



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:53 PM UTC

PDB ID : 3DL5 / pdb_00003dl5
Title : Crystal Structure of the A287F Active Site Mutant of TS-DHFR from *Cryptosporidium hominis*
Authors : Vargo, M.A.; Martucci, W.E.; Anderson, K.S.
Deposited on : 2008-06-26
Resolution : 2.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

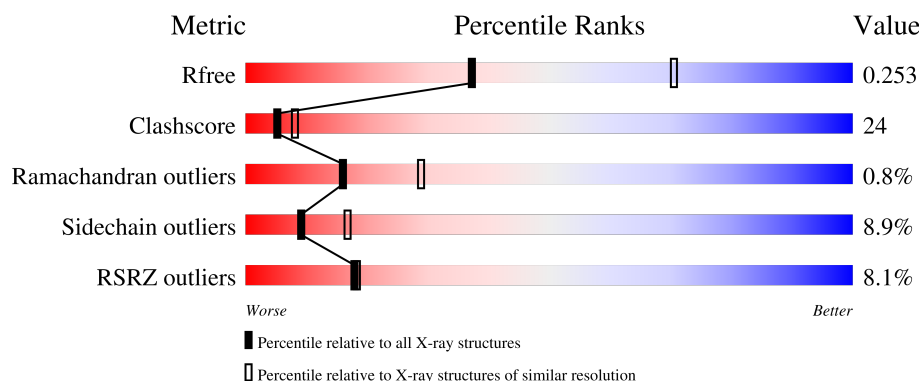
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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

Mol	Chain	Length	Quality of chain
1	A	521	4% 60% 31% 6% ..
1	B	521	3% 62% 29% 6% ..
1	C	521	7% 56% 34% 7% ..
1	D	521	6% 52% 37% 8% ..
1	E	521	20% 53% 37% 7% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CB3	D	616	X	-	X	-
3	CB3	E	620	X	-	X	-
4	DHF	A	605	X	-	-	-
4	DHF	B	609	X	-	X	-
4	DHF	C	613	-	-	X	-
4	DHF	D	617	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21793 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

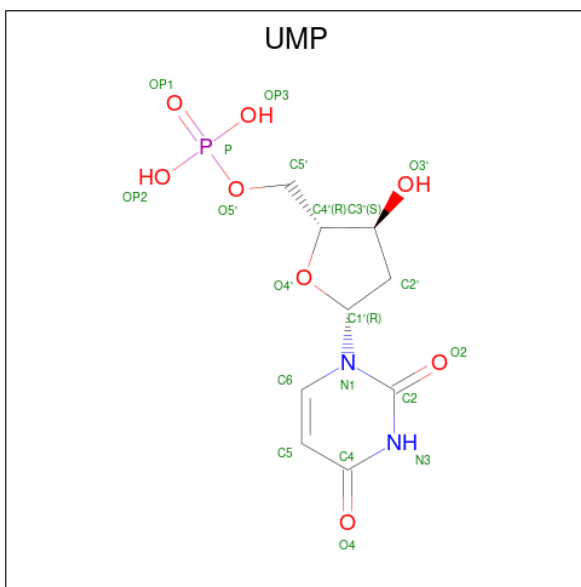
- Molecule 1 is a protein called Dihydrofolate reductase, DHFR.

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

There are 5 discrepancies between the modelled and reference sequences:

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

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



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

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (CCD ID: CB3) (formula: $C_{24}H_{23}N_5O_6$).

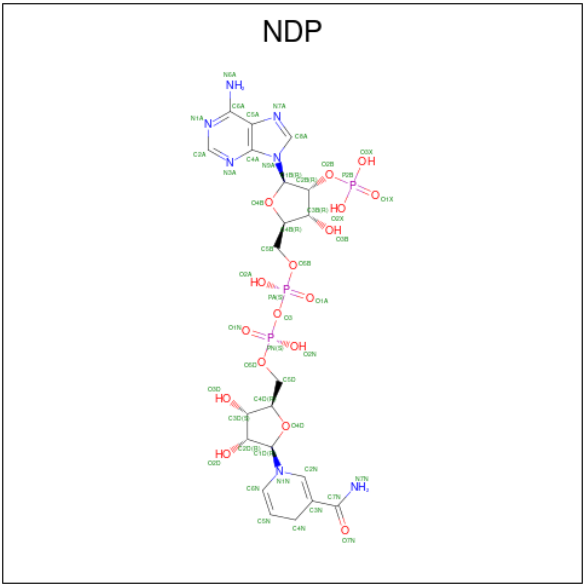


- Molecule 4 is DIHYDROFOLIC ACID (CCD ID: DHF) (formula: $C_{19}H_{21}N_7O_6$).



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 (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

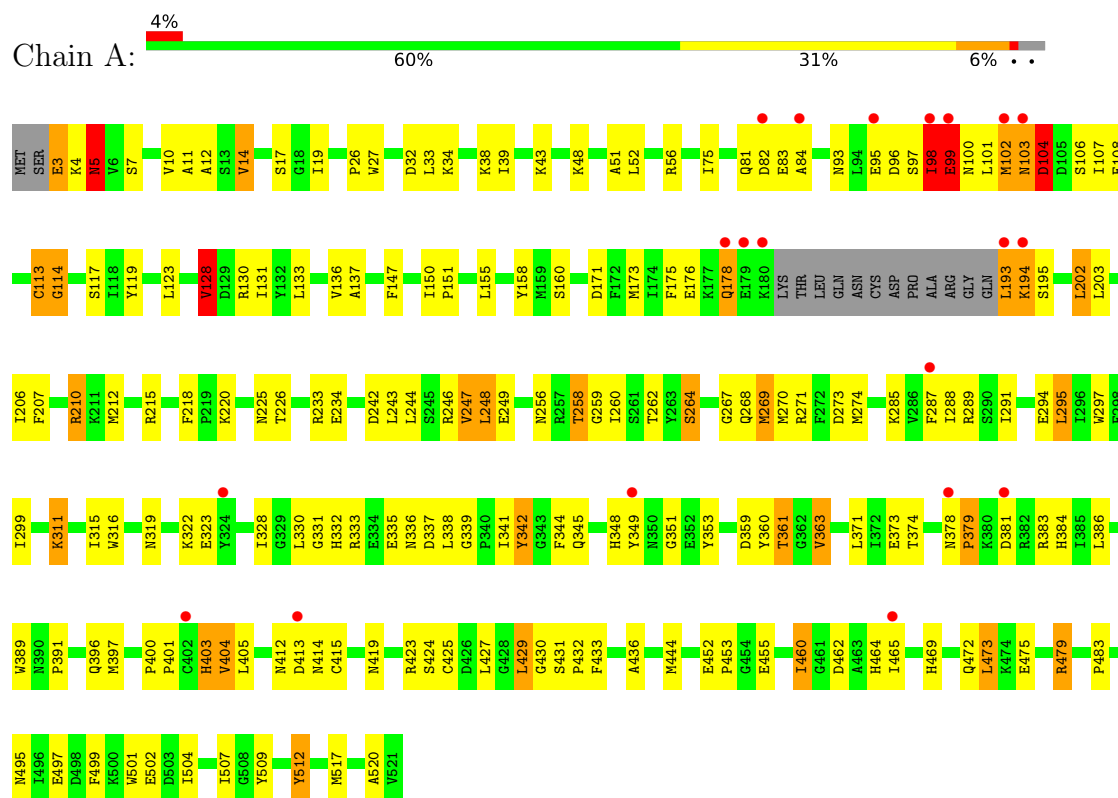
- Molecule 6 is water.

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

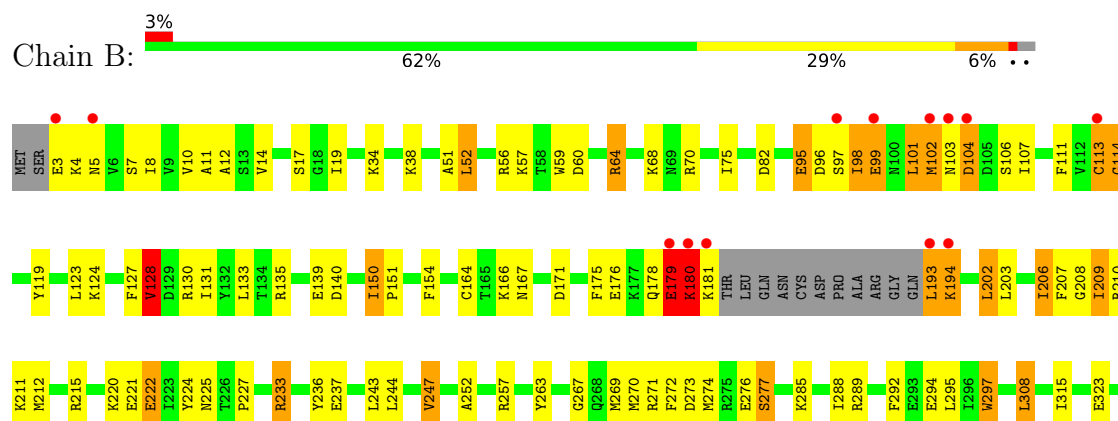
3 Residue-property plots

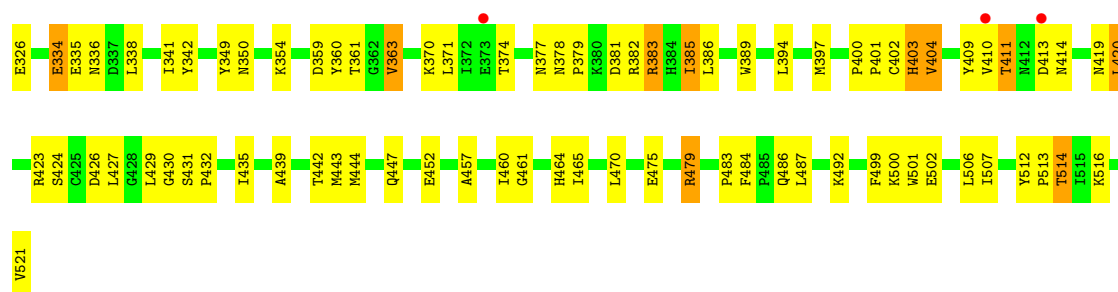
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

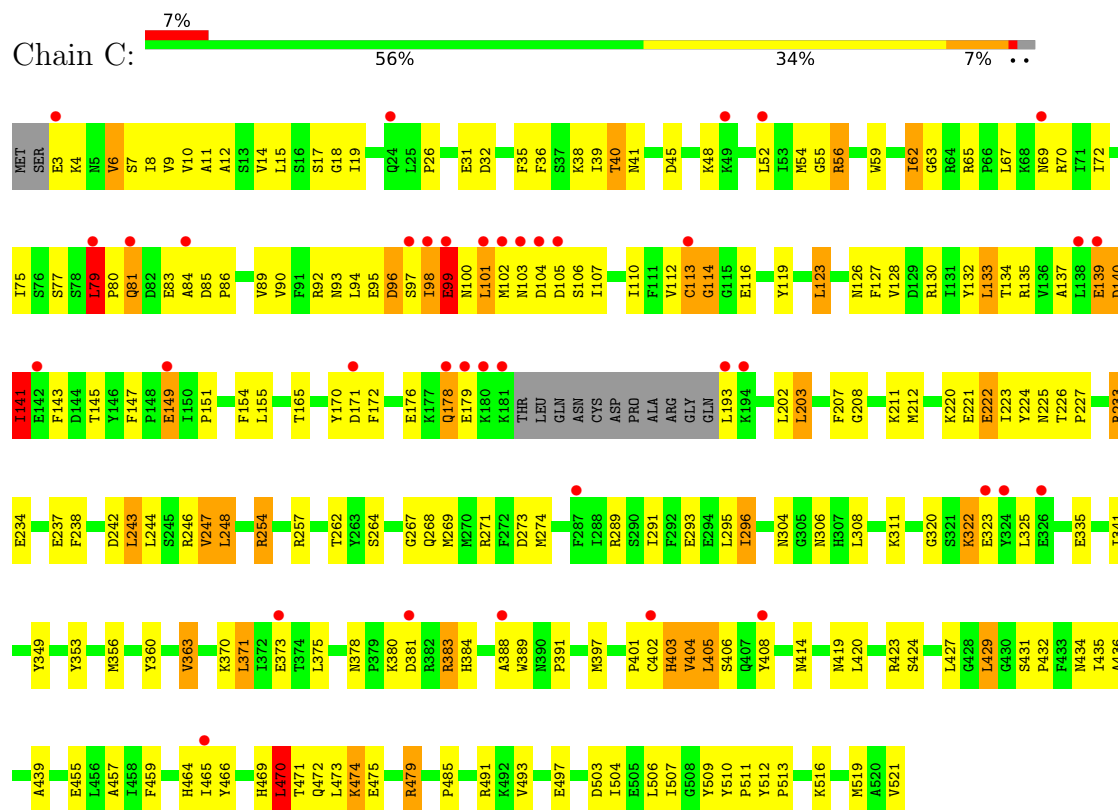


• Molecule 1: Dihydrofolate reductase, DHFR

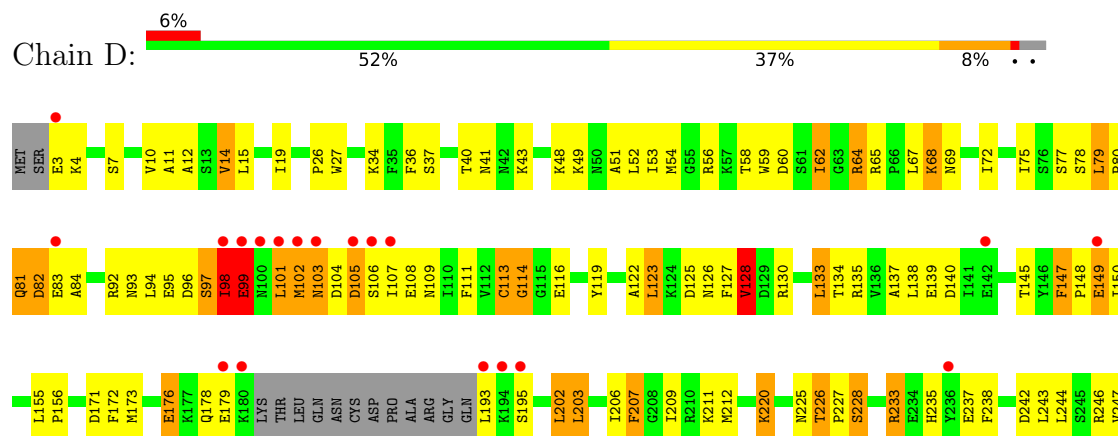


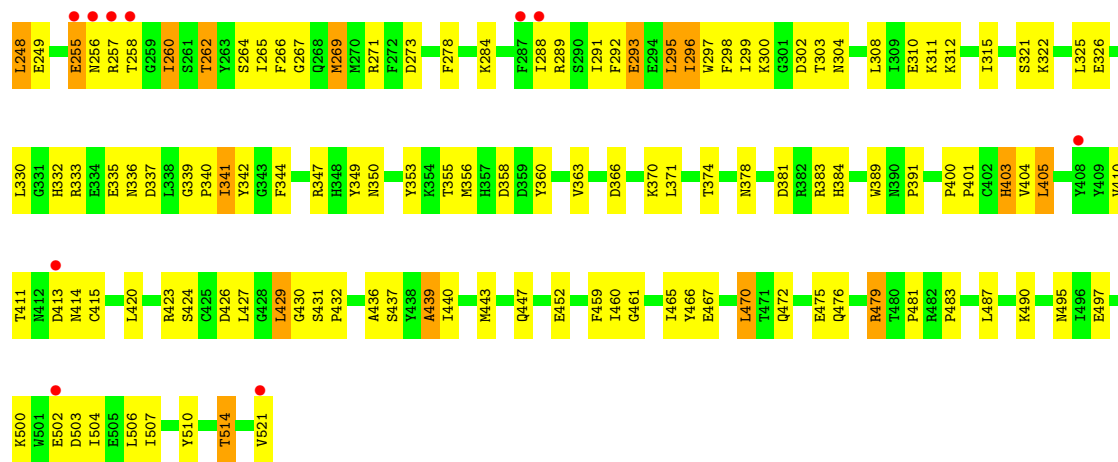


• Molecule 1: Dihydrofolate reductase, DHFR

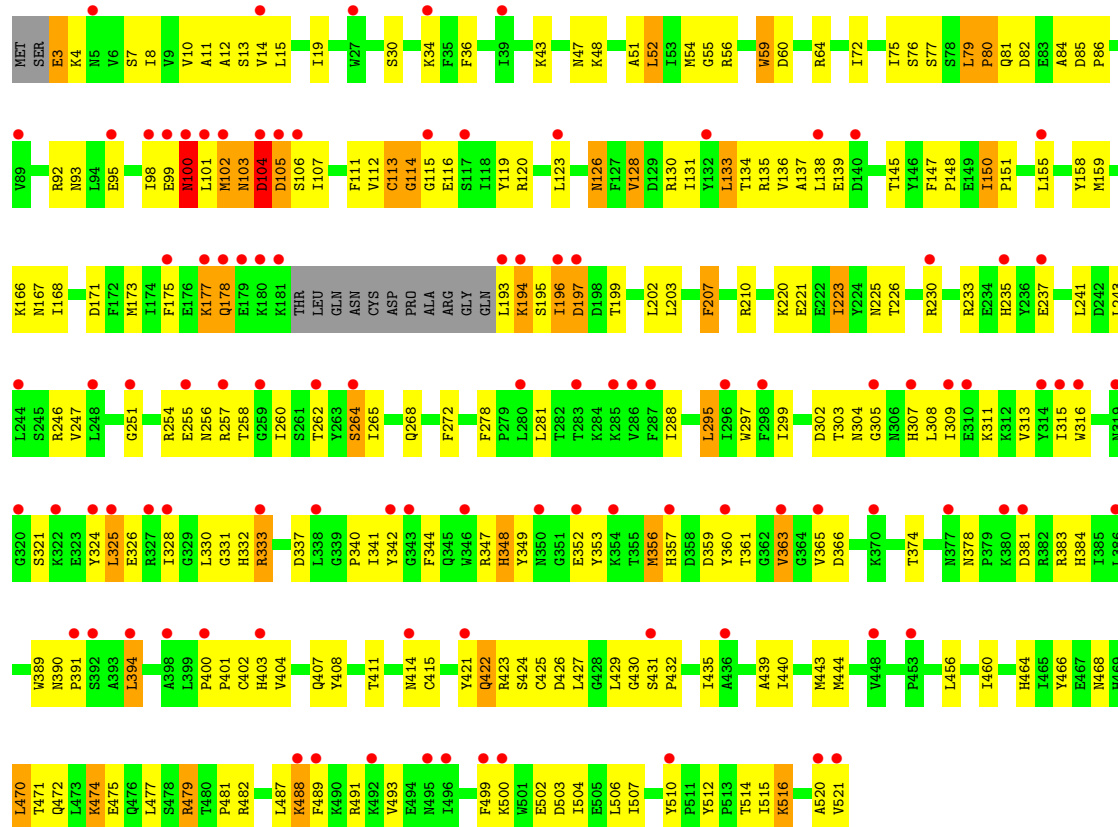


• Molecule 1: Dihydrofolate reductase, DHFR





• 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	214.81Å 116.54Å 219.21Å 90.00° 95.21° 90.00°	Depositor
Resolution (Å)	45.40 – 2.74 45.40 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.40-2.74) 99.8 (45.40-2.74)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.73Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.245 0.225 , 0.253	Depositor DCC
R_{free} test set	7223 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21793	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.45	0/4226	0.97	23/5711 (0.4%)
1	B	0.48	0/4239	0.98	20/5727 (0.3%)
1	C	0.42	0/4231	0.93	11/5718 (0.2%)
1	D	0.42	0/4226	0.92	12/5711 (0.2%)
1	E	0.38	1/4231 (0.0%)	0.94	19/5718 (0.3%)
All	All	0.43	1/21153 (0.0%)	0.95	85/28585 (0.3%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	226	THR	CA-CB	5.12	1.56	1.52

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	VAL	N-CA-C	10.20	121.02	110.72
1	A	14	VAL	N-CA-C	7.72	118.47	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	VAL	N-CA-C	7.35	118.46	108.17
1	D	264	SER	N-CA-C	7.28	120.14	109.07
1	A	351	GLY	N-CA-C	-7.22	103.30	112.54
1	B	14	VAL	N-CA-C	6.98	117.74	110.62
1	D	14	VAL	N-CA-C	6.98	117.69	110.36
1	E	150	ILE	N-CA-C	6.76	116.33	108.96
1	D	439	ALA	N-CA-C	-6.62	104.14	111.36
1	B	5	ASN	N-CA-C	6.59	119.53	110.24
1	D	507	ILE	N-CA-C	6.55	117.30	107.80
1	C	79	LEU	N-CA-CB	-6.52	101.70	110.77
1	C	507	ILE	N-CA-C	6.51	117.24	107.80
1	B	507	ILE	N-CA-C	6.43	117.13	107.80
1	C	243	LEU	N-CA-C	-6.43	104.20	111.14
1	E	221	GLU	N-CA-C	6.41	120.20	112.38
1	D	226	THR	CA-C-N	6.34	127.77	119.84
1	D	226	THR	C-N-CA	6.34	127.77	119.84
1	B	150	ILE	CA-C-N	6.30	126.27	119.78
1	B	150	ILE	C-N-CA	6.30	126.27	119.78
1	A	104	ASP	N-CA-C	-6.27	103.18	111.02
1	A	243	LEU	N-CA-C	-6.27	104.53	111.36
1	A	512	TYR	N-CA-C	-6.21	102.98	110.13
1	C	207	PHE	N-CA-C	6.21	120.93	113.23
1	E	223	ILE	N-CA-C	6.21	118.14	112.43
1	D	179	GLU	N-CA-CB	-6.17	105.85	111.59
1	D	243	LEU	N-CA-C	-6.17	104.67	111.82
1	B	59	TRP	N-CA-C	-6.12	104.61	111.28
1	E	113	CYS	N-CA-C	6.12	120.75	113.16
1	B	68	LYS	N-CA-C	6.11	118.85	110.24
1	D	207	PHE	N-CA-C	6.09	120.78	113.23
1	B	104	ASP	N-CA-C	-6.04	103.06	111.39
1	A	259	GLY	N-CA-C	-6.02	106.21	114.64
1	A	342	TYR	CB-CA-C	-5.91	100.94	110.74
1	C	470	LEU	N-CA-C	5.89	118.18	111.11
1	C	474	LYS	N-CA-C	-5.85	104.98	111.36
1	E	357	HIS	CB-CA-C	-5.84	100.33	110.09
1	B	470	LEU	N-CA-C	5.81	117.28	111.07
1	B	475	GLU	N-CA-C	-5.78	104.89	111.07
1	E	114	GLY	N-CA-C	5.75	121.70	111.01
1	A	328	ILE	N-CA-C	5.74	117.02	111.91
1	C	439	ALA	N-CA-C	-5.72	104.42	111.40
1	B	403	HIS	CA-C-N	5.70	128.52	120.42
1	B	403	HIS	C-N-CA	5.70	128.52	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	59	TRP	N-CA-C	-5.67	105.09	111.28
1	E	126	ASN	N-CA-C	5.67	119.01	111.30
1	B	394	LEU	N-CA-C	5.65	118.17	111.33
1	A	507	ILE	N-CA-C	5.62	116.40	108.36
1	A	342	TYR	N-CA-C	5.61	120.62	111.37
1	B	128	VAL	N-CA-C	5.61	117.06	108.71
1	C	221	GLU	N-CA-C	5.60	118.16	111.71
1	E	507	ILE	N-CA-C	5.57	116.33	108.36
1	E	504	ILE	N-CA-C	5.53	116.26	108.36
1	A	460	ILE	N-CA-C	5.50	116.51	108.53
1	C	464	HIS	N-CA-C	5.47	117.29	109.14
1	A	504	ILE	N-CA-C	5.46	116.45	108.58
1	D	128	VAL	N-CA-C	5.43	117.12	108.87
1	E	207	PHE	N-CA-C	5.42	120.17	113.50
1	E	230	ARG	N-CA-C	5.41	119.83	112.04
1	A	258	THR	N-CA-C	5.40	117.24	111.36
1	A	210	ARG	N-CA-C	-5.39	106.20	112.89
1	B	297	TRP	N-CA-C	-5.37	105.33	111.07
1	A	226	THR	CA-C-N	5.36	126.53	119.84
1	A	226	THR	C-N-CA	5.36	126.53	119.84
1	B	430	GLY	N-CA-C	5.34	118.95	112.49
1	B	377	ASN	N-CA-C	5.34	116.90	111.14
1	D	147	PHE	N-CA-C	-5.33	103.35	110.07
1	A	147	PHE	N-CA-C	-5.32	101.91	109.62
1	E	460	ILE	N-CA-C	5.27	116.07	108.48
1	E	414	ASN	N-CA-C	5.26	118.88	111.52
1	D	460	ILE	N-CA-C	5.25	116.86	108.89
1	E	237	GLU	N-CA-C	-5.23	106.87	113.20
1	C	504	ILE	N-CA-C	5.23	116.11	108.58
1	A	218	PHE	N-CA-C	-5.21	103.21	109.83
1	A	14	VAL	CB-CA-C	-5.20	105.23	111.88
1	B	464	HIS	N-CA-C	5.20	116.88	109.14
1	E	243	LEU	N-CA-C	-5.19	105.80	111.82
1	C	353	TYR	N-CA-C	5.18	117.99	109.76
1	B	334	GLU	N-CA-C	-5.16	102.84	110.48
1	E	104	ASP	N-CA-C	-5.11	105.07	111.92
1	A	412	ASN	N-CA-C	-5.09	106.33	112.54
1	A	5	ASN	N-CA-C	5.08	117.81	110.28
1	E	474	LYS	N-CA-C	-5.05	105.86	112.23
1	E	325	LEU	N-CA-C	-5.04	106.96	113.01
1	A	464	HIS	N-CA-C	5.01	116.80	109.24

There are no chirality outliers.

All (23) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4057	171	0
1	B	4143	0	4074	172	0
1	C	4135	0	4059	201	1
1	D	4130	0	4057	243	0
1	E	4135	0	4059	234	2
2	A	20	0	11	4	0
2	B	20	0	11	3	0
2	C	20	0	11	3	0
2	D	20	0	11	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	20	0	11	6	0
3	A	35	0	21	4	0
3	B	35	0	21	3	0
3	C	35	0	21	2	0
3	D	35	0	21	9	0
3	E	35	0	21	13	0
4	A	32	0	19	6	0
4	B	32	0	19	10	0
4	C	32	0	19	9	0
4	D	32	0	19	9	0
4	E	32	0	19	5	0
5	A	48	0	26	7	0
5	B	48	0	26	8	0
5	C	48	0	26	11	0
5	D	48	0	26	6	0
5	E	48	0	26	12	0
6	A	114	0	0	18	0
6	B	150	0	0	7	0
6	C	95	0	0	9	0
6	D	62	0	0	12	0
6	E	24	0	0	5	0
All	All	21793	0	20691	1024	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1024) 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:B:179:GLU:C	1:B:180:LYS:HG3	1.52	1.27
1:D:104:ASP:O	1:D:106:SER:N	1.63	1.26
1:E:79:LEU:HD23	1:E:80:PRO:CD	1.68	1.21
1:E:79:LEU:CD2	1:E:80:PRO:HD2	1.71	1.18
1:E:178:GLN:OE1	1:E:178:GLN:HA	1.43	1.16
1:E:196:ILE:N	1:E:196:ILE:HD12	1.56	1.13
1:D:255:GLU:CD	1:D:255:GLU:H	1.55	1.11
1:E:196:ILE:H	1:E:196:ILE:CD1	1.51	1.11
1:A:4:LYS:HG2	1:A:101:LEU:HD23	1.34	1.09
1:D:98:ILE:O	1:D:99:GLU:HB3	1.49	1.09
1:B:209:ILE:HD12	1:B:209:ILE:H	1.14	1.07
1:D:102:MET:O	1:D:102:MET:HE3	1.53	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:THR:HG22	1:A:384:HIS:HE1	1.18	1.07
1:B:179:GLU:O	1:B:180:LYS:HG3	1.57	1.04
1:C:171:ASP:OD1	6:C:642:HOH:O	1.72	1.03
1:C:92:ARG:O	5:C:614:NDP:H2A	1.59	1.03
1:A:374:THR:HG22	1:A:384:HIS:CE1	1.93	1.03
3:E:620:CB3:OE2	3:E:620:CB3:HA	1.55	1.03
1:D:104:ASP:O	1:D:107:ILE:N	1.92	1.01
1:E:82:ASP:OD2	1:E:84:ALA:HB2	1.61	1.00
1:E:195:SER:OG	1:E:196:ILE:HD12	1.61	0.99
1:D:337:ASP:HA	1:D:356:MET:HE3	1.38	0.98
2:A:603:UMP:H5	6:A:679:HOH:O	1.42	0.98
3:E:620:CB3:O	3:E:620:CB3:HB1	1.62	0.97
1:D:104:ASP:C	1:D:106:SER:N	2.23	0.96
1:D:77:SER:C	1:D:92:ARG:NH1	2.24	0.95
1:E:195:SER:OG	1:E:196:ILE:CD1	2.14	0.95
1:E:196:ILE:HD12	1:E:196:ILE:H	0.78	0.94
1:E:3:GLU:HB2	1:E:101:LEU:HD22	1.50	0.94
1:E:196:ILE:O	1:E:197:ASP:HB2	1.65	0.94
1:C:269:MET:HE2	1:D:269:MET:HE2	1.49	0.93
1:B:179:GLU:C	1:B:180:LYS:CG	2.36	0.93
1:A:3:GLU:HA	6:A:680:HOH:O	1.69	0.92
1:B:359:ASP:OD2	1:B:361:THR:HG23	1.68	0.92
1:C:77:SER:N	5:C:614:NDP:O1X	2.02	0.92
1:C:98:ILE:O	1:C:99:GLU:HG3	1.68	0.92
1:C:4:LYS:HB2	1:C:101:LEU:HD23	1.51	0.92
1:C:405:LEU:C	1:C:405:LEU:HD23	1.95	0.92
1:B:257:ARG:HD3	2:B:607:UMP:OP2	1.70	0.91
1:D:62:ILE:HD11	4:D:617:DHF:C12	2.00	0.91
1:E:54:MET:HE3	1:E:72:ILE:HG23	1.52	0.90
1:C:140:ASP:O	1:C:141:ILE:HG22	1.72	0.90
1:D:96:ASP:O	1:D:99:GLU:HG2	1.72	0.90
1:D:62:ILE:HD11	4:D:617:DHF:C11	2.03	0.89
1:D:304:ASN:HA	1:D:356:MET:HE2	1.54	0.89
1:D:77:SER:O	1:D:92:ARG:NH1	2.04	0.89
1:B:285:LYS:HB3	1:B:514:THR:HG22	1.55	0.88
1:E:82:ASP:OD2	1:E:84:ALA:CB	2.22	0.88
1:D:342:TYR:CE1	1:D:403:HIS:CE1	2.63	0.87
1:A:258:THR:HG22	1:A:260:ILE:H	1.39	0.87
4:C:613:DHF:HB2	4:C:613:DHF:O	1.73	0.87
1:C:140:ASP:C	1:C:141:ILE:CG2	2.47	0.86
1:E:488:LYS:HD3	1:E:489:PHE:H	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:PHE:O	1:C:40:THR:HB	1.75	0.86
1:D:330:LEU:HA	6:D:648:HOH:O	1.75	0.85
1:D:360:TYR:O	1:D:363:VAL:HG12	1.76	0.85
1:C:349:TYR:CE2	1:D:391:PRO:HD2	2.12	0.85
1:A:4:LYS:HG2	1:A:101:LEU:CD2	2.05	0.85
1:B:209:ILE:H	1:B:209:ILE:CD1	1.90	0.85
1:E:4:LYS:H	1:E:101:LEU:CD2	1.90	0.85
1:E:115:GLY:HA3	5:E:622:NDP:O1A	1.77	0.85
1:B:103:ASN:CG	1:B:104:ASP:H	1.85	0.84
1:D:255:GLU:CD	1:D:255:GLU:N	2.32	0.84
1:B:411:THR:CG2	1:B:413:ASP:HB2	2.09	0.83
1:E:155:LEU:HD12	1:E:178:GLN:NE2	1.94	0.83
1:D:104:ASP:C	1:D:106:SER:H	1.86	0.82
1:D:77:SER:C	1:D:92:ARG:HH11	1.87	0.82
4:C:613:DHF:C6	5:C:614:NDP:H42N	2.10	0.81
1:C:211:LYS:HE3	6:C:635:HOH:O	1.81	0.81
1:E:257:ARG:HD3	2:E:619:UMP:OP2	1.80	0.81
1:D:339:GLY:HA2	1:D:353:TYR:CE2	2.16	0.81
1:E:516:LYS:HE3	1:E:516:LYS:H	1.45	0.81
1:E:100:ASN:O	1:E:103:ASN:O	1.96	0.81
1:A:258:THR:HG21	1:A:520:ALA:HB1	1.63	0.81
1:C:403:HIS:HB2	1:C:420:LEU:HD11	1.63	0.80
1:C:380:LYS:HE2	6:C:636:HOH:O	1.80	0.80
1:B:4:LYS:HE2	1:B:107:ILE:O	1.82	0.80
4:B:609:DHF:C7	5:B:610:NDP:H42N	2.12	0.80
1:D:102:MET:HE3	1:D:102:MET:C	2.06	0.80
1:C:140:ASP:C	1:C:141:ILE:HG23	2.04	0.80
1:D:104:ASP:O	1:D:106:SER:CA	2.30	0.80
1:D:104:ASP:HB3	1:D:107:ILE:HD13	1.62	0.80
1:B:378:ASN:ND2	1:B:381:ASP:HB2	1.97	0.80
1:A:96:ASP:O	1:A:99:GLU:HG2	1.82	0.79
1:D:337:ASP:CA	1:D:356:MET:HE3	2.12	0.79
1:E:15:LEU:HD12	1:E:139:GLU:HG3	1.64	0.79
1:D:104:ASP:O	1:D:105:ASP:C	2.24	0.79
1:A:333:ARG:HA	6:A:626:HOH:O	1.83	0.78
1:E:102:MET:O	1:E:103:ASN:HB2	1.83	0.78
4:B:609:DHF:H72	5:B:610:NDP:H42N	1.64	0.78
2:A:603:UMP:OP1	1:B:383:ARG:NH1	2.17	0.78
1:C:40:THR:HG23	1:C:70:ARG:HD3	1.65	0.78
1:D:149:GLU:H	1:D:149:GLU:CD	1.90	0.78
1:C:178:GLN:OE1	1:C:178:GLN:HA	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:620:CB3:O	3:E:620:CB3:CB	2.31	0.77
1:C:98:ILE:O	1:C:99:GLU:CG	2.31	0.77
1:C:123:LEU:HD12	1:C:128:VAL:HG11	1.67	0.77
1:E:324:TYR:O	1:E:328:ILE:HG12	1.84	0.77
1:E:75:ILE:O	5:E:622:NDP:H1B	1.85	0.76
1:C:104:ASP:C	1:C:106:SER:H	1.92	0.76
1:C:40:THR:CG2	1:C:70:ARG:HD3	2.15	0.76
1:D:332:HIS:HD2	6:D:648:HOH:O	1.69	0.76
1:D:405:LEU:C	1:D:405:LEU:HD23	2.11	0.76
1:E:374:THR:HB	6:E:646:HOH:O	1.86	0.75
3:D:616:CB3:O	3:D:616:CB3:HB1	1.87	0.75
1:A:114:GLY:HA3	1:A:119:TYR:CZ	2.21	0.75
1:E:516:LYS:H	1:E:516:LYS:CE	1.99	0.75
1:A:247:VAL:CG2	1:A:465:ILE:HD12	2.17	0.74
1:A:289:ARG:HG3	1:A:501:TRP:CE2	2.23	0.74
1:C:54:MET:HE3	1:C:72:ILE:HG23	1.69	0.74
1:D:103:ASN:CG	1:D:104:ASP:H	1.95	0.74
1:B:500:LYS:HE3	6:B:734:HOH:O	1.87	0.74
1:C:98:ILE:O	1:C:99:GLU:CB	2.35	0.74
1:E:93:ASN:HD21	1:E:95:GLU:HB3	1.51	0.74
3:E:620:CB3:OE2	3:E:620:CB3:CA	2.35	0.74
1:E:93:ASN:ND2	1:E:95:GLU:HB3	2.02	0.74
1:C:225:ASN:O	1:C:233:ARG:NH2	2.21	0.74
1:D:102:MET:O	1:D:102:MET:CE	2.36	0.74
1:C:92:ARG:O	5:C:614:NDP:C2A	2.35	0.74
1:C:360:TYR:O	1:C:363:VAL:HG13	1.87	0.74
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.22	0.74
1:B:178:GLN:C	1:B:179:GLU:HG2	2.12	0.73
1:E:4:LYS:N	1:E:101:LEU:HD21	2.03	0.73
1:C:140:ASP:O	1:C:141:ILE:CG2	2.36	0.73
1:E:14:VAL:HG23	1:E:15:LEU:HG	1.70	0.73
1:B:411:THR:HG22	1:B:413:ASP:N	2.04	0.73
1:D:260:ILE:HD12	1:D:260:ILE:N	2.03	0.73
1:A:19:ILE:O	5:A:606:NDP:H2N	1.88	0.73
1:A:98:ILE:O	1:A:99:GLU:HB3	1.88	0.73
1:C:193:LEU:HA	6:C:626:HOH:O	1.88	0.73
1:A:26:PRO:HB2	1:A:27:TRP:CE3	2.24	0.73
1:C:139:GLU:HB2	1:C:510:TYR:CZ	2.24	0.73
1:E:4:LYS:H	1:E:101:LEU:HD21	1.54	0.73
1:C:40:THR:HG21	1:C:70:ARG:HH11	1.53	0.72
1:A:225:ASN:O	1:A:233:ARG:NH2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:PRO:HD2	6:A:644:HOH:O	1.88	0.72
1:E:79:LEU:HD23	1:E:80:PRO:HD2	0.82	0.72
1:E:297:TRP:CD1	1:E:302:ASP:HB3	2.25	0.72
1:B:179:GLU:O	1:B:180:LYS:CG	2.33	0.72
1:B:114:GLY:HA3	1:B:119:TYR:CZ	2.25	0.72
1:B:4:LYS:HB2	1:B:101:LEU:CD2	2.19	0.72
1:B:209:ILE:HD12	1:B:209:ILE:N	1.97	0.72
1:D:257:ARG:NH2	1:D:521:VAL:OXT	2.23	0.72
1:D:342:TYR:CD1	1:D:403:HIS:CE1	2.77	0.71
1:D:495:ASN:OD1	1:D:497:GLU:HG2	1.90	0.71
1:C:79:LEU:HD23	1:C:80:PRO:HD2	1.72	0.71
1:B:178:GLN:O	1:B:179:GLU:HG2	1.89	0.71
1:C:4:LYS:HB2	1:C:101:LEU:CD2	2.20	0.71
1:D:255:GLU:HG3	6:D:675:HOH:O	1.89	0.71
1:D:257:ARG:HD3	2:D:615:UMP:OP2	1.89	0.71
1:D:52:LEU:HB3	1:D:113:CYS:SG	2.30	0.71
1:E:155:LEU:HD12	1:E:178:GLN:HE21	1.56	0.71
1:A:38:LYS:HB3	1:B:202:LEU:HG	1.70	0.71
1:E:402:CYS:SG	2:E:619:UMP:C6	2.83	0.71
1:E:207:PHE:HB3	1:E:210:ARG:HB2	1.72	0.71
1:D:82:ASP:OD1	1:D:84:ALA:CB	2.38	0.71
1:D:439:ALA:O	1:D:443:MET:HG3	1.91	0.70
4:D:617:DHF:C6	5:D:618:NDP:H42N	2.21	0.70
1:C:75:ILE:O	5:C:614:NDP:H1B	1.91	0.70
1:B:52:LEU:HB3	1:B:113:CYS:SG	2.31	0.70
1:A:52:LEU:HB3	1:A:113:CYS:SG	2.31	0.70
1:C:178:GLN:OE1	1:C:178:GLN:CA	2.39	0.70
1:E:430:GLY:HA2	3:E:620:CB3:CP3	2.22	0.70
1:B:3:GLU:O	1:B:101:LEU:HD22	1.90	0.70
1:B:60:ASP:OD1	1:B:64:ARG:NH1	2.24	0.70
1:E:430:GLY:CA	3:E:620:CB3:CP3	2.70	0.70
1:B:411:THR:HG22	1:B:413:ASP:H	1.54	0.70
1:C:349:TYR:HH	1:D:349:TYR:HH	1.36	0.70
1:A:220:LYS:HE2	1:A:249:GLU:OE1	1.91	0.69
1:E:196:ILE:O	1:E:197:ASP:CB	2.40	0.69
1:C:149:GLU:CD	1:C:149:GLU:H	1.99	0.69
1:E:34:LYS:HE2	6:E:633:HOH:O	1.91	0.69
1:E:194:LYS:H	1:E:194:LYS:HD3	1.56	0.69
1:D:514:THR:HG22	6:D:628:HOH:O	1.91	0.69
1:A:330:LEU:C	1:A:332:HIS:H	2.00	0.69
1:E:101:LEU:C	1:E:103:ASN:H	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:TYR:OH	1:B:402:CYS:N	2.22	0.68
1:C:267:GLY:O	1:D:271:ARG:NH2	2.25	0.68
1:E:472:GLN:O	1:E:475:GLU:HB3	1.94	0.68
1:A:4:LYS:H	1:A:101:LEU:HD22	1.58	0.68
1:A:32:ASP:OD2	4:A:605:DHF:N3	2.26	0.68
1:E:101:LEU:O	1:E:103:ASN:N	2.27	0.68
1:D:130:ARG:HG3	1:D:176:GLU:OE1	1.93	0.68
1:C:99:GLU:C	1:C:99:GLU:CD	2.62	0.68
1:E:138:LEU:HD11	1:E:168:ILE:HD13	1.76	0.68
1:C:391:PRO:HD2	1:D:349:TYR:CE2	2.29	0.68
1:E:52:LEU:HB3	1:E:113:CYS:SG	2.33	0.68
1:B:98:ILE:HG23	1:B:98:ILE:O	1.93	0.67
1:E:304:ASN:HA	1:E:356:MET:HE2	1.75	0.67
1:E:384:HIS:HB2	1:E:408:TYR:O	1.94	0.67
1:B:99:GLU:OE2	1:B:102:MET:SD	2.52	0.67
1:A:258:THR:CG2	1:A:520:ALA:HB1	2.23	0.67
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.30	0.67
1:B:297:TRP:HH2	1:B:338:LEU:HD12	1.60	0.67
1:C:370:LYS:HA	1:C:373:GLU:HG2	1.77	0.67
1:D:178:GLN:HA	1:D:178:GLN:OE1	1.94	0.67
1:D:97:SER:O	1:D:99:GLU:HG3	1.94	0.67
1:D:342:TYR:CE1	1:D:403:HIS:NE2	2.63	0.67
1:A:256:ASN:OD1	1:A:258:THR:HB	1.95	0.66
1:B:82:ASP:OD1	1:B:82:ASP:C	2.38	0.66
1:C:155:LEU:HD12	1:C:178:GLN:NE2	2.09	0.66
1:C:104:ASP:C	1:C:106:SER:N	2.53	0.66
1:E:360:TYR:HB3	1:E:363:VAL:HG12	1.77	0.66
1:A:431:SER:HB3	1:A:432:PRO:HD3	1.76	0.66
1:C:402:CYS:SG	2:C:611:UMP:C6	2.89	0.66
1:D:225:ASN:O	1:D:233:ARG:NH2	2.27	0.66
1:A:82:ASP:N	6:A:659:HOH:O	2.29	0.66
1:D:96:ASP:O	1:D:99:GLU:CG	2.42	0.66
1:D:337:ASP:CG	1:D:356:MET:HG2	2.20	0.65
1:C:133:LEU:HD22	1:C:134:THR:N	2.12	0.65
1:D:96:ASP:O	1:D:99:GLU:HB3	1.96	0.65
1:B:103:ASN:CG	1:B:104:ASP:N	2.55	0.65
1:B:360:TYR:O	1:B:363:VAL:HG13	1.96	0.65
1:E:114:GLY:HA2	1:E:119:TYR:CZ	2.32	0.65
1:E:330:LEU:C	1:E:332:HIS:H	2.04	0.65
1:E:359:ASP:OD2	1:E:361:THR:HG22	1.97	0.65
1:E:488:LYS:HD3	1:E:489:PHE:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:ARG:HD3	1:D:171:ASP:OD2	1.96	0.65
1:E:347:ARG:O	1:E:366:ASP:HA	1.96	0.65
1:E:297:TRP:CG	1:E:308:LEU:HD21	2.32	0.65
1:E:430:GLY:CA	3:E:620:CB3:HP3	2.26	0.65
1:A:495:ASN:OD1	1:A:497:GLU:HG3	1.97	0.65
1:B:34:LYS:HE2	6:B:758:HOH:O	1.96	0.65
1:A:97:SER:O	1:A:99:GLU:HG3	1.96	0.64
1:A:202:LEU:HG	1:B:38:LYS:HB3	1.78	0.64
1:B:411:THR:CG2	1:B:413:ASP:CB	2.75	0.64
1:D:26:PRO:HG2	1:D:27:TRP:CZ3	2.31	0.64
1:C:405:LEU:C	1:C:405:LEU:CD2	2.69	0.64
1:A:14:VAL:HG23	1:A:137:ALA:HA	1.79	0.64
1:B:98:ILE:O	1:B:98:ILE:CG2	2.46	0.64
1:D:77:SER:C	1:D:92:ARG:HH12	2.04	0.64
1:A:258:THR:HG22	1:A:260:ILE:N	2.11	0.64
1:D:374:THR:HG22	1:D:384:HIS:CE1	2.33	0.64
1:D:452:GLU:HG2	6:D:679:HOH:O	1.96	0.64
1:B:411:THR:CG2	1:B:413:ASP:H	2.11	0.64
1:B:411:THR:HG21	1:B:413:ASP:HB2	1.79	0.64
1:B:315:ILE:HB	3:B:608:CB3:C15	2.28	0.64
1:D:430:GLY:HA2	3:D:616:CB3:CP3	2.28	0.64
1:C:269:MET:CE	1:D:269:MET:HE2	2.26	0.63
1:D:220:LYS:HD3	1:D:249:GLU:OE1	1.98	0.63
1:B:209:ILE:HG13	6:B:708:HOH:O	1.98	0.63
1:C:99:GLU:OE1	1:C:100:ASN:N	2.32	0.63
4:E:621:DHF:C6	5:E:622:NDP:H42N	2.28	0.63
1:A:349:TYR:HH	1:B:349:TYR:HH	1.45	0.63
1:E:330:LEU:O	1:E:332:HIS:N	2.31	0.63
1:A:378:ASN:ND2	1:A:381:ASP:HB2	2.13	0.63
1:B:370:LYS:O	1:B:374:THR:HG23	1.97	0.63
1:C:75:ILE:HG22	5:C:614:NDP:C4A	2.29	0.63
1:C:323:GLU:H	1:C:323:GLU:CD	2.05	0.63
1:E:155:LEU:CD1	1:E:178:GLN:HE21	2.11	0.63
1:E:260:ILE:N	1:E:260:ILE:HD12	2.14	0.63
4:B:609:DHF:C6	5:B:610:NDP:H42N	2.28	0.63
1:A:93:ASN:ND2	1:A:95:GLU:HB3	2.13	0.63
1:E:92:ARG:O	5:E:622:NDP:H2A	1.99	0.63
1:A:5:ASN:HB2	6:A:696:HOH:O	1.98	0.63
1:A:14:VAL:CG2	1:A:137:ALA:HA	2.29	0.62
1:C:114:GLY:HA3	1:C:119:TYR:CZ	2.34	0.62
1:D:405:LEU:HD23	1:D:405:LEU:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:GLU:C	1:C:99:GLU:OE1	2.42	0.62
1:E:104:ASP:OD2	1:E:107:ILE:HD13	2.00	0.62
1:E:135:ARG:HD2	1:E:173:MET:SD	2.39	0.62
1:C:79:LEU:H	1:C:92:ARG:HH12	1.45	0.62
1:D:123:LEU:HD12	1:D:128:VAL:CG1	2.29	0.62
1:E:101:LEU:C	1:E:103:ASN:N	2.57	0.62
1:A:359:ASP:OD1	1:A:361:THR:HG22	2.00	0.62
1:C:52:LEU:HB3	1:C:113:CYS:SG	2.39	0.62
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.80	0.62
1:D:237:GLU:HG2	1:D:481:PRO:HB3	1.79	0.62
1:D:502:GLU:CD	1:D:502:GLU:H	2.08	0.62
1:A:374:THR:CG2	1:A:384:HIS:CE1	2.76	0.62
4:B:609:DHF:HB1	4:B:609:DHF:O	2.00	0.62
1:D:60:ASP:OD1	1:D:64:ARG:NH1	2.33	0.62
1:A:194:LYS:HG2	1:A:195:SER:N	2.13	0.62
1:A:233:ARG:NH1	1:A:242:ASP:OD1	2.32	0.62
4:B:609:DHF:H72	5:B:610:NDP:C4N	2.28	0.62
1:D:4:LYS:N	1:D:101:LEU:HD21	2.15	0.62
1:E:51:ALA:C	1:E:52:LEU:HD23	2.25	0.61
1:B:209:ILE:HA	6:B:708:HOH:O	2.00	0.61
1:A:338:LEU:HB3	1:A:341:ILE:HD13	1.82	0.61
1:D:103:ASN:CG	1:D:104:ASP:N	2.58	0.61
1:D:289:ARG:NH2	1:D:311:LYS:O	2.32	0.61
1:E:3:GLU:HB2	1:E:101:LEU:CD2	2.28	0.61
1:A:269:MET:HE2	1:B:269:MET:SD	2.40	0.61
1:B:379:PRO:HB2	1:B:410:VAL:HG11	1.81	0.61
1:C:403:HIS:H	1:C:403:HIS:CD2	2.18	0.61
1:E:115:GLY:CA	5:E:622:NDP:O1A	2.47	0.61
1:D:62:ILE:HD11	4:D:617:DHF:C13	2.30	0.61
1:D:284:LYS:HE3	6:D:630:HOH:O	1.99	0.61
1:E:297:TRP:CD2	1:E:308:LEU:HD21	2.35	0.61
1:E:104:ASP:O	1:E:106:SER:N	2.34	0.61
1:D:81:GLN:OE1	1:D:92:ARG:NE	2.30	0.61
1:D:147:PHE:CD2	1:D:148:PRO:HD2	2.36	0.61
1:B:276:GLU:O	1:B:277:SER:HB3	1.99	0.60
1:C:378:ASN:ND2	1:C:381:ASP:HB2	2.16	0.60
1:A:155:LEU:HD12	1:A:178:GLN:HG2	1.82	0.60
1:C:293:GLU:HA	1:C:296:ILE:HD11	1.83	0.60
1:C:98:ILE:O	1:C:99:GLU:HB3	1.99	0.60
1:E:135:ARG:HD3	1:E:171:ASP:HB2	1.83	0.59
1:A:383:ARG:NE	1:B:400:PRO:HG2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ASN:O	1:B:233:ARG:NH2	2.25	0.59
1:C:254:ARG:NH2	1:D:410:VAL:O	2.35	0.59
1:C:100:ASN:HB2	1:C:110:ILE:HD11	1.83	0.59
1:D:103:ASN:O	1:D:104:ASP:HB2	2.01	0.59
1:D:296:ILE:HD12	1:D:297:TRP:N	2.17	0.59
1:A:158:TYR:O	1:A:173:MET:HB2	2.02	0.59
1:A:322:LYS:HD3	1:A:335:GLU:HB2	1.84	0.59
1:E:337:ASP:CG	1:E:356:MET:HG2	2.27	0.59
1:E:466:TYR:OH	2:E:619:UMP:O3'	2.21	0.59
1:D:378:ASN:ND2	1:D:381:ASP:HB2	2.17	0.59
1:C:98:ILE:C	1:C:99:GLU:HG3	2.27	0.59
4:D:617:DHF:N10	6:D:634:HOH:O	2.26	0.59
1:E:155:LEU:CG	1:E:178:GLN:HE21	2.16	0.59
1:A:4:LYS:CG	1:A:101:LEU:HD23	2.22	0.58
1:D:291:ILE:HD13	1:D:436:ALA:HB3	1.84	0.58
1:E:3:GLU:CB	1:E:101:LEU:HD22	2.27	0.58
2:A:603:UMP:C5	6:A:679:HOH:O	2.33	0.58
1:B:179:GLU:CA	1:B:180:LYS:HG3	2.30	0.58
1:C:304:ASN:HA	1:C:356:MET:SD	2.43	0.58
1:B:99:GLU:OE1	1:B:99:GLU:N	2.36	0.58
1:B:431:SER:HB3	1:B:432:PRO:HD3	1.84	0.58
1:D:347:ARG:HH21	1:D:366:ASP:CG	2.11	0.58
1:A:271:ARG:HG2	1:B:212:MET:HE1	1.85	0.58
1:D:104:ASP:O	1:D:106:SER:C	2.46	0.58
1:D:347:ARG:NH2	1:D:366:ASP:OD1	2.36	0.58
1:D:62:ILE:CD1	4:D:617:DHF:C12	2.78	0.58
1:A:14:VAL:HG23	1:A:136:VAL:O	2.02	0.58
1:B:179:GLU:CB	1:B:180:LYS:HG3	2.33	0.58
1:C:225:ASN:O	1:C:226:THR:C	2.46	0.58
1:E:4:LYS:HE3	1:E:101:LEU:HD23	1.85	0.58
1:E:516:LYS:H	1:E:516:LYS:CD	2.15	0.58
1:B:19:ILE:O	5:B:610:NDP:H2N	2.03	0.58
4:E:621:DHF:C7	5:E:622:NDP:H42N	2.34	0.58
1:D:114:GLY:HA3	1:D:119:TYR:CZ	2.39	0.58
1:C:31:GLU:HG2	1:D:207:PHE:CE1	2.39	0.58
1:D:426:ASP:HB2	2:D:615:UMP:O3'	2.04	0.58
1:C:257:ARG:NH2	1:C:521:VAL:OXT	2.37	0.57
1:C:404:VAL:HG11	1:D:405:LEU:HD11	1.86	0.57
1:E:103:ASN:CG	1:E:104:ASP:H	2.11	0.57
1:A:75:ILE:O	5:A:606:NDP:H1B	2.04	0.57
1:B:479:ARG:NH2	1:B:513:PRO:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:C	1:A:99:GLU:OE1	2.47	0.57
1:C:291:ILE:HD13	1:C:436:ALA:HB3	1.86	0.57
1:D:48:LYS:HB3	1:D:106:SER:O	2.04	0.57
1:E:4:LYS:N	1:E:101:LEU:CD2	2.60	0.57
1:A:4:LYS:H	1:A:101:LEU:CD2	2.17	0.57
1:D:82:ASP:OD1	1:D:84:ALA:HB3	2.04	0.57
1:B:402:CYS:SG	2:B:607:UMP:C6	2.98	0.57
1:C:116:GLU:HB2	1:C:145:THR:HG23	1.86	0.57
1:C:419:ASN:ND2	1:C:457:ALA:HB3	2.20	0.57
1:D:4:LYS:H	1:D:101:LEU:HD21	1.70	0.57
1:D:116:GLU:HB2	1:D:145:THR:HG23	1.85	0.57
1:B:114:GLY:CA	1:B:119:TYR:CZ	2.88	0.56
1:D:108:GLU:HG2	1:D:109:ASN:ND2	2.19	0.56
1:A:3:GLU:HB3	6:A:618:HOH:O	2.04	0.56
1:A:288:ILE:HG23	1:A:501:TRP:HH2	1.70	0.56
1:C:56:ARG:O	1:C:59:TRP:HB3	2.05	0.56
1:C:96:ASP:O	1:C:99:GLU:HG3	2.05	0.56
1:D:156:PRO:O	1:D:228:SER:HB2	2.06	0.56
1:D:332:HIS:CD2	6:D:648:HOH:O	2.52	0.56
1:E:378:ASN:OD1	1:E:381:ASP:HB2	2.06	0.56
1:B:374:THR:O	1:B:378:ASN:O	2.24	0.56
1:D:98:ILE:CG2	1:D:101:LEU:HD12	2.36	0.56
1:A:289:ARG:NH2	1:A:311:LYS:O	2.37	0.56
1:B:285:LYS:HD3	1:B:514:THR:HG22	1.87	0.56
1:C:247:VAL:CG2	1:C:465:ILE:HD12	2.36	0.56
3:E:620:CB3:C6	3:E:620:CB3:H15	2.36	0.56
1:A:271:ARG:NH2	1:B:267:GLY:O	2.39	0.56
1:D:54:MET:HE3	1:D:72:ILE:HG23	1.88	0.56
1:D:62:ILE:HD11	4:D:617:DHF:C16	2.35	0.56
1:D:149:GLU:OE2	1:D:149:GLU:N	2.39	0.56
1:D:389:TRP:CE3	1:D:401:PRO:HG2	2.41	0.56
1:A:104:ASP:C	1:A:106:SER:H	2.13	0.56
1:B:270:MET:HE2	1:B:460:ILE:HD11	1.88	0.56
1:C:100:ASN:O	1:C:103:ASN:O	2.23	0.56
1:C:7:SER:HB3	1:C:130:ARG:HB3	1.87	0.56
1:D:262:THR:HG21	6:D:626:HOH:O	2.06	0.56
1:E:119:TYR:O	1:E:123:LEU:HD23	2.06	0.56
1:B:3:GLU:O	1:B:4:LYS:HB2	2.06	0.55
1:C:9:VAL:HG12	4:C:613:DHF:HN1	1.71	0.55
1:E:7:SER:HB3	1:E:130:ARG:HB3	1.88	0.55
1:B:326:GLU:HG3	6:B:682:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:GLY:HA2	5:E:622:NDP:O5D	2.06	0.55
1:E:423:ARG:HG3	1:E:424:SER:N	2.20	0.55
1:D:123:LEU:HD12	1:D:128:VAL:HG11	1.88	0.55
1:D:149:GLU:HA	6:D:672:HOH:O	2.05	0.55
1:E:8:ILE:HG12	1:E:112:VAL:HB	1.87	0.55
1:E:514:THR:HG22	1:E:515:ILE:N	2.22	0.55
1:E:378:ASN:ND2	6:E:634:HOH:O	2.40	0.55
4:C:613:DHF:C7	5:C:614:NDP:H42N	2.35	0.55
1:D:4:LYS:N	1:D:101:LEU:CD2	2.70	0.55
1:E:81:GLN:C	6:E:625:HOH:O	2.48	0.55
4:E:621:DHF:H72	5:E:622:NDP:H42N	1.88	0.55
1:B:342:TYR:OH	1:B:401:PRO:HA	2.06	0.55
1:D:123:LEU:CD1	1:D:128:VAL:HG11	2.36	0.55
1:D:256:ASN:O	1:D:257:ARG:C	2.50	0.55
1:E:256:ASN:ND2	1:E:262:THR:HG23	2.20	0.55
1:E:360:TYR:O	1:E:361:THR:C	2.50	0.55
1:E:491:ARG:HD3	1:E:503:ASP:OD2	2.07	0.55
1:B:411:THR:HG22	1:B:413:ASP:CB	2.37	0.55
1:D:304:ASN:HA	1:D:356:MET:CE	2.31	0.55
1:D:322:LYS:O	1:D:326:GLU:HB2	2.06	0.55
1:E:241:LEU:HD11	1:E:481:PRO:HG3	1.89	0.55
1:E:440:ILE:CG2	1:E:444:MET:HE3	2.37	0.55
1:C:423:ARG:HG3	1:C:424:SER:N	2.20	0.55
1:A:246:ARG:HG2	6:A:670:HOH:O	2.06	0.54
1:A:247:VAL:HG22	1:A:465:ILE:HD12	1.87	0.54
1:D:256:ASN:ND2	1:D:260:ILE:O	2.39	0.54
1:E:79:LEU:CD2	1:E:80:PRO:CD	2.55	0.54
1:A:342:TYR:CD2	1:A:403:HIS:CE1	2.95	0.54
1:C:8:ILE:HG12	1:C:112:VAL:HB	1.88	0.54
1:E:422:GLN:CD	1:E:425:CYS:HB2	2.33	0.54
1:C:93:ASN:OD1	1:C:95:GLU:HB3	2.07	0.54
1:D:423:ARG:HG3	1:D:424:SER:N	2.21	0.54
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.90	0.54
1:B:419:ASN:OD1	1:B:457:ALA:HB3	2.07	0.54
1:C:55:GLY:HA3	5:C:614:NDP:PA	2.48	0.54
1:E:135:ARG:NH2	1:E:482:ARG:HA	2.22	0.54
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.89	0.54
1:A:335:GLU:O	1:A:336:ASN:HB2	2.07	0.54
1:B:292:PHE:C	1:B:292:PHE:CD2	2.85	0.54
1:B:342:TYR:HH	1:B:402:CYS:H	1.51	0.54
1:C:360:TYR:C	1:C:363:VAL:HG13	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ASP:OD1	1:D:483:PRO:HG3	2.08	0.54
1:E:391:PRO:HA	1:E:394:LEU:HD23	1.90	0.54
1:E:426:ASP:N	2:E:619:UMP:O2	2.39	0.54
1:E:479:ARG:HG2	1:E:512:TYR:CD2	2.43	0.54
1:A:465:ILE:HG21	1:A:473:LEU:HD23	1.90	0.54
1:C:94:LEU:HD12	1:C:97:SER:OG	2.08	0.54
1:C:389:TRP:CE3	1:C:401:PRO:HG2	2.43	0.54
1:E:10:VAL:HG22	1:E:11:ALA:N	2.22	0.54
1:E:337:ASP:N	1:E:356:MET:HE3	2.23	0.54
1:A:114:GLY:CA	1:A:119:TYR:CZ	2.91	0.53
4:A:605:DHF:C6	5:A:606:NDP:H42N	2.38	0.53
1:D:96:ASP:O	1:D:99:GLU:CB	2.55	0.53
1:C:123:LEU:HD12	1:C:128:VAL:CG1	2.38	0.53
1:D:311:LYS:O	1:D:312:LYS:HB2	2.06	0.53
1:A:56:ARG:NH1	5:A:606:NDP:O3X	2.42	0.53
1:D:59:TRP:CE2	1:D:64:ARG:HG3	2.43	0.53
1:E:4:LYS:H	1:E:101:LEU:HD23	1.71	0.53
1:A:99:GLU:O	1:A:103:ASN:ND2	2.42	0.53
1:C:405:LEU:HD23	1:C:406:SER:N	2.23	0.53
1:A:207:PHE:O	1:A:210:ARG:HB2	2.08	0.53
1:D:296:ILE:O	1:D:300:LYS:HG2	2.08	0.53
1:E:82:ASP:OD2	1:E:84:ALA:HB3	2.09	0.53
1:B:479:ARG:HG2	1:B:512:TYR:CD2	2.43	0.53
1:D:147:PHE:HE1	1:D:150:ILE:HD11	1.74	0.53
1:E:440:ILE:HG22	1:E:444:MET:HE3	1.91	0.53
1:A:502:GLU:HB2	6:A:651:HOH:O	2.09	0.53
1:B:289:ARG:HG3	1:B:501:TRP:CE2	2.44	0.53
1:D:321:SER:O	1:D:325:LEU:HD13	2.08	0.53
1:E:321:SER:O	1:E:325:LEU:HD13	2.09	0.53
1:E:427:LEU:HD23	1:E:464:HIS:O	2.08	0.53
1:B:4:LYS:HB2	1:B:101:LEU:HD23	1.88	0.53
1:B:171:ASP:OD2	1:B:483:PRO:HG3	2.08	0.53
1:C:220:LYS:O	1:C:223:ILE:HG13	2.09	0.53
1:E:260:ILE:HD12	1:E:260:ILE:H	1.71	0.53
1:E:520:ALA:O	1:E:521:VAL:C	2.52	0.53
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.90	0.53
1:A:472:GLN:OE1	1:A:472:GLN:N	2.38	0.52
1:D:133:LEU:HD13	1:D:135:ARG:HG3	1.90	0.52
1:B:444:MET:HE2	1:B:499:PHE:CG	2.44	0.52
1:C:137:ALA:O	1:C:510:TYR:HE2	1.92	0.52
1:A:104:ASP:HB3	1:A:107:ILE:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:VAL:HG22	1:C:11:ALA:N	2.24	0.52
1:C:113:CYS:HB3	4:C:613:DHF:H71	1.90	0.52
1:E:255:GLU:CD	1:E:255:GLU:H	2.17	0.52
1:A:330:LEU:C	1:A:332:HIS:N	2.66	0.52
1:C:7:SER:CB	1:C:130:ARG:HB3	2.39	0.52
1:C:79:LEU:HD23	1:C:80:PRO:CD	2.39	0.52
1:A:264:SER:OG	1:B:409:TYR:OH	2.25	0.52
1:D:260:ILE:HD12	1:D:260:ILE:H	1.72	0.52
1:D:467:GLU:HA	1:D:470:LEU:CD2	2.40	0.52
1:E:471:THR:HB	1:E:472:GLN:OE1	2.09	0.52
3:E:620:CB3:C6	3:E:620:CB3:C15	2.87	0.52
1:B:75:ILE:O	5:B:610:NDP:H1B	2.10	0.52
1:B:57:LYS:O	1:B:60:ASP:HB2	2.09	0.52
1:D:82:ASP:OD1	1:D:84:ALA:N	2.43	0.52
1:E:48:LYS:HB3	1:E:106:SER:O	2.10	0.52
1:E:104:ASP:C	1:E:106:SER:N	2.66	0.52
1:A:3:GLU:HB2	1:A:101:LEU:HD22	1.91	0.52
1:C:384:HIS:HB2	1:C:408:TYR:O	2.09	0.52
1:D:247:VAL:HG12	1:D:265:ILE:HG12	1.91	0.52
1:E:30:SER:HB2	6:E:644:HOH:O	2.08	0.52
1:B:439:ALA:O	1:B:443:MET:HG3	2.10	0.51
1:D:341:ILE:O	1:D:342:TYR:C	2.52	0.51
1:E:12:ALA:HB2	1:E:19:ILE:HG22	1.91	0.51
1:E:100:ASN:OD1	1:E:100:ASN:N	2.36	0.51
1:C:40:THR:CG2	1:C:70:ARG:HH11	2.23	0.51
1:D:415:CYS:HA	1:D:452:GLU:O	2.10	0.51
1:E:85:ASP:OD1	1:E:86:PRO:HD2	2.11	0.51
1:E:133:LEU:HD22	1:E:134:THR:N	2.26	0.51
1:E:423:ARG:NH2	2:E:619:UMP:OP1	2.38	0.51
1:B:285:LYS:CB	1:B:514:THR:HG22	2.33	0.51
1:C:10:VAL:HG11	1:C:147:PHE:CE2	2.45	0.51
1:E:60:ASP:OD1	1:E:64:ARG:NH1	2.41	0.51
1:E:126:ASN:OD1	1:E:177:LYS:HE3	2.10	0.51
1:E:348:HIS:HB3	1:E:363:VAL:O	2.10	0.51
1:C:89:VAL:HG12	1:C:90:VAL:N	2.26	0.51
1:A:315:ILE:HB	3:A:604:CB3:C15	2.41	0.51
1:B:502:GLU:H	1:B:502:GLU:CD	2.19	0.51
1:D:256:ASN:O	1:D:258:THR:O	2.29	0.51
1:E:337:ASP:CA	1:E:356:MET:HE3	2.41	0.51
1:A:360:TYR:O	1:A:363:VAL:CG1	2.58	0.51
1:A:397:MET:SD	1:A:401:PRO:HD3	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:GLU:CD	1:C:222:GLU:H	2.19	0.51
1:C:113:CYS:O	4:C:613:DHF:H72	2.11	0.51
1:D:490:LYS:HD2	1:D:502:GLU:O	2.11	0.51
1:B:342:TYR:CZ	1:B:401:PRO:HA	2.46	0.51
1:C:320:GLY:O	1:C:335:GLU:O	2.28	0.51
1:E:195:SER:OG	1:E:196:ILE:HD11	2.07	0.51
1:A:82:ASP:O	1:A:84:ALA:N	2.40	0.51
1:C:233:ARG:NH1	1:C:242:ASP:OD1	2.43	0.51
1:D:149:GLU:CD	1:D:149:GLU:N	2.67	0.51
1:B:12:ALA:HB1	1:B:17:SER:HA	1.92	0.50
1:C:431:SER:O	1:C:435:ILE:HG13	2.11	0.50
1:C:135:ARG:HD3	1:C:171:ASP:OD2	2.11	0.50
1:E:116:GLU:HB2	1:E:145:THR:HG23	1.93	0.50
1:A:114:GLY:HA2	1:A:119:TYR:CE1	2.47	0.50
1:C:40:THR:HG21	1:C:70:ARG:NH1	2.23	0.50
1:E:315:ILE:HG13	1:E:316:TRP:N	2.27	0.50
1:E:488:LYS:CD	1:E:489:PHE:H	2.20	0.50
1:A:104:ASP:C	1:A:106:SER:N	2.68	0.50
1:A:270:MET:HE2	1:A:460:ILE:HD11	1.93	0.50
1:C:151:PRO:HG2	1:C:154:PHE:HD2	1.76	0.50
1:A:383:ARG:CZ	1:B:400:PRO:HG2	2.41	0.50
1:C:212:MET:SD	1:D:273:ASP:HB2	2.51	0.50
1:A:323:GLU:N	1:A:323:GLU:OE1	2.44	0.50
1:E:4:LYS:HG2	1:E:101:LEU:CD2	2.42	0.50
1:D:19:ILE:HB	5:D:618:NDP:N7N	2.27	0.50
1:D:93:ASN:ND2	1:D:96:ASP:OD2	2.39	0.50
1:D:472:GLN:O	1:D:475:GLU:HB3	2.12	0.50
1:D:476:GLN:O	1:D:479:ARG:HG2	2.12	0.50
1:A:233:ARG:NH1	1:A:242:ASP:CG	2.69	0.50
1:B:95:GLU:HG3	1:B:127:PHE:HZ	1.77	0.50
1:C:38:LYS:HB3	1:D:202:LEU:HG	1.92	0.50
1:E:347:ARG:HB2	1:E:348:HIS:CD2	2.47	0.50
1:A:400:PRO:HG2	1:A:423:ARG:NH2	2.26	0.49
1:B:3:GLU:OE2	1:B:3:GLU:HA	2.11	0.49
1:C:62:ILE:HD11	1:C:67:LEU:HD11	1.94	0.49
1:C:134:THR:HA	1:C:171:ASP:O	2.12	0.49
1:C:491:ARG:NH1	1:C:503:ASP:OD1	2.45	0.49
1:D:10:VAL:HG13	1:D:133:LEU:HD23	1.94	0.49
1:E:303:THR:HG21	1:E:344:PHE:HB2	1.92	0.49
1:B:10:VAL:HG22	1:B:11:ALA:N	2.28	0.49
1:B:193:LEU:HD22	1:B:194:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:PRO:HB2	1:B:423:ARG:NH2	2.28	0.49
1:C:509:TYR:CE1	1:C:511:PRO:HG3	2.47	0.49
1:C:512:TYR:HB3	1:C:513:PRO:HD2	1.95	0.49
1:E:307:HIS:O	1:E:311:LYS:HD2	2.13	0.49
1:A:330:LEU:O	1:A:332:HIS:N	2.46	0.49
1:C:26:PRO:HG2	1:C:143:PHE:HE1	1.77	0.49
1:C:323:GLU:CD	1:C:323:GLU:N	2.70	0.49
1:D:297:TRP:CD1	1:D:302:ASP:HB3	2.47	0.49
1:D:495:ASN:HB2	6:D:650:HOH:O	2.12	0.49
1:E:193:LEU:HD12	1:E:194:LYS:HD3	1.94	0.49
1:E:431:SER:O	1:E:435:ILE:HG13	2.12	0.49
1:B:224:TYR:O	1:B:227:PRO:HD3	2.13	0.49
1:B:285:LYS:HD3	1:B:514:THR:CG2	2.42	0.49
1:D:82:ASP:OD1	1:D:84:ALA:HB2	2.11	0.49
1:E:430:GLY:HA3	3:E:620:CB3:HP3	1.94	0.49
4:C:613:DHF:HG2	4:C:613:DHF:O1	2.11	0.49
1:C:123:LEU:CD1	1:C:128:VAL:HG11	2.39	0.49
1:D:62:ILE:CG2	1:D:62:ILE:O	2.60	0.49
1:D:288:ILE:HA	1:D:291:ILE:HD12	1.94	0.49
1:B:487:LEU:HD23	1:B:487:LEU:C	2.37	0.49
1:E:98:ILE:HG22	1:E:98:ILE:O	2.11	0.49
1:A:233:ARG:NH1	1:A:242:ASP:OD2	2.44	0.49
2:A:603:UMP:P	1:B:383:ARG:HH11	2.36	0.49
1:C:405:LEU:HD23	1:C:405:LEU:O	2.11	0.49
1:A:7:SER:HB3	1:A:130:ARG:HB3	1.94	0.49
1:B:257:ARG:NH2	1:B:521:VAL:OXT	2.46	0.49
1:A:271:ARG:NH1	6:A:666:HOH:O	2.45	0.48
1:A:287:PHE:HB2	6:A:712:HOH:O	2.12	0.48
1:D:94:LEU:O	1:D:97:SER:OG	2.28	0.48
1:D:403:HIS:O	1:D:403:HIS:ND1	2.46	0.48
1:A:444:MET:HE2	1:A:499:PHE:CG	2.48	0.48
1:B:52:LEU:HD13	1:B:113:CYS:SG	2.53	0.48
1:C:32:ASP:O	1:C:35:PHE:HB3	2.14	0.48
1:C:370:LYS:HA	1:C:373:GLU:CG	2.41	0.48
1:E:330:LEU:C	1:E:332:HIS:N	2.69	0.48
1:B:171:ASP:CG	1:B:483:PRO:HG3	2.37	0.48
1:B:411:THR:HG21	1:B:413:ASP:CB	2.42	0.48
1:C:130:ARG:HG3	1:C:130:ARG:HH11	1.79	0.48
1:C:243:LEU:HD11	1:C:268:GLN:HG3	1.94	0.48
1:E:241:LEU:CD1	1:E:481:PRO:HG3	2.42	0.48
1:E:390:ASN:O	1:E:394:LEU:HD22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:472:GLN:OE1	1:E:472:GLN:N	2.46	0.48
1:A:100:ASN:O	1:A:103:ASN:O	2.31	0.48
1:A:339:GLY:HA2	1:A:353:TYR:CE2	2.48	0.48
4:A:605:DHF:H72	5:A:606:NDP:H42N	1.95	0.48
1:C:429:LEU:HD22	1:C:469:HIS:CE1	2.48	0.48
1:E:59:TRP:CD1	1:E:64:ARG:HG2	2.47	0.48
1:B:403:HIS:HB2	1:B:420:LEU:HD11	1.96	0.48
1:D:59:TRP:NE1	1:D:64:ARG:HG3	2.28	0.48
1:A:114:GLY:CA	1:A:119:TYR:CE1	2.97	0.48
1:A:291:ILE:HD13	1:A:436:ALA:HB3	1.94	0.48
1:C:85:ASP:OD2	1:C:86:PRO:HD2	2.14	0.48
1:D:67:LEU:HD22	4:D:617:DHF:CT	2.44	0.48
1:A:93:ASN:ND2	1:A:96:ASP:H	2.11	0.48
1:B:51:ALA:C	1:B:52:LEU:HD23	2.39	0.48
3:B:608:CB3:C14	3:B:608:CB3:C5	2.91	0.48
1:D:37:SER:O	1:D:41:ASN:HB2	2.14	0.48
1:E:77:SER:O	1:E:92:ARG:NH1	2.46	0.48
1:A:360:TYR:O	1:A:363:VAL:HG12	2.13	0.48
4:A:605:DHF:O	4:A:605:DHF:HB1	2.12	0.48
1:B:193:LEU:CD2	1:B:194:LYS:HG2	2.43	0.48
1:B:247:VAL:HG22	1:B:465:ILE:HD12	1.95	0.48
1:B:447:GLN:NE2	1:B:492:LYS:HA	2.28	0.48
1:C:389:TRP:HE3	1:C:401:PRO:HG2	1.78	0.48
1:D:3:GLU:N	1:D:101:LEU:HD22	2.29	0.48
1:D:36:PHE:O	1:D:40:THR:HG23	2.14	0.48
1:E:255:GLU:CD	1:E:255:GLU:N	2.70	0.48
1:E:333:ARG:HG2	1:E:333:ARG:HH11	1.79	0.48
1:E:431:SER:HB3	1:E:432:PRO:HD3	1.95	0.48
1:E:470:LEU:O	1:E:474:LYS:HG3	2.14	0.48
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.96	0.48
1:D:7:SER:O	1:D:111:PHE:HA	2.14	0.48
1:D:135:ARG:HD2	1:D:173:MET:SD	2.54	0.48
1:E:104:ASP:O	1:E:107:ILE:N	2.35	0.48
1:E:502:GLU:CD	1:E:502:GLU:H	2.21	0.48
1:C:434:ASN:OD1	3:C:612:CB3:HP3	2.14	0.47
1:E:14:VAL:HG23	1:E:15:LEU:N	2.28	0.47
1:A:333:ARG:HG2	1:A:337:ASP:HB3	1.96	0.47
4:A:605:DHF:C7	5:A:606:NDP:H42N	2.44	0.47
1:C:15:LEU:HB2	1:C:139:GLU:CD	2.39	0.47
1:C:225:ASN:OD1	1:C:238:PHE:HE1	1.97	0.47
1:D:431:SER:HB3	1:D:432:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:SER:N	1:D:92:ARG:HH12	2.13	0.47
1:E:196:ILE:N	1:E:196:ILE:CD1	2.31	0.47
1:E:254:ARG:HD2	1:E:264:SER:CB	2.45	0.47
1:E:340:PRO:HD3	1:E:353:TYR:CD2	2.49	0.47
1:A:123:LEU:HD23	1:A:128:VAL:CG1	2.44	0.47
1:A:3:GLU:CB	1:A:101:LEU:HD22	2.45	0.47
1:C:18:GLY:HA3	1:C:143:PHE:CD1	2.50	0.47
1:D:98:ILE:HG22	1:D:101:LEU:HD12	1.97	0.47
1:D:226:THR:N	1:D:227:PRO:HD3	2.29	0.47
1:D:295:LEU:O	1:D:299:ILE:HG13	2.15	0.47
1:A:34:LYS:HB3	1:B:206:ILE:HG12	1.96	0.47
1:A:315:ILE:HG13	1:A:316:TRP:CD1	2.49	0.47
1:A:342:TYR:CE2	1:A:403:HIS:CE1	3.02	0.47
1:B:426:ASP:OD2	1:B:426:ASP:C	2.58	0.47
1:C:97:SER:O	1:C:100:ASN:OD1	2.32	0.47
1:D:94:LEU:O	1:D:95:GLU:C	2.58	0.47
1:D:209:ILE:O	1:D:209:ILE:HG22	2.14	0.47
1:E:55:GLY:HA3	5:E:622:NDP:O5B	2.15	0.47
1:E:159:MET:SD	1:E:235:HIS:HD2	2.36	0.47
1:E:425:CYS:HA	2:E:619:UMP:O2	2.14	0.47
1:B:349:TYR:O	1:B:350:ASN:HB2	2.15	0.47
1:C:234:GLU:OE2	1:D:211:LYS:NZ	2.48	0.47
1:C:135:ARG:HD3	1:C:171:ASP:HB3	1.97	0.47
1:B:297:TRP:CH2	1:B:338:LEU:HD12	2.45	0.47
1:D:248:LEU:HD13	1:D:465:ILE:HD12	1.96	0.46
1:D:360:TYR:HD1	1:D:363:VAL:HG11	1.81	0.46
1:A:130:ARG:NH1	1:A:176:GLU:OE2	2.42	0.46
1:A:423:ARG:HG3	1:A:424:SER:N	2.31	0.46
1:B:423:ARG:HG3	1:B:424:SER:N	2.31	0.46
1:C:96:ASP:O	1:C:98:ILE:O	2.33	0.46
1:C:512:TYR:HB3	1:C:513:PRO:CD	2.46	0.46
5:E:622:NDP:O1X	5:E:622:NDP:O3B	2.30	0.46
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.80	0.46
1:B:385:ILE:CG2	1:B:386:LEU:N	2.78	0.46
1:D:330:LEU:C	1:D:332:HIS:H	2.23	0.46
1:C:273:ASP:HB2	1:D:212:MET:SD	2.55	0.46
1:E:104:ASP:C	1:E:106:SER:H	2.22	0.46
1:E:195:SER:CB	1:E:196:ILE:HD12	2.44	0.46
1:E:342:TYR:CD1	1:E:403:HIS:CE1	3.03	0.46
1:E:493:VAL:HG21	1:E:499:PHE:CE1	2.50	0.46
1:E:423:ARG:NH1	1:E:424:SER:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLY:HA2	1:B:119:TYR:CE1	2.50	0.46
1:B:164:CYS:HB2	1:B:486:GLN:NE2	2.30	0.46
1:E:347:ARG:O	1:E:366:ASP:CA	2.64	0.46
1:A:455:GLU:OE2	1:B:215:ARG:NH2	2.48	0.46
1:C:75:ILE:CG2	5:C:614:NDP:C4A	2.94	0.46
1:C:102:MET:HE2	1:C:102:MET:HA	1.98	0.46
1:E:113:CYS:O	4:E:621:DHF:H72	2.15	0.46
1:A:52:LEU:HD13	1:A:113:CYS:SG	2.56	0.46
3:D:616:CB3:H5	3:D:616:CB3:C14	2.46	0.46
1:E:85:ASP:OD1	1:E:85:ASP:C	2.58	0.46
1:E:120:ARG:HG2	1:E:148:PRO:HB3	1.97	0.46
1:E:430:GLY:C	3:E:620:CB3:HP3	2.41	0.46
1:E:516:LYS:HD2	1:E:516:LYS:N	2.31	0.46
1:A:102:MET:CE	6:A:618:HOH:O	2.64	0.46
1:B:237:GLU:HB2	1:B:484:PHE:CZ	2.50	0.46
1:B:378:ASN:CG	1:B:381:ASP:HB2	2.40	0.46
1:D:340:PRO:HD3	1:D:353:TYR:CD2	2.50	0.46
1:A:160:SER:HA	1:A:234:GLU:HB3	1.98	0.45
1:C:248:LEU:HD12	1:C:248:LEU:HA	1.84	0.45
1:C:404:VAL:HG11	1:D:405:LEU:CD1	2.46	0.45
1:E:105:ASP:N	1:E:105:ASP:OD1	2.48	0.45
1:C:172:PHE:CE2	1:D:203:LEU:HD11	2.51	0.45
1:C:203:LEU:HD11	1:D:172:PHE:CE2	2.50	0.45
1:C:335:GLU:O	1:C:335:GLU:HG3	2.16	0.45
1:D:247:VAL:HG21	1:D:465:ILE:HG13	1.98	0.45
3:D:616:CB3:C14	3:D:616:CB3:C5	2.94	0.45
1:E:305:GLY:O	1:E:309:ILE:HG12	2.15	0.45
1:E:516:LYS:CD	1:E:516:LYS:N	2.77	0.45
1:A:82:ASP:C	1:A:84:ALA:H	2.22	0.45
1:A:99:GLU:H	1:A:101:LEU:H	1.64	0.45
1:B:180:LYS:O	1:B:181:LYS:CB	2.64	0.45
1:C:289:ARG:NH2	1:C:311:LYS:O	2.48	0.45
1:C:293:GLU:HG3	6:C:622:HOH:O	2.15	0.45
1:C:402:CYS:SG	2:C:611:UMP:H5''	2.57	0.45
1:C:479:ARG:NH2	1:C:513:PRO:O	2.49	0.45
1:D:19:ILE:O	5:D:618:NDP:H2N	2.17	0.45
1:D:342:TYR:CZ	1:D:403:HIS:NE2	2.84	0.45
1:E:13:SER:HA	1:E:136:VAL:O	2.17	0.45
1:E:147:PHE:CD2	1:E:148:PRO:HD2	2.50	0.45
3:E:620:CB3:C5	3:E:620:CB3:C14	2.93	0.45
1:A:337:ASP:OD2	1:A:337:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:PHE:O	1:A:348:HIS:N	2.45	0.45
1:A:345:GLN:OE1	1:A:349:TYR:CD1	2.70	0.45
1:A:429:LEU:HD11	1:A:517:MET:HB2	1.97	0.45
1:E:199:THR:O	1:E:203:LEU:HB2	2.17	0.45
1:A:43:LYS:HB2	1:A:108:GLU:OE1	2.16	0.45
1:B:139:GLU:O	1:B:140:ASP:HB2	2.16	0.45
1:C:36:PHE:CD1	1:C:36:PHE:C	2.94	0.45
1:D:51:ALA:C	1:D:52:LEU:HD23	2.41	0.45
1:D:411:THR:OG1	1:D:413:ASP:OD1	2.31	0.45
1:E:247:VAL:HG22	1:E:265:ILE:HG12	1.99	0.45
1:B:56:ARG:HD3	5:B:610:NDP:O1X	2.17	0.45
4:B:609:DHF:O	4:B:609:DHF:CB	2.64	0.45
1:D:426:ASP:C	1:D:426:ASP:OD2	2.59	0.45
1:A:288:ILE:HG23	1:A:501:TRP:CH2	2.52	0.45
1:D:62:ILE:O	1:D:62:ILE:HG23	2.17	0.45
1:D:178:GLN:OE1	1:D:178:GLN:CA	2.61	0.45
1:D:293:GLU:HA	1:D:296:ILE:HD11	1.99	0.45
1:D:296:ILE:HD12	1:D:297:TRP:H	1.80	0.45
1:B:7:SER:O	1:B:111:PHE:HA	2.17	0.45
1:E:114:GLY:HA2	1:E:119:TYR:CE2	2.52	0.45
1:E:487:LEU:C	1:E:487:LEU:HD23	2.42	0.45
1:C:40:THR:CG2	1:C:70:ARG:CD	2.90	0.44
1:C:237:GLU:O	1:C:237:GLU:HG3	2.18	0.44
1:D:155:LEU:HB2	1:D:178:GLN:NE2	2.32	0.44
1:D:298:PHE:CE1	1:D:342:TYR:HB2	2.52	0.44
1:D:403:HIS:HB2	1:D:420:LEU:HD11	1.99	0.44
1:E:123:LEU:N	1:E:123:LEU:HD22	2.33	0.44
1:E:246:ARG:NH1	1:E:268:GLN:OE1	2.50	0.44
1:E:402:CYS:O	1:E:404:VAL:HG23	2.17	0.44
1:B:113:CYS:O	4:B:609:DHF:H72	2.17	0.44
1:C:54:MET:HE3	1:C:72:ILE:CG2	2.42	0.44
1:D:133:LEU:HD22	1:D:134:THR:N	2.33	0.44
1:D:292:PHE:CD1	1:D:504:ILE:HD11	2.52	0.44
1:E:123:LEU:HD13	1:E:128:VAL:HG11	2.00	0.44
1:D:125:ASP:HB2	1:D:127:PHE:CE1	2.52	0.44
1:E:56:ARG:O	1:E:59:TRP:HB3	2.17	0.44
1:E:103:ASN:O	1:E:104:ASP:CB	2.65	0.44
1:E:390:ASN:O	1:E:394:LEU:CD2	2.66	0.44
4:E:621:DHF:H72	5:E:622:NDP:C4N	2.46	0.44
1:A:43:LYS:NZ	1:A:48:LYS:O	2.35	0.44
1:A:294:GLU:O	1:A:297:TRP:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:MET:O	1:B:103:ASN:HB3	2.17	0.44
1:C:151:PRO:HG2	1:C:154:PHE:CD2	2.53	0.44
1:E:137:ALA:O	1:E:510:TYR:HE2	1.99	0.44
1:E:155:LEU:HB2	1:E:178:GLN:NE2	2.33	0.44
1:E:258:THR:HG21	1:E:520:ALA:HB1	1.99	0.44
1:E:491:ARG:HH11	1:E:503:ASP:CG	2.25	0.44
1:A:171:ASP:OD2	1:A:483:PRO:HG3	2.16	0.44
1:C:402:CYS:SG	1:C:424:SER:HB3	2.58	0.44
1:D:296:ILE:H	1:D:296:ILE:HG13	1.66	0.44
1:D:467:GLU:O	1:D:470:LEU:HD23	2.18	0.44
1:D:500:LYS:O	1:D:503:ASP:HB2	2.16	0.44
1:A:171:ASP:CG	1:A:483:PRO:HG3	2.43	0.44
1:A:264:SER:HB2	1:A:462:ASP:OD1	2.17	0.44
1:B:397:MET:SD	1:B:401:PRO:HD3	2.57	0.44
1:C:130:ARG:HD2	1:C:132:TYR:CE1	2.53	0.44
1:C:271:ARG:NH2	1:D:267:GLY:O	2.48	0.44
1:C:383:ARG:CZ	1:D:400:PRO:HG3	2.48	0.44
1:C:485:PRO:HB3	1:C:509:TYR:CA	2.48	0.44
4:D:617:DHF:C7	5:D:618:NDP:H42N	2.48	0.44
1:A:117:SER:OG	5:A:606:NDP:O1A	2.24	0.44
1:B:209:ILE:CD1	1:B:209:ILE:N	2.68	0.44
1:C:4:LYS:HE3	1:C:107:ILE:O	2.18	0.44
1:C:6:VAL:HG11	1:C:127:PHE:O	2.18	0.44
1:C:465:ILE:CG2	1:C:473:LEU:HD12	2.48	0.44
1:D:58:THR:OG1	5:D:618:NDP:H6N	2.17	0.44
1:D:99:GLU:OE2	1:D:99:GLU:O	2.35	0.44
3:A:604:CB3:C5	3:A:604:CB3:C14	2.93	0.44
1:B:95:GLU:HB2	6:B:666:HOH:O	2.18	0.44
1:C:14:VAL:HG13	1:C:15:LEU:N	2.32	0.44
1:D:389:TRP:HE3	1:D:401:PRO:HG2	1.83	0.44
1:A:93:ASN:HD21	1:A:95:GLU:HB3	1.81	0.44
1:B:96:ASP:O	1:B:99:GLU:HB2	2.17	0.44
1:B:222:GLU:OE1	1:B:222:GLU:N	2.49	0.44
1:C:304:ASN:OD1	1:C:306:ASN:HB2	2.18	0.44
1:D:12:ALA:HB2	1:D:19:ILE:HG22	1.99	0.44
1:D:49:LYS:O	1:D:107:ILE:HA	2.18	0.44
1:D:288:ILE:O	1:D:291:ILE:HB	2.17	0.44
1:E:150:ILE:HA	1:E:151:PRO:HD3	1.82	0.44
1:E:281:LEU:HD12	1:E:432:PRO:HB3	2.00	0.44
1:A:123:LEU:HD23	1:A:128:VAL:HG13	2.00	0.43
1:A:246:ARG:NH1	1:A:268:GLN:OE1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:THR:HG21	1:A:260:ILE:HB	2.00	0.43
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.83	0.43
3:C:612:CB3:C5	3:C:612:CB3:C14	2.93	0.43
1:D:335:GLU:O	1:D:336:ASN:HB2	2.17	0.43
1:A:396:GLN:HG3	6:A:668:HOH:O	2.16	0.43
1:B:400:PRO:HB2	1:B:423:ARG:HH21	1.82	0.43
1:C:172:PHE:CD2	1:D:203:LEU:HD21	2.53	0.43
1:D:466:TYR:HE2	2:D:615:UMP:O3'	1.99	0.43
1:D:36:PHE:CD1	1:D:36:PHE:C	2.96	0.43
1:D:220:LYS:HE2	1:D:220:LYS:HB2	1.68	0.43
1:D:260:ILE:N	1:D:260:ILE:CD1	2.74	0.43
1:D:400:PRO:HG2	1:D:423:ARG:NH2	2.32	0.43
1:E:303:THR:CG2	1:E:344:PHE:HB2	2.47	0.43
1:E:333:ARG:HG2	1:E:333:ARG:NH1	2.34	0.43
1:E:337:ASP:HA	1:E:356:MET:HE3	2.00	0.43
1:C:274:MET:HE2	1:C:455:GLU:C	2.44	0.43
1:C:471:THR:HG23	6:C:651:HOH:O	2.18	0.43
1:D:14:VAL:HG13	1:D:15:LEU:N	2.33	0.43
1:D:62:ILE:HD13	1:D:62:ILE:HA	1.67	0.43
1:E:330:LEU:HD23	1:E:332:HIS:HE1	1.83	0.43
1:E:464:HIS:CD2	1:E:466:TYR:CE2	3.07	0.43
1:A:462:ASP:OD2	1:B:382:ARG:HG2	2.19	0.43
1:C:81:GLN:HE22	1:C:92:ARG:HH21	1.67	0.43
1:C:472:GLN:O	1:C:475:GLU:HB3	2.18	0.43
1:D:336:ASN:O	1:D:356:MET:CE	2.66	0.43
1:E:352:GLU:HA	1:E:352:GLU:OE2	2.19	0.43
1:C:62:ILE:O	1:C:62:ILE:HG23	2.17	0.43
1:C:243:LEU:CD1	1:C:268:GLN:HG3	2.48	0.43
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.87	0.43
1:C:63:GLY:O	1:C:65:ARG:HG2	2.18	0.43
1:C:246:ARG:NH1	1:C:268:GLN:OE1	2.45	0.43
1:C:262:THR:HG22	1:C:466:TYR:HA	1.99	0.43
1:D:137:ALA:O	1:D:510:TYR:HE2	2.02	0.43
1:C:12:ALA:HB2	1:C:19:ILE:HG22	2.01	0.43
1:C:178:GLN:OE1	1:C:178:GLN:N	2.52	0.43
1:C:224:TYR:O	1:C:227:PRO:HG3	2.19	0.43
1:D:43:LYS:NZ	1:D:48:LYS:O	2.46	0.43
1:D:56:ARG:O	1:D:59:TRP:HB3	2.19	0.43
1:D:242:ASP:O	1:D:246:ARG:HB2	2.19	0.43
1:D:256:ASN:O	1:D:258:THR:N	2.52	0.43
1:D:355:THR:OG1	1:D:358:ASP:OD1	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:SER:O	1:E:111:PHE:HA	2.19	0.43
1:A:479:ARG:HG2	1:A:512:TYR:CD2	2.54	0.43
1:A:509:TYR:HA	6:A:667:HOH:O	2.18	0.43
1:B:52:LEU:HD23	1:B:52:LEU:N	2.34	0.43
1:D:220:LYS:HD3	1:D:249:GLU:CD	2.44	0.43
1:D:429:LEU:HB3	3:D:616:CB3:O4	2.18	0.43
1:D:430:GLY:CA	3:D:616:CB3:HP3	2.49	0.43
1:E:178:GLN:OE1	1:E:178:GLN:CA	2.30	0.43
1:A:386:LEU:O	1:A:405:LEU:HA	2.18	0.43
1:A:415:CYS:HA	1:A:452:GLU:O	2.19	0.43
1:C:98:ILE:C	1:C:99:GLU:CG	2.89	0.43
1:C:402:CYS:SG	2:C:611:UMP:H2'	2.58	0.43
1:D:430:GLY:CA	3:D:616:CB3:CP3	2.96	0.43
1:E:123:LEU:HD13	1:E:128:VAL:CG1	2.49	0.43
1:A:273:ASP:HB2	1:B:212:MET:SD	2.58	0.42
1:B:4:LYS:HD2	1:B:101:LEU:HA	2.01	0.42
1:C:193:LEU:HD12	6:C:626:HOH:O	2.19	0.42
1:E:98:ILE:N	1:E:98:ILE:HD12	2.33	0.42
1:E:295:LEU:HD22	1:E:299:ILE:HD11	2.00	0.42
1:E:360:TYR:HB3	1:E:363:VAL:CG1	2.47	0.42
1:B:166:LYS:O	1:B:167:ASN:HB2	2.19	0.42
1:B:452:GLU:OE2	1:B:452:GLU:HA	2.19	0.42
1:D:122:ALA:O	1:D:127:PHE:HB2	2.19	0.42
1:E:155:LEU:HG	1:E:178:GLN:HE21	1.83	0.42
1:A:33:LEU:HB3	4:A:605:DHF:HG1	2.01	0.42
1:A:425:CYS:SG	1:A:431:SER:HB2	2.59	0.42
1:B:4:LYS:CB	1:B:101:LEU:HD23	2.49	0.42
1:B:335:GLU:O	1:B:336:ASN:HB2	2.19	0.42
1:C:140:ASP:N	1:C:141:ILE:HG23	2.34	0.42
4:C:613:DHF:H91	5:C:614:NDP:C5N	2.49	0.42
1:D:171:ASP:CG	1:D:483:PRO:HG3	2.45	0.42
1:D:244:LEU:O	1:D:247:VAL:HG22	2.19	0.42
2:D:615:UMP:C4	3:D:616:CB3:CP3	3.02	0.42
1:E:225:ASN:HB2	1:E:477:LEU:HD23	2.01	0.42
1:E:272:PHE:HB2	1:E:456:LEU:HB3	2.01	0.42
1:B:150:ILE:HA	1:B:151:PRO:HD3	1.83	0.42
1:B:207:PHE:O	1:B:210:ARG:HB2	2.20	0.42
1:B:243:LEU:O	1:B:247:VAL:HG12	2.19	0.42
1:D:330:LEU:C	1:D:332:HIS:N	2.77	0.42
1:D:349:TYR:O	1:D:350:ASN:HB2	2.18	0.42
1:E:400:PRO:HA	1:E:401:PRO:HD3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:520:ALA:HB3	3:E:620:CB3:HN21	1.84	0.42
1:A:103:ASN:CG	1:A:104:ASP:N	2.76	0.42
1:B:70:ARG:NH1	4:B:609:DHF:O2	2.42	0.42
1:E:10:VAL:CG2	1:E:11:ALA:N	2.83	0.42
1:E:76:SER:OG	1:E:79:LEU:HB2	2.19	0.42
1:A:81:GLN:HA	6:A:659:HOH:O	2.19	0.42
1:A:193:LEU:HD22	1:A:195:SER:H	1.85	0.42
1:B:104:ASP:C	1:B:106:SER:N	2.75	0.42
1:C:18:GLY:HA3	1:C:143:PHE:CG	2.55	0.42
1:C:155:LEU:HD12	1:C:178:GLN:HE21	1.84	0.42
1:C:459:PHE:CD2	1:D:459:PHE:CD2	3.08	0.42
1:E:133:LEU:HD13	1:E:135:ARG:HG3	2.00	0.42
1:A:10:VAL:HG22	1:A:11:ALA:N	2.35	0.42
1:A:472:GLN:O	1:A:475:GLU:HB3	2.19	0.42
1:B:272:PHE:CZ	1:B:435:ILE:HD13	2.54	0.42
1:C:10:VAL:CG2	1:C:11:ALA:N	2.82	0.42
1:C:48:LYS:HE2	1:C:105:ASP:O	2.20	0.42
1:A:430:GLY:O	1:A:433:PHE:N	2.49	0.42
1:C:35:PHE:HA	1:D:206:ILE:HD11	2.01	0.42
1:C:104:ASP:O	1:C:106:SER:N	2.52	0.42
1:D:53:ILE:HG23	1:D:75:ILE:HD13	2.02	0.42
1:E:313:VAL:HG12	1:E:315:ILE:HG12	2.01	0.42
1:A:12:ALA:HB1	1:A:17:SER:HA	2.01	0.42
1:A:413:ASP:O	1:A:414:ASN:HB2	2.19	0.42
1:B:323:GLU:H	1:B:323:GLU:CD	2.28	0.42
1:C:83:GLU:O	1:C:84:ALA:C	2.62	0.42
1:E:114:GLY:HA3	5:E:622:NDP:H5N	2.02	0.42
1:A:212:MET:SD	1:B:273:ASP:HB2	2.59	0.42
1:C:45:ASP:OD2	1:C:48:LYS:HE3	2.20	0.42
5:C:614:NDP:O2N	5:C:614:NDP:O1A	2.38	0.42
1:D:107:ILE:HG22	1:D:107:ILE:O	2.18	0.42
1:D:429:LEU:HD12	1:D:429:LEU:HA	1.82	0.42
1:E:85:ASP:OD1	1:E:86:PRO:CD	2.68	0.42
1:E:254:ARG:HD2	1:E:264:SER:HB2	2.02	0.42
1:E:349:TYR:HB3	1:E:365:VAL:HB	2.02	0.42
1:A:104:ASP:OD2	1:A:106:SER:OG	2.38	0.41
1:A:469:HIS:HB3	1:A:473:LEU:HD22	2.01	0.41
1:B:135:ARG:NH1	1:B:171:ASP:OD2	2.43	0.41
1:B:274:MET:HE1	1:B:442:THR:HG21	2.01	0.41
4:B:609:DHF:H72	5:B:610:NDP:C5N	2.50	0.41
1:C:193:LEU:CD1	6:C:626:HOH:O	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:THR:N	1:C:227:PRO:HD3	2.35	0.41
1:D:96:ASP:O	1:D:98:ILE:O	2.37	0.41
1:D:193:LEU:C	1:D:195:SER:N	2.78	0.41
1:A:345:GLN:O	1:A:349:TYR:HB2	2.20	0.41
1:C:203:LEU:HD12	1:C:203:LEU:HA	1.91	0.41
1:C:485:PRO:HB3	1:C:509:TYR:HA	2.01	0.41
1:C:519:MET:HE2	1:C:519:MET:HB3	2.00	0.41
1:D:114:GLY:HA3	1:D:119:TYR:CE1	2.55	0.41
1:D:193:LEU:HG	1:D:195:SER:CB	2.50	0.41
1:D:203:LEU:HD12	1:D:203:LEU:HA	1.96	0.41
1:D:333:ARG:HD3	1:D:337:ASP:O	2.20	0.41
1:E:324:TYR:C	1:E:326:GLU:H	2.28	0.41
1:E:348:HIS:CD2	1:E:348:HIS:N	2.88	0.41
1:A:51:ALA:C	1:A:52:LEU:HD23	2.45	0.41
1:A:256:ASN:HD21	1:A:262:THR:HG23	1.84	0.41
1:A:360:TYR:HB3	1:A:363:VAL:HG13	2.02	0.41
1:B:99:GLU:OE1	1:B:99:GLU:CA	2.68	0.41
1:B:389:TRP:HE3	1:B:401:PRO:HG2	1.84	0.41
1:C:371:LEU:HD22	1:C:375:LEU:HG	2.01	0.41
1:D:10:VAL:HG22	1:D:11:ALA:N	2.35	0.41
1:D:77:SER:OG	5:D:618:NDP:O1X	2.32	0.41
1:D:360:TYR:C	1:D:363:VAL:HG12	2.43	0.41
1:D:466:TYR:HE2	2:D:615:UMP:HO3'	1.65	0.41
1:E:36:PHE:CD1	1:E:36:PHE:C	2.97	0.41
1:E:297:TRP:NE1	1:E:302:ASP:HB3	2.35	0.41
1:C:41:ASN:HD21	1:C:69:ASN:HB2	1.86	0.41
1:C:41:ASN:ND2	1:C:69:ASN:HB2	2.35	0.41
1:C:431:SER:HB3	1:C:432:PRO:HD3	2.02	0.41
1:D:139:GLU:O	1:D:140:ASP:HB2	2.19	0.41
1:E:499:PHE:O	1:E:500:LYS:HE3	2.20	0.41
1:A:93:ASN:HD21	1:A:96:ASP:H	1.68	0.41
1:B:4:LYS:HB2	1:B:101:LEU:HD22	1.98	0.41
1:B:128:VAL:HG22	1:B:154:PHE:HZ	1.85	0.41
1:B:402:CYS:SG	2:B:607:UMP:H2'	2.61	0.41
1:E:107:ILE:O	1:E:107:ILE:HG22	2.21	0.41
1:E:126:ASN:OD1	1:E:177:LYS:CE	2.69	0.41
1:A:267:GLY:O	1:B:271:ARG:NH2	2.49	0.41
1:A:319:ASN:OD1	3:A:604:CB3:H8	2.20	0.41
1:A:383:ARG:CD	1:B:400:PRO:HG2	2.50	0.41
1:D:3:GLU:CA	1:D:101:LEU:CD2	2.98	0.41
1:A:99:GLU:C	1:A:99:GLU:CD	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:NH2	6:A:687:HOH:O	2.54	0.41
1:A:383:ARG:HD3	1:B:400:PRO:HG2	2.02	0.41
1:E:166:LYS:O	1:E:167:ASN:HB2	2.20	0.41
1:E:324:TYR:C	1:E:326:GLU:N	2.78	0.41
1:E:425:CYS:SG	1:E:431:SER:HB2	2.61	0.41
1:B:208:GLY:C	1:B:210:ARG:N	2.77	0.41
1:B:288:ILE:HG23	1:B:501:TRP:HH2	1.85	0.41
1:B:294:GLU:OE2	3:B:608:CB3:HP11	2.20	0.41
1:B:389:TRP:CE3	1:B:401:PRO:HG2	2.55	0.41
1:C:247:VAL:HG22	1:C:465:ILE:HD12	2.03	0.41
4:C:613:DHF:C6	4:C:613:DHF:H15	2.50	0.41
1:E:315:ILE:HG13	1:E:316:TRP:H	1.85	0.41
1:E:342:TYR:CE1	1:E:403:HIS:CE1	3.08	0.41
1:A:465:ILE:CG2	1:A:473:LEU:HD23	2.51	0.41
1:B:178:GLN:C	1:B:179:GLU:CG	2.90	0.41
1:B:271:ARG:HD2	6:B:731:HOH:O	2.20	0.41
1:B:411:THR:HG22	1:B:413:ASP:CA	2.51	0.41
1:C:3:GLU:HA	1:C:3:GLU:OE2	2.20	0.41
1:C:8:ILE:CG2	1:C:9:VAL:N	2.83	0.41
1:C:133:LEU:HD22	1:C:133:LEU:C	2.46	0.41
1:C:491:ARG:NH2	1:C:493:VAL:HG12	2.35	0.41
1:D:102:MET:O	1:D:103:ASN:HB2	2.21	0.41
1:D:278:PHE:CE1	1:D:439:ALA:HB3	2.55	0.41
1:E:7:SER:CB	1:E:130:ARG:HB3	2.50	0.41
1:E:158:TYR:O	1:E:173:MET:HA	2.21	0.41
1:E:288:ILE:HD11	1:E:440:ILE:HD11	2.03	0.41
1:A:3:GLU:HB2	1:A:4:LYS:H	1.77	0.41
4:B:609:DHF:C6	4:B:609:DHF:H15	2.50	0.41
1:C:12:ALA:HB1	1:C:17:SER:C	2.45	0.41
1:C:322:LYS:HD3	1:C:335:GLU:OE1	2.21	0.41
1:E:220:LYS:O	1:E:223:ILE:HG12	2.21	0.41
1:E:488:LYS:CD	1:E:489:PHE:N	2.82	0.41
1:A:212:MET:HB3	1:B:236:TYR:OH	2.21	0.40
6:A:622:HOH:O	1:B:211:LYS:HG2	2.20	0.40
1:B:252:ALA:O	1:B:263:TYR:HA	2.21	0.40
1:D:363:VAL:CG2	6:D:625:HOH:O	2.69	0.40
1:A:150:ILE:HA	1:A:151:PRO:HD3	1.89	0.40
1:B:135:ARG:HB2	1:B:171:ASP:HB2	2.04	0.40
1:B:334:GLU:O	1:B:335:GLU:C	2.65	0.40
1:B:379:PRO:CB	1:B:410:VAL:HG21	2.51	0.40
1:D:248:LEU:HD12	1:D:248:LEU:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:PHE:HA	1:D:461:GLY:O	2.20	0.40
1:D:303:THR:HG21	1:D:344:PHE:HB2	2.04	0.40
1:E:439:ALA:O	1:E:443:MET:HG3	2.21	0.40
1:A:295:LEU:O	1:A:299:ILE:HG13	2.21	0.40
3:A:604:CB3:C14	3:A:604:CB3:H5	2.51	0.40
1:B:130:ARG:HH11	1:B:130:ARG:HG3	1.86	0.40
1:C:208:GLY:HA3	6:C:701:HOH:O	2.20	0.40
1:C:470:LEU:HD12	1:C:470:LEU:HA	1.91	0.40
1:D:79:LEU:HA	1:D:80:PRO:HD3	1.75	0.40
1:E:43:LYS:NZ	1:E:48:LYS:O	2.43	0.40
1:E:278:PHE:CZ	1:E:440:ILE:HG13	2.57	0.40
1:E:411:THR:OG1	1:E:415:CYS:HB2	2.20	0.40
1:A:274:MET:O	1:A:453:PRO:HB2	2.22	0.40
1:A:323:GLU:H	1:A:323:GLU:CD	2.29	0.40
1:B:98:ILE:HG22	1:B:99:GLU:OE1	2.22	0.40
1:B:104:ASP:C	1:B:106:SER:H	2.28	0.40
1:C:397:MET:SD	1:C:401:PRO:HD3	2.61	0.40
1:D:68:LYS:O	1:D:69:ASN:HB2	2.22	0.40
1:D:235:HIS:O	1:D:238:PHE:CD2	2.74	0.40
1:A:99:GLU:OE1	1:A:99:GLU:O	2.40	0.40
1:A:419:ASN:ND2	1:B:461:GLY:HA2	2.37	0.40
1:B:97:SER:C	1:B:99:GLU:H	2.29	0.40
1:B:102:MET:H	1:B:102:MET:HG2	1.49	0.40
1:C:388:ALA:O	1:C:401:PRO:HG3	2.22	0.40
1:D:315:ILE:HB	3:D:616:CB3:C15	2.51	0.40
1:D:436:ALA:O	1:D:440:ILE:HG13	2.22	0.40
1:E:104:ASP:O	1:E:105:ASP:C	2.64	0.40
1:E:500:LYS:N	1:E:503:ASP:OD1	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ARG:NH2	1:E:251:GLY:O[2_466]	2.11	0.09
1:E:407:GLN:OE1	1:E:421:TYR:OH[2_457]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	503/521 (96%)	476 (95%)	23 (5%)	4 (1%)	16	29
1	B	504/521 (97%)	477 (95%)	23 (5%)	4 (1%)	16	29
1	C	504/521 (97%)	473 (94%)	28 (6%)	3 (1%)	21	36
1	D	503/521 (96%)	469 (93%)	30 (6%)	4 (1%)	16	29
1	E	504/521 (97%)	460 (91%)	38 (8%)	6 (1%)	10	19
All	All	2518/2605 (97%)	2355 (94%)	142 (6%)	21 (1%)	16	29

All (21) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	457/471 (97%)	425 (93%)	32 (7%)	14	26
1	B	459/471 (98%)	417 (91%)	42 (9%)	8	16
1	C	457/471 (97%)	408 (89%)	49 (11%)	6	12
1	D	457/471 (97%)	407 (89%)	50 (11%)	6	11
1	E	457/471 (97%)	426 (93%)	31 (7%)	14	27
All	All	2287/2355 (97%)	2083 (91%)	204 (9%)	9	17

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	5	ASN
1	A	39	ILE
1	A	98	ILE
1	A	99	GLU
1	A	102	MET
1	A	103	ASN
1	A	104	ASP
1	A	128	VAL
1	A	133	LEU
1	A	178	GLN
1	A	193	LEU
1	A	194	LYS
1	A	202	LEU
1	A	203	LEU
1	A	244	LEU
1	A	247	VAL
1	A	248	LEU
1	A	264	SER
1	A	269	MET
1	A	285	LYS
1	A	295	LEU
1	A	311	LYS

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Mol	Chain	Res	Type
1	A	361	THR
1	A	363	VAL
1	A	371	LEU
1	A	373	GLU
1	A	404	VAL
1	A	427	LEU
1	A	429	LEU
1	A	473	LEU
1	A	479	ARG
1	B	8	ILE
1	B	52	LEU
1	B	64	ARG
1	B	95	GLU
1	B	98	ILE
1	B	99	GLU
1	B	102	MET
1	B	123	LEU
1	B	124	LYS
1	B	128	VAL
1	B	133	LEU
1	B	176	GLU
1	B	179	GLU
1	B	180	LYS
1	B	193	LEU
1	B	194	LYS
1	B	202	LEU
1	B	203	LEU
1	B	209	ILE
1	B	220	LYS
1	B	221	GLU
1	B	222	GLU
1	B	233	ARG
1	B	244	LEU
1	B	247	VAL
1	B	295	LEU
1	B	308	LEU
1	B	354	LYS
1	B	363	VAL
1	B	371	LEU
1	B	383	ARG
1	B	385	ILE
1	B	404	VAL

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Mol	Chain	Res	Type
1	B	411	THR
1	B	414	ASN
1	B	420	LEU
1	B	427	LEU
1	B	429	LEU
1	B	479	ARG
1	B	506	LEU
1	B	514	THR
1	B	516	LYS
1	C	6	VAL
1	C	39	ILE
1	C	40	THR
1	C	56	ARG
1	C	62	ILE
1	C	79	LEU
1	C	81	GLN
1	C	96	ASP
1	C	98	ILE
1	C	99	GLU
1	C	101	LEU
1	C	123	LEU
1	C	126	ASN
1	C	133	LEU
1	C	139	GLU
1	C	140	ASP
1	C	141	ILE
1	C	149	GLU
1	C	165	THR
1	C	176	GLU
1	C	178	GLN
1	C	202	LEU
1	C	203	LEU
1	C	222	GLU
1	C	233	ARG
1	C	244	LEU
1	C	247	VAL
1	C	248	LEU
1	C	254	ARG
1	C	264	SER
1	C	295	LEU
1	C	296	ILE
1	C	308	LEU

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Mol	Chain	Res	Type
1	C	322	LYS
1	C	325	LEU
1	C	363	VAL
1	C	371	LEU
1	C	383	ARG
1	C	404	VAL
1	C	405	LEU
1	C	414	ASN
1	C	427	LEU
1	C	429	LEU
1	C	470	LEU
1	C	474	LYS
1	C	479	ARG
1	C	497	GLU
1	C	506	LEU
1	C	516	LYS
1	D	34	LYS
1	D	62	ILE
1	D	64	ARG
1	D	65	ARG
1	D	68	LYS
1	D	79	LEU
1	D	81	GLN
1	D	83	GLU
1	D	97	SER
1	D	98	ILE
1	D	99	GLU
1	D	101	LEU
1	D	102	MET
1	D	123	LEU
1	D	126	ASN
1	D	128	VAL
1	D	133	LEU
1	D	138	LEU
1	D	149	GLU
1	D	176	GLU
1	D	202	LEU
1	D	203	LEU
1	D	220	LYS
1	D	228	SER
1	D	233	ARG
1	D	248	LEU

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Mol	Chain	Res	Type
1	D	255	GLU
1	D	260	ILE
1	D	262	THR
1	D	269	MET
1	D	293	GLU
1	D	295	LEU
1	D	296	ILE
1	D	308	LEU
1	D	310	GLU
1	D	370	LYS
1	D	371	LEU
1	D	383	ARG
1	D	404	VAL
1	D	405	LEU
1	D	414	ASN
1	D	427	LEU
1	D	429	LEU
1	D	437	SER
1	D	447	GLN
1	D	470	LEU
1	D	479	ARG
1	D	487	LEU
1	D	506	LEU
1	D	514	THR
1	E	3	GLU
1	E	47	ASN
1	E	52	LEU
1	E	79	LEU
1	E	99	GLU
1	E	100	ASN
1	E	104	ASP
1	E	105	ASP
1	E	128	VAL
1	E	133	LEU
1	E	178	GLN
1	E	194	LYS
1	E	196	ILE
1	E	202	LEU
1	E	233	ARG
1	E	264	SER
1	E	295	LEU
1	E	333	ARG

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Mol	Chain	Res	Type
1	E	348	HIS
1	E	356	MET
1	E	363	VAL
1	E	383	ARG
1	E	394	LEU
1	E	422	GLN
1	E	429	LEU
1	E	468	ASN
1	E	470	LEU
1	E	479	ARG
1	E	488	LYS
1	E	506	LEU
1	E	516	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	47	ASN
1	A	69	ASN
1	A	81	GLN
1	A	345	GLN
1	A	377	ASN
1	A	384	HIS
1	B	5	ASN
1	B	69	ASN
1	B	81	GLN
1	B	100	ASN
1	B	396	GLN
1	B	476	GLN
1	C	87	ASN
1	C	345	GLN
1	C	396	GLN
1	C	495	ASN
1	D	5	ASN
1	D	69	ASN
1	D	345	GLN
1	D	384	HIS
1	D	396	GLN
1	E	87	ASN
1	E	109	ASN
1	E	178	GLN

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Mol	Chain	Res	Type
1	E	216	HIS
1	E	348	HIS
1	E	378	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CB3	A	604	-	37,37,37	1.89	5 (13%)	50,51,51	1.24	4 (8%)
5	NDP	E	622	-	51,52,52	1.40	5 (9%)	71,80,80	1.64	9 (12%)
2	UMP	E	619	-	21,21,21	2.35	3 (14%)	30,31,31	2.42	9 (30%)
3	CB3	C	612	-	37,37,37	1.92	6 (16%)	50,51,51	1.49	6 (12%)
2	UMP	D	615	-	21,21,21	2.35	3 (14%)	30,31,31	2.40	9 (30%)
2	UMP	C	611	-	21,21,21	2.33	3 (14%)	30,31,31	2.41	9 (30%)
2	UMP	B	607	-	21,21,21	2.34	3 (14%)	30,31,31	2.38	8 (26%)
4	DHF	E	621	-	32,34,34	1.13	3 (9%)	38,47,47	1.23	4 (10%)
4	DHF	B	609	-	32,34,34	1.29	4 (12%)	38,47,47	1.16	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NDP	B	610	-	51,52,52	1.39	6 (11%)	71,80,80	1.54	13 (18%)
3	CB3	B	608	-	37,37,37	1.93	5 (13%)	50,51,51	1.18	5 (10%)
2	UMP	A	603	-	21,21,21	2.33	3 (14%)	30,31,31	2.41	9 (30%)
5	NDP	A	606	-	51,52,52	1.43	7 (13%)	71,80,80	1.47	10 (14%)
3	CB3	D	616	-	37,37,37	1.88	4 (10%)	50,51,51	1.14	5 (10%)
5	NDP	C	614	-	51,52,52	1.38	5 (9%)	71,80,80	1.54	9 (12%)
4	DHF	A	605	-	32,34,34	1.25	3 (9%)	38,47,47	1.29	6 (15%)
3	CB3	E	620	-	37,37,37	1.88	4 (10%)	50,51,51	1.22	5 (10%)
4	DHF	D	617	-	32,34,34	1.23	3 (9%)	38,47,47	1.29	4 (10%)
4	DHF	C	613	-	32,34,34	1.21	3 (9%)	38,47,47	1.36	4 (10%)
5	NDP	D	618	-	51,52,52	1.41	5 (9%)	71,80,80	1.54	10 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CB3	A	604	-	-	4/27/28/28	0/3/3/3
5	NDP	E	622	-	-	5/34/77/77	0/5/5/5
2	UMP	E	619	-	-	3/10/22/22	0/2/2/2
3	CB3	C	612	-	-	4/27/28/28	0/3/3/3
2	UMP	D	615	-	-	3/10/22/22	0/2/2/2
2	UMP	C	611	-	-	2/10/22/22	0/2/2/2
2	UMP	B	607	-	-	3/10/22/22	0/2/2/2
4	DHF	E	621	-	-	2/20/31/31	0/3/3/3
4	DHF	B	609	-	1/1/5/8	5/20/31/31	0/3/3/3
5	NDP	B	610	-	-	4/34/77/77	0/5/5/5
3	CB3	B	608	-	-	6/27/28/28	0/3/3/3
2	UMP	A	603	-	-	1/10/22/22	0/2/2/2
5	NDP	A	606	-	-	3/34/77/77	0/5/5/5
3	CB3	D	616	-	1/1/5/6	5/27/28/28	0/3/3/3
5	NDP	C	614	-	-	4/34/77/77	0/5/5/5
4	DHF	A	605	-	1/1/5/8	5/20/31/31	0/3/3/3
3	CB3	E	620	-	1/1/5/6	6/27/28/28	0/3/3/3
4	DHF	D	617	-	-	1/20/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DHF	C	613	-	-	3/20/31/31	0/3/3/3
5	NDP	D	618	-	-	2/34/77/77	0/5/5/5

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	619	UMP	C6-C5	7.93	1.53	1.35
2	B	607	UMP	C6-C5	7.92	1.53	1.35
2	D	615	UMP	C6-C5	7.91	1.53	1.35
2	A	603	UMP	C6-C5	7.87	1.53	1.35
2	C	611	UMP	C6-C5	7.87	1.53	1.35
3	E	620	CB3	O4-C4	7.42	1.36	1.23
3	B	608	CB3	O4-C4	7.32	1.35	1.23
3	D	616	CB3	O4-C4	7.21	1.35	1.23
3	A	604	CB3	O4-C4	7.18	1.35	1.23
3	C	612	CB3	O4-C4	7.15	1.35	1.23
5	E	622	NDP	C4N-C3N	-6.27	1.38	1.50
5	C	614	NDP	C4N-C3N	-6.26	1.38	1.50
5	D	618	NDP	C4N-C3N	-6.17	1.38	1.50
3	D	616	CB3	C4A-C4	-5.97	1.38	1.48
3	C	612	CB3	C4A-C4	-5.88	1.38	1.48
3	B	608	CB3	C4A-C4	-5.82	1.38	1.48
3	A	604	CB3	C4A-C4	-5.78	1.38	1.48
3	E	620	CB3	C4A-C4	-5.60	1.38	1.48
5	A	606	NDP	C4N-C3N	-5.57	1.39	1.50
5	B	610	NDP	C4N-C3N	-5.56	1.39	1.50
2	D	615	UMP	C5-C4	4.52	1.53	1.43
2	E	619	UMP	C5-C4	4.51	1.53	1.43
2	C	611	UMP	C5-C4	4.46	1.53	1.43
2	B	607	UMP	C5-C4	4.44	1.53	1.43
2	E	619	UMP	C6-N1	4.41	1.48	1.38
2	A	603	UMP	C5-C4	4.41	1.53	1.43
2	B	607	UMP	C6-N1	4.40	1.48	1.38
2	C	611	UMP	C6-N1	4.38	1.48	1.38
2	D	615	UMP	C6-N1	4.37	1.48	1.38
2	A	603	UMP	C6-N1	4.34	1.48	1.38
5	E	622	NDP	C4N-C5N	-4.18	1.38	1.49
5	D	618	NDP	C4N-C5N	-4.16	1.38	1.49
5	C	614	NDP	C4N-C5N	-4.10	1.38	1.49
5	B	610	NDP	C4N-C5N	-3.77	1.39	1.49
5	A	606	NDP	C4N-C5N	-3.66	1.39	1.49
3	E	620	CB3	CP2-CP3	3.38	1.28	1.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	609	DHF	C4A-C8A	-3.33	1.38	1.43
3	A	604	CB3	CP2-CP3	3.26	1.27	1.18
3	D	616	CB3	CP2-CP3	3.25	1.27	1.18
3	B	608	CB3	C8A-N1	-3.24	1.34	1.39
3	E	620	CB3	C8A-N1	-3.23	1.34	1.39
3	A	604	CB3	C8A-N1	-3.22	1.34	1.39
3	C	612	CB3	C8A-N1	-3.19	1.34	1.39
5	A	606	NDP	C5A-N7A	-3.18	1.33	1.39
4	D	617	DHF	C4A-C8A	-3.13	1.38	1.43
3	B	608	CB3	CP2-CP3	3.11	1.27	1.18
4	A	605	DHF	C4A-C8A	-3.08	1.38	1.43
4	C	613	DHF	C4A-C8A	-3.07	1.38	1.43
3	C	612	CB3	CP2-CP3	3.03	1.27	1.18
4	B	609	DHF	C4-C4A	-2.96	1.37	1.45
4	E	621	DHF	C4A-C8A	-2.94	1.38	1.43
4	A	605	DHF	C4-C4A	-2.92	1.37	1.45
3	D	616	CB3	C8A-N1	-2.84	1.35	1.39
4	D	617	DHF	C4-C4A	-2.65	1.37	1.45
4	C	613	DHF	C4-C4A	-2.64	1.37	1.45
5	D	618	NDP	C5A-N7A	-2.62	1.34	1.39
5	B	610	NDP	C5A-N7A	-2.58	1.34	1.39
5	E	622	NDP	C5A-N7A	-2.40	1.34	1.39
4	E	621	DHF	C4-C4A	-2.40	1.38	1.45
4	B	609	DHF	C4-N3	-2.38	1.33	1.38
5	C	614	NDP	C5A-N7A	-2.38	1.34	1.39
5	D	618	NDP	C8A-N9A	-2.35	1.33	1.37
4	A	605	DHF	C4-N3	-2.35	1.34	1.38
5	A	606	NDP	C8A-N9A	-2.29	1.33	1.37
5	D	618	NDP	C4A-N9A	-2.24	1.33	1.37
5	C	614	NDP	C8A-N9A	-2.22	1.33	1.37
5	E	622	NDP	C8A-N9A	-2.22	1.33	1.37
3	A	604	CB3	C4-N3	-2.20	1.34	1.38
5	A	606	NDP	C7N-C3N	2.18	1.53	1.48
3	C	612	CB3	C4-N3	-2.14	1.34	1.38
5	E	622	NDP	C4A-N9A	-2.13	1.33	1.37
3	B	608	CB3	C4-N3	-2.12	1.34	1.38
5	B	610	NDP	C6N-C5N	2.09	1.39	1.33
5	C	614	NDP	C4A-N9A	-2.08	1.33	1.37
5	A	606	NDP	C6N-C5N	2.08	1.39	1.33
5	A	606	NDP	C4A-N9A	-2.07	1.33	1.37
4	D	617	DHF	C4-N3	-2.06	1.34	1.38
4	B	609	DHF	C8A-N1	-2.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	621	DHF	C4-N3	-2.02	1.34	1.38
4	C	613	DHF	O2-CT	-2.02	1.24	1.30
3	C	612	CB3	C4A-C8A	-2.01	1.37	1.41
5	B	610	NDP	PA-O3	2.01	1.61	1.59
5	B	610	NDP	C7N-C3N	2.01	1.53	1.48

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	611	UMP	C6-C5-C4	-6.62	111.08	119.53
2	B	607	UMP	C6-C5-C4	-6.56	111.16	119.53
2	A	603	UMP	C5-C6-N1	-6.35	111.52	121.84
2	D	615	UMP	C6-C5-C4	-6.26	111.53	119.53
2	A	603	UMP	C6-C5-C4	-6.25	111.55	119.53
2	E	619	UMP	C6-C5-C4	-6.24	111.56	119.53
2	E	619	UMP	C5-C6-N1	-6.20	111.76	121.84
2	D	615	UMP	C5-C6-N1	-6.14	111.86	121.84
3	C	612	CB3	CB-CA-N	-6.10	98.83	110.91
2	C	611	UMP	C5-C6-N1	-6.08	111.95	121.84
2	B	607	UMP	C5-C6-N1	-5.97	112.14	121.84
5	E	622	NDP	C2B-C1B-N9A	-5.47	104.74	113.75
5	D	618	NDP	C5A-C4A-N3A	-5.37	119.32	126.72
5	E	622	NDP	C5A-C4A-N3A	-5.37	119.32	126.72
5	C	614	NDP	C5A-C4A-N3A	-5.34	119.36	126.72
3	A	604	CB3	CP2-CP1-N10	-5.08	108.77	113.45
2	E	619	UMP	C4-N3-C2	-4.87	120.57	126.61
5	A	606	NDP	C5A-C4A-N3A	-4.84	120.05	126.72
4	D	617	DHF	CB-CA-N	-4.82	101.37	110.91
2	D	615	UMP	C4-N3-C2	-4.79	120.67	126.61
5	E	622	NDP	N3A-C2A-N1A	-4.77	121.36	128.58
5	A	606	NDP	N3A-C2A-N1A	-4.76	121.37	128.58
2	C	611	UMP	C4-N3-C2	-4.76	120.70	126.61
2	A	603	UMP	C4-N3-C2	-4.75	120.71	126.61
5	C	614	NDP	C2B-C1B-N9A	-4.66	106.08	113.75
5	D	618	NDP	N3A-C2A-N1A	-4.62	121.59	128.58
5	C	614	NDP	N3A-C2A-N1A	-4.60	121.61	128.58
2	B	607	UMP	C4-N3-C2	-4.60	120.91	126.61
4	C	613	DHF	CB-CA-N	-4.57	101.86	110.91
5	B	610	NDP	N3A-C2A-N1A	-4.47	121.82	128.58
2	E	619	UMP	N3-C2-N1	4.28	120.47	114.89
5	B	610	NDP	C5A-C4A-N3A	-4.25	120.87	126.72
2	D	615	UMP	N3-C2-N1	4.20	120.36	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	UMP	N3-C2-N1	4.19	120.35	114.89
5	D	618	NDP	C2B-C1B-N9A	-4.17	106.88	113.75
3	C	612	CB3	CP2-CP1-N10	-4.12	109.65	113.45
3	E	620	CB3	C6-C9-N10	-4.01	107.63	114.13
2	C	611	UMP	N3-C2-N1	3.97	120.06	114.89
2	B	607	UMP	N3-C2-N1	3.93	120.01	114.89
2	B	607	UMP	C5-C4-N3	3.83	120.17	114.80
2	D	615	UMP	C5-C4-N3	3.81	120.13	114.80
2	C	611	UMP	C5-C4-N3	3.80	120.12	114.80
3	B	608	CB3	CP2-CP1-N10	-3.77	109.97	113.45
2	E	619	UMP	C5-C4-N3	3.70	119.98	114.80
5	A	606	NDP	C2B-C1B-N9A	-3.69	107.67	113.75
2	A	603	UMP	C5-C4-N3	3.67	119.94	114.80
3	E	620	CB3	CP2-CP1-N10	-3.66	110.08	113.45
5	B	610	NDP	C4A-C5A-N7A	-3.62	106.44	110.58
5	D	618	NDP	N3A-C4A-N9A	3.53	133.18	127.17
5	A	606	NDP	C2A-N3A-C4A	3.50	120.39	111.83
5	B	610	NDP	N9A-C8A-N7A	-3.50	108.97	113.94
5	E	622	NDP	C2A-N3A-C4A	3.49	120.35	111.83
5	E	622	NDP	N3A-C4A-N9A	3.48	133.09	127.17
5	D	618	NDP	C2A-N3A-C4A	3.44	120.23	111.83
5	C	614	NDP	C2A-N3A-C4A	3.43	120.20	111.83
5	E	622	NDP	N9A-C8A-N7A	-3.43	109.07	113.94
5	B	610	NDP	C5A-N7A-C8A	3.41	108.81	103.45
4	A	605	DHF	CT-CA-N	3.38	118.41	110.57
5	C	614	NDP	N9A-C8A-N7A	-3.38	109.14	113.94
5	D	618	NDP	N9A-C8A-N7A	-3.34	109.19	113.94
5	C	614	NDP	N3A-C4A-N9A	3.34	132.85	127.17
5	A	606	NDP	N3A-C4A-N9A	3.30	132.79	127.17
5	B	610	NDP	C2A-N3A-C4A	3.26	119.80	111.83
2	B	607	UMP	O4-C4-C5	-3.19	119.67	125.16
4	A	605	DHF	CA-N-C	3.13	129.06	121.56
5	A	606	NDP	N9A-C8A-N7A	-3.11	109.53	113.94
2	A	603	UMP	O4-C4-C5	-3.10	119.81	125.16
2	C	611	UMP	O4-C4-C5	-3.06	119.88	125.16
2	D	615	UMP	O4-C4-C5	-3.06	119.89	125.16
2	B	607	UMP	O5'-P-OP1	3.04	114.66	106.44
2	E	619	UMP	O4-C4-C5	-3.04	119.92	125.16
5	B	610	NDP	C2B-C1B-N9A	-2.97	108.86	113.75
4	B	609	DHF	CT-CA-N	2.96	117.45	110.57
2	C	611	UMP	O5'-P-OP1	2.85	114.15	106.44
3	D	616	CB3	CT-CA-N	2.85	117.18	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606	NDP	C5A-N7A-C8A	2.83	107.90	103.45
4	E	621	DHF	CB-CA-N	-2.83	105.31	110.91
5	B	610	NDP	O4B-C1B-N9A	2.81	113.48	108.09
2	A	603	UMP	O5'-P-OP1	2.80	114.00	106.44
5	A	606	NDP	C4A-C5A-N7A	-2.79	107.39	110.58
5	C	614	NDP	C4A-C5A-N7A	-2.79	107.39	110.58
3	B	608	CB3	C13-C14-N10	-2.74	117.58	121.39
2	D	615	UMP	O5'-P-OP1	2.72	113.79	106.44
2	E	619	UMP	O2-C2-N1	-2.70	119.28	122.80
3	B	608	CB3	CB-CA-N	-2.69	105.58	110.91
4	C	613	DHF	C4A-C8A-N8	2.67	121.38	115.89
4	B	609	DHF	CA-N-C	2.65	127.91	121.56
4	D	617	DHF	C4A-C8A-N8	2.63	121.28	115.89
4	E	621	DHF	C4A-N5-C6	2.62	121.44	116.24
2	E	619	UMP	O5'-P-OP1	2.60	113.47	106.44
5	B	610	NDP	N3A-C4A-N9A	2.60	131.59	127.17
2	A	603	UMP	O2-C2-N1	-2.60	119.42	122.80
5	E	622	NDP	C4A-N9A-C8A	2.54	108.40	105.74
5	C	614	NDP	C5A-N7A-C8A	2.53	107.43	103.45
5	D	618	NDP	C4A-C5A-N7A	-2.52	107.70	110.58
4	E	621	DHF	C4A-C8A-N8	2.51	121.06	115.89
2	D	615	UMP	O2-C2-N1	-2.51	119.53	122.80
3	C	612	CB3	CB-CG-CD	-2.50	105.81	112.49
2	B	607	UMP	O2-C2-N1	-2.50	119.54	122.80
5	D	618	NDP	C4A-N9A-C8A	2.49	108.36	105.74
5	E	622	NDP	C4A-C5A-N7A	-2.49	107.74	110.58
4	A	605	DHF	C4A-C8A-N8	2.46	120.94	115.89
4	A	605	DHF	CG-CB-CA	-2.46	108.63	113.16
2	C	611	UMP	O2-C2-N1	-2.43	119.64	122.80
3	E	620	CB3	C13-C14-N10	-2.42	118.03	121.39
5	D	618	NDP	C5A-N7A-C8A	2.42	107.25	103.45
3	A	604	CB3	C13-C14-N10	-2.41	118.04	121.39
3	D	616	CB3	CP1-N10-C9	2.41	119.62	117.19
5	C	614	NDP	C4A-N9A-C8A	2.40	108.25	105.74
5	E	622	NDP	C5A-N7A-C8A	2.39	107.20	103.45
5	B	610	NDP	C4A-N9A-C8A	2.38	108.24	105.74
3	A	604	CB3	CB-CA-N	-2.37	106.22	110.91
4	B	609	DHF	C4A-C8A-N8	2.34	120.69	115.89
3	D	616	CB3	CB-CA-N	-2.33	106.30	110.91
5	B	610	NDP	C6A-C5A-N7A	2.31	136.54	132.09
3	A	604	CB3	C6-C9-N10	-2.30	110.40	114.13
4	C	613	DHF	C4A-N5-C6	2.29	120.79	116.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	613	DHF	C11-C-N	2.29	121.29	117.04
4	B	609	DHF	C4A-N5-C6	2.28	120.77	116.24
4	A	605	DHF	C4A-N5-C6	2.27	120.75	116.24
3	B	608	CB3	C9-N10-C14	2.26	124.64	120.72
4	D	617	DHF	C4A-N5-C6	2.23	120.66	116.24
4	E	621	DHF	CB-CG-CD	-2.22	106.58	112.49
3	B	608	CB3	C6-C9-N10	-2.19	110.57	114.13
5	A	606	NDP	C4A-N9A-C8A	2.17	108.02	105.74
3	E	620	CB3	CB-CA-N	-2.17	106.62	110.91
3	E	620	CB3	CP1-N10-C9	2.16	119.37	117.19
4	D	617	DHF	C4A-C8A-N1	2.16	120.32	115.89
3	C	612	CB3	C13-C14-N10	-2.15	118.41	121.39
3	D	616	CB3	C6-C9-N10	-2.14	110.65	114.13
2	C	611	UMP	C2'-C3'-C4'	-2.12	98.51	102.80
2	A	603	UMP	C3'-C2'-C1'	-2.09	97.47	102.60
4	A	605	DHF	CB-CA-CT	2.09	115.31	110.35
5	D	618	NDP	O3X-P2B-O2X	2.08	115.61	107.80
3	D	616	CB3	CP2-CP1-N10	-2.08	111.53	113.45
2	E	619	UMP	C3'-C2'-C1'	-2.07	97.53	102.60
5	A	606	NDP	C3N-C2N-N1N	-2.07	120.17	123.20
3	C	612	CB3	C6-C9-N10	-2.07	110.78	114.13
5	B	610	NDP	C4A-N9A-C1B	-2.06	121.81	126.63
2	D	615	UMP	C3'-C2'-C1'	-2.05	97.59	102.60
3	C	612	CB3	CB-CA-CT	-2.02	105.57	110.35
5	B	610	NDP	P2B-O2B-C2B	-2.01	118.08	123.43

All (4) chirality outliers are listed below:

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

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	607	UMP	C5'-O5'-P-OP2
2	B	607	UMP	C5'-O5'-P-OP3
2	D	615	UMP	C5'-O5'-P-OP1
2	D	615	UMP	C5'-O5'-P-OP2
2	D	615	UMP	C5'-O5'-P-OP3

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Mol	Chain	Res	Type	Atoms
2	E	619	UMP	C5'-O5'-P-OP1
2	E	619	UMP	C5'-O5'-P-OP2
2	E	619	UMP	C5'-O5'-P-OP3
3	E	620	CB3	CB-CA-N-C
3	E	620	CB3	N-CA-CB-CG
4	A	605	DHF	CB-CA-N-C
4	B	609	DHF	CB-CA-N-C
5	E	622	NDP	C5B-O5B-PA-O1A
5	E	622	NDP	C5B-O5B-PA-O3
5	E	622	NDP	PA-O3-PN-O5D
3	D	616	CB3	CB-CA-N-C
3	A	604	CB3	N-CA-CB-CG
3	C	612	CB3	N-CA-CB-CG
3	E	620	CB3	CA-CB-CG-CD
3	C	612	CB3	CT-CA-CB-CG
3	A	604	CB3	CT-CA-CB-CG
3	E	620	CB3	CT-CA-CB-CG
4	A	605	DHF	CT-CA-CB-CG
4	C	613	DHF	CB-CA-N-C
4	A	605	DHF	CA-CB-CG-CD
4	B	609	DHF	CA-CB-CG-CD
3	B	608	CB3	N-CA-CB-CG
5	C	614	NDP	C3B-C4B-C5B-O5B
3	B	608	CB3	C6-C9-N10-C14
5	E	622	NDP	O4D-C1D-N1N-C2N
3	B	608	CB3	CT-CA-CB-CG
4	E	621	DHF	CT-CA-CB-CG
5	D	618	NDP	O4D-C1D-N1N-C2N
5	C	614	NDP	C5D-O5D-PN-O1N
5	E	622	NDP	C5B-O5B-PA-O2A
4	B	609	DHF	CB-CA-CT-O1
2	C	611	UMP	C3'-C4'-C5'-O5'
4	B	609	DHF	CB-CA-CT-O2
5	C	614	NDP	C2B-O2B-P2B-O3X
5	D	618	NDP	C2B-O2B-P2B-O3X
5	A	606	NDP	O4D-C1D-N1N-C2N
5	B	610	NDP	O4D-C1D-N1N-C2N
5	C	614	NDP	O4D-C1D-N1N-C2N
4	E	621	DHF	N-CA-CB-CG
2	C	611	UMP	O4'-C4'-C5'-O5'
3	D	616	CB3	OE1-CD-CG-CB
5	A	606	NDP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
4	A	605	DHF	CB-CA-CT-O1
3	D	616	CB3	OE2-CD-CG-CB
3	E	620	CB3	CB-CA-CT-O1
3	B	608	CB3	C6-C9-N10-CP1
3	E	620	CB3	CB-CA-CT-O2
5	B	610	NDP	C2D-C1D-N1N-C2N
4	B	609	DHF	CT-CA-CB-CG
2	B	607	UMP	O4'-C4'-C5'-O5'
3	D	616	CB3	CB-CA-CT-O2
4	A	605	DHF	CB-CA-CT-O2
3	C	612	CB3	C6-C9-N10-C14
3	C	612	CB3	C6-C9-N10-CP1
4	C	613	DHF	OE1-CD-CG-CB
5	B	610	NDP	C2B-O2B-P2B-O3X
3	D	616	CB3	CB-CA-CT-O1
4	C	613	DHF	OE2-CD-CG-CB
3	A	604	CB3	C6-C9-N10-C14
5	B	610	NDP	C2B-O2B-P2B-O1X
3	A	604	CB3	C6-C9-N10-CP1
3	B	608	CB3	OE2-CD-CG-CB
5	A	606	NDP	C2D-C1D-N1N-C2N
4	D	617	DHF	OE1-CD-CG-CB
3	B	608	CB3	OE1-CD-CG-CB
2	A	603	UMP	O4'-C4'-C5'-O5'

There are no ring outliers.

20 monomers are involved in 117 short contacts:

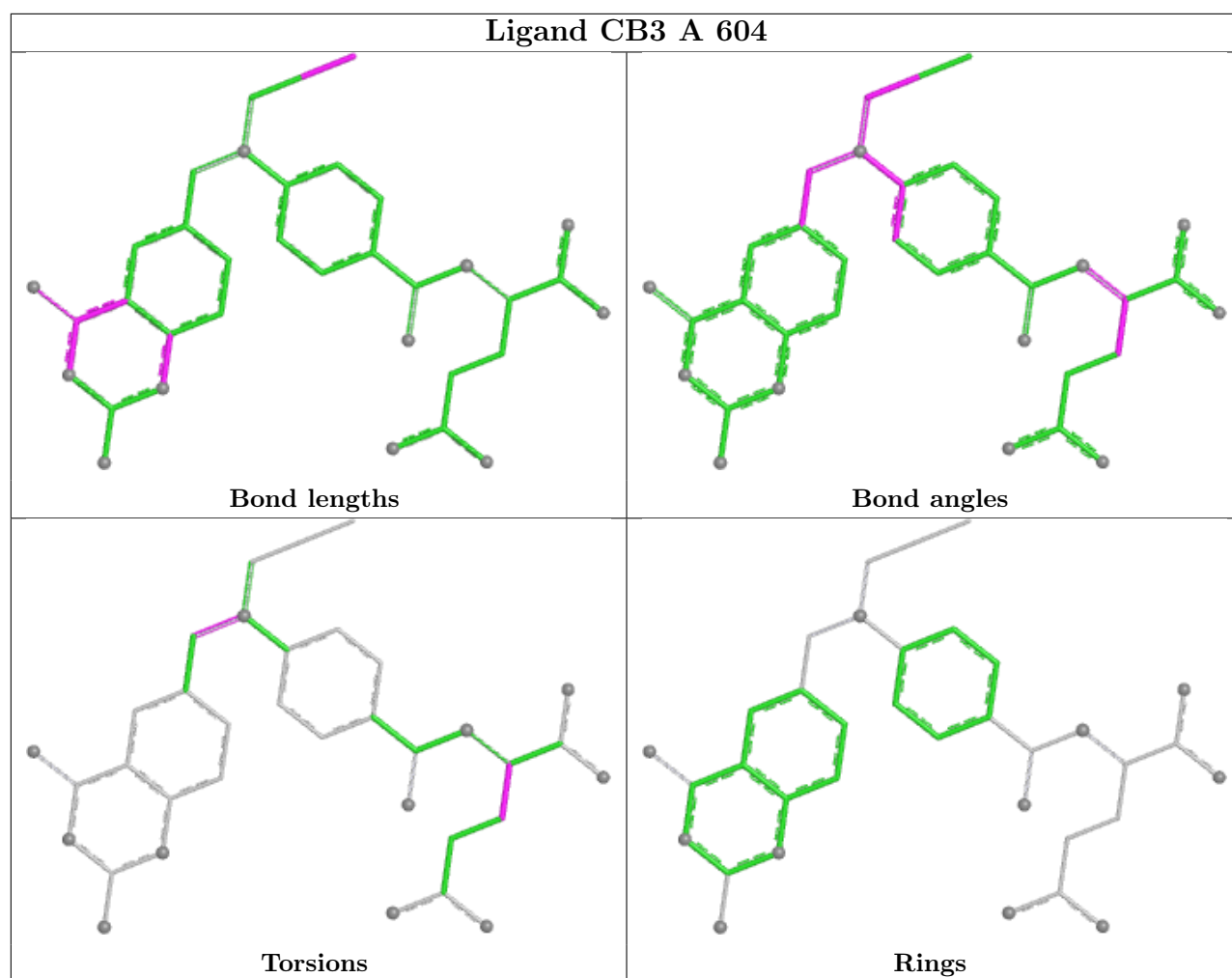
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	CB3	4	0
5	E	622	NDP	12	0
2	E	619	UMP	6	0
3	C	612	CB3	2	0
2	D	615	UMP	5	0
2	C	611	UMP	3	0
2	B	607	UMP	3	0
4	E	621	DHF	5	0
4	B	609	DHF	10	0
5	B	610	NDP	8	0
3	B	608	CB3	3	0
2	A	603	UMP	4	0
5	A	606	NDP	7	0

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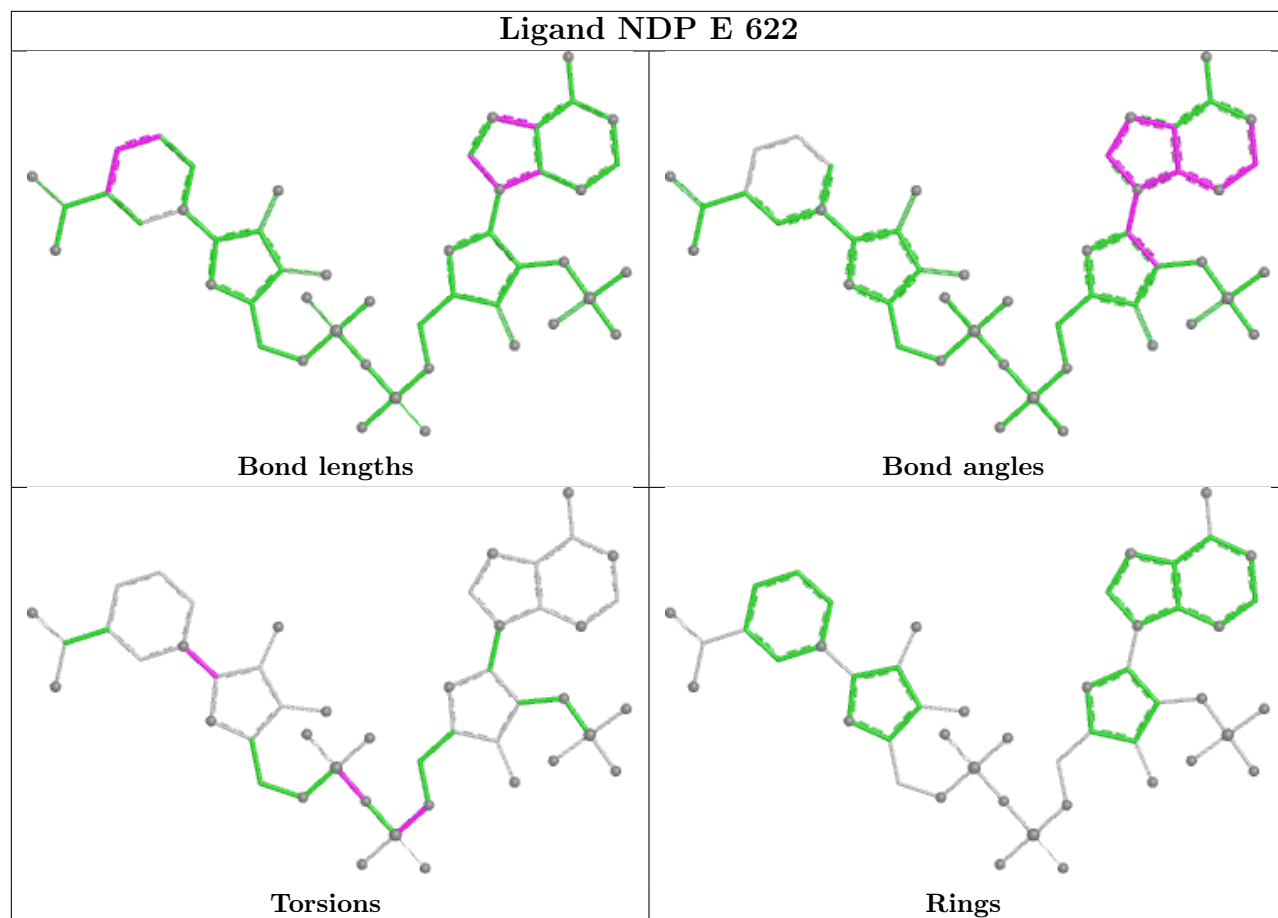
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	616	CB3	9	0
5	C	614	NDP	11	0
4	A	605	DHF	6	0
3	E	620	CB3	13	0
4	D	617	DHF	9	0
4	C	613	DHF	9	0
5	D	618	NDP	6	0

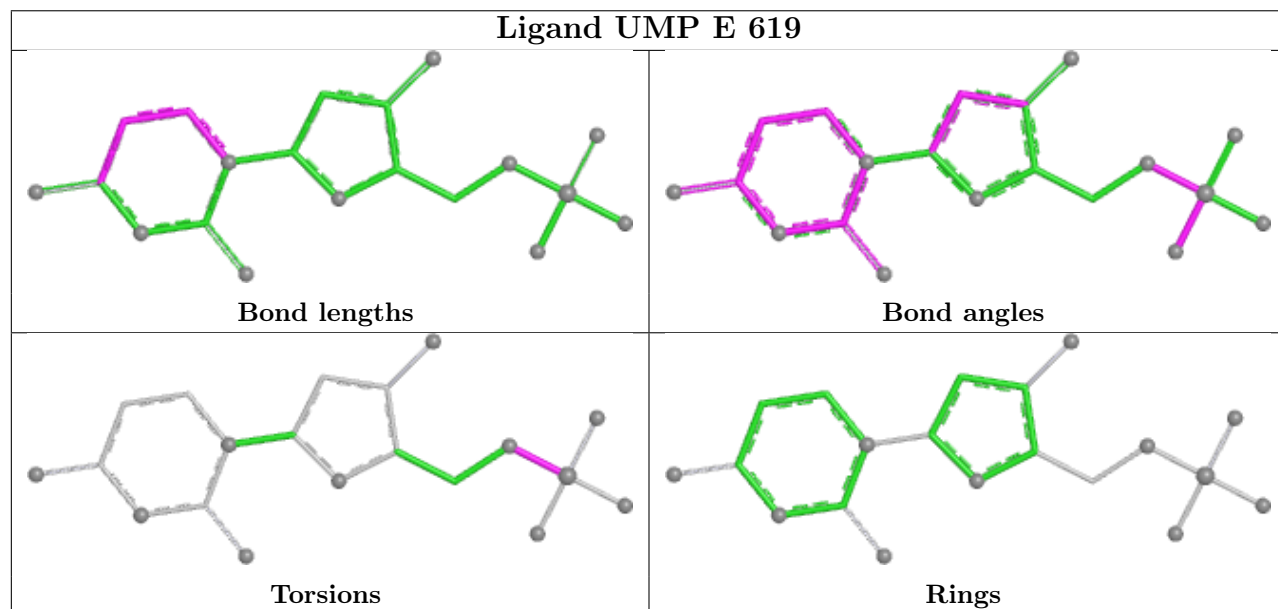
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



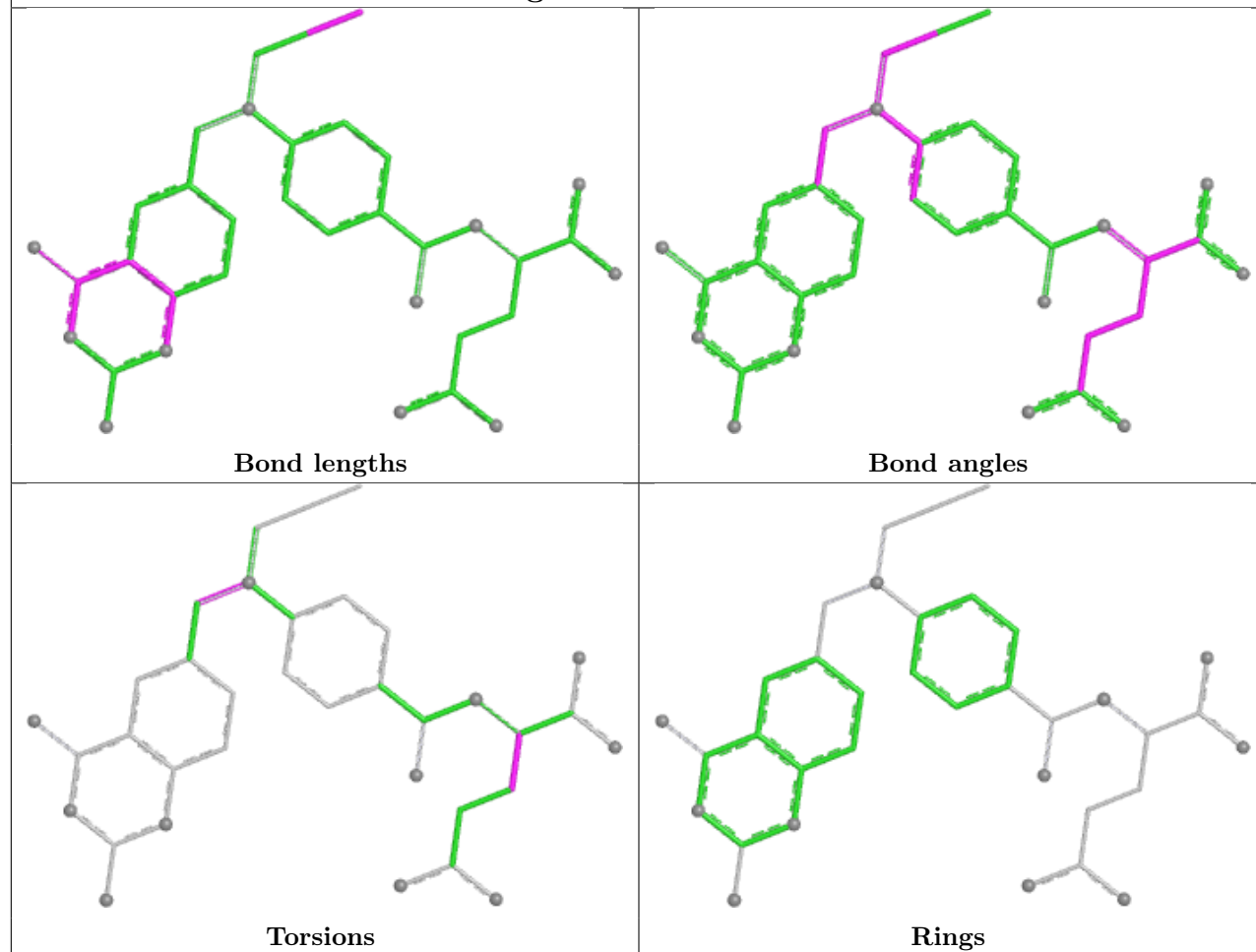
Ligand NDP E 622



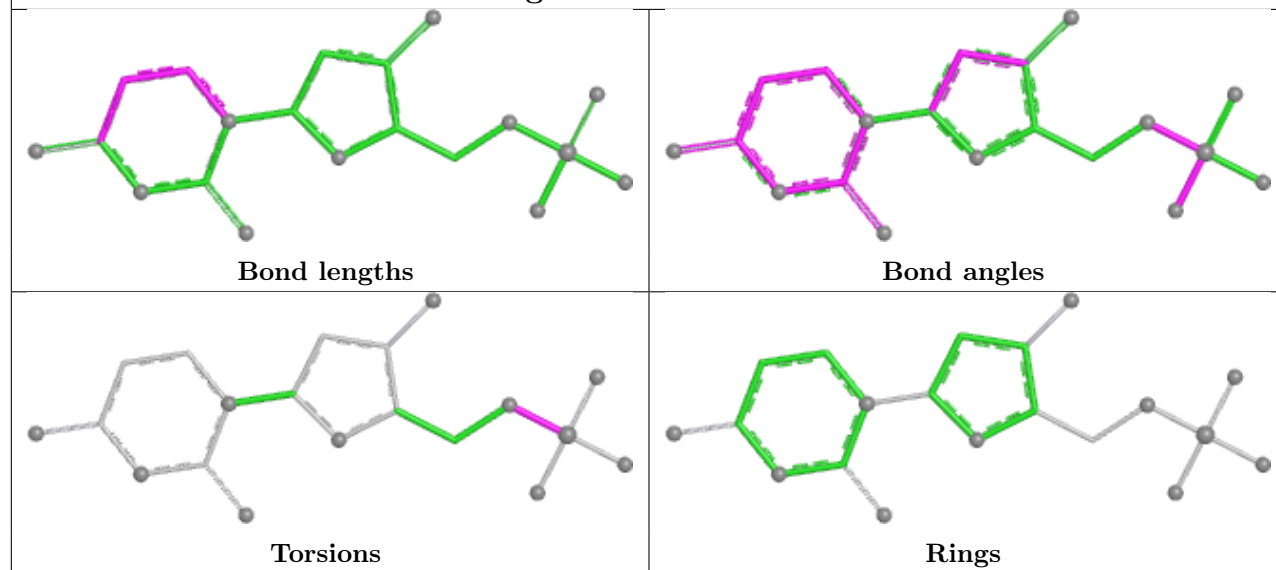
Ligand UMP E 619

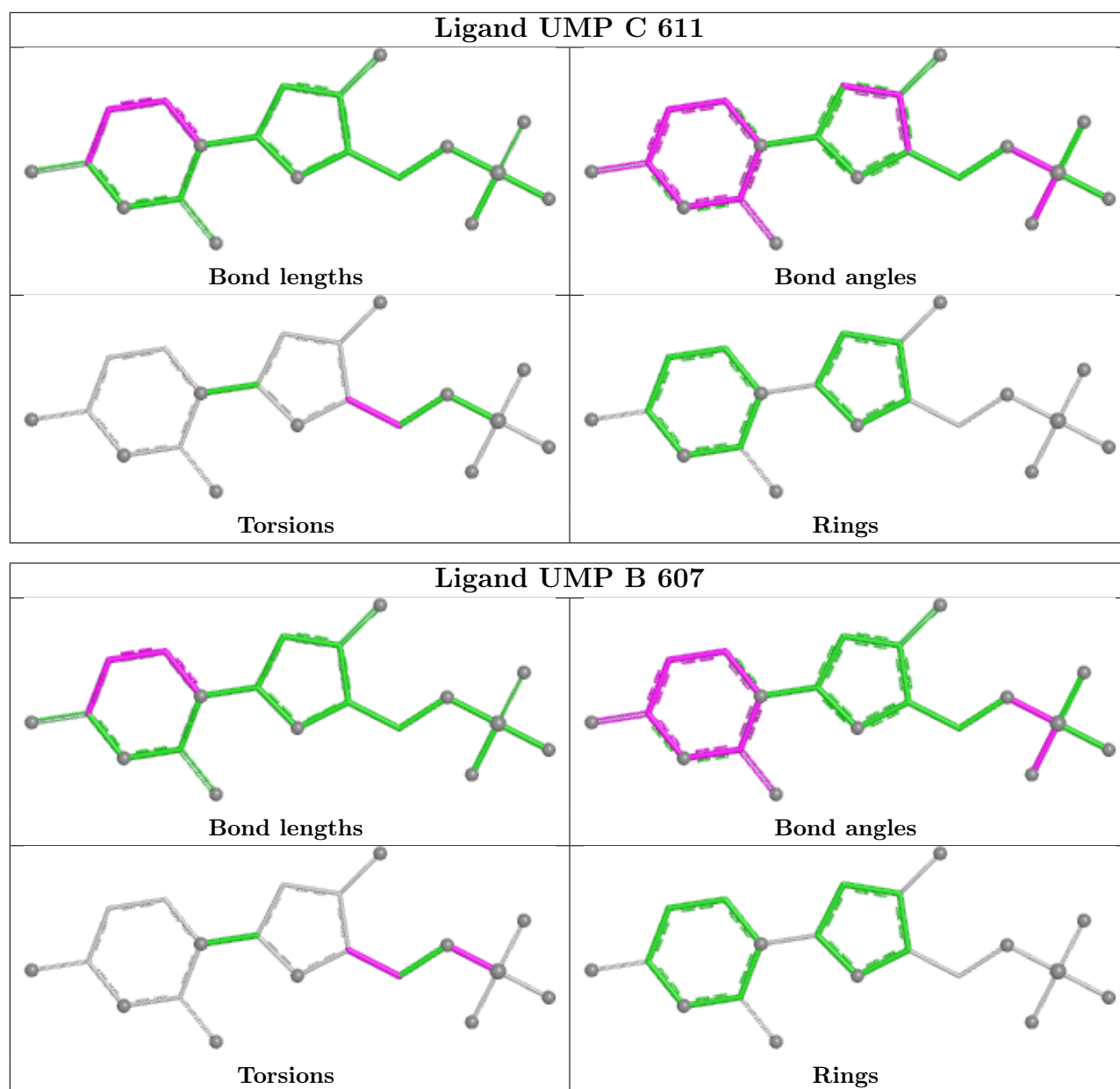


Ligand CB3 C 612

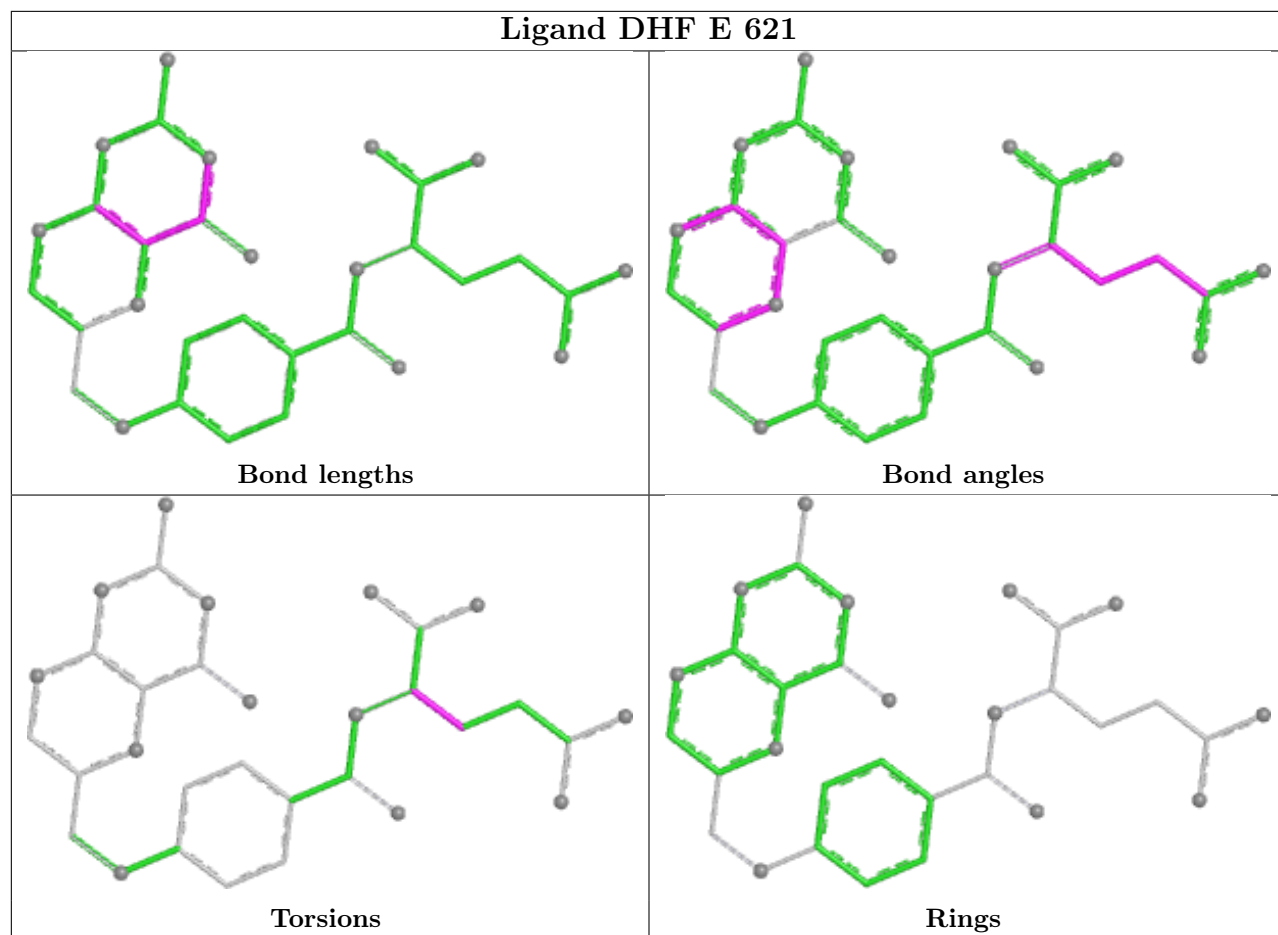


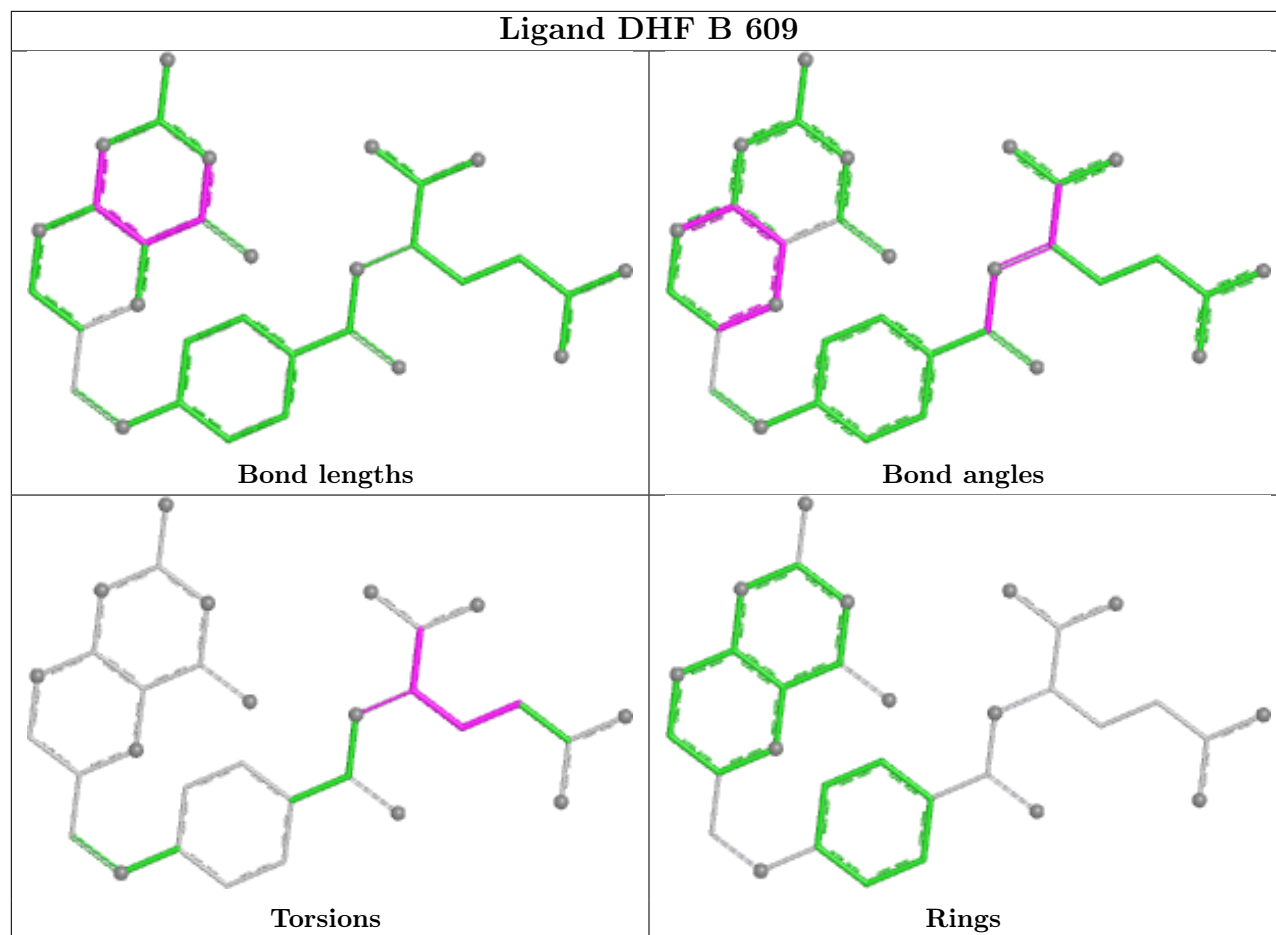
Ligand UMP D 615

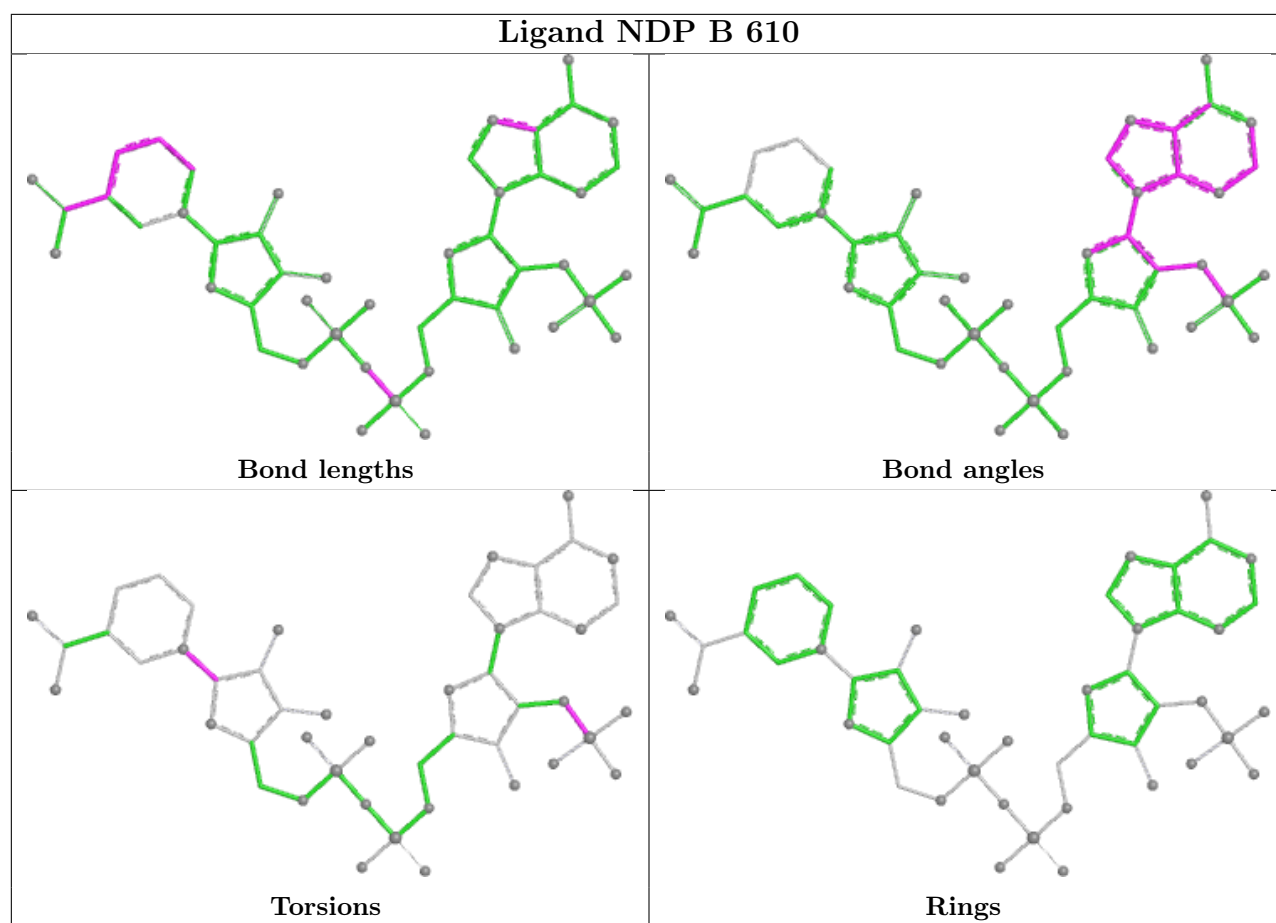




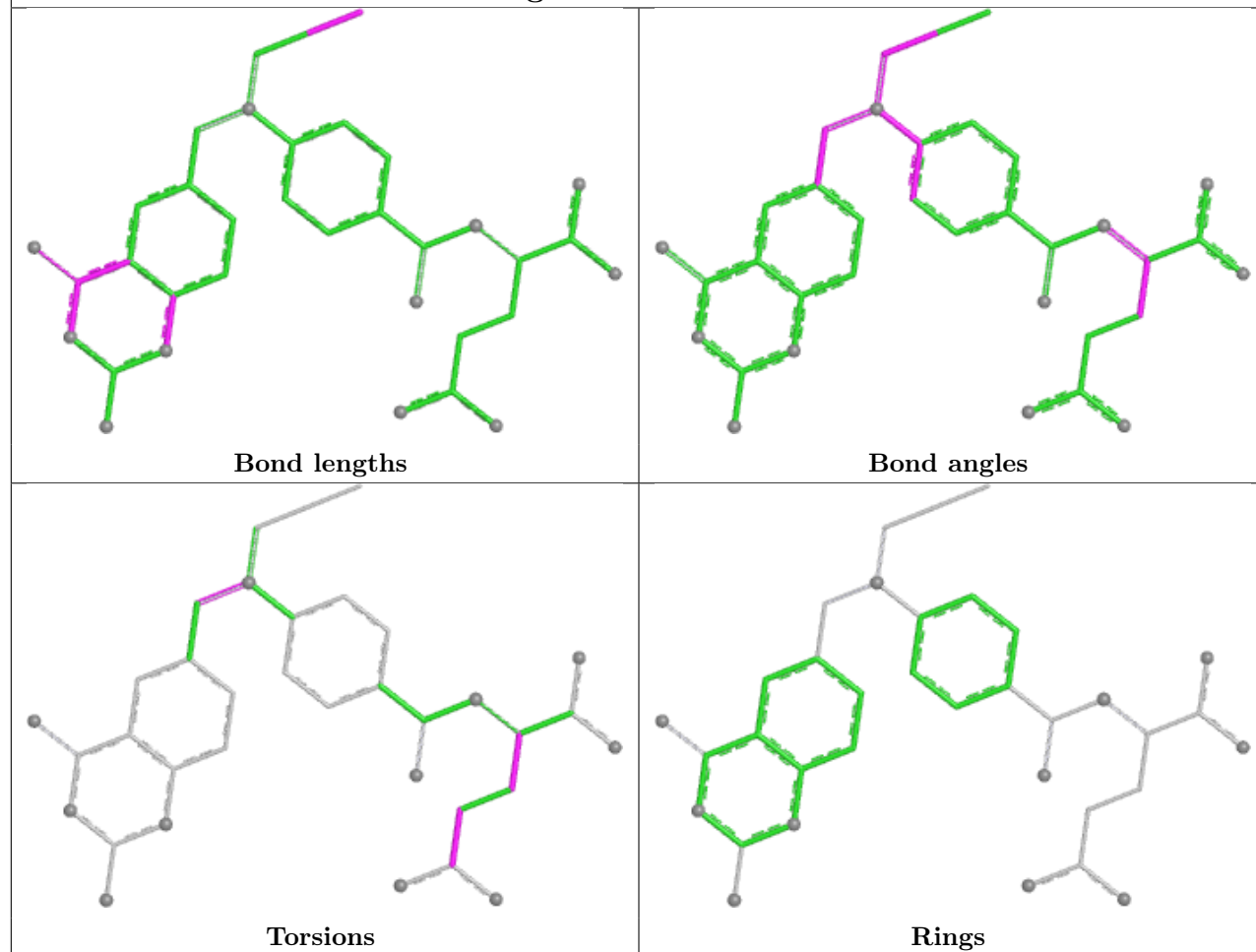
Ligand DHF E 621



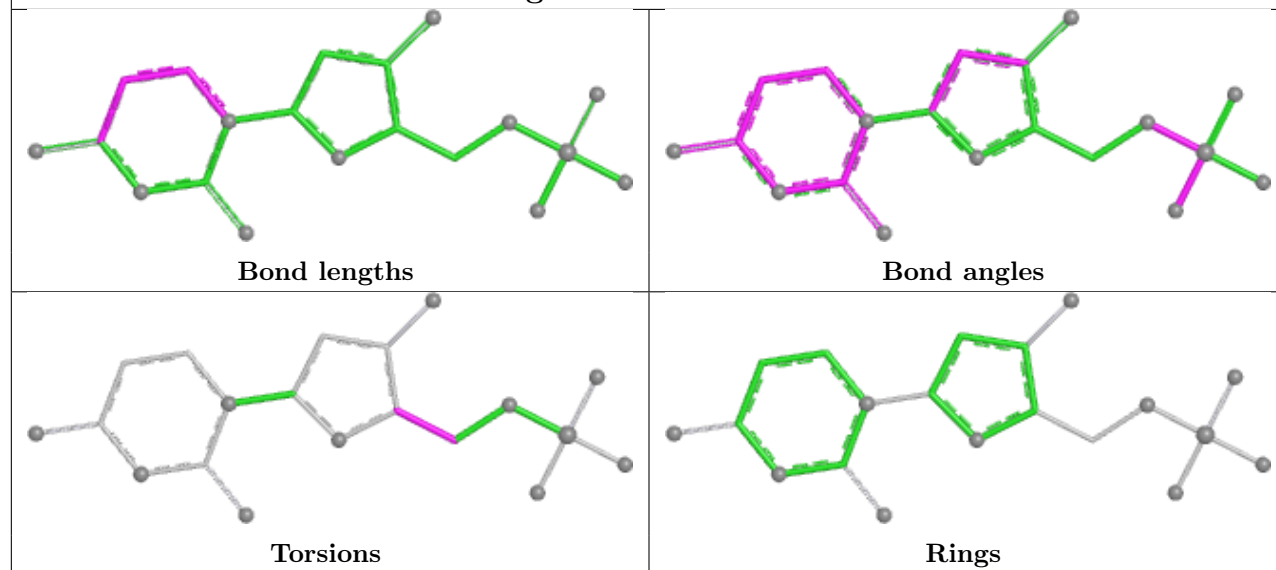


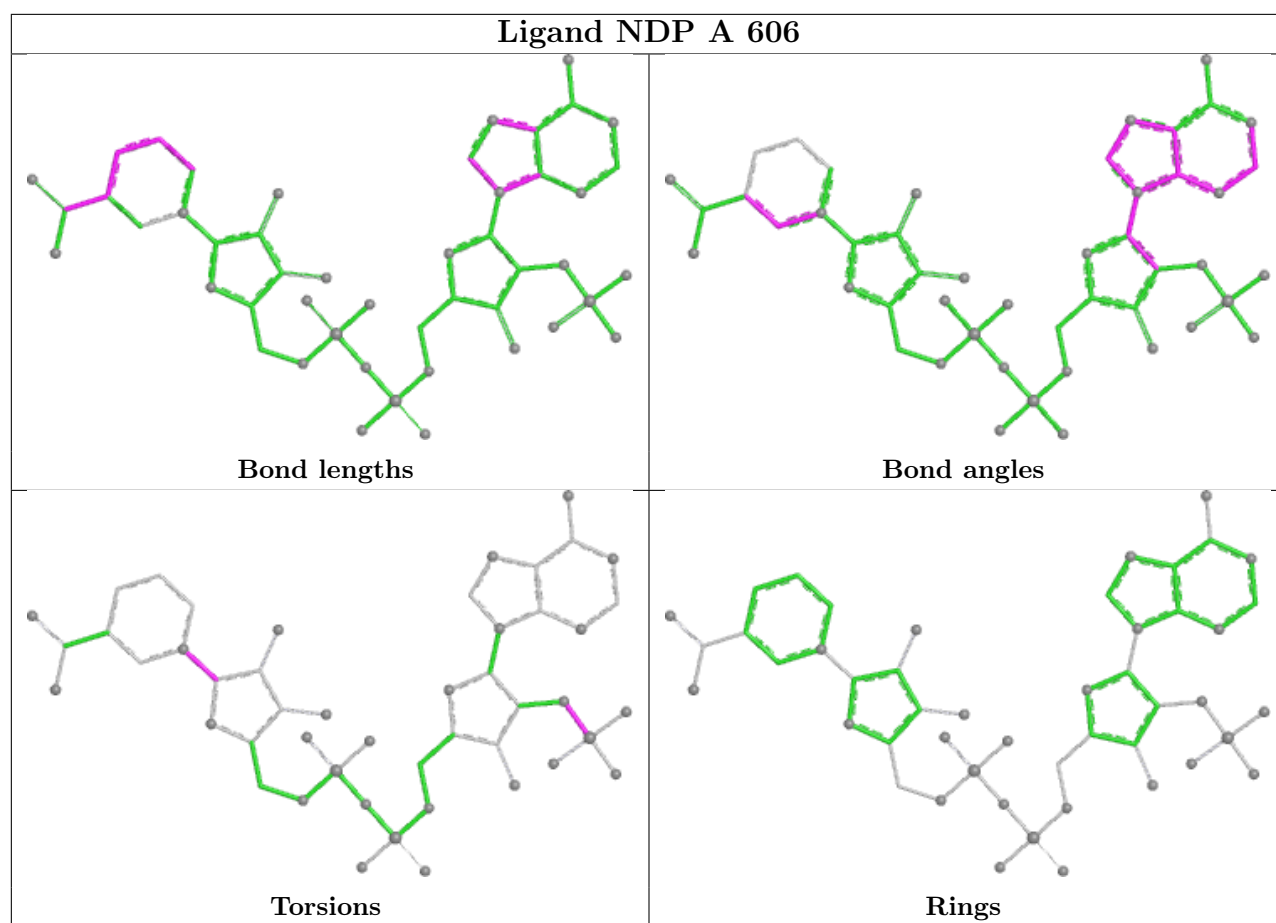


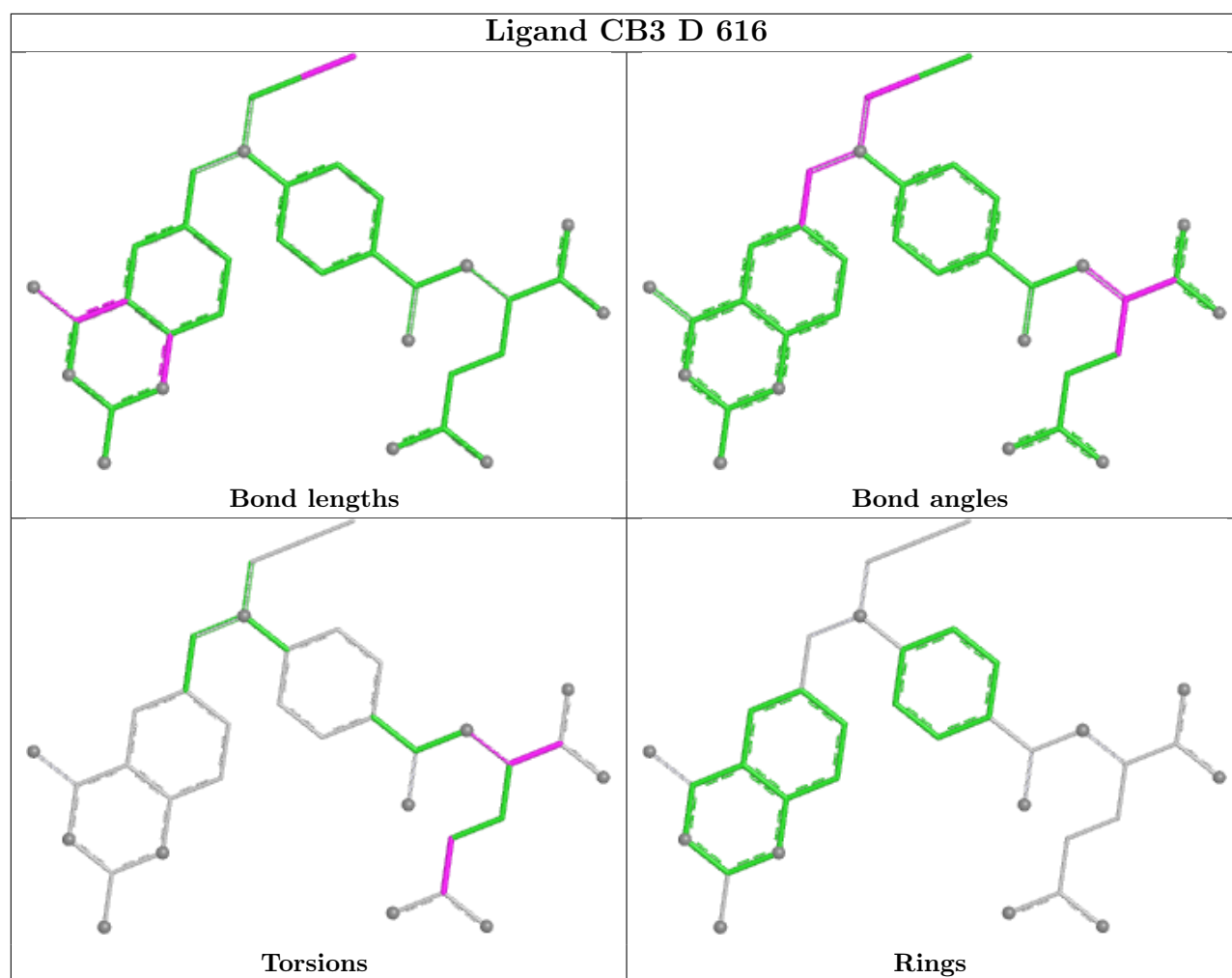
Ligand CB3 B 608

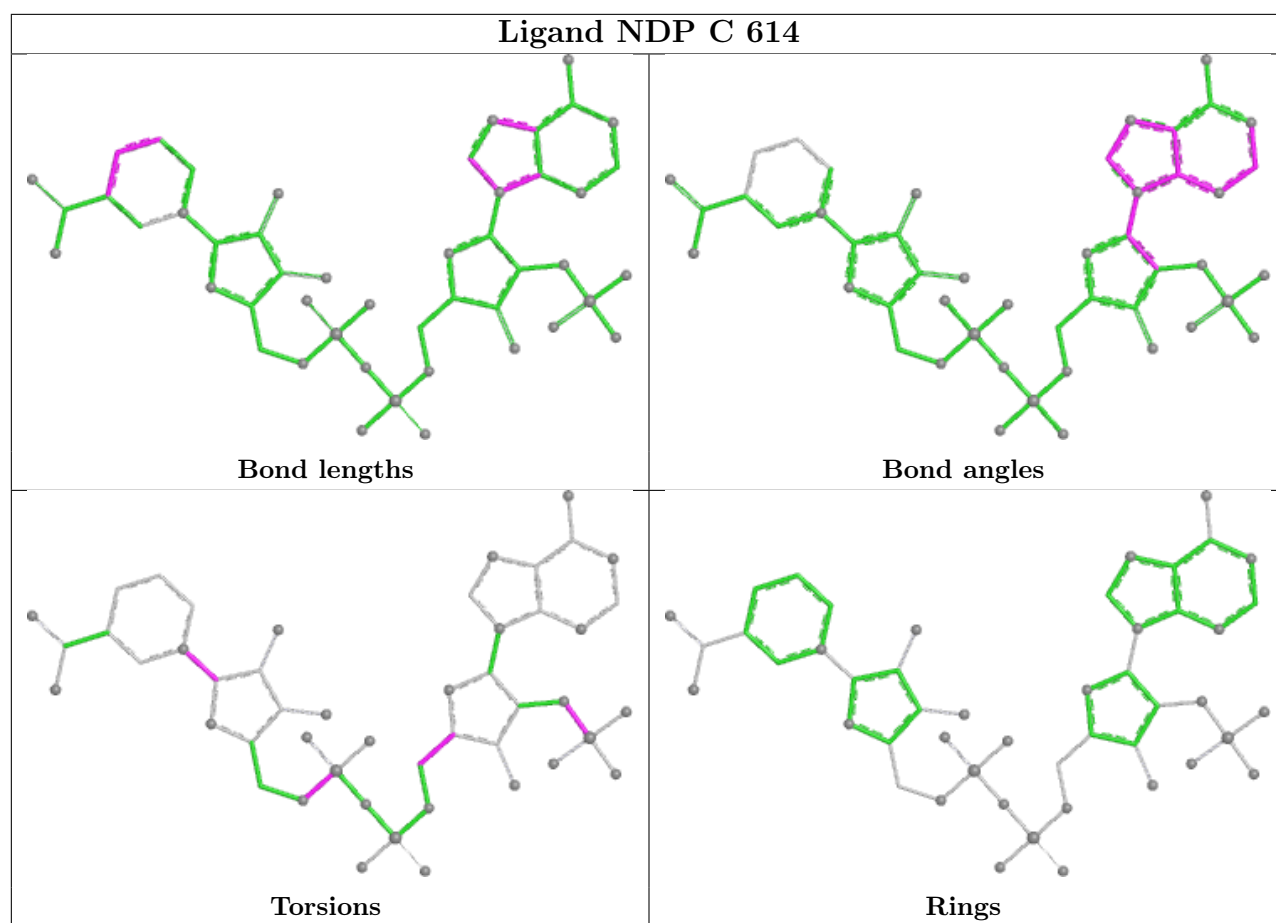


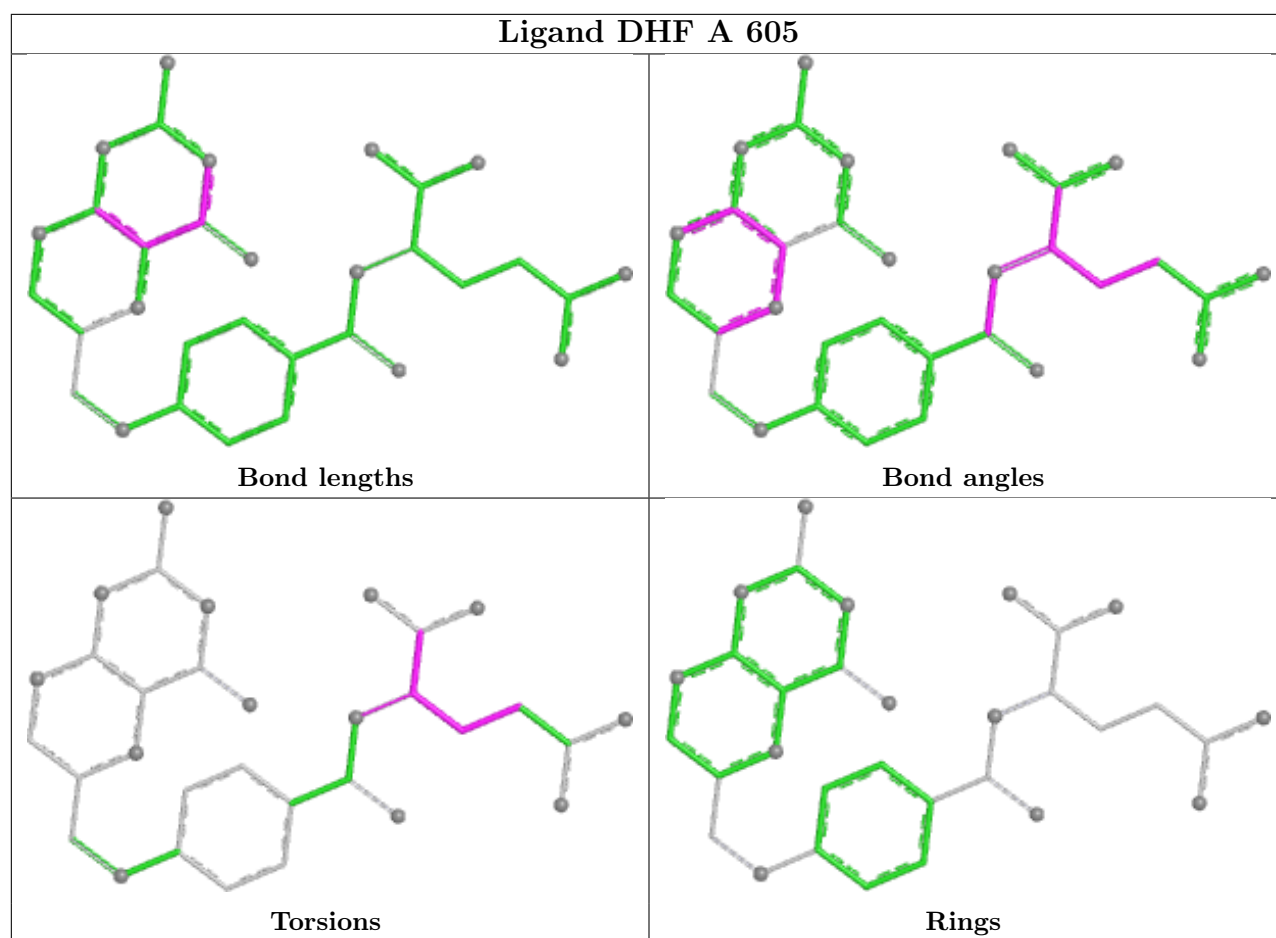
Ligand UMP A 603

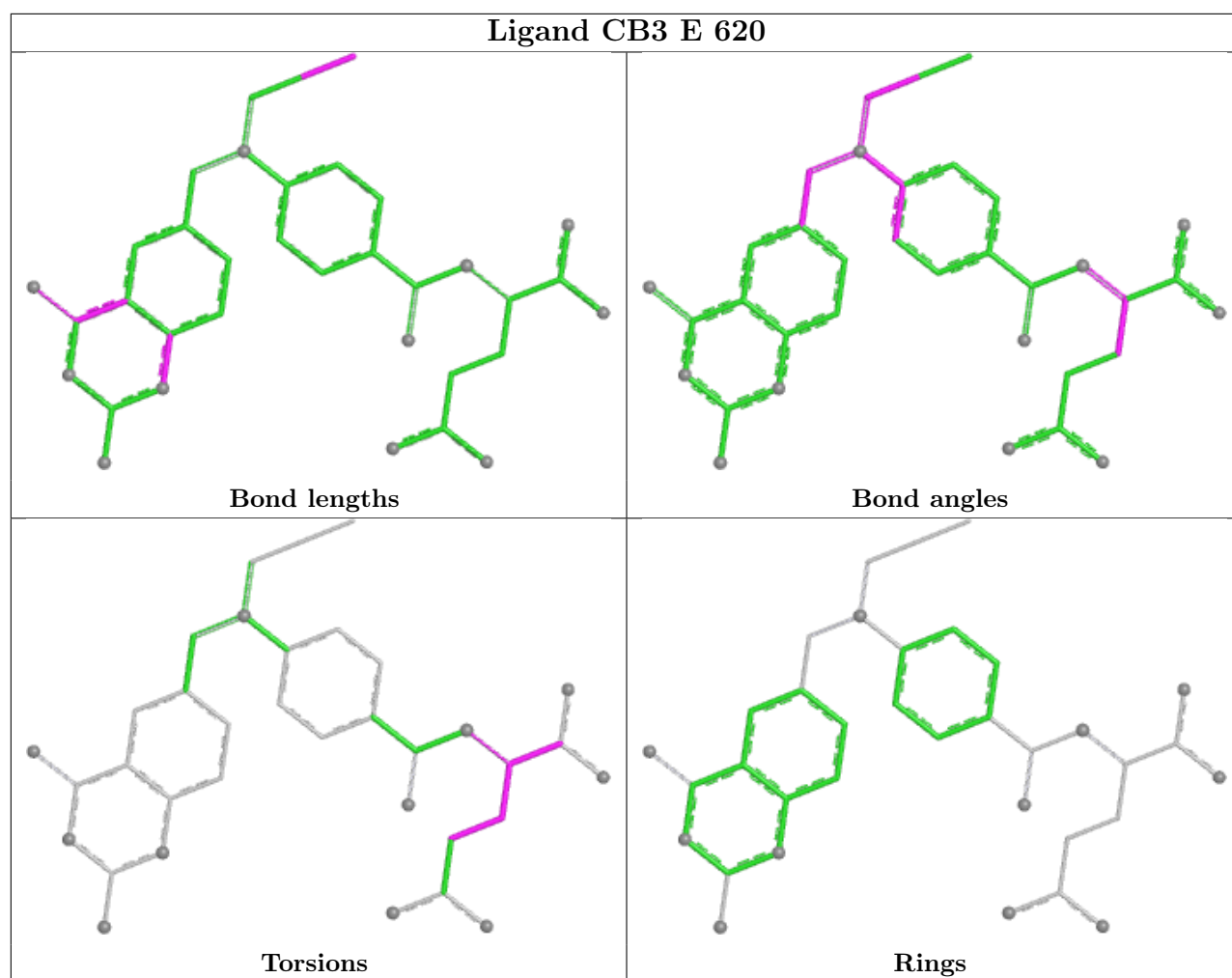


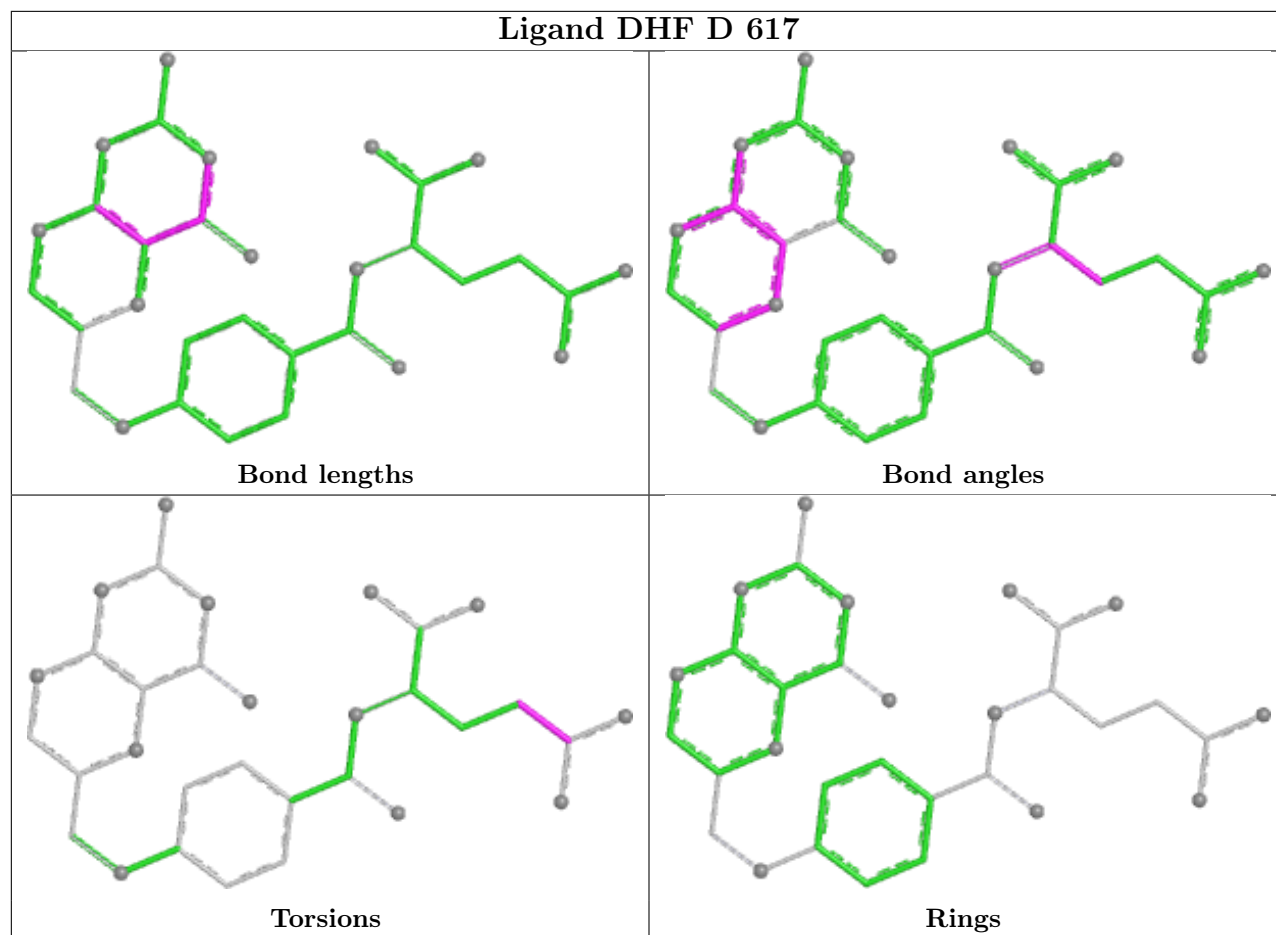


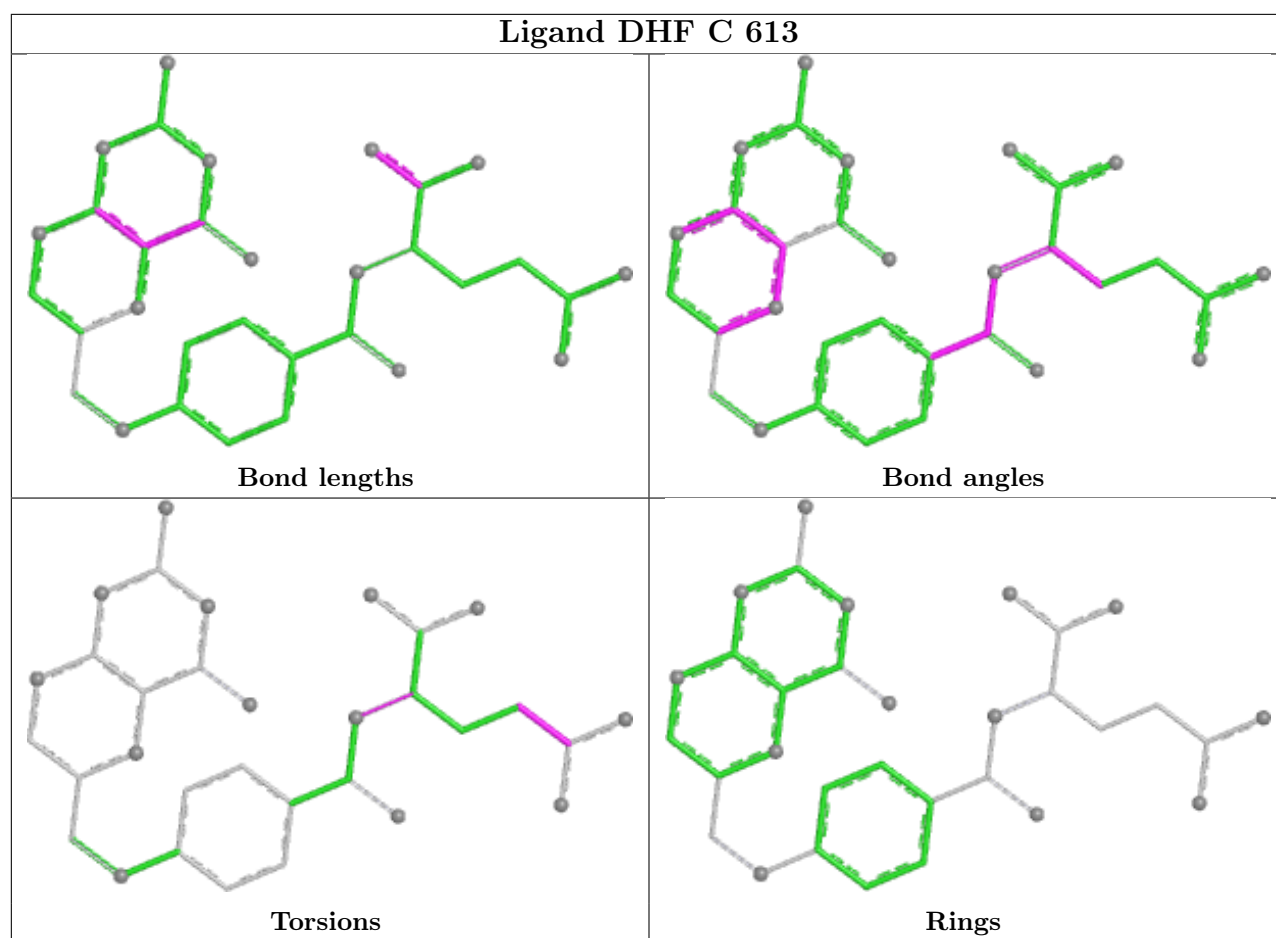


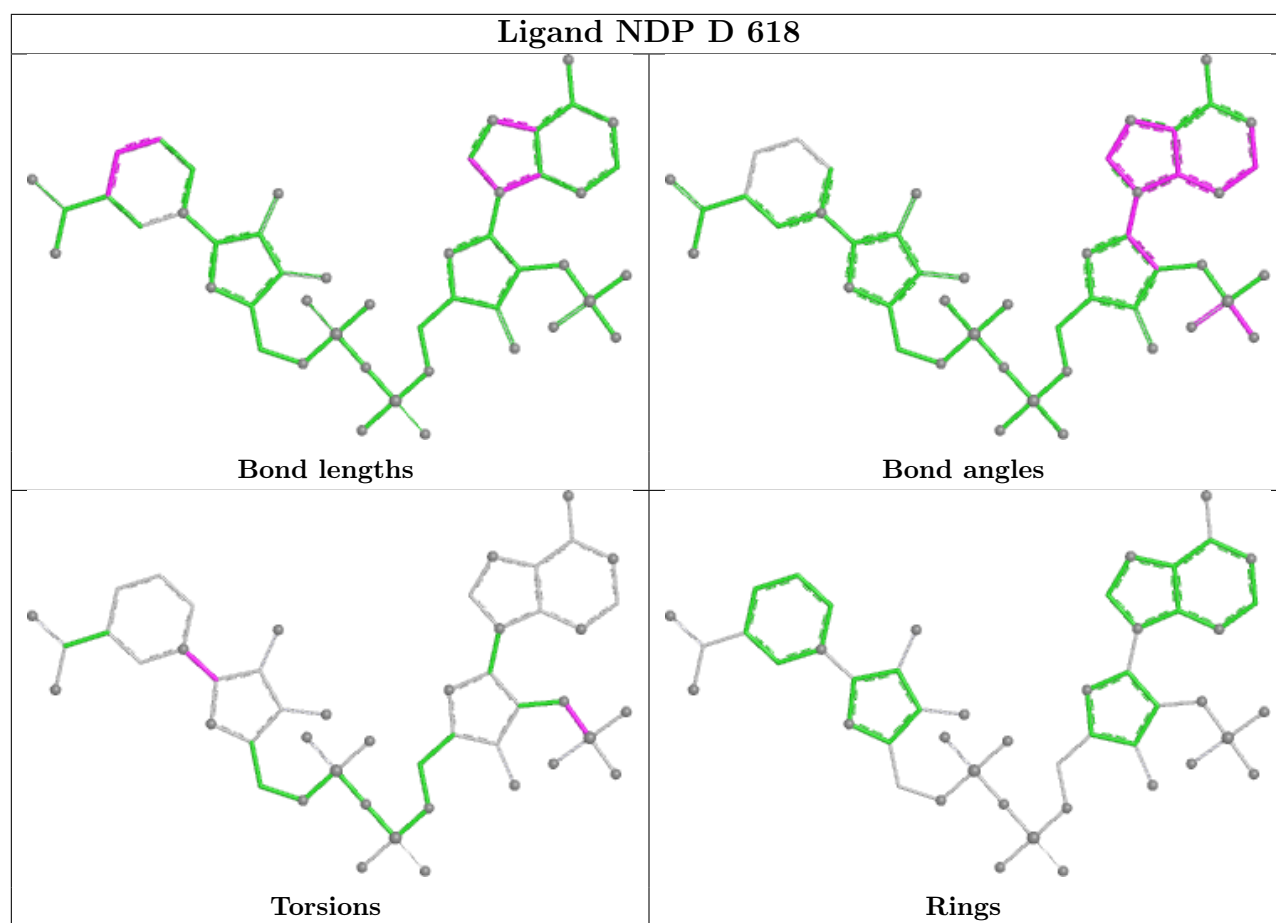












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	507/521 (97%)	0.34	20 (3%)	43	41	23, 39, 74, 118	0
1	B	508/521 (97%)	0.05	16 (3%)	51	49	20, 34, 62, 135	0
1	C	508/521 (97%)	0.59	38 (7%)	20	20	26, 47, 90, 131	0
1	D	507/521 (97%)	0.73	29 (5%)	29	29	29, 50, 84, 158	0
1	E	508/521 (97%)	1.45	103 (20%)	3	2	45, 72, 112, 149	0
All	All	2538/2605 (97%)	0.63	206 (8%)	18	18	20, 48, 96, 158	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	521	VAL	8.1
1	D	193	LEU	8.0
1	D	179	GLU	7.6
1	B	193	LEU	7.2
1	E	179	GLU	7.0
1	E	193	LEU	6.7
1	D	180	LYS	6.5
1	B	102	MET	6.3
1	A	180	LYS	6.2
1	C	193	LEU	5.9
1	E	194	LYS	5.8
1	A	102	MET	5.8
1	E	180	LYS	5.8
1	D	102	MET	5.7
1	B	180	LYS	5.4
1	E	102	MET	5.2
1	A	179	GLU	5.2
1	C	181	LYS	5.1
1	A	193	LEU	4.9
1	B	103	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	181	LYS	4.7
1	E	255	GLU	4.7
1	C	179	GLU	4.6
1	C	102	MET	4.6
1	E	181	LYS	4.5
1	E	287	PHE	4.3
1	E	196	ILE	4.2
1	C	180	LYS	4.1
1	E	520	ALA	4.0
1	E	316	TRP	3.9
1	C	408	TYR	3.9
1	E	175	PHE	3.7
1	A	82	ASP	3.6
1	E	500	LYS	3.5
1	B	413	ASP	3.5
1	A	84	ALA	3.5
1	E	322	LYS	3.5
1	A	103	ASN	3.4
1	D	408	TYR	3.3
1	D	98	ILE	3.3
1	E	100	ASN	3.3
1	D	194	LYS	3.2
1	D	288	ILE	3.2
1	A	194	LYS	3.1
1	C	99	GLU	3.1
1	E	259	GLY	3.1
1	E	328	ILE	3.1
1	A	324	TYR	3.1
1	E	178	GLN	3.1
1	B	104	ASP	3.1
1	D	105	ASP	3.0
1	E	380	LYS	3.0
1	C	98	ILE	3.0
1	A	349	TYR	3.0
1	E	488	LYS	3.0
1	A	465	ILE	3.0
1	E	363	VAL	3.0
1	E	309	ILE	2.9
1	D	287	PHE	2.9
1	E	104	ASP	2.9
1	C	373	GLU	2.9
1	E	392	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	105	ASP	2.9
1	D	236	TYR	2.9
1	A	413	ASP	2.9
1	E	197	ASP	2.9
1	E	343	GLY	2.8
1	B	113	CYS	2.8
1	A	287	PHE	2.8
1	E	352	GLU	2.8
1	E	5	ASN	2.8
1	E	338	LEU	2.8
1	E	386	LEU	2.8
1	D	521	VAL	2.8
1	E	436	ALA	2.8
1	E	98	ILE	2.7
1	E	280	LEU	2.7
1	E	357	HIS	2.7
1	D	258	THR	2.7
1	B	97	SER	2.7
1	D	256	ASN	2.7
1	E	495	ASN	2.7
1	D	99	GLU	2.7
1	E	314	TYR	2.7
1	C	97	SER	2.7
1	D	255	GLU	2.7
1	E	257	ARG	2.7
1	B	99	GLU	2.7
1	C	104	ASP	2.7
1	E	324	TYR	2.6
1	D	100	ASN	2.6
1	E	285	LYS	2.6
1	E	106	SER	2.6
1	C	287	PHE	2.6
1	E	132	TYR	2.6
1	A	402	CYS	2.6
1	E	370	LYS	2.6
1	C	324	TYR	2.6
1	E	327	ARG	2.6
1	E	492	LYS	2.6
1	E	320	GLY	2.6
1	E	296	ILE	2.6
1	C	101	LEU	2.6
1	E	496	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	101	LEU	2.5
1	E	360	TYR	2.5
1	E	315	ILE	2.5
1	C	194	LYS	2.5
1	C	142	GLU	2.5
1	E	123	LEU	2.5
1	E	95	GLU	2.5
1	D	103	ASN	2.5
1	E	177	LYS	2.5
1	E	354	LYS	2.5
1	A	98	ILE	2.5
1	E	381	ASP	2.5
1	B	179	GLU	2.5
1	E	391	PRO	2.5
1	B	410	VAL	2.5
1	E	298	PHE	2.5
1	E	319	ASN	2.4
1	E	394	LEU	2.4
1	D	142	GLU	2.4
1	A	178	GLN	2.4
1	E	499	PHE	2.4
1	C	79	LEU	2.4
1	C	139	GLU	2.4
1	D	502	GLU	2.4
1	E	237	GLU	2.4
1	E	115	GLY	2.4
1	C	52	LEU	2.4
1	E	101	LEU	2.4
1	C	3	GLU	2.4
1	C	402	CYS	2.4
1	D	257	ARG	2.4
1	C	103	ASN	2.4
1	E	264	SER	2.4
1	C	381	ASP	2.4
1	C	113	CYS	2.4
1	E	453	PRO	2.4
1	A	378	ASN	2.3
1	E	400	PRO	2.3
1	E	248	LEU	2.3
1	E	39	ILE	2.3
1	E	342	TYR	2.3
1	E	350	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	99	GLU	2.3
1	E	99	GLU	2.3
1	C	84	ALA	2.3
1	E	333	ARG	2.3
1	E	14	VAL	2.3
1	E	138	LEU	2.3
1	C	465	ILE	2.3
1	B	5	ASN	2.3
1	C	171	ASP	2.3
1	E	346	TRP	2.3
1	C	138	LEU	2.3
1	C	149	GLU	2.2
1	C	323	GLU	2.2
1	E	377	ASN	2.2
1	C	81	GLN	2.2
1	E	89	VAL	2.2
1	E	286	VAL	2.2
1	C	388	ALA	2.2
1	D	3	GLU	2.2
1	E	140	ASP	2.2
1	E	305	GLY	2.2
1	D	107	ILE	2.2
1	E	489	PHE	2.2
1	E	283	THR	2.2
1	D	195	SER	2.2
1	E	403	HIS	2.2
1	D	149	GLU	2.2
1	E	310	GLU	2.2
1	E	510	TYR	2.2
1	C	24	GLN	2.2
1	C	49	LYS	2.2
1	E	325	LEU	2.2
1	A	381	ASP	2.2
1	D	106	SER	2.2
1	E	235	HIS	2.2
1	E	365	VAL	2.2
1	E	262	THR	2.1
1	E	421	TYR	2.1
1	E	251	GLY	2.1
1	B	194	LYS	2.1
1	E	307	HIS	2.1
1	D	413	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	431	SER	2.1
1	B	3	GLU	2.1
1	E	27	TRP	2.1
1	E	230	ARG	2.1
1	B	373	GLU	2.1
1	E	155	LEU	2.1
1	E	244	LEU	2.1
1	E	414	ASN	2.1
1	E	448	VAL	2.1
1	E	105	ASP	2.0
1	C	326	GLU	2.0
1	D	83	GLU	2.0
1	E	117	SER	2.0
1	C	69	ASN	2.0
1	A	95	GLU	2.0
1	E	34	LYS	2.0
1	E	398	ALA	2.0
1	C	178	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CB3	E	620	35/35	0.71	0.21	93,98,107,108	0
3	CB3	D	616	35/35	0.76	0.21	69,75,87,89	0
4	DHF	C	613	32/32	0.82	0.14	29,35,44,48	0
2	UMP	E	619	20/20	0.83	0.15	80,88,89,89	0
4	DHF	E	621	32/32	0.83	0.13	30,33,42,47	0

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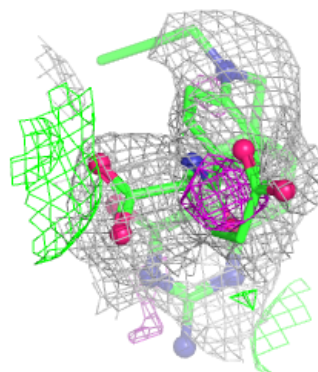
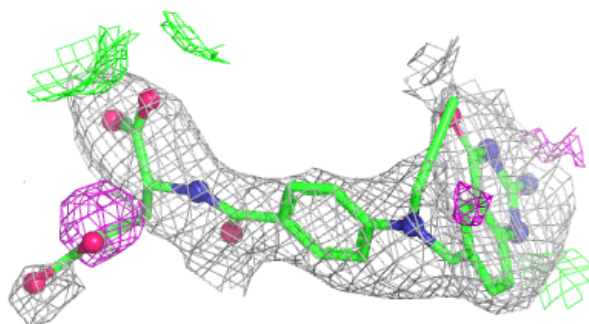
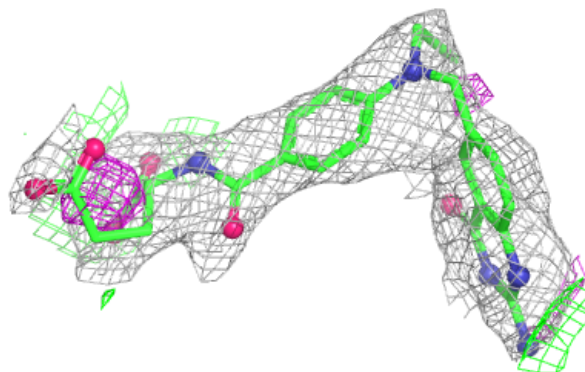
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CB3	A	604	35/35	0.84	0.17	60,67,76,77	0
3	CB3	C	612	35/35	0.84	0.16	49,60,71,73	0
4	DHF	B	609	32/32	0.85	0.14	23,26,39,44	0
4	DHF	D	617	32/32	0.88	0.12	23,31,41,47	0
4	DHF	A	605	32/32	0.88	0.12	23,28,38,48	0
5	NDP	C	614	48/48	0.88	0.14	65,77,95,95	0
2	UMP	B	607	20/20	0.89	0.15	27,44,48,51	0
5	NDP	E	622	48/48	0.89	0.14	66,77,90,92	0
2	UMP	A	603	20/20	0.90	0.15	46,57,61,63	0
2	UMP	D	615	20/20	0.90	0.15	53,66,73,73	0
5	NDP	D	618	48/48	0.91	0.13	50,61,74,76	0
3	CB3	B	608	35/35	0.91	0.12	45,50,68,69	0
2	UMP	C	611	20/20	0.92	0.13	39,50,55,58	0
5	NDP	B	610	48/48	0.95	0.10	31,37,42,43	0
5	NDP	A	606	48/48	0.95	0.10	31,40,43,44	0

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

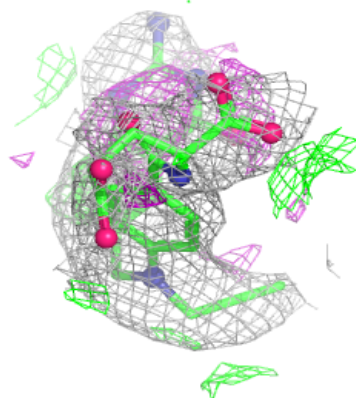
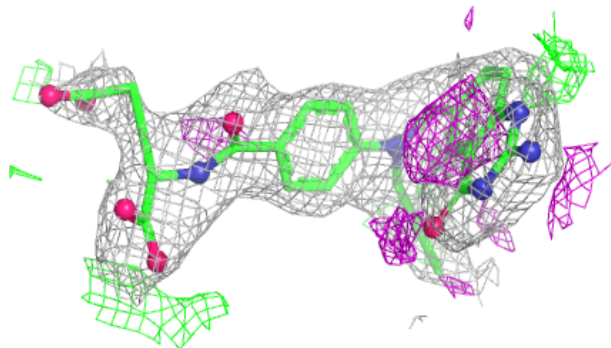
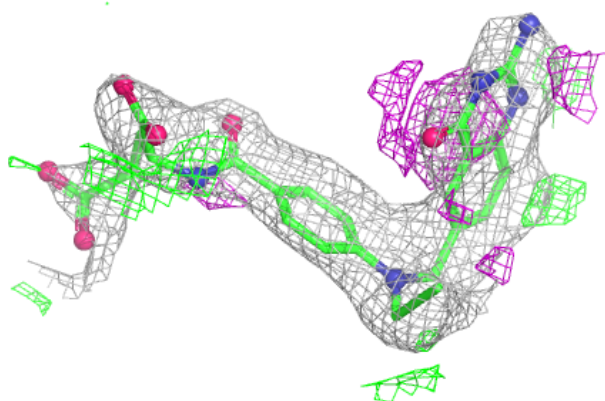
Electron density around CB3 E 620:

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

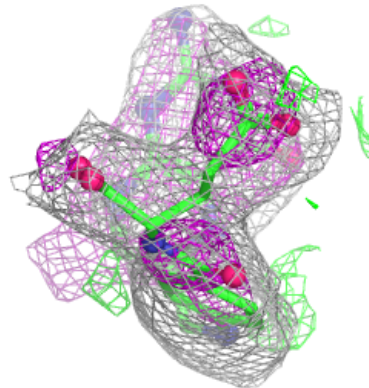
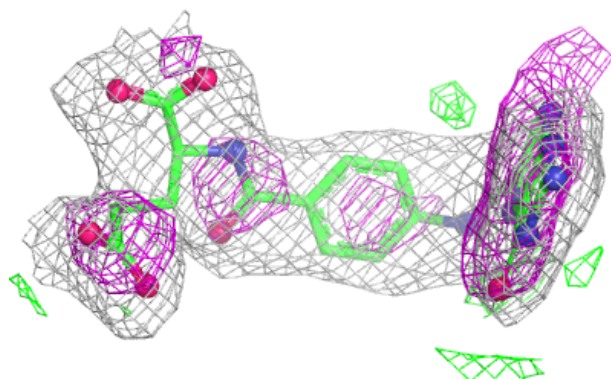
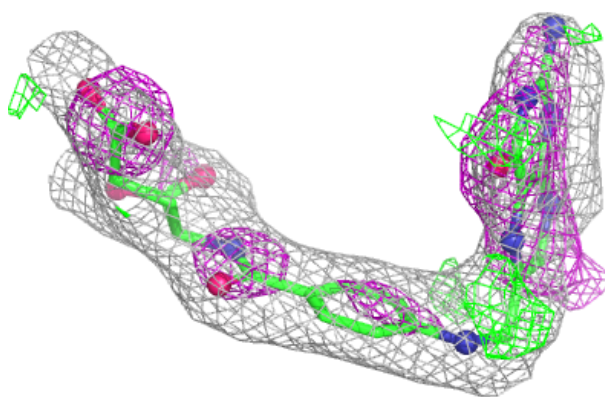


Electron density around CB3 D 616:

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

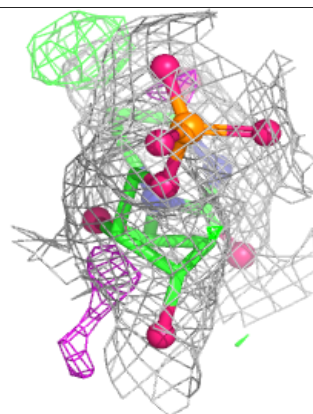
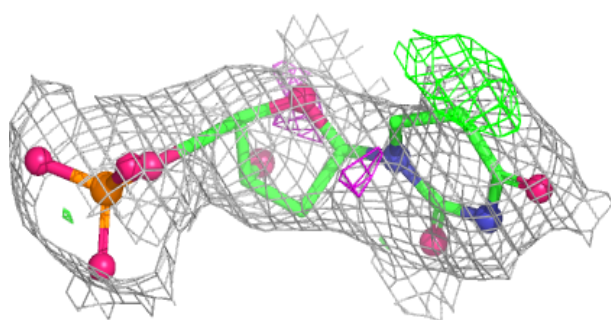
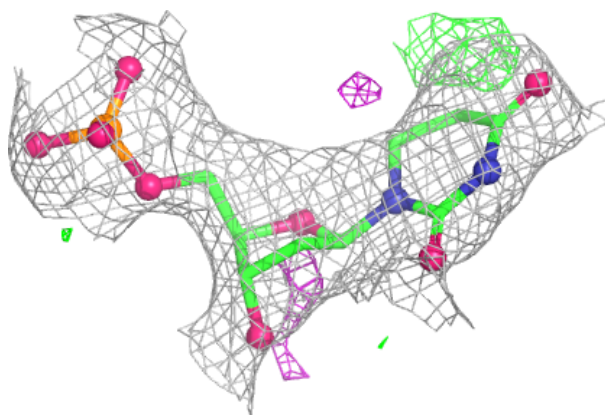
**Electron density around DHF C 613:**

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



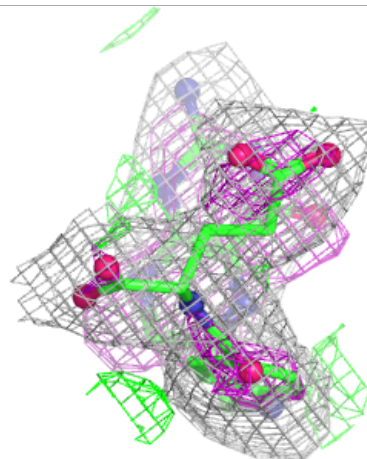
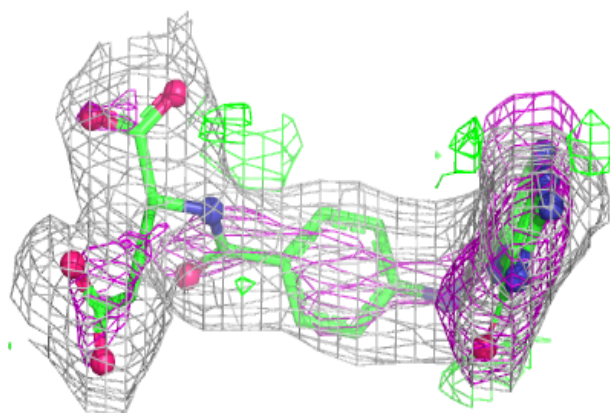
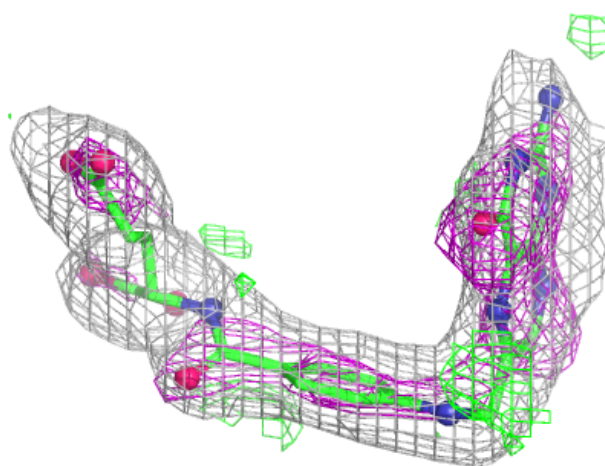
Electron density around UMP E 619:

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



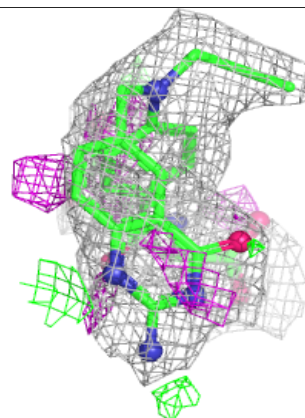
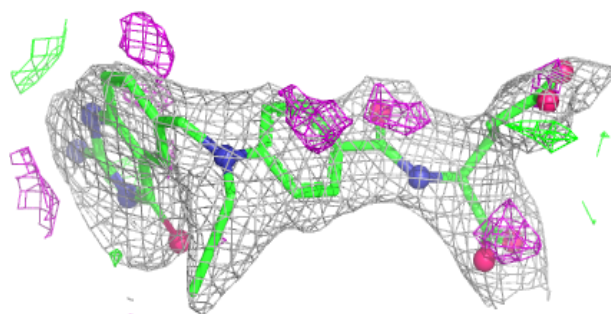
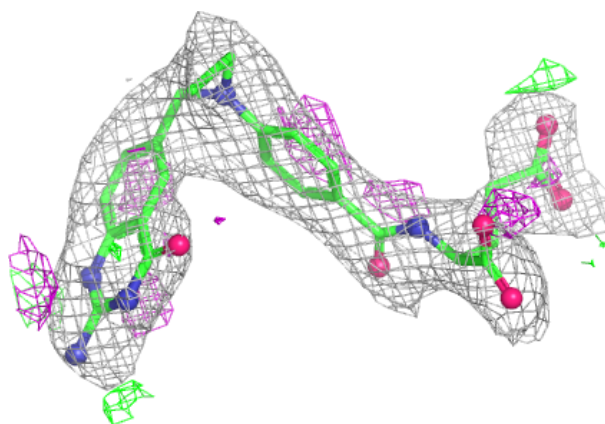
Electron density around DHF E 621:

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

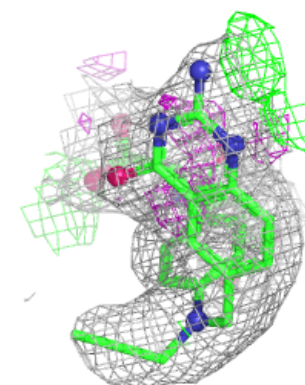
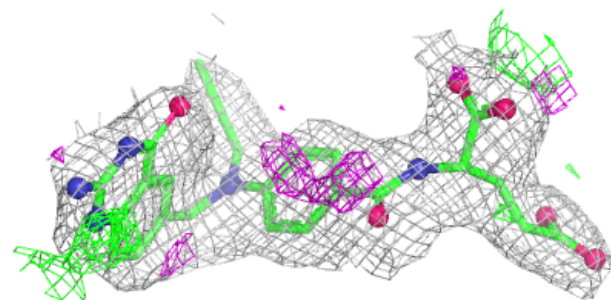
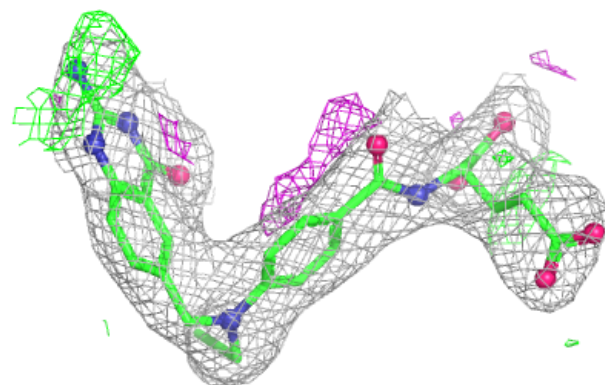


Electron density around CB3 A 604:

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

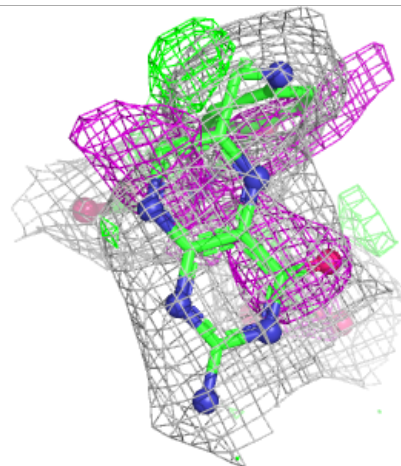
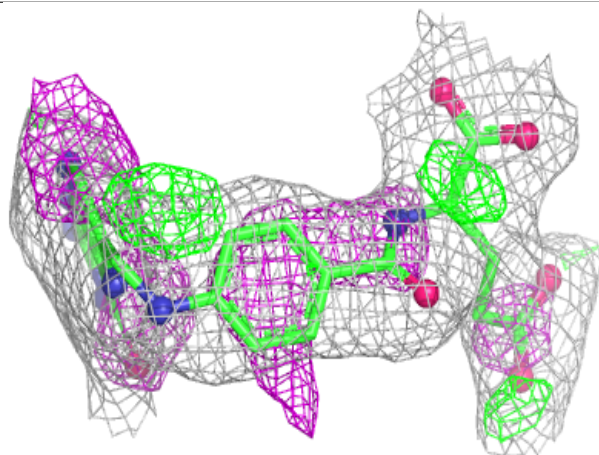
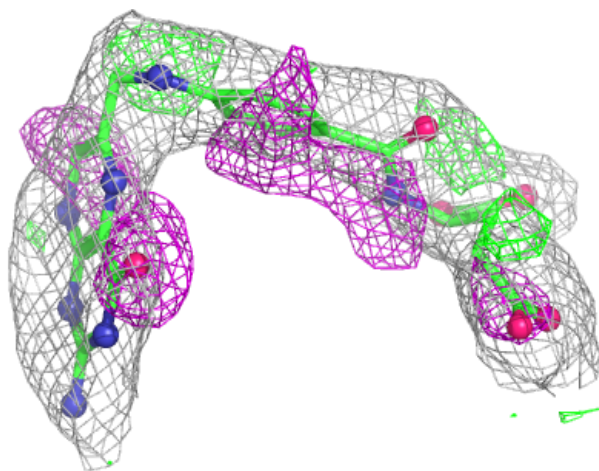
**Electron density around CB3 C 612:**

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



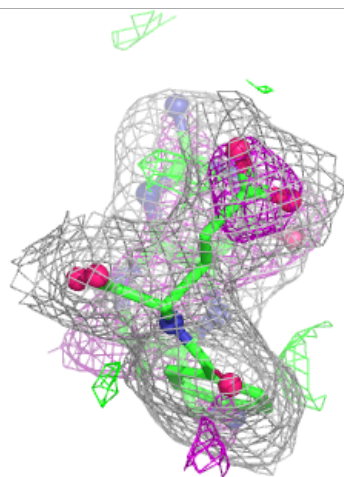
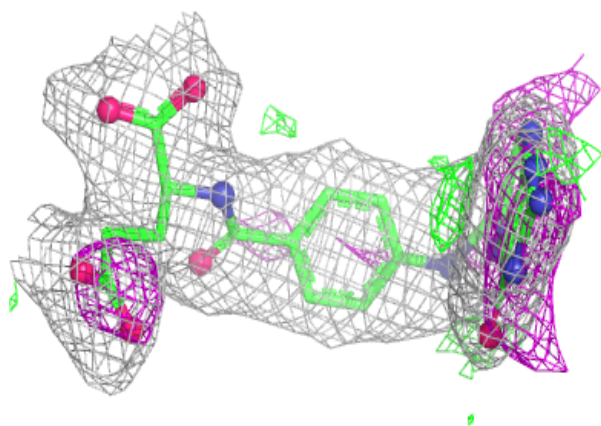
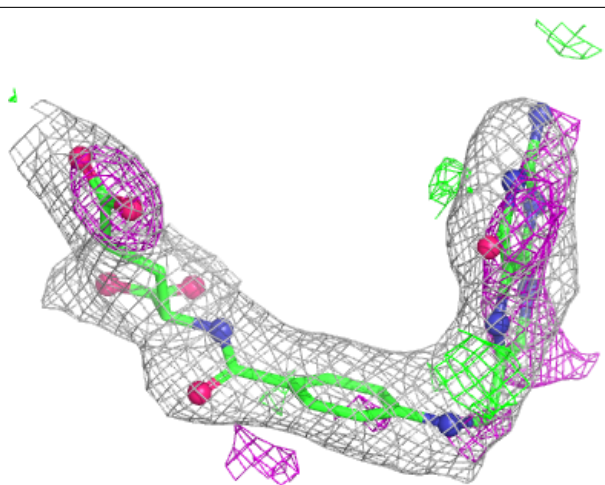
Electron density around DHF B 609:

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



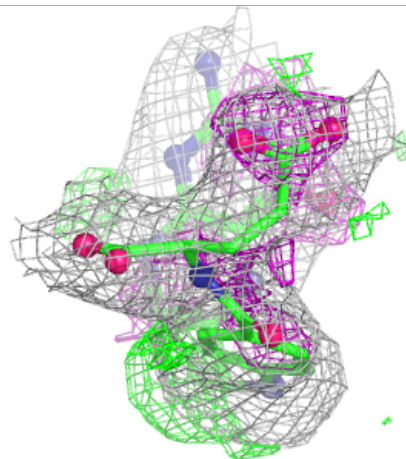
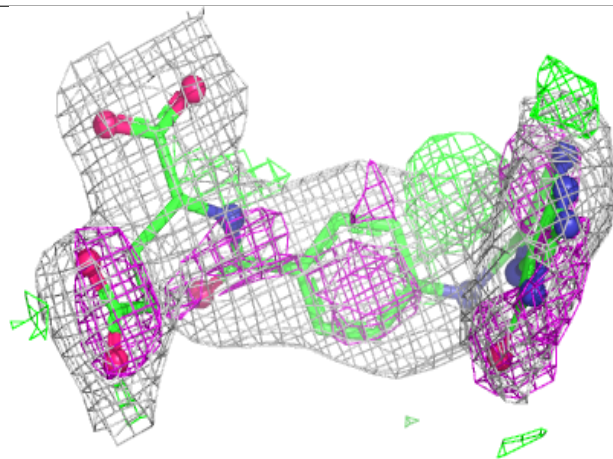
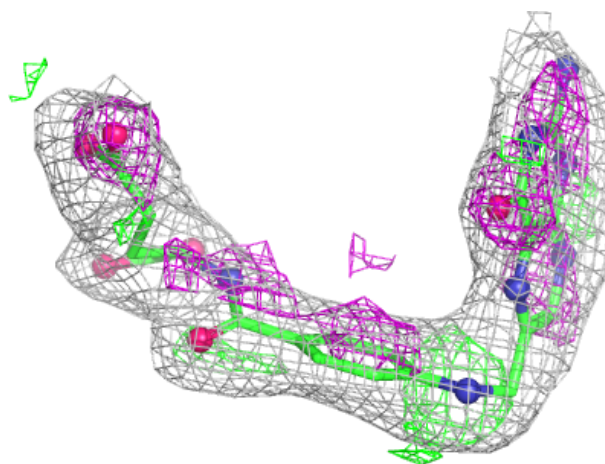
Electron density around DHF D 617:

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



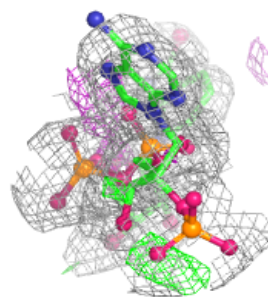
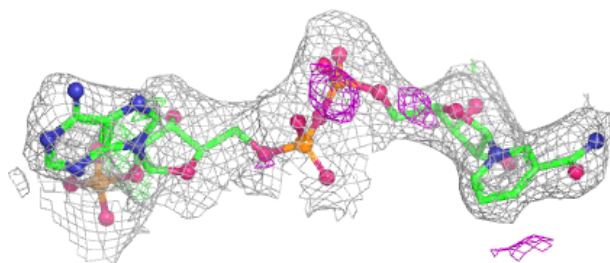
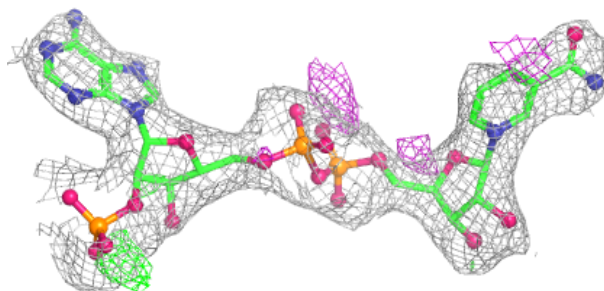
Electron density around DHF A 605:

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

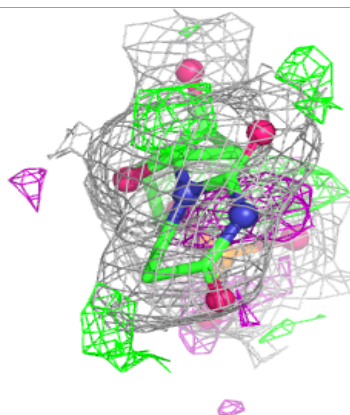
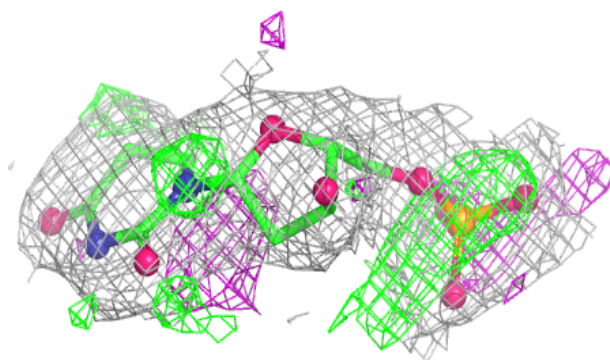
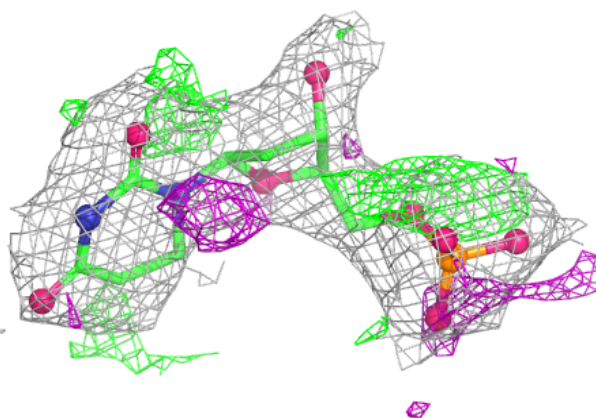


Electron density around NDP C 614:

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

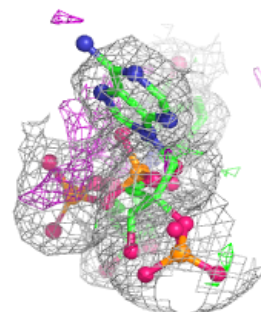
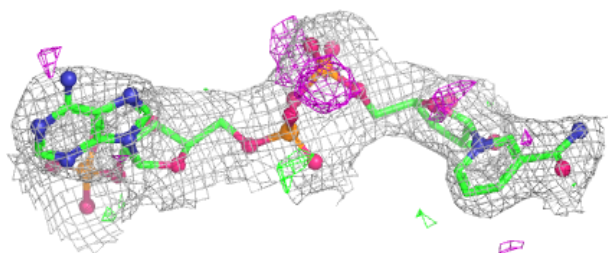
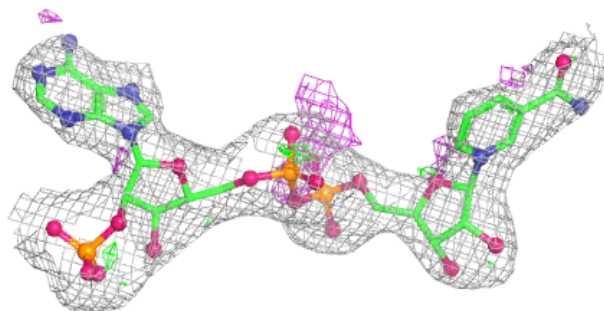
**Electron density around UMP B 607:**

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

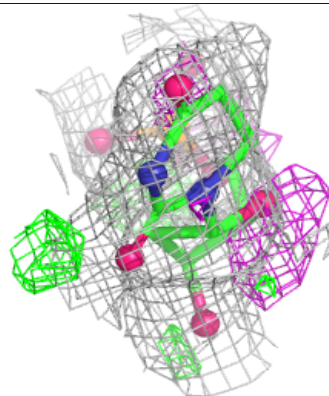
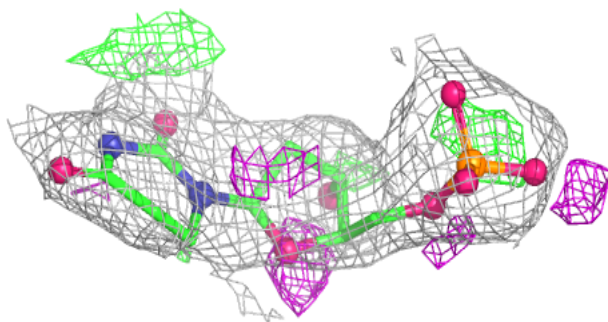
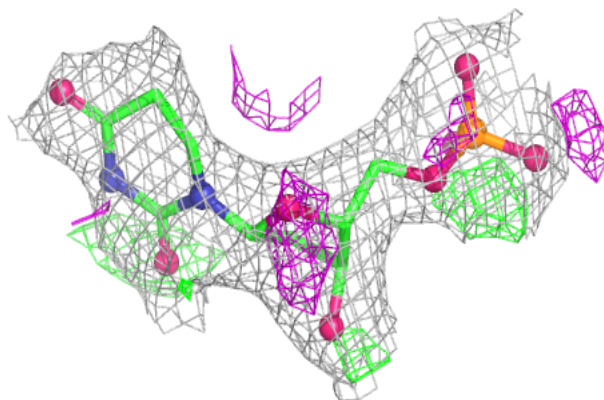


Electron density around NDP E 622:

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

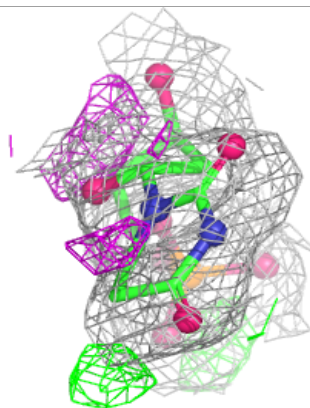
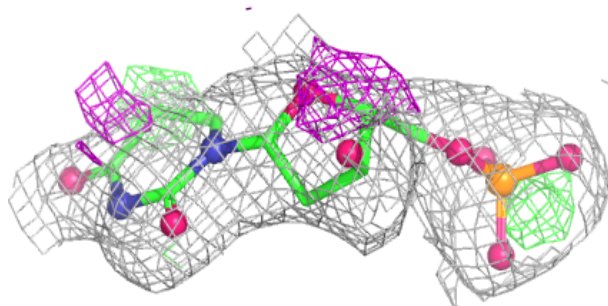
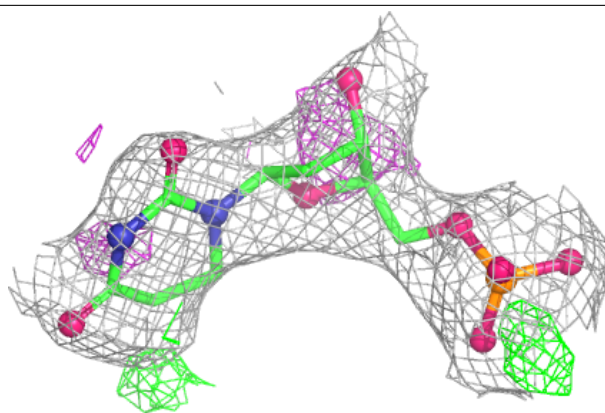
**Electron density around UMP A 603:**

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

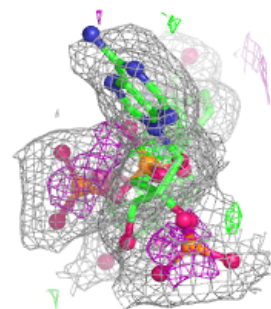
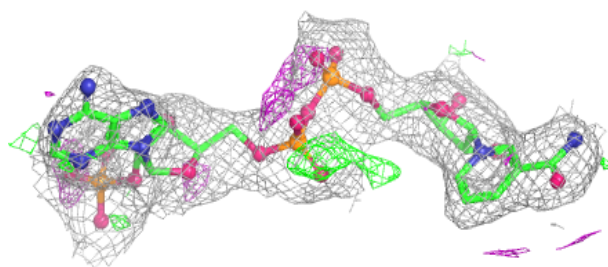
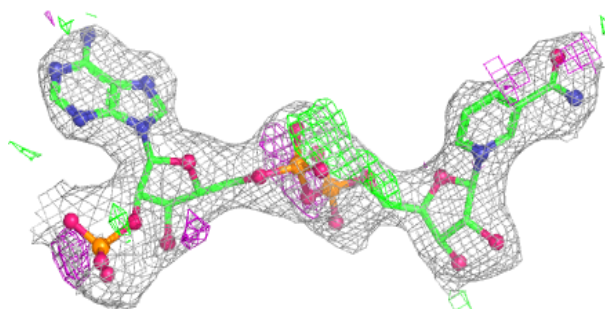


Electron density around UMP D 615:

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

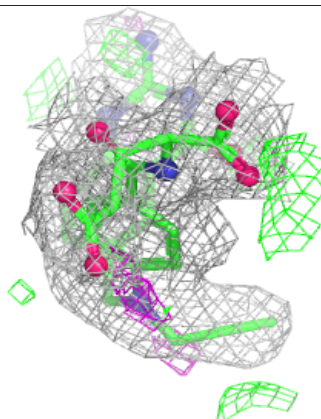
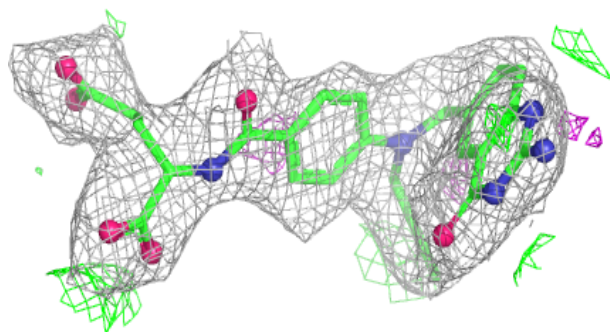
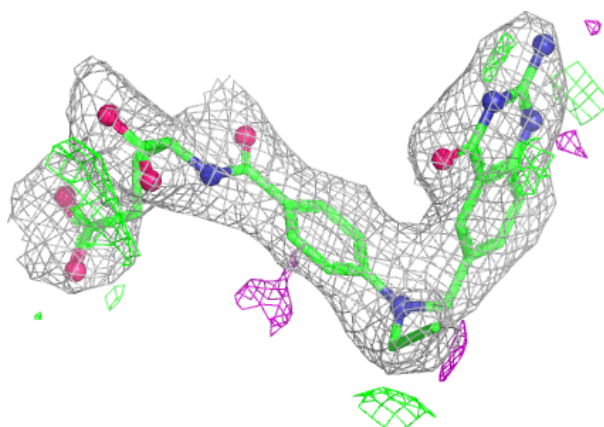
**Electron density around NDP D 618:**

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



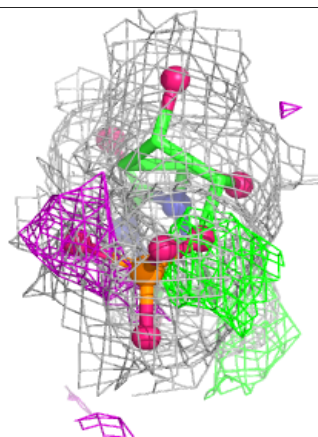
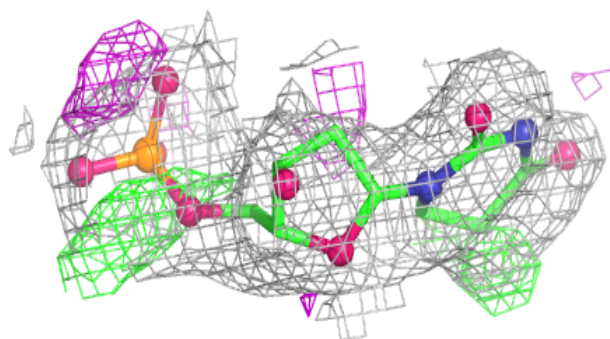
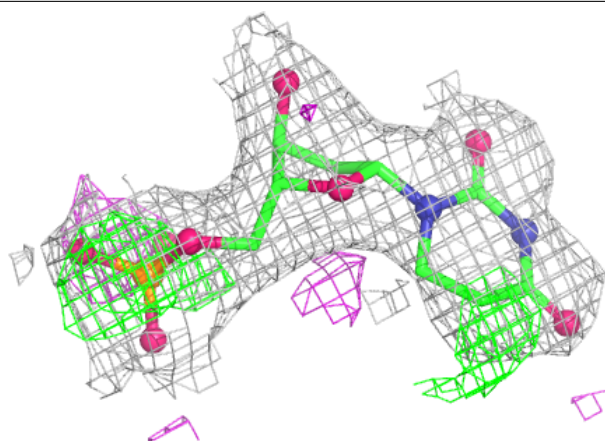
Electron density around CB3 B 608:

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

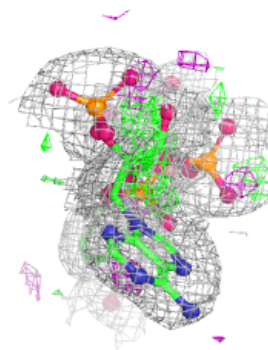
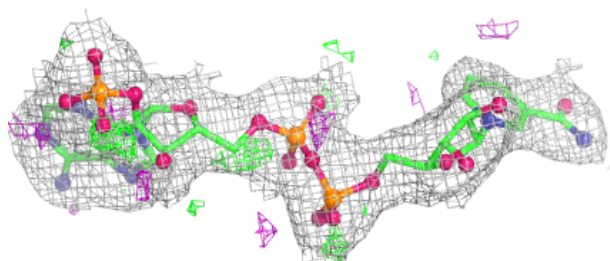
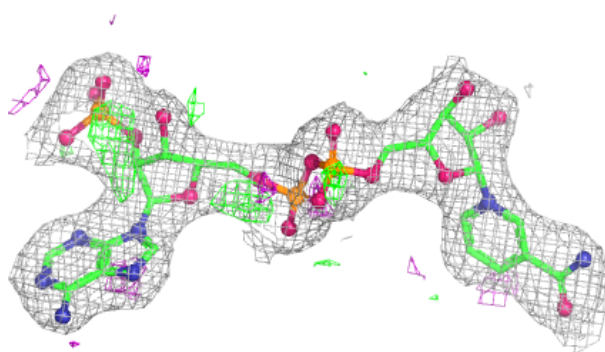


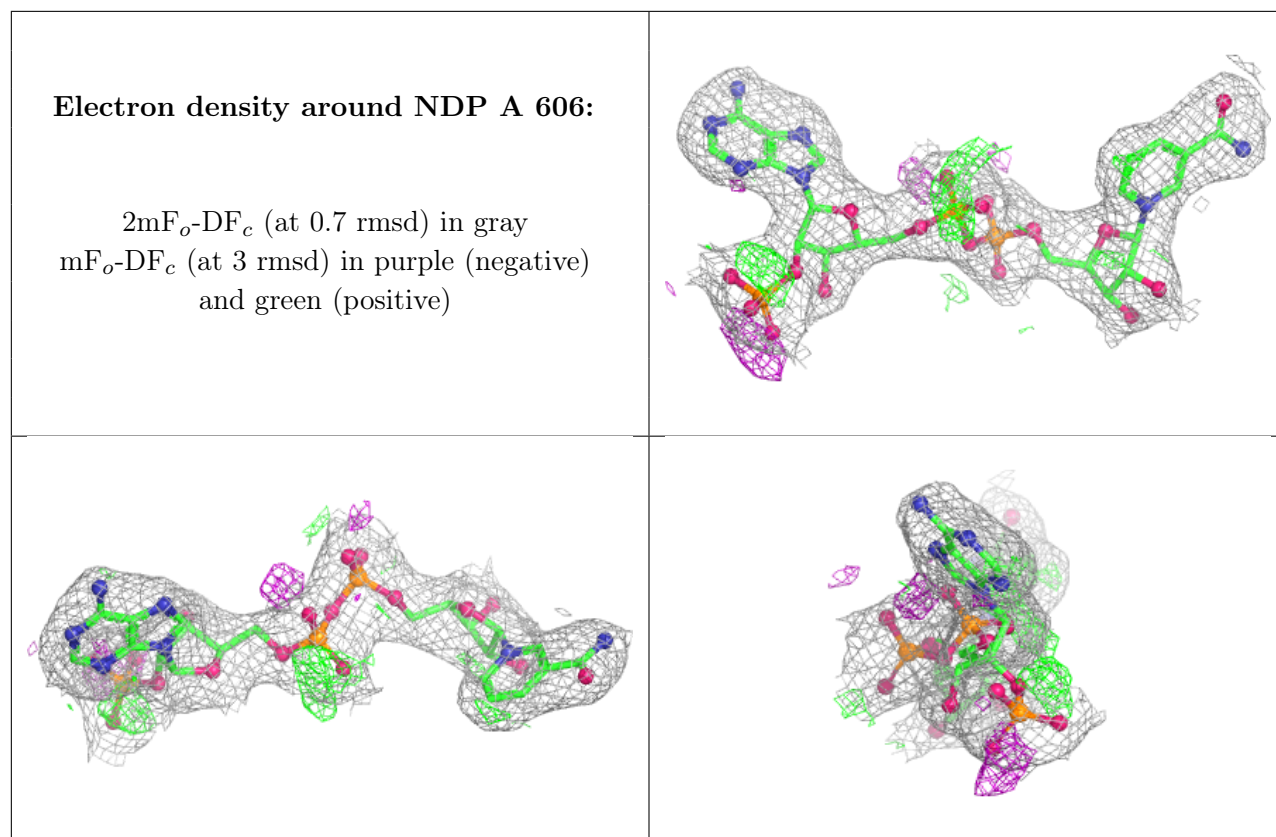
Electron density around UMP C 611:

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

**Electron density around NDP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.