



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 02:07 PM EDT

PDB ID : 2OIP  
Title : Crystal Structure of the S290G Active Site Mutant of TS-DHFR from *Cryptosporidium hominis*  
Authors : Martucci, W.E.; Vargo, M.A.  
Deposited on : 2007-01-11  
Resolution : 2.80 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](mailto: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.

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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	:	2.23.2
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)	:	2.23.2

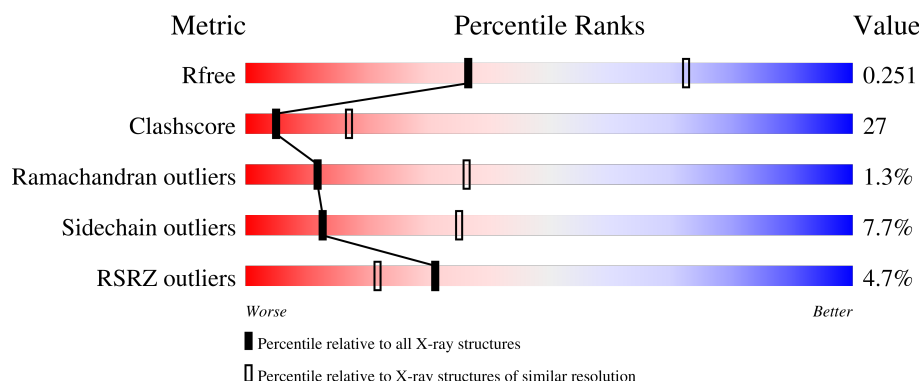
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	519	<div> <div>3%</div> <div>61%</div> <div>34%</div> <div>• •</div> </div>
1	B	519	<div> <div>2%</div> <div>65%</div> <div>29%</div> <div>5%</div> <div>•</div> </div>
1	C	519	<div> <div>5%</div> <div>53%</div> <div>39%</div> <div>6%</div> <div>•</div> </div>
1	D	519	<div> <div>2%</div> <div>55%</div> <div>38%</div> <div>6%</div> <div>•</div> </div>
1	E	519	<div> <div>12%</div> <div>44%</div> <div>50%</div> <div>5%</div> <div>•</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UMP	E	619	-	-	X	-
3	CB3	C	612	X	-	X	-
3	CB3	E	620	X	-	X	X
4	MTX	E	621	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21931 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.

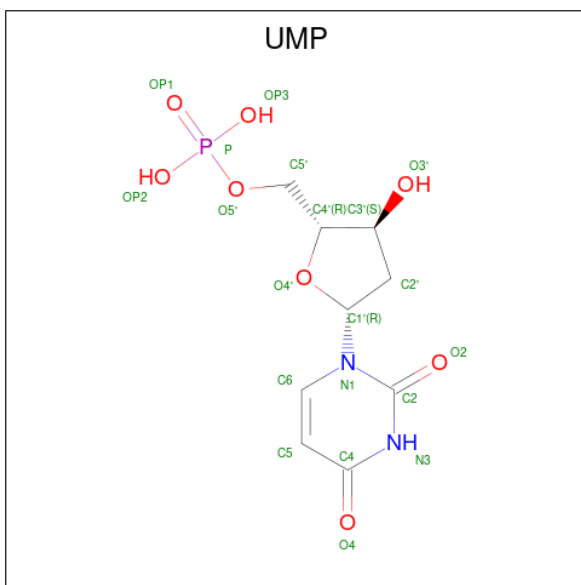
- Molecule 1 is a protein called Chain A, crystal structure of Dhfr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4182	2669	706	784	23			
1	B	516	Total	C	N	O	S	0	0	0
			4189	2674	707	786	22			
1	C	514	Total	C	N	O	S	0	0	0
			4164	2660	703	779	22			
1	D	515	Total	C	N	O	S	0	0	0
			4167	2662	702	781	22			
1	E	511	Total	C	N	O	S	0	0	0
			4145	2648	697	778	22			

There are 5 discrepancies between the modelled and reference sequences:

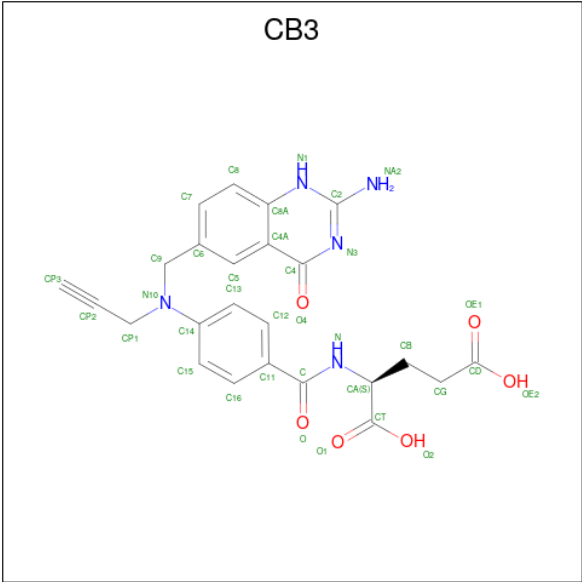
Chain	Residue	Modelled	Actual	Comment	Reference
A	290	GLY	SER	engineered mutation	UNP Q5CGA3
B	290	GLY	SER	engineered mutation	UNP Q5CGA3
C	290	GLY	SER	engineered mutation	UNP Q5CGA3
D	290	GLY	SER	engineered mutation	UNP Q5CGA3
E	290	GLY	SER	engineered mutation	UNP Q5CGA3

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: C<sub>9</sub>H<sub>13</sub>N<sub>2</sub>O<sub>8</sub>P).



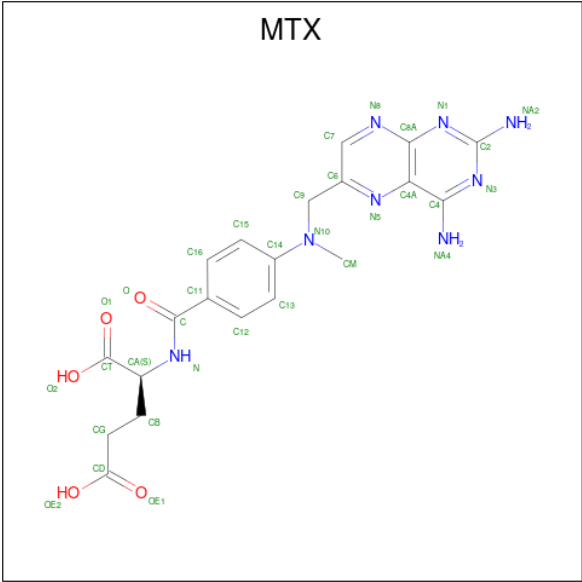
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: C<sub>24</sub>H<sub>23</sub>N<sub>5</sub>O<sub>6</sub>).



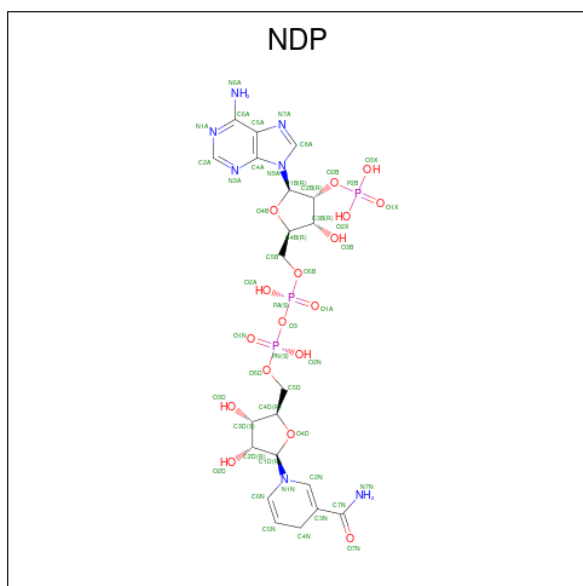
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		
3	D	1	Total	C	N	O	0	0
			35	24	5	6		
3	E	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is METHOTREXATE (three-letter code: MTX) (formula: C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 33	C 20	N 8	O 5	0	0
4	B	1	Total 33	C 20	N 8	O 5	0	0
4	C	1	Total 33	C 20	N 8	O 5	0	0
4	D	1	Total 33	C 20	N 8	O 5	0	0
4	E	1	Total 33	C 20	N 8	O 5	0	0

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	E	1	Total 48	C 21	N 7	O 17	P 3	0	0

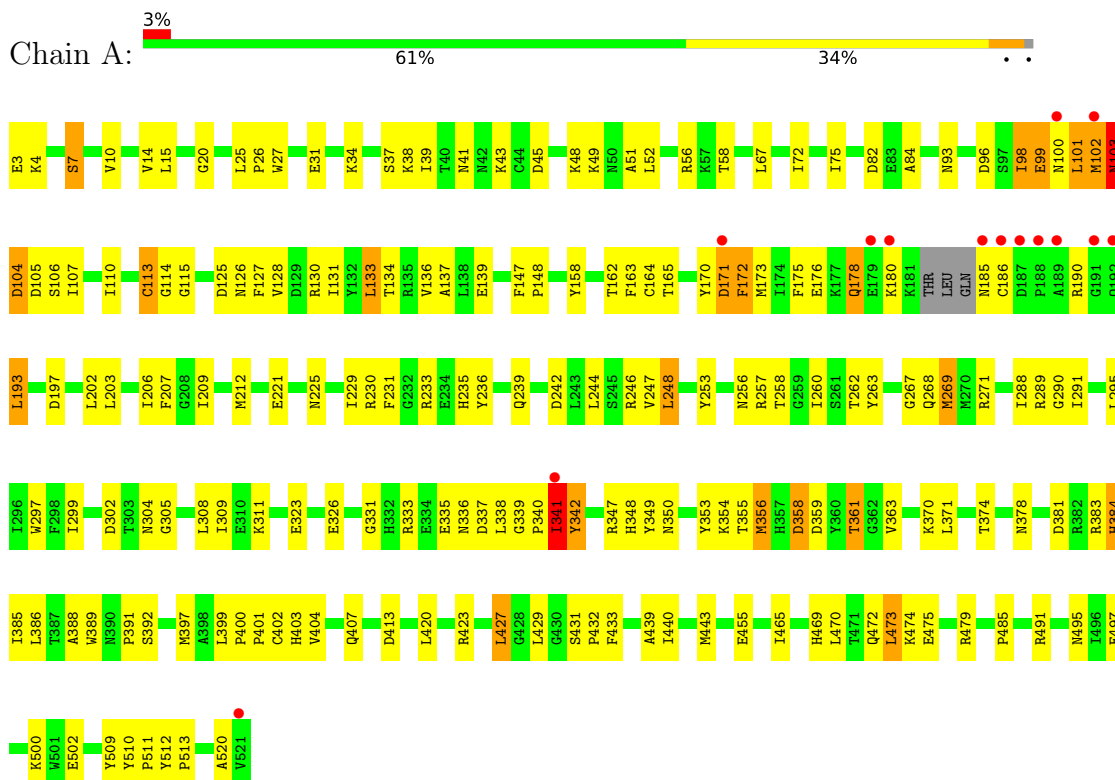
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	113	Total 113	O 113	0	0
6	B	143	Total 143	O 143	0	0
6	C	68	Total 68	O 68	0	0
6	D	61	Total 61	O 61	0	0
6	E	19	Total 19	O 19	0	0

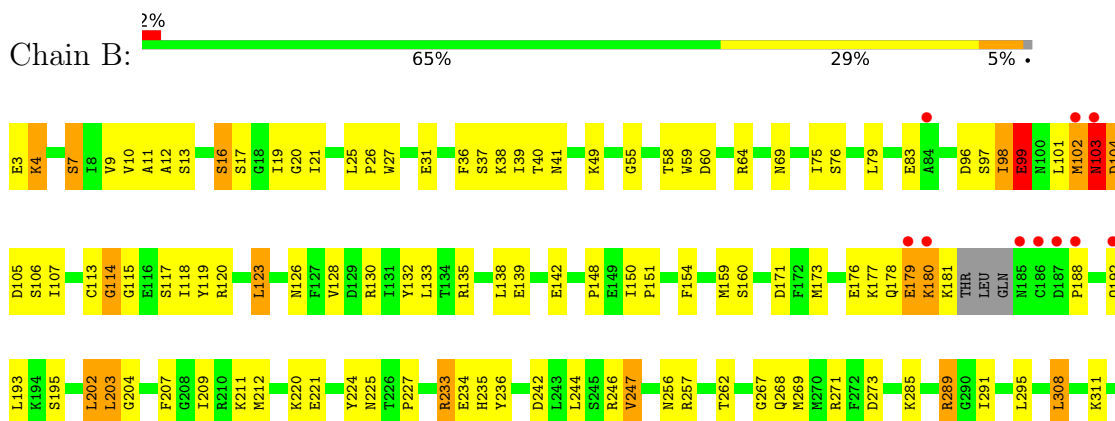
### 3 Residue-property plots

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

#### • Molecule 1: Chain A, crystal structure of Dhfr



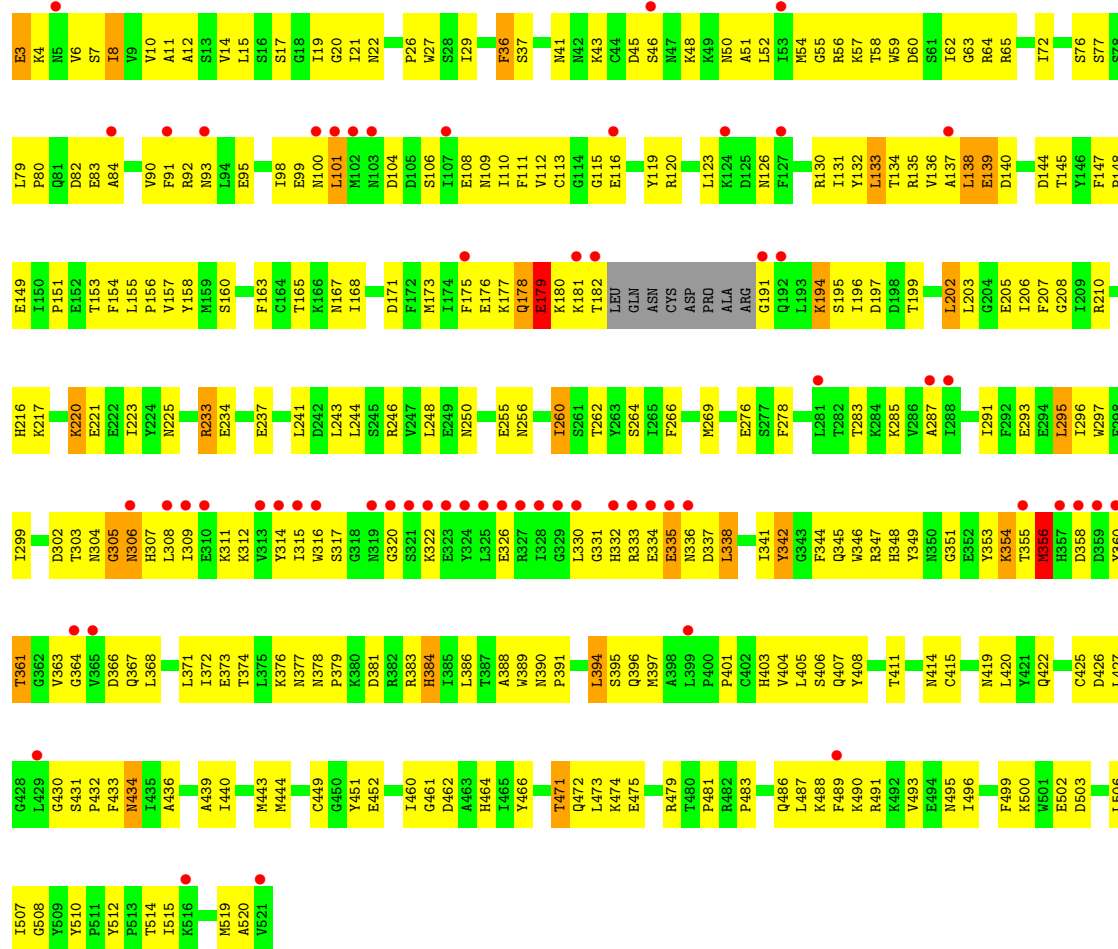
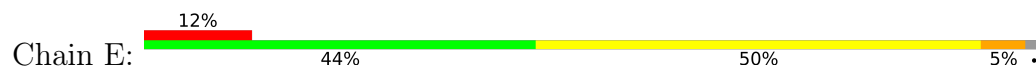
#### • Molecule 1: Chain A, crystal structure of Dhfr







• Molecule 1: Chain A, crystal structure of Dhfr



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	215.03Å 116.20Å 216.60Å 90.00° 94.27° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.80) 99.3 (49.74-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.20 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.222 , 0.259 0.215 , 0.251	Depositor DCC
$R_{free}$ test set	6550 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.9	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 63.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21931	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UMP, MTX, NDP, CB3

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.40	0/4278	0.66	0/5782
1	B	0.43	0/4285	0.68	2/5790 (0.0%)
1	C	0.37	0/4260	0.61	0/5758
1	D	0.36	0/4263	0.62	0/5763
1	E	0.35	0/4240	0.63	0/5730
All	All	0.38	0/21326	0.64	2/28823 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	6
1	D	0	3
1	E	0	5
All	All	0	23

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	B	104	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	CYS	Peptide
1	A	114	GLY	Peptide
1	A	171	ASP	Peptide
1	A	340	PRO	Peptide
1	A	341	ILE	Peptide
1	B	102	MET	Peptide
1	B	113	CYS	Peptide
1	B	114	GLY	Peptide
1	B	99	GLU	Peptide
1	C	104	ASP	Peptide
1	C	112	VAL	Peptide
1	C	113	CYS	Peptide
1	C	136	VAL	Peptide
1	C	254	ARG	Sidechain
1	C	403	HIS	Peptide
1	D	113	CYS	Peptide
1	D	403	HIS	Peptide
1	D	99	GLU	Peptide
1	E	179	GLU	Peptide
1	E	180	LYS	Peptide
1	E	305	GLY	Peptide
1	E	351	GLY	Peptide
1	E	356	MET	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4182	0	4100	201	0
1	B	4189	0	4112	159	0
1	C	4164	0	4085	266	0
1	D	4167	0	4082	226	0
1	E	4145	0	4064	291	1
2	A	20	0	11	3	0
2	B	20	0	11	2	0
2	C	20	0	11	5	0
2	D	20	0	11	5	0
2	E	20	0	11	8	0
3	A	35	0	21	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	35	0	21	7	0
3	C	35	0	20	9	0
3	D	35	0	21	4	0
3	E	35	0	21	17	0
4	A	33	0	19	6	0
4	B	33	0	19	8	0
4	C	33	0	20	6	0
4	D	33	0	20	7	0
4	E	33	0	20	10	0
5	A	48	0	26	5	0
5	B	48	0	26	8	0
5	C	48	0	26	12	0
5	D	48	0	26	7	0
5	E	48	0	26	12	0
6	A	113	0	0	12	0
6	B	143	0	0	6	0
6	C	68	0	0	9	0
6	D	61	0	0	9	0
6	E	19	0	0	3	0
All	All	21931	0	20830	1148	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 27.

All (1148) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ASN:CA	1:C:103:ASN:HB2	1.03	1.50
1:C:100:ASN:HA	1:C:103:ASN:CB	0.91	1.36
1:A:43:LYS:HE3	1:A:48:LYS:O	1.36	1.23
1:C:100:ASN:C	1:C:103:ASN:HB2	1.64	1.16
1:C:99:GLU:CD	1:C:103:ASN:HD21	1.49	1.16
1:A:4:LYS:HG2	1:A:101:LEU:HD23	1.15	1.15
1:C:100:ASN:HA	1:C:103:ASN:CG	1.67	1.12
1:C:96:ASP:O	1:C:99:GLU:HG2	1.47	1.12
1:C:99:GLU:C	1:C:103:ASN:HD22	1.52	1.11
1:B:411:THR:HG22	1:B:413:ASP:H	1.07	1.08
1:A:341:ILE:HA	1:A:397:MET:CE	1.82	1.08
1:C:104:ASP:OD2	1:C:106:SER:N	1.88	1.05
1:A:186:CYS:HA	1:A:230:ARG:HD2	1.40	1.03
1:A:258:THR:HG22	1:A:260:ILE:H	1.20	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:ASP:HB2	1:E:356:MET:SD	1.99	1.01
1:B:4:LYS:HB3	1:B:101:LEU:CD2	1.90	1.01
1:A:341:ILE:HA	1:A:397:MET:HE2	1.02	0.99
1:D:102:MET:HE3	1:D:102:MET:HA	1.40	0.99
1:B:103:ASN:ND2	1:B:104:ASP:H	1.59	0.99
1:E:100:ASN:O	1:E:104:ASP:HB3	1.63	0.98
1:C:100:ASN:HA	1:C:103:ASN:HB3	1.43	0.98
1:E:426:ASP:HB2	2:E:619:UMP:H2''	1.44	0.98
1:C:99:GLU:C	1:C:103:ASN:ND2	2.16	0.97
1:C:391:PRO:HD2	1:D:349:TYR:CE2	1.98	0.96
1:D:56:ARG:HB2	1:D:76:SER:OG	1.65	0.96
1:C:335:GLU:O	1:C:336:ASN:HB2	1.63	0.96
1:A:4:LYS:HG2	1:A:101:LEU:CD2	1.95	0.95
1:E:8:ILE:HG12	1:E:112:VAL:HB	1.49	0.94
1:C:100:ASN:CA	1:C:103:ASN:CB	1.85	0.94
1:A:4:LYS:H	1:A:101:LEU:HD22	1.32	0.94
1:C:138:LEU:H	1:C:138:LEU:CD2	1.79	0.94
1:D:4:LYS:HE2	1:D:101:LEU:HA	1.50	0.94
1:E:191:GLY:HA2	1:E:197:ASP:OD2	1.69	0.92
1:A:304:ASN:HA	1:A:356:MET:HE3	1.49	0.92
1:B:179:GLU:O	1:B:180:LYS:HG3	1.71	0.91
3:D:616:CB3:O	3:D:616:CB3:HB1	1.68	0.91
1:D:102:MET:HA	1:D:102:MET:CE	1.97	0.91
1:C:137:ALA:O	1:C:510:TYR:HE2	1.53	0.90
2:E:619:UMP:H1'	3:E:620:CB3:C2	2.02	0.89
1:D:96:ASP:O	1:D:99:GLU:HG2	1.73	0.89
1:A:341:ILE:CA	1:A:397:MET:HE2	1.98	0.89
1:A:4:LYS:H	1:A:101:LEU:CD2	1.85	0.88
1:D:337:ASP:HA	1:D:356:MET:HE3	1.55	0.88
1:B:180:LYS:HD3	1:B:181:LYS:N	1.88	0.88
1:B:209:ILE:HD12	1:B:209:ILE:H	1.34	0.88
1:D:54:MET:HA	1:D:114:GLY:HA2	1.55	0.88
1:D:399:LEU:HD12	1:D:400:PRO:HD2	1.56	0.88
1:C:190:ARG:HB3	1:C:190:ARG:HH11	1.39	0.88
1:B:103:ASN:CG	1:B:104:ASP:H	1.76	0.88
4:E:621:MTX:HG1	4:E:621:MTX:O1	1.74	0.87
1:A:271:ARG:NH2	1:B:267:GLY:O	2.09	0.86
1:E:304:ASN:CG	1:E:356:MET:HE2	1.95	0.86
1:D:220:LYS:HD3	1:D:249:GLU:OE1	1.75	0.86
1:A:104:ASP:HB3	1:A:107:ILE:HG12	1.56	0.85
1:A:326:GLU:HA	6:A:609:HOH:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:SER:HB2	4:E:621:MTX:HG2	1.58	0.85
1:E:196:ILE:HG22	1:E:197:ASP:N	1.93	0.84
1:D:75:ILE:O	5:D:618:NDP:H1B	1.77	0.84
1:E:304:ASN:HA	1:E:356:MET:HE3	1.59	0.84
1:A:333:ARG:HG2	1:A:337:ASP:HB3	1.58	0.84
1:E:336:ASN:O	1:E:338:LEU:HD23	1.78	0.83
1:D:82:ASP:OD1	1:D:84:ALA:HB3	1.77	0.83
1:C:99:GLU:CD	1:C:103:ASN:ND2	2.31	0.83
1:E:79:LEU:HD23	1:E:80:PRO:HD2	1.59	0.83
3:D:616:CB3:CP2	3:D:616:CB3:H13	2.09	0.82
1:B:411:THR:HG22	1:B:413:ASP:N	1.93	0.82
1:B:4:LYS:HB3	1:B:101:LEU:HD22	1.60	0.81
1:B:411:THR:CG2	1:B:413:ASP:HB2	2.10	0.81
1:C:319:ASN:ND2	3:C:612:CB3:H8	1.94	0.81
1:C:102:MET:O	1:C:103:ASN:O	1.97	0.81
1:C:360:TYR:O	1:C:363:VAL:HG12	1.81	0.81
1:E:334:GLU:HG3	1:E:335:GLU:H	1.44	0.81
1:A:103:ASN:HD22	1:A:103:ASN:C	1.84	0.81
1:C:100:ASN:N	1:C:103:ASN:ND2	2.28	0.80
1:E:338:LEU:HD23	1:E:338:LEU:N	1.97	0.80
4:D:617:MTX:HG2	4:D:617:MTX:O1	1.79	0.80
1:A:349:TYR:CE2	1:B:391:PRO:HD2	2.16	0.80
1:E:151:PRO:HG2	1:E:154:PHE:HD2	1.47	0.80
2:E:619:UMP:H2'	2:E:619:UMP:O2	1.80	0.80
1:E:302:ASP:OD2	1:E:307:HIS:CD2	2.35	0.80
1:E:422:GLN:HG2	1:E:425:CYS:HB2	1.63	0.80
1:E:207:PHE:HB3	1:E:210:ARG:HB2	1.63	0.80
1:C:62:ILE:HD13	1:C:62:ILE:O	1.81	0.80
1:C:190:ARG:HB3	1:C:190:ARG:NH1	1.96	0.80
1:B:103:ASN:ND2	1:B:104:ASP:N	2.29	0.79
2:E:619:UMP:H1'	3:E:620:CB3:N3	1.96	0.79
1:C:158:TYR:HB3	1:C:174:ILE:HG23	1.64	0.79
1:C:349:TYR:CE2	1:D:391:PRO:HD2	2.17	0.79
1:E:306:ASN:O	1:E:309:ILE:HB	1.83	0.79
1:D:4:LYS:CB	1:D:101:LEU:HD23	2.12	0.78
4:E:621:MTX:O1	4:E:621:MTX:CG	2.30	0.78
1:B:285:LYS:HB3	1:B:514:THR:HG22	1.65	0.78
1:C:138:LEU:H	1:C:138:LEU:HD22	1.48	0.78
1:D:25:LEU:HD11	4:D:617:MTX:H7	1.64	0.78
1:C:151:PRO:HG2	1:C:154:PHE:HD2	1.49	0.78
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:THR:HG21	1:B:413:ASP:HB2	1.66	0.78
1:C:123:LEU:HD12	1:C:128:VAL:HG11	1.66	0.78
1:E:196:ILE:O	1:E:197:ASP:HB2	1.84	0.78
1:E:378:ASN:ND2	1:E:381:ASP:HB2	1.99	0.78
1:A:14:VAL:HG23	1:A:136:VAL:O	1.83	0.77
1:A:38:LYS:HB3	1:B:202:LEU:HG	1.66	0.77
1:C:55:GLY:HA3	5:C:614:NDP:O2A	1.84	0.77
1:A:258:THR:HG21	1:A:520:ALA:HB1	1.66	0.77
3:B:608:CB3:HG2	3:B:608:CB3:O1	1.85	0.77
1:D:82:ASP:OD1	1:D:84:ALA:CB	2.32	0.77
1:E:314:TYR:HB3	1:E:317:SER:HB2	1.67	0.77
1:C:79:LEU:HD23	1:C:80:PRO:HD2	1.65	0.77
1:A:163:PHE:HB2	1:A:170:TYR:CE2	2.19	0.76
1:E:58:THR:CG2	4:E:621:MTX:HM2	2.15	0.76
1:A:43:LYS:CE	1:A:48:LYS:O	2.26	0.76
1:A:103:ASN:C	1:A:103:ASN:ND2	2.37	0.76
1:C:26:PRO:HB2	1:C:27:TRP:CE3	2.21	0.76
1:C:171:ASP:OD2	1:C:483:PRO:HG3	1.86	0.76
1:E:196:ILE:CG2	1:E:197:ASP:N	2.49	0.75
1:B:103:ASN:O	1:B:104:ASP:C	2.24	0.75
1:C:79:LEU:HD23	1:C:80:PRO:CD	2.16	0.75
1:E:391:PRO:O	1:E:394:LEU:HD11	1.87	0.75
1:C:138:LEU:H	1:C:138:LEU:HD23	1.52	0.75
1:A:82:ASP:OD2	1:A:84:ALA:HB3	1.86	0.75
1:D:304:ASN:HA	1:D:356:MET:HE2	1.67	0.74
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.68	0.74
2:D:615:UMP:H5	6:D:667:HOH:O	1.69	0.74
1:C:19:ILE:O	5:C:614:NDP:H2N	1.87	0.74
1:E:243:LEU:HA	1:E:246:ARG:NH1	2.03	0.74
1:A:258:THR:CG2	1:A:520:ALA:HB1	2.18	0.74
1:D:342:TYR:CE1	1:D:403:HIS:CE1	2.76	0.74
1:E:264:SER:HB3	1:E:464:HIS:HB3	1.67	0.74
1:E:56:ARG:HD3	5:E:622:NDP:O1X	1.88	0.73
1:E:304:ASN:HA	1:E:356:MET:CE	2.18	0.73
1:A:258:THR:HG22	1:A:260:ILE:N	2.01	0.73
1:C:209:ILE:HD13	1:C:209:ILE:H	1.53	0.73
1:A:374:THR:HG22	1:A:384:HIS:CE1	2.23	0.73
1:A:102:MET:O	1:A:103:ASN:HB3	1.86	0.73
1:C:4:LYS:H	1:C:101:LEU:HD22	1.54	0.73
1:E:76:SER:HA	5:E:622:NDP:O2X	1.89	0.73
1:C:333:ARG:HG2	1:C:333:ARG:HH11	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:ARG:HH21	1:E:57:LYS:HG2	1.53	0.73
1:E:302:ASP:OD2	1:E:307:HIS:HD2	1.72	0.73
1:B:225:ASN:O	1:B:233:ARG:NH2	2.22	0.73
1:D:100:ASN:HB2	1:D:110:ILE:HD11	1.69	0.73
1:E:153:THR:O	1:E:177:LYS:HD2	1.88	0.73
1:D:135:ARG:NH2	1:D:482:ARG:HA	2.04	0.72
1:C:138:LEU:CD2	1:C:138:LEU:N	2.50	0.72
1:D:289:ARG:HG3	1:D:501:TRP:CE2	2.24	0.72
1:E:342:TYR:O	1:E:345:GLN:HB2	1.88	0.72
1:C:135:ARG:NH2	1:C:482:ARG:HA	2.04	0.72
1:E:337:ASP:HB2	1:E:356:MET:CG	2.19	0.72
1:D:26:PRO:HB2	1:D:27:TRP:CE3	2.23	0.72
1:D:62:ILE:HD11	4:D:617:MTX:C14	2.20	0.72
1:E:79:LEU:HD23	1:E:80:PRO:CD	2.19	0.72
1:D:137:ALA:O	1:D:510:TYR:HE2	1.73	0.71
1:C:225:ASN:O	1:C:233:ARG:NH2	2.22	0.71
1:C:419:ASN:ND2	1:C:457:ALA:HB3	2.05	0.71
1:E:115:GLY:HA3	5:E:622:NDP:O1A	1.91	0.71
1:B:102:MET:O	1:B:103:ASN:HB3	1.91	0.71
1:C:254:ARG:NH2	1:D:410:VAL:O	2.23	0.71
1:E:336:ASN:O	1:E:338:LEU:CD2	2.38	0.71
1:A:500:LYS:HE3	6:A:714:HOH:O	1.90	0.71
1:D:337:ASP:CA	1:D:356:MET:HE3	2.20	0.71
1:D:224:TYR:O	1:D:227:PRO:HG3	1.90	0.70
1:A:172:PHE:CD1	1:A:172:PHE:N	2.59	0.70
1:D:514:THR:HG22	6:D:622:HOH:O	1.91	0.70
1:D:126:ASN:CG	1:D:177:LYS:HZ1	1.93	0.70
3:D:616:CB3:O	3:D:616:CB3:CB	2.38	0.70
1:A:102:MET:O	1:A:103:ASN:CB	2.38	0.70
1:C:52:LEU:HD11	1:C:70:ARG:HD2	1.71	0.70
1:E:337:ASP:HB2	1:E:356:MET:HG2	1.74	0.70
1:E:363:VAL:HG13	1:E:364:GLY:H	1.54	0.70
1:D:257:ARG:HH11	2:D:615:UMP:P	2.15	0.70
1:E:179:GLU:HG2	6:E:635:HOH:O	1.92	0.70
1:A:374:THR:HG22	1:A:384:HIS:HE1	1.56	0.69
1:E:430:GLY:HA2	3:E:620:CB3:CP3	2.22	0.69
4:D:617:MTX:O1	4:D:617:MTX:CG	2.40	0.69
1:E:283:THR:O	1:E:512:TYR:HB2	1.93	0.69
1:E:374:THR:HG22	1:E:384:HIS:CE1	2.26	0.69
4:B:609:MTX:O1	4:B:609:MTX:CG	2.39	0.69
1:C:114:GLY:HA2	1:C:119:TYR:CZ	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:GLY:HA2	3:E:620:CB3:HP3	1.75	0.69
1:D:225:ASN:O	1:D:233:ARG:NH2	2.24	0.69
1:E:296:ILE:HD12	1:E:297:TRP:N	2.07	0.69
1:B:360:TYR:O	1:B:363:VAL:HG13	1.92	0.68
1:D:97:SER:O	1:D:99:GLU:HG3	1.93	0.68
1:B:103:ASN:CG	1:B:104:ASP:N	2.46	0.68
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.73	0.68
1:D:255:GLU:CD	1:D:255:GLU:H	1.96	0.68
1:A:7:SER:HB3	1:A:130:ARG:HB3	1.75	0.68
1:E:507:ILE:HD12	1:E:507:ILE:N	2.08	0.68
1:A:289:ARG:NH2	1:A:311:LYS:O	2.27	0.68
1:C:226:THR:O	1:C:226:THR:HG22	1.93	0.68
1:A:130:ARG:NH1	1:A:176:GLU:OE2	2.27	0.68
1:D:130:ARG:HG3	1:D:176:GLU:OE1	1.94	0.68
1:C:335:GLU:O	1:C:336:ASN:CB	2.42	0.67
1:B:209:ILE:H	1:B:209:ILE:CD1	2.07	0.67
1:C:104:ASP:CG	1:C:106:SER:H	1.98	0.67
1:E:256:ASN:HD21	1:E:262:THR:HG23	1.60	0.67
1:D:257:ARG:NH1	2:D:615:UMP:O5'	2.28	0.67
1:D:490:LYS:HD2	1:D:502:GLU:O	1.94	0.67
1:E:135:ARG:HD3	1:E:171:ASP:HB2	1.75	0.67
1:E:439:ALA:O	1:E:443:MET:HG3	1.94	0.67
5:E:622:NDP:O2X	5:E:622:NDP:H1B	1.95	0.67
1:A:48:LYS:HB3	1:A:106:SER:O	1.95	0.67
1:A:399:LEU:HD12	1:A:400:PRO:HD2	1.76	0.67
1:D:94:LEU:O	1:D:98:ILE:HG12	1.94	0.67
1:E:363:VAL:HG13	1:E:364:GLY:N	2.09	0.67
1:E:56:ARG:O	1:E:59:TRP:HB3	1.95	0.66
1:E:160:SER:HA	1:E:234:GLU:HB3	1.77	0.66
1:E:135:ARG:CD	1:E:171:ASP:HB2	2.24	0.66
1:C:156:PRO:O	1:C:228:SER:HB2	1.95	0.66
1:C:160:SER:HA	1:C:234:GLU:HB3	1.77	0.66
1:C:319:ASN:HD21	3:C:612:CB3:H8	1.58	0.66
1:B:470:LEU:O	1:B:474:LYS:HG2	1.96	0.66
3:B:608:CB3:C6	3:B:608:CB3:H15	2.24	0.66
1:C:100:ASN:CA	1:C:103:ASN:CG	2.44	0.66
1:D:467:GLU:HA	1:D:470:LEU:CD2	2.26	0.66
1:E:391:PRO:HA	1:E:394:LEU:HD21	1.76	0.66
1:E:394:LEU:HD12	1:E:395:SER:H	1.61	0.66
1:A:56:ARG:NH1	5:A:606:NDP:O2X	2.29	0.66
1:C:285:LYS:HB3	1:C:514:THR:CG2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:612:CB3:O	3:C:612:CB3:CB	2.42	0.66
1:E:20:GLY:HA2	1:E:26:PRO:HD3	1.77	0.66
1:B:209:ILE:HD12	1:B:209:ILE:N	2.10	0.66
1:C:10:VAL:HG22	1:C:11:ALA:N	2.11	0.66
1:C:389:TRP:HE3	1:C:401:PRO:HG2	1.60	0.66
1:C:51:ALA:C	1:C:52:LEU:HD23	2.16	0.66
1:D:98:ILE:O	1:D:99:GLU:HB3	1.97	0.65
1:E:194:LYS:HD3	1:E:195:SER:H	1.60	0.65
1:E:260:ILE:HD13	1:E:466:TYR:HD1	1.62	0.65
1:C:37:SER:O	1:C:41:ASN:HB2	1.97	0.65
1:D:360:TYR:O	1:D:363:VAL:HG12	1.97	0.65
1:B:20:GLY:HA2	1:B:26:PRO:HD3	1.79	0.65
1:B:247:VAL:HG22	1:B:465:ILE:HD12	1.79	0.65
1:C:99:GLU:CG	1:C:103:ASN:HD21	2.09	0.65
2:C:611:UMP:OP1	1:D:383:ARG:NH1	2.26	0.65
1:D:155:LEU:HB2	1:D:178:GLN:NE2	2.12	0.65
1:C:54:MET:HE3	1:C:72:ILE:HD13	1.78	0.64
1:E:374:THR:HG22	1:E:384:HIS:HE1	1.60	0.64
1:A:162:THR:HA	1:A:171:ASP:OD1	1.96	0.64
1:D:4:LYS:HB3	1:D:101:LEU:HD23	1.79	0.64
1:E:55:GLY:HA3	5:E:622:NDP:O1A	1.97	0.64
1:E:444:MET:HG2	1:E:489:PHE:CZ	2.32	0.64
1:E:479:ARG:HG2	1:E:512:TYR:CD2	2.32	0.64
1:A:190:ARG:NH1	1:A:190:ARG:HB3	2.13	0.64
1:A:58:THR:CG2	4:A:605:MTX:HM2	2.28	0.64
3:E:620:CB3:C5	3:E:620:CB3:C15	2.76	0.64
1:A:348:HIS:HB3	1:A:363:VAL:O	1.98	0.64
1:D:20:GLY:HA2	1:D:26:PRO:HD3	1.80	0.64
1:E:79:LEU:CD2	1:E:80:PRO:HD2	2.27	0.64
3:E:620:CB3:C14	3:E:620:CB3:H5	2.27	0.64
1:A:4:LYS:HE3	1:A:101:LEU:HA	1.80	0.64
1:B:180:LYS:HD3	1:B:181:LYS:CB	2.27	0.64
1:D:123:LEU:HD12	1:D:128:VAL:HG11	1.78	0.64
1:C:38:LYS:HB3	1:D:202:LEU:HG	1.80	0.64
1:C:105:ASP:N	1:C:105:ASP:OD1	2.30	0.64
1:E:330:LEU:O	1:E:332:HIS:N	2.30	0.64
3:B:608:CB3:C6	3:B:608:CB3:C15	2.74	0.64
1:E:334:GLU:HG3	1:E:335:GLU:N	2.13	0.64
1:C:206:ILE:HD11	1:D:35:PHE:HA	1.80	0.63
1:D:248:LEU:HD13	1:D:465:ILE:HD12	1.79	0.63
1:D:342:TYR:CZ	1:D:403:HIS:NE2	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:GLU:HG3	6:E:631:HOH:O	1.98	0.63
1:E:167:ASN:HD21	1:E:488:LYS:HG3	1.63	0.63
1:A:99:GLU:O	1:A:103:ASN:ND2	2.31	0.63
1:C:104:ASP:OD2	1:C:106:SER:HB3	1.98	0.63
1:C:285:LYS:HB3	1:C:514:THR:HG22	1.81	0.63
1:C:389:TRP:CE3	1:C:401:PRO:HG2	2.33	0.63
1:E:260:ILE:HD12	1:E:260:ILE:H	1.63	0.63
1:D:65:ARG:HD3	6:D:643:HOH:O	1.99	0.63
1:B:479:ARG:HG2	1:B:512:TYR:CD2	2.33	0.63
1:C:82:ASP:OD2	1:C:84:ALA:HB2	1.98	0.63
1:D:123:LEU:HD12	1:D:128:VAL:CG1	2.29	0.63
1:E:225:ASN:ND2	1:E:241:LEU:HD13	2.12	0.63
1:E:426:ASP:HB2	2:E:619:UMP:C2'	2.26	0.63
1:A:133:LEU:C	1:A:133:LEU:HD22	2.19	0.63
1:A:288:ILE:HD11	1:A:440:ILE:HD11	1.80	0.63
1:D:467:GLU:HA	1:D:470:LEU:HD23	1.79	0.63
1:E:14:VAL:HG23	1:E:15:LEU:HG	1.79	0.63
1:E:295:LEU:O	1:E:299:ILE:HG12	1.99	0.63
1:E:519:MET:HG2	1:E:520:ALA:N	2.13	0.63
1:C:19:ILE:HB	5:C:614:NDP:N7N	2.14	0.62
1:C:99:GLU:O	1:C:103:ASN:N	2.25	0.62
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.79	0.62
1:D:293:GLU:HA	1:D:296:ILE:HD11	1.81	0.62
1:A:212:MET:SD	1:B:273:ASP:HB2	2.39	0.62
1:C:104:ASP:HB3	1:C:107:ILE:HG13	1.81	0.62
1:E:431:SER:HB3	1:E:432:PRO:HD3	1.81	0.62
1:B:64:ARG:NH2	1:B:79:LEU:HD21	2.14	0.62
1:C:4:LYS:NZ	1:C:100:ASN:O	2.33	0.62
1:E:217:LYS:HZ1	1:E:220:LYS:HE3	1.65	0.62
1:E:344:PHE:O	1:E:348:HIS:O	2.17	0.62
1:D:56:ARG:CB	1:D:76:SER:OG	2.45	0.61
1:E:305:GLY:HA3	1:E:336:ASN:O	1.99	0.61
1:E:338:LEU:N	1:E:338:LEU:CD2	2.62	0.61
1:B:257:ARG:HD3	2:B:607:UMP:OP2	2.00	0.61
1:B:25:LEU:HD11	4:B:609:MTX:H7	1.83	0.61
1:B:58:THR:CG2	4:B:609:MTX:HM2	2.30	0.61
1:C:35:PHE:HA	1:D:206:ILE:HD11	1.82	0.61
1:C:74:VAL:O	1:C:75:ILE:HD12	2.00	0.61
1:B:180:LYS:CD	1:B:181:LYS:N	2.62	0.61
1:B:335:GLU:O	1:B:336:ASN:HB2	1.99	0.61
1:B:413:ASP:O	1:B:414:ASN:CB	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ARG:HG2	1:C:333:ARG:NH1	2.15	0.61
1:C:342:TYR:CZ	1:C:403:HIS:NE2	2.68	0.61
1:D:260:ILE:HD12	1:D:260:ILE:N	2.15	0.61
1:A:341:ILE:CA	1:A:397:MET:CE	2.69	0.61
1:A:4:LYS:N	1:A:101:LEU:HD22	2.11	0.61
4:B:609:MTX:O1	4:B:609:MTX:HG2	2.00	0.61
1:B:178:GLN:HB2	6:B:742:HOH:O	2.00	0.61
1:B:224:TYR:O	1:B:227:PRO:HD3	2.01	0.61
1:B:342:TYR:CZ	1:B:403:HIS:NE2	2.69	0.61
1:C:334:GLU:O	1:C:336:ASN:N	2.34	0.61
1:E:433:PHE:CZ	3:E:620:CB3:H12	2.36	0.61
1:B:378:ASN:ND2	1:B:381:ASP:HB2	2.16	0.60
1:E:333:ARG:HH22	1:E:396:GLN:HB3	1.66	0.60
1:C:13:SER:HB2	1:C:139:GLU:OE1	2.01	0.60
1:C:19:ILE:HB	5:C:614:NDP:H71N	1.65	0.60
1:C:269:MET:HE2	1:D:269:MET:CE	2.31	0.60
1:E:14:VAL:HG13	1:E:136:VAL:O	2.00	0.60
1:A:52:LEU:HB3	1:A:113:CYS:SG	2.41	0.60
1:B:160:SER:HA	1:B:234:GLU:HB3	1.84	0.60
1:C:133:LEU:HD22	1:C:134:THR:N	2.17	0.60
3:C:612:CB3:HG2	3:C:612:CB3:O1	2.00	0.60
1:D:114:GLY:HA3	1:D:118:ILE:HB	1.84	0.60
1:A:495:ASN:OD1	1:A:497:GLU:HG3	2.01	0.60
1:E:260:ILE:HD13	1:E:466:TYR:CD1	2.37	0.60
1:D:133:LEU:HD13	1:D:135:ARG:HG3	1.84	0.60
1:D:247:VAL:HG21	1:D:465:ILE:HG13	1.83	0.60
1:E:191:GLY:HA2	1:E:197:ASP:CG	2.22	0.60
2:E:619:UMP:O2	2:E:619:UMP:C2'	2.50	0.60
1:C:100:ASN:N	1:C:100:ASN:OD1	2.30	0.60
1:D:296:ILE:HD12	1:D:297:TRP:N	2.17	0.60
1:E:157:VAL:HG11	1:E:176:GLU:HG3	1.82	0.60
2:A:603:UMP:P	1:B:383:ARG:HH11	2.25	0.59
1:A:101:LEU:O	1:A:103:ASN:N	2.35	0.59
2:A:603:UMP:P	1:B:383:ARG:NH1	2.74	0.59
1:B:104:ASP:OD2	1:B:106:SER:OG	2.20	0.59
1:C:137:ALA:O	1:C:510:TYR:CE2	2.44	0.59
1:D:58:THR:HG23	4:D:617:MTX:HM2	1.83	0.59
1:A:225:ASN:O	1:A:233:ARG:NH2	2.36	0.59
1:C:4:LYS:H	1:C:101:LEU:CD2	2.14	0.59
1:B:99:GLU:O	1:B:103:ASN:ND2	2.35	0.59
1:D:262:THR:HG23	1:D:464:HIS:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:LEU:HD11	1:E:168:ILE:HD13	1.85	0.59
1:A:4:LYS:CG	1:A:101:LEU:HD23	2.10	0.59
3:B:608:CB3:C14	3:B:608:CB3:C5	2.76	0.59
1:D:292:PHE:CD1	1:D:504:ILE:HD11	2.37	0.59
1:E:52:LEU:HB3	1:E:113:CYS:SG	2.42	0.59
1:A:304:ASN:CA	1:A:356:MET:HE3	2.29	0.59
1:C:291:ILE:HG12	1:C:433:PHE:CD2	2.37	0.59
1:E:305:GLY:H	1:E:356:MET:HE3	1.67	0.59
1:E:386:LEU:HB3	1:E:406:SER:HB2	1.83	0.59
1:C:138:LEU:HD13	1:C:168:ILE:HD13	1.85	0.59
1:E:126:ASN:HD22	1:E:177:LYS:NZ	2.00	0.59
1:C:75:ILE:O	5:C:614:NDP:H1B	2.02	0.59
1:C:439:ALA:O	1:C:443:MET:HG3	2.02	0.59
1:E:217:LYS:NZ	1:E:220:LYS:HE3	2.16	0.59
1:C:208:GLY:C	1:C:210:ARG:H	2.06	0.59
1:E:264:SER:CB	1:E:464:HIS:HB3	2.32	0.59
1:A:341:ILE:O	1:A:397:MET:HE3	2.03	0.58
1:D:7:SER:HB3	1:D:130:ARG:HB3	1.83	0.58
1:E:225:ASN:O	1:E:233:ARG:NH2	2.29	0.58
1:D:342:TYR:CD1	1:D:403:HIS:CE1	2.90	0.58
1:D:439:ALA:O	1:D:443:MET:HG3	2.04	0.58
1:E:394:LEU:HD12	1:E:395:SER:N	2.17	0.58
1:B:7:SER:HB3	1:B:130:ARG:HB3	1.84	0.58
1:E:303:THR:HG21	1:E:344:PHE:HB2	1.85	0.58
1:C:403:HIS:HD2	2:C:611:UMP:O4	1.87	0.58
1:E:116:GLU:HB2	1:E:145:THR:HG23	1.85	0.58
1:E:126:ASN:HD22	1:E:177:LYS:HZ2	1.50	0.58
1:E:123:LEU:HD12	1:E:151:PRO:HG3	1.85	0.58
1:E:430:GLY:CA	3:E:620:CB3:HP3	2.33	0.58
1:A:10:VAL:HG13	1:A:133:LEU:HD23	1.85	0.58
1:D:147:PHE:CD2	1:D:148:PRO:HD2	2.38	0.58
1:C:104:ASP:OD2	1:C:106:SER:CB	2.52	0.58
1:A:193:LEU:HD23	6:A:607:HOH:O	2.02	0.57
1:C:15:LEU:HB2	1:C:139:GLU:HG2	1.86	0.57
1:C:37:SER:HB2	4:C:613:MTX:HG2	1.86	0.57
3:E:620:CB3:C6	3:E:620:CB3:H15	2.33	0.57
1:C:360:TYR:HB3	1:C:363:VAL:CG1	2.34	0.57
1:E:151:PRO:HG2	1:E:154:PHE:CD2	2.33	0.57
1:A:75:ILE:O	5:A:606:NDP:H1B	2.04	0.57
1:C:136:VAL:HG12	1:C:138:LEU:HD22	1.87	0.57
1:E:4:LYS:HG2	1:E:101:LEU:CD2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:HH12	1:A:242:ASP:CG	2.07	0.57
1:C:342:TYR:CE1	1:C:403:HIS:CE1	2.92	0.57
1:E:56:ARG:NH2	1:E:57:LYS:HG2	2.19	0.57
2:E:619:UMP:C1'	3:E:620:CB3:C2	2.79	0.57
4:A:605:MTX:HG2	4:A:605:MTX:O1	2.04	0.57
1:C:495:ASN:HB2	1:C:498:ASP:OD1	2.05	0.57
1:D:257:ARG:NH1	2:D:615:UMP:P	2.77	0.57
1:E:341:ILE:HA	1:E:397:MET:CE	2.35	0.57
6:C:649:HOH:O	1:D:262:THR:HG21	2.04	0.57
1:D:247:VAL:HG12	1:D:265:ILE:HG12	1.87	0.57
1:A:178:GLN:HE21	1:A:178:GLN:N	2.02	0.56
1:B:21:ILE:HD13	1:B:142:GLU:HB3	1.86	0.56
1:B:211:LYS:HE3	6:B:699:HOH:O	2.05	0.56
1:C:74:VAL:C	1:C:75:ILE:HD12	2.26	0.56
1:D:194:LYS:HE3	1:D:198:ASP:OD1	2.03	0.56
1:E:440:ILE:HG12	1:E:487:LEU:CD2	2.35	0.56
1:A:342:TYR:CE2	1:A:403:HIS:CE1	2.94	0.56
1:D:226:THR:HG22	1:D:226:THR:O	2.05	0.56
1:D:244:LEU:CD1	1:D:427:LEU:HB3	2.34	0.56
1:D:495:ASN:HB2	6:D:670:HOH:O	2.06	0.56
1:E:58:THR:HG23	4:E:621:MTX:HM2	1.86	0.56
1:E:179:GLU:N	1:E:179:GLU:OE1	2.37	0.56
1:E:360:TYR:O	1:E:363:VAL:HG12	2.05	0.56
1:B:37:SER:O	1:B:41:ASN:HB2	2.05	0.56
1:B:411:THR:HG22	1:B:413:ASP:HB2	1.86	0.56
1:D:103:ASN:O	1:D:104:ASP:C	2.44	0.56
1:E:297:TRP:CD2	1:E:308:LEU:HD21	2.41	0.56
1:B:99:GLU:CA	1:B:99:GLU:OE1	2.53	0.56
1:C:114:GLY:HA2	1:C:119:TYR:CE1	2.40	0.56
1:A:331:GLY:N	6:A:609:HOH:O	2.38	0.56
1:E:444:MET:HG2	1:E:489:PHE:HZ	1.70	0.56
1:C:350:ASN:HA	6:C:642:HOH:O	2.06	0.56
1:D:82:ASP:OD2	1:D:82:ASP:C	2.43	0.56
1:E:19:ILE:HB	5:E:622:NDP:N7N	2.21	0.56
1:E:283:THR:HA	1:E:512:TYR:HD1	1.70	0.56
1:B:289:ARG:NH2	1:B:311:LYS:O	2.39	0.56
1:B:423:ARG:HG3	1:B:424:SER:N	2.19	0.56
1:C:90:VAL:HG12	1:C:91:PHE:N	2.21	0.56
1:C:104:ASP:OD1	1:C:106:SER:OG	2.20	0.56
4:D:617:MTX:N5	5:D:618:NDP:H42N	2.21	0.56
1:E:138:LEU:CD1	1:E:168:ILE:HD13	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:621:MTX:N5	5:E:622:NDP:H42N	2.21	0.56
1:C:26:PRO:HB2	1:C:27:TRP:HE3	1.70	0.55
1:C:135:ARG:HH21	1:C:482:ARG:HA	1.70	0.55
1:D:396:GLN:HG3	6:D:644:HOH:O	2.05	0.55
1:E:391:PRO:HA	1:E:394:LEU:CD2	2.36	0.55
1:A:186:CYS:HA	1:A:230:ARG:CD	2.26	0.55
1:D:4:LYS:HB2	1:D:101:LEU:HD23	1.87	0.55
1:E:244:LEU:CD1	1:E:427:LEU:HB3	2.35	0.55
1:E:135:ARG:HD2	1:E:173:MET:HG3	1.89	0.55
1:B:58:THR:HG23	4:B:609:MTX:HM2	1.87	0.55
1:B:402:CYS:SG	2:B:607:UMP:C6	3.00	0.55
1:D:99:GLU:OE2	1:D:99:GLU:C	2.45	0.55
1:D:342:TYR:CE1	1:D:403:HIS:NE2	2.75	0.55
1:B:4:LYS:CB	1:B:101:LEU:CD2	2.76	0.55
4:B:609:MTX:N5	5:B:610:NDP:H42N	2.21	0.55
1:C:32:ASP:O	1:C:35:PHE:HB3	2.06	0.55
1:C:360:TYR:HD1	1:C:363:VAL:HG11	1.71	0.55
1:E:120:ARG:HG2	1:E:120:ARG:HH11	1.72	0.55
1:B:188:PRO:O	1:B:192:GLN:NE2	2.40	0.55
1:B:502:GLU:H	1:B:502:GLU:CD	2.10	0.55
1:C:12:ALA:HB1	1:C:17:SER:HA	1.89	0.55
1:C:133:LEU:HD11	1:C:135:ARG:HG3	1.89	0.55
1:D:104:ASP:C	1:D:106:SER:H	2.08	0.55
1:E:337:ASP:CB	1:E:356:MET:SD	2.85	0.55
1:C:409:TYR:HH	1:D:264:SER:HG	1.53	0.55
1:B:411:THR:HG22	1:B:412:ASN:N	2.20	0.55
1:C:138:LEU:HD23	1:C:138:LEU:N	2.18	0.55
4:C:613:MTX:O1	4:C:613:MTX:HG1	2.07	0.55
1:B:76:SER:OG	5:B:610:NDP:O3X	2.22	0.55
1:E:179:GLU:N	1:E:179:GLU:CD	2.60	0.55
1:E:304:ASN:ND2	1:E:356:MET:HE2	2.22	0.55
1:A:341:ILE:HG13	1:A:342:TYR:O	2.07	0.55
3:B:608:CB3:C15	3:B:608:CB3:C5	2.85	0.55
1:C:99:GLU:CG	1:C:103:ASN:ND2	2.70	0.55
1:E:304:ASN:OD1	1:E:306:ASN:HB2	2.07	0.55
1:A:99:GLU:C	1:A:99:GLU:OE1	2.45	0.54
1:C:81:GLN:HB2	1:C:92:ARG:HH21	1.72	0.54
1:D:171:ASP:HB2	1:D:483:PRO:HG3	1.88	0.54
1:E:43:LYS:NZ	1:E:46:SER:HA	2.22	0.54
1:B:334:GLU:OE2	1:B:357:HIS:NE2	2.32	0.54
1:E:119:TYR:HB3	1:E:148:PRO:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:ARG:HD3	1:E:368:LEU:HD23	1.89	0.54
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.42	0.54
1:C:52:LEU:HB3	1:C:113:CYS:SG	2.48	0.54
1:C:97:SER:O	1:C:100:ASN:OD1	2.25	0.54
1:A:104:ASP:O	1:A:107:ILE:N	2.21	0.54
1:A:470:LEU:O	1:A:474:LYS:HG3	2.07	0.54
1:B:413:ASP:O	1:B:414:ASN:HB2	2.07	0.54
1:E:296:ILE:HA	1:E:299:ILE:CG1	2.38	0.54
1:A:139:GLU:HB2	1:A:510:TYR:CE1	2.42	0.54
1:A:185:ASN:O	1:A:230:ARG:NH1	2.39	0.54
1:B:83:GLU:OE2	1:B:83:GLU:HA	2.06	0.54
1:D:104:ASP:OD2	1:D:106:SER:OG	2.25	0.54
1:A:335:GLU:O	1:A:336:ASN:HB2	2.08	0.54
1:E:389:TRP:CZ3	1:E:401:PRO:HD2	2.41	0.54
1:A:403:HIS:H	1:A:403:HIS:CD2	2.26	0.54
1:B:36:PHE:O	1:B:39:ILE:HG22	2.07	0.54
1:C:57:LYS:HA	1:C:60:ASP:OD2	2.07	0.54
1:C:360:TYR:HB3	1:C:363:VAL:HG12	1.88	0.54
1:D:330:LEU:O	1:D:332:HIS:N	2.41	0.54
1:A:342:TYR:CZ	1:A:403:HIS:NE2	2.76	0.54
1:C:133:LEU:CD1	1:C:135:ARG:HG3	2.38	0.54
1:D:100:ASN:HB2	1:D:110:ILE:CD1	2.36	0.54
1:D:123:LEU:CD1	1:D:128:VAL:HG11	2.38	0.54
1:E:440:ILE:HG12	1:E:487:LEU:HD21	1.89	0.54
1:C:123:LEU:CD1	1:C:128:VAL:HG11	2.35	0.54
1:E:296:ILE:HA	1:E:299:ILE:HG12	1.90	0.54
1:E:335:GLU:OE1	1:E:335:GLU:O	2.26	0.54
1:A:186:CYS:HB2	6:A:613:HOH:O	2.08	0.53
1:C:186:CYS:HA	1:C:230:ARG:HE	1.72	0.53
1:E:287:ALA:O	1:E:291:ILE:HG13	2.08	0.53
1:A:331:GLY:C	1:A:333:ARG:H	2.09	0.53
1:C:97:SER:O	1:C:99:GLU:HG3	2.08	0.53
1:C:114:GLY:CA	1:C:119:TYR:CZ	2.91	0.53
1:D:337:ASP:CG	1:D:356:MET:HG2	2.28	0.53
1:E:407:GLN:HB3	1:E:419:ASN:HB2	1.90	0.53
1:E:471:THR:HA	1:E:474:LYS:HE3	1.90	0.53
1:E:347:ARG:O	1:E:366:ASP:HA	2.09	0.53
1:A:34:LYS:O	1:A:38:LYS:HG2	2.07	0.53
1:C:490:LYS:HD3	1:C:502:GLU:O	2.09	0.53
1:E:21:ILE:HD12	1:E:144:ASP:OD2	2.08	0.53
1:E:171:ASP:OD2	1:E:483:PRO:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:ALA:O	1:C:401:PRO:HG3	2.09	0.53
1:E:354:LYS:O	1:E:355:THR:HG23	2.09	0.53
1:E:472:GLN:O	1:E:475:GLU:HB3	2.09	0.53
1:E:512:TYR:HA	6:E:639:HOH:O	2.09	0.53
1:C:400:PRO:HD2	1:D:383:ARG:NH1	2.24	0.53
1:D:470:LEU:O	1:D:474:LYS:HD3	2.09	0.53
1:A:14:VAL:HG23	1:A:137:ALA:HA	1.89	0.52
1:C:98:ILE:O	1:C:99:GLU:HB3	2.09	0.52
1:C:350:ASN:N	6:C:642:HOH:O	2.38	0.52
1:D:171:ASP:OD2	1:D:483:PRO:HG3	2.09	0.52
1:E:3:GLU:O	1:E:4:LYS:HB3	2.09	0.52
1:E:82:ASP:C	1:E:84:ALA:H	2.12	0.52
1:E:196:ILE:CG2	1:E:197:ASP:H	2.20	0.52
1:E:496:ILE:O	1:E:499:PHE:HD1	1.92	0.52
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.91	0.52
1:C:56:ARG:HB3	5:C:614:NDP:O3B	2.09	0.52
1:C:342:TYR:CD1	1:C:403:HIS:CE1	2.96	0.52
1:C:472:GLN:HB3	1:C:515:ILE:HG21	1.91	0.52
3:C:612:CB3:O1	3:C:612:CB3:CG	2.46	0.52
1:D:37:SER:O	1:D:41:ASN:HB2	2.09	0.52
1:E:304:ASN:CG	1:E:356:MET:CE	2.75	0.52
1:E:330:LEU:C	1:E:332:HIS:H	2.13	0.52
1:E:507:ILE:HD12	1:E:507:ILE:H	1.72	0.52
1:C:59:TRP:O	1:C:62:ILE:HG22	2.09	0.52
1:C:102:MET:C	1:C:103:ASN:O	2.48	0.52
1:C:209:ILE:HD13	1:C:209:ILE:N	2.24	0.52
1:E:77:SER:O	1:E:92:ARG:NH1	2.43	0.52
1:E:167:ASN:ND2	1:E:488:LYS:HG3	2.25	0.52
1:A:388:ALA:O	1:A:401:PRO:HG2	2.10	0.52
1:D:467:GLU:O	1:D:470:LEU:HD23	2.10	0.52
1:E:10:VAL:HG22	1:E:11:ALA:N	2.24	0.52
1:E:320:GLY:O	1:E:335:GLU:O	2.27	0.52
1:A:3:GLU:HA	1:A:101:LEU:HD22	1.91	0.52
1:C:99:GLU:OE2	1:C:103:ASN:ND2	2.34	0.52
1:D:102:MET:CE	1:D:102:MET:CA	2.76	0.52
1:D:201:ASP:O	1:D:205:GLU:HG3	2.09	0.52
1:D:262:THR:CG2	1:D:464:HIS:HB2	2.38	0.52
1:D:321:SER:O	1:D:325:LEU:HD13	2.09	0.52
1:A:45:ASP:OD2	1:A:48:LYS:HE3	2.10	0.52
1:A:99:GLU:CA	6:A:674:HOH:O	2.56	0.52
1:B:411:THR:HG23	6:B:632:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:ASN:CA	1:E:356:MET:CE	2.87	0.52
1:A:512:TYR:HB3	1:A:513:PRO:HD2	1.92	0.52
1:B:115:GLY:HA2	5:B:610:NDP:O5D	2.10	0.52
1:C:192:GLN:HG3	1:D:231:PHE:CD2	2.44	0.52
1:A:37:SER:O	1:A:41:ASN:HB2	2.10	0.52
1:B:204:GLY:O	1:B:207:PHE:O	2.28	0.52
1:B:291:ILE:HG12	1:B:433:PHE:CD2	2.45	0.52
1:D:137:ALA:O	1:D:510:TYR:CE2	2.57	0.52
1:D:155:LEU:HB2	1:D:178:GLN:HE21	1.74	0.52
1:E:19:ILE:HB	5:E:622:NDP:H71N	1.75	0.52
1:E:303:THR:CG2	1:E:344:PHE:HB2	2.40	0.52
2:E:619:UMP:H1'	3:E:620:CB3:C4	2.39	0.52
1:C:6:VAL:HG11	1:C:127:PHE:O	2.10	0.52
1:C:381:ASP:HB3	1:C:384:HIS:CE1	2.45	0.52
1:D:447:GLN:NE2	1:D:492:LYS:HA	2.25	0.52
1:E:425:CYS:SG	1:E:431:SER:HB2	2.50	0.52
1:B:16:SER:O	1:B:17:SER:HB2	2.10	0.51
1:C:231:PHE:CE2	1:D:192:GLN:HG3	2.45	0.51
4:A:605:MTX:N5	5:A:606:NDP:H42N	2.24	0.51
1:E:342:TYR:O	1:E:345:GLN:N	2.43	0.51
1:E:403:HIS:CD2	1:E:403:HIS:H	2.27	0.51
1:A:104:ASP:C	1:A:106:SER:N	2.64	0.51
1:A:342:TYR:CD1	1:A:342:TYR:N	2.78	0.51
1:D:139:GLU:O	1:D:140:ASP:HB2	2.10	0.51
1:E:178:GLN:CD	1:E:178:GLN:H	2.05	0.51
1:A:4:LYS:N	1:A:101:LEU:CD2	2.67	0.51
1:C:350:ASN:CA	6:C:642:HOH:O	2.57	0.51
1:D:102:MET:HE3	1:D:102:MET:CA	2.28	0.51
1:E:178:GLN:HA	1:E:179:GLU:OE1	2.10	0.51
1:A:385:ILE:CG2	1:A:386:LEU:N	2.73	0.51
1:B:342:TYR:CE1	1:B:403:HIS:NE2	2.79	0.51
1:C:243:LEU:O	1:C:247:VAL:HG13	2.11	0.51
1:D:288:ILE:HG23	1:D:501:TRP:HH2	1.76	0.51
1:D:82:ASP:CG	1:D:84:ALA:H	2.13	0.51
1:D:135:ARG:O	1:D:170:TYR:HA	2.11	0.51
1:C:98:ILE:O	1:C:99:GLU:CB	2.59	0.51
1:C:194:LYS:HE3	1:C:198:ASP:OD1	2.10	0.51
1:D:126:ASN:ND2	1:D:177:LYS:HZ1	2.09	0.51
1:E:178:GLN:OE1	1:E:178:GLN:N	2.32	0.51
1:A:297:TRP:CD1	1:A:302:ASP:HB3	2.45	0.51
1:C:104:ASP:CB	1:C:107:ILE:HG13	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:372:ILE:O	1:E:376:LYS:HG2	2.10	0.51
1:B:447:GLN:HG3	6:B:751:HOH:O	2.10	0.51
1:C:211:LYS:NZ	1:D:234:GLU:OE1	2.44	0.51
1:E:50:ASN:OD1	1:E:109:ASN:HB2	2.11	0.51
1:E:322:LYS:O	1:E:326:GLU:HB2	2.11	0.51
1:B:39:ILE:HG23	1:B:40:THR:N	2.26	0.51
1:C:138:LEU:HD22	1:C:138:LEU:N	2.20	0.51
1:E:7:SER:O	1:E:111:PHE:HA	2.11	0.51
1:E:21:ILE:HA	1:E:144:ASP:OD2	2.11	0.51
1:E:79:LEU:HD22	1:E:90:VAL:HG21	1.93	0.51
1:A:51:ALA:C	1:A:52:LEU:HD23	2.30	0.50
3:A:604:CB3:CP2	3:A:604:CB3:H13	2.25	0.50
4:C:613:MTX:O1	4:C:613:MTX:CG	2.59	0.50
1:A:93:ASN:ND2	1:A:96:ASP:H	2.10	0.50
1:A:115:GLY:HA3	5:A:606:NDP:O1A	2.11	0.50
1:E:243:LEU:HA	1:E:246:ARG:HH12	1.74	0.50
1:A:25:LEU:HD11	4:A:605:MTX:H7	1.93	0.50
1:B:342:TYR:CD1	1:B:403:HIS:CE1	2.99	0.50
1:B:411:THR:CG2	1:B:412:ASN:N	2.74	0.50
1:C:100:ASN:N	1:C:103:ASN:CG	2.62	0.50
1:C:231:PHE:CD2	1:D:192:GLN:HG3	2.45	0.50
1:B:10:VAL:HG22	1:B:11:ALA:N	2.26	0.50
1:B:128:VAL:HG22	1:B:154:PHE:HZ	1.76	0.50
1:C:48:LYS:HA	1:C:106:SER:O	2.10	0.50
1:D:62:ILE:HD11	4:D:617:MTX:C15	2.42	0.50
1:E:153:THR:OG1	1:E:177:LYS:HE3	2.11	0.50
1:E:216:HIS:HA	1:E:250:ASN:ND2	2.26	0.50
1:E:237:GLU:O	1:E:241:LEU:HG	2.11	0.50
1:A:469:HIS:HB3	1:A:473:LEU:HD22	1.92	0.50
1:B:407:GLN:HG2	1:B:408:TYR:N	2.26	0.50
1:B:415:CYS:HA	1:B:452:GLU:O	2.12	0.50
1:B:431:SER:O	1:B:435:ILE:HG13	2.11	0.50
1:C:10:VAL:CG2	1:C:11:ALA:N	2.74	0.50
1:C:237:GLU:OE2	1:C:283:THR:HG23	2.12	0.50
1:C:404:VAL:HG11	1:D:405:LEU:HD11	1.93	0.50
1:D:405:LEU:C	1:D:405:LEU:HD23	2.31	0.50
3:E:620:CB3:C5	3:E:620:CB3:C14	2.87	0.50
4:E:621:MTX:H92	5:E:622:NDP:H42N	1.93	0.50
1:C:56:ARG:NH1	5:C:614:NDP:O2X	2.43	0.50
1:C:419:ASN:HD22	1:C:457:ALA:HB3	1.74	0.50
4:C:613:MTX:N5	5:C:614:NDP:H42N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:THR:HA	1:D:171:ASP:O	2.11	0.50
1:E:181:LYS:O	1:E:182:THR:CB	2.60	0.50
1:A:349:TYR:O	1:A:350:ASN:HB2	2.12	0.50
1:C:475:GLU:OE2	1:C:479:ARG:HD3	2.12	0.50
5:D:618:NDP:O2N	5:D:618:NDP:O1A	2.30	0.50
1:E:297:TRP:CG	1:E:308:LEU:HD21	2.47	0.50
1:E:355:THR:OG1	1:E:358:ASP:OD1	2.30	0.50
1:A:14:VAL:CG2	1:A:137:ALA:HA	2.42	0.50
1:A:291:ILE:HG12	1:A:433:PHE:CD2	2.46	0.50
1:E:299:ILE:HG23	1:E:368:LEU:HD21	1.93	0.50
1:A:233:ARG:NH1	1:A:242:ASP:OD2	2.45	0.50
1:B:59:TRP:NE1	1:B:64:ARG:HG2	2.27	0.50
1:C:10:VAL:HG22	1:C:11:ALA:H	1.76	0.49
1:A:339:GLY:O	1:A:341:ILE:HG23	2.11	0.49
1:B:98:ILE:HG23	1:B:98:ILE:O	2.11	0.49
1:B:372:ILE:HG22	1:B:376:LYS:HE2	1.94	0.49
1:C:48:LYS:HG2	1:C:106:SER:HA	1.94	0.49
1:C:172:PHE:CD2	1:D:203:LEU:HD21	2.47	0.49
1:A:358:ASP:N	1:A:358:ASP:OD1	2.45	0.49
1:D:337:ASP:OD1	1:D:356:MET:HG2	2.12	0.49
3:D:616:CB3:CP2	3:D:616:CB3:C13	2.77	0.49
1:E:126:ASN:ND2	1:E:177:LYS:NZ	2.60	0.49
1:A:333:ARG:CG	1:A:337:ASP:HB3	2.39	0.49
1:C:203:LEU:HD11	1:D:172:PHE:CE2	2.47	0.49
1:C:342:TYR:CE1	1:C:403:HIS:NE2	2.81	0.49
1:E:147:PHE:CD2	1:E:148:PRO:HD2	2.48	0.49
1:E:486:GLN:O	1:E:506:LEU:HD23	2.12	0.49
1:E:495:ASN:ND2	1:E:496:ILE:H	2.10	0.49
1:B:403:HIS:CD2	1:B:403:HIS:H	2.28	0.49
1:E:311:LYS:O	1:E:312:LYS:HB2	2.12	0.49
1:A:231:PHE:CD2	1:B:192:GLN:HG2	2.48	0.49
1:C:208:GLY:C	1:C:210:ARG:N	2.65	0.49
1:A:359:ASP:OD1	1:A:361:THR:HG22	2.12	0.49
1:C:212:MET:SD	1:D:273:ASP:HB2	2.52	0.49
1:A:58:THR:HG23	4:A:605:MTX:HM2	1.94	0.49
1:C:199:THR:O	1:C:203:LEU:HB2	2.12	0.49
1:D:149:GLU:HG2	6:D:632:HOH:O	2.13	0.49
1:D:242:ASP:O	1:D:246:ARG:HB2	2.13	0.49
1:A:269:MET:HE1	1:B:269:MET:HG2	1.95	0.49
1:B:99:GLU:OE1	1:B:99:GLU:HA	2.13	0.49
1:E:305:GLY:N	1:E:356:MET:HE3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLU:OE1	1:A:323:GLU:N	2.44	0.48
1:D:330:LEU:C	1:D:332:HIS:H	2.16	0.48
1:D:385:ILE:CG2	1:D:386:LEU:N	2.76	0.48
1:E:264:SER:HB2	1:E:462:ASP:OD2	2.12	0.48
1:A:256:ASN:OD1	1:A:258:THR:HB	2.12	0.48
1:A:455:GLU:HG3	6:A:657:HOH:O	2.13	0.48
1:B:359:ASP:OD2	1:B:361:THR:HG23	2.13	0.48
1:C:378:ASN:O	1:C:384:HIS:CE1	2.66	0.48
1:D:138:LEU:HD21	1:D:168:ILE:HD13	1.95	0.48
1:E:60:ASP:OD1	1:E:64:ARG:NH1	2.46	0.48
1:D:62:ILE:CG2	1:D:62:ILE:O	2.62	0.48
1:E:241:LEU:HD11	1:E:481:PRO:HG3	1.95	0.48
1:C:103:ASN:O	1:C:104:ASP:C	2.52	0.48
1:D:266:PHE:HA	1:D:461:GLY:O	2.13	0.48
1:A:231:PHE:CE2	1:B:192:GLN:HG2	2.49	0.48
1:A:439:ALA:O	1:A:443:MET:HG3	2.14	0.48
1:B:60:ASP:OD1	1:B:64:ARG:NH1	2.47	0.48
1:C:100:ASN:CB	1:C:103:ASN:CB	2.82	0.48
1:C:203:LEU:HD11	1:D:172:PHE:CD2	2.48	0.48
1:D:39:ILE:CG2	1:D:40:THR:N	2.76	0.48
1:E:12:ALA:HB1	1:E:17:SER:C	2.34	0.48
1:E:37:SER:CB	4:E:621:MTX:HG2	2.38	0.48
1:E:434:ASN:N	1:E:434:ASN:HD22	2.12	0.48
1:A:99:GLU:HA	6:A:674:HOH:O	2.14	0.48
1:B:19:ILE:O	5:B:610:NDP:H2N	2.14	0.48
1:C:55:GLY:CA	5:C:614:NDP:O2A	2.59	0.48
1:E:37:SER:O	1:E:41:ASN:ND2	2.46	0.48
1:E:449:CYS:HB3	1:E:451:TYR:CE1	2.48	0.48
1:A:98:ILE:O	1:A:98:ILE:CG2	2.61	0.48
1:B:102:MET:O	1:B:103:ASN:CB	2.60	0.48
1:C:72:ILE:HG13	6:C:676:HOH:O	2.14	0.48
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.95	0.48
1:D:388:ALA:O	1:D:401:PRO:HG2	2.14	0.48
1:A:402:CYS:O	1:A:404:VAL:HG23	2.14	0.48
1:B:130:ARG:HG3	1:B:130:ARG:HH11	1.79	0.48
1:B:342:TYR:CZ	1:B:403:HIS:CD2	3.02	0.48
1:E:373:GLU:O	1:E:377:ASN:HB2	2.14	0.48
1:A:52:LEU:HD23	1:A:52:LEU:N	2.29	0.48
1:B:55:GLY:N	1:B:118:ILE:HG13	2.29	0.48
1:D:405:LEU:HD23	1:D:406:SER:N	2.29	0.48
1:E:493:VAL:HG21	1:E:499:PHE:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ALA:O	1:A:510:TYR:HE2	1.97	0.47
1:A:190:ARG:HA	1:A:197:ASP:OD1	2.14	0.47
1:A:407:GLN:HB3	1:B:421:TYR:OH	2.13	0.47
4:A:605:MTX:O1	4:A:605:MTX:CG	2.61	0.47
1:D:100:ASN:CB	1:D:110:ILE:HD11	2.39	0.47
1:E:15:LEU:HD12	1:E:139:GLU:HG2	1.94	0.47
1:C:289:ARG:HG3	1:C:501:TRP:CE2	2.49	0.47
1:E:36:PHE:CD1	1:E:36:PHE:C	2.87	0.47
1:E:60:ASP:O	1:E:63:GLY:N	2.43	0.47
1:E:407:GLN:HG3	1:E:408:TYR:N	2.29	0.47
1:B:323:GLU:CD	1:B:323:GLU:H	2.17	0.47
1:B:384:HIS:O	1:B:407:GLN:HA	2.14	0.47
2:D:615:UMP:C5	6:D:667:HOH:O	2.56	0.47
1:C:23:GLY:HA2	5:C:614:NDP:O3D	2.15	0.47
1:C:354:LYS:HE2	1:C:358:ASP:OD2	2.14	0.47
1:D:135:ARG:HD2	1:D:173:MET:SD	2.54	0.47
1:D:291:ILE:HD13	1:D:436:ALA:HB3	1.97	0.47
1:D:436:ALA:O	1:D:440:ILE:HG13	2.14	0.47
1:E:21:ILE:HG13	1:E:22:ASN:ND2	2.29	0.47
1:E:93:ASN:ND2	1:E:95:GLU:HB3	2.29	0.47
1:E:98:ILE:HG22	1:E:98:ILE:O	2.14	0.47
1:E:217:LYS:NZ	1:E:217:LYS:HB3	2.30	0.47
1:B:135:ARG:HB2	1:B:171:ASP:HB2	1.97	0.47
1:B:359:ASP:OD1	1:B:361:THR:HG22	2.14	0.47
1:C:151:PRO:HG2	1:C:154:PHE:CD2	2.39	0.47
1:C:209:ILE:H	1:C:209:ILE:CD1	2.24	0.47
1:E:223:ILE:HD12	1:E:248:LEU:HB3	1.97	0.47
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.76	0.47
1:E:244:LEU:HD21	1:E:473:LEU:HD22	1.96	0.47
1:E:341:ILE:HA	1:E:397:MET:HE2	1.96	0.47
1:A:248:LEU:HD13	1:A:465:ILE:HD12	1.97	0.47
1:A:333:ARG:HD3	1:A:337:ASP:O	2.14	0.47
1:B:103:ASN:N	1:B:103:ASN:HD22	2.13	0.47
1:D:348:HIS:HB3	1:D:363:VAL:O	2.15	0.47
1:C:244:LEU:HD21	1:C:473:LEU:HD22	1.97	0.47
1:C:323:GLU:OE2	1:C:323:GLU:N	2.37	0.47
1:D:135:ARG:HD3	1:D:171:ASP:HB3	1.97	0.47
1:D:223:ILE:O	1:D:245:SER:HB2	2.14	0.47
1:E:278:PHE:CZ	1:E:487:LEU:HD22	2.50	0.47
1:B:3:GLU:O	1:B:4:LYS:CB	2.62	0.47
1:B:130:ARG:HD2	1:B:132:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASP:OD2	1:B:483:PRO:HG3	2.15	0.47
1:D:309:ILE:HG23	1:D:314:TYR:CE1	2.50	0.47
1:E:43:LYS:HB3	1:E:50:ASN:HD21	1.80	0.47
1:E:210:ARG:HH11	1:E:210:ARG:HG3	1.79	0.47
1:E:390:ASN:O	1:E:394:LEU:HG	2.15	0.47
1:C:99:GLU:CB	1:C:103:ASN:ND2	2.78	0.47
1:C:472:GLN:HB3	1:C:515:ILE:CG2	2.45	0.47
1:D:423:ARG:HG3	1:D:424:SER:N	2.29	0.47
1:E:490:LYS:HD3	1:E:502:GLU:O	2.15	0.47
1:A:267:GLY:O	1:B:271:ARG:NH2	2.48	0.46
1:A:479:ARG:HG2	1:A:512:TYR:CD2	2.51	0.46
1:D:180:LYS:CB	6:D:629:HOH:O	2.62	0.46
1:D:327:ARG:HH11	1:D:327:ARG:HB2	1.79	0.46
1:D:248:LEU:HD12	1:D:248:LEU:HA	1.76	0.46
1:D:335:GLU:O	1:D:336:ASN:HB2	2.14	0.46
1:B:114:GLY:HA2	1:B:119:TYR:CZ	2.50	0.46
1:B:257:ARG:NH2	1:B:521:VAL:OXT	2.48	0.46
1:D:475:GLU:OE2	1:D:479:ARG:HD3	2.15	0.46
1:E:120:ARG:HG2	1:E:120:ARG:NH1	2.31	0.46
1:E:158:TYR:O	1:E:173:MET:HA	2.14	0.46
1:E:208:GLY:C	1:E:210:ARG:H	2.18	0.46
1:A:202:LEU:HG	1:B:38:LYS:HB3	1.96	0.46
1:C:36:PHE:CE1	1:C:40:THR:HG21	2.51	0.46
1:D:126:ASN:ND2	1:D:177:LYS:NZ	2.64	0.46
1:D:255:GLU:OE1	1:D:255:GLU:N	2.37	0.46
1:A:67:LEU:HD12	1:A:72:ILE:HD11	1.98	0.46
1:A:509:TYR:CE1	1:A:511:PRO:HG3	2.51	0.46
3:B:608:CB3:C14	3:B:608:CB3:H5	2.46	0.46
1:C:138:LEU:HD23	1:C:138:LEU:O	2.16	0.46
1:C:267:GLY:O	1:D:271:ARG:NH2	2.49	0.46
1:D:244:LEU:HD21	1:D:473:LEU:HD22	1.98	0.46
1:E:291:ILE:HG12	1:E:433:PHE:CD2	2.51	0.46
1:A:212:MET:HB3	1:B:236:TYR:OH	2.15	0.46
1:D:256:ASN:O	1:D:257:ARG:C	2.53	0.46
1:E:337:ASP:CB	1:E:356:MET:HG2	2.45	0.46
1:A:163:PHE:HB2	1:A:170:TYR:CZ	2.50	0.46
1:B:12:ALA:HB1	1:B:17:SER:HA	1.98	0.46
1:C:96:ASP:O	1:C:99:GLU:CG	2.40	0.46
1:E:304:ASN:HB3	1:E:307:HIS:NE2	2.31	0.46
1:A:402:CYS:SG	2:A:603:UMP:C6	3.09	0.46
1:E:29:ILE:HG23	1:E:165:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:TYR:CE2	1:B:212:MET:HE1	2.51	0.46
1:B:103:ASN:O	1:B:105:ASP:N	2.49	0.46
1:B:139:GLU:HB2	1:B:510:TYR:CE1	2.50	0.46
1:D:12:ALA:HB2	1:D:19:ILE:HG22	1.98	0.46
1:E:51:ALA:C	1:E:52:LEU:HD23	2.37	0.46
1:E:378:ASN:O	1:E:384:HIS:CE1	2.69	0.46
1:E:405:LEU:O	1:E:420:LEU:HD12	2.16	0.46
1:E:490:LYS:HG3	1:E:503:ASP:O	2.15	0.46
1:B:394:LEU:HA	1:B:397:MET:HE3	1.98	0.45
1:C:10:VAL:CG2	1:C:11:ALA:H	2.29	0.45
1:C:135:ARG:HD2	1:C:173:MET:SD	2.55	0.45
1:D:514:THR:HG21	6:D:633:HOH:O	2.17	0.45
1:E:3:GLU:CA	1:E:3:GLU:OE2	2.63	0.45
1:B:180:LYS:HE2	1:B:180:LYS:HB2	1.76	0.45
1:E:26:PRO:HB2	1:E:27:TRP:CE3	2.52	0.45
1:E:338:LEU:HD23	1:E:338:LEU:H	1.79	0.45
1:A:98:ILE:C	1:A:100:ASN:H	2.19	0.45
1:A:158:TYR:O	1:A:173:MET:HB2	2.16	0.45
1:C:193:LEU:HG	1:C:195:SER:OG	2.17	0.45
1:E:260:ILE:HD12	1:E:260:ILE:N	2.31	0.45
1:E:299:ILE:HD13	1:E:346:TRP:HZ3	1.82	0.45
1:A:133:LEU:HD22	1:A:134:THR:N	2.31	0.45
1:A:163:PHE:CB	1:A:170:TYR:CZ	2.99	0.45
1:A:207:PHE:CE1	1:B:31:GLU:HG2	2.52	0.45
1:A:172:PHE:N	1:A:172:PHE:HD1	2.14	0.45
1:C:459:PHE:CD2	1:D:459:PHE:CD2	3.05	0.45
1:D:19:ILE:HB	5:D:618:NDP:N7N	2.32	0.45
1:D:394:LEU:HD23	1:D:397:MET:HE1	1.99	0.45
3:E:620:CB3:C15	3:E:620:CB3:H5	2.46	0.45
1:A:26:PRO:HB2	1:A:27:TRP:CE3	2.51	0.45
1:A:246:ARG:HG2	6:A:632:HOH:O	2.16	0.45
1:A:337:ASP:OD2	1:A:353:TYR:OH	2.29	0.45
1:C:402:CYS:SG	2:C:611:UMP:C6	3.10	0.45
1:D:171:ASP:CG	1:D:483:PRO:HG3	2.37	0.45
1:E:367:GLN:O	1:E:371:LEU:N	2.49	0.45
1:A:392:SER:CB	1:B:350:ASN:HD22	2.29	0.45
1:C:56:ARG:CG	1:C:76:SER:OG	2.65	0.45
1:C:59:TRP:C	1:C:62:ILE:HG22	2.37	0.45
1:C:74:VAL:HG12	1:C:75:ILE:N	2.31	0.45
1:C:431:SER:O	1:C:435:ILE:HG13	2.15	0.45
3:C:612:CB3:O	3:C:612:CB3:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:ARG:NH2	1:D:311:LYS:O	2.50	0.45
1:E:48:LYS:HB3	1:E:106:SER:O	2.17	0.45
1:E:225:ASN:CG	1:E:241:LEU:HD13	2.36	0.45
3:E:620:CB3:C5	3:E:620:CB3:H15	2.46	0.45
1:A:100:ASN:HB2	1:A:110:ILE:HD11	1.98	0.45
1:B:192:GLN:HA	1:B:192:GLN:OE1	2.16	0.45
1:C:4:LYS:HD3	1:C:101:LEU:HA	1.99	0.45
1:C:59:TRP:CD1	1:C:64:ARG:HG2	2.52	0.45
1:C:79:LEU:H	1:C:92:ARG:HH12	1.65	0.45
1:C:315:ILE:HG13	1:C:316:TRP:CD1	2.52	0.45
1:C:502:GLU:CD	1:C:502:GLU:H	2.20	0.45
1:E:304:ASN:CA	1:E:356:MET:HE3	2.39	0.45
1:E:422:GLN:HB3	1:E:460:ILE:HD13	1.98	0.45
1:A:134:THR:HG23	1:A:171:ASP:O	2.16	0.45
1:A:178:GLN:HE21	1:A:178:GLN:CA	2.28	0.45
1:A:383:ARG:HD3	1:B:400:PRO:HG2	1.98	0.45
1:B:120:ARG:HG3	1:B:148:PRO:HG3	1.99	0.45
1:C:130:ARG:HD2	1:C:132:TYR:CE1	2.52	0.45
1:C:333:ARG:HH22	1:C:339:GLY:HA3	1.81	0.45
1:A:246:ARG:NH1	1:A:268:GLN:OE1	2.43	0.45
1:A:253:TYR:HD2	1:A:263:TYR:CZ	2.34	0.45
1:A:257:ARG:HE	1:B:383:ARG:HH12	1.65	0.45
1:A:258:THR:HG23	1:A:520:ALA:HB1	1.97	0.45
1:B:4:LYS:HG2	1:B:101:LEU:HD23	1.99	0.45
1:C:71:ILE:HD12	1:C:71:ILE:N	2.32	0.45
1:C:400:PRO:HG2	1:D:383:ARG:CZ	2.47	0.45
1:E:163:PHE:HA	1:E:276:GLU:HB3	1.98	0.45
1:E:381:ASP:HB3	1:E:384:HIS:NE2	2.32	0.45
1:A:256:ASN:HD21	1:A:262:THR:HG23	1.82	0.44
1:A:260:ILE:N	1:A:260:ILE:HD12	2.32	0.44
1:B:180:LYS:HD3	1:B:181:LYS:CA	2.47	0.44
1:E:427:LEU:HD23	1:E:464:HIS:O	2.17	0.44
1:A:209:ILE:HG12	1:A:209:ILE:O	2.18	0.44
1:C:20:GLY:HA2	1:C:26:PRO:HD3	1.99	0.44
1:E:305:GLY:N	1:E:356:MET:CE	2.80	0.44
1:A:96:ASP:O	1:A:99:GLU:HG3	2.18	0.44
1:A:104:ASP:C	1:A:106:SER:H	2.20	0.44
1:C:94:LEU:HA	1:C:97:SER:OG	2.18	0.44
1:C:100:ASN:C	1:C:103:ASN:CB	2.56	0.44
1:C:193:LEU:HD21	1:D:176:GLU:OE2	2.16	0.44
1:A:15:LEU:HD12	1:A:139:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLY:C	1:A:333:ARG:N	2.70	0.44
1:A:509:TYR:CZ	1:A:511:PRO:HB3	2.52	0.44
1:B:26:PRO:HB2	1:B:27:TRP:CE3	2.53	0.44
1:C:293:GLU:OE2	1:C:296:ILE:HD11	2.18	0.44
1:C:423:ARG:HA	1:D:407:GLN:OE1	2.18	0.44
1:D:10:VAL:HG22	1:D:11:ALA:N	2.32	0.44
1:D:261:SER:HB2	1:D:467:GLU:OE2	2.17	0.44
1:E:202:LEU:HA	1:E:205:GLU:OE1	2.18	0.44
1:E:293:GLU:O	1:E:297:TRP:HB2	2.17	0.44
1:B:115:GLY:HA3	5:B:610:NDP:PA	2.58	0.44
1:C:233:ARG:HG3	6:C:626:HOH:O	2.17	0.44
1:C:421:TYR:OH	1:D:407:GLN:HB3	2.17	0.44
1:E:137:ALA:O	1:E:510:TYR:CE2	2.70	0.44
1:E:285:LYS:HE2	1:E:514:THR:OG1	2.17	0.44
1:A:389:TRP:HB2	1:A:404:VAL:CG1	2.44	0.44
1:B:117:SER:OG	5:B:610:NDP:H8A	2.17	0.44
1:C:471:THR:HG23	6:C:659:HOH:O	2.17	0.44
1:D:48:LYS:HB3	1:D:106:SER:O	2.17	0.44
1:D:330:LEU:C	1:D:332:HIS:N	2.69	0.44
1:D:431:SER:O	1:D:435:ILE:HG13	2.18	0.44
1:E:337:ASP:OD2	1:E:353:TYR:OH	2.33	0.44
1:A:20:GLY:HA2	1:A:26:PRO:HD3	1.99	0.44
1:B:479:ARG:NH2	1:B:513:PRO:O	2.50	0.44
1:C:246:ARG:NH1	1:C:268:GLN:OE1	2.50	0.44
1:C:345:GLN:O	1:C:349:TYR:HB2	2.18	0.44
1:C:519:MET:HG2	1:C:520:ALA:N	2.31	0.44
1:E:100:ASN:OD1	1:E:101:LEU:N	2.51	0.44
1:A:178:GLN:CA	1:A:178:GLN:NE2	2.81	0.44
1:B:96:ASP:O	1:B:99:GLU:HB2	2.18	0.44
1:D:171:ASP:CB	1:D:483:PRO:HG3	2.48	0.44
1:E:63:GLY:O	1:E:65:ARG:HG3	2.18	0.44
1:A:239:GLN:HG3	1:A:271:ARG:O	2.18	0.44
1:B:342:TYR:CE1	1:B:403:HIS:CE1	3.05	0.44
1:C:14:VAL:HG13	1:C:15:LEU:N	2.32	0.44
1:C:104:ASP:OD2	1:C:106:SER:CA	2.66	0.44
1:C:131:ILE:O	1:C:174:ILE:HA	2.18	0.44
1:C:405:LEU:C	1:C:405:LEU:HD23	2.38	0.44
1:D:27:TRP:CE2	1:D:136:VAL:HG21	2.53	0.44
1:D:129:ASP:OD2	1:D:129:ASP:N	2.50	0.44
1:D:303:THR:HG21	1:D:344:PHE:HB2	2.00	0.44
1:E:58:THR:O	1:E:62:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:622:NDP:C5D	5:E:622:NDP:O2A	2.65	0.44
1:A:31:GLU:HG2	1:B:207:PHE:CE1	2.53	0.43
1:A:512:TYR:HB3	1:A:513:PRO:CD	2.48	0.43
1:C:36:PHE:HE2	4:C:613:MTX:NA4	2.16	0.43
1:C:479:ARG:NH2	1:C:513:PRO:O	2.50	0.43
3:C:612:CB3:HN	3:C:612:CB3:H12	1.41	0.43
1:D:208:GLY:C	1:D:210:ARG:N	2.71	0.43
1:D:233:ARG:NH1	1:D:242:ASP:OD1	2.51	0.43
1:E:283:THR:HA	1:E:512:TYR:CD1	2.51	0.43
1:D:311:LYS:O	1:D:312:LYS:HB2	2.17	0.43
1:E:422:GLN:HB3	1:E:460:ILE:CD1	2.48	0.43
1:A:233:ARG:NH1	1:A:242:ASP:CG	2.72	0.43
1:C:224:TYR:CZ	1:C:233:ARG:NH1	2.86	0.43
1:C:467:GLU:HA	1:C:470:LEU:HD22	2.00	0.43
1:D:100:ASN:HB3	1:D:107:ILE:HG21	2.00	0.43
1:D:147:PHE:HE1	1:D:150:ILE:HD11	1.83	0.43
1:E:244:LEU:HD12	1:E:427:LEU:HB3	1.99	0.43
1:E:278:PHE:CE1	1:E:487:LEU:HD22	2.52	0.43
1:E:295:LEU:CD2	1:E:299:ILE:HD11	2.48	0.43
1:E:304:ASN:ND2	1:E:356:MET:HB2	2.34	0.43
1:A:305:GLY:O	1:A:309:ILE:HG13	2.19	0.43
1:A:472:GLN:OE1	1:A:472:GLN:N	2.49	0.43
1:B:193:LEU:CD2	1:B:195:SER:OG	2.66	0.43
1:B:246:ARG:NE	1:B:268:GLN:OE1	2.49	0.43
1:B:262:THR:HG22	1:B:466:TYR:HA	2.01	0.43
1:C:133:LEU:HD22	1:C:133:LEU:C	2.38	0.43
1:C:285:LYS:HB3	1:C:514:THR:HG23	1.99	0.43
1:C:423:ARG:HG3	1:C:424:SER:N	2.33	0.43
1:D:58:THR:OG1	5:D:618:NDP:H6N	2.19	0.43
1:D:98:ILE:O	1:D:99:GLU:CB	2.62	0.43
1:E:8:ILE:HD12	1:E:123:LEU:HD21	2.01	0.43
1:A:381:ASP:HB3	1:A:384:HIS:CE1	2.53	0.43
1:A:502:GLU:CD	1:A:502:GLU:H	2.22	0.43
1:C:98:ILE:C	1:C:99:GLU:CG	2.86	0.43
1:C:402:CYS:SG	2:C:611:UMP:H2'	2.58	0.43
1:A:288:ILE:O	1:A:291:ILE:HB	2.18	0.43
1:A:472:GLN:O	1:A:475:GLU:HB3	2.19	0.43
1:D:4:LYS:HD2	1:D:107:ILE:O	2.19	0.43
1:D:248:LEU:CD1	1:D:465:ILE:HD12	2.47	0.43
1:A:125:ASP:HB2	1:A:127:PHE:CE1	2.53	0.43
1:A:400:PRO:HG2	1:A:423:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LYS:HE3	1:B:101:LEU:HA	1.99	0.43
1:C:48:LYS:CA	1:C:106:SER:O	2.66	0.43
1:E:130:ARG:HD2	1:E:132:TYR:CZ	2.53	0.43
1:E:315:ILE:HG13	1:E:316:TRP:CD1	2.54	0.43
1:C:56:ARG:HB2	1:C:76:SER:OG	2.19	0.43
1:A:98:ILE:O	1:A:98:ILE:HG22	2.19	0.42
1:B:115:GLY:HA3	5:B:610:NDP:O2A	2.18	0.42
1:B:335:GLU:O	1:B:336:ASN:CB	2.67	0.42
1:B:359:ASP:OD2	1:B:361:THR:CG2	2.67	0.42
1:C:304:ASN:OD1	1:C:306:ASN:HB2	2.19	0.42
1:D:472:GLN:O	1:D:475:GLU:HB3	2.18	0.42
1:E:411:THR:OG1	1:E:415:CYS:HB2	2.20	0.42
1:E:434:ASN:ND2	3:E:620:CB3:CP3	2.82	0.42
1:A:236:TYR:CE2	1:B:212:MET:CE	3.02	0.42
1:C:38:LYS:O	1:C:42:ASN:HB2	2.19	0.42
1:C:187:ASP:HA	1:C:188:PRO:HD3	1.91	0.42
1:C:254:ARG:HD2	1:C:264:SER:HB3	2.02	0.42
1:D:342:TYR:CZ	1:D:403:HIS:CD2	3.06	0.42
1:E:378:ASN:HD21	1:E:381:ASP:HB2	1.82	0.42
4:E:621:MTX:C6	5:E:622:NDP:H42N	2.49	0.42
1:A:115:GLY:HA3	5:A:606:NDP:PA	2.60	0.42
1:A:258:THR:HG21	1:A:520:ALA:CB	2.41	0.42
1:C:123:LEU:HD12	1:C:128:VAL:CG1	2.40	0.42
1:C:226:THR:N	1:C:227:PRO:HD3	2.34	0.42
1:C:339:GLY:HA2	1:C:353:TYR:CE2	2.54	0.42
1:D:36:PHE:CD1	1:D:36:PHE:C	2.93	0.42
1:D:52:LEU:HD23	1:D:52:LEU:N	2.34	0.42
1:D:133:LEU:HD22	1:D:134:THR:N	2.35	0.42
1:E:54:MET:CE	1:E:72:ILE:HG23	2.50	0.42
1:E:361:THR:HG23	1:E:361:THR:O	2.18	0.42
1:C:158:TYR:HB3	1:C:174:ILE:CG2	2.42	0.42
1:D:59:TRP:CD1	1:D:64:ARG:HG2	2.55	0.42
1:E:3:GLU:OE2	1:E:3:GLU:HA	2.19	0.42
1:E:6:VAL:HG22	1:E:110:ILE:HB	2.02	0.42
1:E:208:GLY:C	1:E:210:ARG:N	2.71	0.42
1:A:206:ILE:HG13	1:B:38:LYS:NZ	2.35	0.42
1:B:315:ILE:HB	3:B:608:CB3:C15	2.50	0.42
1:C:135:ARG:NH2	1:C:481:PRO:O	2.51	0.42
1:C:226:THR:HG22	1:C:229:ILE:HG13	2.01	0.42
1:B:150:ILE:HA	1:B:151:PRO:HD3	1.86	0.42
1:D:8:ILE:HG12	1:D:112:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ILE:HG12	1:D:433:PHE:CD2	2.54	0.42
1:E:8:ILE:CG1	1:E:112:VAL:HB	2.36	0.42
1:E:363:VAL:CG1	1:E:364:GLY:N	2.79	0.42
1:A:49:LYS:O	1:A:107:ILE:HA	2.19	0.42
1:A:290:GLY:HA3	6:A:718:HOH:O	2.19	0.42
1:D:208:GLY:C	1:D:210:ARG:H	2.23	0.42
1:E:43:LYS:HZ2	1:E:46:SER:HA	1.82	0.42
1:E:56:ARG:HG3	1:E:79:LEU:HD12	2.01	0.42
1:C:179:GLU:HA	6:C:651:HOH:O	2.20	0.42
1:C:190:ARG:HH11	1:C:190:ARG:CB	2.20	0.42
1:D:49:LYS:HD2	1:D:71:ILE:HD11	2.01	0.42
1:D:226:THR:N	1:D:227:PRO:HD3	2.34	0.42
1:D:243:LEU:HA	1:D:246:ARG:NH1	2.35	0.42
1:D:258:THR:HG22	1:D:521:VAL:O	2.20	0.42
1:E:223:ILE:HB	1:E:248:LEU:HD23	2.01	0.42
1:E:472:GLN:HB3	1:E:515:ILE:CG2	2.50	0.42
1:B:123:LEU:HD12	1:B:123:LEU:HA	1.87	0.42
1:B:347:ARG:O	1:B:366:ASP:HA	2.20	0.42
1:C:391:PRO:HD2	1:D:349:TYR:CD2	2.52	0.42
1:E:452:GLU:OE2	1:E:452:GLU:HA	2.20	0.42
1:A:427:LEU:HD12	1:A:427:LEU:HA	1.85	0.42
1:B:400:PRO:HA	1:B:401:PRO:HD3	1.91	0.42
1:B:426:ASP:OD2	1:B:426:ASP:C	2.58	0.42
1:C:26:PRO:HG2	1:C:143:PHE:HE1	1.85	0.42
1:C:347:ARG:O	1:C:366:ASP:HA	2.20	0.42
3:C:612:CB3:O	3:C:612:CB3:HB1	2.14	0.42
3:C:612:CB3:HP12	3:C:612:CB3:H13	1.63	0.42
1:D:501:TRP:HA	1:D:501:TRP:CE3	2.55	0.42
1:E:246:ARG:HB2	1:E:246:ARG:HH11	1.85	0.42
1:B:39:ILE:CG2	1:B:40:THR:N	2.81	0.41
1:B:49:LYS:O	1:B:107:ILE:HA	2.20	0.41
1:D:302:ASP:OD2	1:D:307:HIS:ND1	2.53	0.41
1:E:43:LYS:HB2	1:E:108:GLU:OE1	2.20	0.41
1:E:133:LEU:HD23	1:E:134:THR:N	2.35	0.41
1:E:348:HIS:CE1	1:E:360:TYR:O	2.73	0.41
1:C:157:VAL:HG23	1:D:196:ILE:HD11	2.01	0.41
1:C:257:ARG:NH1	2:C:611:UMP:O5'	2.53	0.41
1:C:295:LEU:HD22	1:C:299:ILE:HD11	2.01	0.41
1:D:53:ILE:HG23	1:D:75:ILE:HD13	2.03	0.41
1:D:103:ASN:O	1:D:105:ASP:N	2.53	0.41
1:E:155:LEU:HA	1:E:156:PRO:HD3	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:PHE:HA	1:E:461:GLY:O	2.20	0.41
4:B:609:MTX:O1	4:B:609:MTX:HG1	2.19	0.41
1:C:180:LYS:CB	6:C:650:HOH:O	2.68	0.41
1:C:267:GLY:HA2	1:C:460:ILE:O	2.20	0.41
1:C:360:TYR:CD1	1:C:363:VAL:HG11	2.53	0.41
1:C:381:ASP:HB3	1:C:384:HIS:NE2	2.35	0.41
1:C:419:ASN:HD22	1:C:419:ASN:HA	1.58	0.41
1:D:400:PRO:HG2	1:D:423:ARG:NH2	2.35	0.41
1:E:90:VAL:HG12	1:E:91:PHE:N	2.34	0.41
1:E:171:ASP:OD2	1:E:483:PRO:HD3	2.20	0.41
1:E:389:TRP:HB2	1:E:404:VAL:CG1	2.44	0.41
1:A:48:LYS:CB	1:A:106:SER:O	2.67	0.41
1:A:102:MET:O	1:A:103:ASN:CG	2.59	0.41
1:A:163:PHE:CB	1:A:170:TYR:CE2	2.97	0.41
1:A:164:CYS:SG	6:A:667:HOH:O	2.63	0.41
1:A:323:GLU:H	1:A:323:GLU:CD	2.22	0.41
3:A:604:CB3:C15	3:A:604:CB3:C6	2.98	0.41
1:B:75:ILE:O	5:B:610:NDP:H1B	2.20	0.41
1:B:203:LEU:HD12	1:B:203:LEU:HA	1.95	0.41
1:C:236:TYR:OH	1:D:212:MET:HB3	2.21	0.41
5:C:614:NDP:O3B	5:C:614:NDP:O2X	2.30	0.41
1:D:7:SER:O	1:D:111:PHE:HA	2.21	0.41
1:D:90:VAL:HG12	1:D:91:PHE:N	2.36	0.41
1:D:104:ASP:C	1:D:106:SER:N	2.73	0.41
1:E:76:SER:CA	5:E:622:NDP:O2X	2.64	0.41
1:A:171:ASP:C	1:A:172:PHE:CD1	2.94	0.41
1:A:248:LEU:HD13	1:A:465:ILE:CD1	2.51	0.41
1:B:193:LEU:HD23	1:B:195:SER:H	1.86	0.41
1:C:79:LEU:HD23	1:C:80:PRO:CG	2.49	0.41
1:C:403:HIS:CD2	1:C:403:HIS:H	2.37	0.41
1:D:506:LEU:HD23	1:D:506:LEU:HA	1.90	0.41
1:E:433:PHE:CE2	3:E:620:CB3:H12	2.56	0.41
1:C:115:GLY:O	1:C:116:GLU:C	2.59	0.41
1:C:248:LEU:HD12	1:C:248:LEU:HA	1.86	0.41
1:C:291:ILE:HG12	1:C:433:PHE:CE2	2.55	0.41
1:D:68:LYS:HE2	1:D:69:ASN:OD1	2.21	0.41
1:D:360:TYR:HB3	1:D:363:VAL:CG1	2.51	0.41
1:E:4:LYS:HG2	1:E:101:LEU:HD23	2.00	0.41
1:E:135:ARG:HD3	1:E:171:ASP:OD2	2.20	0.41
1:E:371:LEU:HD13	1:E:371:LEU:C	2.41	0.41
1:E:436:ALA:O	1:E:439:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PHE:CD2	1:A:148:PRO:HD2	2.55	0.41
1:D:3:GLU:OE2	1:D:3:GLU:HA	2.21	0.41
1:D:92:ARG:O	5:D:618:NDP:C2A	2.67	0.41
1:E:199:THR:O	1:E:203:LEU:HB2	2.21	0.41
1:E:388:ALA:O	1:E:401:PRO:HG2	2.20	0.41
1:B:9:VAL:O	4:B:609:MTX:NA4	2.47	0.41
1:C:77:SER:H	5:C:614:NDP:P2B	2.43	0.41
1:D:10:VAL:HB	1:D:119:TYR:CZ	2.56	0.41
1:D:294:GLU:O	1:D:297:TRP:HB3	2.21	0.41
1:D:431:SER:HB3	1:D:432:PRO:HD3	2.03	0.41
1:E:135:ARG:CG	1:E:171:ASP:HB2	2.50	0.41
1:A:165:THR:N	1:A:170:TYR:HE1	2.19	0.41
1:A:180:LYS:N	6:A:614:HOH:O	2.54	0.41
1:A:299:ILE:O	1:A:347:ARG:NH1	2.51	0.41
1:A:403:HIS:HB2	1:A:420:LEU:HD11	2.02	0.41
1:A:431:SER:HB3	1:A:432:PRO:HD3	2.02	0.41
1:C:269:MET:HE2	1:D:269:MET:HE2	2.03	0.41
1:C:391:PRO:HD2	1:D:349:TYR:HE2	1.71	0.41
1:D:12:ALA:HB2	1:D:19:ILE:CG2	2.51	0.41
1:D:62:ILE:O	1:D:62:ILE:HG23	2.21	0.41
1:D:235:HIS:ND1	1:D:235:HIS:C	2.74	0.41
1:D:495:ASN:OD1	1:D:497:GLU:HG3	2.21	0.41
1:E:59:TRP:O	1:E:62:ILE:HB	2.20	0.41
1:E:337:ASP:OD2	1:E:337:ASP:C	2.59	0.41
1:E:341:ILE:HA	1:E:397:MET:HE3	2.03	0.41
1:E:347:ARG:HA	1:E:366:ASP:OD2	2.21	0.41
1:A:258:THR:CG2	1:A:260:ILE:HB	2.51	0.41
1:B:233:ARG:NH1	1:B:242:ASP:OD1	2.54	0.41
1:C:8:ILE:HD11	1:C:123:LEU:HD13	2.03	0.41
1:C:100:ASN:O	1:C:103:ASN:HB2	2.14	0.41
1:C:405:LEU:HD11	1:D:404:VAL:HG11	2.02	0.41
1:D:297:TRP:HH2	1:D:338:LEU:HD12	1.86	0.41
1:E:14:VAL:HG13	1:E:136:VAL:C	2.41	0.41
1:E:100:ASN:HA	1:E:104:ASP:CB	2.50	0.41
1:A:98:ILE:CG2	1:A:101:LEU:HD12	2.51	0.40
1:C:297:TRP:HH2	1:C:338:LEU:HD12	1.85	0.40
1:C:385:ILE:CG2	1:C:386:LEU:N	2.84	0.40
1:C:491:ARG:CZ	1:C:493:VAL:HG12	2.51	0.40
1:D:470:LEU:HD13	1:D:470:LEU:HA	1.95	0.40
1:A:229:ILE:HG22	1:A:233:ARG:HG2	2.03	0.40
1:B:256:ASN:HB3	6:B:748:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:LYS:HD3	1:B:514:THR:HG22	2.02	0.40
1:D:97:SER:C	1:D:99:GLU:HG3	2.40	0.40
1:D:274:MET:SD	1:D:439:ALA:HA	2.61	0.40
1:E:255:GLU:H	1:E:255:GLU:CD	2.25	0.40
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.86	0.40
1:A:297:TRP:CE3	1:A:308:LEU:HD11	2.56	0.40
1:B:193:LEU:HD21	6:B:660:HOH:O	2.21	0.40
1:C:120:ARG:NH1	1:C:148:PRO:HB3	2.36	0.40
1:D:49:LYS:HD2	1:D:71:ILE:CD1	2.51	0.40
1:E:206:ILE:HG22	1:E:207:PHE:N	2.36	0.40
1:E:508:GLY:O	1:E:510:TYR:CD2	2.74	0.40
1:A:333:ARG:CD	1:A:337:ASP:O	2.70	0.40
1:B:97:SER:C	1:B:99:GLU:H	2.25	0.40
1:C:25:LEU:HD11	4:C:613:MTX:H7	2.04	0.40
1:D:135:ARG:HH22	1:D:482:ARG:HA	1.82	0.40
1:E:62:ILE:HD11	4:E:621:MTX:C13	2.51	0.40
1:E:434:ASN:HD21	3:E:620:CB3:CP3	2.34	0.40
1:A:39:ILE:HD13	1:A:39:ILE:HA	1.86	0.40
1:A:258:THR:HG21	1:A:260:ILE:HB	2.03	0.40
1:A:485:PRO:HB3	1:A:509:TYR:HA	2.03	0.40
1:B:159:MET:HE2	1:B:173:MET:SD	2.62	0.40
1:B:291:ILE:HD13	1:B:436:ALA:HB3	2.02	0.40
1:C:4:LYS:HB2	1:C:101:LEU:HD23	2.03	0.40
1:C:93:ASN:OD1	1:C:95:GLU:HB3	2.22	0.40
1:D:57:LYS:HB2	5:D:618:NDP:O3	2.22	0.40
1:D:479:ARG:NH2	1:D:513:PRO:O	2.55	0.40
1:E:299:ILE:O	1:E:347:ARG:HD3	2.21	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:E:349:TYR:OH	1:E:349:TYR:OH[2_457]	1.93	0.27

## 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	A	512/519 (99%)	481 (94%)	24 (5%)	7 (1%)	11	34
1	B	512/519 (99%)	482 (94%)	25 (5%)	5 (1%)	15	44
1	C	510/519 (98%)	468 (92%)	37 (7%)	5 (1%)	15	44
1	D	511/519 (98%)	464 (91%)	38 (7%)	9 (2%)	8	28
1	E	507/519 (98%)	458 (90%)	42 (8%)	7 (1%)	11	34
All	All	2552/2595 (98%)	2353 (92%)	166 (6%)	33 (1%)	12	36

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	MET
1	A	103	ASN
1	B	103	ASN
1	B	342	TYR
1	C	103	ASN
1	C	335	GLU
1	C	336	ASN
1	C	342	TYR
1	D	99	GLU
1	D	257	ARG
1	D	342	TYR
1	E	331	GLY
1	E	342	TYR
1	A	105	ASP
1	B	414	ASN
1	C	99	GLU
1	D	105	ASP
1	B	69	ASN
1	D	102	MET
1	D	194	LYS
1	D	331	GLY
1	E	83	GLU
1	A	384	HIS
1	E	140	ASP
1	E	361	THR
1	E	379	PRO
1	E	384	HIS

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Mol	Chain	Res	Type
1	A	98	ILE
1	A	101	LEU
1	B	4	LYS
1	D	100	ASN
1	D	104	ASP
1	A	341	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	460/467 (98%)	427 (93%)	33 (7%)	14	38
1	B	461/467 (99%)	423 (92%)	38 (8%)	11	33
1	C	457/467 (98%)	420 (92%)	37 (8%)	11	33
1	D	457/467 (98%)	419 (92%)	38 (8%)	11	32
1	E	456/467 (98%)	425 (93%)	31 (7%)	16	42
All	All	2291/2335 (98%)	2114 (92%)	177 (8%)	13	35

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	99	GLU
1	A	103	ASN
1	A	104	ASP
1	A	126	ASN
1	A	128	VAL
1	A	133	LEU
1	A	172	PHE
1	A	178	GLN
1	A	193	LEU
1	A	203	LEU
1	A	221	GLU
1	A	235	HIS

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Mol	Chain	Res	Type
1	A	244	LEU
1	A	247	VAL
1	A	248	LEU
1	A	269	MET
1	A	295	LEU
1	A	341	ILE
1	A	342	TYR
1	A	354	LYS
1	A	355	THR
1	A	356	MET
1	A	358	ASP
1	A	361	THR
1	A	370	LYS
1	A	371	LEU
1	A	378	ASN
1	A	413	ASP
1	A	427	LEU
1	A	429	LEU
1	A	473	LEU
1	A	491	ARG
1	B	7	SER
1	B	13	SER
1	B	16	SER
1	B	98	ILE
1	B	99	GLU
1	B	103	ASN
1	B	123	LEU
1	B	126	ASN
1	B	133	LEU
1	B	138	LEU
1	B	176	GLU
1	B	177	LYS
1	B	179	GLU
1	B	180	LYS
1	B	202	LEU
1	B	203	LEU
1	B	220	LYS
1	B	221	GLU
1	B	233	ARG
1	B	235	HIS
1	B	244	LEU
1	B	247	VAL

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Mol	Chain	Res	Type
1	B	289	ARG
1	B	295	LEU
1	B	308	LEU
1	B	335	GLU
1	B	352	GLU
1	B	361	THR
1	B	363	VAL
1	B	371	LEU
1	B	383	ARG
1	B	404	VAL
1	B	413	ASP
1	B	427	LEU
1	B	429	LEU
1	B	491	ARG
1	B	506	LEU
1	B	514	THR
1	C	5	ASN
1	C	6	VAL
1	C	52	LEU
1	C	62	ILE
1	C	76	SER
1	C	83	GLU
1	C	98	ILE
1	C	99	GLU
1	C	100	ASN
1	C	102	MET
1	C	105	ASP
1	C	123	LEU
1	C	133	LEU
1	C	138	LEU
1	C	171	ASP
1	C	174	ILE
1	C	176	GLU
1	C	209	ILE
1	C	228	SER
1	C	233	ARG
1	C	235	HIS
1	C	247	VAL
1	C	257	ARG
1	C	295	LEU
1	C	308	LEU
1	C	325	LEU

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Mol	Chain	Res	Type
1	C	333	ARG
1	C	371	LEU
1	C	383	ARG
1	C	427	LEU
1	C	470	LEU
1	C	474	LYS
1	C	479	ARG
1	C	497	GLU
1	C	505	GLU
1	C	506	LEU
1	C	516	LYS
1	D	7	SER
1	D	52	LEU
1	D	76	SER
1	D	79	LEU
1	D	82	ASP
1	D	83	GLU
1	D	96	ASP
1	D	99	GLU
1	D	105	ASP
1	D	113	CYS
1	D	123	LEU
1	D	128	VAL
1	D	129	ASP
1	D	133	LEU
1	D	138	LEU
1	D	149	GLU
1	D	171	ASP
1	D	176	GLU
1	D	202	LEU
1	D	203	LEU
1	D	221	GLU
1	D	233	ARG
1	D	235	HIS
1	D	248	LEU
1	D	256	ASN
1	D	262	THR
1	D	264	SER
1	D	293	GLU
1	D	295	LEU
1	D	308	LEU
1	D	310	GLU

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Mol	Chain	Res	Type
1	D	371	LEU
1	D	383	ARG
1	D	414	ASN
1	D	422	GLN
1	D	437	SER
1	D	479	ARG
1	D	514	THR
1	E	3	GLU
1	E	8	ILE
1	E	36	PHE
1	E	45	ASP
1	E	99	GLU
1	E	101	LEU
1	E	133	LEU
1	E	138	LEU
1	E	139	GLU
1	E	178	GLN
1	E	179	GLU
1	E	194	LYS
1	E	202	LEU
1	E	220	LYS
1	E	221	GLU
1	E	233	ARG
1	E	260	ILE
1	E	269	MET
1	E	295	LEU
1	E	306	ASN
1	E	335	GLU
1	E	338	LEU
1	E	354	LYS
1	E	356	MET
1	E	383	ARG
1	E	394	LEU
1	E	414	ASN
1	E	434	ASN
1	E	471	THR
1	E	491	ARG
1	E	500	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	69	ASN
1	A	103	ASN
1	A	167	ASN
1	A	178	GLN
1	A	192	GLN
1	A	384	HIS
1	A	447	GLN
1	B	100	ASN
1	B	103	ASN
1	B	422	GLN
1	C	5	ASN
1	C	24	GLN
1	C	41	ASN
1	C	69	ASN
1	C	103	ASN
1	C	319	ASN
1	C	377	ASN
1	C	384	HIS
1	C	419	ASN
1	C	422	GLN
1	D	178	GLN
1	D	256	ASN
1	D	306	ASN
1	D	419	ASN
1	D	422	GLN
1	E	22	ASN
1	E	24	GLN
1	E	69	ASN
1	E	126	ASN
1	E	167	ASN
1	E	214	ASN
1	E	307	HIS
1	E	377	ASN
1	E	378	ASN
1	E	384	HIS
1	E	396	GLN
1	E	403	HIS
1	E	434	ASN
1	E	495	ASN

### 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 ⓘ

20 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	$\# Z  > 2$
4	MTX	B	609	-	29,35,35	1.45	3 (10%)	38,49,49	1.91	9 (23%)
5	NDP	A	606	-	45,52,52	1.42	3 (6%)	53,80,80	1.14	3 (5%)
4	MTX	E	621	-	29,35,35	1.34	2 (6%)	38,49,49	1.86	8 (21%)
4	MTX	D	617	-	29,35,35	1.42	2 (6%)	38,49,49	1.99	10 (26%)
4	MTX	C	613	-	29,35,35	1.36	2 (6%)	38,49,49	1.87	8 (21%)
5	NDP	C	614	-	45,52,52	1.31	3 (6%)	53,80,80	1.29	3 (5%)
3	CB3	C	612	-	30,37,37	2.73	18 (60%)	38,51,51	3.16	18 (47%)
3	CB3	A	604	-	30,37,37	2.34	13 (43%)	38,51,51	3.05	19 (50%)
3	CB3	E	620	-	30,37,37	1.26	2 (6%)	38,51,51	2.27	7 (18%)
2	UMP	E	619	-	18,21,21	3.14	3 (16%)	21,31,31	1.08	1 (4%)
5	NDP	B	610	-	45,52,52	1.45	3 (6%)	53,80,80	1.14	3 (5%)
2	UMP	B	607	-	18,21,21	3.11	3 (16%)	21,31,31	0.92	1 (4%)
2	UMP	D	615	1	18,21,21	3.10	3 (16%)	21,31,31	0.93	2 (9%)
3	CB3	D	616	-	30,37,37	2.22	16 (53%)	38,51,51	2.35	12 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	UMP	C	611	-	18,21,21	3.10	3 (16%)	21,31,31	0.97	1 (4%)
4	MTX	A	605	-	29,35,35	1.46	3 (10%)	38,49,49	2.08	12 (31%)
3	CB3	B	608	-	30,37,37	3.37	24 (80%)	38,51,51	3.18	17 (44%)
5	NDP	D	618	-	45,52,52	1.42	3 (6%)	53,80,80	1.21	3 (5%)
2	UMP	A	603	1	18,21,21	3.09	3 (16%)	21,31,31	0.96	2 (9%)
5	NDP	E	622	-	45,52,52	1.38	3 (6%)	53,80,80	1.19	2 (3%)

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
4	MTX	B	609	-	-	7/19/25/25	0/3/3/3
5	NDP	A	606	-	-	4/30/77/77	0/5/5/5
4	MTX	E	621	-	-	8/19/25/25	0/3/3/3
4	MTX	D	617	-	-	7/19/25/25	0/3/3/3
4	MTX	C	613	-	-	6/19/25/25	0/3/3/3
5	NDP	C	614	-	-	15/30/77/77	0/5/5/5
3	CB3	C	612	-	1/1/5/6	5/21/28/28	0/3/3/3
3	CB3	A	604	-	-	5/21/28/28	0/3/3/3
3	CB3	E	620	-	1/1/5/6	6/21/28/28	0/3/3/3
2	UMP	E	619	-	-	5/7/22/22	0/2/2/2
5	NDP	B	610	-	-	3/30/77/77	0/5/5/5
2	UMP	B	607	-	-	2/7/22/22	0/2/2/2
2	UMP	D	615	1	-	5/7/22/22	0/2/2/2
3	CB3	D	616	-	-	5/21/28/28	0/3/3/3
2	UMP	C	611	-	-	2/7/22/22	0/2/2/2
4	MTX	A	605	-	-	5/19/25/25	0/3/3/3
3	CB3	B	608	-	-	6/21/28/28	0/3/3/3
5	NDP	D	618	-	-	2/30/77/77	0/5/5/5
2	UMP	A	603	1	-	3/7/22/22	0/2/2/2
5	NDP	E	622	-	-	14/30/77/77	0/5/5/5

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	619	UMP	C6-N1	9.99	1.48	1.35
2	B	607	UMP	C6-N1	9.92	1.48	1.35
2	D	615	UMP	C6-N1	9.89	1.48	1.35
2	C	611	UMP	C6-N1	9.88	1.48	1.35
2	A	603	UMP	C6-N1	9.87	1.48	1.35
3	B	608	CB3	CP1-N10	-7.71	1.38	1.46
2	E	619	UMP	C6-C5	7.13	1.53	1.38
2	B	607	UMP	C6-C5	6.99	1.53	1.38
2	D	615	UMP	C6-C5	6.97	1.53	1.38
2	A	603	UMP	C6-C5	6.95	1.53	1.38
2	C	611	UMP	C6-C5	6.95	1.53	1.38
3	C	612	CB3	CB-CA	-6.27	1.45	1.53
5	B	610	NDP	C4N-C3N	-6.19	1.37	1.49
5	D	618	NDP	C4N-C3N	-6.08	1.38	1.49
5	A	606	NDP	C4N-C3N	-6.01	1.38	1.49
5	E	622	NDP	C4N-C3N	-5.98	1.38	1.49
5	C	614	NDP	C4N-C3N	-5.43	1.39	1.49
3	D	616	CB3	CP1-N10	-5.16	1.41	1.46
3	B	608	CB3	C12-C11	-4.88	1.30	1.39
3	E	620	CB3	O4-C4	4.80	1.36	1.24
3	B	608	CB3	C8A-N1	-4.68	1.29	1.37
4	E	621	MTX	O-C	4.67	1.32	1.23
4	C	613	MTX	O-C	4.62	1.32	1.23
3	C	612	CB3	C4A-C8A	-4.59	1.32	1.41
4	D	617	MTX	O-C	4.55	1.32	1.23
4	B	609	MTX	O-C	4.52	1.32	1.23
3	C	612	CB3	C5-C4A	-4.50	1.32	1.41
4	A	605	MTX	O-C	4.44	1.32	1.23
2	C	611	UMP	C4-N3	4.42	1.40	1.33
2	E	619	UMP	C4-N3	4.41	1.40	1.33
2	B	607	UMP	C4-N3	4.40	1.40	1.33
2	D	615	UMP	C4-N3	4.34	1.40	1.33
3	B	608	CB3	C4A-C8A	-4.33	1.33	1.41
2	A	603	UMP	C4-N3	4.33	1.40	1.33
3	A	604	CB3	C8-C8A	-4.31	1.34	1.41
3	C	612	CB3	CP1-N10	-4.15	1.42	1.46
5	B	610	NDP	C4N-C5N	-4.14	1.38	1.48
5	A	606	NDP	C4N-C5N	-4.13	1.38	1.48
3	A	604	CB3	CP1-N10	-4.10	1.42	1.46
3	C	612	CB3	CP1-CP2	-4.10	1.41	1.47
5	D	618	NDP	C4N-C5N	-4.09	1.38	1.48
3	B	608	CB3	C15-C14	-4.07	1.31	1.39
4	A	605	MTX	C-N	-4.05	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	609	MTX	C-N	-4.04	1.25	1.34
3	B	608	CB3	C9-N10	-4.03	1.40	1.46
3	B	608	CB3	C5-C4A	-4.02	1.33	1.41
3	B	608	CB3	O-C	-4.00	1.15	1.23
4	D	617	MTX	C-N	-3.97	1.25	1.34
5	E	622	NDP	C4N-C5N	-3.95	1.38	1.48
4	C	613	MTX	C-N	-3.86	1.25	1.34
3	A	604	CB3	C15-C14	-3.83	1.31	1.39
3	B	608	CB3	C-N	-3.81	1.25	1.34
3	B	608	CB3	C2-N3	-3.78	1.28	1.35
4	E	621	MTX	C-N	-3.77	1.26	1.34
5	C	614	NDP	C4N-C5N	-3.69	1.39	1.48
3	B	608	CB3	C8-C8A	-3.64	1.35	1.41
3	A	604	CB3	CP2-CP3	3.56	1.28	1.18
3	B	608	CB3	C11-C	-3.55	1.42	1.50
3	A	604	CB3	C4A-C8A	-3.51	1.34	1.41
5	C	614	NDP	C6N-C5N	3.43	1.39	1.33
3	E	620	CB3	CP2-CP3	3.39	1.28	1.18
3	C	612	CB3	C12-C11	-3.36	1.33	1.39
3	A	604	CB3	C13-C14	-3.34	1.32	1.39
3	D	616	CB3	CP1-CP2	-3.33	1.42	1.47
3	D	616	CB3	O-C	-3.26	1.16	1.23
3	A	604	CB3	C8A-N1	-3.26	1.32	1.37
3	B	608	CB3	C9-C6	-3.25	1.45	1.51
3	A	604	CB3	C5-C4A	-3.25	1.35	1.41
3	D	616	CB3	O4-C4	3.23	1.32	1.24
3	D	616	CB3	C8-C8A	-3.20	1.36	1.41
5	E	622	NDP	C6N-C5N	3.12	1.38	1.33
3	C	612	CB3	C8A-N1	-3.07	1.32	1.37
5	D	618	NDP	C6N-C5N	3.04	1.38	1.33
3	B	608	CB3	CA-N	-3.04	1.42	1.46
3	A	604	CB3	C2-N3	-3.01	1.30	1.35
3	D	616	CB3	C-N	-3.01	1.27	1.34
3	D	616	CB3	C4A-C8A	-2.95	1.35	1.41
3	B	608	CB3	C7-C6	-2.85	1.32	1.38
3	C	612	CB3	C2-N3	-2.83	1.30	1.35
3	C	612	CB3	C8-C8A	-2.83	1.36	1.41
3	B	608	CB3	CP1-CP2	-2.82	1.43	1.47
3	B	608	CB3	O4-C4	2.82	1.31	1.24
3	C	612	CB3	C-N	-2.78	1.28	1.34
5	B	610	NDP	C6N-C5N	2.78	1.38	1.33
3	C	612	CB3	C11-C	-2.77	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	612	CB3	O-C	-2.75	1.17	1.23
3	B	608	CB3	CB-CA	-2.72	1.50	1.53
3	C	612	CB3	C9-C6	-2.65	1.46	1.51
5	A	606	NDP	C6N-C5N	2.63	1.38	1.33
3	C	612	CB3	O4-C4	2.60	1.31	1.24
3	B	608	CB3	C13-C12	-2.59	1.34	1.38
3	B	608	CB3	C2-NA2	-2.57	1.28	1.33
3	A	604	CB3	O-C	-2.55	1.18	1.23
3	B	608	CB3	C16-C15	-2.54	1.34	1.38
3	B	608	CB3	C16-C11	-2.52	1.35	1.39
3	D	616	CB3	C12-C11	-2.49	1.35	1.39
3	B	608	CB3	C13-C14	-2.46	1.34	1.39
3	D	616	CB3	C11-C	-2.40	1.45	1.50
3	D	616	CB3	C16-C11	-2.39	1.35	1.39
3	D	616	CB3	C5-C4A	-2.39	1.36	1.41
3	D	616	CB3	CP2-CP3	2.35	1.25	1.18
3	D	616	CB3	C8A-N1	-2.33	1.33	1.37
3	D	616	CB3	C9-N10	-2.30	1.43	1.46
3	A	604	CB3	C16-C11	-2.29	1.35	1.39
3	C	612	CB3	CA-N	-2.25	1.43	1.46
3	A	604	CB3	O4-C4	2.23	1.30	1.24
4	A	605	MTX	C8A-N8	-2.19	1.34	1.37
3	A	604	CB3	C14-N10	-2.17	1.33	1.38
3	C	612	CB3	C13-C14	-2.14	1.35	1.39
3	D	616	CB3	C7-C6	-2.08	1.34	1.38
3	C	612	CB3	C2-NA2	-2.08	1.29	1.33
3	D	616	CB3	C13-C14	-2.07	1.35	1.39
3	B	608	CB3	CP2-CP3	2.07	1.24	1.18
4	B	609	MTX	C8A-N8	-2.04	1.34	1.37
3	C	612	CB3	C9-N10	-2.02	1.43	1.46

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	608	CB3	C4A-C8A-N1	-12.96	116.56	123.60
3	C	612	CB3	C4A-C8A-N1	-11.18	117.53	123.60
3	D	616	CB3	C4A-C4-N3	-8.14	118.73	124.40
3	B	608	CB3	C4A-C4-N3	-7.79	118.97	124.40
3	E	620	CB3	C4A-C8A-N1	-7.45	119.56	123.60
3	E	620	CB3	C4A-C4-N3	-7.09	119.46	124.40
3	A	604	CB3	CP1-N10-C9	6.95	123.72	117.10
3	C	612	CB3	CB-CA-N	-6.90	100.14	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	616	CB3	C4A-C8A-N1	-6.31	120.17	123.60
3	A	604	CB3	C4A-C4-N3	-6.26	120.04	124.40
3	A	604	CB3	CP1-N10-C14	-5.76	108.06	119.01
3	A	604	CB3	C13-C14-N10	-5.31	114.06	121.38
3	C	612	CB3	CG-CB-CA	-4.99	102.96	113.04
3	A	604	CB3	N1-C2-N3	-4.90	120.69	127.22
4	B	609	MTX	N1-C2-N3	-4.85	120.75	127.22
3	E	620	CB3	N1-C2-N3	-4.84	120.76	127.22
4	E	621	MTX	N1-C2-N3	-4.80	120.82	127.22
3	A	604	CB3	C4A-C8A-N1	-4.78	121.00	123.60
4	A	605	MTX	N1-C2-N3	-4.78	120.85	127.22
5	D	618	NDP	N3A-C2A-N1A	-4.78	121.21	128.68
5	E	622	NDP	N3A-C2A-N1A	-4.72	121.31	128.68
5	C	614	NDP	N3A-C2A-N1A	-4.66	121.39	128.68
4	D	617	MTX	N1-C2-N3	-4.65	121.02	127.22
5	A	606	NDP	N3A-C2A-N1A	-4.65	121.41	128.68
3	B	608	CB3	C6-C9-N10	-4.59	106.81	114.18
4	D	617	MTX	CB-CA-N	-4.57	103.54	110.19
5	B	610	NDP	N3A-C2A-N1A	-4.54	121.58	128.68
4	C	613	MTX	N1-C2-N3	-4.43	121.31	127.22
3	C	612	CB3	C9-N10-C14	4.39	128.32	120.78
3	A	604	CB3	C9-N10-C14	4.33	128.22	120.78
3	C	612	CB3	C4A-C4-N3	-4.29	121.41	124.40
4	A	605	MTX	C6-C9-N10	-4.25	106.32	113.60
3	C	612	CB3	C13-C14-N10	-4.22	115.56	121.38
3	C	612	CB3	CA-N-C	4.22	127.78	122.34
4	C	613	MTX	C2-N1-C8A	4.21	120.16	115.36
4	D	617	MTX	C6-C9-N10	-4.19	106.41	113.60
3	A	604	CB3	C11-C-N	4.17	125.06	117.06
3	D	616	CB3	N1-C2-N3	-4.16	121.67	127.22
4	D	617	MTX	C2-N1-C8A	4.14	120.08	115.36
5	D	618	NDP	PN-O3-PA	-4.13	118.65	132.83
3	B	608	CB3	CB-CA-N	-4.08	104.25	110.19
4	E	621	MTX	C2-N1-C8A	4.07	120.01	115.36
4	A	605	MTX	CB-CA-N	-4.05	104.29	110.19
4	B	609	MTX	C2-N1-C8A	4.05	119.98	115.36
4	A	605	MTX	C2-N1-C8A	4.03	119.95	115.36
4	B	609	MTX	C6-C9-N10	-3.99	106.76	113.60
4	B	609	MTX	N8-C8A-N1	3.97	120.35	115.82
4	A	605	MTX	N8-C8A-N1	3.96	120.34	115.82
3	C	612	CB3	C15-C14-N10	3.93	126.80	121.38
4	C	613	MTX	C6-C9-N10	-3.91	106.89	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	613	MTX	N8-C8A-N1	3.91	120.28	115.82
4	D	617	MTX	N8-C8A-N1	3.83	120.19	115.82
3	A	604	CB3	O-C-N	-3.76	115.53	122.45
3	A	604	CB3	C15-C14-N10	3.73	126.52	121.38
3	B	608	CB3	C13-C12-C11	-3.73	116.44	120.78
3	C	612	CB3	C11-C-N	-3.70	109.98	117.06
3	A	604	CB3	CB-CG-CD	-3.67	105.71	113.59
3	A	604	CB3	C16-C11-C12	-3.65	113.39	118.59
3	A	604	CB3	C4-N3-C2	3.61	121.66	115.93
5	C	614	NDP	PN-O3-PA	-3.59	120.49	132.83
3	E	620	CB3	CB-CA-N	-3.57	105.00	110.19
3	D	616	CB3	C9-N10-C14	3.54	126.86	120.78
4	E	621	MTX	N8-C8A-N1	3.49	119.81	115.82
4	E	621	MTX	C6-C9-N10	-3.48	107.64	113.60
5	E	622	NDP	PN-O3-PA	-3.44	121.01	132.83
3	A	604	CB3	CB-CA-N	3.41	115.16	110.19
3	B	608	CB3	C12-C13-C14	3.24	124.59	120.32
3	C	612	CB3	NA2-C2-N3	3.18	122.19	117.25
3	B	608	CB3	C9-N10-C14	3.14	126.17	120.78
3	D	616	CB3	O-C-N	-3.13	116.70	122.45
4	C	613	MTX	CB-CA-N	-3.12	105.65	110.19
4	C	613	MTX	C7-N8-C8A	3.08	119.78	116.69
3	E	620	CB3	CP1-N10-C9	3.04	120.00	117.10
4	C	613	MTX	C6-C7-N8	-3.02	120.17	123.13
3	B	608	CB3	N1-C2-N3	-3.00	123.22	127.22
5	A	606	NDP	PN-O3-PA	-2.98	122.61	132.83
3	E	620	CB3	C6-C9-N10	-2.96	109.43	114.18
3	A	604	CB3	C6-C5-C4A	-2.94	118.25	122.65
4	A	605	MTX	C7-N8-C8A	2.93	119.64	116.69
3	B	608	CB3	CG-CB-CA	2.93	118.96	113.04
4	B	609	MTX	CB-CA-N	-2.92	105.94	110.19
4	E	621	MTX	C7-N8-C8A	2.92	119.63	116.69
3	E	620	CB3	C4-N3-C2	2.91	120.55	115.93
4	B	609	MTX	C7-N8-C8A	2.88	119.58	116.69
2	E	619	UMP	O5'-P-OP1	2.88	114.54	106.47
3	C	612	CB3	N1-C2-N3	-2.87	123.39	127.22
4	E	621	MTX	C6-C7-N8	-2.84	120.34	123.13
3	D	616	CB3	C4-N3-C2	2.83	120.42	115.93
4	A	605	MTX	C13-C14-N10	-2.82	117.56	121.62
3	D	616	CB3	C13-C14-N10	-2.72	117.63	121.38
4	D	617	MTX	C6-C7-N8	-2.71	120.47	123.13
4	E	621	MTX	C4A-C4-N3	-2.68	119.25	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	621	MTX	CB-CA-N	-2.68	106.29	110.19
4	D	617	MTX	C7-N8-C8A	2.68	119.39	116.69
3	B	608	CB3	C8-C8A-C4A	2.67	123.73	120.05
3	D	616	CB3	C11-C-N	2.65	122.15	117.06
3	D	616	CB3	CA-N-C	-2.65	118.92	122.34
4	A	605	MTX	C4A-C4-N3	-2.64	119.27	121.01
4	B	609	MTX	C4A-C4-N3	-2.62	119.29	121.01
5	B	610	NDP	PN-O3-PA	-2.61	123.86	132.83
2	C	611	UMP	O5'-P-OP1	2.61	113.80	106.47
3	C	612	CB3	C4-C4A-C8A	2.61	120.86	118.59
3	C	612	CB3	C8-C8A-N1	2.61	122.67	118.69
4	B	609	MTX	C6-C7-N8	-2.59	120.58	123.13
4	A	605	MTX	C6-C7-N8	-2.58	120.59	123.13
2	B	607	UMP	O5'-P-OP1	2.58	113.72	106.47
2	A	603	UMP	O5'-P-OP1	2.56	113.67	106.47
3	C	612	CB3	C6-C9-N10	-2.56	110.06	114.18
3	B	608	CB3	C4-C4A-C8A	2.56	120.82	118.59
5	C	614	NDP	C3D-C2D-C1D	2.54	106.25	101.43
3	B	608	CB3	CA-N-C	-2.52	119.09	122.34
4	D	617	MTX	C13-C14-N10	-2.51	118.01	121.62
3	A	604	CB3	C15-C16-C11	2.47	123.66	120.78
4	A	605	MTX	CB-CG-CD	-2.47	108.27	113.59
4	D	617	MTX	CB-CG-CD	-2.42	108.38	113.59
4	A	605	MTX	CA-N-C	2.41	125.45	122.34
4	D	617	MTX	C4A-C4-N3	-2.39	119.44	121.01
3	A	604	CB3	CG-CB-CA	2.39	117.87	113.04
3	C	612	CB3	C12-C13-C14	2.37	123.44	120.32
3	B	608	CB3	C7-C6-C5	2.37	123.44	118.85
3	C	612	CB3	O-C-C11	2.36	125.15	120.94
3	B	608	CB3	C8-C7-C6	-2.35	116.30	121.14
4	A	605	MTX	CM-N10-C9	2.30	120.96	114.84
4	C	613	MTX	C13-C14-N10	-2.28	118.34	121.62
4	B	609	MTX	CM-N10-C9	2.28	120.90	114.84
3	B	608	CB3	NA2-C2-N3	2.26	120.76	117.25
3	B	608	CB3	C2-N1-C8A	2.25	121.89	116.33
2	D	615	UMP	O5'-P-OP1	2.23	112.73	106.47
3	D	616	CB3	C8-C8A-N1	2.23	122.09	118.69
5	A	606	NDP	O3X-P2B-O2X	2.21	116.06	107.64
3	D	616	CB3	NA2-C2-N3	2.19	120.65	117.25
3	B	608	CB3	CP1-N10-C9	-2.18	115.03	117.10
3	D	616	CB3	CP1-N10-C14	-2.15	114.92	119.01
3	A	604	CB3	C13-C12-C11	2.13	123.25	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	612	CB3	NA2-C2-N1	-2.09	114.38	117.79
3	C	612	CB3	CP1-N10-C14	-2.07	115.07	119.01
3	A	604	CB3	C6-C9-N10	-2.07	110.86	114.18
5	D	618	NDP	O3X-P2B-O2X	2.05	115.45	107.64
5	B	610	NDP	O3X-P2B-O2X	2.04	115.41	107.64
2	D	615	UMP	C5-C6-N1	-2.02	116.18	120.68
2	A	603	UMP	C5-C6-N1	-2.01	116.20	120.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	612	CB3	CA
3	E	620	CB3	CA

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	615	UMP	C3'-C4'-C5'-O5'
2	D	615	UMP	C5'-O5'-P-OP1
2	D	615	UMP	C5'-O5'-P-OP2
2	D	615	UMP	C5'-O5'-P-OP3
2	E	619	UMP	C3'-C4'-C5'-O5'
2	E	619	UMP	C5'-O5'-P-OP2
2	E	619	UMP	C5'-O5'-P-OP3
3	A	604	CB3	CT-CA-CB-CG
3	A	604	CB3	CA-CB-CG-CD
3	B	608	CB3	N-CA-CB-CG
3	B	608	CB3	CT-CA-CB-CG
3	B	608	CB3	CA-CB-CG-CD
3	C	612	CB3	CB-CA-N-C
3	D	616	CB3	CB-CA-N-C
3	D	616	CB3	CT-CA-N-C
3	D	616	CB3	CA-CB-CG-CD
3	E	620	CB3	CB-CA-N-C
3	E	620	CB3	CT-CA-CB-CG
4	A	605	MTX	CT-CA-N-C
4	B	609	MTX	CT-CA-N-C
4	B	609	MTX	CT-CA-CB-CG
4	C	613	MTX	CT-CA-N-C
4	C	613	MTX	CT-CA-CB-CG
4	D	617	MTX	C13-C14-N10-CM
4	D	617	MTX	C15-C14-N10-CM

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Mol	Chain	Res	Type	Atoms
4	D	617	MTX	CT-CA-N-C
4	E	621	MTX	CT-CA-N-C
4	E	621	MTX	CT-CA-CB-CG
5	B	610	NDP	C2B-O2B-P2B-O2X
5	C	614	NDP	O4B-C4B-C5B-O5B
5	C	614	NDP	C3B-C4B-C5B-O5B
5	C	614	NDP	C5D-O5D-PN-O3
5	C	614	NDP	C5D-O5D-PN-O1N
5	C	614	NDP	C5D-O5D-PN-O2N
5	C	614	NDP	C3D-C4D-C5D-O5D
5	E	622	NDP	C3B-C4B-C5B-O5B
5	E	622	NDP	C2B-O2B-P2B-O3X
5	E	622	NDP	C5D-O5D-PN-O2N
3	A	604	CB3	N-CA-CB-CG
4	C	613	MTX	N-CA-CB-CG
2	B	607	UMP	O4'-C4'-C5'-O5'
2	D	615	UMP	O4'-C4'-C5'-O5'
3	B	608	CB3	C6-C9-N10-C14
5	E	622	NDP	C1B-C2B-O2B-P2B
3	A	604	CB3	C6-C9-N10-C14
5	E	622	NDP	C3B-C2B-O2B-P2B
2	A	603	UMP	C3'-C4'-C5'-O5'
2	B	607	UMP	C3'-C4'-C5'-O5'
2	E	619	UMP	O4'-C4'-C5'-O5'
5	C	614	NDP	O4D-C4D-C5D-O5D
5	E	622	NDP	O4B-C4B-C5B-O5B
4	C	613	MTX	C13-C14-N10-CM
4	C	613	MTX	C15-C14-N10-CM
2	A	603	UMP	O4'-C4'-C5'-O5'
2	E	619	UMP	C5'-O5'-P-OP1
5	E	622	NDP	PN-O3-PA-O1A
4	B	609	MTX	C13-C14-N10-CM
4	E	621	MTX	C13-C14-N10-CM
4	A	605	MTX	CB-CA-N-C
4	B	609	MTX	CB-CA-N-C
4	C	613	MTX	CB-CA-N-C
4	D	617	MTX	CB-CA-N-C
4	E	621	MTX	CB-CA-N-C
5	E	622	NDP	C3D-C4D-C5D-O5D
4	E	621	MTX	N-CA-CB-CG
4	B	609	MTX	C15-C14-N10-CM
4	E	621	MTX	C15-C14-N10-CM

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Mol	Chain	Res	Type	Atoms
3	C	612	CB3	N-CA-CB-CG
3	E	620	CB3	N-CA-CB-CG
5	A	606	NDP	PA-O3-PN-O5D
2	C	611	UMP	O4'-C4'-C5'-O5'
5	A	606	NDP	C2B-O2B-P2B-O2X
5	E	622	NDP	C5D-O5D-PN-O3
2	C	611	UMP	C3'-C4'-C5'-O5'
3	B	608	CB3	C6-C9-N10-CP1
5	C	614	NDP	C4B-C5B-O5B-PA
5	C	614	NDP	C5B-O5B-PA-O2A
5	E	622	NDP	C5D-O5D-PN-O1N
4	A	605	MTX	C6-C9-N10-CM
4	B	609	MTX	C6-C9-N10-CM
4	D	617	MTX	C6-C9-N10-CM
4	E	621	MTX	C6-C9-N10-CM
5	C	614	NDP	O4D-C1D-N1N-C2N
3	A	604	CB3	C6-C9-N10-CP1
3	C	612	CB3	C6-C9-N10-CP1
2	A	603	UMP	C5'-O5'-P-OP1
3	C	612	CB3	C6-C9-N10-C14
3	D	616	CB3	C6-C9-N10-C14
5	C	614	NDP	C2D-C1D-N1N-C2N
5	A	606	NDP	O4D-C1D-N1N-C2N
5	B	610	NDP	O4D-C1D-N1N-C2N
5	E	622	NDP	O4D-C1D-N1N-C2N
5	E	622	NDP	PN-O3-PA-O2A
3	C	612	CB3	CA-CB-CG-CD
5	D	618	NDP	O4D-C1D-N1N-C2N
4	D	617	MTX	C13-C14-N10-C9
3	D	616	CB3	C6-C9-N10-CP1
5	B	610	NDP	C2D-C1D-N1N-C2N
4	A	605	MTX	C15-C14-N10-CM
3	E	620	CB3	C5-C6-C9-N10
4	B	609	MTX	N-CA-CB-CG
4	A	605	MTX	C13-C14-N10-CM
4	D	617	MTX	C15-C14-N10-C9
5	C	614	NDP	C2D-C1D-N1N-C6N
3	E	620	CB3	CT-CA-N-C
5	C	614	NDP	O4D-C1D-N1N-C6N
3	E	620	CB3	C7-C6-C9-N10
5	A	606	NDP	C2B-O2B-P2B-O3X
5	C	614	NDP	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
4	E	621	MTX	CA-CB-CG-CD
5	D	618	NDP	C2N-C3N-C7N-N7N
5	E	622	NDP	C2N-C3N-C7N-N7N
3	B	608	CB3	CT-CA-N-C
5	C	614	NDP	C3B-C2B-O2B-P2B
5	E	622	NDP	C4D-C5D-O5D-PN

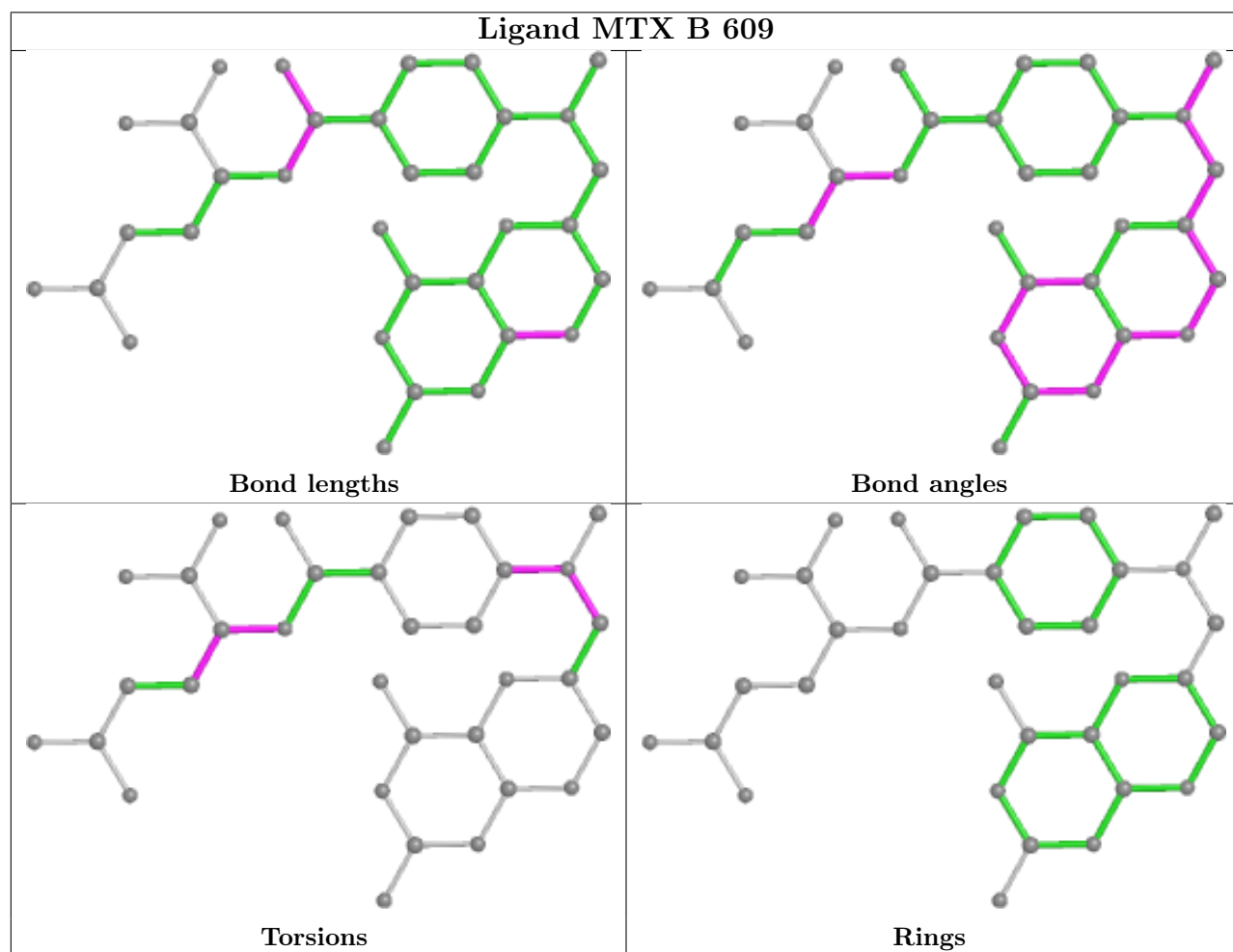
There are no ring outliers.

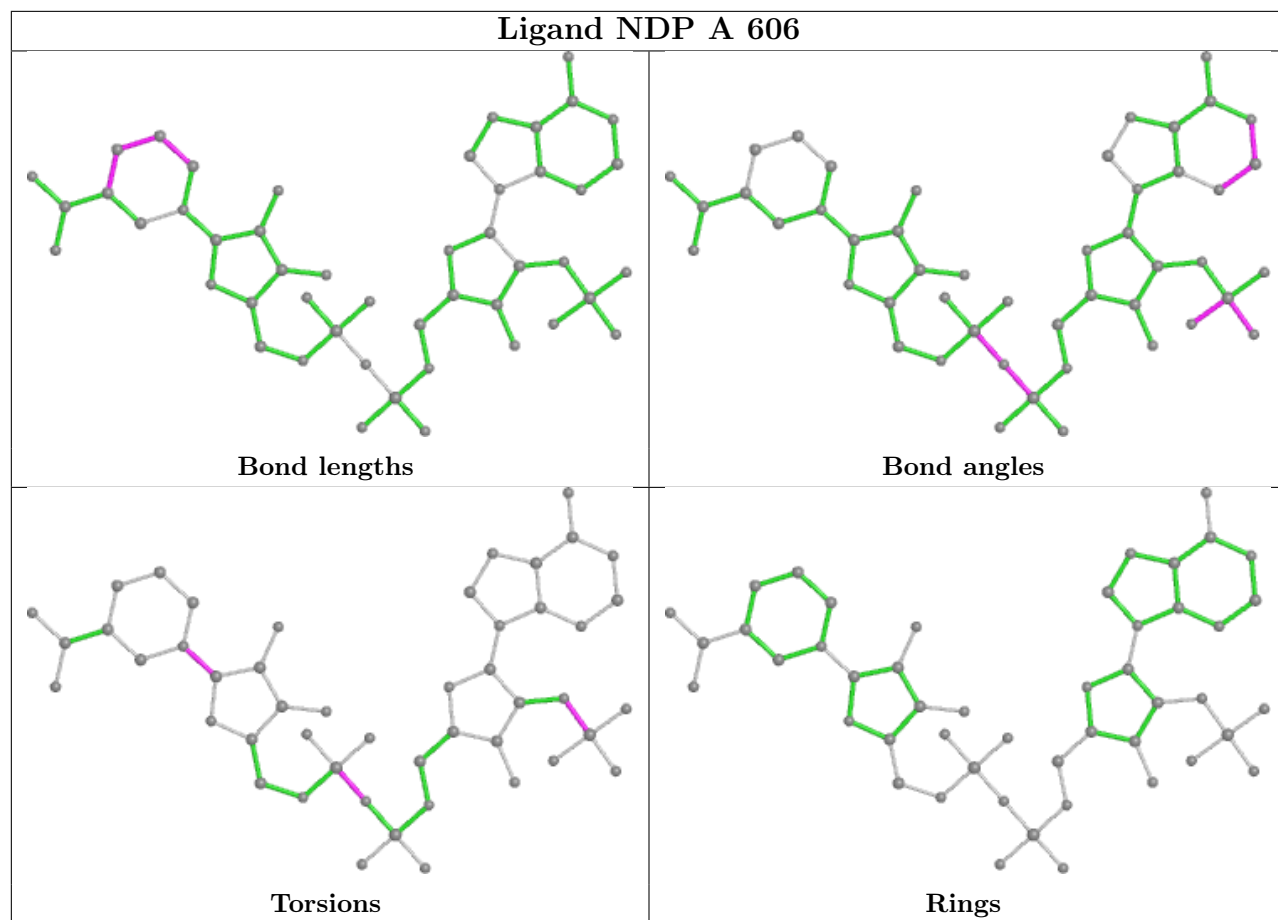
20 monomers are involved in 132 short contacts:

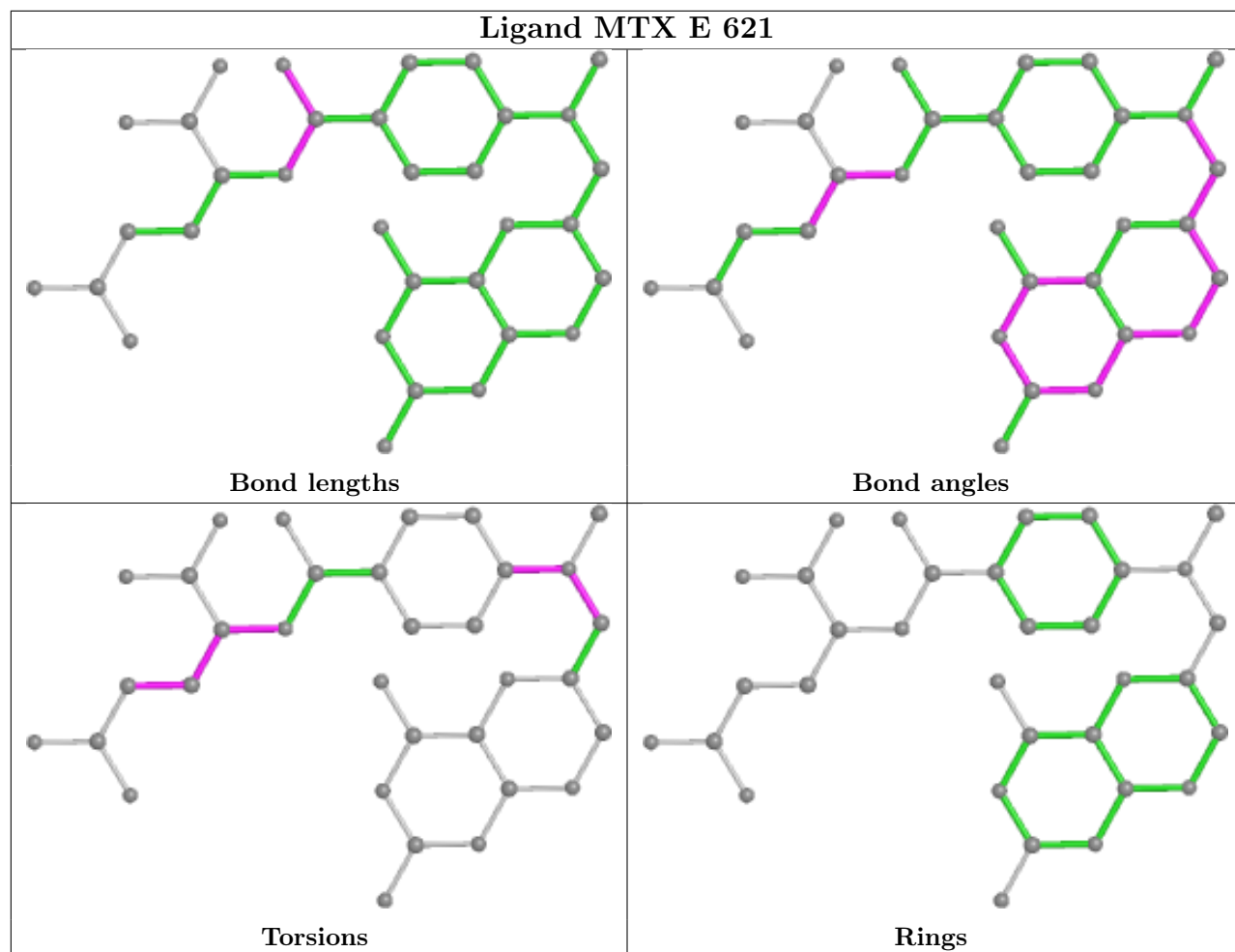
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	609	MTX	8	0
5	A	606	NDP	5	0
4	E	621	MTX	10	0
4	D	617	MTX	7	0
4	C	613	MTX	6	0
5	C	614	NDP	12	0
3	C	612	CB3	9	0
3	A	604	CB3	2	0
3	E	620	CB3	17	0
2	E	619	UMP	8	0
5	B	610	NDP	8	0
2	B	607	UMP	2	0
2	D	615	UMP	5	0
3	D	616	CB3	4	0
2	C	611	UMP	5	0
4	A	605	MTX	6	0
3	B	608	CB3	7	0
5	D	618	NDP	7	0
2	A	603	UMP	3	0
5	E	622	NDP	12	0

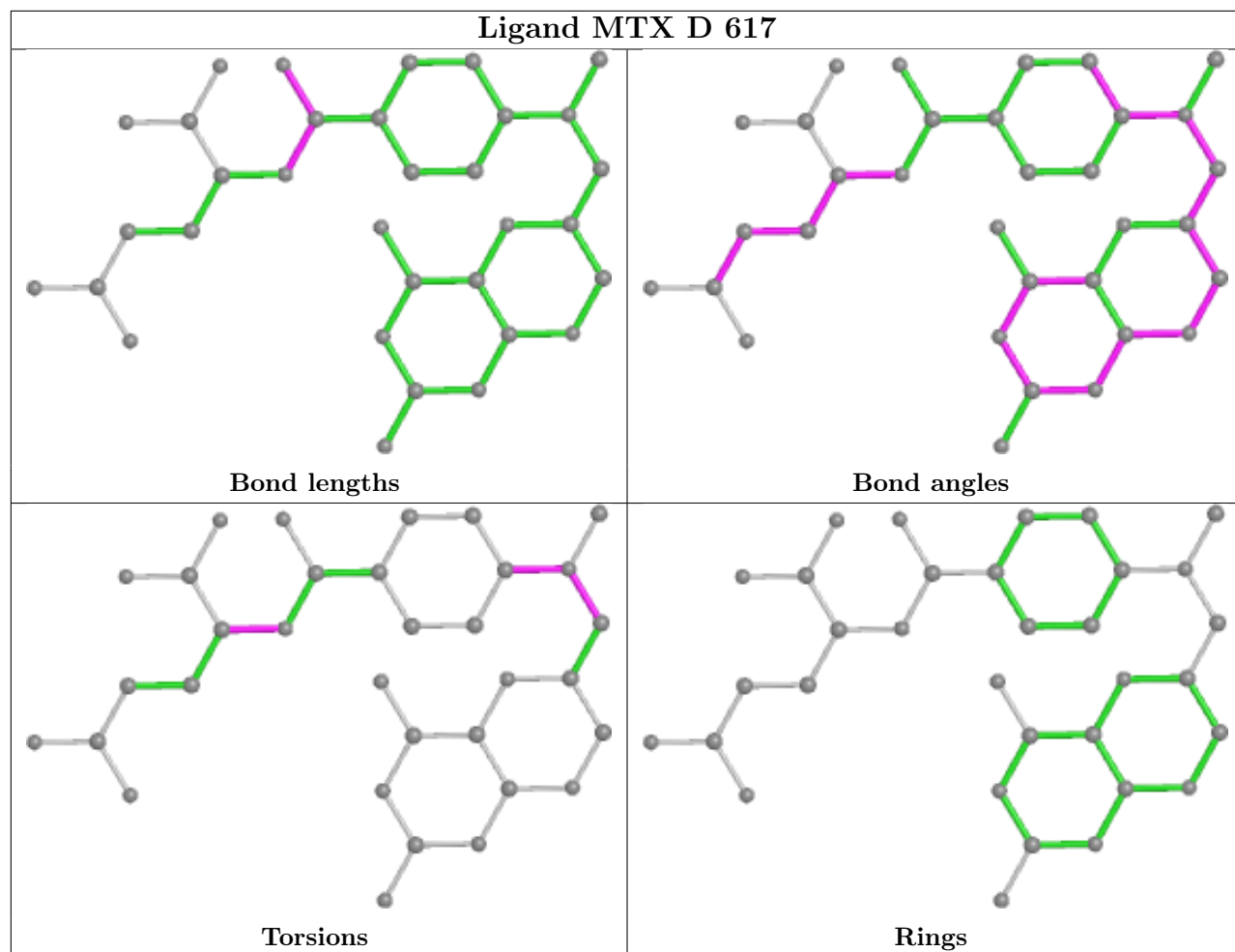
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

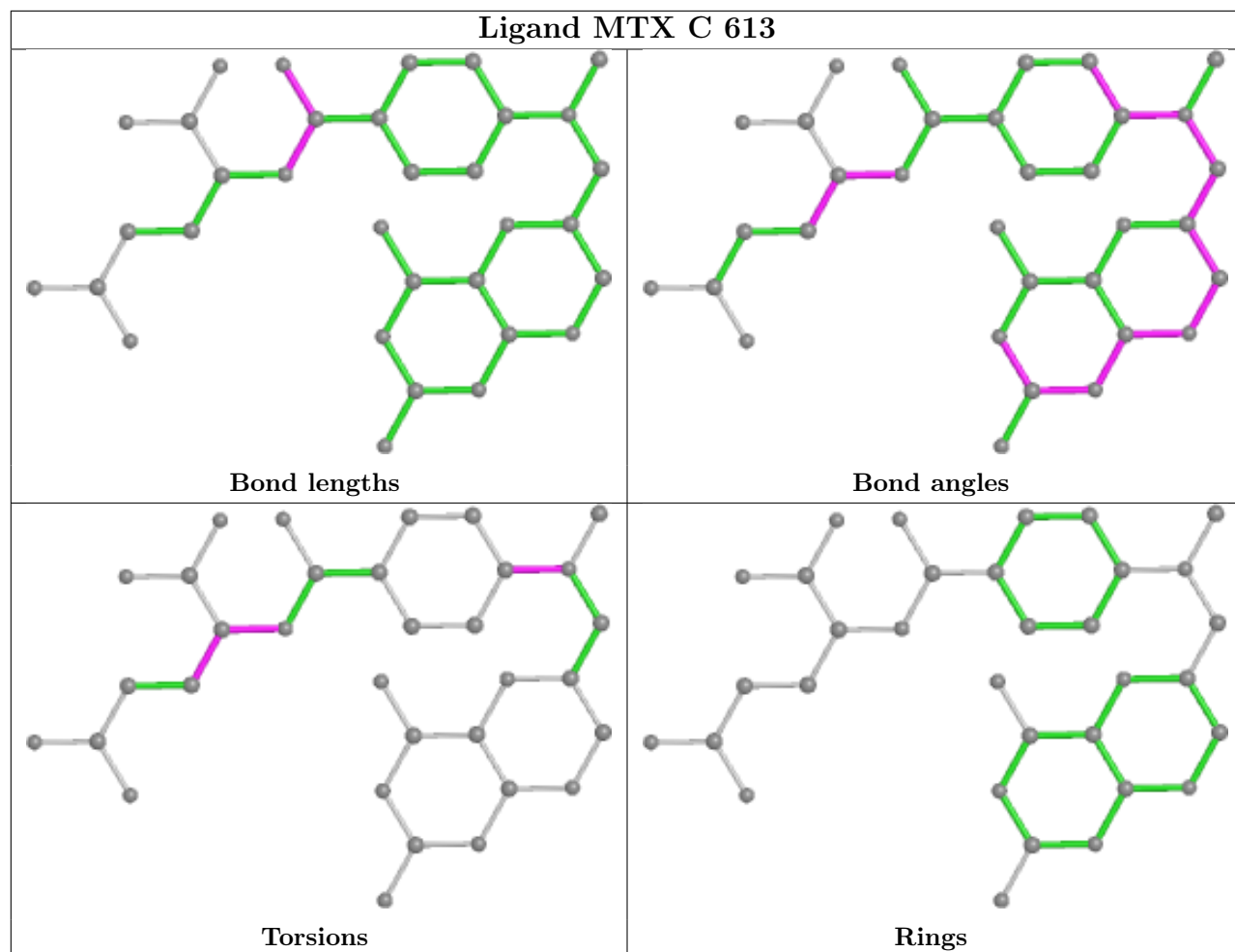
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

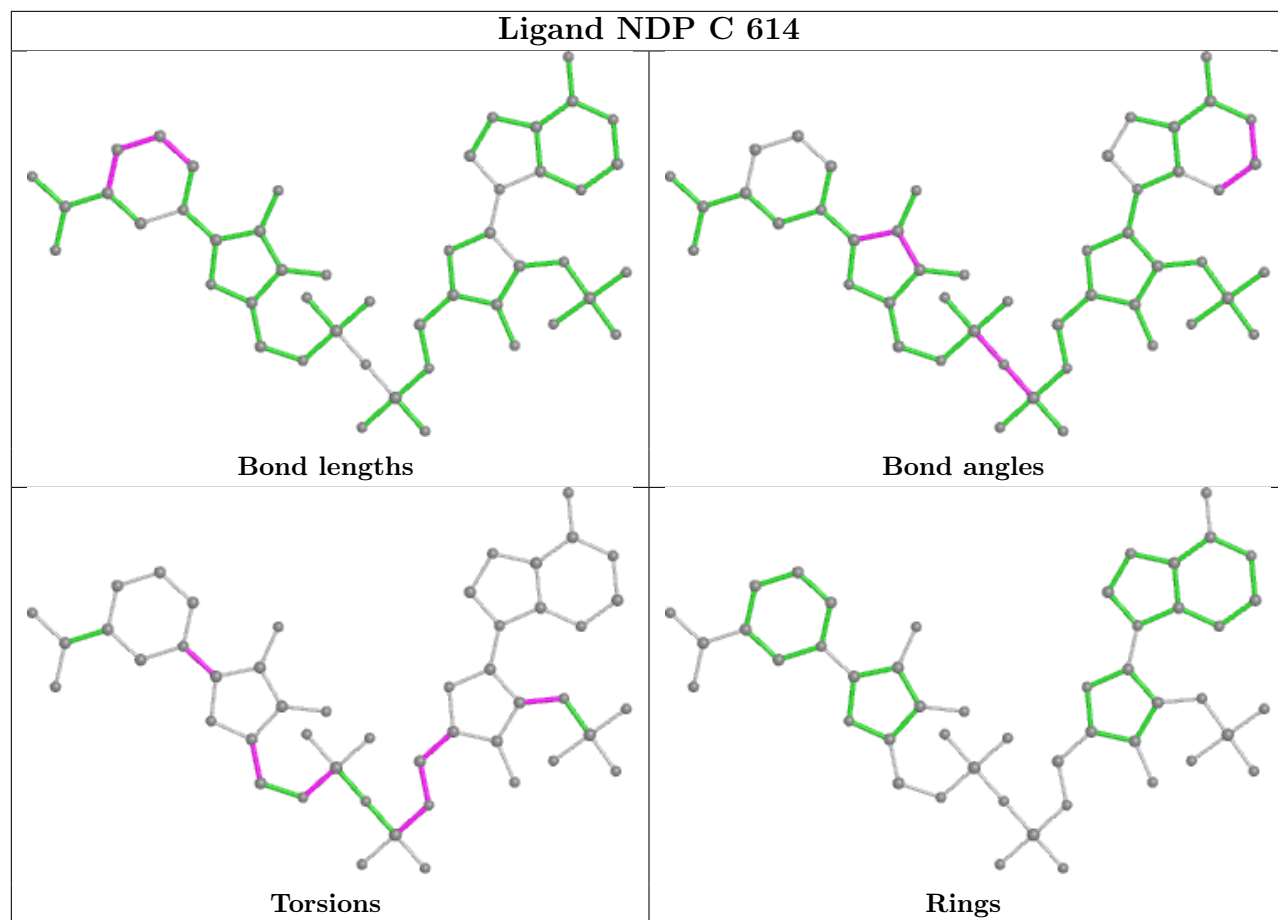


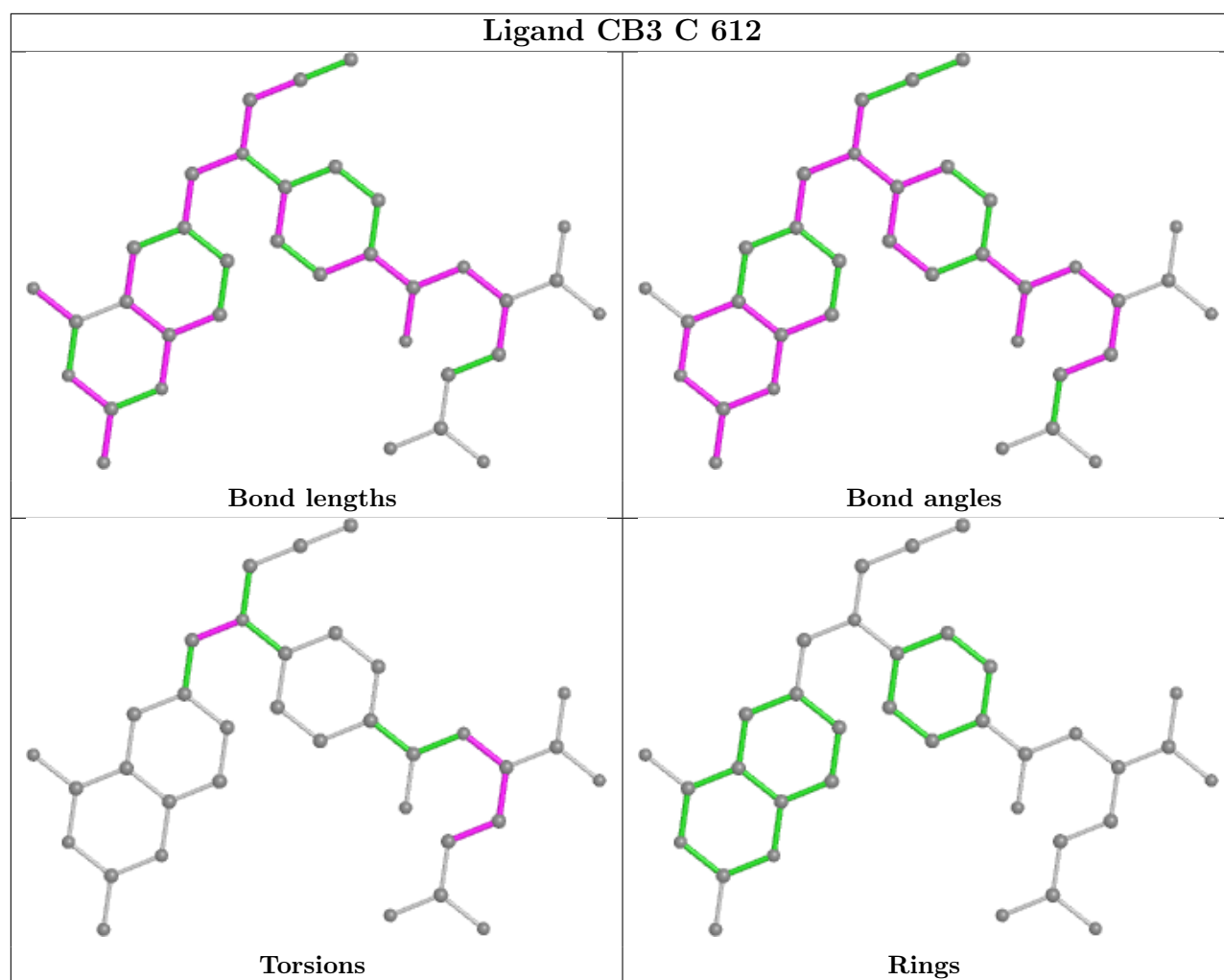


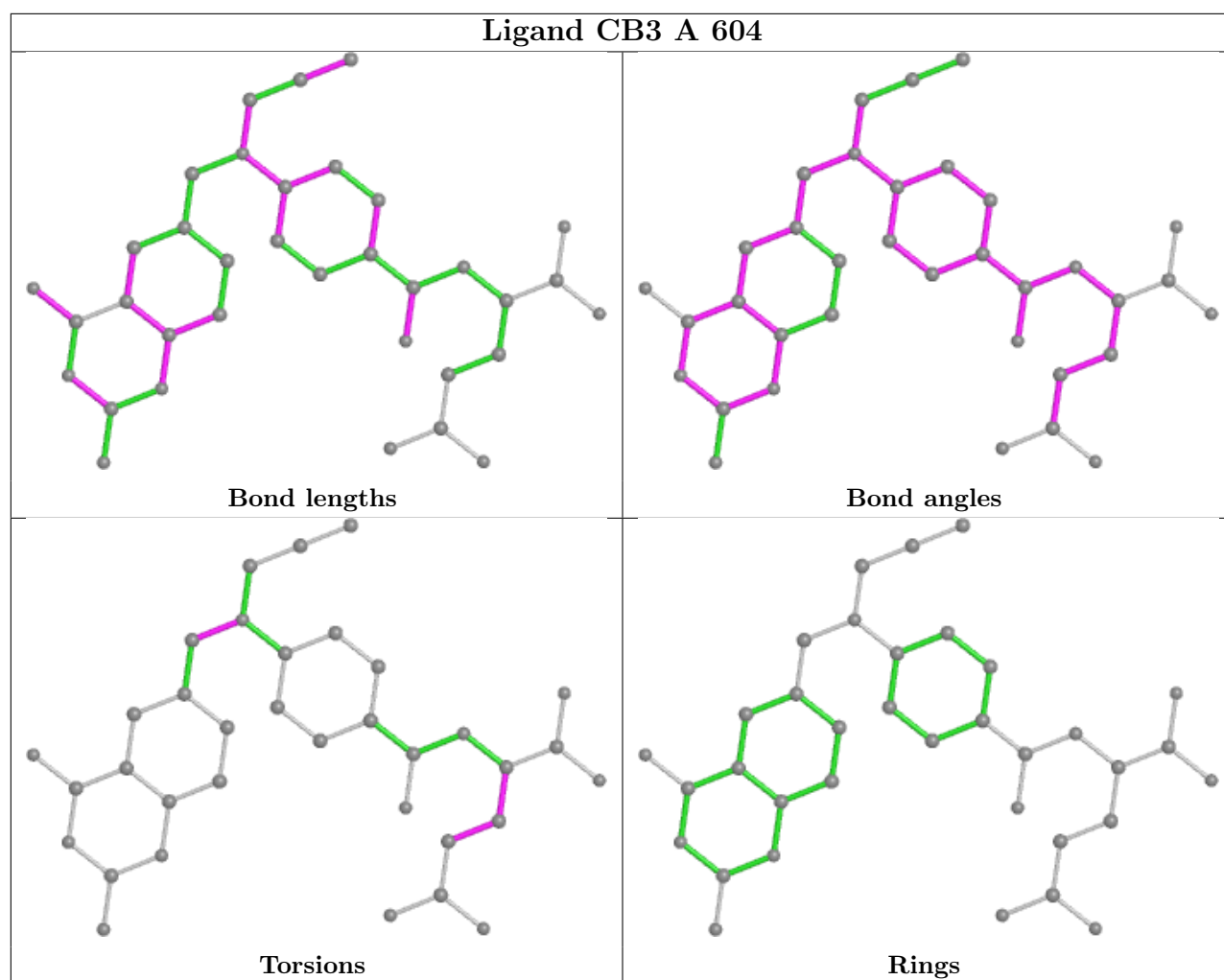




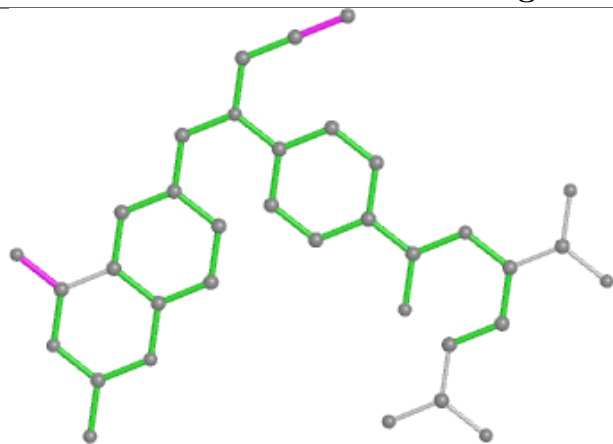




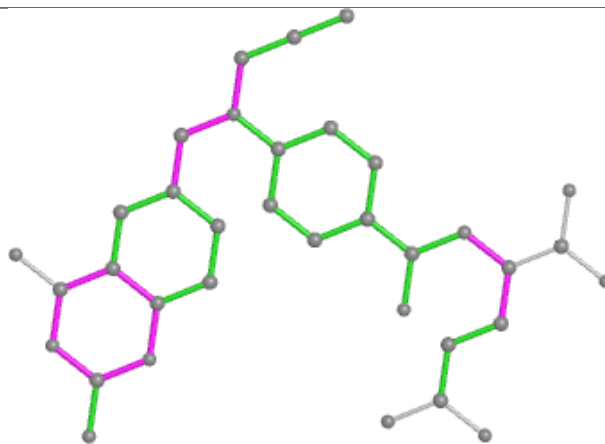




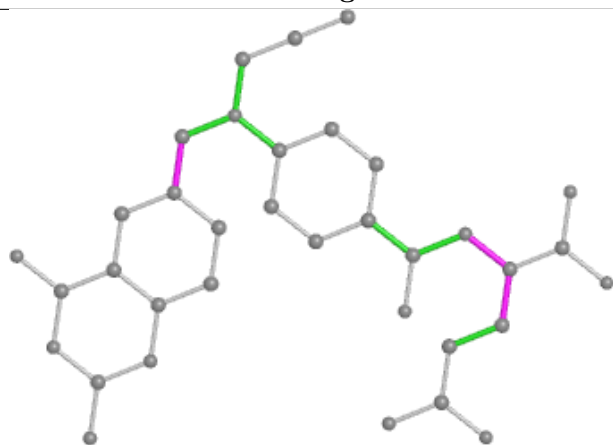
## Ligand CB3 E 620



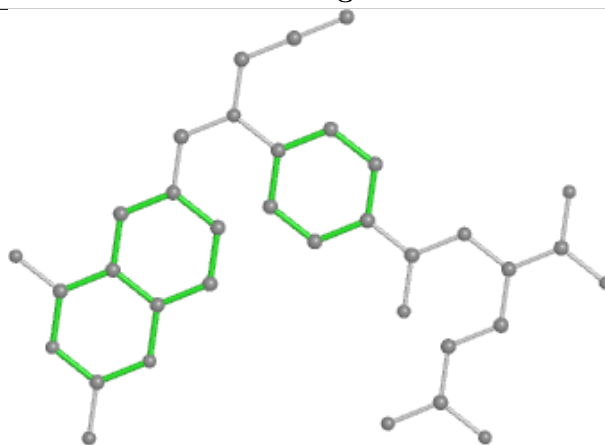
Bond lengths



Bond angles

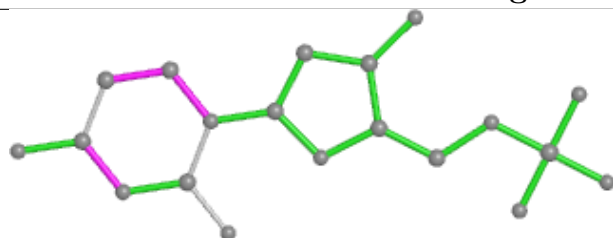


Torsions

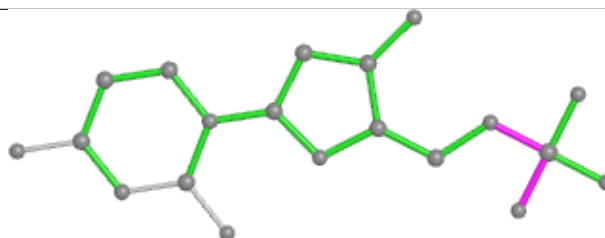


Rings

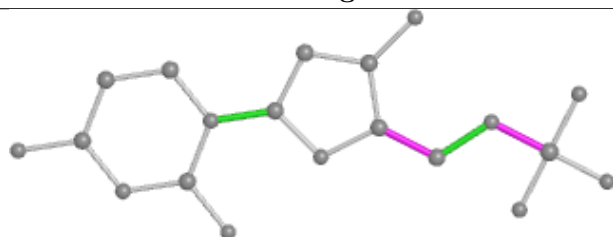
## Ligand UMP E 619



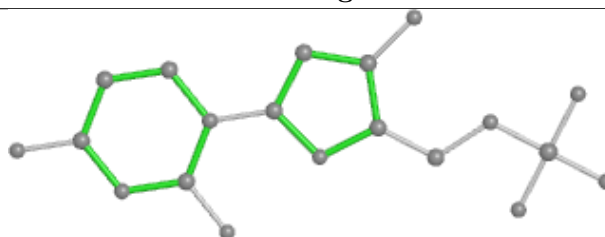
Bond lengths



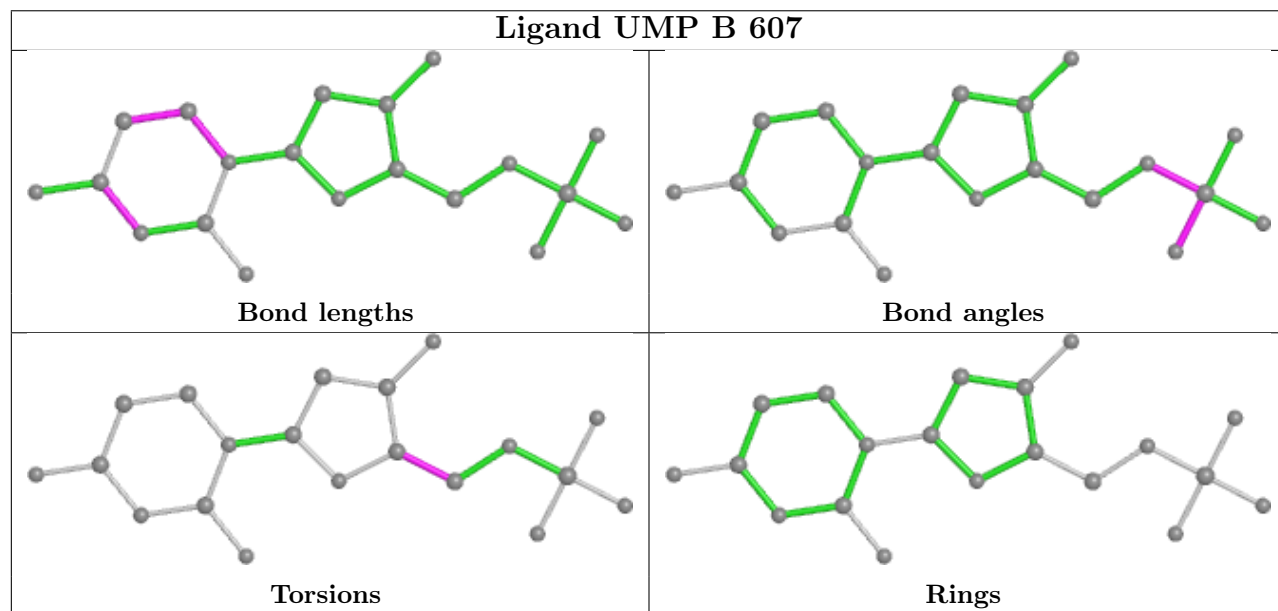
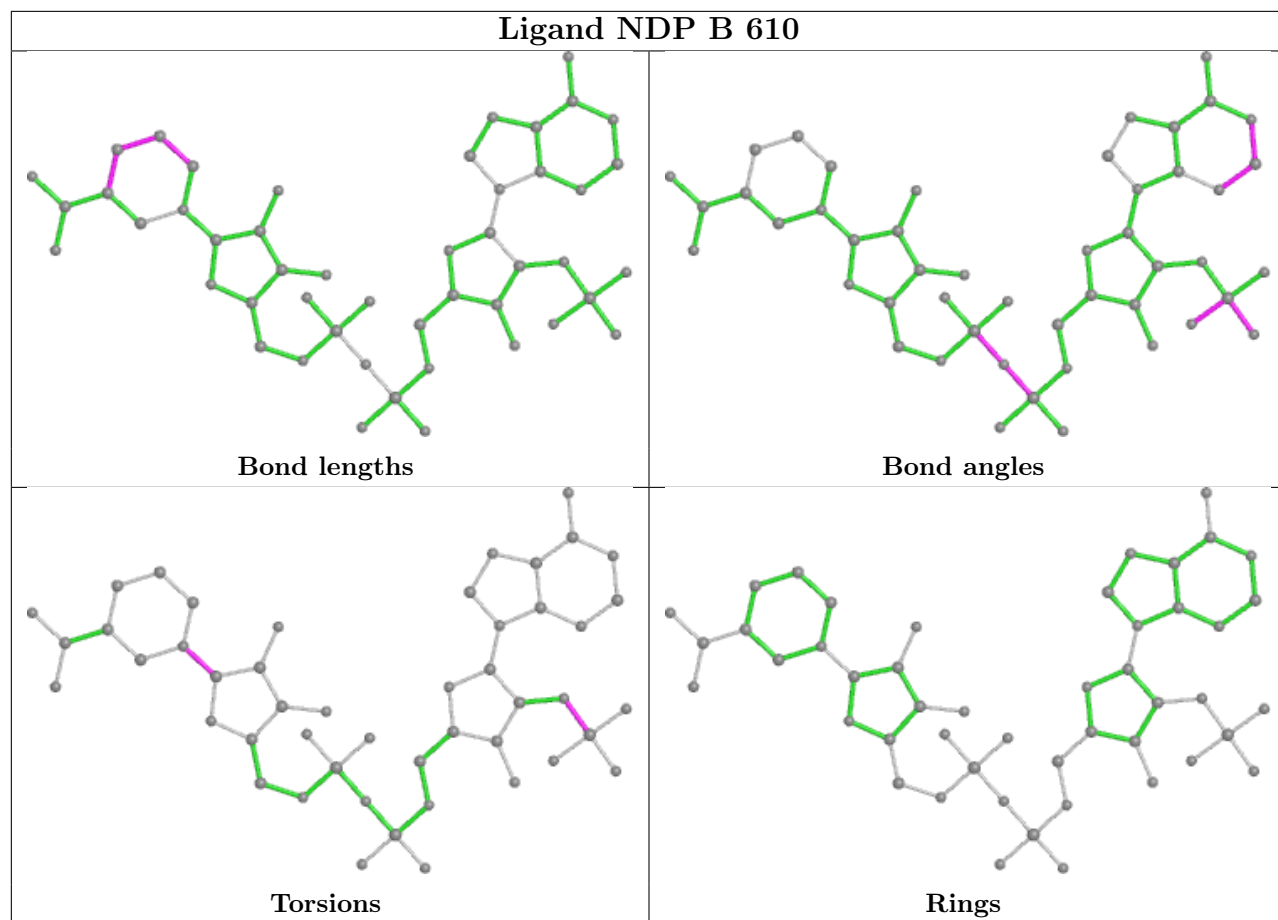
Bond angles

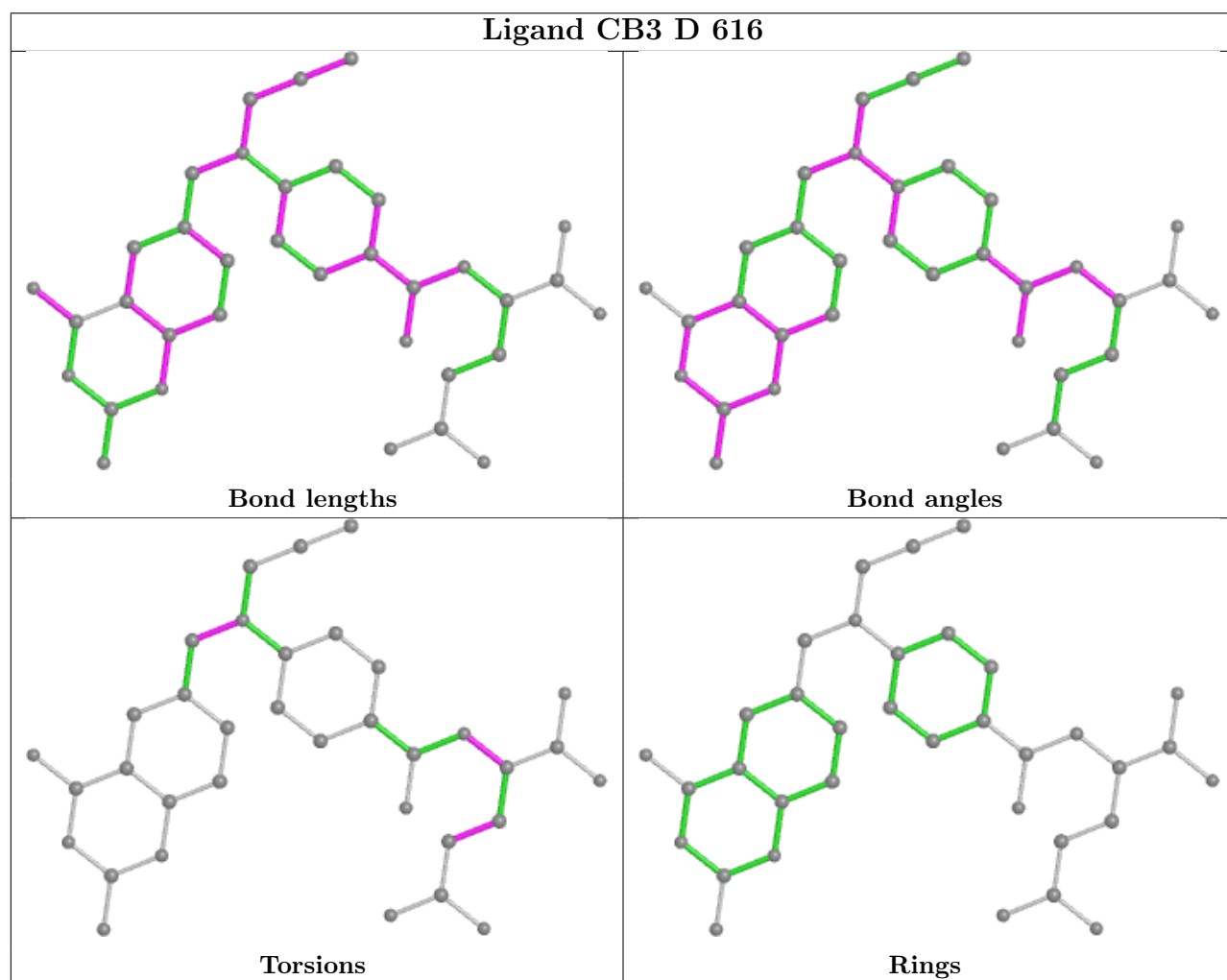
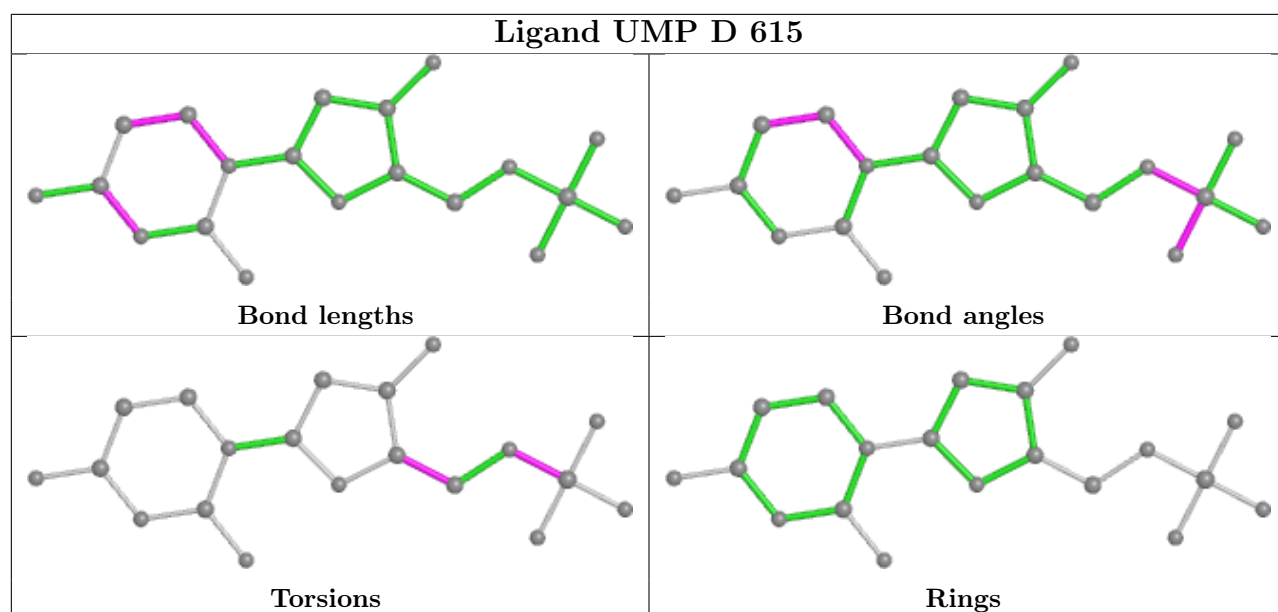


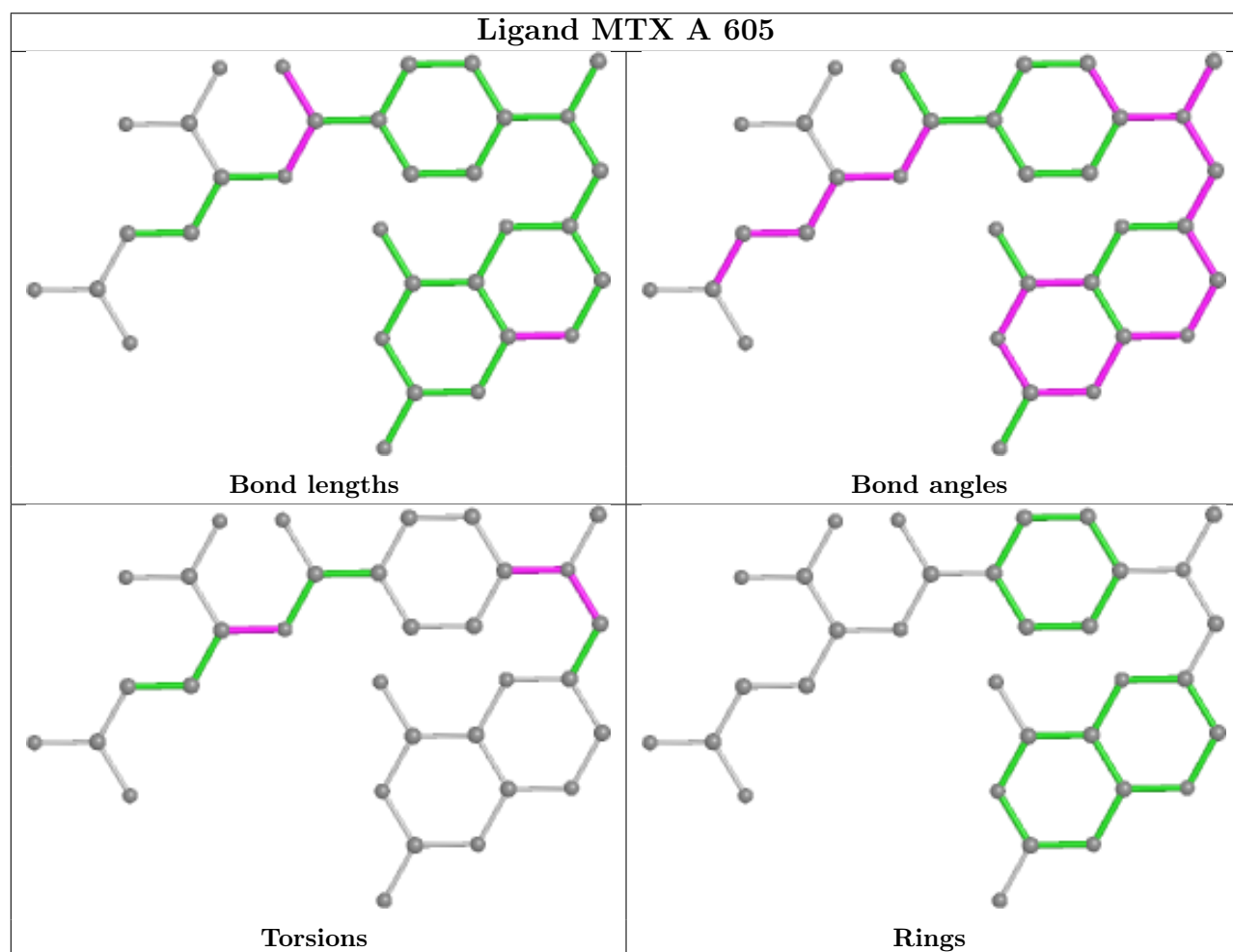
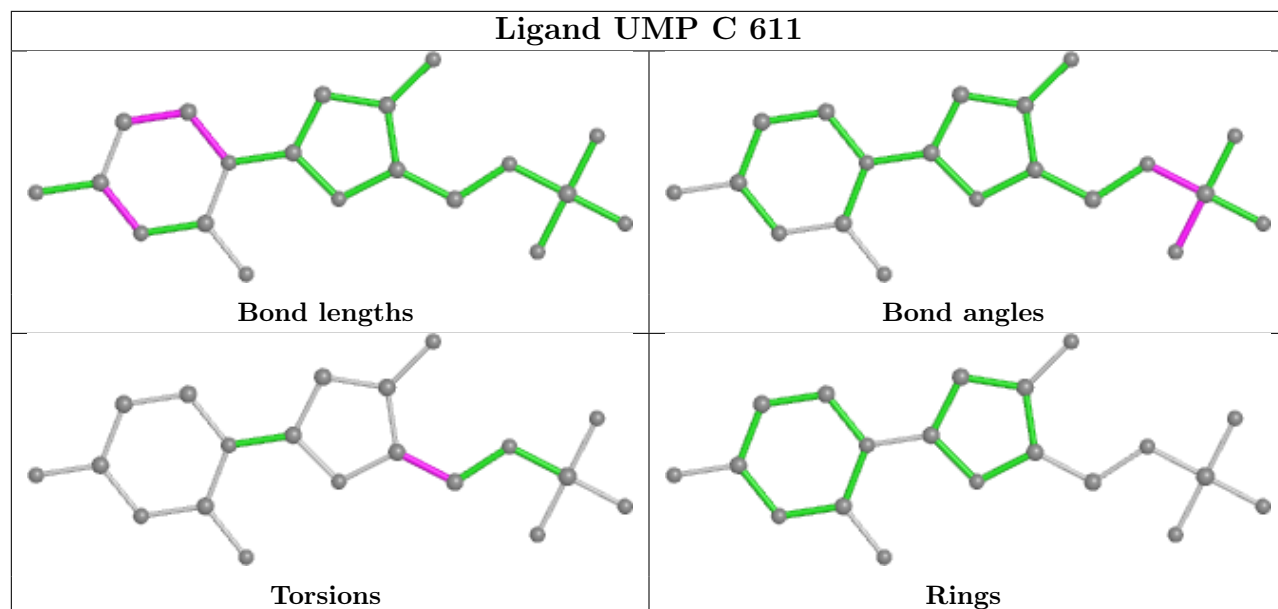
Torsions



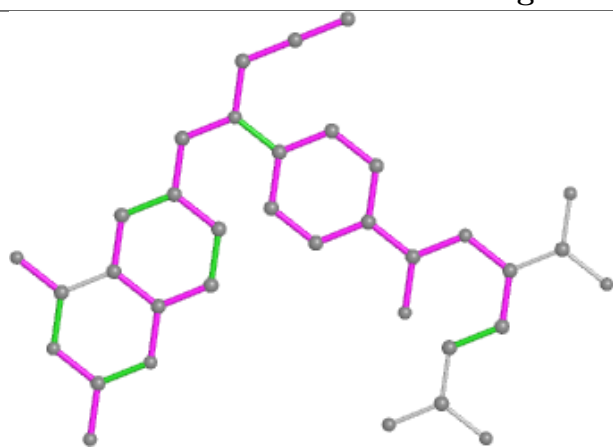
Rings



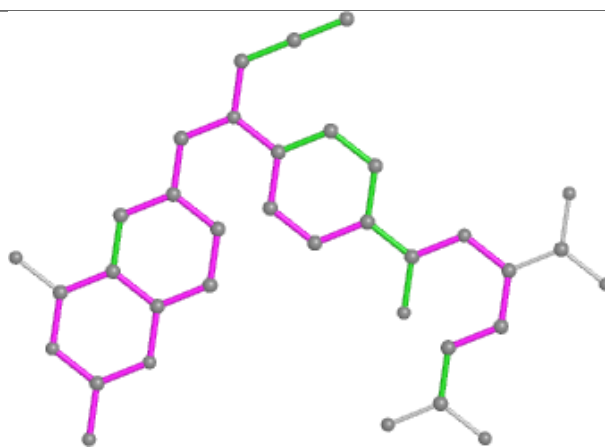




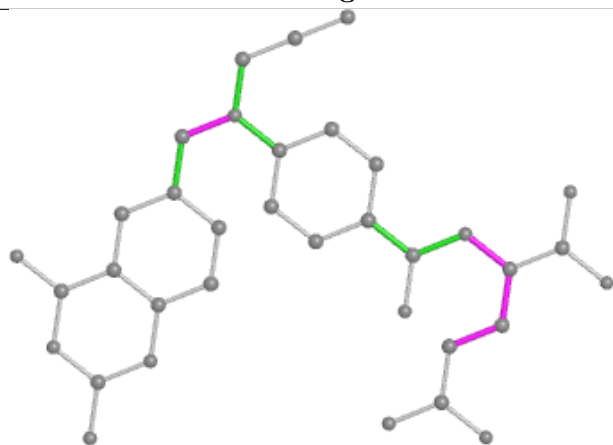
## Ligand CB3 B 608



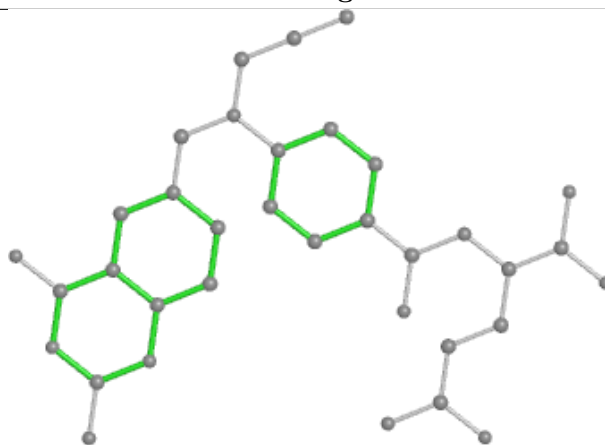
Bond lengths



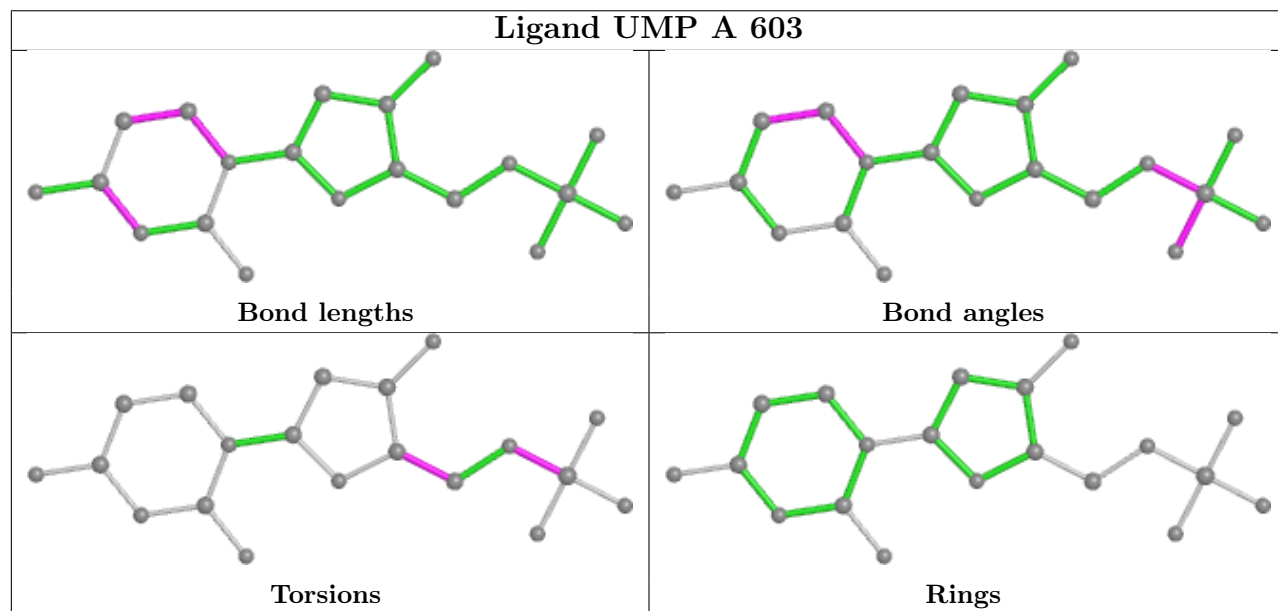
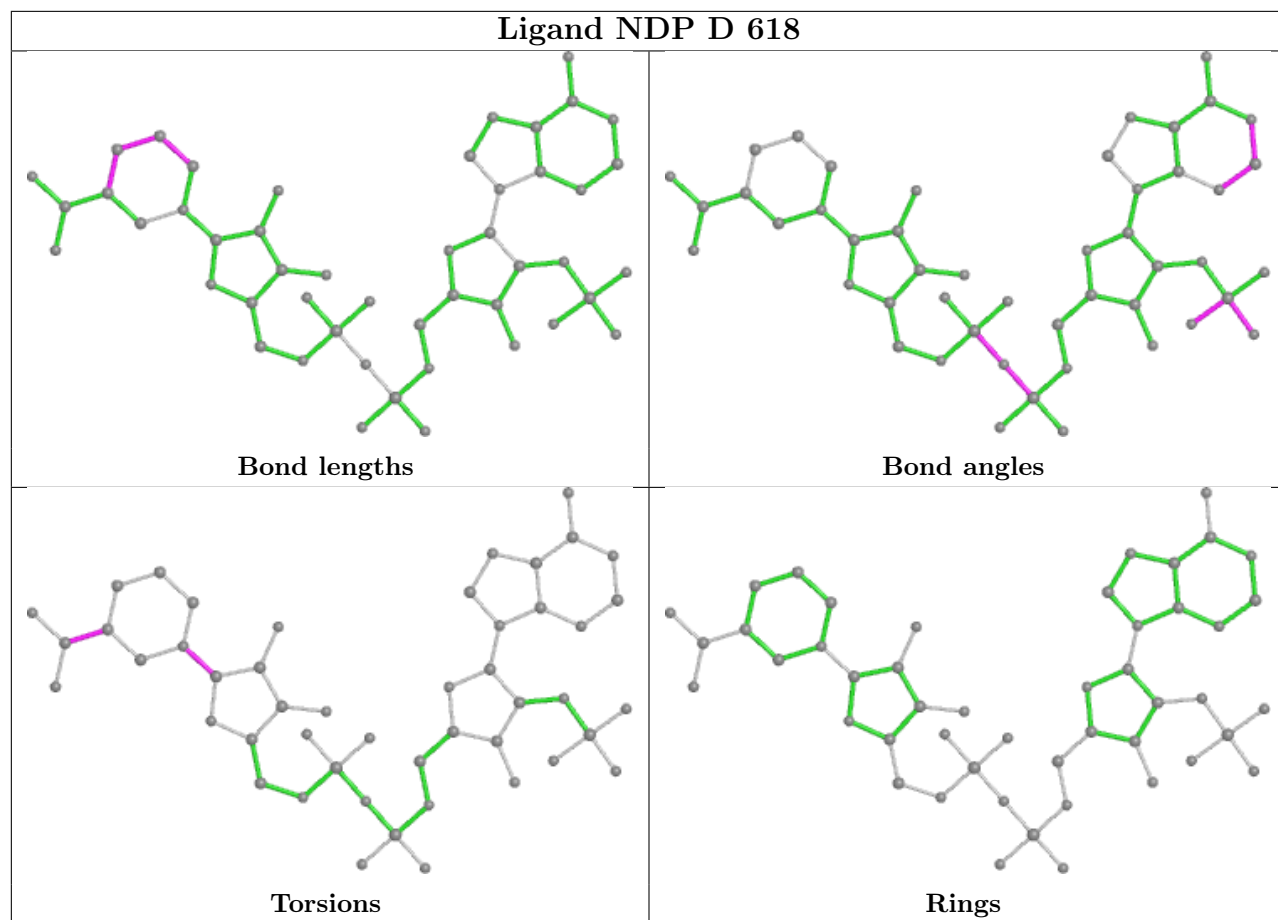
Bond angles

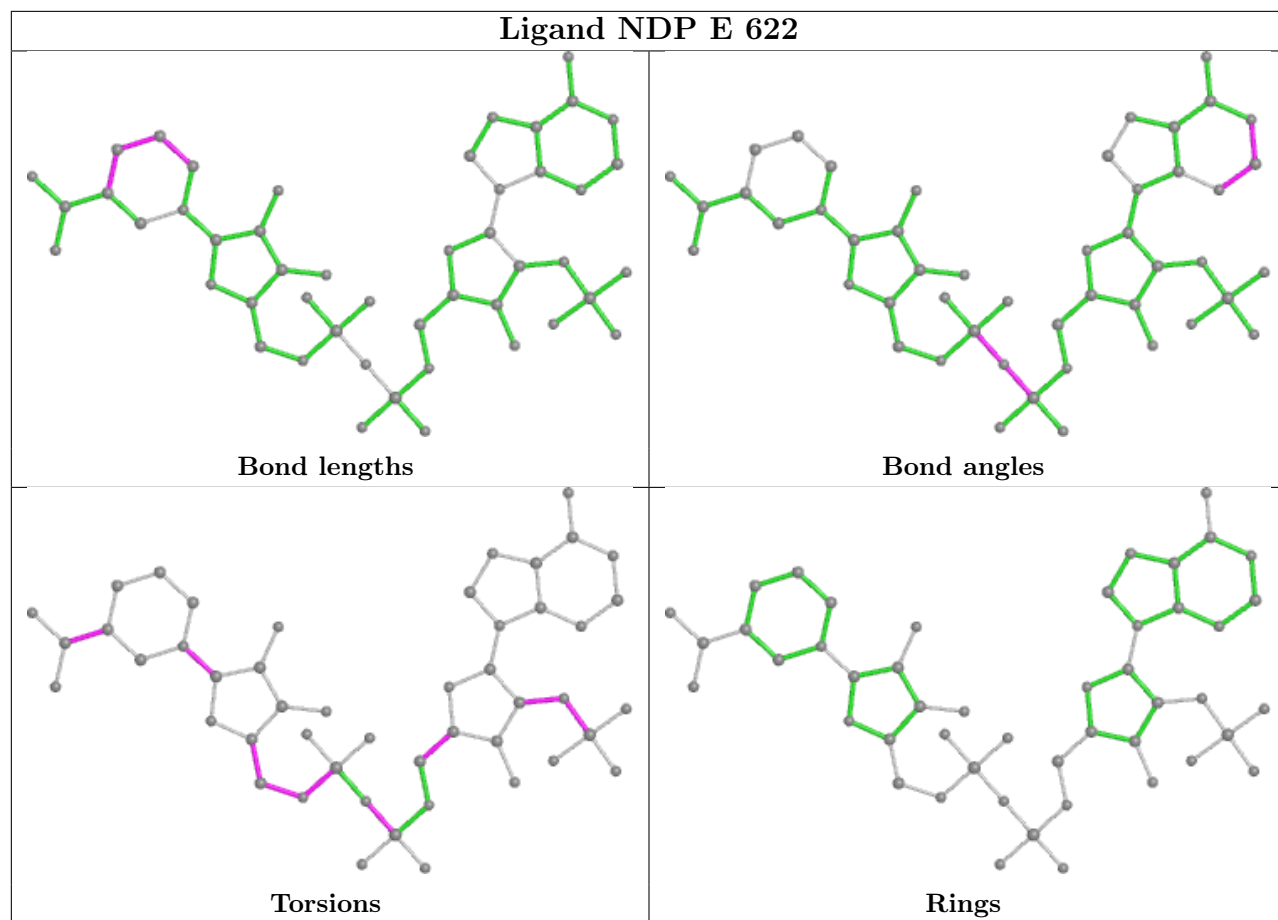


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	516/519 (99%)	-0.07	14 (2%) 54 44	26, 45, 92, 140	0
1	B	516/519 (99%)	-0.20	10 (1%) 66 59	23, 39, 77, 139	0
1	C	514/519 (99%)	0.06	25 (4%) 29 20	34, 60, 111, 148	0
1	D	515/519 (99%)	0.06	12 (2%) 60 51	36, 60, 103, 136	0
1	E	511/519 (98%)	0.69	60 (11%) 4 2	65, 101, 146, 167	0
All	All	2572/2595 (99%)	0.11	121 (4%) 31 22	23, 58, 123, 167	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	CYS	7.7
1	E	103	ASN	6.5
1	D	103	ASN	6.2
1	E	364	GLY	6.1
1	D	192	GLN	5.9
1	D	191	GLY	5.8
1	D	186	CYS	5.3
1	A	186	CYS	5.2
1	E	327	ARG	5.0
1	C	186	CYS	4.8
1	E	137	ALA	4.7
1	D	190	ARG	4.6
1	B	185	ASN	4.5
1	E	314	TYR	4.5
1	C	191	GLY	4.4
1	E	320	GLY	4.4
1	A	191	GLY	4.4
1	E	521	VAL	4.3
1	A	185	ASN	4.3
1	C	189	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	335	GLU	4.0
1	D	100	ASN	4.0
1	E	321	SER	3.9
1	B	102	MET	3.8
1	A	192	GLN	3.8
1	E	357	HIS	3.8
1	E	310	GLU	3.7
1	E	323	GLU	3.7
1	A	341	ILE	3.7
1	C	47	ASN	3.5
1	E	330	LEU	3.5
1	E	328	ILE	3.5
1	E	334	GLU	3.5
1	E	324	TYR	3.4
1	E	181	LYS	3.4
1	C	101	LEU	3.4
1	E	326	GLU	3.3
1	E	319	ASN	3.3
1	E	107	ILE	3.3
1	E	333	ARG	3.3
1	A	100	ASN	3.3
1	E	329	GLY	3.3
1	D	188	PRO	3.2
1	B	192	GLN	3.1
1	C	192	GLN	3.1
1	E	287	ALA	3.1
1	C	107	ILE	3.1
1	E	313	VAL	3.0
1	E	191	GLY	3.0
1	E	127	PHE	3.0
1	E	316	TRP	3.0
1	B	103	ASN	3.0
1	E	5	ASN	2.9
1	E	102	MET	2.9
1	A	188	PRO	2.9
1	E	182	THR	2.8
1	E	192	GLN	2.8
1	C	45	ASP	2.8
1	B	188	PRO	2.8
1	C	53	ILE	2.8
1	E	100	ASN	2.8
1	C	93	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	102	MET	2.7
1	D	107	ILE	2.7
1	C	3	GLU	2.7
1	A	187	ASP	2.6
1	C	105	ASP	2.6
1	A	521	VAL	2.6
1	C	100	ASN	2.6
1	A	189	ALA	2.6
1	E	516	LYS	2.6
1	C	110	ILE	2.6
1	C	4	LYS	2.6
1	E	53	ILE	2.6
1	E	358	ASP	2.6
1	C	190	ARG	2.5
1	E	91	PHE	2.5
1	E	101	LEU	2.5
1	A	102	MET	2.5
1	A	171	ASP	2.5
1	D	105	ASP	2.5
1	E	306	ASN	2.5
1	E	309	ILE	2.5
1	E	429	LEU	2.5
1	E	489	PHE	2.4
1	D	330	LEU	2.4
1	E	336	ASN	2.4
1	E	360	TYR	2.4
1	B	84	ALA	2.4
1	E	84	ALA	2.4
1	E	332	HIS	2.3
1	E	322	LYS	2.3
1	B	187	ASP	2.3
1	C	188	PRO	2.3
1	D	181	LYS	2.3
1	D	101	LEU	2.3
1	E	308	LEU	2.2
1	B	180	LYS	2.2
1	E	325	LEU	2.2
1	E	124	LYS	2.2
1	C	94	LEU	2.2
1	C	123	LEU	2.2
1	C	98	ILE	2.2
1	E	355	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	187	ASP	2.2
1	C	84	ALA	2.2
1	A	180	LYS	2.1
1	C	71	ILE	2.1
1	C	109	ASN	2.1
1	E	315	ILE	2.1
1	E	288	ILE	2.1
1	E	46	SER	2.1
1	E	281	LEU	2.1
1	B	179	GLU	2.1
1	E	175	PHE	2.1
1	E	399	LEU	2.1
1	E	359	ASP	2.1
1	E	365	VAL	2.1
1	E	93	ASN	2.0
1	A	179	GLU	2.0
1	E	116	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CB3	E	620	35/35	0.65	0.53	131,134,135,135	0
3	CB3	D	616	35/35	0.82	0.34	107,110,114,115	0
4	MTX	C	613	33/33	0.85	0.27	75,83,87,87	0
2	UMP	E	619	20/20	0.86	0.18	125,131,135,135	0
4	MTX	E	621	33/33	0.86	0.25	96,102,103,104	0
5	NDP	C	614	48/48	0.86	0.24	92,96,111,112	0

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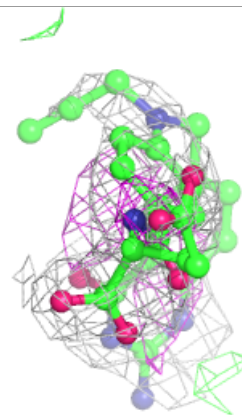
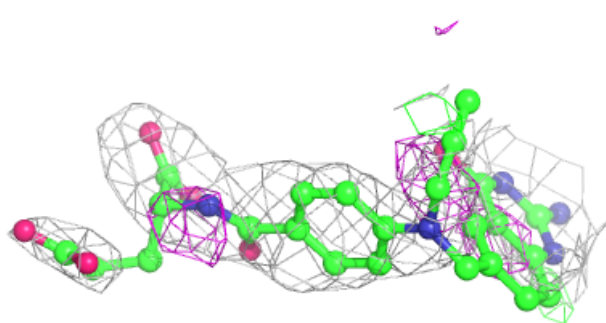
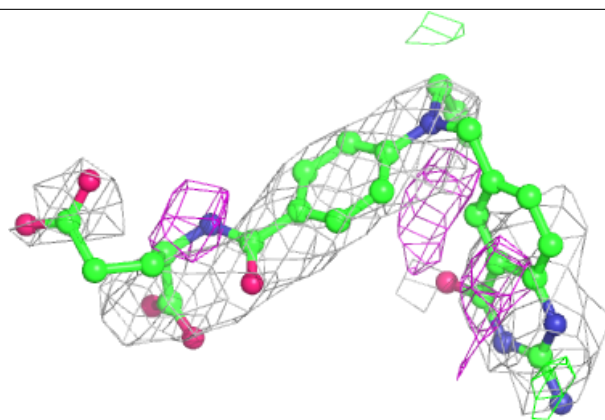
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CB3	A	604	35/35	0.88	0.30	68,77,89,90	0
3	CB3	C	612	35/35	0.89	0.23	59,71,80,82	0
5	NDP	E	622	48/48	0.90	0.18	85,89,105,106	0
2	UMP	D	615	20/20	0.93	0.18	77,82,86,88	0
3	CB3	B	608	35/35	0.93	0.21	44,52,63,66	0
4	MTX	D	617	33/33	0.93	0.21	61,68,71,71	0
5	NDP	D	618	48/48	0.94	0.17	49,64,75,75	0
2	UMP	B	607	20/20	0.95	0.18	37,43,46,50	0
2	UMP	A	603	20/20	0.95	0.17	53,58,63,68	0
4	MTX	B	609	33/33	0.95	0.19	44,50,51,54	0
2	UMP	C	611	20/20	0.96	0.19	44,62,68,70	0
4	MTX	A	605	33/33	0.96	0.18	42,48,50,52	0
5	NDP	B	610	48/48	0.96	0.15	33,41,45,46	0
5	NDP	A	606	48/48	0.97	0.15	41,46,50,50	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.

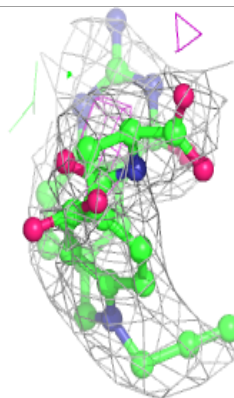
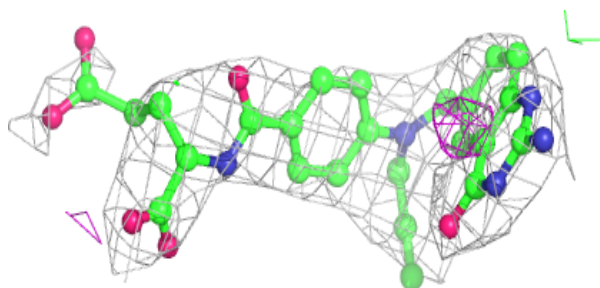
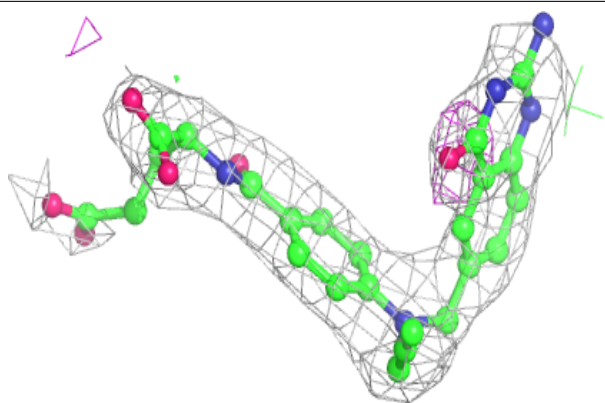
#### Electron density around CB3 E 620:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

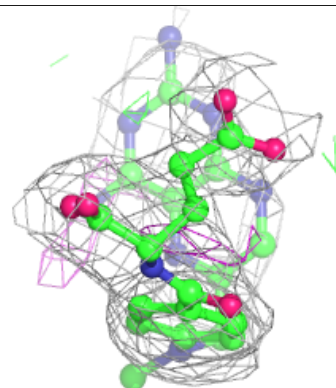
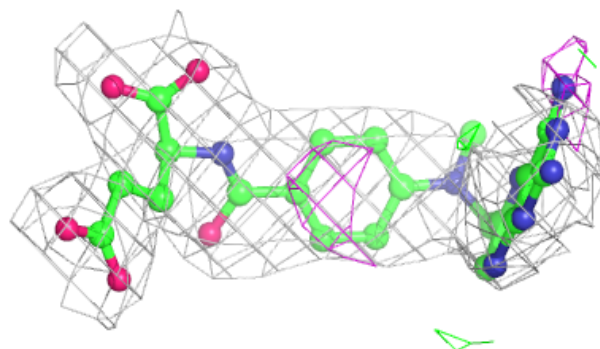
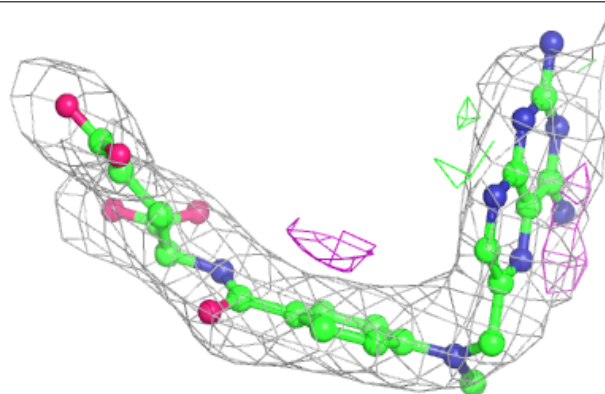


**Electron density around CB3 D 616:**

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

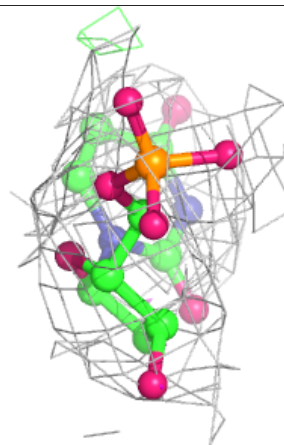
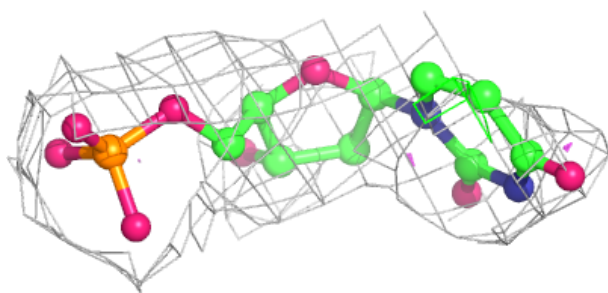
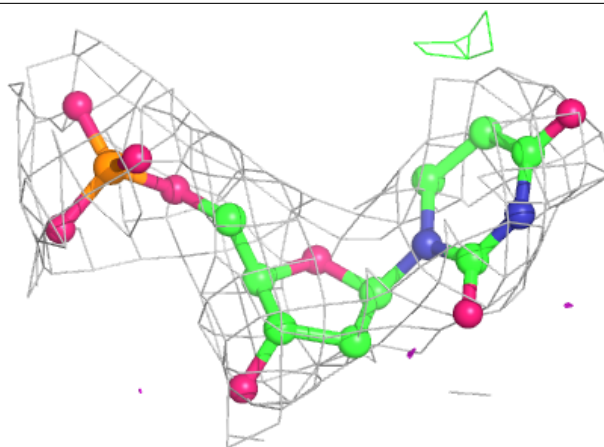
**Electron density around MTX C 613:**

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



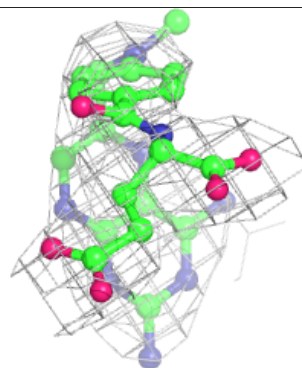
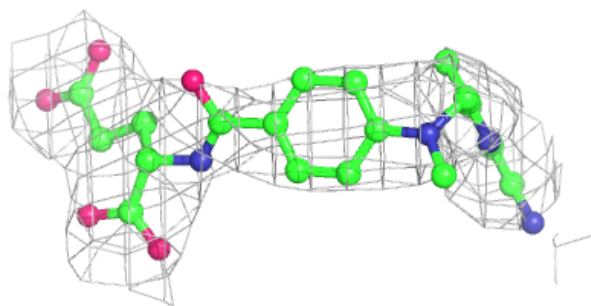
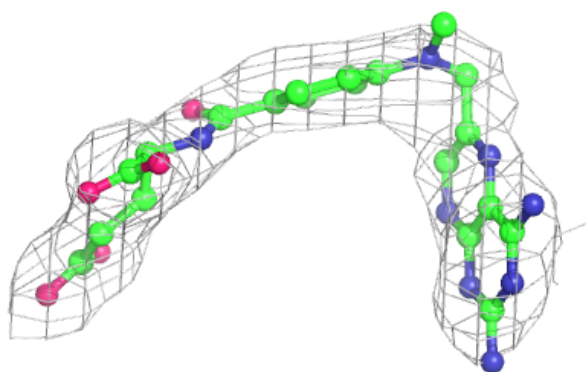
**Electron density around UMP E 619:**

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

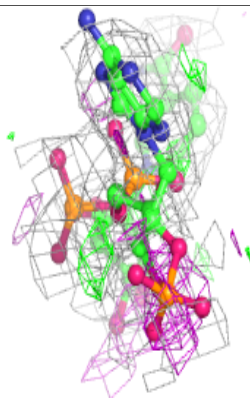
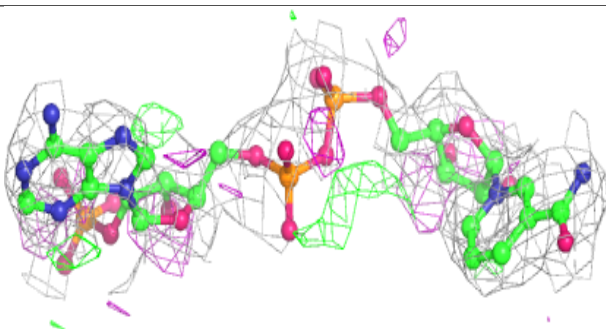
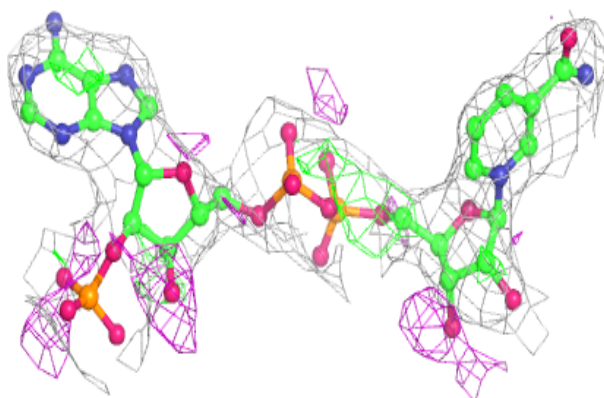


**Electron density around MTX E 621:**

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

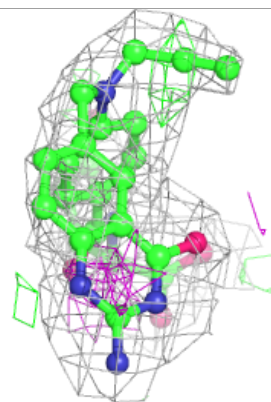
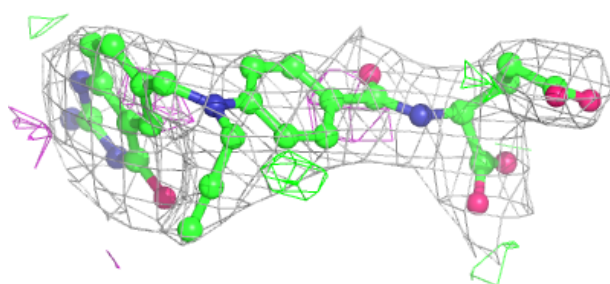
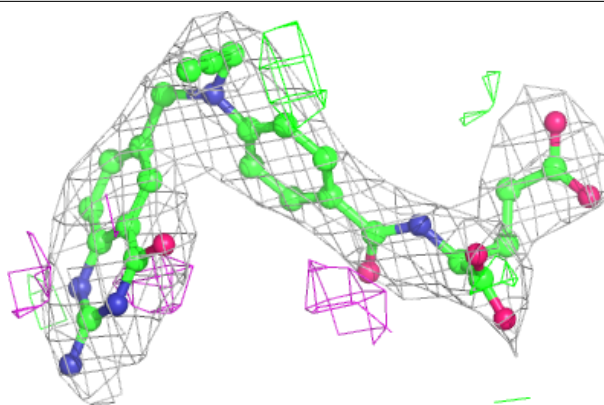
**Electron density around NDP C 614:**

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

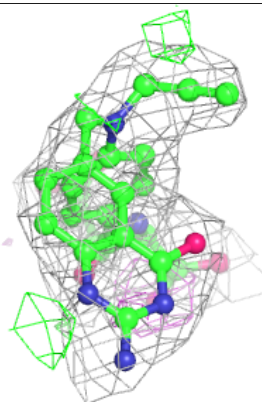
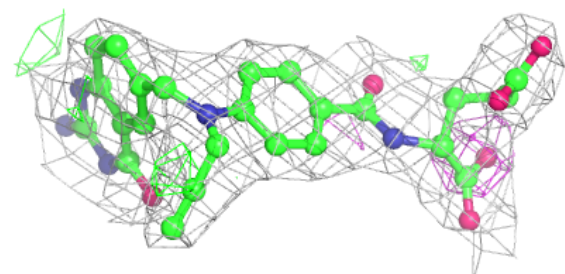
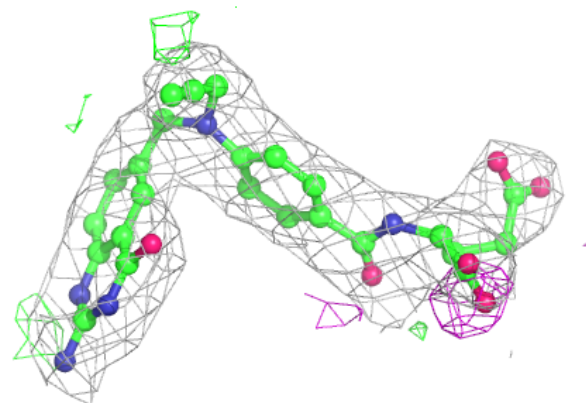


**Electron density around CB3 A 604:**

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

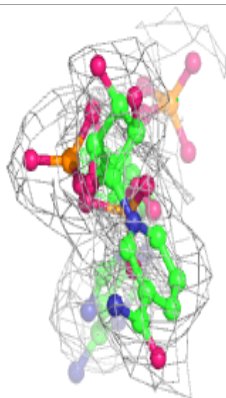
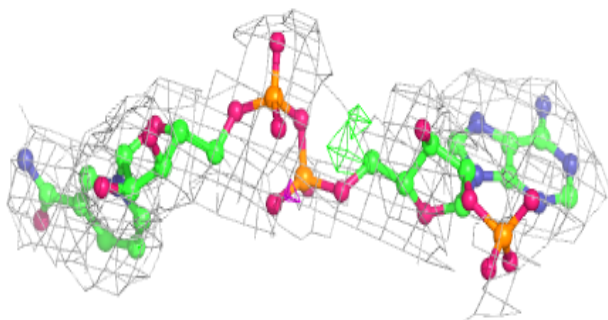
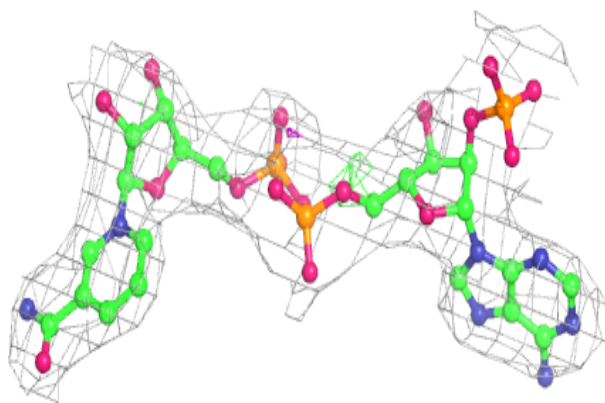
**Electron density around CB3 C 612:**

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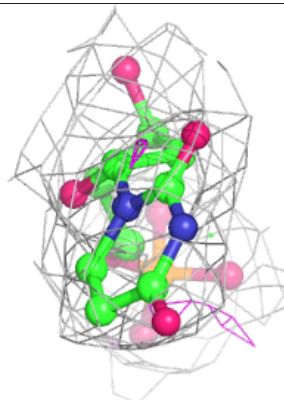
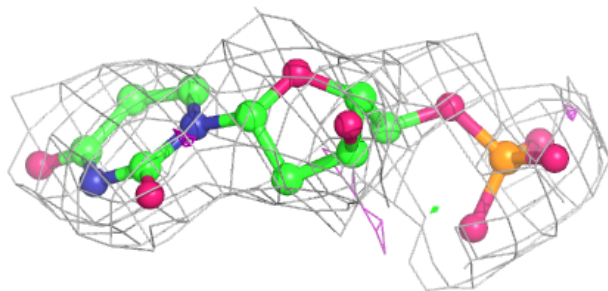
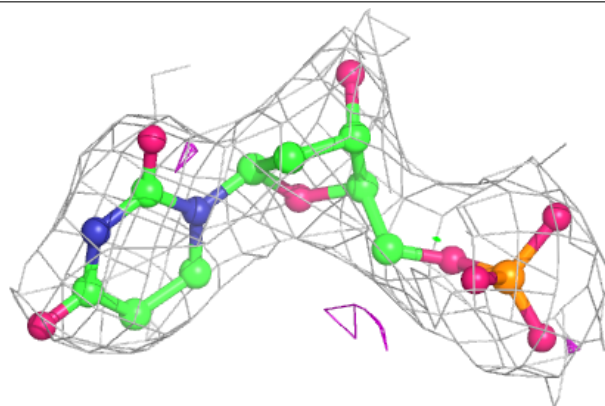


**Electron density around NDP E 622:**

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and green (positive)

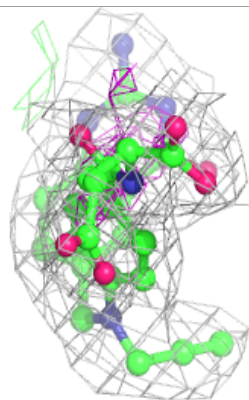
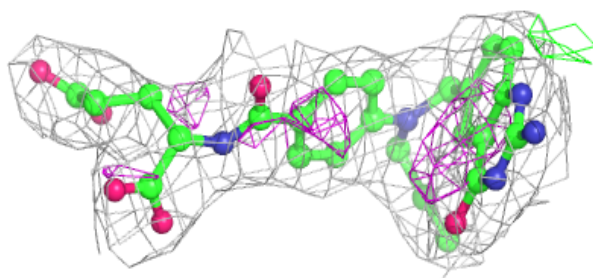
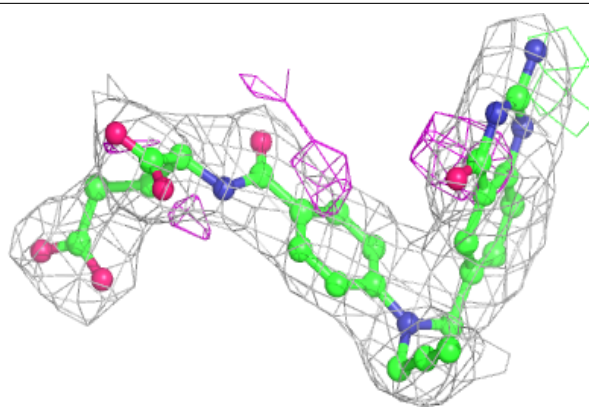
**Electron density around UMP D 615:**

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



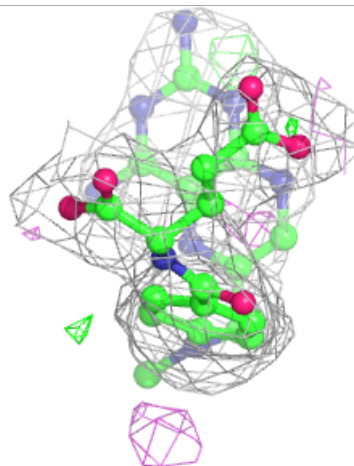
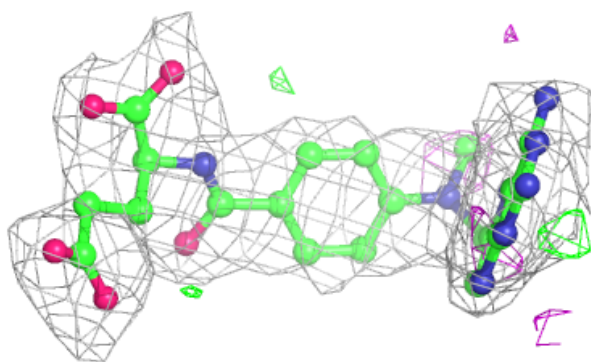
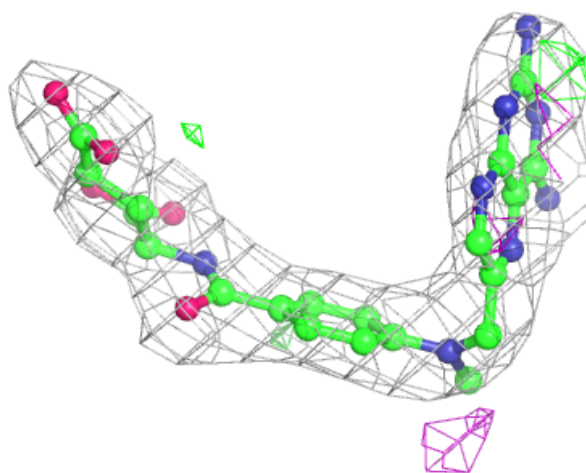
**Electron density around CB3 B 608:**

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



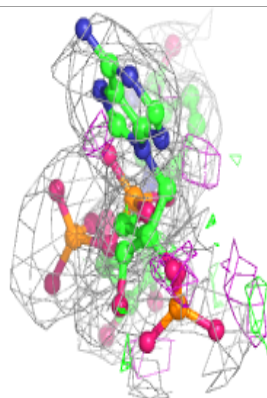
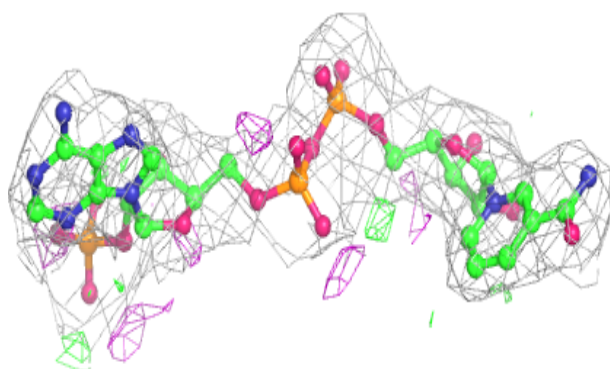
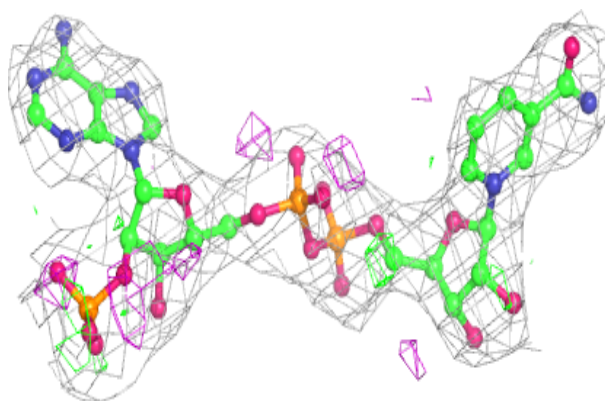
**Electron density around MTX D 617:**

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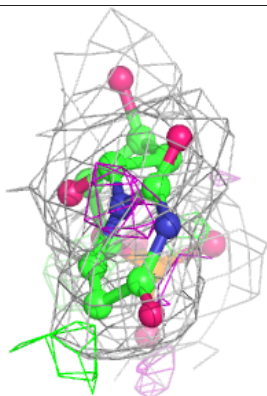
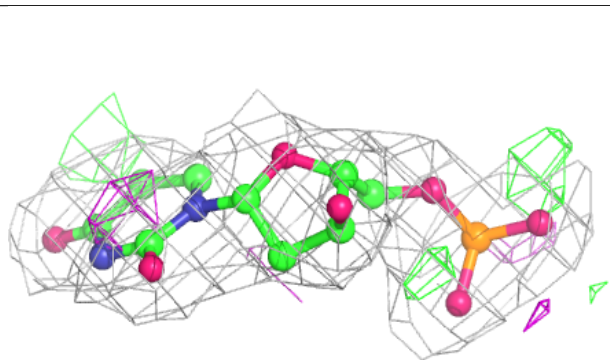
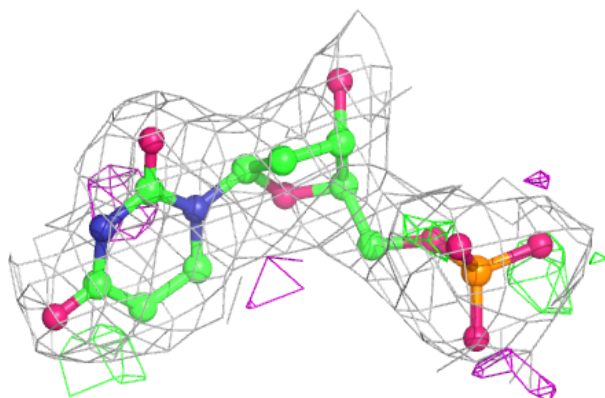


**Electron density around NDP D 618:**

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and green (positive)

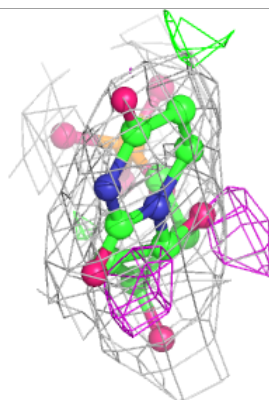
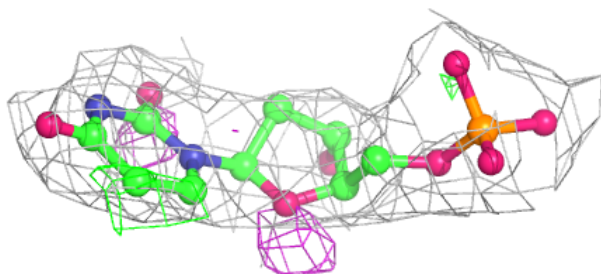
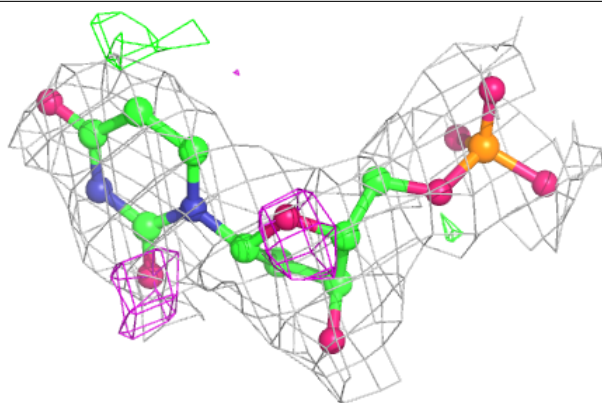
**Electron density around UMP B 607:**

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and green (positive)

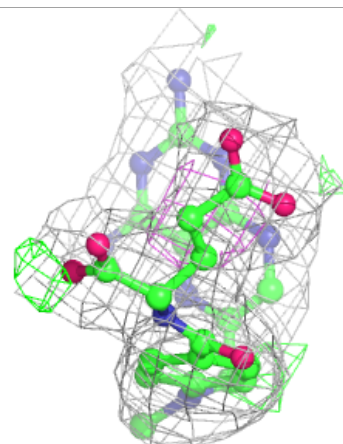
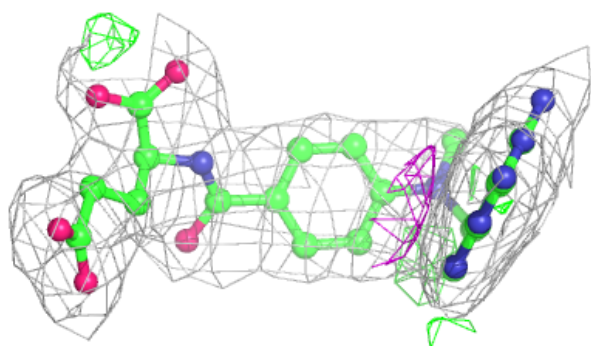
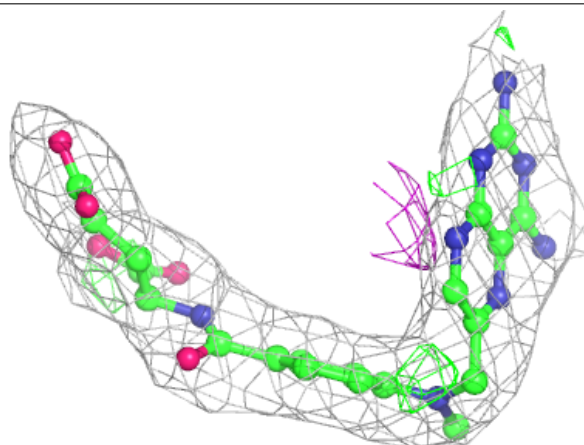


**Electron density around UMP A 603:**

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and green (positive)

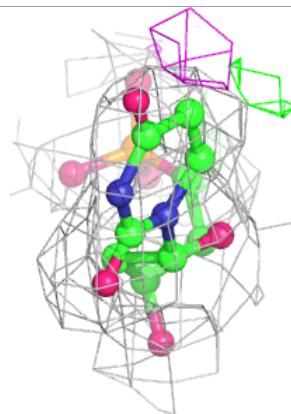
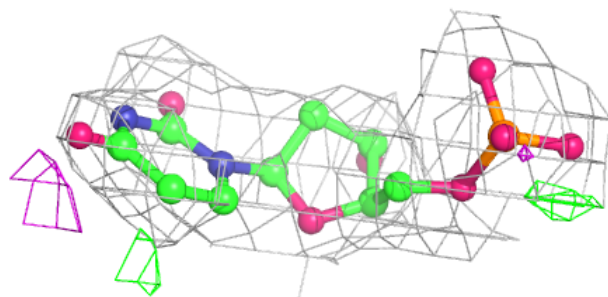
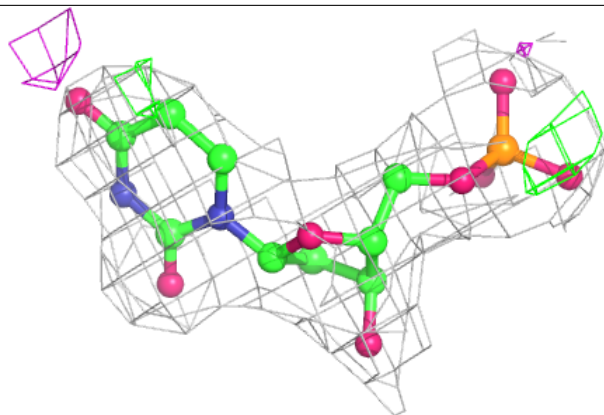
**Electron density around MTX B 609:**

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and green (positive)



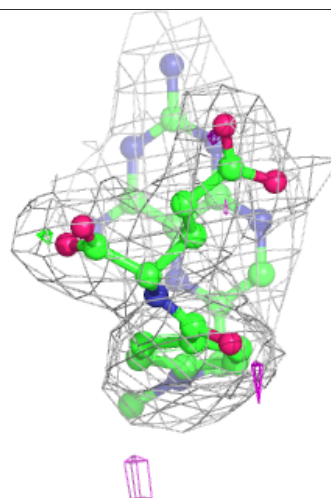
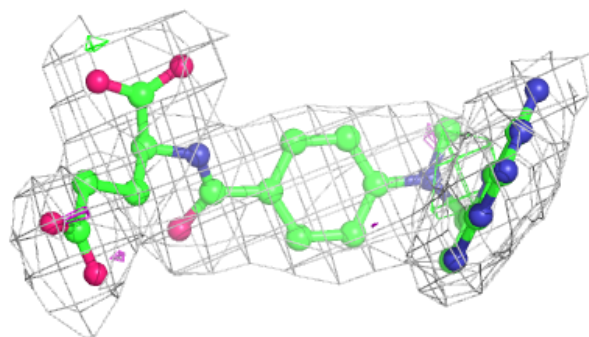
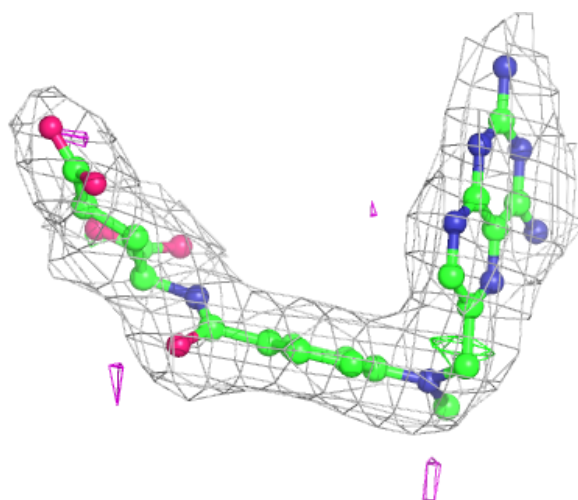
**Electron density around UMP C 611:**

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and green (positive)



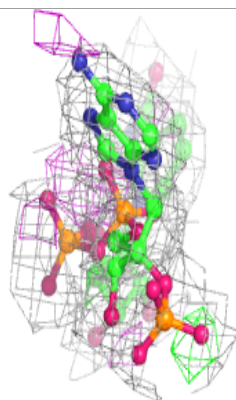
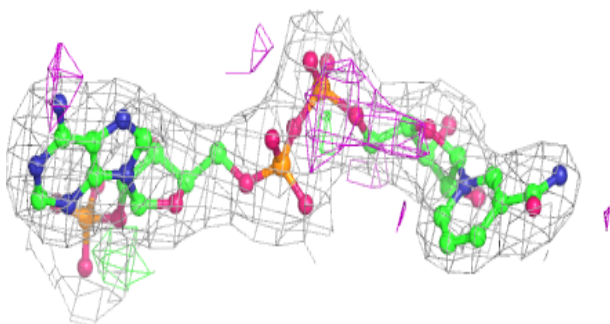
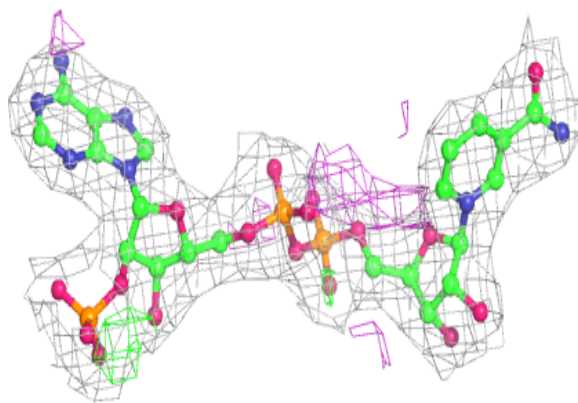
**Electron density around MTX A 605:**

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

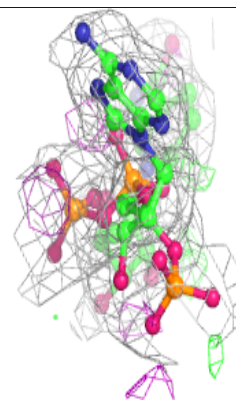
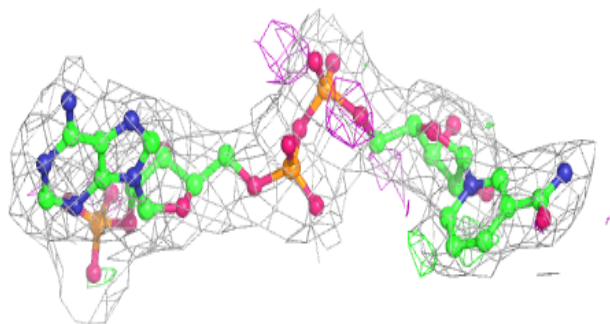
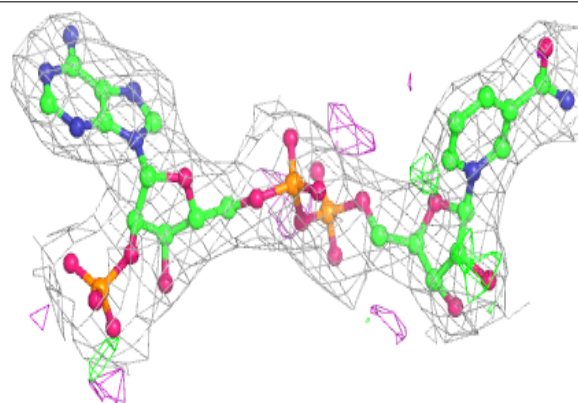


**Electron density around NDP B 610:**

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

**Electron density around NDP A 606:**

$2mF_o-DF_c$  (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.