



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 08:07 AM EDT

PDB ID : 3DL5
Title : Crystal Structure of the A287F Active Site Mutant of TS-DHFR from *Cryptosporidium hominis*
Authors : Vargo, M.A.; Martucci, W.E.; Anderson, K.S.
Deposited on : 2008-06-26
Resolution : 2.74 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

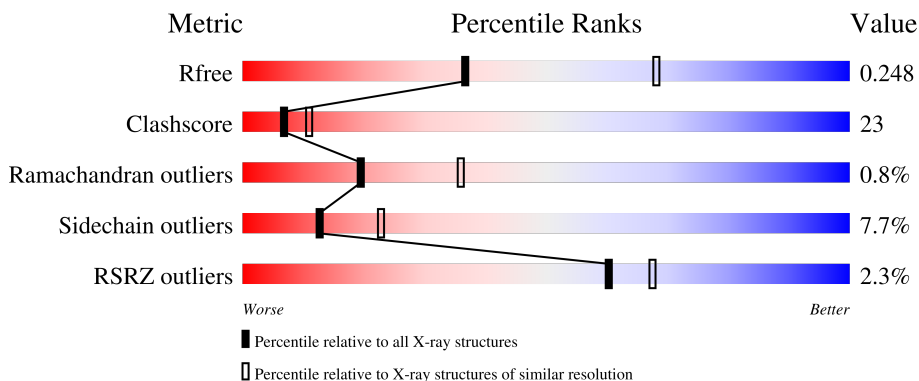
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	521	 63% 29% 5% .
1	B	521	 66% 26% . .
1	C	521	 2% 60% 31% 6% .
1	D	521	 54% 37% 6% .
1	E	521	 6% 55% 38% . .

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
3	CB3	D	616	X	-	X	-
3	CB3	E	620	X	-	X	-
4	DHF	A	605	X	-	-	-
4	DHF	B	609	X	-	X	-
4	DHF	C	613	-	-	X	-
4	DHF	D	617	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21793 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.

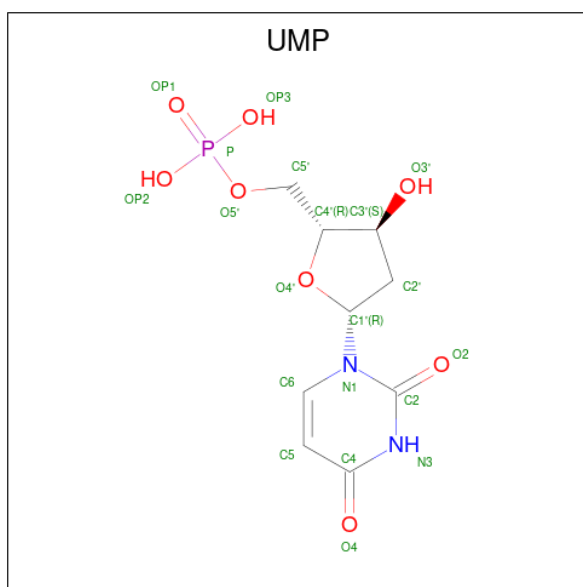
- Molecule 1 is a protein called Dihydrofolate reductase, DHFR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	507	4130	2642	693	773	22	0	0	0
1	B	508	4143	2650	695	776	22	0	0	0
1	C	508	4135	2645	694	774	22	0	0	0
1	D	507	4130	2642	693	773	22	0	0	0
1	E	508	4135	2645	694	774	22	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

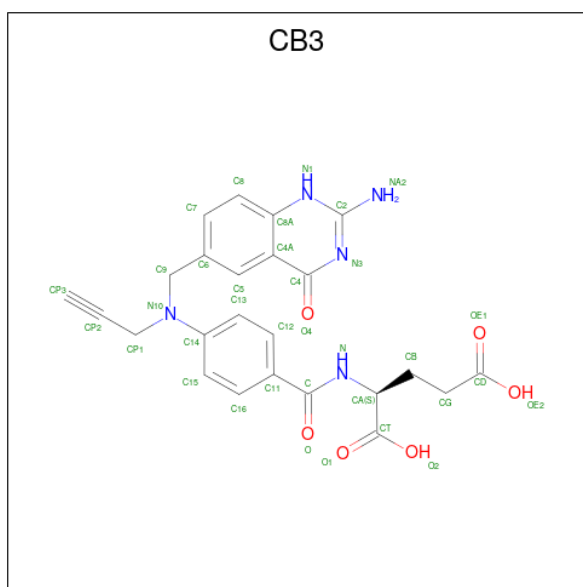
Chain	Residue	Modelled	Actual	Comment	Reference
A	287	PHE	ALA	engineered mutation	UNP Q5CGA3
B	287	PHE	ALA	engineered mutation	UNP Q5CGA3
C	287	PHE	ALA	engineered mutation	UNP Q5CGA3
D	287	PHE	ALA	engineered mutation	UNP Q5CGA3
E	287	PHE	ALA	engineered mutation	UNP Q5CGA3

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: C₉H₁₃N₂O₈P).



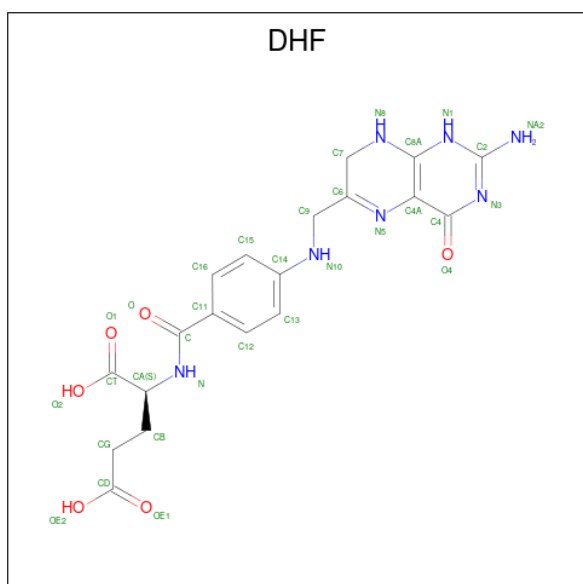
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: C₂₄H₂₃N₅O₆).



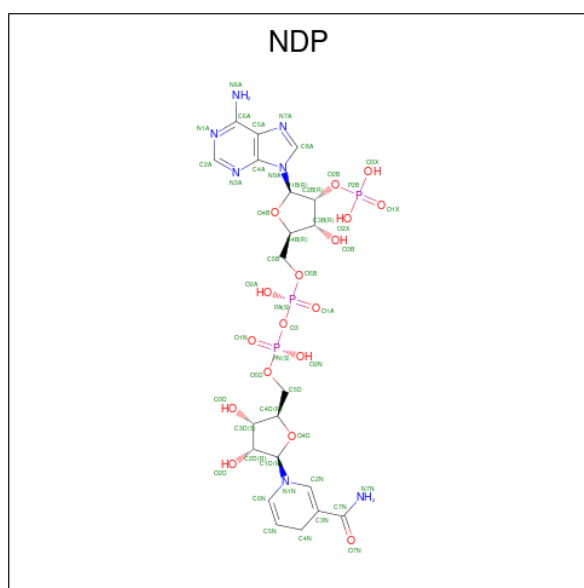
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		
3	D	1	Total	C	N	O	0	0
			35	24	5	6		
3	E	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is DIHYDROFOLIC ACID (three-letter code: DHF) (formula: $C_{19}H_{21}N_7O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total 32	C 19	N 7	O 6	0	0
4	B	1	Total 32	C 19	N 7	O 6	0	0
4	C	1	Total 32	C 19	N 7	O 6	0	0
4	D	1	Total 32	C 19	N 7	O 6	0	0
4	E	1	Total 32	C 19	N 7	O 6	0	0

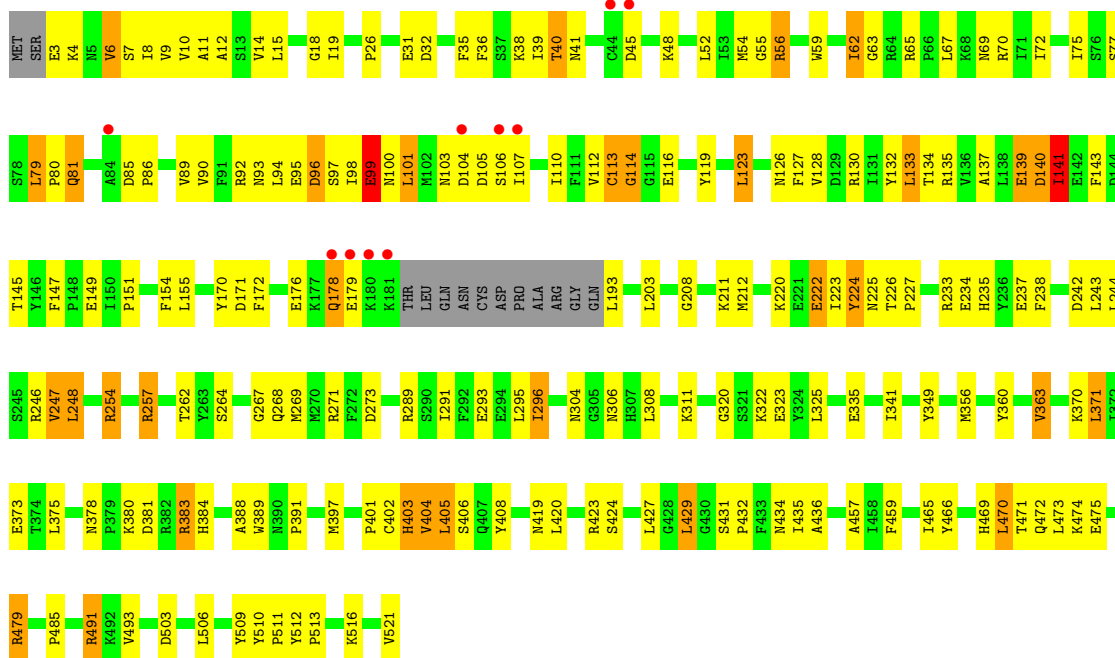
- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



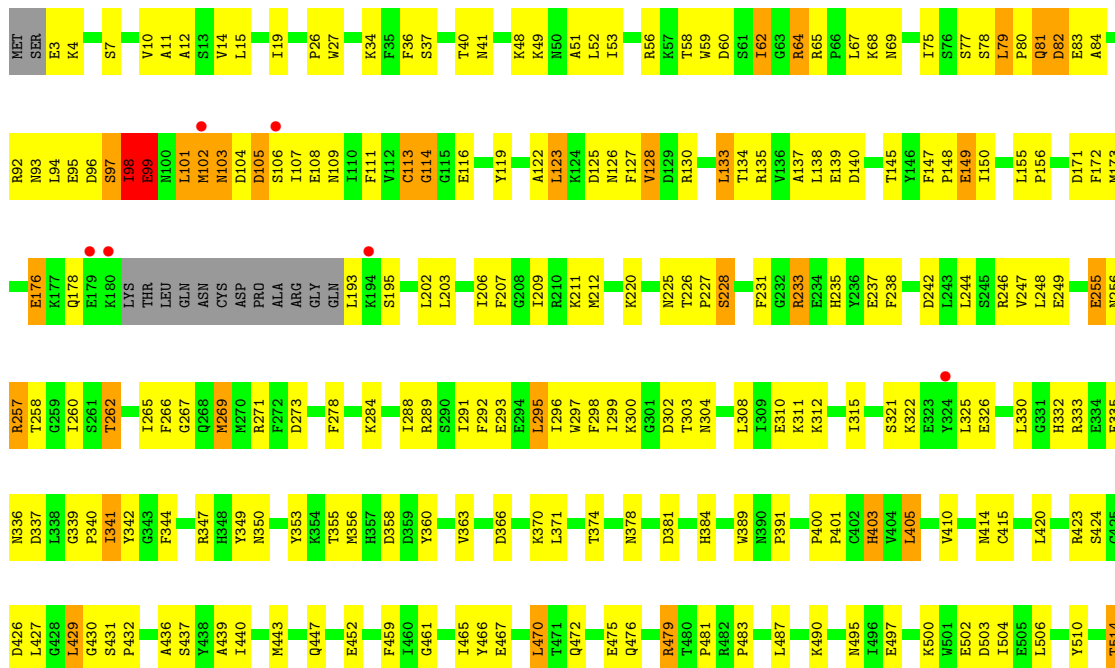
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	114	Total 114	O 114	0	0
6	B	150	Total 150	O 150	0	0
6	C	95	Total 95	O 95	0	0
6	D	62	Total 62	O 62	0	0
6	E	24	Total 24	O 24	0	0



● Molecule 1: Dihydrofolate reductase, DHFR

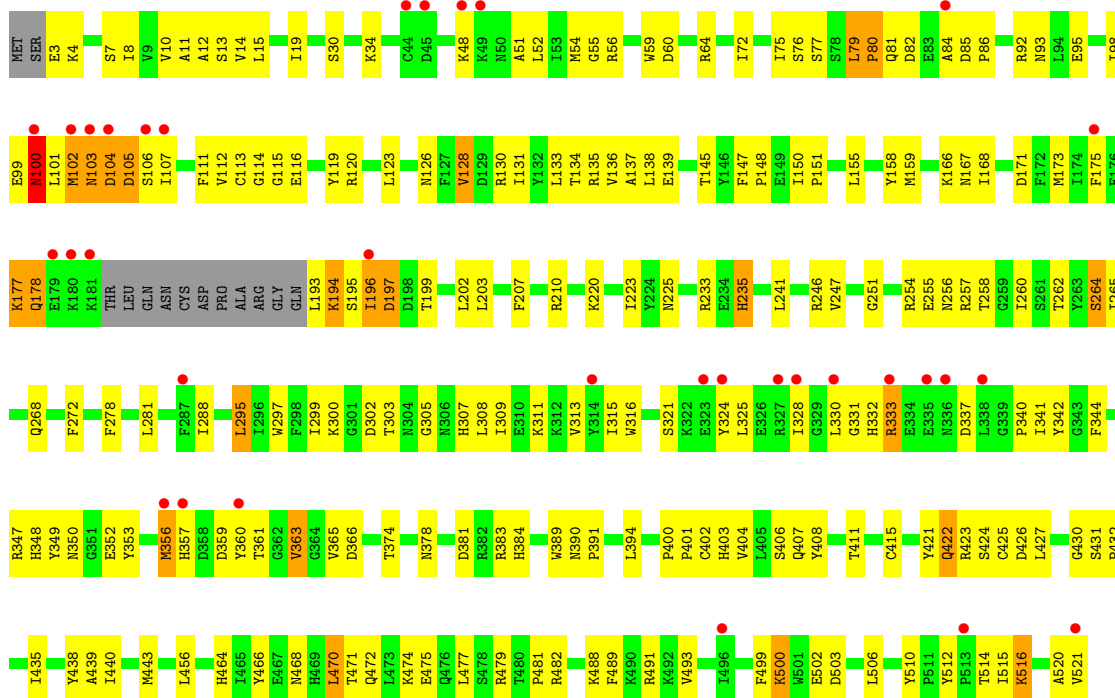


● Molecule 1: Dihydrofolate reductase, DHFR





• Molecule 1: Dihydrofolate reductase, DHFR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.81Å 116.54Å 219.21Å 90.00° 95.21° 90.00°	Depositor
Resolution (Å)	45.40 – 2.74 45.48 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.40-2.74) 99.4 (45.48-2.72)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.73Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.245 0.218 , 0.248	Depositor DCC
R_{free} test set	7223 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtrriage
Anisotropy	0.363	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21793	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	0.38	0/4226	0.65	0/5711
1	B	0.41	0/4239	0.67	0/5727
1	C	0.36	0/4231	0.62	0/5718
1	D	0.36	0/4226	0.61	0/5711
1	E	0.34	0/4231	0.62	1/5718 (0.0%)
All	All	0.37	0/21153	0.63	1/28585 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	4
1	C	0	5
1	D	0	6
1	E	0	2
All	All	0	23

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	357	HIS	CB-CA-C	-5.04	100.33	110.40

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	206	ILE	Peptide
1	A	403	HIS	Peptide
1	A	98	ILE	Peptide
1	A	99	GLU	Peptide
1	B	113	CYS	Peptide
1	B	114	GLY	Peptide
1	B	179	GLU	Peptide
1	B	206	ILE	Peptide
1	C	113	CYS	Peptide
1	C	114	GLY	Peptide
1	C	170	TYR	Peptide
1	C	179	GLU	Peptide
1	C	403	HIS	Peptide
1	D	103	ASN	Peptide
1	D	113	CYS	Peptide
1	D	114	GLY	Peptide
1	D	403	HIS	Peptide
1	D	98	ILE	Peptide
1	D	99	GLU	Peptide
1	E	100	ASN	Peptide
1	E	177	LYS	Peptide

5.2 Too-close contacts [i](#)

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	4130	0	4057	164	0
1	B	4143	0	4074	160	0
1	C	4135	0	4059	193	1
1	D	4130	0	4057	231	0
1	E	4135	0	4059	224	2
2	A	20	0	11	4	0
2	B	20	0	11	3	0
2	C	20	0	11	3	0
2	D	20	0	11	4	0
2	E	20	0	11	6	0
3	A	35	0	21	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	35	0	21	3	0
3	C	35	0	21	2	0
3	D	35	0	21	9	0
3	E	35	0	21	13	0
4	A	32	0	19	6	0
4	B	32	0	19	10	0
4	C	32	0	19	9	0
4	D	32	0	19	9	0
4	E	32	0	19	5	0
5	A	48	0	26	7	0
5	B	48	0	26	8	0
5	C	48	0	26	11	0
5	D	48	0	26	5	0
5	E	48	0	26	12	0
6	A	114	0	0	18	0
6	B	150	0	0	7	0
6	C	95	0	0	9	0
6	D	62	0	0	12	0
6	E	24	0	0	5	0
All	All	21793	0	20691	976	2

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 23.

All (976) 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:D:104:ASP:O	1:D:106:SER:N	1.63	1.26
1:B:179:GLU:C	1:B:180:LYS:HG3	1.52	1.23
1:E:79:LEU:HD23	1:E:80:PRO:CD	1.68	1.21
1:E:79:LEU:CD2	1:E:80:PRO:HD2	1.71	1.18
1:E:178:GLN:OE1	1:E:178:GLN:HA	1.43	1.16
1:E:196:ILE:N	1:E:196:ILE:HD12	1.56	1.13
1:E:196:ILE:H	1:E:196:ILE:CD1	1.51	1.11
1:A:4:LYS:HG2	1:A:101:LEU:HD23	1.34	1.09
1:D:98:ILE:O	1:D:99:GLU:HB3	1.49	1.09
1:B:209:ILE:HD12	1:B:209:ILE:H	1.14	1.07
1:D:337:ASP:HA	1:D:356:MET:HE3	1.35	1.07
1:A:374:THR:HG22	1:A:384:HIS:HE1	1.18	1.07
1:D:255:GLU:CD	1:D:255:GLU:H	1.55	1.06
1:B:179:GLU:O	1:B:180:LYS:HG3	1.57	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ASP:OD1	6:C:642:HOH:O	1.72	1.03
1:C:92:ARG:O	5:C:614:NDP:H2A	1.59	1.03
1:A:374:THR:HG22	1:A:384:HIS:CE1	1.93	1.03
3:E:620:CB3:OE2	3:E:620:CB3:HA	1.55	1.03
1:D:104:ASP:O	1:D:107:ILE:N	1.92	1.01
1:E:82:ASP:OD2	1:E:84:ALA:HB2	1.61	1.00
1:E:195:SER:OG	1:E:196:ILE:HD12	1.61	0.99
2:A:603:UMP:H5	6:A:679:HOH:O	1.42	0.98
3:E:620:CB3:O	3:E:620:CB3:HB1	1.62	0.97
1:E:195:SER:OG	1:E:196:ILE:CD1	2.14	0.95
1:E:196:ILE:HD12	1:E:196:ILE:H	0.78	0.94
1:E:3:GLU:HB2	1:E:101:LEU:HD22	1.50	0.94
1:E:196:ILE:O	1:E:197:ASP:HB2	1.65	0.94
1:D:304:ASN:HA	1:D:356:MET:HE2	1.48	0.94
1:A:3:GLU:HA	6:A:680:HOH:O	1.69	0.92
1:B:359:ASP:OD2	1:B:361:THR:HG23	1.68	0.92
1:C:77:SER:N	5:C:614:NDP:O1X	2.02	0.92
1:C:98:ILE:O	1:C:99:GLU:HG3	1.68	0.92
1:C:4:LYS:HB2	1:C:101:LEU:HD23	1.51	0.92
1:B:257:ARG:HD3	2:B:607:UMP:OP2	1.70	0.91
1:D:62:ILE:HD11	4:D:617:DHF:C12	2.00	0.91
1:D:104:ASP:C	1:D:106:SER:N	2.23	0.91
1:D:77:SER:C	1:D:92:ARG:NH1	2.24	0.90
1:C:140:ASP:O	1:C:141:ILE:HG22	1.72	0.90
1:D:96:ASP:O	1:D:99:GLU:HG2	1.72	0.90
1:B:179:GLU:C	1:B:180:LYS:CG	2.36	0.89
1:D:62:ILE:HD11	4:D:617:DHF:C11	2.03	0.89
1:D:77:SER:O	1:D:92:ARG:NH1	2.04	0.89
1:B:285:LYS:HB3	1:B:514:THR:HG22	1.55	0.88
1:E:82:ASP:OD2	1:E:84:ALA:CB	2.22	0.88
1:D:342:TYR:CE1	1:D:403:HIS:CE1	2.63	0.87
1:A:258:THR:HG22	1:A:260:ILE:H	1.39	0.87
4:C:613:DHF:HB2	4:C:613:DHF:O	1.73	0.87
1:C:405:LEU:C	1:C:405:LEU:HD23	1.95	0.87
1:E:488:LYS:HD3	1:E:489:PHE:H	1.40	0.86
1:C:36:PHE:O	1:C:40:THR:HB	1.75	0.86
1:D:330:LEU:HA	6:D:648:HOH:O	1.75	0.85
1:D:360:TYR:O	1:D:363:VAL:HG12	1.76	0.85
1:C:349:TYR:CE2	1:D:391:PRO:HD2	2.12	0.85
1:A:4:LYS:HG2	1:A:101:LEU:CD2	2.05	0.85
1:B:209:ILE:H	1:B:209:ILE:CD1	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:LYS:H	1:E:101:LEU:CD2	1.90	0.85
1:E:115:GLY:HA3	5:E:622:NDP:O1A	1.77	0.85
1:B:411:THR:CG2	1:B:413:ASP:HB2	2.09	0.83
1:E:155:LEU:HD12	1:E:178:GLN:NE2	1.94	0.83
4:C:613:DHF:C6	5:C:614:NDP:H42N	2.10	0.81
1:C:140:ASP:C	1:C:141:ILE:CG2	2.47	0.81
1:C:211:LYS:HE3	6:C:635:HOH:O	1.81	0.81
1:E:257:ARG:HD3	2:E:619:UMP:OP2	1.80	0.81
1:D:339:GLY:HA2	1:D:353:TYR:CE2	2.16	0.81
1:E:516:LYS:HE3	1:E:516:LYS:H	1.45	0.81
1:E:100:ASN:O	1:E:103:ASN:O	1.96	0.81
1:A:258:THR:HG21	1:A:520:ALA:HB1	1.63	0.81
1:C:403:HIS:HB2	1:C:420:LEU:HD11	1.63	0.80
1:C:380:LYS:HE2	6:C:636:HOH:O	1.80	0.80
1:B:4:LYS:HE2	1:B:107:ILE:O	1.82	0.80
1:B:103:ASN:CG	1:B:104:ASP:H	1.85	0.80
4:B:609:DHF:C7	5:B:610:NDP:H42N	2.12	0.80
1:D:255:GLU:CD	1:D:255:GLU:N	2.32	0.80
1:D:104:ASP:O	1:D:106:SER:CA	2.30	0.80
1:D:104:ASP:HB3	1:D:107:ILE:HD13	1.62	0.80
1:B:378:ASN:ND2	1:B:381:ASP:HB2	1.97	0.80
1:A:96:ASP:O	1:A:99:GLU:HG2	1.82	0.79
1:E:15:LEU:HD12	1:E:139:GLU:HG3	1.64	0.79
1:A:333:ARG:HA	6:A:626:HOH:O	1.83	0.78
1:E:102:MET:O	1:E:103:ASN:HB2	1.83	0.78
1:D:102:MET:O	1:D:102:MET:HE3	1.83	0.78
4:B:609:DHF:H72	5:B:610:NDP:H42N	1.64	0.78
2:A:603:UMP:OP1	1:B:383:ARG:NH1	2.17	0.78
1:C:40:THR:HG23	1:C:70:ARG:HD3	1.65	0.78
1:D:104:ASP:C	1:D:106:SER:H	1.86	0.78
1:C:178:GLN:OE1	1:C:178:GLN:HA	1.84	0.77
1:D:77:SER:C	1:D:92:ARG:HH11	1.87	0.77
3:E:620:CB3:O	3:E:620:CB3:CB	2.31	0.77
1:C:98:ILE:O	1:C:99:GLU:CG	2.31	0.77
1:C:123:LEU:HD12	1:C:128:VAL:HG11	1.67	0.77
1:E:324:TYR:O	1:E:328:ILE:HG12	1.84	0.77
1:B:179:GLU:O	1:B:180:LYS:CG	2.33	0.77
1:E:75:ILE:O	5:E:622:NDP:H1B	1.85	0.76
1:D:337:ASP:CA	1:D:356:MET:HE3	2.12	0.76
1:C:40:THR:CG2	1:C:70:ARG:HD3	2.15	0.76
1:D:332:HIS:HD2	6:D:648:HOH:O	1.69	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:374:THR:HB	6:E:646:HOH:O	1.86	0.75
1:C:140:ASP:C	1:C:141:ILE:HG23	2.04	0.75
3:D:616:CB3:O	3:D:616:CB3:HB1	1.87	0.75
1:A:114:GLY:HA3	1:A:119:TYR:CZ	2.21	0.75
1:E:516:LYS:H	1:E:516:LYS:CE	1.99	0.75
1:D:104:ASP:O	1:D:105:ASP:C	2.24	0.74
1:A:247:VAL:CG2	1:A:465:ILE:HD12	2.17	0.74
1:A:289:ARG:HG3	1:A:501:TRP:CE2	2.23	0.74
1:B:500:LYS:HE3	6:B:734:HOH:O	1.87	0.74
1:C:98:ILE:O	1:C:99:GLU:CB	2.35	0.74
1:E:93:ASN:HD21	1:E:95:GLU:HB3	1.51	0.74
3:E:620:CB3:OE2	3:E:620:CB3:CA	2.35	0.74
1:E:93:ASN:ND2	1:E:95:GLU:HB3	2.02	0.74
1:C:225:ASN:O	1:C:233:ARG:NH2	2.21	0.74
1:C:54:MET:HE3	1:C:72:ILE:HG23	1.69	0.74
1:D:102:MET:O	1:D:102:MET:CE	2.36	0.74
1:C:92:ARG:O	5:C:614:NDP:C2A	2.35	0.74
1:C:360:TYR:O	1:C:363:VAL:HG13	1.87	0.74
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.22	0.74
1:E:4:LYS:N	1:E:101:LEU:HD21	2.03	0.73
1:C:140:ASP:O	1:C:141:ILE:CG2	2.36	0.73
1:E:14:VAL:HG23	1:E:15:LEU:HG	1.70	0.73
1:C:104:ASP:C	1:C:106:SER:H	1.92	0.73
1:B:411:THR:HG22	1:B:413:ASP:N	2.04	0.73
1:D:260:ILE:HD12	1:D:260:ILE:N	2.03	0.73
1:A:19:ILE:O	5:A:606:NDP:H2N	1.88	0.73
1:A:98:ILE:O	1:A:99:GLU:HB3	1.88	0.73
1:C:193:LEU:HA	6:C:626:HOH:O	1.88	0.73
1:A:26:PRO:HB2	1:A:27:TRP:CE3	2.24	0.73
1:C:139:GLU:HB2	1:C:510:TYR:CZ	2.24	0.73
1:E:4:LYS:H	1:E:101:LEU:HD21	1.54	0.73
1:C:40:THR:HG21	1:C:70:ARG:HH11	1.53	0.72
1:A:225:ASN:O	1:A:233:ARG:NH2	2.22	0.72
1:A:379:PRO:HD2	6:A:644:HOH:O	1.88	0.72
1:E:79:LEU:HD23	1:E:80:PRO:HD2	0.82	0.72
1:E:297:TRP:CD1	1:E:302:ASP:HB3	2.25	0.72
1:B:114:GLY:HA3	1:B:119:TYR:CZ	2.25	0.72
1:B:4:LYS:HB2	1:B:101:LEU:CD2	2.19	0.72
1:B:209:ILE:HD12	1:B:209:ILE:N	1.97	0.72
1:D:149:GLU:H	1:D:149:GLU:CD	1.90	0.72
1:D:257:ARG:NH2	1:D:521:VAL:OXT	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:TYR:CD1	1:D:403:HIS:CE1	2.77	0.71
1:D:495:ASN:OD1	1:D:497:GLU:HG2	1.90	0.71
1:C:79:LEU:HD23	1:C:80:PRO:HD2	1.72	0.71
1:B:178:GLN:O	1:B:179:GLU:HG2	1.89	0.71
1:C:4:LYS:HB2	1:C:101:LEU:CD2	2.20	0.71
1:D:255:GLU:HG3	6:D:675:HOH:O	1.89	0.71
1:D:257:ARG:HD3	2:D:615:UMP:OP2	1.89	0.71
1:D:52:LEU:HB3	1:D:113:CYS:SG	2.30	0.71
1:E:155:LEU:HD12	1:E:178:GLN:HE21	1.56	0.71
1:A:38:LYS:HB3	1:B:202:LEU:HG	1.70	0.71
1:E:402:CYS:SG	2:E:619:UMP:C6	2.83	0.71
1:E:207:PHE:HB3	1:E:210:ARG:HB2	1.72	0.71
1:D:405:LEU:C	1:D:405:LEU:HD23	2.11	0.71
1:C:349:TYR:HH	1:D:349:TYR:HH	1.35	0.71
1:D:82:ASP:OD1	1:D:84:ALA:CB	2.38	0.71
1:D:439:ALA:O	1:D:443:MET:HG3	1.91	0.70
4:D:617:DHF:C6	5:D:618:NDP:H42N	2.21	0.70
1:C:75:ILE:O	5:C:614:NDP:H1B	1.91	0.70
1:B:52:LEU:HB3	1:B:113:CYS:SG	2.31	0.70
1:A:52:LEU:HB3	1:A:113:CYS:SG	2.31	0.70
1:C:178:GLN:OE1	1:C:178:GLN:CA	2.39	0.70
1:E:430:GLY:HA2	3:E:620:CB3:CP3	2.22	0.70
1:B:3:GLU:O	1:B:101:LEU:HD22	1.90	0.70
1:B:60:ASP:OD1	1:B:64:ARG:NH1	2.24	0.70
1:E:430:GLY:CA	3:E:620:CB3:CP3	2.70	0.70
1:B:411:THR:HG22	1:B:413:ASP:H	1.54	0.70
1:A:220:LYS:HE2	1:A:249:GLU:OE1	1.91	0.69
1:E:196:ILE:O	1:E:197:ASP:CB	2.40	0.69
1:D:103:ASN:CG	1:D:104:ASP:H	1.95	0.69
1:E:34:LYS:HE2	6:E:633:HOH:O	1.91	0.69
1:E:194:LYS:H	1:E:194:LYS:HD3	1.56	0.69
1:D:514:THR:HG22	6:D:628:HOH:O	1.91	0.69
1:B:178:GLN:C	1:B:179:GLU:HG2	2.12	0.69
1:B:342:TYR:OH	1:B:402:CYS:N	2.22	0.68
1:C:267:GLY:O	1:D:271:ARG:NH2	2.25	0.68
1:E:472:GLN:O	1:E:475:GLU:HB3	1.94	0.68
1:A:4:LYS:H	1:A:101:LEU:HD22	1.58	0.68
1:A:32:ASP:OD2	4:A:605:DHF:N3	2.26	0.68
1:B:98:ILE:HG23	1:B:98:ILE:O	1.93	0.68
1:E:101:LEU:O	1:E:103:ASN:N	2.27	0.68
1:D:130:ARG:HG3	1:D:176:GLU:OE1	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:LEU:HD11	1:E:168:ILE:HD13	1.76	0.68
1:C:391:PRO:HD2	1:D:349:TYR:CE2	2.29	0.68
1:E:52:LEU:HB3	1:E:113:CYS:SG	2.33	0.68
1:E:384:HIS:HB2	1:E:408:TYR:O	1.94	0.67
1:B:99:GLU:OE2	1:B:102:MET:SD	2.52	0.67
1:A:258:THR:CG2	1:A:520:ALA:HB1	2.23	0.67
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.30	0.67
1:B:297:TRP:HH2	1:B:338:LEU:HD12	1.60	0.67
1:C:370:LYS:HA	1:C:373:GLU:HG2	1.77	0.67
1:D:178:GLN:HA	1:D:178:GLN:OE1	1.94	0.67
1:D:97:SER:O	1:D:99:GLU:HG3	1.94	0.67
1:D:342:TYR:CE1	1:D:403:HIS:NE2	2.63	0.67
1:A:256:ASN:OD1	1:A:258:THR:HB	1.95	0.66
1:C:155:LEU:HD12	1:C:178:GLN:NE2	2.09	0.66
1:E:360:TYR:HB3	1:E:363:VAL:HG12	1.77	0.66
1:A:431:SER:HB3	1:A:432:PRO:HD3	1.76	0.66
1:C:402:CYS:SG	2:C:611:UMP:C6	2.89	0.66
1:D:225:ASN:O	1:D:233:ARG:NH2	2.27	0.66
1:A:82:ASP:N	6:A:659:HOH:O	2.29	0.66
1:D:96:ASP:O	1:D:99:GLU:CG	2.42	0.66
1:C:133:LEU:HD22	1:C:134:THR:N	2.12	0.65
1:D:96:ASP:O	1:D:99:GLU:HB3	1.96	0.65
1:B:360:TYR:O	1:B:363:VAL:HG13	1.96	0.65
1:E:114:GLY:HA2	1:E:119:TYR:CZ	2.32	0.65
1:E:359:ASP:OD2	1:E:361:THR:HG22	1.97	0.65
1:E:488:LYS:HD3	1:E:489:PHE:N	2.11	0.65
1:D:135:ARG:HD3	1:D:171:ASP:OD2	1.96	0.65
1:E:347:ARG:O	1:E:366:ASP:HA	1.96	0.65
1:E:297:TRP:CG	1:E:308:LEU:HD21	2.32	0.65
1:E:430:GLY:CA	3:E:620:CB3:HP3	2.26	0.65
1:A:495:ASN:OD1	1:A:497:GLU:HG3	1.97	0.65
1:B:34:LYS:HE2	6:B:758:HOH:O	1.96	0.65
1:A:97:SER:O	1:A:99:GLU:HG3	1.96	0.64
1:A:202:LEU:HG	1:B:38:LYS:HB3	1.78	0.64
1:B:411:THR:CG2	1:B:413:ASP:CB	2.75	0.64
1:D:26:PRO:HG2	1:D:27:TRP:CZ3	2.31	0.64
1:A:330:LEU:C	1:A:332:HIS:H	2.00	0.64
1:A:14:VAL:HG23	1:A:137:ALA:HA	1.79	0.64
1:B:98:ILE:O	1:B:98:ILE:CG2	2.46	0.64
1:A:258:THR:HG22	1:A:260:ILE:N	2.11	0.64
1:D:374:THR:HG22	1:D:384:HIS:CE1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:GLU:HG2	6:D:679:HOH:O	1.96	0.64
1:B:411:THR:CG2	1:B:413:ASP:H	2.11	0.64
1:B:411:THR:HG21	1:B:413:ASP:HB2	1.79	0.64
1:B:315:ILE:HB	3:B:608:CB3:C15	2.28	0.64
1:C:149:GLU:CD	1:C:149:GLU:H	1.99	0.64
1:D:430:GLY:HA2	3:D:616:CB3:CP3	2.28	0.64
1:D:220:LYS:HD3	1:D:249:GLU:OE1	1.98	0.63
1:B:209:ILE:HG13	6:B:708:HOH:O	1.98	0.63
1:C:99:GLU:OE1	1:C:100:ASN:N	2.32	0.63
1:E:101:LEU:C	1:E:103:ASN:H	2.00	0.63
4:E:621:DHF:C6	5:E:622:NDP:H42N	2.28	0.63
1:A:349:TYR:HH	1:B:349:TYR:HH	1.45	0.63
1:E:330:LEU:O	1:E:332:HIS:N	2.31	0.63
1:A:378:ASN:ND2	1:A:381:ASP:HB2	2.13	0.63
1:B:370:LYS:O	1:B:374:THR:HG23	1.97	0.63
1:C:75:ILE:HG22	5:C:614:NDP:C4A	2.29	0.63
1:E:155:LEU:CD1	1:E:178:GLN:HE21	2.11	0.63
1:E:260:ILE:N	1:E:260:ILE:HD12	2.14	0.63
4:B:609:DHF:C6	5:B:610:NDP:H42N	2.28	0.63
1:A:93:ASN:ND2	1:A:95:GLU:HB3	2.13	0.63
1:E:92:ARG:O	5:E:622:NDP:H2A	1.99	0.63
1:A:5:ASN:HB2	6:A:696:HOH:O	1.98	0.63
1:A:14:VAL:CG2	1:A:137:ALA:HA	2.29	0.62
1:C:114:GLY:HA3	1:C:119:TYR:CZ	2.34	0.62
1:D:405:LEU:HD23	1:D:405:LEU:O	1.99	0.62
1:E:104:ASP:OD2	1:E:107:ILE:HD13	2.00	0.62
1:E:135:ARG:HD2	1:E:173:MET:SD	2.39	0.62
1:C:79:LEU:H	1:C:92:ARG:HH12	1.45	0.62
1:D:123:LEU:HD12	1:D:128:VAL:CG1	2.29	0.62
1:A:359:ASP:OD1	1:A:361:THR:HG22	2.00	0.62
1:C:52:LEU:HB3	1:C:113:CYS:SG	2.39	0.62
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.80	0.62
1:D:237:GLU:HG2	1:D:481:PRO:HB3	1.79	0.62
1:A:374:THR:CG2	1:A:384:HIS:CE1	2.76	0.62
4:B:609:DHF:HB1	4:B:609:DHF:O	2.00	0.62
1:D:60:ASP:OD1	1:D:64:ARG:NH1	2.33	0.62
1:A:194:LYS:HG2	1:A:195:SER:N	2.13	0.62
1:A:233:ARG:NH1	1:A:242:ASP:OD1	2.32	0.62
1:B:82:ASP:OD1	1:B:82:ASP:C	2.38	0.62
4:B:609:DHF:H72	5:B:610:NDP:C4N	2.28	0.62
1:D:4:LYS:N	1:D:101:LEU:HD21	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ILE:HA	6:B:708:HOH:O	2.00	0.61
1:A:338:LEU:HB3	1:A:341:ILE:HD13	1.82	0.61
1:D:289:ARG:NH2	1:D:311:LYS:O	2.32	0.61
1:E:3:GLU:HB2	1:E:101:LEU:CD2	2.28	0.61
1:C:104:ASP:C	1:C:106:SER:N	2.53	0.61
1:B:379:PRO:HB2	1:B:410:VAL:HG11	1.81	0.61
1:C:403:HIS:H	1:C:403:HIS:CD2	2.18	0.61
1:E:115:GLY:CA	5:E:622:NDP:O1A	2.47	0.61
1:D:62:ILE:HD11	4:D:617:DHF:C13	2.30	0.61
1:D:284:LYS:HE3	6:D:630:HOH:O	1.99	0.61
1:E:297:TRP:CD2	1:E:308:LEU:HD21	2.35	0.61
1:D:337:ASP:CG	1:D:356:MET:HG2	2.20	0.61
1:E:104:ASP:O	1:E:106:SER:N	2.34	0.61
1:D:81:GLN:OE1	1:D:92:ARG:NE	2.30	0.61
1:D:147:PHE:CD2	1:D:148:PRO:HD2	2.36	0.61
1:B:103:ASN:CG	1:B:104:ASP:N	2.55	0.60
1:B:276:GLU:O	1:B:277:SER:HB3	1.99	0.60
1:C:378:ASN:ND2	1:C:381:ASP:HB2	2.16	0.60
1:A:155:LEU:HD12	1:A:178:GLN:HG2	1.82	0.60
1:C:293:GLU:HA	1:C:296:ILE:HD11	1.83	0.60
1:E:330:LEU:C	1:E:332:HIS:H	2.04	0.60
1:C:98:ILE:O	1:C:99:GLU:HB3	1.99	0.60
1:D:77:SER:C	1:D:92:ARG:HH12	2.04	0.60
1:E:135:ARG:HD3	1:E:171:ASP:HB2	1.83	0.59
1:A:383:ARG:NE	1:B:400:PRO:HG2	2.17	0.59
1:B:225:ASN:O	1:B:233:ARG:NH2	2.25	0.59
1:C:254:ARG:NH2	1:D:410:VAL:O	2.35	0.59
1:C:100:ASN:HB2	1:C:110:ILE:HD11	1.83	0.59
1:D:103:ASN:O	1:D:104:ASP:HB2	2.01	0.59
1:D:296:ILE:HD12	1:D:297:TRP:N	2.17	0.59
1:A:158:TYR:O	1:A:173:MET:HB2	2.02	0.59
1:A:322:LYS:HD3	1:A:335:GLU:HB2	1.84	0.59
1:D:378:ASN:ND2	1:D:381:ASP:HB2	2.17	0.59
1:E:466:TYR:OH	2:E:619:UMP:O3'	2.21	0.59
4:D:617:DHF:N10	6:D:634:HOH:O	2.26	0.59
1:B:179:GLU:CA	1:B:180:LYS:HG3	2.30	0.59
1:E:155:LEU:CG	1:E:178:GLN:HE21	2.16	0.59
1:A:4:LYS:CG	1:A:101:LEU:HD23	2.22	0.58
1:D:291:ILE:HD13	1:D:436:ALA:HB3	1.84	0.58
1:E:3:GLU:CB	1:E:101:LEU:HD22	2.27	0.58
2:A:603:UMP:C5	6:A:679:HOH:O	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:ASN:HA	1:C:356:MET:SD	2.43	0.58
1:B:99:GLU:OE1	1:B:99:GLU:N	2.36	0.58
1:B:431:SER:HB3	1:B:432:PRO:HD3	1.84	0.58
1:C:99:GLU:OE1	1:C:99:GLU:C	2.42	0.58
1:C:99:GLU:C	1:C:99:GLU:CD	2.62	0.58
1:C:323:GLU:H	1:C:323:GLU:CD	2.05	0.58
1:D:347:ARG:NH2	1:D:366:ASP:OD1	2.36	0.58
1:D:62:ILE:CD1	4:D:617:DHF:C12	2.78	0.58
1:A:14:VAL:HG23	1:A:136:VAL:O	2.02	0.58
1:B:179:GLU:CB	1:B:180:LYS:HG3	2.33	0.58
1:E:4:LYS:HE3	1:E:101:LEU:HD23	1.85	0.58
1:E:516:LYS:H	1:E:516:LYS:CD	2.15	0.58
1:B:19:ILE:O	5:B:610:NDP:H2N	2.03	0.58
4:E:621:DHF:C7	5:E:622:NDP:H42N	2.34	0.58
1:D:114:GLY:HA3	1:D:119:TYR:CZ	2.39	0.58
1:C:31:GLU:HG2	1:D:207:PHE:CE1	2.39	0.58
1:D:426:ASP:HB2	2:D:615:UMP:O3'	2.04	0.58
1:C:257:ARG:NH2	1:C:521:VAL:OXT	2.37	0.57
1:E:101:LEU:C	1:E:103:ASN:N	2.57	0.57
1:C:404:VAL:HG11	1:D:405:LEU:HD11	1.86	0.57
1:D:103:ASN:CG	1:D:104:ASP:N	2.58	0.57
1:D:502:GLU:CD	1:D:502:GLU:H	2.08	0.57
1:A:75:ILE:O	5:A:606:NDP:H1B	2.04	0.57
1:B:479:ARG:NH2	1:B:513:PRO:O	2.37	0.57
1:C:291:ILE:HD13	1:C:436:ALA:HB3	1.86	0.57
1:D:48:LYS:HB3	1:D:106:SER:O	2.04	0.57
1:E:4:LYS:N	1:E:101:LEU:CD2	2.60	0.57
1:A:4:LYS:H	1:A:101:LEU:CD2	2.17	0.57
1:D:82:ASP:OD1	1:D:84:ALA:HB3	2.04	0.57
1:B:402:CYS:SG	2:B:607:UMP:C6	2.98	0.57
1:C:116:GLU:HB2	1:C:145:THR:HG23	1.86	0.57
1:C:419:ASN:ND2	1:C:457:ALA:HB3	2.20	0.57
1:D:4:LYS:H	1:D:101:LEU:HD21	1.70	0.57
1:D:116:GLU:HB2	1:D:145:THR:HG23	1.85	0.57
1:E:51:ALA:C	1:E:52:LEU:HD23	2.25	0.57
1:B:114:GLY:CA	1:B:119:TYR:CZ	2.88	0.56
1:D:108:GLU:HG2	1:D:109:ASN:ND2	2.19	0.56
1:A:3:GLU:HB3	6:A:618:HOH:O	2.04	0.56
1:A:288:ILE:HG23	1:A:501:TRP:HH2	1.70	0.56
1:C:56:ARG:O	1:C:59:TRP:HB3	2.05	0.56
1:C:96:ASP:O	1:C:99:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:PRO:O	1:D:228:SER:HB2	2.06	0.56
1:D:332:HIS:CD2	6:D:648:HOH:O	2.52	0.56
1:E:378:ASN:OD1	1:E:381:ASP:HB2	2.06	0.56
1:B:374:THR:O	1:B:378:ASN:O	2.24	0.56
1:D:98:ILE:CG2	1:D:101:LEU:HD12	2.36	0.56
1:A:289:ARG:NH2	1:A:311:LYS:O	2.37	0.56
1:B:285:LYS:HD3	1:B:514:THR:HG22	1.87	0.56
1:C:247:VAL:CG2	1:C:465:ILE:HD12	2.36	0.56
3:E:620:CB3:C6	3:E:620:CB3:H15	2.36	0.56
1:A:271:ARG:NH2	1:B:267:GLY:O	2.39	0.56
1:D:62:ILE:HD11	4:D:617:DHF:C16	2.35	0.56
1:D:149:GLU:OE2	1:D:149:GLU:N	2.39	0.56
1:D:389:TRP:CE3	1:D:401:PRO:HG2	2.41	0.56
1:C:100:ASN:O	1:C:103:ASN:O	2.23	0.56
1:C:7:SER:HB3	1:C:130:ARG:HB3	1.87	0.56
1:D:262:THR:HG21	6:D:626:HOH:O	2.06	0.56
1:E:119:TYR:O	1:E:123:LEU:HD23	2.06	0.56
1:B:3:GLU:O	1:B:4:LYS:HB2	2.06	0.55
1:C:9:VAL:HG12	4:C:613:DHF:HN1	1.71	0.55
1:E:7:SER:HB3	1:E:130:ARG:HB3	1.88	0.55
1:B:326:GLU:HG3	6:B:682:HOH:O	2.06	0.55
1:E:115:GLY:HA2	5:E:622:NDP:O5D	2.06	0.55
1:E:423:ARG:HG3	1:E:424:SER:N	2.20	0.55
1:D:123:LEU:HD12	1:D:128:VAL:HG11	1.88	0.55
1:D:149:GLU:HA	6:D:672:HOH:O	2.05	0.55
1:E:8:ILE:HG12	1:E:112:VAL:HB	1.87	0.55
1:E:514:THR:HG22	1:E:515:ILE:N	2.22	0.55
1:E:378:ASN:ND2	6:E:634:HOH:O	2.40	0.55
4:C:613:DHF:C7	5:C:614:NDP:H42N	2.35	0.55
1:D:4:LYS:N	1:D:101:LEU:CD2	2.70	0.55
4:E:621:DHF:H72	5:E:622:NDP:H42N	1.88	0.55
1:B:342:TYR:OH	1:B:401:PRO:HA	2.06	0.55
1:D:123:LEU:CD1	1:D:128:VAL:HG11	2.36	0.55
1:E:256:ASN:ND2	1:E:262:THR:HG23	2.20	0.55
1:E:491:ARG:HD3	1:E:503:ASP:OD2	2.07	0.55
1:B:411:THR:HG22	1:B:413:ASP:CB	2.37	0.55
1:D:304:ASN:HA	1:D:356:MET:CE	2.31	0.55
1:D:322:LYS:O	1:D:326:GLU:HB2	2.06	0.55
1:E:241:LEU:HD11	1:E:481:PRO:HG3	1.89	0.55
1:C:423:ARG:HG3	1:C:424:SER:N	2.20	0.55
1:A:246:ARG:HG2	6:A:670:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:VAL:HG22	1:A:465:ILE:HD12	1.87	0.54
1:D:256:ASN:ND2	1:D:260:ILE:O	2.39	0.54
1:E:79:LEU:CD2	1:E:80:PRO:CD	2.55	0.54
1:E:337:ASP:CG	1:E:356:MET:HG2	2.27	0.54
1:A:342:TYR:CD2	1:A:403:HIS:CE1	2.95	0.54
1:C:8:ILE:HG12	1:C:112:VAL:HB	1.88	0.54
1:C:93:ASN:OD1	1:C:95:GLU:HB3	2.07	0.54
1:C:98:ILE:C	1:C:99:GLU:HG3	2.27	0.54
1:D:423:ARG:HG3	1:D:424:SER:N	2.21	0.54
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.90	0.54
1:B:419:ASN:OD1	1:B:457:ALA:HB3	2.07	0.54
1:C:55:GLY:HA3	5:C:614:NDP:PA	2.48	0.54
1:E:135:ARG:NH2	1:E:482:ARG:HA	2.22	0.54
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.89	0.54
1:A:335:GLU:O	1:A:336:ASN:HB2	2.07	0.54
1:D:171:ASP:OD1	1:D:483:PRO:HG3	2.08	0.54
1:D:347:ARG:HH21	1:D:366:ASP:CG	2.11	0.54
1:E:391:PRO:HA	1:E:394:LEU:HD23	1.90	0.54
1:E:426:ASP:N	2:E:619:UMP:O2	2.39	0.54
1:E:479:ARG:HG2	1:E:512:TYR:CD2	2.43	0.54
1:A:465:ILE:HG21	1:A:473:LEU:HD23	1.90	0.54
1:C:94:LEU:HD12	1:C:97:SER:OG	2.08	0.54
1:C:389:TRP:CE3	1:C:401:PRO:HG2	2.43	0.54
1:D:104:ASP:O	1:D:106:SER:C	2.46	0.54
1:E:10:VAL:HG22	1:E:11:ALA:N	2.22	0.54
1:A:114:GLY:CA	1:A:119:TYR:CZ	2.91	0.53
4:A:605:DHF:C6	5:A:606:NDP:H42N	2.38	0.53
1:D:96:ASP:O	1:D:99:GLU:CB	2.55	0.53
1:C:123:LEU:HD12	1:C:128:VAL:CG1	2.38	0.53
1:C:225:ASN:O	1:C:226:THR:C	2.46	0.53
1:D:311:LYS:O	1:D:312:LYS:HB2	2.06	0.53
1:A:56:ARG:NH1	5:A:606:NDP:O3X	2.42	0.53
1:D:59:TRP:CE2	1:D:64:ARG:HG3	2.43	0.53
1:E:4:LYS:H	1:E:101:LEU:HD23	1.71	0.53
1:A:99:GLU:O	1:A:103:ASN:ND2	2.42	0.53
1:C:405:LEU:HD23	1:C:406:SER:N	2.23	0.53
1:A:207:PHE:O	1:A:210:ARG:HB2	2.08	0.53
1:D:296:ILE:O	1:D:300:LYS:HG2	2.08	0.53
1:E:82:ASP:OD2	1:E:84:ALA:HB3	2.09	0.53
1:B:479:ARG:HG2	1:B:512:TYR:CD2	2.43	0.53
1:D:147:PHE:HE1	1:D:150:ILE:HD11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLU:HB2	6:A:651:HOH:O	2.09	0.53
1:B:289:ARG:HG3	1:B:501:TRP:CE2	2.44	0.53
1:D:321:SER:O	1:D:325:LEU:HD13	2.08	0.53
1:E:103:ASN:CG	1:E:104:ASP:H	2.11	0.53
1:E:321:SER:O	1:E:325:LEU:HD13	2.09	0.53
1:E:427:LEU:HD23	1:E:464:HIS:O	2.08	0.53
1:B:4:LYS:HB2	1:B:101:LEU:HD23	1.88	0.53
1:B:171:ASP:OD2	1:B:483:PRO:HG3	2.08	0.53
1:C:220:LYS:O	1:C:223:ILE:HG13	2.09	0.53
1:E:260:ILE:HD12	1:E:260:ILE:H	1.71	0.53
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.90	0.53
1:C:405:LEU:C	1:C:405:LEU:CD2	2.69	0.53
1:A:472:GLN:OE1	1:A:472:GLN:N	2.38	0.52
1:D:133:LEU:HD13	1:D:135:ARG:HG3	1.90	0.52
1:A:99:GLU:C	1:A:99:GLU:OE1	2.47	0.52
1:C:137:ALA:O	1:C:510:TYR:HE2	1.92	0.52
1:A:104:ASP:HB3	1:A:107:ILE:HG12	1.90	0.52
1:C:10:VAL:HG22	1:C:11:ALA:N	2.24	0.52
1:C:113:CYS:HB3	4:C:613:DHF:H71	1.90	0.52
1:C:7:SER:CB	1:C:130:ARG:HB3	2.39	0.52
1:C:79:LEU:HD23	1:C:80:PRO:CD	2.39	0.52
1:D:260:ILE:HD12	1:D:260:ILE:H	1.72	0.52
1:D:467:GLU:HA	1:D:470:LEU:CD2	2.40	0.52
1:E:471:THR:HB	1:E:472:GLN:OE1	2.09	0.52
3:E:620:CB3:C6	3:E:620:CB3:C15	2.87	0.52
1:B:75:ILE:O	5:B:610:NDP:H1B	2.10	0.52
1:B:57:LYS:O	1:B:60:ASP:HB2	2.09	0.52
1:D:82:ASP:OD1	1:D:84:ALA:N	2.43	0.52
1:E:48:LYS:HB3	1:E:106:SER:O	2.10	0.52
1:A:3:GLU:HB2	1:A:101:LEU:HD22	1.91	0.52
1:C:384:HIS:HB2	1:C:408:TYR:O	2.09	0.52
1:D:247:VAL:HG12	1:D:265:ILE:HG12	1.91	0.52
1:E:30:SER:HB2	6:E:644:HOH:O	2.08	0.52
1:B:439:ALA:O	1:B:443:MET:HG3	2.10	0.51
1:E:12:ALA:HB2	1:E:19:ILE:HG22	1.91	0.51
1:E:100:ASN:OD1	1:E:100:ASN:N	2.36	0.51
1:C:40:THR:CG2	1:C:70:ARG:HH11	2.23	0.51
1:D:415:CYS:HA	1:D:452:GLU:O	2.10	0.51
1:E:85:ASP:OD1	1:E:86:PRO:HD2	2.11	0.51
1:E:133:LEU:HD22	1:E:134:THR:N	2.26	0.51
1:E:423:ARG:NH2	2:E:619:UMP:OP1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:LYS:CB	1:B:514:THR:HG22	2.33	0.51
1:C:10:VAL:HG11	1:C:147:PHE:CE2	2.45	0.51
1:E:60:ASP:OD1	1:E:64:ARG:NH1	2.41	0.51
1:E:126:ASN:OD1	1:E:177:LYS:HE3	2.10	0.51
1:E:348:HIS:HB3	1:E:363:VAL:O	2.10	0.51
1:C:89:VAL:HG12	1:C:90:VAL:N	2.26	0.51
1:A:104:ASP:C	1:A:106:SER:H	2.13	0.51
1:A:315:ILE:HB	3:A:604:CB3:C15	2.41	0.51
1:D:256:ASN:O	1:D:258:THR:O	2.29	0.51
1:A:360:TYR:O	1:A:363:VAL:CG1	2.58	0.51
1:A:397:MET:SD	1:A:401:PRO:HD3	2.50	0.51
1:C:113:CYS:O	4:C:613:DHF:H72	2.11	0.51
1:D:490:LYS:HD2	1:D:502:GLU:O	2.11	0.51
1:B:342:TYR:CZ	1:B:401:PRO:HA	2.46	0.51
1:C:320:GLY:O	1:C:335:GLU:O	2.28	0.51
1:E:195:SER:OG	1:E:196:ILE:HD11	2.07	0.51
1:A:82:ASP:O	1:A:84:ALA:N	2.40	0.51
1:C:233:ARG:NH1	1:C:242:ASP:OD1	2.43	0.51
1:B:12:ALA:HB1	1:B:17:SER:HA	1.92	0.50
1:C:431:SER:O	1:C:435:ILE:HG13	2.11	0.50
1:E:81:GLN:C	6:E:625:HOH:O	2.48	0.50
1:C:135:ARG:HD3	1:C:171:ASP:OD2	2.11	0.50
1:D:256:ASN:O	1:D:257:ARG:C	2.50	0.50
1:E:116:GLU:HB2	1:E:145:THR:HG23	1.93	0.50
1:E:360:TYR:O	1:E:361:THR:C	2.50	0.50
1:A:114:GLY:HA2	1:A:119:TYR:CE1	2.47	0.50
1:C:40:THR:HG21	1:C:70:ARG:NH1	2.23	0.50
1:E:315:ILE:HG13	1:E:316:TRP:N	2.27	0.50
1:E:488:LYS:CD	1:E:489:PHE:H	2.20	0.50
1:C:151:PRO:HG2	1:C:154:PHE:HD2	1.76	0.50
1:A:383:ARG:CZ	1:B:400:PRO:HG2	2.41	0.50
1:C:212:MET:SD	1:D:273:ASP:HB2	2.51	0.50
1:A:323:GLU:N	1:A:323:GLU:OE1	2.44	0.50
1:E:4:LYS:HG2	1:E:101:LEU:CD2	2.42	0.50
1:D:19:ILE:HB	5:D:618:NDP:N7N	2.27	0.50
1:D:93:ASN:ND2	1:D:96:ASP:OD2	2.39	0.50
1:D:472:GLN:O	1:D:475:GLU:HB3	2.12	0.50
1:D:476:GLN:O	1:D:479:ARG:HG2	2.12	0.50
1:B:95:GLU:HG3	1:B:127:PHE:HZ	1.77	0.50
1:C:38:LYS:HB3	1:D:202:LEU:HG	1.92	0.50
1:E:347:ARG:HB2	1:E:348:HIS:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:PRO:HG2	1:A:423:ARG:NH2	2.26	0.49
1:B:3:GLU:OE2	1:B:3:GLU:HA	2.11	0.49
1:C:62:ILE:HD11	1:C:67:LEU:HD11	1.94	0.49
1:C:134:THR:HA	1:C:171:ASP:O	2.12	0.49
1:C:491:ARG:NH1	1:C:503:ASP:OD1	2.45	0.49
1:D:10:VAL:HG13	1:D:133:LEU:HD23	1.94	0.49
1:E:303:THR:HG21	1:E:344:PHE:HB2	1.92	0.49
1:B:10:VAL:HG22	1:B:11:ALA:N	2.28	0.49
1:B:193:LEU:HD22	1:B:194:LYS:HG2	1.94	0.49
1:B:400:PRO:HB2	1:B:423:ARG:NH2	2.28	0.49
1:C:509:TYR:CE1	1:C:511:PRO:HG3	2.47	0.49
1:C:512:TYR:HB3	1:C:513:PRO:HD2	1.95	0.49
1:E:307:HIS:O	1:E:311:LYS:HD2	2.13	0.49
1:A:330:LEU:O	1:A:332:HIS:N	2.46	0.49
1:C:26:PRO:HG2	1:C:143:PHE:HE1	1.77	0.49
1:D:297:TRP:CD1	1:D:302:ASP:HB3	2.47	0.49
1:D:495:ASN:HB2	6:D:650:HOH:O	2.12	0.49
1:E:193:LEU:HD12	1:E:194:LYS:HD3	1.94	0.49
1:E:422:GLN:CD	1:E:425:CYS:HB2	2.33	0.49
1:E:431:SER:O	1:E:435:ILE:HG13	2.12	0.49
1:B:224:TYR:O	1:B:227:PRO:HD3	2.13	0.49
1:B:285:LYS:HD3	1:B:514:THR:CG2	2.42	0.49
1:D:82:ASP:OD1	1:D:84:ALA:HB2	2.11	0.49
1:E:430:GLY:HA3	3:E:620:CB3:HP3	1.94	0.49
4:C:613:DHF:HG2	4:C:613:DHF:O1	2.11	0.49
1:B:292:PHE:C	1:B:292:PHE:CD2	2.85	0.49
1:C:123:LEU:CD1	1:C:128:VAL:HG11	2.39	0.49
1:C:360:TYR:C	1:C:363:VAL:HG13	2.32	0.49
1:D:62:ILE:CG2	1:D:62:ILE:O	2.60	0.49
1:D:288:ILE:HA	1:D:291:ILE:HD12	1.94	0.49
1:E:98:ILE:HG22	1:E:98:ILE:O	2.11	0.49
1:A:233:ARG:NH1	1:A:242:ASP:OD2	2.44	0.49
2:A:603:UMP:P	1:B:383:ARG:HH11	2.36	0.49
1:C:405:LEU:HD23	1:C:405:LEU:O	2.11	0.49
1:A:7:SER:HB3	1:A:130:ARG:HB3	1.94	0.49
1:A:271:ARG:HG2	1:B:212:MET:HE1	1.95	0.49
1:B:257:ARG:NH2	1:B:521:VAL:OXT	2.46	0.49
1:A:271:ARG:NH1	6:A:666:HOH:O	2.45	0.48
1:A:287:PHE:HB2	6:A:712:HOH:O	2.12	0.48
1:D:94:LEU:O	1:D:97:SER:OG	2.28	0.48
1:D:403:HIS:O	1:D:403:HIS:ND1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:VAL:HG23	1:E:15:LEU:N	2.28	0.48
1:A:269:MET:HE1	1:B:269:MET:HG2	1.94	0.48
1:B:52:LEU:HD13	1:B:113:CYS:SG	2.53	0.48
1:C:32:ASP:O	1:C:35:PHE:HB3	2.14	0.48
1:C:370:LYS:HA	1:C:373:GLU:CG	2.41	0.48
1:E:54:MET:CE	1:E:72:ILE:HG23	2.44	0.48
1:B:411:THR:HG21	1:B:413:ASP:CB	2.42	0.48
1:C:130:ARG:HG3	1:C:130:ARG:HH11	1.79	0.48
1:C:243:LEU:HD11	1:C:268:GLN:HG3	1.94	0.48
1:E:241:LEU:CD1	1:E:481:PRO:HG3	2.42	0.48
1:E:390:ASN:O	1:E:394:LEU:HD22	2.13	0.48
1:E:472:GLN:OE1	1:E:472:GLN:N	2.46	0.48
1:A:100:ASN:O	1:A:103:ASN:O	2.31	0.48
1:A:339:GLY:HA2	1:A:353:TYR:CE2	2.48	0.48
4:A:605:DHF:H72	5:A:606:NDP:H42N	1.95	0.48
1:C:429:LEU:HD22	1:C:469:HIS:CE1	2.48	0.48
1:E:59:TRP:CD1	1:E:64:ARG:HG2	2.47	0.48
1:B:403:HIS:HB2	1:B:420:LEU:HD11	1.96	0.48
1:D:59:TRP:NE1	1:D:64:ARG:HG3	2.28	0.48
1:A:114:GLY:CA	1:A:119:TYR:CE1	2.97	0.48
1:A:291:ILE:HD13	1:A:436:ALA:HB3	1.94	0.48
1:C:85:ASP:OD2	1:C:86:PRO:HD2	2.14	0.48
1:D:67:LEU:HD22	4:D:617:DHF:CT	2.44	0.48
1:A:93:ASN:ND2	1:A:96:ASP:H	2.11	0.48
3:B:608:CB3:C14	3:B:608:CB3:C5	2.91	0.48
1:D:37:SER:O	1:D:41:ASN:HB2	2.14	0.48
1:E:77:SER:O	1:E:92:ARG:NH1	2.46	0.48
1:A:360:TYR:O	1:A:363:VAL:HG12	2.13	0.48
4:A:605:DHF:O	4:A:605:DHF:HB1	2.12	0.48
1:B:193:LEU:CD2	1:B:194:LYS:HG2	2.43	0.48
1:B:247:VAL:HG22	1:B:465:ILE:HD12	1.95	0.48
1:B:447:GLN:NE2	1:B:492:LYS:HA	2.28	0.48
1:C:389:TRP:HE3	1:C:401:PRO:HG2	1.78	0.48
1:D:3:GLU:N	1:D:101:LEU:HD22	2.29	0.48
1:D:36:PHE:O	1:D:40:THR:HG23	2.14	0.48
1:E:333:ARG:HG2	1:E:333:ARG:HH11	1.79	0.48
1:E:431:SER:HB3	1:E:432:PRO:HD3	1.95	0.48
1:E:470:LEU:O	1:E:474:LYS:HG3	2.14	0.48
1:E:520:ALA:O	1:E:521:VAL:C	2.52	0.48
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.96	0.48
1:D:7:SER:O	1:D:111:PHE:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:ARG:HD2	1:D:173:MET:SD	2.54	0.48
1:E:104:ASP:O	1:E:107:ILE:N	2.35	0.48
1:C:434:ASN:OD1	3:C:612:CB3:HP3	2.14	0.47
1:E:255:GLU:CD	1:E:255:GLU:H	2.17	0.47
1:A:333:ARG:HG2	1:A:337:ASP:HB3	1.96	0.47
4:A:605:DHF:C7	5:A:606:NDP:H42N	2.44	0.47
1:C:225:ASN:OD1	1:C:238:PHE:HE1	1.97	0.47
1:D:431:SER:HB3	1:D:432:PRO:HD3	1.97	0.47
1:D:78:SER:N	1:D:92:ARG:HH12	2.13	0.47
1:E:196:ILE:N	1:E:196:ILE:CD1	2.31	0.47
1:E:254:ARG:HD2	1:E:264:SER:CB	2.45	0.47
1:E:340:PRO:HD3	1:E:353:TYR:CD2	2.49	0.47
1:A:123:LEU:HD23	1:A:128:VAL:CG1	2.44	0.47
1:E:406:SER:HG	1:E:438:TYR:HE1	1.58	0.47
1:A:3:GLU:CB	1:A:101:LEU:HD22	2.45	0.47
1:C:18:GLY:HA3	1:C:143:PHE:CD1	2.50	0.47
1:D:98:ILE:HG22	1:D:101:LEU:HD12	1.97	0.47
1:D:226:THR:N	1:D:227:PRO:HD3	2.29	0.47
1:D:295:LEU:O	1:D:299:ILE:HG13	2.15	0.47
1:A:34:LYS:HB3	1:B:206:ILE:HG12	1.96	0.47
1:A:315:ILE:HG13	1:A:316:TRP:CD1	2.49	0.47
1:A:342:TYR:CE2	1:A:403:HIS:CE1	3.02	0.47
1:C:97:SER:O	1:C:100:ASN:OD1	2.32	0.47
1:D:209:ILE:O	1:D:209:ILE:HG22	2.14	0.47
1:E:55:GLY:HA3	5:E:622:NDP:O5B	2.15	0.47
1:E:104:ASP:C	1:E:106:SER:N	2.66	0.47
1:E:159:MET:SD	1:E:235:HIS:HD2	2.36	0.47
1:E:425:CYS:HA	2:E:619:UMP:O2	2.14	0.47
1:B:349:TYR:O	1:B:350:ASN:HB2	2.15	0.47
1:C:234:GLU:OE2	1:D:211:LYS:NZ	2.48	0.47
1:D:341:ILE:O	1:D:342:TYR:C	2.52	0.47
1:A:104:ASP:C	1:A:106:SER:N	2.68	0.47
1:C:135:ARG:HD3	1:C:171:ASP:HB3	1.97	0.47
1:B:297:TRP:CH2	1:B:338:LEU:HD12	2.45	0.47
1:D:248:LEU:HD13	1:D:465:ILE:HD12	1.96	0.46
1:D:360:TYR:HD1	1:D:363:VAL:HG11	1.81	0.46
1:A:130:ARG:NH1	1:A:176:GLU:OE2	2.42	0.46
1:A:423:ARG:HG3	1:A:424:SER:N	2.31	0.46
1:B:423:ARG:HG3	1:B:424:SER:N	2.31	0.46
1:C:96:ASP:O	1:C:98:ILE:O	2.33	0.46
1:C:512:TYR:HB3	1:C:513:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:622:NDP:O1X	5:E:622:NDP:O3B	2.30	0.46
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.80	0.46
1:B:385:ILE:CG2	1:B:386:LEU:N	2.78	0.46
1:B:502:GLU:H	1:B:502:GLU:CD	2.19	0.46
1:C:222:GLU:CD	1:C:222:GLU:H	2.19	0.46
1:C:273:ASP:HB2	1:D:212:MET:SD	2.55	0.46
1:E:195:SER:CB	1:E:196:ILE:HD12	2.44	0.46
1:E:342:TYR:CD1	1:E:403:HIS:CE1	3.03	0.46
1:E:493:VAL:HG21	1:E:499:PHE:CE1	2.50	0.46
1:E:423:ARG:NH1	1:E:424:SER:HB2	2.30	0.46
1:B:114:GLY:HA2	1:B:119:TYR:CE1	2.50	0.46
1:B:164:CYS:HB2	1:B:486:GLN:NE2	2.30	0.46
1:E:347:ARG:O	1:E:366:ASP:CA	2.64	0.46
1:A:455:GLU:OE2	1:B:215:ARG:NH2	2.48	0.46
1:C:75:ILE:CG2	5:C:614:NDP:C4A	2.94	0.46
1:E:113:CYS:O	4:E:621:DHF:H72	2.15	0.46
1:A:52:LEU:HD13	1:A:113:CYS:SG	2.56	0.46
3:D:616:CB3:H5	3:D:616:CB3:C14	2.46	0.46
1:E:120:ARG:HG2	1:E:148:PRO:HB3	1.97	0.46
1:E:516:LYS:HD2	1:E:516:LYS:N	2.31	0.46
1:A:102:MET:CE	6:A:618:HOH:O	2.64	0.46
1:B:237:GLU:HB2	1:B:484:PHE:CZ	2.50	0.46
1:D:102:MET:HE2	1:D:102:MET:HB3	1.59	0.46
1:D:340:PRO:HD3	1:D:353:TYR:CD2	2.50	0.46
1:A:160:SER:HA	1:A:234:GLU:HB3	1.98	0.45
1:C:248:LEU:HD12	1:C:248:LEU:HA	1.84	0.45
1:C:404:VAL:HG11	1:D:405:LEU:CD1	2.46	0.45
1:E:105:ASP:N	1:E:105:ASP:OD1	2.48	0.45
1:C:172:PHE:CE2	1:D:203:LEU:HD11	2.51	0.45
1:C:203:LEU:HD11	1:D:172:PHE:CE2	2.50	0.45
1:C:335:GLU:O	1:C:335:GLU:HG3	2.16	0.45
1:D:247:VAL:HG21	1:D:465:ILE:HG13	1.98	0.45
3:D:616:CB3:C14	3:D:616:CB3:C5	2.94	0.45
1:E:305:GLY:O	1:E:309:ILE:HG12	2.15	0.45
1:E:516:LYS:CD	1:E:516:LYS:N	2.77	0.45
1:A:99:GLU:H	1:A:101:LEU:H	1.64	0.45
1:B:180:LYS:O	1:B:181:LYS:CB	2.64	0.45
1:C:289:ARG:NH2	1:C:311:LYS:O	2.48	0.45
1:C:293:GLU:HG3	6:C:622:HOH:O	2.15	0.45
1:C:402:CYS:SG	2:C:611:UMP:H5"	2.57	0.45
1:C:479:ARG:NH2	1:C:513:PRO:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ILE:O	5:D:618:NDP:H2N	2.17	0.45
1:D:342:TYR:CZ	1:D:403:HIS:NE2	2.84	0.45
1:E:13:SER:HA	1:E:136:VAL:O	2.17	0.45
1:E:147:PHE:CD2	1:E:148:PRO:HD2	2.50	0.45
3:E:620:CB3:C5	3:E:620:CB3:C14	2.93	0.45
1:A:344:PHE:O	1:A:348:HIS:N	2.45	0.45
1:A:233:ARG:NH1	1:A:242:ASP:CG	2.69	0.45
1:A:345:GLN:OE1	1:A:349:TYR:CD1	2.70	0.45
1:A:429:LEU:HD11	1:A:517:MET:HB2	1.97	0.45
1:E:199:THR:O	1:E:203:LEU:HB2	2.17	0.45
1:A:43:LYS:HB2	1:A:108:GLU:OE1	2.16	0.45
1:B:139:GLU:O	1:B:140:ASP:HB2	2.16	0.45
1:E:247:VAL:HG22	1:E:265:ILE:HG12	1.99	0.45
1:B:56:ARG:HD3	5:B:610:NDP:O1X	2.17	0.45
4:B:609:DHF:O	4:B:609:DHF:CB	2.64	0.45
1:C:269:MET:HB3	1:D:269:MET:HE2	1.99	0.45
1:D:149:GLU:CD	1:D:149:GLU:N	2.67	0.45
1:A:288:ILE:HG23	1:A:501:TRP:CH2	2.52	0.45
1:D:62:ILE:O	1:D:62:ILE:HG23	2.17	0.45
1:D:178:GLN:OE1	1:D:178:GLN:CA	2.61	0.45
1:D:293:GLU:HA	1:D:296:ILE:HD11	1.99	0.45
1:D:296:ILE:HD12	1:D:297:TRP:H	1.80	0.45
1:B:102:MET:O	1:B:103:ASN:HB3	2.17	0.45
1:B:7:SER:O	1:B:111:PHE:HA	2.17	0.45
1:E:114:GLY:HA2	1:E:119:TYR:CE2	2.52	0.45
1:C:40:THR:CG2	1:C:70:ARG:CD	2.90	0.44
1:C:54:MET:HE3	1:C:72:ILE:CG2	2.42	0.44
1:C:237:GLU:O	1:C:237:GLU:HG3	2.18	0.44
1:D:155:LEU:HB2	1:D:178:GLN:NE2	2.32	0.44
1:D:298:PHE:CE1	1:D:342:TYR:HB2	2.52	0.44
1:D:403:HIS:HB2	1:D:420:LEU:HD11	1.99	0.44
1:E:123:LEU:N	1:E:123:LEU:HD22	2.33	0.44
1:E:246:ARG:NH1	1:E:268:GLN:OE1	2.50	0.44
1:E:402:CYS:O	1:E:404:VAL:HG23	2.17	0.44
1:B:113:CYS:O	4:B:609:DHF:H72	2.17	0.44
1:D:133:LEU:HD22	1:D:134:THR:N	2.33	0.44
1:D:292:PHE:CD1	1:D:504:ILE:HD11	2.52	0.44
1:E:123:LEU:HD13	1:E:128:VAL:HG11	2.00	0.44
1:D:125:ASP:HB2	1:D:127:PHE:CE1	2.52	0.44
1:E:56:ARG:O	1:E:59:TRP:HB3	2.17	0.44
1:E:103:ASN:O	1:E:104:ASP:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:390:ASN:O	1:E:394:LEU:CD2	2.66	0.44
4:E:621:DHF:H72	5:E:622:NDP:C4N	2.46	0.44
1:A:43:LYS:NZ	1:A:48:LYS:O	2.35	0.44
1:A:294:GLU:O	1:A:297:TRP:HB3	2.17	0.44
1:C:151:PRO:HG2	1:C:154:PHE:CD2	2.53	0.44
1:E:137:ALA:O	1:E:510:TYR:HE2	1.99	0.44
1:E:155:LEU:HB2	1:E:178:GLN:NE2	2.33	0.44
1:E:258:THR:HG21	1:E:520:ALA:HB1	1.99	0.44
1:A:171:ASP:OD2	1:A:483:PRO:HG3	2.16	0.44
1:B:487:LEU:HD23	1:B:487:LEU:C	2.37	0.44
1:C:402:CYS:SG	1:C:424:SER:HB3	2.58	0.44
1:D:296:ILE:H	1:D:296:ILE:HG13	1.66	0.44
1:D:467:GLU:O	1:D:470:LEU:HD23	2.18	0.44
1:D:500:LYS:O	1:D:503:ASP:HB2	2.16	0.44
1:A:264:SER:HB2	1:A:462:ASP:OD1	2.17	0.44
1:B:397:MET:SD	1:B:401:PRO:HD3	2.57	0.44
1:C:130:ARG:HD2	1:C:132:TYR:CE1	2.53	0.44
1:C:271:ARG:NH2	1:D:267:GLY:O	2.48	0.44
1:C:383:ARG:CZ	1:D:400:PRO:HG3	2.48	0.44
1:C:485:PRO:HB3	1:C:509:TYR:CA	2.48	0.44
4:D:617:DHF:C7	5:D:618:NDP:H42N	2.48	0.44
1:A:117:SER:OG	5:A:606:NDP:O1A	2.24	0.44
1:B:209:ILE:CD1	1:B:209:ILE:N	2.68	0.44
1:C:4:LYS:HE3	1:C:107:ILE:O	2.18	0.44
1:C:6:VAL:HG11	1:C:127:PHE:O	2.18	0.44
1:C:465:ILE:CG2	1:C:473:LEU:HD12	2.48	0.44
1:D:58:THR:OG1	5:D:618:NDP:H6N	2.17	0.44
1:D:99:GLU:OE2	1:D:99:GLU:O	2.35	0.44
1:E:330:LEU:C	1:E:332:HIS:N	2.69	0.44
3:A:604:CB3:C5	3:A:604:CB3:C14	2.93	0.44
1:B:95:GLU:HB2	6:B:666:HOH:O	2.18	0.44
1:B:171:ASP:CG	1:B:483:PRO:HG3	2.37	0.44
1:C:14:VAL:HG13	1:C:15:LEU:N	2.32	0.44
1:D:389:TRP:HE3	1:D:401:PRO:HG2	1.83	0.44
1:A:93:ASN:HD21	1:A:95:GLU:HB3	1.81	0.44
1:B:96:ASP:O	1:B:99:GLU:HB2	2.17	0.44
1:B:222:GLU:OE1	1:B:222:GLU:N	2.49	0.44
1:C:304:ASN:OD1	1:C:306:ASN:HB2	2.18	0.44
1:D:12:ALA:HB2	1:D:19:ILE:HG22	1.99	0.44
1:D:49:LYS:O	1:D:107:ILE:HA	2.18	0.44
1:D:288:ILE:O	1:D:291:ILE:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:ILE:HA	1:E:151:PRO:HD3	1.82	0.44
1:E:281:LEU:HD12	1:E:432:PRO:HB3	2.00	0.44
1:A:123:LEU:HD23	1:A:128:VAL:HG13	2.00	0.43
1:A:246:ARG:NH1	1:A:268:GLN:OE1	2.47	0.43
1:A:258:THR:HG21	1:A:260:ILE:HB	2.00	0.43
1:A:264:SER:OG	1:B:409:TYR:OH	2.25	0.43
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.83	0.43
3:C:612:CB3:C5	3:C:612:CB3:C14	2.93	0.43
1:D:335:GLU:O	1:D:336:ASN:HB2	2.17	0.43
1:A:330:LEU:C	1:A:332:HIS:N	2.66	0.43
1:A:396:GLN:HG3	6:A:668:HOH:O	2.16	0.43
1:B:400:PRO:HB2	1:B:423:ARG:HH21	1.82	0.43
1:C:172:PHE:CD2	1:D:203:LEU:HD21	2.53	0.43
1:D:466:TYR:HE2	2:D:615:UMP:O3'	1.99	0.43
1:D:220:LYS:HE2	1:D:220:LYS:HB2	1.68	0.43
1:D:260:ILE:N	1:D:260:ILE:CD1	2.74	0.43
1:D:400:PRO:HG2	1:D:423:ARG:NH2	2.32	0.43
1:E:303:THR:CG2	1:E:344:PHE:HB2	2.47	0.43
1:E:333:ARG:HG2	1:E:333:ARG:NH1	2.34	0.43
1:C:471:THR:HG23	6:C:651:HOH:O	2.18	0.43
1:D:14:VAL:HG13	1:D:15:LEU:N	2.33	0.43
1:D:62:ILE:HD13	1:D:62:ILE:HA	1.67	0.43
1:E:255:GLU:CD	1:E:255:GLU:N	2.70	0.43
1:E:330:LEU:HD23	1:E:332:HIS:HE1	1.83	0.43
1:E:464:HIS:CD2	1:E:466:TYR:CE2	3.07	0.43
1:A:462:ASP:OD2	1:B:382:ARG:HG2	2.19	0.43
1:B:51:ALA:C	1:B:52:LEU:HD23	2.39	0.43
1:C:81:GLN:HE22	1:C:92:ARG:HH21	1.67	0.43
1:C:472:GLN:O	1:C:475:GLU:HB3	2.18	0.43
1:D:336:ASN:O	1:D:356:MET:CE	2.66	0.43
1:E:352:GLU:HA	1:E:352:GLU:OE2	2.19	0.43
1:C:62:ILE:O	1:C:62:ILE:HG23	2.17	0.43
1:C:243:LEU:CD1	1:C:268:GLN:HG3	2.48	0.43
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.87	0.43
1:C:63:GLY:O	1:C:65:ARG:HG2	2.18	0.43
1:C:246:ARG:NH1	1:C:268:GLN:OE1	2.45	0.43
1:C:262:THR:HG22	1:C:466:TYR:HA	1.99	0.43
1:D:137:ALA:O	1:D:510:TYR:HE2	2.02	0.43
1:E:502:GLU:CD	1:E:502:GLU:H	2.21	0.43
1:C:12:ALA:HB2	1:C:19:ILE:HG22	2.01	0.43
1:C:178:GLN:OE1	1:C:178:GLN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:TYR:O	1:C:227:PRO:HG3	2.19	0.43
1:D:56:ARG:O	1:D:59:TRP:HB3	2.19	0.43
1:D:242:ASP:O	1:D:246:ARG:HB2	2.19	0.43
1:D:256:ASN:O	1:D:258:THR:N	2.52	0.43
1:D:355:THR:OG1	1:D:358:ASP:OD1	2.29	0.43
1:E:7:SER:O	1:E:111:PHE:HA	2.19	0.43
1:A:479:ARG:HG2	1:A:512:TYR:CD2	2.54	0.43
1:A:509:TYR:HA	6:A:667:HOH:O	2.18	0.43
1:B:52:LEU:HD23	1:B:52:LEU:N	2.34	0.43
1:C:15:LEU:HB2	1:C:139:GLU:CD	2.39	0.43
1:D:429:LEU:HB3	3:D:616:CB3:O4	2.18	0.43
1:D:430:GLY:CA	3:D:616:CB3:HP3	2.49	0.43
1:E:178:GLN:OE1	1:E:178:GLN:CA	2.30	0.43
1:A:386:LEU:O	1:A:405:LEU:HA	2.18	0.43
1:A:415:CYS:HA	1:A:452:GLU:O	2.19	0.43
1:C:402:CYS:SG	2:C:611:UMP:H2'	2.58	0.43
1:D:430:GLY:CA	3:D:616:CB3:CP3	2.96	0.43
1:E:123:LEU:HD13	1:E:128:VAL:CG1	2.49	0.43
1:A:273:ASP:HB2	1:B:212:MET:SD	2.58	0.42
1:B:4:LYS:HD2	1:B:101:LEU:HA	2.01	0.42
1:C:193:LEU:HD12	6:C:626:HOH:O	2.19	0.42
1:E:98:ILE:N	1:E:98:ILE:HD12	2.33	0.42
1:E:295:LEU:HD22	1:E:299:ILE:HD11	2.00	0.42
1:E:360:TYR:HB3	1:E:363:VAL:CG1	2.47	0.42
1:B:166:LYS:O	1:B:167:ASN:HB2	2.19	0.42
1:B:452:GLU:OE2	1:B:452:GLU:HA	2.19	0.42
1:D:122:ALA:O	1:D:127:PHE:HB2	2.19	0.42
1:E:155:LEU:HG	1:E:178:GLN:HE21	1.83	0.42
1:E:337:ASP:N	1:E:356:MET:HE3	2.35	0.42
1:A:33:LEU:HB3	4:A:605:DHF:HG1	2.01	0.42
1:A:425:CYS:SG	1:A:431:SER:HB2	2.59	0.42
1:B:4:LYS:CB	1:B:101:LEU:HD23	2.49	0.42
1:B:335:GLU:O	1:B:336:ASN:HB2	2.19	0.42
1:C:140:ASP:N	1:C:141:ILE:HG23	2.34	0.42
4:C:613:DHF:H91	5:C:614:NDP:C5N	2.49	0.42
1:D:244:LEU:O	1:D:247:VAL:HG22	2.19	0.42
2:D:615:UMP:C4	3:D:616:CB3:CP3	3.02	0.42
1:E:225:ASN:HB2	1:E:477:LEU:HD23	2.01	0.42
1:E:272:PHE:HB2	1:E:456:LEU:HB3	2.01	0.42
1:B:150:ILE:HA	1:B:151:PRO:HD3	1.83	0.42
1:B:207:PHE:O	1:B:210:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:LEU:O	1:B:247:VAL:HG12	2.19	0.42
1:C:104:ASP:O	1:C:106:SER:N	2.52	0.42
1:D:94:LEU:O	1:D:95:GLU:C	2.58	0.42
1:D:349:TYR:O	1:D:350:ASN:HB2	2.18	0.42
1:E:400:PRO:HA	1:E:401:PRO:HD3	1.94	0.42
1:E:520:ALA:HB3	3:E:620:CB3:HN21	1.84	0.42
1:B:70:ARG:NH1	4:B:609:DHF:O2	2.42	0.42
1:B:426:ASP:OD2	1:B:426:ASP:C	2.58	0.42
1:E:10:VAL:CG2	1:E:11:ALA:N	2.83	0.42
1:E:76:SER:OG	1:E:79:LEU:HB2	2.19	0.42
1:A:81:GLN:HA	6:A:659:HOH:O	2.19	0.42
1:A:193:LEU:HD22	1:A:195:SER:H	1.85	0.42
1:C:18:GLY:HA3	1:C:143:PHE:CG	2.55	0.42
1:C:155:LEU:HD12	1:C:178:GLN:HE21	1.84	0.42
1:C:459:PHE:CD2	1:D:459:PHE:CD2	3.08	0.42
1:E:133:LEU:HD13	1:E:135:ARG:HG3	2.00	0.42
1:A:10:VAL:HG22	1:A:11:ALA:N	2.35	0.42
1:A:472:GLN:O	1:A:475:GLU:HB3	2.19	0.42
1:B:272:PHE:CZ	1:B:435:ILE:HD13	2.54	0.42
1:C:10:VAL:CG2	1:C:11:ALA:N	2.82	0.42
1:C:48:LYS:HE2	1:C:105:ASP:O	2.20	0.42
1:D:330:LEU:C	1:D:332:HIS:H	2.23	0.42
1:A:430:GLY:O	1:A:433:PHE:N	2.49	0.42
1:C:35:PHE:HA	1:D:206:ILE:HD11	2.01	0.42
1:D:53:ILE:HG23	1:D:75:ILE:HD13	2.02	0.42
1:E:313:VAL:HG12	1:E:315:ILE:HG12	2.01	0.42
1:A:12:ALA:HB1	1:A:17:SER:HA	2.01	0.42
1:A:413:ASP:O	1:A:414:ASN:HB2	2.19	0.42
1:E:104:ASP:C	1:E:106:SER:H	2.22	0.42
1:E:114:GLY:HA3	5:E:622:NDP:H5N	2.02	0.42
1:A:212:MET:SD	1:B:273:ASP:HB2	2.59	0.42
1:C:45:ASP:OD2	1:C:48:LYS:HE3	2.20	0.42
5:C:614:NDP:O2N	5:C:614:NDP:O1A	2.38	0.42
1:D:107:ILE:HG22	1:D:107:ILE:O	2.18	0.42
1:D:429:LEU:HD12	1:D:429:LEU:HA	1.82	0.42
1:E:85:ASP:OD1	1:E:86:PRO:CD	2.68	0.42
1:E:254:ARG:HD2	1:E:264:SER:HB2	2.02	0.42
1:E:349:TYR:HB3	1:E:365:VAL:HB	2.02	0.42
1:A:104:ASP:OD2	1:A:106:SER:OG	2.38	0.41
1:A:469:HIS:HB3	1:A:473:LEU:HD22	2.01	0.41
1:B:135:ARG:NH1	1:B:171:ASP:OD2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:609:DHF:H72	5:B:610:NDP:C5N	2.50	0.41
1:C:193:LEU:CD1	6:C:626:HOH:O	2.67	0.41
1:C:226:THR:N	1:C:227:PRO:HD3	2.35	0.41
1:D:96:ASP:O	1:D:98:ILE:O	2.37	0.41
1:A:345:GLN:O	1:A:349:TYR:HB2	2.20	0.41
1:C:203:LEU:HD12	1:C:203:LEU:HA	1.91	0.41
1:C:323:GLU:CD	1:C:323:GLU:N	2.70	0.41
1:C:485:PRO:HB3	1:C:509:TYR:HA	2.01	0.41
1:D:114:GLY:HA3	1:D:119:TYR:CE1	2.55	0.41
1:D:193:LEU:HG	1:D:195:SER:CB	2.50	0.41
1:D:203:LEU:HD12	1:D:203:LEU:HA	1.96	0.41
1:D:333:ARG:HD3	1:D:337:ASP:O	2.20	0.41
1:E:348:HIS:CD2	1:E:348:HIS:N	2.88	0.41
1:A:256:ASN:HD21	1:A:262:THR:HG23	1.84	0.41
1:A:360:TYR:HB3	1:A:363:VAL:HG13	2.02	0.41
1:B:99:GLU:OE1	1:B:99:GLU:CA	2.68	0.41
1:B:389:TRP:HE3	1:B:401:PRO:HG2	1.84	0.41
1:C:371:LEU:HD22	1:C:375:LEU:HG	2.01	0.41
1:D:10:VAL:HG22	1:D:11:ALA:N	2.35	0.41
1:E:297:TRP:NE1	1:E:302:ASP:HB3	2.35	0.41
1:C:41:ASN:HD21	1:C:69:ASN:HB2	1.86	0.41
1:C:41:ASN:ND2	1:C:69:ASN:HB2	2.35	0.41
1:C:431:SER:HB3	1:C:432:PRO:HD3	2.02	0.41
1:D:139:GLU:O	1:D:140:ASP:HB2	2.19	0.41
1:E:499:PHE:O	1:E:500:LYS:HE3	2.20	0.41
1:A:93:ASN:HD21	1:A:96:ASP:H	1.68	0.41
1:B:4:LYS:HB2	1:B:101:LEU:HD22	1.98	0.41
1:B:128:VAL:HG22	1:B:154:PHE:HZ	1.85	0.41
1:B:402:CYS:SG	2:B:607:UMP:H2'	2.61	0.41
1:E:107:ILE:O	1:E:107:ILE:HG22	2.21	0.41
1:E:126:ASN:OD1	1:E:177:LYS:CE	2.69	0.41
1:A:267:GLY:O	1:B:271:ARG:NH2	2.49	0.41
1:A:319:ASN:OD1	3:A:604:CB3:H8	2.20	0.41
1:A:383:ARG:CD	1:B:400:PRO:HG2	2.50	0.41
1:D:3:GLU:CA	1:D:101:LEU:CD2	2.98	0.41
1:A:215:ARG:NH2	6:A:687:HOH:O	2.54	0.41
1:A:383:ARG:HD3	1:B:400:PRO:HG2	2.02	0.41
1:E:166:LYS:O	1:E:167:ASN:HB2	2.20	0.41
1:E:425:CYS:SG	1:E:431:SER:HB2	2.61	0.41
1:E:430:GLY:C	3:E:620:CB3:HP3	2.41	0.41
1:B:288:ILE:HG23	1:B:501:TRP:HH2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLU:OE2	3:B:608:CB3:HP11	2.20	0.41
1:B:389:TRP:CE3	1:B:401:PRO:HG2	2.55	0.41
1:C:247:VAL:HG22	1:C:465:ILE:HD12	2.03	0.41
4:C:613:DHF:C6	4:C:613:DHF:H15	2.50	0.41
1:E:85:ASP:OD1	1:E:85:ASP:C	2.58	0.41
1:E:315:ILE:HG13	1:E:316:TRP:H	1.85	0.41
1:E:342:TYR:CE1	1:E:403:HIS:CE1	3.08	0.41
1:A:465:ILE:CG2	1:A:473:LEU:HD23	2.51	0.41
1:B:271:ARG:HD2	6:B:731:HOH:O	2.20	0.41
1:B:411:THR:HG22	1:B:413:ASP:CA	2.51	0.41
1:C:3:GLU:HA	1:C:3:GLU:OE2	2.20	0.41
1:C:8:ILE:CG2	1:C:9:VAL:N	2.83	0.41
1:C:491:ARG:NH2	1:C:493:VAL:HG12	2.35	0.41
1:D:51:ALA:C	1:D:52:LEU:HD23	2.41	0.41
1:D:102:MET:O	1:D:103:ASN:HB2	2.21	0.41
1:D:278:PHE:CE1	1:D:439:ALA:HB3	2.55	0.41
1:E:7:SER:CB	1:E:130:ARG:HB3	2.50	0.41
1:E:158:TYR:O	1:E:173:MET:HA	2.21	0.41
1:E:288:ILE:HD11	1:E:440:ILE:HD11	2.03	0.41
1:A:3:GLU:HB2	1:A:4:LYS:H	1.77	0.41
1:A:337:ASP:C	1:A:337:ASP:OD2	2.59	0.41
4:B:609:DHF:C6	4:B:609:DHF:H15	2.50	0.41
1:C:322:LYS:HD3	1:C:335:GLU:OE1	2.21	0.41
1:E:220:LYS:O	1:E:223:ILE:HG12	2.21	0.41
1:E:488:LYS:CD	1:E:489:PHE:N	2.82	0.41
1:A:82:ASP:C	1:A:84:ALA:H	2.22	0.40
1:A:212:MET:HB3	1:B:236:TYR:OH	2.21	0.40
6:A:622:HOH:O	1:B:211:LYS:HG2	2.20	0.40
1:B:252:ALA:O	1:B:263:TYR:HA	2.21	0.40
1:D:363:VAL:CG2	6:D:625:HOH:O	2.69	0.40
1:A:150:ILE:HA	1:A:151:PRO:HD3	1.89	0.40
1:B:135:ARG:HB2	1:B:171:ASP:HB2	2.04	0.40
1:B:379:PRO:CB	1:B:410:VAL:HG21	2.51	0.40
1:D:248:LEU:HD12	1:D:248:LEU:HA	1.86	0.40
1:D:266:PHE:HA	1:D:461:GLY:O	2.20	0.40
1:D:303:THR:HG21	1:D:344:PHE:HB2	2.04	0.40
1:E:349:TYR:O	1:E:350:ASN:HB2	2.21	0.40
1:E:439:ALA:O	1:E:443:MET:HG3	2.21	0.40
1:A:295:LEU:O	1:A:299:ILE:HG13	2.21	0.40
3:A:604:CB3:C14	3:A:604:CB3:H5	2.51	0.40
1:B:130:ARG:HH11	1:B:130:ARG:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:PHE:CD1	1:C:36:PHE:C	2.94	0.40
1:C:208:GLY:HA3	6:C:701:HOH:O	2.20	0.40
1:C:470:LEU:HD12	1:C:470:LEU:HA	1.91	0.40
1:D:79:LEU:HA	1:D:80:PRO:HD3	1.75	0.40
1:E:278:PHE:CZ	1:E:440:ILE:HG13	2.57	0.40
1:E:411:THR:OG1	1:E:415:CYS:HB2	2.20	0.40
1:A:274:MET:O	1:A:453:PRO:HB2	2.22	0.40
1:B:98:ILE:HG22	1:B:99:GLU:OE1	2.22	0.40
1:C:397:MET:SD	1:C:401:PRO:HD3	2.61	0.40
1:D:68:LYS:O	1:D:69:ASN:HB2	2.22	0.40
1:D:235:HIS:O	1:D:238:PHE:CD2	2.74	0.40
1:D:426:ASP:OD2	1:D:426:ASP:C	2.59	0.40
1:A:99:GLU:O	1:A:99:GLU:OE1	2.40	0.40
1:A:419:ASN:ND2	1:B:461:GLY:HA2	2.37	0.40
1:B:102:MET:H	1:B:102:MET:HG2	1.49	0.40
1:C:388:ALA:O	1:C:401:PRO:HG3	2.22	0.40
1:D:315:ILE:HB	3:D:616:CB3:C15	2.51	0.40
1:D:436:ALA:O	1:D:440:ILE:HG13	2.22	0.40
1:E:500:LYS:N	1:E:503:ASP:OD1	2.54	0.40

All (2) 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:C:65:ARG:NH2	1:E:251:GLY:O[2_466]	2.11	0.09
1:E:407:GLN:OE1	1:E:421:TYR:OH[2_457]	2.19	0.01

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	503/521 (96%)	476 (95%)	23 (5%)	4 (1%)	19 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	504/521 (97%)	477 (95%)	23 (5%)	4 (1%)	19	36
1	C	504/521 (97%)	473 (94%)	28 (6%)	3 (1%)	25	44
1	D	503/521 (96%)	469 (93%)	30 (6%)	4 (1%)	19	36
1	E	504/521 (97%)	460 (91%)	38 (8%)	6 (1%)	13	24
All	All	2518/2605 (97%)	2355 (94%)	142 (6%)	21 (1%)	19	36

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	LYS
1	C	99	GLU
1	D	105	ASP
1	E	103	ASN
1	A	99	GLU
1	A	331	GLY
1	D	99	GLU
1	E	102	MET
1	E	331	GLY
1	E	197	ASP
1	A	379	PRO
1	B	277	SER
1	D	82	ASP
1	B	101	LEU
1	C	341	ILE
1	A	83	GLU
1	C	141	ILE
1	E	341	ILE
1	B	341	ILE
1	D	341	ILE
1	E	80	PRO

5.3.2 Protein sidechains [i](#)

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	457/471 (97%)	427 (93%)	30 (7%)	16	29
1	B	459/471 (98%)	425 (93%)	34 (7%)	13	24
1	C	457/471 (97%)	413 (90%)	44 (10%)	8	15
1	D	457/471 (97%)	415 (91%)	42 (9%)	9	17
1	E	457/471 (97%)	432 (94%)	25 (6%)	21	37
All	All	2287/2355 (97%)	2112 (92%)	175 (8%)	13	23

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	5	ASN
1	A	98	ILE
1	A	99	GLU
1	A	102	MET
1	A	103	ASN
1	A	104	ASP
1	A	128	VAL
1	A	133	LEU
1	A	178	GLN
1	A	193	LEU
1	A	194	LYS
1	A	202	LEU
1	A	203	LEU
1	A	244	LEU
1	A	247	VAL
1	A	248	LEU
1	A	264	SER
1	A	269	MET
1	A	285	LYS
1	A	295	LEU
1	A	361	THR
1	A	363	VAL
1	A	371	LEU
1	A	373	GLU
1	A	427	LEU
1	A	429	LEU
1	A	433	PHE
1	A	473	LEU
1	A	479	ARG
1	B	95	GLU

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Mol	Chain	Res	Type
1	B	98	ILE
1	B	99	GLU
1	B	102	MET
1	B	123	LEU
1	B	128	VAL
1	B	133	LEU
1	B	176	GLU
1	B	179	GLU
1	B	180	LYS
1	B	193	LEU
1	B	194	LYS
1	B	202	LEU
1	B	203	LEU
1	B	209	ILE
1	B	221	GLU
1	B	233	ARG
1	B	235	HIS
1	B	244	LEU
1	B	247	VAL
1	B	257	ARG
1	B	295	LEU
1	B	308	LEU
1	B	354	LYS
1	B	363	VAL
1	B	371	LEU
1	B	383	ARG
1	B	413	ASP
1	B	414	ASN
1	B	427	LEU
1	B	429	LEU
1	B	506	LEU
1	B	514	THR
1	B	516	LYS
1	C	6	VAL
1	C	39	ILE
1	C	40	THR
1	C	56	ARG
1	C	62	ILE
1	C	79	LEU
1	C	81	GLN
1	C	96	ASP
1	C	99	GLU

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Mol	Chain	Res	Type
1	C	101	LEU
1	C	123	LEU
1	C	126	ASN
1	C	133	LEU
1	C	139	GLU
1	C	140	ASP
1	C	141	ILE
1	C	176	GLU
1	C	178	GLN
1	C	222	GLU
1	C	224	TYR
1	C	235	HIS
1	C	244	LEU
1	C	247	VAL
1	C	248	LEU
1	C	254	ARG
1	C	257	ARG
1	C	264	SER
1	C	295	LEU
1	C	296	ILE
1	C	308	LEU
1	C	325	LEU
1	C	363	VAL
1	C	371	LEU
1	C	383	ARG
1	C	404	VAL
1	C	405	LEU
1	C	427	LEU
1	C	429	LEU
1	C	470	LEU
1	C	474	LYS
1	C	479	ARG
1	C	491	ARG
1	C	506	LEU
1	C	516	LYS
1	D	34	LYS
1	D	62	ILE
1	D	64	ARG
1	D	65	ARG
1	D	79	LEU
1	D	81	GLN
1	D	83	GLU

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Mol	Chain	Res	Type
1	D	97	SER
1	D	98	ILE
1	D	99	GLU
1	D	101	LEU
1	D	102	MET
1	D	123	LEU
1	D	126	ASN
1	D	128	VAL
1	D	133	LEU
1	D	138	LEU
1	D	149	GLU
1	D	176	GLU
1	D	228	SER
1	D	231	PHE
1	D	233	ARG
1	D	255	GLU
1	D	257	ARG
1	D	262	THR
1	D	269	MET
1	D	295	LEU
1	D	308	LEU
1	D	310	GLU
1	D	370	LYS
1	D	371	LEU
1	D	405	LEU
1	D	414	ASN
1	D	427	LEU
1	D	429	LEU
1	D	437	SER
1	D	447	GLN
1	D	470	LEU
1	D	479	ARG
1	D	487	LEU
1	D	506	LEU
1	D	514	THR
1	E	79	LEU
1	E	99	GLU
1	E	100	ASN
1	E	104	ASP
1	E	105	ASP
1	E	128	VAL
1	E	178	GLN

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Mol	Chain	Res	Type
1	E	194	LYS
1	E	196	ILE
1	E	202	LEU
1	E	233	ARG
1	E	235	HIS
1	E	264	SER
1	E	295	LEU
1	E	300	LYS
1	E	333	ARG
1	E	356	MET
1	E	363	VAL
1	E	383	ARG
1	E	422	GLN
1	E	468	ASN
1	E	470	LEU
1	E	500	LYS
1	E	506	LEU
1	E	516	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	235	HIS
1	A	345	GLN
1	A	384	HIS
1	B	100	ASN
1	C	419	ASN
1	C	422	GLN
1	D	109	ASN
1	D	384	HIS
1	E	178	GLN
1	E	348	HIS

5.3.3 RNA

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 monosaccharides 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
4	DHF	D	617	-	29,34,34	0.92	0	35,47,47	1.78	6 (17%)
2	UMP	D	615	-	21,21,21	2.33	3 (14%)	31,31,31	2.27	8 (25%)
3	CB3	B	608	-	36,37,37	1.29	2 (5%)	46,51,51	2.12	9 (19%)
5	NDP	C	614	-	45,52,52	1.39	3 (6%)	53,80,80	1.12	2 (3%)
3	CB3	C	612	-	36,37,37	1.30	3 (8%)	46,51,51	2.19	9 (19%)
4	DHF	A	605	-	29,34,34	0.89	1 (3%)	35,47,47	1.83	9 (25%)
5	NDP	D	618	-	45,52,52	1.40	3 (6%)	53,80,80	1.13	3 (5%)
5	NDP	E	622	-	45,52,52	1.39	3 (6%)	53,80,80	1.22	2 (3%)
4	DHF	C	613	-	29,34,34	0.88	0	35,47,47	1.90	7 (20%)
2	UMP	E	619	-	21,21,21	2.34	3 (14%)	31,31,31	2.28	8 (25%)
5	NDP	B	610	-	45,52,52	1.39	5 (11%)	53,80,80	1.20	4 (7%)
4	DHF	E	621	-	29,34,34	0.81	0	35,47,47	1.72	7 (20%)
3	CB3	D	616	-	36,37,37	1.23	2 (5%)	46,51,51	2.08	9 (19%)
3	CB3	E	620	-	36,37,37	1.26	2 (5%)	46,51,51	2.02	10 (21%)
2	UMP	A	603	-	21,21,21	2.31	3 (14%)	31,31,31	2.27	9 (29%)
2	UMP	C	611	-	21,21,21	2.32	3 (14%)	31,31,31	2.28	9 (29%)
3	CB3	A	604	-	36,37,37	1.26	2 (5%)	46,51,51	1.99	8 (17%)
4	DHF	B	609	-	29,34,34	0.93	1 (3%)	35,47,47	1.75	7 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NDP	A	606	-	45,52,52	1.41	5 (11%)	53,80,80	1.10	3 (5%)
2	UMP	B	607	-	21,21,21	2.33	3 (14%)	31,31,31	2.26	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DHF	D	617	-	-	2/20/31/31	0/3/3/3
2	UMP	D	615	-	-	4/10/22/22	0/2/2/2
3	CB3	B	608	-	-	6/27/28/28	0/3/3/3
5	NDP	C	614	-	-	6/30/77/77	0/5/5/5
3	CB3	C	612	-	-	4/27/28/28	0/3/3/3
4	DHF	A	605	-	1/1/5/8	5/20/31/31	0/3/3/3
5	NDP	D	618	-	-	2/30/77/77	0/5/5/5
5	NDP	E	622	-	-	5/30/77/77	0/5/5/5
4	DHF	C	613	-	-	4/20/31/31	0/3/3/3
2	UMP	E	619	-	-	4/10/22/22	0/2/2/2
5	NDP	B	610	-	-	4/30/77/77	0/5/5/5
4	DHF	E	621	-	-	2/20/31/31	0/3/3/3
3	CB3	D	616	-	1/1/5/6	5/27/28/28	0/3/3/3
3	CB3	E	620	-	1/1/5/6	6/27/28/28	0/3/3/3
2	UMP	A	603	-	-	1/10/22/22	0/2/2/2
2	UMP	C	611	-	-	2/10/22/22	0/2/2/2
3	CB3	A	604	-	-	6/27/28/28	0/3/3/3
4	DHF	B	609	-	1/1/5/8	5/20/31/31	0/3/3/3
5	NDP	A	606	-	-	3/30/77/77	0/5/5/5
2	UMP	B	607	-	-	3/10/22/22	0/2/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	619	UMP	C6-C5	7.90	1.53	1.35
2	B	607	UMP	C6-C5	7.90	1.53	1.35
2	D	615	UMP	C6-C5	7.89	1.53	1.35
2	A	603	UMP	C6-C5	7.85	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	611	UMP	C6-C5	7.85	1.53	1.35
5	E	622	NDP	C4N-C3N	-5.99	1.38	1.49
5	C	614	NDP	C4N-C3N	-5.98	1.38	1.49
5	D	618	NDP	C4N-C3N	-5.89	1.38	1.49
5	A	606	NDP	C4N-C3N	-5.32	1.39	1.49
5	B	610	NDP	C4N-C3N	-5.31	1.39	1.49
3	E	620	CB3	O4-C4	4.55	1.36	1.24
3	B	608	CB3	O4-C4	4.49	1.35	1.24
2	D	615	UMP	C5-C4	4.46	1.53	1.43
2	E	619	UMP	C5-C4	4.46	1.53	1.43
3	D	616	CB3	O4-C4	4.42	1.35	1.24
2	C	611	UMP	C5-C4	4.40	1.53	1.43
3	A	604	CB3	O4-C4	4.40	1.35	1.24
2	E	619	UMP	C6-N1	4.39	1.48	1.38
2	B	607	UMP	C6-N1	4.39	1.48	1.38
2	B	607	UMP	C5-C4	4.38	1.53	1.43
3	C	612	CB3	O4-C4	4.37	1.35	1.24
2	C	611	UMP	C6-N1	4.36	1.48	1.38
2	D	615	UMP	C6-N1	4.35	1.48	1.38
2	A	603	UMP	C5-C4	4.35	1.53	1.43
2	A	603	UMP	C6-N1	4.32	1.48	1.38
5	E	622	NDP	C4N-C5N	-4.11	1.38	1.48
5	D	618	NDP	C4N-C5N	-4.09	1.38	1.48
5	C	614	NDP	C4N-C5N	-4.02	1.38	1.48
5	B	610	NDP	C4N-C5N	-3.70	1.39	1.48
5	A	606	NDP	C4N-C5N	-3.59	1.39	1.48
5	B	610	NDP	C6N-C5N	3.42	1.39	1.33
5	A	606	NDP	C6N-C5N	3.41	1.39	1.33
3	E	620	CB3	CP2-CP3	3.32	1.28	1.18
3	A	604	CB3	CP2-CP3	3.20	1.27	1.18
3	D	616	CB3	CP2-CP3	3.19	1.27	1.18
5	C	614	NDP	C6N-C5N	3.09	1.38	1.33
3	B	608	CB3	CP2-CP3	3.06	1.27	1.18
3	C	612	CB3	CP2-CP3	2.97	1.27	1.18
5	E	622	NDP	C6N-C5N	2.92	1.38	1.33
5	D	618	NDP	C6N-C5N	2.88	1.38	1.33
5	B	610	NDP	O4B-C1B	2.71	1.44	1.41
5	A	606	NDP	O4B-C1B	2.35	1.44	1.41
4	B	609	DHF	C4A-N5	-2.27	1.34	1.38
5	A	606	NDP	C7N-C3N	2.18	1.53	1.48
4	A	605	DHF	C4A-N5	-2.07	1.34	1.38
3	C	612	CB3	C8-C8A	-2.06	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	610	NDP	C7N-C3N	2.01	1.53	1.48

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	608	CB3	C4A-C8A-N1	-7.92	119.30	123.60
3	A	604	CB3	C4A-C8A-N1	-7.62	119.46	123.60
3	B	608	CB3	C4A-C4-N3	-7.53	119.16	124.40
3	D	616	CB3	C4A-C4-N3	-7.45	119.20	124.40
3	E	620	CB3	C4A-C4-N3	-7.36	119.27	124.40
3	C	612	CB3	C4A-C8A-N1	-7.14	119.72	123.60
3	D	616	CB3	C4A-C8A-N1	-7.11	119.74	123.60
3	C	612	CB3	C4A-C4-N3	-6.88	119.61	124.40
4	A	605	DHF	C8A-C4A-C4	6.79	118.97	114.53
4	B	609	DHF	C8A-C4A-C4	6.74	118.94	114.53
3	A	604	CB3	C4A-C4-N3	-6.67	119.75	124.40
3	E	620	CB3	C4A-C8A-N1	-6.49	120.08	123.60
4	C	613	DHF	C8A-C4A-C4	6.44	118.74	114.53
2	C	611	UMP	C6-C5-C4	-6.17	111.08	119.52
2	A	603	UMP	C5-C6-N1	-6.14	111.52	121.81
2	B	607	UMP	C6-C5-C4	-6.12	111.16	119.52
2	E	619	UMP	C5-C6-N1	-6.00	111.76	121.81
4	E	621	DHF	C8A-C4A-C4	5.97	118.43	114.53
3	C	612	CB3	CB-CA-N	-5.96	98.83	110.88
2	D	615	UMP	C5-C6-N1	-5.94	111.86	121.81
4	D	617	DHF	C8A-C4A-C4	5.93	118.41	114.53
2	C	611	UMP	C5-C6-N1	-5.89	111.95	121.81
2	D	615	UMP	C6-C5-C4	-5.84	111.53	119.52
2	A	603	UMP	C6-C5-C4	-5.83	111.55	119.52
2	E	619	UMP	C6-C5-C4	-5.82	111.56	119.52
2	B	607	UMP	C5-C6-N1	-5.77	112.14	121.81
3	D	616	CB3	N1-C2-N3	-4.74	120.91	127.22
4	D	617	DHF	CB-CA-N	-4.70	101.37	110.88
5	E	622	NDP	N3A-C2A-N1A	-4.68	121.36	128.68
5	A	606	NDP	N3A-C2A-N1A	-4.68	121.37	128.68
2	E	619	UMP	C4-N3-C2	-4.56	120.57	126.58
5	D	618	NDP	N3A-C2A-N1A	-4.54	121.59	128.68
5	C	614	NDP	N3A-C2A-N1A	-4.52	121.61	128.68
3	C	612	CB3	N1-C2-N3	-4.51	121.20	127.22
2	D	615	UMP	C4-N3-C2	-4.48	120.67	126.58
3	A	604	CB3	N1-C2-N3	-4.48	121.25	127.22
4	C	613	DHF	CB-CA-N	-4.46	101.86	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	611	UMP	C4-N3-C2	-4.45	120.70	126.58
2	A	603	UMP	C4-N3-C2	-4.45	120.71	126.58
3	B	608	CB3	N1-C2-N3	-4.39	121.37	127.22
5	B	610	NDP	N3A-C2A-N1A	-4.39	121.82	128.68
3	E	620	CB3	N1-C2-N3	-4.37	121.40	127.22
2	B	607	UMP	C4-N3-C2	-4.30	120.91	126.58
2	E	619	UMP	N3-C2-N1	4.20	120.47	114.89
2	D	615	UMP	N3-C2-N1	4.12	120.36	114.89
2	A	603	UMP	N3-C2-N1	4.11	120.35	114.89
3	E	620	CB3	C6-C9-N10	-4.07	107.63	114.18
2	C	611	UMP	N3-C2-N1	3.90	120.06	114.89
2	B	607	UMP	N3-C2-N1	3.86	120.01	114.89
5	E	622	NDP	PN-O3-PA	-3.80	119.78	132.83
2	B	607	UMP	C5-C4-N3	3.56	120.17	114.84
2	D	615	UMP	C5-C4-N3	3.54	120.13	114.84
2	C	611	UMP	C5-C4-N3	3.53	120.12	114.84
2	E	619	UMP	C5-C4-N3	3.44	119.98	114.84
2	A	603	UMP	C5-C4-N3	3.41	119.94	114.84
4	A	605	DHF	CT-CA-N	3.32	118.41	110.55
5	C	614	NDP	PN-O3-PA	-3.30	121.49	132.83
5	D	618	NDP	PN-O3-PA	-3.30	121.52	132.83
2	B	607	UMP	O4-C4-C5	-3.12	119.67	125.16
5	B	610	NDP	PN-O3-PA	-3.09	122.22	132.83
3	D	616	CB3	C2-N3-C4	3.05	120.77	115.93
4	A	605	DHF	CA-N-C	3.05	129.06	121.60
2	A	603	UMP	O4-C4-C5	-3.04	119.81	125.16
4	C	613	DHF	N1-C2-N3	-3.02	120.68	125.42
2	C	611	UMP	O4-C4-C5	-3.00	119.88	125.16
2	D	615	UMP	O4-C4-C5	-3.00	119.89	125.16
2	E	619	UMP	O4-C4-C5	-2.98	119.92	125.16
4	C	613	DHF	C2-N3-C4	2.96	120.64	115.93
2	B	607	UMP	O5'-P-OP1	2.92	114.66	106.47
4	B	609	DHF	CT-CA-N	2.91	117.45	110.55
4	E	621	DHF	N1-C2-N3	-2.91	120.86	125.42
4	E	621	DHF	C2-N3-C4	2.88	120.50	115.93
5	A	606	NDP	PN-O3-PA	-2.86	123.00	132.83
4	C	613	DHF	C4A-C4-N3	-2.85	119.53	123.43
5	B	610	NDP	C4A-C5A-N7A	-2.84	106.44	109.40
4	D	617	DHF	C2-N3-C4	2.83	120.43	115.93
4	D	617	DHF	C4A-C4-N3	-2.80	119.60	123.43
3	D	616	CB3	CT-CA-N	2.80	117.18	110.55
3	B	608	CB3	C2-N3-C4	2.77	120.32	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	608	CB3	C13-C14-N10	-2.75	117.58	121.38
5	B	610	NDP	C1B-N9A-C4A	-2.75	121.81	126.64
4	E	621	DHF	CB-CA-N	-2.75	105.31	110.88
2	C	611	UMP	O5'-P-OP1	2.74	114.15	106.47
3	E	620	CB3	C2-N3-C4	2.72	120.26	115.93
4	B	609	DHF	N1-C2-N3	-2.72	121.16	125.42
2	A	603	UMP	O5'-P-OP1	2.68	114.00	106.47
4	D	617	DHF	N1-C2-N3	-2.67	121.22	125.42
4	C	613	DHF	C2-N1-C8A	2.67	120.53	114.54
4	A	605	DHF	C2-N3-C4	2.66	120.16	115.93
4	B	609	DHF	C2-N3-C4	2.66	120.16	115.93
4	E	621	DHF	C2-N1-C8A	2.66	120.50	114.54
3	C	612	CB3	C2-N3-C4	2.65	120.14	115.93
3	D	616	CB3	CP1-N10-C9	2.64	119.62	117.10
4	A	605	DHF	C4A-C4-N3	-2.64	119.82	123.43
2	E	619	UMP	O2-C2-N1	-2.64	119.28	122.79
3	B	608	CB3	CB-CA-N	-2.62	105.58	110.88
2	D	615	UMP	O5'-P-OP1	2.61	113.79	106.47
3	A	604	CB3	C2-N3-C4	2.59	120.05	115.93
4	B	609	DHF	CA-N-C	2.58	127.91	121.60
4	B	609	DHF	C4A-C4-N3	-2.57	119.91	123.43
4	A	605	DHF	N1-C2-N3	-2.55	121.42	125.42
2	A	603	UMP	O2-C2-N1	-2.53	119.42	122.79
4	E	621	DHF	C4A-C4-N3	-2.53	119.97	123.43
3	C	612	CB3	CB-CG-CD	-2.52	105.81	112.51
4	B	609	DHF	C2-N1-C8A	2.50	120.14	114.54
2	E	619	UMP	O5'-P-OP1	2.49	113.47	106.47
2	D	615	UMP	O2-C2-N1	-2.45	119.53	122.79
4	D	617	DHF	C2-N1-C8A	2.44	120.01	114.54
2	B	607	UMP	O2-C2-N1	-2.44	119.54	122.79
3	E	620	CB3	C13-C14-N10	-2.43	118.03	121.38
3	A	604	CB3	C13-C14-N10	-2.42	118.04	121.38
4	A	605	DHF	CG-CB-CA	-2.42	108.63	113.16
3	E	620	CB3	CP1-N10-C9	2.38	119.37	117.10
2	C	611	UMP	O2-C2-N1	-2.37	119.64	122.79
3	A	604	CB3	C6-C9-N10	-2.36	110.40	114.18
4	A	605	DHF	C2-N1-C8A	2.35	119.82	114.54
3	C	612	CB3	C6-C5-C4A	-2.35	119.14	122.65
3	A	604	CB3	CB-CA-N	-2.30	106.22	110.88
3	D	616	CB3	CB-CA-N	-2.26	106.30	110.88
3	E	620	CB3	NA2-C2-N3	2.25	120.75	117.25
3	E	620	CB3	C6-C5-C4A	-2.25	119.28	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	608	CB3	C9-N10-C14	2.25	124.64	120.78
3	B	608	CB3	C6-C9-N10	-2.25	110.57	114.18
4	E	621	DHF	CB-CG-CD	-2.23	106.58	112.51
3	B	608	CB3	C6-C5-C4A	-2.22	119.33	122.65
4	C	613	DHF	C11-C-N	2.20	121.29	117.06
3	D	616	CB3	C6-C9-N10	-2.20	110.65	114.18
3	C	612	CB3	C13-C14-N10	-2.16	118.41	121.38
3	C	612	CB3	C6-C9-N10	-2.12	110.78	114.18
3	E	620	CB3	CB-CA-N	-2.10	106.62	110.88
3	D	616	CB3	C6-C5-C4A	-2.09	119.53	122.65
5	D	618	NDP	O3X-P2B-O2X	2.09	115.61	107.64
3	A	604	CB3	C6-C5-C4A	-2.09	119.53	122.65
4	A	605	DHF	CB-CA-CT	2.06	115.31	110.35
5	A	606	NDP	C3N-C2N-N1N	-2.05	120.17	123.10
2	C	611	UMP	C2'-C3'-C4'	-2.04	98.51	102.76
2	A	603	UMP	C3'-C2'-C1'	-2.02	97.47	102.54

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	616	CB3	CA
3	E	620	CB3	CA
4	A	605	DHF	CA
4	B	609	DHF	CA

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	607	UMP	C5'-O5'-P-OP2
2	B	607	UMP	C5'-O5'-P-OP3
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-OP1
2	E	619	UMP	C5'-O5'-P-OP2
2	E	619	UMP	C5'-O5'-P-OP3
3	E	620	CB3	CB-CA-N-C
3	E	620	CB3	N-CA-CB-CG
4	A	605	DHF	CB-CA-N-C
4	B	609	DHF	CB-CA-N-C
5	A	606	NDP	C2B-O2B-P2B-O1X
5	C	614	NDP	C2B-O2B-P2B-O3X

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Mol	Chain	Res	Type	Atoms
5	D	618	NDP	C2B-O2B-P2B-O3X
5	E	622	NDP	C5B-O5B-PA-O1A
5	E	622	NDP	C5B-O5B-PA-O3
5	E	622	NDP	PA-O3-PN-O5D
3	D	616	CB3	CB-CA-N-C
3	A	604	CB3	N-CA-CB-CG
3	E	620	CB3	CA-CB-CG-CD
3	C	612	CB3	N-CA-CB-CG
3	A	604	CB3	CT-CA-CB-CG
3	C	612	CB3	CT-CA-CB-CG
3	E	620	CB3	CT-CA-CB-CG
4	A	605	DHF	CA-CB-CG-CD
4	A	605	DHF	CT-CA-CB-CG
4	C	613	DHF	CB-CA-N-C
4	B	609	DHF	CA-CB-CG-CD
3	B	608	CB3	C6-C9-N10-C14
3	B	608	CB3	N-CA-CB-CG
5	C	614	NDP	C3B-C4B-C5B-O5B
5	B	610	NDP	C2B-O2B-P2B-O1X
3	B	608	CB3	CT-CA-CB-CG
5	B	610	NDP	C2B-O2B-P2B-O3X
2	C	611	UMP	O4'-C4'-C5'-O5'
5	E	622	NDP	O4D-C1D-N1N-C2N
5	E	622	NDP	C5B-O5B-PA-O2A
4	B	609	DHF	CB-CA-CT-O1
2	C	611	UMP	C3'-C4'-C5'-O5'
5	D	618	NDP	O4D-C1D-N1N-C2N
4	E	621	DHF	CT-CA-CB-CG
4	B	609	DHF	CB-CA-CT-O2
5	A	606	NDP	O4D-C1D-N1N-C2N
5	B	610	NDP	O4D-C1D-N1N-C2N
5	C	614	NDP	O4D-C1D-N1N-C2N
4	A	605	DHF	CB-CA-CT-O1
4	E	621	DHF	N-CA-CB-CG
3	B	608	CB3	C6-C9-N10-CP1
3	D	616	CB3	OE1-CD-CG-CB
2	B	607	UMP	O4'-C4'-C5'-O5'
3	E	620	CB3	CB-CA-CT-O1
3	A	604	CB3	C6-C9-N10-C14
3	C	612	CB3	C6-C9-N10-C14
3	D	616	CB3	OE2-CD-CG-CB
3	C	612	CB3	C6-C9-N10-CP1

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Mol	Chain	Res	Type	Atoms
5	B	610	NDP	C2D-C1D-N1N-C2N
3	D	616	CB3	CB-CA-CT-O1
3	D	616	CB3	CB-CA-CT-O2
3	E	620	CB3	CB-CA-CT-O2
4	A	605	DHF	CB-CA-CT-O2
4	C	613	DHF	OE1-CD-CG-CB
3	A	604	CB3	C6-C9-N10-CP1
4	B	609	DHF	CT-CA-CB-CG
2	A	603	UMP	O4'-C4'-C5'-O5'
4	C	613	DHF	OE2-CD-CG-CB
5	C	614	NDP	C5D-O5D-PN-O3
4	C	613	DHF	CT-CA-N-C
5	A	606	NDP	C2D-C1D-N1N-C2N
3	B	608	CB3	OE2-CD-CG-CB
5	C	614	NDP	C5D-O5D-PN-O1N
2	D	615	UMP	O4'-C4'-C5'-O5'
2	E	619	UMP	O4'-C4'-C5'-O5'
4	D	617	DHF	OE1-CD-CG-CB
3	B	608	CB3	OE1-CD-CG-CB
4	D	617	DHF	OE2-CD-CG-CB
3	A	604	CB3	OE1-CD-CG-CB
3	A	604	CB3	OE2-CD-CG-CB
5	C	614	NDP	C2D-C1D-N1N-C2N

There are no ring outliers.

20 monomers are involved in 115 short contacts:

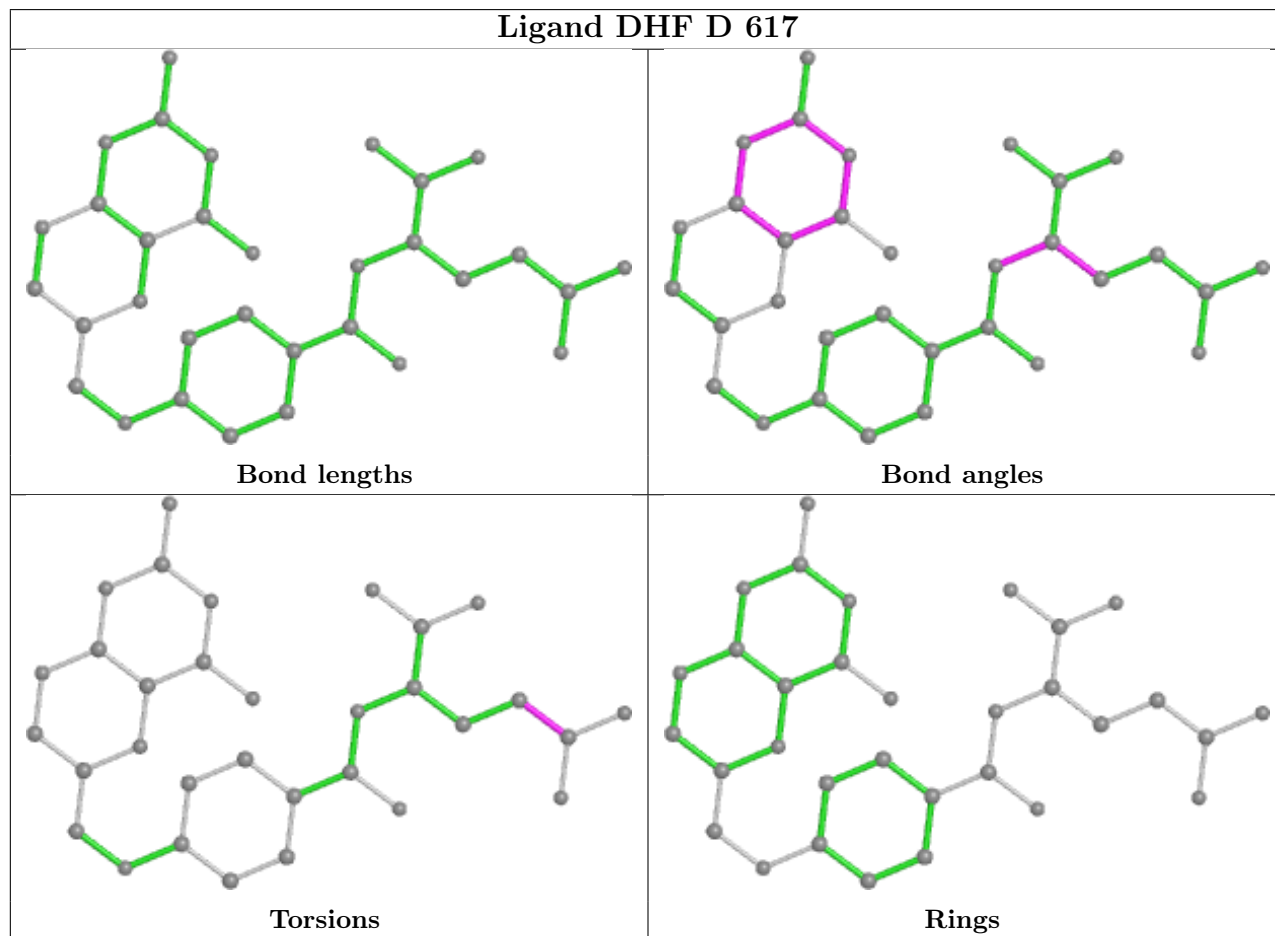
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	617	DHF	9	0
2	D	615	UMP	4	0
3	B	608	CB3	3	0
5	C	614	NDP	11	0
3	C	612	CB3	2	0
4	A	605	DHF	6	0
5	D	618	NDP	5	0
5	E	622	NDP	12	0
4	C	613	DHF	9	0
2	E	619	UMP	6	0
5	B	610	NDP	8	0
4	E	621	DHF	5	0
3	D	616	CB3	9	0
3	E	620	CB3	13	0

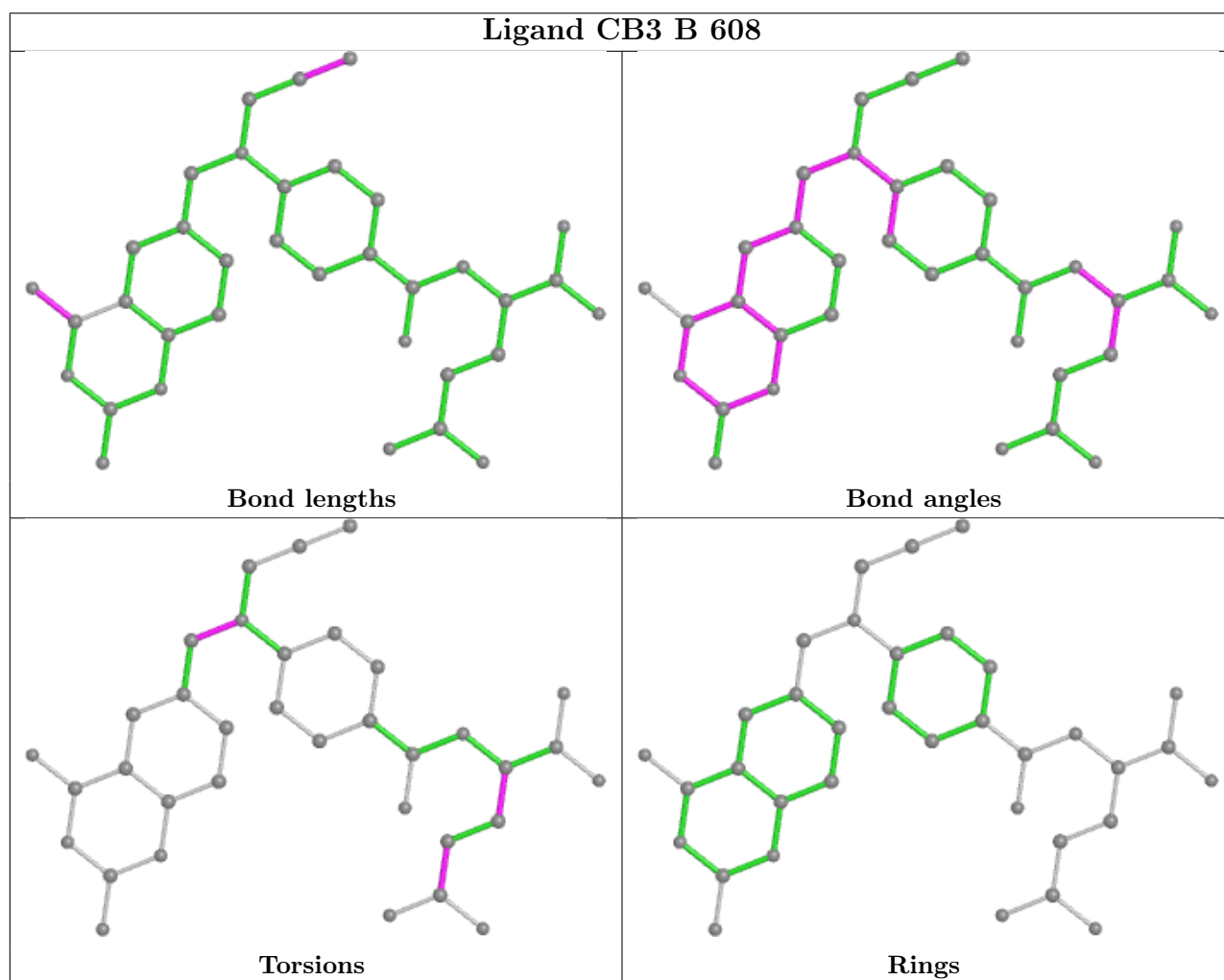
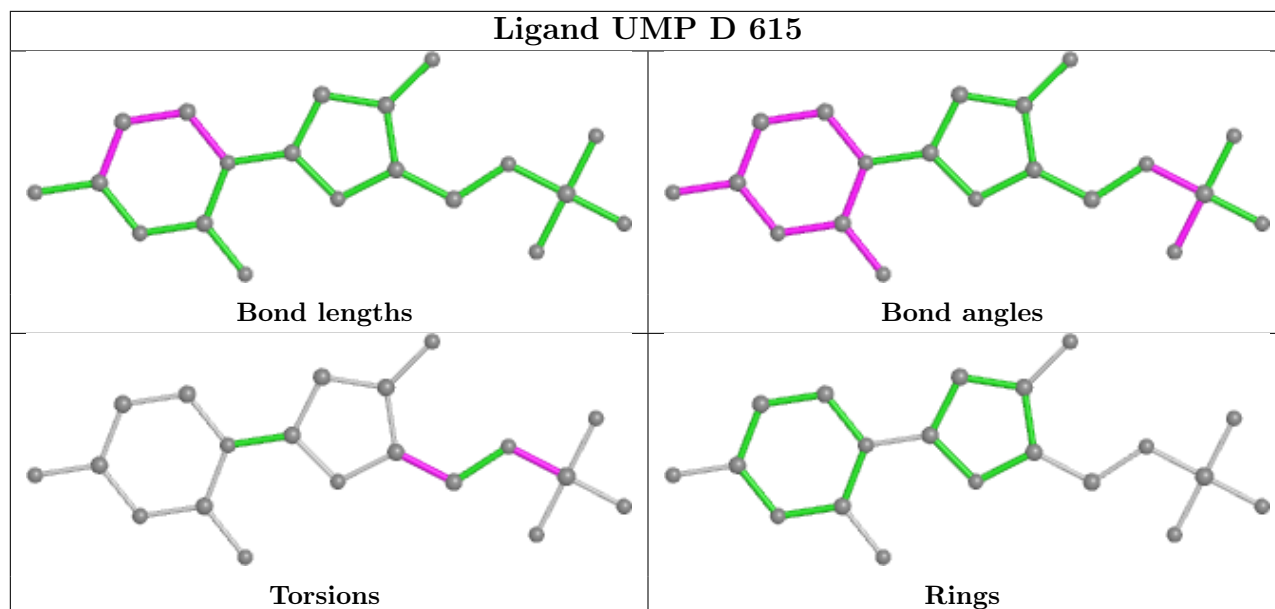
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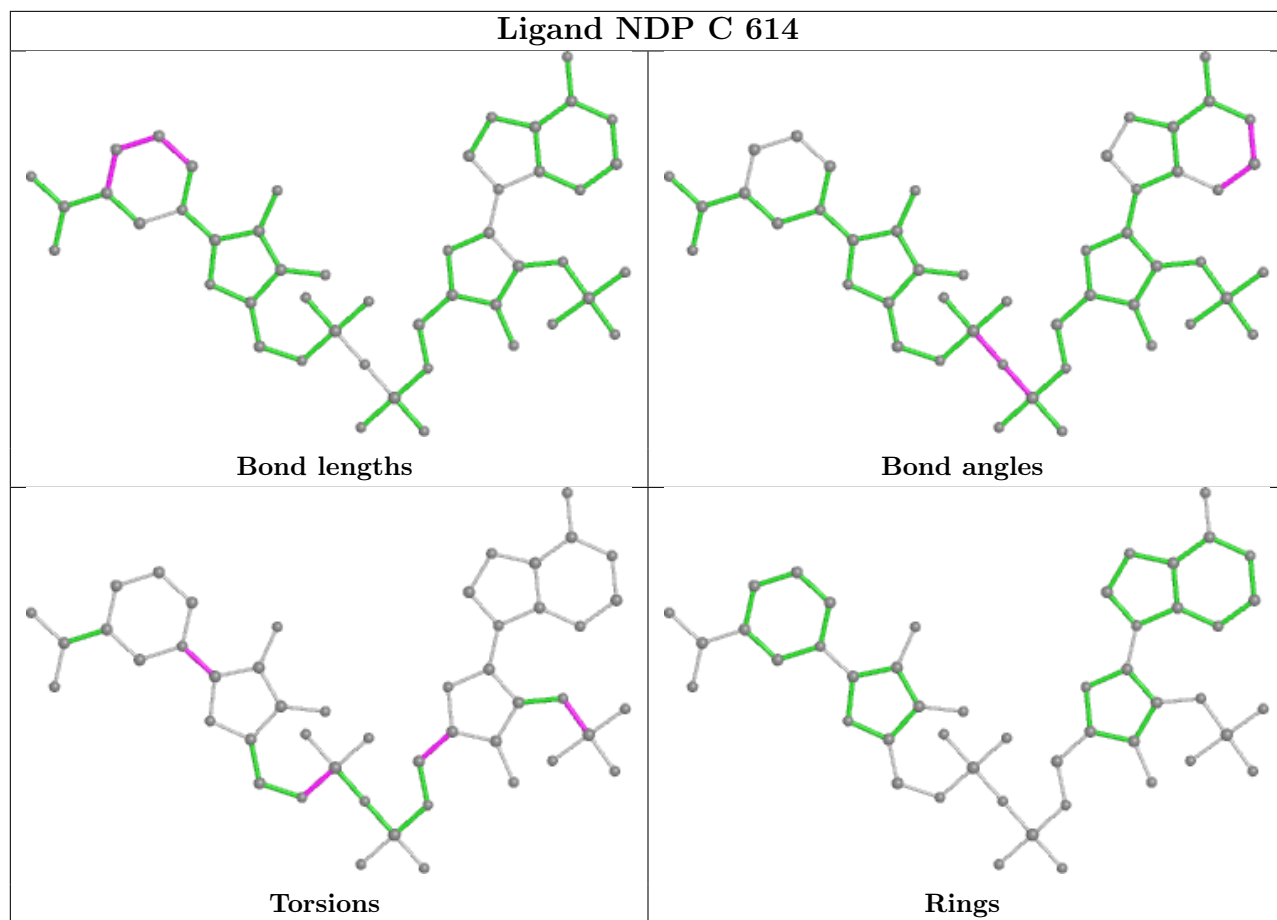
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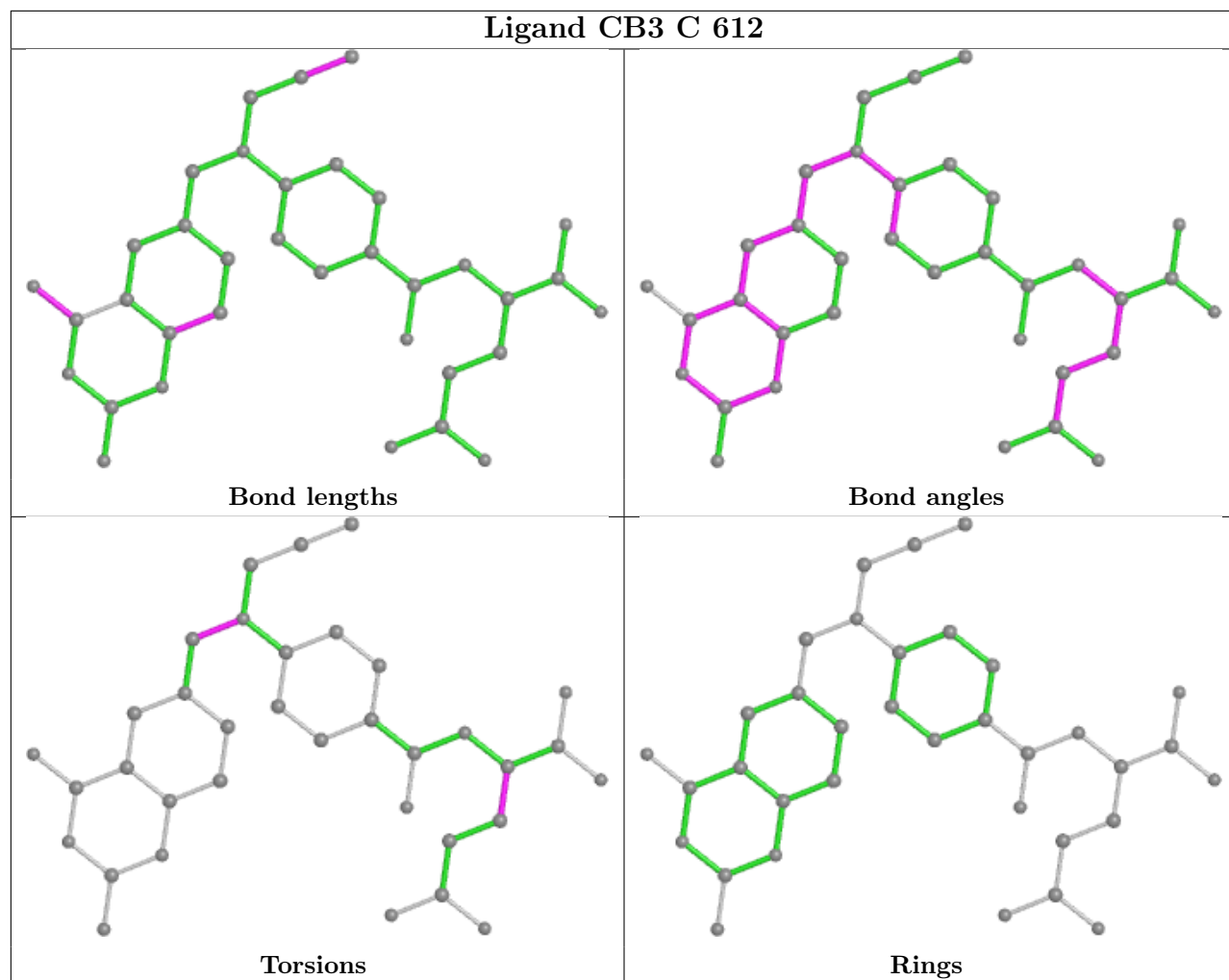
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	UMP	4	0
2	C	611	UMP	3	0
3	A	604	CB3	4	0
4	B	609	DHF	10	0
5	A	606	NDP	7	0
2	B	607	UMP	3	0

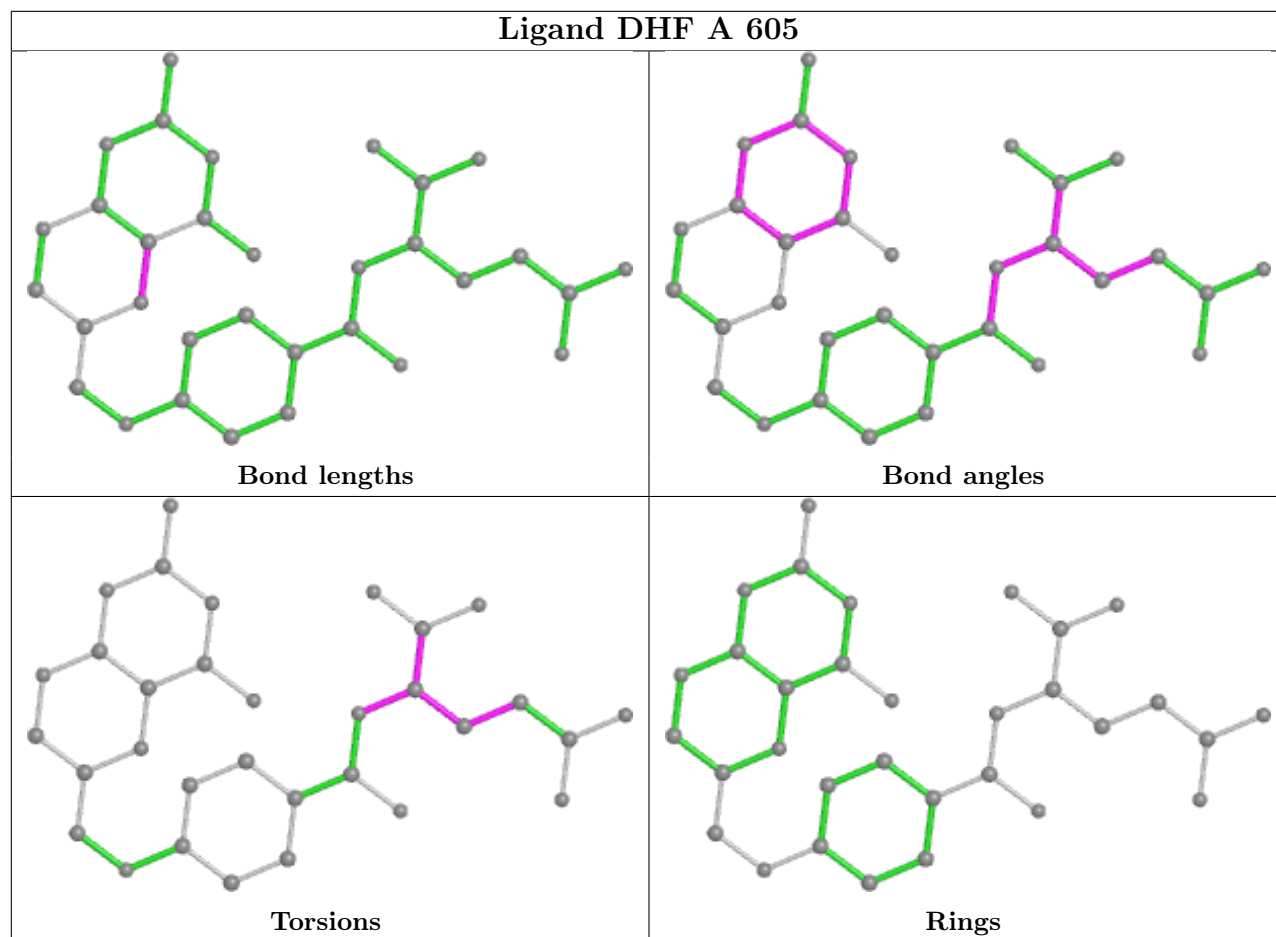
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

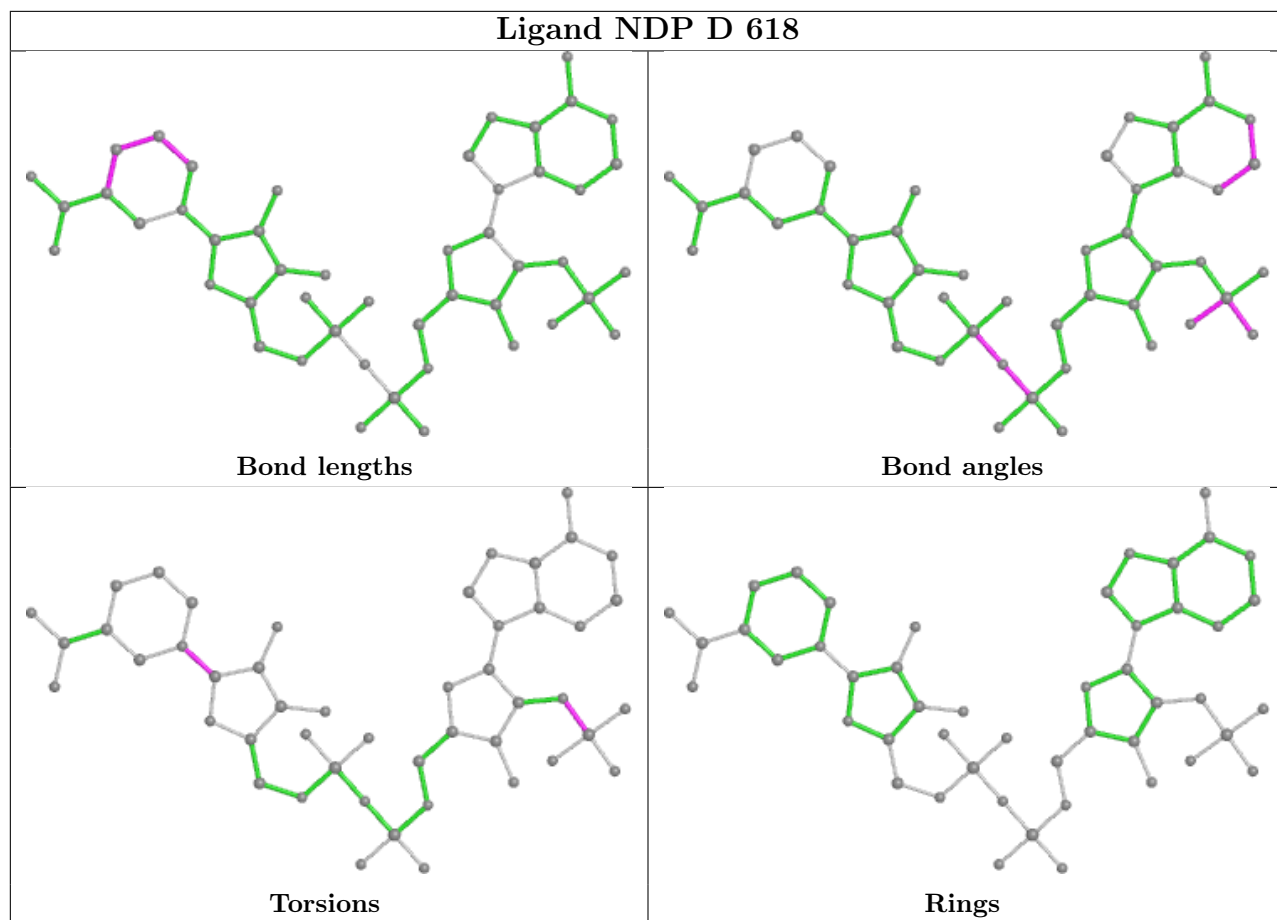


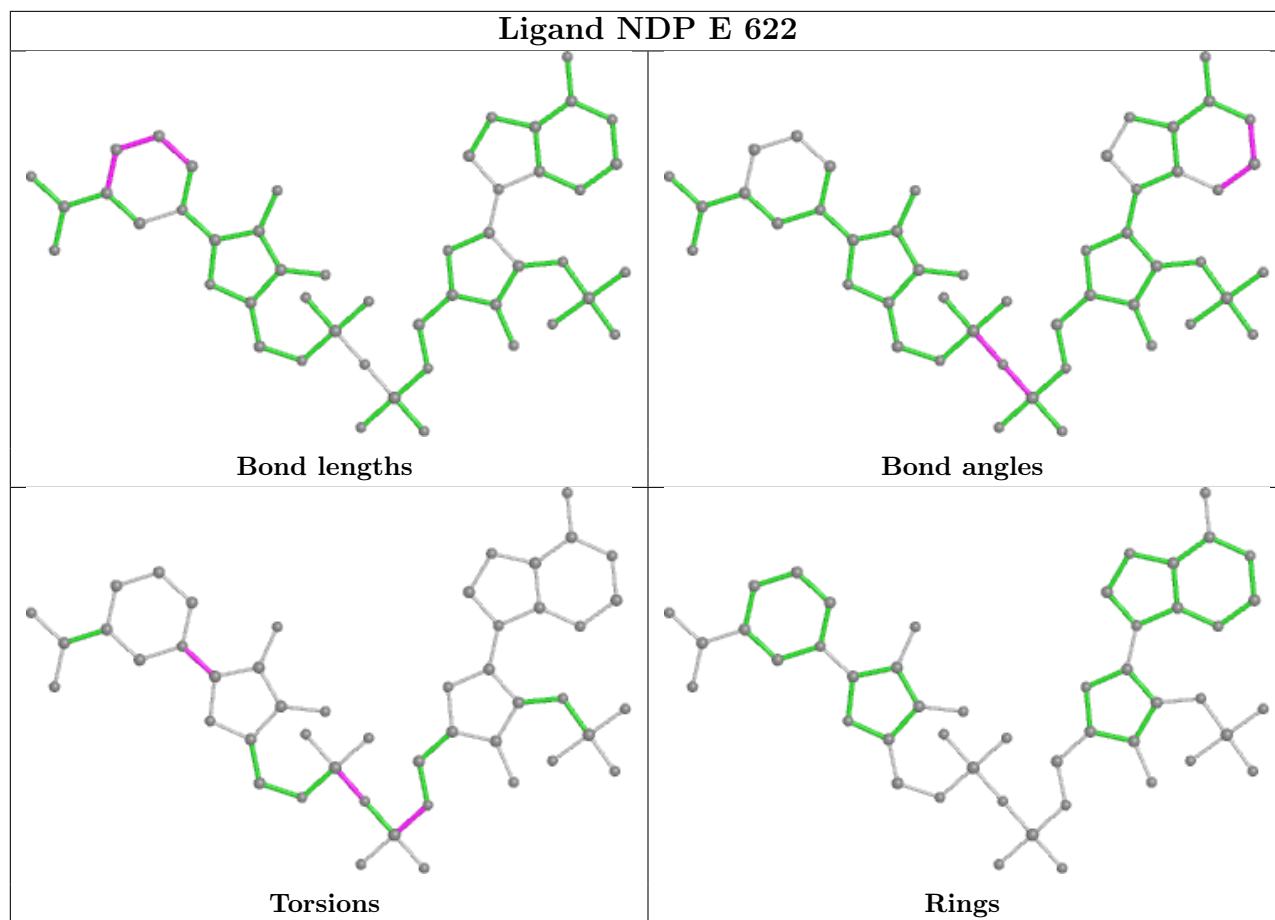


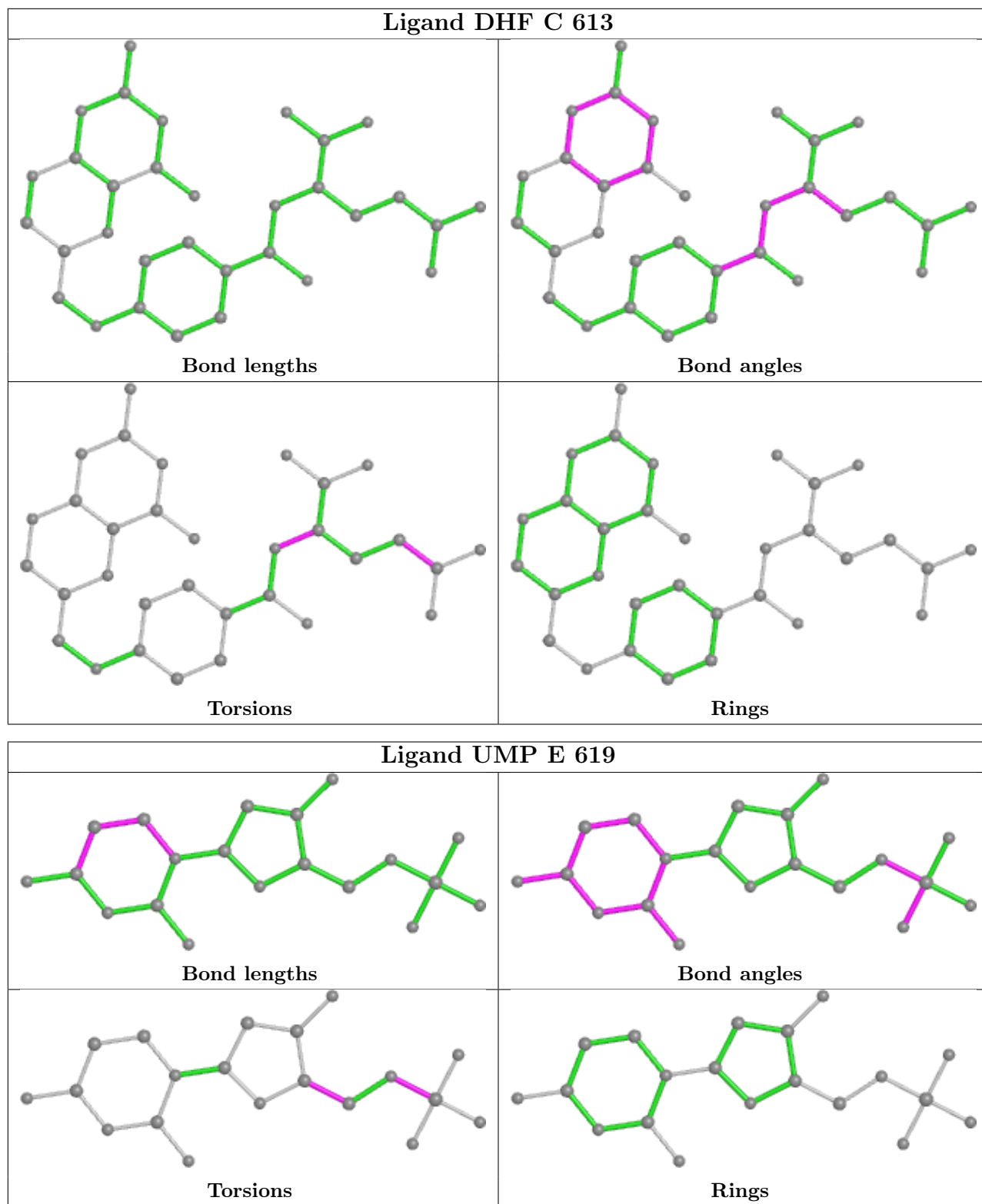


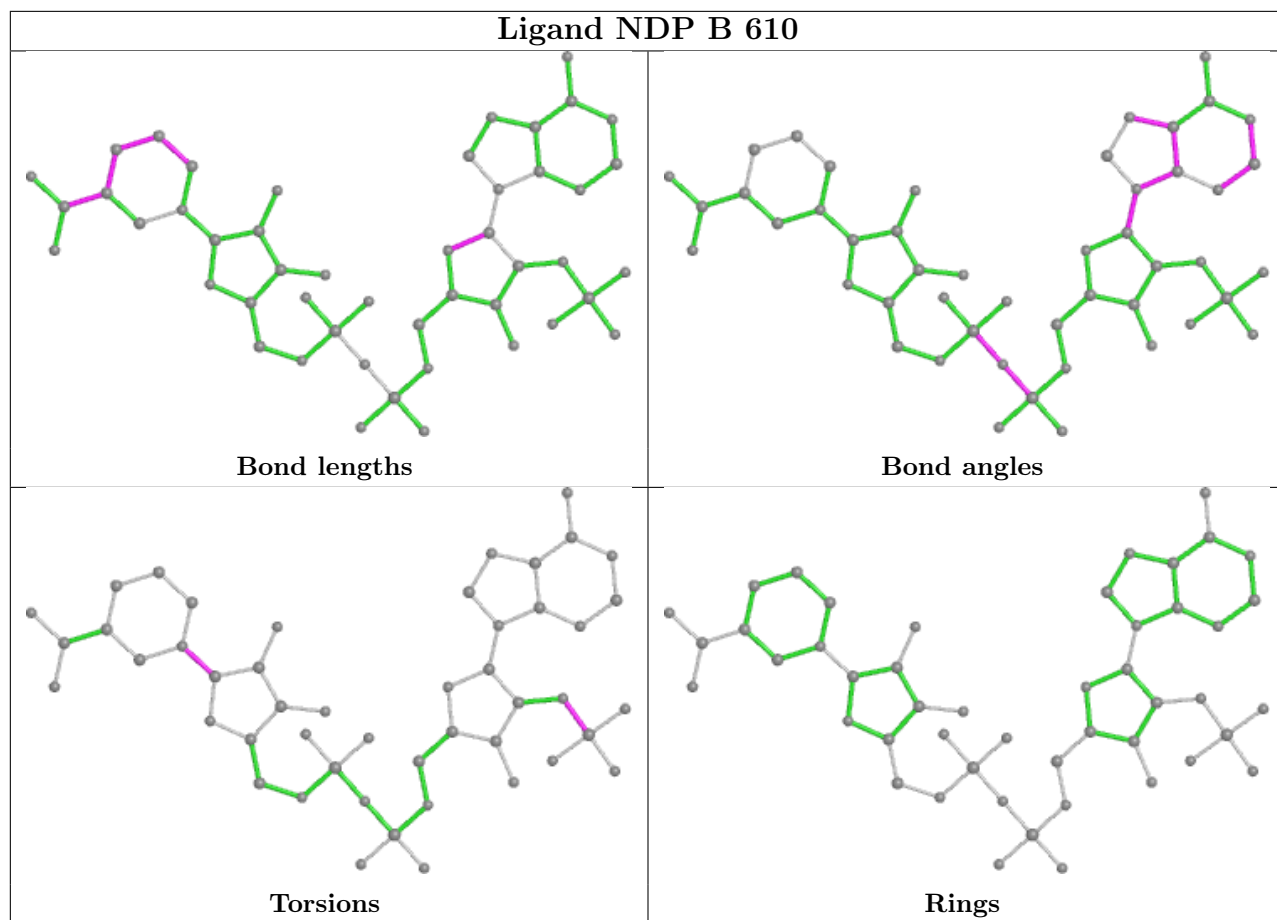


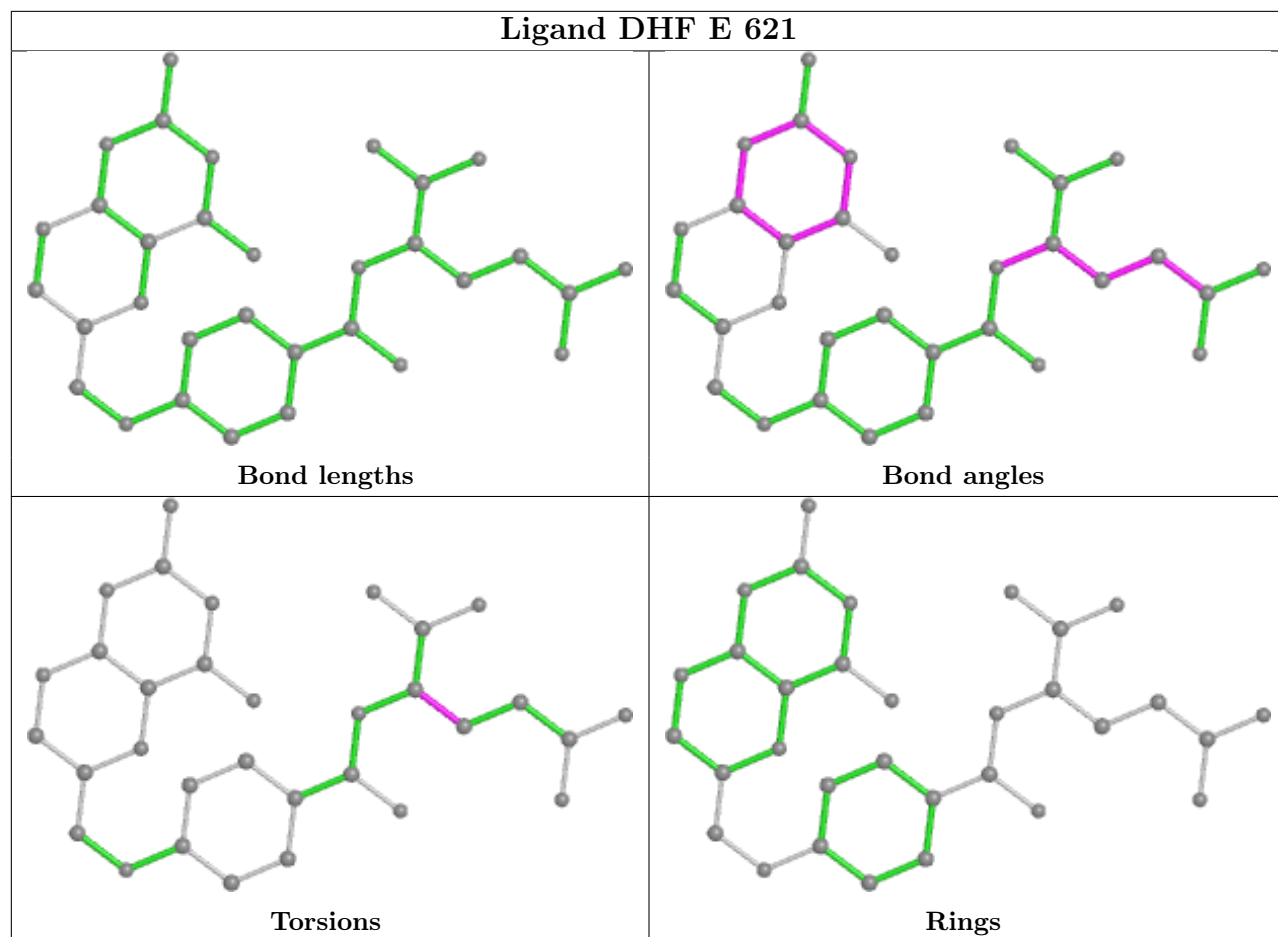


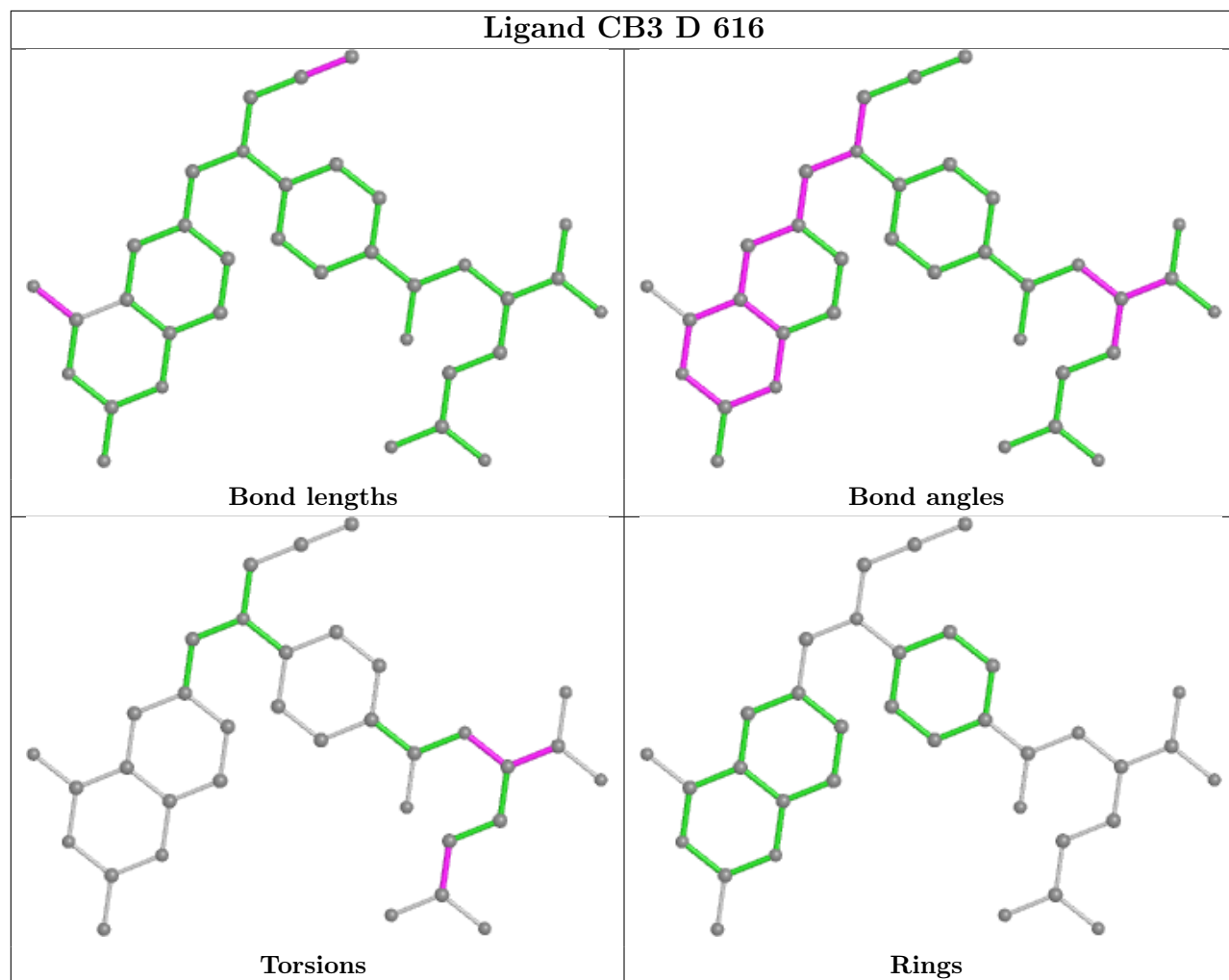


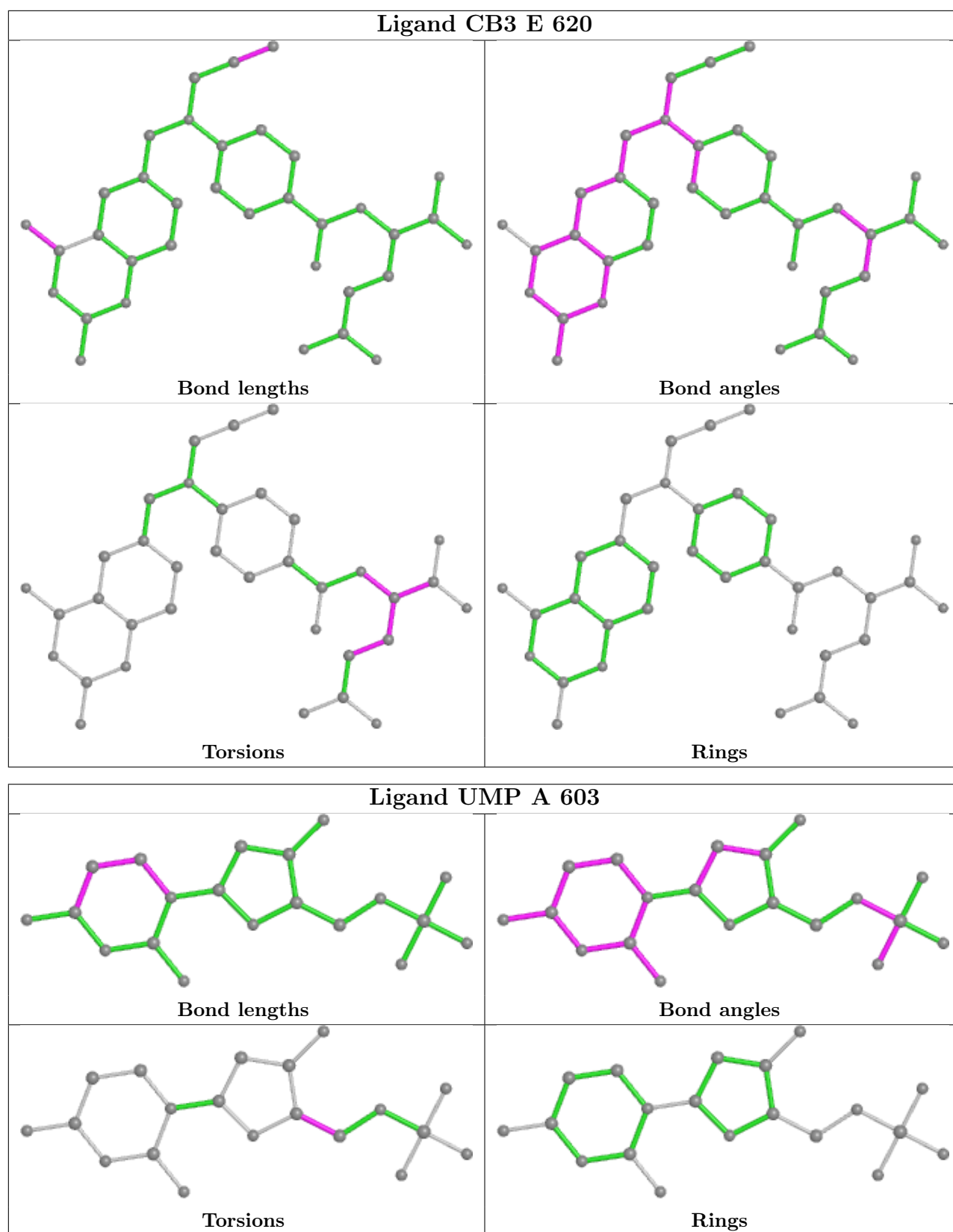


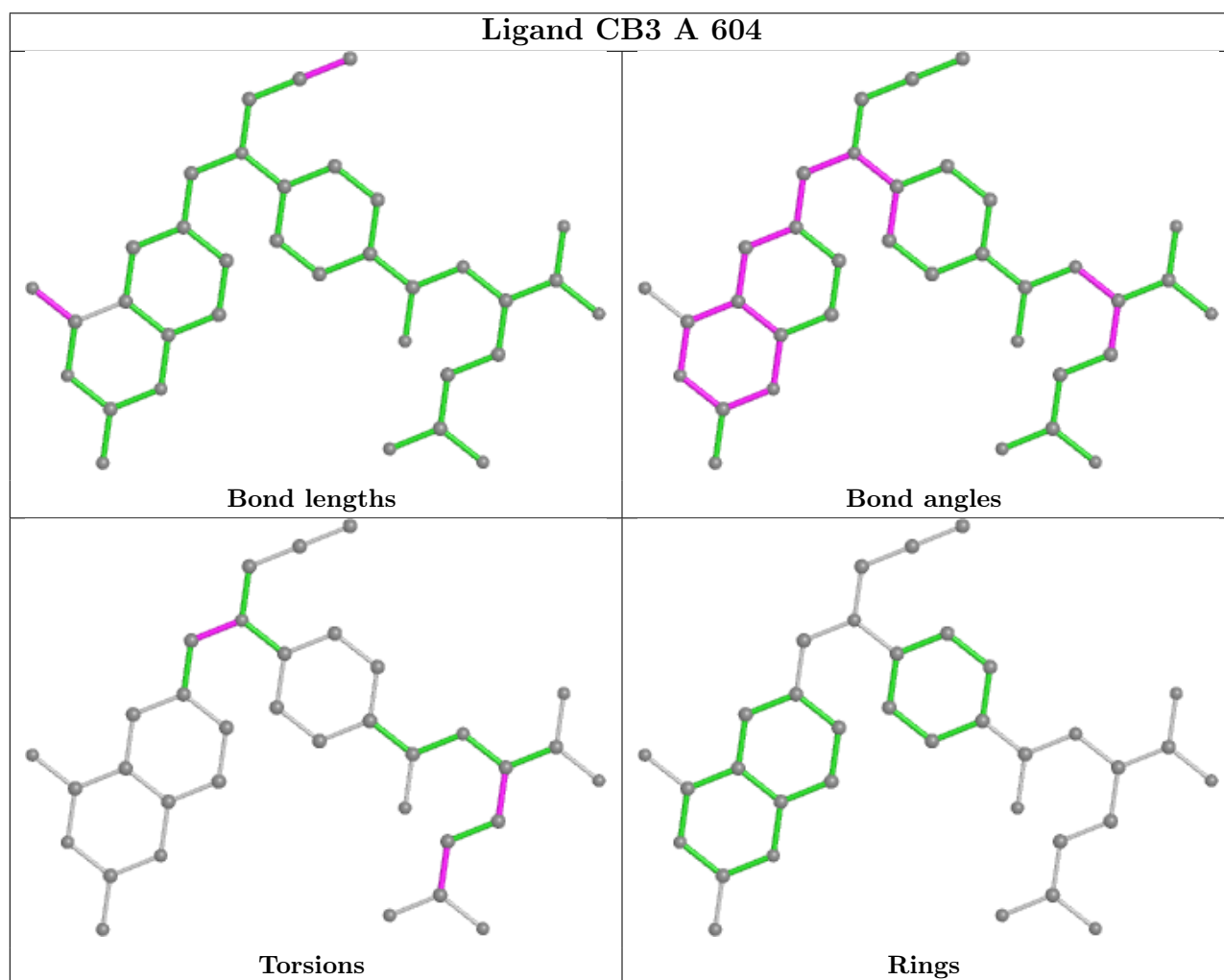
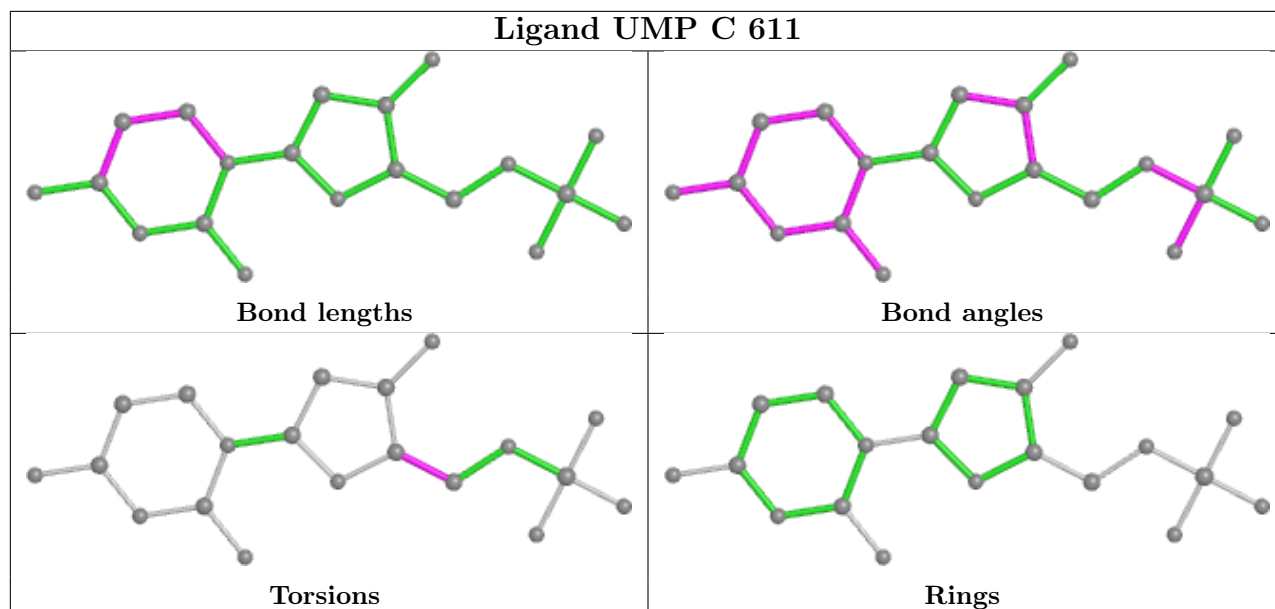


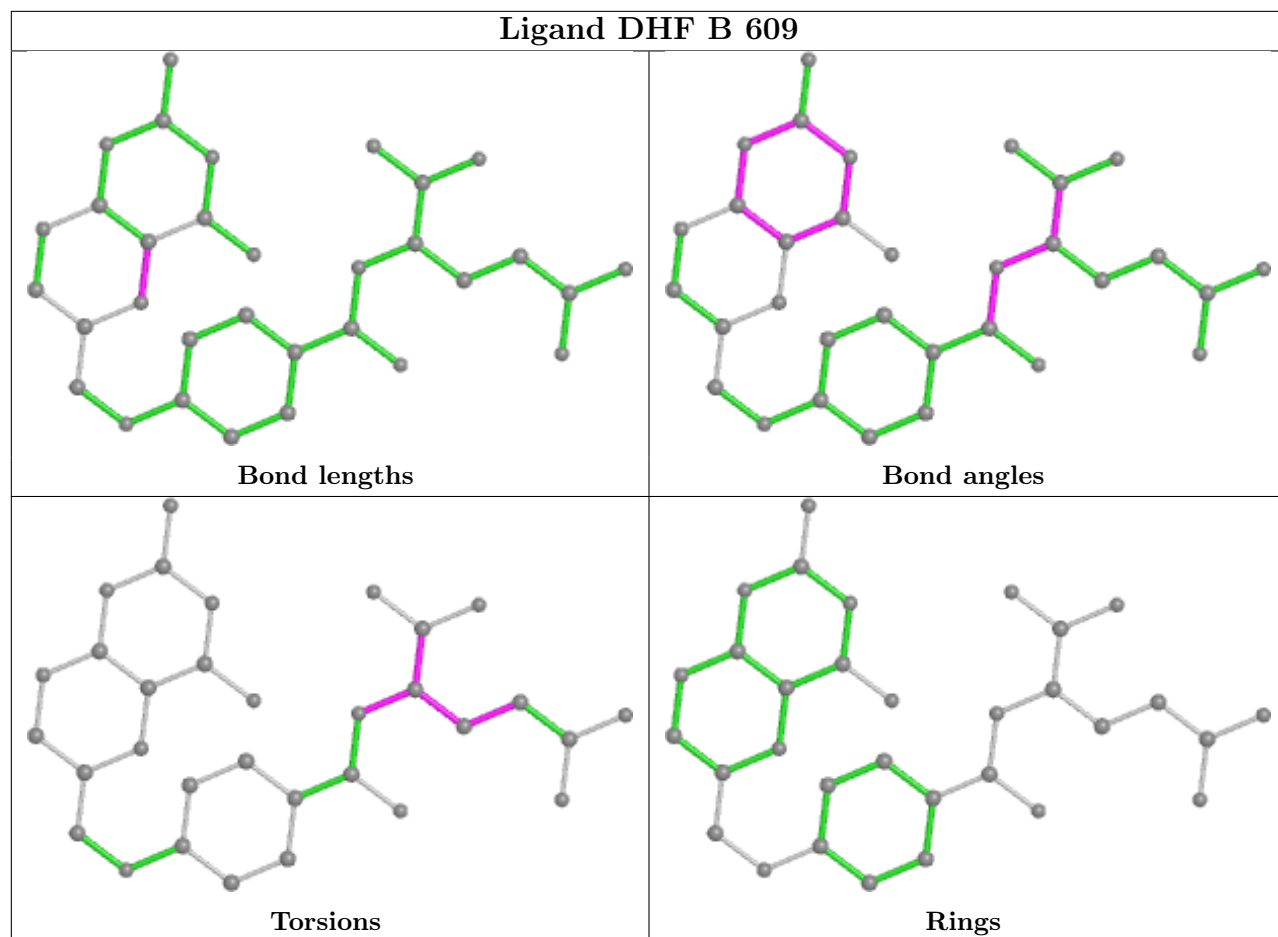


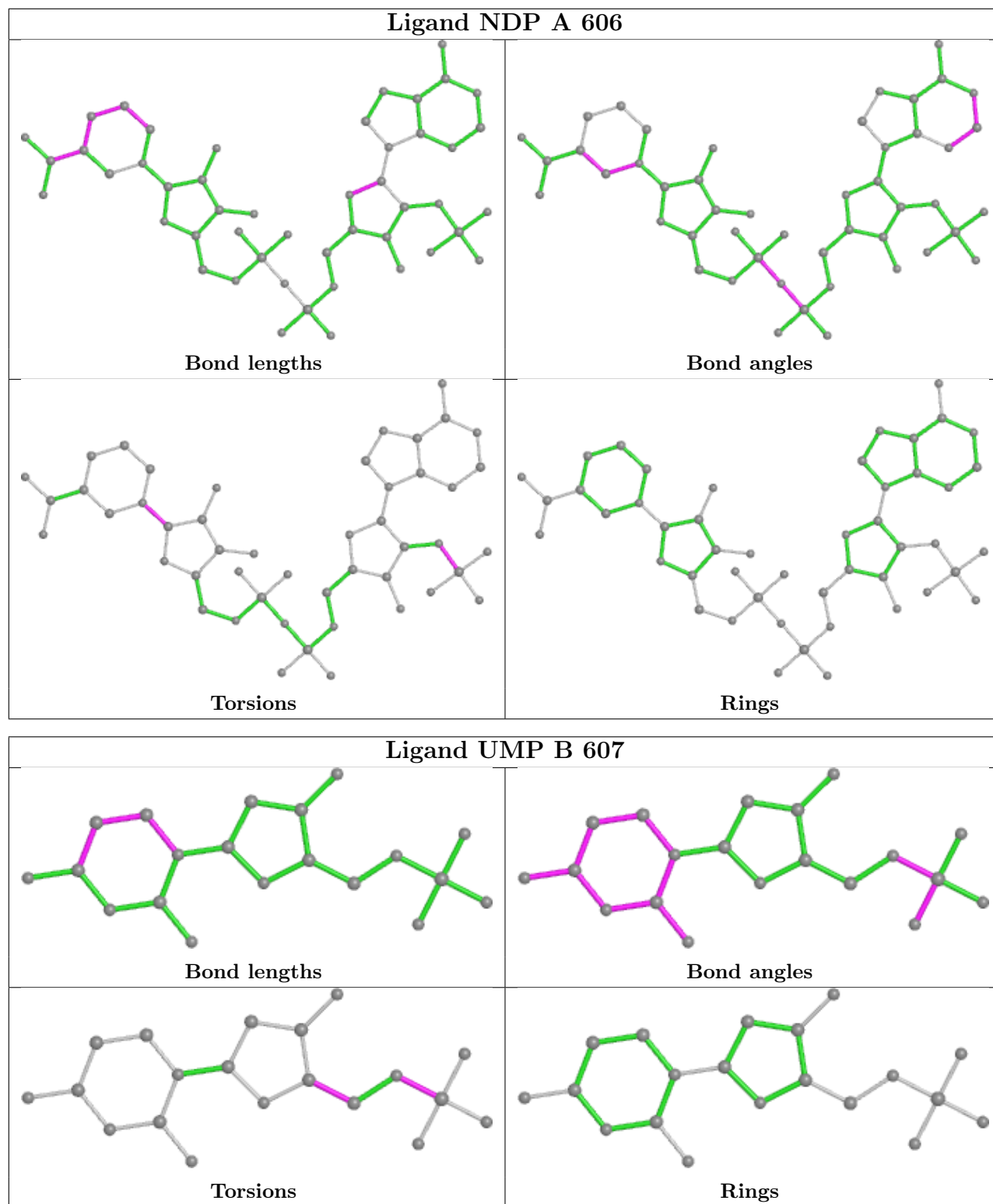












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	507/521 (97%)	-0.16	3 (0%) 89 91	23, 39, 74, 118	0
1	B	508/521 (97%)	-0.30	5 (0%) 82 86	20, 34, 62, 135	0
1	C	508/521 (97%)	-0.09	10 (1%) 65 72	26, 47, 90, 131	0
1	D	507/521 (97%)	0.01	7 (1%) 75 80	29, 50, 84, 158	0
1	E	508/521 (97%)	0.49	33 (6%) 18 21	45, 72, 112, 149	0
All	All	2538/2605 (97%)	-0.01	58 (2%) 60 67	20, 48, 96, 158	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	521	VAL	5.1
1	E	324	TYR	3.9
1	E	179	GLU	3.8
1	E	106	SER	3.6
1	C	181	LYS	3.4
1	E	323	GLU	3.4
1	E	102	MET	3.3
1	E	333	ARG	3.2
1	C	179	GLU	3.2
1	D	102	MET	3.1
1	E	327	ARG	3.1
1	E	45	ASP	3.0
1	E	180	LYS	3.0
1	C	180	LYS	2.9
1	E	44	CYS	2.9
1	D	194	LYS	2.9
1	D	179	GLU	2.9
1	C	45	ASP	2.9
1	E	107	ILE	2.8
1	B	180	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	102	MET	2.7
1	E	104	ASP	2.7
1	B	103	ASN	2.7
1	B	179	GLU	2.7
1	E	84	ALA	2.6
1	A	402	CYS	2.6
1	A	102	MET	2.6
1	D	180	LYS	2.5
1	E	49	LYS	2.5
1	B	181	LYS	2.5
1	E	181	LYS	2.5
1	D	521	VAL	2.4
1	E	175	PHE	2.4
1	E	330	LEU	2.4
1	E	357	HIS	2.4
1	E	328	ILE	2.3
1	E	335	GLU	2.3
1	E	100	ASN	2.3
1	E	360	TYR	2.3
1	C	106	SER	2.2
1	C	84	ALA	2.2
1	C	44	CYS	2.2
1	D	106	SER	2.2
1	C	104	ASP	2.2
1	E	314	TYR	2.2
1	C	107	ILE	2.2
1	A	179	GLU	2.2
1	C	178	GLN	2.2
1	E	338	LEU	2.2
1	E	287	PHE	2.1
1	E	103	ASN	2.1
1	E	48	LYS	2.1
1	E	336	ASN	2.1
1	E	356	MET	2.1
1	E	196	ILE	2.0
1	E	496	ILE	2.0
1	D	324	TYR	2.0
1	E	513	PRO	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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

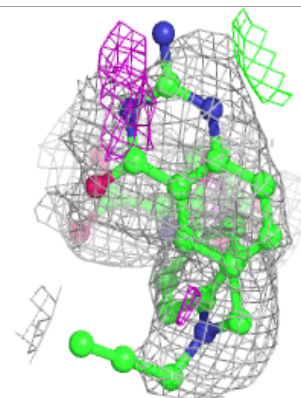
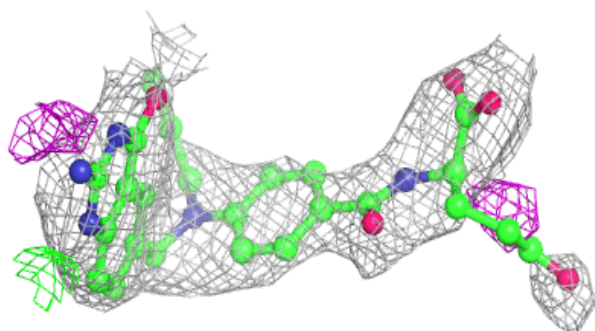
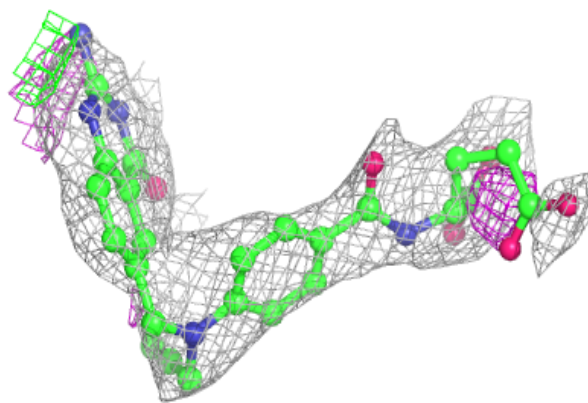
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CB3	E	620	35/35	0.73	0.31	93,98,107,108	0
3	CB3	D	616	35/35	0.78	0.33	69,75,87,89	0
3	CB3	A	604	35/35	0.84	0.24	60,67,76,77	0
2	UMP	E	619	20/20	0.88	0.19	80,88,89,89	0
3	CB3	C	612	35/35	0.90	0.21	49,60,71,73	0
4	DHF	B	609	32/32	0.91	0.18	23,26,39,44	0
4	DHF	C	613	32/32	0.91	0.22	29,35,44,48	0
5	NDP	C	614	48/48	0.91	0.18	65,77,95,95	0
4	DHF	A	605	32/32	0.92	0.16	23,28,38,48	0
2	UMP	A	603	20/20	0.92	0.22	46,57,61,63	0
2	UMP	D	615	20/20	0.92	0.20	53,66,73,73	0
4	DHF	D	617	32/32	0.92	0.16	23,31,41,47	0
3	CB3	B	608	35/35	0.92	0.20	45,50,68,69	0
5	NDP	E	622	48/48	0.92	0.18	66,77,90,92	0
4	DHF	E	621	32/32	0.93	0.22	30,33,42,47	0
2	UMP	C	611	20/20	0.93	0.18	39,50,55,58	0
5	NDP	D	618	48/48	0.93	0.18	50,61,74,76	0
2	UMP	B	607	20/20	0.93	0.19	27,44,48,51	0
5	NDP	A	606	48/48	0.96	0.14	31,40,43,44	0
5	NDP	B	610	48/48	0.97	0.15	31,37,42,43	0

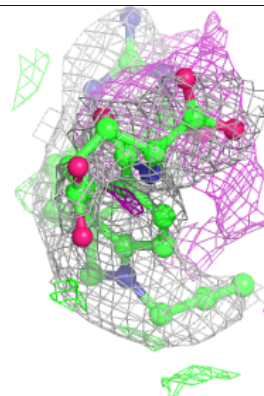
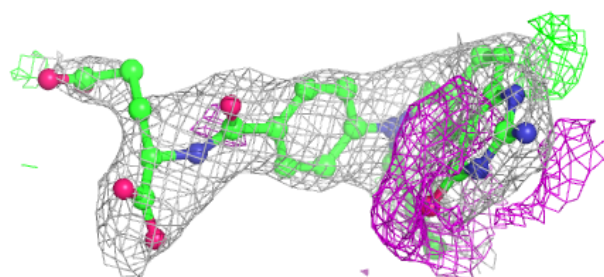
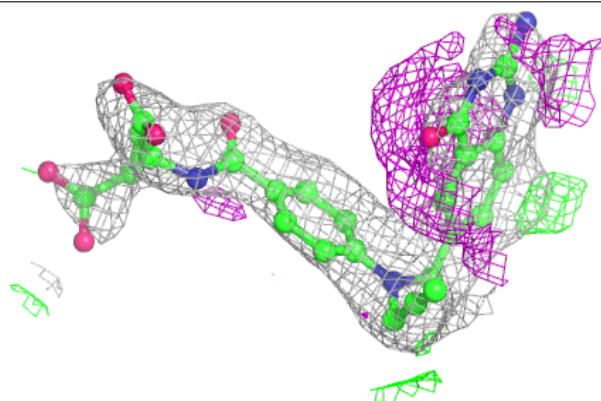
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

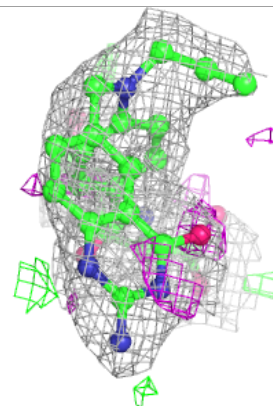
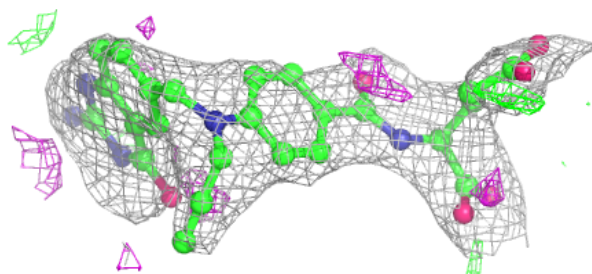
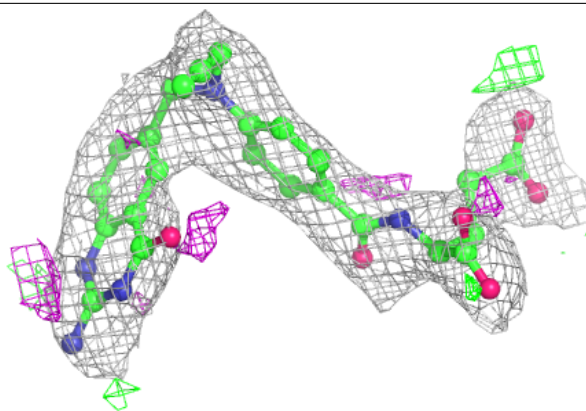
**Electron density around CB3 D 616:**

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

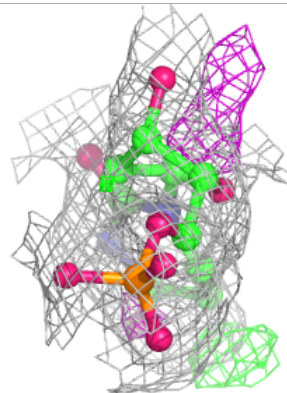
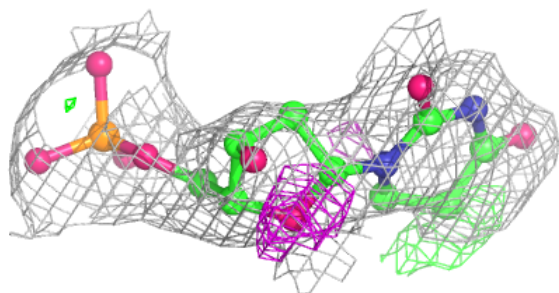
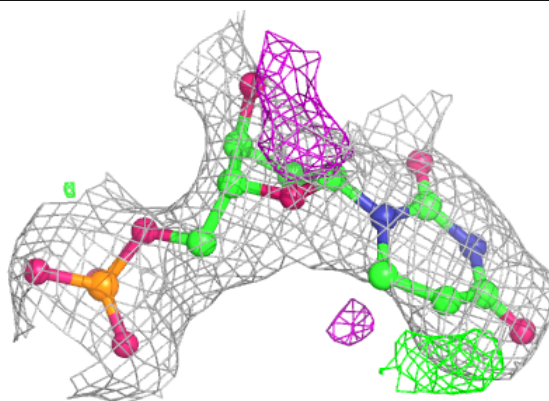


Electron density around CB3 A 604:

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

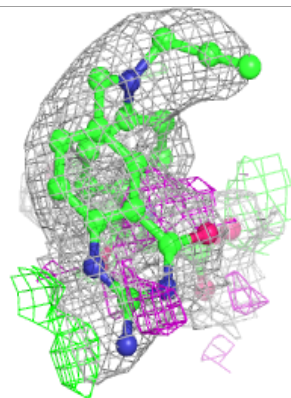
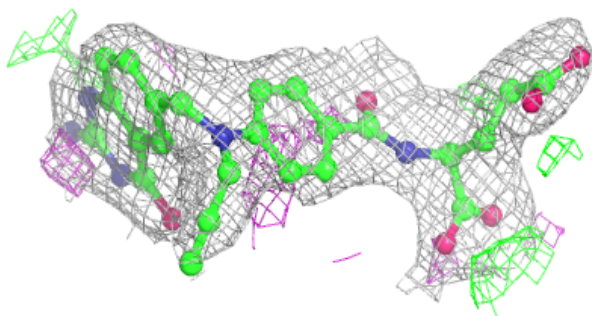
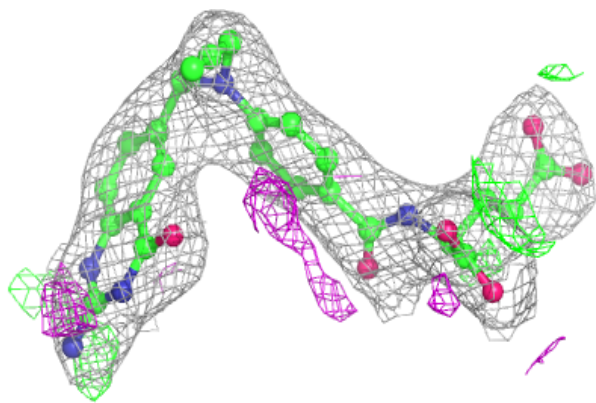
**Electron density around UMP E 619:**

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



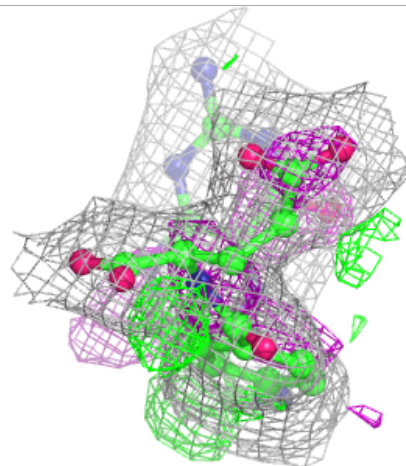
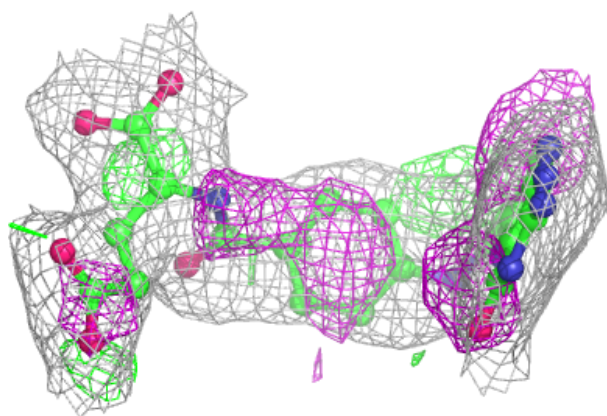
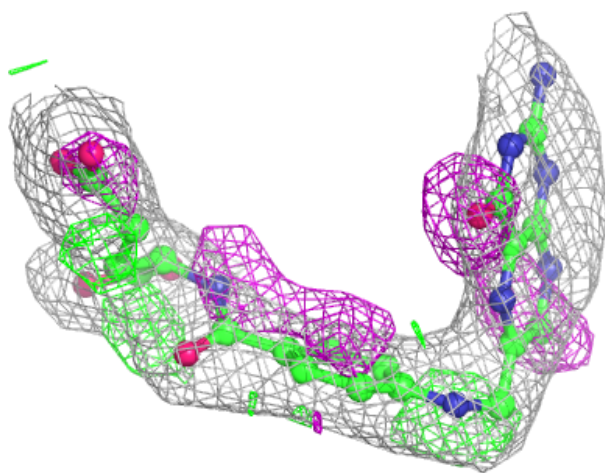
Electron density around CB3 C 612:

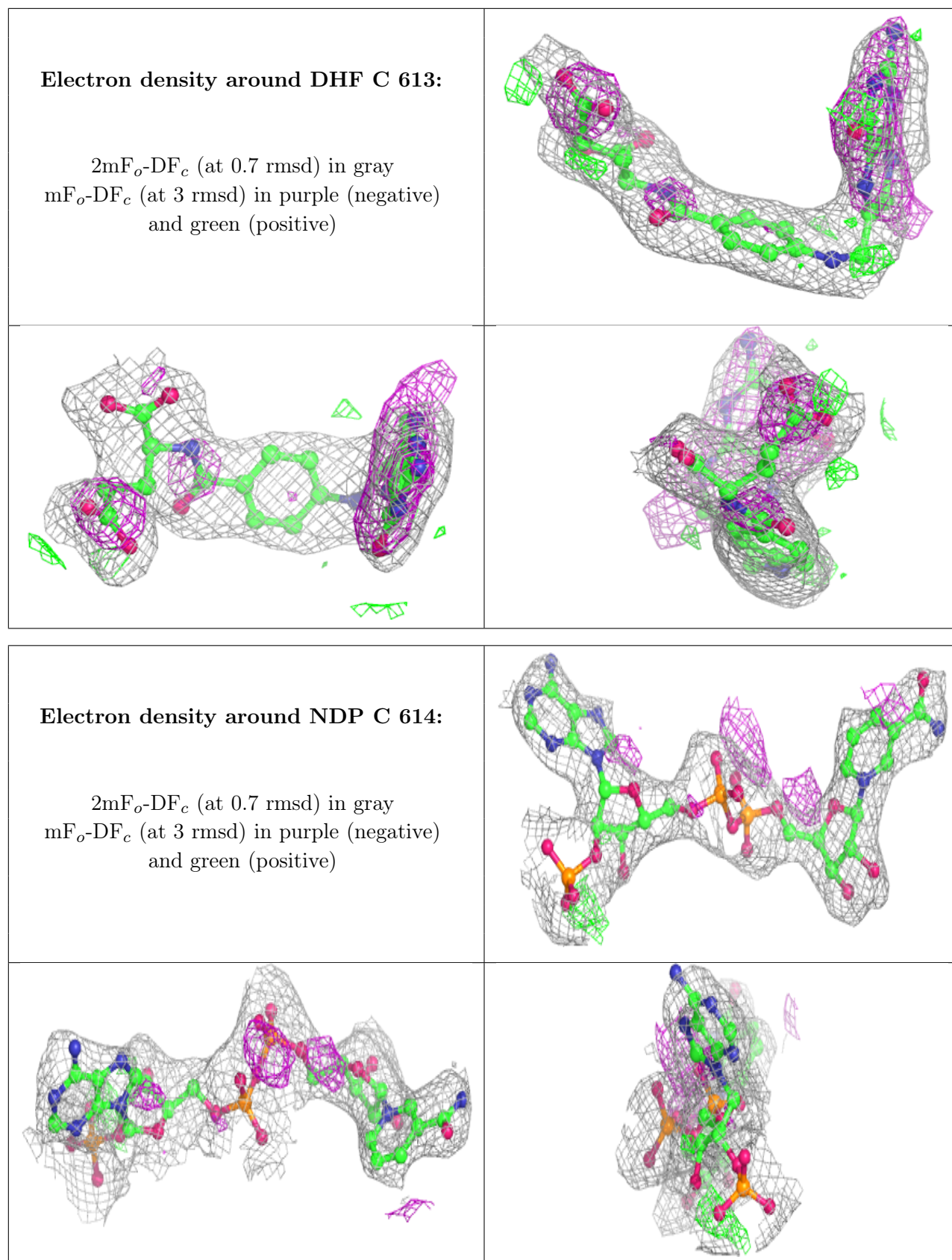
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DHF B 609:

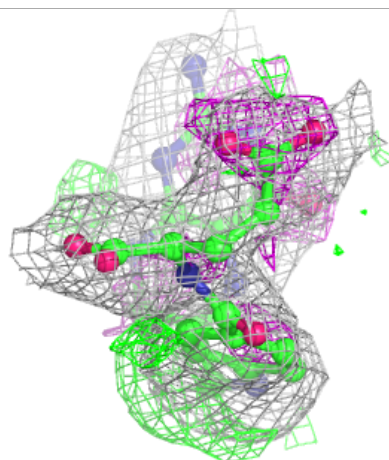
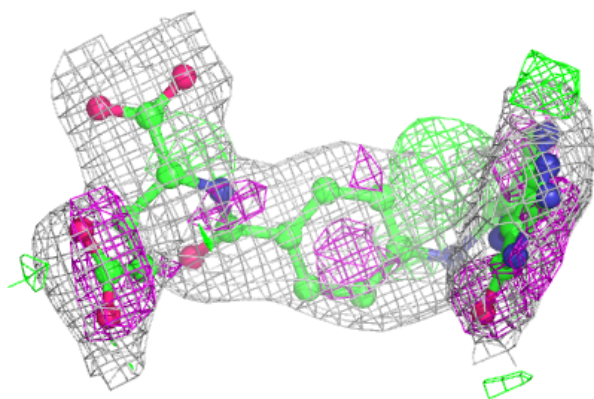
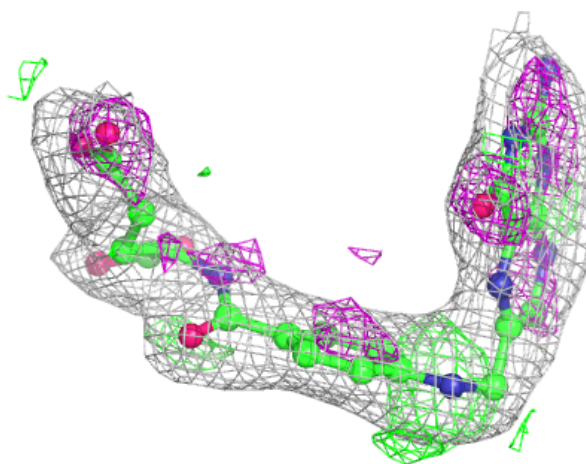
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





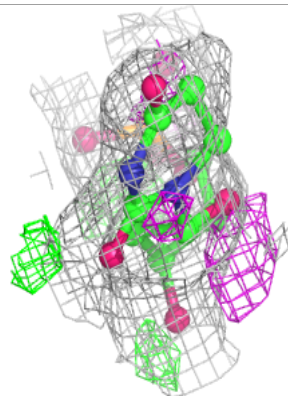
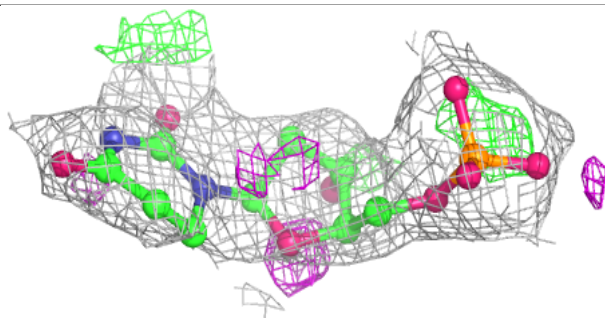
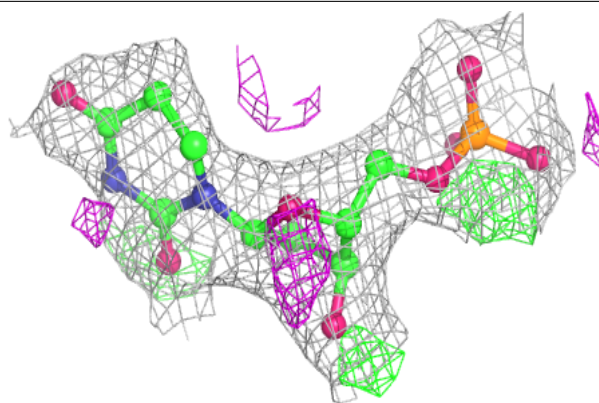
Electron density around DHF A 605:

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

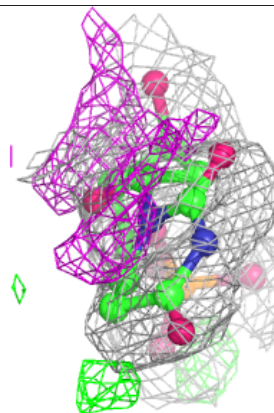
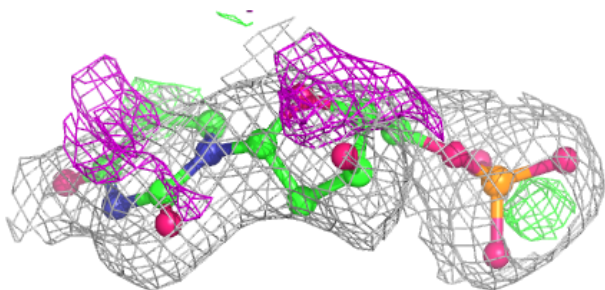
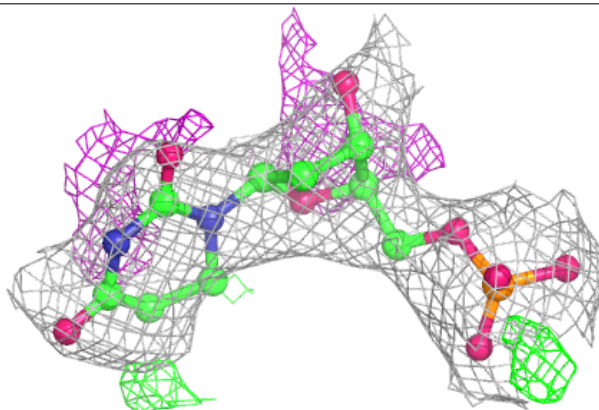


Electron density around UMP A 603:

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

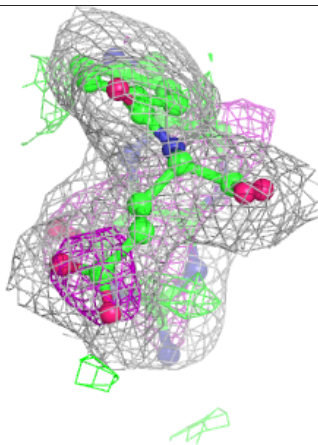
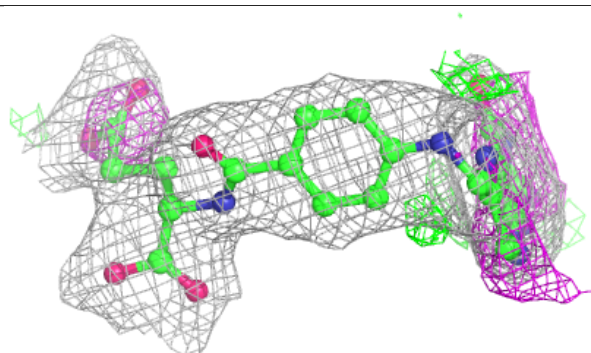
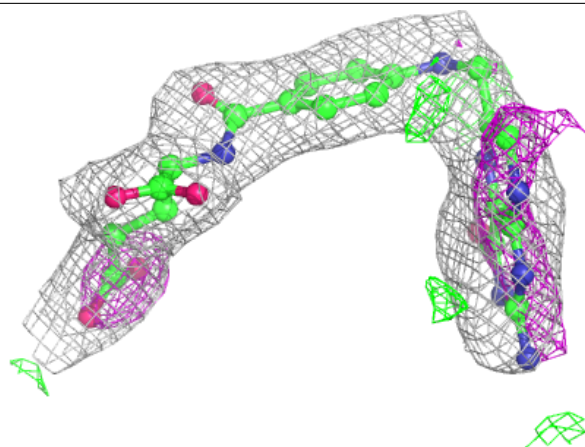
**Electron density around UMP D 615:**

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



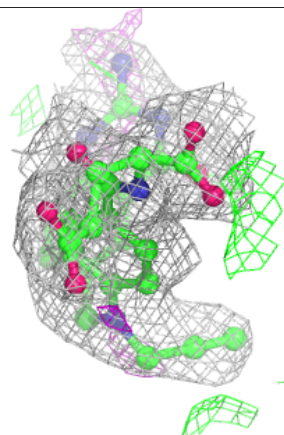
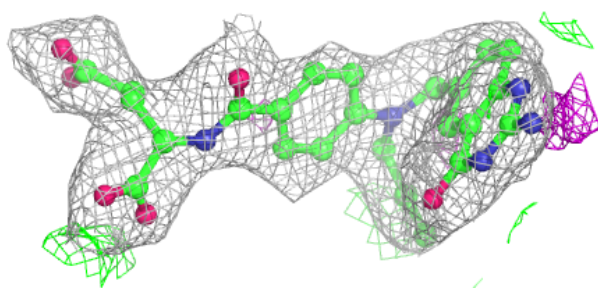
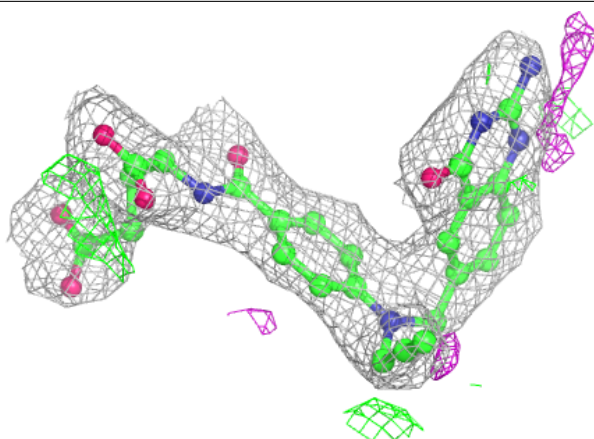
Electron density around DHF D 617:

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

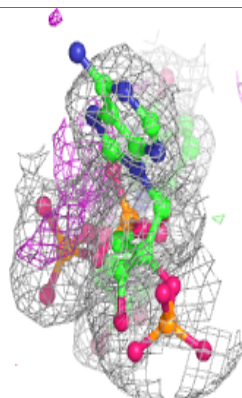
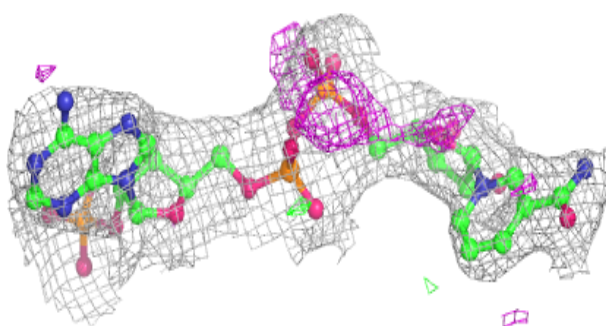
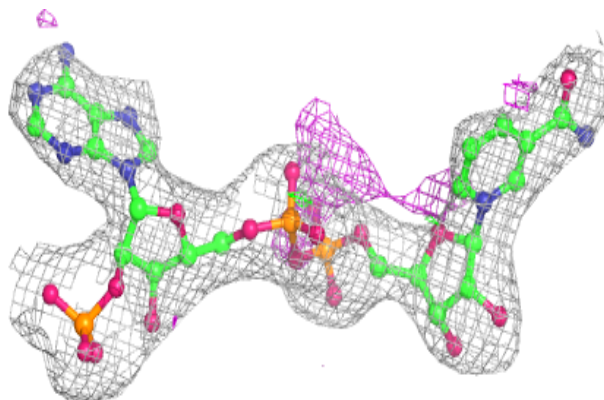


Electron density around CB3 B 608:

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

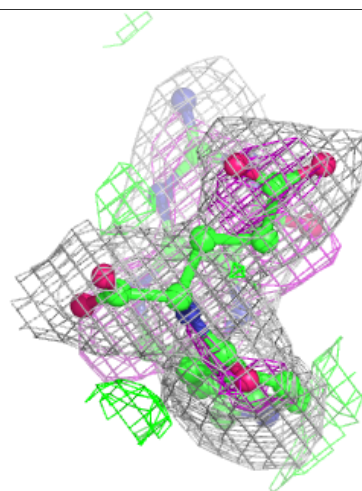
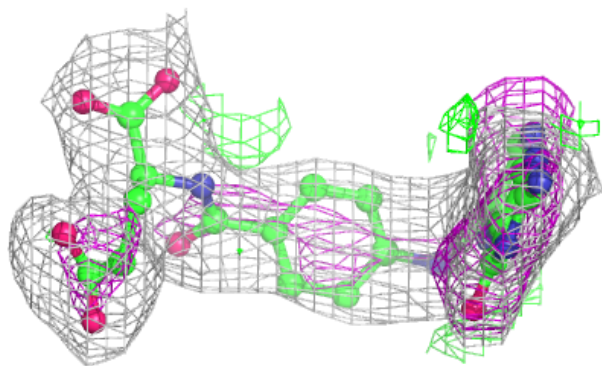
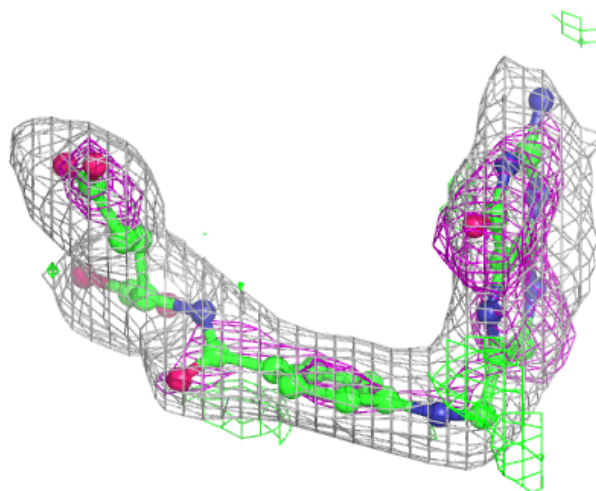
**Electron density around NDP E 622:**

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



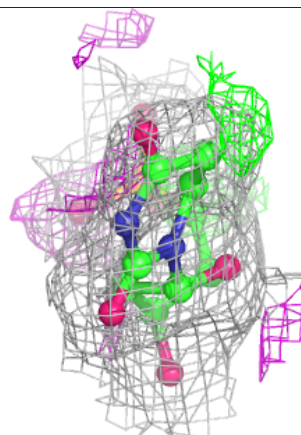
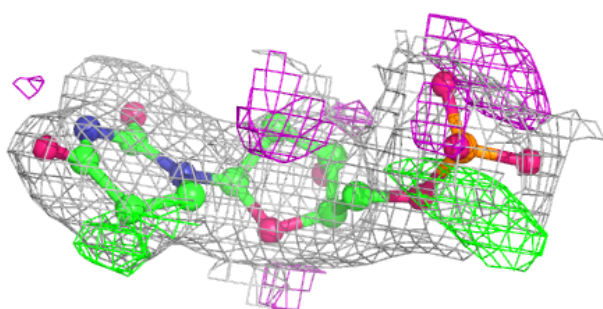
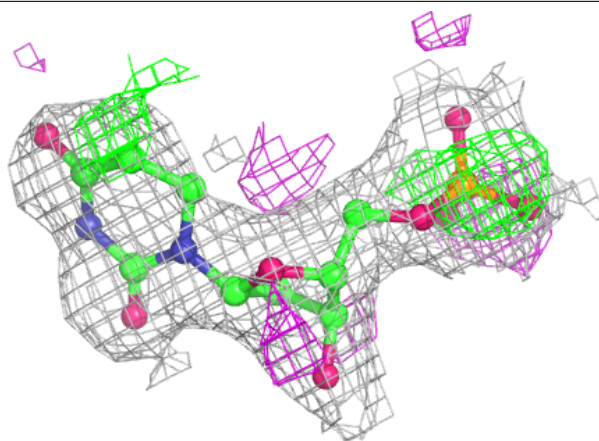
Electron density around DHF E 621:

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

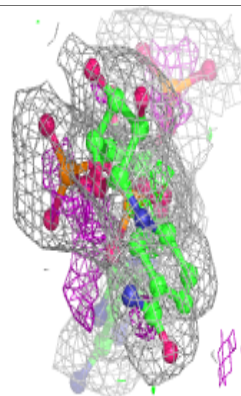
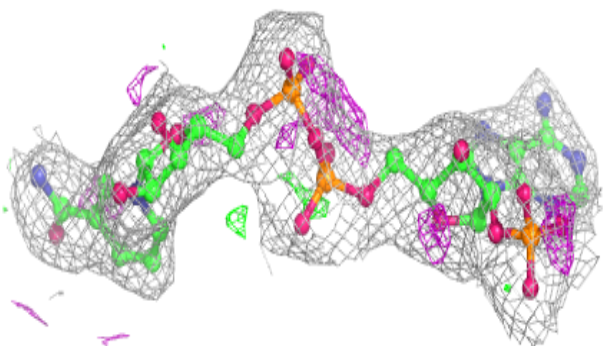
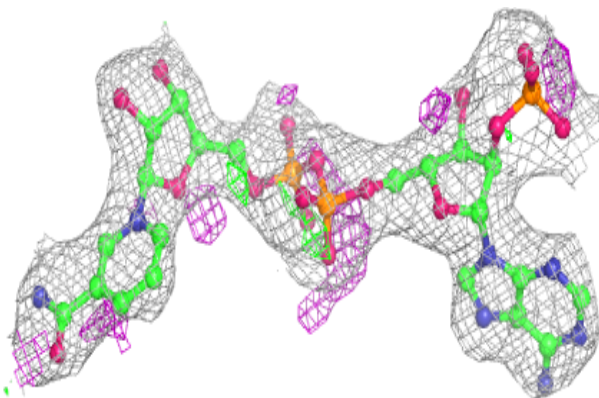


Electron density around UMP C 611:

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

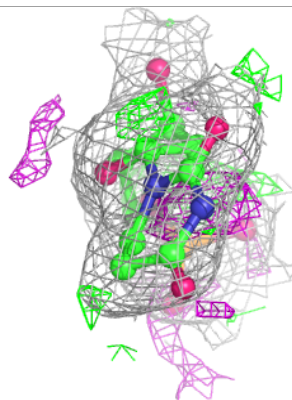
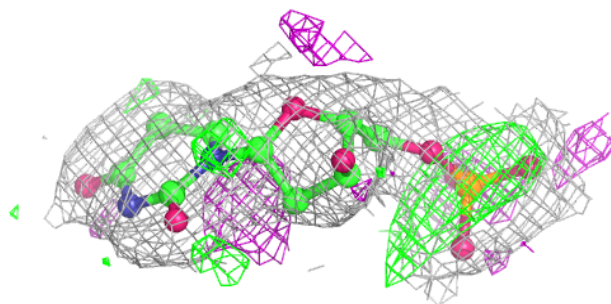
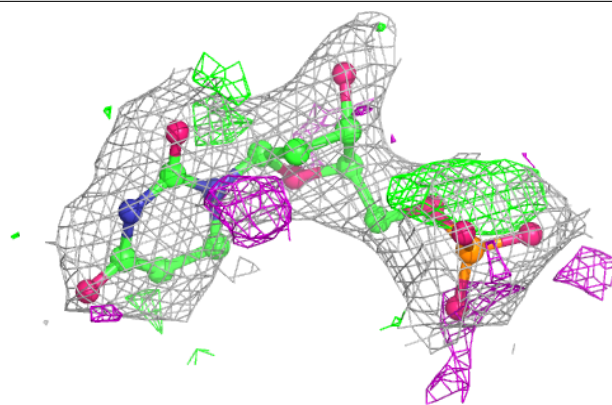
**Electron density around NDP D 618:**

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

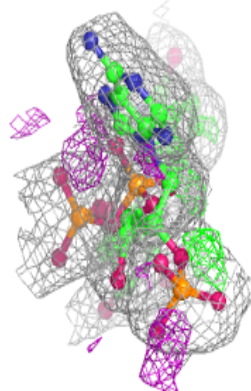
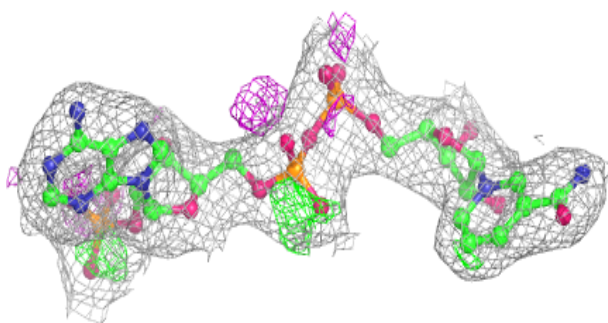
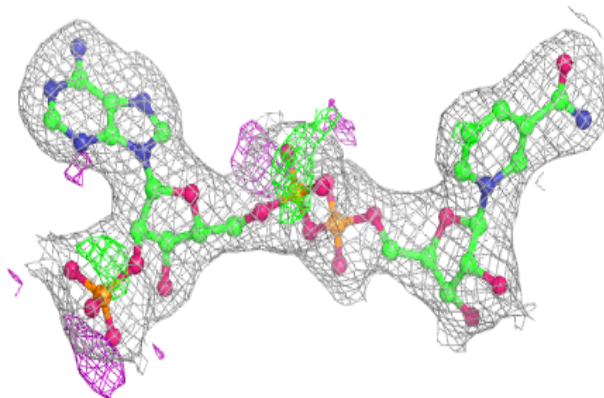


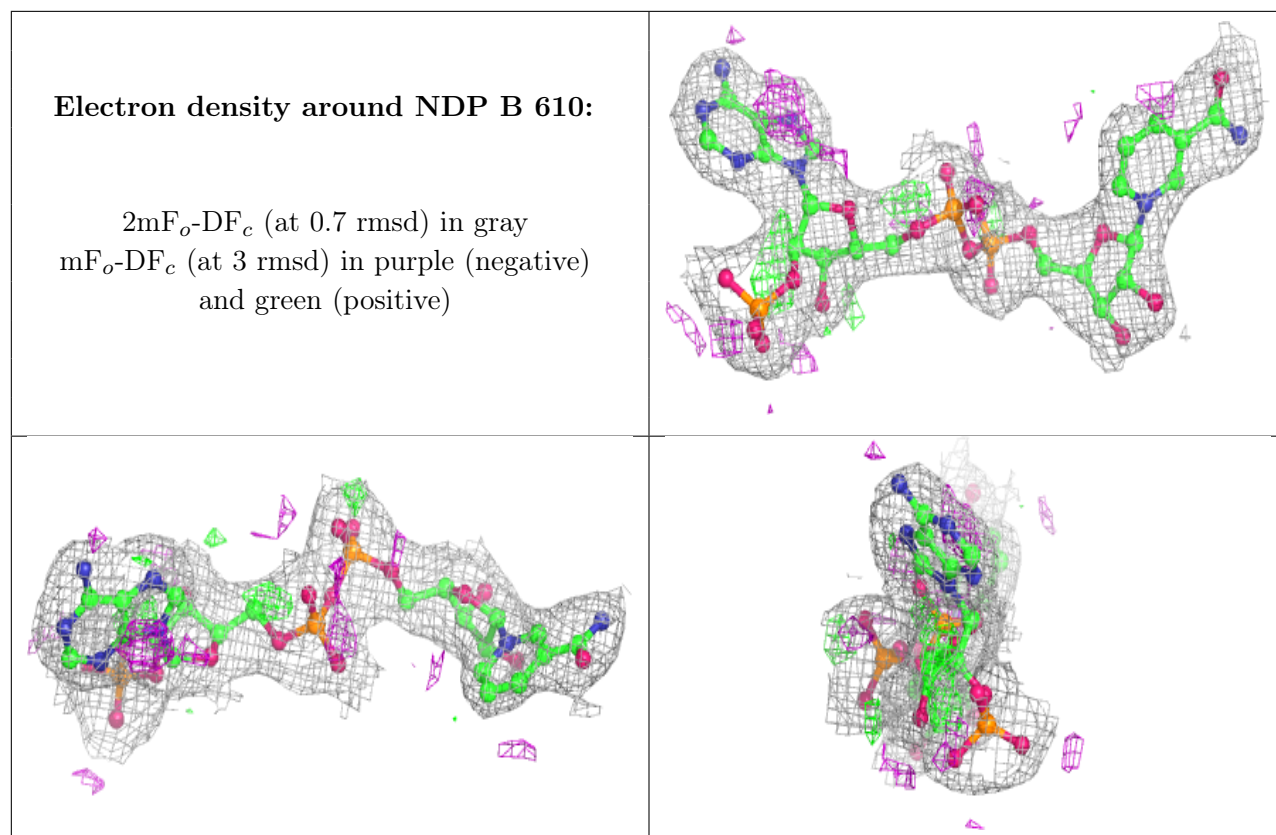
Electron density around UMP B 607:

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

**Electron density around NDP 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.