



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:34 PM BST

PDB ID : 2FHH
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

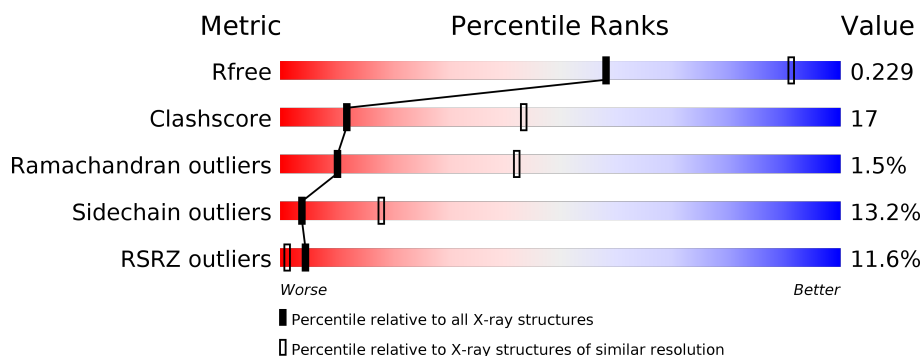
1 Overall quality at a glance i

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	251	<div> <div>23%</div> <div>54%</div> <div>30%</div> <div>•</div> <div>12%</div> </div>
1	A	251	<div> <div>6%</div> <div>55%</div> <div>29%</div> <div>•</div> <div>12%</div> </div>
1	B	251	<div> <div>12%</div> <div>53%</div> <div>30%</div> <div>•</div> <div>12%</div> </div>
1	D	251	<div> <div>16%</div> <div>54%</div> <div>30%</div> <div>•</div> <div>12%</div> </div>
1	F	251	<div> <div>14%</div> <div>53%</div> <div>29%</div> <div>5%</div> <div>12%</div> </div>
1	I	251	<div> <div>12%</div> <div>53%</div> <div>30%</div> <div>•</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
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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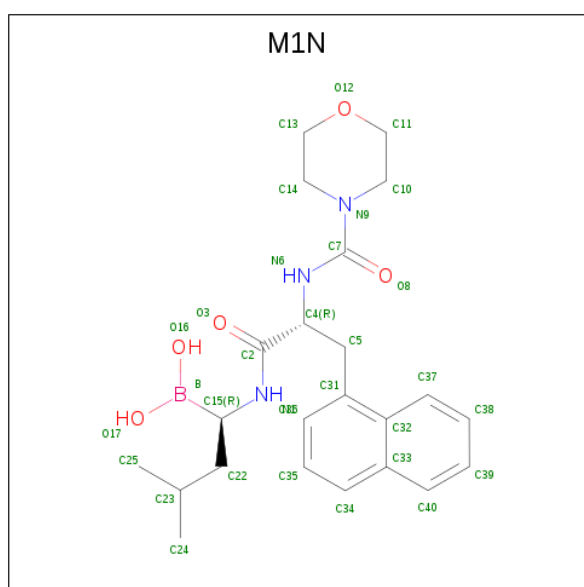
Chain	Residue	Modelled	Actual	Comment	Reference
N	535	HIS	-	EXPRESSION TAG	GB 13881852
N	536	HIS	-	EXPRESSION TAG	GB 13881852
N	537	HIS	-	EXPRESSION TAG	GB 13881852
N	538	HIS	-	EXPRESSION TAG	GB 13881852
N	539	HIS	-	EXPRESSION TAG	GB 13881852
N	540	HIS	-	EXPRESSION TAG	GB 13881852
P	535	HIS	-	EXPRESSION 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 (three-letter code: 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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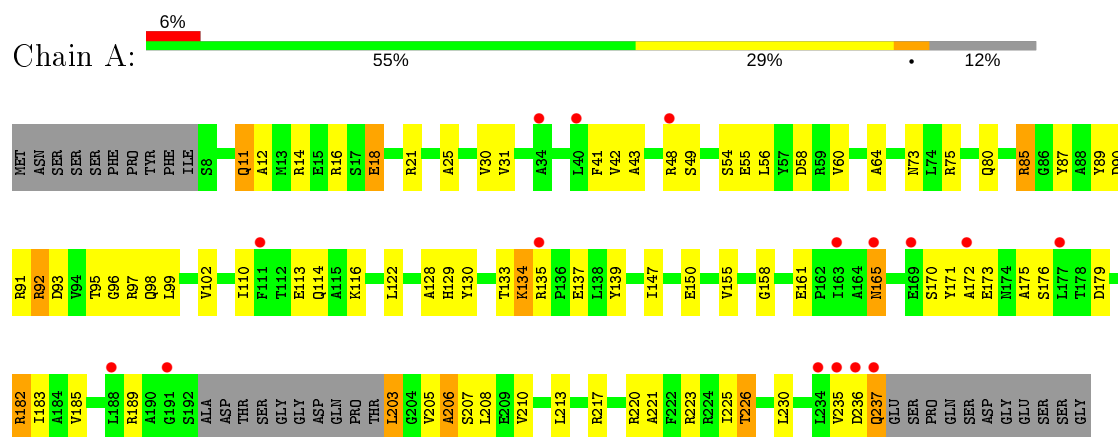
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	13	Total 13	O 13	0	0
4	N	12	Total 12	O 12	0	0
4	O	15	Total 15	O 15	0	0
4	P	15	Total 15	O 15	0	0
4	Q	6	Total 6	O 6	0	0
4	R	12	Total 12	O 12	0	0
4	S	5	Total 5	O 5	0	0
4	T	8	Total 8	O 8	0	0
4	U	2	Total 2	O 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

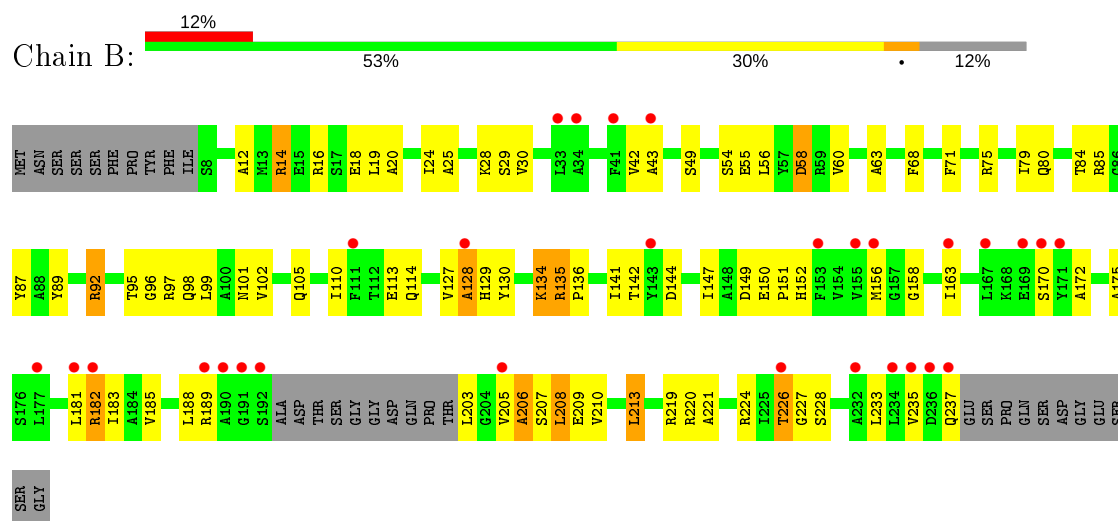
3 Residue-property plots [i](#)

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

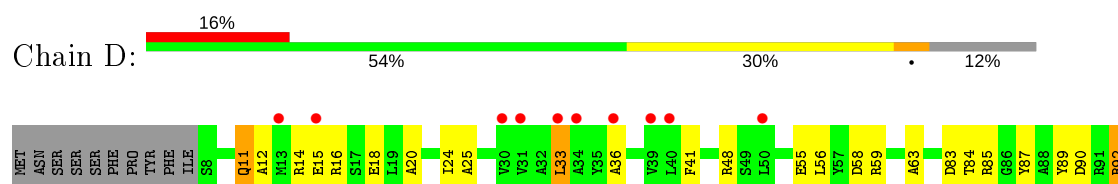
- Molecule 1: 20S proteasome, alpha and beta subunits

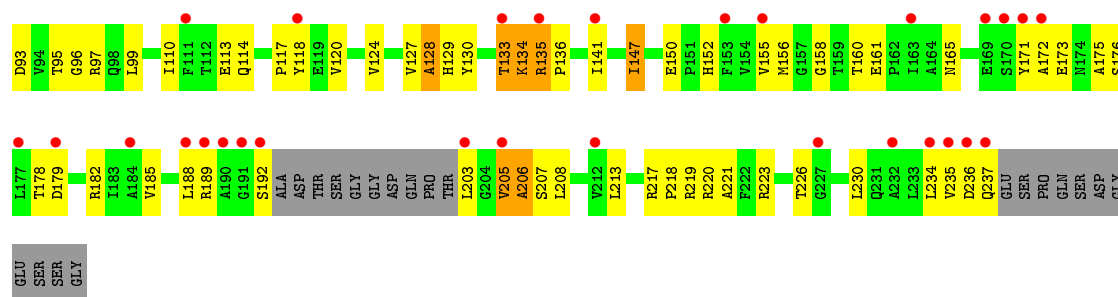


- Molecule 1: 20S proteasome, alpha and beta subunits

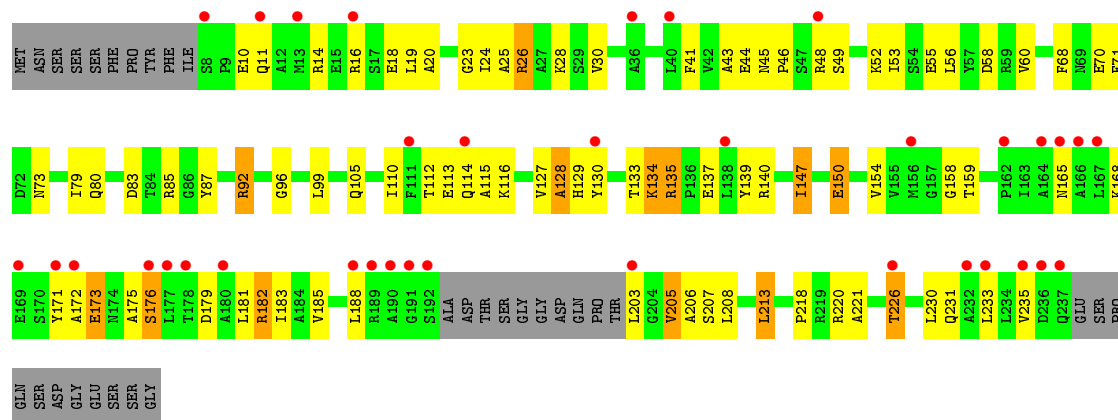


- Molecule 1: 20S proteasome, alpha and beta subunits

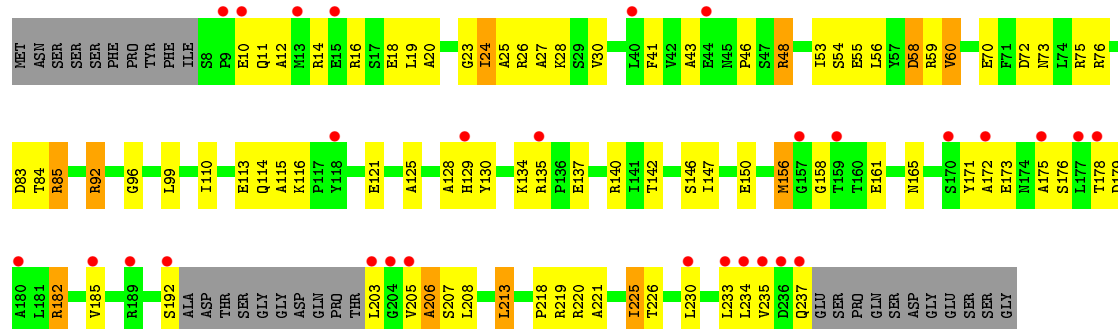




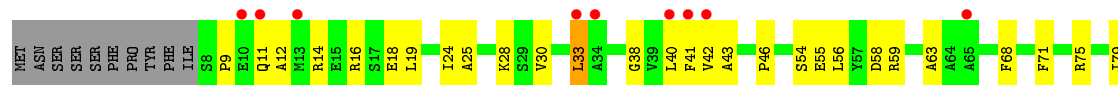
- Molecule 1: 20S proteasome, alpha and beta subunits

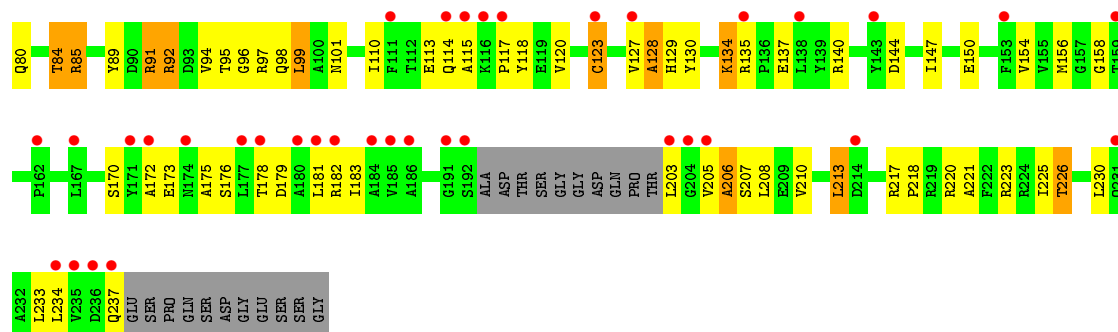


- Molecule 1: 20S proteasome, alpha and beta subunits

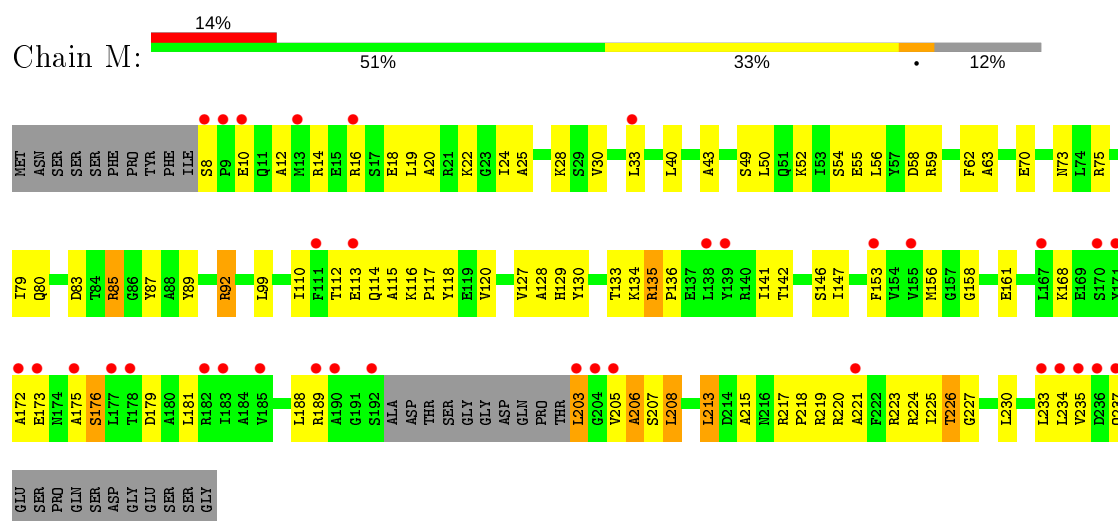


- Molecule 1: 20S proteasome, alpha and beta subunits

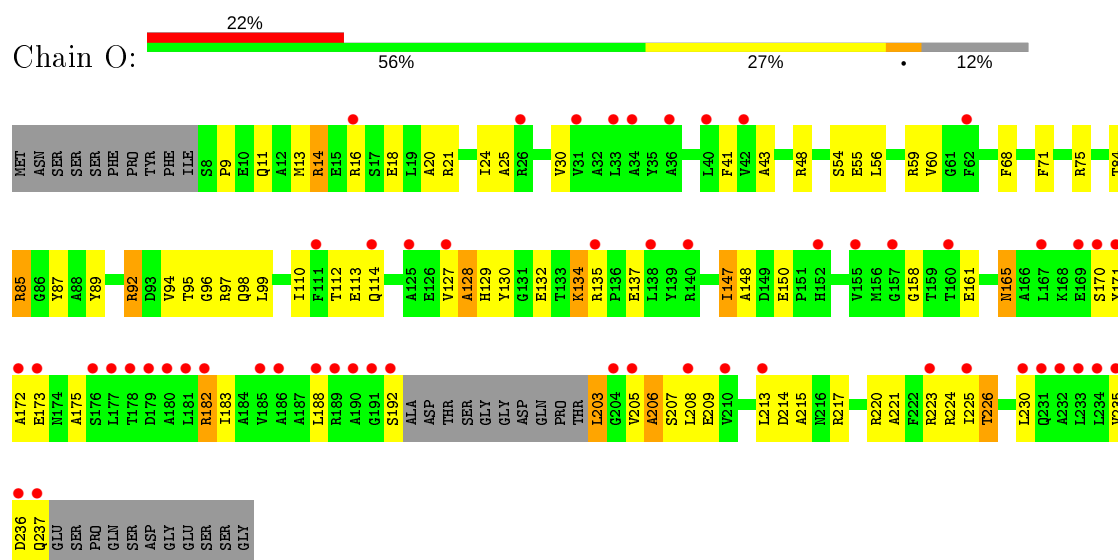




- Molecule 1: 20S proteasome, alpha and beta subunits

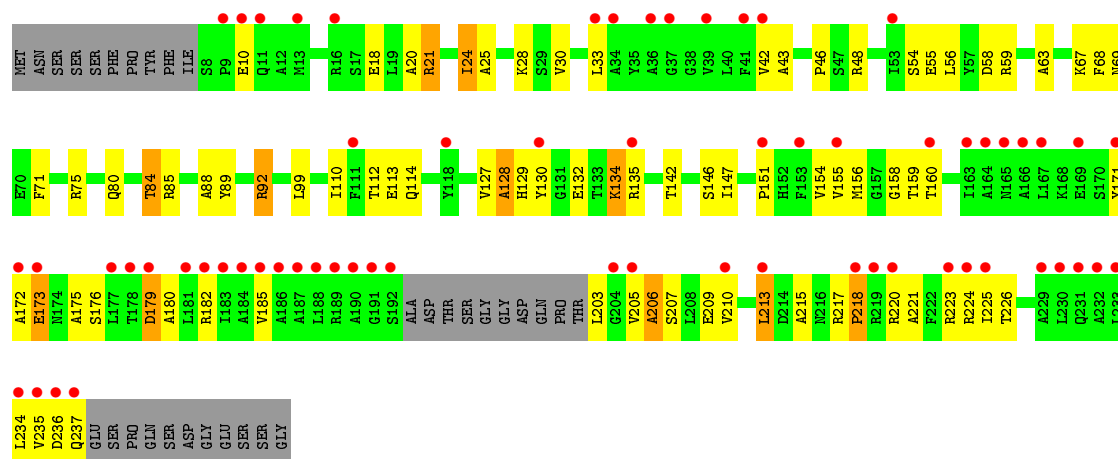


- Molecule 1: 20S proteasome, alpha and beta subunits

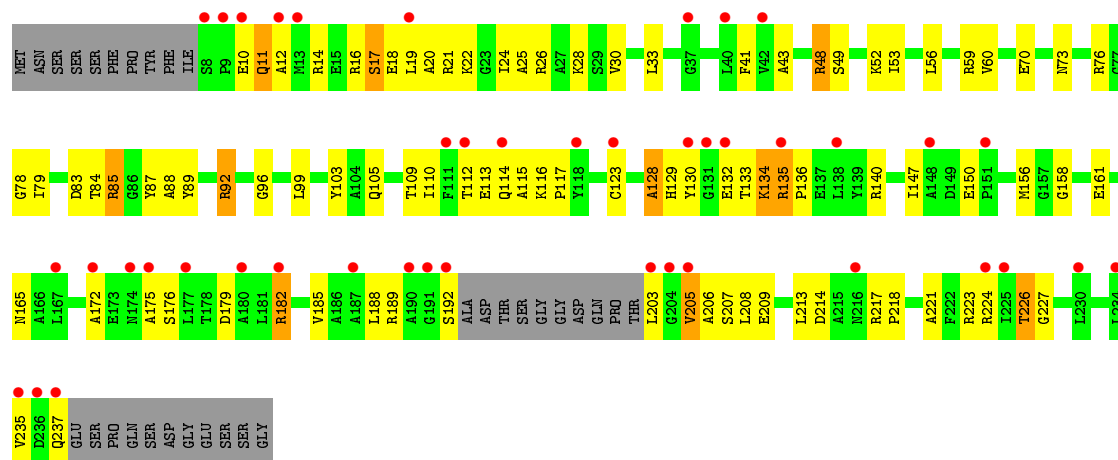


- Molecule 1: 20S proteasome, alpha and beta subunits

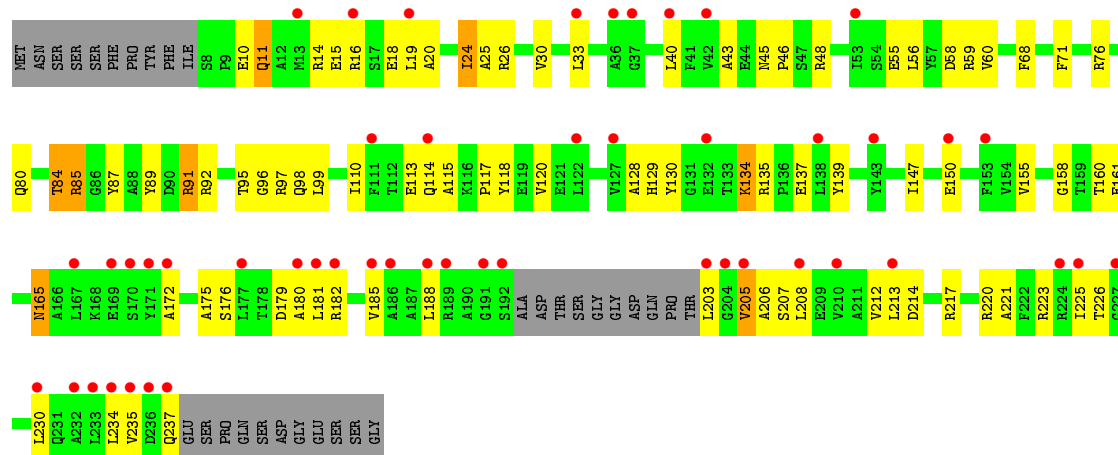




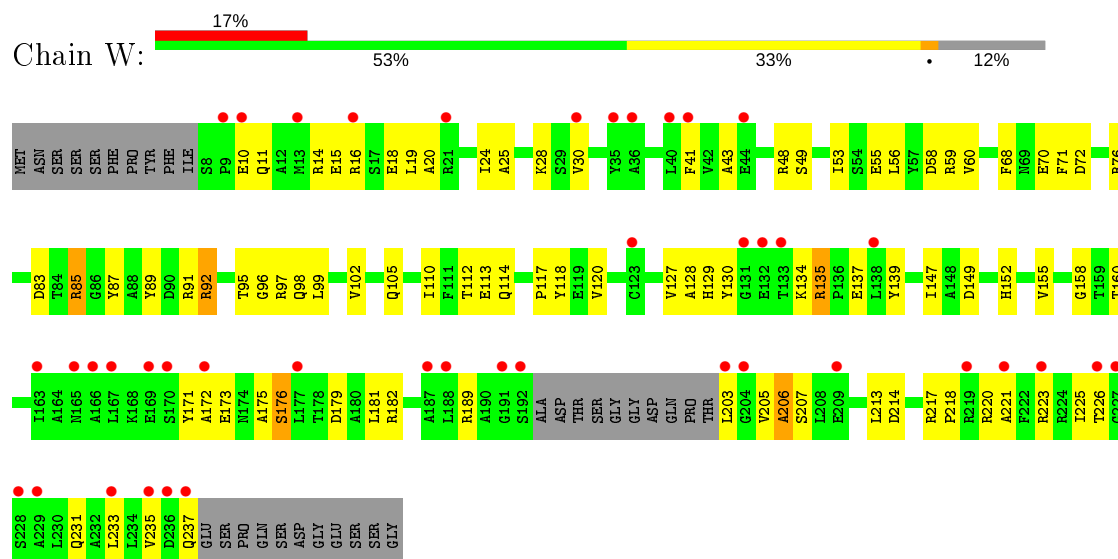
- Molecule 1: 20S proteasome, alpha and beta subunits



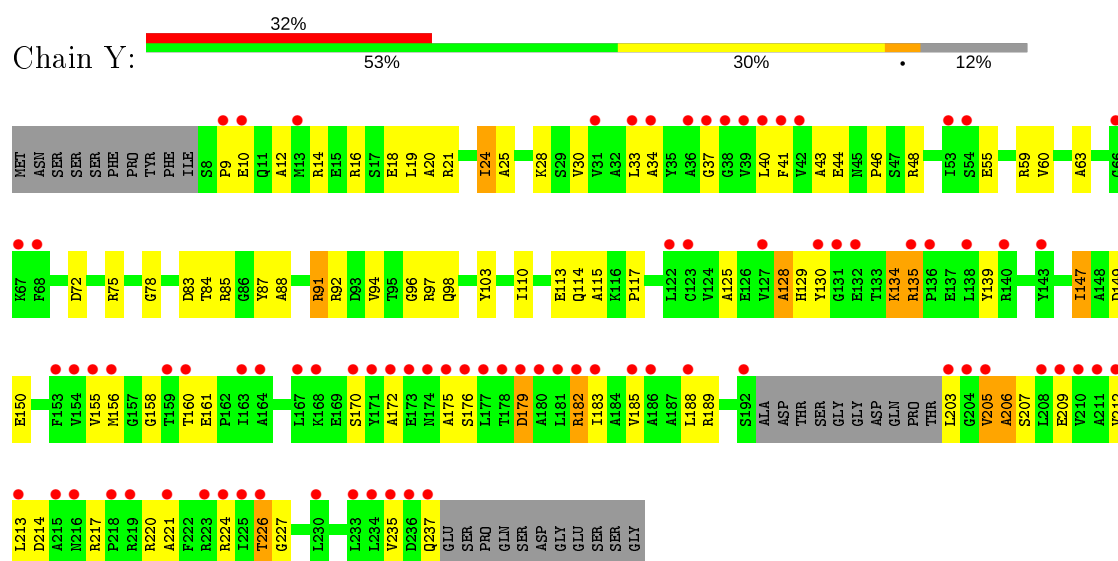
- Molecule 1: 20S proteasome, alpha and beta subunits



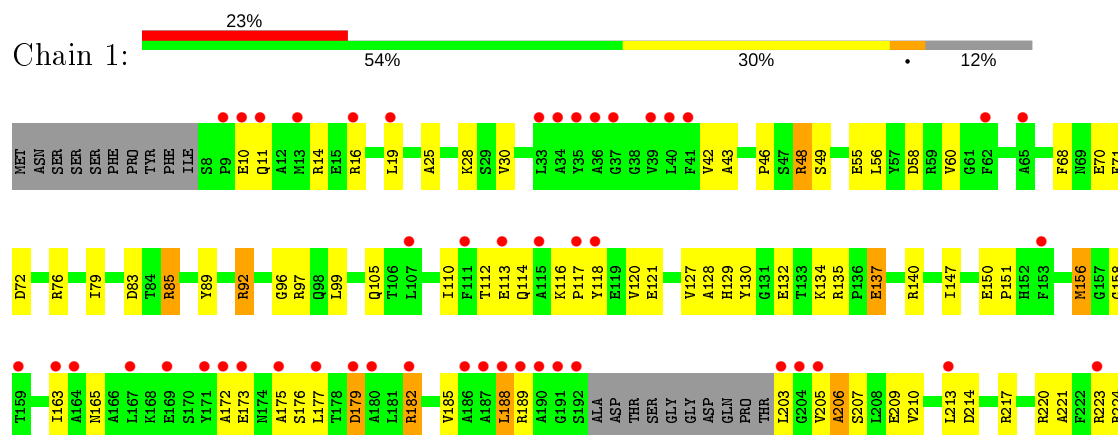
- Molecule 1: 20S proteasome, alpha and beta subunits

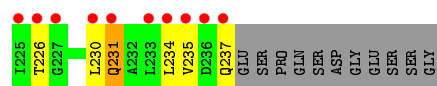


- Molecule 1: 20S proteasome, alpha and beta subunits

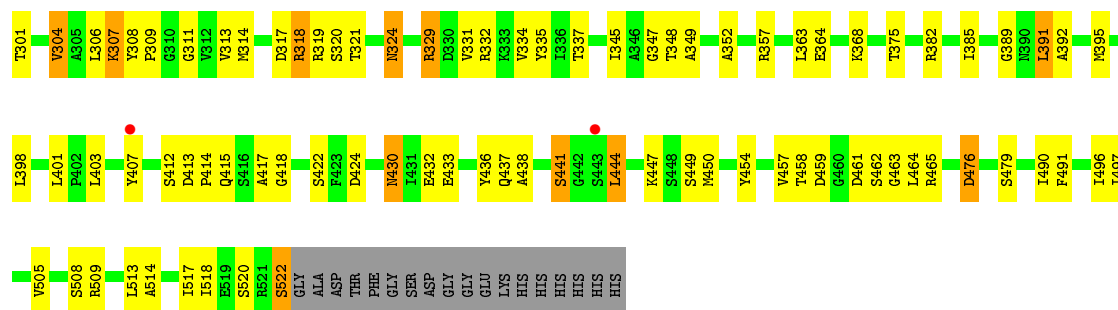


- Molecule 1: 20S proteasome, alpha and beta subunits

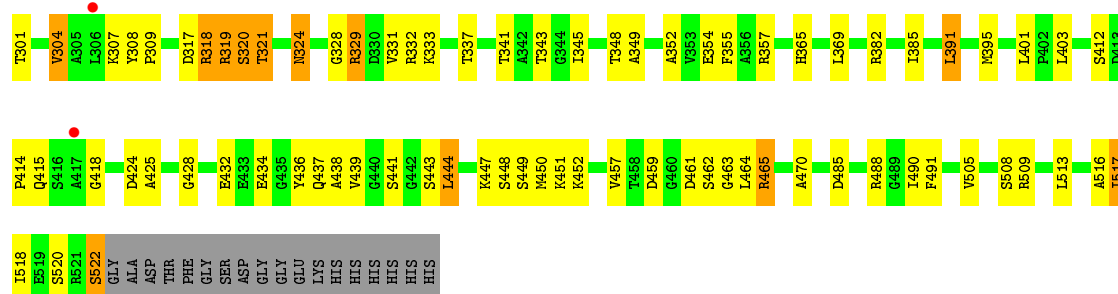




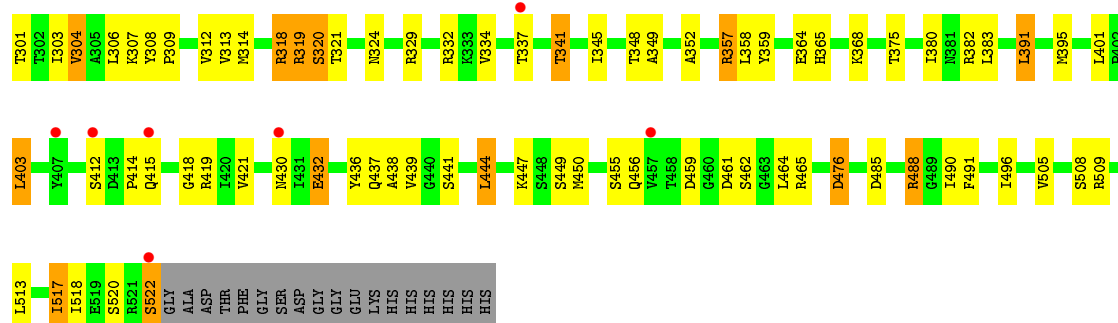
- Molecule 2: proteasome, beta subunit



- Molecule 2: proteasome, beta subunit

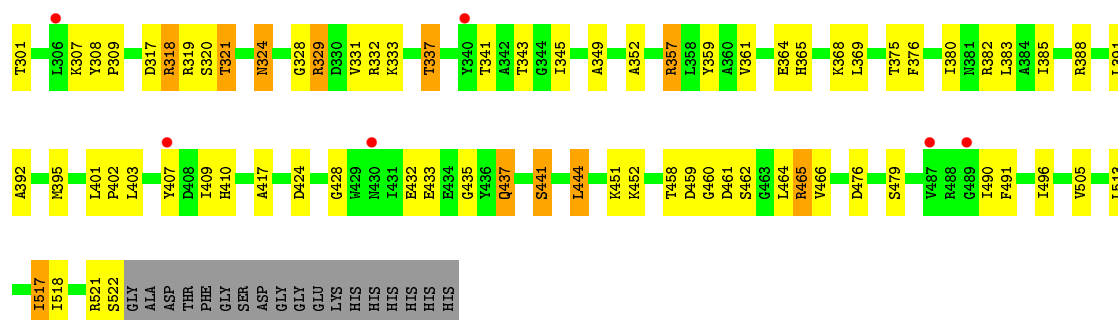


- Molecule 2: proteasome, beta subunit

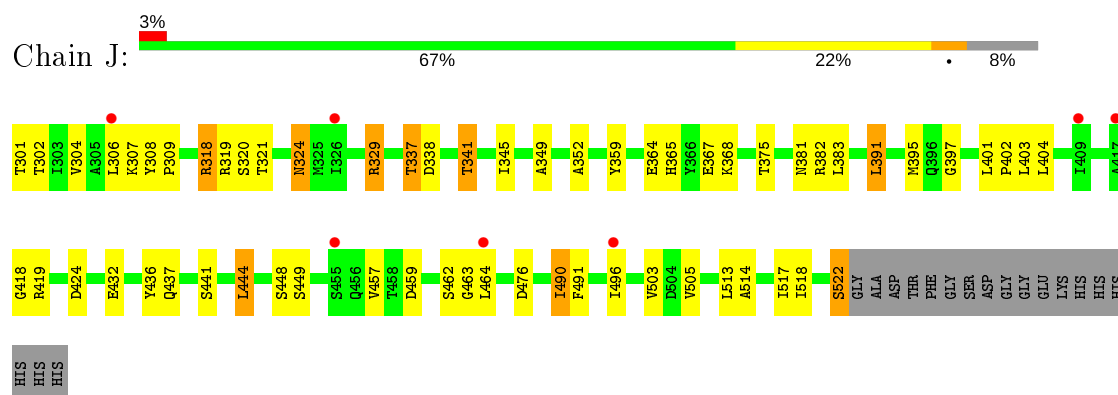


- Molecule 2: proteasome, beta subunit

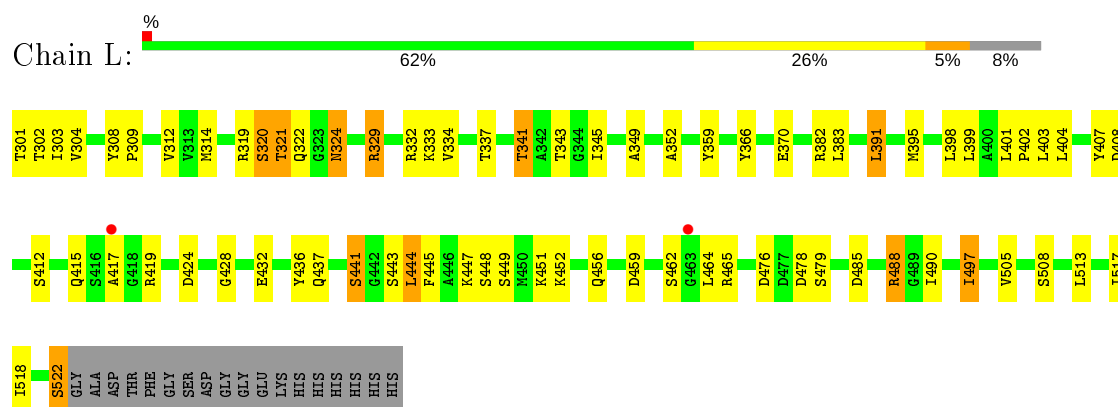




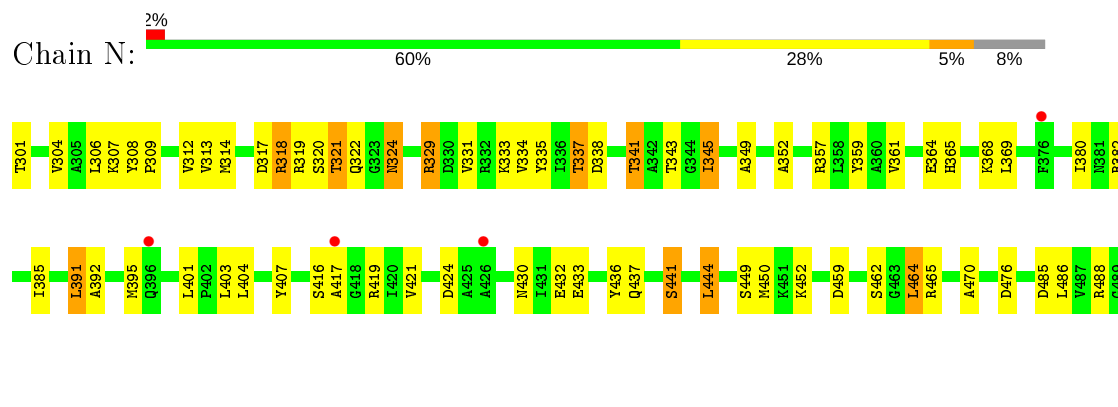
- Molecule 2: proteasome, beta subunit



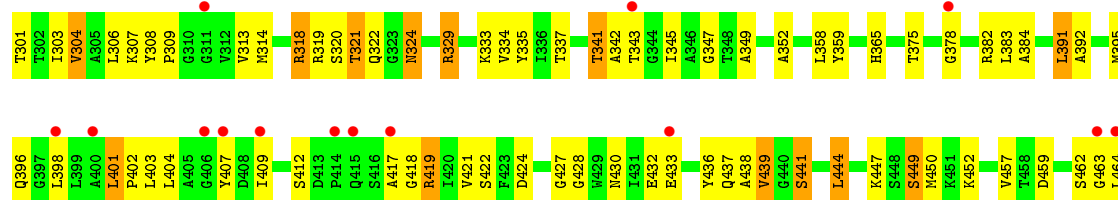
- Molecule 2: proteasome, beta subunit



- 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 49.77 – 2.99	Depositor EDS
% Data completeness (in resolution range)	94.1 (50.00-2.99) 94.1 (49.77-2.99)	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 , 88.1	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	0.92	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	0.49	0/1717	0.62	0/2320
1	A	0.45	0/1717	0.61	0/2320
1	B	0.45	0/1717	0.64	0/2320
1	D	0.48	0/1717	0.63	1/2320 (0.0%)
1	F	0.45	0/1717	0.63	0/2320
1	I	0.46	0/1717	0.61	0/2320
1	K	0.46	0/1717	0.63	0/2320
1	M	0.45	0/1717	0.63	0/2320
1	O	0.47	0/1717	0.62	0/2320
1	Q	0.49	0/1717	0.61	0/2320
1	S	0.47	0/1717	0.61	0/2320
1	U	0.47	0/1717	0.63	0/2320
1	W	0.62	2/1717 (0.1%)	0.64	1/2320 (0.0%)
1	Y	0.45	0/1717	0.61	0/2320
2	2	0.55	0/1662	0.71	0/2254
2	C	0.53	0/1662	0.72	0/2254
2	E	0.51	0/1662	0.72	0/2254
2	G	0.51	0/1662	0.69	0/2254
2	H	0.55	0/1662	0.71	0/2254
2	J	0.51	0/1662	0.69	0/2254
2	L	0.53	0/1662	0.70	0/2254
2	N	0.52	0/1662	0.69	0/2254
2	P	0.53	0/1662	0.73	0/2254
2	R	0.60	1/1662 (0.1%)	0.71	0/2254
2	T	0.54	1/1662 (0.1%)	0.68	0/2254
2	V	0.50	0/1662	0.69	0/2254
2	X	0.50	0/1662	0.69	0/2254
2	Z	0.52	0/1662	0.71	0/2254
All	All	0.50	4/47306 (0.0%)	0.66	2/64036 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	173	GLU	CD-OE1	13.22	1.40	1.25
2	R	412	SER	CB-OG	12.49	1.58	1.42
1	W	173	GLU	CD-OE2	11.28	1.38	1.25
2	T	456	GLN	CD-NE2	5.50	1.46	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	33	LEU	CA-CB-CG	5.71	128.44	115.30
1	W	173	GLU	OE1-CD-OE2	5.57	129.98	123.30

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	68	0
1	A	1692	0	1688	53	1
1	B	1692	0	1688	55	0
1	D	1692	0	1688	54	1
1	F	1692	0	1688	64	0
1	I	1692	0	1688	53	0
1	K	1692	0	1688	64	0
1	M	1692	0	1688	68	0
1	O	1692	0	1688	59	0
1	Q	1692	0	1688	45	0
1	S	1692	0	1688	65	0
1	U	1692	0	1688	53	0
1	W	1692	0	1688	60	0
1	Y	1692	0	1688	54	0
2	2	1638	0	1629	76	0
2	C	1638	0	1629	68	0
2	E	1638	0	1629	55	0
2	G	1638	0	1629	68	0
2	H	1638	0	1629	64	0
2	J	1638	0	1629	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1638	0	1629	67	0
2	N	1638	0	1629	80	0
2	P	1638	0	1629	56	0
2	R	1638	0	1629	55	0
2	T	1638	0	1629	55	0
2	V	1638	0	1629	65	0
2	X	1638	0	1629	73	0
2	Z	1638	0	1629	60	0
3	2	32	0	32	9	0
3	C	32	0	32	12	0
3	E	32	0	32	14	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
3	Z	32	0	32	17	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1629	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 17.

All (1629) 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: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:O16	3:N:273:M1N:H221	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
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:HH11	2:C:465:ARG:HG3	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:HH11	1:O:85:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:M:85:ARG:HG2	1.35	0.88
1:O:85:ARG:HH11	1:O:85:ARG:HG2	1.37	0.88
3:Z:273:M1N:O16	3:Z:273:M1N:H221	1.74	0.88
2:L:337:THR:OG1	2:L:343:THR:HG22	1.74	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: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:N:304:VAL:HG21	2:N:450:MET:HE1	1.55	0.86
2:Z:437:GLN:OE1	2:Z:447:LYS:HD3	1.76	0.85
2:N:349:ALA:N	3:N:273:M1N:H35	1.91	0.85
2:C:444:LEU:HD12	2:R:444:LEU:HD12	1.59	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
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
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:HG3	2:H:465:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:92:ARG:HD2	1:1:129:HIS:CE1	2.15	0.80
2:V:301:THR:N	2:V:441:SER:HG	1.80	0.80
2:T:301:THR:N	2:T:441:SER:HG	1.80	0.79
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: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
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:485:ASP:OD2	2:X:488:ARG:HB2	1.84	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:T:382:ARG:HD3	1:1:89:TYR:CD1	2.20	0.77
2:L:444:LEU:CD1	2:P:444:LEU:HD12	2.14	0.77
2:Z:349:ALA:HB2	3:Z:273:M1N:H252	1.67	0.76
3:E:273:M1N:C25	3:E:273:M1N:HN1	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
1:1:14:ARG:HH11	1:1:14:ARG:HB3	1.49	0.75
3:C:273:M1N:H221	3:C:273:M1N:O16	1.85	0.75
2:H:324:ASN:H	2:H:324:ASN:ND2	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:11:GLN:HG2	1:D:14:ARG:NH1	2.01	0.74
2:H:324:ASN:HD22	2:H:324:ASN:H	1.35	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
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:208:LEU:HB3	4:B:251:HOH:O	1.89	0.73
1:B:42:VAL:HG22	1:B:210:VAL:HG22	1.70	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
2:N:304:VAL:HG21	2:N:450:MET:HE3	1.69	0.73
1:I:92:ARG:HD2	1:I:129:HIS:CE1	2.24	0.73
2:N:304:VAL:CG2	2:N:450:MET:HE1	2.19	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:H252	3:E:273:M1N:HN1	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
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:HH11	1:S:85:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:465:ARG:NH1	2:C:465:ARG:HG3	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
2:2:464:LEU:HD12	2:2:496:ILE:HD11	1.73	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:G:321:THR:O	3:G:273:M1N:H51	1.91	0.71
2:T:337:THR:HG21	2:T:359:TYR:CD2	2.24	0.71
3:V:273:M1N:H221	3:V:273:M1N:O16	1.89	0.71
2:2:301:THR:N	2:2:441:SER:HG	1.88	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
1:1:217:ARG:HH21	1:1:223:ARG:HG3	1.56	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:J:301:THR:HG21	3:J:273:M1N:O16	1.91	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:HH11	1:W:85:ARG:HG2	1.57	0.70
2:2:485:ASP:OD2	2:2:488:ARG:HB2	1.92	0.69
2:C:318:ARG:HG2	4:C:551:HOH:O	1.90	0.69
2:L:301:THR:N	2:L:441:SER:HG	1.89	0.69
1:Y:72:ASP:OD2	4:Y:258:HOH:O	2.10	0.69
2:T:382:ARG:HD3	1:1:89:TYR:HD1	1.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:Z:465:ARG:HB2	2:Z:513:LEU:CD2	2.22	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
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:I: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:M:92:ARG:HH11	1:M:92:ARG:HB2	1.59	0.68
2:L:314:MET:CE	2:L:334:VAL:HG13	2.24	0.68
2:L:518:ILE:O	2:L:522:SER:HB2	1.93	0.68
1:I:14:ARG:HB3	1:I:14:ARG:NH1	2.07	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: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:H:321:THR:O	3:H:273:M1N:H37	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
2:N:304:VAL:CG2	2:N:450:MET:CE	2.70	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
2:T:314:MET:CE	2:T:334:VAL:HG13	2.24	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
2:T:318:ARG:HD3	2:T:491:PHE:O	1.93	0.67
1:O:9:PRO:HD2	1:U:15:GLU:OE1	1.95	0.67
2:C:308:TYR:HB2	2:C:309:PRO:HD2	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:16:ARG:HE	1:1:117:PRO:HD3	1.60	0.66
2:C:329:ARG:NH2	2:E:476:ASP:O	2.28	0.66
2:J:391:LEU:O	2:J:395:MET:HG2	1.95	0.66
2:P:375:THR:HB	2:P:378:GLY:H	1.60	0.66
1:Y:75:ARG:NH2	4:Y:254:HOH:O	2.28	0.66
3:R:273:M1N:N1	3:R:273:M1N:H252	2.09	0.66
2:2:375:THR:HB	2:2:378:GLY:H	1.60	0.66
2:G:437:GLN:HA	2:G:437:GLN:OE1	1.94	0.66
2:J:324:ASN:ND2	2:J:324:ASN:H	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:C:459:ASP:H	2:C:462:SER:HB3	1.61	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
2:R:301:THR:N	2:R:441:SER:HG	1.94	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: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
2:2:459:ASP:H	2:2:462:SER:HB3	1.59	0.65
3:P:273:M1N:H253	3:P:273:M1N:HN1	1.61	0.65
2:G:337:THR:HG21	2:G:359:TYR:CD2	2.31	0.65
2:H:459:ASP:H	2:H:462:SER:HB3	1.62	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
1:1:205:VAL:HG12	1:1:206:ALA:H	1.62	0.65
2:J:341:THR:HG22	2:J:404:LEU:HD11	1.76	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
2:N:301:THR:N	2:N:441:SER:HG	1.95	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
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:HH11	1:S:140:ARG:HB3	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
1:F:165:ASN:HD22	1:F:168:LYS:NZ	1.95	0.64
1:F:56:LEU:HD13	1:F:99:LEU:HD22	1.79	0.64
3:L:273:M1N:HN1	3:L:273:M1N:C25	2.10	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:C:301:THR:HG21	3:C:273:M1N:H16	1.63	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
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
1:1:30:VAL:HG13	1:1:43:ALA:HB2	1.80	0.63
1:D:90:ASP:HB3	1:D:93:ASP:OD1	1.98	0.63
2:X:464:LEU:HD12	2:X:496:ILE:HD11	1.80	0.63
1:M:189:ARG:HH22	1:M:235:VAL:HG13	1.63	0.63
2:X:424:ASP:HB3	2:X:428:GLY:H	1.62	0.63
2:C:304:VAL:HG21	2:C:450:MET:CE	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
1:1:217:ARG:NH2	1:1:223:ARG:HG3	2.14	0.63
2:N:321:THR:O	3:N:273:M1N:H52	1.99	0.63
2:2:518:ILE:O	2:2:522:SER:HB2	1.98	0.63
1:A:170:SER:HB2	1:A:183:ILE:HD12	1.80	0.63
1:A:87:TYR:O	2:H:357:ARG:NH2	2.32	0.63
2:C:391:LEU:O	2:C:395:MET:HG2	1.99	0.63
2:J:459:ASP:H	2:J:462:SER:HB3	1.63	0.63
1:D:48:ARG:HD2	1:K:137:GLU:OE2	1.99	0.63
2:N:324:ASN:H	2:N:324:ASN:ND2	1.92	0.63
1:U:95:THR:OG1	1:U:98:GLN:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:444:LEU:CD1	2:V:444:LEU:HD12	2.22	0.63
1:S:14:ARG:HB2	1:S:14:ARG:NH1	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:110:ILE:HG23	1:W:114:GLN:HG3	1.80	0.63
1:W:14:ARG:NH1	1:W:14:ARG:HB3	2.14	0.63
1:W:189:ARG:NH2	1:W:237:GLN:HB3	2.14	0.63
2:Z:324:ASN:H	2:Z:324:ASN:HD22	1.47	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:NH1	1:O:85:ARG:CG	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
2:L:314:MET:HE3	2:L:334:VAL:HG13	1.79	0.62
2:R:457:VAL:HG22	2:R:463:GLY:HA2	1.80	0.62
1:U:89:TYR:CD1	2:2:382:ARG:HD3	2.34	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
3:R:273:M1N:C25	3:R:273:M1N:N1	2.63	0.62
2:R:459:ASP:H	2:R:462:SER:HB3	1.63	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
1:1:60: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:C25	3:R:273:M1N:HN1	2.13	0.62
2:2:308:TYR:HB2	2:2:309:PRO:HD2	1.80	0.61
2:G:518:ILE:O	2:G:522:SER:HB2	1.99	0.61
1:F:73:ASN:HD22	1:W:105:GLN:NE2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:324:ASN:C	2:2:324:ASN:HD22	2.04	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
1:1:230:LEU:HD21	1:1:234:LEU:HD13	1.81	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
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:O:205:VAL:C	1:O:207:SER:H	2.03	0.61
1:Q:56:LEU:HD13	1:Q:99:LEU:HD22	1.81	0.61
2:2:441:SER:HB2	2:2:478:ASP:OD2	2.00	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:H:324:ASN:HD22	2:H:324:ASN:N	1.95	0.61
2:X:307:LYS:HD2	2:X:418:GLY:O	2.01	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
2:H:395:MET:HA	2:H:395:MET:CE	2.31	0.61
3:J:273:M1N:C25	3:J:273:M1N:HN1	2.14	0.61
1:Y:25:ALA:O	1:Y:158:GLY:HA2	2.00	0.61
2:2:345:ILE:HD13	2:2:352:ALA:HB1	1.83	0.60
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
3:L:273:M1N:H252	3:L:273:M1N:HN1	1.66	0.60
2:L:456:GLN:NE2	2:L:465:ARG:NH1	2.49	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:N:318:ARG:HD3	2:N:491:PHE:O	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:321:THR:O	3:J:273:M1N:C5	2.49	0.60
2:2:419:ARG:HH11	2:2:419:ARG:HG3	1.66	0.60
1:F:20:ALA:O	1:F:24:ILE:HG12	2.01	0.60
1:B:19:LEU:HD12	1:I:10:GLU:HA	1.83	0.60
1:O:14:ARG:HH11	1:O:14:ARG:CB	2.14	0.60
2:E:318:ARG:HD3	2:E:491:PHE:O	2.01	0.60
1:U:11:GLN:CG	1:U:14:ARG:HH12	2.11	0.60
2:G:444:LEU:HD12	2:2:444:LEU:CD1	2.31	0.60
2:2:515:ARG:HA	2:2:518:ILE:HD12	1.84	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
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
1:D:110:ILE:HG23	1:D:114:GLN:HG3	1.81	0.60
2:T:473:ASP:HA	4:X:20:HOH:O	2.01	0.60
1:Q:89:TYR:CD1	2:Z:382:ARG:HD3	2.37	0.60
3:H:273:M1N:H40	2:P:424:ASP:OD1	2.02	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:Y:205:VAL:C	1:Y:207:SER:H	2.05	0.59
1:O:217:ARG:NH2	1:O:223:ARG:HG3	2.15	0.59
2:R:324:ASN:HD22	2:R:324:ASN:C	2.06	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:NH1	1:S:85:ARG:HG2	2.18	0.59
1:U:55:GLU:OE2	1:U:220:ARG:HD2	2.02	0.59
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:349:ALA:HB2	3:2:273:M1N:H252	1.84	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: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
1:I:205:VAL:C	1:I:207:SER:H	2.05	0.58
2:X:430:ASN:ND2	4:X:16:HOH:O	2.31	0.58
2:C:301:THR:N	2:C:441:SER:OG	2.36	0.58
2:H:407:TYR:CE1	2:H:417:ALA:HB3	2.38	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
1:1:11:GLN:HG2	1:1:14:ARG:HH12	1.68	0.58
2:2:419:ARG:CG	2:2:419:ARG:HH11	2.16	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
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
2:2:419:ARG:NH1	2:2:419:ARG:HG3	2.17	0.58
1:1:14:ARG:CB	1:1:14:ARG:HH11	2.16	0.58
1:K:205:VAL:C	1:K:207:SER:H	2.07	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
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:C25	3:P:273:M1N:HN1	2.16	0.58
1:U:96:GLY:HA2	1:U:99:LEU:HD13	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:304:VAL:HG21	2:C:450:MET:HE3	1.85	0.57
2:H:465:ARG:HG3	2:H:465:ARG:NH1	2.18	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
1:I:92:ARG:HD2	1:I:129:HIS:ND1	2.18	0.57
1:M:205:VAL:C	1:M:207:SER:H	2.07	0.57
2:R:409:ILE:HG13	2:R:410:HIS:HD2	1.69	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:S:205:VAL:C	1:S:207:SER:H	2.06	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
2:2:391:LEU:O	2:2:395:MET:HG2	2.04	0.57
2:C:513:LEU:O	2:C:517:ILE:HG12	2.04	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
1:F:19:LEU:HD12	1:W:10:GLU:HA	1.85	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
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.86	0.57
1:U:205:VAL:C	1:U:207:SER:H	2.08	0.57
2:G:383:LEU:HD21	2:G:402:PRO:CG	2.35	0.57
1:Q:205:VAL:C	1:Q:207:SER:H	2.08	0.57
2:T:308:TYR:HB2	2:T:309:PRO:HD2	1.87	0.57
1:A:205:VAL:C	1:A:207:SER:H	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:K:19:LEU:HD12	1:M:10:GLU:HA	1.86	0.56
2:R:321:THR:O	3:R:273:M1N:C5	2.48	0.56
1:I:73:ASN:HB2	1:S:105:GLN:HE22	1.70	0.56
1:W:41:PHE:HB3	1:W:53:ILE:HD13	1.87	0.56
1:F:110:ILE:HG23	1:F:114:GLN:HG3	1.87	0.56
2:H:391:LEU:O	2:H:395:MET:HG2	2.05	0.56
2:J:383:LEU:HD21	2:J:402:PRO:HG2	1.86	0.56
1:M:230:LEU:HD21	1:M:234:LEU:HD13	1.85	0.56
2:N:395:MET:HA	2:N:395:MET:CE	2.34	0.56
2:P:388:ARG:NH1	4:P:551:HOH:O	2.39	0.56
2:Z:335:TYR:HE1	2:Z:345:ILE:HD11	1.71	0.56
1:I:182:ARG:HH11	1:I:182:ARG:HB2	1.69	0.56
2:G:444:LEU:CD1	2:2:444:LEU:HD12	2.31	0.56
3:E:273:M1N:C22	3:E:273:M1N:O16	2.53	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:I:121:GLU:OE2	1:I:156:MET:HB3	2.06	0.56
2:2:329:ARG:O	2:2:490:ILE:HG21	2.06	0.56
1:A:25:ALA:O	1:A:158:GLY:HA2	2.04	0.56
1:F:205:VAL:C	1:F:207:SER:H	2.09	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:349:ALA:H	3:N:273:M1N:C36	2.18	0.56
2:V:321:THR:O	3:V:273:M1N:C5	2.53	0.56
1:I:213:LEU:HA	1:I:221:ALA:O	2.06	0.56
2:2:341:THR:HG22	2:2:404:LEU:HD11	1.88	0.56
2:H:461:ASP:OD1	2:H:509:ARG:HD2	2.06	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:182:ARG:HB2	1:B:182:ARG:NH1	2.21	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
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:Z:317:ASP:OD1	2:Z:333:LYS:NZ	2.37	0.56
2:2:462:SER:O	2:2:465:ARG:HG2	2.06	0.56
2:E:314:MET:HE2	2:E:334:VAL:HG13	1.88	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:O	2:T:345:ILE:HD12	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
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:J:444:LEU:CD1	2:Z:444:LEU:HD12	2.21	0.55
1:D:161:GLU:H	1:D:161:GLU:CD	2.10	0.55
1:D:205:VAL:C	1:D:207:SER:H	2.09	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
2:L:337:THR:OG1	2:L:343:THR:CG2	2.51	0.55
1:1:205:VAL:C	1:1:207:SER:H	2.10	0.55
1:D:87:TYR:O	2:E:357:ARG:NH2	2.39	0.55
2:2:314:MET:CE	2:2:334:VAL:HG13	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:349:ALA:H	3:L:273:M1N:H35	1.71	0.55
1:S:161:GLU:O	1:S:165:ASN:HB2	2.06	0.55
1:1:110:ILE:HA	1:1:114:GLN:HG2	1.88	0.55
2:2:341:THR:CG2	2:2:404:LEU:HD11	2.37	0.55
2:J:324:ASN:N	2:J:324:ASN:HD22	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:W:205:VAL:C	1:W:207:SER:H	2.10	0.55
2:2:459:ASP:HB2	4:2:552:HOH:O	2.07	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
1:1:205:VAL:HG12	1:1:206:ALA:N	2.21	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
2:2:432:GLU:HG3	2:2:437:GLN:HB2	1.87	0.54
1:O:92:ARG:HH11	1:O:92:ARG:HB2	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
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
1:U:213:LEU:HA	1:U:221:ALA:O	2.07	0.54
1:U:33:LEU:HD11	1:U:180:ALA:HB1	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:337:THR:HG21	2:2:359:TYR:CD2	2.43	0.54
3:E:273:M1N:N1	3:E:273:M1N:C25	2.71	0.54
2:H:307:LYS:HD2	2:H:418:GLY:O	2.06	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:X:314:MET:HE3	2:X:334:VAL:HG13	1.89	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
1:D:36:ALA:HA	4:D:250:HOH:O	2.07	0.54
2:H:301:THR:N	2:H:441:SER:OG	2.41	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: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
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
2:G:521:ARG:HH22	2:2:452:LYS:NZ	2.06	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CZ	1:U:14:ARG:HB3	2.38	0.53
2:V:432:GLU:HG3	2:V:437:GLN:HB2	1.90	0.53
1:W:55:GLU:OE2	1:W:220:ARG:HD2	2.08	0.53
2:G:424:ASP:OD2	3:X:273:M1N:H34	2.07	0.53
1:B:205:VAL:C	1:B:207:SER:H	2.11	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:Q:63:ALA:O	1:Q:156:MET:HE1	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
2:2:345:ILE:HB	2:2:352:ALA:HB1	1.91	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
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
2:G:451:LYS:NZ	2:2:473:ASP:OD1	2.38	0.53
1:A:176:SER:HB3	1:A:179:ASP:OD1	2.09	0.53
2:C:457:VAL:HG22	2:C:463:GLY:HA2	1.90	0.53
1:D:219:ARG:HH11	1:D:219:ARG:HG2	1.73	0.53
2:H:457:VAL:HG22	2:H:463:GLY:HA2	1.91	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:D:89:TYR:CE1	2:R:382:ARG:HD3	2.44	0.53
1:Y:41:PHE:HE2	1:Y:213:LEU:HD13	1.73	0.53
1:1:140:ARG:NH1	1:1:140:ARG:HB3	2.24	0.53
1:1:72:ASP:O	1:1:76:ARG:HG3	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:450:MET:HE3	2:C:470:ALA:CB	2.38	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
2:T:314:MET:HE3	2:T:334:VAL:HG13	1.89	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
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
1:A:12:ALA:O	1:A:16:ARG:HG2	2.09	0.52
1:F:165:ASN:ND2	1:F:168:LYS:HZ1	2.08	0.52
1:K:176:SER:HB3	1:K:179:ASP:OD1	2.09	0.52
1:K:92:ARG:HB2	1:K:92:ARG:HH11	1.73	0.52
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
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:64:ALA:CB	1:A:122:LEU:HD12	2.40	0.52
1:A:54:SER:CB	1:A:75:ARG:HD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:118:TYR:HB3	1:M:120:VAL:HG22	1.92	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
2:X:314:MET:HE2	2:X:342:ALA:CB	2.40	0.52
1:F:165:ASN:ND2	1:F:168:LYS:NZ	2.57	0.52
1:F:16:ARG:NH2	1:F:114:GLN:O	2.43	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:HN1	3:T:273:M1N:C25	2.23	0.52
2:X:395:MET:HA	2:X:395:MET:CE	2.39	0.52
2:P:439:VAL:HG11	4:P:548:HOH:O	2.09	0.52
1:F:48:ARG:NH2	1:W:135:ARG:HD2	2.25	0.52
1:W:60:VAL:HG21	1:W:96:GLY:HA3	1.92	0.52
1:I:55:GLU:OE2	1:I:220:ARG:HD2	2.10	0.51
1:F:182:ARG:HH11	1:F:182:ARG:HB2	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:A:90:ASP:HB3	1:A:93:ASP:OD1	2.10	0.51
1:D:63:ALA:O	1:D:156:MET:HE1	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:223:ARG:HA	4:W:253:HOH:O	2.10	0.51
1:W:87:TYR:HA	2:X:357:ARG:HH21	1.75	0.51
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:HG3	1:O:85:ARG:HH11	1.70	0.51
1:I:209:GLU:OE2	1:I:224:ARG:NH2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:92:ARG:HB2	1:W:92:ARG:HH11	1.75	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
2:T:314:MET:HE2	2:T:334:VAL:HG13	1.93	0.51
2:2:513:LEU:O	2:2:517:ILE:HG12	2.10	0.51
1:M:85:ARG:NH1	1:M:85:ARG:CG	2.59	0.51
1:Y:226:THR:HG23	1:Y:227:GLY:N	2.26	0.51
1:1:132:GLU:HA	4:1:252:HOH:O	2.11	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:V:345:ILE:HD13	2:V:352:ALA:HB1	1.91	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
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
2:Z:304:VAL:HG21	2:Z:450: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
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:F:165:ASN:HD22	1:F:168:LYS:HZ3	1.57	0.50
1:D:15:GLU:OE1	1:K:9:PRO:HD2	2.11	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
1:O:112:THR:HG22	1:U:115:ALA:HB3	1.92	0.50
2:Z:319:ARG:HG3	2:Z:320:SER:N	2.27	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:324:ASN:HD22	2:X:324:ASN:C	2.14	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
2:X:314:MET:HE2	2:X:342:ALA:HB1	1.93	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
3:Z:273:M1N:H221	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: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:H:513:LEU:O	2:H:517:ILE:HG12	2.11	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
2:T:324:ASN:HD22	2:T:324:ASN:C	2.15	0.50
1:D:92:ARG:CD	1:D:129:HIS:CE1	2.92	0.49
2:H:462:SER:O	2:H:465:ARG:HG2	2.12	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
2:2:437:GLN:OE1	2:2:447:LYS:HD3	2.12	0.49
2:N:465:ARG:HB2	2:N:513:LEU:HD22	1.94	0.49
1:O:85:ARG:NH1	1:O:85:ARG:HG2	2.16	0.49
2:C:452:LYS:HE2	2:R:521:ARG:HH22	1.78	0.49
1:S:60:VAL:HG21	1:S:96:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:63:ALA:O	1:B:156:MET:HE1	2.13	0.49
2:E:301:THR:N	2:E:441:SER:OG	2.46	0.49
2:E:395:MET:CE	2:E:395:MET:HA	2.42	0.49
1:B:181:LEU:HD23	1:B:233:LEU:HB3	1.95	0.49
2:N:322:GLN:O	2:N:322:GLN:HG2	2.13	0.49
1:M:83:ASP:OD2	2:N:365:HIS:CD2	2.65	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:HH11	1:B:14:ARG:HB3	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:322:GLN:HE21	3:X:273:M1N:C38	2.26	0.49
2:X:321:THR:O	3:X:273:M1N:H37	2.12	0.49
2:X:358:LEU:HD23	4:X:141:HOH:O	2.12	0.49
2:2:392:ALA:O	2:2:395:MET:HB2	2.12	0.49
1:A:172:ALA:HB3	1:A:175:ALA:HB2	1.95	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
2:H:382:ARG:HD3	1:B:89:TYR:CD1	2.48	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
1:1:56:LEU:HB2	1:1:60:VAL:HG13	1.95	0.49
1:A:11:GLN:HG2	1:A:14:ARG:HH12	1.77	0.49
1:I:161:GLU:O	1:I:165:ASN:HB2	2.13	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
1:K:42:VAL:HG22	1:K:210:VAL:HG22	1.93	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
1:1:182:ARG:NH1	1:1:182:ARG:HB2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:83:ASP:OD2	2:2:365:HIS:HD2	1.95	0.49
2:2:304:VAL:HG23	2:2:438:ALA:HB2	1.95	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
1:1:30:VAL:HG22	1:1:43:ALA:HB1	1.94	0.49
2:G:357:ARG:O	2:G:361:VAL:HG23	2.12	0.49
1:K:85:ARG:NH1	1:K:85:ARG:CG	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
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
1:1:85:ARG:HH11	1:1:85:ARG:HG2	1.76	0.48
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
1:1:110:ILE:HG21	1:1:118:TYR:CD1	2.47	0.48
2:E:465:ARG:NH1	2:E:465:ARG:HG3	2.25	0.48
2:H:364:GLU:HG2	2:H:368:LYS:HE2	1.95	0.48
1:I:115:ALA:HB3	1:S:112:THR:HG22	1.94	0.48
2:H:331:VAL:HG11	3:H:273:M1N:H251	1.93	0.48
2:J:349:ALA:N	3:J:273:M1N:H35	2.28	0.48
2:P:424:ASP:HB3	2:P:428:GLY:H	1.76	0.48
1:B:185:VAL:HB	1:B:235:VAL:HG11	1.94	0.48
1:I:92:ARG:HH11	1:I:92:ARG:HB2	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
1:1:177:LEU:CB	4:1:251:HOH:O	2.60	0.48
1:B:209:GLU:OE2	1:B:224:ARG:NH2	2.46	0.48
2:C:324:ASN:HD22	2:C:324:ASN:C	2.15	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:F:48:ARG:HH22	1:W:135:ARG:HD2	1.78	0.48
1:W:56:LEU:HB2	1:W:60:VAL:HG13	1.96	0.48
2:2:321:THR:O	3:2:273:M1N:C5	2.56	0.48
2:2:395:MET:HA	2:2:395:MET:CE	2.42	0.48
2:E:337:THR:HG21	2:E:359:TYR:CD2	2.49	0.48
2:E:304:VAL:HG23	2:E:438:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1:1:48: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
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
1:1:42:VAL:HG22	1:1:210:VAL:HG22	1.95	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
1:1:118:TYR:HB3	1:1:120:VAL:HG22	1.94	0.48
1:1:214:ASP:OD2	1:1:217:ARG:HG2	2.13	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:K:63:ALA:O	1:K:156:MET:HE1	2.14	0.48
1:M:205:VAL:CG1	1:M:206:ALA:N	2.77	0.48
1:Q:176:SER:H	1:Q:179:ASP:HB2	1.77	0.48
1:Q:127:VAL:HG11	1:Q:213:LEU:HB3	1.96	0.48
2:R:341:THR:CG2	2:R:404:LEU:HD11	2.44	0.48
2:2:457:VAL:HG22	2:2:463:GLY:HA2	1.94	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
2:X:308:TYR:HB2	2:X:309:PRO:HD2	1.96	0.48
1:1:189:ARG:NH2	1:1:237:GLN:HB3	2.29	0.47
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
2:L:314:MET:HE2	2:L:334:VAL:HG13	1.93	0.47
1:Q:112:THR:HG22	1:Y:115:ALA:HB3	1.96	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: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
2:N:395:MET:HA	2:N:395:MET:HE1	1.96	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:U:80:GLN:O	1:U:84:THR:OG1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:450:MET:HE2	2:N:470:ALA:CB	2.45	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
2:2:314:MET:HE2	2:2:334:VAL:HG13	1.96	0.47
1:B:135:ARG:HH22	1:B:152:HIS:CD2	2.32	0.47
1:O:161:GLU:O	1:O:165:ASN:HB2	2.14	0.47
1:O:85:ARG:HG3	1:O:85:ARG:NH1	2.28	0.47
1:S:226:THR:HG23	1:S:227:GLY:N	2.29	0.47
2:G:424:ASP:CG	3:X:273:M1N:H40	2.34	0.47
2:C:424:ASP:HB3	2:C:428:GLY:H	1.80	0.47
2:H:514:ALA:O	2:H:518:ILE:HG13	2.14	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
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:E:304:VAL:HG21	2:E:450:MET:HE3	1.97	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:335:TYR:HE1	2:H:345:ILE:HD11	1.79	0.47
1:I:97:ARG:HH11	1:I:97:ARG:HG3	1.80	0.47
2:2:335:TYR:HE1	2:2:345:ILE:HD11	1.80	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
2:H:337:THR:HG22	2:H:363:LEU:HD12	1.96	0.47
1:I:142:THR:OG1	1:I:146:SER:HB2	2.15	0.47
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:185:VAL:HB	1:1:235:VAL:CG1	2.45	0.47
2:2:349:ALA:CB	3:2:273:M1N:H252	2.45	0.47
2:2:318:ARG:HD3	2:2:491:PHE:O	2.15	0.47
1:D:141:ILE:HG13	1:D:147:ILE:HG12	1.97	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
2:X:344:GLY:C	4:X:58:HOH:O	2.48	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
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
1:W:72:ASP:O	1:W:76:ARG:HG3	2.15	0.46
1:W:19:LEU:HD12	1:Y:10:GLU:HA	1.97	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:329:ARG:O	2:H:490:ILE:HG21	2.15	0.46
1:K:59:ARG:HG3	1:K:129:HIS:CD2	2.43	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
2:2:314:MET:HE1	2:2:342:ALA:HB1	1.96	0.46
2:H:432:GLU:HG3	2:H:437:GLN:HB2	1.96	0.46
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:N:314:MET:CE	2:N:334:VAL:HG13	2.45	0.46
2:C:320:SER:HB3	2:C:328:GLY:HA3	1.98	0.46
2:C:318:ARG:HB3	2:C:331:VAL:O	2.15	0.46
1:F:28:LYS:HE3	1:F:44:GLU:HG3	1.97	0.46
2:G:301:THR:N	2:G:441:SER:HG	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:137:GLU:HG2	1:A:139:TYR:CE2	2.51	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
2:P:324:ASN:C	2:P:324:ASN:HD22	2.18	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
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
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:CE	2:Z:395:MET:HA	2.45	0.46
1:B:110:ILE:HA	1:B:114:GLN:HG2	1.98	0.46
2:C:349:ALA:H	3:C:273:M1N:C36	2.29	0.46
2:C:307:LYS:HD2	2:C:418:GLY:O	2.15	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:H:392:ALA:O	2:H:395:MET:HB2	2.16	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
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:L:319:ARG:HG3	2:L:320:SER:N	2.31	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
1:1:96:GLY:HA2	1:1:99:LEU:HB2	1.97	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
2:V:349:ALA:HB3	3:V:273:M1N:C34	2.46	0.46
2:V:345:ILE:HB	2:V:352:ALA:HB1	1.97	0.46
1:B:226:THR:OG1	1:B:227:GLY:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:301:THR:N	2:H:441:SER:HG	2.13	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
3:T:273:M1N:H36	3:T:273:M1N:H4	1.86	0.45
2:T:349:ALA:HB2	3:T:273:M1N:H252	1.98	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
1:F:115:ALA:HB3	1:W:112:THR:CG2	2.46	0.45
2:G:437:GLN:CA	2:G:437:GLN:OE1	2.63	0.45
2:H:304:VAL:HG21	2:H:450:MET:HE3	1.97	0.45
2:H:307:LYS:NZ	2:H:433:GLU:HA	2.31	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:K:24:ILE:HD11	1:K:120:VAL:C	2.37	0.45
1:O:16:ARG:NH2	1:O:114:GLN:O	2.48	0.45
2:P:345:ILE:O	2:P:345:ILE:HD12	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:S:135:ARG:HA	1:S:136:PRO:HD2	1.87	0.45
3:T:273:M1N:O16	3:T:273:M1N:C22	2.64	0.45
1:S:87:TYR:O	2:T:357:ARG:NH2	2.49	0.45
1:U:214:ASP:OD2	1:U:217:ARG:HG2	2.17	0.45
1:O:137:GLU:OE2	1:U:48:ARG:HD2	2.15	0.45
2:X:304:VAL:HG21	2:X:450:MET:HE3	1.97	0.45
2:G:521:ARG:NH2	2:2:452:LYS:NZ	2.65	0.45
1:D:230:LEU:HD21	1:D:234:LEU:HD13	1.97	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:U:182:ARG:HB2	1:U:182:ARG:NH1	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:185:VAL:HG12	1:Y:189:ARG:NH1	2.31	0.45
1:Y:30:VAL:HG22	1:Y:43:ALA:HB1	1.98	0.45
2:2:424:ASP:HB2	4:2:545:HOH:O	2.16	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
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:ND2	2:N:324:ASN:N	2.55	0.45
2:N:338:ASP:C	2:N:338:ASP:OD1	2.55	0.45
1:Q:128:ALA:HB2	1:Q:134:LYS:HB3	1.98	0.45
1:Y:41:PHE:HZ	1:Y:125:ALA:HB3	1.82	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
1:B:170:SER:HB2	1:B:183:ILE:HD12	1.99	0.45
1:B:60:VAL:HG21	1:B:96:GLY:HA3	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: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:HD23	2:T:383:LEU:O	2.17	0.45
2:T:444:LEU:HD12	2:X:444:LEU:CD1	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
2:H:496:ILE:HG12	2:H:505:VAL:CG2	2.47	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
2:2:322:GLN:O	2:2:322:GLN:HG2	2.16	0.45
3:L:273:M1N:H221	3:L:273:M1N:O16	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
1:W:41:PHE:HE2	1:W:213:LEU:HD13	1.81	0.45
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:I:112:THR:HG23	1.99	0.44
2:2:314:MET:HE3	2:2:334:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:308:TYR:HB2	2:N:309:PRO:HD2	1.98	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
1:1:163:ILE:HG23	1:1:188:LEU:HA	1.98	0.44
1:1:70:GLU:OE2	1:1:116:LYS:NZ	2.50	0.44
1:D:16:ARG:HE	1:D:117:PRO:HD3	1.83	0.44
2:H:436:TYR:HB2	2:H:450:MET:SD	2.57	0.44
1:I:56:LEU:HD13	1:I:99:LEU:CD2	2.47	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
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
2:2:319:ARG:O	2:2:333:LYS:NZ	2.45	0.44
2:2:464:LEU:HD11	2:2:505:VAL:HG11	1.99	0.44
2:H:318:ARG:HB3	2:H:331:VAL:O	2.17	0.44
2:L:341:THR:HG22	2:L:404:LEU:HD11	1.99	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
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
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: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
2:Z:304:VAL:CG2	2:Z:450:MET:SD	3.06	0.44
1:F:172:ALA:HB3	1:F:175:ALA:HB2	1.99	0.44
1:F:70:GLU:OE2	1:F:116:LYS:NZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:518:ILE:HG23	2:V:487:VAL:CG2	2.48	0.44
1:W:127:VAL:HG13	1:W:127:VAL:O	2.16	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
1:I:92:ARG:HD2	1:I:129:HIS:NE2	2.31	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:179:ASP:O	1:F:183:ILE:HG12	2.18	0.44
1:F:45:ASN:HA	1:F:46:PRO:HD2	1.91	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:N	1:B:141:ILE:HD12	2.33	0.43
2:J:349:ALA:N	3:J:273:M1N:C35	2.78	0.43
2:J:301:THR:HG21	3:J:273:M1N:H16	1.82	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: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:H:395:MET:HE1	2:H:395:MET:HA	2.00	0.43
2:H:309:PRO:HG2	2:H:458:THR:O	2.17	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
1:Y:63:ALA:O	1:Y:156:MET:HE1	2.18	0.43
2:Z:337:THR:OG1	2:Z:343:THR:HG22	2.17	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:B:142:THR:OG1	1:B:144:ASP:OD1	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:273:M1N:C22	3:H:273:M1N:O16	2.54	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
2:Z:488:ARG:HB3	2:Z:490:ILE:HG12	2.00	0.43
1:D:97:ARG:HB2	4:D:249:HOH:O	2.17	0.43
2:E:364:GLU:HG2	2:E:368:LYS:HE2	2.00	0.43
2:E:439:VAL:HG23	2:E:439:VAL:O	2.18	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:139:TYR:CD2	1:W:149:ASP:HB3	2.53	0.43
1:W:48:ARG:HH22	1:Y:135:ARG:HD2	1.81	0.43
1:Y:205:VAL:HG12	1:Y:206:ALA:H	1.83	0.43
1:A:92:ARG:HD2	1:A:129:HIS:CE1	2.53	0.43
1:A:73:ASN:HD22	1:B:105:GLN:NE2	2.16	0.43
2:C:465:ARG:HH11	2:C:465:ARG:CB	2.31	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:63:ALA:O	1:M:156:MET:HE1	2.18	0.43
1:M:189:ARG:CZ	1:M:237:GLN:HB3	2.48	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:C:450:MET:CE	2:C:470:ALA:CB	2.97	0.43
2:E:403:LEU:HG	2:E:439:VAL:HG13	2.01	0.43
3:J:273:M1N:HN1	3:J:273:M1N:H252	1.83	0.43
1:M:30:VAL:HG22	1:M:43:ALA:CB	2.49	0.43
1:S:70:GLU:OE2	1:S:116:LYS:NZ	2.51	0.43
1:U:95:THR:C	1:U:97:ARG:H	2.22	0.43
1:Y:91:ARG:HE	1:Y:91:ARG:HB3	1.68	0.43
2:2:401:LEU:HA	2:2:402:PRO:HD3	1.88	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:HD23	2:L:464:LEU:O	2.19	0.43
3:N:273:M1N:H4	3:N:273:M1N:H36	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
1:B:30:VAL:HG22	1:B:43:ALA:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:349:ALA:HB2	3:E:273:M1N:H252	2.00	0.43
1:K:54:SER:OG	1:K:55:GLU:N	2.52	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
2:N:338:ASP:OD1	2:N:341:THR:OG1	2.28	0.43
1:U:30:VAL:HG22	1:U:43:ALA:HB1	2.00	0.43
2:V:395:MET:HA	2:V:395:MET:CE	2.48	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: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
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:182:ARG:HB2	1:S:182:ARG:HH11	1.84	0.43
1:S:28:LYS:HB2	1:S:52:LYS:NZ	2.33	0.43
2:X:302:THR:O	2:X:303:ILE:HD13	2.18	0.43
2:Z:301:THR:HG21	3:Z:273:M1N:H16	1.83	0.43
1:A:171:TYR:CE2	1:A:173:GLU:HA	2.54	0.43
1:D:155:VAL:HG12	1:D:160:THR:HG22	2.01	0.43
2:H:437:GLN:OE1	2:H:447:LYS:HD3	2.19	0.43
2:H:306:LEU:CD2	2:H:454:TYR:HE1	2.31	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
1:1:176:SER:H	1:1:179:ASP:HB2	1.83	0.42
2:E:306:LEU:HB2	2:E:313:VAL:CG1	2.49	0.42
2:G:317:ASP:OD1	2:G:333:LYS:NZ	2.51	0.42
2:H:465:ARG:HA	2:H:513:LEU:HD13	2.00	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: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
2:2:513:LEU:O	2:2:516:ALA:HB3	2.19	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
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:Z:461:ASP:OD1	2:Z:509:ARG:HD2	2.19	0.42
1:A:183:ILE:HD13	1:A:183:ILE:HA	1.84	0.42
2:G:324:ASN:C	2:G:324:ASN:HD22	2.21	0.42
2:L:383:LEU:HD21	2:L:402:PRO:CG	2.50	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	1:1:89:TYR:CE1	2.53	0.42
2:X:335:TYR:HE1	2:X:345:ILE:HD11	1.83	0.42
2:Z:349:ALA:N	3:Z:273:M1N:C35	2.79	0.42
2:X:424:ASP:OD2	3:Z:273:M1N:H34	2.19	0.42
1:B:127:VAL:O	1:B:127:VAL:HG13	2.20	0.42
1:D:41:PHE:HE2	1:D:213:LEU:HD13	1.83	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
2:V:301:THR:HG21	3:V:273:M1N:H16	1.80	0.42
2:X:401:LEU:HA	2:X:401:LEU:HD12	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: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
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
1:1:97:ARG:NH1	1:1:97:ARG:HG3	2.34	0.42
2:C:301:THR:CG2	3:C:273:M1N:H16	2.29	0.42
3:E:273:M1N:H221	3:E:273:M1N:O16	2.18	0.42
1:F:83:ASP:OD2	2:G:365:HIS:HD2	2.02	0.42
3:G:273:M1N:C25	3:G:273:M1N:HN1	2.31	0.42
2:G:329:ARG:HB3	2:G:329:ARG:HE	1.64	0.42
2:H:464:LEU:HD23	2:H:513:LEU:HD12	2.01	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
2:X:392:ALA:O	2:X:395:MET:HB2	2.20	0.42
1:1:28:LYS:HE2	1:1:46:PRO:HD3	2.02	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:205:VAL:C	1:O:207:SER:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:H:273:M1N:HN1	3:H:273:M1N:C25	2.32	0.42
1:I:171:TYR:CE2	1:I:173:GLU:HA	2.54	0.42
1:K:170:SER:HB2	1:K:183:ILE:HD12	2.01	0.42
1:K:54:SER:HB3	1:K:75:ARG:HD2	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
1:I:177:LEU:HB2	4:I:251:HOH:O	2.18	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:D:95:THR:C	1:D:97:ARG:H	2.23	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:M:127:VAL:O	1:M:127:VAL:HG13	2.20	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
1:F:49:SER:HB2	1:W:97:ARG:HH11	1.85	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
2:H:321:THR:O	3:H:273:M1N:H51	2.20	0.42
1:M:217:ARG:NH2	1:M:223:ARG:HG3	2.34	0.42
1:U:68:PHE:HA	1:U:71:PHE:CE2	2.55	0.42
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: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:F:181:LEU:HD23	1:F:233:LEU:HB3	2.01	0.41
1:I:30:VAL:HG13	1:I:43:ALA:HB2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:92:ARG:HB2	1:1:92:ARG:HH11	1.85	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:F:10:GLU:OE2	1:M:22:LYS:HD2	2.19	0.41
2:N:314:MET:HE3	2:N:334:VAL:HG13	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
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: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
2:X:349:ALA:H	3:X:273:M1N:C36	2.34	0.41
1:1:127:VAL:HG11	1:1:213:LEU:HB3	2.01	0.41
1:A:41:PHE:HE2	1:A:213:LEU:HD13	1.85	0.41
2:C:345:ILE:O	2:C:345:ILE:HD12	2.20	0.41
2:E:345:ILE:HD12	2:E:345:ILE:O	2.20	0.41
2:G:383:LEU:HD21	2:G:402:PRO:HG2	2.03	0.41
3:J:273:M1N:H36	3:J:273:M1N:H4	1.76	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
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
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:A:203:LEU:HG	1:A:237:GLN:OE1	2.19	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:HH11	1:F:92:ARG:HB2	1.85	0.41
2:G:424:ASP:HB3	2:G:428:GLY:N	2.35	0.41
2:H:314:MET:CE	2:H:334:VAL:HG13	2.50	0.41
2:H:304:VAL:HG23	2:H:438:ALA:HB2	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:O:95:THR:C	1:O:97:ARG:H	2.24	0.41
1:Q:234:LEU:HG	1:Q:235:VAL:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:R:306:LEU:HB2	2:R:313:VAL:CG1	2.50	0.41
2:R:330:ASP:OD1	2:R:330:ASP:N	2.54	0.41
1:U:85:ARG:HH11	1:U:89:TYR:HE2	1.69	0.41
1:W:95:THR:C	1:W:97:ARG:H	2.24	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:T:395:MET:CE	2:T:395:MET:HA	2.50	0.41
1:A:31:VAL:HG22	1:A:155:VAL:HG13	2.03	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
2:G:395:MET:CE	2:G:395:MET:HA	2.51	0.41
2:H:306:LEU:CD2	2:H:454:TYR:CE1	3.04	0.41
1:M:127:VAL:HG22	1:M:215:ALA:HB2	2.02	0.41
2:N:345:ILE:HD12	2:N:345:ILE:O	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
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
2:2:306:LEU:HB2	2:2:313:VAL:CG1	2.50	0.41
2:2:407:TYR:CE1	2:2:417:ALA:HB3	2.56	0.41
1:I:28:LYS:HE2	1:I:46:PRO:HD3	2.01	0.41
1:K:91:ARG:HB3	1:K:91:ARG:HE	1.65	0.41
1:M:208:LEU:HB3	4:M:254:HOH:O	2.19	0.41
2:N:407:TYR:CE1	2:N:417:ALA:HB3	2.55	0.41
1:O:24:ILE:H	1:O:24:ILE:HG12	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:87:TYR:OH	2:V:354:GLU:HG2	2.20	0.41
2:Z:320:SER:HB3	2:Z:331:VAL:HG21	2.03	0.41
1:B:205:VAL:CG1	1:B:206:ALA:H	2.31	0.41
1:D:171:TYR:CE2	1:D:173:GLU:HA	2.56	0.41
1:D:89:TYR:CD1	2:R:382:ARG:HD3	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
2:H:324:ASN:N	2:H:324:ASN:ND2	2.49	0.41
2:H:348:THR:HA	3:H:273:M1N:H36	2.03	0.41
1:I:205:VAL:C	1:I:207:SER:N	2.73	0.41
1:I:30:VAL:HG22	1:I:43:ALA:CB	2.51	0.41
2:L:424:ASP:HB3	2:L:428:GLY:H	1.86	0.41
1:M:153:PHE:HZ	1:M:168:LYS:HG2	1.86	0.41
1:M:226:THR:OG1	1:M:227:GLY:N	2.53	0.41
2:P:513:LEU:O	2:P:516:ALA:HB3	2.21	0.41
2:V:329:ARG:O	2:V:490:ILE:HG21	2.21	0.41
2:V:344:GLY:C	4:V:553:HOH:O	2.59	0.41
2:V:441:SER:HB2	2:V:478:ASP:OD2	2.21	0.41
1:Y:182:ARG:HA	1:Y:235:VAL:HB	2.03	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
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
1:M:205:VAL:C	1:M:207:SER:N	2.74	0.41
2:N:345:ILE:HD11	4:N:549:HOH:O	2.21	0.41
3:R:273:M1N:H40	2:Z:424:ASP:OD1	2.21	0.41
2:R:392:ALA:HB3	4:R:159:HOH:O	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
2:Z:514:ALA:O	2:Z:518:ILE:HG13	2.21	0.41
1:1:68:PHE:HA	1:1:71:PHE:CE2	2.56	0.40
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:433:GLU:O	2:P:433:GLU:HG3	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:ARG:HA	1:D:136:PRO:HD2	1.88	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:N:452:LYS:HZ3	2:V:449:SER:HB2	1.85	0.40
3:Z:273:M1N:H36	3:Z:273:M1N:H4	1.97	0.40
2:Z:382:ARG:NH1	2:Z:385:ILE:HD13	2.37	0.40
2:2:384:ALA:HB1	2:2:427:GLY:O	2.22	0.40
1:B:95:THR:C	1:B:97:ARG:H	2.25	0.40
1:F:92:ARG:HD2	1:F:129:HIS:ND1	2.35	0.40
1:I:54:SER:CB	1:I:75:ARG:HD2	2.51	0.40
2:J:432:GLU:HG3	2:J:437:GLN:HB2	2.04	0.40
2:J:306:LEU:CD2	2:J:436:TYR:HB3	2.51	0.40
1:K:123:CYS:HB3	1:K:156:MET:CE	2.51	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:O	1:S:207:SER:N	2.54	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
2:2:452:LYS:HA	2:2:452:LYS:HD3	1.85	0.40
1:A:96:GLY:HA2	1:A:99:LEU:HB2	2.02	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:H:321:THR:HG22	4:H:542:HOH:O	2.20	0.40
2:H:313:VAL:HB	2:H:496:ILE:HD13	2.03	0.40
2:J:395:MET:HA	2:J:395:MET:CE	2.51	0.40
2:J:496:ILE:HG13	2:J:505:VAL:CG2	2.51	0.40
2:P:388:ARG:HD3	4:P:544:HOH:O	2.21	0.40
2:R:388:ARG:C	2:R:390:ASN:H	2.24	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
1:1:165:ASN:HA	1:1:165:ASN:HD22	1.74	0.40
1:A:95:THR:C	1:A:97:ARG:H	2.25	0.40
2:H:347:GLY:H	3:H:273:M1N:H16	1.69	0.40
1:K:95:THR:C	1:K:97:ARG:H	2.25	0.40
2:L:322:GLN:O	2:L:322:GLN:HG2	2.21	0.40
1:M:161:GLU:H	1:M:161:GLU:CD	2.25	0.40
2:N:357:ARG:O	2:N:361:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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%)	6	30
1	A	216/251 (86%)	190 (88%)	21 (10%)	5 (2%)	6	30
1	B	216/251 (86%)	189 (88%)	22 (10%)	5 (2%)	6	30
1	D	216/251 (86%)	188 (87%)	22 (10%)	6 (3%)	5	25
1	F	216/251 (86%)	192 (89%)	18 (8%)	6 (3%)	5	25
1	I	216/251 (86%)	188 (87%)	22 (10%)	6 (3%)	5	25
1	K	216/251 (86%)	190 (88%)	20 (9%)	6 (3%)	5	25
1	M	216/251 (86%)	190 (88%)	21 (10%)	5 (2%)	6	30
1	O	216/251 (86%)	189 (88%)	22 (10%)	5 (2%)	6	30
1	Q	216/251 (86%)	189 (88%)	20 (9%)	7 (3%)	4	22
1	S	216/251 (86%)	188 (87%)	22 (10%)	6 (3%)	5	25
1	U	216/251 (86%)	188 (87%)	23 (11%)	5 (2%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	216/251 (86%)	187 (87%)	23 (11%)	6 (3%)	5	25
1	Y	216/251 (86%)	188 (87%)	24 (11%)	4 (2%)	8	36
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%)	29	68
2	H	220/240 (92%)	201 (91%)	17 (8%)	2 (1%)	17	55
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%)	29	68
2	P	220/240 (92%)	202 (92%)	17 (8%)	1 (0%)	29	68
2	R	220/240 (92%)	204 (93%)	13 (6%)	3 (1%)	11	43
2	T	220/240 (92%)	202 (92%)	18 (8%)	0	100	100
2	V	220/240 (92%)	202 (92%)	16 (7%)	2 (1%)	17	55
2	X	220/240 (92%)	200 (91%)	18 (8%)	2 (1%)	17	55
2	Z	220/240 (92%)	199 (90%)	20 (9%)	1 (0%)	29	68
All	All	6104/6874 (89%)	5457 (89%)	557 (9%)	90 (2%)	10	42

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	I	58	ASP
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%)	152 (90%)	17 (10%)	7	29
1	A	169/195 (87%)	151 (89%)	18 (11%)	6	26
1	B	169/195 (87%)	149 (88%)	20 (12%)	5	22
1	D	169/195 (87%)	148 (88%)	21 (12%)	4	20
1	F	169/195 (87%)	149 (88%)	20 (12%)	5	22
1	I	169/195 (87%)	147 (87%)	22 (13%)	4	19
1	K	169/195 (87%)	148 (88%)	21 (12%)	4	20
1	M	169/195 (87%)	151 (89%)	18 (11%)	6	26
1	O	169/195 (87%)	148 (88%)	21 (12%)	4	20
1	Q	169/195 (87%)	150 (89%)	19 (11%)	6	24
1	S	169/195 (87%)	147 (87%)	22 (13%)	4	19
1	U	169/195 (87%)	150 (89%)	19 (11%)	6	24
1	W	169/195 (87%)	154 (91%)	15 (9%)	9	35
1	Y	169/195 (87%)	147 (87%)	22 (13%)	4	19
2	2	165/178 (93%)	138 (84%)	27 (16%)	2	11
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%)	145 (88%)	20 (12%)	5	21
2	H	165/178 (93%)	140 (85%)	25 (15%)	3	14
2	J	165/178 (93%)	144 (87%)	21 (13%)	4	19
2	L	165/178 (93%)	141 (86%)	24 (14%)	3	15
2	N	165/178 (93%)	143 (87%)	22 (13%)	4	17
2	P	165/178 (93%)	142 (86%)	23 (14%)	3	16
2	R	165/178 (93%)	135 (82%)	30 (18%)	1	9
2	T	165/178 (93%)	139 (84%)	26 (16%)	2	12
2	V	165/178 (93%)	137 (83%)	28 (17%)	2	10
2	X	165/178 (93%)	146 (88%)	19 (12%)	5	24
2	Z	165/178 (93%)	143 (87%)	22 (13%)	4	17
All	All	4676/5222 (90%)	4060 (87%)	616 (13%)	4	18

All (616) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	18	GLU
1	A	60	VAL
1	A	80	GLN
1	A	85	ARG
1	A	91	ARG
1	A	92	ARG
1	A	113	GLU
1	A	116	LYS
1	A	134	LYS
1	A	135	ARG
1	A	147	ILE
1	A	150	GLU
1	A	165	ASN
1	A	182	ARG
1	A	203	LEU
1	A	208	LEU
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	332	ARG
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	508	SER
2	H	520	SER
2	H	522	SER

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Mol	Chain	Res	Type
1	B	14	ARG
1	B	18	GLU
1	B	28	LYS
1	B	29	SER
1	B	49	SER
1	B	80	GLN
1	B	84	THR
1	B	85	ARG
1	B	92	ARG
1	B	113	GLU
1	B	134	LYS
1	B	135	ARG
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	228	SER
2	C	304	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	332	ARG
2	C	341	THR
2	C	354	GLU
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	461	ASP
2	C	465	ARG
2	C	490	ILE

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Mol	Chain	Res	Type
2	C	508	SER
2	C	517	ILE
2	C	522	SER
1	D	11	GLN
1	D	18	GLU
1	D	33	LEU
1	D	84	THR
1	D	85	ARG
1	D	92	ARG
1	D	113	GLU
1	D	133	THR
1	D	134	LYS
1	D	135	ARG
1	D	147	ILE
1	D	150	GLU
1	D	165	ASN
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	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	332	ARG
2	E	341	THR
2	E	357	ARG
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	415	GLN
2	E	419	ARG

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Mol	Chain	Res	Type
2	E	432	GLU
2	E	444	LEU
2	E	449	SER
2	E	455	SER
2	E	476	ASP
2	E	488	ARG
2	E	490	ILE
2	E	508	SER
2	E	517	ILE
2	E	520	SER
2	E	522	SER
1	F	18	GLU
1	F	26	ARG
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
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	357	ARG
2	G	375	THR
2	G	391	LEU
2	G	401	LEU

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Mol	Chain	Res	Type
2	G	403	LEU
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	517	ILE
1	I	18	GLU
1	I	24	ILE
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	135	ARG
1	I	137	GLU
1	I	140	ARG
1	I	147	ILE
1	I	150	GLU
1	I	156	MET
1	I	182	ARG
1	I	192	SER
1	I	203	LEU
1	I	208	LEU
1	I	213	LEU
1	I	225	ILE
1	I	237	GLN
2	J	304	VAL
2	J	318	ARG
2	J	319	ARG
2	J	320	SER
2	J	324	ASN
2	J	329	ARG
2	J	337	THR
2	J	341	THR
2	J	375	THR
2	J	391	LEU
2	J	401	LEU

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Mol	Chain	Res	Type
2	J	403	LEU
2	J	419	ARG
2	J	424	ASP
2	J	444	LEU
2	J	448	SER
2	J	449	SER
2	J	476	ASP
2	J	490	ILE
2	J	503	VAL
2	J	522	SER
1	K	18	GLU
1	K	33	LEU
1	K	84	THR
1	K	85	ARG
1	K	91	ARG
1	K	92	ARG
1	K	99	LEU
1	K	113	GLU
1	K	123	CYS
1	K	134	LYS
1	K	135	ARG
1	K	144	ASP
1	K	147	ILE
1	K	150	GLU
1	K	173	GLU
1	K	178	THR
1	K	203	LEU
1	K	208	LEU
1	K	213	LEU
1	K	225	ILE
1	K	237	GLN
2	L	304	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	391	LEU
2	L	398	LEU
2	L	403	LEU
2	L	412	SER

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Mol	Chain	Res	Type
2	L	415	GLN
2	L	419	ARG
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	488	ARG
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	113	GLU
1	M	133	THR
1	M	134	LYS
1	M	135	ARG
1	M	147	ILE
1	M	173	GLU
1	M	176	SER
1	M	188	LEU
1	M	203	LEU
1	M	208	LEU
1	M	213	LEU
2	N	307	LYS
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	337	THR
2	N	341	THR
2	N	345	ILE

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Mol	Chain	Res	Type
2	N	391	LEU
2	N	401	LEU
2	N	403	LEU
2	N	416	SER
2	N	419	ARG
2	N	430	ASN
2	N	441	SER
2	N	444	LEU
2	N	449	SER
2	N	464	LEU
2	N	476	ASP
1	O	11	GLN
1	O	14	ARG
1	O	18	GLU
1	O	21	ARG
1	O	48	ARG
1	O	84	THR
1	O	85	ARG
1	O	92	ARG
1	O	113	GLU
1	O	134	LYS
1	O	135	ARG
1	O	147	ILE
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	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

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Mol	Chain	Res	Type
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	488	ARG
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
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	159	THR
1	Q	173	GLU
1	Q	179	ASP
1	Q	203	LEU
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	329	ARG
2	R	337	THR
2	R	341	THR

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Mol	Chain	Res	Type
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	419	ARG
2	R	424	ASP
2	R	434	GLU
2	R	436	TYR
2	R	444	LEU
2	R	449	SER
2	R	461	ASP
2	R	476	ASP
2	R	481	THR
2	R	488	ARG
2	R	490	ILE
2	R	503	VAL
2	R	508	SER
2	R	520	SER
1	S	11	GLN
1	S	17	SER
1	S	18	GLU
1	S	33	LEU
1	S	48	ARG
1	S	49	SER
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	135	ARG
1	S	147	ILE
1	S	150	GLU
1	S	182	ARG
1	S	188	LEU
1	S	192	SER
1	S	203	LEU
1	S	205	VAL
1	S	208	LEU

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Mol	Chain	Res	Type
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	357	ARG
2	T	391	LEU
2	T	398	LEU
2	T	401	LEU
2	T	403	LEU
2	T	415	GLN
2	T	419	ARG
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
2	T	522	SER
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	135	ARG
1	U	147	ILE
1	U	150	GLU
1	U	165	ASN
1	U	188	LEU
1	U	203	LEU

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Mol	Chain	Res	Type
1	U	205	VAL
1	U	208	LEU
1	U	237	GLN
2	V	303	ILE
2	V	304	VAL
2	V	312	VAL
2	V	318	ARG
2	V	319	ARG
2	V	320	SER
2	V	324	ASN
2	V	329	ARG
2	V	345	ILE
2	V	355	PHE
2	V	375	THR
2	V	383	LEU
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	448	SER
2	V	449	SER
2	V	476	ASP
2	V	479	SER
2	V	490	ILE
2	V	508	SER
2	V	513	LEU
1	W	11	GLN
1	W	18	GLU
1	W	28	LYS
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

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Mol	Chain	Res	Type
1	W	176	SER
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	358	LEU
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	430	ASN
2	X	444	LEU
2	X	448	SER
2	X	458	THR
2	X	476	ASP
2	X	490	ILE
2	X	522	SER
1	Y	14	ARG
1	Y	18	GLU
1	Y	21	ARG
1	Y	24	ILE
1	Y	33	LEU
1	Y	48	ARG
1	Y	84	THR
1	Y	85	ARG
1	Y	91	ARG
1	Y	92	ARG
1	Y	113	GLU
1	Y	134	LYS
1	Y	135	ARG
1	Y	147	ILE
1	Y	150	GLU
1	Y	161	GLU
1	Y	179	ASP
1	Y	182	ARG
1	Y	188	LEU

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Mol	Chain	Res	Type
1	Y	203	LEU
1	Y	205	VAL
1	Y	237	GLN
2	Z	318	ARG
2	Z	319	ARG
2	Z	320	SER
2	Z	321	THR
2	Z	324	ASN
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	419	ARG
2	Z	444	LEU
2	Z	448	SER
2	Z	476	ASP
2	Z	479	SER
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	231	GLN

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Mol	Chain	Res	Type
2	2	304	VAL
2	2	318	ARG
2	2	320	SER
2	2	321	THR
2	2	324	ASN
2	2	329	ARG
2	2	341	THR
2	2	358	LEU
2	2	383	LEU
2	2	391	LEU
2	2	396	GLN
2	2	398	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	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	73	ASN
1	A	98	GLN
1	A	105	GLN
1	A	165	ASN
1	A	231	GLN
2	H	324	ASN
2	H	365	HIS
2	H	410	HIS
2	H	415	GLN
2	H	456	GLN

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Mol	Chain	Res	Type
1	B	51	GLN
1	B	73	ASN
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
2	E	324	ASN
2	E	365	HIS
2	E	456	GLN
1	F	51	GLN
1	F	80	GLN
1	F	98	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	51	GLN
1	I	98	GLN
1	I	105	GLN
1	I	129	HIS
1	I	165	ASN
2	J	324	ASN
2	J	365	HIS
2	J	415	GLN
2	J	456	GLN
1	K	51	GLN
1	K	73	ASN

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Mol	Chain	Res	Type
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	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	98	GLN
1	O	129	HIS
1	O	165	ASN
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
1	S	80	GLN
1	S	98	GLN
1	S	105	GLN
1	S	114	GLN
1	S	129	HIS
1	S	165	ASN
2	T	324	ASN
2	T	365	HIS

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Mol	Chain	Res	Type
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	80	GLN
1	W	98	GLN
1	W	105	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	105	GLN
1	Y	129	HIS
1	Y	165	ASN
1	Y	231	GLN
2	Z	324	ASN
2	Z	365	HIS
1	1	51	GLN
1	1	105	GLN
1	1	129	HIS
1	1	152	HIS
1	1	165	ASN
1	1	231	GLN
2	2	324	ASN
2	2	365	HIS

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Mol	Chain	Res	Type
2	2	456	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	M1N	T	273	2	30,34,34	2.95	15 (50%)	39,46,46	4.39	16 (41%)
3	M1N	V	273	2	30,34,34	2.75	15 (50%)	39,46,46	4.22	15 (38%)
3	M1N	X	273	2	30,34,34	2.95	16 (53%)	39,46,46	4.45	16 (41%)
3	M1N	Z	273	2	30,34,34	2.82	13 (43%)	39,46,46	4.04	15 (38%)
3	M1N	2	273	2	30,34,34	2.95	14 (46%)	39,46,46	4.78	18 (46%)
3	M1N	C	273	2	30,34,34	2.60	12 (40%)	39,46,46	4.40	17 (43%)
3	M1N	E	273	2	30,34,34	2.71	13 (43%)	39,46,46	4.61	18 (46%)
3	M1N	G	273	2	30,34,34	2.94	15 (50%)	39,46,46	4.36	15 (38%)
3	M1N	H	273	2	30,34,34	2.71	12 (40%)	39,46,46	4.48	16 (41%)
3	M1N	J	273	2	30,34,34	2.78	13 (43%)	39,46,46	4.17	16 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	M1N	L	273	2	30,34,34	2.69	13 (43%)	39,46,46	4.61	16 (41%)
3	M1N	N	273	2	30,34,34	2.76	14 (46%)	39,46,46	4.26	17 (43%)
3	M1N	P	273	2	30,34,34	2.82	12 (40%)	39,46,46	4.50	18 (46%)
3	M1N	R	273	2	30,34,34	2.95	14 (46%)	39,46,46	4.39	13 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	M1N	T	273	2	-	8/22/36/36	0/3/3/3
3	M1N	V	273	2	-	11/22/36/36	0/3/3/3
3	M1N	X	273	2	-	10/22/36/36	0/3/3/3
3	M1N	Z	273	2	-	11/22/36/36	0/3/3/3
3	M1N	2	273	2	-	10/22/36/36	0/3/3/3
3	M1N	C	273	2	-	9/22/36/36	0/3/3/3
3	M1N	E	273	2	-	8/22/36/36	0/3/3/3
3	M1N	G	273	2	-	10/22/36/36	0/3/3/3
3	M1N	H	273	2	-	8/22/36/36	0/3/3/3
3	M1N	J	273	2	-	9/22/36/36	0/3/3/3
3	M1N	L	273	2	-	10/22/36/36	0/3/3/3
3	M1N	N	273	2	-	10/22/36/36	0/3/3/3
3	M1N	P	273	2	-	11/22/36/36	0/3/3/3
3	M1N	R	273	2	-	12/22/36/36	0/3/3/3

All (191) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	273	M1N	C5-C4	-6.78	1.37	1.54
3	P	273	M1N	C5-C4	-6.76	1.37	1.54
3	G	273	M1N	C5-C4	-6.66	1.37	1.54
3	J	273	M1N	C5-C4	-6.60	1.37	1.54
3	N	273	M1N	C5-C4	-6.52	1.37	1.54
3	H	273	M1N	C5-C4	-6.49	1.37	1.54
3	R	273	M1N	C5-C4	-6.39	1.38	1.54
3	C	273	M1N	C5-C4	-6.36	1.38	1.54
3	Z	273	M1N	C5-C4	-6.30	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	273	M1N	C5-C4	-6.23	1.38	1.54
3	V	273	M1N	C5-C4	-6.14	1.38	1.54
3	L	273	M1N	C5-C4	-6.13	1.38	1.54
3	2	273	M1N	C5-C4	-6.11	1.38	1.54
3	T	273	M1N	C5-C4	-5.97	1.39	1.54
3	2	273	M1N	C7-N9	5.26	1.46	1.36
3	X	273	M1N	C2-N1	5.19	1.45	1.34
3	T	273	M1N	C38-C37	5.19	1.48	1.36
3	R	273	M1N	O8-C7	5.18	1.32	1.23
3	T	273	M1N	O8-C7	5.17	1.32	1.23
3	G	273	M1N	O8-C7	5.14	1.32	1.23
3	2	273	M1N	C2-N1	5.12	1.45	1.34
3	R	273	M1N	C38-C37	5.10	1.48	1.36
3	T	273	M1N	C2-N1	5.10	1.45	1.34
3	X	273	M1N	O8-C7	5.08	1.32	1.23
3	Z	273	M1N	O8-C7	5.05	1.32	1.23
3	2	273	M1N	C38-C37	5.01	1.48	1.36
3	P	273	M1N	C2-N1	4.95	1.44	1.34
3	2	273	M1N	O8-C7	4.92	1.32	1.23
3	R	273	M1N	C7-N6	4.87	1.46	1.35
3	G	273	M1N	C2-N1	4.82	1.44	1.34
3	P	273	M1N	C38-C37	4.82	1.47	1.36
3	N	273	M1N	C2-N1	4.81	1.44	1.34
3	X	273	M1N	C7-N6	4.80	1.46	1.35
3	L	273	M1N	C2-N1	4.75	1.44	1.34
3	N	273	M1N	C38-C37	4.74	1.47	1.36
3	J	273	M1N	O8-C7	4.73	1.31	1.23
3	G	273	M1N	C38-C37	4.71	1.47	1.36
3	V	273	M1N	C2-N1	4.70	1.44	1.34
3	Z	273	M1N	C38-C37	4.70	1.47	1.36
3	R	273	M1N	C2-N1	4.68	1.44	1.34
3	N	273	M1N	O8-C7	4.66	1.31	1.23
3	H	273	M1N	C2-N1	4.65	1.44	1.34
3	V	273	M1N	C38-C37	4.64	1.47	1.36
3	2	273	M1N	C7-N6	4.63	1.45	1.35
3	G	273	M1N	C7-N6	4.61	1.45	1.35
3	X	273	M1N	C38-C37	4.60	1.47	1.36
3	P	273	M1N	O8-C7	4.58	1.31	1.23
3	J	273	M1N	C38-C37	4.57	1.47	1.36
3	H	273	M1N	O8-C7	4.55	1.31	1.23
3	V	273	M1N	O8-C7	4.54	1.31	1.23
3	E	273	M1N	O8-C7	4.52	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	273	M1N	C2-N1	4.47	1.43	1.34
3	L	273	M1N	C38-C37	4.47	1.46	1.36
3	T	273	M1N	C7-N6	4.46	1.45	1.35
3	T	273	M1N	C7-N9	4.37	1.44	1.36
3	E	273	M1N	C38-C37	4.36	1.46	1.36
3	C	273	M1N	C2-N1	4.36	1.43	1.34
3	Z	273	M1N	C7-N9	4.34	1.44	1.36
3	R	273	M1N	C7-N9	4.31	1.44	1.36
3	Z	273	M1N	C2-N1	4.30	1.43	1.34
3	C	273	M1N	C38-C37	4.29	1.46	1.36
3	L	273	M1N	O8-C7	4.27	1.30	1.23
3	J	273	M1N	C2-N1	4.26	1.43	1.34
3	2	273	M1N	C10-N9	4.21	1.54	1.47
3	Z	273	M1N	C7-N6	4.20	1.44	1.35
3	H	273	M1N	C7-N6	4.20	1.44	1.35
3	H	273	M1N	C38-C37	4.18	1.46	1.36
3	L	273	M1N	C35-C36	4.16	1.47	1.38
3	H	273	M1N	C35-C36	4.16	1.47	1.38
3	C	273	M1N	O8-C7	4.14	1.30	1.23
3	X	273	M1N	C35-C36	4.13	1.47	1.38
3	L	273	M1N	C7-N6	4.12	1.44	1.35
3	J	273	M1N	C7-N9	4.08	1.44	1.36
3	G	273	M1N	C7-N9	4.07	1.44	1.36
3	J	273	M1N	C7-N6	4.06	1.44	1.35
3	G	273	M1N	C35-C36	4.05	1.47	1.38
3	P	273	M1N	C7-N9	4.04	1.43	1.36
3	P	273	M1N	C35-C36	4.03	1.47	1.38
3	X	273	M1N	C7-N9	3.99	1.43	1.36
3	N	273	M1N	C7-N6	3.97	1.44	1.35
3	H	273	M1N	C7-N9	3.92	1.43	1.36
3	2	273	M1N	C35-C36	3.92	1.47	1.38
3	T	273	M1N	C35-C36	3.90	1.47	1.38
3	V	273	M1N	C7-N6	3.89	1.43	1.35
3	C	273	M1N	C7-N6	3.89	1.43	1.35
3	R	273	M1N	C35-C36	3.88	1.47	1.38
3	P	273	M1N	C7-N6	3.87	1.43	1.35
3	E	273	M1N	C35-C36	3.84	1.47	1.38
3	J	273	M1N	C35-C36	3.84	1.47	1.38
3	Z	273	M1N	C35-C36	3.80	1.46	1.38
3	V	273	M1N	C35-C36	3.78	1.46	1.38
3	E	273	M1N	C7-N6	3.77	1.43	1.35
3	X	273	M1N	C10-N9	3.74	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	273	M1N	C7-N9	3.72	1.43	1.36
3	C	273	M1N	C35-C36	3.71	1.46	1.38
3	J	273	M1N	C35-C34	3.69	1.45	1.36
3	Z	273	M1N	C10-N9	3.68	1.53	1.47
3	L	273	M1N	C7-N9	3.68	1.43	1.36
3	N	273	M1N	C35-C36	3.67	1.46	1.38
3	V	273	M1N	C7-N9	3.65	1.43	1.36
3	E	273	M1N	C35-C34	3.65	1.45	1.36
3	R	273	M1N	C4-C2	-3.62	1.43	1.52
3	E	273	M1N	C7-N9	3.61	1.43	1.36
3	R	273	M1N	C35-C34	3.57	1.44	1.36
3	T	273	M1N	C10-N9	3.48	1.53	1.47
3	G	273	M1N	C35-C34	3.47	1.44	1.36
3	J	273	M1N	C10-N9	3.47	1.53	1.47
3	V	273	M1N	C10-N9	3.45	1.53	1.47
3	C	273	M1N	C35-C34	3.44	1.44	1.36
3	T	273	M1N	C14-N9	3.40	1.53	1.47
3	Z	273	M1N	C4-C2	-3.39	1.44	1.52
3	G	273	M1N	C10-N9	3.37	1.53	1.47
3	X	273	M1N	C35-C34	3.37	1.44	1.36
3	P	273	M1N	C35-C34	3.36	1.44	1.36
3	L	273	M1N	C10-N9	3.36	1.53	1.47
3	G	273	M1N	C4-C2	-3.35	1.44	1.52
3	H	273	M1N	C4-C2	-3.33	1.44	1.52
3	T	273	M1N	C35-C34	3.33	1.44	1.36
3	C	273	M1N	C4-C2	-3.33	1.44	1.52
3	T	273	M1N	C4-C2	-3.32	1.44	1.52
3	P	273	M1N	C10-N9	3.31	1.52	1.47
3	L	273	M1N	C35-C34	3.30	1.44	1.36
3	L	273	M1N	C4-C2	-3.29	1.44	1.52
3	Z	273	M1N	C35-C34	3.23	1.44	1.36
3	C	273	M1N	C7-N9	3.22	1.42	1.36
3	H	273	M1N	C35-C34	3.18	1.43	1.36
3	G	273	M1N	C14-N9	3.17	1.52	1.47
3	N	273	M1N	C10-N9	3.16	1.52	1.47
3	R	273	M1N	C10-N9	3.15	1.52	1.47
3	E	273	M1N	C4-C2	-3.15	1.44	1.52
3	X	273	M1N	C14-N9	3.14	1.52	1.47
3	N	273	M1N	C35-C34	3.13	1.43	1.36
3	C	273	M1N	C10-N9	3.12	1.52	1.47
3	E	273	M1N	C10-N9	3.11	1.52	1.47
3	Z	273	M1N	C14-N9	3.09	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	273	M1N	C4-C2	-3.01	1.45	1.52
3	P	273	M1N	C14-N9	3.01	1.52	1.47
3	J	273	M1N	C4-C2	-3.01	1.45	1.52
3	J	273	M1N	C14-N9	3.00	1.52	1.47
3	2	273	M1N	C35-C34	3.00	1.43	1.36
3	H	273	M1N	C10-N9	2.98	1.52	1.47
3	N	273	M1N	C4-C2	-2.97	1.45	1.52
3	V	273	M1N	C35-C34	2.94	1.43	1.36
3	V	273	M1N	C14-N9	2.94	1.52	1.47
3	N	273	M1N	C14-N9	2.90	1.52	1.47
3	R	273	M1N	C14-N9	2.88	1.52	1.47
3	X	273	M1N	C4-C2	-2.85	1.45	1.52
3	L	273	M1N	C14-N9	2.73	1.51	1.47
3	Z	273	M1N	O12-C11	2.65	1.53	1.42
3	X	273	M1N	O12-C11	2.65	1.53	1.42
3	T	273	M1N	C32-C33	2.64	1.47	1.43
3	2	273	M1N	C14-N9	2.64	1.51	1.47
3	V	273	M1N	O12-C11	2.63	1.53	1.42
3	X	273	M1N	C36-C31	2.59	1.42	1.37
3	G	273	M1N	C36-C31	2.58	1.42	1.37
3	T	273	M1N	C36-C31	2.53	1.42	1.37
3	2	273	M1N	C4-C2	-2.53	1.46	1.52
3	N	273	M1N	C32-C33	2.53	1.47	1.43
3	H	273	M1N	C14-N9	2.53	1.51	1.47
3	C	273	M1N	C14-N9	2.52	1.51	1.47
3	R	273	M1N	O12-C11	2.49	1.52	1.42
3	V	273	M1N	C32-C33	2.48	1.47	1.43
3	P	273	M1N	O12-C11	2.48	1.52	1.42
3	G	273	M1N	C32-C33	2.44	1.47	1.43
3	V	273	M1N	C4-C2	-2.43	1.46	1.52
3	2	273	M1N	O12-C11	2.43	1.52	1.42
3	E	273	M1N	C14-N9	2.40	1.51	1.47
3	G	273	M1N	C31-C32	2.40	1.48	1.42
3	G	273	M1N	O12-C11	2.38	1.52	1.42
3	V	273	M1N	C31-C32	2.37	1.48	1.42
3	C	273	M1N	O12-C11	2.37	1.52	1.42
3	T	273	M1N	O12-C11	2.36	1.52	1.42
3	E	273	M1N	O12-C11	2.36	1.52	1.42
3	R	273	M1N	C32-C33	2.36	1.47	1.43
3	J	273	M1N	O12-C11	2.34	1.52	1.42
3	2	273	M1N	C36-C31	2.33	1.41	1.37
3	T	273	M1N	C31-C32	2.33	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	273	M1N	C32-C33	2.32	1.47	1.43
3	N	273	M1N	O12-C11	2.30	1.52	1.42
3	H	273	M1N	O12-C11	2.27	1.51	1.42
3	X	273	M1N	C31-C32	2.26	1.47	1.42
3	L	273	M1N	O12-C11	2.26	1.51	1.42
3	X	273	M1N	C4-N6	2.22	1.50	1.45
3	Z	273	M1N	C36-C31	2.17	1.41	1.37
3	N	273	M1N	C31-C32	2.16	1.47	1.42
3	R	273	M1N	C36-C31	2.15	1.41	1.37
3	V	273	M1N	C36-C31	2.15	1.41	1.37
3	J	273	M1N	C32-C33	2.15	1.46	1.43
3	2	273	M1N	C32-C33	2.10	1.46	1.43
3	L	273	M1N	C36-C31	2.03	1.41	1.37
3	E	273	M1N	C36-C31	2.02	1.41	1.37

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	273	M1N	C15-C22-C23	19.99	140.51	115.39
3	T	273	M1N	C15-C22-C23	19.39	139.76	115.39
3	2	273	M1N	C15-C22-C23	19.25	139.58	115.39
3	L	273	M1N	C15-C22-C23	18.81	139.02	115.39
3	G	273	M1N	C15-C22-C23	18.46	138.59	115.39
3	P	273	M1N	C15-C22-C23	18.23	138.29	115.39
3	X	273	M1N	C15-C22-C23	18.01	138.02	115.39
3	R	273	M1N	C15-C22-C23	17.71	137.64	115.39
3	N	273	M1N	C15-C22-C23	17.52	137.41	115.39
3	H	273	M1N	C15-C22-C23	17.41	137.26	115.39
3	J	273	M1N	C15-C22-C23	17.06	136.83	115.39
3	C	273	M1N	C15-C22-C23	16.76	136.45	115.39
3	V	273	M1N	C15-C22-C23	16.23	135.78	115.39
3	Z	273	M1N	C15-C22-C23	15.24	134.54	115.39
3	L	273	M1N	O8-C7-N9	-12.43	104.31	121.78
3	X	273	M1N	O8-C7-N9	-11.97	104.96	121.78
3	C	273	M1N	O8-C7-N9	-11.72	105.31	121.78
3	2	273	M1N	N6-C7-N9	11.51	138.14	117.21
3	H	273	M1N	O8-C7-N9	-11.47	105.66	121.78
3	R	273	M1N	O8-C7-N9	-11.37	105.80	121.78
3	E	273	M1N	O8-C7-N9	-11.07	106.23	121.78
3	V	273	M1N	O8-C7-N9	-10.85	106.54	121.78
3	2	273	M1N	O8-C7-N9	-10.76	106.66	121.78
3	Z	273	M1N	O8-C7-N9	-10.52	106.99	121.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	273	M1N	O8-C7-N9	-10.47	107.07	121.78
3	L	273	M1N	N6-C7-N9	10.37	136.07	117.21
3	T	273	M1N	O8-C7-N9	-10.37	107.21	121.78
3	P	273	M1N	O8-C7-N9	-10.19	107.46	121.78
3	H	273	M1N	N6-C7-N9	10.11	135.59	117.21
3	E	273	M1N	N6-C7-N9	10.06	135.50	117.21
3	C	273	M1N	N6-C7-N9	9.99	135.37	117.21
3	N	273	M1N	O8-C7-N9	-9.94	107.82	121.78
3	J	273	M1N	O8-C7-N9	-9.76	108.07	121.78
3	Z	273	M1N	N6-C7-N9	9.74	134.92	117.21
3	R	273	M1N	N6-C7-N9	9.49	134.46	117.21
3	P	273	M1N	N6-C7-N9	9.47	134.42	117.21
3	X	273	M1N	N6-C7-N9	9.46	134.41	117.21
3	V	273	M1N	N6-C7-N9	9.29	134.10	117.21
3	J	273	M1N	N6-C7-N9	8.65	132.94	117.21
3	G	273	M1N	C4-C2-N1	8.58	135.53	116.70
3	T	273	M1N	N6-C7-N9	8.50	132.66	117.21
3	2	273	M1N	C4-C2-N1	8.47	135.27	116.70
3	C	273	M1N	C4-C2-N1	8.32	134.95	116.70
3	P	273	M1N	C4-C2-N1	8.29	134.88	116.70
3	H	273	M1N	C4-C2-N1	8.19	134.65	116.70
3	L	273	M1N	C4-C2-N1	8.18	134.65	116.70
3	R	273	M1N	C4-C2-N1	8.16	134.60	116.70
3	N	273	M1N	N6-C7-N9	7.96	131.68	117.21
3	N	273	M1N	C4-C2-N1	7.93	134.09	116.70
3	G	273	M1N	N6-C7-N9	7.80	131.39	117.21
3	V	273	M1N	C4-C2-N1	7.48	133.10	116.70
3	J	273	M1N	C4-C2-N1	7.44	133.03	116.70
3	T	273	M1N	C4-C2-N1	7.32	132.76	116.70
3	X	273	M1N	C4-C2-N1	7.31	132.74	116.70
3	Z	273	M1N	C4-C2-N1	7.16	132.40	116.70
3	2	273	M1N	O3-C2-N1	-6.90	110.14	122.93
3	E	273	M1N	C4-C2-N1	6.79	131.60	116.70
3	V	273	M1N	O3-C2-N1	-6.72	110.49	122.93
3	C	273	M1N	O3-C2-N1	-6.10	111.62	122.93
3	P	273	M1N	O3-C2-N1	-6.07	111.69	122.93
3	N	273	M1N	O3-C2-N1	-6.00	111.81	122.93
3	G	273	M1N	O3-C2-N1	-5.74	112.29	122.93
3	J	273	M1N	O3-C2-N1	-5.74	112.29	122.93
3	H	273	M1N	O3-C2-N1	-5.42	112.90	122.93
3	2	273	M1N	C5-C4-N6	-5.37	99.48	110.79
3	T	273	M1N	C14-N9-C7	-5.30	102.41	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	273	M1N	O3-C2-N1	-5.17	113.36	122.93
3	G	273	M1N	C14-N9-C7	-5.16	102.93	121.94
3	P	273	M1N	C14-N9-C7	-5.13	103.05	121.94
3	X	273	M1N	C14-N9-C7	-5.08	103.23	121.94
3	X	273	M1N	O3-C2-N1	-5.07	113.53	122.93
3	N	273	M1N	C14-N9-C7	-4.96	103.66	121.94
3	L	273	M1N	O3-C2-N1	-4.93	113.79	122.93
3	V	273	M1N	C14-N9-C7	-4.91	103.85	121.94
3	R	273	M1N	C14-N9-C7	-4.91	103.86	121.94
3	P	273	M1N	C5-C4-N6	-4.90	100.47	110.79
3	E	273	M1N	C14-N9-C7	-4.89	103.92	121.94
3	Z	273	M1N	O3-C2-N1	-4.83	113.98	122.93
3	C	273	M1N	C14-N9-C7	-4.78	104.33	121.94
3	R	273	M1N	O3-C2-N1	-4.73	114.17	122.93
3	J	273	M1N	C14-N9-C7	-4.67	104.73	121.94
3	T	273	M1N	O3-C2-N1	-4.65	114.33	122.93
3	H	273	M1N	C14-N9-C7	-4.62	104.91	121.94
3	L	273	M1N	C14-N9-C7	-4.54	105.23	121.94
3	H	273	M1N	C5-C31-C32	-4.52	113.61	120.76
3	2	273	M1N	C14-N9-C7	-4.51	105.31	121.94
3	R	273	M1N	O3-C2-C4	-4.39	111.22	120.45
3	H	273	M1N	C5-C31-C36	4.34	127.26	119.86
3	L	273	M1N	O3-C2-C4	-4.23	111.55	120.45
3	Z	273	M1N	C14-N9-C7	-4.13	106.74	121.94
3	E	273	M1N	C5-C31-C32	-4.00	114.44	120.76
3	J	273	M1N	C10-N9-C14	3.97	120.27	112.62
3	G	273	M1N	O3-C2-C4	-3.96	112.11	120.45
3	R	273	M1N	C5-C31-C32	-3.93	114.55	120.76
3	X	273	M1N	C5-C31-C32	-3.89	114.62	120.76
3	H	273	M1N	O3-C2-C4	-3.83	112.40	120.45
3	Z	273	M1N	C5-C31-C32	-3.78	114.78	120.76
3	2	273	M1N	C5-C31-C32	-3.70	114.92	120.76
3	X	273	M1N	C10-N9-C14	3.67	119.69	112.62
3	P	273	M1N	C5-C31-C32	-3.65	114.99	120.76
3	2	273	M1N	C5-C31-C36	3.63	126.03	119.86
3	T	273	M1N	O3-C2-C4	-3.60	112.88	120.45
3	X	273	M1N	C5-C31-C36	3.51	125.84	119.86
3	C	273	M1N	C5-C31-C32	-3.51	115.22	120.76
3	R	273	M1N	C15-N1-C2	-3.39	114.01	122.77
3	C	273	M1N	O3-C2-C4	-3.39	113.32	120.45
3	P	273	M1N	O3-C2-C4	-3.37	113.37	120.45
3	J	273	M1N	C5-C31-C32	-3.33	115.50	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	273	M1N	O3-C2-C4	-3.30	113.52	120.45
3	N	273	M1N	C15-N1-C2	-3.28	114.28	122.77
3	Z	273	M1N	C5-C31-C36	3.27	125.42	119.86
3	V	273	M1N	C5-C4-N6	-3.26	103.91	110.79
3	2	273	M1N	C15-N1-C2	-3.23	114.42	122.77
3	C	273	M1N	C5-C4-N6	-3.21	104.02	110.79
3	X	273	M1N	O3-C2-C4	-3.21	113.70	120.45
3	N	273	M1N	C40-C33-C32	3.18	123.31	119.12
3	C	273	M1N	C5-C31-C36	3.17	125.26	119.86
3	2	273	M1N	C31-C5-C4	3.15	119.61	113.45
3	G	273	M1N	C5-C31-C32	-3.12	115.83	120.76
3	V	273	M1N	C31-C5-C4	3.11	119.54	113.45
3	R	273	M1N	C5-C31-C36	3.11	125.15	119.86
3	E	273	M1N	C5-C31-C36	3.06	125.08	119.86
3	E	273	M1N	C5-C4-N6	-3.05	104.36	110.79
3	P	273	M1N	C15-N1-C2	-3.02	114.96	122.77
3	N	273	M1N	O3-C2-C4	-3.02	114.09	120.45
3	L	273	M1N	C40-C33-C32	2.99	123.06	119.12
3	T	273	M1N	C15-N1-C2	-2.99	115.05	122.77
3	H	273	M1N	C31-C5-C4	2.99	119.29	113.45
3	H	273	M1N	C11-O12-C13	2.97	119.81	109.89
3	G	273	M1N	C15-N1-C2	-2.96	115.11	122.77
3	V	273	M1N	C5-C31-C36	2.96	124.90	119.86
3	G	273	M1N	C5-C31-C36	2.94	124.86	119.86
3	Z	273	M1N	C11-O12-C13	2.92	119.64	109.89
3	Z	273	M1N	C11-C10-N9	-2.92	103.62	109.84
3	P	273	M1N	C5-C31-C36	2.82	124.66	119.86
3	2	273	M1N	O8-C7-N6	-2.81	115.19	123.05
3	2	273	M1N	O3-C2-C4	-2.80	114.57	120.45
3	P	273	M1N	C40-C33-C32	2.79	122.79	119.12
3	E	273	M1N	C15-N1-C2	-2.78	115.58	122.77
3	G	273	M1N	C10-N9-C14	2.78	117.98	112.62
3	X	273	M1N	C11-O12-C13	2.78	119.17	109.89
3	J	273	M1N	O3-C2-C4	-2.75	114.66	120.45
3	P	273	M1N	C31-C5-C4	2.73	118.80	113.45
3	H	273	M1N	C5-C4-N6	-2.73	105.03	110.79
3	2	273	M1N	O12-C13-C14	-2.72	105.80	111.80
3	V	273	M1N	C5-C31-C32	-2.72	116.47	120.76
3	N	273	M1N	C5-C31-C32	-2.72	116.47	120.76
3	E	273	M1N	C11-O12-C13	2.70	118.91	109.89
3	J	273	M1N	C5-C4-N6	-2.70	105.10	110.79
3	J	273	M1N	C5-C31-C36	2.69	124.44	119.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	273	M1N	C11-C10-N9	-2.67	104.15	109.84
3	L	273	M1N	C40-C33-C34	-2.67	116.95	123.19
3	J	273	M1N	C40-C33-C32	2.67	122.63	119.12
3	T	273	M1N	C40-C33-C32	2.63	122.59	119.12
3	C	273	M1N	C40-C33-C32	2.63	122.58	119.12
3	N	273	M1N	C40-C33-C34	-2.60	117.12	123.19
3	E	273	M1N	O3-C2-C4	-2.60	114.99	120.45
3	L	273	M1N	C10-N9-C14	2.57	117.56	112.62
3	V	273	M1N	C11-O12-C13	2.54	118.38	109.89
3	V	273	M1N	C40-C33-C32	2.54	122.47	119.12
3	T	273	M1N	C10-N9-C14	2.53	117.50	112.62
3	N	273	M1N	C5-C4-N6	-2.53	105.46	110.79
3	E	273	M1N	C2-C4-N6	2.51	117.99	111.16
3	R	273	M1N	C10-N9-C7	-2.51	112.71	121.94
3	T	273	M1N	C5-C31-C36	2.50	124.11	119.86
3	N	273	M1N	C5-C31-C36	2.47	124.07	119.86
3	E	273	M1N	C10-N9-C7	-2.46	112.86	121.94
3	T	273	M1N	C5-C31-C32	-2.43	116.92	120.76
3	L	273	M1N	C5-C31-C36	2.42	123.98	119.86
3	C	273	M1N	C10-N9-C14	2.41	117.27	112.62
3	H	273	M1N	C10-N9-C14	2.40	117.24	112.62
3	X	273	M1N	C2-C4-N6	2.39	117.67	111.16
3	X	273	M1N	C31-C5-C4	2.38	118.11	113.45
3	Z	273	M1N	C10-N9-C14	2.38	117.21	112.62
3	C	273	M1N	C2-C4-N6	2.37	117.61	111.16
3	Z	273	M1N	C2-C4-N6	2.36	117.60	111.16
3	R	273	M1N	C10-N9-C14	2.36	117.17	112.62
3	2	273	M1N	C10-N9-C7	-2.36	113.27	121.94
3	E	273	M1N	C40-C33-C32	2.34	122.20	119.12
3	V	273	M1N	C40-C33-C34	-2.34	117.72	123.19
3	P	273	M1N	C40-C33-C34	-2.34	117.73	123.19
3	C	273	M1N	C40-C33-C34	-2.33	117.73	123.19
3	X	273	M1N	C40-C33-C32	2.32	122.18	119.12
3	C	273	M1N	C11-O12-C13	2.32	117.65	109.89
3	H	273	M1N	C10-N9-C7	-2.32	113.39	121.94
3	R	273	M1N	C11-O12-C13	2.31	117.59	109.89
3	L	273	M1N	C11-O12-C13	2.28	117.52	109.89
3	J	273	M1N	C40-C33-C34	-2.28	117.86	123.19
3	G	273	M1N	C11-O12-C13	2.27	117.45	109.89
3	L	273	M1N	C10-N9-C7	-2.26	113.62	121.94
3	T	273	M1N	C40-C33-C34	-2.25	117.92	123.19
3	N	273	M1N	C10-N9-C14	2.24	116.94	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	273	M1N	C5-C31-C32	-2.23	117.23	120.76
3	H	273	M1N	C40-C33-C34	-2.23	117.98	123.19
3	2	273	M1N	C2-C4-N6	2.22	117.22	111.16
3	P	273	M1N	C10-N9-C14	2.22	116.90	112.62
3	Z	273	M1N	C31-C5-C4	2.20	117.74	113.45
3	2	273	M1N	C40-C33-C34	-2.18	118.09	123.19
3	P	273	M1N	C11-O12-C13	2.18	117.17	109.89
3	T	273	M1N	O12-C13-C14	-2.18	107.00	111.80
3	V	273	M1N	C5-C4-C2	2.15	115.84	110.25
3	P	273	M1N	C35-C36-C31	-2.12	117.72	121.48
3	L	273	M1N	C11-C10-N9	-2.12	105.33	109.84
3	E	273	M1N	C40-C33-C34	-2.12	118.24	123.19
3	Z	273	M1N	C5-C4-N6	-2.11	106.33	110.79
3	T	273	M1N	C11-C10-N9	-2.11	105.36	109.84
3	C	273	M1N	C15-N1-C2	-2.10	117.34	122.77
3	N	273	M1N	O12-C13-C14	-2.10	107.18	111.80
3	E	273	M1N	C11-C10-N9	-2.10	105.38	109.84
3	X	273	M1N	C40-C33-C34	-2.09	118.29	123.19
3	T	273	M1N	C10-N9-C7	-2.09	114.25	121.94
3	X	273	M1N	C10-N9-C7	-2.08	114.27	121.94
3	2	273	M1N	C40-C33-C32	2.08	121.86	119.12
3	G	273	M1N	C40-C33-C34	-2.06	118.36	123.19
3	N	273	M1N	C34-C35-C36	2.06	124.28	120.99
3	L	273	M1N	C15-N1-C2	-2.06	117.45	122.77
3	G	273	M1N	C11-C10-N9	-2.06	105.46	109.84
3	J	273	M1N	C11-C10-N9	-2.04	105.50	109.84
3	J	273	M1N	C11-O12-C13	2.04	116.70	109.89
3	G	273	M1N	C40-C33-C32	2.04	121.81	119.12
3	E	273	M1N	C10-N9-C14	2.03	116.53	112.62
3	C	273	M1N	C10-N9-C7	-2.03	114.46	121.94
3	H	273	M1N	C15-N1-C2	-2.02	117.54	122.77
3	V	273	M1N	C10-N9-C7	-2.02	114.51	121.94
3	J	273	M1N	C5-C4-C2	2.01	115.46	110.25
3	P	273	M1N	C11-C10-N9	-2.00	105.58	109.84

There are no chirality outliers.

All (137) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	273	M1N	O3-C2-N1-C15
3	T	273	M1N	C4-C2-N1-C15
3	T	273	M1N	C2-C4-C5-C31

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Mol	Chain	Res	Type	Atoms
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
3	V	273	M1N	C4-C2-N1-C15
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	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	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	C15-C22-C23-C24
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	C	273	M1N	O3-C2-N1-C15
3	C	273	M1N	C4-C2-N1-C15
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
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

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Mol	Chain	Res	Type	Atoms
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	H	273	M1N	O3-C2-N1-C15
3	H	273	M1N	C4-C2-N1-C15
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	J	273	M1N	O3-C2-N1-C15
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	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	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	2	273	M1N	N6-C4-C5-C31
3	C	273	M1N	N6-C4-C5-C31
3	V	273	M1N	C2-C4-C5-C31

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

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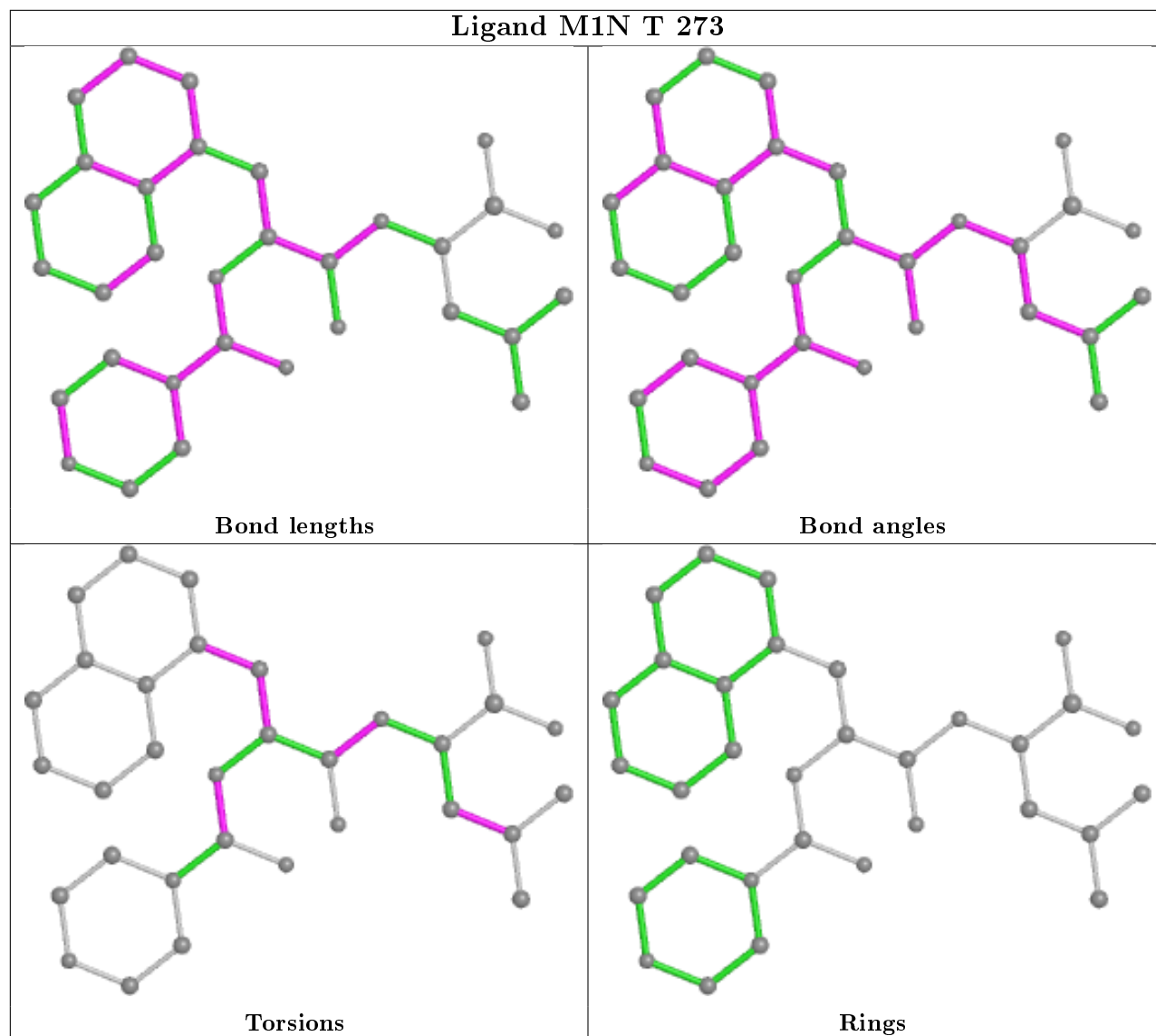
Mol	Chain	Res	Type	Atoms
3	P	273	M1N	N6-C7-N9-C14
3	N	273	M1N	N1-C15-C22-C23
3	X	273	M1N	N1-C15-C22-C23
3	R	273	M1N	O8-C7-N9-C10
3	G	273	M1N	N6-C7-N9-C14
3	R	273	M1N	N6-C7-N9-C10
3	Z	273	M1N	N1-C15-C22-C23
3	Z	273	M1N	C15-C22-C23-C24

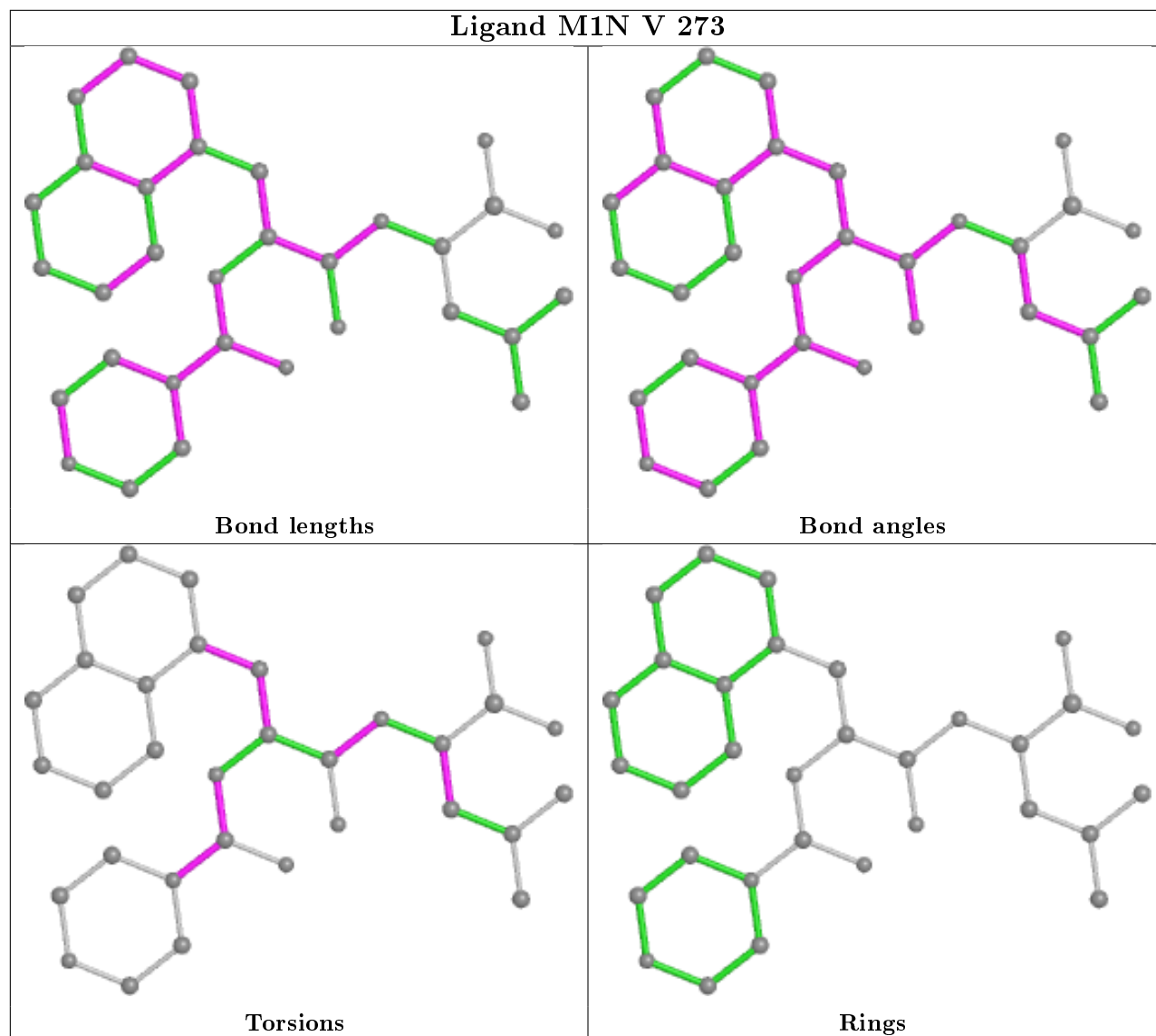
There are no ring outliers.

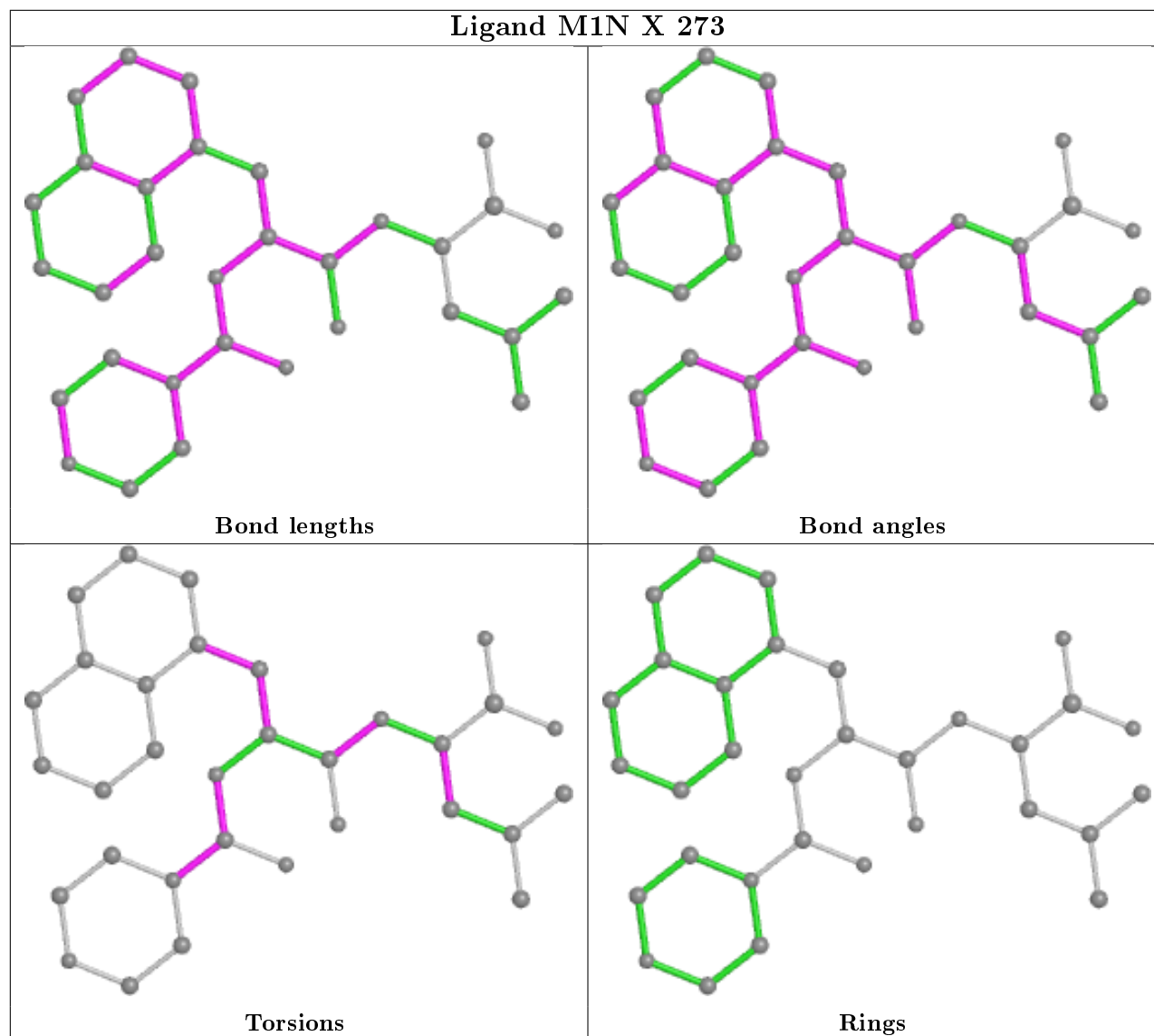
14 monomers are involved in 188 short contacts:

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

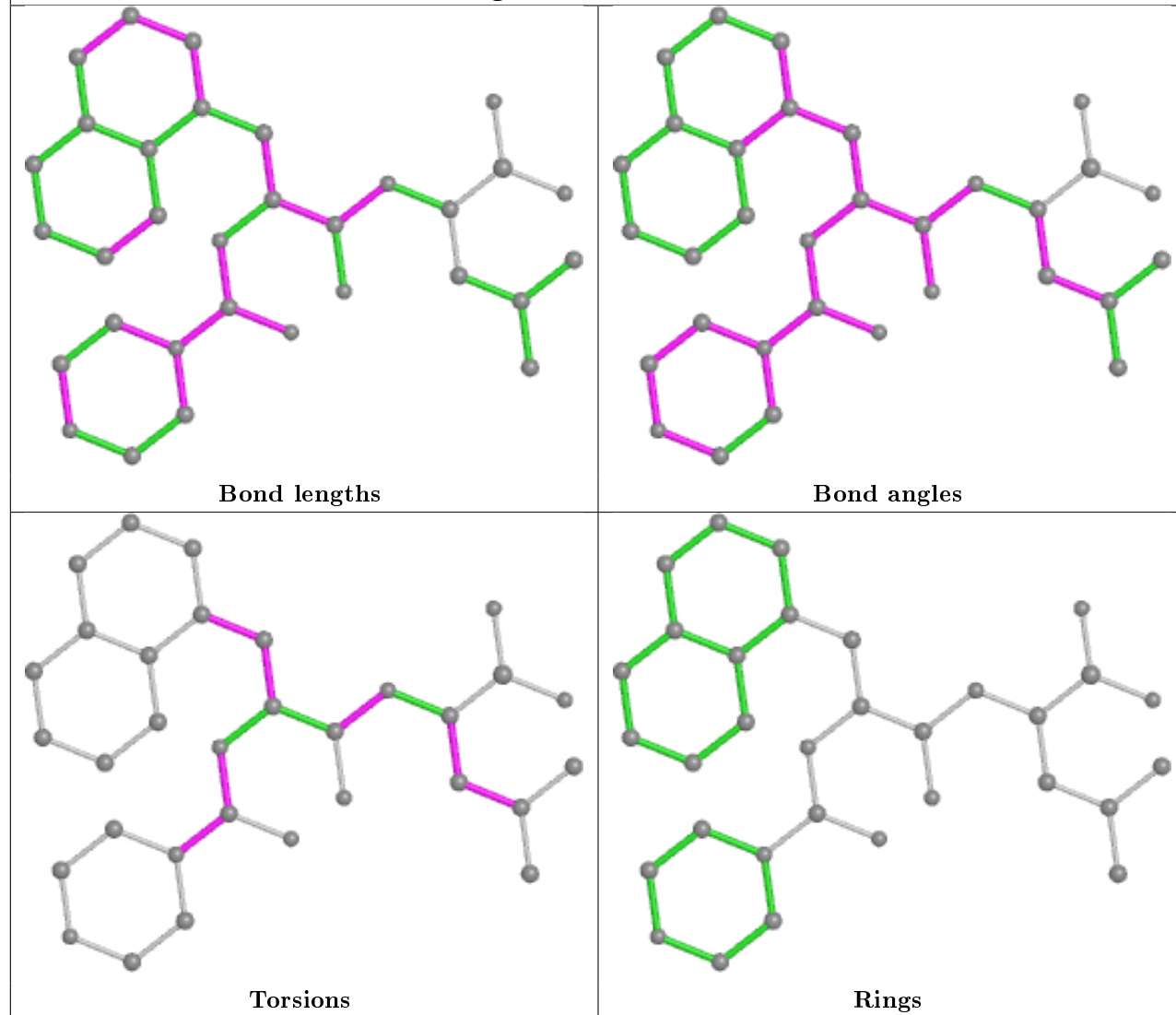
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



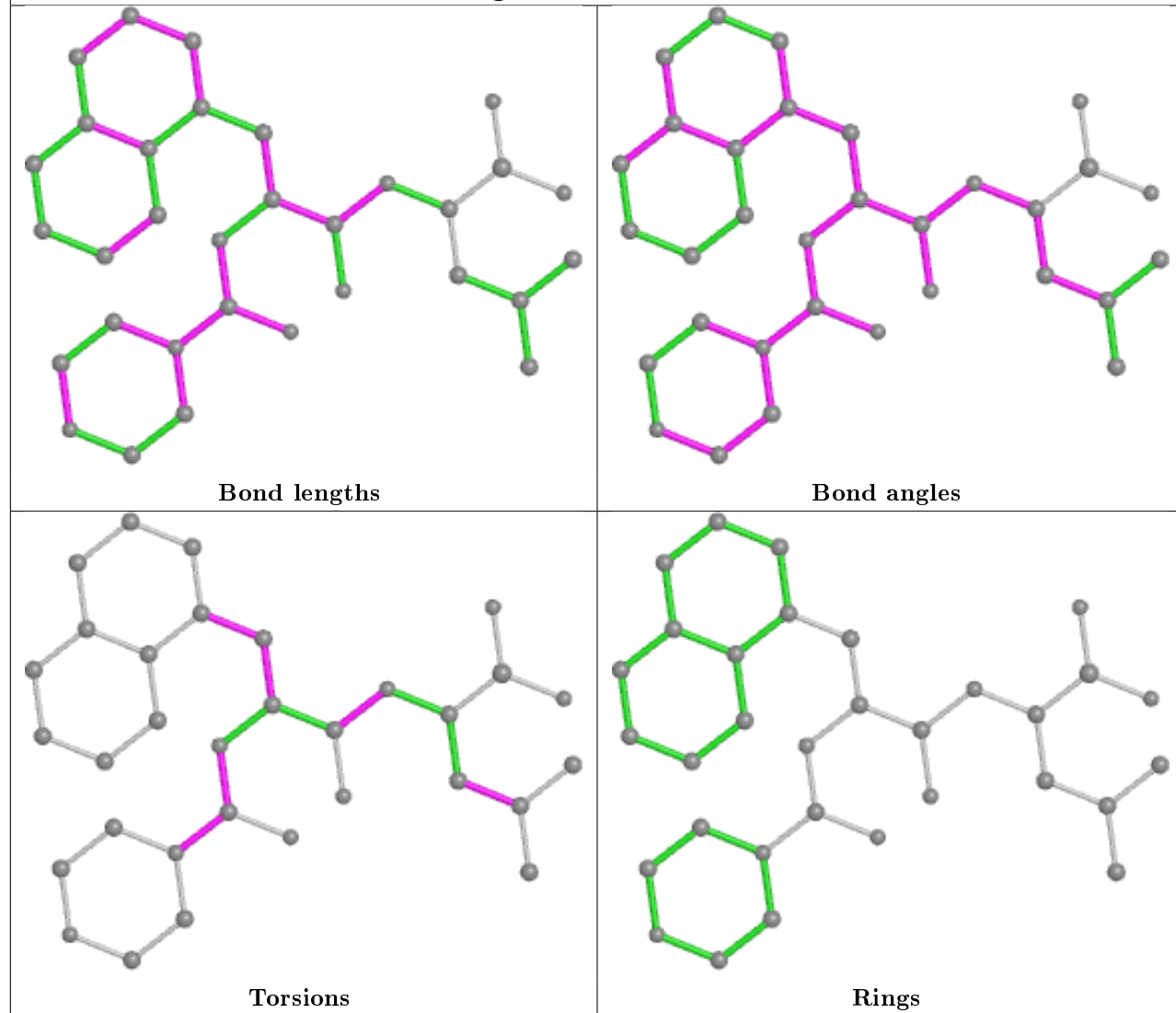




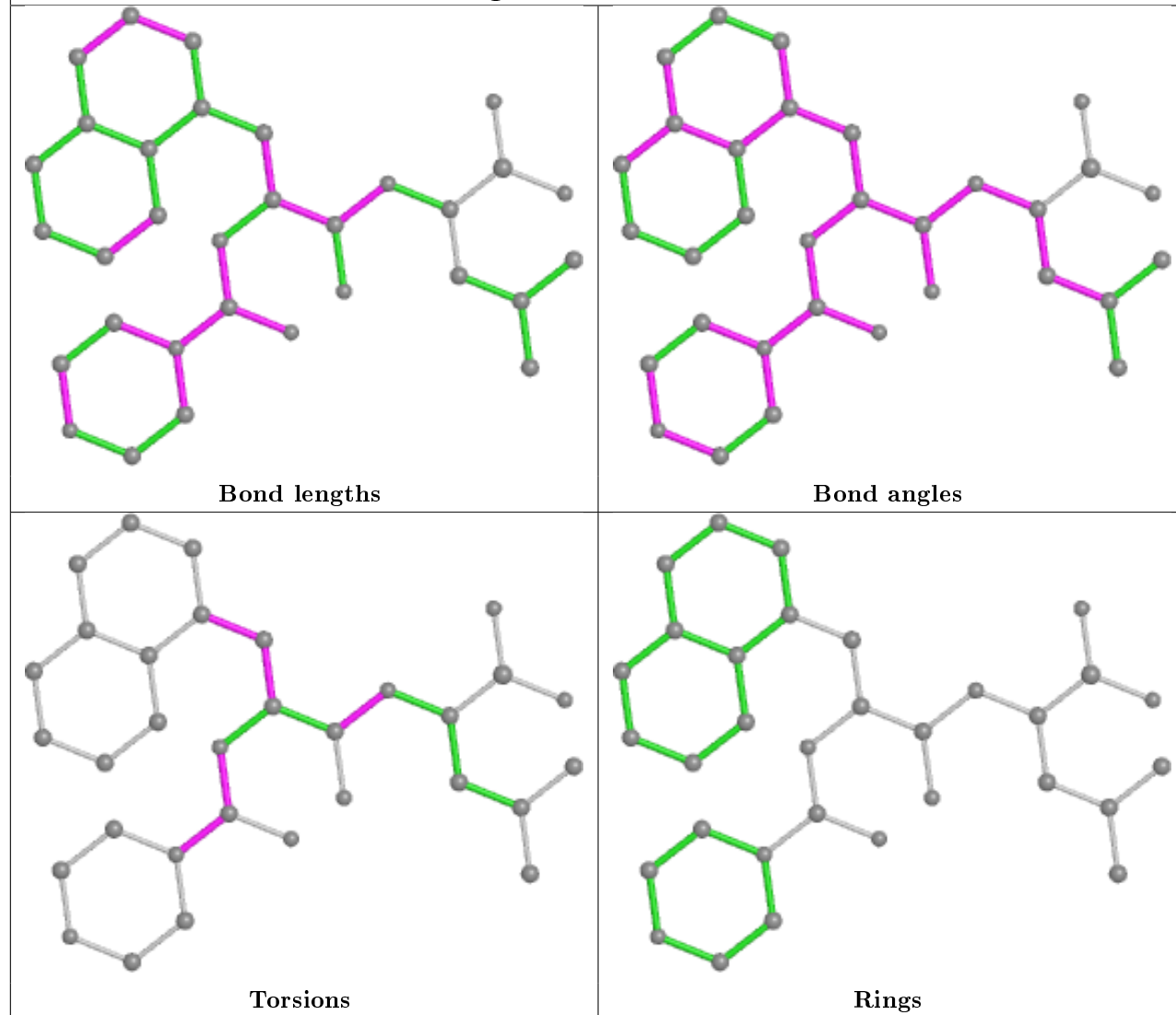
Ligand M1N Z 273



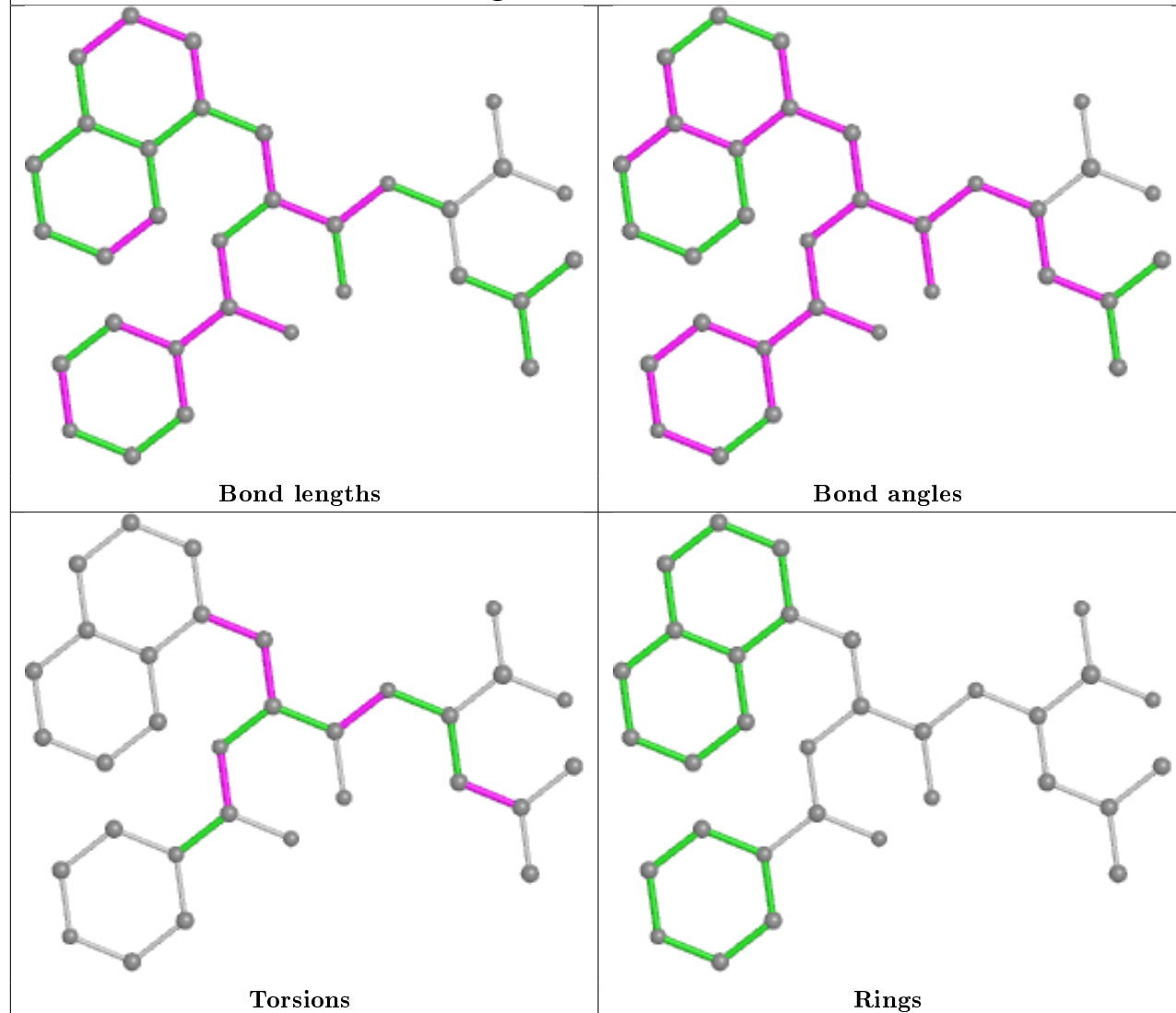
Ligand M1N 2 273

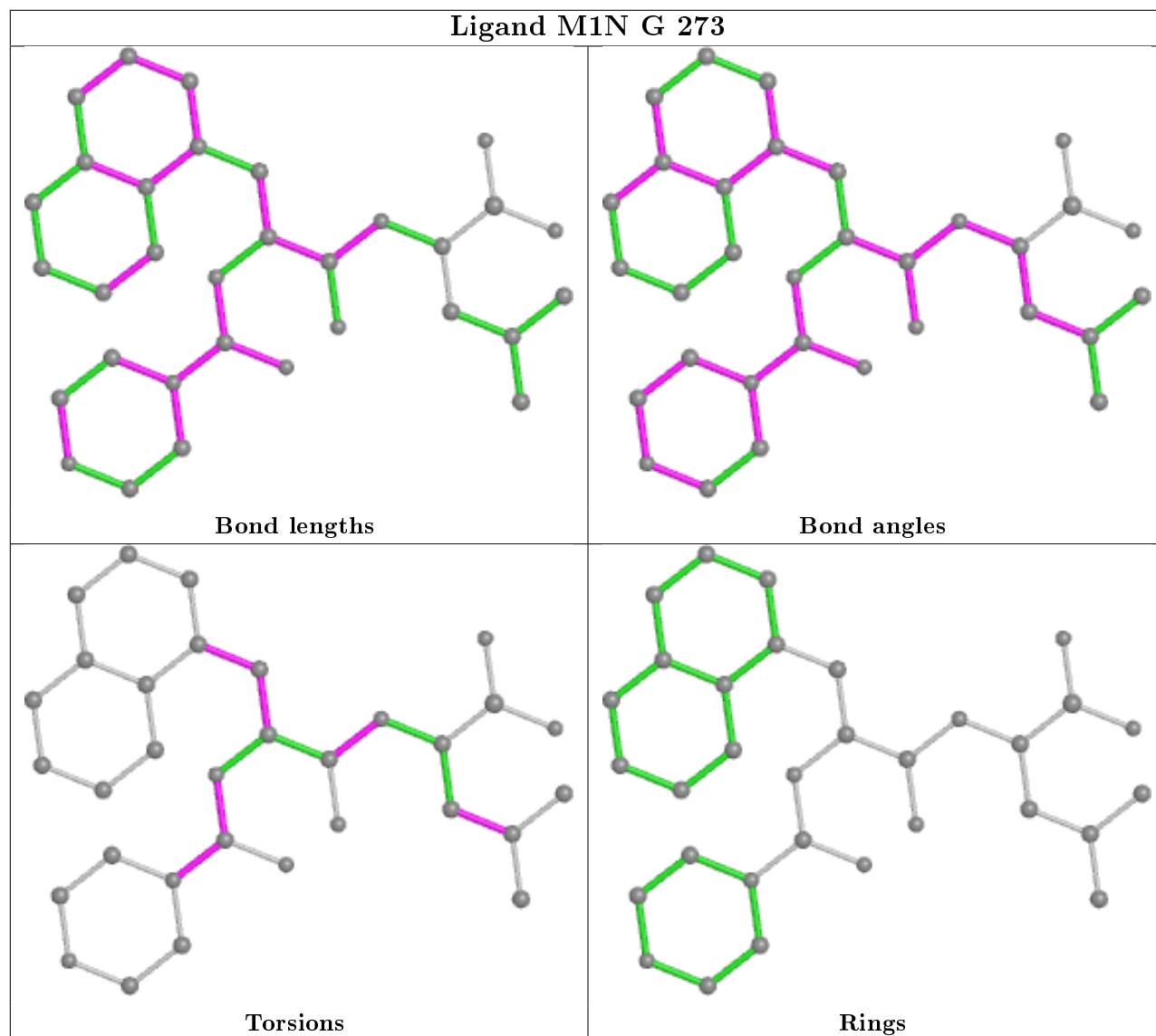


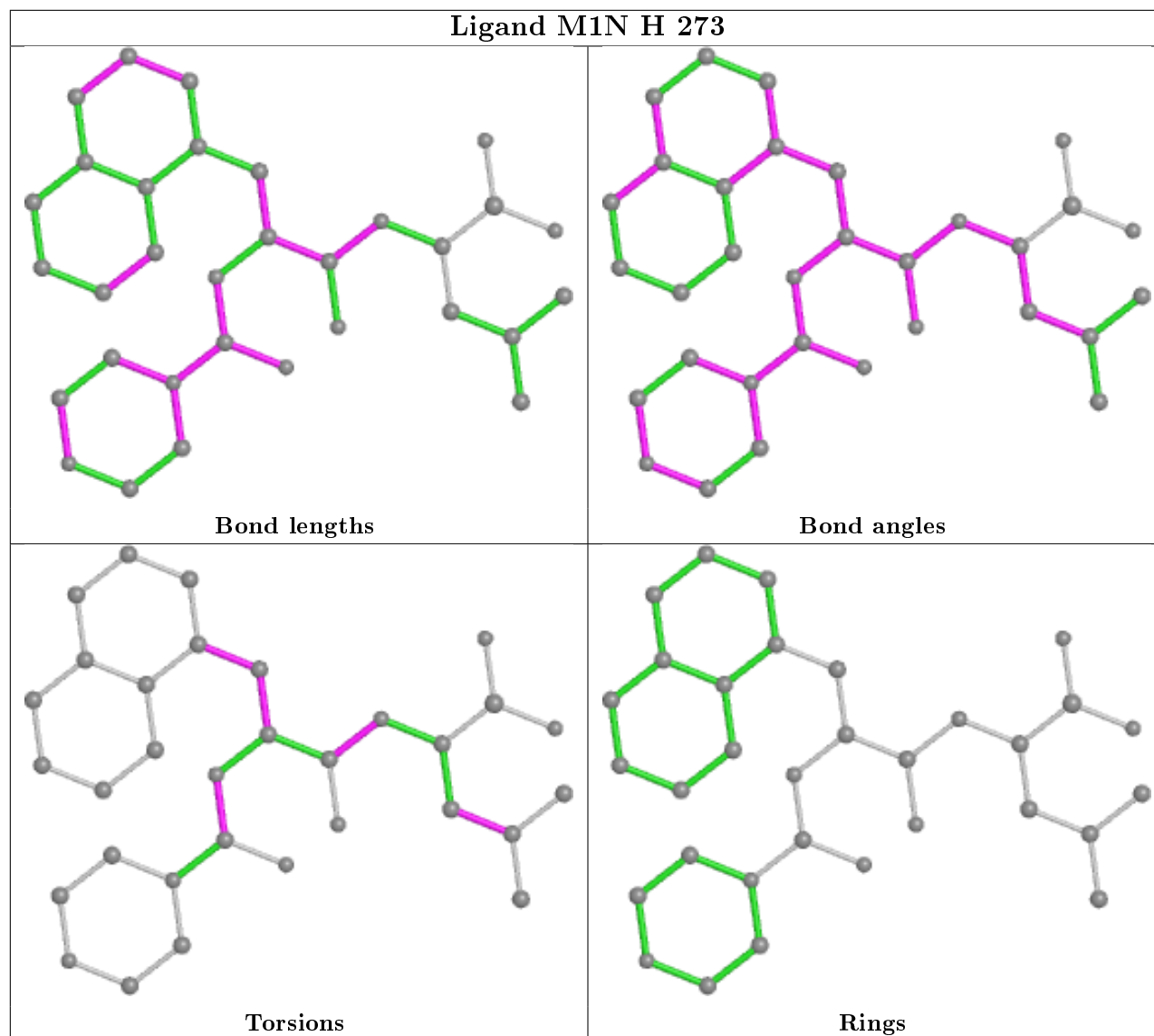
Ligand M1N C 273



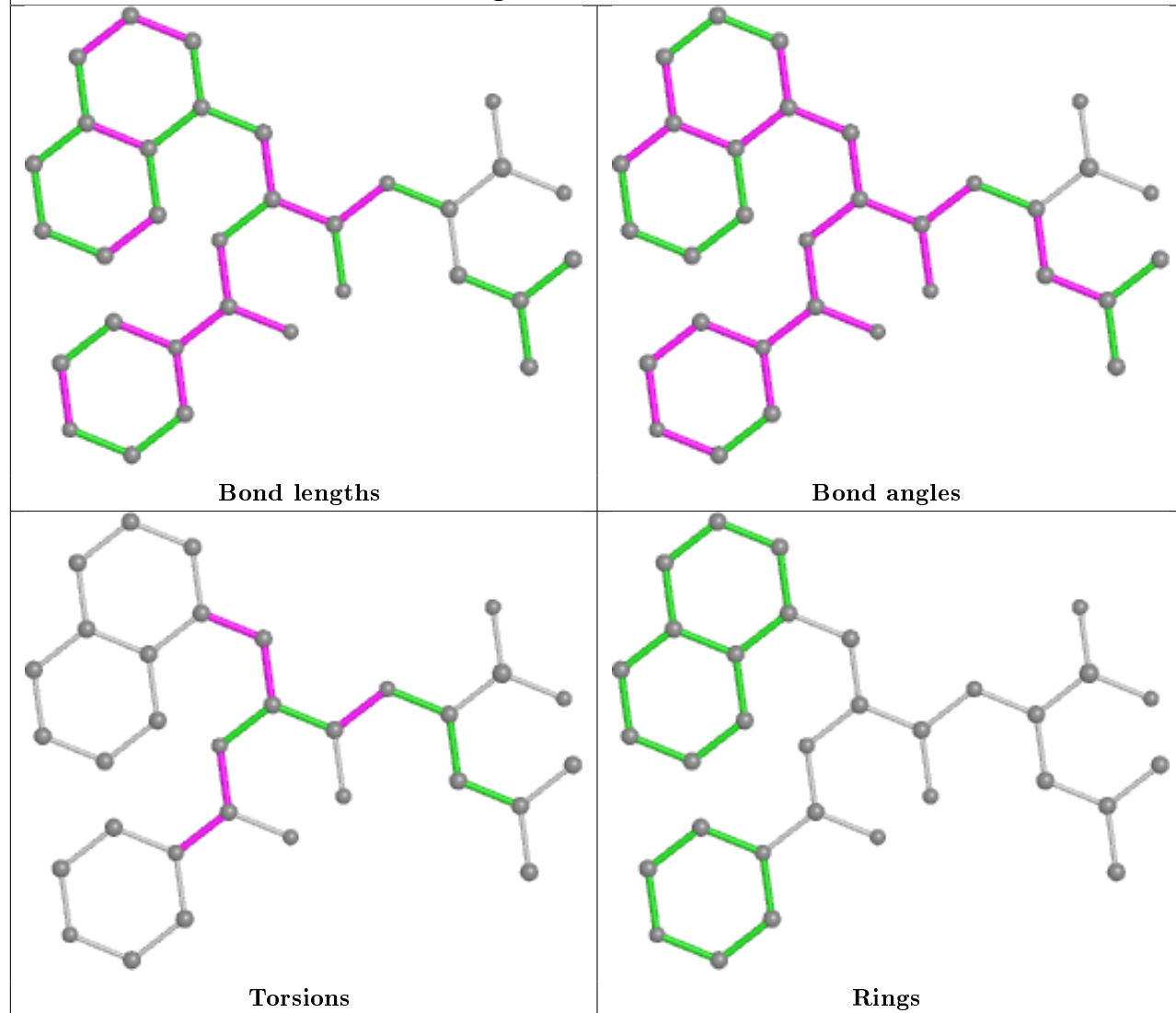
Ligand M1N E 273



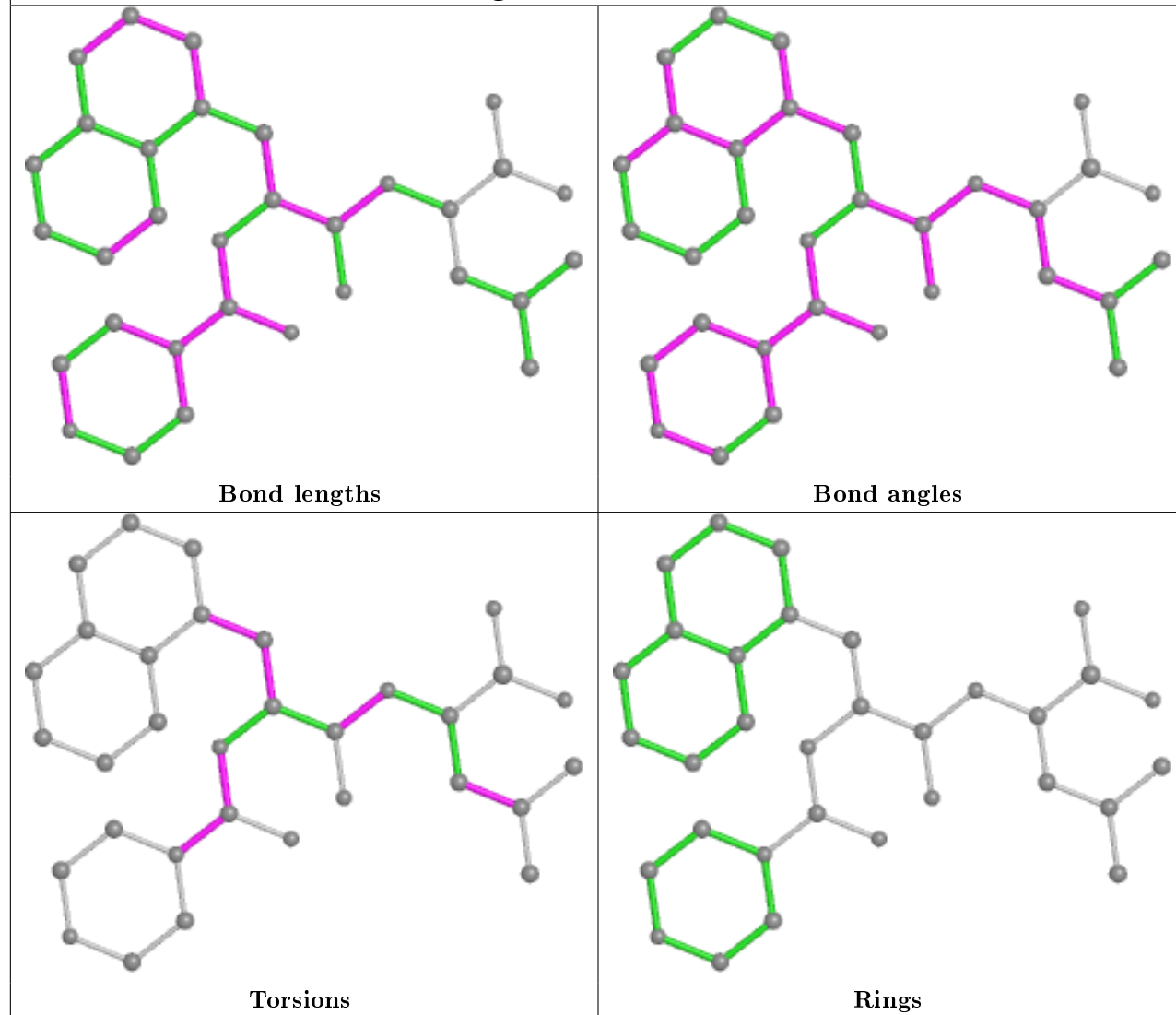


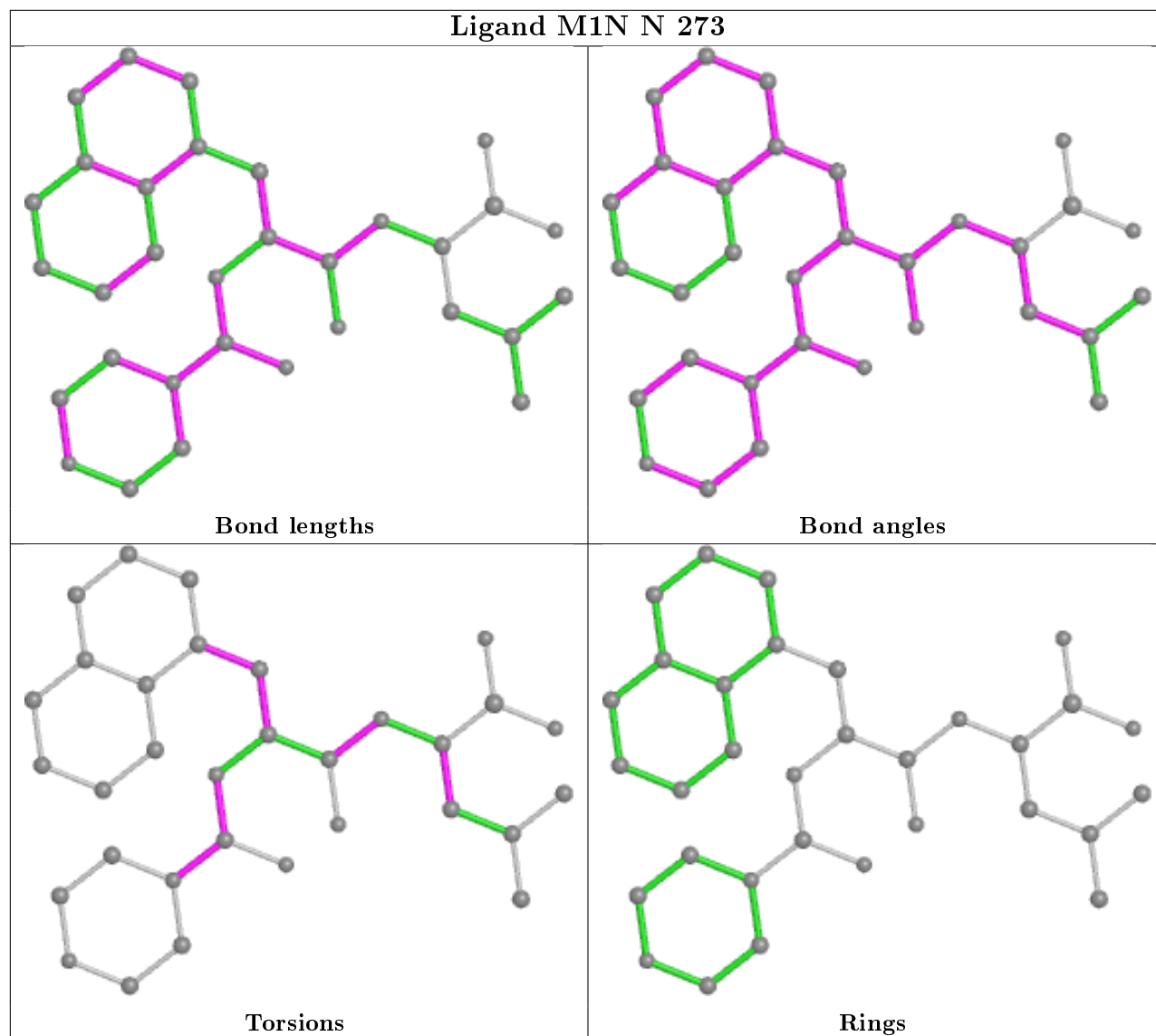


Ligand M1N J 273

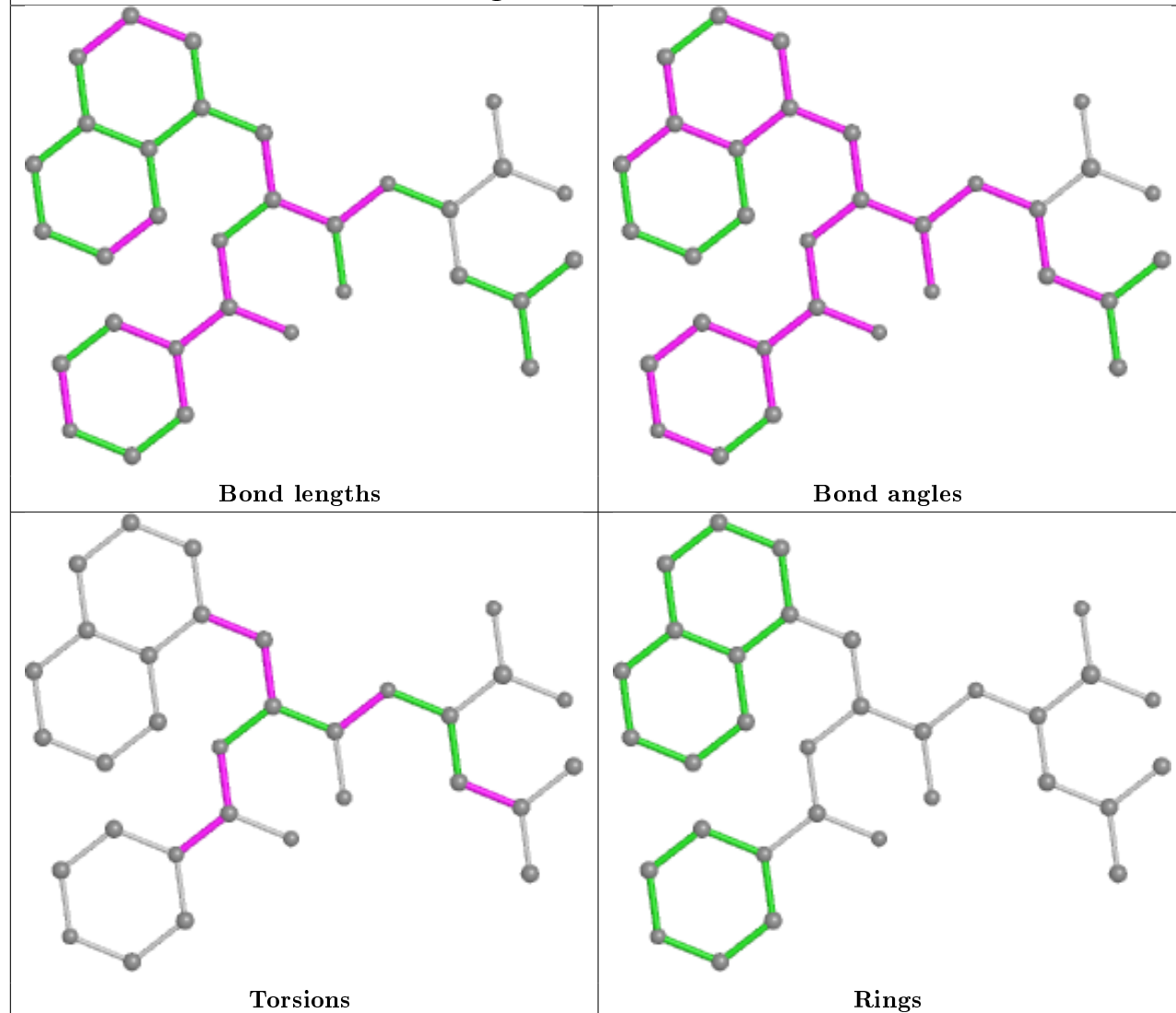


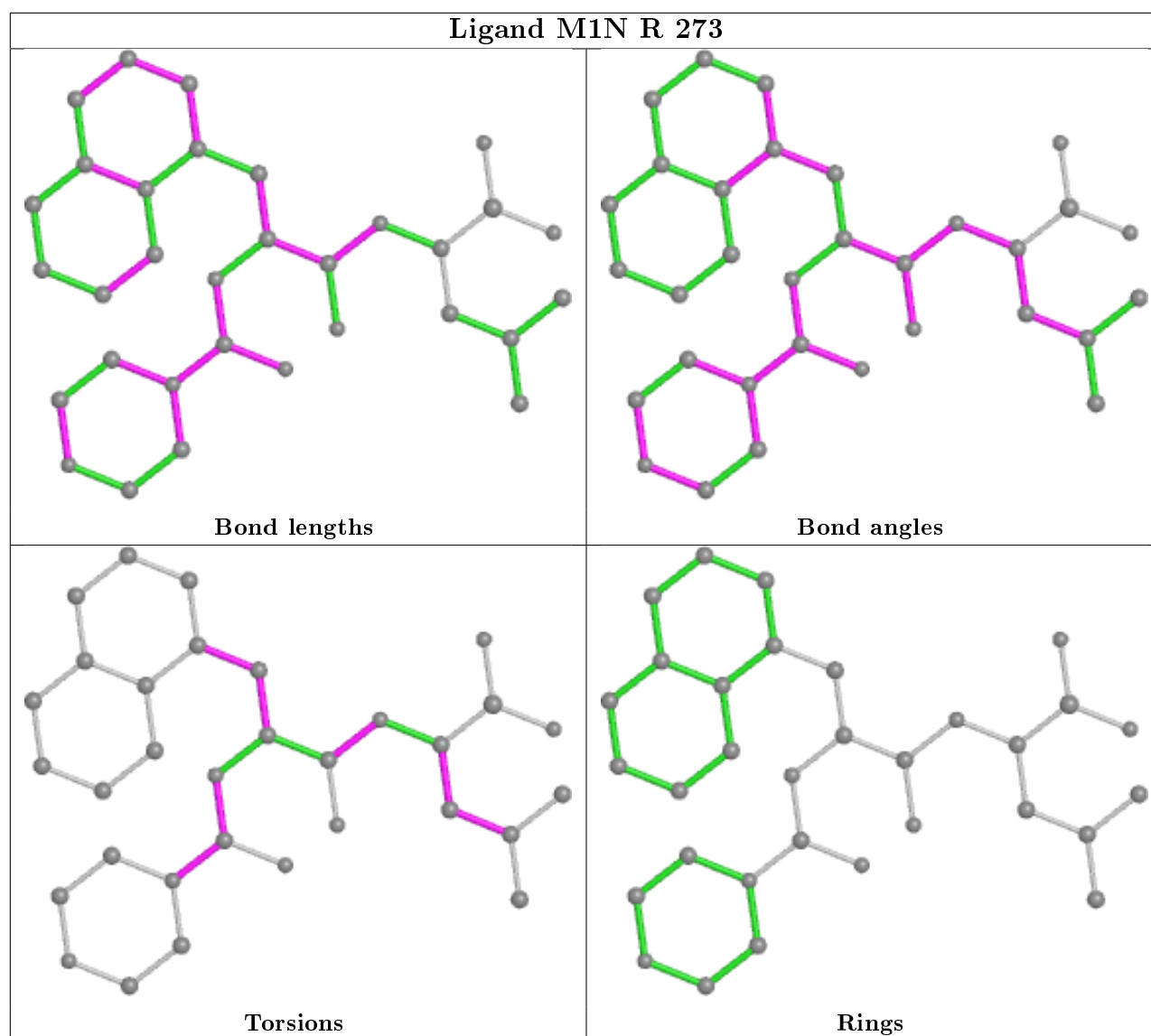
Ligand M1N L 273





Ligand M1N P 273





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%)	1.34	58 (26%) 0 0	75, 100, 100, 100	0
1	A	220/251 (87%)	0.76	16 (7%) 15 4	74, 100, 100, 100	0
1	B	220/251 (87%)	0.98	29 (13%) 3 1	74, 100, 100, 100	0
1	D	220/251 (87%)	1.11	39 (17%) 1 0	74, 100, 100, 100	0
1	F	220/251 (87%)	1.09	36 (16%) 1 0	74, 100, 100, 100	0
1	I	220/251 (87%)	1.01	29 (13%) 3 1	74, 100, 100, 100	0
1	K	220/251 (87%)	1.38	45 (20%) 1 0	74, 100, 100, 100	0
1	M	220/251 (87%)	1.04	35 (15%) 1 1	74, 100, 100, 100	0
1	O	220/251 (87%)	1.35	55 (25%) 0 0	74, 100, 100, 100	0
1	Q	220/251 (87%)	1.44	64 (29%) 0 0	74, 100, 100, 100	0
1	S	220/251 (87%)	1.16	43 (19%) 1 0	74, 100, 100, 100	0
1	U	220/251 (87%)	1.23	49 (22%) 0 0	74, 100, 100, 100	0
1	W	220/251 (87%)	1.18	42 (19%) 1 0	74, 100, 100, 100	0
1	Y	220/251 (87%)	1.68	81 (36%) 0 0	74, 100, 100, 100	0
2	2	222/240 (92%)	0.49	17 (7%) 13 4	52, 72, 91, 100	0
2	C	222/240 (92%)	0.58	2 (0%) 84 63	53, 72, 91, 100	0
2	E	222/240 (92%)	0.46	7 (3%) 47 20	52, 72, 92, 100	0
2	G	222/240 (92%)	0.37	6 (2%) 54 26	52, 72, 91, 100	0
2	H	222/240 (92%)	0.54	2 (0%) 84 63	52, 72, 91, 100	0
2	J	222/240 (92%)	0.43	7 (3%) 47 20	53, 72, 92, 100	0
2	L	222/240 (92%)	0.47	2 (0%) 84 63	53, 72, 92, 100	0
2	N	222/240 (92%)	0.39	5 (2%) 60 31	52, 72, 91, 100	0
2	P	222/240 (92%)	0.41	2 (0%) 84 63	53, 72, 91, 100	0
2	R	222/240 (92%)	0.47	12 (5%) 25 9	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%)	0.50	12 (5%) 25 9	53, 72, 92, 100	0
2	V	222/240 (92%)	0.43	5 (2%) 60 31	53, 72, 92, 100	0
2	X	222/240 (92%)	0.51	14 (6%) 20 6	53, 72, 91, 100	0
2	Z	222/240 (92%)	0.41	6 (2%) 54 26	53, 72, 92, 100	0
All	All	6188/6874 (90%)	0.83	720 (11%) 4 1	52, 88, 100, 100	0

All (720) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	235	VAL	21.3
1	K	236	ASP	19.4
1	S	235	VAL	17.4
1	W	235	VAL	14.7
1	W	236	ASP	14.6
1	M	236	ASP	14.6
1	1	235	VAL	14.5
1	F	236	ASP	12.7
1	U	236	ASP	12.4
1	I	235	VAL	11.7
1	1	236	ASP	11.6
1	M	235	VAL	11.4
1	A	235	VAL	11.1
1	I	237	GLN	10.7
1	Q	235	VAL	10.7
1	M	237	GLN	10.6
1	U	237	GLN	10.3
1	S	234	LEU	10.0
1	I	236	ASP	10.0
1	U	235	VAL	9.9
1	I	203	LEU	9.6
1	Q	236	ASP	9.5
1	O	237	GLN	9.4
1	B	235	VAL	9.4
1	S	236	ASP	9.3
2	2	414	PRO	9.1
1	U	192	SER	9.0
1	O	33	LEU	8.9
1	D	236	ASP	8.9
1	A	237	GLN	8.7
1	O	236	ASP	8.4
1	1	188	LEU	8.4

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Mol	Chain	Res	Type	RSRZ
1	Q	237	GLN	8.3
1	K	237	GLN	8.0
1	F	167	LEU	7.9
1	B	236	ASP	7.8
1	F	177	LEU	7.7
1	Q	234	LEU	7.1
1	Y	237	GLN	7.0
1	S	237	GLN	7.0
1	D	188	LEU	7.0
1	Y	188	LEU	6.8
1	F	237	GLN	6.8
1	K	191	GLY	6.8
1	I	234	LEU	6.6
1	Q	191	GLY	6.5
1	K	13	MET	6.5
1	K	167	LEU	6.5
1	1	227	GLY	6.4
1	B	237	GLN	6.4
1	K	234	LEU	6.3
1	A	177	LEU	6.3
1	I	204	GLY	6.3
1	M	172	ALA	6.2
1	O	230	LEU	6.2
1	F	235	VAL	6.1
1	1	205	VAL	6.1
1	O	172	ALA	6.0
1	O	188	LEU	6.0
1	U	232	ALA	6.0
1	Q	230	LEU	5.9
1	A	236	ASP	5.9
1	Y	177	LEU	5.9
1	Q	118	TYR	5.8
1	Q	177	LEU	5.8
1	Y	235	VAL	5.7
1	B	192	SER	5.7
1	K	177	LEU	5.7
1	Q	33	LEU	5.7
1	O	191	GLY	5.7
1	M	182	ARG	5.6
1	Y	171	TYR	5.6
1	K	111	PHE	5.5
1	Y	230	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	M	192	SER	5.5
1	W	228	SER	5.5
1	Q	192	SER	5.4
1	1	237	GLN	5.4
1	S	19	LEU	5.4
1	1	234	LEU	5.4
1	U	234	LEU	5.3
1	D	235	VAL	5.3
1	1	115	ALA	5.3
1	D	111	PHE	5.3
1	D	237	GLN	5.3
1	D	170	SER	5.3
1	O	232	ALA	5.3
1	Y	10	GLU	5.3
1	D	177	LEU	5.2
1	K	172	ALA	5.2
1	S	204	GLY	5.2
1	U	230	LEU	5.2
1	K	185	VAL	5.2
1	O	177	LEU	5.1
1	Y	236	ASP	5.1
1	Y	156	MET	5.1
1	Y	9	PRO	5.1
2	2	407	TYR	5.1
1	U	111	PHE	5.0
1	Q	163	ILE	5.0
1	Y	192	SER	5.0
1	Y	39	VAL	5.0
1	Y	213	LEU	4.9
1	Q	232	ALA	4.9
1	B	205	VAL	4.9
1	D	171	TYR	4.9
2	X	407	TYR	4.9
1	D	191	GLY	4.9
1	Y	31	VAL	4.8
1	1	9	PRO	4.8
2	Z	417	ALA	4.8
1	Y	167	LEU	4.8
1	Q	171	TYR	4.8
1	K	127	VAL	4.8
1	K	181	LEU	4.8
1	O	235	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	Y	34	ALA	4.8
1	1	177	LEU	4.7
1	O	234	LEU	4.7
1	W	229	ALA	4.7
1	Q	9	PRO	4.7
1	S	9	PRO	4.7
1	M	8	SER	4.7
1	Y	122	LEU	4.6
1	Y	204	GLY	4.6
1	1	225	ILE	4.6
1	Q	190	ALA	4.6
1	B	191	GLY	4.6
1	1	172	ALA	4.6
1	1	191	GLY	4.6
1	U	171	TYR	4.6
1	Y	233	LEU	4.5
1	M	189	ARG	4.5
1	S	192	SER	4.5
1	O	169	GLU	4.5
1	B	153	PHE	4.5
1	U	191	GLY	4.5
1	Y	38	GLY	4.5
1	O	185	VAL	4.5
1	Y	210	VAL	4.5
1	O	138	LEU	4.5
1	Q	188	LEU	4.5
1	K	34	ALA	4.4
1	W	163	ILE	4.4
1	Y	160	THR	4.4
1	Y	182	ARG	4.4
1	F	171	TYR	4.4
1	O	192	SER	4.4
1	M	177	LEU	4.4
1	D	203	LEU	4.4
1	1	40	LEU	4.4
1	K	33	LEU	4.3
1	Y	172	ALA	4.3
1	K	171	TYR	4.3
1	O	225	ILE	4.3
1	U	169	GLU	4.3
1	M	9	PRO	4.3
1	K	204	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	I	135	ARG	4.3
1	B	171	TYR	4.3
1	Y	176	SER	4.2
1	Q	220	ARG	4.2
1	Q	155	VAL	4.2
1	Y	42	VAL	4.2
1	K	143	TYR	4.2
1	1	171	TYR	4.2
2	T	340	TYR	4.2
1	F	164	ALA	4.2
1	U	177	LEU	4.2
1	U	181	LEU	4.2
1	M	171	TYR	4.2
1	S	203	LEU	4.1
1	W	167	LEU	4.1
1	S	205	VAL	4.1
1	M	204	GLY	4.1
2	R	460	GLY	4.1
1	I	233	LEU	4.1
1	U	33	LEU	4.1
1	Q	182	ARG	4.1
1	U	40	LEU	4.1
1	D	36	ALA	4.1
1	S	13	MET	4.0
1	S	135	ARG	4.0
1	M	234	LEU	4.0
1	F	191	GLY	4.0
1	S	151	PRO	4.0
1	Y	40	LEU	4.0
1	B	167	LEU	4.0
1	K	203	LEU	4.0
1	U	205	VAL	4.0
1	W	237	GLN	3.9
1	Y	155	VAL	3.9
1	Y	41	PHE	3.9
1	Y	180	ALA	3.9
2	N	417	ALA	3.9
1	Y	208	LEU	3.9
1	M	170	SER	3.9
1	O	152	HIS	3.9
1	Q	225	ILE	3.8
1	U	188	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	W	188	LEU	3.8
1	M	178	THR	3.8
1	1	35	TYR	3.8
1	S	175	ALA	3.8
1	K	205	VAL	3.8
1	Q	233	LEU	3.7
1	1	230	LEU	3.7
1	D	234	LEU	3.7
1	F	233	LEU	3.7
1	D	163	ILE	3.7
1	O	155	VAL	3.7
1	W	177	LEU	3.7
1	S	172	ALA	3.7
1	Q	135	ARG	3.7
1	D	33	LEU	3.7
1	Y	175	ALA	3.6
1	Y	33	LEU	3.6
1	S	114	GLN	3.6
1	1	182	ARG	3.6
1	D	30	VAL	3.6
2	C	417	ALA	3.6
1	B	163	ILE	3.6
1	Y	205	VAL	3.6
1	1	39	VAL	3.6
1	K	159	THR	3.6
1	O	233	LEU	3.6
2	R	308	TYR	3.6
1	I	192	SER	3.6
1	K	186	ALA	3.6
1	O	181	LEU	3.6
1	Y	136	PRO	3.6
1	F	188	LEU	3.5
1	S	40	LEU	3.5
1	M	13	MET	3.5
1	Q	169	GLU	3.5
1	I	172	ALA	3.5
1	Y	212	VAL	3.5
1	K	114	GLN	3.5
1	I	44	GLU	3.5
1	Q	186	ALA	3.5
1	M	183	ILE	3.5
1	Y	67	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	V	510	ILE	3.5
1	O	167	LEU	3.5
1	S	177	LEU	3.5
1	D	155	VAL	3.5
1	O	160	THR	3.5
1	1	33	LEU	3.5
1	1	153	PHE	3.5
1	I	9	PRO	3.5
1	M	173	GLU	3.5
1	Q	187	ALA	3.5
1	S	224	ARG	3.5
1	W	36	ALA	3.5
1	1	117	PRO	3.4
1	Q	189	ARG	3.4
1	U	213	LEU	3.4
1	1	186	ALA	3.4
1	Y	185	VAL	3.4
1	1	204	GLY	3.4
1	K	115	ALA	3.4
1	K	180	ALA	3.4
2	T	486	LEU	3.4
1	F	172	ALA	3.4
1	Y	13	MET	3.4
1	U	143	TYR	3.4
1	W	10	GLU	3.4
1	W	16	ARG	3.4
1	I	177	LEU	3.4
1	S	182	ARG	3.4
1	Y	234	LEU	3.4
1	A	169	GLU	3.4
1	U	225	ILE	3.4
1	F	176	SER	3.3
1	S	8	SER	3.3
1	Y	179	ASP	3.3
1	S	138	LEU	3.3
1	S	12	ALA	3.3
2	L	417	ALA	3.3
1	Y	132	GLU	3.3
1	O	111	PHE	3.3
1	Y	223	ARG	3.3
1	O	179	ASP	3.3
1	M	167	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	31	VAL	3.3
1	O	205	VAL	3.3
1	U	172	ALA	3.3
1	1	192	SER	3.3
1	U	138	LEU	3.3
1	Y	225	ILE	3.3
1	O	178	THR	3.3
1	1	167	LEU	3.3
1	U	53	ILE	3.3
1	W	191	GLY	3.3
1	F	40	LEU	3.3
1	B	170	SER	3.2
1	Y	170	SER	3.2
1	Q	130	TYR	3.2
1	W	165	ASN	3.2
1	Q	167	LEU	3.2
1	O	180	ALA	3.2
1	M	185	VAL	3.2
1	Q	36	ALA	3.2
1	Q	205	VAL	3.2
1	M	10	GLU	3.2
1	Y	218	PRO	3.2
2	X	491	PHE	3.2
1	1	10	GLU	3.2
1	Y	211	ALA	3.2
1	O	204	GLY	3.2
2	2	415	GLN	3.2
1	B	155	VAL	3.1
1	Y	178	THR	3.1
2	2	464	LEU	3.1
1	F	189	ARG	3.1
1	F	13	MET	3.1
2	T	464	LEU	3.1
1	B	43	ALA	3.1
1	D	227	GLY	3.1
1	M	111	PHE	3.1
1	1	163	ILE	3.1
1	D	135	ARG	3.1
1	U	203	LEU	3.1
1	F	8	SER	3.1
1	M	190	ALA	3.1
1	Q	164	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	U	208	LEU	3.1
1	B	156	MET	3.1
1	Y	226	THR	3.1
1	A	163	ILE	3.1
1	O	223	ARG	3.1
1	K	10	GLU	3.1
1	1	159	THR	3.0
1	Y	154	VAL	3.0
1	U	186	ALA	3.0
1	1	164	ALA	3.0
1	A	188	LEU	3.0
1	1	13	MET	3.0
2	R	415	GLN	3.0
1	D	118	TYR	3.0
1	Y	140	ARG	3.0
1	Q	173	GLU	3.0
1	Y	186	ALA	3.0
1	Q	181	LEU	3.0
1	S	131	GLY	3.0
1	I	175	ALA	3.0
1	K	174	ASN	3.0
1	Q	224	ARG	3.0
1	1	118	TYR	3.0
1	Y	135	ARG	3.0
1	W	169	GLU	3.0
1	O	42	VAL	3.0
1	O	208	LEU	2.9
1	1	16	ARG	2.9
1	K	214	ASP	2.9
1	O	16	ARG	2.9
1	S	191	GLY	2.9
1	K	153	PHE	2.9
1	Y	68	PHE	2.9
1	1	65	ALA	2.9
2	R	306	LEU	2.9
2	2	463	GLY	2.9
1	I	10	GLU	2.9
1	A	111	PHE	2.9
1	F	190	ALA	2.9
1	F	203	LEU	2.9
1	W	203	LEU	2.9
1	Q	218	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	11	GLN	2.9
1	Y	174	ASN	2.9
1	U	189	ARG	2.9
1	I	205	VAL	2.9
1	Q	34	ALA	2.9
1	U	153	PHE	2.9
1	K	178	THR	2.9
2	2	343	THR	2.9
1	K	138	LEU	2.9
1	Y	36	ALA	2.9
1	1	113	GLU	2.9
2	T	519	GLU	2.9
1	D	169	GLU	2.9
1	I	157	GLY	2.9
1	W	44	GLU	2.9
1	Y	159	THR	2.9
2	V	464	LEU	2.9
1	O	189	ARG	2.9
1	S	111	PHE	2.9
1	Y	153	PHE	2.9
1	M	138	LEU	2.9
1	U	233	LEU	2.9
1	1	180	ALA	2.9
1	Y	163	ILE	2.9
2	R	340	TYR	2.9
2	J	464	LEU	2.9
1	1	179	ASP	2.8
2	N	426	ALA	2.8
1	O	125	ALA	2.8
1	D	192	SER	2.8
1	W	13	MET	2.8
1	W	9	PRO	2.8
1	Q	160	THR	2.8
1	Q	42	VAL	2.8
1	Y	181	LEU	2.8
1	U	36	ALA	2.8
1	D	13	MET	2.8
1	Q	231	GLN	2.8
2	T	414	PRO	2.8
1	B	189	ARG	2.8
1	Y	143	TYR	2.8
1	D	190	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	1	187	ALA	2.8
1	W	187	ALA	2.8
2	T	497	ILE	2.8
2	T	460	GLY	2.7
1	Q	223	ARG	2.7
1	I	185	VAL	2.7
1	Q	185	VAL	2.7
1	1	203	LEU	2.7
1	O	186	ALA	2.7
1	Y	221	ALA	2.7
1	M	153	PHE	2.7
2	2	398	LEU	2.7
1	F	226	THR	2.7
1	I	13	MET	2.7
1	Y	216	ASN	2.7
1	D	34	ALA	2.7
1	U	204	GLY	2.7
2	Z	460	GLY	2.7
1	D	172	ALA	2.7
1	I	129	HIS	2.7
2	X	511	ALA	2.7
2	J	455	SER	2.7
1	Q	41	PHE	2.7
1	Q	178	THR	2.7
2	2	409	ILE	2.7
1	K	40	LEU	2.7
1	1	213	LEU	2.7
1	O	34	ALA	2.7
1	U	180	ALA	2.7
2	X	514	ALA	2.7
1	F	192	SER	2.7
1	Y	173	GLU	2.7
1	Q	39	VAL	2.7
1	1	189	ARG	2.7
1	1	169	GLU	2.6
1	W	123	CYS	2.6
1	I	170	SER	2.6
2	X	340	TYR	2.6
1	D	179	ASP	2.6
2	2	521	ARG	2.6
1	K	65	ALA	2.6
1	O	36	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	O	62	PHE	2.6
1	O	31	VAL	2.6
1	A	34	ALA	2.6
1	K	231	GLN	2.6
2	T	415	GLN	2.6
1	S	167	LEU	2.6
1	Q	229	ALA	2.6
1	M	33	LEU	2.6
2	X	510	ILE	2.6
1	D	39	VAL	2.6
1	W	132	GLU	2.6
1	Y	54	SER	2.6
2	Z	519	GLU	2.6
1	D	153	PHE	2.6
1	F	36	ALA	2.6
1	Q	166	ALA	2.6
1	U	16	ARG	2.6
1	D	141	ILE	2.6
1	S	112	THR	2.6
1	W	40	LEU	2.6
1	U	185	VAL	2.6
1	Y	209	GLU	2.6
2	R	498	ASP	2.6
1	I	189	ARG	2.6
1	1	231	GLN	2.5
1	Y	203	LEU	2.5
1	O	171	TYR	2.5
1	Y	130	TYR	2.5
1	M	175	ALA	2.5
1	1	41	PHE	2.5
1	O	213	LEU	2.5
1	1	233	LEU	2.5
1	U	182	ARG	2.5
2	G	487	VAL	2.5
1	F	114	GLN	2.5
1	Y	131	GLY	2.5
1	1	34	ALA	2.5
1	Y	219	ARG	2.5
1	F	138	LEU	2.5
1	Y	164	ALA	2.5
2	X	417	ALA	2.5
1	1	226	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	Q	10	GLU	2.5
1	K	182	ARG	2.5
1	F	232	ALA	2.5
1	1	36	ALA	2.5
2	G	407	TYR	2.5
1	K	117	PRO	2.5
1	U	170	SER	2.5
1	W	30	VAL	2.5
2	2	491	PHE	2.5
1	B	232	ALA	2.5
1	Y	53	ILE	2.5
2	H	407	TYR	2.5
1	W	170	SER	2.5
2	X	521	ARG	2.5
1	W	133	THR	2.5
1	1	19	LEU	2.5
1	S	10	GLU	2.4
1	Q	153	PHE	2.4
1	D	184	ALA	2.4
2	R	411	ALA	2.4
1	F	178	THR	2.4
1	B	234	LEU	2.4
1	O	140	ARG	2.4
1	O	173	GLU	2.4
1	W	233	LEU	2.4
1	O	170	SER	2.4
1	M	155	VAL	2.4
1	F	180	ALA	2.4
2	2	417	ALA	2.4
2	R	407	TYR	2.4
1	B	111	PHE	2.4
1	Y	215	ALA	2.4
1	I	40	LEU	2.4
1	Q	53	ILE	2.4
2	T	407	TYR	2.4
1	K	123	CYS	2.4
1	S	123	CYS	2.4
1	U	13	MET	2.4
1	B	128	ALA	2.4
1	I	180	ALA	2.4
1	S	187	ALA	2.4
1	K	116	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	407	TYR	2.4
1	Q	213	LEU	2.4
1	Q	204	GLY	2.4
1	Y	127	VAL	2.4
2	E	522	SER	2.4
1	W	166	ALA	2.4
1	A	191	GLY	2.4
1	W	209	GLU	2.4
1	W	192	SER	2.4
2	2	499	ALA	2.4
1	D	50	LEU	2.4
1	W	223	ARG	2.4
1	D	205	VAL	2.4
1	I	15	GLU	2.4
1	S	42	VAL	2.4
1	S	118	TYR	2.4
1	U	42	VAL	2.4
1	M	233	LEU	2.4
1	Q	183	ILE	2.4
2	R	465	ARG	2.4
2	X	399	LEU	2.4
2	G	489	GLY	2.3
1	U	132	GLU	2.3
1	K	42	VAL	2.3
1	M	205	VAL	2.3
2	T	506	PRO	2.3
1	M	221	ALA	2.3
1	A	165	ASN	2.3
1	I	230	LEU	2.3
1	Y	123	CYS	2.3
2	X	518	ILE	2.3
1	F	111	PHE	2.3
1	A	48	ARG	2.3
1	B	177	LEU	2.3
1	D	133	THR	2.3
1	W	219	ARG	2.3
1	F	130	TYR	2.3
1	W	172	ALA	2.3
1	D	40	LEU	2.3
1	U	227	GLY	2.3
1	W	21	ARG	2.3
1	D	212	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	Q	151	PRO	2.3
1	F	162	PRO	2.3
1	S	190	ALA	2.3
1	W	138	LEU	2.3
1	Y	66	GLY	2.3
1	1	111	PHE	2.3
1	Q	165	ASN	2.3
1	W	226	THR	2.3
1	K	162	PRO	2.3
1	B	34	ALA	2.3
1	1	223	ARG	2.3
2	X	464	LEU	2.3
1	1	37	GLY	2.3
2	N	376	PHE	2.3
1	F	169	GLU	2.3
1	S	174	ASN	2.3
1	U	210	VAL	2.3
1	D	232	ALA	2.3
1	U	122	LEU	2.3
1	Y	138	LEU	2.3
1	M	139	TYR	2.3
1	O	135	ARG	2.2
1	F	156	MET	2.2
1	M	203	LEU	2.2
1	Y	168	LYS	2.2
2	R	315	ALA	2.2
2	X	453	LEU	2.2
1	Y	183	ILE	2.2
2	R	497	ILE	2.2
2	2	378	GLY	2.2
2	J	409	ILE	2.2
2	X	517	ILE	2.2
2	Z	491	PHE	2.2
1	K	135	ARG	2.2
1	M	16	ARG	2.2
1	O	210	VAL	2.2
1	S	225	ILE	2.2
1	1	175	ALA	2.2
2	2	433	GLU	2.2
1	Q	16	ARG	2.2
1	Q	210	VAL	2.2
1	U	127	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	457	VAL	2.2
1	A	234	LEU	2.2
1	B	181	LEU	2.2
1	1	173	GLU	2.2
1	Q	111	PHE	2.2
2	N	396	GLN	2.2
2	G	340	TYR	2.2
1	U	37	GLY	2.2
1	W	204	GLY	2.2
1	I	178	THR	2.2
1	Q	184	ALA	2.2
1	Q	219	ARG	2.2
1	U	224	ARG	2.2
2	J	417	ALA	2.2
2	N	496	ILE	2.2
2	T	468	VAL	2.2
1	M	113	GLU	2.2
2	2	406	GLY	2.2
1	Y	224	ARG	2.2
1	O	114	GLN	2.2
2	V	457	VAL	2.2
1	Q	179	ASP	2.2
1	A	172	ALA	2.2
1	K	184	ALA	2.2
1	O	190	ALA	2.2
1	O	176	SER	2.2
1	U	114	GLN	2.2
1	1	11	GLN	2.2
1	B	143	TYR	2.2
1	F	48	ARG	2.2
1	O	157	GLY	2.2
1	W	131	GLY	2.2
1	U	19	LEU	2.2
1	Q	172	ALA	2.2
1	S	216	ASN	2.2
2	2	400	ALA	2.2
1	O	127	VAL	2.2
1	S	37	GLY	2.1
1	Y	37	GLY	2.1
1	B	33	LEU	2.1
2	G	306	LEU	2.1
1	F	166	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	11	GLN	2.1
1	O	231	GLN	2.1
2	P	407	TYR	2.1
1	S	230	LEU	2.1
2	J	306	LEU	2.1
2	Z	521	ARG	2.1
1	W	41	PHE	2.1
2	C	306	LEU	2.1
1	B	190	ALA	2.1
1	Q	11	GLN	2.1
2	G	430	ASN	2.1
2	R	310	GLY	2.1
1	A	40	LEU	2.1
1	O	40	LEU	2.1
1	I	107	LEU	2.1
1	D	189	ARG	2.1
2	J	326	ILE	2.1
2	T	490	ILE	2.1
1	Q	13	MET	2.1
1	A	135	ARG	2.1
1	I	159	THR	2.1
1	W	35	TYR	2.1
2	J	496	ILE	2.1
1	Q	37	GLY	2.1
1	F	16	ARG	2.1
1	O	182	ARG	2.1
1	B	41	PHE	2.1
1	U	150	GLU	2.1
2	E	430	ASN	2.1
1	K	192	SER	2.1
1	I	62	PHE	2.1
2	P	430	ASN	2.1
2	V	430	ASN	2.1
1	S	130	TYR	2.1
1	W	227	GLY	2.1
1	D	15	GLU	2.1
2	H	443	SER	2.0
1	S	132	GLU	2.0
1	U	167	LEU	2.0
1	B	182	ARG	2.0
1	S	180	ALA	2.0
2	Z	510	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	2	311	GLY	2.0
2	E	337	THR	2.0
1	F	165	ASN	2.0
1	K	41	PHE	2.0
1	O	26	ARG	2.0
1	B	169	GLU	2.0
1	W	221	ALA	2.0
2	E	412	SER	2.0
1	B	226	THR	2.0
2	V	465	ARG	2.0
1	1	190	ALA	2.0
2	L	463	GLY	2.0
2	X	497	ILE	2.0
1	S	148	ALA	2.0
1	I	118	TYR	2.0
2	E	415	GLN	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 monosaccharides 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	0.84	0.30	65,76,78,79	0
3	M1N	V	273	32/32	0.85	0.30	65,76,78,78	0
3	M1N	T	273	32/32	0.85	0.30	64,77,78,79	0
3	M1N	P	273	32/32	0.85	0.24	65,76,78,79	0
3	M1N	J	273	32/32	0.86	0.31	64,76,77,78	0
3	M1N	X	273	32/32	0.87	0.31	65,76,78,79	0
3	M1N	Z	273	32/32	0.88	0.24	66,76,78,78	0

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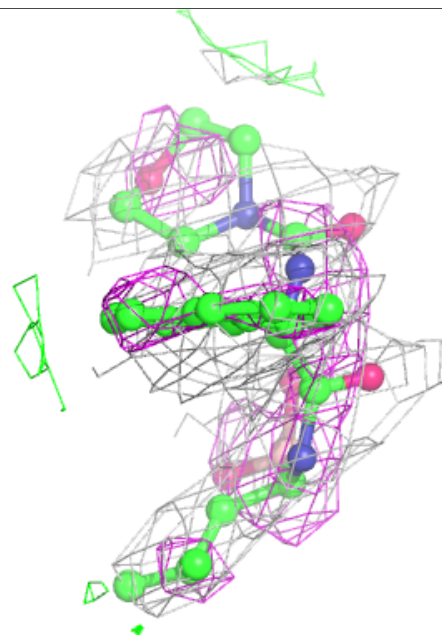
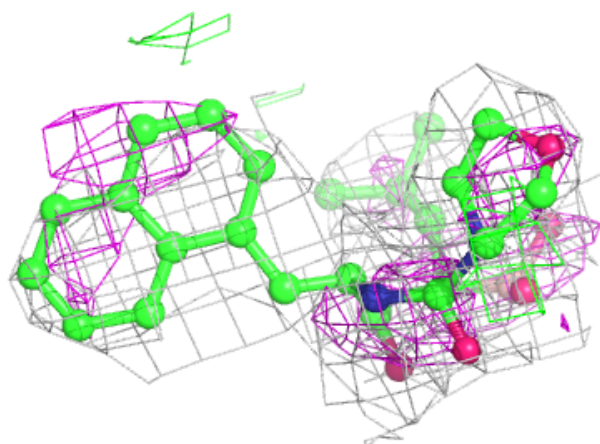
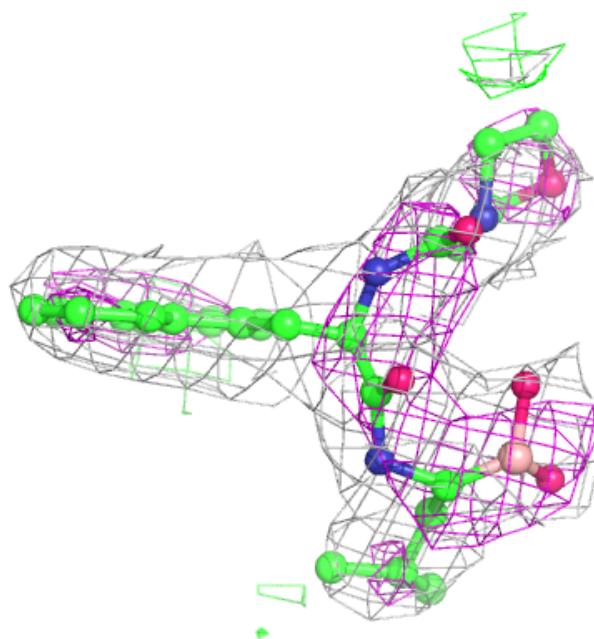
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	M1N	G	273	32/32	0.89	0.21	64,75,77,78	0
3	M1N	C	273	32/32	0.89	0.24	63,75,77,78	0
3	M1N	E	273	32/32	0.89	0.26	63,76,78,78	0
3	M1N	R	273	32/32	0.90	0.24	64,76,78,78	0
3	M1N	N	273	32/32	0.91	0.24	65,76,77,78	0
3	M1N	H	273	32/32	0.91	0.25	64,75,77,78	0
3	M1N	L	273	32/32	0.91	0.24	65,75,77,78	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.

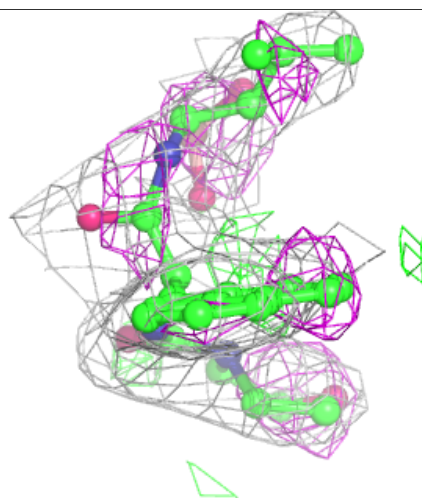
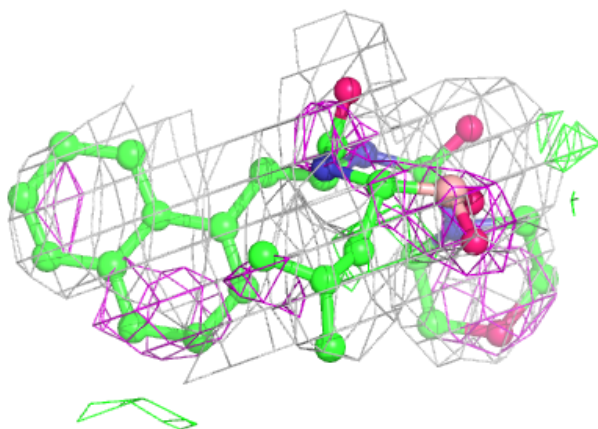
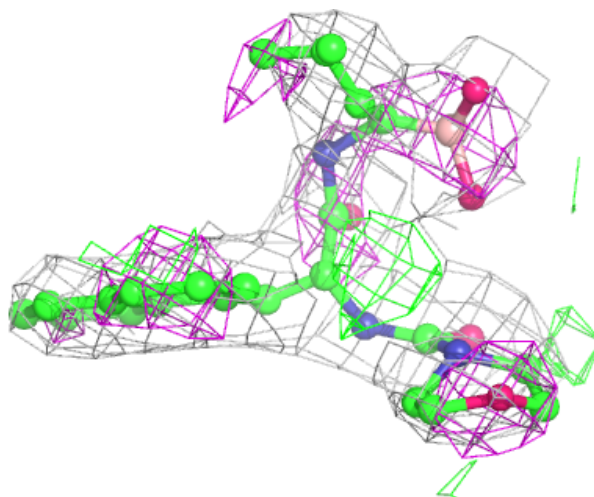
Electron density around M1N 2 273:

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



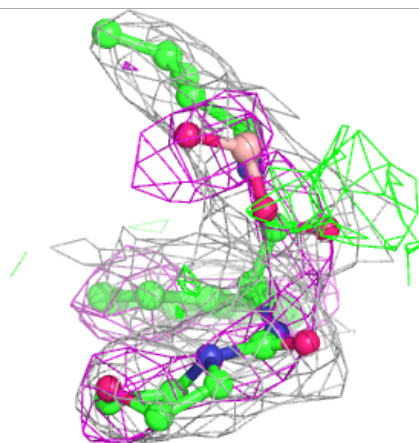
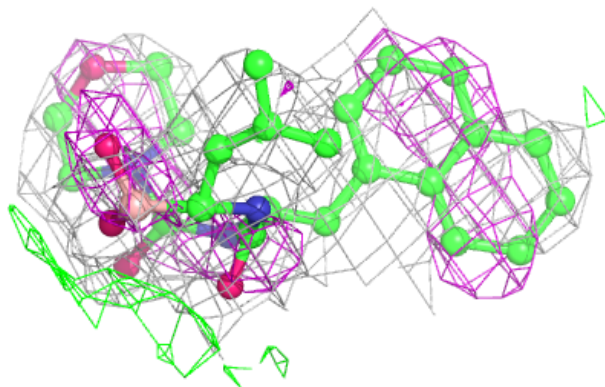
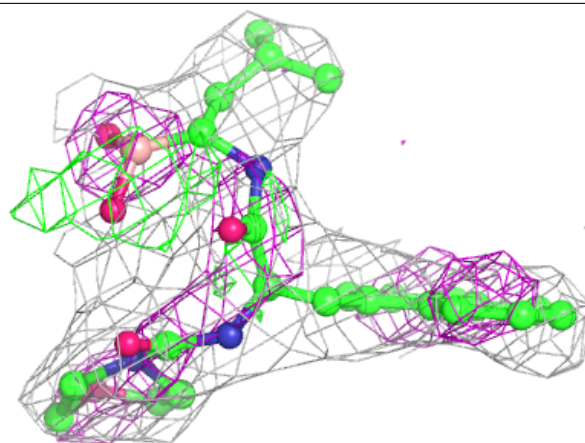
Electron density around M1N V 273:

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



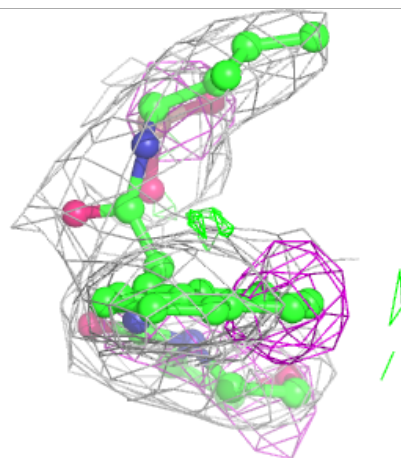
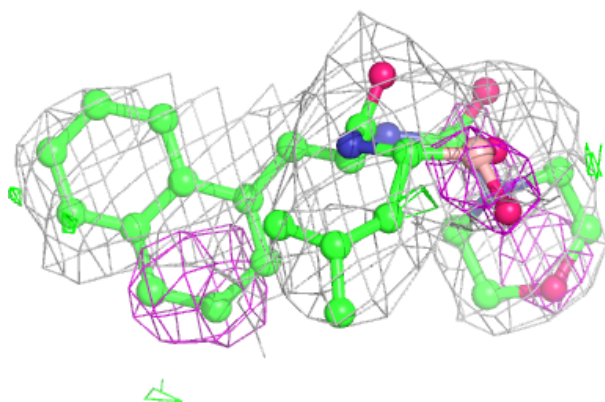
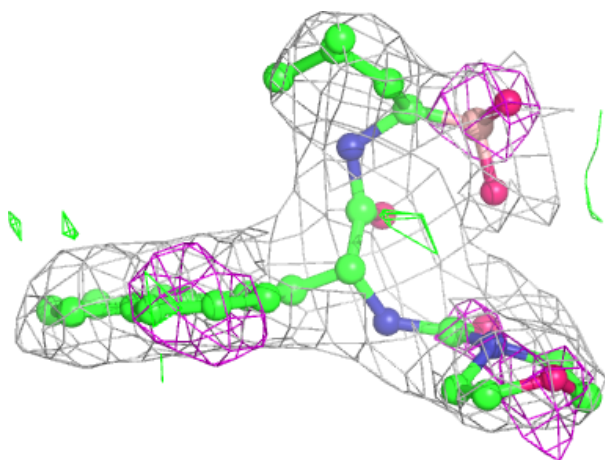
Electron density around M1N T 273:

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



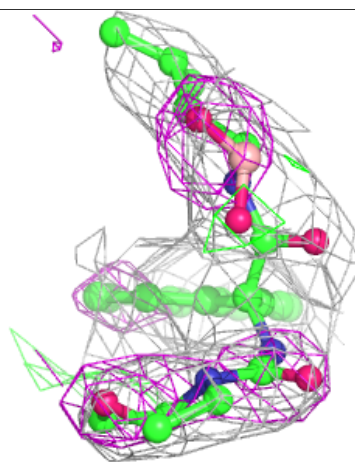
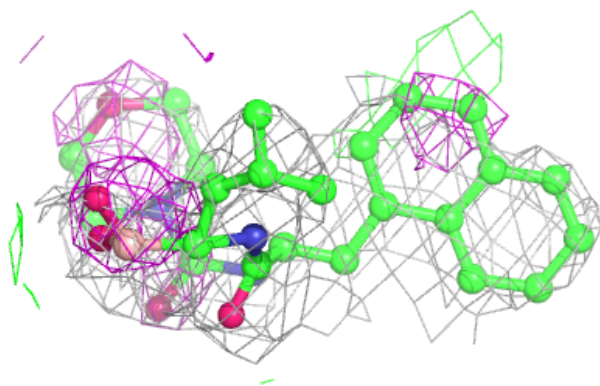
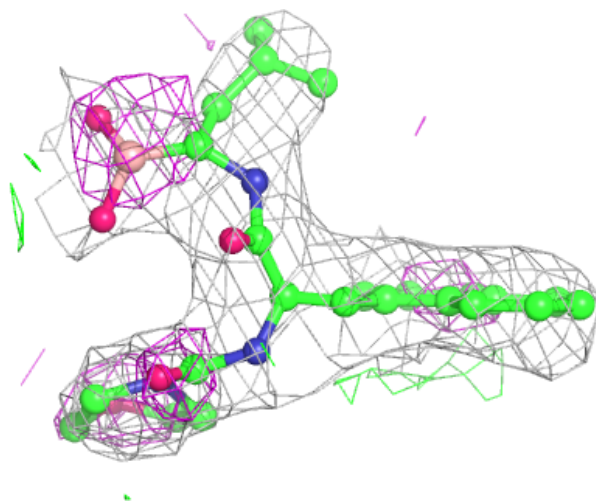
Electron density around M1N P 273:

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



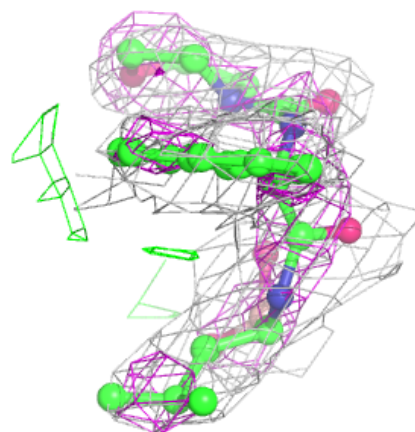
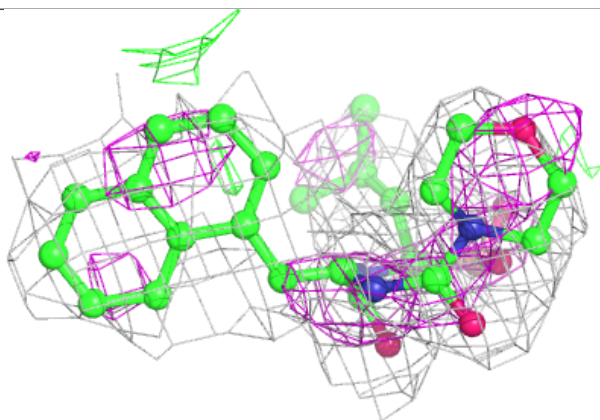
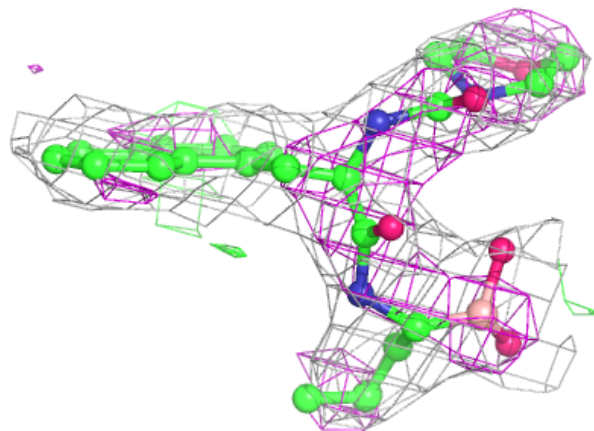
Electron density around M1N J 273:

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



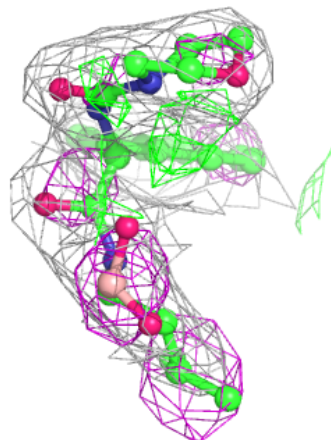
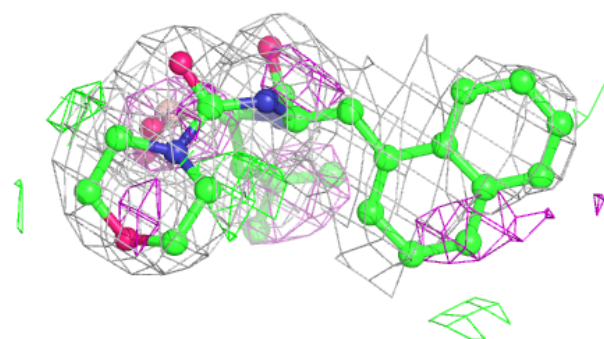
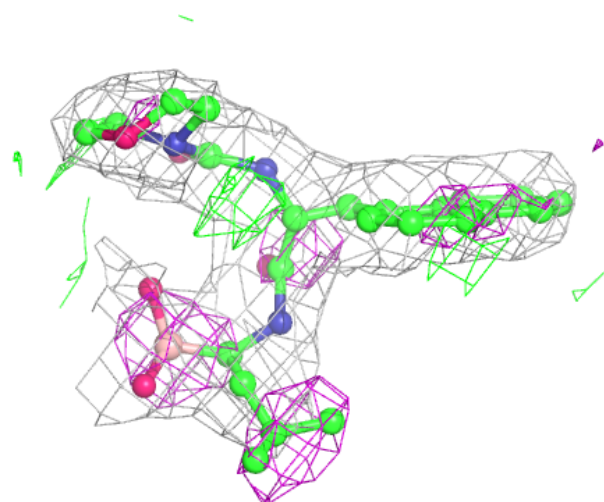
Electron density around M1N X 273:

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



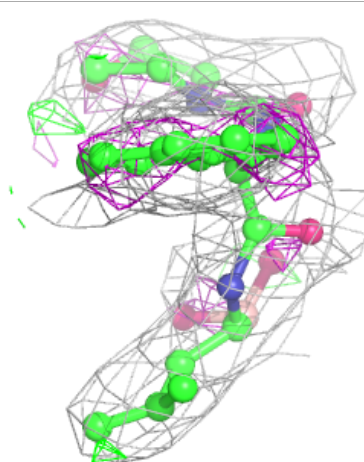
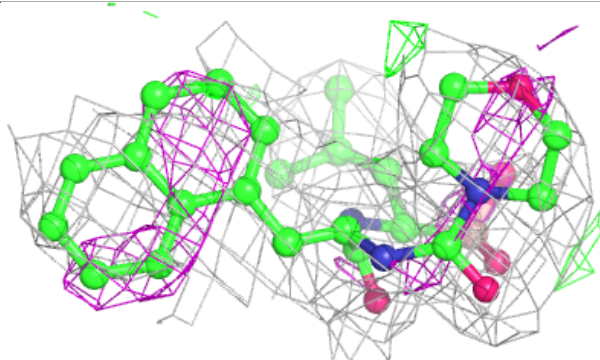
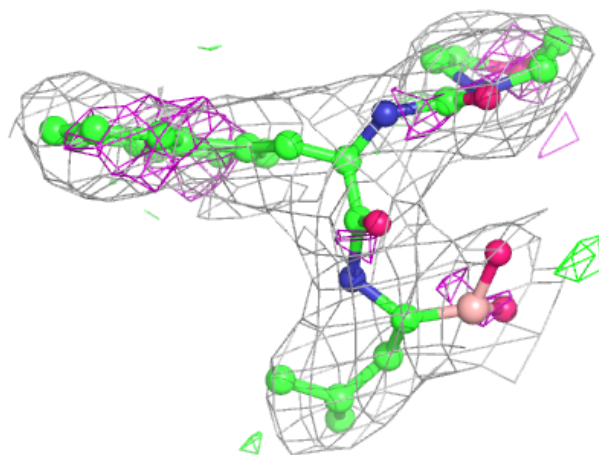
Electron density around M1N Z 273:

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



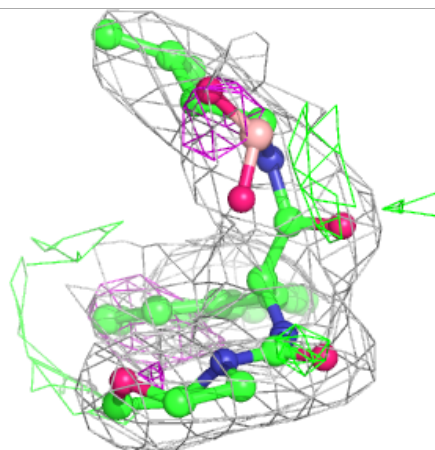
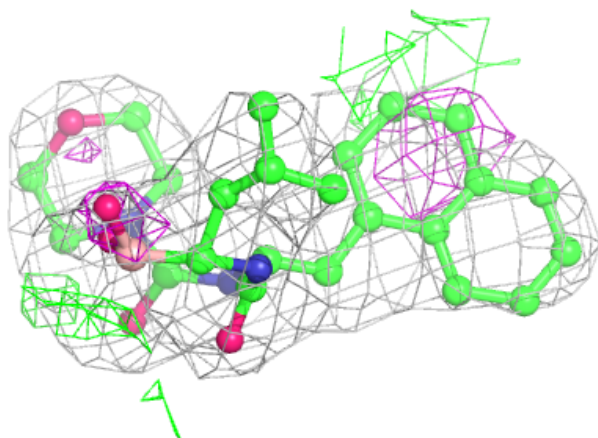
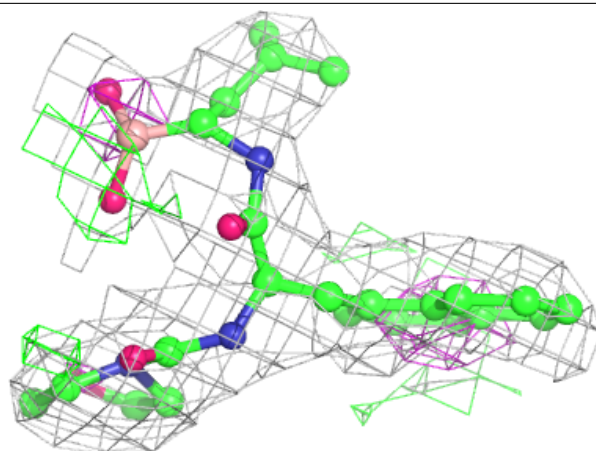
Electron density around M1N G 273:

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



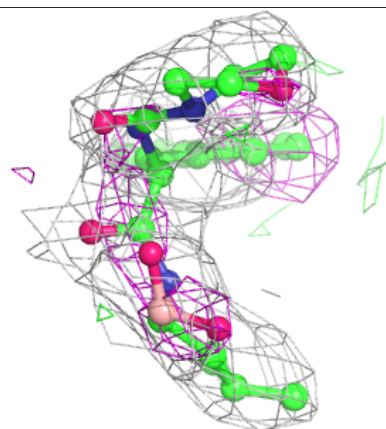
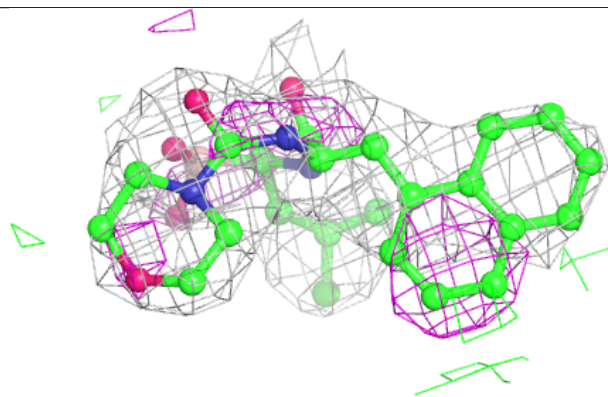
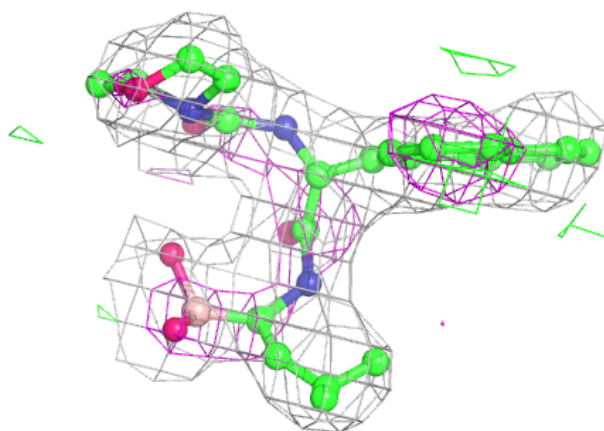
Electron density around M1N C 273:

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



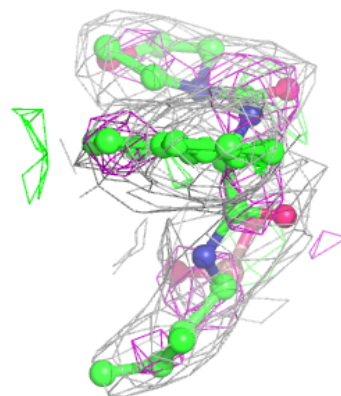
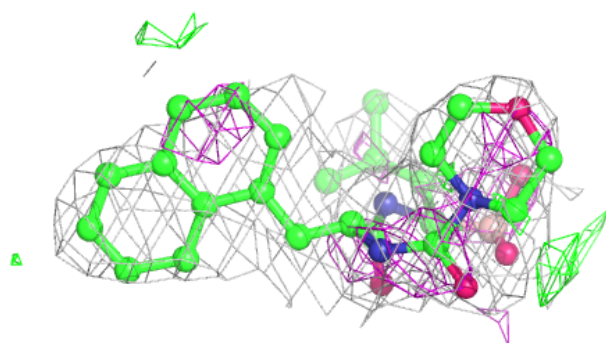
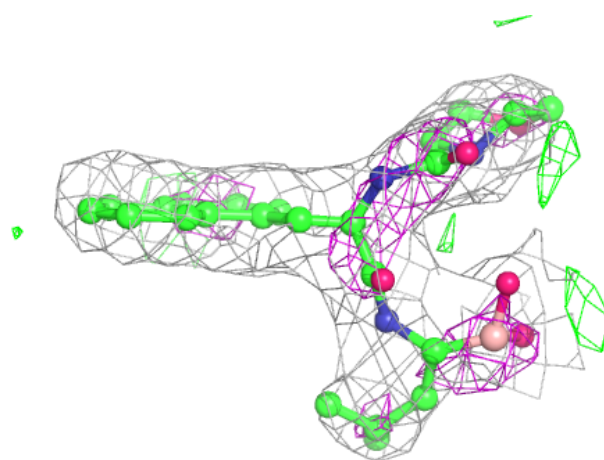
Electron density around M1N E 273:

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



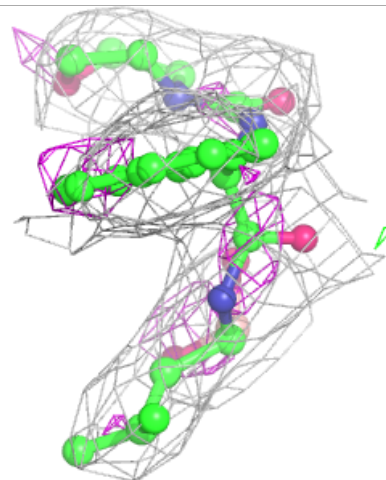
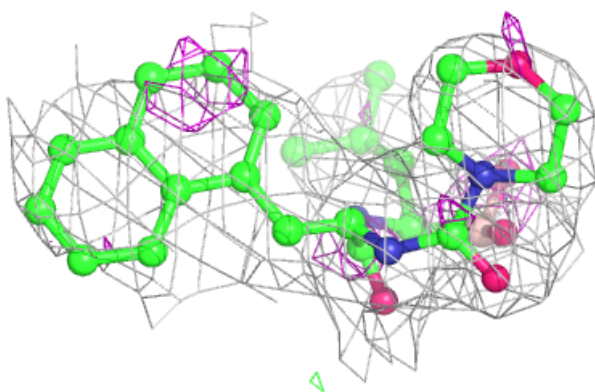
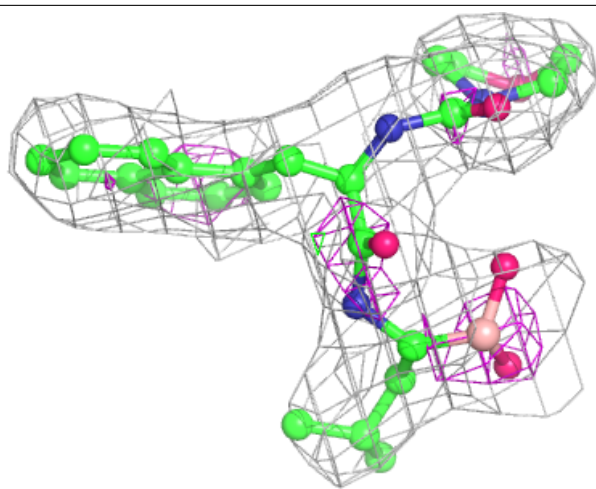
Electron density around M1N R 273:

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



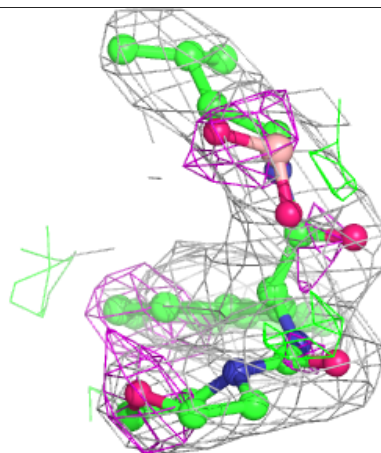
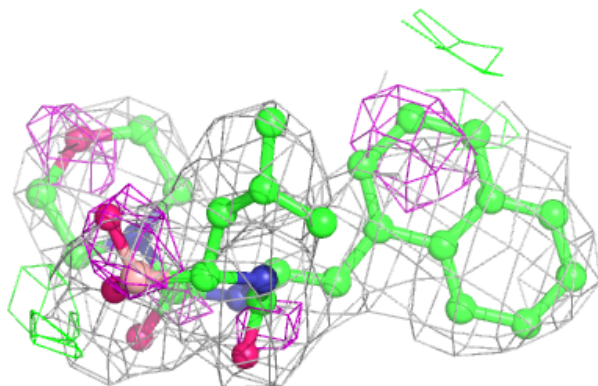
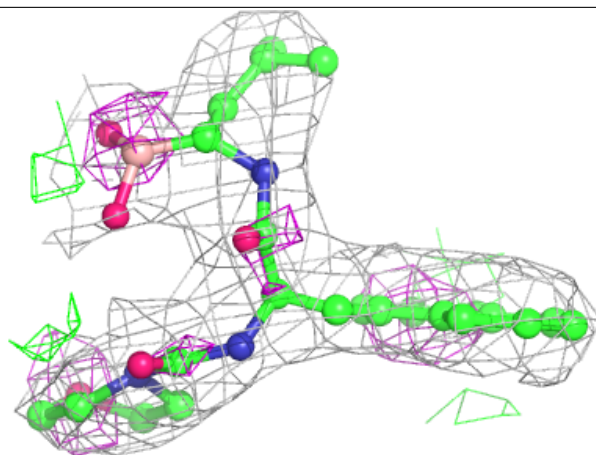
Electron density around M1N N 273:

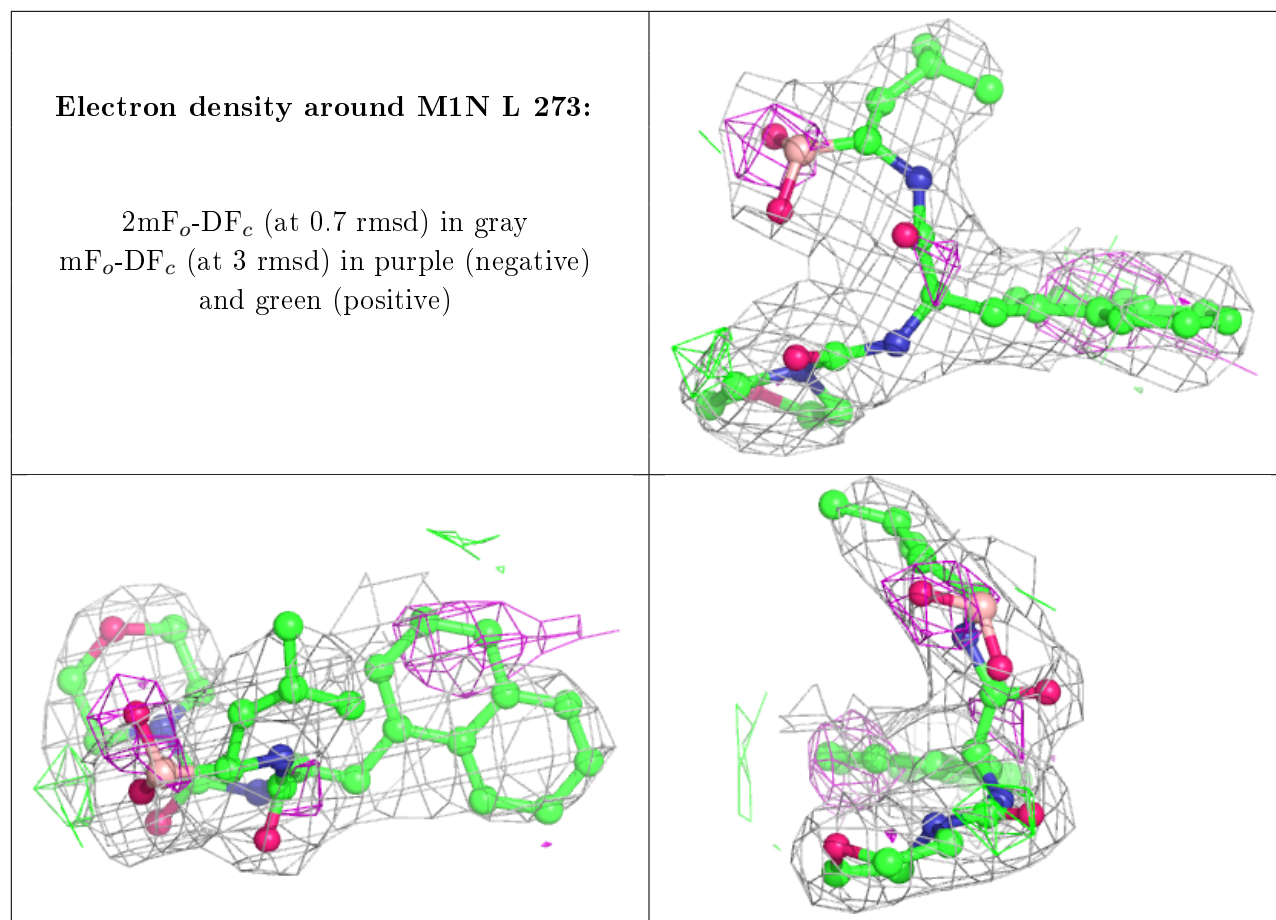
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around M1N 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.