



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 05:58 AM EDT

PDB ID : 3DL6
Title : Crystal Structure of the A287F/S290G Active Site Mutant of TS-DHFR from *Cryptosporidium hominis*
Authors : Martucci, W.E.; Vargo, M.A.; Anderson, K.S.
Deposited on : 2008-06-26
Resolution : 3.25 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

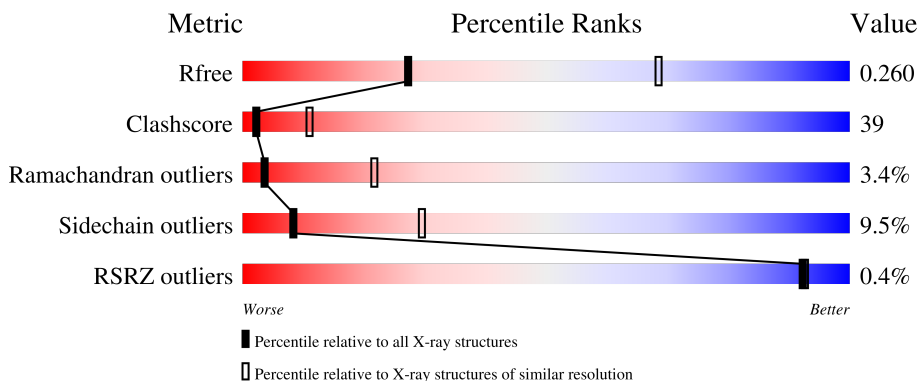
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


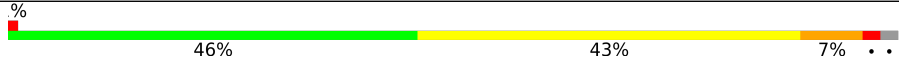

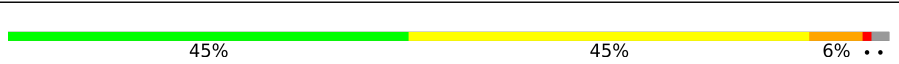
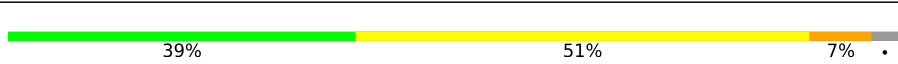
The reported resolution of this entry is 3.25 Å.

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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	
1	B	521	
1	C	521	
1	D	521	
1	E	521	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UMP	A	603	-	-	X	-
2	UMP	B	607	-	-	X	-
2	UMP	E	619	-	-	X	-
3	CB3	B	608	-	-	X	-
3	CB3	C	612	-	-	X	-
3	CB3	D	616	-	-	X	-
3	CB3	E	620	-	-	X	-
4	DHF	A	605	-	-	X	-
4	DHF	B	609	X	-	X	-
4	DHF	C	613	-	-	X	-
4	DHF	D	617	-	-	X	X
4	DHF	E	621	-	-	X	-
5	NDP	C	614	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21446 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.

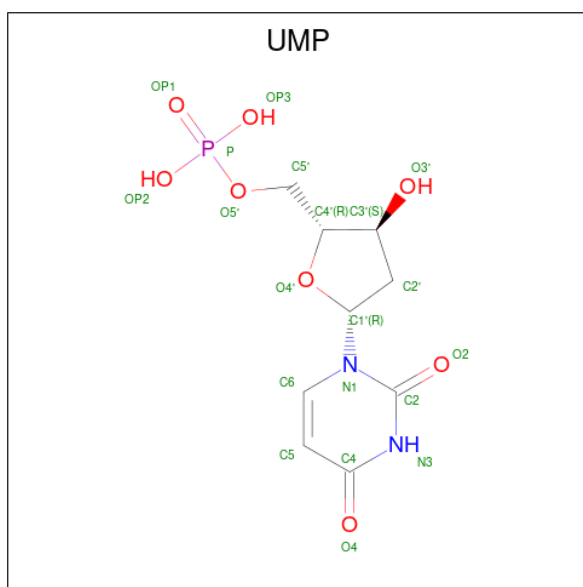
- Molecule 1 is a protein called Dihydrofolate reductase, DHFR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	505	4111	2629	690	770	22	0	0	0
1	B	508	4126	2638	693	773	22	0	0	0
1	C	508	4133	2644	694	773	22	0	0	0
1	D	508	4137	2646	694	775	22	0	0	0
1	E	507	4121	2635	692	772	22	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

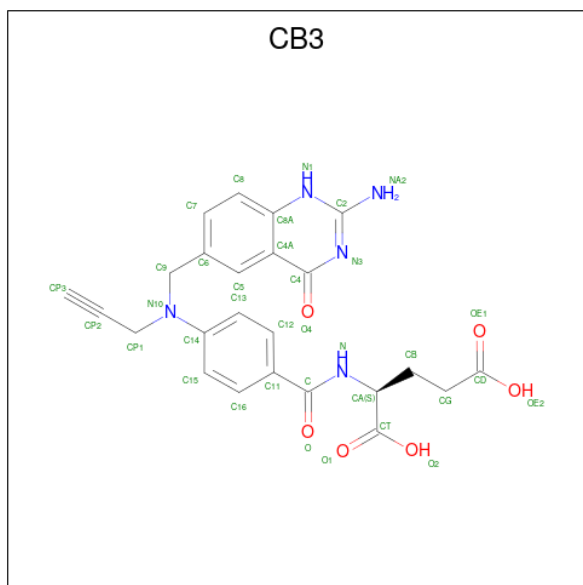
Chain	Residue	Modelled	Actual	Comment	Reference
A	287	PHE	ALA	engineered mutation	UNP Q5CGA3
A	290	GLY	SER	engineered mutation	UNP Q5CGA3
B	287	PHE	ALA	engineered mutation	UNP Q5CGA3
B	290	GLY	SER	engineered mutation	UNP Q5CGA3
C	287	PHE	ALA	engineered mutation	UNP Q5CGA3
C	290	GLY	SER	engineered mutation	UNP Q5CGA3
D	287	PHE	ALA	engineered mutation	UNP Q5CGA3
D	290	GLY	SER	engineered mutation	UNP Q5CGA3
E	287	PHE	ALA	engineered mutation	UNP Q5CGA3
E	290	GLY	SER	engineered mutation	UNP Q5CGA3

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



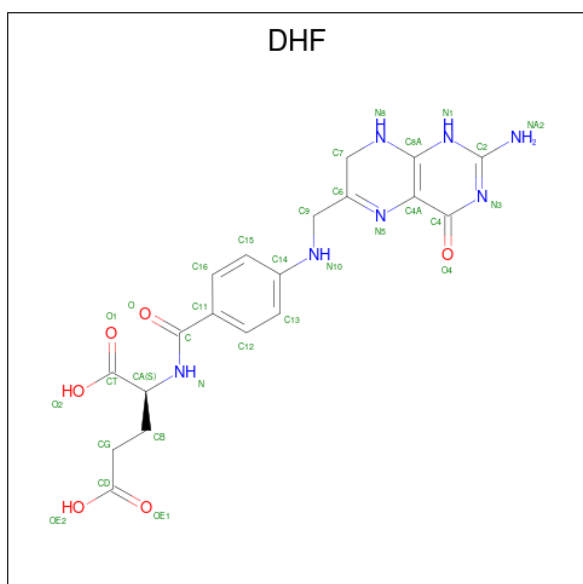
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			
2	A	1	Total	20	9	2	8	1	0	0
2	B	1	Total	20	9	2	8	1	0	0
2	C	1	Total	20	9	2	8	1	0	0
2	D	1	Total	20	9	2	8	1	0	0
2	E	1	Total	20	9	2	8	1	0	0

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



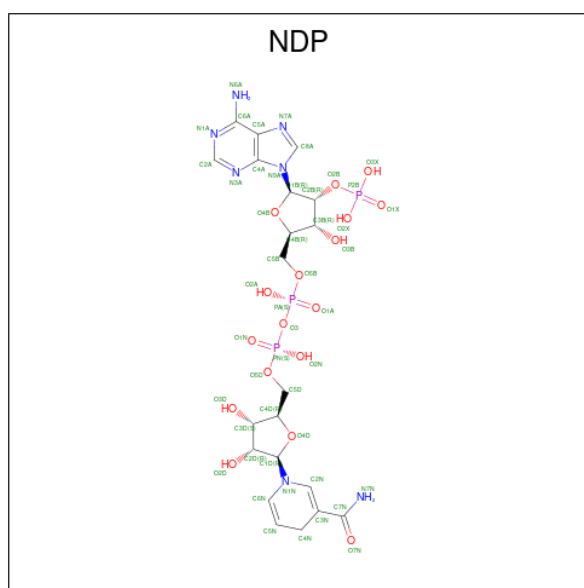
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		
3	D	1	Total	C	N	O	0	0
			35	24	5	6		
3	E	1	Total	C	N	O	0	0
			35	24	5	6		

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



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

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



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

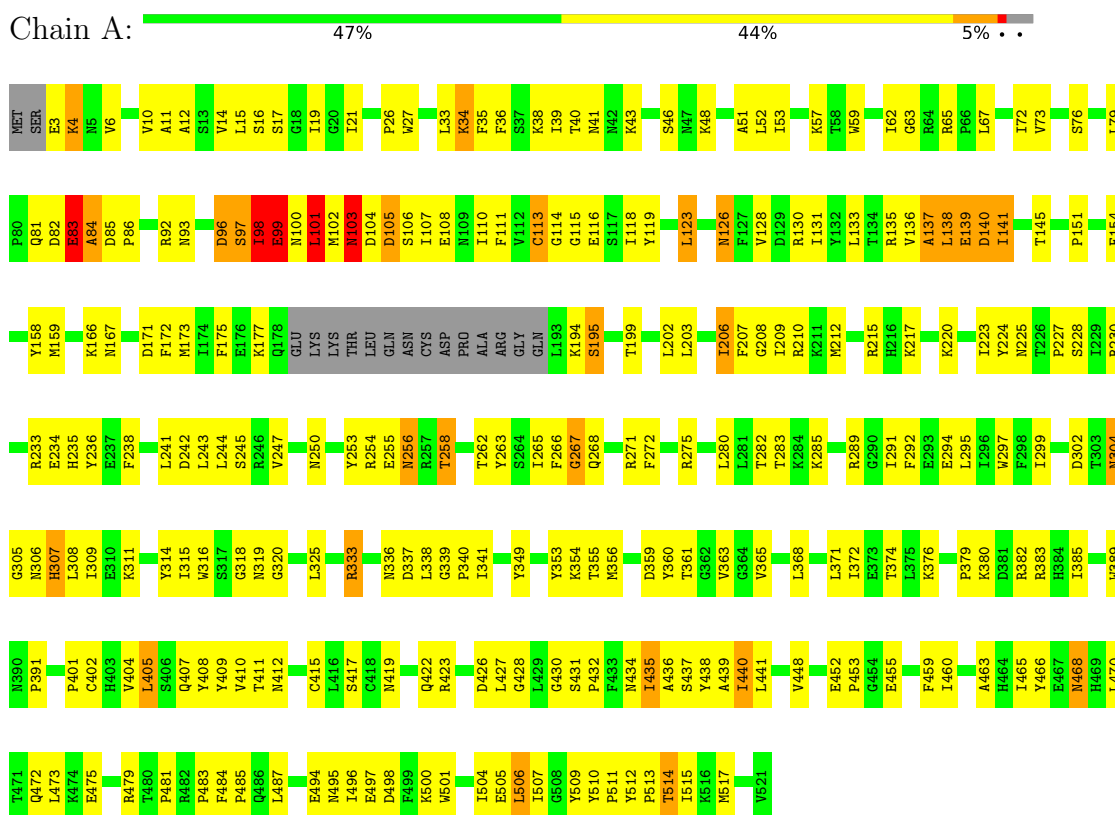
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	35	Total 35	O 35	0	0
6	B	48	Total 48	O 48	0	0
6	C	22	Total 22	O 22	0	0
6	D	23	Total 23	O 23	0	0
6	E	15	Total 15	O 15	0	0

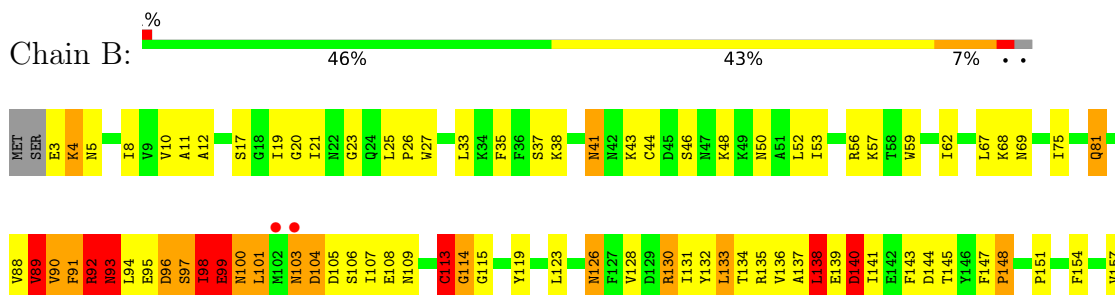
3 Residue-property plots

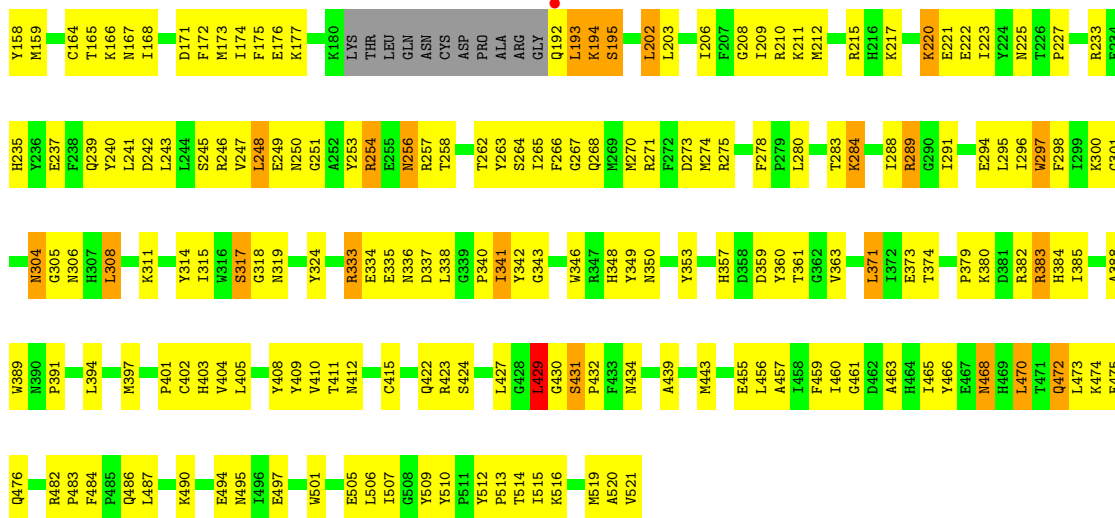
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Dihydrofolate reductase, DHFR

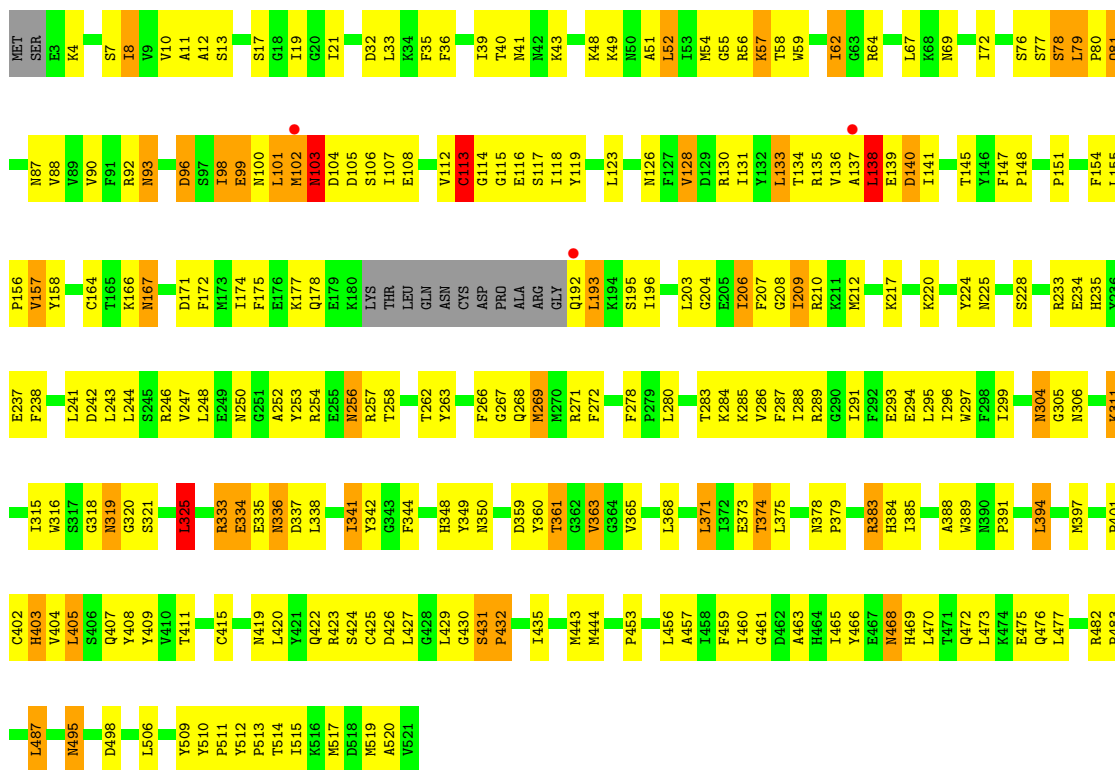


- Molecule 1: Dihydrofolate reductase, DHFR

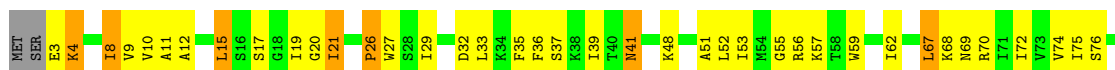


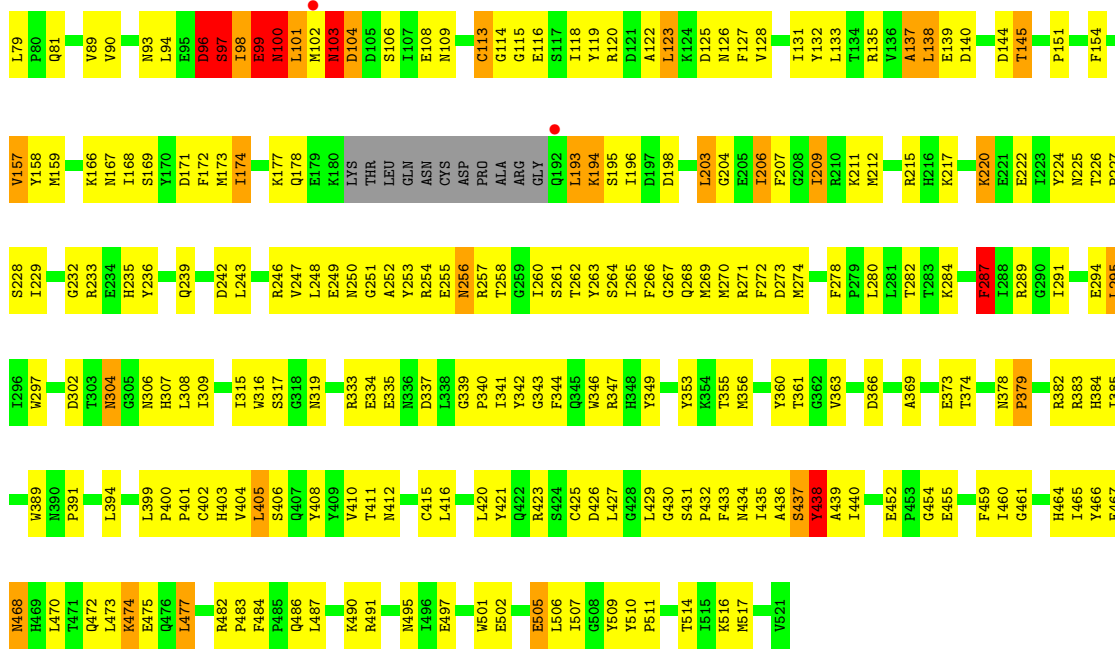


● Molecule 1: Dihydrofolate reductase, DHFR

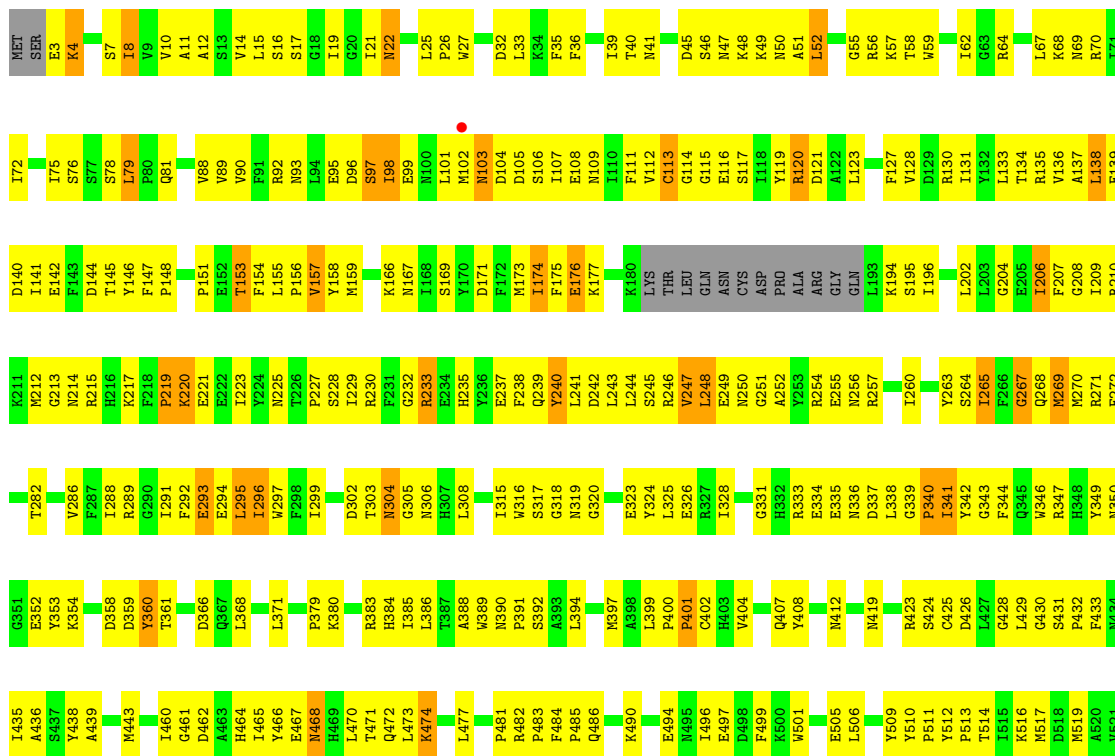
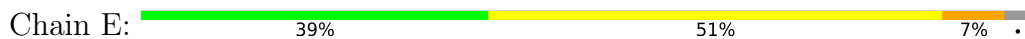


● Molecule 1: Dihydrofolate reductase, DHFR





● 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	214.91Å 116.92Å 220.95Å 90.00° 95.94° 90.00°	Depositor
Resolution (Å)	3.45 – 3.25 46.21 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.2 (3.45-3.25) 98.2 (46.21-3.26)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 3.25Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.276 0.211 , 0.260	Depositor DCC
R_{free} test set	4159 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtrriage
Anisotropy	0.359	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	21446	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/4207	0.68	0/5686
1	B	0.39	0/4222	0.65	0/5707
1	C	0.39	0/4229	0.66	0/5715
1	D	0.38	1/4233 (0.0%)	0.65	0/5720
1	E	0.35	0/4217	0.65	0/5700
All	All	0.38	1/21108 (0.0%)	0.66	0/28528

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	7
1	B	0	9
1	C	0	3
1	D	0	5
1	E	0	2
All	All	0	26

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	379	PRO	N-CD	5.38	1.55	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	LEU	Peptide
1	A	113	CYS	Peptide
1	A	138	LEU	Peptide
1	A	140	ASP	Peptide
1	A	81	GLN	Peptide
1	A	83	GLU	Peptide
1	A	98	ILE	Peptide
1	B	100	ASN	Peptide
1	B	113	CYS	Peptide
1	B	114	GLY	Peptide
1	B	138	LEU	Peptide
1	B	429	LEU	Peptide
1	B	90	VAL	Peptide
1	B	91	PHE	Peptide
1	B	92	ARG	Peptide
1	B	98	ILE	Peptide
1	C	112	VAL	Peptide
1	C	113	CYS	Peptide
1	C	138	LEU	Peptide
1	D	100	ASN	Peptide
1	D	113	CYS	Peptide
1	D	438	TYR	Peptide
1	D	97	SER	Peptide
1	D	98	ILE	Peptide
1	E	112	VAL	Peptide
1	E	113	CYS	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	4111	0	4031	311	0
1	B	4126	0	4036	325	0
1	C	4133	0	4057	332	0
1	D	4137	0	4061	343	0
1	E	4121	0	4035	332	0
2	A	20	0	11	8	0
2	B	20	0	11	10	0
2	C	20	0	10	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	20	0	11	3	0
2	E	20	0	11	10	0
3	A	35	0	21	5	0
3	B	35	0	21	14	0
3	C	35	0	21	15	0
3	D	35	0	21	14	0
3	E	35	0	21	13	0
4	A	32	0	19	9	0
4	B	32	0	19	18	0
4	C	32	0	19	24	0
4	D	32	0	19	33	0
4	E	32	0	19	20	0
5	A	48	0	26	18	0
5	B	48	0	26	13	0
5	C	48	0	26	23	0
5	D	48	0	26	14	0
5	E	48	0	26	19	0
6	A	35	0	0	2	0
6	B	48	0	0	1	0
6	C	22	0	0	1	0
6	D	23	0	0	5	0
6	E	15	0	0	1	0
All	All	21446	0	20604	1630	0

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 39.

All (1630) 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:A:349:TYR:CE2	1:B:391:PRO:HD2	1.31	1.63
1:C:349:TYR:CE2	1:D:391:PRO:HD2	1.57	1.39
1:B:81:GLN:OE1	1:B:92:ARG:NH1	1.59	1.34
1:B:67:LEU:HD22	4:B:609:DHF:O2	1.24	1.31
1:D:67:LEU:CD2	4:D:617:DHF:O2	1.81	1.26
1:B:67:LEU:CD2	4:B:609:DHF:O2	1.84	1.24
1:B:138:LEU:HD13	1:B:168:ILE:CD1	1.68	1.23
1:A:349:TYR:CZ	1:B:391:PRO:HD2	1.75	1.21
1:D:99:GLU:O	1:D:102:MET:N	1.71	1.20
1:E:33:LEU:CD2	4:E:621:DHF:H12	1.70	1.20
1:A:349:TYR:CE2	1:B:391:PRO:CD	2.23	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LYS:HB2	5:D:618:NDP:O1A	1.38	1.19
1:D:430:GLY:HA2	3:D:616:CB3:CP3	1.75	1.17
1:B:4:LYS:HB3	1:B:101:LEU:CD2	1.76	1.15
1:C:62:ILE:HD11	4:C:613:DHF:C16	1.76	1.15
1:D:67:LEU:HD23	4:D:617:DHF:O2	1.39	1.14
1:C:62:ILE:CG1	4:C:613:DHF:H15	1.78	1.14
1:E:26:PRO:HB2	1:E:27:TRP:CE3	1.84	1.12
1:C:4:LYS:HB3	1:C:101:LEU:HD23	1.25	1.12
1:C:115:GLY:HA3	5:C:614:NDP:O2A	1.47	1.11
1:C:430:GLY:HA2	3:C:612:CB3:HP3	1.29	1.11
1:B:402:CYS:SG	2:B:607:UMP:C6	2.44	1.11
1:C:33:LEU:HD22	4:C:613:DHF:H12	1.32	1.10
1:C:62:ILE:HG12	4:C:613:DHF:H15	1.34	1.10
1:B:139:GLU:O	1:B:140:ASP:HB2	1.51	1.10
1:C:93:ASN:HD21	1:C:96:ASP:HB2	0.94	1.08
1:E:21:ILE:HD12	1:E:142:GLU:O	1.53	1.08
1:C:62:ILE:HD11	4:C:613:DHF:H16	1.29	1.08
1:A:33:LEU:HD22	4:A:605:DHF:H16	1.28	1.07
1:C:93:ASN:ND2	1:C:96:ASP:HB2	1.68	1.06
1:B:4:LYS:HB3	1:B:101:LEU:HD23	1.08	1.06
1:D:15:LEU:HB2	1:D:139:GLU:HG2	1.35	1.06
1:D:430:GLY:HA2	3:D:616:CB3:HP3	1.15	1.06
1:B:26:PRO:HG2	1:B:27:TRP:CE3	1.90	1.06
1:E:430:GLY:O	3:E:620:CB3:HP3	1.57	1.05
1:B:137:ALA:O	1:B:510:TYR:HE2	1.40	1.05
4:D:617:DHF:C16	4:D:617:DHF:HB2	1.87	1.05
1:C:193:LEU:HD23	1:C:193:LEU:N	1.67	1.04
1:E:3:GLU:HG3	1:E:4:LYS:H	1.22	1.04
1:B:209:ILE:HD12	1:B:209:ILE:H	1.20	1.03
1:D:430:GLY:CA	3:D:616:CB3:HP3	1.88	1.03
1:B:26:PRO:HG2	1:B:27:TRP:CZ3	1.93	1.03
1:C:383:ARG:NH1	2:D:615:UMP:OP1	1.90	1.02
4:C:613:DHF:H72	5:C:614:NDP:H42N	1.42	1.01
1:D:97:SER:O	1:D:99:GLU:HG3	1.58	1.01
1:D:455:GLU:HA	6:D:640:HOH:O	1.58	1.01
1:B:138:LEU:HD13	1:B:168:ILE:HD12	1.43	1.00
1:C:4:LYS:HB3	1:C:101:LEU:CD2	1.90	1.00
1:D:33:LEU:HB3	4:D:617:DHF:HG2	1.02	1.00
5:A:606:NDP:H1B	5:A:606:NDP:O2X	1.60	0.99
1:B:139:GLU:HB3	1:B:510:TYR:CZ	1.98	0.99
4:B:609:DHF:HA	4:B:609:DHF:C12	1.93	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:TYR:O	1:D:363:VAL:HG12	1.63	0.99
1:E:116:GLU:HB2	1:E:145:THR:HG23	1.42	0.98
1:C:62:ILE:HD11	4:C:613:DHF:C15	1.93	0.98
1:A:217:LYS:H	1:A:250:ASN:HD21	1.10	0.98
1:D:33:LEU:HB3	4:D:617:DHF:CG	1.92	0.98
1:C:79:LEU:HD23	1:C:80:PRO:HD2	1.45	0.98
1:E:116:GLU:HB2	1:E:145:THR:CG2	1.94	0.98
1:B:472:GLN:H	1:B:472:GLN:HE21	1.09	0.98
1:A:349:TYR:CZ	1:B:391:PRO:CD	2.44	0.97
1:B:402:CYS:SG	2:B:607:UMP:H6	1.87	0.97
1:C:476:GLN:HE21	1:C:515:ILE:HD12	1.30	0.97
1:B:4:LYS:CB	1:B:101:LEU:HD23	1.93	0.97
1:B:217:LYS:H	1:B:250:ASN:HD21	1.05	0.97
1:E:33:LEU:HD21	4:E:621:DHF:H12	1.40	0.96
1:B:138:LEU:CD1	1:B:168:ILE:CD1	2.42	0.96
1:D:67:LEU:HD21	4:D:617:DHF:O2	1.64	0.96
1:D:33:LEU:CB	4:D:617:DHF:HG2	1.95	0.96
1:C:319:ASN:OD1	3:C:612:CB3:H8	1.65	0.95
1:D:15:LEU:CB	1:D:139:GLU:HG2	1.95	0.95
1:B:304:ASN:C	1:B:304:ASN:HD22	1.68	0.95
1:C:430:GLY:HA2	3:C:612:CB3:CP3	1.94	0.95
1:C:430:GLY:CA	3:C:612:CB3:HP3	1.97	0.95
1:E:3:GLU:HG3	1:E:4:LYS:N	1.81	0.95
1:E:217:LYS:H	1:E:250:ASN:HD21	1.10	0.94
2:A:603:UMP:OP1	1:B:383:ARG:NH1	2.00	0.94
1:A:67:LEU:HD21	4:A:605:DHF:H12	1.47	0.94
1:A:102:MET:O	1:A:103:ASN:HB3	1.64	0.94
1:A:57:LYS:HD3	5:A:606:NDP:O2N	1.68	0.93
4:D:617:DHF:O2	4:D:617:DHF:H12	1.68	0.93
1:E:67:LEU:HD12	1:E:72:ILE:HD11	1.50	0.93
1:A:349:TYR:HE2	1:B:391:PRO:HD2	1.30	0.92
1:B:94:LEU:O	1:B:94:LEU:HD12	1.69	0.92
1:B:304:ASN:ND2	1:B:306:ASN:H	1.65	0.92
1:D:15:LEU:HB2	1:D:139:GLU:CG	2.00	0.92
1:D:468:ASN:H	1:D:468:ASN:HD22	1.10	0.92
1:C:62:ILE:CD1	4:C:613:DHF:H15	1.99	0.92
1:A:468:ASN:HD22	1:A:468:ASN:H	1.17	0.92
4:D:617:DHF:HB2	4:D:617:DHF:C11	1.97	0.91
1:C:349:TYR:CE2	1:D:391:PRO:CD	2.50	0.91
1:C:62:ILE:CD1	4:C:613:DHF:C15	2.48	0.91
1:B:137:ALA:O	1:B:510:TYR:CE2	2.23	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.53	0.91
1:E:430:GLY:HA2	3:E:620:CB3:CP3	2.01	0.90
1:A:512:TYR:HB3	1:A:513:PRO:HD2	1.51	0.90
1:C:33:LEU:CD2	4:C:613:DHF:H12	2.02	0.90
1:B:430:GLY:O	3:B:608:CB3:HP3	1.72	0.89
1:E:225:ASN:O	1:E:233:ARG:NH2	2.06	0.89
1:E:468:ASN:HD22	1:E:468:ASN:H	1.16	0.89
1:D:67:LEU:HD12	1:D:72:ILE:HD11	1.54	0.88
1:D:3:GLU:HG3	1:D:4:LYS:H	1.38	0.88
1:D:114:GLY:HA3	1:D:119:TYR:CZ	2.09	0.88
1:E:62:ILE:HG13	4:E:621:DHF:C15	2.04	0.87
1:B:289:ARG:NH2	1:B:311:LYS:O	2.07	0.87
1:C:217:LYS:H	1:C:250:ASN:HD21	1.20	0.87
1:A:115:GLY:HA3	5:A:606:NDP:O2A	1.74	0.87
1:E:52:LEU:HB3	1:E:113:CYS:SG	2.14	0.87
1:B:37:SER:HB2	4:B:609:DHF:HG2	1.55	0.87
1:A:139:GLU:HB3	1:A:510:TYR:CZ	2.10	0.86
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.40	0.86
1:E:137:ALA:O	1:E:510:TYR:HE2	1.58	0.86
1:E:151:PRO:HG2	1:E:154:PHE:HD2	1.40	0.86
1:E:426:ASP:N	2:E:619:UMP:O2	2.06	0.86
1:E:333:ARG:HG3	1:E:337:ASP:HB3	1.58	0.86
1:D:52:LEU:HB3	1:D:113:CYS:SG	2.15	0.85
1:B:97:SER:O	1:B:100:ASN:ND2	2.09	0.85
1:C:193:LEU:HD23	1:C:193:LEU:H	1.37	0.85
1:D:10:VAL:N	4:D:617:DHF:HN21	1.74	0.85
1:C:62:ILE:CD1	4:C:613:DHF:C16	2.54	0.85
1:D:67:LEU:HD21	4:D:617:DHF:H12	1.58	0.85
1:E:26:PRO:HB2	1:E:27:TRP:CZ3	2.11	0.85
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.58	0.85
1:A:304:ASN:ND2	1:A:306:ASN:H	1.74	0.84
1:D:217:LYS:H	1:D:250:ASN:HD21	1.22	0.84
1:A:4:LYS:CE	1:A:101:LEU:HA	2.06	0.84
1:E:423:ARG:HG3	1:E:423:ARG:HH11	1.43	0.84
1:C:243:LEU:HD11	1:C:268:GLN:HG3	1.59	0.83
1:A:3:GLU:HG3	1:A:4:LYS:H	1.42	0.83
1:C:304:ASN:C	1:C:304:ASN:HD22	1.82	0.83
1:E:116:GLU:OE2	1:E:145:THR:HG23	1.78	0.83
1:B:138:LEU:HD13	1:B:168:ILE:HD11	1.59	0.83
1:B:67:LEU:HD21	4:B:609:DHF:O2	1.77	0.83
1:C:156:PRO:HG3	1:C:175:PHE:CE2	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:613:DHF:C7	5:C:614:NDP:H42N	2.09	0.83
1:E:252:ALA:O	1:E:254:ARG:HG3	1.78	0.83
1:B:359:ASP:OD1	1:B:361:THR:HG22	1.77	0.82
1:D:118:ILE:HD11	5:D:618:NDP:C8A	2.09	0.82
1:A:67:LEU:HD12	1:A:72:ILE:HD11	1.59	0.82
1:B:48:LYS:HE2	1:B:105:ASP:O	1.79	0.82
1:A:33:LEU:CD2	4:A:605:DHF:H16	2.10	0.82
1:E:3:GLU:CG	1:E:4:LYS:H	1.92	0.82
1:C:304:ASN:ND2	1:C:306:ASN:H	1.77	0.81
1:B:314:TYR:O	1:B:317:SER:OG	1.96	0.81
4:B:609:DHF:HA	4:B:609:DHF:H12	1.63	0.81
1:E:359:ASP:O	1:E:360:TYR:C	2.19	0.81
1:B:171:ASP:OD2	1:B:483:PRO:HG3	1.79	0.81
1:B:262:THR:HG22	1:B:466:TYR:HA	1.63	0.81
1:A:360:TYR:O	1:A:363:VAL:HG12	1.80	0.81
1:C:62:ILE:CD1	4:C:613:DHF:H16	2.10	0.81
1:A:114:GLY:HA2	1:A:119:TYR:CE1	2.15	0.81
1:A:104:ASP:C	1:A:106:SER:H	1.84	0.81
1:E:248:LEU:HD13	1:E:465:ILE:HD12	1.63	0.81
1:E:430:GLY:HA2	3:E:620:CB3:HP3	1.62	0.81
1:C:349:TYR:HE2	1:D:391:PRO:HD2	1.39	0.80
1:D:94:LEU:O	1:D:97:SER:HB3	1.80	0.80
3:E:620:CB3:C6	3:E:620:CB3:H15	2.10	0.80
1:C:115:GLY:CA	5:C:614:NDP:O2A	2.29	0.80
1:D:262:THR:HG22	1:D:466:TYR:HA	1.62	0.80
1:D:75:ILE:O	5:D:618:NDP:H1B	1.82	0.80
1:C:133:LEU:HD22	1:C:134:THR:N	1.97	0.80
1:C:206:ILE:HD11	1:D:35:PHE:HA	1.63	0.80
4:D:617:DHF:O2	4:D:617:DHF:C12	2.30	0.80
1:B:3:GLU:HG3	1:B:4:LYS:H	1.45	0.80
1:C:254:ARG:NH2	1:D:410:VAL:O	2.15	0.80
1:B:139:GLU:HB3	1:B:510:TYR:CE1	2.17	0.79
1:A:171:ASP:OD2	1:A:483:PRO:HG3	1.82	0.79
1:B:158:TYR:O	1:B:173:MET:HB2	1.82	0.79
1:D:151:PRO:HG2	1:D:154:PHE:HD2	1.47	0.79
1:B:62:ILE:HD11	4:B:609:DHF:C13	2.13	0.79
1:D:304:ASN:ND2	1:D:306:ASN:H	1.80	0.79
1:E:19:ILE:HB	5:E:622:NDP:N7N	1.97	0.79
1:A:304:ASN:HD22	1:A:304:ASN:C	1.86	0.78
1:C:512:TYR:HB3	1:C:513:PRO:HD2	1.65	0.78
1:D:374:THR:HG22	1:D:384:HIS:CE1	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:ARG:NH1	5:E:622:NDP:O1X	2.16	0.78
1:B:209:ILE:H	1:B:209:ILE:CD1	1.96	0.78
1:E:4:LYS:HB3	1:E:101:LEU:CD2	2.13	0.78
1:E:137:ALA:O	1:E:510:TYR:CE2	2.35	0.78
1:A:57:LYS:HG3	5:A:606:NDP:O3B	1.84	0.78
5:A:606:NDP:O2X	5:A:606:NDP:C1B	2.31	0.78
1:C:196:ILE:HD11	1:D:157:VAL:HG23	1.66	0.78
1:E:468:ASN:H	1:E:468:ASN:ND2	1.82	0.78
1:C:62:ILE:HG12	4:C:613:DHF:C15	2.14	0.78
1:C:193:LEU:N	1:C:193:LEU:CD2	2.42	0.78
4:D:617:DHF:C11	4:D:617:DHF:CB	2.60	0.78
1:B:217:LYS:N	1:B:250:ASN:HD21	1.80	0.77
1:B:468:ASN:H	1:B:468:ASN:HD22	1.32	0.77
1:B:237:GLU:OE2	1:B:283:THR:HG23	1.85	0.77
1:D:304:ASN:C	1:D:304:ASN:HD22	1.87	0.77
1:C:468:ASN:HD22	1:C:468:ASN:H	1.33	0.77
1:D:209:ILE:O	1:D:209:ILE:HG22	1.83	0.76
1:B:472:GLN:H	1:B:472:GLN:NE2	1.83	0.76
4:C:613:DHF:HB2	4:C:613:DHF:O	1.84	0.76
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.19	0.76
1:A:426:ASP:N	2:A:603:UMP:O2	2.17	0.76
1:C:403:HIS:H	1:C:403:HIS:CD2	2.03	0.76
1:B:217:LYS:H	1:B:250:ASN:ND2	1.82	0.76
1:B:67:LEU:HD22	4:B:609:DHF:CT	2.16	0.76
1:E:430:GLY:CA	3:E:620:CB3:HP3	2.16	0.76
4:E:621:DHF:O	4:E:621:DHF:CB	2.34	0.76
1:E:388:ALA:O	1:E:401:PRO:HG2	1.84	0.76
1:E:430:GLY:C	3:E:620:CB3:HP3	2.06	0.75
1:B:468:ASN:HD22	1:B:468:ASN:N	1.83	0.75
1:A:139:GLU:O	1:A:140:ASP:HB2	1.86	0.75
1:B:147:PHE:CD2	1:B:148:PRO:HD2	2.21	0.75
1:C:391:PRO:HA	1:C:394:LEU:HD12	1.68	0.75
1:E:217:LYS:H	1:E:250:ASN:ND2	1.84	0.75
1:D:20:GLY:HA3	1:D:145:THR:OG1	1.85	0.75
1:D:468:ASN:H	1:D:468:ASN:ND2	1.83	0.75
1:A:262:THR:HG22	1:A:466:TYR:HA	1.69	0.75
1:C:304:ASN:HD21	1:C:306:ASN:HB2	1.51	0.75
1:E:133:LEU:CD1	1:E:135:ARG:HG2	2.17	0.75
1:B:380:LYS:HE3	1:B:412:ASN:ND2	2.00	0.74
1:D:209:ILE:CD1	1:D:209:ILE:N	2.49	0.74
1:C:174:ILE:HG13	1:C:174:ILE:O	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:TRP:HB2	1:D:404:VAL:HG13	1.67	0.74
1:C:10:VAL:HG22	1:C:11:ALA:N	2.02	0.74
1:D:209:ILE:N	1:D:209:ILE:HD12	2.01	0.74
1:E:295:LEU:HD22	1:E:295:LEU:O	1.86	0.74
1:B:220:LYS:HD3	1:B:249:GLU:OE1	1.87	0.74
1:C:126:ASN:HD21	1:C:177:LYS:NZ	1.84	0.74
1:D:67:LEU:CD2	4:D:617:DHF:CT	2.66	0.74
1:A:209:ILE:HD12	1:A:209:ILE:N	2.01	0.74
1:C:151:PRO:HG2	1:C:154:PHE:CD2	2.22	0.74
1:C:151:PRO:HG2	1:C:154:PHE:HD2	1.51	0.74
1:A:115:GLY:HA3	5:A:606:NDP:PA	2.27	0.74
1:C:334:GLU:O	1:C:336:ASN:N	2.20	0.73
1:C:389:TRP:HB2	1:C:404:VAL:HG13	1.70	0.73
1:E:21:ILE:HD12	1:E:142:GLU:C	2.08	0.73
1:A:85:ASP:OD1	1:A:86:PRO:HD2	1.88	0.73
1:A:468:ASN:H	1:A:468:ASN:ND2	1.86	0.73
1:B:294:GLU:O	1:B:297:TRP:HB3	1.88	0.73
1:E:429:LEU:HD11	1:E:517:MET:HB2	1.69	0.73
1:C:423:ARG:HD3	1:D:385:ILE:HD11	1.70	0.73
1:D:10:VAL:C	4:D:617:DHF:NA2	2.42	0.73
1:B:225:ASN:O	1:B:233:ARG:NH2	2.21	0.73
1:E:464:HIS:NE2	2:E:619:UMP:O3'	2.09	0.73
4:E:621:DHF:O	4:E:621:DHF:HB2	1.88	0.73
1:B:98:ILE:HA	1:B:100:ASN:H	1.53	0.73
1:C:62:ILE:HD11	4:C:613:DHF:H15	1.64	0.72
1:D:118:ILE:HD11	5:D:618:NDP:H8A	1.71	0.72
1:E:62:ILE:HG13	4:E:621:DHF:H15	1.72	0.72
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.71	0.72
1:E:391:PRO:HA	1:E:394:LEU:HD13	1.69	0.72
1:E:423:ARG:HG3	1:E:423:ARG:NH1	2.02	0.72
1:C:35:PHE:HA	1:D:206:ILE:HD11	1.70	0.72
1:C:509:TYR:CE1	1:C:511:PRO:HG3	2.25	0.72
1:A:135:ARG:HH12	1:A:159:MET:HE1	1.55	0.72
1:E:217:LYS:N	1:E:250:ASN:HD21	1.85	0.72
1:A:505:GLU:HG2	1:A:507:ILE:HD11	1.71	0.72
1:E:257:ARG:HD3	2:E:619:UMP:OP2	1.89	0.72
1:B:304:ASN:HD22	1:B:306:ASN:H	1.38	0.71
1:C:62:ILE:CG1	4:C:613:DHF:C15	2.66	0.71
1:D:225:ASN:O	1:D:233:ARG:NH2	2.23	0.71
1:E:114:GLY:HA2	1:E:119:TYR:CE1	2.25	0.71
1:B:95:GLU:C	1:B:97:SER:H	1.93	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:PRO:HD2	1:D:349:TYR:CE2	2.26	0.71
1:D:178:GLN:HA	1:D:178:GLN:HE21	1.56	0.71
1:D:246:ARG:HH11	1:D:268:GLN:HE21	1.39	0.71
1:E:57:LYS:HB2	5:E:622:NDP:PA	2.31	0.71
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.26	0.71
1:A:271:ARG:NH2	1:B:267:GLY:O	2.24	0.71
1:D:123:LEU:CD1	1:D:128:VAL:HG11	2.20	0.71
1:E:21:ILE:CD1	1:E:142:GLU:O	2.37	0.71
1:B:26:PRO:CG	1:B:27:TRP:CZ3	2.74	0.71
1:E:115:GLY:HA2	5:E:622:NDP:O5D	1.89	0.71
1:A:19:ILE:O	5:A:606:NDP:H2N	1.91	0.70
1:C:430:GLY:O	3:C:612:CB3:HP3	1.91	0.70
1:A:215:ARG:CZ	1:B:275:ARG:HD2	2.20	0.70
1:A:307:HIS:O	1:A:311:LYS:HD2	1.90	0.70
4:C:613:DHF:H72	5:C:614:NDP:C4N	2.20	0.70
1:A:430:GLY:O	3:A:604:CB3:HP3	1.90	0.70
1:E:59:TRP:O	1:E:62:ILE:HG22	1.90	0.70
1:E:62:ILE:HG13	4:E:621:DHF:C16	2.20	0.70
5:B:610:NDP:C5D	5:B:610:NDP:O2A	2.39	0.70
1:C:304:ASN:HD22	1:C:306:ASN:H	1.38	0.70
1:D:96:ASP:O	1:D:98:ILE:N	2.25	0.70
1:E:470:LEU:O	1:E:474:LYS:HB2	1.90	0.70
1:E:519:MET:SD	3:E:620:CB3:H16	2.32	0.70
1:C:321:SER:O	1:C:325:LEU:HB2	1.92	0.70
1:E:19:ILE:HB	5:E:622:NDP:H71N	1.54	0.70
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.72	0.69
1:C:140:ASP:O	1:C:141:ILE:CG2	2.40	0.69
1:E:116:GLU:CB	1:E:145:THR:HG23	2.21	0.69
1:E:304:ASN:ND2	1:E:306:ASN:H	1.90	0.69
5:E:622:NDP:O2X	5:E:622:NDP:C1B	2.40	0.69
1:A:333:ARG:HG2	1:A:333:ARG:NH1	2.07	0.69
1:B:403:HIS:CD2	1:B:403:HIS:H	2.09	0.69
1:C:79:LEU:HD23	1:C:80:PRO:CD	2.22	0.69
1:C:271:ARG:NH2	1:D:267:GLY:O	2.25	0.69
1:B:225:ASN:ND2	1:B:241:LEU:HD13	2.07	0.69
1:E:114:GLY:HA2	1:E:119:TYR:CZ	2.28	0.69
1:B:411:THR:OG1	1:B:415:CYS:HB2	1.92	0.69
1:E:380:LYS:HE3	1:E:412:ASN:ND2	2.07	0.69
4:E:621:DHF:H72	5:E:622:NDP:H42N	1.73	0.69
1:C:4:LYS:HE2	1:C:101:LEU:HA	1.74	0.69
1:C:246:ARG:HH11	1:C:268:GLN:NE2	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:ARG:HH11	1:D:268:GLN:NE2	1.90	0.69
1:C:360:TYR:O	1:C:363:VAL:CG1	2.41	0.69
1:A:103:ASN:C	1:A:103:ASN:ND2	2.46	0.69
1:A:135:ARG:NH1	1:A:159:MET:CE	2.55	0.69
1:A:145:THR:HG21	5:A:606:NDP:H52N	1.73	0.68
3:C:612:CB3:C6	3:C:612:CB3:H15	2.22	0.68
1:E:425:CYS:HA	2:E:619:UMP:O2	1.93	0.68
1:A:254:ARG:NH2	1:B:410:VAL:O	2.27	0.68
1:A:256:ASN:HD22	1:A:258:THR:H	1.40	0.68
1:A:294:GLU:O	1:A:297:TRP:HB3	1.93	0.68
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.28	0.68
1:E:104:ASP:HB3	1:E:107:ILE:HD13	1.75	0.68
1:A:224:TYR:O	1:A:227:PRO:HG3	1.94	0.68
4:B:609:DHF:C12	4:B:609:DHF:CA	2.71	0.68
1:E:297:TRP:CG	1:E:308:LEU:HD21	2.28	0.68
1:A:35:PHE:HA	1:B:206:ILE:HD11	1.76	0.68
1:A:472:GLN:O	1:A:475:GLU:HB3	1.93	0.68
1:D:436:ALA:O	1:D:438:TYR:N	2.25	0.68
1:D:99:GLU:OE2	1:D:99:GLU:C	2.31	0.68
1:D:158:TYR:O	1:D:173:MET:HB2	1.93	0.68
1:D:304:ASN:HD21	1:D:306:ASN:HB2	1.59	0.68
1:D:430:GLY:O	3:D:616:CB3:HP3	1.94	0.68
1:A:97:SER:O	1:A:99:GLU:HG3	1.93	0.68
1:A:304:ASN:HD22	1:A:306:ASN:H	1.42	0.68
1:E:98:ILE:HG22	1:E:98:ILE:O	1.93	0.68
1:E:214:ASN:HB3	1:E:217:LYS:HZ2	1.58	0.68
1:D:256:ASN:C	1:D:256:ASN:HD22	1.97	0.68
1:B:208:GLY:C	1:B:210:ARG:H	1.96	0.67
1:B:389:TRP:HB2	1:B:404:VAL:HG22	1.76	0.67
1:B:468:ASN:H	1:B:468:ASN:ND2	1.91	0.67
1:D:26:PRO:HG2	1:D:27:TRP:CZ3	2.28	0.67
1:A:427:LEU:HD21	1:A:463:ALA:HB1	1.76	0.67
1:B:304:ASN:C	1:B:304:ASN:ND2	2.43	0.67
1:B:380:LYS:HE3	1:B:412:ASN:HD21	1.56	0.67
1:A:404:VAL:HG11	1:B:405:LEU:HD11	1.76	0.67
1:A:99:GLU:OE2	1:A:99:GLU:C	2.33	0.67
1:C:154:PHE:CE1	1:C:177:LYS:HB2	2.30	0.67
1:C:424:SER:OG	2:C:611:UMP:H3'	1.94	0.67
2:C:611:UMP:H5'	1:D:382:ARG:NH2	2.08	0.67
1:A:48:LYS:HB3	1:A:106:SER:O	1.94	0.67
1:B:138:LEU:CD2	1:B:141:ILE:HD13	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:GLU:HA	1:E:296:ILE:CD1	2.24	0.67
3:E:620:CB3:C5	3:E:620:CB3:C15	2.72	0.67
1:C:262:THR:HG22	1:C:466:TYR:HA	1.75	0.67
1:E:468:ASN:HD22	1:E:468:ASN:N	1.81	0.67
1:A:383:ARG:NH1	2:B:607:UMP:OP1	2.24	0.67
1:B:402:CYS:HB2	2:B:607:UMP:C5	2.30	0.67
1:C:67:LEU:HD22	4:C:613:DHF:O2	1.95	0.67
3:E:620:CB3:C6	3:E:620:CB3:C15	2.70	0.67
1:E:297:TRP:CD1	1:E:302:ASP:HB3	2.30	0.67
1:E:402:CYS:SG	2:E:619:UMP:C6	2.88	0.67
1:D:104:ASP:C	1:D:106:SER:H	1.97	0.67
1:B:476:GLN:HE21	1:B:515:ILE:HD12	1.60	0.66
1:E:223:ILE:O	1:E:245:SER:HB3	1.94	0.66
1:C:103:ASN:C	1:C:103:ASN:ND2	2.48	0.66
1:C:56:ARG:N	5:C:614:NDP:H4B	2.09	0.66
1:D:411:THR:OG1	1:D:415:CYS:HB2	1.95	0.66
1:E:130:ARG:HG3	1:E:176:GLU:HG3	1.77	0.66
1:E:295:LEU:O	1:E:299:ILE:HG13	1.96	0.66
1:E:296:ILE:HD12	1:E:296:ILE:H	1.59	0.66
1:A:225:ASN:O	1:A:233:ARG:NH2	2.28	0.66
3:B:608:CB3:C6	3:B:608:CB3:H15	2.24	0.66
1:A:315:ILE:HB	3:A:604:CB3:C15	2.26	0.66
1:D:294:GLU:O	1:D:297:TRP:HB3	1.96	0.66
1:E:257:ARG:HD3	2:E:619:UMP:P	2.36	0.66
1:E:33:LEU:HD21	4:E:621:DHF:C12	2.23	0.66
1:A:243:LEU:HD23	1:A:427:LEU:HD11	1.78	0.66
1:D:217:LYS:N	1:D:250:ASN:HD21	1.93	0.66
1:D:243:LEU:HD11	1:D:268:GLN:HG3	1.77	0.66
1:D:59:TRP:O	1:D:62:ILE:HG22	1.96	0.65
1:E:151:PRO:HG2	1:E:154:PHE:CD2	2.29	0.65
1:A:154:PHE:CE1	1:A:177:LYS:HB2	2.31	0.65
1:C:267:GLY:O	1:D:271:ARG:NH2	2.29	0.65
1:D:126:ASN:HB2	6:D:636:HOH:O	1.95	0.65
1:C:4:LYS:CB	1:C:101:LEU:HD23	2.15	0.65
1:D:115:GLY:HA3	5:D:618:NDP:O2A	1.97	0.65
1:D:297:TRP:CD2	1:D:308:LEU:HD21	2.31	0.65
5:B:610:NDP:N3A	5:B:610:NDP:O3X	2.30	0.65
1:C:293:GLU:CG	1:C:311:LYS:HD3	2.25	0.65
1:C:404:VAL:HG11	1:D:405:LEU:HD11	1.79	0.65
1:D:98:ILE:O	1:D:101:LEU:HB2	1.97	0.65
1:A:6:VAL:HG22	1:A:110:ILE:HB	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ASN:C	1:C:256:ASN:HD22	1.99	0.65
1:D:430:GLY:C	3:D:616:CB3:HP3	2.17	0.65
1:E:4:LYS:HB3	1:E:101:LEU:HD23	1.79	0.65
1:D:67:LEU:HD21	4:D:617:DHF:C12	2.25	0.65
1:E:10:VAL:HG22	1:E:11:ALA:N	2.11	0.65
1:E:136:VAL:HG12	1:E:138:LEU:HD23	1.78	0.65
5:A:606:NDP:O2X	5:A:606:NDP:N3A	2.30	0.64
1:B:21:ILE:HD12	1:B:144:ASP:OD2	1.96	0.64
1:C:12:ALA:HB1	1:C:17:SER:HA	1.77	0.64
1:D:57:LYS:H	5:D:618:NDP:H4B	1.62	0.64
1:C:140:ASP:O	1:C:141:ILE:HG22	1.97	0.64
1:E:98:ILE:O	1:E:98:ILE:CG2	2.46	0.64
1:A:139:GLU:HB3	1:A:510:TYR:OH	1.96	0.64
1:A:460:ILE:HG21	1:A:463:ALA:HB2	1.78	0.64
1:C:174:ILE:O	1:C:174:ILE:CG1	2.45	0.64
1:A:57:LYS:H	5:A:606:NDP:H4B	1.62	0.64
1:A:243:LEU:HD11	1:A:268:GLN:HG3	1.79	0.64
1:A:431:SER:HB3	1:A:432:PRO:HD3	1.78	0.64
1:C:423:ARG:HD3	1:D:385:ILE:CD1	2.27	0.64
1:D:15:LEU:HB2	1:D:139:GLU:CD	2.16	0.64
1:D:151:PRO:HG2	1:D:154:PHE:CD2	2.30	0.64
1:E:359:ASP:O	1:E:361:THR:N	2.30	0.64
1:A:209:ILE:HD12	1:A:209:ILE:H	1.61	0.64
1:A:215:ARG:NH1	1:B:275:ARG:HD2	2.12	0.64
1:A:430:GLY:O	3:A:604:CB3:CP3	2.46	0.64
1:A:26:PRO:HG2	1:A:27:TRP:CZ3	2.32	0.64
1:A:297:TRP:CD1	1:A:302:ASP:HB3	2.32	0.64
1:C:247:VAL:HG21	1:C:465:ILE:HG13	1.78	0.64
1:B:341:ILE:HA	1:B:397:MET:HE2	1.79	0.64
1:B:133:LEU:HD13	1:B:135:ARG:HG2	1.80	0.64
1:B:138:LEU:CD1	1:B:168:ILE:HD11	2.20	0.64
1:B:209:ILE:HD12	1:B:209:ILE:N	2.05	0.64
1:D:436:ALA:C	1:D:438:TYR:H	2.01	0.64
1:E:237:GLU:OE1	1:E:481:PRO:HB3	1.98	0.64
1:B:95:GLU:O	1:B:97:SER:N	2.31	0.64
1:B:319:ASN:ND2	3:B:608:CB3:H8	2.13	0.64
4:B:609:DHF:H12	4:B:609:DHF:CA	2.28	0.64
1:C:225:ASN:O	1:C:233:ARG:NH2	2.30	0.64
1:C:288:ILE:HA	1:C:291:ILE:HD12	1.78	0.64
1:D:319:ASN:ND2	1:D:399:LEU:HD13	2.13	0.64
1:A:85:ASP:OD1	1:A:86:PRO:CD	2.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:VAL:O	1:B:254:ARG:NH2	2.32	0.63
1:D:243:LEU:CD1	1:D:268:GLN:HG3	2.28	0.63
1:A:272:PHE:CE2	1:A:435:ILE:CG2	2.82	0.63
1:C:98:ILE:HG22	1:C:98:ILE:O	1.97	0.63
1:C:114:GLY:HA2	1:C:119:TYR:CE1	2.33	0.63
1:D:287:PHE:O	1:D:291:ILE:HG13	1.98	0.63
1:A:52:LEU:HB3	1:A:113:CYS:SG	2.38	0.63
1:C:103:ASN:C	1:C:103:ASN:HD22	2.00	0.63
1:C:137:ALA:O	1:C:510:TYR:CE2	2.50	0.63
1:E:12:ALA:HB1	1:E:17:SER:HA	1.80	0.63
1:C:10:VAL:HG22	1:C:11:ALA:H	1.63	0.63
1:C:56:ARG:H	5:C:614:NDP:H4B	1.61	0.63
1:D:10:VAL:O	4:D:617:DHF:NA2	2.31	0.63
4:E:621:DHF:HG2	4:E:621:DHF:O1	1.97	0.63
1:A:243:LEU:CD2	1:A:427:LEU:HD11	2.29	0.63
1:B:430:GLY:CA	3:B:608:CB3:HP3	2.29	0.63
1:B:472:GLN:HE21	1:B:472:GLN:N	1.88	0.63
1:D:225:ASN:HB2	1:D:477:LEU:HD23	1.81	0.63
1:B:139:GLU:O	1:B:140:ASP:CB	2.37	0.63
1:C:241:LEU:HD11	1:C:283:THR:HG21	1.81	0.63
1:A:151:PRO:HG2	1:A:154:PHE:HD2	1.63	0.63
1:B:115:GLY:HA3	5:B:610:NDP:O1A	1.99	0.63
1:C:52:LEU:N	1:C:52:LEU:HD23	2.14	0.63
1:C:87:ASN:O	1:C:88:VAL:HG23	1.99	0.63
1:C:284:LYS:HD2	6:C:623:HOH:O	1.98	0.63
1:D:304:ASN:ND2	1:D:304:ASN:C	2.52	0.63
1:A:99:GLU:O	1:A:102:MET:N	2.32	0.63
1:A:206:ILE:HG22	1:A:207:PHE:N	2.12	0.63
1:A:297:TRP:NE1	1:A:302:ASP:HB3	2.13	0.63
1:A:423:ARG:NH1	1:B:383:ARG:HG3	2.13	0.63
1:D:319:ASN:HD22	1:D:399:LEU:HD13	1.64	0.63
1:A:468:ASN:HD22	1:A:468:ASN:N	1.80	0.62
1:C:334:GLU:O	1:C:335:GLU:C	2.36	0.62
1:D:67:LEU:HD12	1:D:72:ILE:CD1	2.27	0.62
5:E:622:NDP:O2X	5:E:622:NDP:H1B	1.98	0.62
1:D:333:ARG:HH11	1:D:333:ARG:HG2	1.65	0.62
1:E:56:ARG:O	1:E:59:TRP:HB3	2.00	0.62
1:C:266:PHE:HA	1:C:461:GLY:O	1.98	0.62
1:C:246:ARG:HH11	1:C:268:GLN:HE22	1.47	0.62
1:C:403:HIS:H	1:C:403:HIS:HD2	1.46	0.62
1:E:255:GLU:CD	1:E:255:GLU:H	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASN:C	1:A:103:ASN:HD22	2.03	0.62
1:C:10:VAL:HG11	1:C:147:PHE:CD2	2.34	0.62
1:D:128:VAL:HG22	1:D:154:PHE:HZ	1.65	0.62
1:D:158:TYR:HB3	1:D:174:ILE:HG23	1.79	0.62
1:D:366:ASP:HB3	1:D:369:ALA:HB3	1.82	0.62
1:A:104:ASP:O	1:A:106:SER:N	2.32	0.62
1:B:164:CYS:HB2	1:B:486:GLN:NE2	2.14	0.62
1:B:243:LEU:O	1:B:247:VAL:HG13	1.99	0.62
1:E:173:MET:HG3	1:E:175:PHE:HE1	1.63	0.62
1:E:208:GLY:C	1:E:210:ARG:H	2.03	0.62
1:A:85:ASP:OD1	1:A:86:PRO:N	2.33	0.62
1:B:384:HIS:HB2	1:B:408:TYR:O	1.99	0.62
1:C:429:LEU:HD11	1:C:517:MET:HB2	1.82	0.62
1:C:304:ASN:ND2	1:C:306:ASN:HB2	2.15	0.62
1:C:405:LEU:C	1:C:405:LEU:HD23	2.19	0.62
1:E:57:LYS:HB2	5:E:622:NDP:O3	2.00	0.62
1:A:247:VAL:HG12	1:A:265:ILE:HG12	1.81	0.62
1:C:349:TYR:HB3	1:C:365:VAL:HB	1.81	0.62
1:E:92:ARG:O	5:E:622:NDP:H2A	2.00	0.62
1:A:104:ASP:C	1:A:106:SER:N	2.48	0.61
1:A:404:VAL:CG2	1:A:423:ARG:HG2	2.30	0.61
1:A:472:GLN:HG2	1:A:517:MET:HG2	1.82	0.61
1:C:54:MET:HE3	1:C:72:ILE:HG23	1.81	0.61
1:D:99:GLU:O	1:D:100:ASN:C	2.39	0.61
1:D:374:THR:HG22	1:D:384:HIS:HE1	1.64	0.61
1:E:347:ARG:O	1:E:366:ASP:HA	1.99	0.61
1:A:67:LEU:CD1	1:A:72:ILE:HD11	2.29	0.61
1:B:243:LEU:HD11	1:B:268:GLN:HG3	1.81	0.61
1:A:3:GLU:O	1:A:4:LYS:HB2	2.00	0.61
1:C:244:LEU:HD21	1:C:473:LEU:HD22	1.81	0.61
1:D:57:LYS:CB	5:D:618:NDP:O1A	2.31	0.61
1:D:99:GLU:OE2	1:D:100:ASN:N	2.33	0.61
1:E:391:PRO:HA	1:E:394:LEU:CD1	2.31	0.61
1:B:505:GLU:HB3	1:B:507:ILE:HD11	1.82	0.61
1:C:51:ALA:C	1:C:52:LEU:HD23	2.20	0.61
1:C:206:ILE:HG22	1:C:207:PHE:N	2.15	0.61
1:D:33:LEU:O	4:D:617:DHF:HG1	2.00	0.61
1:A:4:LYS:HE2	1:A:101:LEU:HA	1.82	0.61
1:B:56:ARG:N	5:B:610:NDP:H4B	2.16	0.61
1:B:138:LEU:HD23	1:B:141:ILE:CD1	2.30	0.61
1:E:62:ILE:CG1	4:E:621:DHF:H15	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ILE:HD13	1:A:436:ALA:HB3	1.82	0.61
1:C:403:HIS:HB2	1:C:420:LEU:HD11	1.83	0.61
3:D:616:CB3:CP2	3:D:616:CB3:H13	2.30	0.61
1:A:405:LEU:C	1:A:405:LEU:HD23	2.21	0.61
1:C:333:ARG:CG	1:C:337:ASP:HB3	2.30	0.61
1:E:10:VAL:CG2	1:E:11:ALA:N	2.64	0.61
1:A:206:ILE:HD11	1:B:35:PHE:HA	1.83	0.61
1:B:247:VAL:HG21	1:B:465:ILE:HG13	1.82	0.61
1:D:137:ALA:HB3	1:D:169:SER:O	2.00	0.61
1:E:169:SER:OG	1:E:486:GLN:HG2	2.01	0.61
1:E:390:ASN:O	1:E:394:LEU:HD12	2.01	0.61
1:E:431:SER:HB3	1:E:432:PRO:HD3	1.81	0.61
1:E:464:HIS:CE1	2:E:619:UMP:HO3'	2.19	0.61
1:B:193:LEU:O	1:B:194:LYS:C	2.39	0.61
1:A:10:VAL:HG22	1:A:11:ALA:N	2.16	0.60
1:A:256:ASN:ND2	1:A:258:THR:HG23	2.16	0.60
1:B:405:LEU:C	1:B:405:LEU:HD23	2.21	0.60
1:D:99:GLU:HG3	1:D:100:ASN:N	2.16	0.60
1:D:509:TYR:CE1	1:D:511:PRO:HG3	2.36	0.60
4:D:617:DHF:C16	4:D:617:DHF:CB	2.73	0.60
1:E:304:ASN:C	1:E:304:ASN:HD22	2.04	0.60
1:A:101:LEU:O	1:A:103:ASN:N	2.34	0.60
1:A:333:ARG:HG3	1:A:337:ASP:HB3	1.84	0.60
1:A:135:ARG:NH1	1:A:159:MET:HE1	2.14	0.60
1:C:81:GLN:HE22	1:C:92:ARG:CZ	2.15	0.60
1:C:430:GLY:C	3:C:612:CB3:HP3	2.21	0.60
1:E:128:VAL:HG23	1:E:154:PHE:HZ	1.65	0.60
1:C:217:LYS:H	1:C:250:ASN:ND2	1.96	0.60
1:D:114:GLY:HA3	1:D:119:TYR:CE1	2.35	0.60
1:B:257:ARG:HD3	2:B:607:UMP:OP2	2.01	0.60
1:C:320:GLY:O	1:C:325:LEU:HD22	2.01	0.60
1:C:405:LEU:HD23	1:C:405:LEU:O	2.02	0.60
1:B:93:ASN:OD1	1:B:96:ASP:HB2	2.02	0.60
1:C:311:LYS:NZ	1:C:311:LYS:HB3	2.16	0.60
1:C:349:TYR:CZ	1:D:391:PRO:HD2	2.29	0.60
1:D:133:LEU:CD1	1:D:135:ARG:HG2	2.32	0.60
1:D:470:LEU:HD12	1:D:470:LEU:H	1.66	0.60
4:E:621:DHF:C7	5:E:622:NDP:H42N	2.31	0.60
1:D:104:ASP:C	1:D:106:SER:N	2.55	0.60
1:C:10:VAL:CG2	1:C:11:ALA:H	2.15	0.60
1:C:243:LEU:HD23	1:C:427:LEU:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:612:CB3:C6	3:C:612:CB3:C15	2.79	0.60
1:E:239:GLN:HG3	1:E:271:ARG:O	2.02	0.60
1:A:114:GLY:HA2	1:A:119:TYR:CZ	2.37	0.60
1:C:133:LEU:HD22	1:C:133:LEU:C	2.21	0.60
1:D:304:ASN:HD22	1:D:306:ASN:H	1.49	0.60
1:E:335:GLU:HG3	1:E:336:ASN:OD1	2.01	0.60
1:E:354:LYS:N	1:E:360:TYR:OH	2.30	0.60
1:C:56:ARG:O	1:C:59:TRP:N	2.34	0.60
1:C:140:ASP:C	1:C:141:ILE:HG23	2.21	0.59
1:C:294:GLU:O	1:C:297:TRP:HB3	2.02	0.59
1:C:116:GLU:HB2	1:C:145:THR:HG23	1.82	0.59
1:E:246:ARG:HE	1:E:268:GLN:NE2	1.99	0.59
1:B:19:ILE:O	5:B:610:NDP:H2N	2.03	0.59
1:C:10:VAL:HG23	5:C:614:NDP:C7N	2.31	0.59
1:D:99:GLU:CG	1:D:100:ASN:N	2.65	0.59
1:E:46:SER:C	1:E:47:ASN:HD22	2.06	0.59
1:C:459:PHE:HB3	1:D:459:PHE:CD1	2.38	0.59
1:D:273:ASP:HA	6:D:640:HOH:O	2.03	0.59
1:E:225:ASN:CG	1:E:241:LEU:HD13	2.22	0.59
1:E:341:ILE:HA	1:E:397:MET:HE3	1.84	0.59
1:C:360:TYR:O	1:C:363:VAL:HG12	2.02	0.59
1:C:56:ARG:H	5:C:614:NDP:C4B	2.15	0.59
4:D:617:DHF:C12	4:D:617:DHF:CT	2.79	0.59
1:E:206:ILE:HG22	1:E:207:PHE:N	2.17	0.59
1:C:126:ASN:ND2	1:C:177:LYS:NZ	2.51	0.59
1:C:158:TYR:HB3	1:C:174:ILE:HG12	1.85	0.59
1:E:248:LEU:HD13	1:E:465:ILE:CD1	2.32	0.59
1:C:384:HIS:HB2	1:C:408:TYR:O	2.03	0.59
1:D:304:ASN:ND2	1:D:306:ASN:HB2	2.17	0.59
1:D:427:LEU:HD23	1:D:464:HIS:O	2.02	0.59
1:D:468:ASN:HD22	1:D:468:ASN:N	1.80	0.59
1:A:349:TYR:HB3	1:A:365:VAL:HB	1.84	0.59
1:B:88:VAL:C	1:B:89:VAL:HG12	2.23	0.59
1:A:409:TYR:HB3	1:A:417:SER:HB2	1.85	0.58
1:C:278:PHE:O	1:C:280:LEU:N	2.32	0.58
1:C:388:ALA:O	1:C:401:PRO:HG2	2.03	0.58
1:D:233:ARG:NH1	1:D:242:ASP:OD2	2.36	0.58
1:E:389:TRP:CZ2	1:E:394:LEU:HD21	2.37	0.58
1:E:433:PHE:HB2	3:E:620:CB3:CP3	2.33	0.58
1:E:472:GLN:HG2	1:E:517:MET:HG2	1.85	0.58
1:B:430:GLY:C	3:B:608:CB3:HP3	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:612:CB3:H13	3:C:612:CB3:CP2	2.33	0.58
4:C:613:DHF:H13	4:C:613:DHF:N5	2.17	0.58
1:D:405:LEU:C	1:D:405:LEU:HD23	2.22	0.58
1:C:114:GLY:HA2	1:C:119:TYR:CZ	2.38	0.58
1:C:482:ARG:HB3	1:C:483:PRO:HD2	1.86	0.58
1:E:128:VAL:HG23	1:E:154:PHE:CZ	2.38	0.58
1:B:297:TRP:HH2	1:B:338:LEU:HD12	1.68	0.58
1:C:10:VAL:CG2	1:C:11:ALA:N	2.65	0.58
1:C:468:ASN:HD22	1:C:468:ASN:N	1.92	0.58
1:A:99:GLU:HG3	1:A:100:ASN:H	1.68	0.58
1:C:407:GLN:NE2	1:D:423:ARG:HB2	2.18	0.58
1:E:33:LEU:HD22	4:E:621:DHF:H12	1.78	0.58
1:E:92:ARG:O	5:E:622:NDP:C2A	2.51	0.58
1:A:104:ASP:HB3	1:A:107:ILE:HD12	1.85	0.58
1:B:114:GLY:HA2	1:B:119:TYR:CE1	2.38	0.58
1:B:334:GLU:HG3	1:B:335:GLU:H	1.68	0.58
1:C:8:ILE:HB	1:C:131:ILE:HG12	1.84	0.58
1:C:423:ARG:CD	1:D:385:ILE:HD11	2.32	0.58
1:D:55:GLY:HA3	5:D:618:NDP:O5B	2.03	0.58
1:E:114:GLY:CA	1:E:119:TYR:CZ	2.86	0.58
1:A:509:TYR:CE1	1:A:511:PRO:HG3	2.39	0.58
1:C:243:LEU:CD1	1:C:268:GLN:HG3	2.33	0.58
1:C:360:TYR:O	1:C:363:VAL:HG13	2.03	0.58
1:A:349:TYR:CE2	1:B:391:PRO:CG	2.87	0.58
1:B:223:ILE:O	1:B:245:SER:HB3	2.04	0.58
1:B:465:ILE:HD13	1:B:473:LEU:HD13	1.86	0.58
1:D:93:ASN:OD1	1:D:96:ASP:OD2	2.22	0.58
1:D:384:HIS:HB2	1:D:408:TYR:O	2.03	0.58
1:E:11:ALA:CB	1:E:134:THR:HB	2.33	0.58
1:A:415:CYS:HA	1:A:452:GLU:O	2.04	0.58
1:B:115:GLY:HA3	5:B:610:NDP:PA	2.44	0.58
1:B:397:MET:HE1	1:B:401:PRO:HD3	1.85	0.58
1:D:123:LEU:HD13	1:D:128:VAL:HG11	1.85	0.58
1:A:59:TRP:O	1:A:62:ILE:HG22	2.02	0.58
1:A:4:LYS:HE3	1:A:101:LEU:HA	1.83	0.57
1:B:288:ILE:HA	1:B:291:ILE:HD12	1.86	0.57
1:B:304:ASN:ND2	1:B:306:ASN:N	2.47	0.57
1:C:39:ILE:HG23	1:C:40:THR:N	2.19	0.57
1:D:391:PRO:HA	1:D:394:LEU:HD12	1.86	0.57
1:A:506:LEU:HD13	1:A:509:TYR:HB2	1.85	0.57
3:B:608:CB3:C5	3:B:608:CB3:C15	2.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LYS:CE	1:B:101:LEU:HA	2.35	0.57
1:B:145:THR:HG21	5:B:610:NDP:O4D	2.04	0.57
1:D:431:SER:HB3	1:D:432:PRO:HD3	1.85	0.57
1:B:138:LEU:CD2	1:B:141:ILE:CD1	2.82	0.57
1:D:403:HIS:H	1:D:403:HIS:CD2	2.21	0.57
1:E:10:VAL:CG2	1:E:11:ALA:H	2.17	0.57
1:B:402:CYS:CB	2:B:607:UMP:C6	2.86	0.57
1:C:344:PHE:O	1:C:348:HIS:O	2.22	0.57
1:D:339:GLY:HA2	1:D:353:TYR:CE2	2.38	0.57
1:E:14:VAL:HG13	1:E:15:LEU:H	1.68	0.57
1:A:468:ASN:ND2	1:A:468:ASN:N	2.50	0.57
1:D:425:CYS:SG	1:D:431:SER:HB2	2.44	0.57
1:D:256:ASN:HD22	1:D:258:THR:H	1.52	0.57
1:B:284:LYS:HD3	1:B:476:GLN:NE2	2.18	0.57
1:B:389:TRP:HB2	1:B:404:VAL:CG2	2.34	0.57
1:D:10:VAL:HG22	1:D:11:ALA:N	2.20	0.57
1:E:33:LEU:HD23	4:E:621:DHF:H12	1.79	0.57
1:B:139:GLU:HB3	1:B:510:TYR:OH	2.04	0.57
1:D:3:GLU:O	1:D:4:LYS:HB2	2.04	0.57
1:D:3:GLU:CG	1:D:4:LYS:H	2.14	0.57
1:A:297:TRP:CD2	1:A:308:LEU:HD21	2.39	0.57
1:C:209:ILE:HG22	1:C:209:ILE:O	2.04	0.56
1:D:99:GLU:HG3	1:D:100:ASN:H	1.70	0.56
1:E:50:ASN:OD1	1:E:109:ASN:HB2	2.05	0.56
1:A:16:SER:O	1:A:17:SER:HB2	2.04	0.56
1:A:422:GLN:OE1	1:A:434:ASN:OD1	2.23	0.56
1:C:293:GLU:HG2	1:C:311:LYS:HD3	1.86	0.56
1:C:304:ASN:ND2	1:C:306:ASN:N	2.50	0.56
1:D:224:TYR:O	1:D:227:PRO:HG3	2.05	0.56
1:E:45:ASP:HB3	1:E:48:LYS:HB2	1.86	0.56
1:A:304:ASN:ND2	1:A:304:ASN:C	2.55	0.56
1:B:56:ARG:H	5:B:610:NDP:C4B	2.19	0.56
1:B:95:GLU:C	1:B:97:SER:N	2.59	0.56
1:C:49:LYS:O	1:C:107:ILE:HA	2.05	0.56
1:C:157:VAL:HG23	1:D:196:ILE:HD11	1.88	0.56
1:C:476:GLN:NE2	1:C:515:ILE:HD12	2.12	0.56
1:B:3:GLU:OE2	1:B:3:GLU:HA	2.05	0.56
1:B:151:PRO:HG2	1:B:154:PHE:HD2	1.71	0.56
1:C:203:LEU:HD21	1:D:172:PHE:CD2	2.40	0.56
1:C:405:LEU:HD11	1:D:404:VAL:HG11	1.86	0.56
1:D:334:GLU:CG	1:D:335:GLU:N	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:GLU:O	1:B:103:ASN:ND2	2.38	0.56
1:D:99:GLU:OE2	1:D:100:ASN:CA	2.53	0.56
1:D:239:GLN:HG3	1:D:271:ARG:O	2.05	0.56
1:A:14:VAL:HG13	1:A:15:LEU:HD23	1.85	0.56
1:A:102:MET:O	1:A:103:ASN:CB	2.44	0.56
1:A:173:MET:HG3	1:A:175:PHE:HE1	1.70	0.56
1:B:304:ASN:HD21	1:B:306:ASN:H	1.49	0.56
1:C:237:GLU:OE2	1:C:283:THR:HG23	2.06	0.56
1:A:295:LEU:O	1:A:299:ILE:HG13	2.06	0.56
1:B:298:PHE:O	1:B:301:GLY:N	2.33	0.56
1:A:212:MET:HG3	1:A:215:ARG:NH2	2.21	0.56
1:B:208:GLY:C	1:B:210:ARG:N	2.58	0.56
1:C:10:VAL:HG11	1:C:147:PHE:CE2	2.41	0.56
1:D:291:ILE:HD13	1:D:436:ALA:HB3	1.88	0.56
1:A:62:ILE:HD12	4:A:605:DHF:H13	1.88	0.56
1:A:295:LEU:O	1:A:295:LEU:HD22	2.06	0.56
1:A:465:ILE:HG21	1:A:473:LEU:HD12	1.88	0.56
1:B:158:TYR:HB3	1:B:174:ILE:HG12	1.88	0.56
1:B:430:GLY:O	3:B:608:CB3:CP3	2.50	0.56
1:C:253:TYR:HD2	1:C:263:TYR:CZ	2.23	0.56
1:C:443:MET:SD	1:C:487:LEU:HD22	2.46	0.56
1:D:334:GLU:HG2	1:D:335:GLU:N	2.20	0.56
1:E:103:ASN:O	1:E:104:ASP:C	2.44	0.56
1:E:108:GLU:HG2	1:E:109:ASN:ND2	2.20	0.56
1:E:133:LEU:HD11	1:E:135:ARG:HG2	1.87	0.56
1:C:385:ILE:CD1	1:D:423:ARG:HD3	2.36	0.56
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.88	0.56
1:B:154:PHE:CE1	1:B:177:LYS:HB2	2.41	0.55
1:A:63:GLY:O	1:A:65:ARG:HG3	2.06	0.55
1:A:195:SER:CB	1:B:130:ARG:NH1	2.69	0.55
1:A:223:ILE:O	1:A:245:SER:HB3	2.06	0.55
1:A:135:ARG:NH1	1:A:159:MET:HE2	2.20	0.55
1:C:128:VAL:HG22	1:C:154:PHE:HZ	1.71	0.55
1:E:229:ILE:CG2	1:E:232:GLY:O	2.55	0.55
1:B:304:ASN:HD21	1:B:306:ASN:HB2	1.71	0.55
1:D:337:ASP:HA	1:D:356:MET:SD	2.46	0.55
3:D:616:CB3:H5	3:D:616:CB3:C14	2.37	0.55
1:A:62:ILE:HG13	4:A:605:DHF:C13	2.37	0.55
1:C:100:ASN:O	1:C:103:ASN:O	2.24	0.55
1:E:333:ARG:CG	1:E:337:ASP:HB3	2.34	0.55
1:E:490:LYS:HD2	1:E:505:GLU:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LYS:HE3	1:B:101:LEU:HA	1.89	0.55
1:D:427:LEU:H	1:D:427:LEU:HD22	1.70	0.55
1:A:36:PHE:O	1:A:40:THR:HG23	2.07	0.55
1:B:130:ARG:HG2	1:B:131:ILE:H	1.72	0.55
1:B:130:ARG:HG2	1:B:131:ILE:N	2.21	0.55
1:C:147:PHE:CG	1:C:148:PRO:HD2	2.42	0.55
1:C:315:ILE:HG13	1:C:316:TRP:CD1	2.41	0.55
1:C:333:ARG:HG2	1:C:333:ARG:HH11	1.72	0.55
1:C:342:TYR:OH	1:C:402:CYS:N	2.31	0.55
1:C:269:MET:HE1	1:D:269:MET:HB3	1.87	0.55
1:C:402:CYS:O	1:C:422:GLN:HA	2.06	0.55
1:D:247:VAL:O	1:D:251:GLY:N	2.36	0.55
1:E:115:GLY:HA3	5:E:622:NDP:O1A	2.06	0.55
1:C:55:GLY:CA	1:C:118:ILE:HG13	2.37	0.55
1:D:53:ILE:HG23	1:D:75:ILE:HD13	1.88	0.55
1:A:145:THR:HG21	5:A:606:NDP:C5D	2.37	0.55
1:B:138:LEU:CD1	1:B:168:ILE:HD13	2.32	0.55
1:D:108:GLU:HG2	1:D:109:ASN:CG	2.27	0.55
1:D:274:MET:N	6:D:640:HOH:O	2.40	0.55
1:D:3:GLU:HG3	1:D:4:LYS:N	2.15	0.54
1:E:494:GLU:HG2	6:E:631:HOH:O	2.06	0.54
1:A:325:LEU:HD23	1:A:333:ARG:HB3	1.88	0.54
1:C:117:SER:OG	5:C:614:NDP:O1A	2.14	0.54
1:C:140:ASP:C	1:C:141:ILE:CG2	2.75	0.54
1:D:154:PHE:CE1	1:D:177:LYS:HB2	2.42	0.54
1:E:316:TRP:CE3	1:E:338:LEU:HD13	2.42	0.54
1:A:76:SER:HB3	1:A:79:LEU:HB2	1.90	0.54
1:B:374:THR:HG22	1:B:384:HIS:CE1	2.43	0.54
1:D:209:ILE:O	1:D:209:ILE:CG2	2.55	0.54
1:D:391:PRO:HA	1:D:394:LEU:CD1	2.37	0.54
1:E:424:SER:OG	2:E:619:UMP:H3'	2.07	0.54
1:C:99:GLU:C	1:C:99:GLU:OE2	2.45	0.54
1:E:119:TYR:O	1:E:121:ASP:N	2.40	0.54
1:E:154:PHE:CE1	1:E:177:LYS:HB2	2.41	0.54
1:A:82:ASP:O	1:A:84:ALA:N	2.41	0.54
1:A:115:GLY:CA	5:A:606:NDP:PA	2.95	0.54
1:E:52:LEU:N	1:E:52:LEU:HD23	2.23	0.54
1:A:411:THR:OG1	1:A:415:CYS:HB2	2.07	0.54
1:B:37:SER:HB2	4:B:609:DHF:CG	2.33	0.54
1:D:137:ALA:O	1:D:510:TYR:HE2	1.90	0.54
1:B:192:GLN:O	1:B:193:LEU:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:GLY:CA	1:C:119:TYR:CZ	2.90	0.54
1:C:287:PHE:O	1:C:291:ILE:HG13	2.08	0.54
1:C:426:ASP:HB2	2:C:611:UMP:H1'	1.90	0.54
1:E:246:ARG:HE	1:E:268:GLN:HE22	1.55	0.54
1:B:133:LEU:CD1	1:B:135:ARG:HG2	2.37	0.54
1:B:151:PRO:HG2	1:B:154:PHE:CD2	2.42	0.54
1:D:169:SER:OG	1:D:486:GLN:HG2	2.07	0.54
1:D:342:TYR:CZ	1:D:403:HIS:NE2	2.76	0.54
1:A:409:TYR:HB2	1:B:266:PHE:CE2	2.41	0.54
1:A:494:GLU:HG3	1:A:495:ASN:N	2.23	0.54
1:C:468:ASN:H	1:C:468:ASN:ND2	2.02	0.54
1:D:21:ILE:HG23	1:D:21:ILE:O	2.06	0.54
1:D:29:ILE:HG22	1:D:32:ASP:H	1.73	0.54
1:D:466:TYR:HH	2:D:615:UMP:HO3'	1.42	0.54
1:D:487:LEU:C	1:D:487:LEU:HD23	2.27	0.54
1:E:3:GLU:O	1:E:4:LYS:HB2	2.07	0.54
1:A:14:VAL:HG13	1:A:15:LEU:CD2	2.38	0.54
1:B:430:GLY:CA	3:B:608:CB3:CP3	2.86	0.54
3:D:616:CB3:C6	3:D:616:CB3:H15	2.38	0.54
1:E:209:ILE:HG22	1:E:209:ILE:O	2.08	0.54
1:D:333:ARG:HG2	1:D:333:ARG:NH1	2.23	0.53
1:D:470:LEU:HD12	1:D:470:LEU:N	2.23	0.53
1:A:505:GLU:HG2	1:A:507:ILE:CD1	2.38	0.53
1:B:104:ASP:C	1:B:106:SER:H	2.11	0.53
1:C:167:ASN:N	1:C:167:ASN:HD22	2.05	0.53
1:E:62:ILE:HD11	4:E:621:DHF:H16	1.90	0.53
1:B:460:ILE:HG21	1:B:463:ALA:HB2	1.89	0.53
1:A:133:LEU:HD11	1:A:135:ARG:HG2	1.90	0.53
1:E:380:LYS:HE3	1:E:412:ASN:HD21	1.73	0.53
1:A:195:SER:HB3	1:B:130:ARG:NH1	2.24	0.53
1:B:360:TYR:O	1:B:363:VAL:HG12	2.09	0.53
1:C:423:ARG:HG3	1:C:424:SER:N	2.23	0.53
1:D:253:TYR:HD2	1:D:263:TYR:CZ	2.27	0.53
1:E:323:GLU:CD	1:E:323:GLU:H	2.12	0.53
1:B:243:LEU:CD1	1:B:268:GLN:HG3	2.38	0.53
1:D:138:LEU:HD13	1:D:168:ILE:HD11	1.90	0.53
1:E:3:GLU:CG	1:E:4:LYS:N	2.54	0.53
1:B:507:ILE:HD12	1:B:507:ILE:N	2.23	0.53
1:D:472:GLN:HG2	1:D:517:MET:HG2	1.89	0.53
1:E:299:ILE:HG23	1:E:368:LEU:HD21	1.91	0.53
1:B:343:GLY:HA2	1:B:346:TRP:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:TYR:HB3	1:B:468:ASN:HD21	1.73	0.53
1:E:26:PRO:HB2	1:E:27:TRP:HE3	1.60	0.53
1:A:349:TYR:CD2	1:B:391:PRO:HB2	2.44	0.53
1:B:138:LEU:HD23	1:B:141:ILE:HD13	1.91	0.53
1:E:269:MET:HG3	1:E:270:MET:N	2.23	0.53
3:E:620:CB3:C5	3:E:620:CB3:C14	2.85	0.53
1:A:255:GLU:CD	1:A:255:GLU:H	2.13	0.53
1:A:272:PHE:CZ	1:A:435:ILE:HG21	2.44	0.53
4:A:605:DHF:H72	5:A:606:NDP:H42N	1.92	0.53
3:B:608:CB3:C6	3:B:608:CB3:C15	2.81	0.53
1:C:116:GLU:HB2	1:C:145:THR:CG2	2.39	0.53
1:C:126:ASN:HD21	1:C:177:LYS:HZ1	1.55	0.53
1:D:470:LEU:O	1:D:474:LYS:HB2	2.08	0.53
1:C:19:ILE:HB	5:C:614:NDP:H2N	1.91	0.52
1:C:244:LEU:HD23	1:C:477:LEU:HD21	1.89	0.52
1:E:401:PRO:O	1:E:404:VAL:HG22	2.08	0.52
1:E:468:ASN:ND2	1:E:468:ASN:N	2.49	0.52
1:B:257:ARG:NH2	1:B:521:VAL:OXT	2.43	0.52
1:D:123:LEU:HD12	1:D:128:VAL:CG1	2.40	0.52
1:D:206:ILE:HG22	1:D:207:PHE:N	2.24	0.52
1:E:394:LEU:HD12	1:E:394:LEU:H	1.74	0.52
1:A:99:GLU:HG3	1:A:100:ASN:N	2.24	0.52
1:A:372:ILE:O	1:A:376:LYS:HG2	2.09	0.52
1:B:50:ASN:OD1	1:B:109:ASN:HB2	2.08	0.52
1:B:103:ASN:O	1:B:104:ASP:C	2.48	0.52
1:B:334:GLU:OE2	1:B:357:HIS:HE1	1.93	0.52
1:B:371:LEU:O	1:B:371:LEU:HD22	2.09	0.52
1:D:10:VAL:CA	4:D:617:DHF:NA2	2.72	0.52
1:D:67:LEU:CD2	4:D:617:DHF:H12	2.36	0.52
1:E:389:TRP:HB2	1:E:404:VAL:CG1	2.35	0.52
1:B:289:ARG:HG3	1:B:501:TRP:CE2	2.45	0.52
1:D:75:ILE:O	5:D:618:NDP:C1B	2.55	0.52
1:E:58:THR:N	5:E:622:NDP:O2A	2.42	0.52
1:A:93:ASN:ND2	1:A:96:ASP:H	2.07	0.52
1:B:423:ARG:HG3	1:B:424:SER:N	2.24	0.52
1:B:490:LYS:HE3	1:B:505:GLU:HG3	1.92	0.52
1:C:206:ILE:HG22	1:C:207:PHE:H	1.74	0.52
1:D:304:ASN:HD21	1:D:306:ASN:CB	2.22	0.52
1:E:14:VAL:HG13	1:E:15:LEU:N	2.25	0.52
1:E:119:TYR:C	1:E:121:ASP:H	2.13	0.52
1:A:53:ILE:HG12	1:A:73:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ASN:HD21	1:A:306:ASN:HB2	1.73	0.52
1:B:98:ILE:HA	1:B:100:ASN:N	2.23	0.52
1:D:171:ASP:OD2	1:D:483:PRO:HB3	2.09	0.52
3:D:616:CB3:CP2	3:D:616:CB3:C13	2.86	0.52
1:E:62:ILE:HD11	1:E:67:LEU:HD11	1.91	0.52
1:A:57:LYS:CD	5:A:606:NDP:O2N	2.52	0.52
1:A:115:GLY:HA2	5:A:606:NDP:H51N	1.91	0.52
1:C:304:ASN:HD22	1:C:306:ASN:N	2.05	0.52
1:D:178:GLN:HA	1:D:178:GLN:NE2	2.23	0.52
1:E:26:PRO:HB3	1:E:141:ILE:HD11	1.92	0.52
1:A:304:ASN:HA	1:A:356:MET:SD	2.50	0.52
1:A:402:CYS:O	1:A:404:VAL:HG23	2.10	0.52
1:A:423:ARG:HB3	1:B:385:ILE:HD11	1.92	0.52
1:B:88:VAL:HG12	1:B:89:VAL:N	2.24	0.52
1:B:107:ILE:HG22	1:B:107:ILE:O	2.08	0.52
1:B:482:ARG:HB3	1:B:483:PRO:CD	2.39	0.52
1:C:192:GLN:C	1:C:193:LEU:HD23	2.29	0.52
1:C:252:ALA:O	1:C:254:ARG:HG3	2.10	0.52
1:C:315:ILE:HB	3:C:612:CB3:C15	2.40	0.52
1:D:74:VAL:HB	1:D:90:VAL:HG22	1.92	0.52
1:D:426:ASP:OD1	3:D:616:CB3:N3	2.43	0.52
1:E:238:PHE:HA	1:E:241:LEU:HB2	1.90	0.52
1:B:402:CYS:CB	2:B:607:UMP:C5	2.93	0.52
1:D:297:TRP:CD1	1:D:302:ASP:HB3	2.45	0.52
1:E:104:ASP:C	1:E:106:SER:N	2.63	0.52
1:E:299:ILE:O	1:E:347:ARG:HD3	2.10	0.52
4:E:621:DHF:H72	5:E:622:NDP:C4N	2.40	0.52
1:B:5:ASN:HD21	1:B:130:ARG:HH21	1.58	0.51
1:D:260:ILE:HD12	1:D:260:ILE:N	2.25	0.51
1:D:340:PRO:HD3	1:D:353:TYR:CG	2.45	0.51
1:E:251:GLY:HA3	1:E:263:TYR:HB3	1.92	0.51
1:A:289:ARG:HG3	1:A:501:TRP:CE2	2.46	0.51
1:E:32:ASP:O	1:E:35:PHE:HB3	2.10	0.51
1:E:225:ASN:ND2	1:E:241:LEU:HD13	2.25	0.51
1:A:233:ARG:NH1	1:A:242:ASP:OD2	2.43	0.51
1:A:304:ASN:HD21	1:A:306:ASN:CB	2.23	0.51
1:A:455:GLU:HG2	1:B:215:ARG:NH2	2.26	0.51
1:C:52:LEU:HB3	1:C:113:CYS:SG	2.50	0.51
1:D:9:VAL:HG12	4:D:617:DHF:NA2	2.25	0.51
1:D:36:PHE:CD1	1:D:36:PHE:C	2.83	0.51
1:D:123:LEU:HD12	1:D:128:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:TYR:CD1	1:E:240:TYR:C	2.83	0.51
1:A:82:ASP:C	1:A:84:ALA:N	2.63	0.51
1:A:114:GLY:CA	1:A:119:TYR:CZ	2.93	0.51
1:C:342:TYR:CZ	1:C:401:PRO:HA	2.45	0.51
1:C:443:MET:HG2	1:C:453:PRO:HG3	1.92	0.51
1:D:137:ALA:CB	1:D:169:SER:O	2.58	0.51
1:E:97:SER:C	1:E:99:GLU:H	2.14	0.51
3:B:608:CB3:C5	3:B:608:CB3:C14	2.87	0.51
1:C:39:ILE:CG2	1:C:40:THR:N	2.73	0.51
1:C:56:ARG:O	1:C:58:THR:N	2.43	0.51
1:C:102:MET:O	1:C:103:ASN:HB3	2.10	0.51
1:C:238:PHE:O	1:C:242:ASP:HB2	2.11	0.51
1:C:402:CYS:SG	2:C:611:UMP:C6	3.04	0.51
1:D:10:VAL:CA	4:D:617:DHF:HN21	2.23	0.51
1:D:97:SER:C	1:D:99:GLU:HG3	2.30	0.51
1:D:255:GLU:HA	1:D:261:SER:OG	2.10	0.51
1:A:455:GLU:HG2	1:B:215:ARG:HH22	1.75	0.51
1:B:114:GLY:HA3	1:B:119:TYR:CZ	2.46	0.51
1:C:293:GLU:HG3	1:C:311:LYS:HD3	1.92	0.51
1:C:473:LEU:O	1:C:477:LEU:HG	2.10	0.51
1:D:108:GLU:HG2	1:D:109:ASN:ND2	2.26	0.51
1:D:126:ASN:HD21	1:D:177:LYS:CE	2.23	0.51
1:E:333:ARG:HG2	1:E:333:ARG:HH11	1.75	0.51
1:B:57:LYS:H	5:B:610:NDP:H4B	1.75	0.51
1:B:247:VAL:O	1:B:251:GLY:N	2.42	0.51
1:C:425:CYS:HB3	1:C:460:ILE:HG21	1.93	0.51
1:D:57:LYS:HG3	5:D:618:NDP:O1N	2.11	0.51
1:D:295:LEU:O	1:D:295:LEU:HD22	2.10	0.51
1:D:431:SER:O	1:D:432:PRO:C	2.48	0.51
1:E:158:TYR:HB3	1:E:174:ILE:HG23	1.91	0.51
1:E:208:GLY:C	1:E:210:ARG:N	2.63	0.51
1:C:130:ARG:O	1:C:131:ILE:HG13	2.11	0.51
1:C:246:ARG:NH1	1:C:268:GLN:NE2	2.58	0.51
1:D:297:TRP:NE1	1:D:302:ASP:HB3	2.26	0.51
1:D:482:ARG:HB3	1:D:483:PRO:HD2	1.93	0.51
3:D:616:CB3:C15	3:D:616:CB3:C5	2.89	0.51
1:A:62:ILE:CD1	4:A:605:DHF:H13	2.40	0.51
1:B:93:ASN:OD1	1:B:96:ASP:OD2	2.29	0.51
1:C:253:TYR:HD2	1:C:263:TYR:CE1	2.29	0.51
1:D:15:LEU:CG	1:D:139:GLU:HG2	2.41	0.51
4:D:617:DHF:HB2	4:D:617:DHF:H16	1.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:512:TYR:HB3	1:E:513:PRO:HD2	1.92	0.51
1:B:23:GLY:HA2	5:B:610:NDP:O3D	2.11	0.51
1:B:133:LEU:HD13	1:B:135:ARG:CG	2.41	0.51
1:B:466:TYR:HB3	1:B:468:ASN:ND2	2.26	0.51
1:A:206:ILE:HG22	1:A:207:PHE:H	1.76	0.50
1:A:297:TRP:CG	1:A:308:LEU:HD21	2.46	0.50
1:C:115:GLY:HA3	5:C:614:NDP:PA	2.48	0.50
3:C:612:CB3:CP2	3:C:612:CB3:C13	2.88	0.50
1:A:10:VAL:HG23	5:A:606:NDP:O7N	2.11	0.50
1:A:304:ASN:ND2	1:A:306:ASN:HB2	2.26	0.50
1:D:93:ASN:ND2	1:D:96:ASP:H	2.10	0.50
1:E:68:LYS:O	1:E:69:ASN:HB2	2.12	0.50
1:E:212:MET:HG3	1:E:215:ARG:NH2	2.26	0.50
1:A:159:MET:HE1	1:A:481:PRO:O	2.12	0.50
1:A:318:GLY:C	1:A:320:GLY:H	2.15	0.50
1:D:15:LEU:HB2	1:D:139:GLU:OE1	2.11	0.50
1:D:229:ILE:HG22	1:D:233:ARG:HG2	1.93	0.50
1:D:334:GLU:CG	1:D:335:GLU:H	2.25	0.50
1:E:151:PRO:HB2	1:E:153:THR:HG23	1.94	0.50
1:E:339:GLY:O	1:E:341:ILE:N	2.42	0.50
1:E:460:ILE:HG22	1:E:461:GLY:N	2.26	0.50
1:A:217:LYS:N	1:A:250:ASN:HD21	1.94	0.50
1:C:206:ILE:CD1	1:D:35:PHE:HA	2.38	0.50
1:E:35:PHE:CE1	1:E:39:ILE:HD13	2.46	0.50
1:C:101:LEU:O	1:C:103:ASN:N	2.44	0.50
1:E:158:TYR:O	1:E:173:MET:HB2	2.11	0.50
1:E:239:GLN:O	1:E:270:MET:HG2	2.12	0.50
1:A:21:ILE:HG23	1:A:21:ILE:O	2.10	0.50
1:A:512:TYR:HB3	1:A:513:PRO:CD	2.32	0.50
1:B:10:VAL:HG13	1:B:133:LEU:HD23	1.94	0.50
1:B:248:LEU:HD13	1:B:465:ILE:HD12	1.93	0.50
1:C:126:ASN:ND2	1:C:177:LYS:HZ2	2.10	0.50
1:A:145:THR:HG21	5:A:606:NDP:C4D	2.42	0.50
1:B:21:ILE:O	1:B:21:ILE:HG23	2.12	0.50
1:B:115:GLY:HA2	5:B:610:NDP:O5D	2.10	0.50
1:C:217:LYS:N	1:C:250:ASN:HD21	1.99	0.50
1:C:286:VAL:CG1	1:C:291:ILE:HD11	2.42	0.50
1:D:436:ALA:C	1:D:438:TYR:N	2.65	0.50
1:A:253:TYR:HD2	1:A:263:TYR:CZ	2.30	0.50
1:A:304:ASN:HD22	1:A:305:GLY:N	2.10	0.50
1:B:166:LYS:O	1:B:167:ASN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:ILE:CD1	1:E:67:LEU:HD11	2.42	0.50
1:E:138:LEU:HG	1:E:138:LEU:O	2.12	0.50
1:E:166:LYS:O	1:E:167:ASN:HB2	2.12	0.50
1:A:209:ILE:N	1:A:209:ILE:CD1	2.71	0.49
1:C:466:TYR:CE1	1:C:520:ALA:CB	2.95	0.49
1:D:10:VAL:HG13	1:D:133:LEU:HD23	1.93	0.49
1:E:247:VAL:HG21	1:E:465:ILE:HG13	1.93	0.49
1:E:385:ILE:HD13	1:E:407:GLN:HB2	1.94	0.49
1:E:95:GLU:HG3	1:E:127:PHE:HZ	1.77	0.49
1:E:289:ARG:O	1:E:292:PHE:HB3	2.12	0.49
1:E:304:ASN:HD22	1:E:305:GLY:N	2.10	0.49
1:E:344:PHE:CE2	1:E:353:TYR:HD1	2.30	0.49
1:A:292:PHE:CD1	1:A:504:ILE:HD11	2.47	0.49
3:B:608:CB3:C14	3:B:608:CB3:H5	2.42	0.49
1:C:272:PHE:HB2	1:C:456:LEU:HB3	1.94	0.49
1:D:33:LEU:HD22	4:D:617:DHF:C16	2.42	0.49
1:D:33:LEU:HD21	4:D:617:DHF:H15	1.94	0.49
1:D:212:MET:HG2	1:D:215:ARG:NH2	2.27	0.49
1:E:145:THR:HG22	1:E:146:TYR:N	2.27	0.49
1:C:59:TRP:NE1	1:C:64:ARG:HD3	2.27	0.49
1:D:289:ARG:HG3	1:D:501:TRP:CE2	2.47	0.49
1:E:343:GLY:HA2	1:E:346:TRP:HB2	1.95	0.49
1:A:382:ARG:NE	2:B:607:UMP:OP3	2.45	0.49
1:B:342:TYR:CE1	1:B:403:HIS:NE2	2.81	0.49
1:B:512:TYR:HB3	1:B:513:PRO:HD2	1.93	0.49
1:C:171:ASP:OD2	1:C:483:PRO:HB3	2.12	0.49
1:C:296:ILE:HG23	1:C:297:TRP:N	2.27	0.49
1:E:51:ALA:C	1:E:52:LEU:HD23	2.32	0.49
1:A:62:ILE:HG12	1:A:62:ILE:O	2.12	0.49
1:A:423:ARG:CB	1:B:385:ILE:HD11	2.42	0.49
1:B:139:GLU:CB	1:B:510:TYR:CZ	2.85	0.49
1:B:494:GLU:HG3	1:B:495:ASN:N	2.27	0.49
1:C:43:LYS:HB2	1:C:108:GLU:OE1	2.12	0.49
1:C:137:ALA:O	1:C:510:TYR:HE2	1.93	0.49
1:E:288:ILE:HA	1:E:291:ILE:HD12	1.94	0.49
1:C:140:ASP:O	1:C:141:ILE:HG23	2.13	0.49
1:D:425:CYS:HB3	1:D:460:ILE:HG21	1.95	0.49
1:D:52:LEU:HD11	1:D:70:ARG:HD2	1.95	0.49
1:D:233:ARG:HH12	1:D:242:ASP:CG	2.16	0.49
1:D:256:ASN:ND2	1:D:258:THR:H	2.11	0.49
1:D:339:GLY:HA2	1:D:353:TYR:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:ASN:HD22	1:E:47:ASN:N	2.10	0.49
1:E:233:ARG:HB3	1:E:238:PHE:CD2	2.48	0.49
1:E:257:ARG:NH1	2:E:619:UMP:H5''	2.28	0.49
1:C:333:ARG:HG2	1:C:333:ARG:NH1	2.28	0.49
4:C:613:DHF:H13	4:C:613:DHF:C6	2.43	0.49
1:D:159:MET:HE2	1:D:173:MET:SD	2.52	0.49
1:D:166:LYS:O	1:D:167:ASN:HB2	2.13	0.49
1:E:48:LYS:HE2	1:E:105:ASP:O	2.13	0.49
1:E:117:SER:O	1:E:121:ASP:HB2	2.13	0.49
1:A:10:VAL:CG2	1:A:11:ALA:N	2.76	0.49
1:B:67:LEU:CD2	4:B:609:DHF:CT	2.81	0.49
1:B:256:ASN:HD22	1:B:258:THR:H	1.61	0.49
1:C:208:GLY:C	1:C:210:ARG:H	2.16	0.49
1:C:286:VAL:HG12	1:C:287:PHE:N	2.28	0.49
1:E:212:MET:HA	1:E:215:ARG:CZ	2.42	0.49
1:C:138:LEU:HG	1:C:138:LEU:O	2.11	0.48
1:C:299:ILE:HG23	1:C:368:LEU:HD21	1.95	0.48
1:E:260:ILE:HG22	1:E:466:TYR:HD1	1.78	0.48
1:A:139:GLU:HB3	1:A:510:TYR:CE2	2.47	0.48
1:A:337:ASP:HA	1:A:356:MET:SD	2.53	0.48
1:B:10:VAL:HG22	1:B:11:ALA:N	2.29	0.48
1:C:4:LYS:HB3	1:C:101:LEU:HD22	1.88	0.48
1:C:425:CYS:SG	1:C:460:ILE:HD13	2.53	0.48
1:E:4:LYS:HE2	1:E:101:LEU:HA	1.94	0.48
1:A:158:TYR:O	1:A:173:MET:HB2	2.13	0.48
1:A:404:VAL:HG23	1:A:423:ARG:HG2	1.94	0.48
1:B:297:TRP:O	1:B:298:PHE:C	2.52	0.48
1:C:256:ASN:C	1:C:256:ASN:ND2	2.66	0.48
1:C:371:LEU:CD2	1:C:375:LEU:HG	2.42	0.48
1:C:405:LEU:CD1	1:D:404:VAL:HG11	2.43	0.48
1:D:235:HIS:ND1	1:D:236:TYR:N	2.62	0.48
1:D:400:PRO:HB2	1:D:423:ARG:HH21	1.77	0.48
1:E:340:PRO:HG3	1:E:353:TYR:CG	2.48	0.48
1:A:234:GLU:CD	1:B:211:LYS:HZ1	2.15	0.48
1:A:280:LEU:HD23	1:A:509:TYR:CE2	2.48	0.48
1:A:339:GLY:HA2	1:A:353:TYR:CE2	2.48	0.48
4:C:613:DHF:H72	5:C:614:NDP:C5N	2.43	0.48
1:D:96:ASP:HB3	1:D:97:SER:H	1.48	0.48
1:E:341:ILE:HA	1:E:397:MET:CE	2.44	0.48
1:E:359:ASP:OD1	1:E:361:THR:HG22	2.14	0.48
4:E:621:DHF:O1	4:E:621:DHF:CG	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ALA:O	1:A:510:TYR:HE2	1.97	0.48
1:C:4:LYS:CE	1:C:101:LEU:HA	2.43	0.48
1:D:103:ASN:N	1:D:103:ASN:HD22	2.11	0.48
1:A:130:ARG:NH1	1:B:195:SER:HB3	2.27	0.48
1:B:113:CYS:O	4:B:609:DHF:H72	2.13	0.48
1:B:138:LEU:HD21	1:B:141:ILE:HD13	1.96	0.48
1:D:96:ASP:O	1:D:97:SER:C	2.52	0.48
1:D:366:ASP:CG	1:D:369:ALA:HB2	2.34	0.48
4:D:617:DHF:H15	4:D:617:DHF:H91	1.67	0.48
1:A:99:GLU:C	1:A:102:MET:H	2.17	0.48
1:A:115:GLY:O	1:A:118:ILE:N	2.46	0.48
1:D:126:ASN:ND2	1:D:177:LYS:HE3	2.28	0.48
1:D:193:LEU:O	1:D:194:LYS:C	2.52	0.48
1:D:209:ILE:CD1	1:D:209:ILE:H	2.26	0.48
1:A:282:THR:O	1:A:511:PRO:HA	2.14	0.48
1:C:338:LEU:HB3	1:C:341:ILE:HD13	1.95	0.48
1:D:68:LYS:O	1:D:69:ASN:HB2	2.14	0.48
1:E:342:TYR:OH	1:E:402:CYS:N	2.45	0.48
1:B:422:GLN:OE1	2:B:607:UMP:N3	2.45	0.48
1:E:229:ILE:HG21	1:E:232:GLY:O	2.13	0.48
1:E:243:LEU:HD11	1:E:268:GLN:HG3	1.95	0.48
1:C:371:LEU:HD22	1:C:375:LEU:HG	1.95	0.48
1:D:98:ILE:O	1:D:98:ILE:HG22	2.14	0.48
1:D:103:ASN:O	1:D:104:ASP:C	2.52	0.48
1:D:194:LYS:HG2	1:D:198:ASP:OD1	2.14	0.48
3:D:616:CB3:C14	3:D:616:CB3:C5	2.89	0.48
1:E:319:ASN:OD1	3:E:620:CB3:H8	2.14	0.48
1:A:431:SER:N	1:A:432:PRO:CD	2.77	0.47
1:B:37:SER:O	1:B:41:ASN:HB2	2.14	0.47
1:B:278:PHE:O	1:B:280:LEU:N	2.42	0.47
1:C:295:LEU:O	1:C:295:LEU:HD22	2.12	0.47
1:D:126:ASN:HD21	1:D:177:LYS:HE3	1.79	0.47
1:E:155:LEU:HD22	1:E:228:SER:OG	2.14	0.47
1:D:306:ASN:O	1:D:309:ILE:N	2.47	0.47
1:A:151:PRO:HG2	1:A:154:PHE:CD2	2.45	0.47
1:A:241:LEU:HD11	1:A:283:THR:HG21	1.95	0.47
1:C:10:VAL:HG23	5:C:614:NDP:O7N	2.14	0.47
1:D:37:SER:O	1:D:41:ASN:HB2	2.14	0.47
1:E:97:SER:O	1:E:99:GLU:N	2.47	0.47
1:E:145:THR:CG2	1:E:146:TYR:N	2.77	0.47
1:B:280:LEU:HD23	1:B:509:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ARG:NH2	1:C:311:LYS:O	2.48	0.47
1:A:99:GLU:OE2	1:A:100:ASN:N	2.48	0.47
1:E:257:ARG:HD3	2:E:619:UMP:OP1	2.14	0.47
1:E:315:ILE:HG13	1:E:316:TRP:HD1	1.78	0.47
1:A:3:GLU:O	1:A:4:LYS:CB	2.63	0.47
1:A:409:TYR:HB2	1:B:266:PHE:CZ	2.49	0.47
1:C:204:GLY:O	1:C:207:PHE:O	2.33	0.47
1:E:11:ALA:HB2	1:E:134:THR:HB	1.97	0.47
1:A:126:ASN:HD22	1:A:126:ASN:C	2.18	0.47
1:B:4:LYS:HD2	1:B:107:ILE:HG22	1.96	0.47
1:B:104:ASP:C	1:B:106:SER:N	2.68	0.47
1:B:138:LEU:HD12	1:B:168:ILE:HD13	1.97	0.47
1:B:239:GLN:O	1:B:270:MET:HG2	2.14	0.47
1:C:233:ARG:NH1	1:C:242:ASP:OD1	2.47	0.47
1:C:403:HIS:CD2	1:C:403:HIS:N	2.77	0.47
1:D:12:ALA:HB1	1:D:17:SER:HA	1.97	0.47
1:D:118:ILE:CD1	5:D:618:NDP:C8A	2.88	0.47
1:D:252:ALA:O	1:D:254:ARG:HG2	2.15	0.47
1:E:67:LEU:CD1	1:E:72:ILE:HD11	2.34	0.47
1:E:156:PRO:O	1:E:229:ILE:HG13	2.15	0.47
1:E:384:HIS:HB2	1:E:408:TYR:O	2.14	0.47
1:A:33:LEU:HD22	4:A:605:DHF:C16	2.21	0.47
1:B:3:GLU:CG	1:B:4:LYS:H	2.19	0.47
1:B:114:GLY:CA	1:B:119:TYR:CZ	2.98	0.47
1:B:388:ALA:O	1:B:401:PRO:HG2	2.14	0.47
1:C:133:LEU:HD13	1:C:135:ARG:HG3	1.97	0.47
1:E:10:VAL:HB	1:E:119:TYR:OH	2.14	0.47
1:E:206:ILE:HG22	1:E:207:PHE:H	1.79	0.47
1:E:304:ASN:HD22	1:E:306:ASN:H	1.62	0.47
3:E:620:CB3:C14	3:E:620:CB3:H5	2.45	0.47
1:B:37:SER:CB	4:B:609:DHF:HG2	2.38	0.47
4:B:609:DHF:CG	4:B:609:DHF:O1	2.60	0.47
1:D:98:ILE:O	1:D:98:ILE:CG2	2.63	0.47
1:D:402:CYS:SG	2:D:615:UMP:C6	3.08	0.47
1:E:159:MET:HE2	1:E:173:MET:SD	2.55	0.47
1:B:93:ASN:OD1	1:B:93:ASN:O	2.33	0.47
1:B:430:GLY:HA2	3:B:608:CB3:CP3	2.45	0.47
1:B:465:ILE:HD13	1:B:473:LEU:CD1	2.43	0.47
1:D:94:LEU:HD21	1:D:122:ALA:HA	1.97	0.47
1:D:266:PHE:HA	1:D:461:GLY:O	2.14	0.47
1:D:347:ARG:HG3	1:D:347:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LEU:O	1:C:299:ILE:HG13	2.15	0.46
1:C:411:THR:OG1	1:C:415:CYS:HB2	2.16	0.46
1:D:3:GLU:OE2	1:D:3:GLU:HA	2.14	0.46
1:E:49:LYS:O	1:E:107:ILE:HA	2.15	0.46
1:B:81:GLN:CD	1:B:92:ARG:HH11	2.17	0.46
1:C:78:SER:O	1:C:79:LEU:C	2.54	0.46
1:C:136:VAL:HG12	1:C:138:LEU:HD23	1.97	0.46
1:C:404:VAL:HG11	1:D:405:LEU:CD1	2.45	0.46
1:D:280:LEU:O	1:D:484:PHE:CD1	2.69	0.46
1:D:343:GLY:HA2	1:D:346:TRP:HB2	1.98	0.46
1:E:16:SER:OG	1:E:139:GLU:OE2	2.23	0.46
1:A:195:SER:HB3	1:B:130:ARG:HH12	1.79	0.46
1:A:203:LEU:HD11	1:B:172:PHE:CD2	2.51	0.46
1:C:321:SER:O	1:C:325:LEU:HD22	2.16	0.46
1:C:403:HIS:CB	1:C:420:LEU:HD11	2.44	0.46
1:E:334:GLU:CG	1:E:335:GLU:H	2.29	0.46
1:B:403:HIS:H	1:B:403:HIS:HD2	1.60	0.46
1:C:288:ILE:HG23	1:C:289:ARG:N	2.30	0.46
1:C:375:LEU:HD23	1:C:375:LEU:HA	1.77	0.46
1:D:137:ALA:CB	1:D:169:SER:HB2	2.45	0.46
1:D:239:GLN:O	1:D:270:MET:HG2	2.15	0.46
1:A:93:ASN:OD1	1:A:96:ASP:HB2	2.16	0.46
1:D:48:LYS:HB3	1:D:106:SER:O	2.16	0.46
1:D:247:VAL:HG12	1:D:265:ILE:CD1	2.45	0.46
1:A:235:HIS:HE1	1:A:484:PHE:CE2	2.34	0.46
1:B:88:VAL:CG1	1:B:89:VAL:N	2.79	0.46
1:C:21:ILE:HG23	1:C:21:ILE:O	2.16	0.46
1:E:62:ILE:CD1	4:E:621:DHF:H16	2.46	0.46
1:B:11:ALA:HB2	4:B:609:DHF:NA2	2.31	0.46
1:C:409:TYR:HB2	1:D:266:PHE:CZ	2.50	0.46
1:C:429:LEU:HD13	1:C:469:HIS:CE1	2.51	0.46
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.98	0.46
1:A:316:TRP:CE3	1:A:338:LEU:HD13	2.51	0.46
1:A:333:ARG:HD2	1:A:337:ASP:CG	2.35	0.46
1:C:166:LYS:C	1:C:167:ASN:HD22	2.19	0.46
1:C:349:TYR:O	1:C:350:ASN:HB2	2.15	0.46
4:C:613:DHF:HG2	4:C:613:DHF:O1	2.15	0.46
1:D:21:ILE:HA	1:D:144:ASP:OD1	2.15	0.46
1:D:284:LYS:HD2	6:D:621:HOH:O	2.16	0.46
1:D:429:LEU:N	1:D:429:LEU:CD1	2.78	0.46
1:E:209:ILE:O	1:E:209:ILE:CG2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:VAL:CG1	1:E:291:ILE:HD11	2.45	0.46
1:E:289:ARG:HG3	1:E:501:TRP:CE2	2.51	0.46
1:A:115:GLY:O	1:A:116:GLU:C	2.54	0.46
1:A:289:ARG:NH2	1:A:311:LYS:O	2.49	0.46
1:C:48:LYS:HE2	1:C:105:ASP:O	2.16	0.46
1:C:427:LEU:HD21	1:C:463:ALA:HB1	1.98	0.46
1:D:193:LEU:N	1:D:193:LEU:HD23	2.29	0.46
1:D:204:GLY:O	1:D:207:PHE:O	2.34	0.46
1:D:256:ASN:C	1:D:256:ASN:ND2	2.67	0.46
1:A:466:TYR:HH	2:A:603:UMP:HO3'	1.60	0.46
1:D:93:ASN:O	1:D:96:ASP:HB2	2.16	0.46
3:D:616:CB3:C6	3:D:616:CB3:C15	2.92	0.46
1:A:466:TYR:CE2	2:A:603:UMP:O3'	2.69	0.45
1:B:334:GLU:CG	1:B:335:GLU:N	2.79	0.45
1:C:35:PHE:HA	1:D:206:ILE:CD1	2.44	0.45
1:A:35:PHE:HA	1:B:206:ILE:CD1	2.43	0.45
1:A:38:LYS:HB3	1:B:202:LEU:HG	1.97	0.45
1:A:85:ASP:OD1	1:A:85:ASP:C	2.53	0.45
1:B:304:ASN:HD21	1:B:306:ASN:CB	2.29	0.45
1:E:339:GLY:C	1:E:341:ILE:H	2.17	0.45
1:A:505:GLU:CG	1:A:507:ILE:HD11	2.43	0.45
1:C:128:VAL:HG22	1:C:154:PHE:CZ	2.50	0.45
1:E:115:GLY:O	1:E:116:GLU:C	2.54	0.45
1:E:297:TRP:CD1	1:E:308:LEU:HD21	2.51	0.45
1:E:496:ILE:O	1:E:499:PHE:HD1	1.99	0.45
1:A:247:VAL:HG12	1:A:265:ILE:CD1	2.46	0.45
1:A:280:LEU:HD23	1:A:509:TYR:CZ	2.51	0.45
1:A:372:ILE:HG22	1:A:376:LYS:HE2	1.97	0.45
1:A:459:PHE:CD1	1:B:459:PHE:HB3	2.52	0.45
1:C:57:LYS:HG3	5:C:614:NDP:O3B	2.17	0.45
1:C:72:ILE:HB	1:C:88:VAL:HG22	1.98	0.45
1:C:349:TYR:CD2	1:D:391:PRO:HD2	2.36	0.45
3:C:612:CB3:C15	3:C:612:CB3:C5	2.94	0.45
1:D:128:VAL:HG22	1:D:154:PHE:CZ	2.47	0.45
1:D:278:PHE:O	1:D:280:LEU:N	2.46	0.45
1:E:39:ILE:CG2	1:E:40:THR:N	2.80	0.45
1:E:272:PHE:CZ	1:E:435:ILE:HD13	2.52	0.45
1:A:136:VAL:C	1:A:138:LEU:H	2.20	0.45
1:B:93:ASN:OD1	1:B:96:ASP:CB	2.64	0.45
1:B:237:GLU:C	1:B:239:GLN:H	2.20	0.45
1:B:317:SER:O	1:B:318:GLY:C	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ASP:O	1:C:35:PHE:HB3	2.17	0.45
1:C:248:LEU:HD13	1:C:465:ILE:HD12	1.98	0.45
1:C:334:GLU:C	1:C:336:ASN:N	2.67	0.45
1:C:419:ASN:ND2	1:C:457:ALA:HB3	2.31	0.45
1:E:10:VAL:HB	1:E:119:TYR:CZ	2.51	0.45
1:A:247:VAL:CG2	1:A:465:ILE:HD12	2.47	0.45
1:C:257:ARG:HG3	1:C:258:THR:N	2.31	0.45
1:D:171:ASP:OD2	1:D:483:PRO:HD3	2.17	0.45
1:D:229:ILE:CG2	1:D:232:GLY:O	2.64	0.45
1:D:374:THR:O	1:D:378:ASN:O	2.35	0.45
1:E:340:PRO:HG3	1:E:353:TYR:CB	2.47	0.45
1:A:130:ARG:CG	1:A:131:ILE:N	2.79	0.45
1:B:273:ASP:OD2	1:B:274:MET:N	2.50	0.45
1:B:296:ILE:O	1:B:300:LYS:HG3	2.17	0.45
1:B:319:ASN:HD21	3:B:608:CB3:H8	1.81	0.45
1:C:19:ILE:HB	5:C:614:NDP:H71N	1.80	0.45
1:C:208:GLY:C	1:C:210:ARG:N	2.70	0.45
1:C:341:ILE:HA	1:C:397:MET:HE3	1.98	0.45
1:C:431:SER:O	1:C:432:PRO:C	2.54	0.45
1:D:133:LEU:HD11	1:D:135:ARG:HG2	1.99	0.45
1:E:4:LYS:CE	1:E:101:LEU:HA	2.47	0.45
1:B:4:LYS:HE2	1:B:101:LEU:HA	1.99	0.45
1:C:76:SER:HA	5:C:614:NDP:N3A	2.32	0.45
1:C:193:LEU:HD12	1:C:195:SER:OG	2.17	0.45
1:D:405:LEU:HD23	1:D:406:SER:N	2.32	0.45
1:E:16:SER:O	1:E:17:SER:HB2	2.17	0.45
1:E:390:ASN:OD1	1:E:392:SER:HB2	2.16	0.45
1:E:423:ARG:NH1	1:E:424:SER:HB2	2.31	0.45
1:B:128:VAL:HG22	1:B:154:PHE:HZ	1.82	0.45
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.81	0.45
1:C:59:TRP:HZ3	1:C:72:ILE:HD12	1.82	0.45
1:D:472:GLN:O	1:D:475:GLU:N	2.50	0.45
1:E:119:TYR:C	1:E:121:ASP:N	2.70	0.45
1:A:247:VAL:HG12	1:A:265:ILE:CG1	2.47	0.45
1:A:389:TRP:CE3	1:A:401:PRO:HD2	2.51	0.45
1:B:53:ILE:HG23	1:B:75:ILE:HD13	1.99	0.45
1:D:118:ILE:CD1	5:D:618:NDP:H8A	2.43	0.45
1:E:220:LYS:NZ	1:E:249:GLU:OE1	2.49	0.45
1:A:304:ASN:ND2	1:A:306:ASN:N	2.54	0.44
1:B:242:ASP:O	1:B:246:ARG:HB2	2.18	0.44
1:E:55:GLY:O	1:E:56:ARG:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:385:ILE:HG22	1:E:386:LEU:N	2.30	0.44
1:E:400:PRO:HA	1:E:401:PRO:HD3	1.84	0.44
1:E:509:TYR:CG	1:E:511:PRO:HD3	2.52	0.44
1:A:138:LEU:CD2	1:A:141:ILE:CD1	2.95	0.44
1:A:202:LEU:HG	1:B:38:LYS:HB3	1.98	0.44
1:C:19:ILE:O	5:C:614:NDP:H2N	2.17	0.44
1:E:8:ILE:HG13	1:E:128:VAL:HG11	2.00	0.44
1:E:243:LEU:CD1	1:E:268:GLN:HG3	2.47	0.44
1:E:349:TYR:O	1:E:350:ASN:HB2	2.17	0.44
1:A:236:TYR:OH	1:B:212:MET:HE2	2.18	0.44
1:B:130:ARG:HD2	1:B:132:TYR:CZ	2.52	0.44
1:B:304:ASN:HD22	1:B:306:ASN:N	2.11	0.44
1:B:333:ARG:HA	1:B:333:ARG:HD3	1.70	0.44
1:E:293:GLU:HA	1:E:296:ILE:HD11	1.97	0.44
1:A:194:LYS:O	1:A:195:SER:C	2.55	0.44
1:B:175:PHE:CD1	1:B:175:PHE:N	2.85	0.44
1:B:256:ASN:HD22	1:B:258:THR:N	2.14	0.44
1:B:348:HIS:O	1:B:349:TYR:C	2.55	0.44
1:C:81:GLN:HE22	1:C:92:ARG:NE	2.15	0.44
1:E:19:ILE:O	5:E:622:NDP:H2N	2.17	0.44
1:E:349:TYR:CE1	1:E:390:ASN:HB2	2.52	0.44
1:A:48:LYS:HE2	1:A:105:ASP:O	2.18	0.44
1:A:285:LYS:HB3	1:A:514:THR:HG22	1.98	0.44
1:B:221:GLU:HG3	1:B:227:PRO:HB3	1.99	0.44
1:B:334:GLU:HG3	1:B:335:GLU:N	2.31	0.44
1:C:320:GLY:O	1:C:335:GLU:O	2.34	0.44
1:C:466:TYR:CZ	1:C:520:ALA:HB3	2.53	0.44
1:D:10:VAL:HG22	1:D:11:ALA:H	1.82	0.44
1:D:337:ASP:OD1	1:D:356:MET:N	2.51	0.44
1:A:39:ILE:HG23	1:A:40:THR:N	2.33	0.44
1:A:99:GLU:OE2	1:A:99:GLU:O	2.36	0.44
1:A:135:ARG:HH12	1:A:159:MET:CE	2.22	0.44
1:A:359:ASP:OD2	1:A:361:THR:HG22	2.17	0.44
1:B:17:SER:O	1:B:19:ILE:HG23	2.18	0.44
1:B:130:ARG:CG	1:B:131:ILE:H	2.31	0.44
1:B:315:ILE:HB	3:B:608:CB3:C16	2.48	0.44
5:B:610:NDP:H52N	5:B:610:NDP:H6N	2.00	0.44
1:C:13:SER:HB2	1:C:139:GLU:OE1	2.17	0.44
1:C:104:ASP:C	1:C:106:SER:H	2.21	0.44
1:C:114:GLY:HA3	1:C:119:TYR:CZ	2.53	0.44
1:C:304:ASN:HD21	1:C:306:ASN:CB	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LYS:O	1:A:355:THR:HG23	2.18	0.44
4:A:605:DHF:C7	5:A:606:NDP:H42N	2.48	0.44
1:B:284:LYS:HD2	6:B:629:HOH:O	2.16	0.44
1:C:56:ARG:O	1:C:57:LYS:C	2.55	0.44
1:C:172:PHE:CD2	1:D:203:LEU:HD21	2.53	0.44
1:C:407:GLN:HB3	1:D:421:TYR:OH	2.17	0.44
1:C:424:SER:HG	2:C:611:UMP:H3'	1.83	0.44
1:D:174:ILE:O	1:D:174:ILE:HG12	2.18	0.44
1:E:67:LEU:HD12	1:E:72:ILE:CD1	2.34	0.44
1:E:242:ASP:C	1:E:244:LEU:N	2.69	0.44
1:E:347:ARG:HG3	1:E:347:ARG:HH11	1.83	0.44
4:E:621:DHF:C6	4:E:621:DHF:H13	2.46	0.44
1:D:51:ALA:C	1:D:52:LEU:HD23	2.38	0.44
1:D:427:LEU:HD22	1:D:427:LEU:N	2.32	0.44
1:E:39:ILE:HG22	1:E:40:THR:N	2.33	0.44
1:E:316:TRP:HE3	1:E:338:LEU:HD13	1.83	0.44
1:A:99:GLU:CG	1:A:100:ASN:N	2.81	0.44
1:A:166:LYS:O	1:A:167:ASN:HB2	2.17	0.44
1:B:56:ARG:H	5:B:610:NDP:H4B	1.77	0.44
1:B:130:ARG:CG	1:B:131:ILE:N	2.81	0.44
1:C:103:ASN:HD22	1:C:103:ASN:N	2.14	0.44
1:C:234:GLU:O	1:C:235:HIS:C	2.56	0.44
1:C:318:GLY:C	1:C:320:GLY:H	2.20	0.44
1:E:104:ASP:C	1:E:106:SER:H	2.21	0.44
1:E:130:ARG:HG2	1:E:131:ILE:H	1.83	0.44
1:E:221:GLU:HG3	1:E:227:PRO:HB3	2.00	0.44
1:E:292:PHE:O	1:E:295:LEU:N	2.47	0.44
1:E:315:ILE:HG13	1:E:316:TRP:N	2.33	0.44
1:E:385:ILE:CD1	1:E:407:GLN:HB2	2.47	0.44
1:E:439:ALA:O	1:E:443:MET:HG3	2.18	0.44
1:A:138:LEU:HD23	1:A:141:ILE:CD1	2.48	0.43
1:A:440:ILE:HG22	1:A:441:LEU:N	2.32	0.43
1:B:266:PHE:HA	1:B:461:GLY:O	2.18	0.43
1:C:296:ILE:CG2	1:C:297:TRP:N	2.80	0.43
1:C:318:GLY:O	1:C:320:GLY:N	2.48	0.43
1:C:342:TYR:OH	1:C:401:PRO:HA	2.18	0.43
1:C:374:THR:O	1:C:378:ASN:O	2.35	0.43
1:D:243:LEU:HD13	1:D:268:GLN:HB3	1.99	0.43
1:E:7:SER:O	1:E:111:PHE:HA	2.18	0.43
1:E:78:SER:O	1:E:79:LEU:C	2.56	0.43
1:E:220:LYS:NZ	1:E:220:LYS:HB2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:GLY:O	1:E:325:LEU:HD13	2.18	0.43
1:A:407:GLN:NE2	1:B:423:ARG:HB2	2.34	0.43
1:B:165:THR:O	1:B:166:LYS:HB2	2.17	0.43
1:C:57:LYS:HB2	5:C:614:NDP:O3	2.17	0.43
1:D:39:ILE:HD11	1:D:132:TYR:CZ	2.53	0.43
1:E:303:THR:HG21	1:E:344:PHE:HB2	2.00	0.43
1:A:405:LEU:HD23	1:A:405:LEU:O	2.17	0.43
1:D:115:GLY:N	1:D:119:TYR:CE2	2.69	0.43
1:D:243:LEU:CD2	1:D:427:LEU:HD11	2.48	0.43
1:E:303:THR:CG2	1:E:344:PHE:HB2	2.48	0.43
4:E:621:DHF:C6	5:E:622:NDP:H42N	2.49	0.43
1:A:83:GLU:H	1:A:83:GLU:HG2	1.40	0.43
1:A:212:MET:HG3	1:B:455:GLU:OE2	2.19	0.43
1:A:409:TYR:HB2	1:B:266:PHE:CD2	2.54	0.43
1:C:429:LEU:HD11	1:C:517:MET:CB	2.47	0.43
1:D:487:LEU:HD23	1:D:487:LEU:O	2.19	0.43
1:D:495:ASN:OD1	1:D:497:GLU:HG2	2.19	0.43
1:E:41:ASN:HD21	1:E:70:ARG:NE	2.16	0.43
1:E:136:VAL:HG12	1:E:138:LEU:CD2	2.47	0.43
1:E:267:GLY:HA2	1:E:460:ILE:O	2.19	0.43
1:A:139:GLU:CB	1:A:510:TYR:CE2	3.01	0.43
1:B:456:LEU:HD12	1:B:457:ALA:H	1.84	0.43
1:D:423:ARG:HG3	1:D:423:ARG:HH11	1.83	0.43
1:A:39:ILE:CG2	1:A:40:THR:N	2.82	0.43
1:A:402:CYS:HB2	2:A:603:UMP:C5	2.53	0.43
1:B:245:SER:HA	1:B:248:LEU:HB2	2.00	0.43
1:C:212:MET:HE3	1:D:455:GLU:CD	2.39	0.43
1:C:234:GLU:OE1	1:D:211:LYS:NZ	2.50	0.43
1:C:254:ARG:HE	1:D:412:ASN:ND2	2.16	0.43
1:C:443:MET:O	1:C:444:MET:C	2.54	0.43
1:C:472:GLN:O	1:C:475:GLU:N	2.49	0.43
1:D:32:ASP:O	1:D:35:PHE:HB3	2.19	0.43
1:D:315:ILE:HG13	1:D:316:TRP:CD1	2.54	0.43
1:E:93:ASN:OD1	1:E:96:ASP:HB2	2.19	0.43
1:E:333:ARG:HG2	1:E:333:ARG:NH1	2.33	0.43
1:A:85:ASP:HA	1:A:86:PRO:HD3	1.84	0.43
1:A:208:GLY:C	1:A:210:ARG:H	2.22	0.43
1:A:267:GLY:O	1:B:271:ARG:NH2	2.39	0.43
1:B:294:GLU:O	1:B:297:TRP:CB	2.61	0.43
1:B:429:LEU:HD12	1:B:429:LEU:HA	1.80	0.43
1:B:487:LEU:HD23	1:B:487:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ARG:HG2	1:D:412:ASN:HD21	1.83	0.43
1:C:385:ILE:HD12	1:D:423:ARG:HD3	2.00	0.43
1:D:10:VAL:N	4:D:617:DHF:NA2	2.56	0.43
1:D:99:GLU:OE2	1:D:100:ASN:HA	2.18	0.43
1:E:173:MET:HG3	1:E:175:PHE:CE1	2.49	0.43
1:E:359:ASP:OD1	1:E:361:THR:CG2	2.67	0.43
1:A:389:TRP:CZ3	1:A:401:PRO:HD2	2.53	0.43
1:A:426:ASP:OD2	1:A:426:ASP:C	2.57	0.43
1:C:155:LEU:HA	1:C:156:PRO:HD3	1.87	0.43
1:C:209:ILE:O	1:C:209:ILE:CG2	2.66	0.43
1:D:360:TYR:C	1:D:363:VAL:HG12	2.37	0.43
1:E:4:LYS:HD2	1:E:108:GLU:O	2.18	0.43
1:E:171:ASP:OD2	1:E:483:PRO:HD3	2.18	0.43
1:E:304:ASN:ND2	1:E:304:ASN:C	2.70	0.43
1:E:428:GLY:C	1:E:429:LEU:HD12	2.38	0.43
3:A:604:CB3:C14	3:A:604:CB3:C5	2.95	0.43
1:C:368:LEU:O	1:C:371:LEU:HB3	2.19	0.43
1:D:209:ILE:H	1:D:209:ILE:HD13	1.84	0.43
1:E:157:VAL:HG22	1:E:174:ILE:HG12	2.01	0.43
1:E:214:ASN:HB3	1:E:217:LYS:NZ	2.29	0.43
1:A:3:GLU:HG3	1:A:4:LYS:N	2.22	0.43
1:B:56:ARG:O	1:B:59:TRP:HB3	2.19	0.43
1:C:10:VAL:HA	5:C:614:NDP:O7N	2.19	0.43
1:C:67:LEU:HD12	1:C:72:ILE:HD11	2.00	0.43
1:C:519:MET:SD	3:C:612:CB3:C8A	3.07	0.43
1:D:264:SER:CB	1:D:464:HIS:HB3	2.49	0.43
1:D:427:LEU:H	1:D:427:LEU:CD2	2.31	0.43
1:E:41:ASN:HD21	1:E:70:ARG:HE	1.66	0.43
1:E:75:ILE:N	1:E:75:ILE:HD12	2.33	0.43
1:E:286:VAL:HG12	1:E:291:ILE:HD11	2.01	0.43
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.88	0.42
1:A:98:ILE:O	1:A:99:GLU:HB3	2.16	0.42
1:A:101:LEU:O	1:A:103:ASN:O	2.37	0.42
1:A:289:ARG:NH1	6:A:611:HOH:O	2.51	0.42
1:A:448:VAL:HG21	1:A:496:ILE:HB	2.01	0.42
1:B:126:ASN:C	1:B:126:ASN:HD22	2.21	0.42
1:C:342:TYR:CZ	1:C:403:HIS:NE2	2.87	0.42
1:D:8:ILE:HB	1:D:131:ILE:HG12	2.00	0.42
1:D:280:LEU:O	1:D:484:PHE:CE1	2.72	0.42
1:E:400:PRO:HB2	1:E:423:ARG:HH21	1.84	0.42
1:E:509:TYR:CD2	1:E:511:PRO:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ASN:HD21	1:B:177:LYS:NZ	2.17	0.42
1:B:431:SER:HB3	1:B:432:PRO:HD3	2.00	0.42
1:D:103:ASN:CG	1:D:104:ASP:N	2.72	0.42
1:E:48:LYS:HD3	1:E:108:GLU:HB2	2.01	0.42
1:E:282:THR:HG21	1:E:482:ARG:O	2.20	0.42
5:E:622:NDP:P2B	5:E:622:NDP:O3B	2.77	0.42
1:A:199:THR:O	1:A:203:LEU:HB2	2.20	0.42
1:B:253:TYR:HA	1:B:262:THR:O	2.19	0.42
1:C:72:ILE:O	1:C:88:VAL:HA	2.19	0.42
1:C:285:LYS:HB3	1:C:514:THR:HG22	2.02	0.42
1:E:12:ALA:HB1	1:E:17:SER:CA	2.49	0.42
1:E:334:GLU:CG	1:E:335:GLU:N	2.82	0.42
1:A:43:LYS:HB2	1:A:108:GLU:OE1	2.20	0.42
1:C:167:ASN:N	1:C:167:ASN:ND2	2.67	0.42
1:D:115:GLY:O	1:D:118:ILE:N	2.52	0.42
1:D:416:LEU:O	1:D:454:GLY:N	2.52	0.42
1:D:490:LYS:HD2	1:D:505:GLU:HG3	2.01	0.42
1:E:108:GLU:HG2	1:E:109:ASN:CG	2.40	0.42
1:A:133:LEU:CD1	1:A:135:ARG:HG2	2.49	0.42
1:A:209:ILE:H	1:A:209:ILE:CD1	2.28	0.42
1:A:292:PHE:CD1	1:A:504:ILE:CD1	3.03	0.42
1:B:43:LYS:HB2	1:B:108:GLU:OE1	2.20	0.42
1:B:62:ILE:HD11	4:B:609:DHF:C14	2.49	0.42
1:B:68:LYS:O	1:B:69:ASN:HB2	2.19	0.42
1:B:340:PRO:HD3	1:B:353:TYR:CG	2.55	0.42
1:B:359:ASP:OD1	1:B:359:ASP:C	2.58	0.42
1:C:77:SER:O	1:C:92:ARG:NH1	2.52	0.42
1:C:96:ASP:O	1:C:99:GLU:HG3	2.18	0.42
1:D:62:ILE:CD1	4:D:617:DHF:H13	2.50	0.42
1:D:470:LEU:H	1:D:470:LEU:CD1	2.29	0.42
1:A:275:ARG:HG2	1:A:453:PRO:O	2.20	0.42
1:C:269:MET:HB2	1:C:459:PHE:HD2	1.84	0.42
1:D:33:LEU:CD2	4:D:617:DHF:C15	2.98	0.42
1:D:473:LEU:O	1:D:477:LEU:HB2	2.20	0.42
1:E:21:ILE:HG23	1:E:21:ILE:O	2.18	0.42
1:E:399:LEU:HA	1:E:400:PRO:HD3	1.92	0.42
1:A:340:PRO:HD3	1:A:353:TYR:CD2	2.54	0.42
1:B:27:TRP:CE2	1:B:136:VAL:HG21	2.55	0.42
1:B:341:ILE:HA	1:B:397:MET:CE	2.46	0.42
1:B:349:TYR:O	1:B:350:ASN:HB2	2.19	0.42
1:D:56:ARG:HB2	1:D:76:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:THR:HA	1:D:465:ILE:O	2.20	0.42
1:D:467:GLU:O	1:D:470:LEU:HD13	2.19	0.42
1:E:21:ILE:O	1:E:22:ASN:C	2.58	0.42
1:E:59:TRP:CE2	1:E:64:ARG:HA	2.55	0.42
1:E:88:VAL:HG12	1:E:89:VAL:N	2.34	0.42
1:E:297:TRP:CH2	1:E:341:ILE:HD11	2.54	0.42
5:E:622:NDP:P2B	5:E:622:NDP:HO3A	2.43	0.42
1:A:426:ASP:O	1:A:427:LEU:C	2.57	0.42
1:A:431:SER:O	1:A:435:ILE:HG12	2.20	0.42
1:B:319:ASN:HA	1:B:324:TYR:CD2	2.55	0.42
1:B:361:THR:HG23	1:B:361:THR:O	2.20	0.42
1:C:389:TRP:CE3	1:C:401:PRO:HD2	2.53	0.42
4:C:613:DHF:C6	4:C:613:DHF:C13	2.95	0.42
1:D:247:VAL:CG2	1:D:248:LEU:N	2.83	0.42
1:D:291:ILE:HG12	1:D:433:PHE:CD2	2.55	0.42
1:E:229:ILE:CG2	1:E:232:GLY:C	2.88	0.42
1:A:407:GLN:HG2	1:A:408:TYR:N	2.34	0.42
1:A:436:ALA:O	1:A:437:SER:C	2.58	0.42
1:B:90:VAL:HG12	1:B:91:PHE:O	2.20	0.42
1:B:422:GLN:OE1	1:B:434:ASN:OD1	2.38	0.42
1:C:101:LEU:C	1:C:103:ASN:H	2.23	0.42
1:C:431:SER:HB3	1:C:432:PRO:HD3	2.02	0.42
1:C:495:ASN:O	1:C:498:ASP:HB2	2.20	0.42
1:D:344:PHE:CE2	1:D:353:TYR:HD1	2.38	0.42
1:D:415:CYS:HA	1:D:452:GLU:O	2.19	0.42
1:D:416:LEU:HD12	1:D:416:LEU:HA	1.78	0.42
1:E:243:LEU:O	1:E:247:VAL:HG13	2.20	0.42
1:E:358:ASP:HB2	1:E:360:TYR:CE2	2.55	0.42
1:A:38:LYS:NZ	1:B:206:ILE:HG13	2.35	0.42
1:A:48:LYS:CB	1:A:106:SER:O	2.65	0.42
1:A:110:ILE:HG22	1:A:111:PHE:N	2.35	0.42
1:A:349:TYR:CD2	1:B:391:PRO:CG	3.03	0.42
1:B:26:PRO:CG	1:B:27:TRP:CE3	2.82	0.42
1:B:130:ARG:HD2	1:B:132:TYR:CE1	2.55	0.42
4:B:609:DHF:H92	4:B:609:DHF:H13	1.73	0.42
1:C:104:ASP:C	1:C:106:SER:N	2.74	0.42
1:D:138:LEU:HD13	1:D:168:ILE:CD1	2.49	0.42
1:D:220:LYS:HD3	1:D:249:GLU:OE1	2.19	0.42
1:E:10:VAL:HG11	1:E:147:PHE:CE2	2.55	0.42
1:E:294:GLU:O	1:E:297:TRP:HB3	2.20	0.42
1:E:318:GLY:C	1:E:320:GLY:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:CYS:SG	2:A:603:UMP:C5	3.13	0.41
1:A:514:THR:HG23	6:A:633:HOH:O	2.20	0.41
1:B:94:LEU:O	1:B:94:LEU:CD1	2.56	0.41
1:D:145:THR:HG21	5:D:618:NDP:H4D	2.02	0.41
1:E:26:PRO:CB	1:E:27:TRP:CZ3	2.94	0.41
1:E:247:VAL:O	1:E:251:GLY:N	2.51	0.41
1:E:423:ARG:HH12	1:E:424:SER:HB2	1.84	0.41
1:A:12:ALA:HB1	1:A:17:SER:HA	2.01	0.41
1:A:236:TYR:CE2	1:B:212:MET:HE1	2.56	0.41
1:D:400:PRO:HA	1:D:401:PRO:HD3	1.91	0.41
1:E:36:PHE:CD1	1:E:36:PHE:C	2.93	0.41
1:E:260:ILE:CG2	1:E:466:TYR:HD1	2.32	0.41
1:A:123:LEU:HD12	1:A:123:LEU:HA	1.93	0.41
1:B:253:TYR:HB2	1:B:263:TYR:CE1	2.55	0.41
1:C:311:LYS:HB3	1:C:311:LYS:HZ3	1.85	0.41
1:D:4:LYS:HE2	1:D:101:LEU:HA	2.03	0.41
1:D:15:LEU:HD12	1:D:139:GLU:HG2	2.03	0.41
1:D:225:ASN:O	1:D:226:THR:C	2.58	0.41
1:E:173:MET:HE2	1:E:175:PHE:CE1	2.55	0.41
1:E:225:ASN:HB2	1:E:477:LEU:HD23	2.02	0.41
1:E:467:GLU:HA	1:E:470:LEU:HD13	2.00	0.41
1:B:52:LEU:HB3	1:B:113:CYS:SG	2.60	0.41
1:B:235:HIS:HE1	1:B:484:PHE:CE2	2.38	0.41
1:D:115:GLY:O	1:D:116:GLU:C	2.59	0.41
1:E:25:LEU:C	1:E:27:TRP:H	2.24	0.41
1:A:93:ASN:HD21	1:A:96:ASP:H	1.69	0.41
1:A:385:ILE:CD1	1:B:423:ARG:HD3	2.51	0.41
1:B:235:HIS:CE1	1:B:237:GLU:HB2	2.55	0.41
1:B:470:LEU:HD12	1:B:470:LEU:HA	1.83	0.41
1:C:175:PHE:H	1:C:175:PHE:HD1	1.69	0.41
1:D:75:ILE:O	1:D:75:ILE:HG22	2.20	0.41
1:D:178:GLN:HE21	1:D:178:GLN:CA	2.22	0.41
1:D:233:ARG:NH1	1:D:242:ASP:CG	2.74	0.41
1:D:405:LEU:O	1:D:420:LEU:HD12	2.20	0.41
1:D:434:ASN:O	1:D:438:TYR:HB2	2.21	0.41
1:E:21:ILE:HA	1:E:144:ASP:OD1	2.20	0.41
1:E:56:ARG:HB2	1:E:76:SER:HB2	2.02	0.41
1:E:219:PRO:HG3	1:E:246:ARG:HA	2.03	0.41
1:E:264:SER:OG	1:E:462:ASP:OD2	2.32	0.41
2:A:603:UMP:OP2	1:B:382:ARG:NH2	2.42	0.41
1:C:56:ARG:C	1:C:58:THR:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:ASP:OD2	1:C:361:THR:HG23	2.21	0.41
1:D:33:LEU:HD22	4:D:617:DHF:C15	2.50	0.41
1:D:125:ASP:HB2	1:D:127:PHE:CE1	2.56	0.41
1:E:120:ARG:O	1:E:120:ARG:HG2	2.20	0.41
1:E:225:ASN:HB2	1:E:477:LEU:CD2	2.50	0.41
1:A:130:ARG:HG3	1:A:131:ILE:N	2.36	0.41
1:A:297:TRP:CD2	1:A:308:LEU:CD2	3.03	0.41
1:A:495:ASN:OD1	1:A:497:GLU:HG2	2.20	0.41
1:B:159:MET:HA	1:B:173:MET:HB3	2.01	0.41
1:C:130:ARG:HG3	1:C:130:ARG:HH11	1.84	0.41
1:D:114:GLY:CA	1:D:119:TYR:CE1	3.01	0.41
1:D:266:PHE:CD1	1:D:461:GLY:O	2.74	0.41
1:A:368:LEU:HA	1:A:368:LEU:HD12	1.83	0.41
1:A:385:ILE:HD11	1:B:423:ARG:HD3	2.02	0.41
1:A:402:CYS:CB	2:A:603:UMP:C5	3.04	0.41
1:B:20:GLY:HA2	1:B:26:PRO:HD3	2.03	0.41
1:B:103:ASN:ND2	1:B:104:ASP:N	2.69	0.41
1:C:19:ILE:HD12	5:C:614:NDP:C2N	2.51	0.41
1:C:466:TYR:HB3	1:C:468:ASN:ND2	2.36	0.41
3:C:612:CB3:C5	3:C:612:CB3:C14	2.96	0.41
1:D:206:ILE:HG22	1:D:207:PHE:H	1.86	0.41
1:E:263:TYR:N	1:E:263:TYR:CD2	2.88	0.41
1:A:309:ILE:HG23	1:A:314:TYR:CD1	2.56	0.41
1:B:33:LEU:HD23	1:B:33:LEU:HA	1.86	0.41
1:B:103:ASN:CG	1:B:104:ASP:N	2.74	0.41
1:B:133:LEU:HD22	1:B:134:THR:N	2.35	0.41
1:B:240:TYR:HA	1:B:270:MET:SD	2.61	0.41
1:B:265:ILE:HG21	1:B:265:ILE:HD13	1.86	0.41
1:C:57:LYS:HG3	5:C:614:NDP:HO3A	1.86	0.41
1:C:304:ASN:HD22	1:C:305:GLY:N	2.19	0.41
1:C:333:ARG:HA	1:C:333:ARG:HD3	1.78	0.41
1:D:9:VAL:HG12	4:D:617:DHF:C2	2.50	0.41
1:D:19:ILE:O	5:D:618:NDP:H2N	2.21	0.41
1:D:247:VAL:C	1:D:249:GLU:N	2.73	0.41
1:D:472:GLN:O	1:D:475:GLU:HB3	2.20	0.41
1:D:491:ARG:HG3	1:D:491:ARG:HH21	1.86	0.41
1:E:171:ASP:OD2	1:E:483:PRO:HB3	2.20	0.41
1:A:104:ASP:CB	1:A:107:ILE:HD12	2.49	0.41
1:A:203:LEU:HD11	1:B:172:PHE:CE2	2.56	0.41
1:A:238:PHE:O	1:A:242:ASP:HB2	2.20	0.41
1:A:404:VAL:HG11	1:B:405:LEU:CD1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASN:HD22	1:A:419:ASN:HA	1.64	0.41
1:A:426:ASP:O	1:A:428:GLY:N	2.54	0.41
1:A:479:ARG:NH2	1:A:515:ILE:HD11	2.36	0.41
1:B:233:ARG:NH1	1:B:242:ASP:OD1	2.54	0.41
1:D:425:CYS:HB3	1:D:460:ILE:CG2	2.51	0.41
1:E:241:LEU:HD23	1:E:241:LEU:HA	1.87	0.41
1:E:244:LEU:HD21	1:E:473:LEU:HD22	2.03	0.41
1:A:33:LEU:O	1:A:34:LYS:C	2.58	0.40
1:A:439:ALA:O	1:A:440:ILE:C	2.60	0.40
1:B:12:ALA:HB1	1:B:17:SER:HA	2.03	0.40
1:B:288:ILE:O	1:B:291:ILE:HB	2.21	0.40
1:B:304:ASN:HD22	1:B:305:GLY:N	2.16	0.40
1:B:342:TYR:CE1	1:B:403:HIS:CD2	3.09	0.40
1:B:519:MET:HG3	1:B:520:ALA:N	2.36	0.40
1:C:35:PHE:O	1:C:36:PHE:C	2.58	0.40
1:D:315:ILE:HB	3:D:616:CB3:C15	2.51	0.40
1:E:194:LYS:O	1:E:195:SER:C	2.59	0.40
1:E:202:LEU:C	1:E:204:GLY:N	2.74	0.40
1:E:324:TYR:CE2	1:E:328:ILE:HD13	2.57	0.40
1:E:334:GLU:HG2	1:E:335:GLU:H	1.86	0.40
1:E:423:ARG:HG3	1:E:424:SER:N	2.36	0.40
1:E:436:ALA:O	1:E:438:TYR:N	2.54	0.40
1:A:243:LEU:CD1	1:A:268:GLN:HG3	2.48	0.40
1:A:292:PHE:CE1	1:A:504:ILE:HD11	2.57	0.40
1:B:237:GLU:C	1:B:239:GLN:N	2.75	0.40
1:C:126:ASN:HD21	1:C:177:LYS:HZ2	1.62	0.40
1:C:175:PHE:CD1	1:C:175:PHE:N	2.89	0.40
1:C:272:PHE:CZ	1:C:435:ILE:HD13	2.56	0.40
1:C:320:GLY:O	1:C:325:LEU:CD2	2.68	0.40
1:C:341:ILE:HA	1:C:397:MET:CE	2.50	0.40
1:D:98:ILE:C	1:D:100:ASN:N	2.74	0.40
1:D:120:ARG:HE	1:D:120:ARG:HB2	1.76	0.40
1:A:92:ARG:HA	1:A:92:ARG:HD3	1.88	0.40
1:A:172:PHE:CD2	1:B:203:LEU:HD21	2.56	0.40
1:A:266:PHE:CE1	1:B:409:TYR:HB2	2.56	0.40
1:B:26:PRO:CB	1:B:143:PHE:HE1	2.34	0.40
1:B:93:ASN:OD1	1:B:93:ASN:C	2.57	0.40
1:B:223:ILE:O	1:B:245:SER:CB	2.69	0.40
1:B:402:CYS:HB2	2:B:607:UMP:C4	2.56	0.40
1:B:434:ASN:HD22	1:B:434:ASN:HA	1.67	0.40
1:D:272:PHE:CZ	1:D:435:ILE:HD13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:VAL:HG22	1:E:90:VAL:N	2.36	0.40
1:E:138:LEU:HD23	1:E:138:LEU:H	1.86	0.40
1:E:243:LEU:HD21	1:E:460:ILE:HD12	2.02	0.40
1:A:51:ALA:C	1:A:52:LEU:HD23	2.41	0.40
1:A:498:ASP:O	1:A:500:LYS:HE3	2.21	0.40
1:C:334:GLU:C	1:C:336:ASN:H	2.24	0.40
1:D:282:THR:HG21	1:D:482:ARG:O	2.22	0.40
1:E:14:VAL:HG22	1:E:15:LEU:HD23	2.03	0.40
1:E:247:VAL:HG12	1:E:265:ILE:HD13	2.03	0.40
1:E:496:ILE:HG23	1:E:497:GLU:N	2.37	0.40
1:A:315:ILE:HG22	3:A:604:CB3:C11	2.52	0.40
1:A:487:LEU:C	1:A:487:LEU:HD23	2.42	0.40
1:B:53:ILE:O	1:B:113:CYS:HB2	2.21	0.40
1:B:439:ALA:O	1:B:443:MET:HG3	2.22	0.40
1:B:505:GLU:HB3	1:B:507:ILE:CD1	2.49	0.40
1:C:55:GLY:HA3	5:C:614:NDP:O5B	2.21	0.40
1:C:79:LEU:HD22	1:C:90:VAL:HG21	2.03	0.40
1:C:520:ALA:HB3	3:C:612:CB3:NA2	2.37	0.40
1:E:212:MET:O	1:E:213:GLY:C	2.60	0.40
1:E:235:HIS:HE1	1:E:484:PHE:CE2	2.39	0.40

There are no symmetry-related clashes.

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	501/521 (96%)	431 (86%)	51 (10%)	19 (4%)	3	19
1	B	504/521 (97%)	435 (86%)	53 (10%)	16 (3%)	4	23
1	C	504/521 (97%)	445 (88%)	46 (9%)	13 (3%)	5	27
1	D	504/521 (97%)	427 (85%)	56 (11%)	21 (4%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	503/521 (96%)	419 (83%)	67 (13%)	17 (3%)	3	22
All	All	2516/2605 (97%)	2157 (86%)	273 (11%)	86 (3%)	3	22

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	84	ALA
1	A	103	ASN
1	A	105	ASP
1	A	206	ILE
1	B	93	ASN
1	B	101	LEU
1	B	193	LEU
1	B	195	SER
1	C	102	MET
1	C	103	ASN
1	C	206	ILE
1	C	394	LEU
1	D	96	ASP
1	D	97	SER
1	D	99	GLU
1	D	100	ASN
1	D	101	LEU
1	D	137	ALA
1	D	206	ILE
1	E	81	GLN
1	E	206	ILE
1	E	360	TYR
1	A	83	GLU
1	A	99	GLU
1	A	139	GLU
1	B	96	ASP
1	B	140	ASP
1	B	148	PRO
1	B	297	TRP
1	C	81	GLN
1	D	287	PHE
1	E	120	ARG
1	E	341	ILE
1	E	352	GLU
1	A	46	SER

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Mol	Chain	Res	Type
1	A	137	ALA
1	A	379	PRO
1	B	99	GLU
1	C	57	LYS
1	C	69	ASN
1	C	319	ASN
1	D	4	LYS
1	D	103	ASN
1	D	195	SER
1	D	257	ARG
1	D	307	HIS
1	D	379	PRO
1	D	437	SER
1	E	22	ASN
1	A	307	HIS
1	A	319	ASN
1	B	194	LYS
1	B	394	LEU
1	D	439	ALA
1	E	4	LYS
1	E	485	PRO
1	A	267	GLY
1	A	380	LYS
1	B	4	LYS
1	B	104	ASP
1	B	341	ILE
1	B	379	PRO
1	C	209	ILE
1	C	325	LEU
1	A	195	SER
1	A	341	ILE
1	C	379	PRO
1	D	26	PRO
1	D	194	LYS
1	D	341	ILE
1	E	148	PRO
1	E	267	GLY
1	E	379	PRO
1	C	341	ILE
1	D	440	ILE
1	E	340	PRO
1	A	440	ILE

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Mol	Chain	Res	Type
1	D	21	ILE
1	E	331	GLY
1	E	401	PRO
1	C	98	ILE
1	A	485	PRO
1	E	219	PRO
1	B	89	VAL
1	E	98	ILE

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	454/470 (97%)	422 (93%)	32 (7%)	15	43
1	B	454/470 (97%)	402 (88%)	52 (12%)	5	22
1	C	456/470 (97%)	407 (89%)	49 (11%)	6	25
1	D	457/470 (97%)	413 (90%)	44 (10%)	8	29
1	E	454/470 (97%)	416 (92%)	38 (8%)	11	35
All	All	2275/2350 (97%)	2060 (90%)	215 (10%)	8	29

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

Mol	Chain	Res	Type
1	A	34	LYS
1	A	41	ASN
1	A	83	GLU
1	A	96	ASP
1	A	97	SER
1	A	98	ILE
1	A	99	GLU
1	A	101	LEU
1	A	103	ASN
1	A	123	LEU
1	A	126	ASN

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Mol	Chain	Res	Type
1	A	128	VAL
1	A	141	ILE
1	A	220	LYS
1	A	228	SER
1	A	230	ARG
1	A	244	LEU
1	A	256	ASN
1	A	258	THR
1	A	304	ASN
1	A	333	ARG
1	A	336	ASN
1	A	371	LEU
1	A	374	THR
1	A	405	LEU
1	A	412	ASN
1	A	435	ILE
1	A	438	TYR
1	A	468	ASN
1	A	470	LEU
1	A	506	LEU
1	A	514	THR
1	B	8	ILE
1	B	25	LEU
1	B	41	ASN
1	B	44	CYS
1	B	46	SER
1	B	81	GLN
1	B	89	VAL
1	B	92	ARG
1	B	93	ASN
1	B	97	SER
1	B	98	ILE
1	B	99	GLU
1	B	103	ASN
1	B	113	CYS
1	B	123	LEU
1	B	126	ASN
1	B	130	ARG
1	B	133	LEU
1	B	138	LEU
1	B	140	ASP
1	B	157	VAL

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Mol	Chain	Res	Type
1	B	176	GLU
1	B	202	LEU
1	B	220	LYS
1	B	222	GLU
1	B	248	LEU
1	B	254	ARG
1	B	256	ASN
1	B	264	SER
1	B	284	LYS
1	B	289	ARG
1	B	295	LEU
1	B	304	ASN
1	B	308	LEU
1	B	317	SER
1	B	333	ARG
1	B	336	ASN
1	B	371	LEU
1	B	373	GLU
1	B	383	ARG
1	B	427	LEU
1	B	429	LEU
1	B	431	SER
1	B	468	ASN
1	B	470	LEU
1	B	472	GLN
1	B	474	LYS
1	B	475	GLU
1	B	497	GLU
1	B	506	LEU
1	B	514	THR
1	B	516	LYS
1	C	7	SER
1	C	8	ILE
1	C	41	ASN
1	C	52	LEU
1	C	62	ILE
1	C	78	SER
1	C	79	LEU
1	C	93	ASN
1	C	96	ASP
1	C	99	GLU
1	C	101	LEU

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Mol	Chain	Res	Type
1	C	103	ASN
1	C	113	CYS
1	C	123	LEU
1	C	128	VAL
1	C	133	LEU
1	C	138	LEU
1	C	140	ASP
1	C	157	VAL
1	C	164	CYS
1	C	167	ASN
1	C	178	GLN
1	C	193	LEU
1	C	220	LYS
1	C	224	TYR
1	C	228	SER
1	C	256	ASN
1	C	269	MET
1	C	304	ASN
1	C	311	LYS
1	C	325	LEU
1	C	333	ARG
1	C	334	GLU
1	C	336	ASN
1	C	361	THR
1	C	363	VAL
1	C	371	LEU
1	C	373	GLU
1	C	374	THR
1	C	383	ARG
1	C	403	HIS
1	C	405	LEU
1	C	431	SER
1	C	432	PRO
1	C	468	ASN
1	C	470	LEU
1	C	487	LEU
1	C	495	ASN
1	C	506	LEU
1	D	8	ILE
1	D	15	LEU
1	D	41	ASN
1	D	67	LEU

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Mol	Chain	Res	Type
1	D	79	LEU
1	D	81	GLN
1	D	89	VAL
1	D	96	ASP
1	D	99	GLU
1	D	103	ASN
1	D	104	ASP
1	D	123	LEU
1	D	138	LEU
1	D	140	ASP
1	D	145	THR
1	D	157	VAL
1	D	174	ILE
1	D	193	LEU
1	D	203	LEU
1	D	209	ILE
1	D	220	LYS
1	D	222	GLU
1	D	228	SER
1	D	256	ASN
1	D	287	PHE
1	D	295	LEU
1	D	304	ASN
1	D	317	SER
1	D	355	THR
1	D	361	THR
1	D	373	GLU
1	D	383	ARG
1	D	405	LEU
1	D	437	SER
1	D	438	TYR
1	D	468	ASN
1	D	474	LYS
1	D	477	LEU
1	D	502	GLU
1	D	505	GLU
1	D	506	LEU
1	D	507	ILE
1	D	514	THR
1	D	516	LYS
1	E	8	ILE
1	E	52	LEU

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Mol	Chain	Res	Type
1	E	79	LEU
1	E	97	SER
1	E	102	MET
1	E	103	ASN
1	E	123	LEU
1	E	138	LEU
1	E	140	ASP
1	E	153	THR
1	E	157	VAL
1	E	174	ILE
1	E	176	GLU
1	E	196	ILE
1	E	220	LYS
1	E	230	ARG
1	E	233	ARG
1	E	240	TYR
1	E	247	VAL
1	E	248	LEU
1	E	256	ASN
1	E	265	ILE
1	E	269	MET
1	E	293	GLU
1	E	295	LEU
1	E	296	ILE
1	E	304	ASN
1	E	317	SER
1	E	326	GLU
1	E	371	LEU
1	E	383	ARG
1	E	419	ASN
1	E	468	ASN
1	E	471	THR
1	E	474	LYS
1	E	506	LEU
1	E	514	THR
1	E	516	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	47	ASN

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Mol	Chain	Res	Type
1	A	69	ASN
1	A	93	ASN
1	A	103	ASN
1	A	126	ASN
1	A	167	ASN
1	A	214	ASN
1	A	216	HIS
1	A	250	ASN
1	A	256	ASN
1	A	268	GLN
1	A	304	ASN
1	A	306	ASN
1	A	336	ASN
1	A	403	HIS
1	A	412	ASN
1	A	419	ASN
1	A	468	ASN
1	A	476	GLN
1	B	5	ASN
1	B	24	GLN
1	B	47	ASN
1	B	100	ASN
1	B	103	ASN
1	B	126	ASN
1	B	167	ASN
1	B	216	HIS
1	B	250	ASN
1	B	256	ASN
1	B	268	GLN
1	B	304	ASN
1	B	306	ASN
1	B	319	ASN
1	B	336	ASN
1	B	350	ASN
1	B	357	HIS
1	B	384	HIS
1	B	412	ASN
1	B	419	ASN
1	B	468	ASN
1	B	472	GLN
1	B	476	GLN
1	C	24	GLN

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Mol	Chain	Res	Type
1	C	47	ASN
1	C	69	ASN
1	C	81	GLN
1	C	93	ASN
1	C	100	ASN
1	C	103	ASN
1	C	126	ASN
1	C	167	ASN
1	C	216	HIS
1	C	250	ASN
1	C	256	ASN
1	C	268	GLN
1	C	304	ASN
1	C	345	GLN
1	C	357	HIS
1	C	377	ASN
1	C	412	ASN
1	C	419	ASN
1	C	468	ASN
1	C	476	GLN
1	D	24	GLN
1	D	41	ASN
1	D	47	ASN
1	D	93	ASN
1	D	103	ASN
1	D	126	ASN
1	D	167	ASN
1	D	178	GLN
1	D	216	HIS
1	D	250	ASN
1	D	256	ASN
1	D	268	GLN
1	D	304	ASN
1	D	306	ASN
1	D	319	ASN
1	D	336	ASN
1	D	345	GLN
1	D	357	HIS
1	D	396	GLN
1	D	412	ASN
1	D	419	ASN
1	D	468	ASN

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Mol	Chain	Res	Type
1	D	476	GLN
1	E	24	GLN
1	E	41	ASN
1	E	47	ASN
1	E	103	ASN
1	E	109	ASN
1	E	167	ASN
1	E	214	ASN
1	E	250	ASN
1	E	268	GLN
1	E	304	ASN
1	E	306	ASN
1	E	319	ASN
1	E	412	ASN
1	E	419	ASN
1	E	434	ASN
1	E	468	ASN
1	E	476	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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
3	CB3	B	608	-	36,37,37	1.29	3 (8%)	46,51,51	2.00	9 (19%)
3	CB3	A	604	-	36,37,37	1.37	3 (8%)	46,51,51	2.22	8 (17%)
3	CB3	E	620	-	36,37,37	1.29	3 (8%)	46,51,51	2.00	9 (19%)
5	NDP	D	618	-	45,52,52	1.31	3 (6%)	53,80,80	1.30	3 (5%)
4	DHF	D	617	-	29,34,34	0.77	0	35,47,47	1.78	6 (17%)
3	CB3	C	612	-	36,37,37	1.29	3 (8%)	46,51,51	2.01	9 (19%)
4	DHF	C	613	-	29,34,34	0.77	0	35,47,47	1.80	6 (17%)
4	DHF	B	609	-	29,34,34	0.76	0	35,47,47	1.78	6 (17%)
5	NDP	B	610	-	45,52,52	1.31	3 (6%)	53,80,80	1.29	3 (5%)
4	DHF	A	605	-	29,34,34	0.77	0	35,47,47	1.79	6 (17%)
3	CB3	D	616	-	36,37,37	1.29	3 (8%)	46,51,51	2.00	9 (19%)
2	UMP	D	615	-	21,21,21	2.36	3 (14%)	31,31,31	2.04	9 (29%)
2	UMP	E	619	-	21,21,21	2.36	3 (14%)	31,31,31	2.41	10 (32%)
2	UMP	A	603	-	21,21,21	2.34	3 (14%)	31,31,31	2.15	8 (25%)
2	UMP	C	611	-	21,21,21	2.35	3 (14%)	31,31,31	3.32	13 (41%)
5	NDP	C	614	-	45,52,52	1.31	3 (6%)	53,80,80	1.29	3 (5%)
4	DHF	E	621	-	29,34,34	0.76	0	35,47,47	1.79	6 (17%)
5	NDP	E	622	-	45,52,52	1.31	3 (6%)	53,80,80	1.30	3 (5%)
5	NDP	A	606	-	45,52,52	1.31	3 (6%)	53,80,80	1.29	3 (5%)
2	UMP	B	607	-	21,21,21	2.34	3 (14%)	31,31,31	2.09	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
3	CB3	B	608	-	-	2/27/28/28	0/3/3/3
3	CB3	A	604	-	-	6/27/28/28	0/3/3/3
3	CB3	E	620	-	-	5/27/28/28	0/3/3/3
5	NDP	D	618	-	-	6/30/77/77	0/5/5/5
4	DHF	D	617	-	-	13/20/31/31	0/3/3/3
3	CB3	C	612	-	-	2/27/28/28	0/3/3/3
4	DHF	C	613	-	-	7/20/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DHF	B	609	-	1/1/5/8	8/20/31/31	0/3/3/3
5	NDP	B	610	-	-	12/30/77/77	0/5/5/5
4	DHF	A	605	-	-	8/20/31/31	0/3/3/3
3	CB3	D	616	-	-	4/27/28/28	0/3/3/3
2	UMP	D	615	-	-	6/10/22/22	0/2/2/2
2	UMP	E	619	-	-	3/10/22/22	0/2/2/2
2	UMP	A	603	-	-	4/10/22/22	0/2/2/2
2	UMP	C	611	-	-	2/10/22/22	0/2/2/2
5	NDP	C	614	-	-	10/30/77/77	0/5/5/5
4	DHF	E	621	-	-	6/20/31/31	0/3/3/3
5	NDP	E	622	-	-	7/30/77/77	0/5/5/5
5	NDP	A	606	-	-	13/30/77/77	0/5/5/5
2	UMP	B	607	-	-	2/10/22/22	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	619	UMP	C6-C5	8.07	1.53	1.35
2	D	615	UMP	C6-C5	7.99	1.53	1.35
2	C	611	UMP	C6-C5	7.98	1.53	1.35
2	A	603	UMP	C6-C5	7.96	1.53	1.35
2	B	607	UMP	C6-C5	7.93	1.53	1.35
5	D	618	NDP	C4N-C3N	-5.46	1.39	1.49
5	B	610	NDP	C4N-C3N	-5.45	1.39	1.49
5	A	606	NDP	C4N-C3N	-5.44	1.39	1.49
5	E	622	NDP	C4N-C3N	-5.43	1.39	1.49
5	C	614	NDP	C4N-C3N	-5.41	1.39	1.49
3	A	604	CB3	O4-C4	4.77	1.36	1.24
2	E	619	UMP	C5-C4	4.51	1.53	1.43
2	D	615	UMP	C5-C4	4.50	1.53	1.43
2	A	603	UMP	C5-C4	4.46	1.53	1.43
2	C	611	UMP	C5-C4	4.45	1.53	1.43
2	E	619	UMP	C6-N1	4.44	1.48	1.38
2	B	607	UMP	C5-C4	4.44	1.53	1.43
2	C	611	UMP	C6-N1	4.44	1.48	1.38
2	D	615	UMP	C6-N1	4.42	1.48	1.38
2	B	607	UMP	C6-N1	4.41	1.48	1.38
2	A	603	UMP	C6-N1	4.40	1.48	1.38
3	C	612	CB3	O-C	4.02	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	616	CB3	O-C	4.02	1.31	1.23
3	B	608	CB3	O-C	4.01	1.31	1.23
3	E	620	CB3	O-C	3.99	1.31	1.23
5	B	610	NDP	C4N-C5N	-3.71	1.39	1.48
5	C	614	NDP	C4N-C5N	-3.70	1.39	1.48
5	A	606	NDP	C4N-C5N	-3.69	1.39	1.48
5	D	618	NDP	C4N-C5N	-3.69	1.39	1.48
5	E	622	NDP	C4N-C5N	-3.68	1.39	1.48
3	E	620	CB3	CP1-CP2	3.47	1.51	1.47
5	C	614	NDP	C6N-C5N	3.45	1.39	1.33
3	D	616	CB3	CP1-CP2	3.43	1.51	1.47
5	E	622	NDP	C6N-C5N	3.43	1.39	1.33
5	A	606	NDP	C6N-C5N	3.42	1.39	1.33
5	D	618	NDP	C6N-C5N	3.42	1.39	1.33
3	C	612	CB3	CP1-CP2	3.41	1.51	1.47
3	A	604	CB3	CP2-CP3	3.39	1.28	1.18
5	B	610	NDP	C6N-C5N	3.39	1.39	1.33
3	B	608	CB3	CP1-CP2	3.37	1.51	1.47
3	B	608	CB3	C4-N3	3.17	1.38	1.33
3	C	612	CB3	C4-N3	3.12	1.38	1.33
3	E	620	CB3	C4-N3	3.08	1.38	1.33
3	D	616	CB3	C4-N3	3.07	1.38	1.33
3	A	604	CB3	CP1-N10	2.64	1.48	1.46

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	611	UMP	P-O5'-C5'	9.55	144.61	118.30
2	C	611	UMP	O4'-C4'-C5'	8.96	138.85	109.37
3	A	604	CB3	C4A-C8A-N1	-7.84	119.34	123.60
3	A	604	CB3	C4A-C4-N3	-7.57	119.12	124.40
4	C	613	DHF	C8A-C4A-C4	7.06	119.14	114.53
4	E	621	DHF	C8A-C4A-C4	6.98	119.10	114.53
4	A	605	DHF	C8A-C4A-C4	6.97	119.09	114.53
4	B	609	DHF	C8A-C4A-C4	6.94	119.07	114.53
4	D	617	DHF	C8A-C4A-C4	6.93	119.06	114.53
3	C	612	CB3	C4A-C8A-N1	-6.84	119.89	123.60
3	E	620	CB3	C4A-C8A-N1	-6.81	119.90	123.60
3	D	616	CB3	C4A-C8A-N1	-6.78	119.92	123.60
3	B	608	CB3	C4A-C8A-N1	-6.75	119.93	123.60
3	C	612	CB3	C4A-C4-N3	-6.56	119.83	124.40
3	D	616	CB3	C4A-C4-N3	-6.53	119.85	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	620	CB3	C4A-C4-N3	-6.53	119.85	124.40
3	B	608	CB3	C4A-C4-N3	-6.51	119.86	124.40
2	C	611	UMP	C6-C5-C4	-5.60	111.86	119.52
2	E	619	UMP	N3-C2-N1	5.55	122.26	114.89
2	B	607	UMP	C6-C5-C4	-5.43	112.09	119.52
3	A	604	CB3	N1-C2-N3	-5.34	120.10	127.22
2	A	603	UMP	C5-C6-N1	-5.34	112.87	121.81
3	D	616	CB3	N1-C2-N3	-5.30	120.16	127.22
3	B	608	CB3	N1-C2-N3	-5.28	120.17	127.22
3	E	620	CB3	N1-C2-N3	-5.28	120.19	127.22
3	C	612	CB3	N1-C2-N3	-5.26	120.21	127.22
2	D	615	UMP	C6-C5-C4	-5.09	112.56	119.52
2	C	611	UMP	C5-C6-N1	-5.03	113.39	121.81
2	B	607	UMP	C5-C6-N1	-4.88	113.64	121.81
2	A	603	UMP	C6-C5-C4	-4.84	112.91	119.52
2	A	603	UMP	N3-C2-N1	4.75	121.20	114.89
2	E	619	UMP	C5-C6-N1	-4.74	113.87	121.81
5	B	610	NDP	N3A-C2A-N1A	-4.71	121.32	128.68
5	E	622	NDP	N3A-C2A-N1A	-4.69	121.34	128.68
5	C	614	NDP	N3A-C2A-N1A	-4.69	121.35	128.68
5	A	606	NDP	N3A-C2A-N1A	-4.69	121.35	128.68
5	D	618	NDP	N3A-C2A-N1A	-4.69	121.35	128.68
2	D	615	UMP	C5-C6-N1	-4.67	113.98	121.81
2	E	619	UMP	O2-C2-N1	-4.63	116.64	122.79
2	B	607	UMP	N3-C2-N1	4.60	121.00	114.89
2	E	619	UMP	C4-N3-C2	-4.56	120.57	126.58
2	D	615	UMP	N3-C2-N1	4.47	120.82	114.89
2	E	619	UMP	C6-C5-C4	-4.45	113.43	119.52
2	C	611	UMP	O3'-C3'-C4'	-4.28	93.73	110.10
2	B	607	UMP	C4-N3-C2	-4.25	120.97	126.58
2	D	615	UMP	C4-N3-C2	-4.23	121.01	126.58
2	C	611	UMP	N3-C2-N1	4.21	120.48	114.89
2	A	603	UMP	C4-N3-C2	-4.20	121.04	126.58
2	C	611	UMP	C4-N3-C2	-4.20	121.04	126.58
2	E	619	UMP	P-O5'-C5'	4.09	129.55	118.30
2	C	611	UMP	O5'-C5'-C4'	3.79	122.05	108.99
2	A	603	UMP	C5-C4-N3	3.79	120.51	114.84
2	E	619	UMP	O4'-C4'-C5'	3.67	121.46	109.37
3	A	604	CB3	C6-C9-N10	-3.67	108.29	114.18
5	D	618	NDP	PN-O3-PA	-3.60	120.47	132.83
5	E	622	NDP	PN-O3-PA	-3.59	120.50	132.83
5	C	614	NDP	PN-O3-PA	-3.59	120.51	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	610	NDP	PN-O3-PA	-3.58	120.54	132.83
5	A	606	NDP	PN-O3-PA	-3.56	120.60	132.83
3	A	604	CB3	C2-N3-C4	3.35	121.25	115.93
3	B	608	CB3	CP1-N10-C9	3.10	120.05	117.10
3	C	612	CB3	CP1-N10-C9	3.06	120.01	117.10
3	E	620	CB3	CP1-N10-C9	3.05	120.00	117.10
2	B	607	UMP	C5-C4-N3	3.04	119.39	114.84
4	E	621	DHF	N1-C2-N3	-3.04	120.66	125.42
4	D	617	DHF	N1-C2-N3	-3.03	120.66	125.42
4	B	609	DHF	N1-C2-N3	-3.03	120.66	125.42
3	D	616	CB3	CP1-N10-C9	3.01	119.97	117.10
4	C	613	DHF	N1-C2-N3	-3.01	120.69	125.42
4	A	605	DHF	N1-C2-N3	-3.00	120.72	125.42
2	D	615	UMP	C5-C4-N3	2.97	119.28	114.84
3	B	608	CB3	C6-C9-N10	-2.95	109.44	114.18
3	C	612	CB3	C6-C9-N10	-2.95	109.44	114.18
3	D	616	CB3	C6-C9-N10	-2.95	109.45	114.18
2	C	611	UMP	C5-C4-N3	2.95	119.25	114.84
2	D	615	UMP	O2-C2-N1	-2.94	118.88	122.79
2	E	619	UMP	O5'-P-OP1	2.93	114.69	106.47
3	E	620	CB3	C6-C9-N10	-2.92	109.49	114.18
4	A	605	DHF	CB-CA-N	-2.91	104.99	110.88
4	D	617	DHF	CB-CA-N	-2.91	105.00	110.88
4	C	613	DHF	CB-CA-N	-2.90	105.00	110.88
2	B	607	UMP	O2-C2-N1	-2.90	118.93	122.79
4	B	609	DHF	CB-CA-N	-2.90	105.02	110.88
4	E	621	DHF	CB-CA-N	-2.89	105.03	110.88
4	B	609	DHF	C2-N3-C4	2.87	120.49	115.93
2	E	619	UMP	O5'-C5'-C4'	2.86	118.82	108.99
4	E	621	DHF	C2-N3-C4	2.83	120.43	115.93
4	C	613	DHF	C2-N3-C4	2.82	120.41	115.93
4	D	617	DHF	C2-N3-C4	2.82	120.41	115.93
4	A	605	DHF	C2-N3-C4	2.82	120.41	115.93
2	E	619	UMP	C5-C4-N3	2.80	119.02	114.84
2	C	611	UMP	O2-C2-N1	-2.79	119.07	122.79
4	C	613	DHF	C2-N1-C8A	2.78	120.78	114.54
4	D	617	DHF	C2-N1-C8A	2.78	120.78	114.54
4	A	605	DHF	C2-N1-C8A	2.77	120.76	114.54
4	E	621	DHF	C2-N1-C8A	2.77	120.75	114.54
4	B	609	DHF	C2-N1-C8A	2.76	120.72	114.54
4	C	613	DHF	C4A-C4-N3	-2.76	119.66	123.43
4	A	605	DHF	C4A-C4-N3	-2.75	119.67	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	609	DHF	C4A-C4-N3	-2.74	119.68	123.43
2	A	603	UMP	O4-C4-C5	-2.74	120.33	125.16
4	E	621	DHF	C4A-C4-N3	-2.72	119.71	123.43
4	D	617	DHF	C4A-C4-N3	-2.70	119.73	123.43
2	A	603	UMP	O2-C2-N1	-2.70	119.20	122.79
3	D	616	CB3	C2-N3-C4	2.68	120.19	115.93
3	B	608	CB3	C2-N3-C4	2.67	120.18	115.93
2	B	607	UMP	O5'-P-OP1	2.67	113.97	106.47
3	E	620	CB3	C2-N3-C4	2.66	120.16	115.93
3	C	612	CB3	C2-N3-C4	2.66	120.16	115.93
2	A	603	UMP	O5'-P-OP1	2.61	113.81	106.47
5	D	618	NDP	C3D-C2D-C1D	2.54	106.26	101.43
5	E	622	NDP	C3D-C2D-C1D	2.54	106.25	101.43
5	C	614	NDP	C3D-C2D-C1D	2.53	106.24	101.43
5	A	606	NDP	C3D-C2D-C1D	2.53	106.23	101.43
5	B	610	NDP	C3D-C2D-C1D	2.52	106.21	101.43
2	C	611	UMP	O5'-P-OP1	2.52	113.54	106.47
2	B	607	UMP	O4-C4-C5	-2.50	120.77	125.16
2	C	611	UMP	O4-C4-C5	-2.47	120.82	125.16
2	D	615	UMP	O4'-C1'-N1	2.41	112.18	107.86
3	A	604	CB3	C13-C14-N10	-2.35	118.14	121.38
2	D	615	UMP	O4-C4-C5	-2.32	121.08	125.16
2	D	615	UMP	O5'-P-OP1	2.31	112.95	106.47
3	B	608	CB3	O2-CT-O1	-2.22	119.04	124.09
3	E	620	CB3	O2-CT-O1	-2.19	119.11	124.09
3	A	604	CB3	CB-CA-N	-2.17	106.50	110.88
3	D	616	CB3	O2-CT-O1	-2.16	119.18	124.09
3	C	612	CB3	O2-CT-O1	-2.16	119.18	124.09
2	C	611	UMP	C2'-C1'-N1	-2.06	109.03	113.77
3	E	620	CB3	O2-CT-CA	2.05	120.20	113.40
3	B	608	CB3	O2-CT-CA	2.05	120.20	113.40
3	C	612	CB3	O2-CT-CA	2.04	120.17	113.40
3	D	616	CB3	O2-CT-CA	2.03	120.16	113.40
3	E	620	CB3	OE2-CD-CG	2.02	120.53	114.03
3	C	612	CB3	OE2-CD-CG	2.02	120.53	114.03
3	D	616	CB3	OE2-CD-CG	2.01	120.48	114.03
3	A	604	CB3	C6-C5-C4A	-2.00	119.65	122.65
3	B	608	CB3	OE2-CD-CG	2.00	120.46	114.03

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
4	B	609	DHF	CA

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	615	UMP	C3'-C4'-C5'-O5'
2	D	615	UMP	C5'-O5'-P-OP1
2	D	615	UMP	C5'-O5'-P-OP2
2	D	615	UMP	C5'-O5'-P-OP3
2	E	619	UMP	C5'-O5'-P-OP1
2	E	619	UMP	C5'-O5'-P-OP2
2	E	619	UMP	C5'-O5'-P-OP3
4	B	609	DHF	C11-C-N-CA
4	B	609	DHF	O-C-N-CA
4	D	617	DHF	C11-C-N-CA
4	D	617	DHF	O-C-N-CA
4	E	621	DHF	CB-CA-N-C
5	A	606	NDP	C5B-O5B-PA-O2A
5	A	606	NDP	C2B-O2B-P2B-O1X
5	B	610	NDP	C5D-O5D-PN-O1N
5	C	614	NDP	C5B-O5B-PA-O1A
5	C	614	NDP	O4B-C4B-C5B-O5B
5	C	614	NDP	C3B-C4B-C5B-O5B
5	C	614	NDP	C2B-O2B-P2B-O1X
5	D	618	NDP	PA-O3-PN-O5D
5	E	622	NDP	C3B-C4B-C5B-O5B
4	D	617	DHF	O-C-C11-C12
4	D	617	DHF	N-C-C11-C12
4	D	617	DHF	O-C-C11-C16
4	D	617	DHF	N-C-C11-C16
4	A	605	DHF	O-C-C11-C16
4	A	605	DHF	N-C-C11-C12
4	A	605	DHF	O-C-C11-C12
4	A	605	DHF	N-C-C11-C16
3	A	604	CB3	N-CA-CB-CG
3	C	612	CB3	N-CA-CB-CG
4	D	617	DHF	N-CA-CB-CG
4	D	617	DHF	CA-CB-CG-CD
2	B	607	UMP	O4'-C4'-C5'-O5'
2	D	615	UMP	O4'-C4'-C5'-O5'
5	A	606	NDP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
5	A	606	NDP	C3B-C4B-C5B-O5B
5	B	610	NDP	O4B-C4B-C5B-O5B
5	B	610	NDP	C3B-C4B-C5B-O5B
5	A	606	NDP	C1B-C2B-O2B-P2B
5	E	622	NDP	C1B-C2B-O2B-P2B
3	D	616	CB3	N-CA-CB-CG
4	A	605	DHF	N-CA-CB-CG
3	A	604	CB3	CT-CA-CB-CG
3	B	608	CB3	CT-CA-CB-CG
3	C	612	CB3	CT-CA-CB-CG
3	D	616	CB3	CT-CA-CB-CG
4	A	605	DHF	CT-CA-CB-CG
4	C	613	DHF	CB-CA-N-C
4	E	621	DHF	O-C-C11-C12
4	E	621	DHF	N-C-C11-C12
5	E	622	NDP	C3B-C2B-O2B-P2B
2	C	611	UMP	C3'-C4'-C5'-O5'
4	C	613	DHF	N-C-C11-C12
4	D	617	DHF	CB-CA-N-C
4	C	613	DHF	O-C-C11-C12
4	E	621	DHF	N-C-C11-C16
4	E	621	DHF	O-C-C11-C16
4	D	617	DHF	CT-CA-CB-CG
2	B	607	UMP	C3'-C4'-C5'-O5'
4	C	613	DHF	O-C-C11-C16
4	B	609	DHF	N-CA-CT-O1
4	C	613	DHF	N-C-C11-C16
2	A	603	UMP	C2'-C1'-N1-C6
5	E	622	NDP	O4B-C4B-C5B-O5B
5	A	606	NDP	C2D-C1D-N1N-C2N
3	A	604	CB3	CT-CA-N-C
4	B	609	DHF	N-CA-CT-O2
5	A	606	NDP	C2D-C1D-N1N-C6N
3	A	604	CB3	CB-CA-N-C
2	C	611	UMP	C4'-C5'-O5'-P
5	B	610	NDP	C1B-C2B-O2B-P2B
5	B	610	NDP	PA-O3-PN-O5D
5	E	622	NDP	PA-O3-PN-O5D
4	B	609	DHF	CA-CB-CG-CD
4	B	609	DHF	C6-C9-N10-C14
5	B	610	NDP	C4D-C5D-O5D-PN
5	A	606	NDP	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
5	B	610	NDP	C5D-O5D-PN-O3
5	C	614	NDP	C5B-O5B-PA-O3
5	B	610	NDP	PN-O3-PA-O2A
5	A	606	NDP	O4D-C1D-N1N-C2N
5	B	610	NDP	O4D-C1D-N1N-C2N
5	E	622	NDP	O4D-C1D-N1N-C2N
5	E	622	NDP	C4D-C5D-O5D-PN
5	B	610	NDP	C5D-O5D-PN-O2N
5	C	614	NDP	C5B-O5B-PA-O2A
3	E	620	CB3	C6-C9-N10-C14
2	A	603	UMP	C2'-C1'-N1-C2
5	A	606	NDP	O4D-C1D-N1N-C6N
2	D	615	UMP	C2'-C1'-N1-C2
3	B	608	CB3	N-CA-CB-CG
5	C	614	NDP	O4D-C1D-N1N-C2N
3	A	604	CB3	C6-C9-N10-CP1
4	C	613	DHF	CB-CA-CT-O1
4	C	613	DHF	CB-CA-CT-O2
2	A	603	UMP	O4'-C4'-C5'-O5'
4	B	609	DHF	CB-CA-CT-O1
5	D	618	NDP	O4D-C1D-N1N-C2N
4	A	605	DHF	OE2-CD-CG-CB
5	C	614	NDP	C3D-C4D-C5D-O5D
4	E	621	DHF	CT-CA-CB-CG
4	B	609	DHF	CB-CA-CT-O2
4	A	605	DHF	OE1-CD-CG-CB
5	A	606	NDP	O4D-C4D-C5D-O5D
3	E	620	CB3	OE2-CD-CG-CB
5	D	618	NDP	PN-O3-PA-O1A
4	D	617	DHF	OE2-CD-CG-CB
2	A	603	UMP	C3'-C4'-C5'-O5'
5	D	618	NDP	O4D-C4D-C5D-O5D
4	D	617	DHF	C6-C9-N10-C14
5	B	610	NDP	C3B-C2B-O2B-P2B
3	E	620	CB3	OE1-CD-CG-CB
4	D	617	DHF	OE1-CD-CG-CB
5	A	606	NDP	C2B-O2B-P2B-O2X
5	D	618	NDP	C2B-O2B-P2B-O2X
3	E	620	CB3	C6-C9-N10-CP1
5	B	610	NDP	PN-O3-PA-O1A
5	A	606	NDP	C5B-O5B-PA-O1A
5	C	614	NDP	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
3	E	620	CB3	CT-CA-N-C
3	D	616	CB3	OE2-CD-CG-CB
5	C	614	NDP	C4D-C5D-O5D-PN
3	A	604	CB3	OE2-CD-CG-CB
3	D	616	CB3	OE1-CD-CG-CB
5	D	618	NDP	C2D-C1D-N1N-C2N

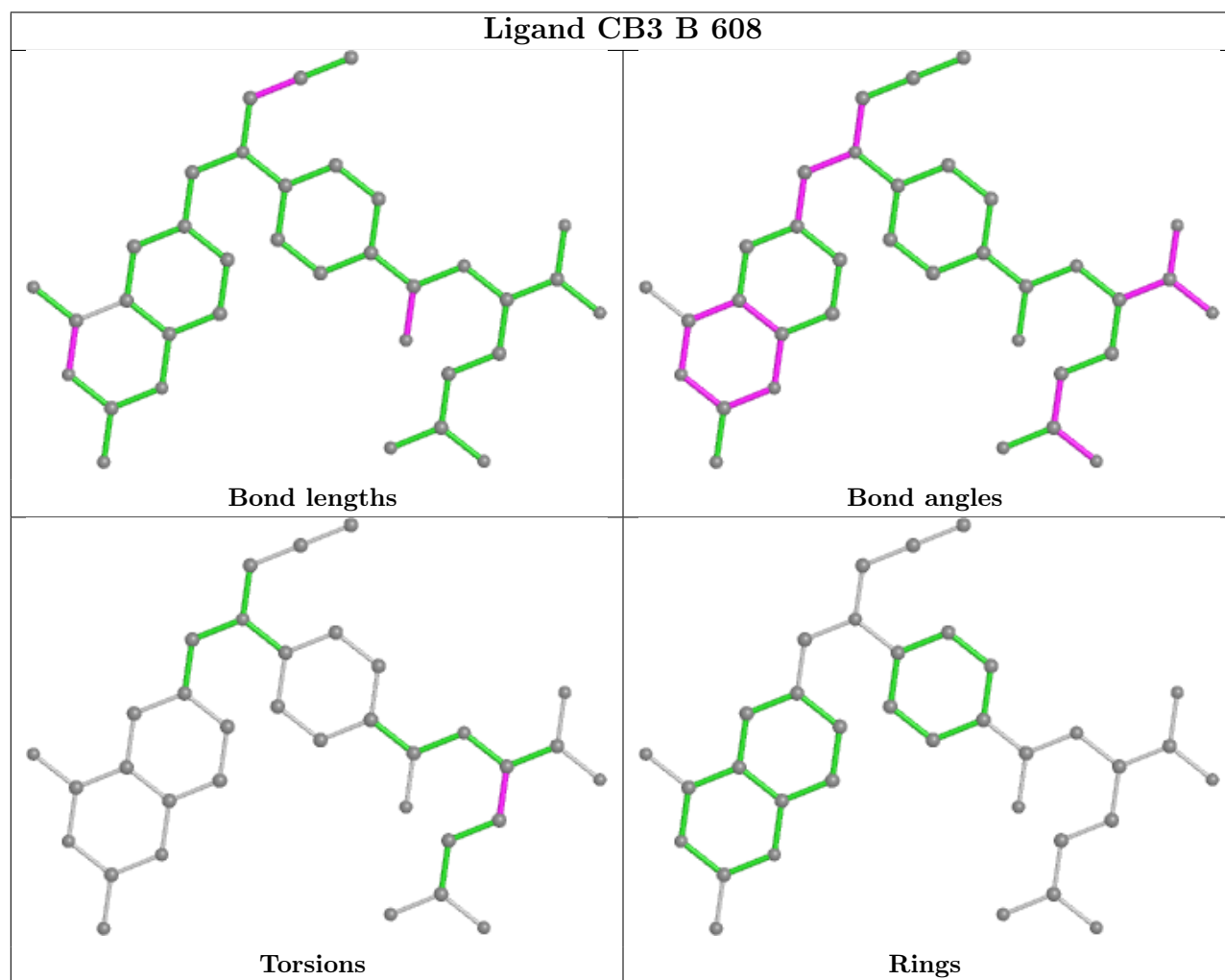
There are no ring outliers.

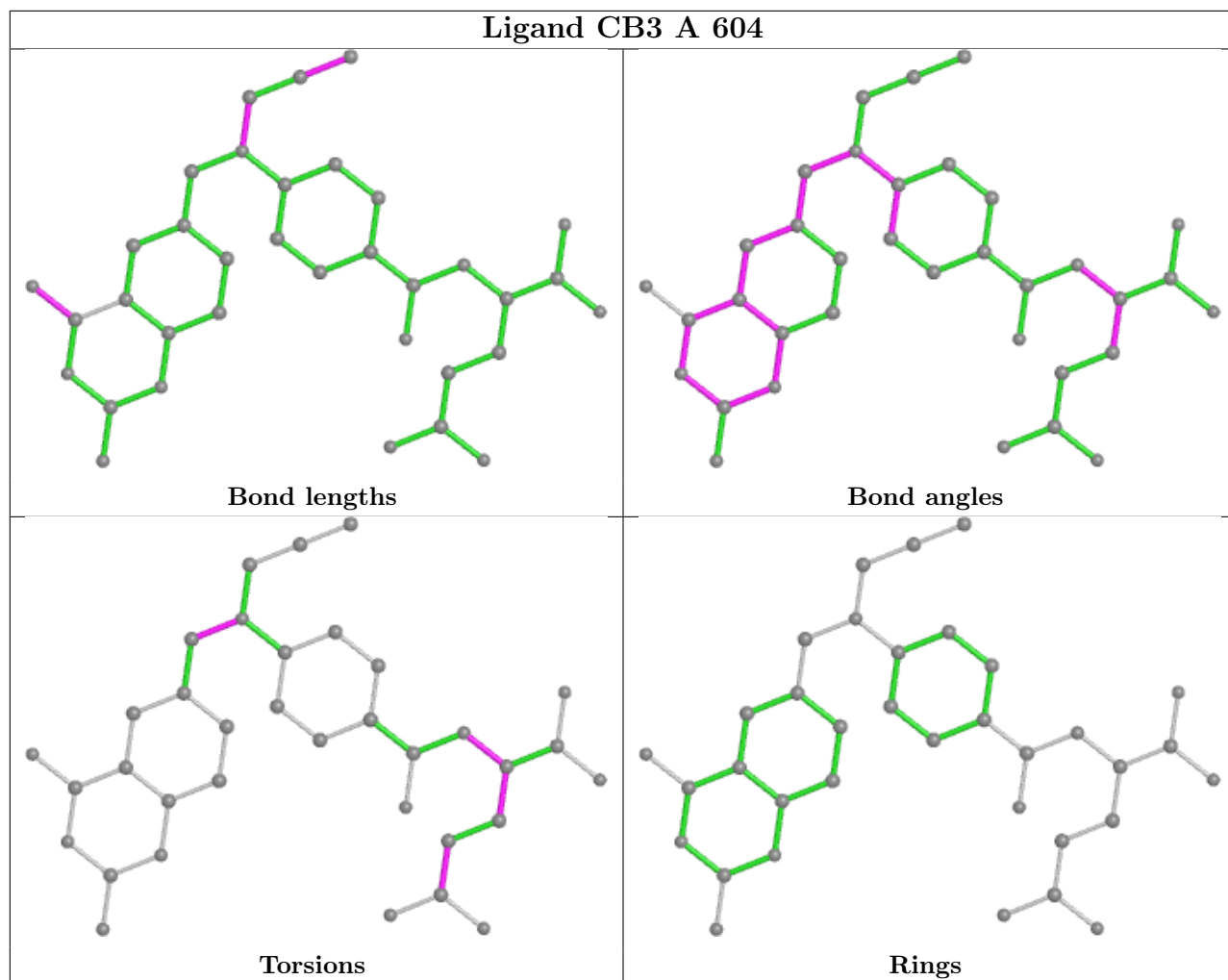
20 monomers are involved in 278 short contacts:

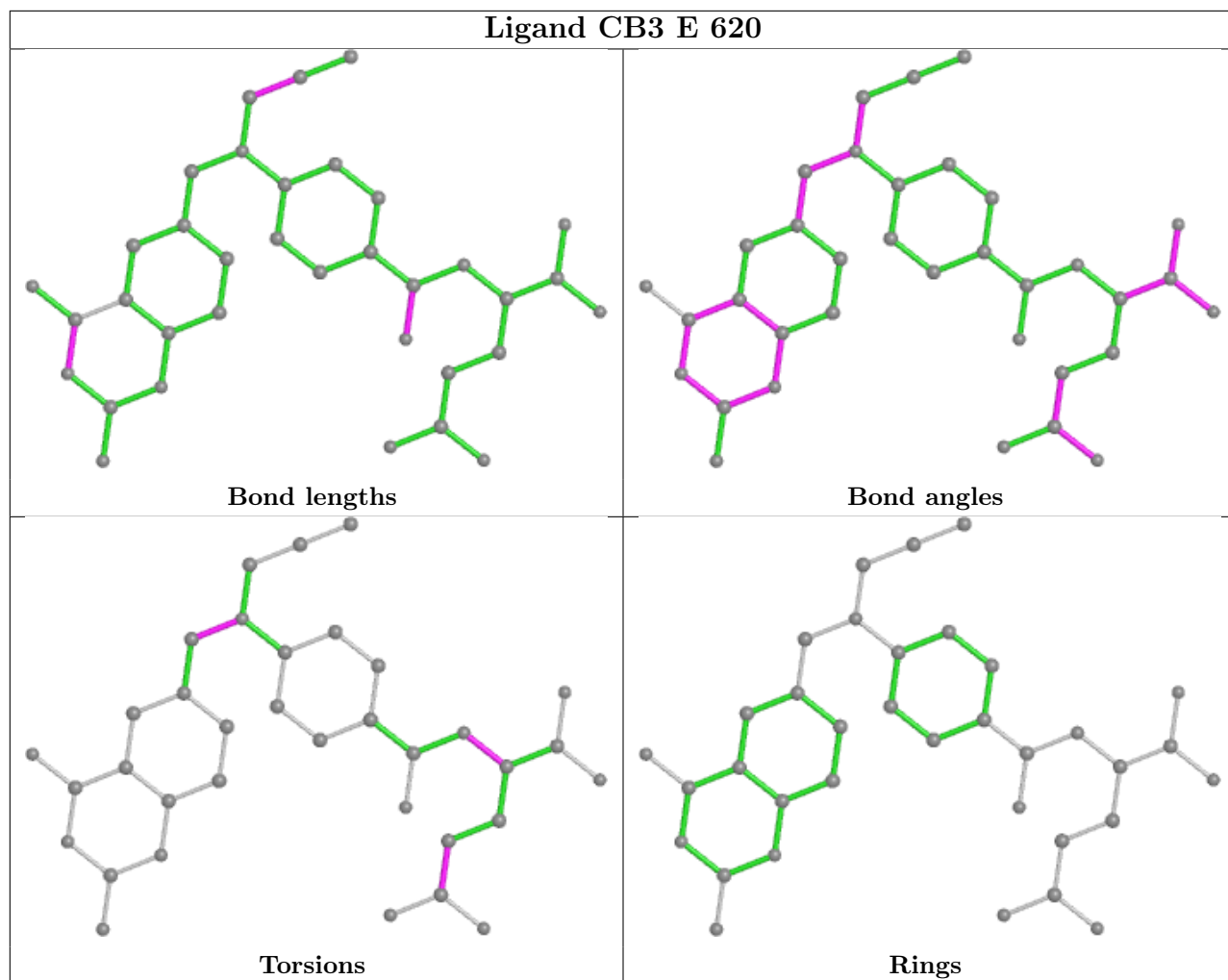
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	608	CB3	14	0
3	A	604	CB3	5	0
3	E	620	CB3	13	0
5	D	618	NDP	14	0
4	D	617	DHF	33	0
3	C	612	CB3	15	0
4	C	613	DHF	24	0
4	B	609	DHF	18	0
5	B	610	NDP	13	0
4	A	605	DHF	9	0
3	D	616	CB3	14	0
2	D	615	UMP	3	0
2	E	619	UMP	10	0
2	A	603	UMP	8	0
2	C	611	UMP	5	0
5	C	614	NDP	23	0
4	E	621	DHF	20	0
5	E	622	NDP	19	0
5	A	606	NDP	18	0
2	B	607	UMP	10	0

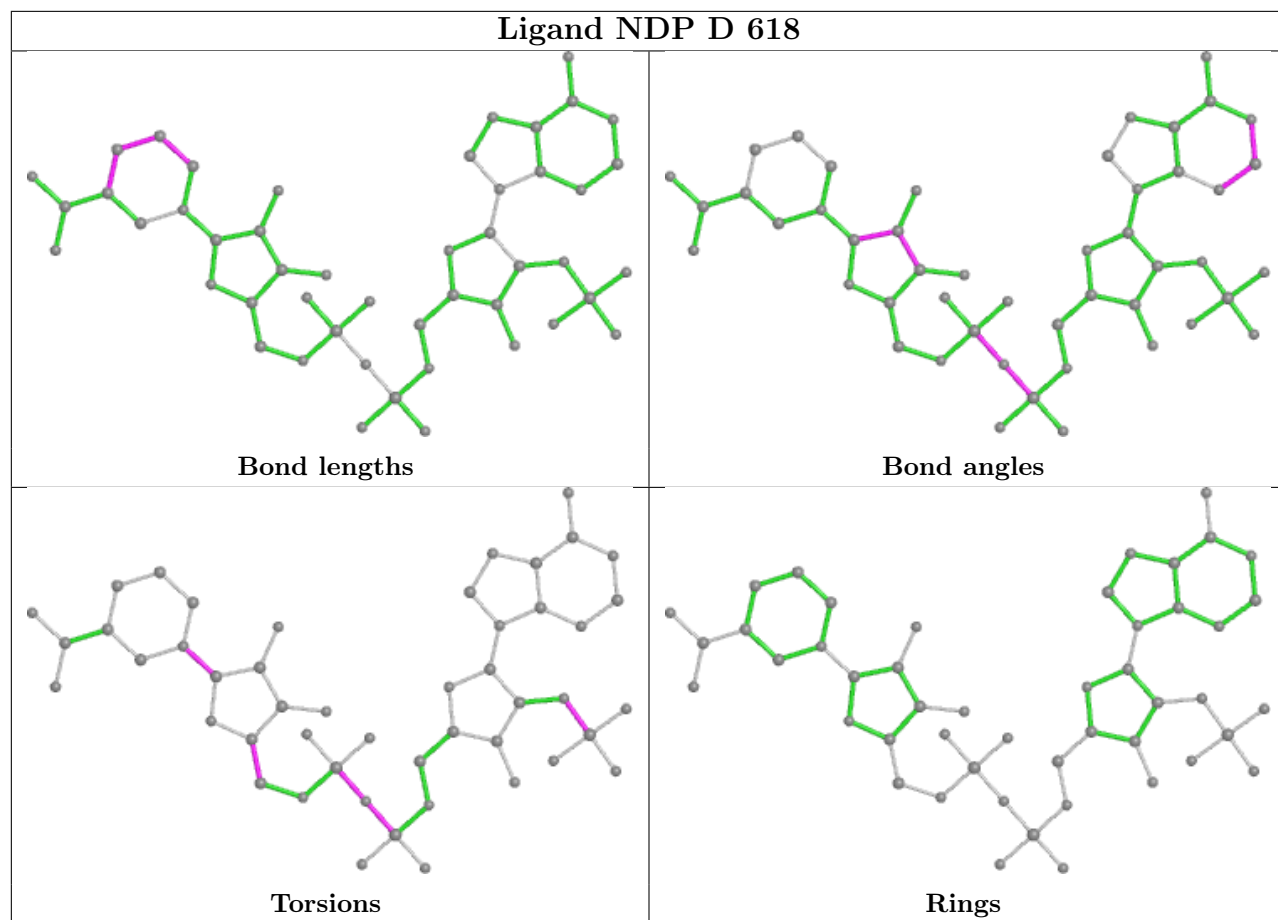
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

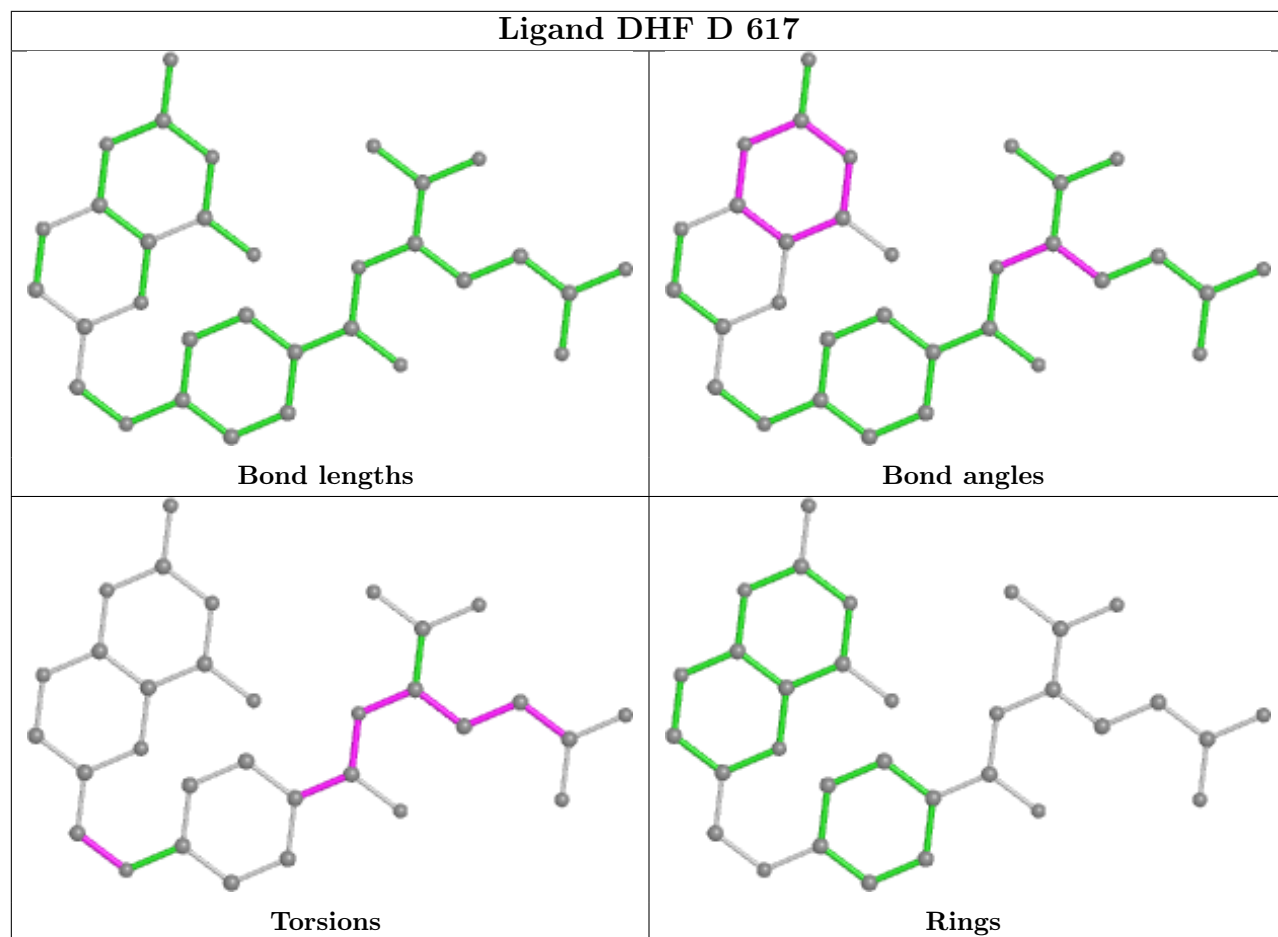
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

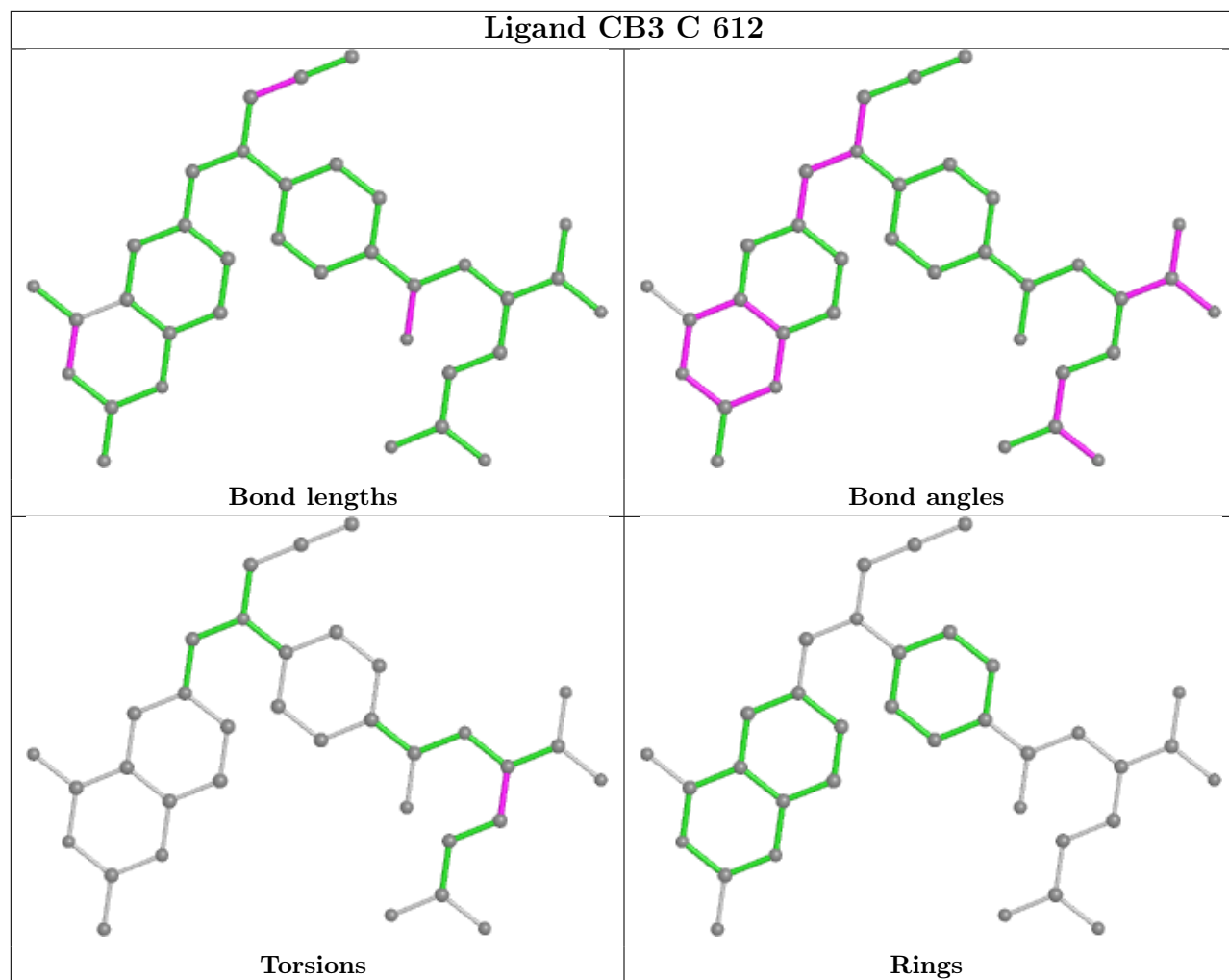


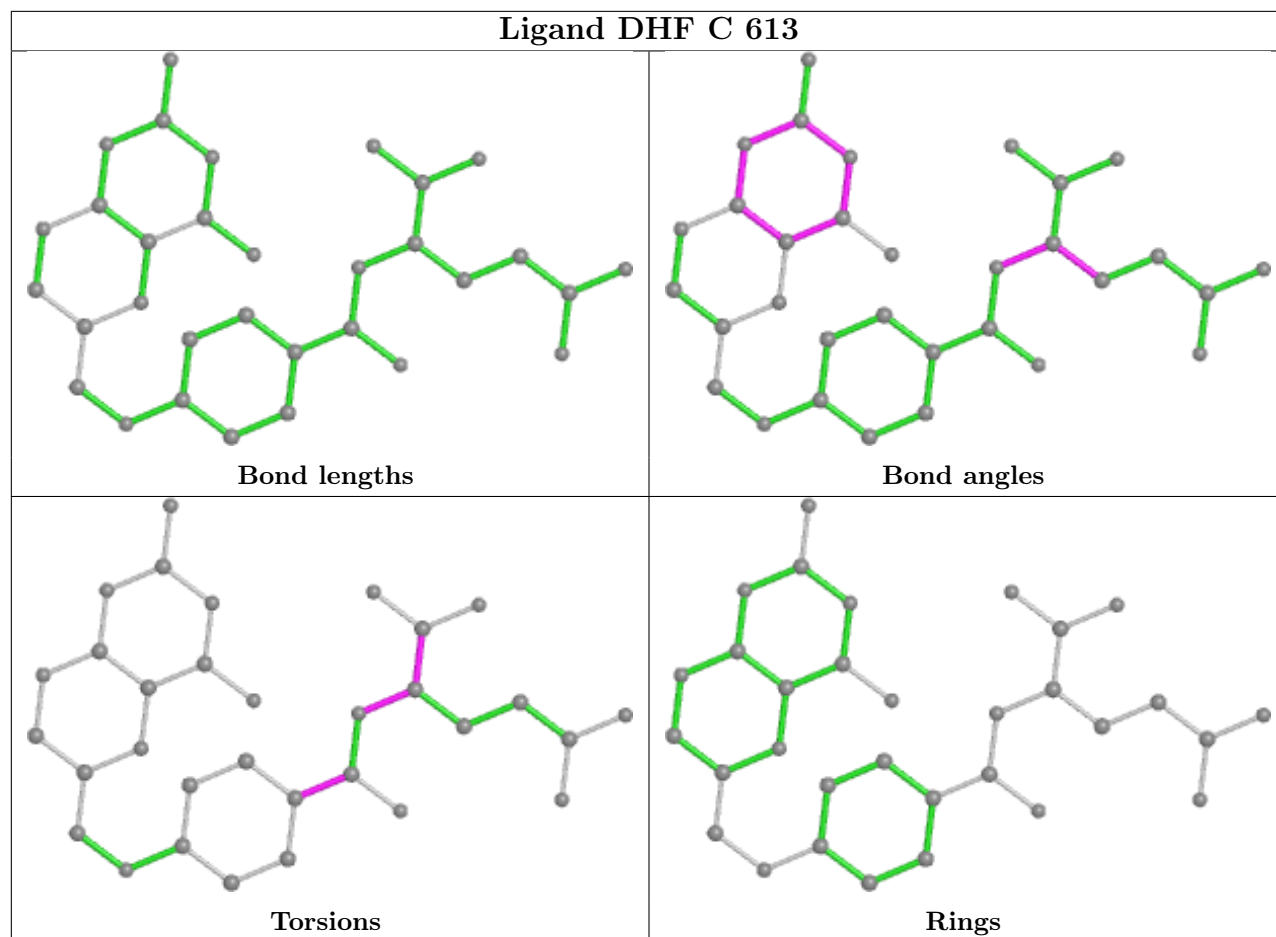


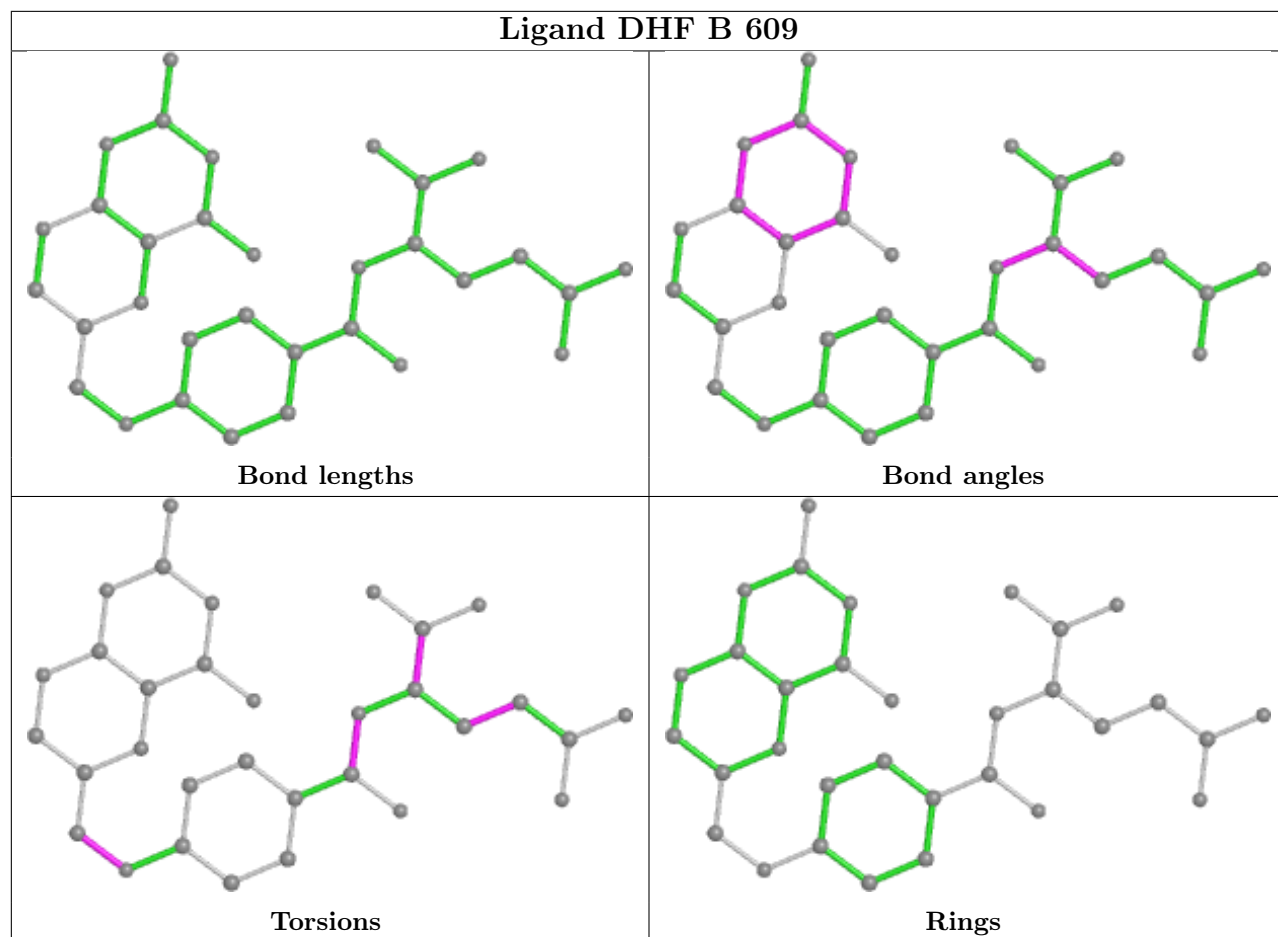


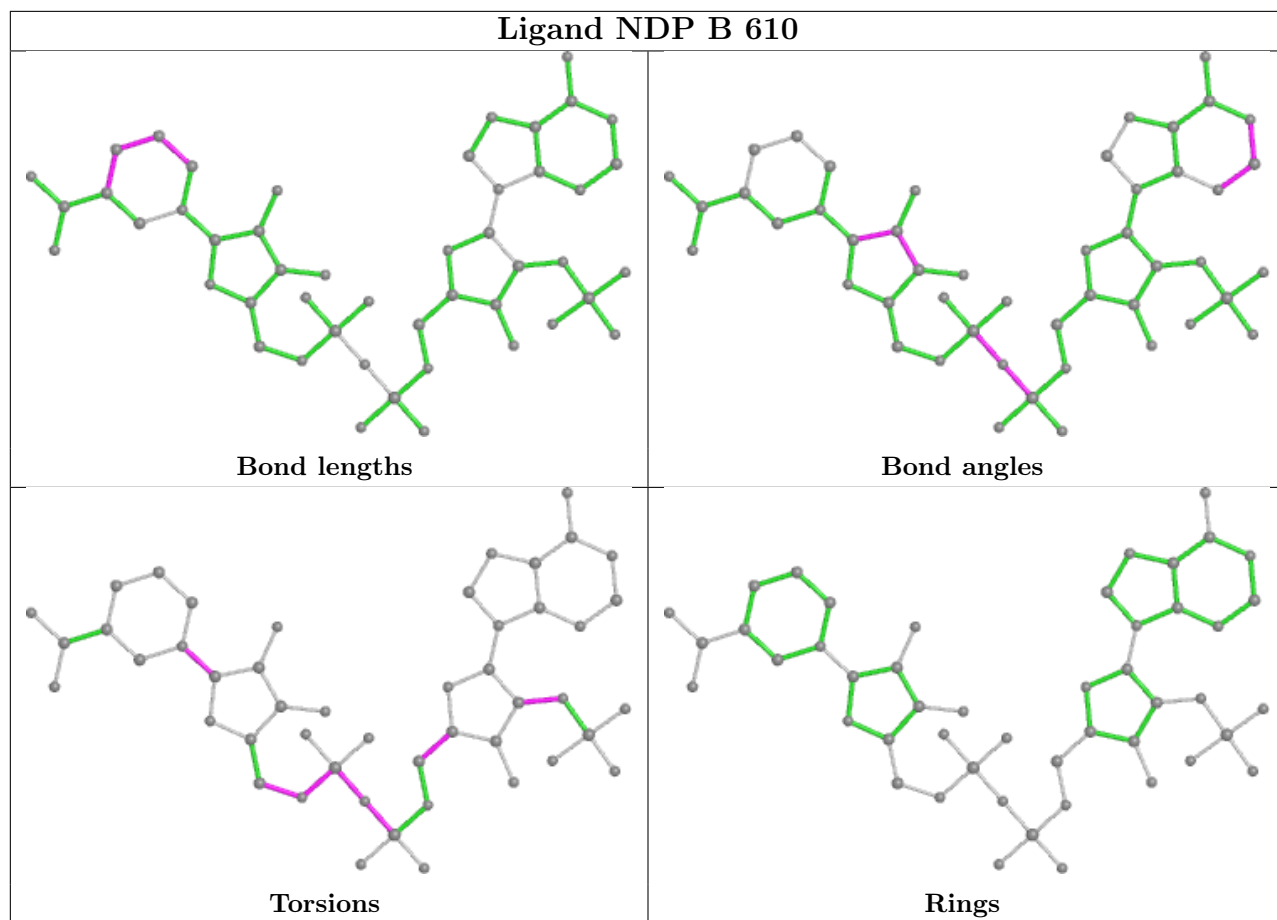


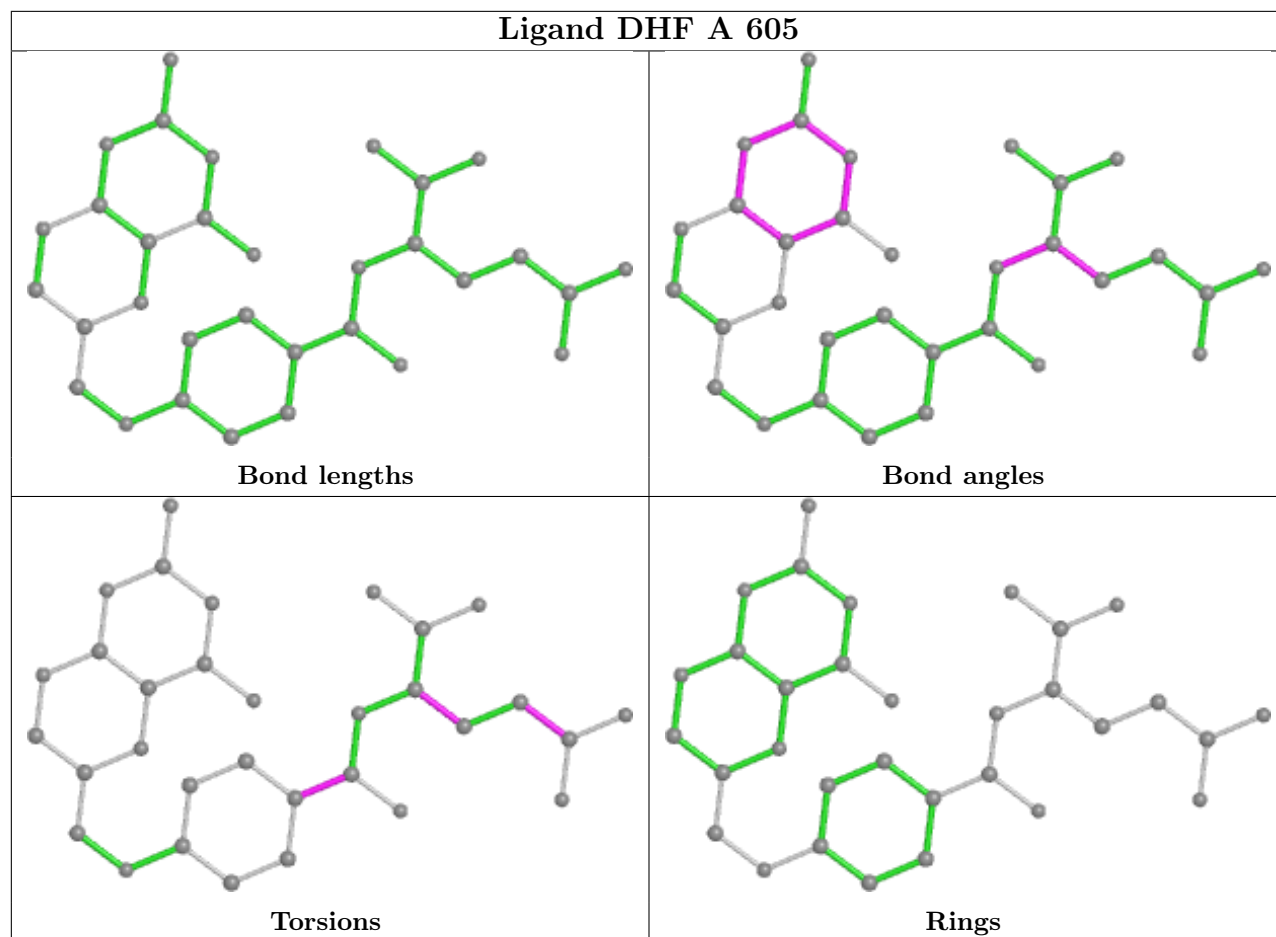


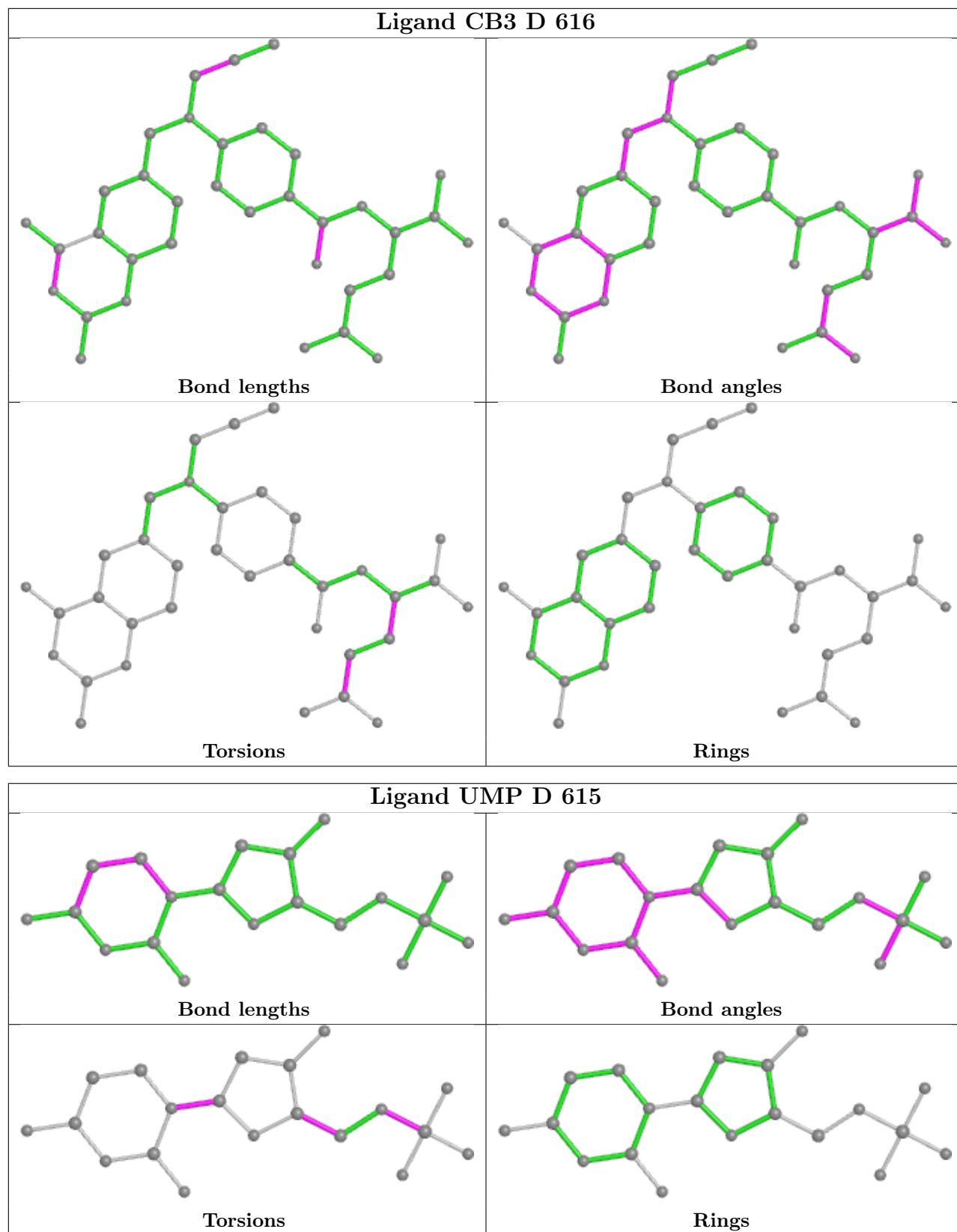


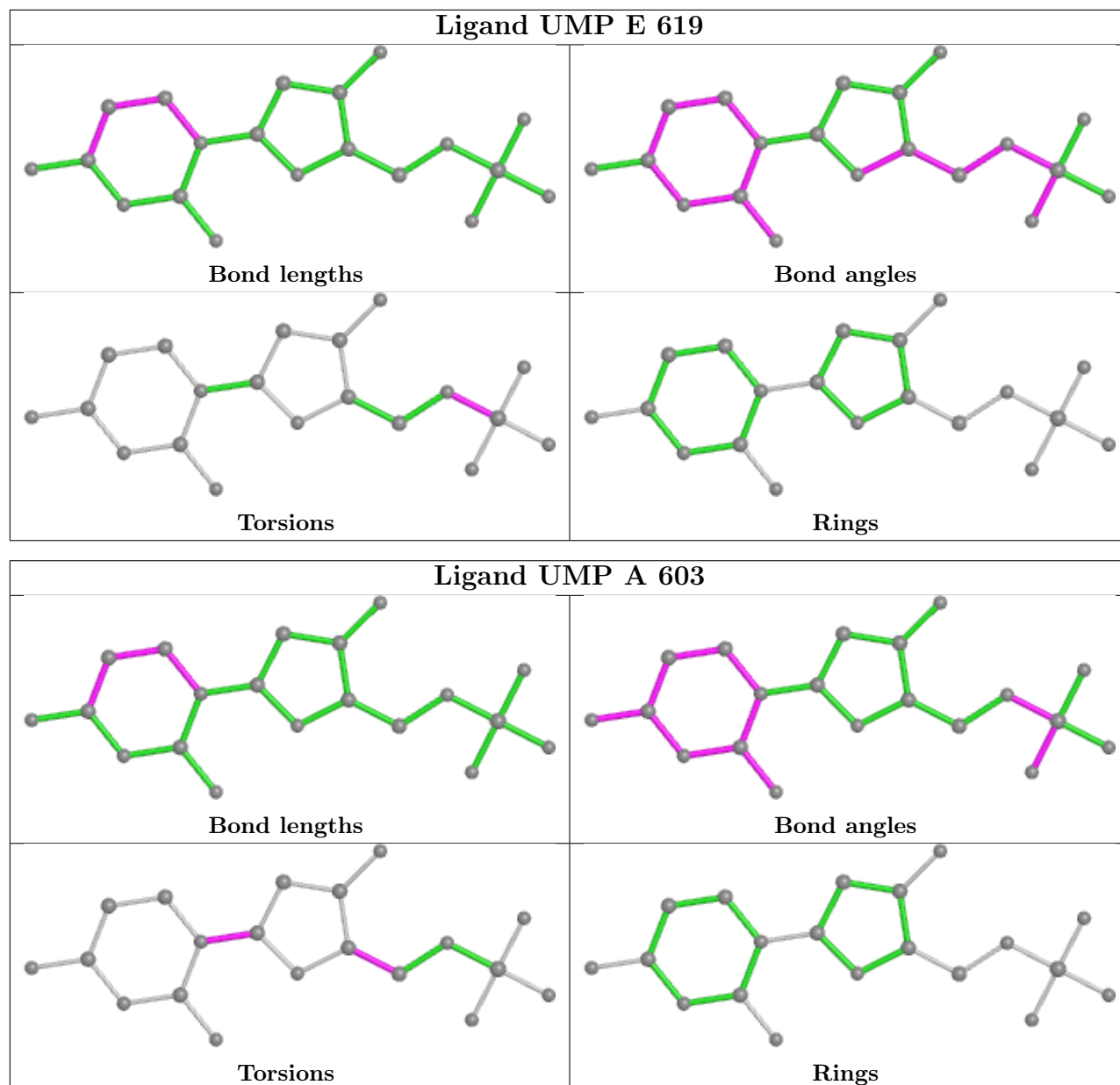


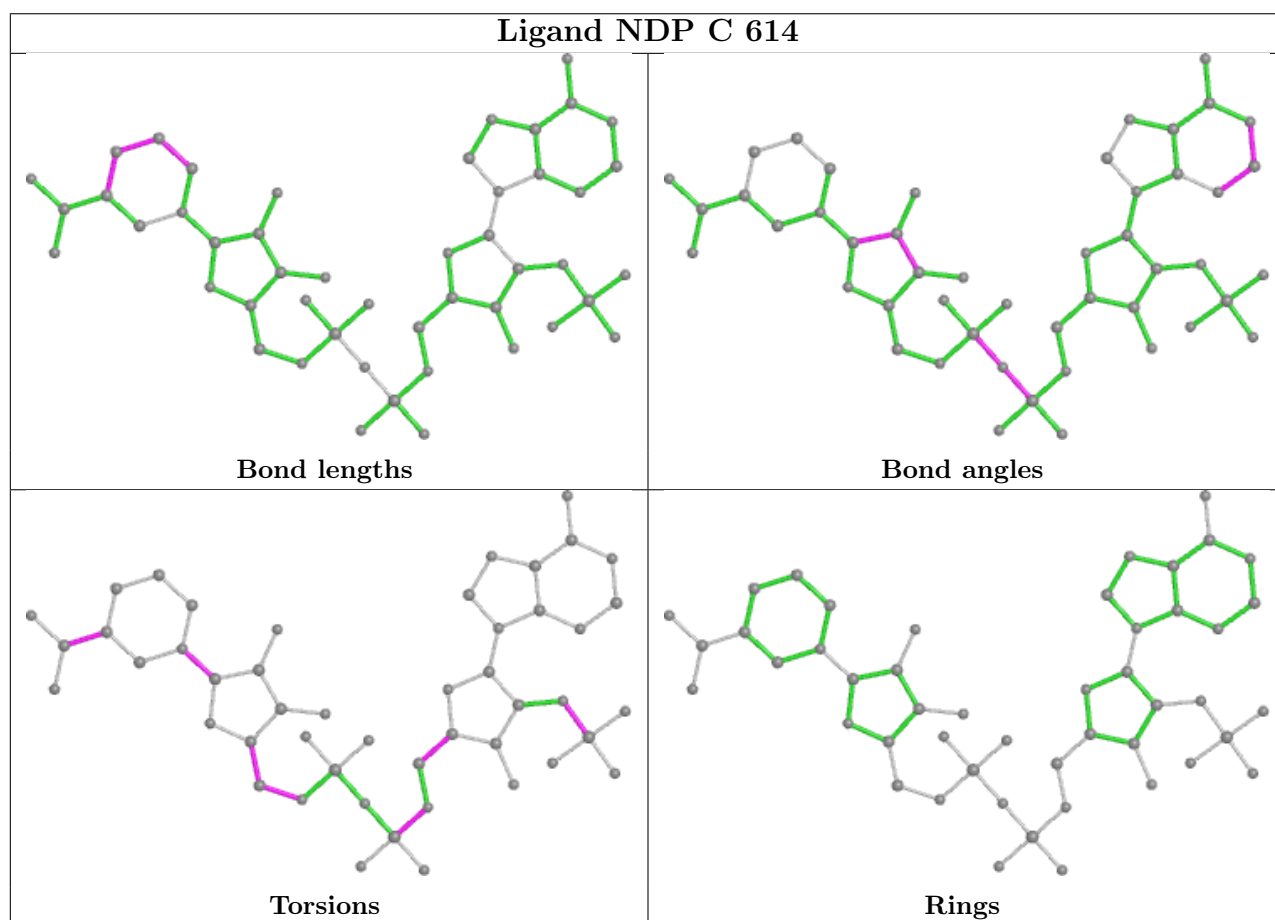
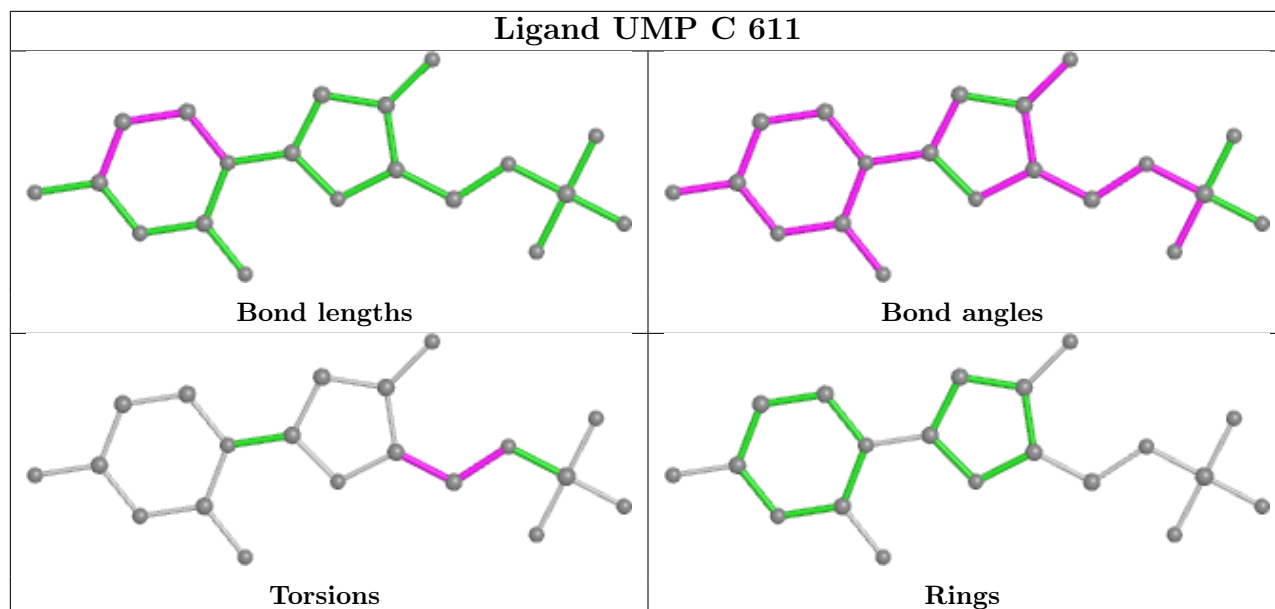


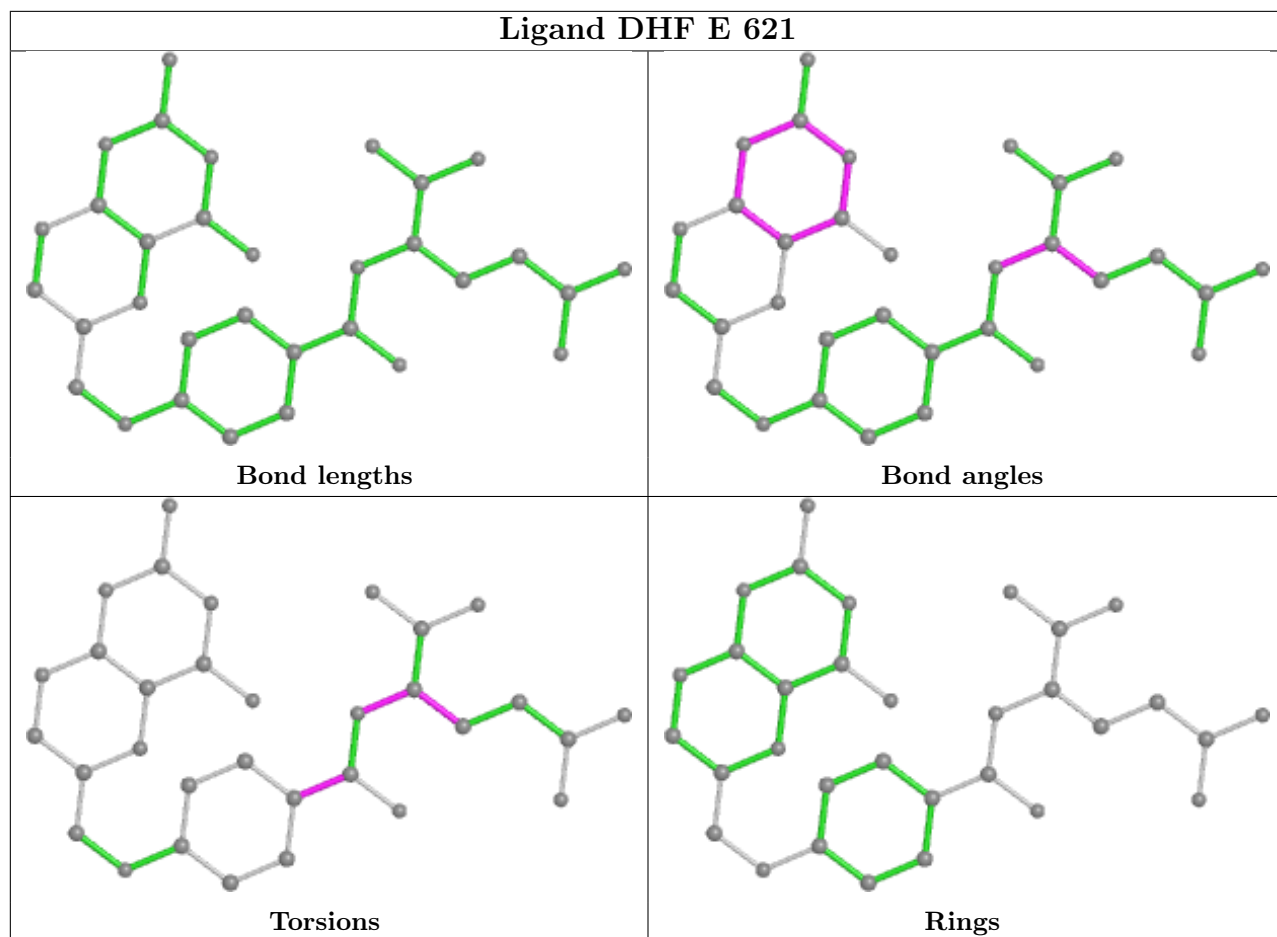


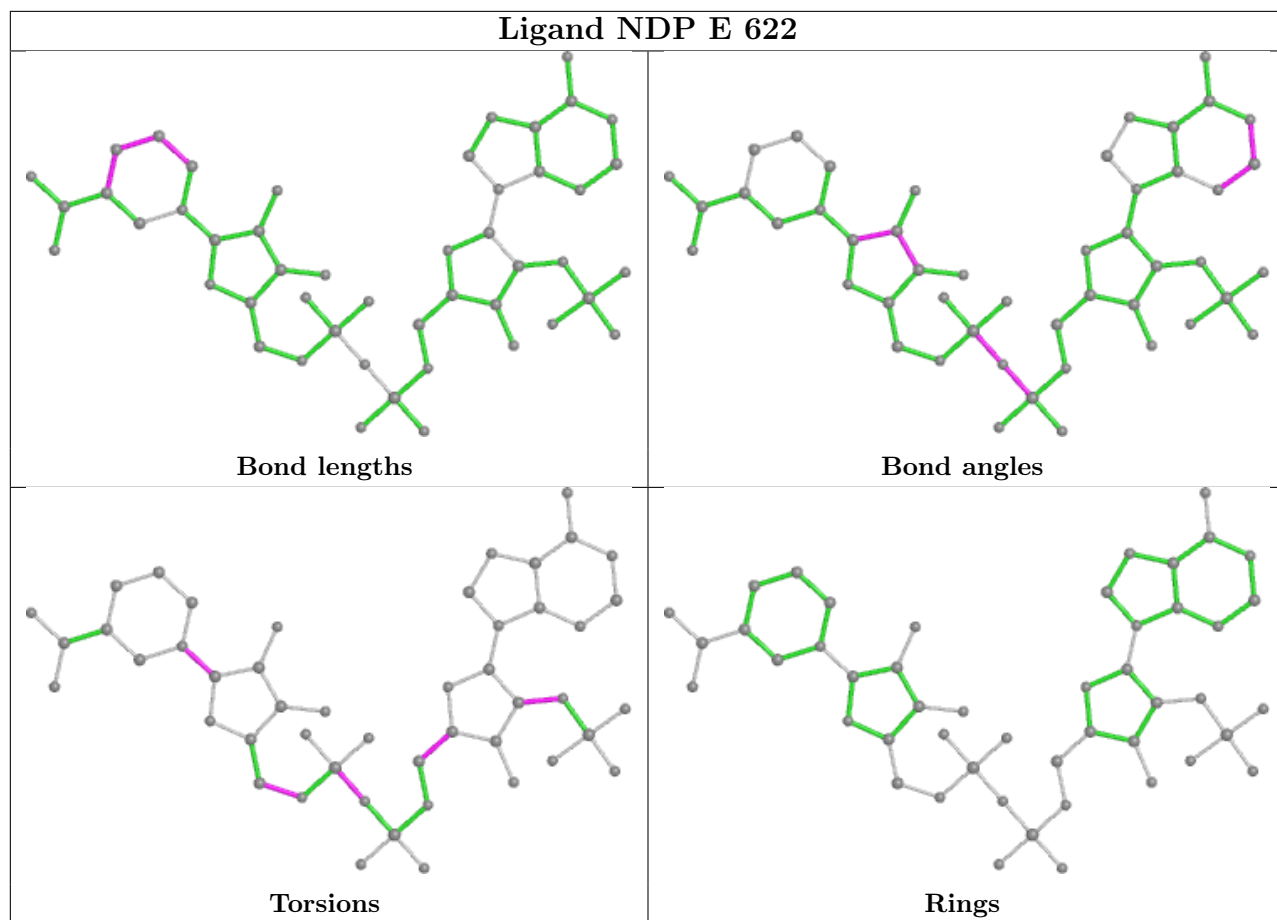


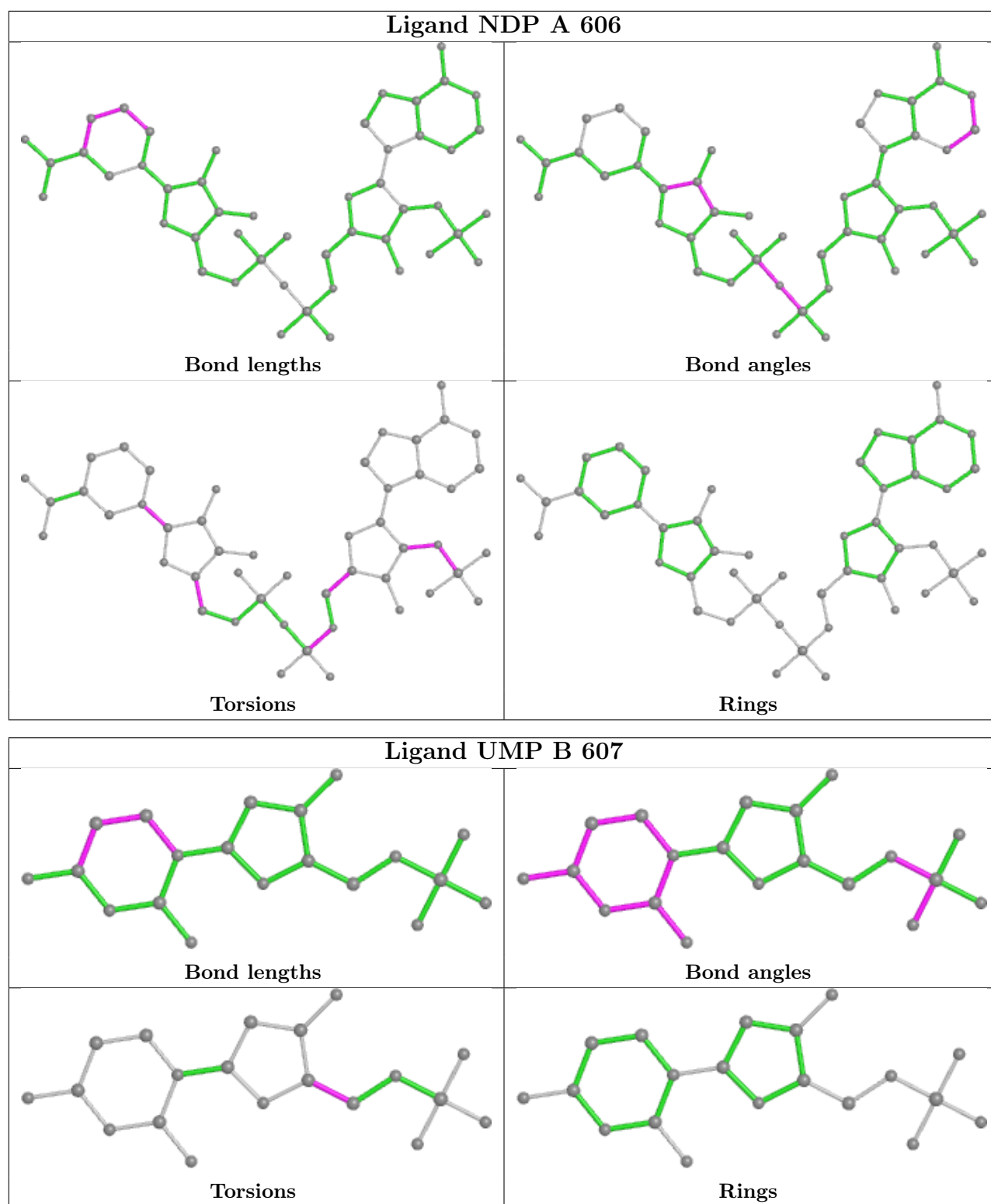












5.7 Other polymers [\(i\)](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	505/521 (96%)	-0.43	0 100 100	22, 52, 94, 157	0
1	B	508/521 (97%)	-0.45	3 (0%) 89 89	20, 47, 94, 157	0
1	C	508/521 (97%)	-0.31	3 (0%) 89 89	27, 57, 110, 189	0
1	D	508/521 (97%)	-0.32	2 (0%) 92 92	25, 60, 110, 172	0
1	E	507/521 (97%)	-0.12	1 (0%) 95 95	36, 75, 125, 181	0
All	All	2536/2605 (97%)	-0.32	9 (0%) 92 92	20, 58, 111, 189	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	192	GLN	3.6
1	B	192	GLN	3.5
1	C	102	MET	3.1
1	D	192	GLN	3.0
1	E	102	MET	2.9
1	B	103	ASN	2.8
1	D	102	MET	2.3
1	B	102	MET	2.3
1	C	137	ALA	2.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

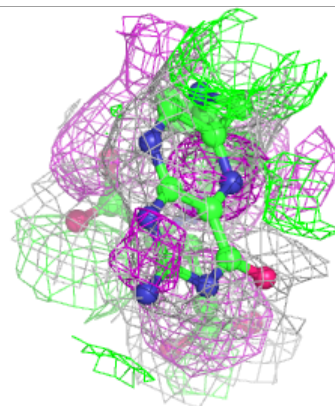
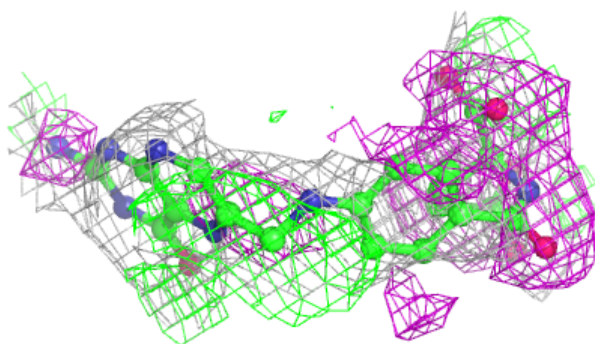
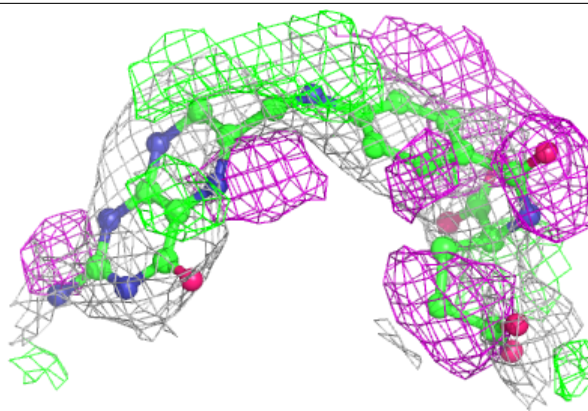
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DHF	D	617	32/32	0.69	0.45	40,63,63,63	0
4	DHF	B	609	32/32	0.79	0.35	33,63,63,63	0
5	NDP	C	614	48/48	0.80	0.39	52,63,92,99	0
3	CB3	E	620	35/35	0.84	0.42	55,66,89,98	0
3	CB3	A	604	35/35	0.85	0.34	60,63,76,80	0
4	DHF	C	613	32/32	0.86	0.28	42,63,63,72	0
5	NDP	D	618	48/48	0.86	0.30	49,63,73,88	0
5	NDP	E	622	48/48	0.86	0.28	56,63,90,94	0
4	DHF	A	605	32/32	0.87	0.27	33,63,63,64	0
5	NDP	A	606	48/48	0.87	0.28	28,63,63,63	0
5	NDP	B	610	48/48	0.87	0.28	28,63,63,65	0
2	UMP	E	619	20/20	0.88	0.24	63,63,81,84	0
3	CB3	D	616	35/35	0.88	0.31	53,63,65,76	0
3	CB3	B	608	35/35	0.89	0.34	44,50,63,63	0
2	UMP	B	607	20/20	0.89	0.24	25,63,63,63	0
3	CB3	C	612	35/35	0.91	0.29	45,58,63,63	0
4	DHF	E	621	32/32	0.92	0.22	41,63,63,81	0
2	UMP	A	603	20/20	0.92	0.22	40,63,66,72	0
2	UMP	C	611	20/20	0.93	0.20	45,63,63,66	0
2	UMP	D	615	20/20	0.95	0.17	57,63,65,84	0

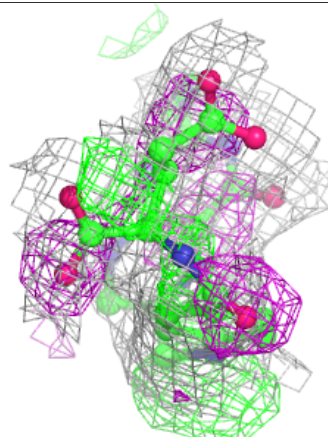
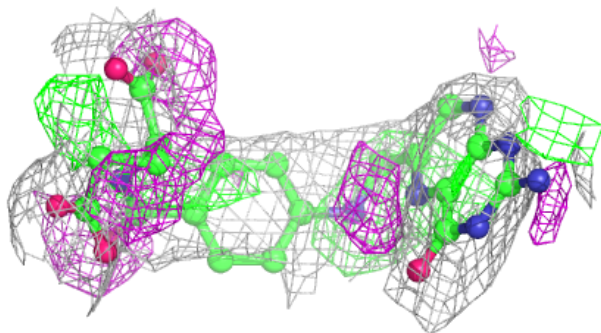
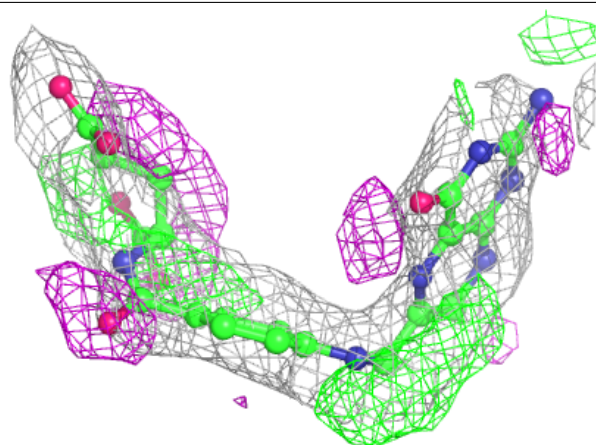
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

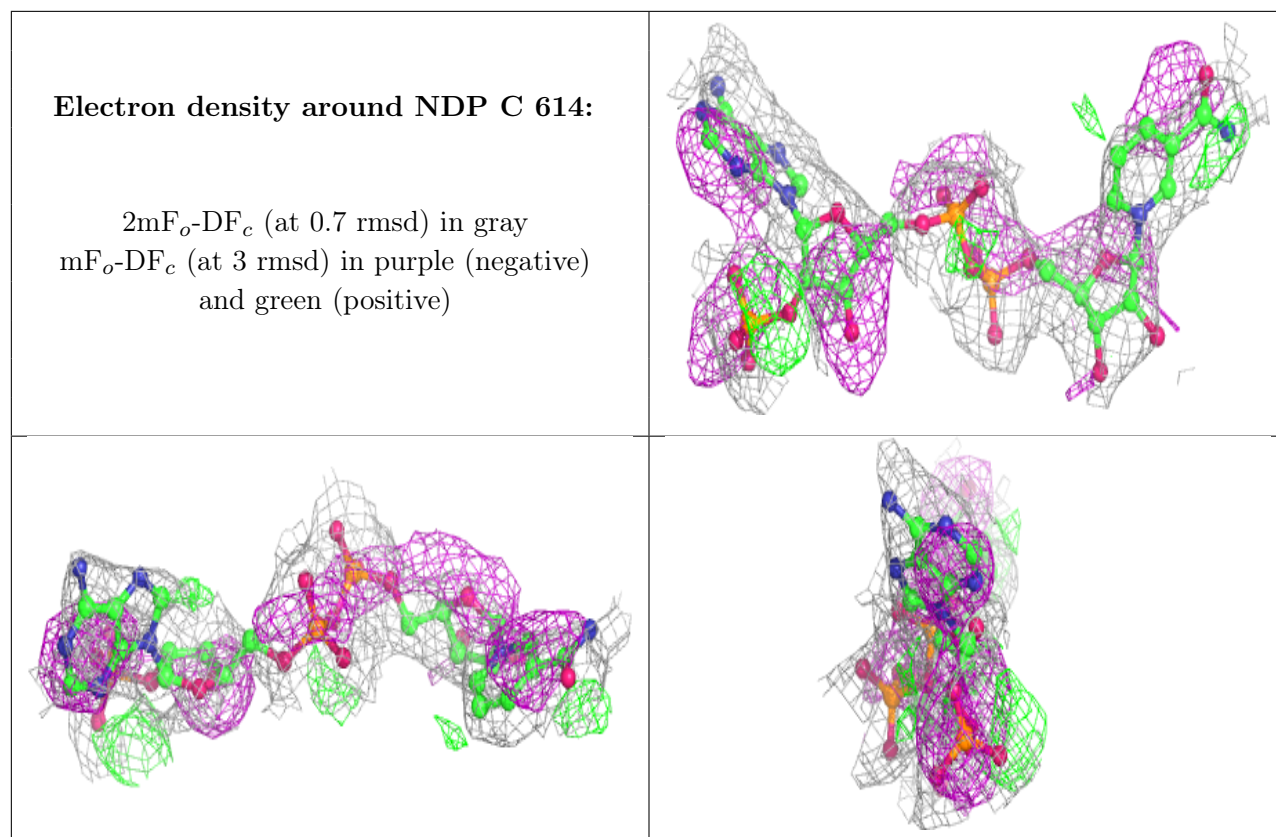
Electron density around DHF D 617:

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

**Electron density around DHF B 609:**

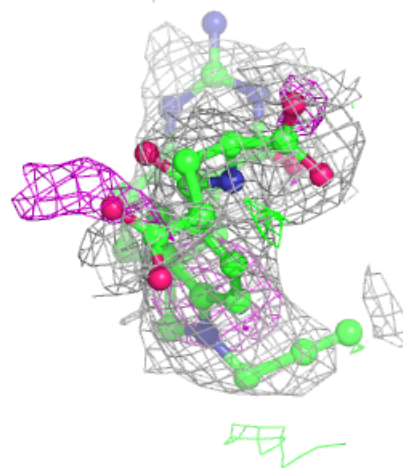
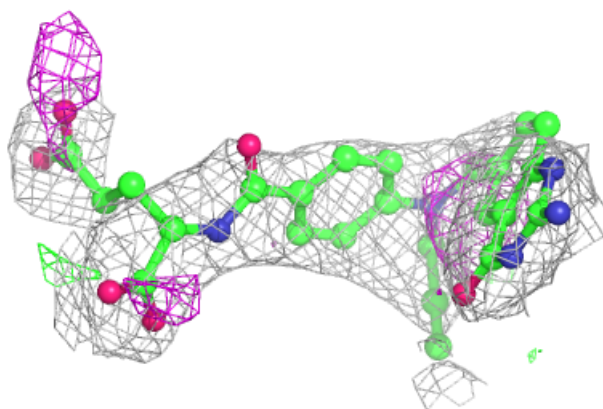
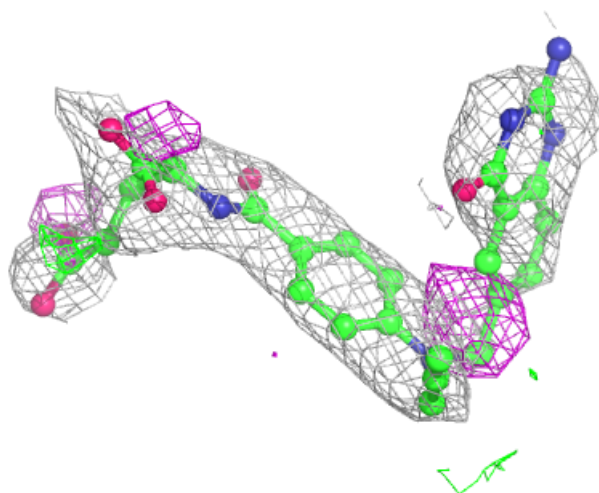
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





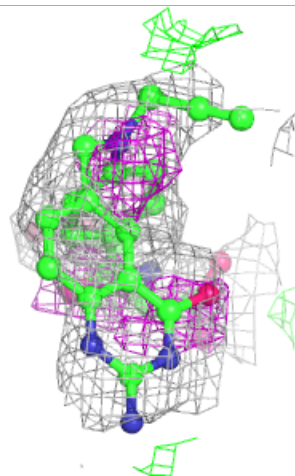
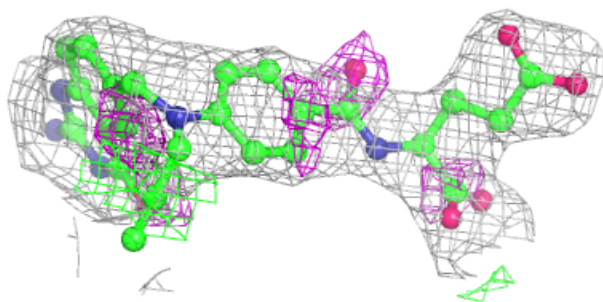
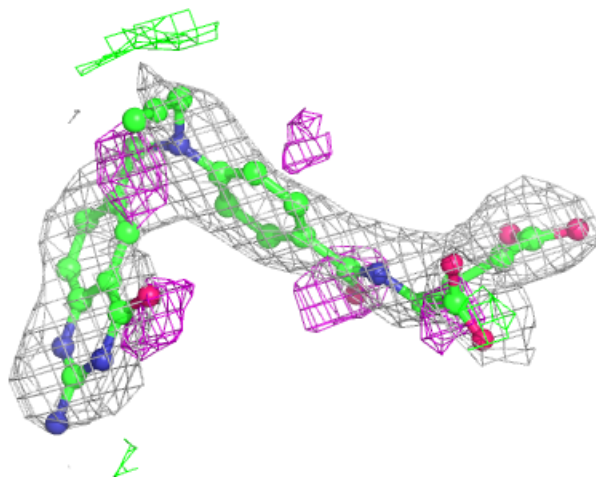
Electron density around CB3 E 620:

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



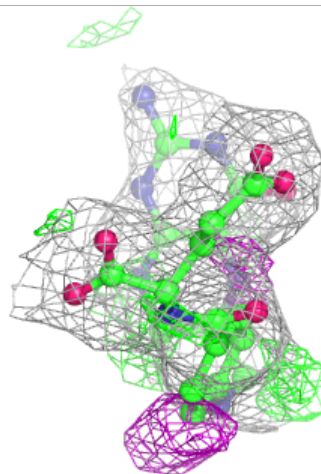
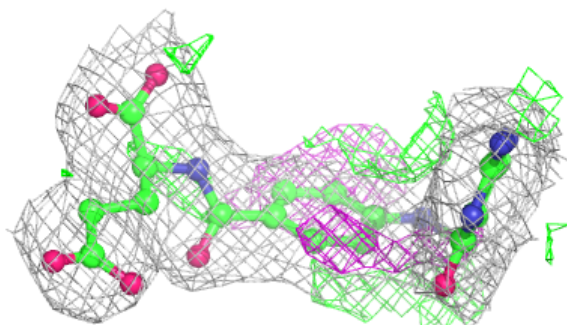
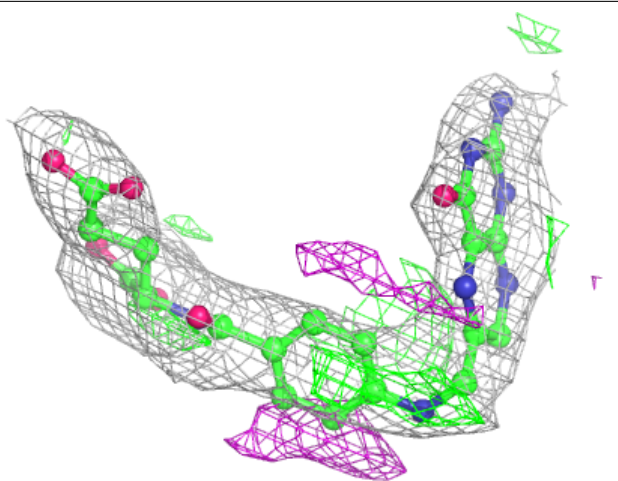
Electron density around CB3 A 604:

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



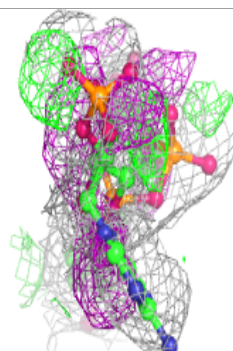
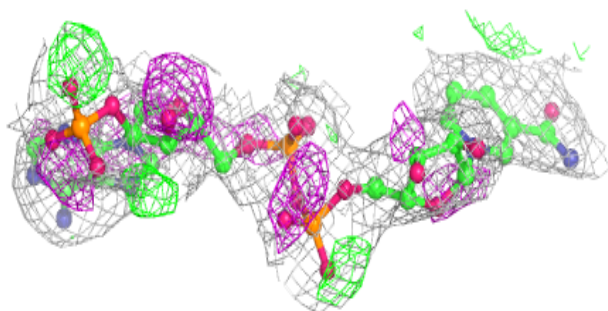
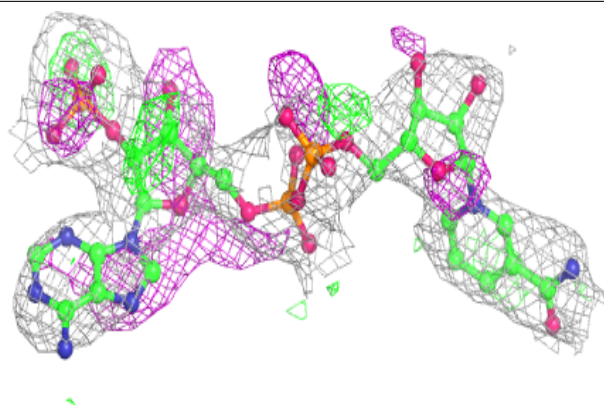
Electron density around DHF C 613:

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

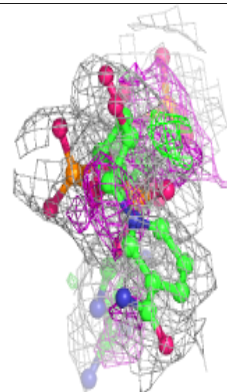
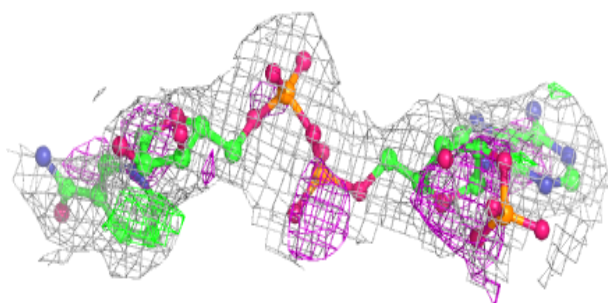
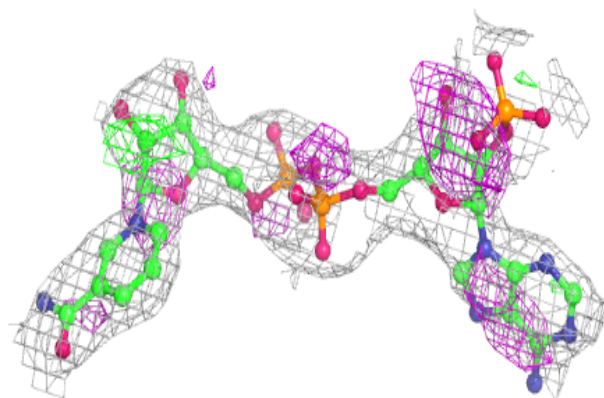


Electron density around NDP D 618:

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

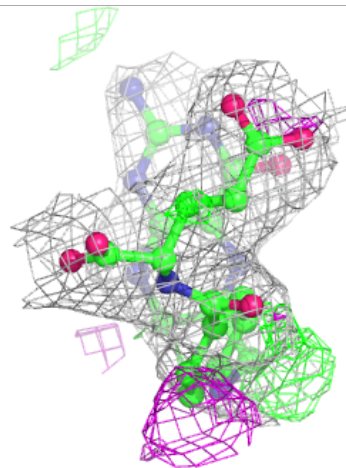
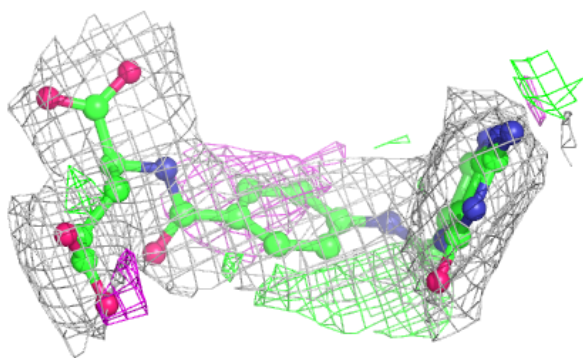
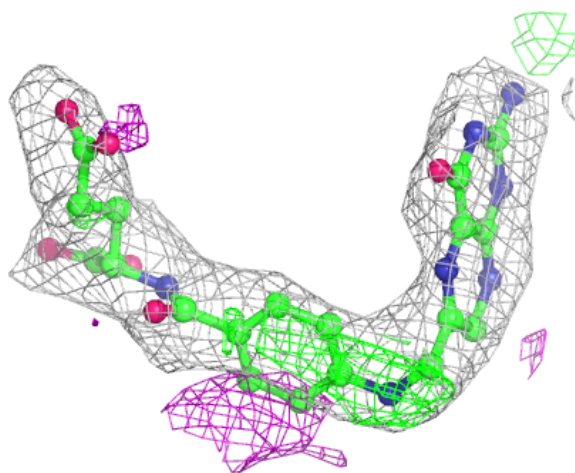
**Electron density around NDP E 622:**

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



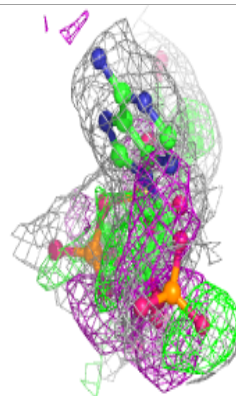
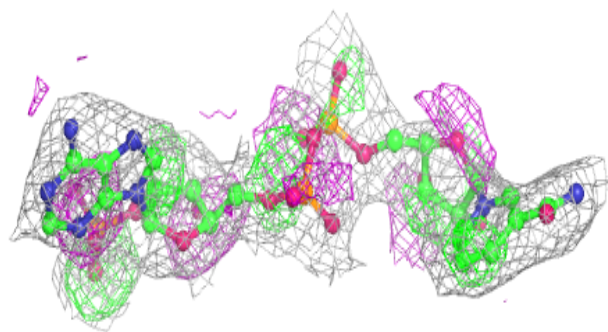
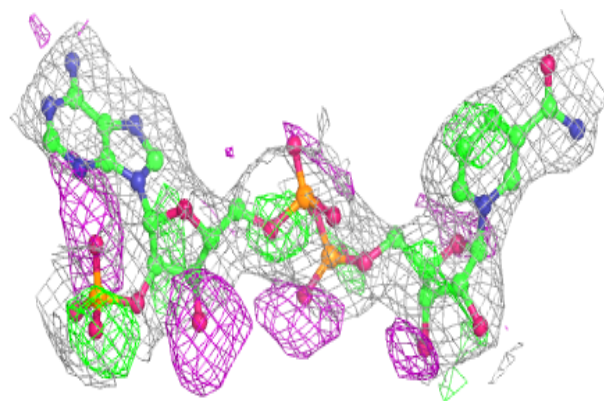
Electron density around DHF A 605:

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

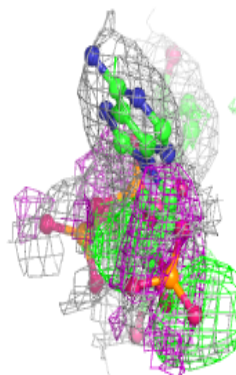
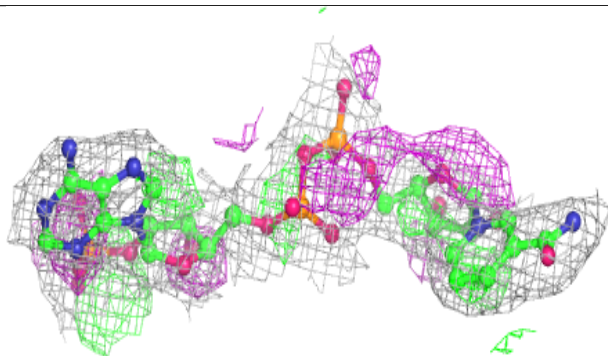
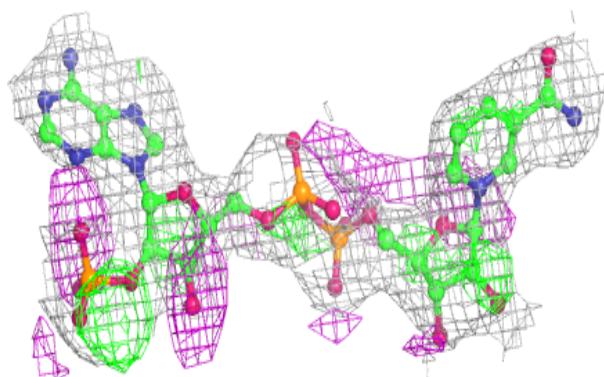


Electron density around NDP A 606:

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

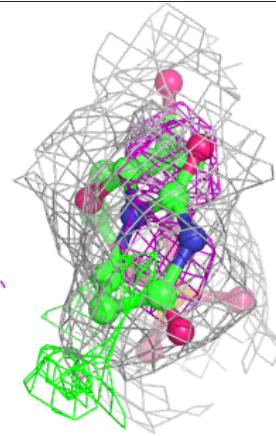
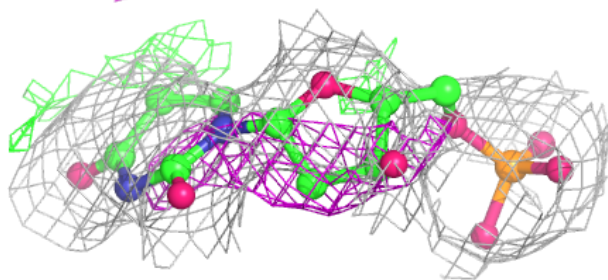
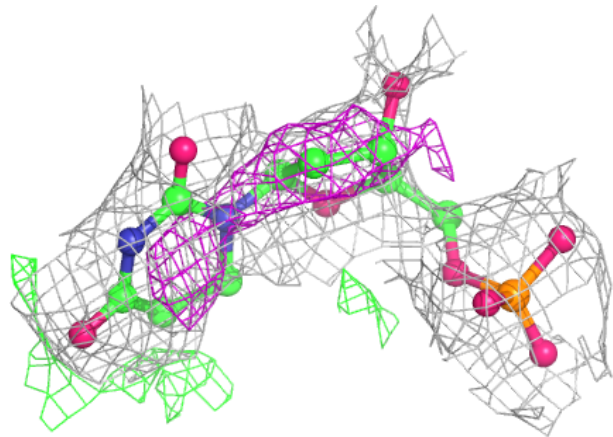
**Electron density around NDP B 610:**

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

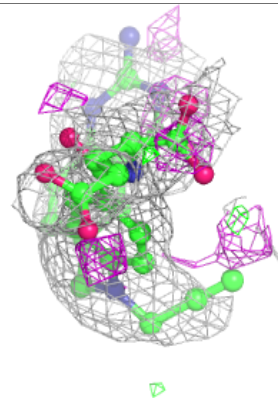
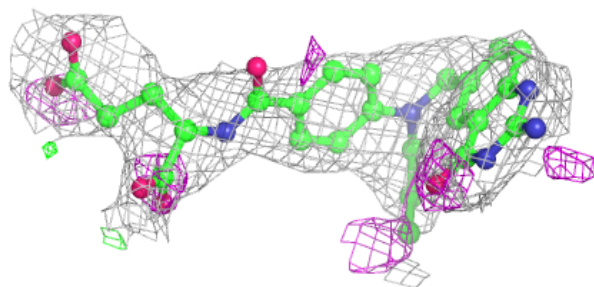
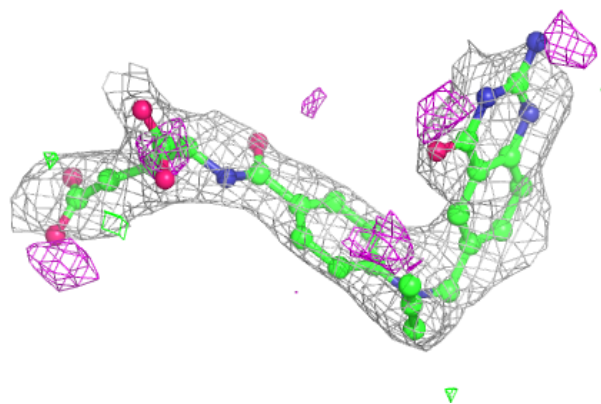


Electron density around UMP E 619:

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

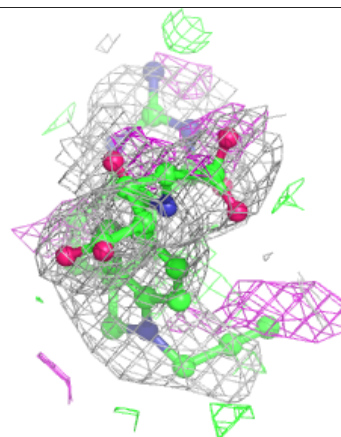
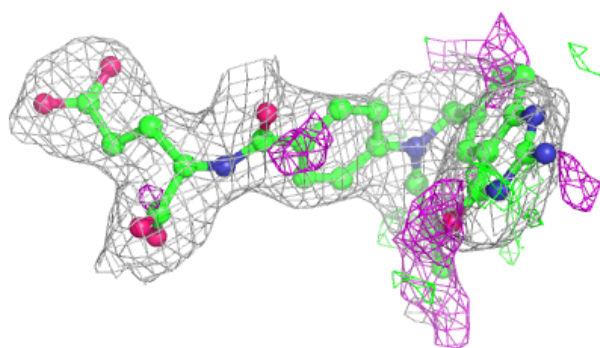
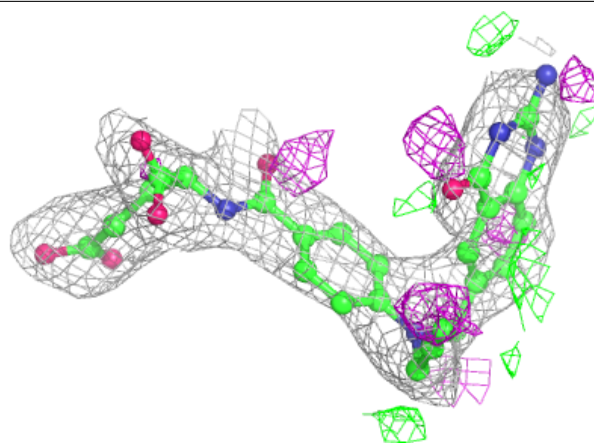
**Electron density around CB3 D 616:**

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

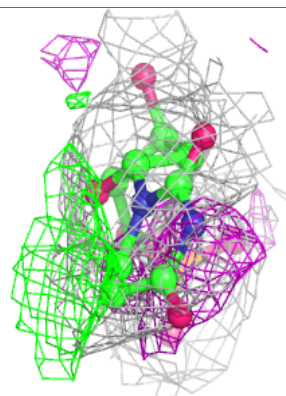
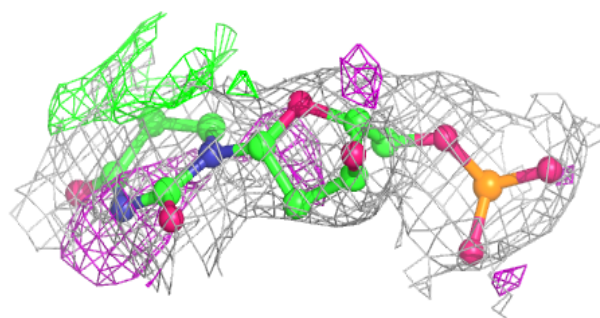
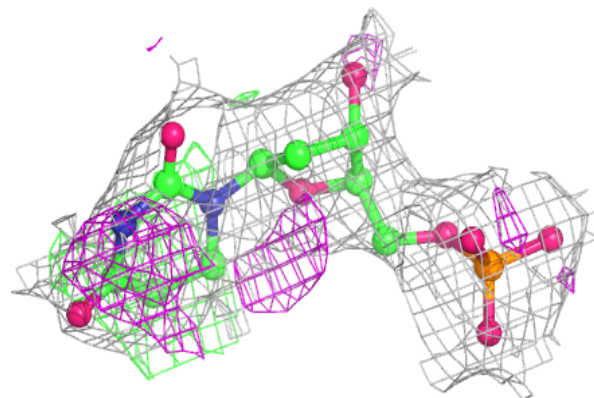


Electron density around CB3 B 608:

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

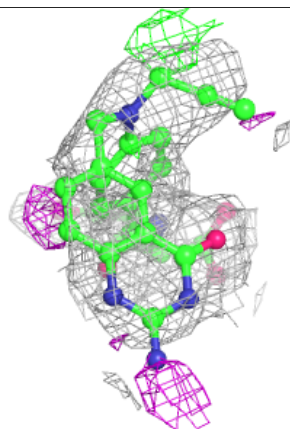
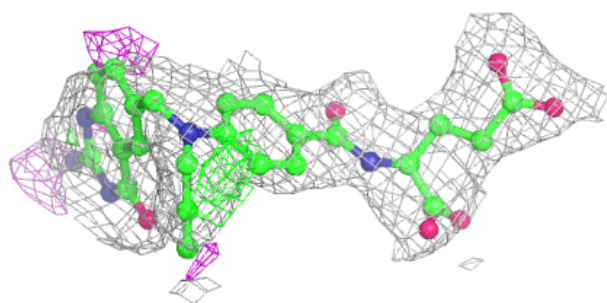
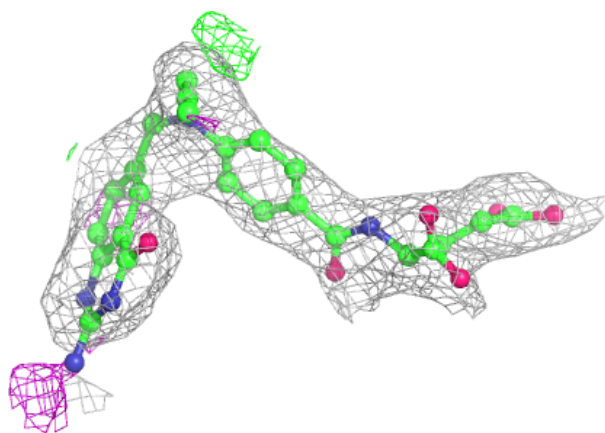
**Electron density around UMP B 607:**

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

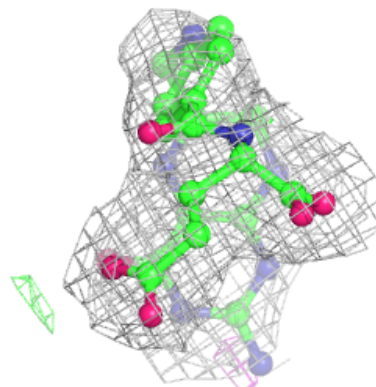
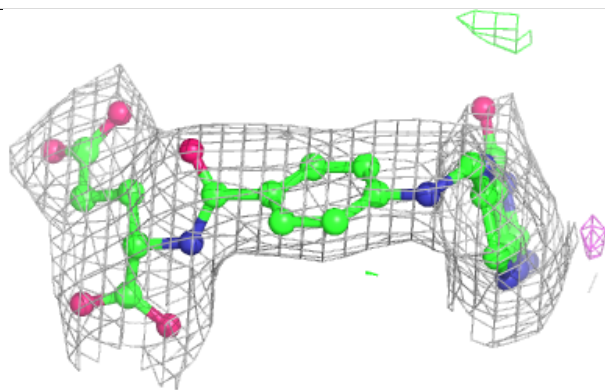
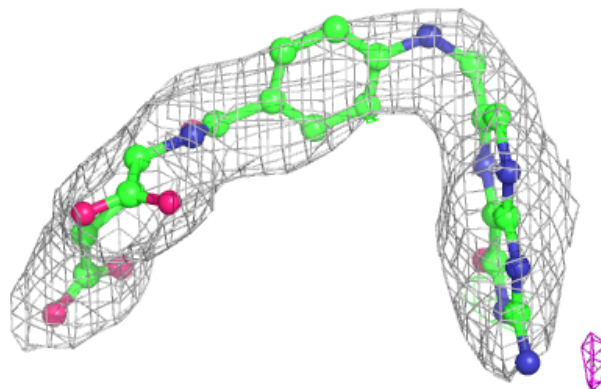


Electron density around CB3 C 612:

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

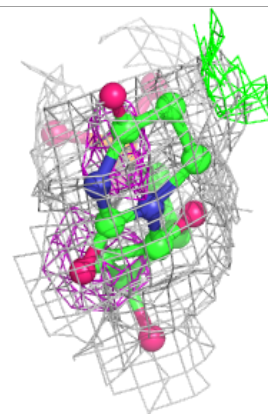
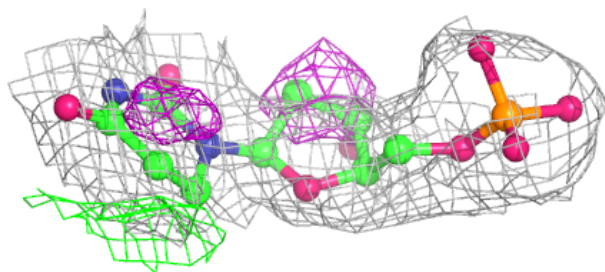
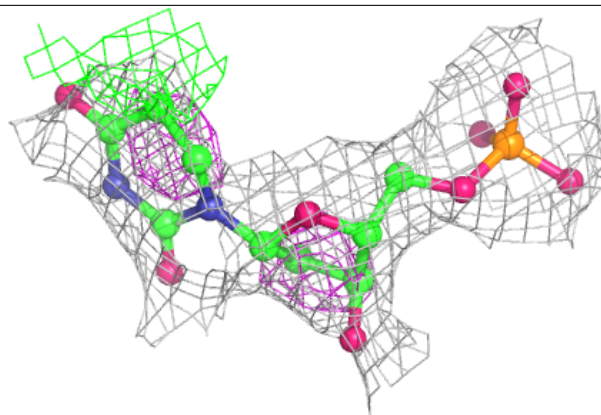
**Electron density around DHF E 621:**

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

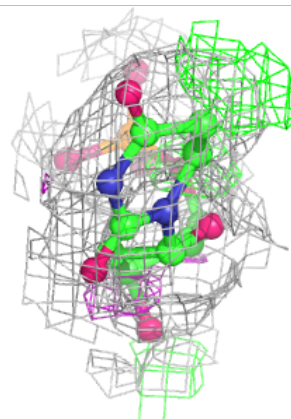
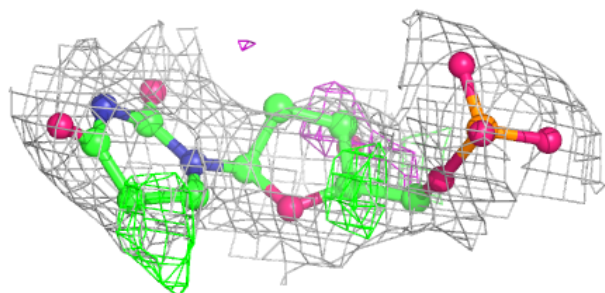
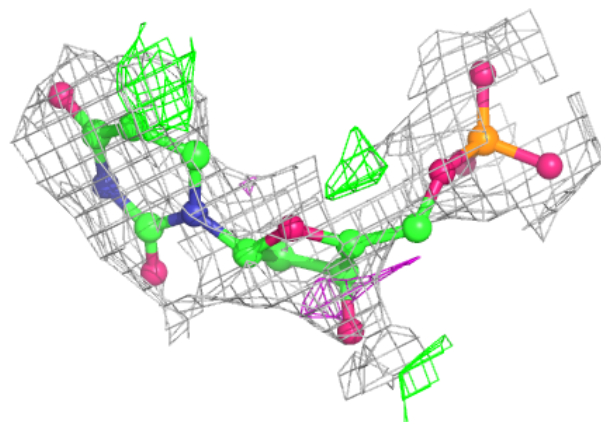


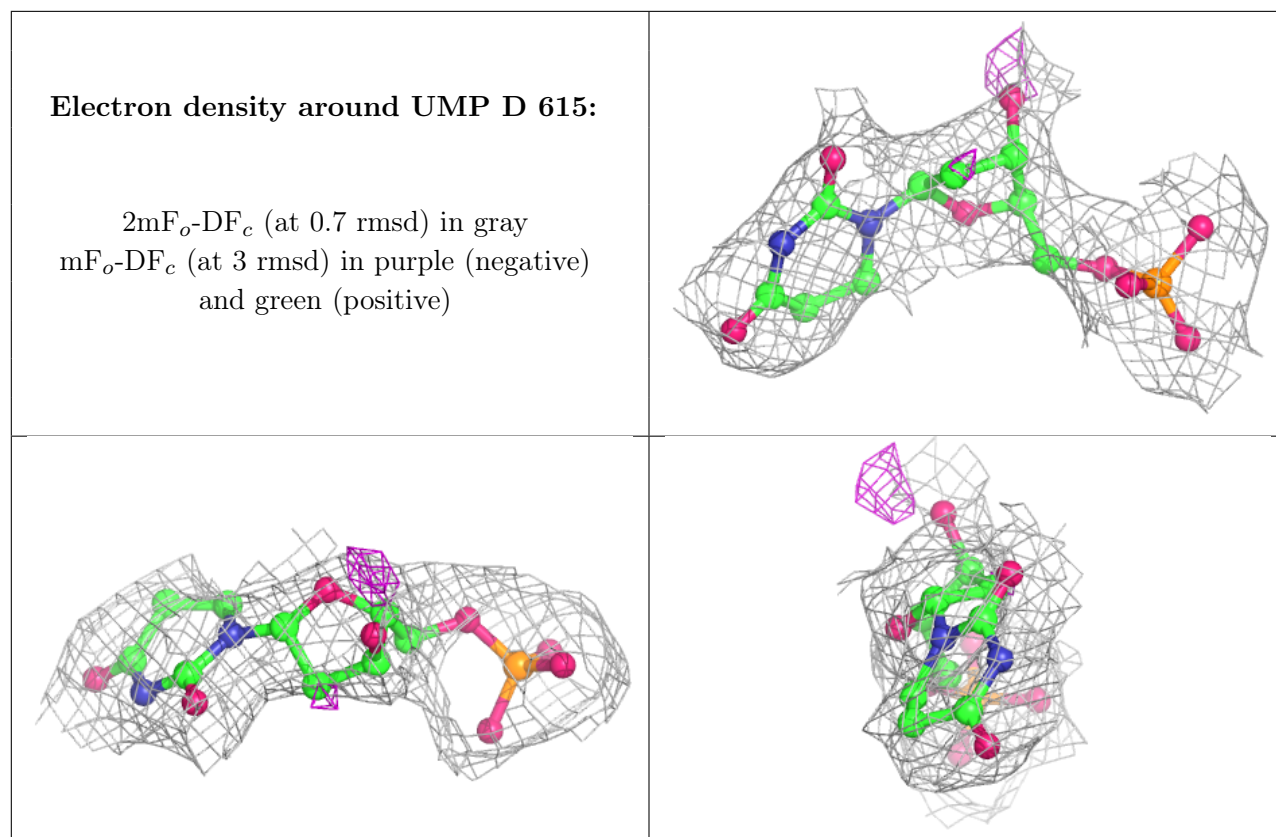
Electron density around UMP A 603:

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

**Electron density around UMP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.