



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:18 AM UTC

PDB ID : 2OIP / pdb_00002oip
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

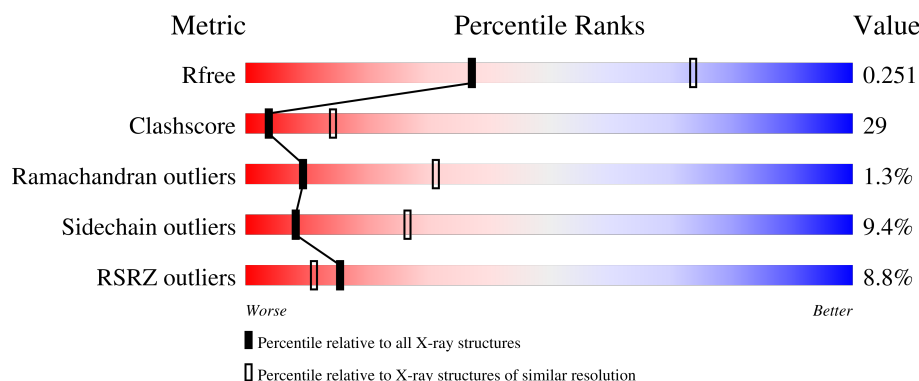
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 ≥ 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	6% 57% 36% 5% ..
1	B	519	4% 61% 31% 6% ..
1	C	519	7% 52% 39% 8% .
1	D	519	7% 50% 39% 8% ..
1	E	519	20% 41% 49% 7% ..

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	B	608	-	X	-	-
3	CB3	C	612	X	X	X	-
3	CB3	E	620	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.

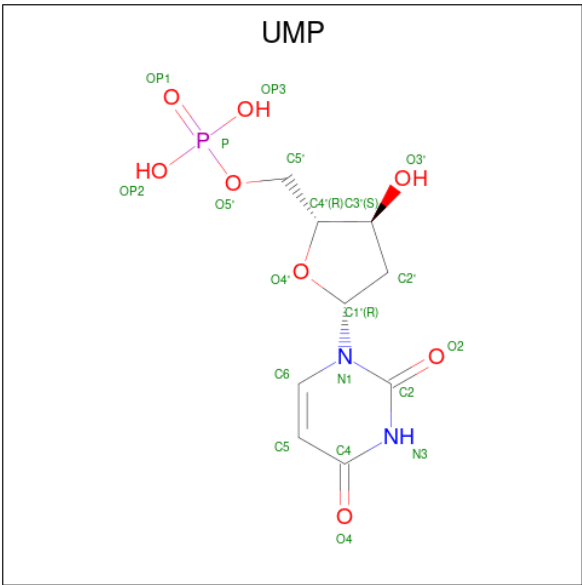
- Molecule 1 is a protein called Chain A, crystal structure of Dhfr.

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:

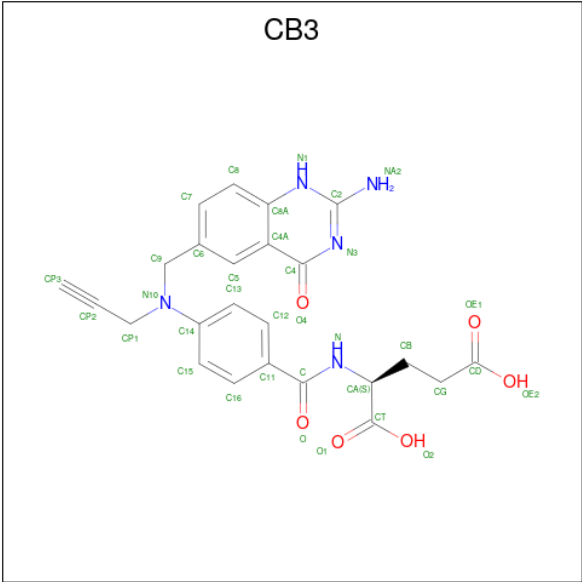
Chain	Residue	Modelled	Actual	Comment	Reference
A	290	GLY	SER	engineered mutation	UNP Q5CGA3
B	290	GLY	SER	engineered mutation	UNP Q5CGA3
C	290	GLY	SER	engineered mutation	UNP Q5CGA3
D	290	GLY	SER	engineered mutation	UNP Q5CGA3
E	290	GLY	SER	engineered mutation	UNP Q5CGA3

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: C₉H₁₃N₂O₈P).



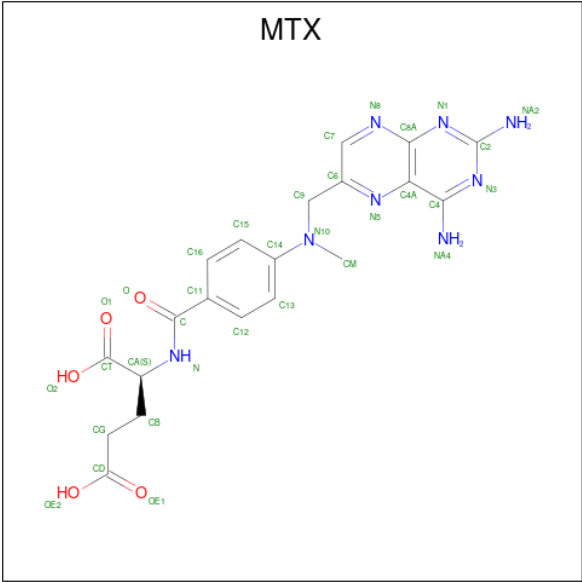
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (CCD ID: CB3) (formula: C₂₄H₂₃N₅O₆).



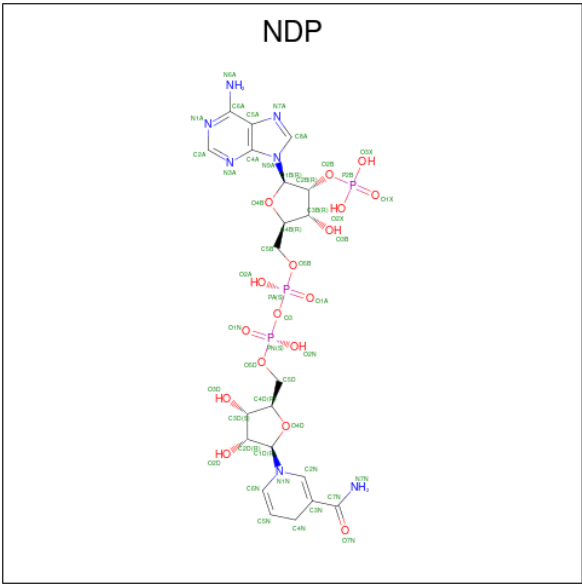
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		
3	D	1	Total	C	N	O	0	0
			35	24	5	6		
3	E	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is METHOTREXATE (CCD ID: MTX) (formula: C₂₀H₂₂N₈O₅).



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

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: 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

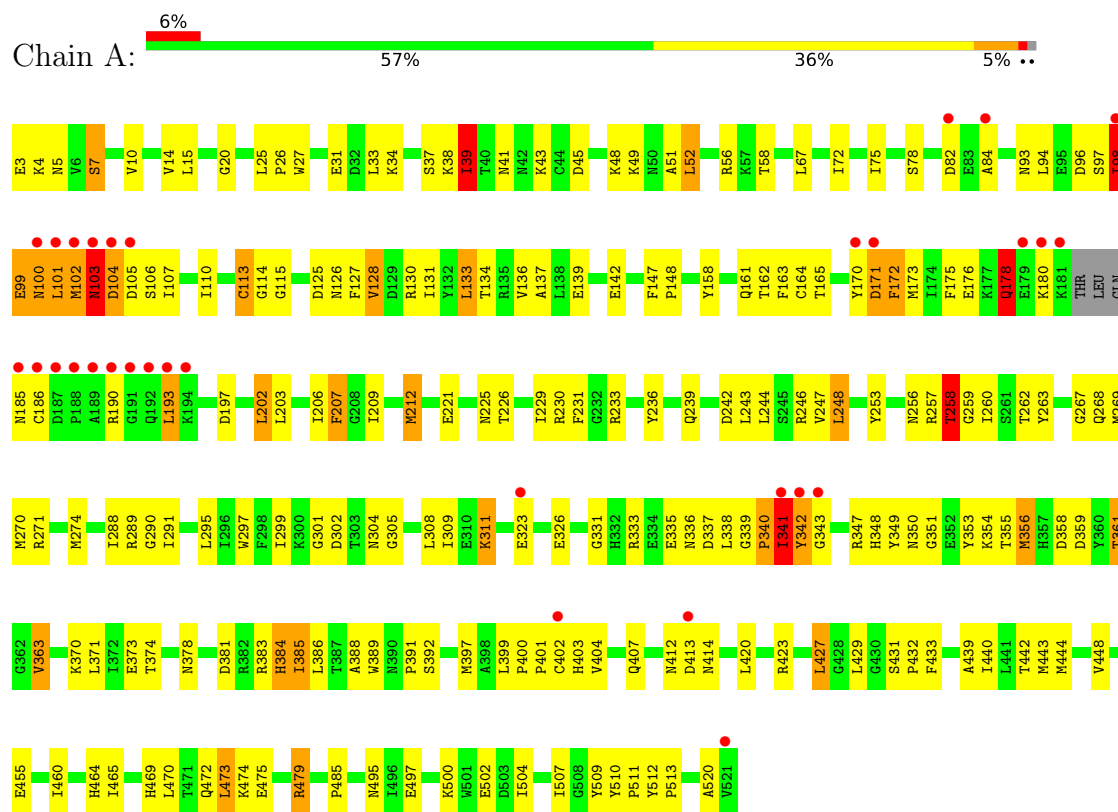
- Molecule 6 is water.

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

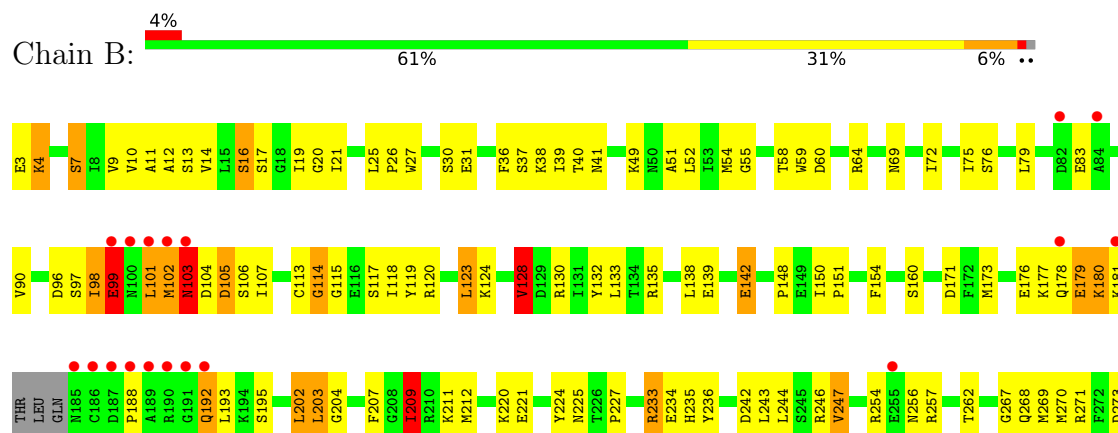
3 Residue-property plots

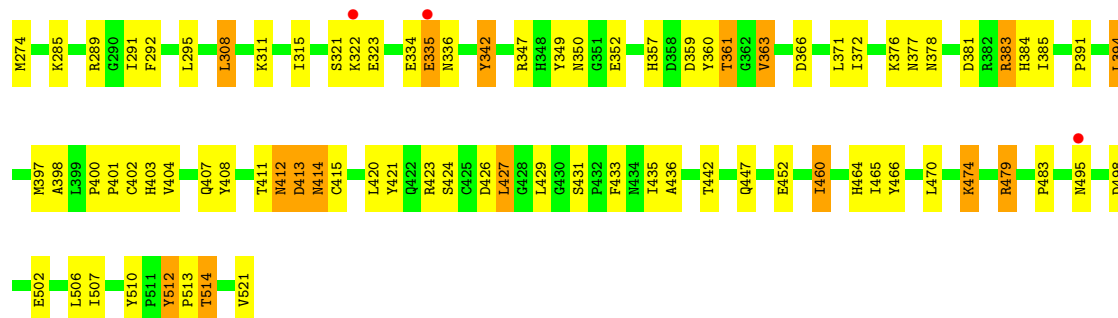
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

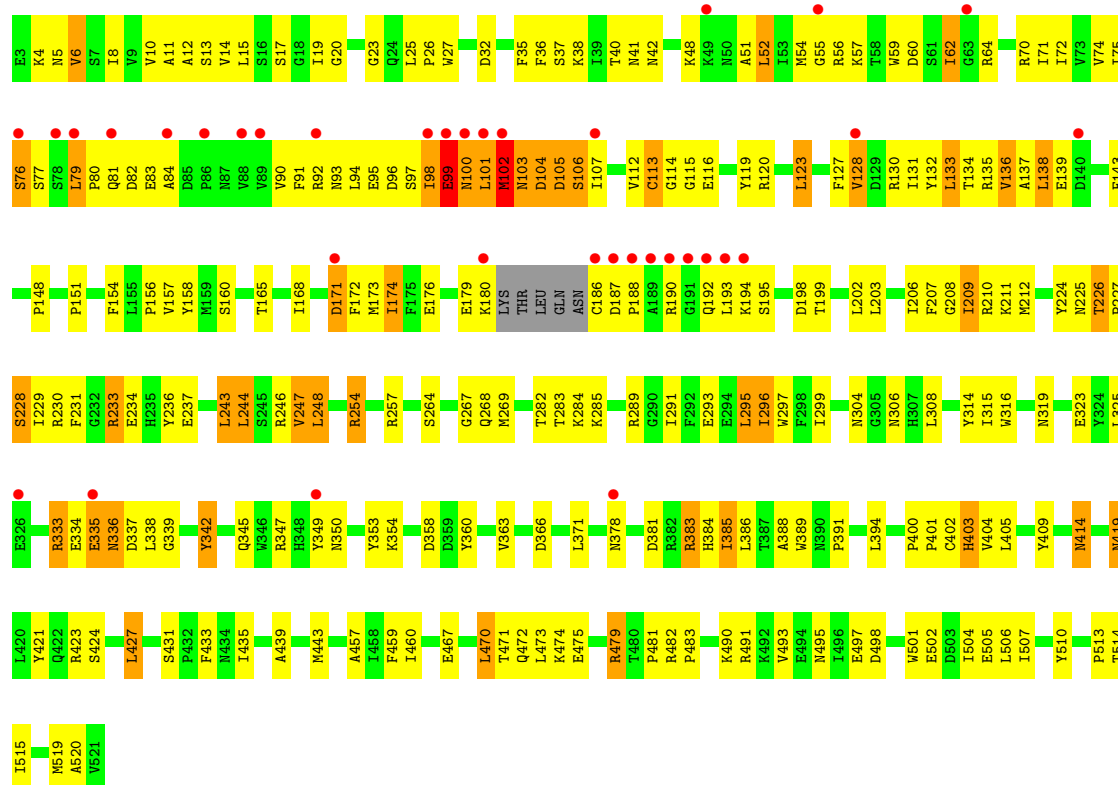


• Molecule 1: Chain A, crystal structure of Dhfr

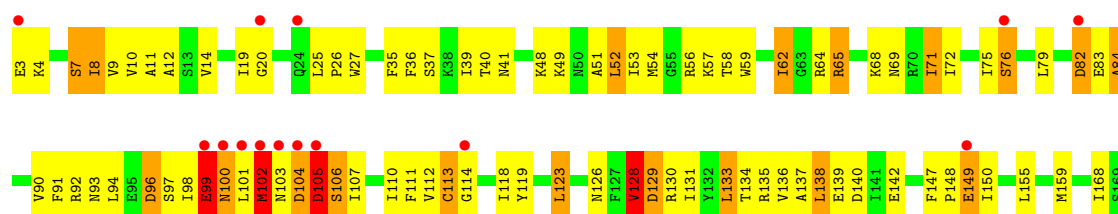


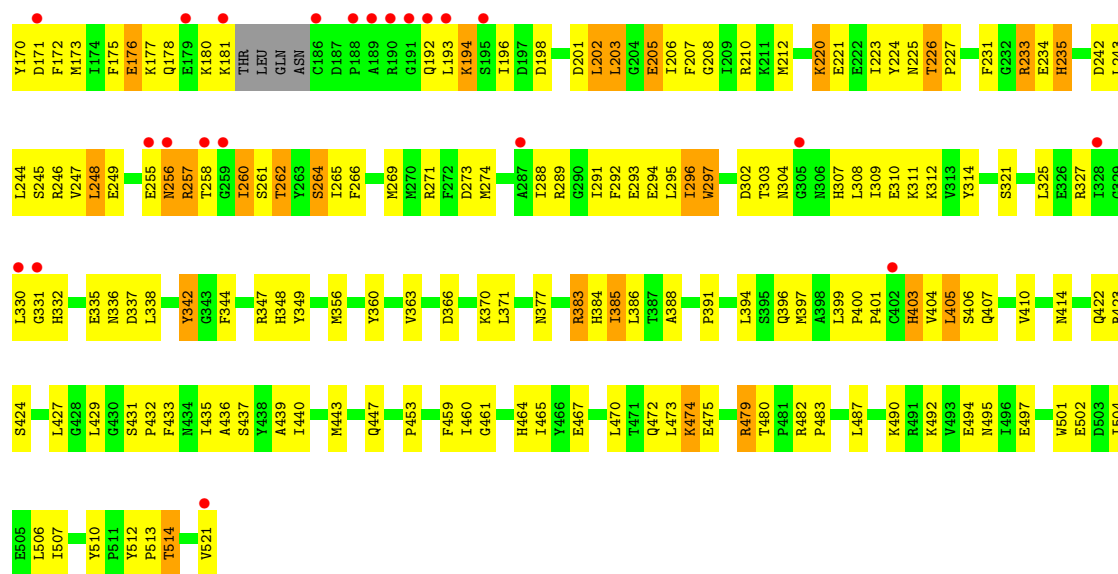


• Molecule 1: Chain A, crystal structure of Dhfr

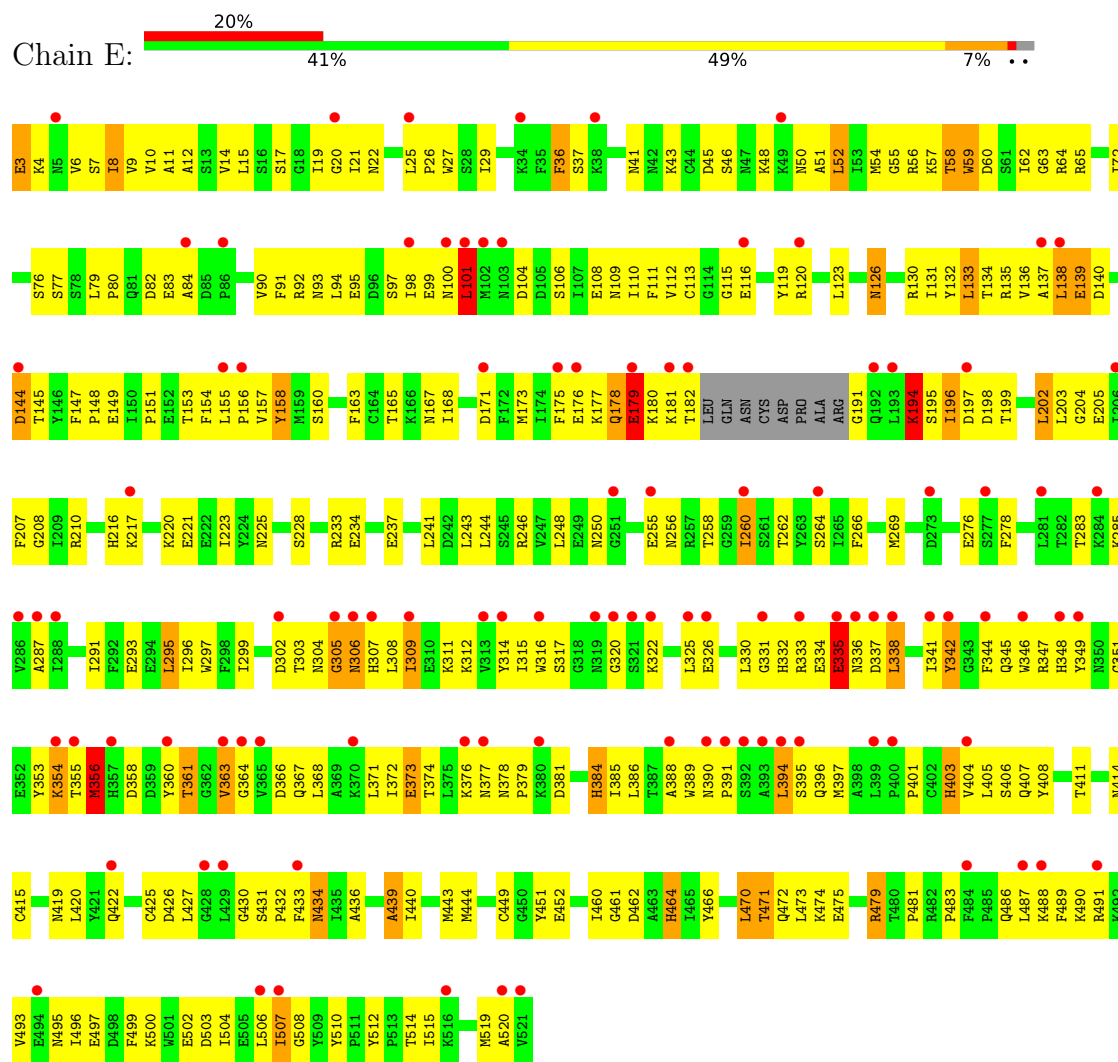


• Molecule 1: Chain A, crystal structure of Dhfr





• 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, α , β , γ	215.03Å 116.20Å 216.60Å 90.00° 94.27° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.80) 99.2 (50.00-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.47	0/4278	0.99	20/5782 (0.3%)
1	B	0.51	0/4285	1.00	22/5790 (0.4%)
1	C	0.43	0/4260	0.95	16/5758 (0.3%)
1	D	0.42	0/4263	0.93	18/5763 (0.3%)
1	E	0.40	0/4240	0.95	17/5730 (0.3%)
All	All	0.45	0/21326	0.97	93/28823 (0.3%)

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 (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ASN	N-CA-C	-9.13	101.41	112.54
1	C	102	MET	N-CA-C	-8.81	101.75	111.36
1	B	507	ILE	N-CA-C	8.41	120.04	107.51
1	E	363	VAL	N-CA-C	8.08	119.08	111.48
1	D	84	ALA	N-CA-C	8.00	120.78	111.02
1	C	101	LEU	N-CA-C	-7.61	102.67	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	106	SER	N-CA-C	-7.53	104.22	113.41
1	A	39	ILE	N-CA-C	7.48	117.60	110.42
1	E	385	ILE	N-CA-C	7.46	119.48	108.45
1	E	335	GLU	N-CA-C	7.30	119.93	111.02
1	A	507	ILE	N-CA-C	7.25	119.02	108.58
1	E	363	VAL	CB-CA-C	-7.20	105.59	111.71
1	D	507	ILE	N-CA-C	7.19	118.22	107.80
1	C	507	ILE	N-CA-C	7.10	118.36	107.99
1	B	209	ILE	N-CA-C	-7.10	102.10	112.04
1	C	128	VAL	N-CA-C	7.04	118.71	108.58
1	D	205	GLU	N-CA-C	-7.03	104.34	113.12
1	B	398	ALA	N-CA-C	-7.00	103.64	111.28
1	B	101	LEU	N-CA-C	6.99	118.79	111.03
1	E	126	ASN	N-CA-C	6.75	120.73	111.54
1	E	470	LEU	N-CA-C	6.73	118.28	111.07
1	B	377	ASN	N-CA-C	6.67	118.63	111.36
1	B	105	ASP	N-CA-C	-6.64	104.93	113.16
1	E	101	LEU	N-CA-C	-6.63	104.13	111.82
1	B	90	VAL	N-CA-C	6.61	118.11	108.53
1	B	512	TYR	N-CA-C	-6.60	102.54	110.13
1	C	385	ILE	N-CA-C	6.49	119.03	108.97
1	E	194	LYS	N-CA-C	6.48	118.00	111.07
1	D	128	VAL	N-CA-C	6.37	118.20	108.71
1	B	460	ILE	N-CA-C	6.28	117.63	108.53
1	B	243	LEU	N-CA-C	-6.25	104.54	111.36
1	B	14	VAL	N-CA-C	6.25	117.74	110.62
1	D	377	ASN	N-CA-C	6.24	118.16	111.36
1	B	474	LYS	N-CA-C	-6.13	104.68	111.36
1	D	512	TYR	N-CA-C	-6.12	103.09	110.13
1	B	427	LEU	N-CA-C	6.12	118.75	111.71
1	B	254	ARG	N-CA-C	6.08	118.66	109.23
1	C	414	ASN	N-CA-C	6.03	119.88	111.74
1	C	207	PHE	N-CA-C	-5.99	101.91	110.59
1	A	5	ASN	N-CA-C	5.98	119.13	110.28
1	C	243	LEU	N-CA-C	-5.97	104.85	111.36
1	C	394	LEU	N-CA-C	5.97	118.27	111.11
1	A	464	HIS	N-CA-C	5.88	117.89	109.14
1	D	14	VAL	N-CA-C	5.87	116.61	110.62
1	B	128	VAL	N-CA-C	5.83	117.39	108.71
1	A	243	LEU	N-CA-C	-5.83	105.01	111.36
1	D	297	TRP	N-CA-C	-5.75	104.91	111.07
1	A	33	LEU	N-CA-C	-5.75	105.09	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	439	ALA	N-CA-C	-5.70	104.99	111.14
1	D	226	THR	CA-C-N	5.65	126.91	119.84
1	D	226	THR	C-N-CA	5.65	126.91	119.84
1	C	314	TYR	N-CA-C	5.65	119.86	112.92
1	A	142	GLU	N-CA-C	5.62	118.70	109.76
1	A	259	GLY	N-CA-C	-5.62	108.00	114.69
1	D	480	THR	CA-C-N	5.57	125.58	119.90
1	D	480	THR	C-N-CA	5.57	125.58	119.90
1	E	158	TYR	N-CA-C	5.54	117.52	108.55
1	D	65	ARG	N-CA-C	-5.51	101.67	110.10
1	A	178	GLN	N-CA-C	5.50	119.20	109.96
1	A	258	THR	N-CA-C	5.48	117.25	111.28
1	B	30	SER	N-CA-C	5.47	117.25	111.28
1	A	226	THR	CA-C-N	5.46	126.66	119.84
1	A	226	THR	C-N-CA	5.46	126.66	119.84
1	D	220	LYS	N-CA-C	-5.45	102.81	110.50
1	A	207	PHE	N-CA-C	5.43	119.97	113.23
1	B	498	ASP	N-CA-C	5.43	119.62	112.89
1	E	144	ASP	N-CA-C	-5.42	107.91	114.75
1	C	427	LEU	N-CA-C	5.41	117.18	111.28
1	A	504	ILE	N-CA-C	5.39	115.86	107.99
1	B	394	LEU	N-CA-C	5.38	117.57	111.11
1	D	460	ILE	N-CA-C	5.38	116.33	108.53
1	B	412	ASN	N-CA-C	-5.36	106.25	112.89
1	B	321	SER	N-CA-C	5.35	117.19	110.24
1	B	464	HIS	N-CA-C	5.34	117.31	109.24
1	A	351	GLY	N-CA-C	-5.30	105.75	112.54
1	A	78	SER	N-CA-C	5.28	119.78	112.45
1	C	106	SER	N-CA-C	-5.27	106.86	113.72
1	E	464	HIS	N-CA-C	5.27	117.20	109.24
1	C	226	THR	CA-C-N	5.24	126.39	119.84
1	C	226	THR	C-N-CA	5.24	126.39	119.84
1	E	58	THR	N-CA-C	-5.24	105.63	112.23
1	E	504	ILE	N-CA-C	5.23	116.11	108.53
1	D	474	LYS	N-CA-C	-5.20	105.70	111.36
1	D	207	PHE	N-CA-C	-5.15	102.90	110.52
1	A	128	VAL	N-CA-C	5.14	115.99	108.53
1	A	412	ASN	N-CA-C	-5.12	106.29	112.54
1	A	161	GLN	N-CA-C	-5.11	103.93	110.53
1	B	142	GLU	N-CA-C	5.11	117.84	110.28
1	E	59	TRP	N-CA-C	-5.10	105.72	111.28
1	E	309	ILE	CB-CA-C	-5.10	105.36	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	504	ILE	N-CA-C	5.07	115.39	107.99
1	E	258	THR	CB-CA-C	-5.07	101.46	111.60
1	C	248	LEU	N-CA-C	-5.01	106.42	112.54

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	219	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4189	0	4112	173	0
1	C	4164	0	4085	275	0
1	D	4167	0	4082	243	0
1	E	4145	0	4064	301	1
2	A	20	0	11	4	0
2	B	20	0	11	2	0
2	C	20	0	11	5	0
2	D	20	0	11	6	0
2	E	20	0	11	8	0
3	A	35	0	21	2	0
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	13	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	1212	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 29.

All (1212) 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	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:GLU:CD	1:C:103:ASN:HD21	1.49	1.20
1:C:100:ASN:HA	1:C:103:ASN:CG	1.67	1.17
1:C:99:GLU:C	1:C:103:ASN:HD22	1.52	1.16
1:A:4:LYS:HG2	1:A:101:LEU:HD23	1.15	1.15
1:A:341:ILE:HA	1:A:397:MET:HE3	1.24	1.14
1:C:96:ASP:O	1:C:99:GLU:HG2	1.47	1.12
1:D:102:MET:HE3	1:D:102:MET:HA	1.28	1.12
2:A:603:UMP:OP1	1:B:383:ARG:NH1	1.85	1.10
1:C:383:ARG:NH1	2:D:615:UMP:OP1	1.85	1.10
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:E:341:ILE:HA	1:E:397:MET:HE3	1.39	1.04
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
1:C:99:GLU:C	1:C:103:ASN:ND2	2.16	1.02
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: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:D:337:ASP:HA	1:D:356:MET:HE3	1.46	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:E:304:ASN:CG	1:E:356:MET:HE2	1.91	0.95
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:B:103:ASN:CG	1:B:104:ASP:H	1.76	0.92
1:A:304:ASN:HA	1:A:356:MET:HE3	1.51	0.92
1:E:304:ASN:HA	1:E:356:MET:HE3	1.48	0.91
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:102:MET:HE3	1:D:102:MET:CA	2.03	0.89
1:A:4:LYS:H	1:A:101:LEU:CD2	1.85	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:D:304:ASN:HA	1:D:356:MET:HE2	1.55	0.88
1:C:190:ARG:HB3	1:C:190:ARG:HH11	1.39	0.88
1:E:54:MET:HE3	1:E:72:ILE:HG23	1.55	0.88
4:E:621:MTX:HG1	4:E:621:MTX:O1	1.74	0.87
1:C:99:GLU:CD	1:C:103:ASN:ND2	2.31	0.87
1:A:341:ILE:CA	1:A:397:MET:HE3	2.04	0.87
1:A:271:ARG:NH2	1:B:267:GLY:O	2.09	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
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: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:A:103:ASN:HD22	1:A:103:ASN:C	1.84	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:A:236:TYR:CE2	1:B:212:MET:HE2	2.15	0.82
1:C:269:MET:HE2	1:D:269:MET:HE2	1.60	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:C	1:A:103:ASN:ND2	2.37	0.81
1:C:100:ASN:N	1:C:103:ASN:ND2	2.28	0.80
1:D:54:MET:HE3	1:D:72:ILE:HG23	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:TYR:CE2	1:B:391:PRO:HD2	2.16	0.80
1:B:103:ASN:O	1:B:104:ASP:C	2.24	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
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:C:54:MET:HE3	1:C:72:ILE:HG23	1.65	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: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:C:79:LEU:HD23	1:C:80:PRO:CD	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:126:ASN:CG	1:D:177:LYS:HZ1	1.93	0.75
1:A:82:ASP:OD2	1:A:84:ALA:HB3	1.86	0.75
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:D:337:ASP:CA	1:D:356:MET:HE3	2.18	0.73
1:A:102:MET:O	1:A:103:ASN:HB3	1.86	0.73
1:B:103:ASN:CG	1:B:104:ASP:N	2.46	0.73
1:C:4:LYS:H	1:C:101:LEU:HD22	1.54	0.73
1:D:255:GLU:CD	1:D:255:GLU:H	1.96	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
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:A:397:MET:HE1	1:A:401:PRO:HG3	1.71	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:C:104:ASP:CG	1:C:106:SER:H	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:51:ALA:C	1:C:52:LEU:HD23	2.16	0.70
1:D:514:THR:HG22	6:D:622:HOH:O	1.91	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:100:ASN:CA	1:C:103:ASN:CG	2.44	0.69
1:C:114:GLY:HA2	1:C:119:TYR:CZ	2.28	0.69
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:A:133:LEU:C	1:A:133:LEU:HD22	2.19	0.68
1:A:341:ILE:HA	1:A:397:MET:HE2	1.75	0.68
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:A:389:TRP:HB2	1:A:404:VAL:HG13	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:394:LEU:HA	1:D:397:MET:HE3	1.77	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: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
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:D:98:ILE:O	1:D:99:GLU:HB3	1.97	0.65
1:C:269:MET:CE	1:D:269:MET:HE2	2.26	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
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:E:191:GLY:HA2	1:E:197:ASP:CG	2.22	0.64
1:E:374:THR:HG22	1:E:384:HIS:HE1	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:208:GLY:C	1:C:210:ARG:H	2.06	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: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:178:GLN:CD	1:E:178:GLN:H	2.05	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:LEU:O	1:E:299:ILE:HG12	1.99	0.63
1:C:99:GLU:CG	1:C:103:ASN:HD21	2.09	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:A:212:MET:HE2	1:B:236:TYR:CE2	2.33	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:A:233:ARG:HH12	1:A:242:ASP:CG	2.07	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:B:274:MET:HE1	1:B:442:THR:HG21	1.82	0.61
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:C:74:VAL:C	1:C:75:ILE:HD12	2.26	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
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:C:54:MET:HE3	1:C:72:ILE:CG2	2.30	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:D:103:ASN:O	1:D:104:ASP:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ASP:OD2	1:D:82:ASP:C	2.43	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: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:A:236:TYR:CZ	1:B:212:MET:HE2	2.37	0.60
1:D:99:GLU:OE2	1:D:99:GLU:C	2.45	0.60
1:E:179:GLU:N	1:E:179:GLU:CD	2.60	0.60
1:E:260:ILE:HD13	1:E:466:TYR:CD1	2.37	0.60
1:A:99:GLU:C	1:A:99:GLU:OE1	2.45	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
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:104:ASP:C	1:D:106:SER:H	2.08	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: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:A:331:GLY:C	1:A:333:ARG:H	2.09	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
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:C:291:ILE:HG12	1:C:433:PHE:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:502:GLU:H	1:B:502:GLU:CD	2.10	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:E:264:SER:CB	1:E:464:HIS:HB3	2.32	0.59
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:D:337:ASP:CG	1:D:356:MET:HG2	2.28	0.58
1:B:104:ASP:OD2	1:B:106:SER:OG	2.20	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
1:E:82:ASP:C	1:E:84:ALA:H	2.12	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
1:E:330:LEU:C	1:E:332:HIS:H	2.13	0.57
4:A:605:MTX:HG2	4:A:605:MTX:O1	2.04	0.57
1:C:102:MET:C	1:C:103:ASN:O	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:269:MET:HE2	1:D:269:MET:CE	2.31	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:E:297:TRP:CD2	1:E:308:LEU:HD21	2.41	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: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:E:397:MET:HE1	1:E:401:PRO:HG3	1.86	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:D:82:ASP:CG	1:D:84:ALA:H	2.13	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:LEU:C	1:D:405:LEU:HD23	2.31	0.55
1:E:244:LEU:CD1	1:E:427:LEU:HB3	2.35	0.55
1:A:51:ALA:C	1:A:52:LEU:HD23	2.30	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:99:GLU:CA	1:B:99:GLU:OE1	2.53	0.55
1:B:402:CYS:SG	2:B:607:UMP:C6	3.00	0.55
1:D:342:TYR:CE1	1:D:403:HIS:NE2	2.75	0.55
1:A:304:ASN:CG	1:A:356:MET:HE2	2.32	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: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:E:304:ASN:CA	1:E:356:MET:HE3	2.32	0.55
1:E:337:ASP:CB	1:E:356:MET:SD	2.85	0.55
1:E:304:ASN:ND2	1:E:356:MET:HE2	2.20	0.55
1:C:100:ASN:N	1:C:103:ASN:CG	2.62	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: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: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:B:411:THR:HG22	1:B:412:ASN:N	2.20	0.54
1:E:119:TYR:HB3	1:E:148:PRO:HG3	1.88	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:269:MET:HE2	1:B:269:MET:HG2	1.90	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:B:54:MET:HE3	1:B:72:ILE:HG23	1.89	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: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: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:103:ASN:O	1:C:104:ASP:C	2.52	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:B:394:LEU:HA	1:B:397:MET:HE3	1.90	0.53
1:E:12:ALA:HB1	1:E:17:SER:C	2.34	0.53
1:E:171:ASP:OD2	1:E:483:PRO:HB3	2.09	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:126:ASN:ND2	1:D:177:LYS:HZ1	2.07	0.52
1:C:56:ARG:HB3	5:C:614:NDP:O3B	2.09	0.52
1:C:101:LEU:HB2	1:C:102:MET:HE3	1.92	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: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:209:ILE:HD13	1:C:209:ILE:N	2.24	0.52
1:D:330:LEU:C	1:D:332:HIS:H	2.16	0.52
1:E:36:PHE:CD1	1:E:36:PHE:C	2.87	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:B:323:GLU:CD	1:B:323:GLU:H	2.17	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:304:ASN:CG	1:E:356:MET:CE	2.75	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:270:MET:HE2	1:A:460:ILE:HD11	1.91	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: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:E:178:GLN:HA	1:E:179:GLU:OE1	2.10	0.51
1:E:208:GLY:C	1:E:210:ARG:H	2.18	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: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: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:99:GLU:OE2	1:C:103:ASN:ND2	2.34	0.51
1:C:104:ASP:CB	1:C:107:ILE:HG13	2.41	0.51
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:C:138:LEU:HD22	1:C:138:LEU:N	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:GLY:C	1:C:210:ARG:N	2.65	0.51
1:D:256:ASN:O	1:D:257:ARG:C	2.53	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:104:ASP:C	1:A:106:SER:N	2.64	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:C:409:TYR:HH	1:D:264:SER:HG	1.54	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:A:212:MET:HE2	1:B:236:TYR:CZ	2.47	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:231:PHE:CD2	1:D:192:GLN:HG3	2.45	0.50
1:E:51:ALA:C	1:E:52:LEU:HD23	2.37	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
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:B:39:ILE:HG23	1:B:40:THR:N	2.26	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
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:98:ILE:C	1:A:100:ASN:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:TRP:C	1:C:62:ILE:HG22	2.37	0.50
1:A:340:PRO:O	1:A:397:MET:HE3	2.11	0.49
1:E:225:ASN:CG	1:E:241:LEU:HD13	2.36	0.49
1:C:10:VAL:HG22	1:C:11:ALA:H	1.76	0.49
1:C:502:GLU:CD	1:C:502:GLU:H	2.20	0.49
1:A:339:GLY:O	1:A:341:ILE:HG23	2.11	0.49
1:B:98:ILE:O	1:B:98:ILE:HG23	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:D:135:ARG:NH1	1:D:159:MET:HE2	2.27	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:A:104:ASP:C	1:A:106:SER:H	2.20	0.49
1:A:269:MET:HE2	1:B:269:MET:SD	2.53	0.49
1:A:331:GLY:C	1:A:333:ARG:N	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:GLU:HG2	6:D:632:HOH:O	2.13	0.49
1:D:171:ASP:CG	1:D:483:PRO:HG3	2.37	0.49
1:D:242:ASP:O	1:D:246:ARG:HB2	2.13	0.49
1:B:99:GLU:OE1	1:B:99:GLU:HA	2.13	0.49
1:C:405:LEU:C	1:C:405:LEU:HD23	2.38	0.49
1:A:323:GLU:OE1	1:A:323:GLU:N	2.44	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:D:330:LEU:C	1:D:332:HIS:N	2.69	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: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:274:MET:HE1	1:A:442:THR:HG21	1.96	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: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:94:LEU:O	1:A:97:SER:OG	2.25	0.48
1:A:99:GLU:HA	6:A:674:HOH:O	2.14	0.48
1:A:233:ARG:NH1	1:A:242:ASP:CG	2.72	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:C:133:LEU:HD22	1:C:133:LEU:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:502:GLU:CD	1:A:502:GLU:H	2.22	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:173:MET:HE3	1:E:175:PHE:CE1	2.49	0.48
1:E:493:VAL:HG21	1:E:499:PHE:CE1	2.49	0.48
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: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: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:C:100:ASN:C	1:C:103:ASN:CB	2.56	0.47
1:D:36:PHE:CD1	1:D:36:PHE:C	2.93	0.47
1:E:244:LEU:HD21	1:E:473:LEU:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ILE:C	1:C:99:GLU:CG	2.86	0.47
1:D:348:HIS:HB3	1:D:363:VAL:O	2.15	0.47
1:E:208:GLY:C	1:E:210:ARG:N	2.71	0.47
1:A:14:VAL:HG23	1:A:136:VAL:C	2.40	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:HH12	1:D:159:MET:HE2	1.79	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
1:B:171:ASP:OD2	1:B:483:PRO:HG3	2.15	0.47
1:B:270:MET:HE2	1:B:460:ILE:HD11	1.96	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:D:104:ASP:C	1:D:106:SER:N	2.73	0.46
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:E:173:MET:HE3	1:E:175:PHE:HE1	1.81	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: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:102:MET:O	1:A:103:ASN:CG	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLU:H	1:A:323:GLU:CD	2.22	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:220:LYS:HD3	1:D:249:GLU:CD	2.41	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:171:ASP:C	1:A:172:PHE:CD1	2.94	0.46
1:A:212:MET:HB3	1:B:236:TYR:OH	2.15	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:C:115:GLY:O	1:C:116:GLU:C	2.59	0.46
1:E:304:ASN:HB3	1:E:307:HIS:NE2	2.31	0.46
1:E:371:LEU:C	1:E:371:LEU:HD13	2.41	0.46
1:A:402:CYS:SG	2:A:603:UMP:C6	3.09	0.46
1:E:14:VAL:HG13	1:E:136:VAL:C	2.41	0.46
1:E:29:ILE:HG23	1:E:165:THR:HG21	1.97	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: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: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:208:GLY:C	1:D:210:ARG:H	2.23	0.45
1:D:514:THR:HG21	6:D:633:HOH:O	2.17	0.45
1:E:3:GLU:OE2	1:E:3:GLU:CA	2.63	0.45
1:B:180:LYS:HE2	1:B:180:LYS:HB2	1.76	0.45
1:D:235:HIS:ND1	1:D:235:HIS:C	2.74	0.45
1:E:26:PRO:HB2	1:E:27:TRP:CE3	2.52	0.45
1:E:337:ASP:OD2	1:E:337:ASP:C	2.59	0.45
1:E:338:LEU:HD23	1:E:338:LEU:H	1.79	0.45
1:A:158:TYR:O	1:A:173:MET:HB2	2.16	0.45
1:B:426:ASP:OD2	1:B:426:ASP:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:304:ASN:CA	1:A:356:MET:HE3	2.36	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:97:SER:C	1:D:99:GLU:HG3	2.40	0.45
1:E:255:GLU:CD	1:E:255:GLU:H	2.25	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:E:367:GLN:O	1:E:371:LEU:N	2.49	0.45
1:A:133:LEU:C	1:A:133:LEU:CD2	2.88	0.45
1:A:392:SER:CB	1:B:350:ASN:HD22	2.29	0.45
1:B:97:SER:C	1:B:99:GLU:H	2.25	0.45
1:C:56:ARG:CG	1:C:76:SER:OG	2.65	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
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
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:A:171:ASP:CG	6:A:612:HOH:O	2.59	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: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:D:35:PHE:O	1:D:36:PHE:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:51:ALA:C	1:B:52:LEU:HD23	2.42	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:D:347:ARG:HE	1:D:366:ASP:CG	2.24	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:C:94:LEU:HA	1:C:97:SER:OG	2.18	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
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:B:192:GLN:OE1	1:B:192:GLN:HA	2.16	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:D:68:LYS:HG2	1:D:69:ASN:CG	2.43	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:208:GLY:C	1:D:210:ARG:N	2.71	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:D:27:TRP:CE2	1:D:136:VAL:HG21	2.53	0.44
1:D:102:MET:CE	1:D:102:MET:CA	2.76	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
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:74:VAL:HG12	1:C:75:ILE:N	2.31	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: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:B:378:ASN:CG	1:B:381:ASP:HB2	2.43	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: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:178:GLN:CD	1:E:178:GLN:N	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:GLY:H	1:E:356:MET:HE3	1.83	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:285:LYS:HB3	1:C:514:THR:HG23	1.99	0.43
1:E:304:ASN:OD1	1:E:356:MET:HE2	2.14	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:E:82:ASP:C	1:E:84:ALA:N	2.75	0.43
1:A:103:ASN:O	1:A:104:ASP:C	2.61	0.43
1:A:381:ASP:HB3	1:A:384:HIS:CE1	2.53	0.43
1:B:292:PHE:CD2	1:B:292:PHE:C	2.96	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:440:ILE:CG2	1:A:444:MET:HE3	2.48	0.43
1:A:472:GLN:O	1:A:475:GLU:HB3	2.19	0.43
1:B:97:SER:C	1:B:99:GLU:N	2.76	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
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:70:ARG:C	1:C:71:ILE:HD12	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:394:LEU:CA	1:D:397:MET:HE3	2.46	0.42
1:E:54:MET:HE3	1:E:72:ILE:CG2	2.39	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:36:PHE:CD1	1:C:36:PHE:C	2.97	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: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:361:THR:HG23	1:E:361:THR:O	2.18	0.42
1:A:98:ILE:C	1:A:100:ASN:N	2.78	0.42
1:B:180:LYS:HD3	1:B:180:LYS:C	2.42	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:6:VAL:HG22	1:E:110:ILE:HB	2.02	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:B:360:TYR:C	1:B:363:VAL:HG13	2.45	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:A:301:GLY:HA2	1:A:343:GLY:C	2.44	0.42
1:B:150:ILE:HA	1:B:151:PRO:HD3	1.86	0.42
1:C:104:ASP:CG	1:C:106:SER:CB	2.92	0.42
1:D:8:ILE:HG12	1:D:112:VAL:HB	2.02	0.42
1:D:291:ILE:HG12	1:D:433:PHE:CD2	2.54	0.42
1:D:443:MET:HE2	1:D:453:PRO:HG2	2.01	0.42
1:E:8:ILE:CG1	1:E:112:VAL:HB	2.36	0.42
1:E:255:GLU:CD	1:E:255:GLU:N	2.78	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:341:ILE:O	1:E:342:TYR:C	2.63	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:202:LEU:C	1:E:204:GLY:H	2.28	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: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:D:384:HIS:C	1:D:385:ILE:HD12	2.45	0.41
1:E:3:GLU:OE2	1:E:3:GLU:HA	2.19	0.41
1:E:155:LEU:HA	1:E:156:PRO:HD3	1.57	0.41
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:99:GLU:C	1:C:101:LEU:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:94:LEU:O	1:E:97:SER:OG	2.35	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: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
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:CG	1:D:107:ILE:HD13	2.46	0.41
1:E:76:SER:CA	5:E:622:NDP:O2X	2.64	0.41
1:E:305:GLY:H	1:E:356:MET:CE	2.33	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:25:LEU:C	1:E:27:TRP:H	2.28	0.41
1:E:433:PHE:CE2	3:E:620:CB3:H12	2.56	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:193:LEU:O	1:D:194:LYS:C	2.64	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:354:LYS:C	1:E:355:THR:HG23	2.46	0.41
1:E:436:ALA:O	1:E:439:ALA:HB3	2.21	0.41
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:B:235:HIS:C	1:B:235:HIS:ND1	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:180:LYS:O	1:D:181:LYS:C	2.62	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:B:173:MET:HE2	1:B:173:MET:HB3	1.98	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: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:347:ARG:HA	1:E:366:ASP:OD2	2.21	0.41
1:A:93:ASN:OD1	1:A:96:ASP:CG	2.64	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:282:THR:C	1:C:284:LYS:H	2.28	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: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:A:304:ASN:CG	1:A:356:MET:CE	2.94	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:51:ALA:C	1:D:52:LEU:HD23	2.46	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
1:B:285:LYS:HD3	1:B:514:THR:HG22	2.02	0.40
1:D:274:MET:SD	1:D:439:ALA:HA	2.61	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:96:ASP:O	1:C:97:SER:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:25:LEU:HD11	4:C:613:MTX:H7	2.04	0.40
1:D:93:ASN:CG	1:D:96:ASP:HB2	2.46	0.40
1:D:135:ARG:HH22	1:D:482:ARG:HA	1.82	0.40
1:D:487:LEU:C	1:D:487:LEU:HD23	2.46	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: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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	9 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	512/519 (99%)	482 (94%)	25 (5%)	5 (1%)	12	38
1	C	510/519 (98%)	468 (92%)	37 (7%)	5 (1%)	12	38
1	D	511/519 (98%)	464 (91%)	38 (7%)	9 (2%)	6	23
1	E	507/519 (98%)	458 (90%)	42 (8%)	7 (1%)	9	30
All	All	2552/2595 (98%)	2353 (92%)	166 (6%)	33 (1%)	9	31

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
1	A	98	ILE
1	A	101	LEU
1	B	4	LYS
1	D	100	ASN
1	D	104	ASP

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Mol	Chain	Res	Type
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%)	418 (91%)	42 (9%)	9	28
1	B	461/467 (99%)	418 (91%)	43 (9%)	8	27
1	C	457/467 (98%)	416 (91%)	41 (9%)	9	28
1	D	457/467 (98%)	408 (89%)	49 (11%)	6	21
1	E	456/467 (98%)	416 (91%)	40 (9%)	9	29
All	All	2291/2335 (98%)	2076 (91%)	215 (9%)	8	27

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	39	ILE
1	A	52	LEU
1	A	98	ILE
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	202	LEU
1	A	203	LEU
1	A	212	MET
1	A	221	GLU
1	A	244	LEU

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Mol	Chain	Res	Type
1	A	247	VAL
1	A	248	LEU
1	A	258	THR
1	A	295	LEU
1	A	311	LYS
1	A	341	ILE
1	A	342	TYR
1	A	354	LYS
1	A	355	THR
1	A	356	MET
1	A	361	THR
1	A	363	VAL
1	A	370	LYS
1	A	371	LEU
1	A	373	GLU
1	A	378	ASN
1	A	385	ILE
1	A	413	ASP
1	A	414	ASN
1	A	427	LEU
1	A	429	LEU
1	A	448	VAL
1	A	473	LEU
1	A	479	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	124	LYS
1	B	128	VAL
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	192	GLN
1	B	202	LEU
1	B	203	LEU

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Mol	Chain	Res	Type
1	B	209	ILE
1	B	220	LYS
1	B	221	GLU
1	B	233	ARG
1	B	244	LEU
1	B	247	VAL
1	B	295	LEU
1	B	308	LEU
1	B	322	LYS
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	385	ILE
1	B	404	VAL
1	B	413	ASP
1	B	420	LEU
1	B	427	LEU
1	B	429	LEU
1	B	479	ARG
1	B	495	ASN
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	79	LEU
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	165	THR
1	C	171	ASP

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Mol	Chain	Res	Type
1	C	174	ILE
1	C	176	GLU
1	C	202	LEU
1	C	209	ILE
1	C	228	SER
1	C	233	ARG
1	C	244	LEU
1	C	247	VAL
1	C	295	LEU
1	C	296	ILE
1	C	308	LEU
1	C	325	LEU
1	C	333	ARG
1	C	371	LEU
1	C	383	ARG
1	C	414	ASN
1	C	419	ASN
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	D	7	SER
1	D	8	ILE
1	D	9	VAL
1	D	52	LEU
1	D	62	ILE
1	D	71	ILE
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	102	MET
1	D	105	ASP
1	D	113	CYS
1	D	123	LEU
1	D	128	VAL
1	D	129	ASP

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Mol	Chain	Res	Type
1	D	133	LEU
1	D	138	LEU
1	D	142	GLU
1	D	149	GLU
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	260	ILE
1	D	262	THR
1	D	264	SER
1	D	295	LEU
1	D	296	ILE
1	D	308	LEU
1	D	310	GLU
1	D	370	LYS
1	D	371	LEU
1	D	383	ARG
1	D	385	ILE
1	D	405	LEU
1	D	414	ASN
1	D	422	GLN
1	D	429	LEU
1	D	437	SER
1	D	479	ARG
1	D	494	GLU
1	D	514	THR
1	E	3	GLU
1	E	8	ILE
1	E	9	VAL
1	E	36	PHE
1	E	45	ASP
1	E	52	LEU
1	E	99	GLU
1	E	101	LEU
1	E	133	LEU
1	E	138	LEU
1	E	139	GLU

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Mol	Chain	Res	Type
1	E	178	GLN
1	E	179	GLU
1	E	194	LYS
1	E	196	ILE
1	E	198	ASP
1	E	202	LEU
1	E	221	GLU
1	E	228	SER
1	E	260	ILE
1	E	269	MET
1	E	295	LEU
1	E	306	ASN
1	E	325	LEU
1	E	335	GLU
1	E	338	LEU
1	E	354	LYS
1	E	356	MET
1	E	373	GLU
1	E	394	LEU
1	E	403	HIS
1	E	414	ASN
1	E	434	ASN
1	E	470	LEU
1	E	471	THR
1	E	479	ARG
1	E	491	ARG
1	E	497	GLU
1	E	500	LYS
1	E	507	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) 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	377	ASN
1	A	384	HIS
1	A	447	GLN

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Mol	Chain	Res	Type
1	A	486	GLN
1	B	100	ASN
1	B	103	ASN
1	B	178	GLN
1	B	345	GLN
1	B	348	HIS
1	B	422	GLN
1	B	486	GLN
1	C	5	ASN
1	C	24	GLN
1	C	41	ASN
1	C	69	ASN
1	C	103	ASN
1	C	225	ASN
1	C	306	ASN
1	C	319	ASN
1	C	336	ASN
1	C	348	HIS
1	C	377	ASN
1	C	384	HIS
1	C	419	ASN
1	C	422	GLN
1	D	178	GLN
1	D	306	ASN
1	D	345	GLN
1	D	348	HIS
1	D	396	GLN
1	D	422	GLN
1	D	434	ASN
1	E	5	ASN
1	E	22	ASN
1	E	24	GLN
1	E	41	ASN
1	E	50	ASN
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

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Mol	Chain	Res	Type
1	E	396	GLN
1	E	403	HIS
1	E	434	ASN
1	E	447	GLN
1	E	486	GLN
1	E	495	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	CB3	C	612	-	37,37,37	3.10	20 (54%)	50,51,51	2.63	19 (38%)
3	CB3	D	616	-	37,37,37	2.67	21 (56%)	50,51,51	1.65	13 (26%)
5	NDP	A	606	-	51,52,52	1.45	5 (9%)	71,80,80	1.63	10 (14%)
3	CB3	E	620	-	37,37,37	1.82	4 (10%)	50,51,51	1.22	4 (8%)
2	UMP	A	603	-	21,21,21	2.27	3 (14%)	30,31,31	2.15	9 (30%)
2	UMP	D	615	-	21,21,21	2.28	3 (14%)	30,31,31	2.13	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MTX	E	621	-	35,35,35	1.24	2 (5%)	47,49,49	1.66	7 (14%)
4	MTX	A	605	-	35,35,35	1.33	3 (8%)	47,49,49	1.82	8 (17%)
3	CB3	B	608	-	37,37,37	3.63	29 (78%)	50,51,51	2.52	16 (32%)
4	MTX	B	609	-	35,35,35	1.34	3 (8%)	47,49,49	1.70	7 (14%)
5	NDP	C	614	-	51,52,52	1.31	5 (9%)	71,80,80	1.58	10 (14%)
5	NDP	E	622	-	51,52,52	1.37	4 (7%)	71,80,80	1.59	9 (12%)
4	MTX	D	617	-	35,35,35	1.30	2 (5%)	47,49,49	1.75	7 (14%)
2	UMP	C	611	-	21,21,21	2.28	3 (14%)	30,31,31	2.11	9 (30%)
4	MTX	C	613	-	35,35,35	1.26	2 (5%)	47,49,49	1.67	7 (14%)
2	UMP	E	619	-	21,21,21	2.32	3 (14%)	30,31,31	2.17	8 (26%)
5	NDP	D	618	-	51,52,52	1.43	5 (9%)	71,80,80	1.61	10 (14%)
3	CB3	A	604	-	37,37,37	2.93	18 (48%)	50,51,51	2.68	21 (42%)
2	UMP	B	607	-	21,21,21	2.29	3 (14%)	30,31,31	2.09	9 (30%)
5	NDP	B	610	-	51,52,52	1.48	5 (9%)	71,80,80	1.59	10 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CB3	C	612	-	1/1/5/6	10/27/28/28	0/3/3/3
3	CB3	D	616	-	-	6/27/28/28	0/3/3/3
5	NDP	A	606	-	-	3/34/77/77	0/5/5/5
3	CB3	E	620	-	1/1/5/6	9/27/28/28	0/3/3/3
2	UMP	D	615	-	-	5/10/22/22	0/2/2/2
2	UMP	A	603	-	-	3/10/22/22	0/2/2/2
4	MTX	E	621	-	-	8/25/25/25	0/3/3/3
4	MTX	A	605	-	-	4/25/25/25	0/3/3/3
3	CB3	B	608	-	-	5/27/28/28	0/3/3/3
4	MTX	B	609	-	-	8/25/25/25	0/3/3/3
5	NDP	C	614	-	-	15/34/77/77	0/5/5/5
5	NDP	E	622	-	-	14/34/77/77	0/5/5/5
4	MTX	D	617	-	-	8/25/25/25	0/3/3/3
2	UMP	C	611	-	-	2/10/22/22	0/2/2/2
4	MTX	C	613	-	-	6/25/25/25	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UMP	E	619	-	-	7/10/22/22	0/2/2/2
5	NDP	D	618	-	-	2/34/77/77	0/5/5/5
3	CB3	A	604	-	-	6/27/28/28	0/3/3/3
2	UMP	B	607	-	-	2/10/22/22	0/2/2/2
5	NDP	B	610	-	-	3/34/77/77	0/5/5/5

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	CB3	C4A-C4	-9.83	1.31	1.48
3	C	612	CB3	C4A-C4	-9.52	1.32	1.48
2	E	619	UMP	C6-C5	8.09	1.53	1.35
2	B	607	UMP	C6-C5	7.95	1.53	1.35
2	D	615	UMP	C6-C5	7.93	1.53	1.35
2	A	603	UMP	C6-C5	7.91	1.53	1.35
2	C	611	UMP	C6-C5	7.91	1.53	1.35
3	B	608	CB3	CP1-N10	-7.82	1.38	1.46
3	E	620	CB3	O4-C4	7.79	1.36	1.23
3	D	616	CB3	C4A-C4	-7.76	1.35	1.48
3	B	608	CB3	C4A-C4	-7.44	1.35	1.48
5	B	610	NDP	C4N-C3N	-6.48	1.37	1.50
5	D	618	NDP	C4N-C3N	-6.36	1.38	1.50
5	A	606	NDP	C4N-C3N	-6.29	1.38	1.50
5	E	622	NDP	C4N-C3N	-6.26	1.38	1.50
3	B	608	CB3	C8A-N1	-5.85	1.29	1.39
5	C	614	NDP	C4N-C3N	-5.68	1.39	1.50
3	B	608	CB3	C12-C11	-5.60	1.30	1.39
3	C	612	CB3	C4A-C8A	-5.50	1.32	1.41
3	D	616	CB3	O4-C4	5.43	1.32	1.23
3	D	616	CB3	CP1-N10	-5.23	1.41	1.46
3	E	620	CB3	C4A-C4	-5.21	1.39	1.48
3	B	608	CB3	C4A-C8A	-5.17	1.33	1.41
3	B	608	CB3	O4-C4	4.80	1.31	1.23
3	C	612	CB3	C5-C4A	-4.50	1.32	1.39
3	A	604	CB3	C8A-N1	-4.48	1.32	1.39
3	C	612	CB3	O4-C4	4.47	1.31	1.23
3	A	604	CB3	C4-N3	-4.43	1.29	1.38
3	B	608	CB3	C4-N3	-4.42	1.29	1.38
3	C	612	CB3	C8A-N1	-4.29	1.32	1.39
3	B	608	CB3	C15-C14	-4.27	1.31	1.39
3	C	612	CB3	C4-N3	-4.23	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	619	UMP	C6-N1	4.23	1.48	1.38
3	B	608	CB3	C2-N1	-4.22	1.27	1.37
5	B	610	NDP	C4N-C5N	-4.22	1.38	1.49
2	E	619	UMP	C5-C4	4.21	1.52	1.43
3	C	612	CB3	CP1-N10	-4.20	1.42	1.46
5	A	606	NDP	C4N-C5N	-4.20	1.38	1.49
2	B	607	UMP	C6-N1	4.19	1.48	1.38
2	D	615	UMP	C5-C4	4.18	1.52	1.43
2	D	615	UMP	C6-N1	4.17	1.48	1.38
2	B	607	UMP	C5-C4	4.17	1.52	1.43
2	C	611	UMP	C6-N1	4.17	1.48	1.38
2	A	603	UMP	C6-N1	4.17	1.48	1.38
5	D	618	NDP	C4N-C5N	-4.16	1.38	1.49
2	A	603	UMP	C5-C4	4.16	1.52	1.43
3	A	604	CB3	CP1-N10	-4.15	1.42	1.46
3	A	604	CB3	C4A-C8A	-4.15	1.34	1.41
2	C	611	UMP	C5-C4	4.13	1.52	1.43
4	E	621	MTX	O-C	4.06	1.32	1.23
3	A	604	CB3	C15-C14	-4.02	1.31	1.39
5	E	622	NDP	C4N-C5N	-4.02	1.38	1.49
4	C	613	MTX	O-C	4.01	1.32	1.23
4	D	617	MTX	O-C	3.96	1.32	1.23
3	B	608	CB3	C9-N10	-3.94	1.40	1.46
3	B	608	CB3	C5-C4A	-3.94	1.33	1.39
4	B	609	MTX	O-C	3.93	1.32	1.23
3	A	604	CB3	O4-C4	3.91	1.30	1.23
3	C	612	CB3	C12-C11	-3.88	1.33	1.39
4	A	605	MTX	O-C	3.86	1.32	1.23
4	A	605	MTX	C-N	-3.83	1.25	1.34
4	B	609	MTX	C-N	-3.83	1.25	1.34
4	D	617	MTX	C-N	-3.76	1.25	1.34
5	C	614	NDP	C4N-C5N	-3.76	1.39	1.49
4	C	613	MTX	C-N	-3.66	1.25	1.34
3	A	604	CB3	CP2-CP3	3.62	1.28	1.18
3	B	608	CB3	C-N	-3.62	1.25	1.34
3	D	616	CB3	C8A-N1	-3.58	1.33	1.39
3	C	612	CB3	CP1-CP2	-3.58	1.41	1.46
4	E	621	MTX	C-N	-3.58	1.26	1.34
3	B	608	CB3	O2-CT	-3.51	1.19	1.30
3	B	608	CB3	O-C	-3.51	1.15	1.23
3	A	604	CB3	C13-C14	-3.51	1.32	1.39
3	C	612	CB3	CB-CA	-3.49	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	616	CB3	C4A-C8A	-3.46	1.35	1.41
3	E	620	CB3	CP2-CP3	3.45	1.28	1.18
3	B	608	CB3	C11-C	-3.38	1.42	1.50
3	A	604	CB3	C8-C8A	-3.30	1.34	1.39
3	A	604	CB3	C2-N1	-3.22	1.29	1.37
3	B	608	CB3	C9-C6	-3.22	1.45	1.51
3	B	608	CB3	C7-C6	-3.16	1.32	1.38
3	B	608	CB3	OE2-CD	-3.13	1.20	1.30
3	C	612	CB3	OE2-CD	-3.13	1.20	1.30
3	A	604	CB3	C5-C4A	-3.03	1.35	1.39
3	B	608	CB3	CA-CT	-3.03	1.45	1.52
3	D	616	CB3	C4-N3	-3.01	1.32	1.38
3	C	612	CB3	C2-N1	-3.00	1.30	1.37
3	B	608	CB3	C13-C12	-2.95	1.34	1.38
3	B	608	CB3	C16-C11	-2.93	1.35	1.39
3	D	616	CB3	CP1-CP2	-2.90	1.42	1.46
3	D	616	CB3	C12-C11	-2.89	1.35	1.39
3	B	608	CB3	C16-C15	-2.89	1.34	1.38
3	D	616	CB3	O-C	-2.86	1.16	1.23
3	D	616	CB3	C-N	-2.86	1.27	1.34
3	D	616	CB3	C16-C11	-2.78	1.35	1.39
3	B	608	CB3	C8-C7	-2.77	1.34	1.38
5	A	606	NDP	C5A-N7A	-2.75	1.34	1.39
3	D	616	CB3	C5-C6	-2.73	1.34	1.39
3	A	604	CB3	OE2-CD	-2.72	1.21	1.30
5	B	610	NDP	C5A-N7A	-2.67	1.34	1.39
3	A	604	CB3	C16-C11	-2.67	1.35	1.39
3	C	612	CB3	C-N	-2.64	1.28	1.34
3	C	612	CB3	C11-C	-2.64	1.44	1.50
3	E	620	CB3	C8A-N1	-2.63	1.35	1.39
3	C	612	CB3	C9-C6	-2.62	1.46	1.51
3	B	608	CB3	C13-C14	-2.58	1.34	1.39
3	B	608	CB3	C8-C8A	-2.58	1.35	1.39
3	C	612	CB3	CA-CT	-2.54	1.46	1.52
3	C	612	CB3	C5-C6	-2.53	1.35	1.39
5	D	618	NDP	C5A-N7A	-2.53	1.34	1.39
3	D	616	CB3	O2-CT	-2.52	1.22	1.30
5	B	610	NDP	C4A-N9A	-2.51	1.32	1.37
3	C	612	CB3	O2-CT	-2.50	1.22	1.30
5	A	606	NDP	C8A-N9A	-2.49	1.33	1.37
5	B	610	NDP	C8A-N9A	-2.49	1.33	1.37
3	B	608	CB3	CP1-CP2	-2.44	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	618	NDP	C8A-N9A	-2.42	1.33	1.37
3	C	612	CB3	O-C	-2.42	1.17	1.23
5	A	606	NDP	C4A-N9A	-2.40	1.32	1.37
3	B	608	CB3	C5-C6	-2.40	1.35	1.39
5	E	622	NDP	C5A-N7A	-2.40	1.34	1.39
3	D	616	CB3	CP2-CP3	2.39	1.25	1.18
3	D	616	CB3	C7-C6	-2.33	1.34	1.38
3	B	608	CB3	C2-NA2	-2.31	1.28	1.34
3	D	616	CB3	C11-C	-2.28	1.45	1.50
5	D	618	NDP	C4A-N9A	-2.28	1.33	1.37
3	A	604	CB3	C8-C7	-2.26	1.35	1.38
3	D	616	CB3	C9-N10	-2.25	1.43	1.46
3	C	612	CB3	C13-C14	-2.25	1.35	1.39
3	A	604	CB3	O-C	-2.25	1.18	1.23
3	D	616	CB3	C2-N1	-2.24	1.32	1.37
4	A	605	MTX	C8A-N8	-2.17	1.34	1.37
3	D	616	CB3	C13-C14	-2.17	1.35	1.39
3	A	604	CB3	O2-CT	-2.16	1.23	1.30
3	A	604	CB3	C14-N10	-2.14	1.33	1.38
3	D	616	CB3	C8-C8A	-2.11	1.36	1.39
3	B	608	CB3	CP2-CP3	2.10	1.24	1.18
5	C	614	NDP	C5A-N7A	-2.10	1.35	1.39
5	C	614	NDP	C6N-C5N	2.09	1.39	1.33
5	C	614	NDP	C8A-N7A	2.08	1.35	1.31
4	B	609	MTX	C8A-N8	-2.03	1.34	1.37
3	D	616	CB3	C5-C4A	-2.02	1.36	1.39
5	E	622	NDP	C8A-N9A	-2.01	1.34	1.37

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	608	CB3	CP2-CP1-N10	-11.39	102.94	113.45
3	C	612	CB3	CT-CA-N	10.03	133.83	110.57
3	A	604	CB3	CP2-CP1-N10	-7.82	106.24	113.45
3	A	604	CB3	CP1-N10-C9	6.49	123.72	117.19
5	A	606	NDP	C2B-C1B-N9A	-6.01	103.87	113.75
3	A	604	CB3	CP1-N10-C14	-5.85	108.06	119.03
3	D	616	CB3	CP2-CP1-N10	-5.82	108.08	113.45
2	E	619	UMP	N3-C2-N1	5.69	122.30	114.89
3	C	612	CB3	CG-CB-CA	-5.53	102.96	113.16
5	E	622	NDP	C5A-C4A-N3A	-5.46	119.19	126.72
5	D	618	NDP	C2B-C1B-N9A	-5.45	104.79	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	612	CB3	CB-CA-N	-5.44	100.14	110.91
5	B	610	NDP	C2B-C1B-N9A	-5.35	104.94	113.75
3	A	604	CB3	C13-C14-N10	-5.28	114.06	121.39
5	C	614	NDP	C5A-C4A-N3A	-5.25	119.48	126.72
2	D	615	UMP	N3-C2-N1	5.22	121.68	114.89
2	A	603	UMP	N3-C2-N1	5.16	121.60	114.89
5	D	618	NDP	C5A-C4A-N3A	-5.10	119.70	126.72
5	A	606	NDP	C5A-C4A-N3A	-5.09	119.71	126.72
4	B	609	MTX	N1-C2-N3	-5.08	120.75	127.21
5	B	610	NDP	C5A-C4A-N3A	-5.07	119.74	126.72
2	B	607	UMP	N3-C2-N1	5.06	121.48	114.89
4	E	621	MTX	N1-C2-N3	-5.03	120.82	127.21
4	A	605	MTX	N1-C2-N3	-5.00	120.85	127.21
2	A	603	UMP	C5-C4-N3	4.94	121.72	114.80
2	C	611	UMP	C5-C4-N3	4.89	121.65	114.80
2	C	611	UMP	N3-C2-N1	4.89	121.25	114.89
4	D	617	MTX	N1-C2-N3	-4.87	121.02	127.21
5	D	618	NDP	N3A-C2A-N1A	-4.87	121.21	128.58
5	E	622	NDP	C2B-C1B-N9A	-4.81	105.84	113.75
5	E	622	NDP	N3A-C2A-N1A	-4.81	121.31	128.58
5	C	614	NDP	N3A-C2A-N1A	-4.75	121.39	128.58
5	A	606	NDP	N3A-C2A-N1A	-4.74	121.41	128.58
2	B	607	UMP	C5-C4-N3	4.72	121.41	114.80
2	D	615	UMP	C5-C4-N3	4.70	121.39	114.80
4	C	613	MTX	N1-C2-N3	-4.64	121.31	127.21
5	B	610	NDP	N3A-C2A-N1A	-4.63	121.58	128.58
3	B	608	CB3	C6-C9-N10	-4.52	106.81	114.13
2	E	619	UMP	C5-C4-N3	4.45	121.03	114.80
3	C	612	CB3	C9-N10-C14	4.39	128.32	120.72
2	A	603	UMP	C4-N3-C2	-4.36	121.20	126.61
4	C	613	MTX	C2-N1-C8A	4.34	120.16	115.48
3	A	604	CB3	C11-C-N	4.33	125.06	117.04
3	A	604	CB3	C9-N10-C14	4.32	128.22	120.72
2	D	615	UMP	C4-N3-C2	-4.28	121.30	126.61
4	D	617	MTX	C2-N1-C8A	4.26	120.08	115.48
3	E	620	CB3	CP2-CP1-N10	-4.25	109.53	113.45
2	E	619	UMP	C4-N3-C2	-4.21	121.39	126.61
4	B	609	MTX	N8-C8A-N1	4.21	120.35	115.77
3	C	612	CB3	C13-C14-N10	-4.20	115.56	121.39
4	E	621	MTX	C2-N1-C8A	4.19	120.01	115.48
4	A	605	MTX	N8-C8A-N1	4.19	120.34	115.77
4	B	609	MTX	C2-N1-C8A	4.17	119.98	115.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	MTX	C2-N1-C8A	4.15	119.95	115.48
4	C	613	MTX	N8-C8A-N1	4.14	120.28	115.77
2	C	611	UMP	O4-C4-C5	-4.14	118.03	125.16
3	B	608	CB3	C13-C12-C11	-4.08	116.44	120.80
3	A	604	CB3	C16-C11-C12	-4.07	113.39	118.57
4	D	617	MTX	N8-C8A-N1	4.06	120.19	115.77
2	B	607	UMP	C4-N3-C2	-4.05	121.59	126.61
2	C	611	UMP	C4-N3-C2	-4.04	121.60	126.61
2	B	607	UMP	O4-C4-C5	-3.95	118.35	125.16
3	C	612	CB3	C15-C14-N10	3.89	126.80	121.39
2	A	603	UMP	O4-C4-C5	-3.88	118.47	125.16
4	A	605	MTX	C6-C9-N10	-3.87	106.32	112.95
2	D	615	UMP	O4-C4-C5	-3.84	118.54	125.16
4	D	617	MTX	C6-C9-N10	-3.82	106.41	112.95
3	C	612	CB3	C11-C-N	-3.81	109.98	117.04
3	A	604	CB3	C5-C4A-C8A	3.75	122.47	119.09
4	D	617	MTX	CB-CA-N	-3.72	103.54	110.91
3	C	612	CB3	O4-C4-C4A	-3.72	115.35	121.33
3	B	608	CB3	C4A-C8A-N1	-3.71	116.56	119.46
4	E	621	MTX	N8-C8A-N1	3.71	119.81	115.77
3	A	604	CB3	C15-C14-N10	3.69	126.52	121.39
3	A	604	CB3	O-C-N	-3.65	115.53	122.47
2	E	619	UMP	O4-C4-C5	-3.64	118.89	125.16
4	B	609	MTX	C6-C9-N10	-3.61	106.76	112.95
5	D	618	NDP	N9A-C8A-N7A	-3.61	108.82	113.94
3	B	608	CB3	C8-C7-C6	-3.58	116.30	121.00
5	E	622	NDP	C2A-N3A-C4A	3.57	120.56	111.83
3	B	608	CB3	C7-C6-C5	3.55	123.44	118.55
3	D	616	CB3	C9-N10-C14	3.54	126.86	120.72
4	C	613	MTX	C6-C9-N10	-3.53	106.89	112.95
5	A	606	NDP	N9A-C8A-N7A	-3.52	108.94	113.94
3	B	608	CB3	C5-C4A-C8A	-3.52	115.93	119.09
2	D	615	UMP	C5-C6-N1	-3.48	116.18	121.84
2	A	603	UMP	C5-C6-N1	-3.47	116.20	121.84
5	C	614	NDP	N9A-C8A-N7A	-3.46	109.03	113.94
5	D	618	NDP	C2A-N3A-C4A	3.46	120.28	111.83
3	A	604	CB3	O2-CT-CA	3.44	125.16	113.51
5	E	622	NDP	N3A-C4A-N9A	3.44	133.02	127.17
5	B	610	NDP	N9A-C8A-N7A	-3.44	109.06	113.94
5	C	614	NDP	C2A-N3A-C4A	3.43	120.22	111.83
5	C	614	NDP	N3A-C4A-N9A	3.39	132.93	127.17
3	B	608	CB3	C12-C13-C14	3.39	124.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606	NDP	C2A-N3A-C4A	3.37	120.07	111.83
3	B	608	CB3	CB-CA-N	-3.36	104.25	110.91
4	A	605	MTX	CB-CA-N	-3.34	104.29	110.91
3	B	608	CB3	C8-C8A-C4A	3.34	123.73	119.37
5	B	610	NDP	C2A-N3A-C4A	3.33	119.96	111.83
5	A	606	NDP	N3A-C4A-N9A	3.28	132.74	127.17
2	E	619	UMP	C5-C6-N1	-3.27	116.53	121.84
5	E	622	NDP	N9A-C8A-N7A	-3.23	109.36	113.94
2	B	607	UMP	C6-C5-C4	-3.22	115.42	119.53
2	C	611	UMP	C5-C6-N1	-3.22	116.61	121.84
2	B	607	UMP	C5-C6-N1	-3.22	116.61	121.84
5	D	618	NDP	N3A-C4A-N9A	3.21	132.63	127.17
3	B	608	CB3	C9-N10-C14	3.15	126.17	120.72
3	B	608	CB3	CG-CB-CA	3.14	118.96	113.16
2	D	615	UMP	O2-C2-N1	-3.10	118.76	122.80
4	E	621	MTX	C6-C9-N10	-3.10	107.64	112.95
2	E	619	UMP	O2-C2-N1	-3.10	118.77	122.80
4	C	613	MTX	C6-C7-N8	-3.09	120.17	123.14
2	A	603	UMP	O2-C2-N1	-3.05	118.83	122.80
5	B	610	NDP	N3A-C4A-N9A	3.04	132.33	127.17
3	D	616	CB3	O-C-N	-3.03	116.70	122.47
2	B	607	UMP	O2-C2-N1	-3.02	118.86	122.80
2	C	611	UMP	C6-C5-C4	-3.02	115.68	119.53
2	E	619	UMP	O5'-P-OP1	3.00	114.54	106.44
3	C	612	CB3	CB-CA-CT	-2.99	103.26	110.35
3	E	620	CB3	CB-CA-N	-2.99	105.00	110.91
4	E	621	MTX	C6-C7-N8	-2.92	120.34	123.14
2	A	603	UMP	C6-C5-C4	-2.92	115.81	119.53
3	E	620	CB3	C6-C9-N10	-2.90	109.43	114.13
4	A	605	MTX	C13-C14-N10	-2.89	117.56	121.59
3	D	616	CB3	O4-C4-C4A	-2.85	116.74	121.33
3	D	616	CB3	O4-C4-N3	2.83	124.53	120.23
2	D	615	UMP	C6-C5-C4	-2.83	115.92	119.53
3	E	620	CB3	CP1-N10-C9	2.79	120.00	117.19
4	D	617	MTX	C6-C7-N8	-2.78	120.47	123.14
5	B	610	NDP	C4A-C5A-N7A	-2.77	107.42	110.58
3	D	616	CB3	C11-C-N	2.76	122.15	117.04
5	D	618	NDP	C4A-C5A-N7A	-2.76	107.43	110.58
3	C	612	CB3	O2-CT-CA	2.74	122.79	113.51
5	C	614	NDP	C4A-C5A-N7A	-2.73	107.46	110.58
2	C	611	UMP	O5'-P-OP1	2.72	113.80	106.44
3	D	616	CB3	C13-C14-N10	-2.71	117.63	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	607	UMP	O5'-P-OP1	2.69	113.72	106.44
5	D	618	NDP	C4A-N9A-C8A	2.68	108.56	105.74
3	A	604	CB3	C15-C16-C11	2.67	123.66	120.80
2	A	603	UMP	O5'-P-OP1	2.67	113.67	106.44
2	E	619	UMP	C6-C5-C4	-2.66	116.13	119.53
4	B	609	MTX	C6-C7-N8	-2.66	120.58	123.14
2	C	611	UMP	O2-C2-N1	-2.66	119.33	122.80
4	C	613	MTX	CB-CA-N	-2.66	105.65	110.91
4	A	605	MTX	C6-C7-N8	-2.65	120.59	123.14
5	C	614	NDP	C2B-C1B-N9A	-2.64	109.41	113.75
5	A	606	NDP	C4A-N9A-C8A	2.63	108.50	105.74
5	C	614	NDP	C5A-N7A-C8A	2.62	107.57	103.45
3	C	612	CB3	CA-N-C	2.59	127.78	121.56
5	E	622	NDP	C4A-C5A-N7A	-2.59	107.62	110.58
5	D	618	NDP	C5A-N7A-C8A	2.59	107.52	103.45
3	D	616	CB3	C5-C4A-C8A	2.57	121.40	119.09
4	D	617	MTX	C13-C14-N10	-2.57	118.01	121.59
3	A	604	CB3	CG-CB-CA	2.55	117.87	113.16
3	A	604	CB3	CB-CG-CD	-2.54	105.71	112.49
5	C	614	NDP	C3D-C2D-C1D	2.53	106.25	101.46
2	C	611	UMP	C1'-N1-C6	-2.52	116.57	121.53
5	A	606	NDP	C4A-C5A-N7A	-2.51	107.71	110.58
4	B	609	MTX	CB-CA-N	-2.51	105.94	110.91
3	C	612	CB3	C6-C9-N10	-2.51	110.06	114.13
5	C	614	NDP	C4A-N9A-C8A	2.50	108.36	105.74
3	C	612	CB3	C12-C13-C14	2.48	123.44	120.30
3	C	612	CB3	C4A-C8A-N1	-2.47	117.53	119.46
5	A	606	NDP	C5A-N7A-C8A	2.45	107.31	103.45
5	B	610	NDP	C5A-N7A-C8A	2.45	107.31	103.45
5	B	610	NDP	C4A-N9A-C8A	2.43	108.29	105.74
5	E	622	NDP	C5A-N7A-C8A	2.43	107.27	103.45
4	E	621	MTX	CB-CA-N	-2.33	106.29	110.91
4	C	613	MTX	C13-C14-N10	-2.33	118.34	121.59
2	D	615	UMP	O5'-P-OP1	2.33	112.73	106.44
3	C	612	CB3	O1-CT-CA	-2.30	114.84	122.26
3	A	604	CB3	C13-C12-C11	2.30	123.25	120.80
3	B	608	CB3	O2-CT-CA	2.29	121.24	113.51
3	B	608	CB3	CB-CA-CT	-2.26	105.00	110.35
4	A	605	MTX	CM-N10-C9	2.25	120.96	115.11
3	A	604	CB3	CB-CA-CT	-2.22	105.08	110.35
4	B	609	MTX	CM-N10-C9	2.22	120.90	115.11
3	C	612	CB3	OE2-CD-CG	2.22	121.03	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	607	UMP	C1'-N1-C6	-2.21	117.18	121.53
5	A	606	NDP	O3X-P2B-O2X	2.20	116.06	107.80
3	D	616	CB3	CP1-N10-C14	-2.19	114.92	119.03
3	A	604	CB3	O1-CT-CA	-2.16	115.30	122.26
3	A	604	CB3	CB-CA-N	2.15	115.16	110.91
3	C	612	CB3	O-C-C11	2.15	125.15	120.90
3	B	608	CB3	CP1-N10-C9	-2.14	115.03	117.19
2	A	603	UMP	C1'-N1-C6	-2.14	117.33	121.53
5	E	622	NDP	C4A-N9A-C8A	2.12	107.96	105.74
3	C	612	CB3	CP1-N10-C14	-2.11	115.07	119.03
3	D	616	CB3	OE2-CD-CG	2.07	120.53	114.00
3	C	612	CB3	C5-C4A-C8A	2.06	120.94	119.09
5	D	618	NDP	O3X-P2B-O2X	2.04	115.45	107.80
5	B	610	NDP	O3X-P2B-O2X	2.03	115.41	107.80
3	D	616	CB3	OE1-CD-CG	-2.03	116.66	123.09
4	E	621	MTX	C13-C14-N10	-2.03	118.77	121.59
3	A	604	CB3	C4A-C5-C6	-2.02	118.25	121.38
3	D	616	CB3	O2-CT-O1	-2.02	119.50	124.08
3	B	608	CB3	OE2-CD-CG	2.02	120.37	114.00
3	A	604	CB3	C6-C9-N10	-2.02	110.86	114.13
3	A	604	CB3	O2-CT-O1	-2.01	119.52	124.08
3	D	616	CB3	CB-CA-CT	2.00	115.11	110.35

All (2) chirality outliers are listed below:

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

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C5'-O5'-P-OP2
2	E	619	UMP	C5'-O5'-P-OP3
3	B	608	CB3	N-CA-CB-CG
3	B	608	CB3	CT-CA-CB-CG
3	C	612	CB3	CB-CA-N-C
4	C	613	MTX	CT-CA-CB-CG
4	E	621	MTX	CT-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
5	C	614	NDP	C5B-O5B-PA-O2A
5	C	614	NDP	O4B-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	E	622	NDP	C5D-O5D-PN-O3
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	E	619	UMP	C2'-C1'-N1-C2
2	D	615	UMP	C3'-C4'-C5'-O5'
2	D	615	UMP	O4'-C4'-C5'-O5'
2	E	619	UMP	C3'-C4'-C5'-O5'
5	C	614	NDP	C3B-C4B-C5B-O5B
5	C	614	NDP	C3D-C4D-C5D-O5D
5	E	622	NDP	C3B-C4B-C5B-O5B
4	D	617	MTX	C13-C14-N10-CM
4	D	617	MTX	C15-C14-N10-CM
3	D	616	CB3	CB-CA-N-C
3	A	604	CB3	CT-CA-CB-CG
3	B	608	CB3	C6-C9-N10-C14
2	E	619	UMP	C2'-C1'-N1-C6
5	E	622	NDP	C1B-C2B-O2B-P2B
4	C	613	MTX	CT-CA-N-C
3	A	604	CB3	C6-C9-N10-C14
4	D	617	MTX	CT-CA-N-C
4	B	609	MTX	CT-CA-CB-CG
2	E	619	UMP	O4'-C4'-C5'-O5'
5	C	614	NDP	O4D-C4D-C5D-O5D
5	E	622	NDP	O4B-C4B-C5B-O5B
5	E	622	NDP	C3B-C2B-O2B-P2B
3	A	604	CB3	CA-CB-CG-CD
4	C	613	MTX	C15-C14-N10-CM
2	E	619	UMP	C5'-O5'-P-OP1
3	E	620	CB3	N-CA-CT-O2
4	C	613	MTX	C13-C14-N10-CM
4	E	621	MTX	N-CA-CB-CG
2	B	607	UMP	O4'-C4'-C5'-O5'
5	E	622	NDP	C3D-C4D-C5D-O5D
3	E	620	CB3	CB-CA-N-C
5	E	622	NDP	PN-O3-PA-O1A
3	E	620	CB3	N-CA-CT-O1

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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
2	A	603	UMP	C3'-C4'-C5'-O5'
2	B	607	UMP	C3'-C4'-C5'-O5'
4	B	609	MTX	C13-C14-N10-CM
4	E	621	MTX	C13-C14-N10-CM
5	A	606	NDP	PA-O3-PN-O5D
3	B	608	CB3	CA-CB-CG-CD
3	E	620	CB3	CT-CA-CB-CG
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	B	609	MTX	C15-C14-N10-CM
4	E	621	MTX	C15-C14-N10-CM
2	A	603	UMP	O4'-C4'-C5'-O5'
4	B	609	MTX	CT-CA-N-C
3	C	612	CB3	N-CA-CT-O2
3	B	608	CB3	C6-C9-N10-CP1
5	A	606	NDP	C5B-O5B-PA-O1A
5	C	614	NDP	C5B-O5B-PA-O3
5	E	622	NDP	C5D-O5D-PN-O1N
5	C	614	NDP	C4B-C5B-O5B-PA
2	A	603	UMP	C5'-O5'-P-OP1
3	C	612	CB3	N-CA-CT-O1
2	C	611	UMP	C3'-C4'-C5'-O5'
3	E	620	CB3	CB-CA-CT-O2
4	D	617	MTX	C13-C14-N10-C9
5	E	622	NDP	PN-O3-PA-O2A
3	A	604	CB3	C6-C9-N10-CP1
3	E	620	CB3	CB-CA-CT-O1
5	B	610	NDP	C2B-O2B-P2B-O2X
5	E	622	NDP	C2B-O2B-P2B-O3X
5	A	606	NDP	O4D-C1D-N1N-C2N
5	B	610	NDP	O4D-C1D-N1N-C2N
5	E	622	NDP	O4D-C1D-N1N-C2N
2	C	611	UMP	O4'-C4'-C5'-O5'
5	C	614	NDP	O4D-C1D-N1N-C2N
5	D	618	NDP	O4D-C1D-N1N-C2N
3	C	612	CB3	C6-C9-N10-CP1
4	B	609	MTX	N-CA-CB-CG
3	D	616	CB3	CA-CB-CG-CD
5	D	618	NDP	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
5	E	622	NDP	C2N-C3N-C7N-N7N
5	C	614	NDP	C2D-C1D-N1N-C2N
4	A	605	MTX	C15-C14-N10-CM
3	C	612	CB3	CB-CA-CT-O1
3	E	620	CB3	C5-C6-C9-N10
3	D	616	CB3	C6-C9-N10-C14
3	C	612	CB3	OE2-CD-CG-CB
4	D	617	MTX	C15-C14-N10-C9
4	E	621	MTX	C6-C9-N10-CM
3	D	616	CB3	C6-C9-N10-CP1
3	C	612	CB3	C6-C9-N10-C14
3	D	616	CB3	OE2-CD-CG-CB
5	B	610	NDP	C2D-C1D-N1N-C2N
3	C	612	CB3	OE1-CD-CG-CB
3	E	620	CB3	C7-C6-C9-N10
3	D	616	CB3	OE1-CD-CG-CB
4	A	605	MTX	C13-C14-N10-CM
4	D	617	MTX	CB-CA-CT-O1
4	D	617	MTX	CB-CA-CT-O2
4	E	621	MTX	CB-CA-CT-O1
4	E	621	MTX	CB-CA-CT-O2
4	A	605	MTX	CT-CA-N-C
4	E	621	MTX	CT-CA-N-C
5	C	614	NDP	O4D-C1D-N1N-C6N
5	C	614	NDP	C2D-C1D-N1N-C6N
5	C	614	NDP	C3B-C2B-O2B-P2B
4	C	613	MTX	CB-CA-N-C
5	E	622	NDP	C4D-C5D-O5D-PN
3	C	612	CB3	CB-CA-CT-O2
4	B	609	MTX	CB-CA-CT-O1
4	B	609	MTX	CB-CA-CT-O2
3	A	604	CB3	OE2-CD-CG-CB

There are no ring outliers.

20 monomers are involved in 134 short contacts:

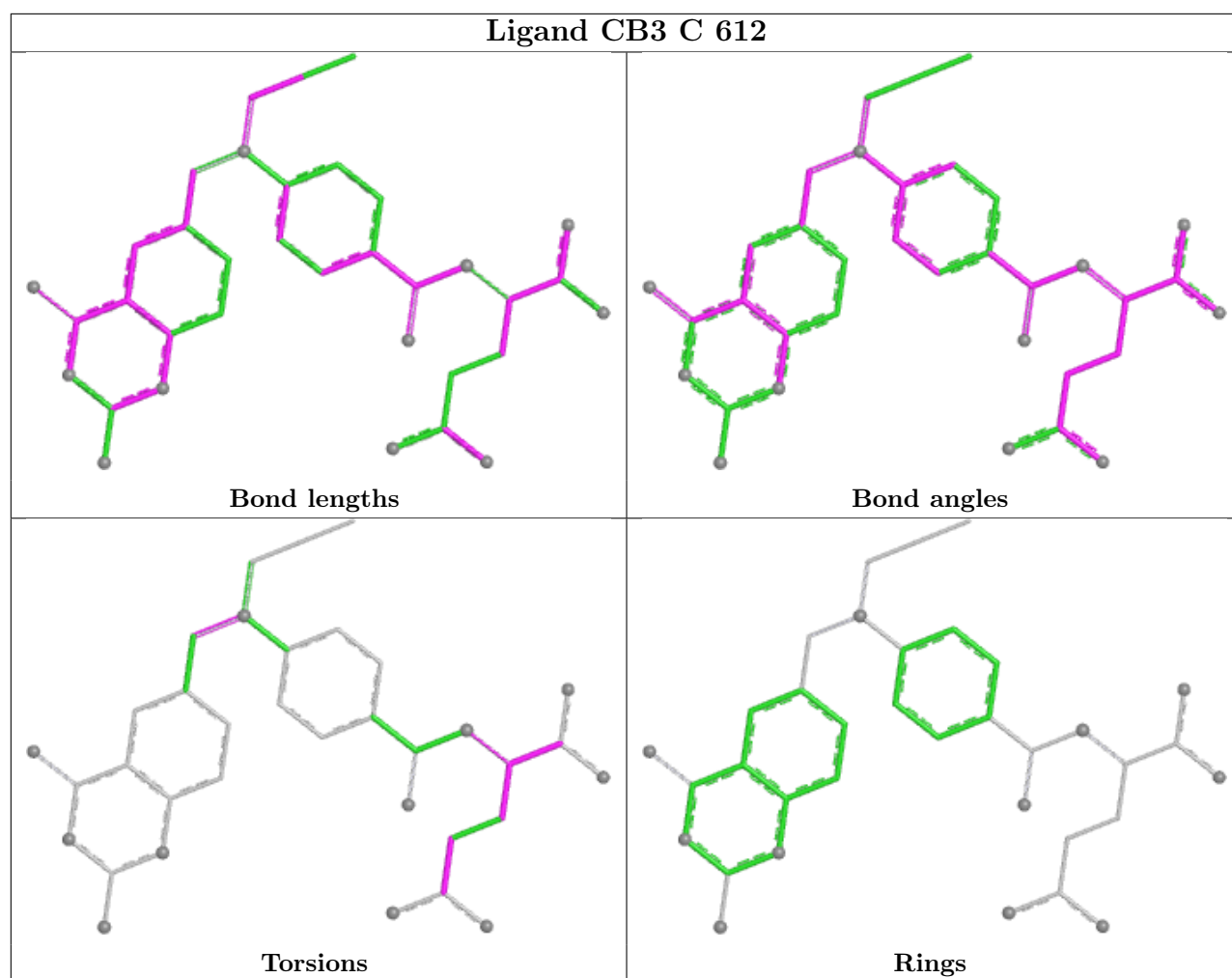
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	612	CB3	9	0
3	D	616	CB3	4	0
5	A	606	NDP	5	0
3	E	620	CB3	17	0
2	A	603	UMP	4	0

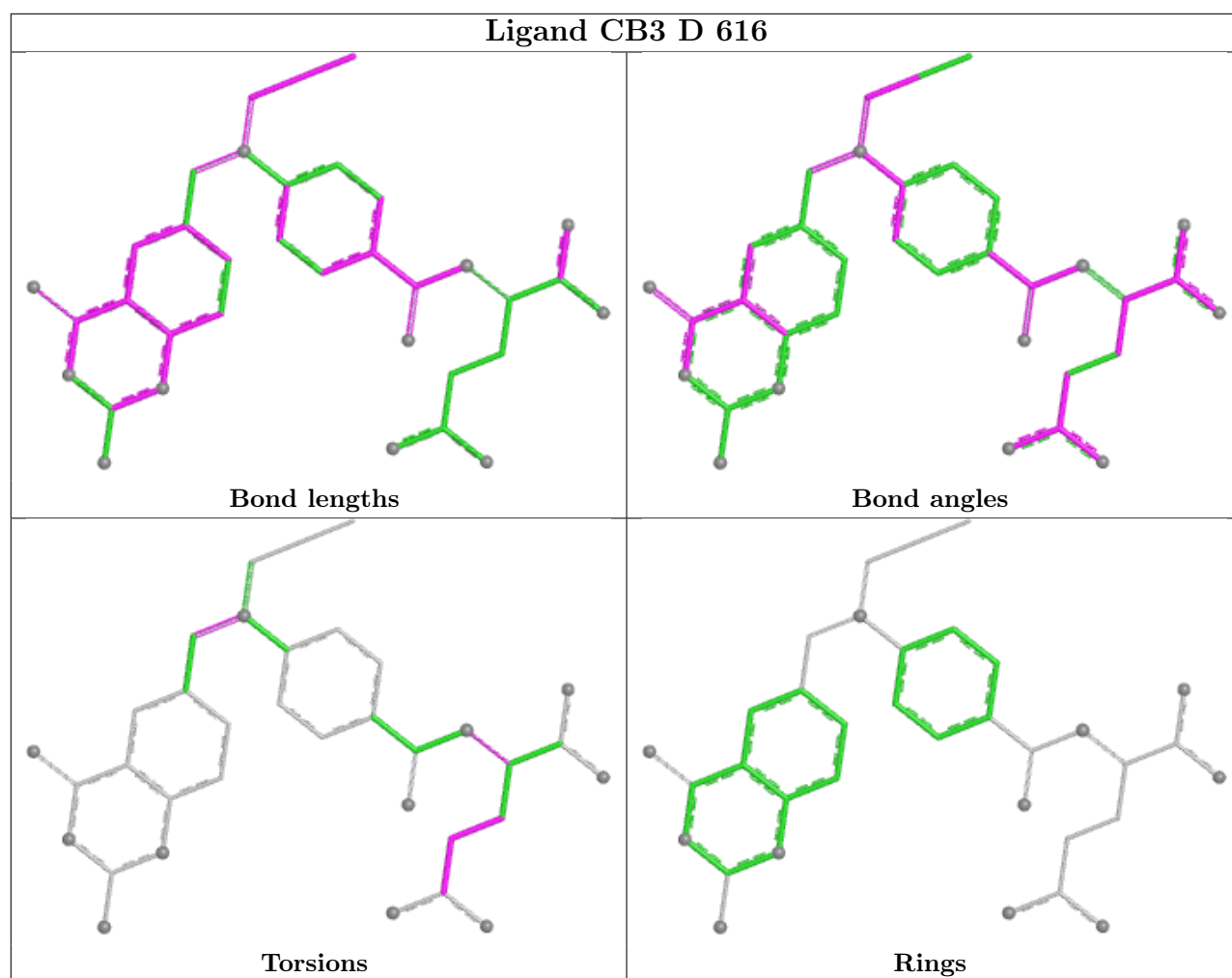
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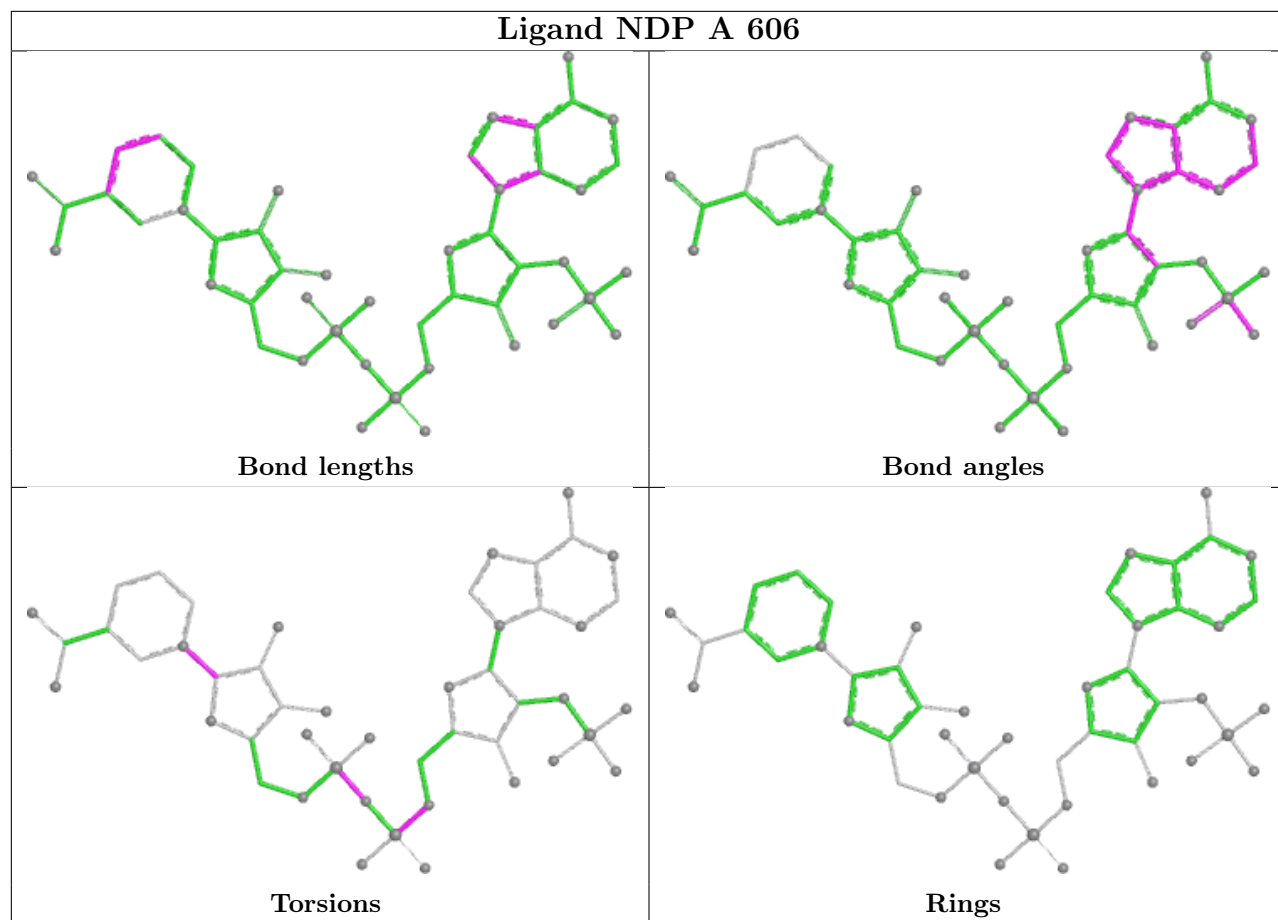
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	615	UMP	6	0
4	E	621	MTX	10	0
4	A	605	MTX	6	0
3	B	608	CB3	7	0
4	B	609	MTX	8	0
5	C	614	NDP	12	0
5	E	622	NDP	12	0
4	D	617	MTX	7	0
2	C	611	UMP	5	0
4	C	613	MTX	6	0
2	E	619	UMP	8	0
5	D	618	NDP	7	0
3	A	604	CB3	2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

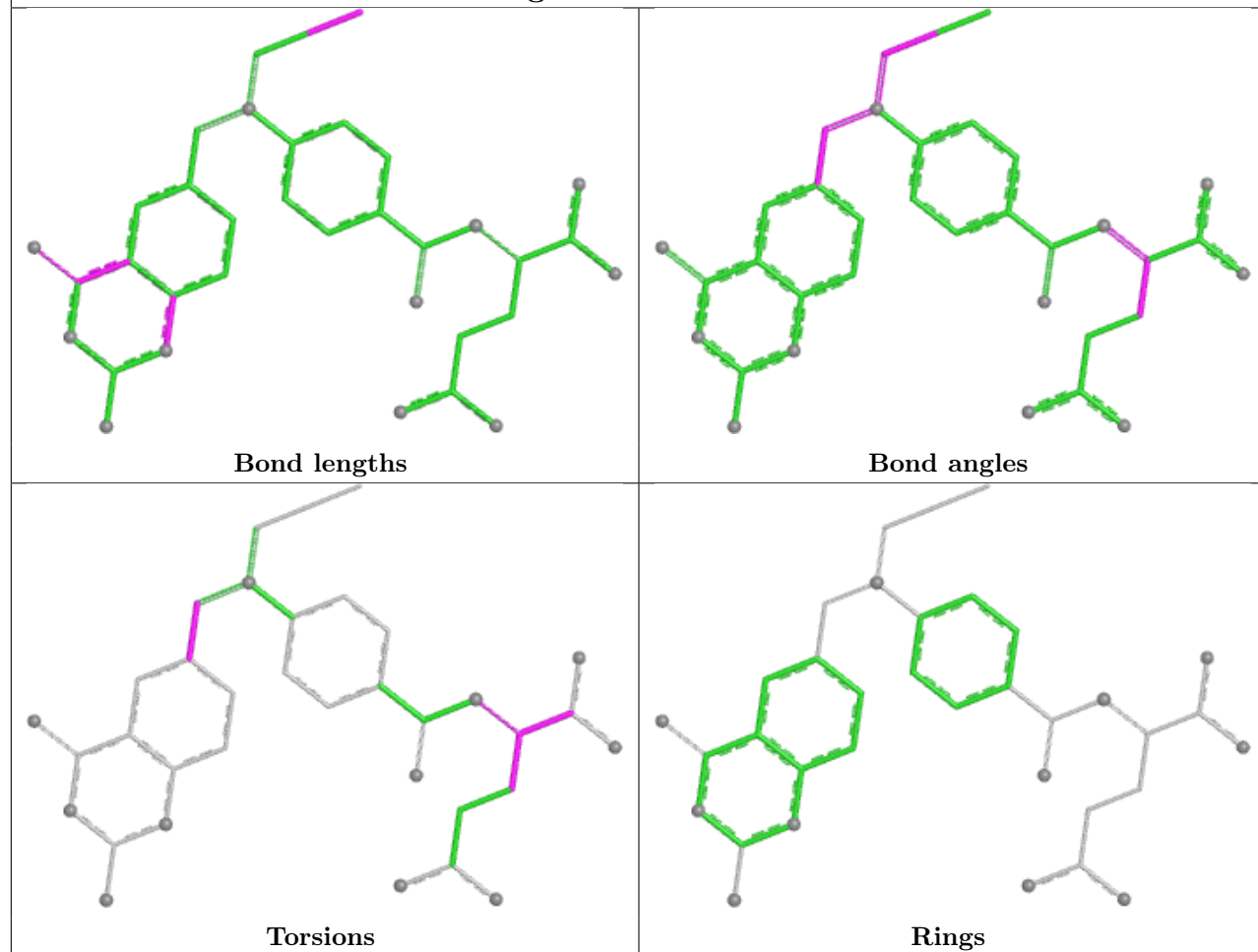
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



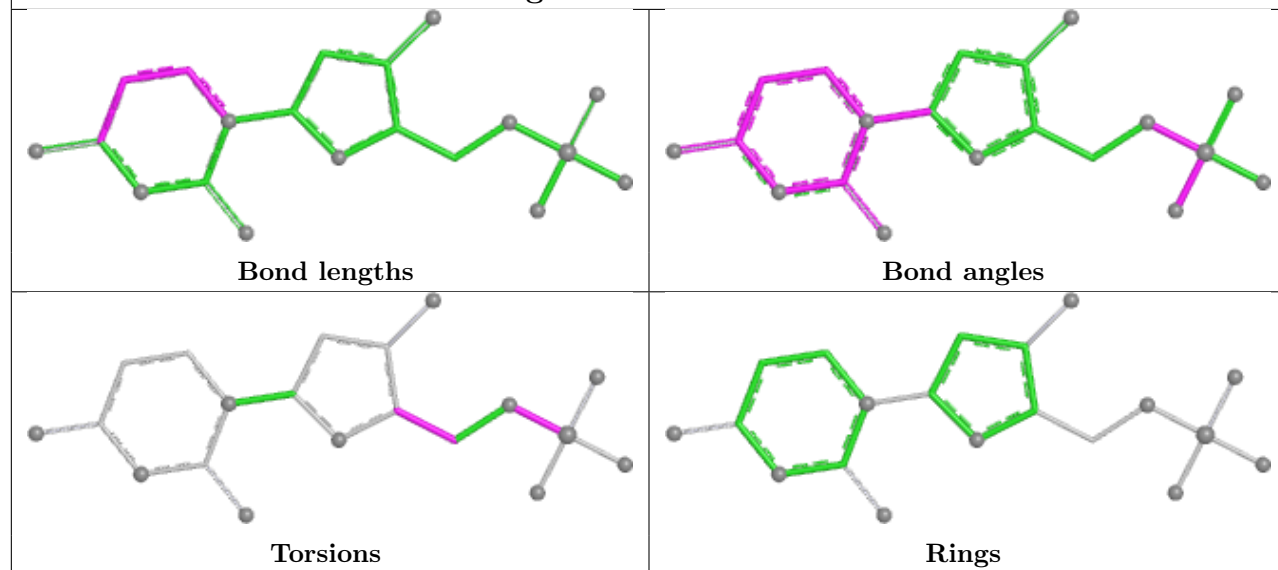


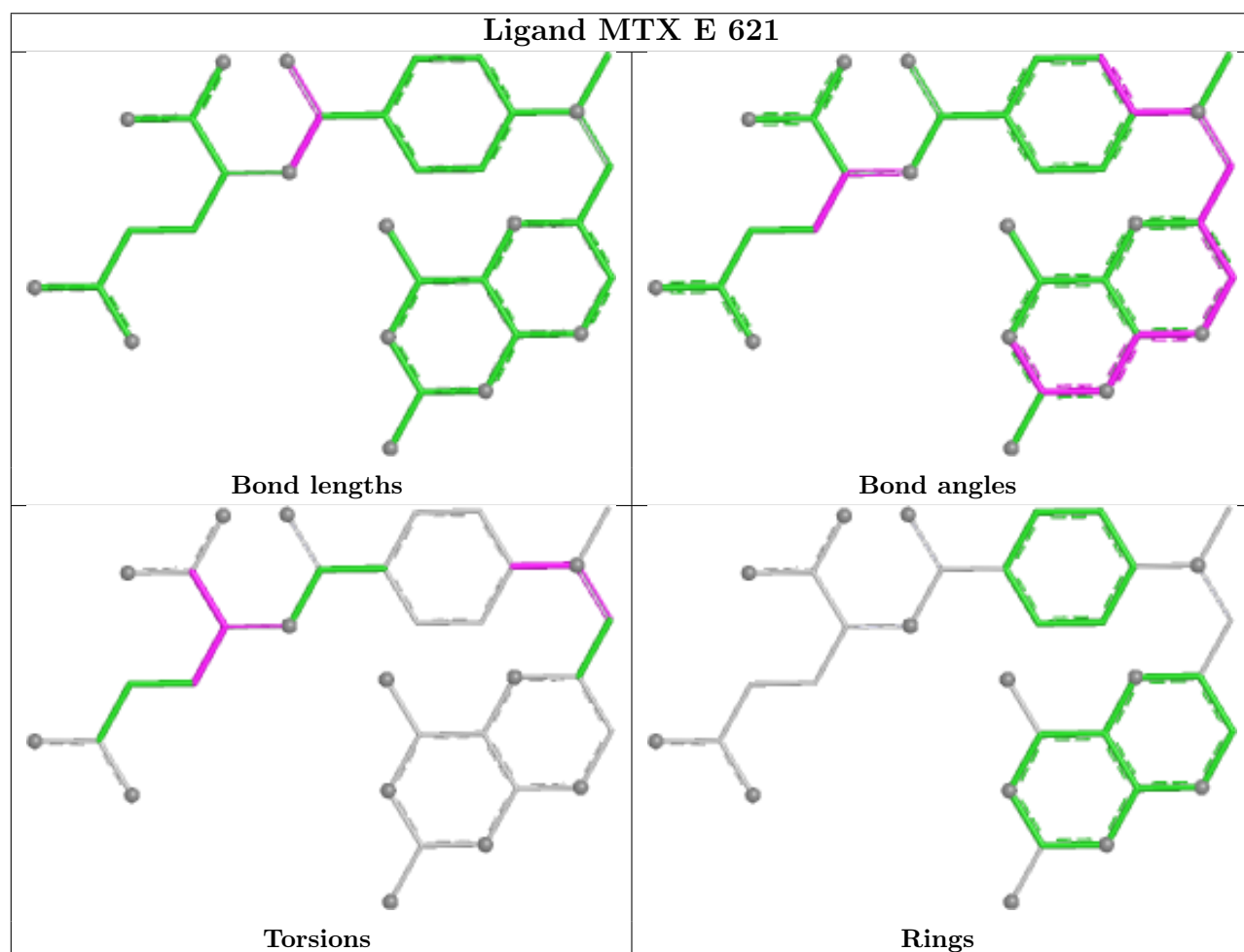
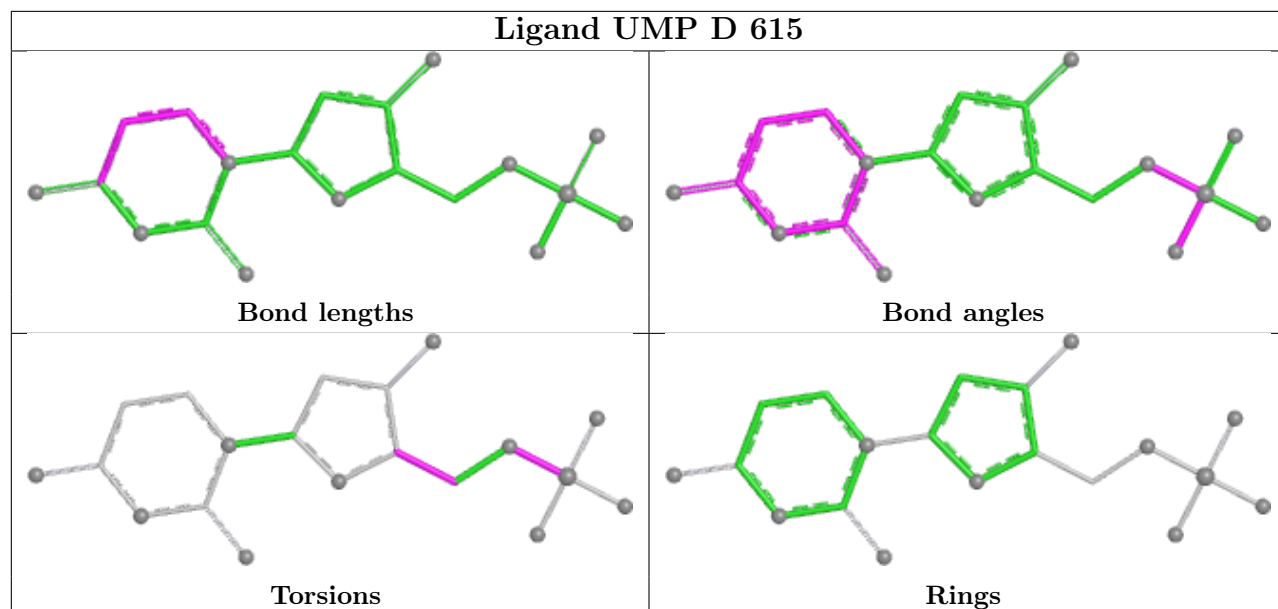


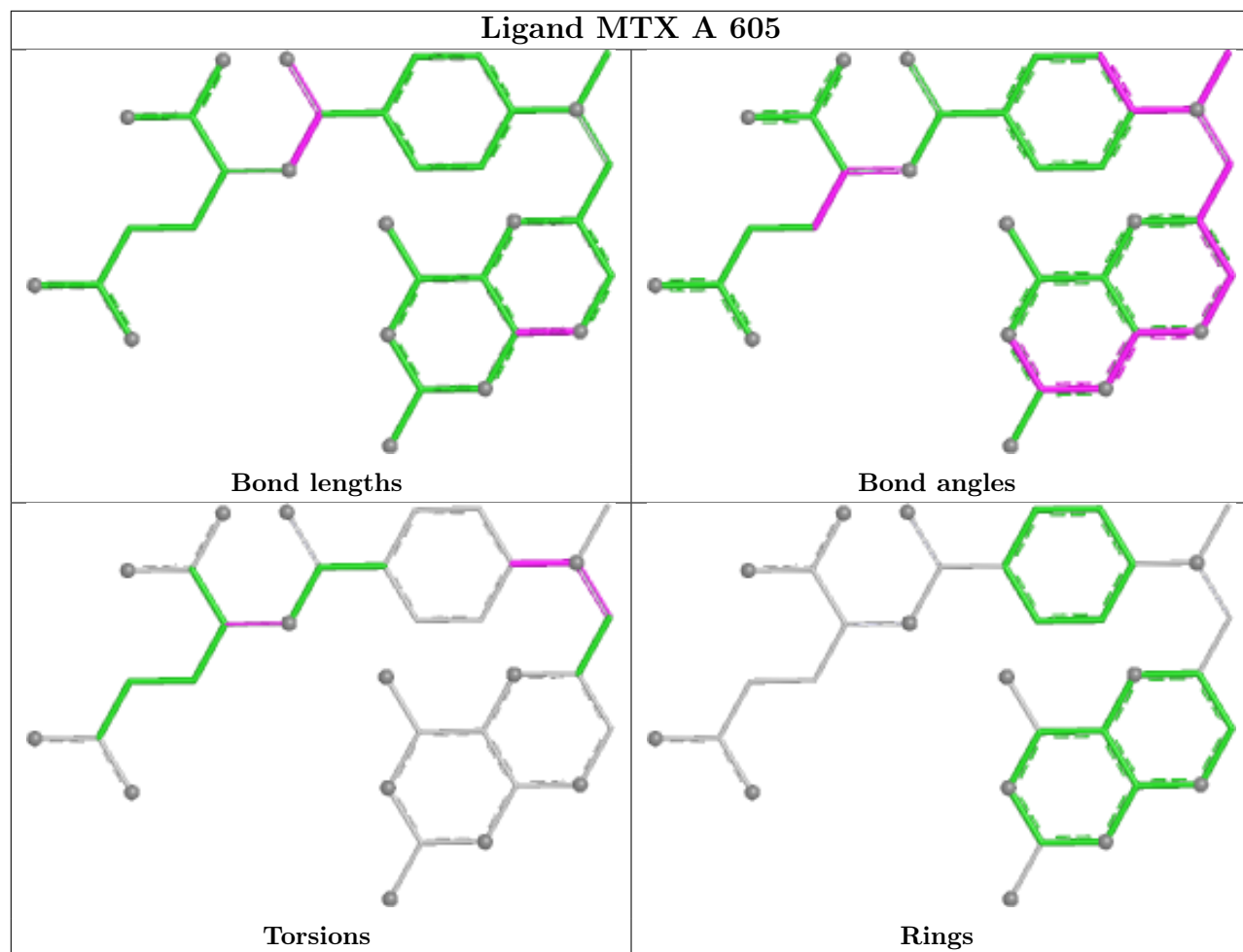
Ligand CB3 E 620

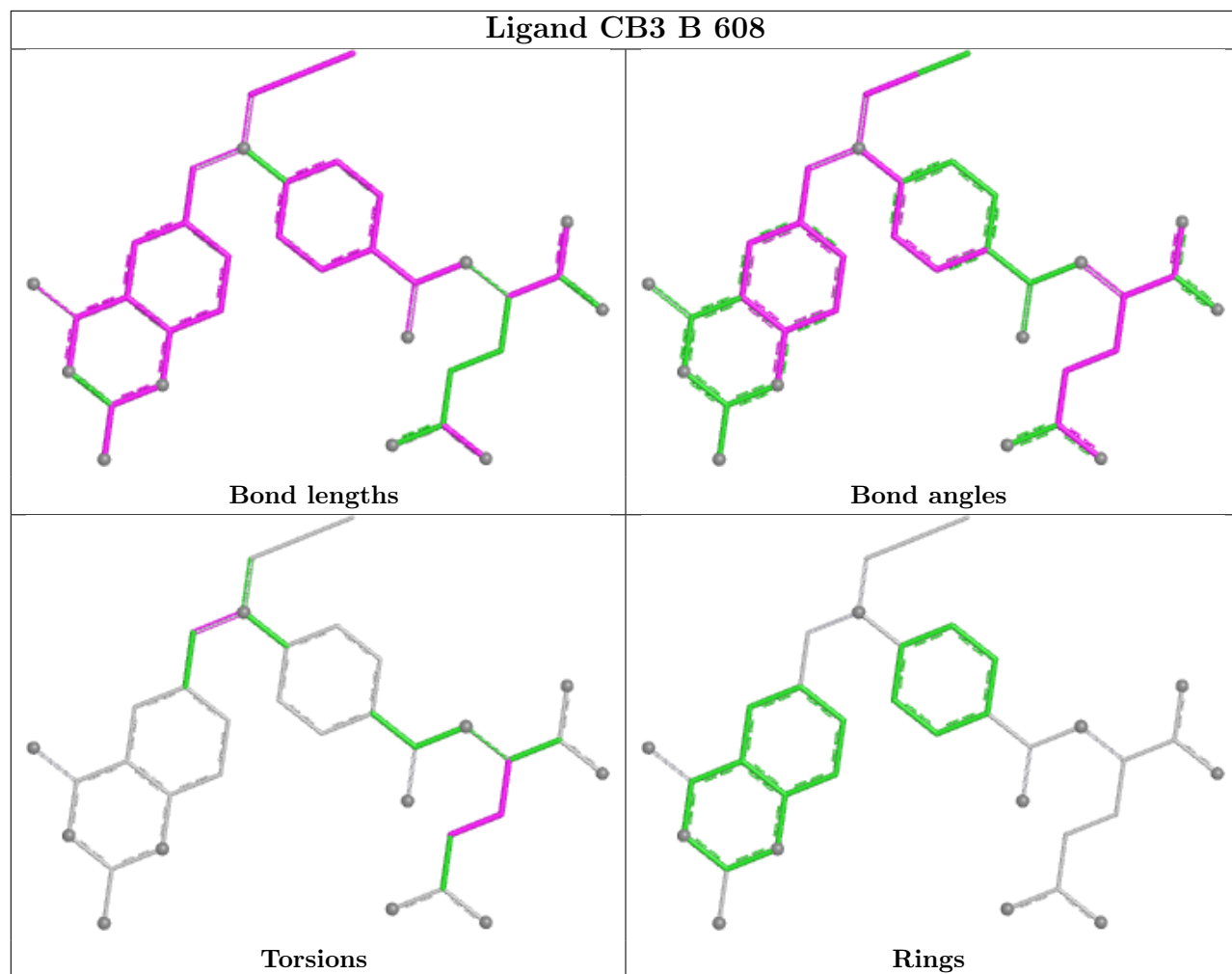


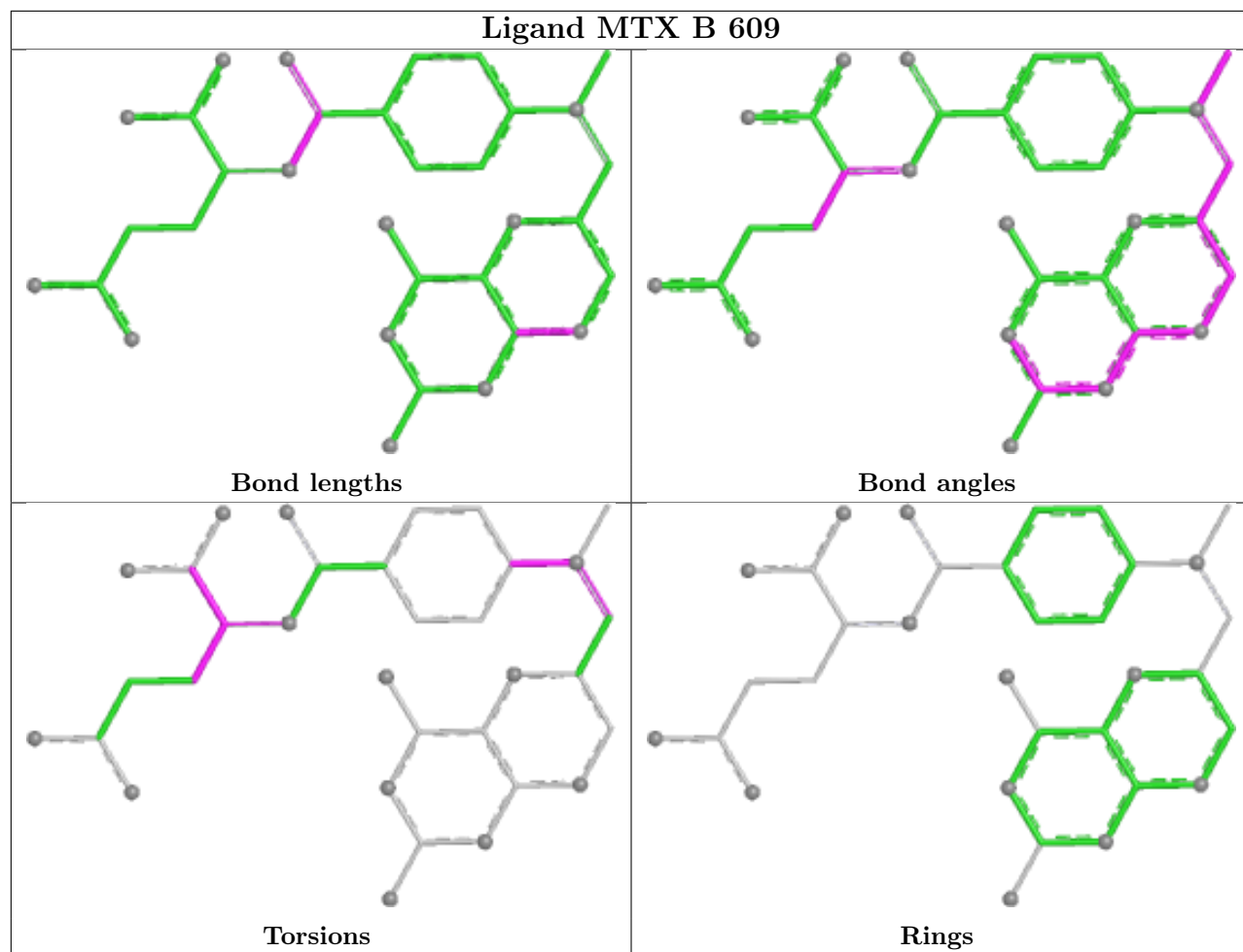
Ligand UMP A 603

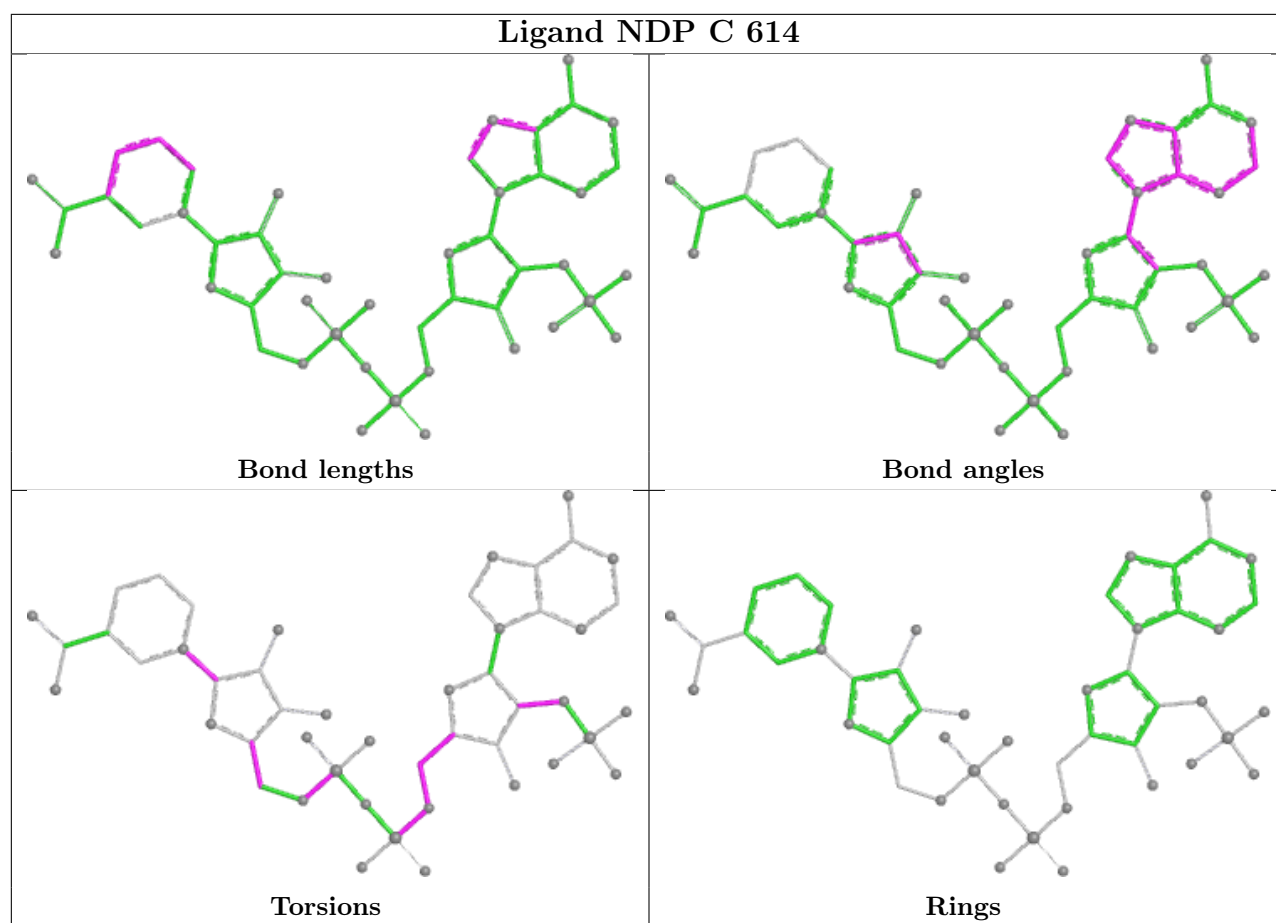


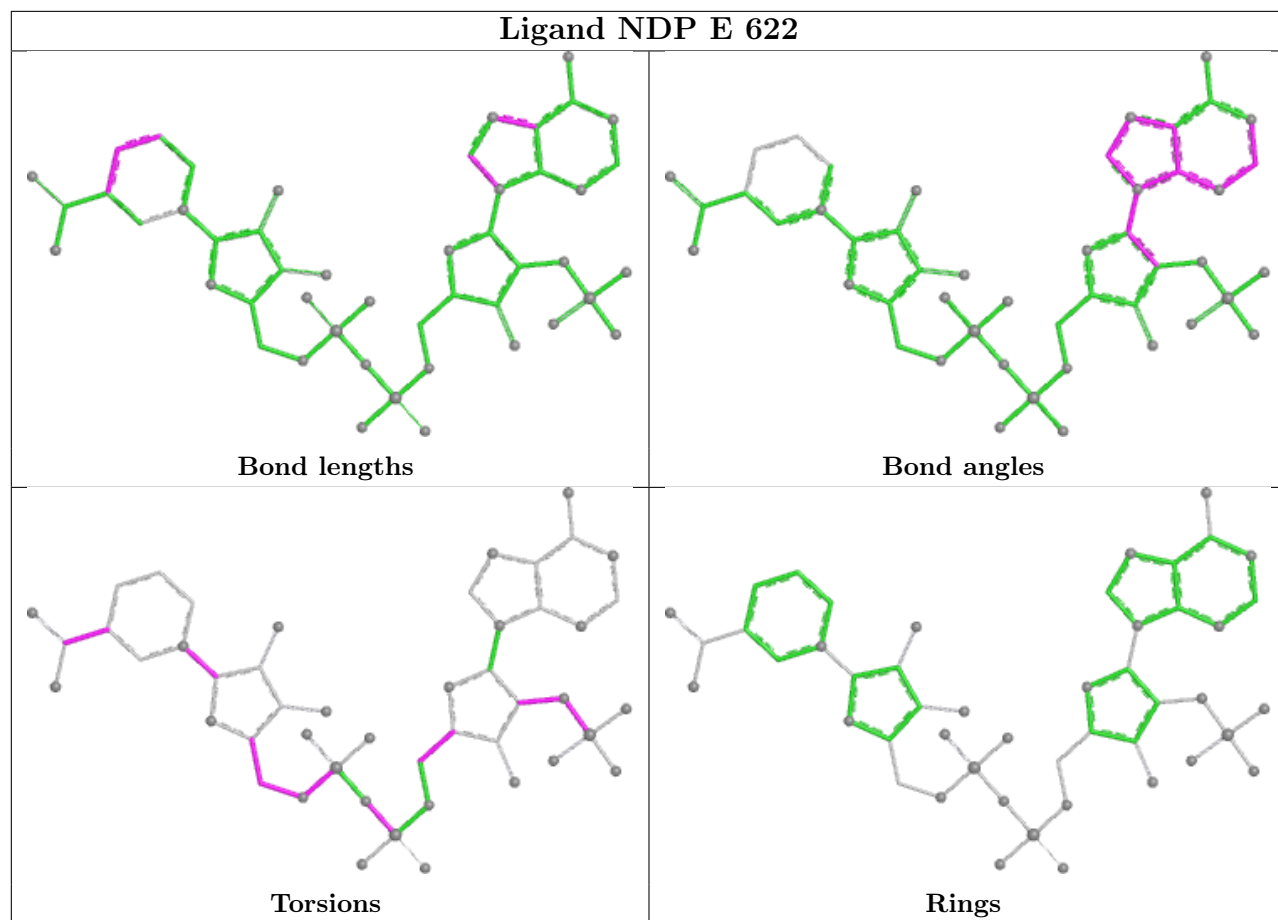


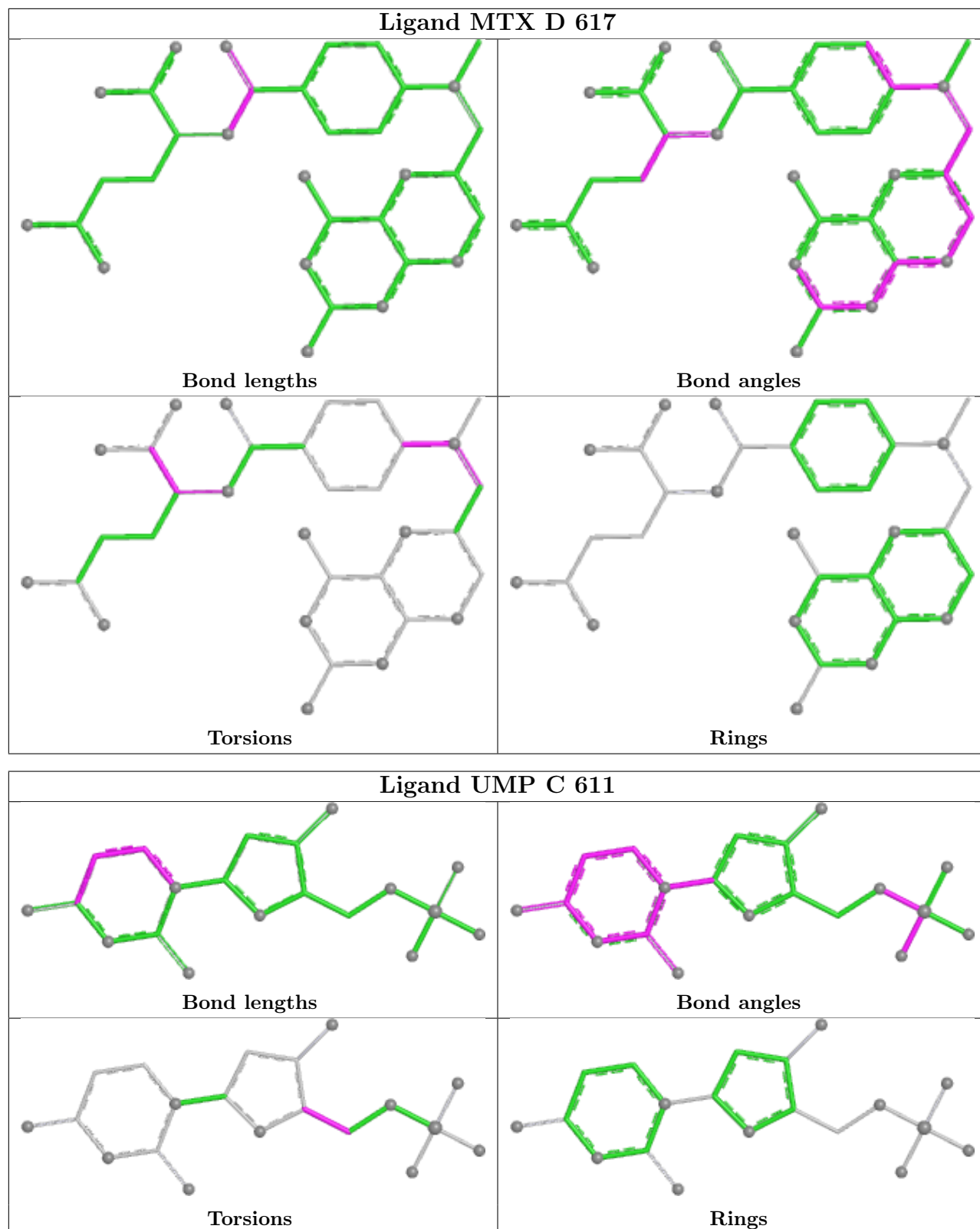


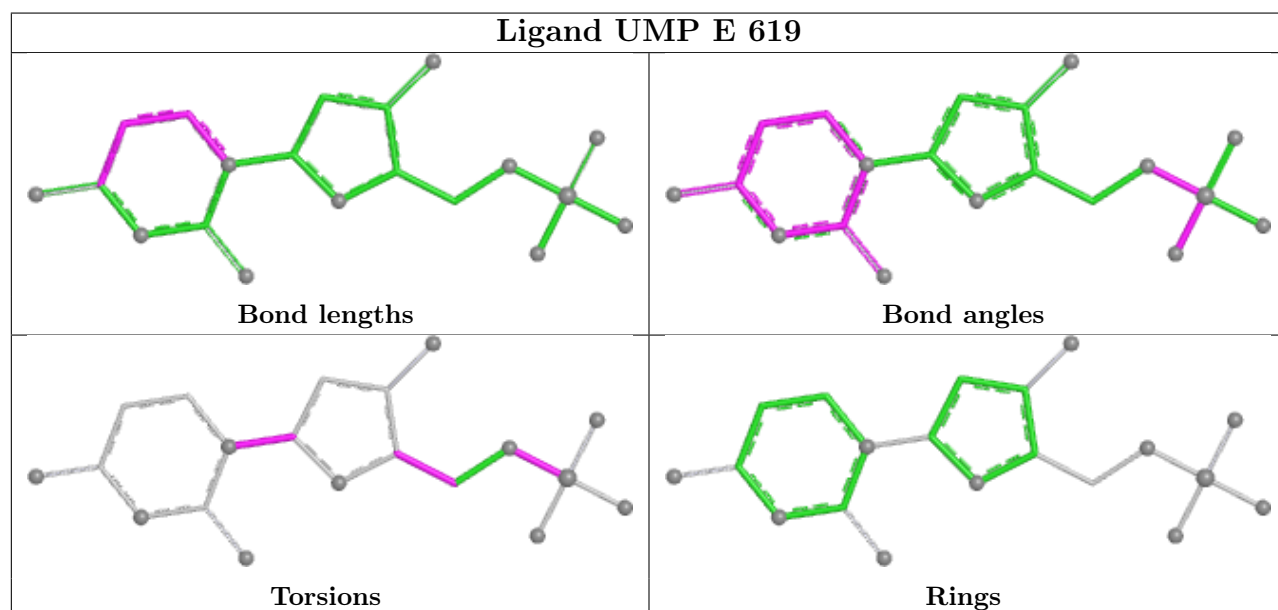
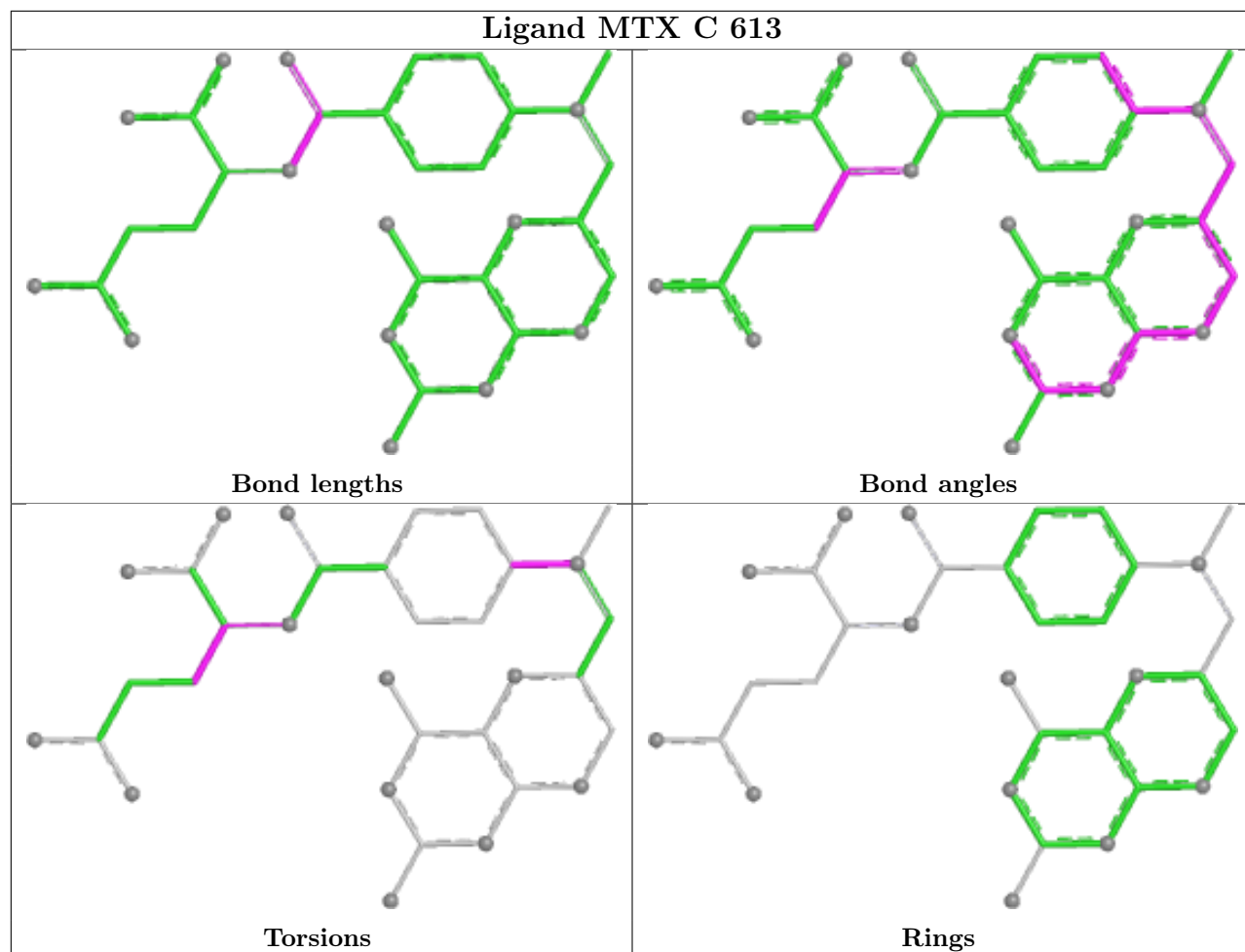


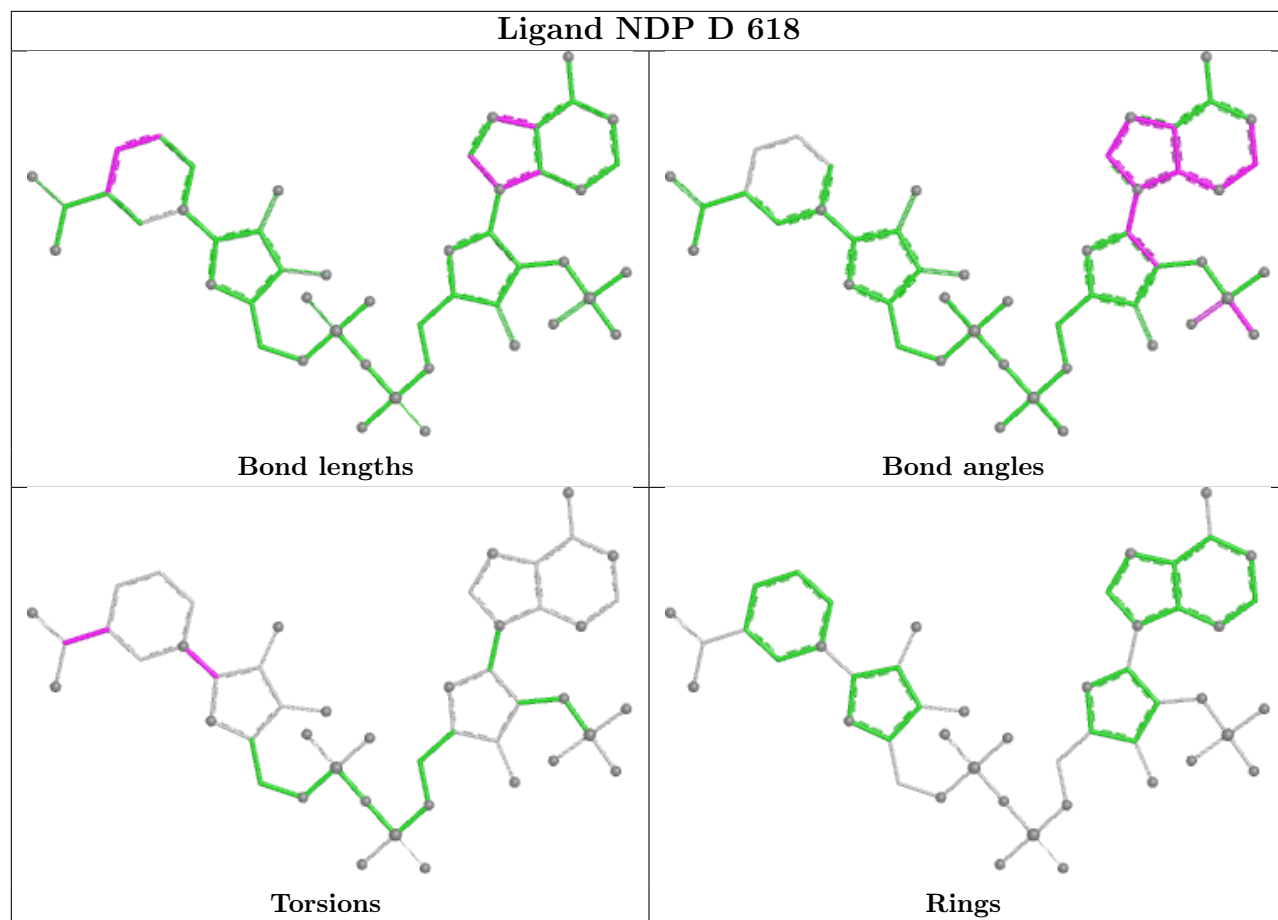




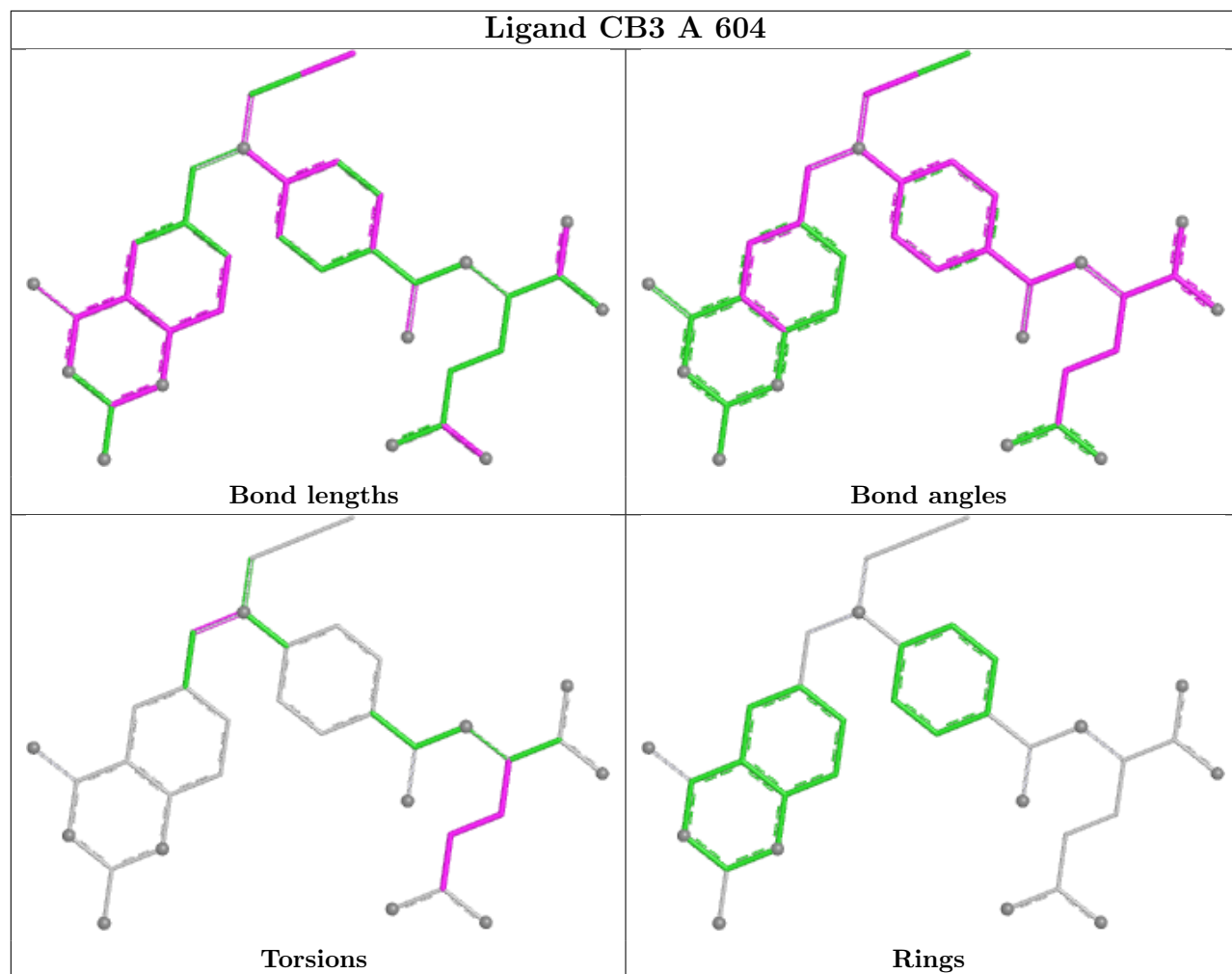




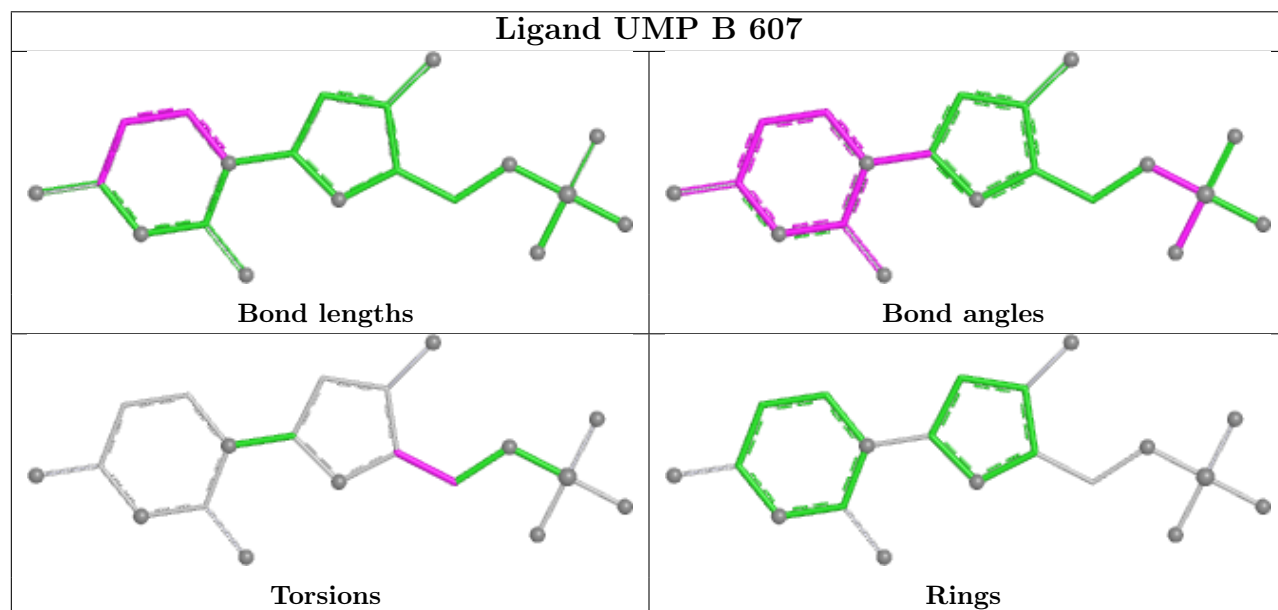


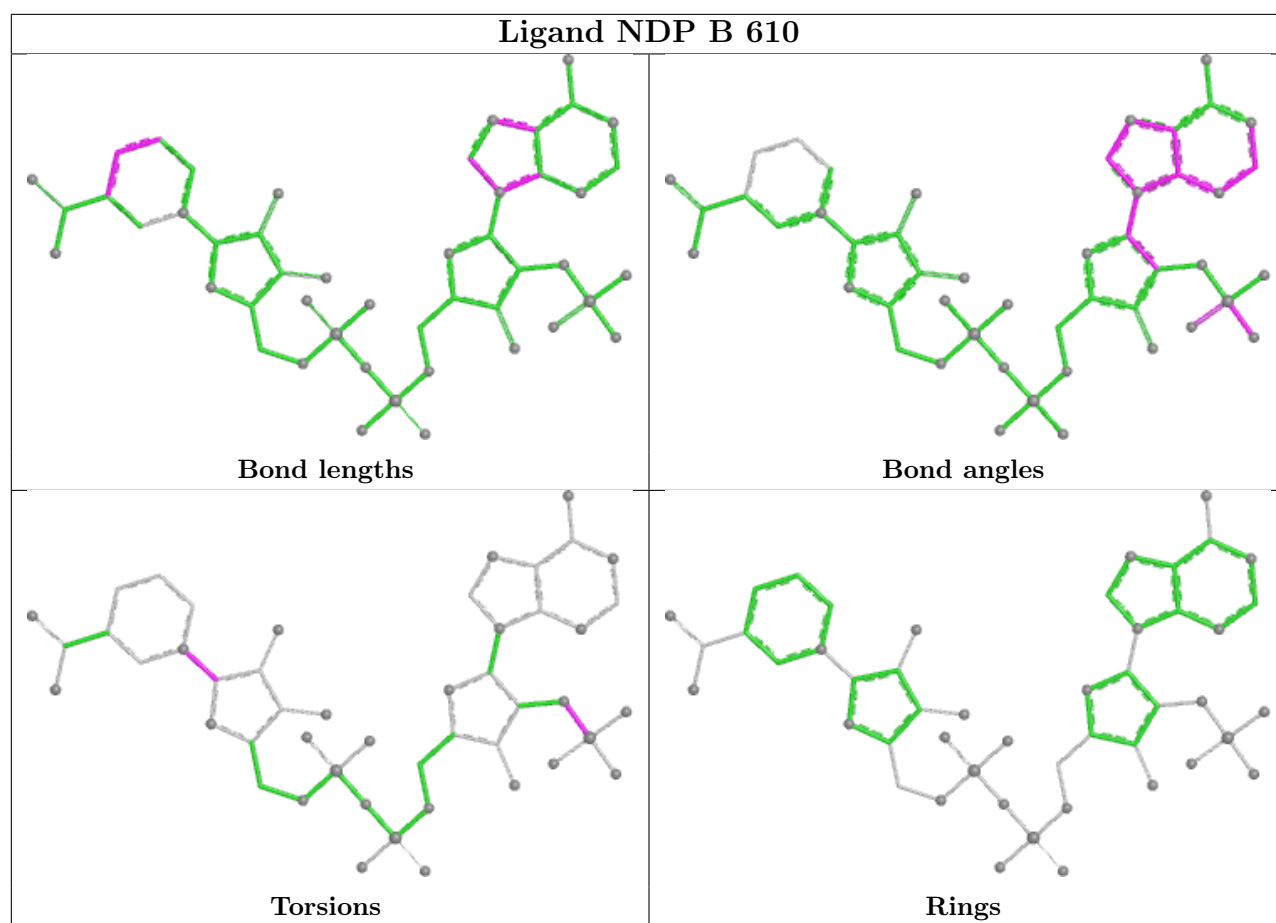


Ligand CB3 A 604



Ligand UMP B 607





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	516/519 (99%)	0.22	31 (6%) 27 21	26, 45, 92, 140	0
1	B	516/519 (99%)	-0.07	21 (4%) 41 33	23, 39, 77, 139	0
1	C	514/519 (99%)	0.58	35 (6%) 23 17	34, 60, 111, 148	0
1	D	515/519 (99%)	0.55	36 (6%) 22 16	36, 60, 103, 136	0
1	E	511/519 (98%)	1.42	103 (20%) 3 2	65, 101, 146, 167	0
All	All	2572/2595 (99%)	0.54	226 (8%) 15 11	23, 58, 123, 167	0

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	103	ASN	11.1
1	A	171	ASP	7.7
1	A	341	ILE	7.2
1	D	191	GLY	7.0
1	A	188	PRO	6.8
1	B	102	MET	6.2
1	B	186	CYS	6.1
1	B	103	ASN	6.1
1	A	191	GLY	5.8
1	B	188	PRO	5.8
1	A	189	ALA	5.7
1	C	189	ALA	5.7
1	E	137	ALA	5.6
1	D	102	MET	5.3
1	A	102	MET	5.3
1	A	190	ARG	5.2
1	E	5	ASN	5.0
1	E	182	THR	4.8
1	A	186	CYS	4.8
1	D	100	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	364	GLY	4.6
1	D	188	PRO	4.5
1	E	138	LEU	4.5
1	E	521	VAL	4.5
1	B	187	ASP	4.5
1	B	185	ASN	4.5
1	E	400	PRO	4.4
1	A	170	TYR	4.4
1	B	189	ALA	4.3
1	D	190	ARG	4.3
1	E	49	LYS	4.3
1	C	186	CYS	4.2
1	B	82	ASP	4.2
1	E	309	ILE	4.2
1	D	186	CYS	4.1
1	D	76	SER	4.1
1	C	188	PRO	4.1
1	C	102	MET	4.1
1	A	192	GLN	4.1
1	C	187	ASP	4.1
1	D	259	GLY	4.0
1	E	305	GLY	3.9
1	D	189	ALA	3.8
1	B	191	GLY	3.8
1	A	100	ASN	3.8
1	C	98	ILE	3.8
1	E	306	ASN	3.7
1	A	187	ASP	3.6
1	D	255	GLU	3.6
1	E	316	TRP	3.6
1	E	363	VAL	3.6
1	E	360	TYR	3.6
1	C	76	SER	3.5
1	E	335	GLU	3.5
1	A	342	TYR	3.5
1	E	102	MET	3.5
1	E	181	LYS	3.5
1	D	192	GLN	3.5
1	E	321	SER	3.5
1	E	428	GLY	3.4
1	A	185	ASN	3.4
1	E	255	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	84	ALA	3.4
1	E	342	TYR	3.4
1	D	114	GLY	3.4
1	B	192	GLN	3.4
1	E	422	GLN	3.4
1	E	86	PRO	3.4
1	C	335	GLU	3.3
1	D	331	GLY	3.3
1	E	520	ALA	3.3
1	A	521	VAL	3.3
1	A	82	ASP	3.2
1	A	194	LYS	3.2
1	E	507	ILE	3.2
1	C	191	GLY	3.2
1	E	34	LYS	3.2
1	E	100	ASN	3.2
1	E	116	GLU	3.1
1	B	335	GLU	3.1
1	B	101	LEU	3.1
1	C	86	PRO	3.1
1	D	171	ASP	3.1
1	E	197	ASP	3.0
1	E	98	ILE	3.0
1	C	101	LEU	3.0
1	D	258	THR	3.0
1	A	343	GLY	3.0
1	C	171	ASP	3.0
1	E	101	LEU	2.9
1	E	314	TYR	2.9
1	D	104	ASP	2.9
1	A	180	LYS	2.9
1	E	217	LYS	2.9
1	A	101	LEU	2.9
1	E	319	ASN	2.8
1	E	171	ASP	2.8
1	E	391	PRO	2.8
1	C	84	ALA	2.8
1	C	190	ARG	2.8
1	D	256	ASN	2.8
1	D	99	GLU	2.8
1	C	193	LEU	2.8
1	E	404	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	107	ILE	2.8
1	C	100	ASN	2.8
1	E	302	ASP	2.8
1	E	38	LYS	2.8
1	E	193	LEU	2.7
1	E	354	LYS	2.7
1	E	488	LYS	2.7
1	E	325	LEU	2.7
1	E	349	TYR	2.7
1	E	284	LYS	2.7
1	A	98	ILE	2.7
1	B	99	GLU	2.7
1	C	78	SER	2.7
1	E	264	SER	2.7
1	C	180	LYS	2.6
1	C	194	LYS	2.6
1	D	193	LEU	2.6
1	E	376	LYS	2.6
1	E	388	ALA	2.6
1	E	322	LYS	2.6
1	A	179	GLU	2.6
1	C	378	ASN	2.6
1	E	390	ASN	2.6
1	E	103	ASN	2.6
1	A	105	ASP	2.6
1	E	20	GLY	2.5
1	E	313	VAL	2.5
1	E	392	SER	2.5
1	E	516	LYS	2.5
1	E	156	PRO	2.5
1	E	346	TRP	2.5
1	E	394	LEU	2.5
1	E	429	LEU	2.5
1	E	355	THR	2.5
1	E	273	ASP	2.5
1	E	281	LEU	2.5
1	C	99	GLU	2.5
1	E	393	ALA	2.5
1	A	181	LYS	2.5
1	D	149	GLU	2.5
1	E	307	HIS	2.5
1	B	100	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	377	ASN	2.5
1	D	101	LEU	2.4
1	E	333	ARG	2.4
1	E	260	ILE	2.4
1	E	286	VAL	2.4
1	E	320	GLY	2.4
1	C	49	LYS	2.4
1	E	175	PHE	2.4
1	E	365	VAL	2.4
1	E	336	ASN	2.4
1	E	120	ARG	2.4
1	A	103	ASN	2.3
1	E	380	LYS	2.3
1	A	104	ASP	2.3
1	E	179	GLU	2.3
1	B	495	ASN	2.3
1	A	323	GLU	2.3
1	D	105	ASP	2.3
1	E	287	ALA	2.3
1	E	357	HIS	2.3
1	C	89	VAL	2.3
1	D	305	GLY	2.3
1	E	433	PHE	2.3
1	D	328	ILE	2.3
1	E	395	SER	2.3
1	D	521	VAL	2.3
1	C	63	GLY	2.3
1	C	326	GLU	2.3
1	C	192	GLN	2.3
1	E	206	ILE	2.3
1	E	277	SER	2.3
1	E	344	PHE	2.2
1	D	181	LYS	2.2
1	E	288	ILE	2.2
1	E	341	ILE	2.2
1	E	192	GLN	2.2
1	E	348	HIS	2.2
1	A	402	CYS	2.2
1	E	155	LEU	2.2
1	E	337	ASP	2.2
1	C	128	VAL	2.2
1	D	20	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	193	LEU	2.2
1	E	25	LEU	2.2
1	B	181	LYS	2.2
1	E	331	GLY	2.2
1	C	92	ARG	2.1
1	E	506	LEU	2.1
1	D	3	GLU	2.1
1	E	491	ARG	2.1
1	E	338	LEU	2.1
1	E	484	PHE	2.1
1	B	84	ALA	2.1
1	D	179	GLU	2.1
1	D	195	SER	2.1
1	D	402	CYS	2.1
1	B	178	GLN	2.1
1	C	55	GLY	2.1
1	C	79	LEU	2.1
1	E	399	LEU	2.1
1	E	487	LEU	2.1
1	E	176	GLU	2.1
1	E	326	GLU	2.1
1	C	81	GLN	2.1
1	E	251	GLY	2.1
1	D	287	ALA	2.1
1	B	255	GLU	2.1
1	E	494	GLU	2.1
1	C	349	TYR	2.1
1	C	88	VAL	2.0
1	D	330	LEU	2.0
1	B	190	ARG	2.0
1	A	84	ALA	2.0
1	A	413	ASP	2.0
1	D	82	ASP	2.0
1	E	370	LYS	2.0
1	D	24	GLN	2.0
1	C	140	ASP	2.0
1	E	144	ASP	2.0
1	B	322	LYS	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

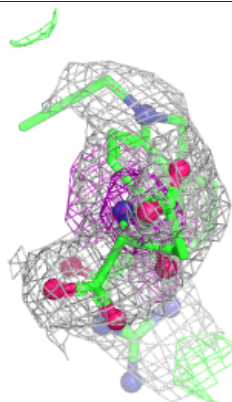
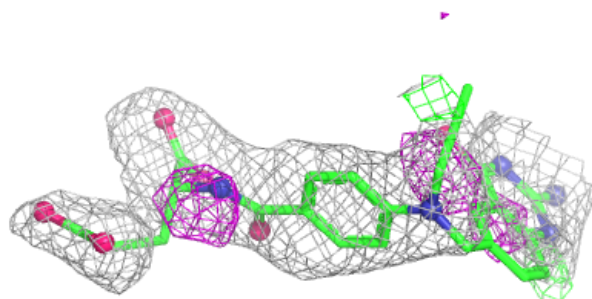
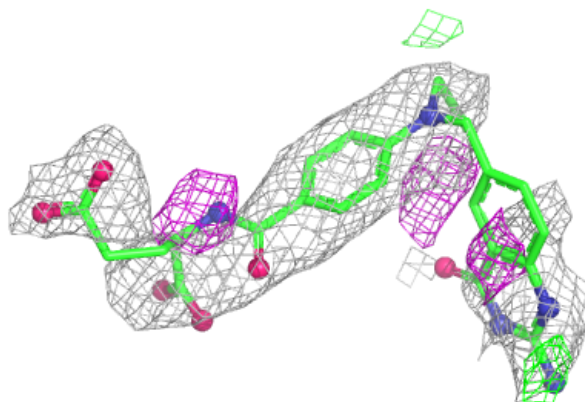
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CB3	E	620	35/35	0.67	0.19	131,134,135,135	0
5	NDP	C	614	48/48	0.83	0.18	92,96,111,112	0
3	CB3	D	616	35/35	0.84	0.17	107,110,114,115	0
3	CB3	A	604	35/35	0.85	0.15	68,77,89,90	0
2	UMP	E	619	20/20	0.86	0.17	125,131,135,135	0
4	MTX	E	621	33/33	0.88	0.15	96,102,103,104	0
3	CB3	C	612	35/35	0.89	0.14	59,71,80,82	0
4	MTX	C	613	33/33	0.89	0.16	75,83,87,87	0
5	NDP	E	622	48/48	0.90	0.14	85,89,105,106	0
3	CB3	B	608	35/35	0.91	0.11	44,52,63,66	0
4	MTX	B	609	33/33	0.93	0.11	44,50,51,54	0
2	UMP	D	615	20/20	0.93	0.13	77,82,86,88	0
5	NDP	D	618	48/48	0.93	0.11	49,64,75,75	0
4	MTX	D	617	33/33	0.93	0.13	61,68,71,71	0
2	UMP	A	603	20/20	0.94	0.12	53,58,63,68	0
4	MTX	A	605	33/33	0.94	0.10	42,48,50,52	0
2	UMP	C	611	20/20	0.94	0.12	44,62,68,70	0
2	UMP	B	607	20/20	0.95	0.11	37,43,46,50	0
5	NDP	B	610	48/48	0.96	0.08	33,41,45,46	0
5	NDP	A	606	48/48	0.96	0.09	41,46,50,50	0

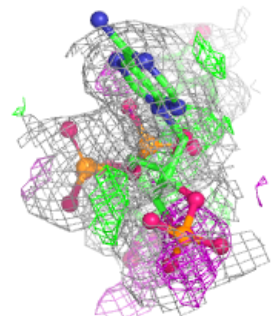
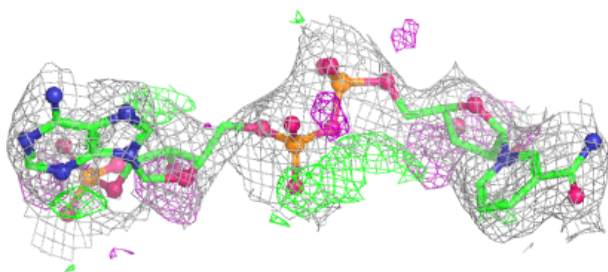
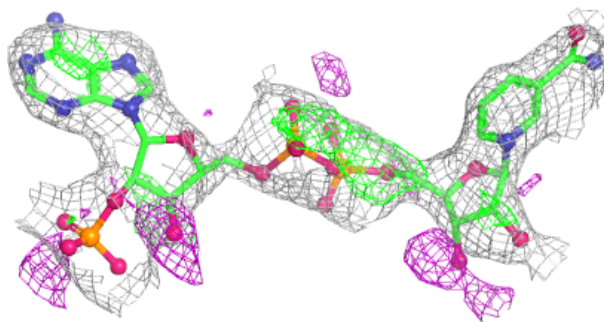
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CB3 E 620:

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

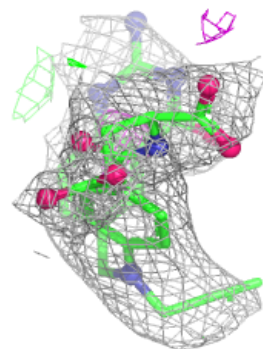
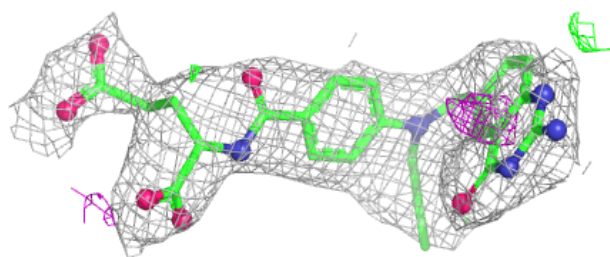
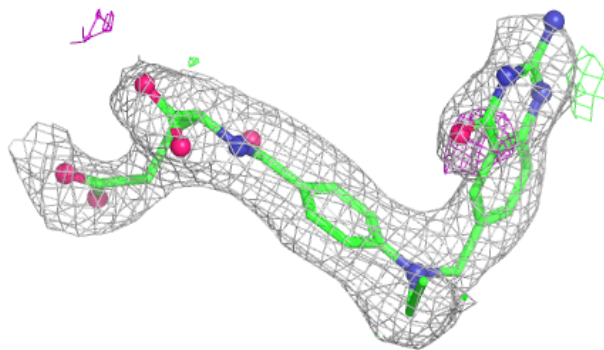
**Electron density around NDP C 614:**

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

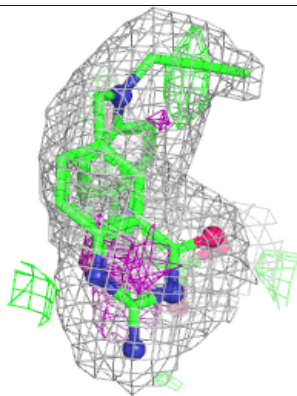
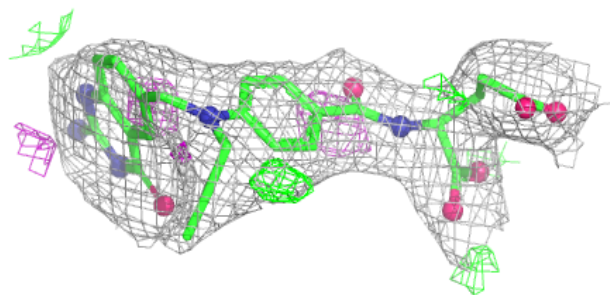
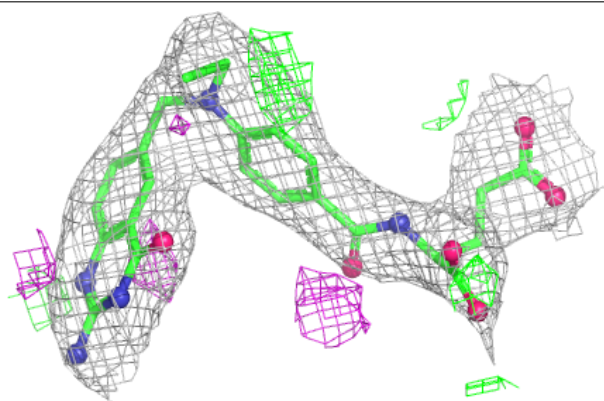


Electron density around CB3 D 616:

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

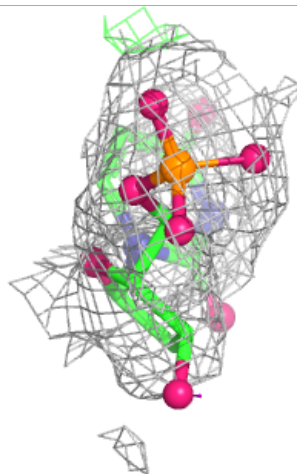
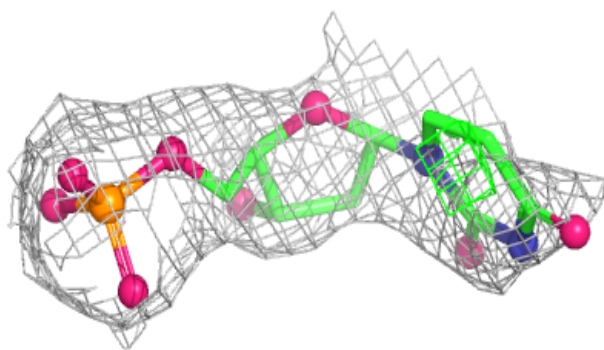
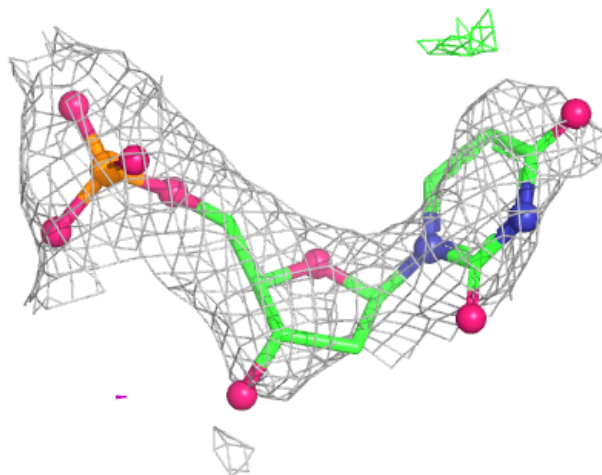
**Electron density around CB3 A 604:**

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



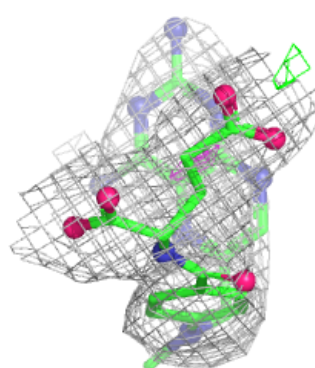
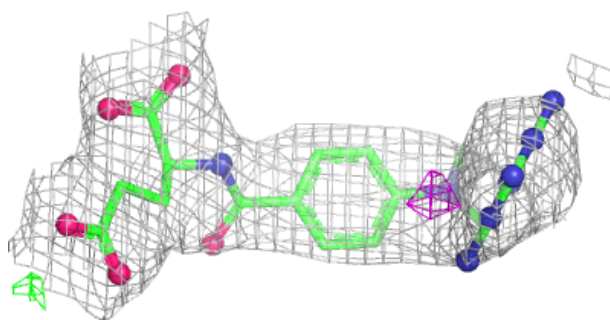
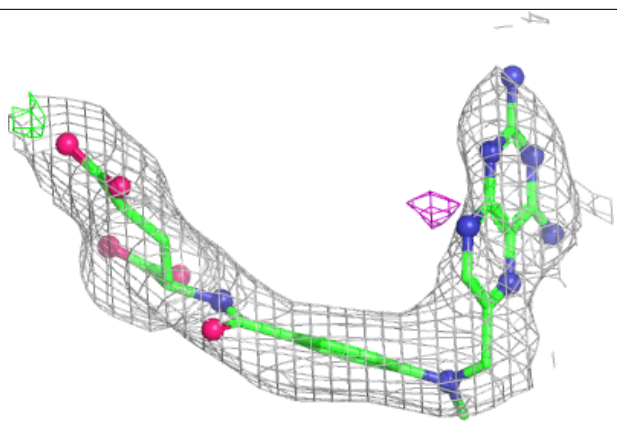
Electron density around UMP E 619:

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

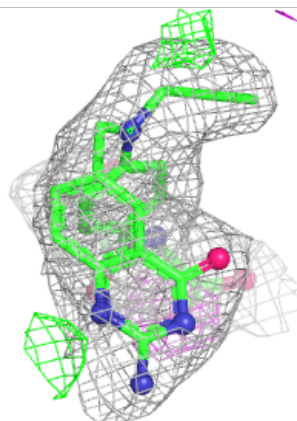
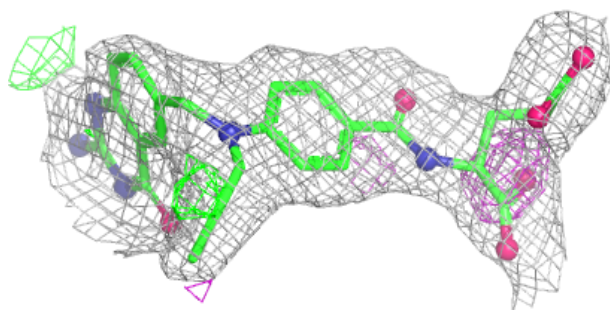
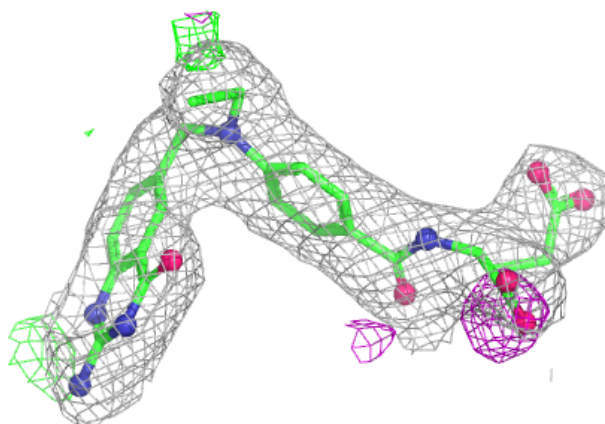


Electron density around MTX E 621:

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

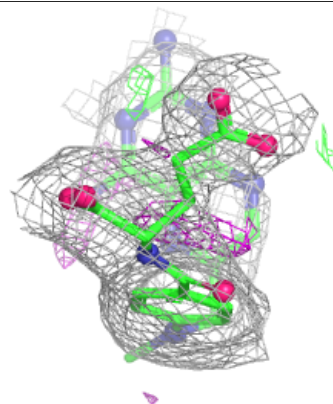
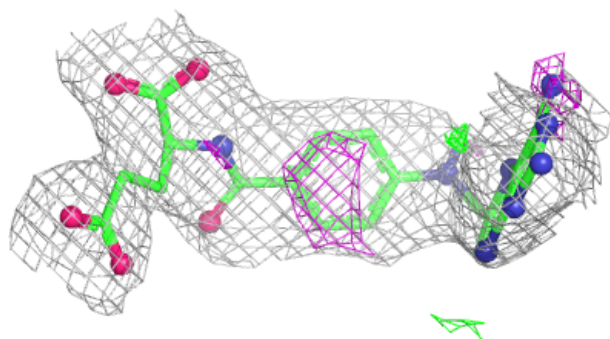
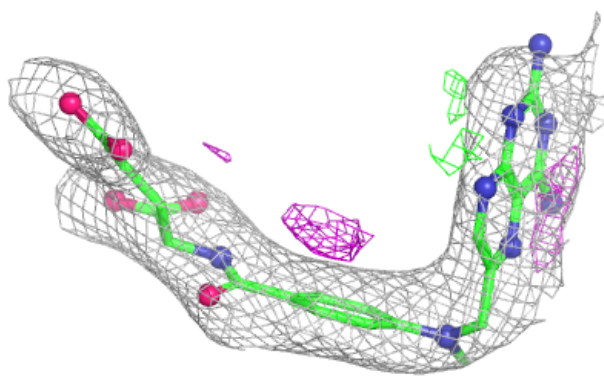
**Electron density around CB3 C 612:**

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

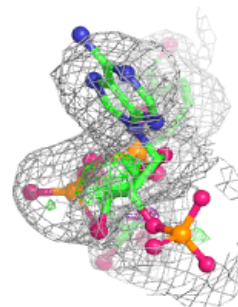
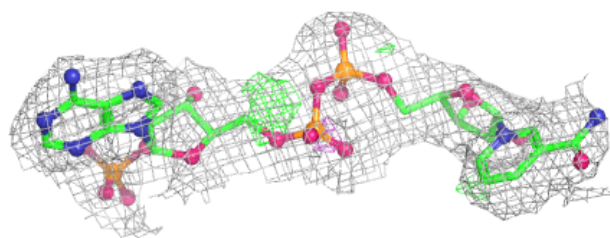
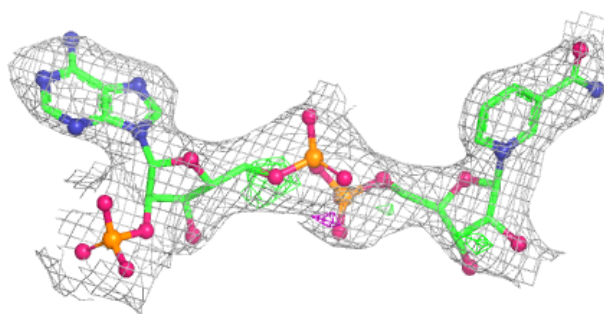


Electron density around MTX C 613:

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

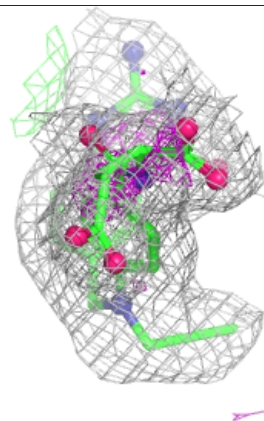
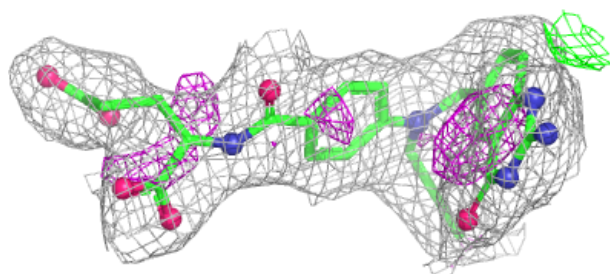
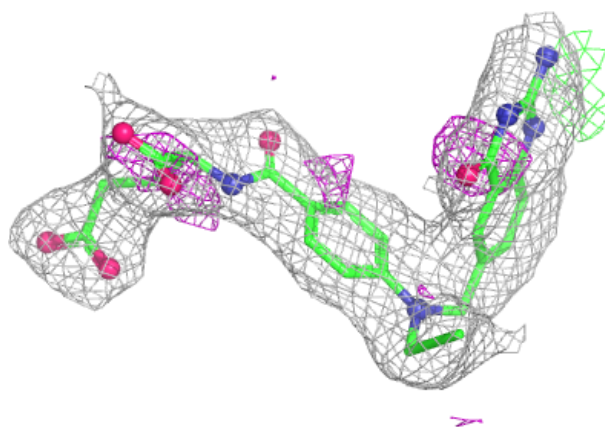
**Electron density around NDP E 622:**

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



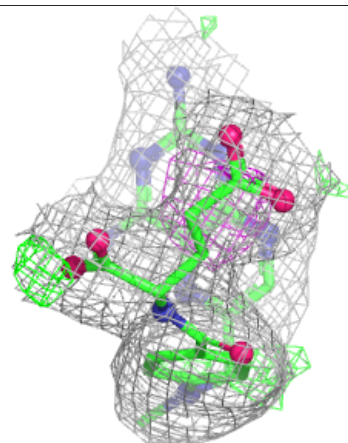
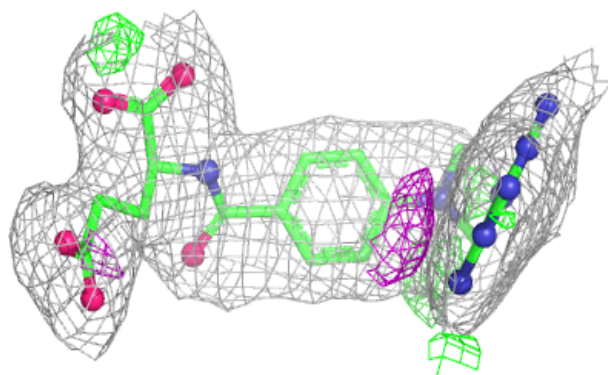
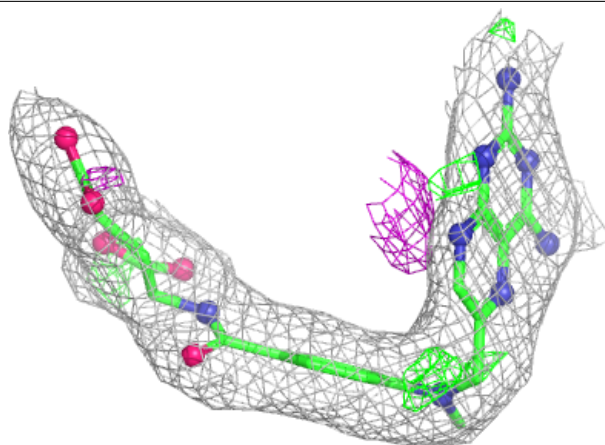
Electron density around CB3 B 608:

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



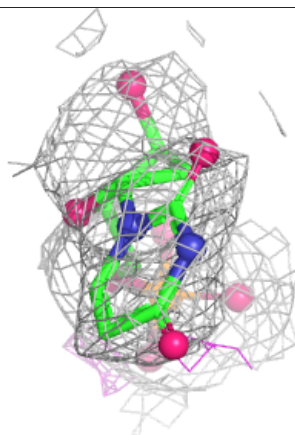
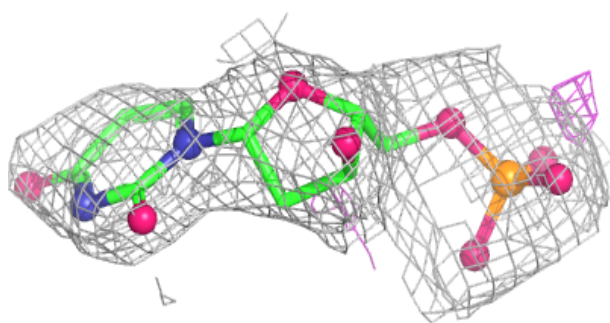
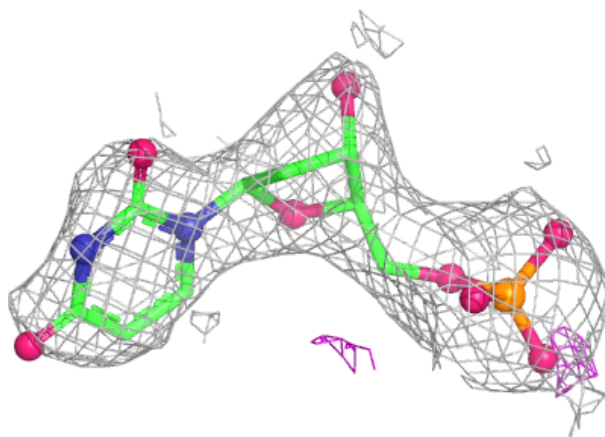
Electron density around MTX B 609:

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

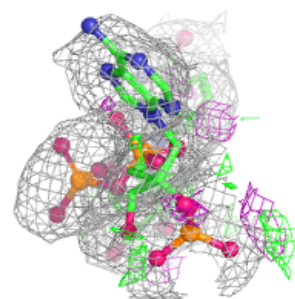
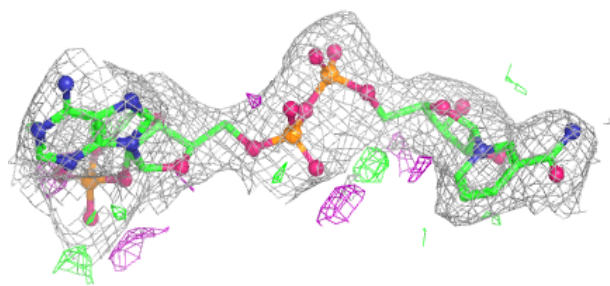
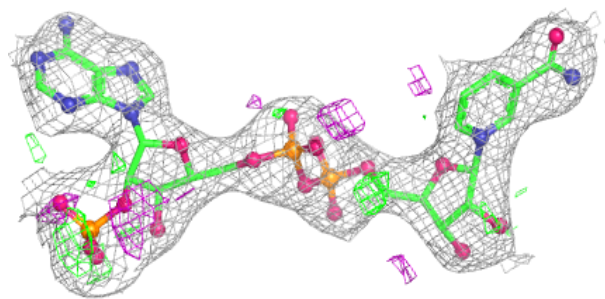


Electron density around UMP D 615:

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

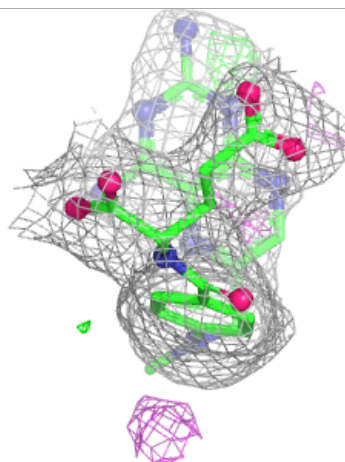
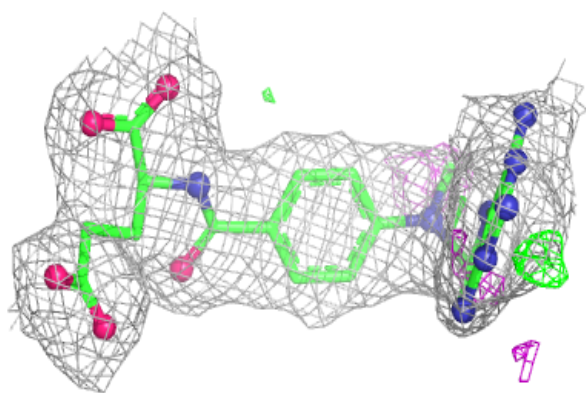
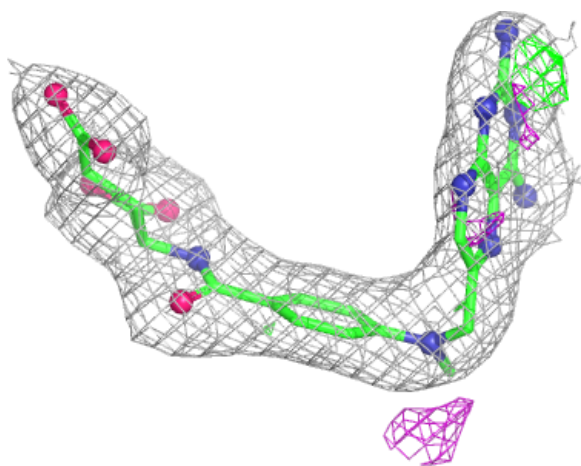
**Electron density around NDP D 618:**

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



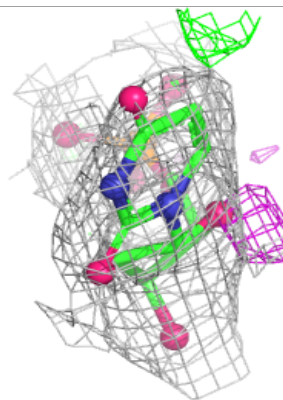
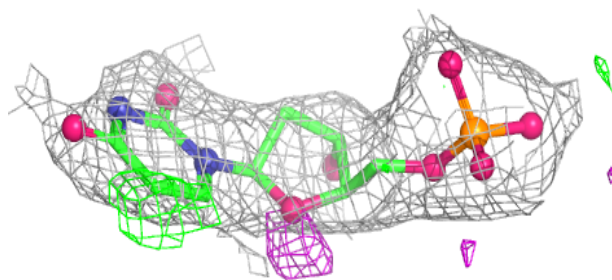
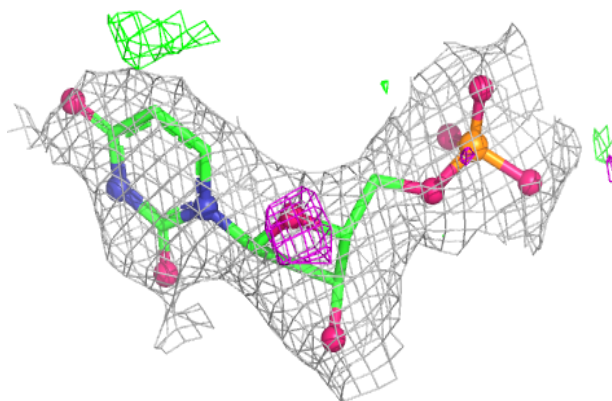
Electron density around MTX D 617:

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



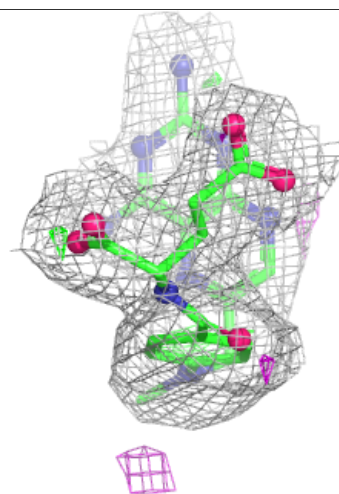
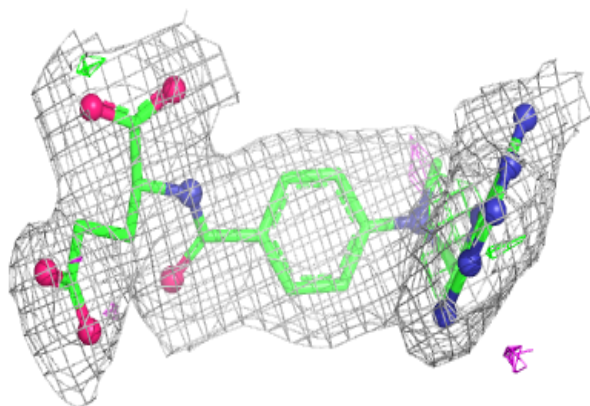
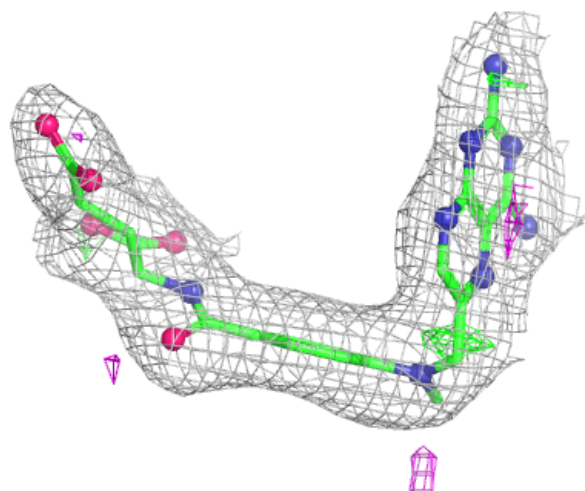
Electron density around UMP A 603:

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



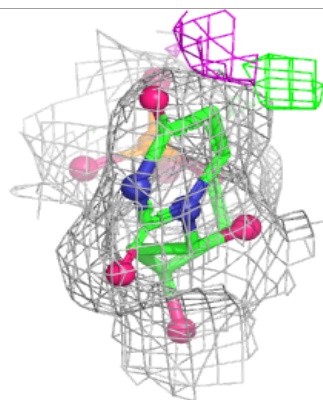
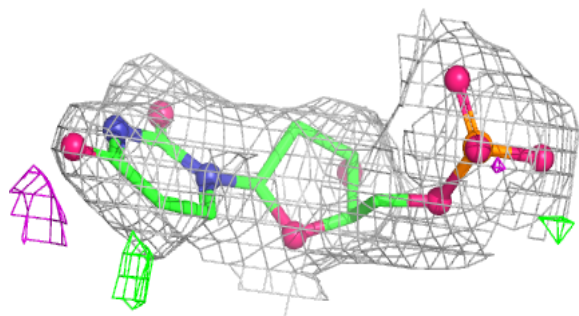
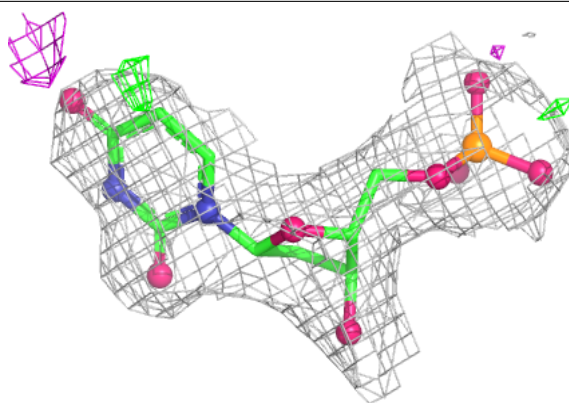
Electron density around MTX A 605:

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

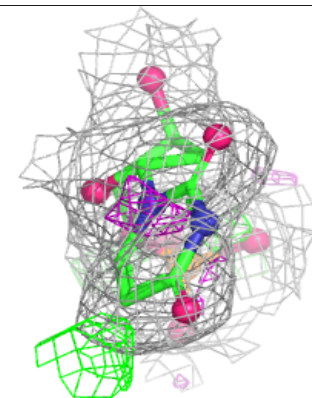
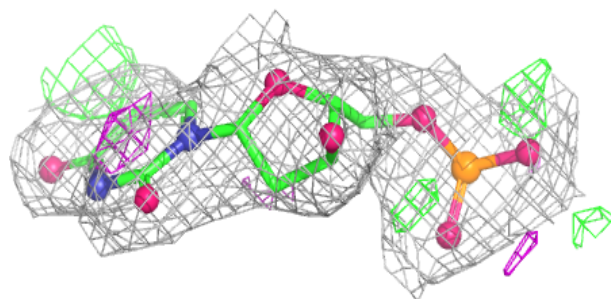
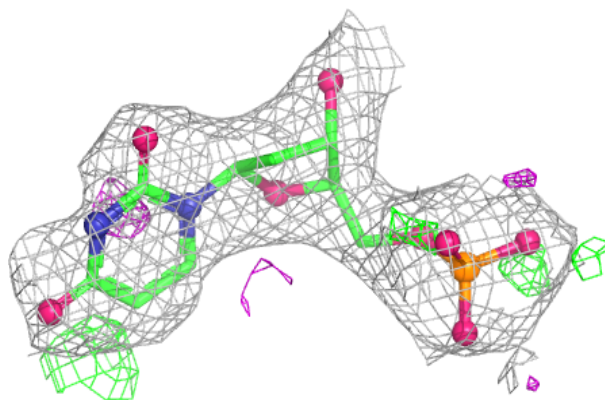


Electron density around UMP C 611:

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

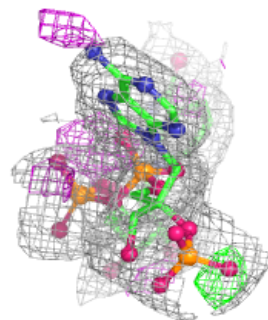
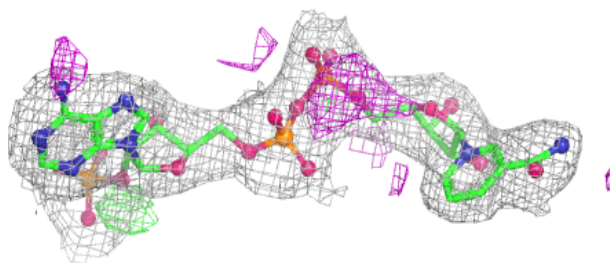
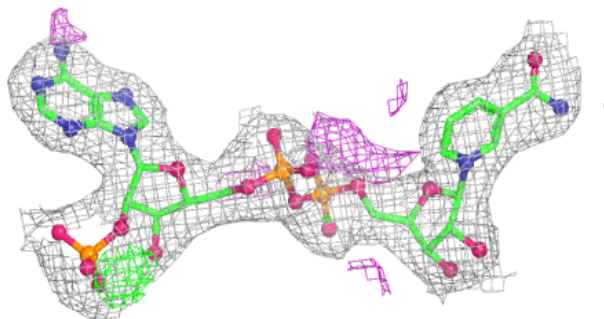
**Electron density around UMP B 607:**

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

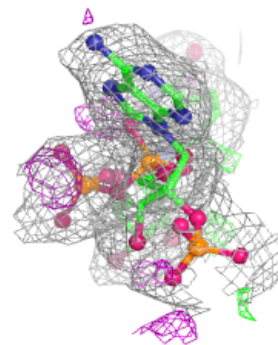
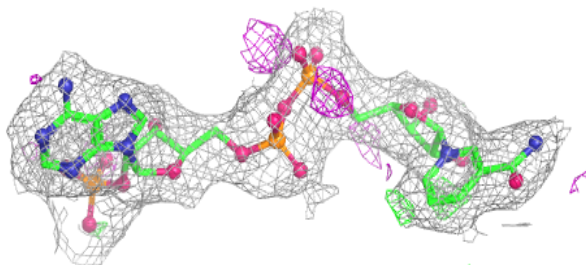
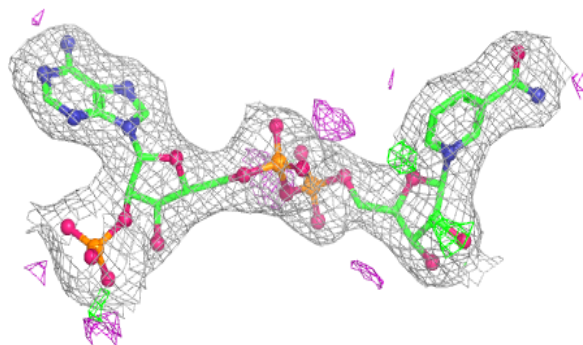


Electron density around NDP B 610:

$2mF_o-DF_c$ (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.