG21	2.21	0.41
1:U:87:TYR:OH	2:V:354:GLU:HG2	2.20	0.41
2:V:329:ARG:O	2:V:490:ILE:HG21	2.21	0.41
2:V:441:SER:HB2	2:V:478:ASP:OD2	2.21	0.41
1:Y:57:TYR:O	1:Y:58:ASP:C	2.64	0.41
1:Y:182:ARG:HA	1:Y:235:VAL:HB	2.03	0.41
2:Z:320:SER:HB3	2:Z:331:VAL:HG21	2.03	0.41
2:2:306:LEU:HB2	2:2:313:VAL:CG1	2.50	0.41
2:2:395:MET:HA	2:2:395:MET:CE	2.42	0.41
2:2:407:TYR:CE1	2:2:417:ALA:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TYR:O	1:A:58:ASP:C	2.63	0.41
1:A:167:LEU:C	1:A:169:GLU:N	2.79	0.41
2:G:321:THR:HG22	4:G:153:HOH:O	2.20	0.41
1:K:96:GLY:HA2	1:K:99:LEU:HB2	2.02	0.41
2:N:345:ILE:HD11	4:N:549:HOH:O	2.21	0.41
2:R:392:ALA:HB3	4:R:159:HOH:O	2.21	0.41
3:R:273:M1N:H40	2:Z:424:ASP:OD1	2.21	0.41
2:T:465:ARG:HB2	2:T:513:LEU:HD22	2.02	0.41
2:V:515:ARG:HA	2:V:518:ILE:HD12	2.03	0.41
1:W:205:VAL:C	1:W:207:SER:N	2.77	0.41
2:Z:514:ALA:O	2:Z:518:ILE:HG13	2.21	0.41
1:1:176:SER:HB3	1:1:179:ASP:HB2	2.01	0.41
2:2:347:GLY:CA	3:2:273:M1N:H132	2.51	0.41
1:A:18:GLU:OE1	1:A:21:ARG:NH2	2.54	0.40
2:H:317:ASP:HB2	4:H:552:HOH:O	2.21	0.40
2:H:413:ASP:HA	2:H:414:PRO:HD3	1.93	0.40
1:I:205:VAL:HG12	1:I:206:ALA:H	1.85	0.40
2:P:383:LEU:HD23	2:P:383:LEU:C	2.46	0.40
2:P:433:GLU:HG3	2:P:433:GLU:O	2.21	0.40
1:U:57:TYR:O	1:U:58:ASP:C	2.64	0.40
2:V:395:MET:HA	2:V:395:MET:CE	2.48	0.40
1:W:152:HIS:CD2	1:W:171:TYR:CE2	3.09	0.40
2:Z:311:GLY:HA3	2:Z:497:ILE:O	2.22	0.40
1:1:68:PHE:HA	1:1:71:PHE:CE2	2.56	0.40
1:A:205:VAL:HG12	1:A:206:ALA:H	1.87	0.40
2:C:464:LEU:HD11	2:C:505:VAL:HG11	2.03	0.40
1:D:92:ARG:CG	1:D:129:HIS:CE1	3.03	0.40
1:D:135:ARG:HA	1:D:136:PRO:HD2	1.88	0.40
1:F:232:ALA:C	1:F:233:LEU:HD12	2.46	0.40
2:G:395:MET:HA	2:G:395:MET:CE	2.51	0.40
1:K:98:GLN:O	1:K:101:ASN:HB2	2.21	0.40
2:L:366:TYR:CZ	2:L:370:GLU:HG3	2.57	0.40
2:N:306:LEU:HB2	2:N:313:VAL:HG13	2.04	0.40
1:Q:185:VAL:HB	1:Q:235:VAL:CG1	2.51	0.40
1:S:185:VAL:HB	1:S:235:VAL:HG11	2.02	0.40
2:V:408:ASP:HA	4:V:551:HOH:O	2.21	0.40
2:Z:382:ARG:NH1	2:Z:385:ILE:HD13	2.37	0.40
3:Z:273:M1N:H36	3:Z:273:M1N:H4	1.97	0.40
1:F:92:ARG:HD2	1:F:129:HIS:ND1	2.35	0.40
2:G:388:ARG:C	2:G:390:ASN:H	2.29	0.40
1:I:54:SER:CB	1:I:75:ARG:HD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:306:LEU:CD2	2:J:436:TYR:HB3	2.51	0.40
2:J:432:GLU:HG3	2:J:437:GLN:HB2	2.04	0.40
2:L:485:ASP:OD2	2:L:488:ARG:HB2	2.22	0.40
2:N:450:MET:CE	2:N:470:ALA:CB	2.99	0.40
1:S:205:VAL:C	1:S:207:SER:N	2.74	0.40
1:S:205:VAL:O	1:S:207:SER:N	2.54	0.40
2:V:338:ASP:OD1	2:V:338:ASP:C	2.64	0.40
2:V:403:LEU:HD12	2:V:439:VAL:HG22	2.03	0.40
2:X:321:THR:HG23	3:X:273:M1N:O3	2.21	0.40
2:2:384:ALA:HB1	2:2:427:GLY:O	2.22	0.40
1:A:96:GLY:HA2	1:A:99:LEU:HB2	2.02	0.40
2:H:313:VAL:HB	2:H:496:ILE:HD13	2.03	0.40
2:H:321:THR:HG22	4:H:542:HOH:O	2.20	0.40
1:B:19:LEU:C	1:B:19:LEU:HD23	2.45	0.40
2:C:438:ALA:CB	2:C:443:SER:HB2	2.51	0.40
2:C:520:SER:HB2	4:C:554:HOH:O	2.21	0.40
2:J:496:ILE:HG13	2:J:505:VAL:CG2	2.51	0.40
1:O:57:TYR:O	1:O:58:ASP:C	2.65	0.40
2:P:388:ARG:HD3	4:P:544:HOH:O	2.21	0.40
1:U:45:ASN:HA	1:U:46:PRO:HD2	1.97	0.40
2:X:320:SER:HB2	2:X:331:VAL:HG21	2.03	0.40
2:2:452:LYS:HA	2:2:452:LYS:HD3	1.85	0.40
2:H:347:GLY:H	3:H:273:M1N:H16	1.69	0.40
1:I:230:LEU:HD23	1:I:230:LEU:C	2.46	0.40
2:L:322:GLN:HG2	2:L:322:GLN:O	2.21	0.40
2:N:357:ARG:O	2:N:361:VAL:HG23	2.22	0.40
1:O:182:ARG:HD3	1:O:235:VAL:CG2	2.52	0.40
1:O:209:GLU:OE2	1:O:224:ARG:NH2	2.55	0.40
2:X:331:VAL:HG11	3:X:273:M1N:H251	2.04	0.40
2:X:390:ASN:HA	4:X:31:HOH:O	2.22	0.40
2:Z:313:VAL:HG23	2:Z:496:ILE:HG12	2.03	0.40
1:1:165:ASN:HD22	1:1:165:ASN:HA	1.74	0.40
2:2:314:MET:HE3	2:2:334:VAL:CG1	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASP:O	1:D:133:THR:OG1[2_655]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	216/251 (86%)	188 (87%)	23 (11%)	5 (2%)	5	25
1	A	216/251 (86%)	190 (88%)	21 (10%)	5 (2%)	5	25
1	B	216/251 (86%)	189 (88%)	22 (10%)	5 (2%)	5	25
1	D	216/251 (86%)	188 (87%)	22 (10%)	6 (3%)	4	21
1	F	216/251 (86%)	192 (89%)	18 (8%)	6 (3%)	4	21
1	I	216/251 (86%)	188 (87%)	22 (10%)	6 (3%)	4	21
1	K	216/251 (86%)	190 (88%)	20 (9%)	6 (3%)	4	21
1	M	216/251 (86%)	190 (88%)	21 (10%)	5 (2%)	5	25
1	O	216/251 (86%)	189 (88%)	22 (10%)	5 (2%)	5	25
1	Q	216/251 (86%)	189 (88%)	20 (9%)	7 (3%)	3	18
1	S	216/251 (86%)	188 (87%)	22 (10%)	6 (3%)	4	21
1	U	216/251 (86%)	188 (87%)	23 (11%)	5 (2%)	5	25
1	W	216/251 (86%)	187 (87%)	23 (11%)	6 (3%)	4	21
1	Y	216/251 (86%)	188 (87%)	24 (11%)	4 (2%)	6	30
2	2	220/240 (92%)	202 (92%)	18 (8%)	0	100	100
2	C	220/240 (92%)	201 (91%)	19 (9%)	0	100	100
2	E	220/240 (92%)	201 (91%)	19 (9%)	0	100	100
2	G	220/240 (92%)	201 (91%)	18 (8%)	1 (0%)	24	60
2	H	220/240 (92%)	201 (91%)	17 (8%)	2 (1%)	14	48
2	J	220/240 (92%)	199 (90%)	21 (10%)	0	100	100
2	L	220/240 (92%)	199 (90%)	21 (10%)	0	100	100
2	N	220/240 (92%)	200 (91%)	19 (9%)	1 (0%)	24	60
2	P	220/240 (92%)	202 (92%)	17 (8%)	1 (0%)	24	60
2	R	220/240 (92%)	204 (93%)	13 (6%)	3 (1%)	9	36
2	T	220/240 (92%)	202 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	220/240 (92%)	202 (92%)	16 (7%)	2 (1%)	14	48
2	X	220/240 (92%)	200 (91%)	18 (8%)	2 (1%)	14	48
2	Z	220/240 (92%)	199 (90%)	20 (9%)	1 (0%)	24	60
All	All	6104/6874 (89%)	5457 (89%)	557 (9%)	90 (2%)	8	35

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ALA
1	B	128	ALA
1	D	128	ALA
1	F	128	ALA
1	I	128	ALA
1	K	128	ALA
1	M	128	ALA
1	M	130	TYR
1	O	128	ALA
1	Q	128	ALA
1	S	128	ALA
1	U	128	ALA
1	W	128	ALA
1	Y	128	ALA
1	1	128	ALA
1	A	130	TYR
1	B	130	TYR
1	B	206	ALA
1	B	226	THR
1	D	130	TYR
1	D	206	ALA
1	F	130	TYR
1	I	130	TYR
1	I	206	ALA
1	K	130	TYR
1	K	206	ALA
1	M	206	ALA
1	M	226	THR
1	O	130	TYR
1	O	206	ALA
1	Q	130	TYR
1	S	130	TYR
1	S	206	ALA

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Mol	Chain	Res	Type
1	S	226	THR
1	U	130	TYR
1	U	206	ALA
1	U	226	THR
1	W	130	TYR
1	Y	130	TYR
1	Y	206	ALA
1	1	130	TYR
1	1	206	ALA
1	1	226	THR
1	A	58	ASP
1	A	206	ALA
1	A	226	THR
1	D	226	THR
1	F	206	ALA
1	F	226	THR
1	I	58	ASP
1	I	226	THR
1	K	58	ASP
1	K	226	THR
1	O	226	THR
1	Q	58	ASP
1	Q	206	ALA
1	Q	226	THR
1	U	58	ASP
1	W	206	ALA
1	W	226	THR
1	Y	226	THR
2	P	398	LEU
2	R	398	LEU
2	R	433	GLU
2	H	398	LEU
1	D	58	ASP
1	F	58	ASP
2	N	433	GLU
1	O	132	GLU
2	R	389	GLY
1	S	132	GLU
2	V	317	ASP
2	V	398	LEU
1	W	58	ASP
1	1	58	ASP

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Mol	Chain	Res	Type
1	B	58	ASP
1	Q	132	GLU
2	X	460	GLY
2	Z	389	GLY
2	H	389	GLY
1	F	218	PRO
1	K	218	PRO
2	G	460	GLY
1	I	218	PRO
1	M	218	PRO
1	W	218	PRO
2	X	389	GLY
1	D	218	PRO
1	Q	218	PRO
1	S	218	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	169/195 (87%)	150 (89%)	19 (11%)	6	24
1	A	169/195 (87%)	146 (86%)	23 (14%)	3	17
1	B	169/195 (87%)	147 (87%)	22 (13%)	4	19
1	D	169/195 (87%)	146 (86%)	23 (14%)	3	17
1	F	169/195 (87%)	145 (86%)	24 (14%)	3	16
1	I	169/195 (87%)	143 (85%)	26 (15%)	2	13
1	K	169/195 (87%)	146 (86%)	23 (14%)	3	17
1	M	169/195 (87%)	152 (90%)	17 (10%)	7	29
1	O	169/195 (87%)	146 (86%)	23 (14%)	3	17
1	Q	169/195 (87%)	147 (87%)	22 (13%)	4	19
1	S	169/195 (87%)	147 (87%)	22 (13%)	4	19
1	U	169/195 (87%)	150 (89%)	19 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	169/195 (87%)	151 (89%)	18 (11%)	6	26
1	Y	169/195 (87%)	145 (86%)	24 (14%)	3	16
2	2	165/178 (93%)	132 (80%)	33 (20%)	1	7
2	C	165/178 (93%)	140 (85%)	25 (15%)	3	14
2	E	165/178 (93%)	136 (82%)	29 (18%)	2	10
2	G	165/178 (93%)	142 (86%)	23 (14%)	3	17
2	H	165/178 (93%)	139 (84%)	26 (16%)	2	13
2	J	165/178 (93%)	139 (84%)	26 (16%)	2	13
2	L	165/178 (93%)	138 (84%)	27 (16%)	2	12
2	N	165/178 (93%)	141 (86%)	24 (14%)	3	15
2	P	165/178 (93%)	138 (84%)	27 (16%)	2	12
2	R	165/178 (93%)	133 (81%)	32 (19%)	1	8
2	T	165/178 (93%)	139 (84%)	26 (16%)	2	13
2	V	165/178 (93%)	138 (84%)	27 (16%)	2	12
2	X	165/178 (93%)	144 (87%)	21 (13%)	4	20
2	Z	165/178 (93%)	144 (87%)	21 (13%)	4	20
All	All	4676/5222 (90%)	4004 (86%)	672 (14%)	3	15

All (672) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	18	GLU
1	A	33	LEU
1	A	60	VAL
1	A	85	ARG
1	A	91	ARG
1	A	92	ARG
1	A	105	GLN
1	A	113	GLU
1	A	116	LYS
1	A	122	LEU
1	A	133	THR
1	A	134	LYS
1	A	135	ARG
1	A	147	ILE

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Mol	Chain	Res	Type
1	A	150	GLU
1	A	165	ASN
1	A	182	ARG
1	A	188	LEU
1	A	203	LEU
1	A	208	LEU
1	A	225	ILE
1	A	237	GLN
2	H	304	VAL
2	H	307	LYS
2	H	318	ARG
2	H	319	ARG
2	H	320	SER
2	H	324	ASN
2	H	329	ARG
2	H	345	ILE
2	H	375	THR
2	H	391	LEU
2	H	401	LEU
2	H	403	LEU
2	H	412	SER
2	H	415	GLN
2	H	422	SER
2	H	424	ASP
2	H	430	ASN
2	H	441	SER
2	H	444	LEU
2	H	449	SER
2	H	476	ASP
2	H	479	SER
2	H	481	THR
2	H	508	SER
2	H	520	SER
2	H	522	SER
1	B	11	GLN
1	B	14	ARG
1	B	18	GLU
1	B	24	ILE
1	B	28	LYS
1	B	49	SER
1	B	80	GLN
1	B	84	THR

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Mol	Chain	Res	Type
1	B	85	ARG
1	B	92	ARG
1	B	113	GLU
1	B	134	LYS
1	B	147	ILE
1	B	149	ASP
1	B	150	GLU
1	B	182	ARG
1	B	203	LEU
1	B	208	LEU
1	B	213	LEU
1	B	225	ILE
1	B	228	SER
1	B	235	VAL
2	C	304	VAL
2	C	312	VAL
2	C	318	ARG
2	C	319	ARG
2	C	320	SER
2	C	321	THR
2	C	324	ASN
2	C	329	ARG
2	C	341	THR
2	C	345	ILE
2	C	355	PHE
2	C	391	LEU
2	C	401	LEU
2	C	403	LEU
2	C	415	GLN
2	C	434	GLU
2	C	439	VAL
2	C	444	LEU
2	C	449	SER
2	C	465	ARG
2	C	490	ILE
2	C	497	ILE
2	C	508	SER
2	C	517	ILE
2	C	522	SER
1	D	11	GLN
1	D	18	GLU
1	D	31	VAL

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Mol	Chain	Res	Type
1	D	33	LEU
1	D	84	THR
1	D	85	ARG
1	D	92	ARG
1	D	105	GLN
1	D	113	GLU
1	D	133	THR
1	D	134	LYS
1	D	147	ILE
1	D	150	GLU
1	D	154	VAL
1	D	178	THR
1	D	182	ARG
1	D	188	LEU
1	D	192	SER
1	D	203	LEU
1	D	205	VAL
1	D	208	LEU
1	D	235	VAL
1	D	236	ASP
2	E	304	VAL
2	E	312	VAL
2	E	318	ARG
2	E	319	ARG
2	E	320	SER
2	E	324	ASN
2	E	329	ARG
2	E	341	THR
2	E	345	ILE
2	E	358	LEU
2	E	375	THR
2	E	383	LEU
2	E	391	LEU
2	E	401	LEU
2	E	403	LEU
2	E	409	ILE
2	E	415	GLN
2	E	432	GLU
2	E	444	LEU
2	E	449	SER
2	E	455	SER
2	E	476	ASP

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Mol	Chain	Res	Type
2	E	488	ARG
2	E	490	ILE
2	E	508	SER
2	E	513	LEU
2	E	517	ILE
2	E	520	SER
2	E	522	SER
1	F	18	GLU
1	F	24	ILE
1	F	33	LEU
1	F	48	ARG
1	F	49	SER
1	F	80	GLN
1	F	85	ARG
1	F	92	ARG
1	F	113	GLU
1	F	133	THR
1	F	134	LYS
1	F	135	ARG
1	F	147	ILE
1	F	150	GLU
1	F	159	THR
1	F	173	GLU
1	F	176	SER
1	F	182	ARG
1	F	188	LEU
1	F	203	LEU
1	F	205	VAL
1	F	208	LEU
1	F	213	LEU
1	F	225	ILE
2	G	318	ARG
2	G	319	ARG
2	G	321	THR
2	G	324	ASN
2	G	329	ARG
2	G	337	THR
2	G	341	THR
2	G	345	ILE
2	G	358	LEU
2	G	375	THR
2	G	391	LEU

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Mol	Chain	Res	Type
2	G	401	LEU
2	G	403	LEU
2	G	415	GLN
2	G	437	GLN
2	G	441	SER
2	G	444	LEU
2	G	461	ASP
2	G	465	ARG
2	G	476	ASP
2	G	479	SER
2	G	497	ILE
2	G	517	ILE
1	I	18	GLU
1	I	24	ILE
1	I	26	ARG
1	I	48	ARG
1	I	60	VAL
1	I	84	THR
1	I	85	ARG
1	I	92	ARG
1	I	113	GLU
1	I	134	LYS
1	I	137	GLU
1	I	138	LEU
1	I	140	ARG
1	I	147	ILE
1	I	150	GLU
1	I	156	MET
1	I	168	LYS
1	I	182	ARG
1	I	192	SER
1	I	203	LEU
1	I	205	VAL
1	I	208	LEU
1	I	213	LEU
1	I	225	ILE
1	I	235	VAL
1	I	237	GLN
2	J	304	VAL
2	J	318	ARG
2	J	319	ARG
2	J	320	SER

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Mol	Chain	Res	Type
2	J	324	ASN
2	J	329	ARG
2	J	337	THR
2	J	341	THR
2	J	345	ILE
2	J	375	THR
2	J	391	LEU
2	J	401	LEU
2	J	403	LEU
2	J	419	ARG
2	J	421	VAL
2	J	424	ASP
2	J	444	LEU
2	J	448	SER
2	J	449	SER
2	J	476	ASP
2	J	481	THR
2	J	490	ILE
2	J	497	ILE
2	J	503	VAL
2	J	517	ILE
2	J	522	SER
1	K	11	GLN
1	K	14	ARG
1	K	18	GLU
1	K	33	LEU
1	K	84	THR
1	K	85	ARG
1	K	92	ARG
1	K	98	GLN
1	K	99	LEU
1	K	113	GLU
1	K	134	LYS
1	K	144	ASP
1	K	147	ILE
1	K	150	GLU
1	K	154	VAL
1	K	173	GLU
1	K	178	THR
1	K	203	LEU
1	K	208	LEU
1	K	213	LEU

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Mol	Chain	Res	Type
1	K	223	ARG
1	K	225	ILE
1	K	237	GLN
2	L	304	VAL
2	L	312	VAL
2	L	320	SER
2	L	321	THR
2	L	324	ASN
2	L	329	ARG
2	L	332	ARG
2	L	341	THR
2	L	345	ILE
2	L	358	LEU
2	L	391	LEU
2	L	398	LEU
2	L	401	LEU
2	L	403	LEU
2	L	412	SER
2	L	415	GLN
2	L	421	VAL
2	L	441	SER
2	L	443	SER
2	L	444	LEU
2	L	448	SER
2	L	449	SER
2	L	476	ASP
2	L	479	SER
2	L	497	ILE
2	L	508	SER
2	L	522	SER
1	M	8	SER
1	M	14	ARG
1	M	18	GLU
1	M	49	SER
1	M	80	GLN
1	M	85	ARG
1	M	92	ARG
1	M	105	GLN
1	M	133	THR
1	M	134	LYS
1	M	135	ARG
1	M	147	ILE

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Mol	Chain	Res	Type
1	M	173	GLU
1	M	188	LEU
1	M	203	LEU
1	M	208	LEU
1	M	213	LEU
2	N	304	VAL
2	N	312	VAL
2	N	318	ARG
2	N	319	ARG
2	N	320	SER
2	N	321	THR
2	N	324	ASN
2	N	329	ARG
2	N	331	VAL
2	N	337	THR
2	N	341	THR
2	N	345	ILE
2	N	391	LEU
2	N	396	GLN
2	N	401	LEU
2	N	403	LEU
2	N	430	ASN
2	N	441	SER
2	N	444	LEU
2	N	449	SER
2	N	464	LEU
2	N	476	ASP
2	N	481	THR
2	N	513	LEU
1	O	11	GLN
1	O	14	ARG
1	O	21	ARG
1	O	24	ILE
1	O	48	ARG
1	O	84	THR
1	O	85	ARG
1	O	92	ARG
1	O	98	GLN
1	O	105	GLN
1	O	113	GLU
1	O	134	LYS
1	O	147	ILE

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Mol	Chain	Res	Type
1	O	150	GLU
1	O	165	ASN
1	O	182	ARG
1	O	188	LEU
1	O	192	SER
1	O	203	LEU
1	O	205	VAL
1	O	208	LEU
1	O	225	ILE
1	O	236	ASP
2	P	304	VAL
2	P	307	LYS
2	P	318	ARG
2	P	319	ARG
2	P	320	SER
2	P	324	ASN
2	P	325	MET
2	P	329	ARG
2	P	332	ARG
2	P	337	THR
2	P	341	THR
2	P	345	ILE
2	P	357	ARG
2	P	375	THR
2	P	391	LEU
2	P	396	GLN
2	P	401	LEU
2	P	403	LEU
2	P	444	LEU
2	P	448	SER
2	P	449	SER
2	P	476	ASP
2	P	481	THR
2	P	488	ARG
2	P	496	ILE
2	P	508	SER
2	P	517	ILE
1	Q	18	GLU
1	Q	21	ARG
1	Q	24	ILE
1	Q	48	ARG
1	Q	84	THR

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Mol	Chain	Res	Type
1	Q	85	ARG
1	Q	92	ARG
1	Q	113	GLU
1	Q	134	LYS
1	Q	135	ARG
1	Q	147	ILE
1	Q	154	VAL
1	Q	159	THR
1	Q	168	LYS
1	Q	173	GLU
1	Q	179	ASP
1	Q	203	LEU
1	Q	205	VAL
1	Q	213	LEU
1	Q	225	ILE
1	Q	236	ASP
1	Q	237	GLN
2	R	304	VAL
2	R	314	MET
2	R	318	ARG
2	R	319	ARG
2	R	320	SER
2	R	321	THR
2	R	324	ASN
2	R	325	MET
2	R	329	ARG
2	R	337	THR
2	R	341	THR
2	R	345	ILE
2	R	355	PHE
2	R	375	THR
2	R	383	LEU
2	R	391	LEU
2	R	401	LEU
2	R	403	LEU
2	R	412	SER
2	R	424	ASP
2	R	434	GLU
2	R	436	TYR
2	R	444	LEU
2	R	449	SER
2	R	461	ASP

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Mol	Chain	Res	Type
2	R	476	ASP
2	R	481	THR
2	R	488	ARG
2	R	490	ILE
2	R	496	ILE
2	R	503	VAL
2	R	508	SER
1	S	17	SER
1	S	49	SER
1	S	80	GLN
1	S	84	THR
1	S	85	ARG
1	S	92	ARG
1	S	109	THR
1	S	113	GLU
1	S	133	THR
1	S	134	LYS
1	S	140	ARG
1	S	147	ILE
1	S	150	GLU
1	S	165	ASN
1	S	182	ARG
1	S	188	LEU
1	S	192	SER
1	S	203	LEU
1	S	205	VAL
1	S	208	LEU
1	S	213	LEU
1	S	235	VAL
2	T	304	VAL
2	T	318	ARG
2	T	319	ARG
2	T	320	SER
2	T	321	THR
2	T	324	ASN
2	T	329	ARG
2	T	337	THR
2	T	341	THR
2	T	345	ILE
2	T	358	LEU
2	T	391	LEU
2	T	398	LEU

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Mol	Chain	Res	Type
2	T	401	LEU
2	T	403	LEU
2	T	409	ILE
2	T	415	GLN
2	T	430	ASN
2	T	439	VAL
2	T	441	SER
2	T	444	LEU
2	T	448	SER
2	T	449	SER
2	T	476	ASP
2	T	508	SER
2	T	517	ILE
1	U	11	GLN
1	U	18	GLU
1	U	24	ILE
1	U	26	ARG
1	U	84	THR
1	U	85	ARG
1	U	91	ARG
1	U	92	ARG
1	U	113	GLU
1	U	134	LYS
1	U	147	ILE
1	U	150	GLU
1	U	188	LEU
1	U	203	LEU
1	U	205	VAL
1	U	208	LEU
1	U	231	GLN
1	U	235	VAL
1	U	237	GLN
2	V	303	ILE
2	V	304	VAL
2	V	312	VAL
2	V	318	ARG
2	V	320	SER
2	V	324	ASN
2	V	329	ARG
2	V	341	THR
2	V	345	ILE
2	V	375	THR

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Mol	Chain	Res	Type
2	V	383	LEU
2	V	385	ILE
2	V	391	LEU
2	V	401	LEU
2	V	403	LEU
2	V	412	SER
2	V	415	GLN
2	V	416	SER
2	V	430	ASN
2	V	441	SER
2	V	444	LEU
2	V	449	SER
2	V	476	ASP
2	V	481	THR
2	V	490	ILE
2	V	508	SER
2	V	513	LEU
1	W	11	GLN
1	W	18	GLU
1	W	24	ILE
1	W	28	LYS
1	W	33	LEU
1	W	85	ARG
1	W	91	ARG
1	W	92	ARG
1	W	113	GLU
1	W	134	LYS
1	W	135	ARG
1	W	137	GLU
1	W	147	ILE
1	W	176	SER
1	W	188	LEU
1	W	203	LEU
1	W	225	ILE
1	W	231	GLN
2	X	319	ARG
2	X	321	THR
2	X	324	ASN
2	X	329	ARG
2	X	337	THR
2	X	345	ILE
2	X	358	LEU

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Mol	Chain	Res	Type
2	X	375	THR
2	X	383	LEU
2	X	391	LEU
2	X	398	LEU
2	X	401	LEU
2	X	403	LEU
2	X	412	SER
2	X	421	VAL
2	X	444	LEU
2	X	458	THR
2	X	476	ASP
2	X	490	ILE
2	X	503	VAL
2	X	522	SER
1	Y	14	ARG
1	Y	18	GLU
1	Y	21	ARG
1	Y	24	ILE
1	Y	48	ARG
1	Y	84	THR
1	Y	85	ARG
1	Y	92	ARG
1	Y	105	GLN
1	Y	107	LEU
1	Y	113	GLU
1	Y	134	LYS
1	Y	147	ILE
1	Y	150	GLU
1	Y	161	GLU
1	Y	179	ASP
1	Y	182	ARG
1	Y	188	LEU
1	Y	203	LEU
1	Y	205	VAL
1	Y	208	LEU
1	Y	225	ILE
1	Y	235	VAL
1	Y	237	GLN
2	Z	318	ARG
2	Z	320	SER
2	Z	321	THR
2	Z	324	ASN

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Mol	Chain	Res	Type
2	Z	329	ARG
2	Z	337	THR
2	Z	345	ILE
2	Z	383	LEU
2	Z	391	LEU
2	Z	401	LEU
2	Z	403	LEU
2	Z	415	GLN
2	Z	416	SER
2	Z	444	LEU
2	Z	448	SER
2	Z	476	ASP
2	Z	479	SER
2	Z	481	THR
2	Z	490	ILE
2	Z	508	SER
2	Z	513	LEU
1	1	48	ARG
1	1	49	SER
1	1	85	ARG
1	1	92	ARG
1	1	113	GLU
1	1	134	LYS
1	1	135	ARG
1	1	137	GLU
1	1	147	ILE
1	1	150	GLU
1	1	156	MET
1	1	173	GLU
1	1	179	ASP
1	1	182	ARG
1	1	188	LEU
1	1	203	LEU
1	1	225	ILE
1	1	231	GLN
1	1	235	VAL
2	2	303	ILE
2	2	304	VAL
2	2	318	ARG
2	2	320	SER
2	2	321	THR
2	2	324	ASN

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Mol	Chain	Res	Type
2	2	329	ARG
2	2	332	ARG
2	2	341	THR
2	2	345	ILE
2	2	358	LEU
2	2	383	LEU
2	2	391	LEU
2	2	396	GLN
2	2	398	LEU
2	2	399	LEU
2	2	401	LEU
2	2	409	ILE
2	2	412	SER
2	2	419	ARG
2	2	421	VAL
2	2	422	SER
2	2	430	ASN
2	2	432	GLU
2	2	439	VAL
2	2	441	SER
2	2	444	LEU
2	2	449	SER
2	2	476	ASP
2	2	497	ILE
2	2	503	VAL
2	2	508	SER
2	2	517	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	51	GLN
1	A	69	ASN
1	A	73	ASN
1	A	80	GLN
1	A	98	GLN
1	A	105	GLN
1	A	165	ASN
1	A	231	GLN
2	H	324	ASN
2	H	365	HIS

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Mol	Chain	Res	Type
2	H	410	HIS
2	H	415	GLN
2	H	456	GLN
1	B	51	GLN
1	B	69	ASN
1	B	80	GLN
1	B	98	GLN
1	B	105	GLN
1	B	152	HIS
1	B	165	ASN
1	B	231	GLN
2	C	324	ASN
2	C	365	HIS
2	C	415	GLN
2	C	456	GLN
1	D	98	GLN
1	D	105	GLN
1	D	129	HIS
1	D	152	HIS
1	D	165	ASN
1	D	231	GLN
2	E	324	ASN
2	E	365	HIS
2	E	415	GLN
2	E	456	GLN
1	F	51	GLN
1	F	80	GLN
1	F	105	GLN
1	F	129	HIS
1	F	165	ASN
1	F	231	GLN
2	G	324	ASN
2	G	365	HIS
2	G	410	HIS
2	G	415	GLN
2	G	456	GLN
1	I	80	GLN
1	I	98	GLN
1	I	129	HIS
1	I	165	ASN
1	I	174	ASN
1	I	237	GLN

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Mol	Chain	Res	Type
2	J	324	ASN
2	J	365	HIS
2	J	415	GLN
2	J	456	GLN
1	K	51	GLN
1	K	73	ASN
1	K	98	GLN
1	K	105	GLN
1	K	129	HIS
1	K	165	ASN
2	L	324	ASN
2	L	365	HIS
2	L	415	GLN
2	L	456	GLN
1	M	51	GLN
1	M	69	ASN
1	M	73	ASN
1	M	129	HIS
1	M	231	GLN
2	N	324	ASN
2	N	365	HIS
2	N	410	HIS
2	N	415	GLN
2	N	456	GLN
1	O	51	GLN
1	O	73	ASN
1	O	129	HIS
1	O	165	ASN
1	O	231	GLN
2	P	324	ASN
2	P	365	HIS
2	P	410	HIS
2	P	456	GLN
1	Q	98	GLN
1	Q	129	HIS
1	Q	165	ASN
1	Q	231	GLN
2	R	324	ASN
2	R	365	HIS
2	R	410	HIS
2	R	415	GLN
2	R	456	GLN

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Mol	Chain	Res	Type
1	S	80	GLN
1	S	98	GLN
1	S	105	GLN
1	S	114	GLN
1	S	129	HIS
1	S	165	ASN
1	S	174	ASN
1	S	237	GLN
2	T	324	ASN
2	T	365	HIS
2	T	390	ASN
2	T	456	GLN
1	U	51	GLN
1	U	98	GLN
1	U	105	GLN
1	U	129	HIS
1	U	165	ASN
1	U	231	GLN
2	V	324	ASN
2	V	410	HIS
2	V	430	ASN
2	V	456	GLN
1	W	51	GLN
1	W	73	ASN
1	W	105	GLN
1	W	114	GLN
1	W	129	HIS
1	W	152	HIS
1	W	165	ASN
1	W	231	GLN
2	X	322	GLN
2	X	324	ASN
2	X	365	HIS
2	X	410	HIS
2	X	456	GLN
1	Y	51	GLN
1	Y	80	GLN
1	Y	98	GLN
1	Y	129	HIS
1	Y	165	ASN
1	Y	231	GLN
2	Z	322	GLN

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Mol	Chain	Res	Type
2	Z	324	ASN
2	Z	365	HIS
1	1	51	GLN
1	1	69	ASN
1	1	105	GLN
1	1	129	HIS
1	1	165	ASN
1	1	174	ASN
1	1	231	GLN
2	2	324	ASN
2	2	365	HIS
2	2	456	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	M1N	T	273	2	30,34,34	3.10	16 (53%)	40,46,46	4.35	17 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	M1N	2	273	2	30,34,34	3.10	15 (50%)	40,46,46	4.78	19 (47%)
3	M1N	P	273	2	30,34,34	2.97	13 (43%)	40,46,46	4.48	19 (47%)
3	M1N	L	273	2	30,34,34	2.84	13 (43%)	40,46,46	4.57	16 (40%)
3	M1N	X	273	2	30,34,34	3.10	17 (56%)	40,46,46	4.45	17 (42%)
3	M1N	G	273	2	30,34,34	3.09	15 (50%)	40,46,46	4.33	15 (37%)
3	M1N	J	273	2	30,34,34	2.93	14 (46%)	40,46,46	4.14	17 (42%)
3	M1N	H	273	2	30,34,34	2.86	13 (43%)	40,46,46	4.47	17 (42%)
3	M1N	V	273	2	30,34,34	2.89	16 (53%)	40,46,46	4.24	18 (45%)
3	M1N	C	273	2	30,34,34	2.74	12 (40%)	40,46,46	4.40	20 (50%)
3	M1N	R	273	2	30,34,34	3.10	15 (50%)	40,46,46	4.36	13 (32%)
3	M1N	N	273	2	30,34,34	2.90	15 (50%)	40,46,46	4.26	19 (47%)
3	M1N	Z	273	2	30,34,34	2.97	13 (43%)	40,46,46	4.07	16 (40%)
3	M1N	E	273	2	30,34,34	2.86	13 (43%)	40,46,46	4.58	17 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	M1N	T	273	2	-	9/23/36/36	0/3/3/3
3	M1N	2	273	2	-	12/23/36/36	0/3/3/3
3	M1N	P	273	2	-	11/23/36/36	0/3/3/3
3	M1N	L	273	2	-	11/23/36/36	0/3/3/3
3	M1N	X	273	2	-	12/23/36/36	0/3/3/3
3	M1N	G	273	2	-	11/23/36/36	0/3/3/3
3	M1N	J	273	2	-	11/23/36/36	0/3/3/3
3	M1N	H	273	2	-	10/23/36/36	0/3/3/3
3	M1N	V	273	2	-	12/23/36/36	0/3/3/3
3	M1N	C	273	2	-	11/23/36/36	0/3/3/3
3	M1N	R	273	2	-	12/23/36/36	0/3/3/3
3	M1N	N	273	2	-	12/23/36/36	0/3/3/3
3	M1N	Z	273	2	-	12/23/36/36	0/3/3/3
3	M1N	E	273	2	-	9/23/36/36	0/3/3/3

All (200) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	273	M1N	C5-C4	-7.05	1.37	1.54
3	P	273	M1N	C5-C4	-7.03	1.37	1.54
3	G	273	M1N	C5-C4	-6.92	1.37	1.54
3	J	273	M1N	C5-C4	-6.86	1.37	1.54
3	N	273	M1N	C5-C4	-6.78	1.37	1.54
3	H	273	M1N	C5-C4	-6.75	1.37	1.54
3	R	273	M1N	C5-C4	-6.64	1.38	1.54
3	C	273	M1N	C5-C4	-6.61	1.38	1.54
3	Z	273	M1N	C5-C4	-6.54	1.38	1.54
3	X	273	M1N	C5-C4	-6.47	1.38	1.54
3	V	273	M1N	C5-C4	-6.38	1.38	1.54
3	L	273	M1N	C5-C4	-6.38	1.38	1.54
3	2	273	M1N	C5-C4	-6.35	1.38	1.54
3	T	273	M1N	C5-C4	-6.21	1.39	1.54
3	T	273	M1N	C38-C37	5.65	1.48	1.36
3	2	273	M1N	C7-N9	5.60	1.46	1.36
3	R	273	M1N	C38-C37	5.56	1.48	1.36
3	2	273	M1N	C38-C37	5.45	1.48	1.36
3	R	273	M1N	O8-C7	5.34	1.32	1.23
3	T	273	M1N	O8-C7	5.33	1.32	1.23
3	X	273	M1N	C2-N1	5.33	1.45	1.34
3	G	273	M1N	O8-C7	5.30	1.32	1.23
3	2	273	M1N	C2-N1	5.26	1.45	1.34
3	P	273	M1N	C38-C37	5.24	1.47	1.36
3	T	273	M1N	C2-N1	5.24	1.45	1.34
3	X	273	M1N	O8-C7	5.24	1.32	1.23
3	Z	273	M1N	O8-C7	5.20	1.32	1.23
3	N	273	M1N	C38-C37	5.16	1.47	1.36
3	L	273	M1N	C35-C36	5.14	1.47	1.38
3	H	273	M1N	C35-C36	5.13	1.47	1.38
3	G	273	M1N	C38-C37	5.13	1.47	1.36
3	Z	273	M1N	C38-C37	5.12	1.47	1.36
3	X	273	M1N	C35-C36	5.09	1.47	1.38
3	P	273	M1N	C2-N1	5.09	1.44	1.34
3	2	273	M1N	O8-C7	5.07	1.32	1.23
3	V	273	M1N	C38-C37	5.05	1.47	1.36
3	R	273	M1N	C7-N6	5.01	1.46	1.35
3	X	273	M1N	C38-C37	5.01	1.47	1.36
3	G	273	M1N	C35-C36	4.99	1.47	1.38
3	P	273	M1N	C35-C36	4.98	1.47	1.38
3	J	273	M1N	C38-C37	4.97	1.47	1.36
3	G	273	M1N	C2-N1	4.95	1.44	1.34
3	N	273	M1N	C2-N1	4.94	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	273	M1N	C7-N6	4.94	1.46	1.35
3	L	273	M1N	C2-N1	4.88	1.44	1.34
3	J	273	M1N	O8-C7	4.87	1.31	1.23
3	L	273	M1N	C38-C37	4.86	1.46	1.36
3	2	273	M1N	C35-C36	4.83	1.47	1.38
3	V	273	M1N	C2-N1	4.83	1.44	1.34
3	T	273	M1N	C35-C36	4.82	1.47	1.38
3	R	273	M1N	C2-N1	4.81	1.44	1.34
3	N	273	M1N	O8-C7	4.80	1.31	1.23
3	R	273	M1N	C35-C36	4.78	1.47	1.38
3	H	273	M1N	C2-N1	4.77	1.44	1.34
3	2	273	M1N	C7-N6	4.77	1.45	1.35
3	G	273	M1N	C7-N6	4.75	1.45	1.35
3	E	273	M1N	C35-C36	4.74	1.47	1.38
3	E	273	M1N	C38-C37	4.74	1.46	1.36
3	J	273	M1N	C35-C36	4.73	1.47	1.38
3	P	273	M1N	O8-C7	4.72	1.31	1.23
3	Z	273	M1N	C35-C36	4.69	1.46	1.38
3	H	273	M1N	O8-C7	4.69	1.31	1.23
3	V	273	M1N	O8-C7	4.67	1.31	1.23
3	V	273	M1N	C35-C36	4.67	1.46	1.38
3	C	273	M1N	C38-C37	4.66	1.46	1.36
3	E	273	M1N	O8-C7	4.65	1.31	1.23
3	T	273	M1N	C7-N9	4.64	1.44	1.36
3	Z	273	M1N	C7-N9	4.61	1.44	1.36
3	E	273	M1N	C2-N1	4.59	1.43	1.34
3	T	273	M1N	C7-N6	4.59	1.45	1.35
3	C	273	M1N	C35-C36	4.58	1.46	1.38
3	R	273	M1N	C7-N9	4.58	1.44	1.36
3	H	273	M1N	C38-C37	4.53	1.46	1.36
3	N	273	M1N	C35-C36	4.53	1.46	1.38
3	C	273	M1N	C2-N1	4.47	1.43	1.34
3	Z	273	M1N	C2-N1	4.42	1.43	1.34
3	L	273	M1N	O8-C7	4.40	1.30	1.23
3	J	273	M1N	C2-N1	4.38	1.43	1.34
3	J	273	M1N	C7-N9	4.33	1.44	1.36
3	G	273	M1N	C7-N9	4.33	1.44	1.36
3	Z	273	M1N	C7-N6	4.33	1.44	1.35
3	H	273	M1N	C7-N6	4.32	1.44	1.35
3	P	273	M1N	C7-N9	4.29	1.43	1.36
3	C	273	M1N	O8-C7	4.26	1.30	1.23
3	L	273	M1N	C7-N6	4.24	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	273	M1N	C7-N9	4.23	1.43	1.36
3	J	273	M1N	C7-N6	4.18	1.44	1.35
3	2	273	M1N	C10-N9	4.17	1.54	1.47
3	H	273	M1N	C7-N9	4.16	1.43	1.36
3	N	273	M1N	C7-N6	4.08	1.44	1.35
3	V	273	M1N	C7-N6	4.01	1.43	1.35
3	J	273	M1N	C35-C34	4.00	1.45	1.36
3	C	273	M1N	C7-N6	4.00	1.43	1.35
3	P	273	M1N	C7-N6	3.98	1.43	1.35
3	E	273	M1N	C35-C34	3.96	1.45	1.36
3	N	273	M1N	C7-N9	3.95	1.43	1.36
3	L	273	M1N	C7-N9	3.90	1.43	1.36
3	E	273	M1N	C7-N6	3.88	1.43	1.35
3	V	273	M1N	C7-N9	3.88	1.43	1.36
3	R	273	M1N	C35-C34	3.87	1.44	1.36
3	E	273	M1N	C7-N9	3.83	1.43	1.36
3	G	273	M1N	C35-C34	3.76	1.44	1.36
3	R	273	M1N	C4-C2	-3.75	1.43	1.52
3	C	273	M1N	C35-C34	3.72	1.44	1.36
3	X	273	M1N	C10-N9	3.70	1.53	1.47
3	Z	273	M1N	C10-N9	3.65	1.53	1.47
3	X	273	M1N	C35-C34	3.64	1.44	1.36
3	P	273	M1N	C35-C34	3.64	1.44	1.36
3	T	273	M1N	C35-C34	3.60	1.44	1.36
3	L	273	M1N	C35-C34	3.57	1.44	1.36
3	Z	273	M1N	C4-C2	-3.51	1.44	1.52
3	Z	273	M1N	C35-C34	3.49	1.44	1.36
3	G	273	M1N	C4-C2	-3.47	1.44	1.52
3	H	273	M1N	C4-C2	-3.45	1.44	1.52
3	C	273	M1N	C4-C2	-3.45	1.44	1.52
3	T	273	M1N	C10-N9	3.45	1.53	1.47
3	J	273	M1N	C10-N9	3.44	1.53	1.47
3	T	273	M1N	C4-C2	-3.44	1.44	1.52
3	H	273	M1N	C35-C34	3.44	1.43	1.36
3	V	273	M1N	C10-N9	3.42	1.53	1.47
3	C	273	M1N	C7-N9	3.41	1.42	1.36
3	L	273	M1N	C4-C2	-3.41	1.44	1.52
3	N	273	M1N	C35-C34	3.38	1.43	1.36
3	T	273	M1N	C14-N9	3.37	1.53	1.47
3	G	273	M1N	C10-N9	3.34	1.53	1.47
3	L	273	M1N	C10-N9	3.33	1.53	1.47
3	P	273	M1N	C10-N9	3.28	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	273	M1N	C4-C2	-3.26	1.44	1.52
3	2	273	M1N	C35-C34	3.24	1.43	1.36
3	V	273	M1N	C35-C34	3.17	1.43	1.36
3	G	273	M1N	C14-N9	3.14	1.52	1.47
3	N	273	M1N	C10-N9	3.13	1.52	1.47
3	P	273	M1N	C4-C2	-3.13	1.45	1.52
3	J	273	M1N	C4-C2	-3.12	1.45	1.52
3	R	273	M1N	C10-N9	3.12	1.52	1.47
3	X	273	M1N	C14-N9	3.11	1.52	1.47
3	C	273	M1N	C10-N9	3.09	1.52	1.47
3	N	273	M1N	C4-C2	-3.08	1.45	1.52
3	E	273	M1N	C10-N9	3.07	1.52	1.47
3	Z	273	M1N	C14-N9	3.06	1.52	1.47
3	P	273	M1N	C14-N9	2.98	1.52	1.47
3	J	273	M1N	C14-N9	2.97	1.52	1.47
3	X	273	M1N	C4-C2	-2.96	1.45	1.52
3	H	273	M1N	C10-N9	2.95	1.52	1.47
3	V	273	M1N	C14-N9	2.91	1.52	1.47
3	N	273	M1N	C14-N9	2.87	1.52	1.47
3	R	273	M1N	C14-N9	2.85	1.52	1.47
3	Z	273	M1N	O12-C11	2.78	1.53	1.42
3	X	273	M1N	O12-C11	2.77	1.53	1.42
3	V	273	M1N	O12-C11	2.75	1.53	1.42
3	L	273	M1N	C14-N9	2.71	1.51	1.47
3	X	273	M1N	C36-C31	2.62	1.42	1.37
3	2	273	M1N	C4-C2	-2.62	1.46	1.52
3	R	273	M1N	O12-C11	2.61	1.52	1.42
3	2	273	M1N	C14-N9	2.61	1.51	1.47
3	G	273	M1N	C36-C31	2.61	1.42	1.37
3	P	273	M1N	O12-C11	2.60	1.52	1.42
3	T	273	M1N	C32-C33	2.58	1.47	1.43
3	T	273	M1N	C36-C31	2.56	1.42	1.37
3	2	273	M1N	O12-C11	2.54	1.52	1.42
3	V	273	M1N	C4-C2	-2.53	1.46	1.52
3	H	273	M1N	C14-N9	2.50	1.51	1.47
3	C	273	M1N	C14-N9	2.49	1.51	1.47
3	G	273	M1N	O12-C11	2.49	1.52	1.42
3	C	273	M1N	O12-C11	2.48	1.52	1.42
3	T	273	M1N	O12-C11	2.47	1.52	1.42
3	E	273	M1N	O12-C11	2.47	1.52	1.42
3	N	273	M1N	C32-C33	2.47	1.47	1.43
3	J	273	M1N	O12-C11	2.45	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	273	M1N	C32-C33	2.43	1.47	1.43
3	N	273	M1N	O12-C11	2.41	1.52	1.42
3	G	273	M1N	C32-C33	2.39	1.47	1.43
3	E	273	M1N	C14-N9	2.38	1.51	1.47
3	H	273	M1N	O12-C11	2.38	1.51	1.42
3	L	273	M1N	O12-C11	2.36	1.51	1.42
3	2	273	M1N	C36-C31	2.36	1.41	1.37
3	G	273	M1N	C31-C32	2.33	1.48	1.42
3	R	273	M1N	C32-C33	2.30	1.47	1.43
3	V	273	M1N	C31-C32	2.30	1.48	1.42
3	X	273	M1N	C32-C33	2.27	1.47	1.43
3	T	273	M1N	C31-C32	2.26	1.47	1.42
3	X	273	M1N	C4-N6	2.24	1.50	1.45
3	2	273	M1N	C38-C39	2.23	1.43	1.38
3	Z	273	M1N	C36-C31	2.20	1.41	1.37
3	X	273	M1N	C31-C32	2.19	1.47	1.42
3	N	273	M1N	C38-C39	2.18	1.43	1.38
3	R	273	M1N	C36-C31	2.18	1.41	1.37
3	V	273	M1N	C36-C31	2.17	1.41	1.37
3	V	273	M1N	C38-C39	2.16	1.43	1.38
3	X	273	M1N	C38-C39	2.13	1.42	1.38
3	N	273	M1N	C31-C32	2.10	1.47	1.42
3	J	273	M1N	C32-C33	2.10	1.46	1.43
3	2	273	M1N	C32-C33	2.06	1.46	1.43
3	L	273	M1N	C36-C31	2.05	1.41	1.37
3	E	273	M1N	C36-C31	2.04	1.41	1.37
3	J	273	M1N	C38-C39	2.02	1.42	1.38
3	H	273	M1N	C36-C31	2.02	1.41	1.37
3	P	273	M1N	C38-C39	2.02	1.42	1.38
3	R	273	M1N	C38-C39	2.01	1.42	1.38
3	T	273	M1N	C38-C39	2.00	1.42	1.38

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	273	M1N	C15-C22-C23	19.73	140.51	115.32
3	T	273	M1N	C15-C22-C23	19.14	139.76	115.32
3	2	273	M1N	C15-C22-C23	19.00	139.58	115.32
3	L	273	M1N	C15-C22-C23	18.57	139.02	115.32
3	G	273	M1N	C15-C22-C23	18.23	138.59	115.32
3	P	273	M1N	C15-C22-C23	17.99	138.29	115.32
3	X	273	M1N	C15-C22-C23	17.78	138.02	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	273	M1N	C15-C22-C23	17.48	137.64	115.32
3	N	273	M1N	C15-C22-C23	17.30	137.41	115.32
3	H	273	M1N	C15-C22-C23	17.19	137.26	115.32
3	J	273	M1N	C15-C22-C23	16.85	136.83	115.32
3	C	273	M1N	C15-C22-C23	16.55	136.45	115.32
3	V	273	M1N	C15-C22-C23	16.03	135.78	115.32
3	Z	273	M1N	C15-C22-C23	15.05	134.54	115.32
3	L	273	M1N	O8-C7-N9	-12.44	104.31	121.67
3	X	273	M1N	O8-C7-N9	-11.98	104.96	121.67
3	C	273	M1N	O8-C7-N9	-11.72	105.31	121.67
3	2	273	M1N	N6-C7-N9	11.71	138.14	117.23
3	H	273	M1N	O8-C7-N9	-11.48	105.66	121.67
3	R	273	M1N	O8-C7-N9	-11.37	105.80	121.67
3	E	273	M1N	O8-C7-N9	-11.07	106.23	121.67
3	V	273	M1N	O8-C7-N9	-10.85	106.54	121.67
3	2	273	M1N	O8-C7-N9	-10.76	106.66	121.67
3	L	273	M1N	N6-C7-N9	10.55	136.07	117.23
3	Z	273	M1N	O8-C7-N9	-10.52	106.99	121.67
3	G	273	M1N	O8-C7-N9	-10.46	107.07	121.67
3	T	273	M1N	O8-C7-N9	-10.36	107.21	121.67
3	H	273	M1N	N6-C7-N9	10.28	135.59	117.23
3	E	273	M1N	N6-C7-N9	10.23	135.50	117.23
3	P	273	M1N	O8-C7-N9	-10.19	107.46	121.67
3	C	273	M1N	N6-C7-N9	10.16	135.37	117.23
3	N	273	M1N	O8-C7-N9	-9.93	107.82	121.67
3	Z	273	M1N	N6-C7-N9	9.91	134.92	117.23
3	J	273	M1N	O8-C7-N9	-9.75	108.07	121.67
3	R	273	M1N	N6-C7-N9	9.65	134.46	117.23
3	P	273	M1N	N6-C7-N9	9.63	134.42	117.23
3	X	273	M1N	N6-C7-N9	9.63	134.41	117.23
3	V	273	M1N	N6-C7-N9	9.45	134.10	117.23
3	G	273	M1N	C4-C2-N1	8.86	135.53	116.63
3	J	273	M1N	N6-C7-N9	8.80	132.94	117.23
3	2	273	M1N	C4-C2-N1	8.74	135.27	116.63
3	T	273	M1N	N6-C7-N9	8.64	132.66	117.23
3	C	273	M1N	C4-C2-N1	8.59	134.95	116.63
3	P	273	M1N	C4-C2-N1	8.56	134.88	116.63
3	H	273	M1N	C4-C2-N1	8.45	134.65	116.63
3	L	273	M1N	C4-C2-N1	8.45	134.65	116.63
3	R	273	M1N	C4-C2-N1	8.43	134.60	116.63
3	N	273	M1N	C4-C2-N1	8.19	134.09	116.63
3	N	273	M1N	N6-C7-N9	8.10	131.68	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	273	M1N	N6-C7-N9	7.93	131.39	117.23
3	V	273	M1N	C4-C2-N1	7.72	133.10	116.63
3	J	273	M1N	C4-C2-N1	7.69	133.03	116.63
3	T	273	M1N	C4-C2-N1	7.56	132.76	116.63
3	X	273	M1N	C4-C2-N1	7.56	132.74	116.63
3	Z	273	M1N	C4-C2-N1	7.39	132.40	116.63
3	2	273	M1N	O3-C2-N1	-7.16	110.14	122.96
3	E	273	M1N	C4-C2-N1	7.02	131.60	116.63
3	V	273	M1N	O3-C2-N1	-6.96	110.49	122.96
3	C	273	M1N	O3-C2-N1	-6.33	111.62	122.96
3	P	273	M1N	O3-C2-N1	-6.29	111.69	122.96
3	N	273	M1N	O3-C2-N1	-6.23	111.81	122.96
3	G	273	M1N	O3-C2-N1	-5.96	112.29	122.96
3	J	273	M1N	O3-C2-N1	-5.96	112.29	122.96
3	H	273	M1N	O3-C2-N1	-5.62	112.90	122.96
3	2	273	M1N	C5-C4-N6	-5.48	99.48	110.83
3	E	273	M1N	O3-C2-N1	-5.36	113.36	122.96
3	T	273	M1N	C14-N9-C7	-5.34	102.41	121.83
3	X	273	M1N	O3-C2-N1	-5.26	113.53	122.96
3	G	273	M1N	C14-N9-C7	-5.20	102.93	121.83
3	P	273	M1N	C14-N9-C7	-5.17	103.05	121.83
3	X	273	M1N	C14-N9-C7	-5.12	103.23	121.83
3	L	273	M1N	O3-C2-N1	-5.12	113.79	122.96
3	Z	273	M1N	O3-C2-N1	-5.02	113.98	122.96
3	H	273	M1N	C5-C31-C32	-5.01	113.61	120.89
3	P	273	M1N	C5-C4-N6	-5.01	100.47	110.83
3	N	273	M1N	C14-N9-C7	-5.00	103.66	121.83
3	V	273	M1N	C14-N9-C7	-4.95	103.85	121.83
3	R	273	M1N	C14-N9-C7	-4.94	103.86	121.83
3	E	273	M1N	C14-N9-C7	-4.93	103.92	121.83
3	R	273	M1N	O3-C2-N1	-4.91	114.17	122.96
3	T	273	M1N	O3-C2-N1	-4.82	114.33	122.96
3	C	273	M1N	C14-N9-C7	-4.81	104.33	121.83
3	J	273	M1N	C14-N9-C7	-4.70	104.73	121.83
3	H	273	M1N	C14-N9-C7	-4.65	104.91	121.83
3	H	273	M1N	C5-C31-C36	4.63	127.26	119.92
3	L	273	M1N	C14-N9-C7	-4.57	105.23	121.83
3	2	273	M1N	C14-N9-C7	-4.54	105.31	121.83
3	E	273	M1N	C5-C31-C32	-4.44	114.44	120.89
3	R	273	M1N	O3-C2-C4	-4.42	111.22	120.48
3	R	273	M1N	C5-C31-C32	-4.37	114.55	120.89
3	X	273	M1N	C5-C31-C32	-4.32	114.62	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	273	M1N	O3-C2-C4	-4.26	111.55	120.48
3	Z	273	M1N	C5-C31-C32	-4.21	114.78	120.89
3	Z	273	M1N	C14-N9-C7	-4.15	106.74	121.83
3	2	273	M1N	C5-C31-C32	-4.11	114.92	120.89
3	P	273	M1N	C5-C31-C32	-4.06	114.99	120.89
3	G	273	M1N	O3-C2-C4	-3.99	112.11	120.48
3	C	273	M1N	C5-C31-C32	-3.90	115.22	120.89
3	Z	273	M1N	B-C15-C22	-3.90	104.96	112.31
3	2	273	M1N	C5-C31-C36	3.86	126.03	119.92
3	H	273	M1N	O3-C2-C4	-3.85	112.40	120.48
3	X	273	M1N	C5-C31-C36	3.74	125.84	119.92
3	J	273	M1N	C10-N9-C14	3.72	120.27	112.68
3	J	273	M1N	C5-C31-C32	-3.71	115.50	120.89
3	T	273	M1N	O3-C2-C4	-3.63	112.88	120.48
3	R	273	M1N	C15-N1-C2	-3.56	114.01	122.99
3	V	273	M1N	B-C15-C22	-3.53	105.65	112.31
3	X	273	M1N	B-C15-C22	-3.52	105.67	112.31
3	G	273	M1N	C5-C31-C32	-3.49	115.83	120.89
3	Z	273	M1N	C5-C31-C36	3.47	125.42	119.92
3	N	273	M1N	C15-N1-C2	-3.45	114.28	122.99
3	X	273	M1N	C10-N9-C14	3.44	119.69	112.68
3	C	273	M1N	O3-C2-C4	-3.42	113.32	120.48
3	2	273	M1N	C15-N1-C2	-3.40	114.42	122.99
3	P	273	M1N	O3-C2-C4	-3.39	113.37	120.48
3	2	273	M1N	C31-C5-C4	3.39	119.61	113.49
3	C	273	M1N	C5-C31-C36	3.37	125.26	119.92
3	V	273	M1N	C31-C5-C4	3.35	119.54	113.49
3	V	273	M1N	C5-C4-N6	-3.34	103.91	110.83
3	Z	273	M1N	O3-C2-C4	-3.32	113.52	120.48
3	R	273	M1N	C5-C31-C36	3.30	125.15	119.92
3	C	273	M1N	C5-C4-N6	-3.29	104.02	110.83
3	E	273	M1N	C5-C31-C36	3.26	125.08	119.92
3	N	273	M1N	C40-C33-C32	3.24	123.31	119.12
3	X	273	M1N	O3-C2-C4	-3.24	113.70	120.48
3	N	273	M1N	B-C15-C22	-3.22	106.23	112.31
3	H	273	M1N	C31-C5-C4	3.21	119.29	113.49
3	P	273	M1N	C15-N1-C2	-3.18	114.96	122.99
3	T	273	M1N	C15-N1-C2	-3.15	115.05	122.99
3	V	273	M1N	C5-C31-C36	3.14	124.90	119.92
3	E	273	M1N	C5-C4-N6	-3.13	104.36	110.83
3	G	273	M1N	C15-N1-C2	-3.12	115.11	122.99
3	G	273	M1N	C5-C31-C36	3.12	124.86	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	273	M1N	C11-O12-C13	3.07	119.81	109.88
3	L	273	M1N	C40-C33-C32	3.05	123.06	119.12
3	N	273	M1N	O3-C2-C4	-3.05	114.09	120.48
3	N	273	M1N	C5-C31-C32	-3.05	116.47	120.89
3	V	273	M1N	C5-C31-C32	-3.05	116.47	120.89
3	Z	273	M1N	C11-O12-C13	3.02	119.64	109.88
3	P	273	M1N	C5-C31-C36	2.99	124.66	119.92
3	P	273	M1N	C31-C5-C4	2.94	118.80	113.49
3	Z	273	M1N	C11-C10-N9	-2.94	103.62	109.82
3	E	273	M1N	C15-N1-C2	-2.94	115.58	122.99
3	X	273	M1N	C11-O12-C13	2.87	119.17	109.88
3	J	273	M1N	C5-C31-C36	2.85	124.44	119.92
3	P	273	M1N	C40-C33-C32	2.84	122.79	119.12
3	2	273	M1N	O3-C2-C4	-2.82	114.57	120.48
3	2	273	M1N	B-C15-C22	-2.81	107.01	112.31
3	2	273	M1N	O8-C7-N6	-2.81	115.19	122.96
3	H	273	M1N	C5-C4-N6	-2.80	105.03	110.83
3	E	273	M1N	C11-O12-C13	2.79	118.91	109.88
3	J	273	M1N	O3-C2-C4	-2.78	114.66	120.48
3	2	273	M1N	O12-C13-C14	-2.77	105.80	111.77
3	J	273	M1N	C5-C4-N6	-2.77	105.10	110.83
3	T	273	M1N	C5-C31-C32	-2.73	116.92	120.89
3	J	273	M1N	C40-C33-C32	2.72	122.63	119.12
3	N	273	M1N	C11-C10-N9	-2.69	104.15	109.82
3	T	273	M1N	C40-C33-C32	2.68	122.59	119.12
3	C	273	M1N	C40-C33-C32	2.68	122.58	119.12
3	L	273	M1N	C40-C33-C34	-2.66	116.95	123.01
3	T	273	M1N	C5-C31-C36	2.64	124.11	119.92
3	V	273	M1N	C11-O12-C13	2.63	118.38	109.88
3	N	273	M1N	C5-C31-C36	2.62	124.07	119.92
3	E	273	M1N	O3-C2-C4	-2.62	114.99	120.48
3	G	273	M1N	C10-N9-C14	2.60	117.98	112.68
3	N	273	M1N	C5-C4-N6	-2.59	105.46	110.83
3	V	273	M1N	C40-C33-C32	2.59	122.47	119.12
3	N	273	M1N	C40-C33-C34	-2.58	117.12	123.01
3	L	273	M1N	C5-C31-C36	2.56	123.98	119.92
3	X	273	M1N	C31-C5-C4	2.56	118.11	113.49
3	E	273	M1N	C2-C4-N6	2.54	117.99	111.11
3	C	273	M1N	B-C15-C22	-2.54	107.51	112.31
3	L	273	M1N	C5-C31-C32	-2.52	117.23	120.89
3	R	273	M1N	C10-N9-C7	-2.51	112.71	121.83
3	E	273	M1N	C10-N9-C7	-2.47	112.86	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	273	M1N	C2-C4-N6	2.42	117.67	111.11
3	C	273	M1N	C11-O12-C13	2.40	117.65	109.88
3	C	273	M1N	C2-C4-N6	2.40	117.61	111.11
3	Z	273	M1N	C2-C4-N6	2.40	117.60	111.11
3	L	273	M1N	C10-N9-C14	2.39	117.56	112.68
3	R	273	M1N	C11-O12-C13	2.39	117.59	109.88
3	E	273	M1N	C40-C33-C32	2.38	122.20	119.12
3	X	273	M1N	C40-C33-C32	2.37	122.18	119.12
3	L	273	M1N	C11-O12-C13	2.36	117.52	109.88
3	T	273	M1N	C10-N9-C14	2.36	117.50	112.68
3	Z	273	M1N	C31-C5-C4	2.36	117.74	113.49
3	2	273	M1N	C10-N9-C7	-2.36	113.27	121.83
3	G	273	M1N	C11-O12-C13	2.34	117.45	109.88
3	H	273	M1N	C10-N9-C7	-2.32	113.39	121.83
3	V	273	M1N	C40-C33-C34	-2.32	117.72	123.01
3	P	273	M1N	C40-C33-C34	-2.32	117.73	123.01
3	C	273	M1N	C40-C33-C34	-2.31	117.73	123.01
3	L	273	M1N	C10-N9-C7	-2.26	113.62	121.83
3	2	273	M1N	C2-C4-N6	2.26	117.22	111.11
3	J	273	M1N	C40-C33-C34	-2.26	117.86	123.01
3	P	273	M1N	C11-O12-C13	2.25	117.17	109.88
3	C	273	M1N	C10-N9-C14	2.25	117.27	112.68
3	C	273	M1N	C15-N1-C2	-2.24	117.34	122.99
3	H	273	M1N	C10-N9-C14	2.23	117.24	112.68
3	T	273	M1N	C40-C33-C34	-2.23	117.92	123.01
3	Z	273	M1N	C10-N9-C14	2.22	117.21	112.68
3	T	273	M1N	O12-C13-C14	-2.22	107.00	111.77
3	H	273	M1N	C40-C33-C34	-2.20	117.98	123.01
3	R	273	M1N	C10-N9-C14	2.20	117.17	112.68
3	L	273	M1N	C15-N1-C2	-2.19	117.45	122.99
3	Z	273	M1N	C5-C4-N6	-2.17	106.33	110.83
3	V	273	M1N	C5-C4-C2	2.16	115.84	110.30
3	H	273	M1N	C15-N1-C2	-2.16	117.54	122.99
3	2	273	M1N	C40-C33-C34	-2.16	118.09	123.01
3	N	273	M1N	C34-C35-C36	2.14	124.28	121.00
3	N	273	M1N	O12-C13-C14	-2.13	107.18	111.77
3	P	273	M1N	C35-C36-C31	-2.13	117.72	121.50
3	L	273	M1N	C11-C10-N9	-2.13	105.33	109.82
3	T	273	M1N	C11-C10-N9	-2.12	105.36	109.82
3	2	273	M1N	C40-C33-C32	2.12	121.86	119.12
3	J	273	M1N	C11-O12-C13	2.11	116.70	109.88
3	E	273	M1N	C11-C10-N9	-2.11	105.38	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	273	M1N	C40-C33-C34	-2.09	118.24	123.01
3	N	273	M1N	C10-N9-C14	2.09	116.94	112.68
3	T	273	M1N	C10-N9-C7	-2.08	114.25	121.83
3	X	273	M1N	C10-N9-C7	-2.08	114.27	121.83
3	G	273	M1N	C40-C33-C32	2.08	121.81	119.12
3	G	273	M1N	C11-C10-N9	-2.07	105.46	109.82
3	X	273	M1N	C40-C33-C34	-2.07	118.29	123.01
3	P	273	M1N	C10-N9-C14	2.07	116.90	112.68
3	T	273	M1N	C31-C5-C4	2.06	117.20	113.49
3	J	273	M1N	C11-C10-N9	-2.05	105.50	109.82
3	C	273	M1N	C31-C5-C4	2.05	117.19	113.49
3	N	273	M1N	C35-C34-C33	-2.05	117.63	120.48
3	C	273	M1N	C24-C23-C22	2.04	118.41	111.08
3	G	273	M1N	C40-C33-C34	-2.04	118.36	123.01
3	J	273	M1N	C15-N1-C2	-2.03	117.85	122.99
3	C	273	M1N	C10-N9-C7	-2.03	114.46	121.83
3	V	273	M1N	C15-N1-C2	-2.02	117.89	122.99
3	V	273	M1N	C2-C4-N6	2.02	116.57	111.11
3	J	273	M1N	C5-C4-C2	2.02	115.46	110.30
3	P	273	M1N	C11-C10-N9	-2.01	105.58	109.82
3	V	273	M1N	C10-N9-C7	-2.01	114.51	121.83
3	P	273	M1N	C2-C4-N6	2.01	116.55	111.11
3	H	273	M1N	C35-C34-C33	-2.00	117.70	120.48

There are no chirality outliers.

All (155) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	273	M1N	O3-C2-N1-C15
3	H	273	M1N	C4-C2-N1-C15
3	H	273	M1N	B-C15-C22-C23
3	H	273	M1N	C2-C4-C5-C31
3	H	273	M1N	N6-C4-C5-C31
3	H	273	M1N	N9-C7-N6-C4
3	H	273	M1N	O8-C7-N6-C4
3	C	273	M1N	O3-C2-N1-C15
3	C	273	M1N	C4-C2-N1-C15
3	C	273	M1N	B-C15-C22-C23
3	C	273	M1N	C2-C4-C5-C31
3	C	273	M1N	N9-C7-N6-C4
3	C	273	M1N	O8-C7-N6-C4
3	E	273	M1N	O3-C2-N1-C15

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Mol	Chain	Res	Type	Atoms
3	E	273	M1N	C2-C4-C5-C31
3	E	273	M1N	N6-C4-C5-C31
3	E	273	M1N	N9-C7-N6-C4
3	E	273	M1N	O8-C7-N6-C4
3	G	273	M1N	O3-C2-N1-C15
3	G	273	M1N	N6-C4-C5-C31
3	G	273	M1N	N9-C7-N6-C4
3	G	273	M1N	O8-C7-N6-C4
3	J	273	M1N	O3-C2-N1-C15
3	J	273	M1N	B-C15-C22-C23
3	J	273	M1N	C2-C4-C5-C31
3	J	273	M1N	N6-C4-C5-C31
3	J	273	M1N	N9-C7-N6-C4
3	J	273	M1N	O8-C7-N6-C4
3	L	273	M1N	O3-C2-N1-C15
3	L	273	M1N	N6-C4-C5-C31
3	L	273	M1N	N9-C7-N6-C4
3	L	273	M1N	O8-C7-N6-C4
3	N	273	M1N	O3-C2-N1-C15
3	N	273	M1N	B-C15-C22-C23
3	N	273	M1N	N9-C7-N6-C4
3	N	273	M1N	O8-C7-N6-C4
3	P	273	M1N	O3-C2-N1-C15
3	P	273	M1N	C4-C2-N1-C15
3	P	273	M1N	C2-C4-C5-C31
3	P	273	M1N	N6-C4-C5-C31
3	P	273	M1N	N9-C7-N6-C4
3	P	273	M1N	O8-C7-N6-C4
3	R	273	M1N	O3-C2-N1-C15
3	R	273	M1N	C15-C22-C23-C25
3	R	273	M1N	C15-C22-C23-C24
3	R	273	M1N	C2-C4-C5-C31
3	R	273	M1N	N6-C4-C5-C31
3	R	273	M1N	N9-C7-N6-C4
3	R	273	M1N	O8-C7-N6-C4
3	T	273	M1N	O3-C2-N1-C15
3	T	273	M1N	C4-C2-N1-C15
3	T	273	M1N	C2-C4-C5-C31
3	T	273	M1N	N6-C4-C5-C31
3	T	273	M1N	N9-C7-N6-C4
3	T	273	M1N	O8-C7-N6-C4
3	V	273	M1N	O3-C2-N1-C15

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Mol	Chain	Res	Type	Atoms
3	V	273	M1N	C4-C2-N1-C15
3	V	273	M1N	B-C15-C22-C23
3	V	273	M1N	N6-C4-C5-C31
3	V	273	M1N	N9-C7-N6-C4
3	V	273	M1N	O8-C7-N6-C4
3	V	273	M1N	O8-C7-N9-C14
3	V	273	M1N	C36-C31-C5-C4
3	V	273	M1N	C32-C31-C5-C4
3	X	273	M1N	O3-C2-N1-C15
3	X	273	M1N	C4-C2-N1-C15
3	X	273	M1N	B-C15-C22-C23
3	X	273	M1N	C2-C4-C5-C31
3	X	273	M1N	N9-C7-N6-C4
3	X	273	M1N	O8-C7-N6-C4
3	X	273	M1N	N6-C7-N9-C14
3	X	273	M1N	O8-C7-N9-C14
3	Z	273	M1N	O3-C2-N1-C15
3	Z	273	M1N	C4-C2-N1-C15
3	Z	273	M1N	B-C15-C22-C23
3	Z	273	M1N	C2-C4-C5-C31
3	Z	273	M1N	N6-C4-C5-C31
3	Z	273	M1N	N9-C7-N6-C4
3	Z	273	M1N	O8-C7-N6-C4
3	2	273	M1N	O3-C2-N1-C15
3	2	273	M1N	C4-C2-N1-C15
3	2	273	M1N	B-C15-C22-C23
3	2	273	M1N	C2-C4-C5-C31
3	2	273	M1N	N9-C7-N6-C4
3	2	273	M1N	O8-C7-N6-C4
3	2	273	M1N	N6-C7-N9-C10
3	2	273	M1N	O8-C7-N9-C10
3	E	273	M1N	C4-C2-N1-C15
3	G	273	M1N	C4-C2-N1-C15
3	L	273	M1N	C4-C2-N1-C15
3	N	273	M1N	C4-C2-N1-C15
3	C	273	M1N	N6-C4-C5-C31
3	2	273	M1N	N6-C4-C5-C31
3	V	273	M1N	C2-C4-C5-C31
3	N	273	M1N	N6-C4-C5-C31
3	J	273	M1N	C4-C2-N1-C15
3	X	273	M1N	N6-C4-C5-C31
3	G	273	M1N	C2-C4-C5-C31

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Mol	Chain	Res	Type	Atoms
3	L	273	M1N	C2-C4-C5-C31
3	R	273	M1N	C4-C2-N1-C15
3	C	273	M1N	O8-C7-N9-C14
3	J	273	M1N	O8-C7-N9-C14
3	L	273	M1N	O8-C7-N9-C14
3	N	273	M1N	O8-C7-N9-C14
3	Z	273	M1N	O8-C7-N9-C14
3	J	273	M1N	N6-C7-N9-C14
3	L	273	M1N	N6-C7-N9-C14
3	N	273	M1N	N6-C7-N9-C14
3	V	273	M1N	N6-C7-N9-C14
3	E	273	M1N	C36-C31-C5-C4
3	P	273	M1N	C36-C31-C5-C4
3	N	273	M1N	C2-C4-C5-C31
3	C	273	M1N	N6-C7-N9-C14
3	Z	273	M1N	N6-C7-N9-C14
3	H	273	M1N	C36-C31-C5-C4
3	C	273	M1N	C36-C31-C5-C4
3	G	273	M1N	C36-C31-C5-C4
3	J	273	M1N	C36-C31-C5-C4
3	L	273	M1N	C36-C31-C5-C4
3	N	273	M1N	C36-C31-C5-C4
3	R	273	M1N	C36-C31-C5-C4
3	T	273	M1N	C36-C31-C5-C4
3	X	273	M1N	C36-C31-C5-C4
3	Z	273	M1N	C36-C31-C5-C4
3	2	273	M1N	C36-C31-C5-C4
3	R	273	M1N	N1-C15-C22-C23
3	H	273	M1N	C15-C22-C23-C25
3	E	273	M1N	C15-C22-C23-C25
3	G	273	M1N	C15-C22-C23-C25
3	L	273	M1N	C15-C22-C23-C25
3	P	273	M1N	C15-C22-C23-C25
3	T	273	M1N	C15-C22-C23-C25
3	2	273	M1N	C15-C22-C23-C24
3	P	273	M1N	O8-C7-N9-C14
3	V	273	M1N	N1-C15-C22-C23
3	P	273	M1N	C32-C31-C5-C4
3	G	273	M1N	O8-C7-N9-C14
3	N	273	M1N	N1-C15-C22-C23
3	P	273	M1N	N6-C7-N9-C14
3	X	273	M1N	N1-C15-C22-C23

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Mol	Chain	Res	Type	Atoms
3	G	273	M1N	N6-C7-N9-C14
3	Z	273	M1N	N1-C15-C22-C23
3	R	273	M1N	N6-C7-N9-C10
3	H	273	M1N	C32-C31-C5-C4
3	C	273	M1N	C32-C31-C5-C4
3	E	273	M1N	C32-C31-C5-C4
3	G	273	M1N	C32-C31-C5-C4
3	J	273	M1N	C32-C31-C5-C4
3	L	273	M1N	C32-C31-C5-C4
3	N	273	M1N	C32-C31-C5-C4
3	R	273	M1N	C32-C31-C5-C4
3	T	273	M1N	C32-C31-C5-C4
3	X	273	M1N	C32-C31-C5-C4
3	Z	273	M1N	C32-C31-C5-C4
3	2	273	M1N	C32-C31-C5-C4

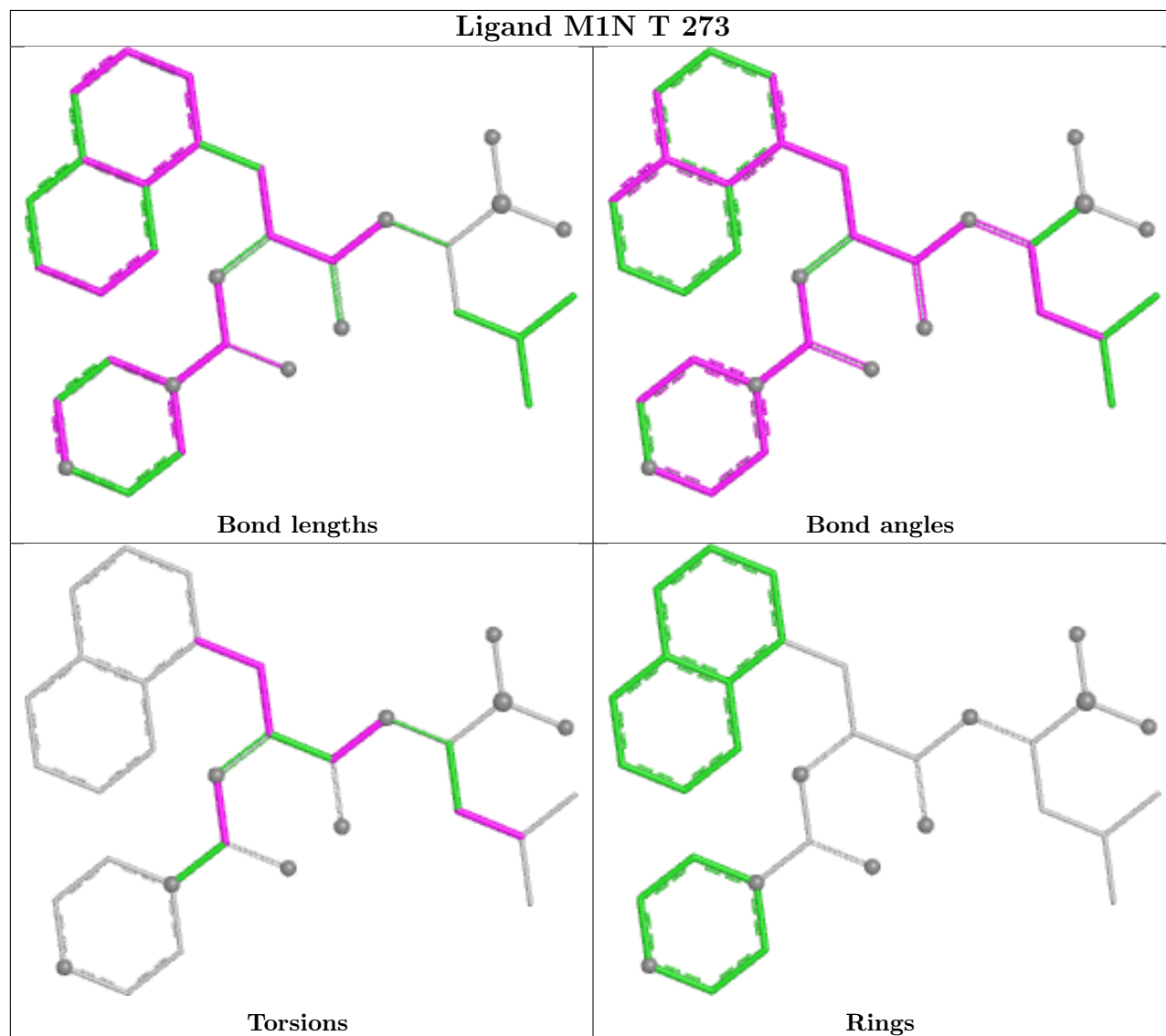
There are no ring outliers.

14 monomers are involved in 189 short contacts:

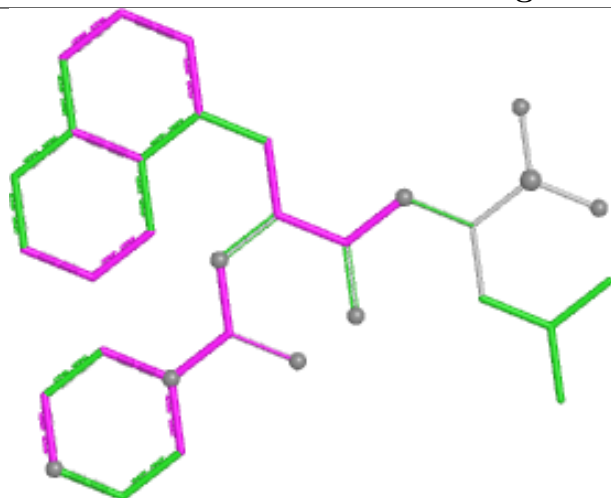
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	273	M1N	11	0
3	2	273	M1N	10	0
3	P	273	M1N	14	0
3	L	273	M1N	16	0
3	X	273	M1N	14	0
3	G	273	M1N	10	0
3	J	273	M1N	17	0
3	H	273	M1N	12	0
3	V	273	M1N	17	0
3	C	273	M1N	12	0
3	R	273	M1N	9	0
3	N	273	M1N	16	0
3	Z	273	M1N	16	0
3	E	273	M1N	15	0

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

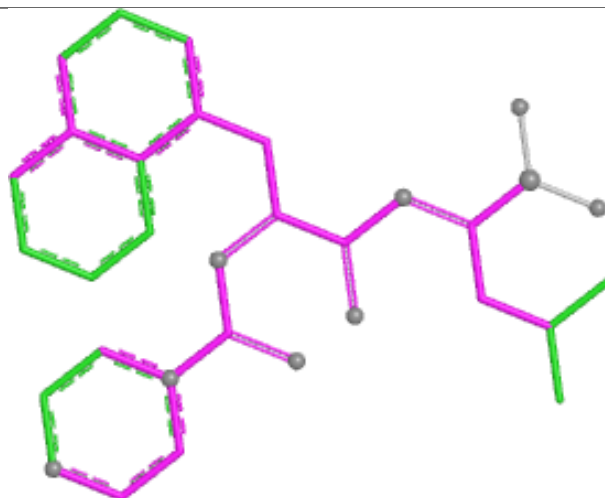
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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



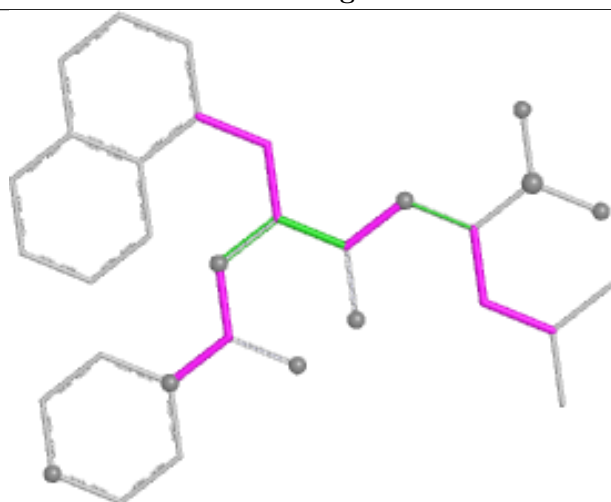
Ligand M1N 2 273



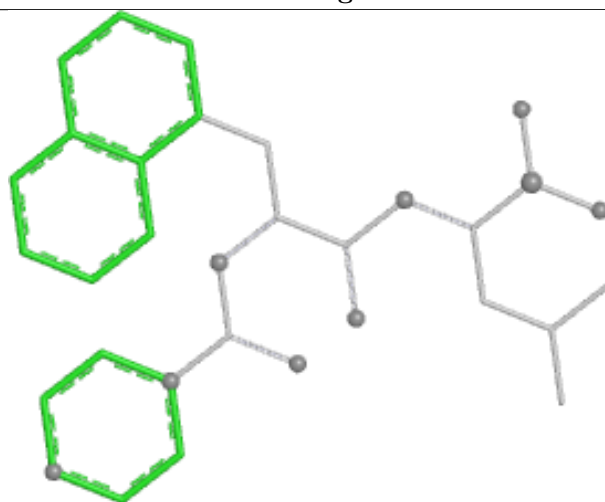
Bond lengths



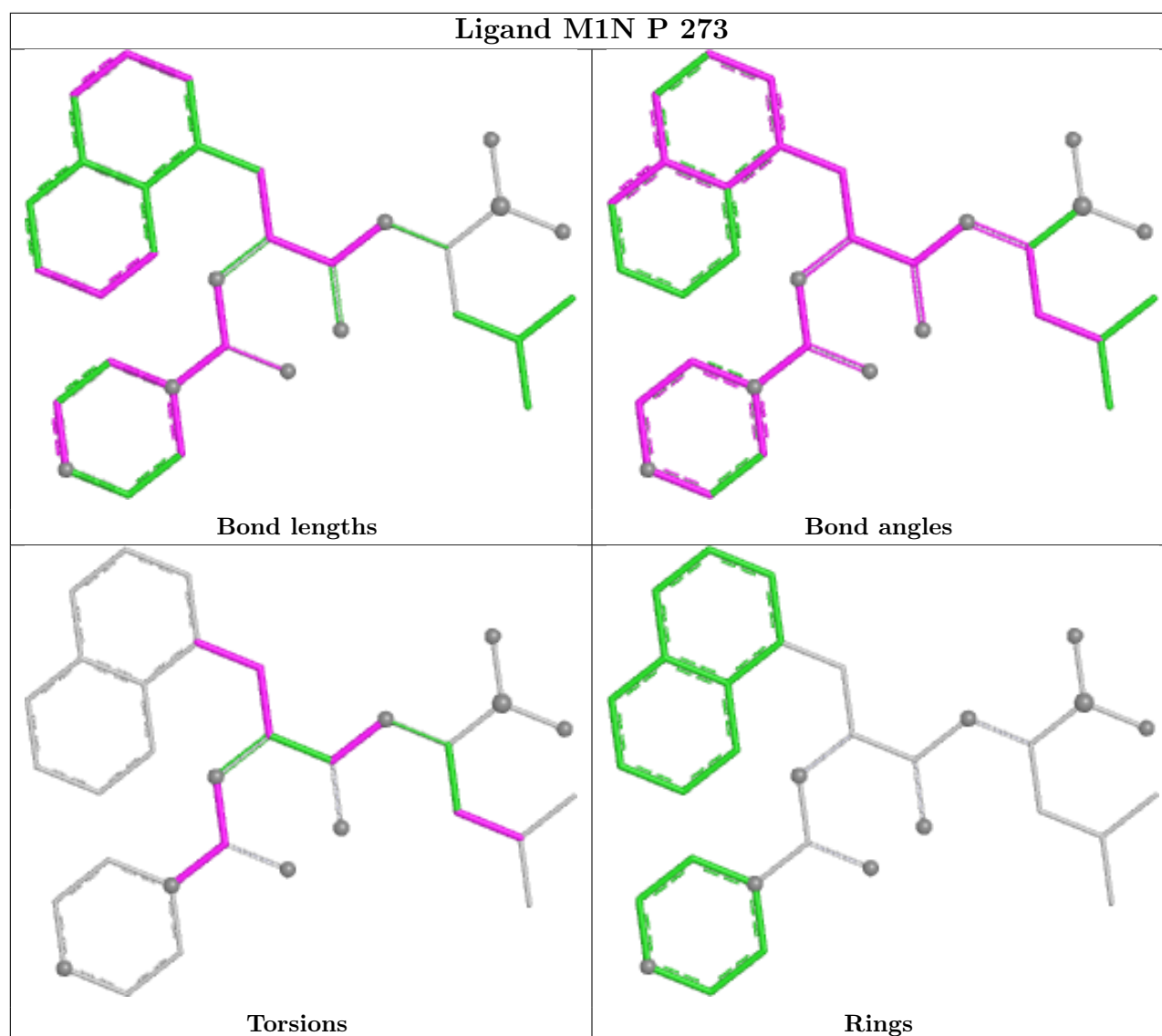
Bond angles



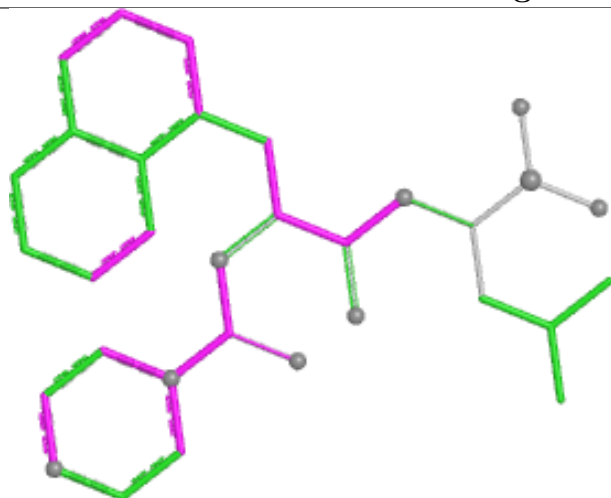
Torsions



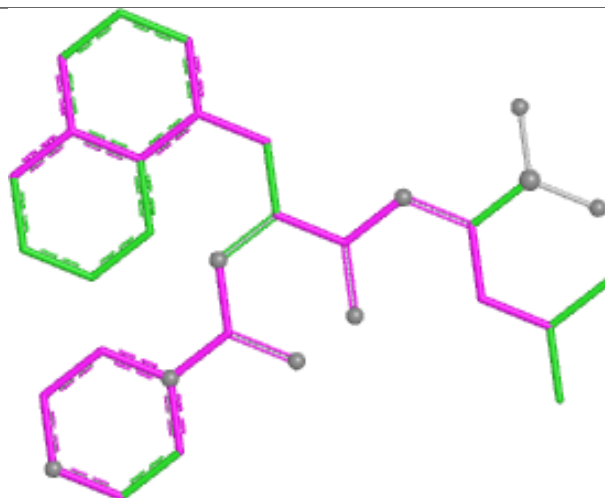
Rings



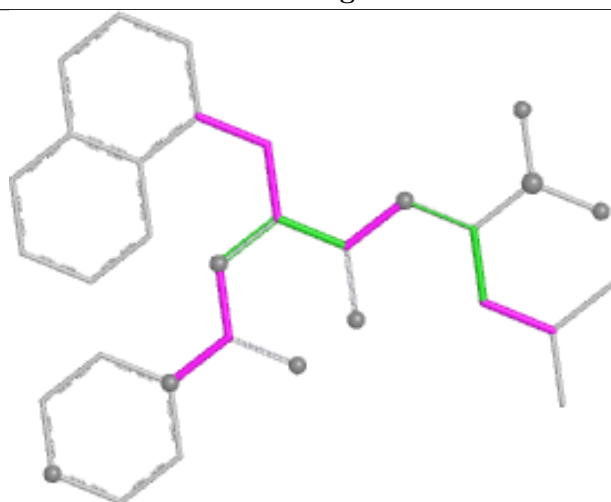
Ligand M1N L 273



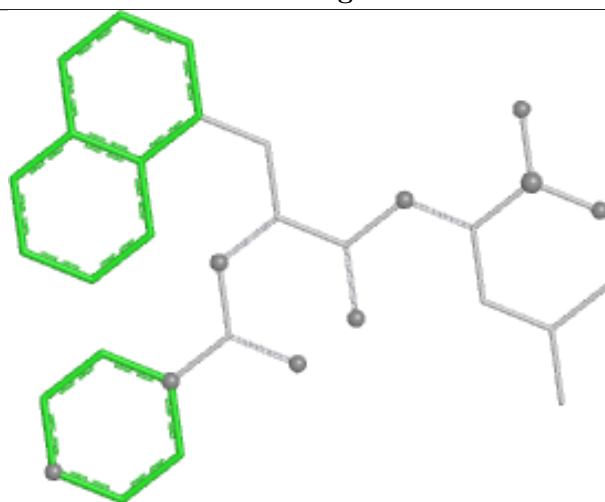
Bond lengths



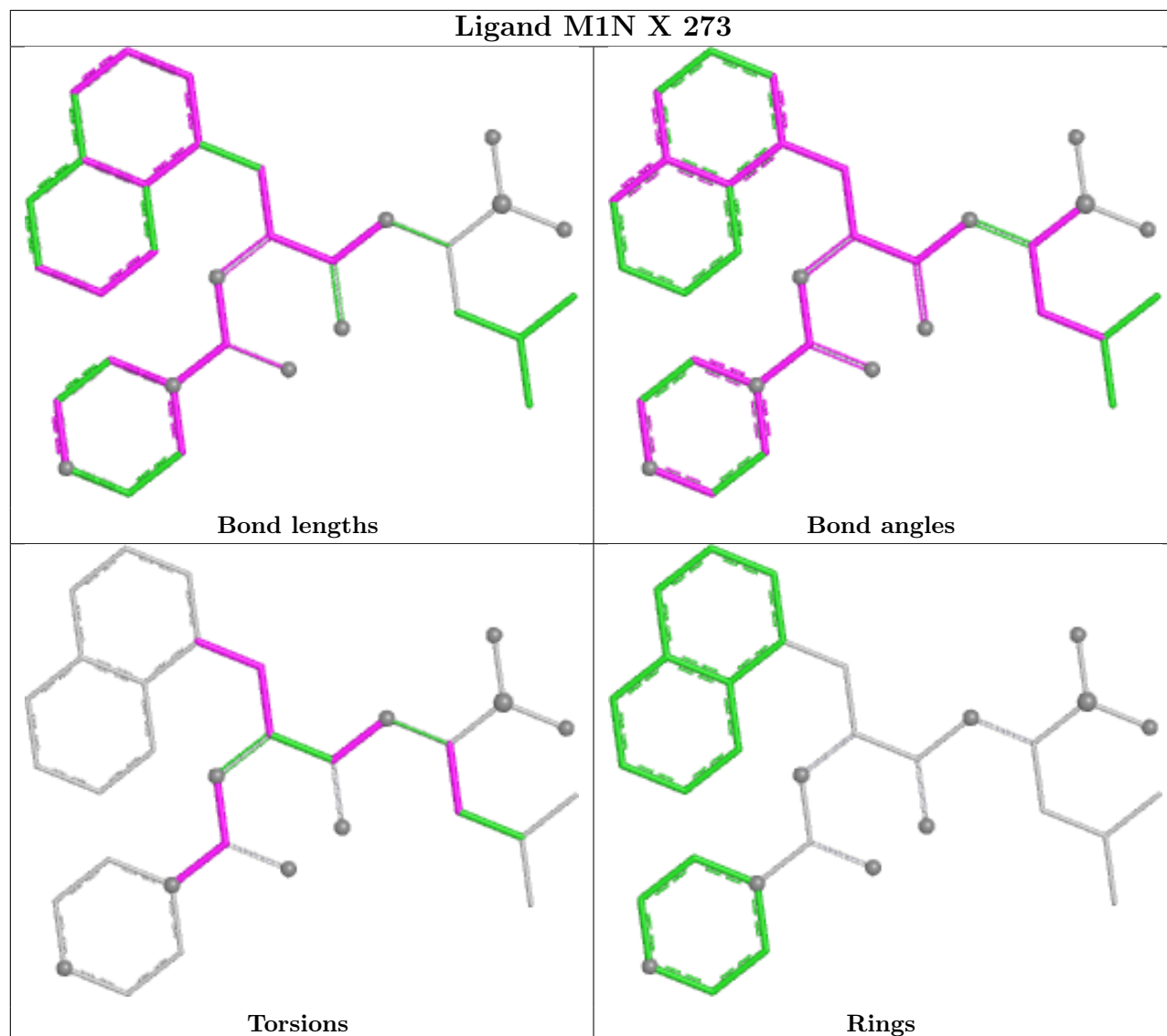
Bond angles

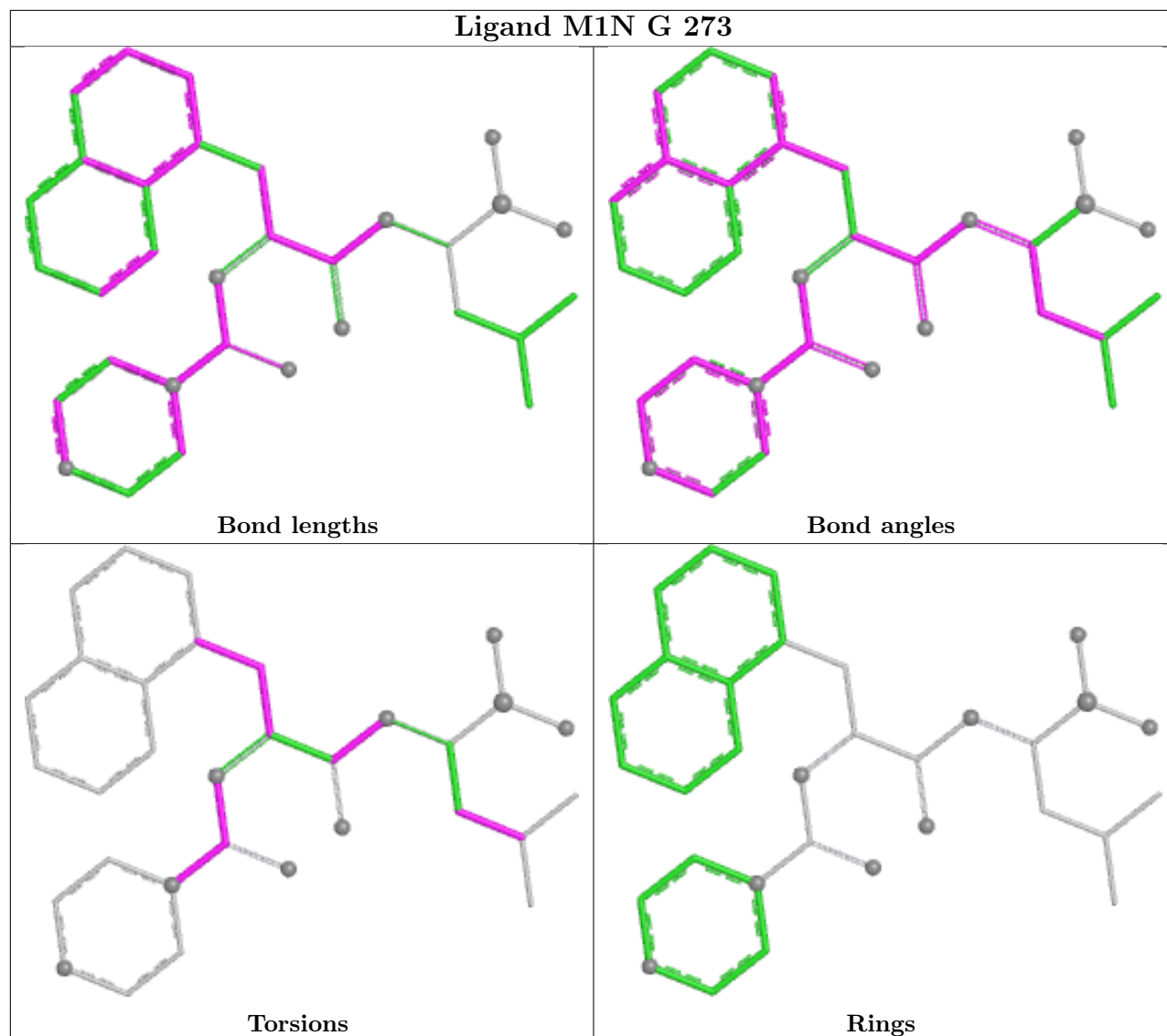


Torsions

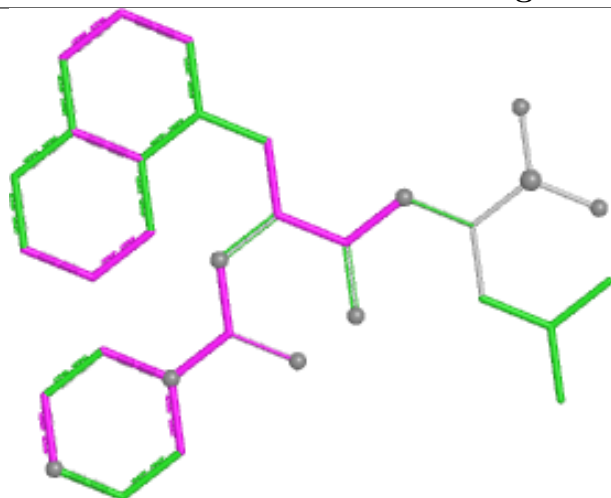


Rings

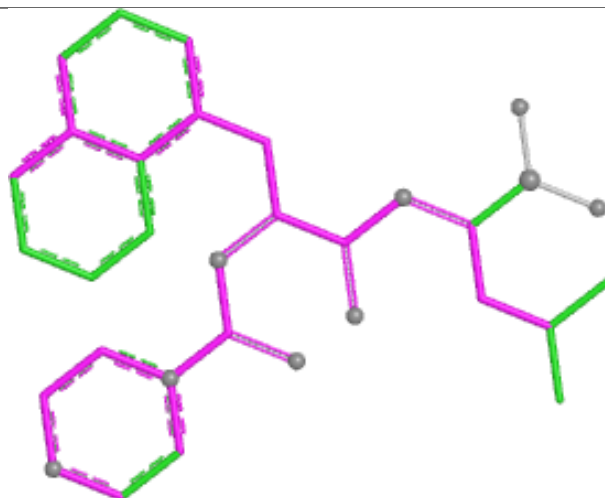




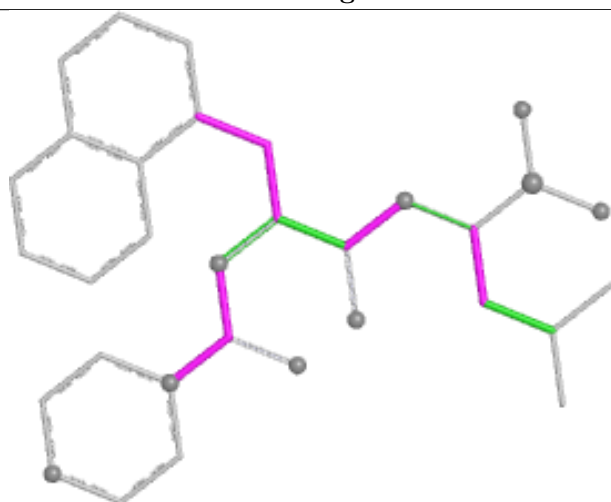
Ligand M1N J 273



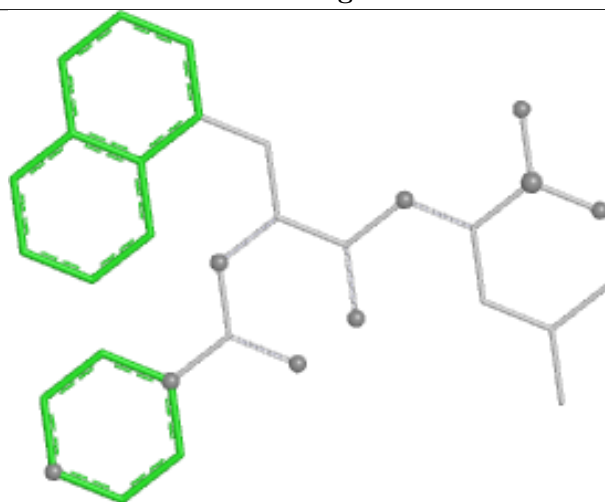
Bond lengths



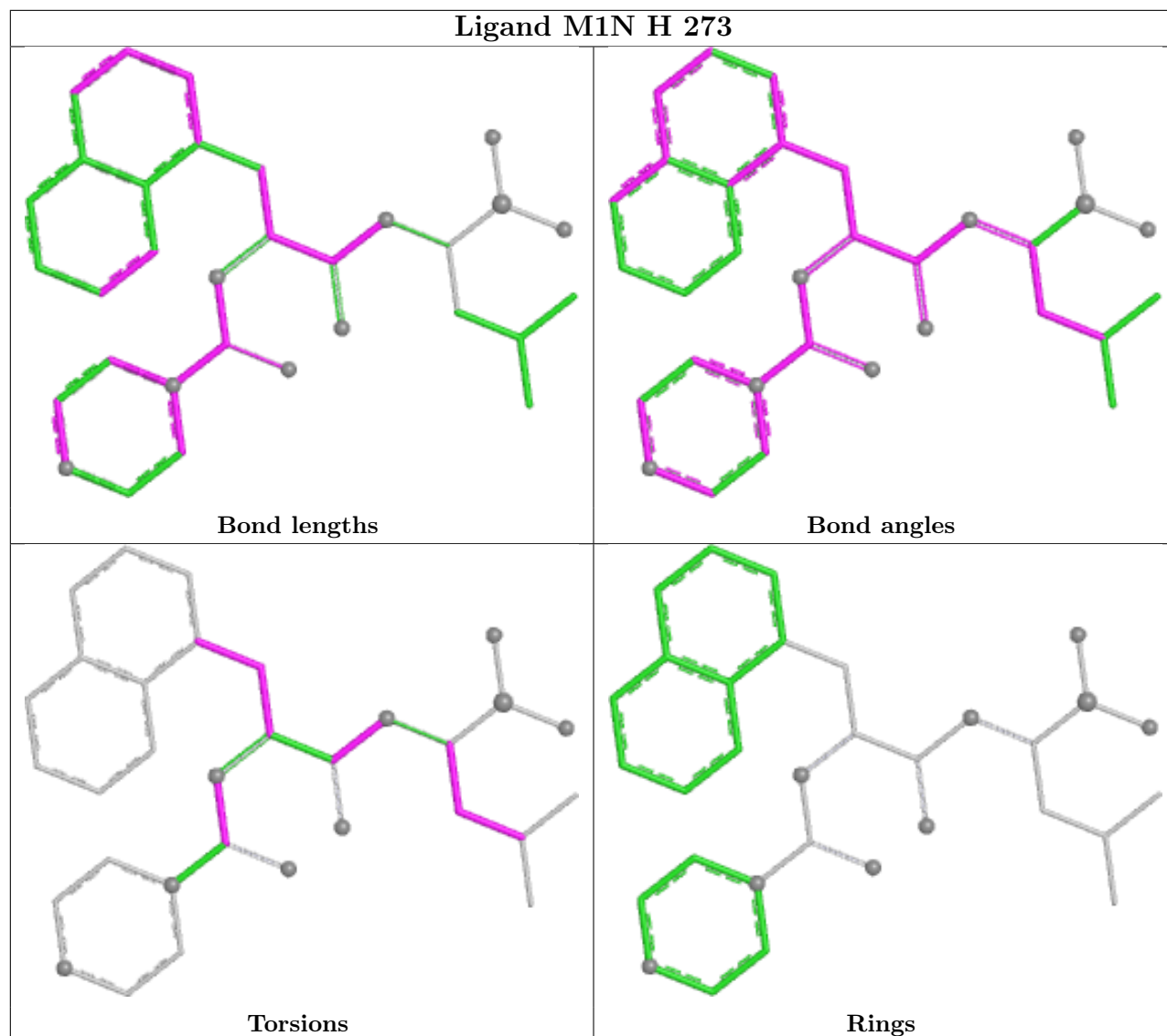
Bond angles

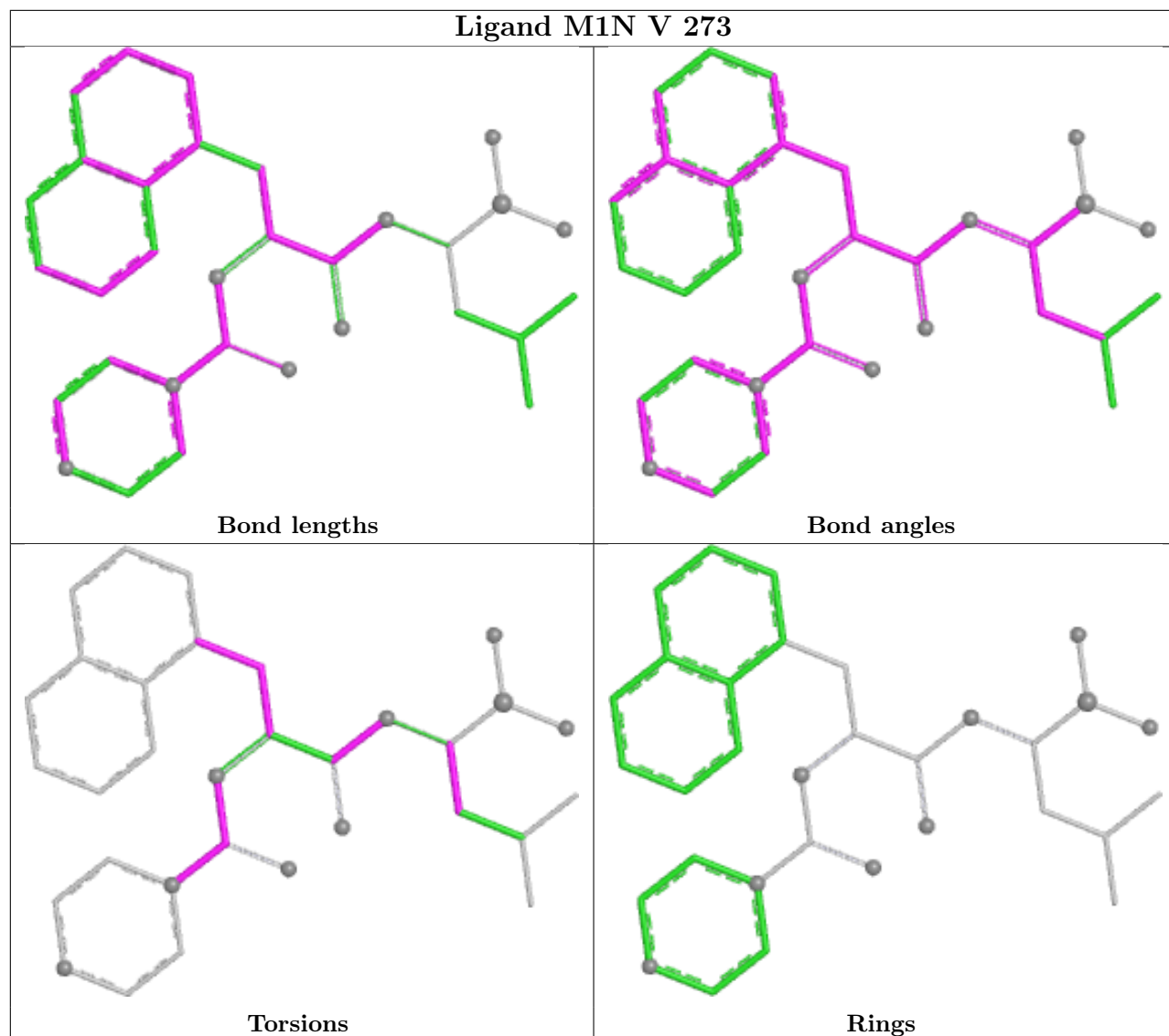


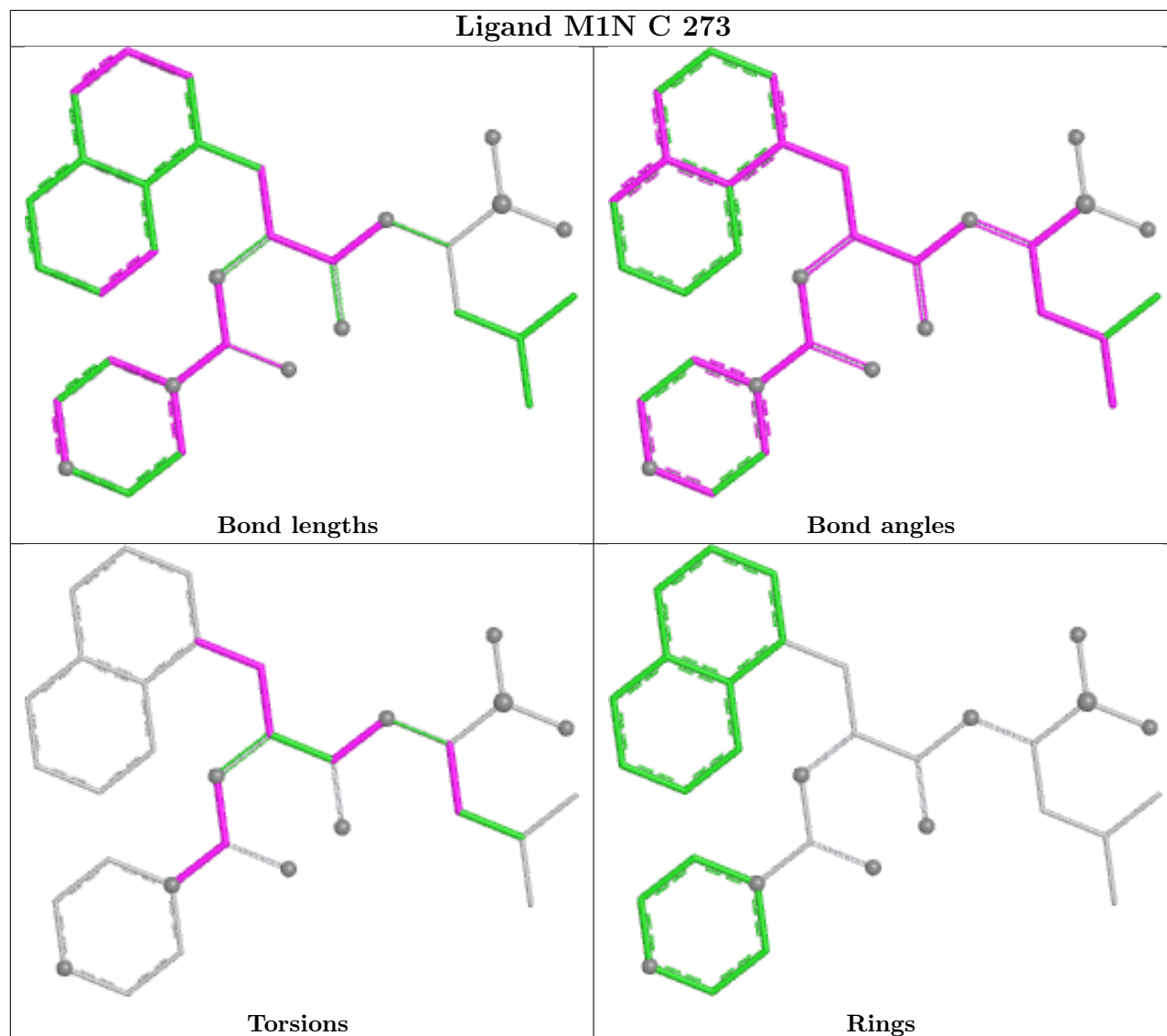
Torsions

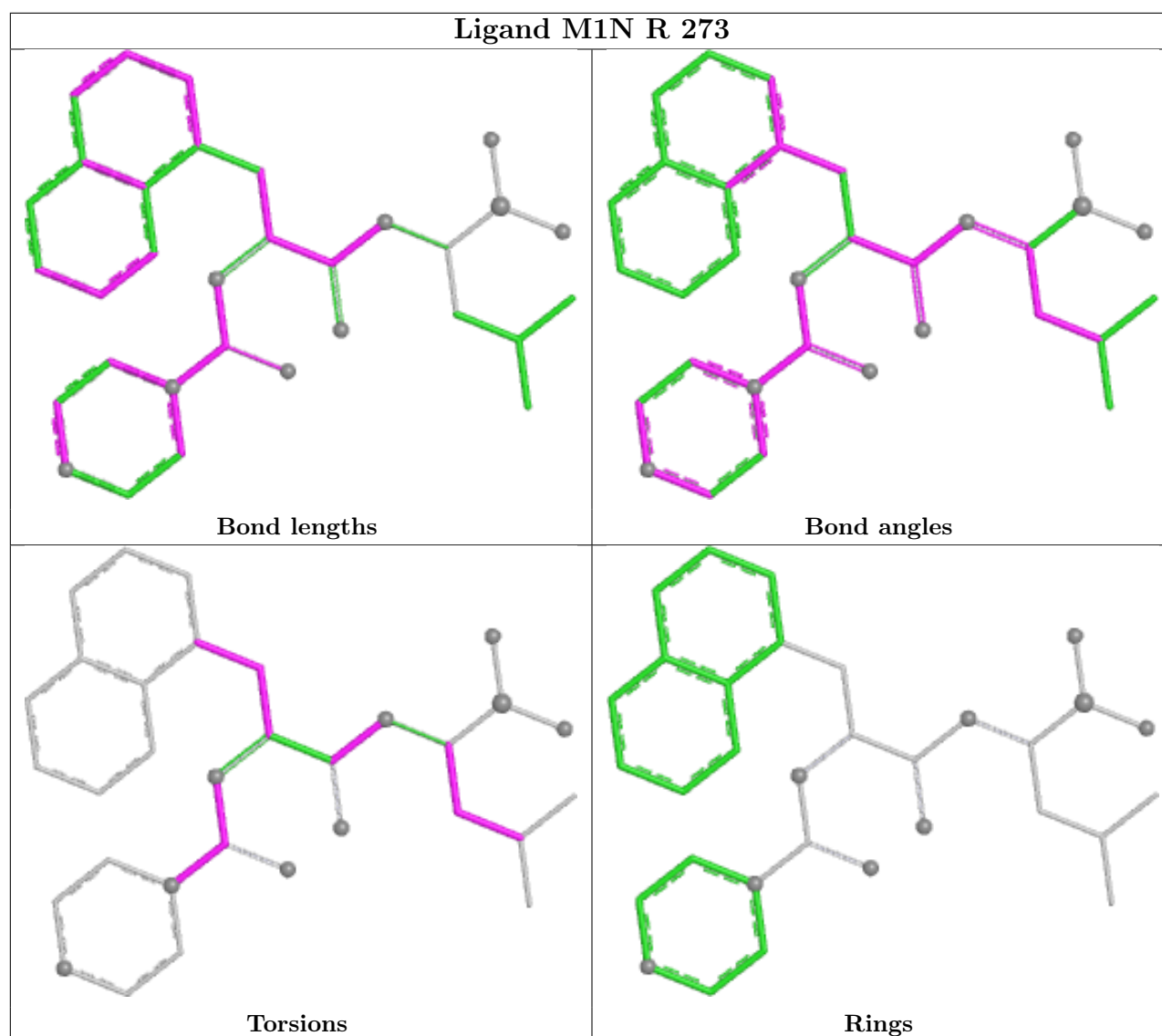


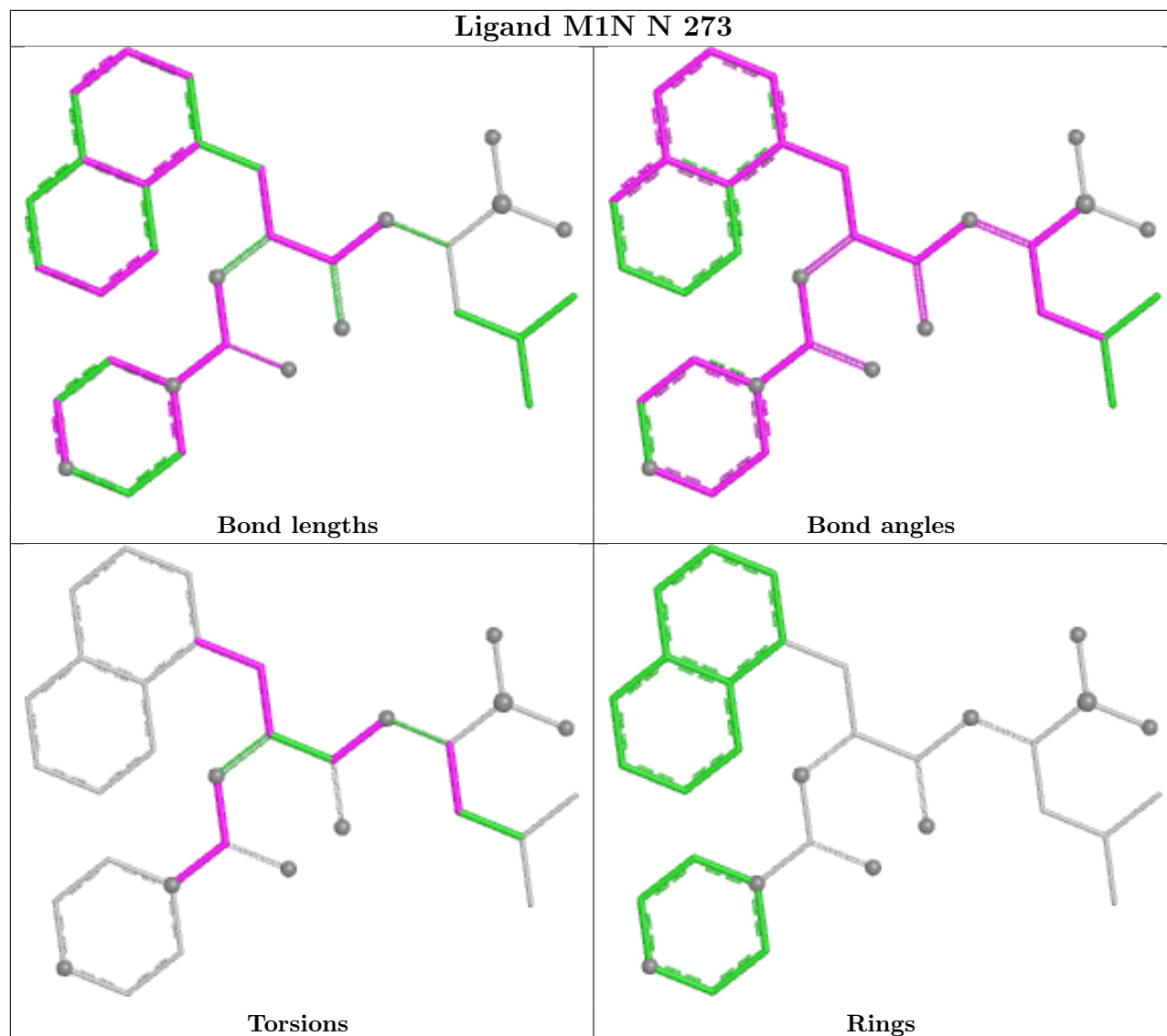
Rings



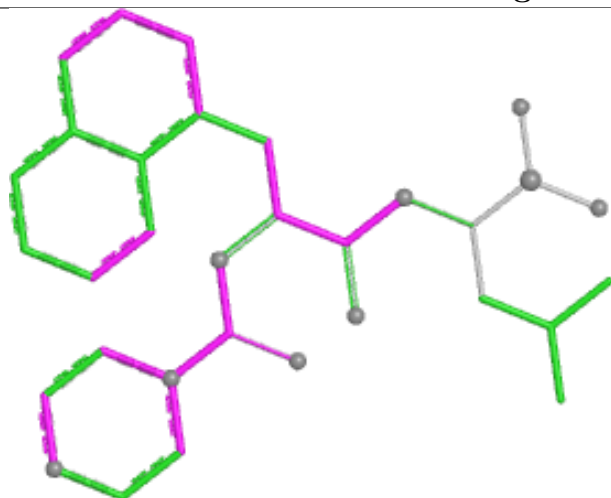




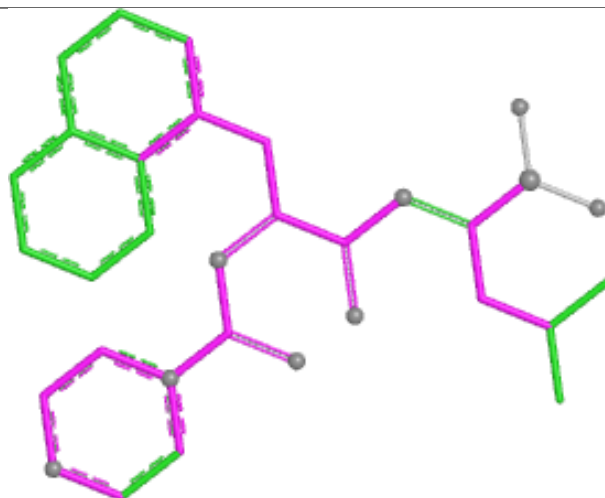




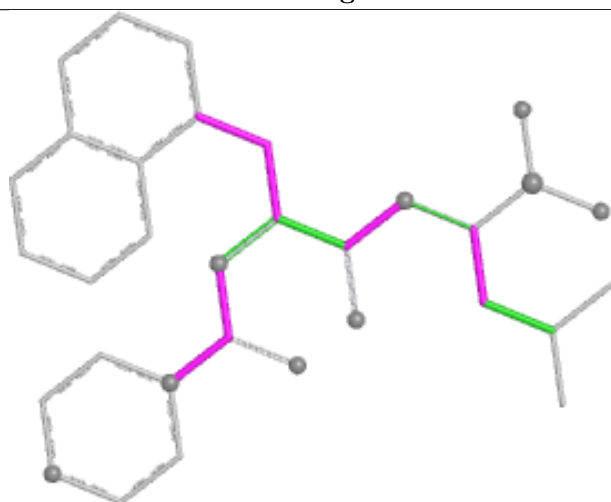
Ligand M1N Z 273



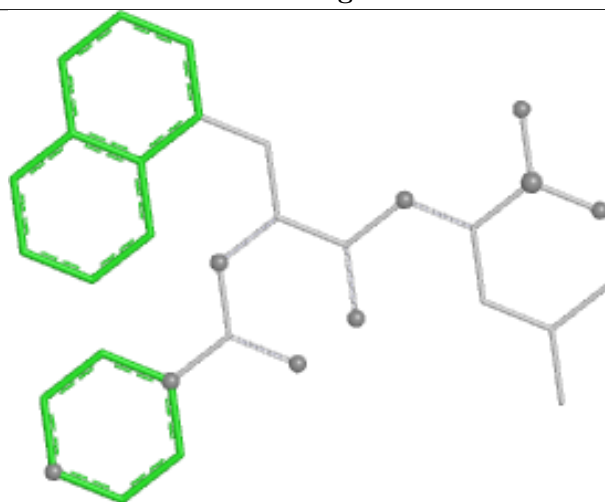
Bond lengths



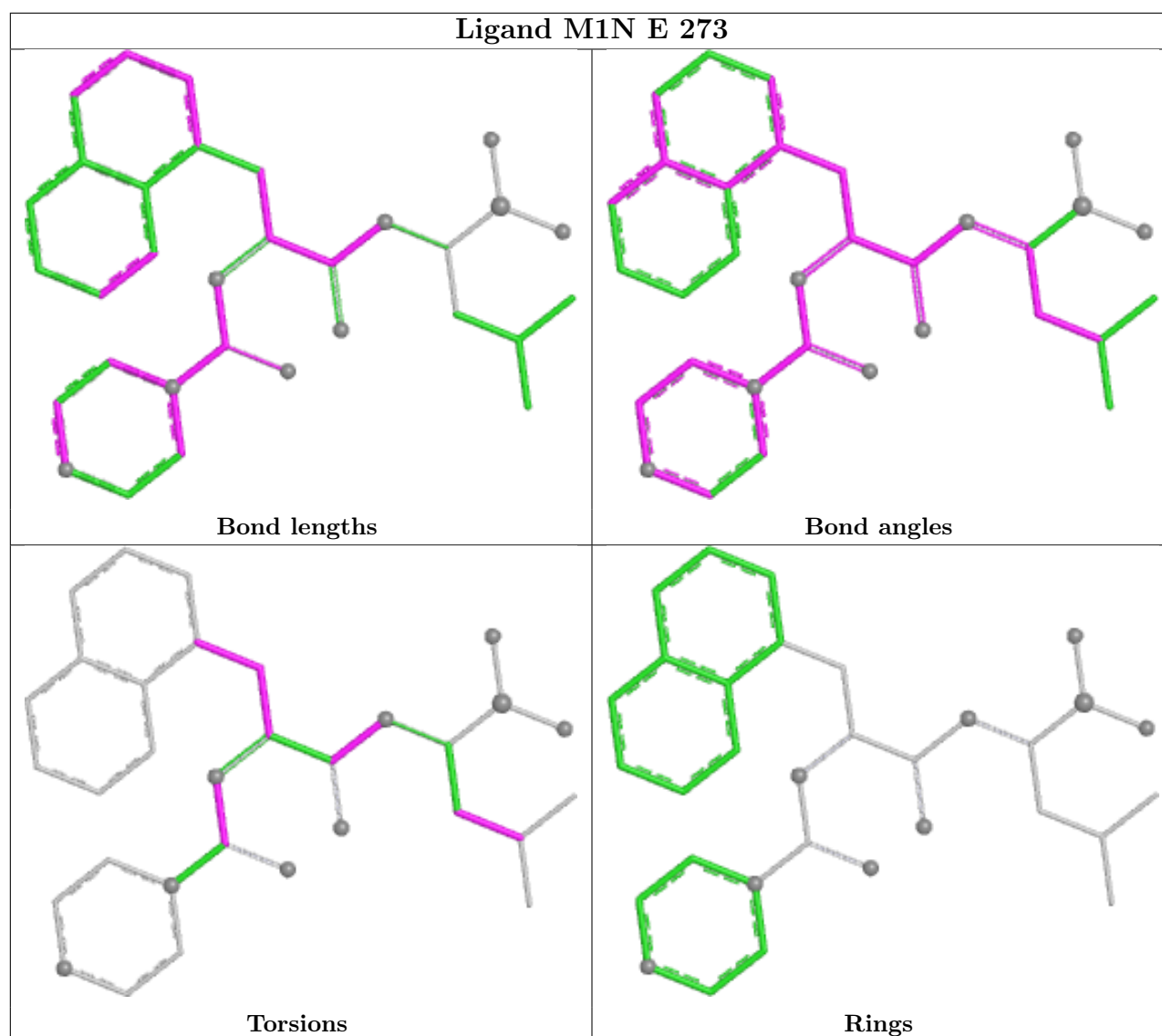
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	220/251 (87%)	0.48	4 (1%) 67 44	75, 100, 100, 100	0
1	A	220/251 (87%)	0.57	5 (2%) 61 38	74, 100, 100, 100	0
1	B	220/251 (87%)	0.33	3 (1%) 73 51	74, 100, 100, 100	0
1	D	220/251 (87%)	0.22	3 (1%) 73 51	74, 100, 100, 100	0
1	F	220/251 (87%)	0.36	6 (2%) 56 33	74, 100, 100, 100	0
1	I	220/251 (87%)	0.39	5 (2%) 61 38	74, 100, 100, 100	0
1	K	220/251 (87%)	0.59	10 (4%) 38 20	74, 100, 100, 100	0
1	M	220/251 (87%)	0.39	8 (3%) 46 26	74, 100, 100, 100	0
1	O	220/251 (87%)	0.34	4 (1%) 67 44	74, 100, 100, 100	0
1	Q	220/251 (87%)	0.29	5 (2%) 61 38	74, 100, 100, 100	0
1	S	220/251 (87%)	0.50	10 (4%) 38 20	74, 100, 100, 100	0
1	U	220/251 (87%)	0.17	3 (1%) 73 51	74, 100, 100, 100	0
1	W	220/251 (87%)	0.59	10 (4%) 38 20	74, 100, 100, 100	0
1	Y	220/251 (87%)	0.75	10 (4%) 38 20	74, 100, 100, 100	0
2	2	222/240 (92%)	0.13	2 (0%) 81 61	52, 72, 91, 100	0
2	C	222/240 (92%)	0.13	1 (0%) 87 72	53, 72, 91, 100	0
2	E	222/240 (92%)	-0.00	1 (0%) 87 72	52, 72, 92, 100	0
2	G	222/240 (92%)	-0.09	0 100 100	52, 72, 91, 100	0
2	H	222/240 (92%)	0.24	3 (1%) 73 51	52, 72, 91, 100	0
2	J	222/240 (92%)	-0.00	0 100 100	53, 72, 92, 100	0
2	L	222/240 (92%)	0.05	0 100 100	53, 72, 92, 100	0
2	N	222/240 (92%)	-0.07	0 100 100	52, 72, 91, 100	0
2	P	222/240 (92%)	0.02	1 (0%) 87 72	53, 72, 91, 100	0
2	R	222/240 (92%)	-0.08	0 100 100	53, 72, 92, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	T	222/240 (92%)	0.05	1 (0%) 87 72	53, 72, 92, 100	0
2	V	222/240 (92%)	-0.08	0 100 100	53, 72, 92, 100	0
2	X	222/240 (92%)	0.13	0 100 100	53, 72, 91, 100	0
2	Z	222/240 (92%)	0.06	1 (0%) 87 72	53, 72, 92, 100	0
All	All	6188/6874 (90%)	0.23	96 (1%) 70 47	52, 88, 100, 100	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	235	VAL	6.8
1	K	236	ASP	5.6
1	S	235	VAL	5.4
1	M	235	VAL	5.1
2	2	414	PRO	4.9
1	A	177	LEU	4.7
1	I	235	VAL	4.6
1	M	236	ASP	4.3
1	B	235	VAL	4.1
1	A	235	VAL	3.8
1	W	235	VAL	3.8
1	Y	115	ALA	3.7
1	W	229	ALA	3.6
1	1	203	LEU	3.5
2	E	522	SER	3.3
1	Y	9	PRO	3.3
1	S	234	LEU	3.1
1	Y	188	LEU	3.1
1	B	236	ASP	3.1
1	1	235	VAL	3.0
1	U	235	VAL	3.0
1	I	203	LEU	2.9
1	K	204	GLY	2.9
1	Y	154	VAL	2.9
2	C	417	ALA	2.9
1	F	235	VAL	2.8
1	A	236	ASP	2.8
1	D	236	ASP	2.8
1	Q	234	LEU	2.7
1	M	172	ALA	2.7
1	W	228	SER	2.7
1	F	167	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	O	203	LEU	2.7
1	D	145	GLY	2.6
1	Y	107	LEU	2.6
1	S	13	MET	2.6
1	S	236	ASP	2.6
1	M	237	GLN	2.5
1	K	186	ALA	2.5
2	Z	417	ALA	2.5
1	F	236	ASP	2.5
1	I	204	GLY	2.5
1	Y	88	ALA	2.5
1	A	203	LEU	2.5
1	S	131	GLY	2.5
1	K	205	VAL	2.5
1	I	44	GLU	2.4
1	S	118	TYR	2.4
1	1	39	VAL	2.4
1	K	203	LEU	2.4
1	O	236	ASP	2.4
1	U	236	ASP	2.4
1	W	236	ASP	2.4
1	S	117	PRO	2.3
1	Y	177	LEU	2.3
1	F	9	PRO	2.3
1	S	94	VAL	2.3
1	F	191	GLY	2.3
1	K	185	VAL	2.3
1	Y	203	LEU	2.3
1	K	234	LEU	2.2
1	M	203	LEU	2.2
2	H	435	GLY	2.2
1	Y	13	MET	2.2
1	D	203	LEU	2.2
1	W	208	LEU	2.2
1	Q	237	GLN	2.2
1	M	13	MET	2.2
1	A	237	GLN	2.2
1	Q	236	ASP	2.2
1	W	9	PRO	2.2
1	O	13	MET	2.2
1	K	9	PRO	2.2
1	S	9	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	460	GLY	2.2
2	T	501	GLY	2.2
1	Q	203	LEU	2.2
1	Y	236	ASP	2.1
1	F	145	GLY	2.1
1	Q	204	GLY	2.1
1	S	203	LEU	2.1
1	W	89	TYR	2.1
1	W	166	ALA	2.1
1	U	13	MET	2.1
1	I	236	ASP	2.1
1	W	33	LEU	2.1
1	M	182	ARG	2.1
1	M	204	GLY	2.1
1	K	41	PHE	2.1
1	O	172	ALA	2.1
1	1	50	LEU	2.0
2	2	430	ASN	2.0
2	H	431	ILE	2.0
1	W	203	LEU	2.0
2	P	430	ASN	2.0
1	B	221	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	M1N	2	273	32/32	0.82	0.17	65,76,78,79	0

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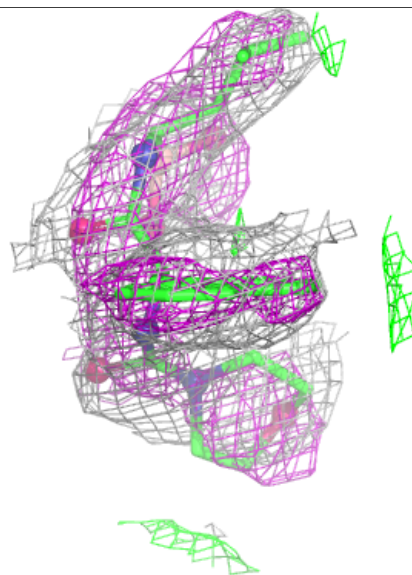
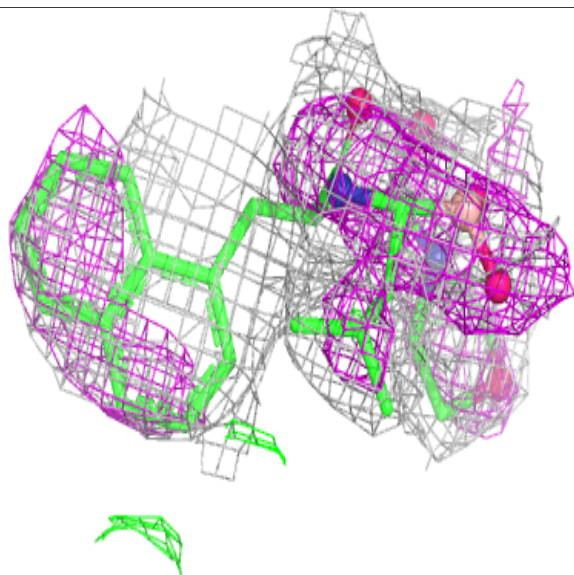
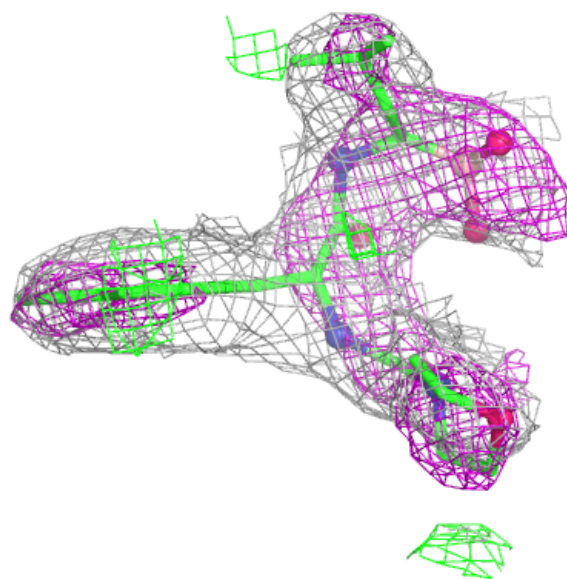
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	M1N	X	273	32/32	0.83	0.17	65,76,78,79	0
3	M1N	V	273	32/32	0.84	0.15	65,76,78,78	0
3	M1N	Z	273	32/32	0.85	0.14	66,76,78,78	0
3	M1N	T	273	32/32	0.85	0.16	64,77,78,79	0
3	M1N	J	273	32/32	0.88	0.14	64,76,77,78	0
3	M1N	P	273	32/32	0.89	0.14	65,76,78,79	0
3	M1N	E	273	32/32	0.89	0.13	63,76,78,78	0
3	M1N	R	273	32/32	0.90	0.14	64,76,78,78	0
3	M1N	L	273	32/32	0.90	0.13	65,75,77,78	0
3	M1N	G	273	32/32	0.90	0.13	64,75,77,78	0
3	M1N	N	273	32/32	0.91	0.13	65,76,77,78	0
3	M1N	C	273	32/32	0.91	0.13	63,75,77,78	0
3	M1N	H	273	32/32	0.93	0.12	64,75,77,78	0

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

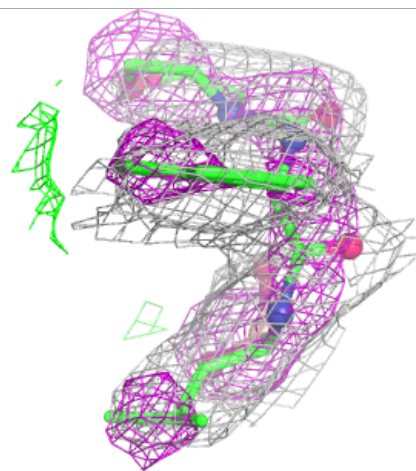
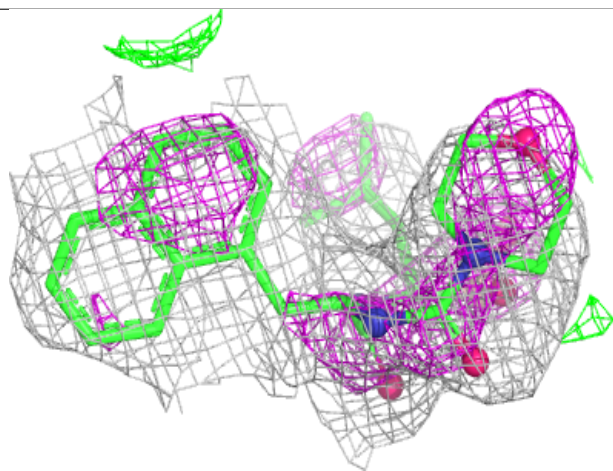
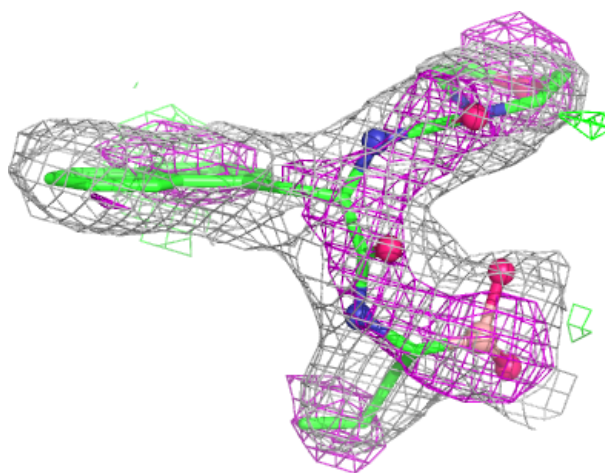
Electron density around M1N 2 273:

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



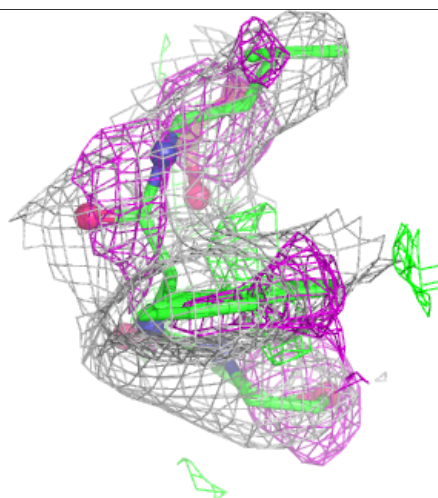
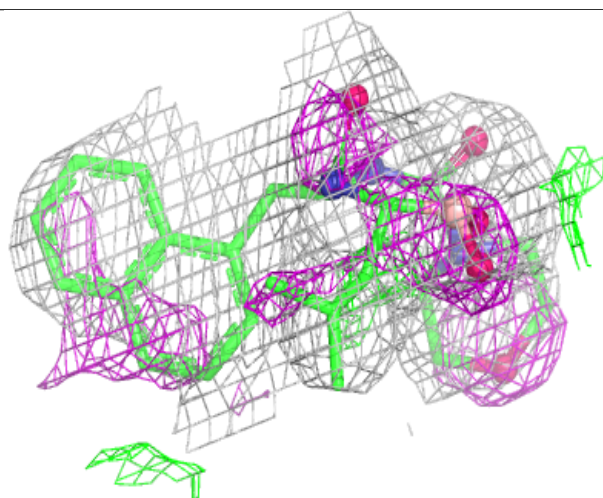
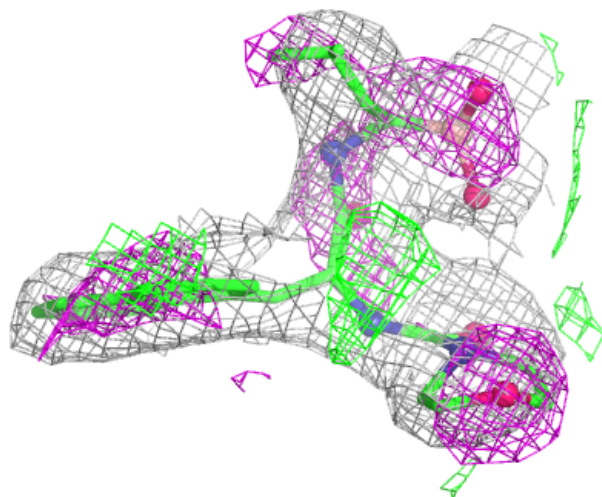
Electron density around M1N X 273:

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



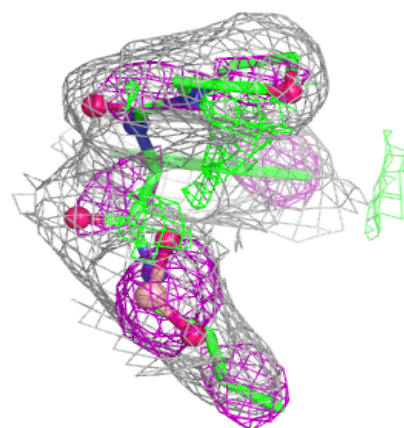
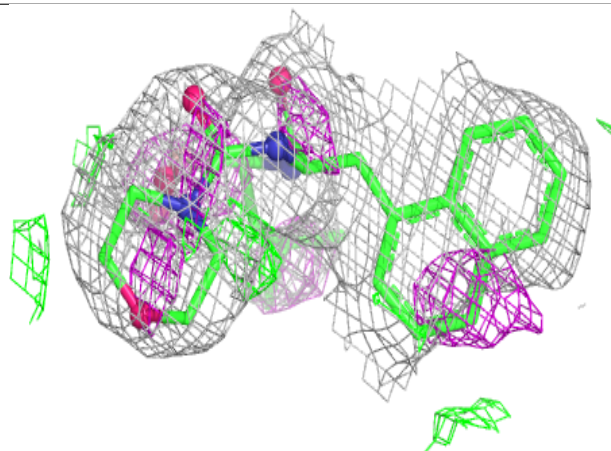
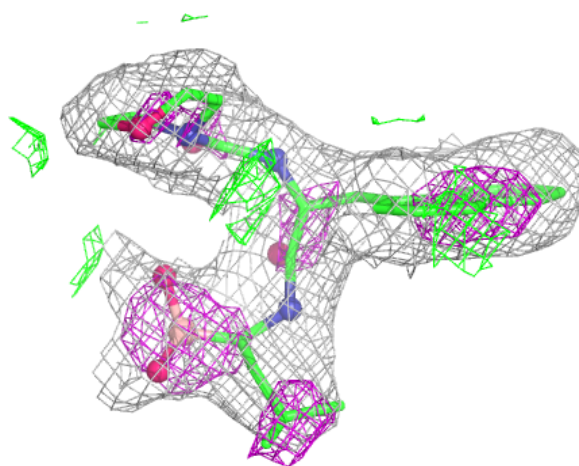
Electron density around M1N V 273:

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



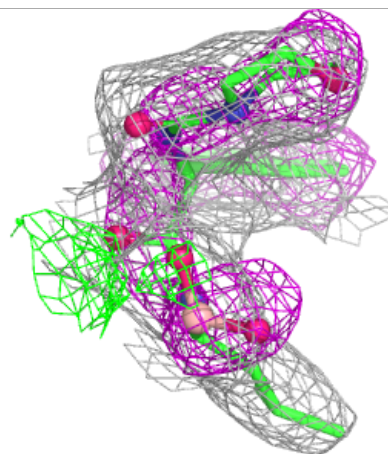
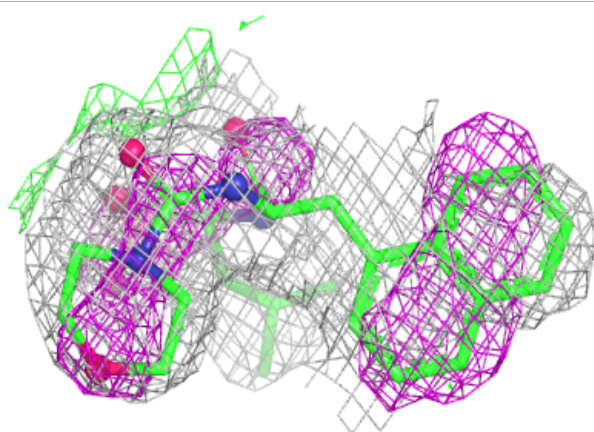
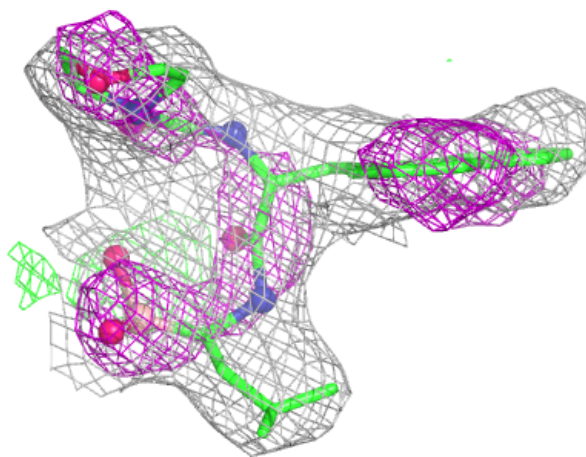
Electron density around M1N Z 273:

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



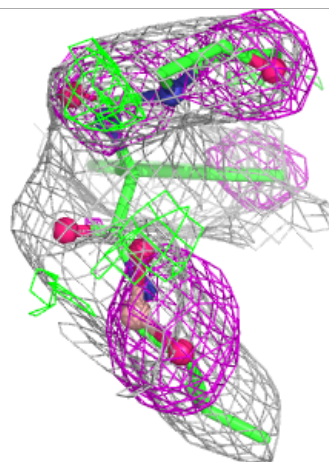
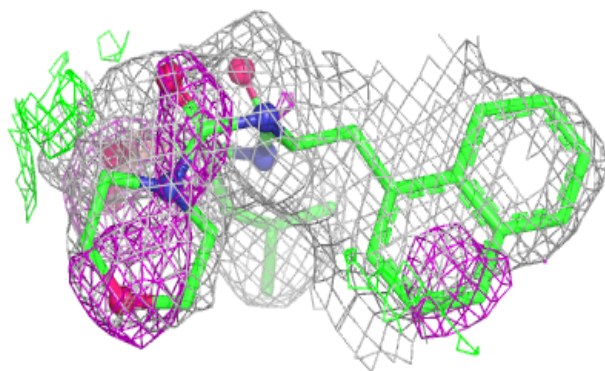
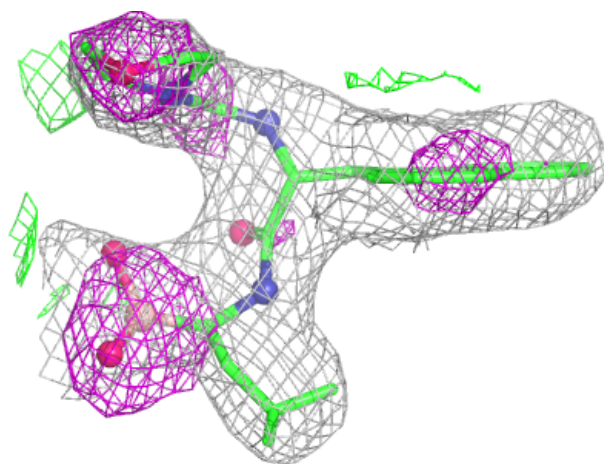
Electron density around M1N T 273:

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



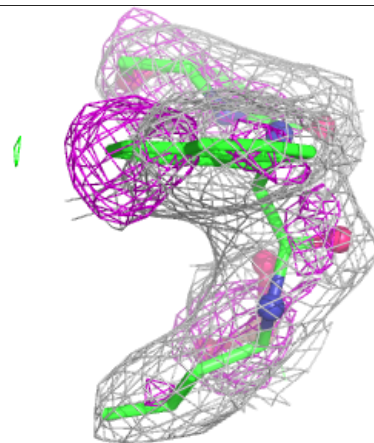
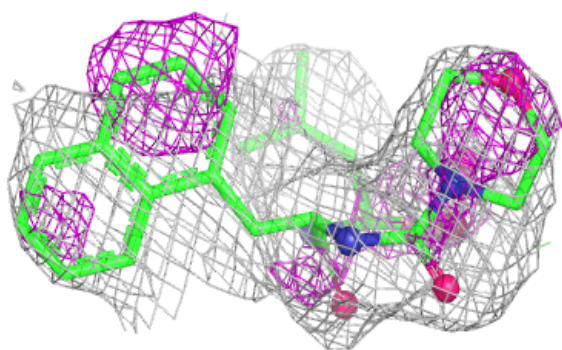
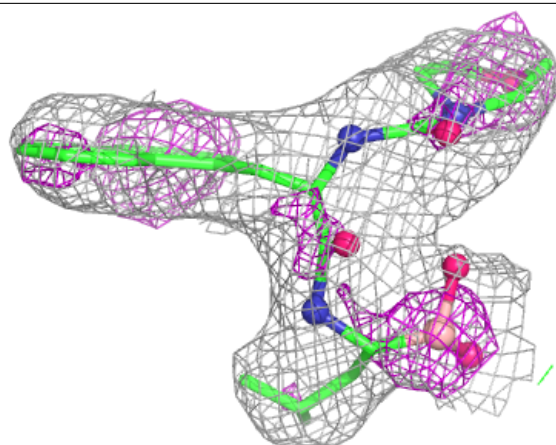
Electron density around M1N J 273:

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



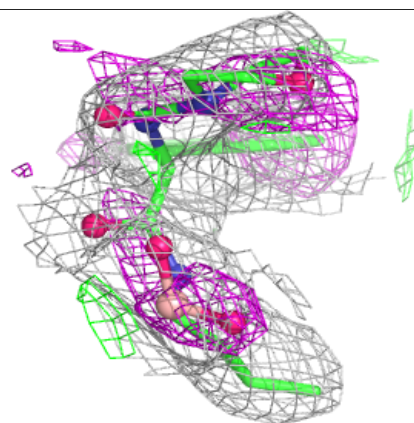
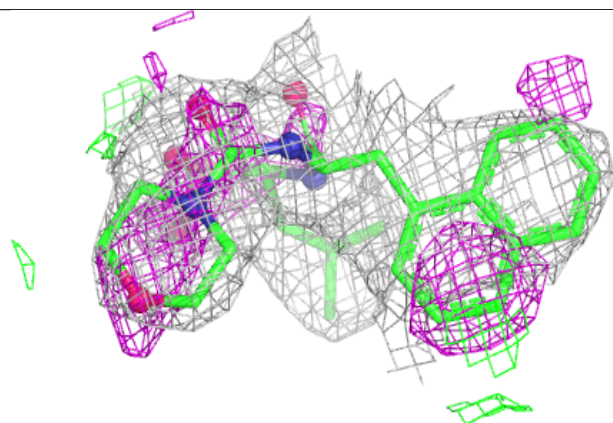
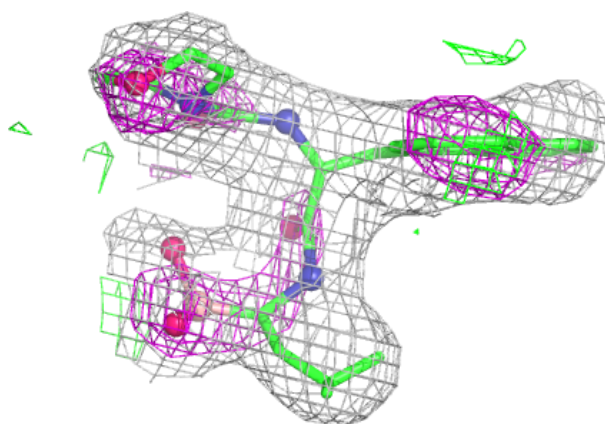
Electron density around M1N P 273:

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



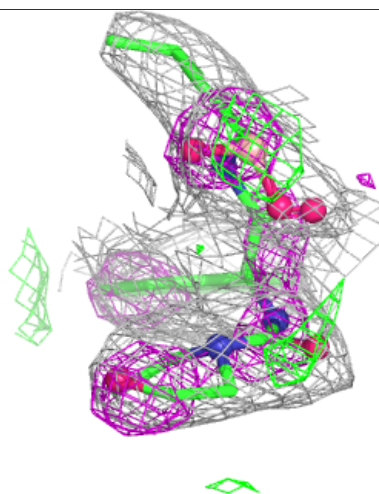
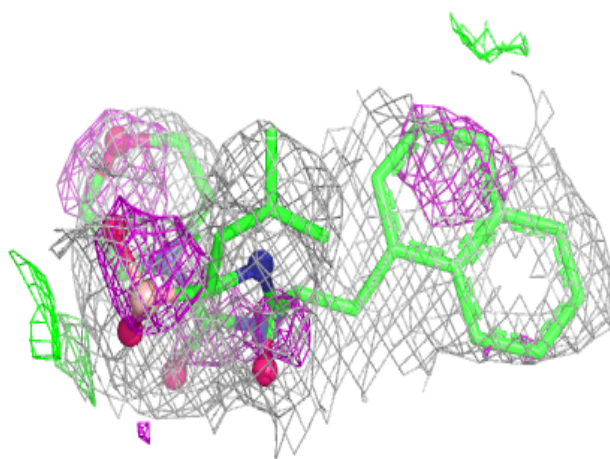
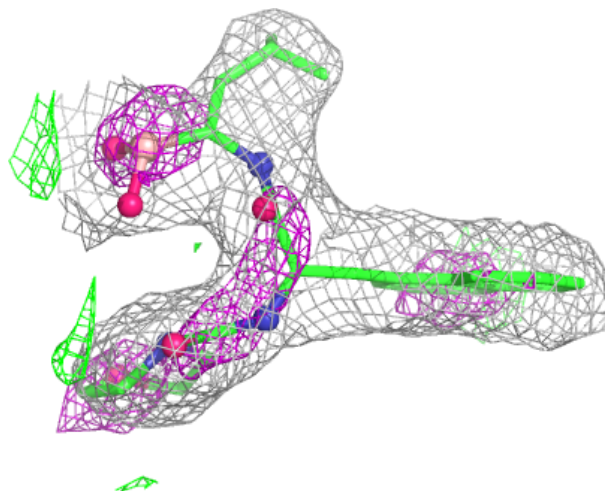
Electron density around M1N E 273:

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



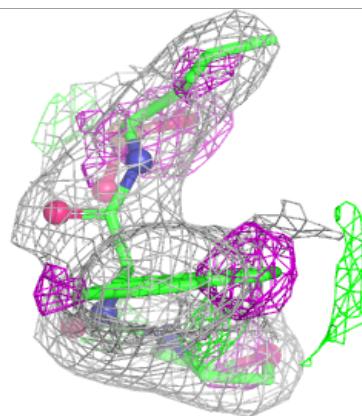
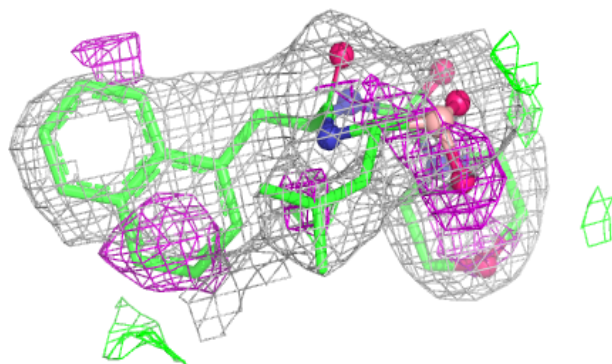
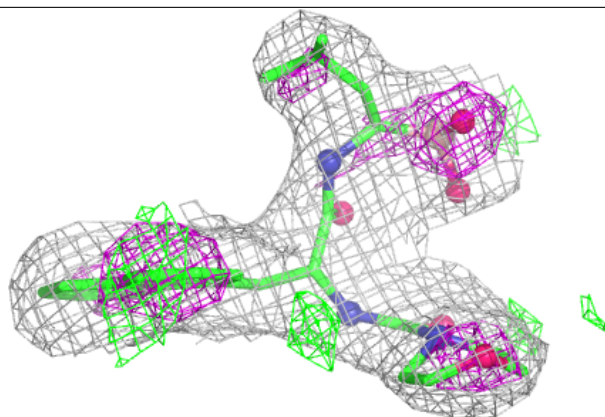
Electron density around M1N R 273:

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



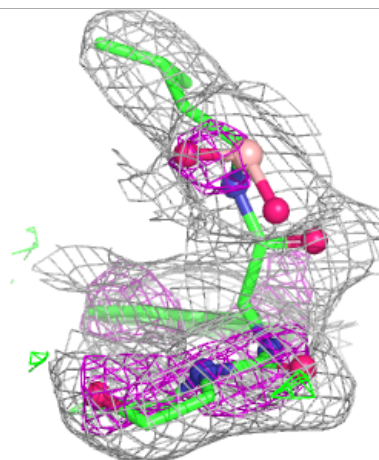
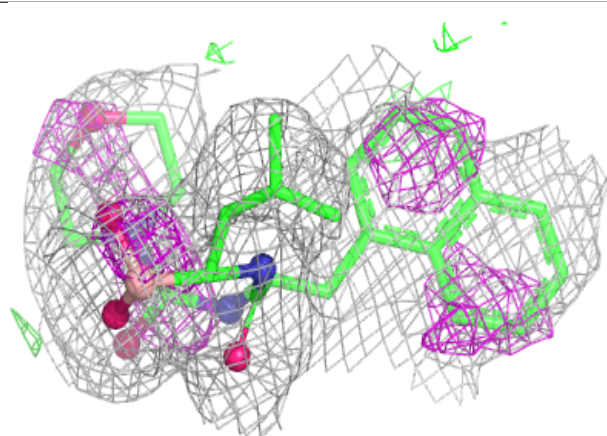
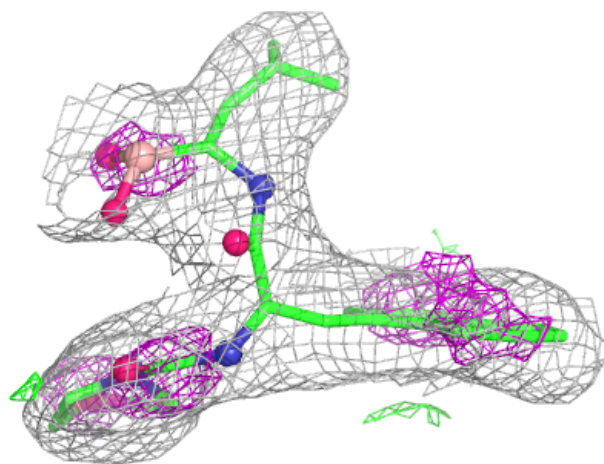
Electron density around M1N L 273:

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



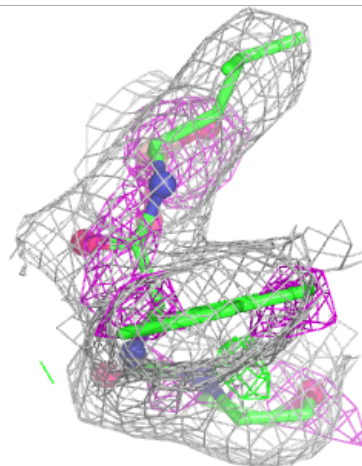
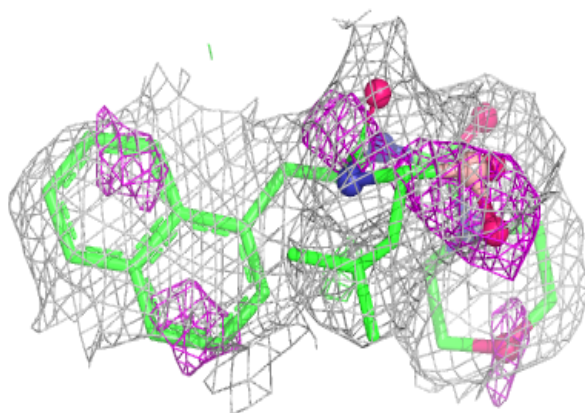
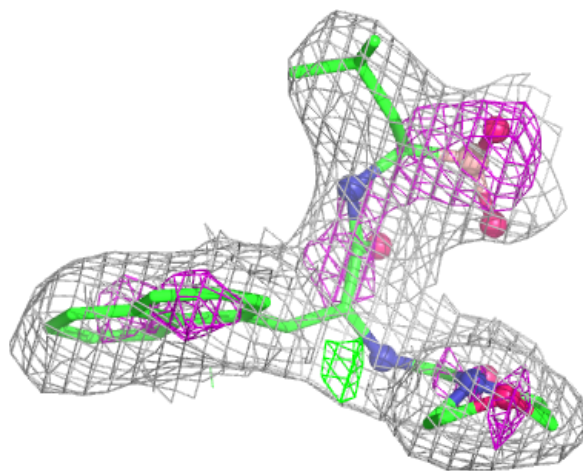
Electron density around M1N G 273:

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



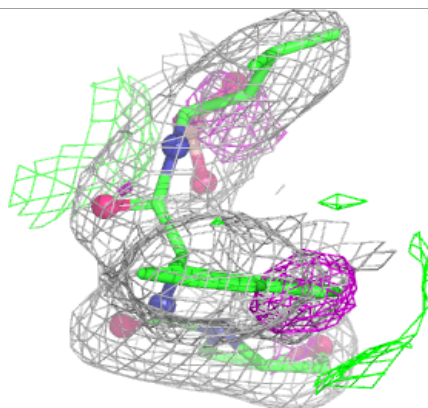
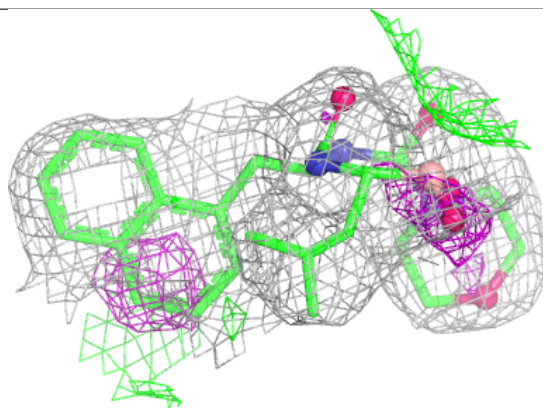
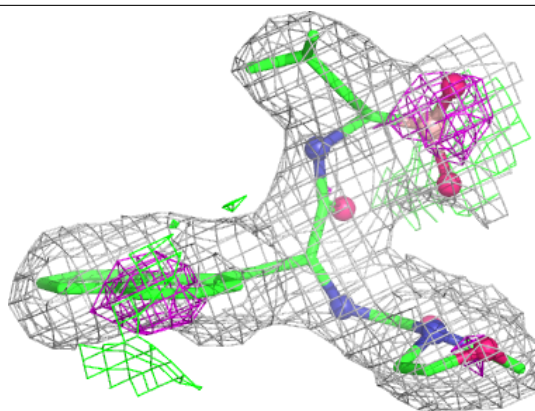
Electron density around M1N N 273:

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

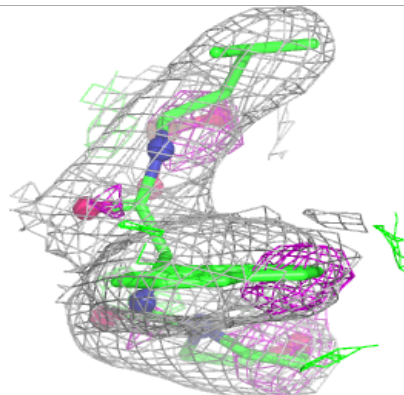
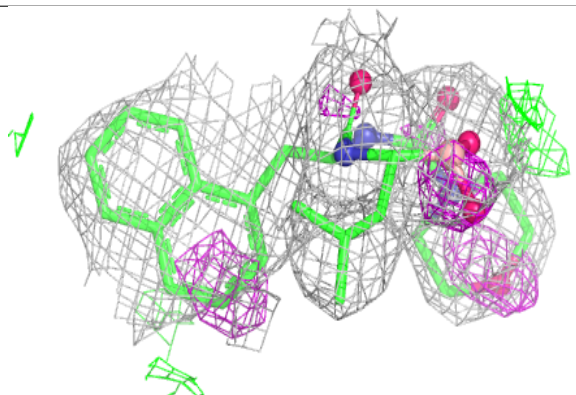
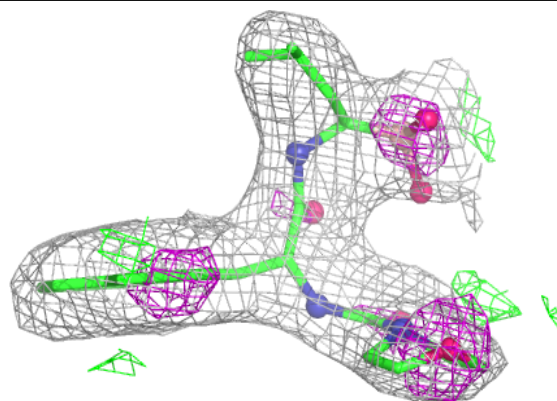


Electron density around M1N C 273:

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

**Electron density around M1N H 273:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.