



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:51 AM UTC

PDB ID : 1QZF / pdb_00001qzf
Title : Crystal structure of DHFR-TS from *Cryptosporidium hominis*
Authors : O'Neil, R.H.; Lilien, R.H.; Donald, B.R.; Stroud, R.M.; Anderson, A.C.
Deposited on : 2003-09-16
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

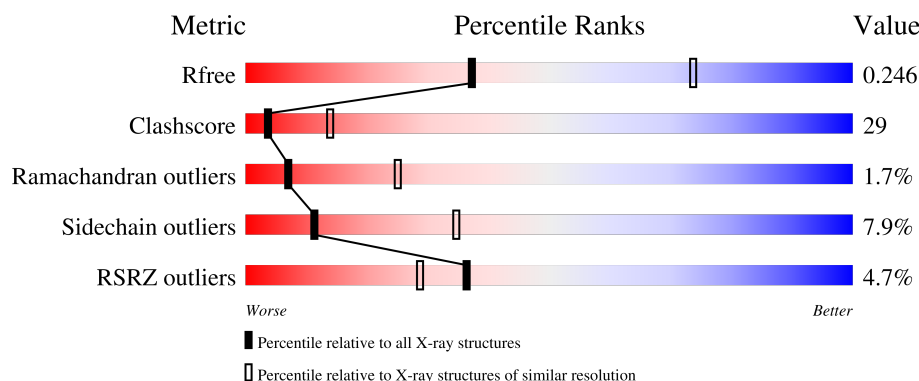
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	521	6% 52% 40% 6%
1	B	521	5% 52% 40% 7%
1	C	521	4% 50% 41% 7%
1	D	521	5% 50% 42% 7%
1	E	521	4% 52% 39% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UMP	A	603	-	-	X	-
2	UMP	B	607	-	-	X	-
2	UMP	C	611	-	-	X	-
3	CB3	A	604	X	-	-	-
3	CB3	B	608	X	-	-	-
3	CB3	C	612	X	-	-	-
3	CB3	D	616	X	-	-	-
3	CB3	E	620	X	-	-	-
4	FOL	A	605	-	-	X	-
4	FOL	D	617	-	-	X	-
4	FOL	E	621	-	-	X	-

2 Entry composition [i](#)

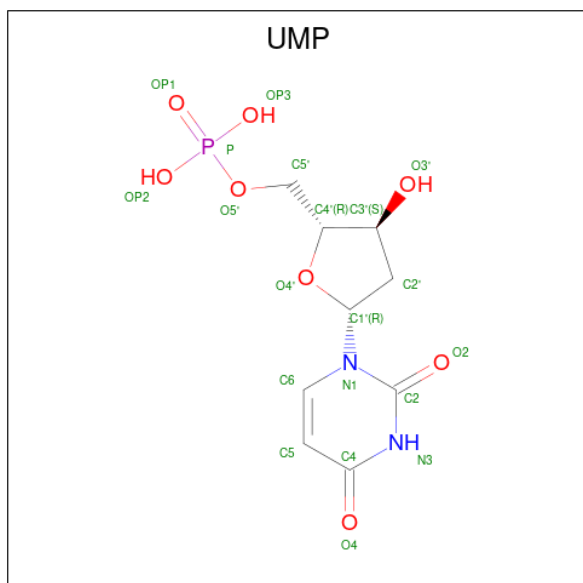
There are 6 unique types of molecules in this entry. The entry contains 22196 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4223	2694	713	793	23			
1	B	519	Total	C	N	O	S	0	0	0
			4223	2694	713	793	23			
1	C	519	Total	C	N	O	S	0	0	0
			4223	2694	713	793	23			
1	D	519	Total	C	N	O	S	0	0	0
			4223	2694	713	793	23			
1	E	519	Total	C	N	O	S	0	0	0
			4223	2694	713	793	23			

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: $C_9H_{13}N_2O_8P$).



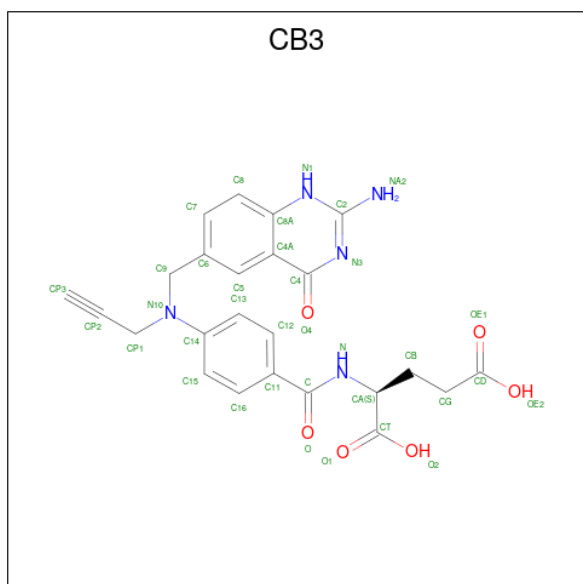
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

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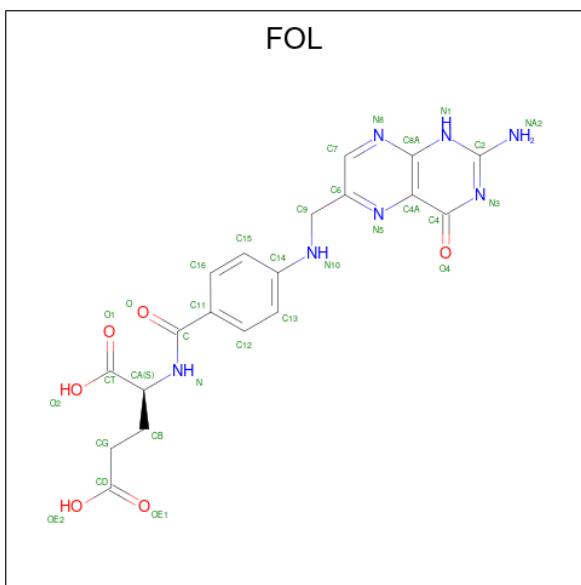
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

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



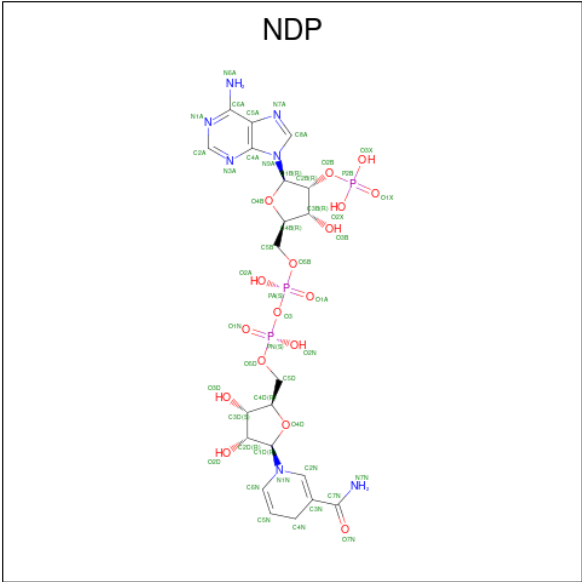
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		
3	D	1	Total	C	N	O	0	0
			35	24	5	6		
3	E	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is FOLIC ACID (CCD ID: FOL) (formula: $C_{19}H_{19}N_7O_6$).



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	C	N	O	P	0	0
			48	21	7	17	3		
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

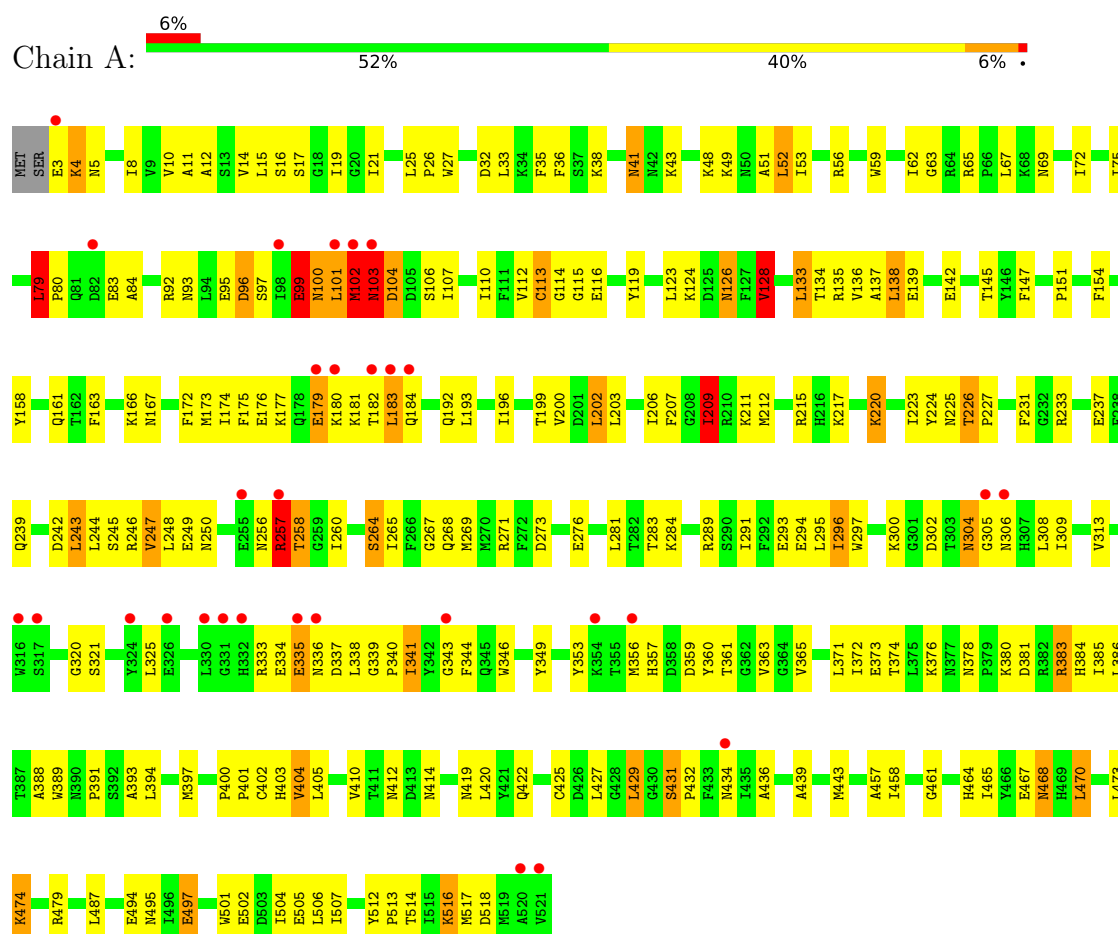
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	101	Total	O	0	0
			101	101		
6	B	116	Total	O	0	0
			116	116		
6	C	83	Total	O	0	0
			83	83		
6	D	71	Total	O	0	0
			71	71		
6	E	35	Total	O	0	0
			35	35		

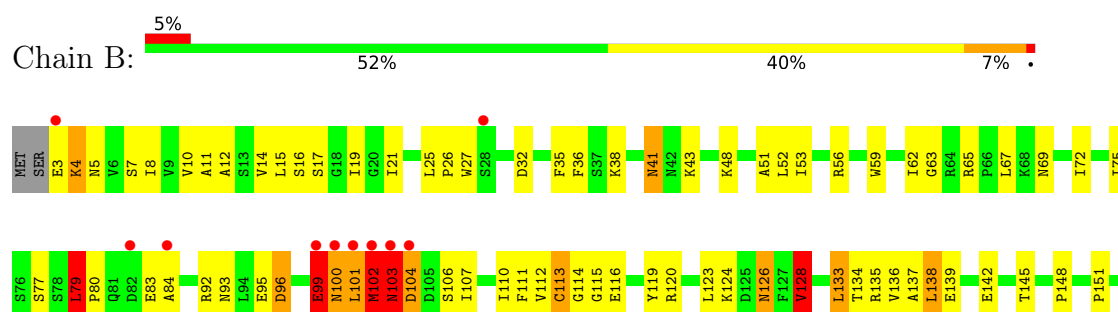
3 Residue-property plots

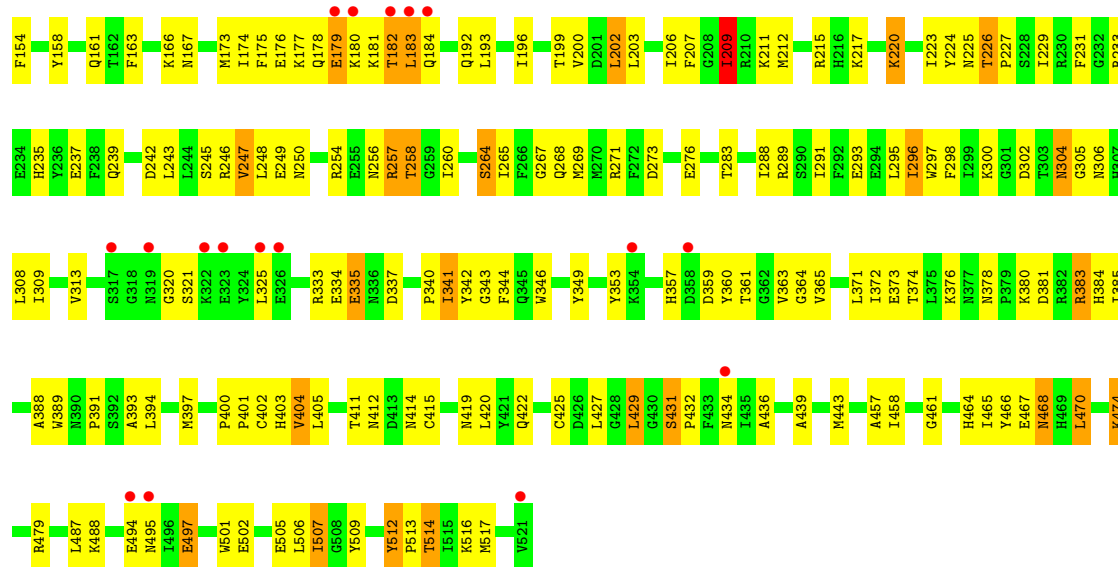
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

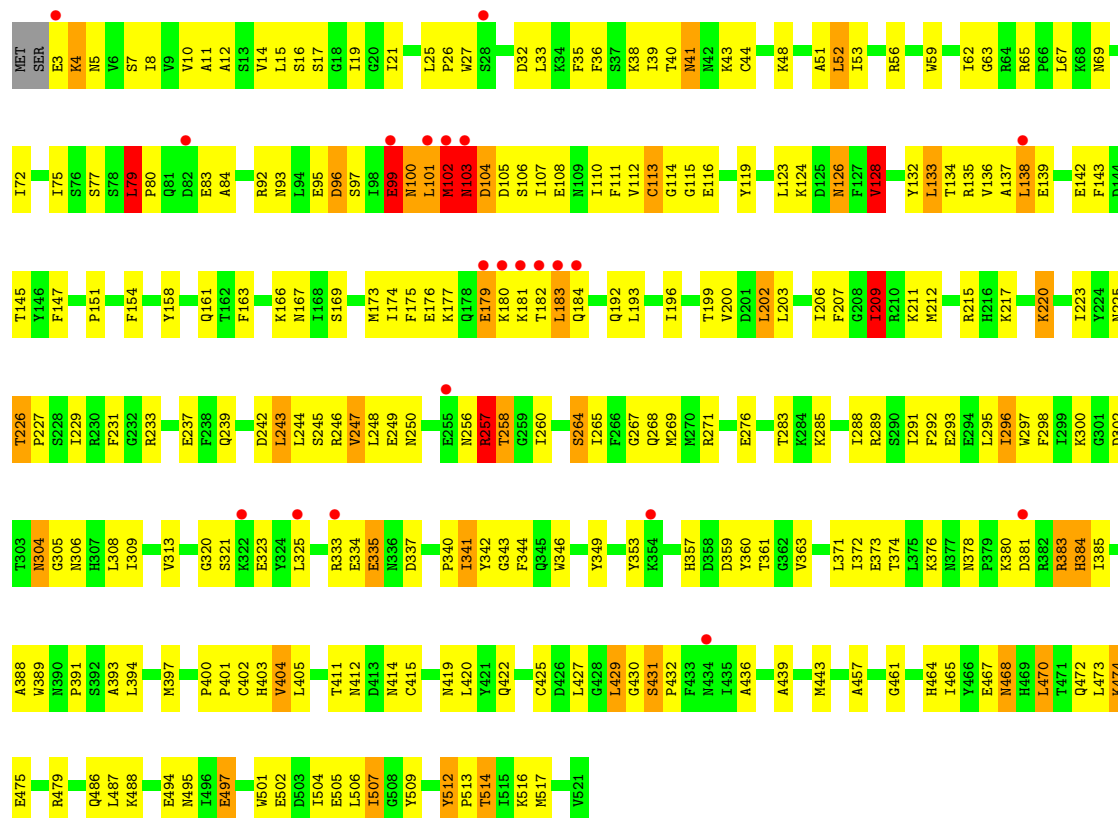


- Molecule 1: bifunctional dihydrofolate reductase-thymidylate synthase



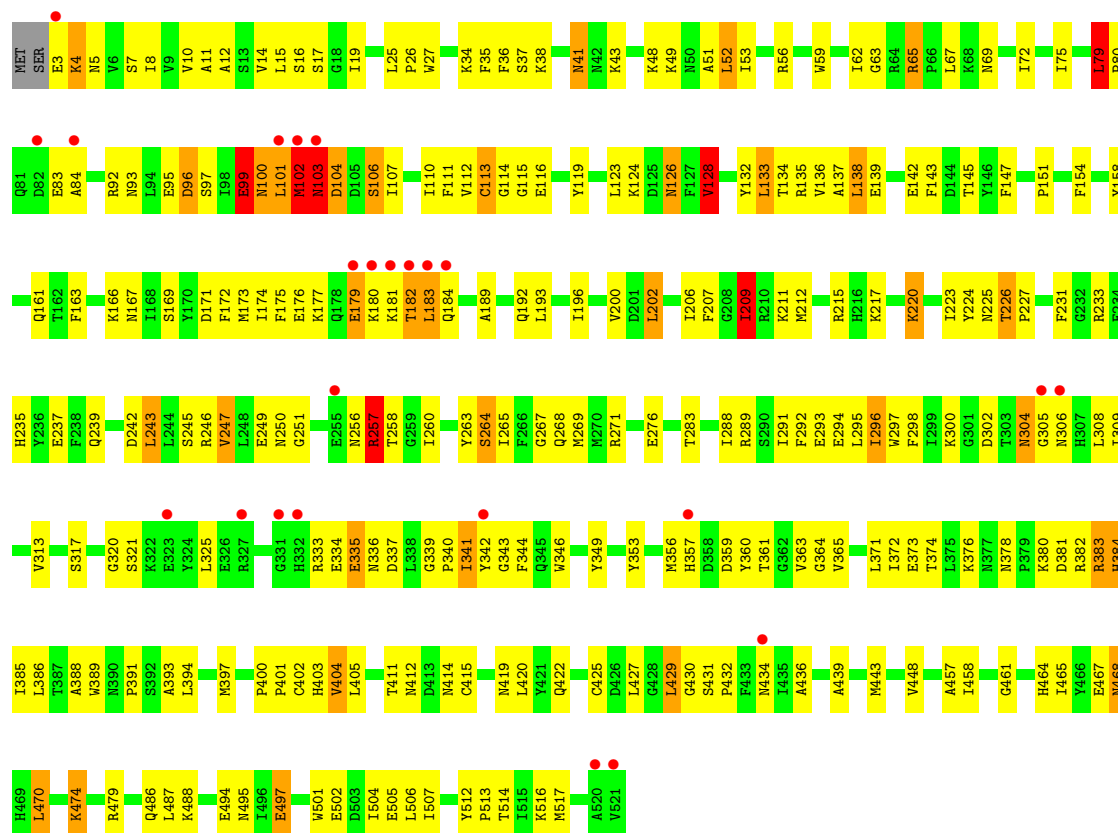


• Molecule 1: bifunctional dihydrofolate reductase-thymidylate synthase

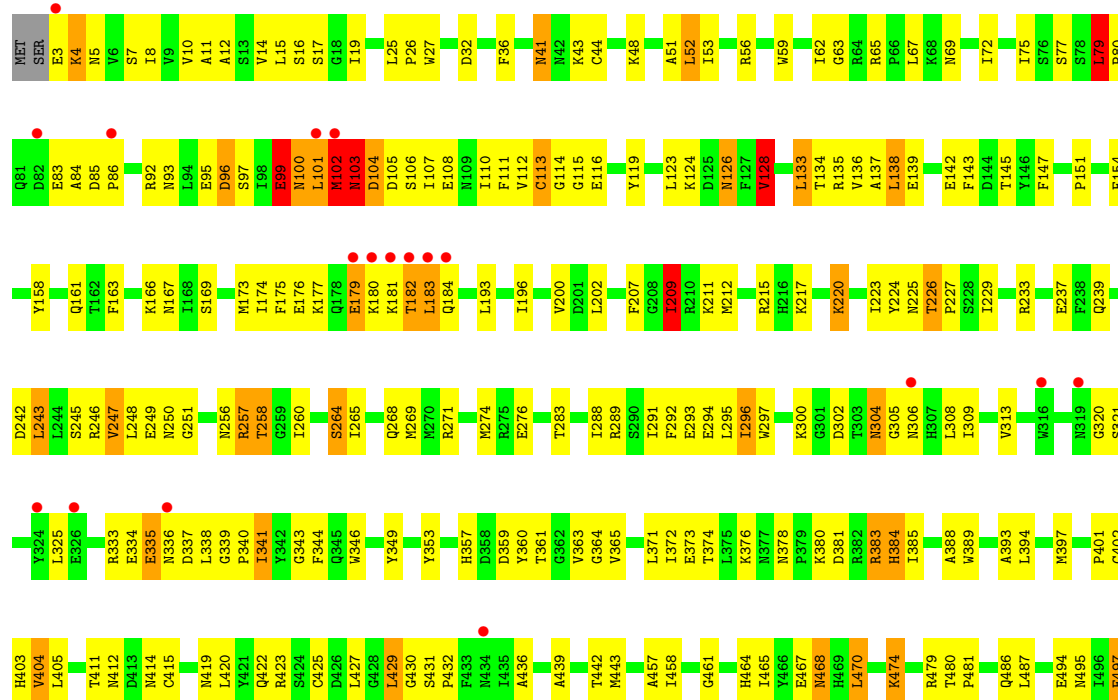


• Molecule 1: bifunctional dihydrofolate reductase-thymidylate synthase





● Molecule 1: bifunctional dihydrofolate reductase-thymidylate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.90Å 116.30Å 219.70Å 90.00° 95.23° 90.00°	Depositor
Resolution (Å)	29.80 – 2.80 29.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.6 (29.80-2.80) 83.6 (29.80-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.245 0.227 , 0.246	Depositor DCC
R_{free} test set	5618 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22196	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.53	1/4320 (0.0%)	1.04	28/5838 (0.5%)
1	B	0.53	1/4320 (0.0%)	1.04	28/5838 (0.5%)
1	C	0.51	0/4320	1.05	30/5838 (0.5%)
1	D	0.51	1/4320 (0.0%)	1.04	30/5838 (0.5%)
1	E	0.50	1/4320 (0.0%)	1.05	31/5838 (0.5%)
All	All	0.52	4/21600 (0.0%)	1.05	147/29190 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	102	MET	SD-CE	6.45	1.95	1.79
1	E	102	MET	SD-CE	5.54	1.93	1.79
1	B	102	MET	SD-CE	5.29	1.92	1.79
1	A	102	MET	SD-CE	5.26	1.92	1.79

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	404	VAL	N-CA-C	11.26	121.23	110.30
1	E	404	VAL	N-CA-C	11.05	121.02	110.30
1	B	404	VAL	N-CA-C	10.89	120.86	110.30
1	D	404	VAL	N-CA-C	10.82	120.79	110.30
1	A	404	VAL	N-CA-C	10.58	120.56	110.30
1	A	100	ASN	N-CA-C	-9.01	100.22	111.75
1	D	100	ASN	N-CA-C	-8.82	100.47	111.75
1	B	100	ASN	N-CA-C	-8.78	100.51	111.75
1	E	100	ASN	N-CA-C	-8.64	100.70	111.75
1	C	100	ASN	N-CA-C	-8.43	100.96	111.75
1	C	113	CYS	N-CA-C	7.77	121.63	112.93
1	E	113	CYS	N-CA-C	7.62	121.46	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	CYS	N-CA-C	7.50	121.32	112.93
1	E	209	ILE	N-CA-C	-7.49	102.88	113.07
1	A	113	CYS	N-CA-C	7.29	121.09	112.93
1	D	113	CYS	N-CA-C	7.24	121.04	112.93
1	C	209	ILE	N-CA-C	-7.14	103.36	113.07
1	B	209	ILE	N-CA-C	-7.05	103.48	113.07
1	A	461	GLY	N-CA-C	-7.05	103.80	110.21
1	D	207	PHE	N-CA-C	-7.01	101.09	110.55
1	E	257	ARG	NE-CZ-NH2	-7.00	112.90	119.20
1	C	25	LEU	N-CA-C	-6.97	100.98	109.83
1	D	461	GLY	N-CA-C	-6.95	103.89	110.21
1	B	128	VAL	N-CA-C	6.88	118.97	108.71
1	E	101	LEU	N-CA-C	-6.86	103.42	111.03
1	D	209	ILE	N-CA-C	-6.83	103.78	113.07
1	A	209	ILE	N-CA-C	-6.82	103.80	113.07
1	B	25	LEU	N-CA-C	-6.80	101.50	109.93
1	B	257	ARG	NE-CZ-NH2	-6.76	113.11	119.20
1	C	461	GLY	N-CA-C	-6.74	104.08	110.21
1	A	101	LEU	N-CA-C	-6.66	103.64	111.03
1	A	226	THR	CA-C-N	6.65	127.18	119.47
1	A	226	THR	C-N-CA	6.65	127.18	119.47
1	C	207	PHE	N-CA-C	-6.63	101.60	110.55
1	D	101	LEU	N-CA-C	-6.63	103.67	111.03
1	C	101	LEU	N-CA-C	-6.61	103.69	111.03
1	A	25	LEU	N-CA-C	-6.60	101.75	109.93
1	E	25	LEU	N-CA-C	-6.59	101.46	109.83
1	B	226	THR	CA-C-N	6.58	127.10	119.47
1	B	226	THR	C-N-CA	6.58	127.10	119.47
1	E	461	GLY	N-CA-C	-6.55	104.25	110.21
1	B	101	LEU	N-CA-C	-6.55	103.76	111.03
1	D	128	VAL	N-CA-C	6.55	118.47	108.71
1	A	128	VAL	N-CA-C	6.55	118.47	108.71
1	E	207	PHE	N-CA-C	-6.51	101.76	110.55
1	B	207	PHE	N-CA-C	-6.45	100.97	110.52
1	C	226	THR	CA-C-N	6.45	126.95	119.47
1	C	226	THR	C-N-CA	6.45	126.95	119.47
1	E	226	THR	CA-C-N	6.44	126.66	119.32
1	E	226	THR	C-N-CA	6.44	126.66	119.32
1	B	461	GLY	N-CA-C	-6.43	104.36	110.21
1	D	257	ARG	NE-CZ-NH2	6.43	124.99	119.20
1	D	25	LEU	N-CA-C	-6.42	101.67	109.83
1	E	128	VAL	N-CA-C	6.42	118.27	108.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	VAL	N-CA-C	6.40	118.25	108.71
1	C	137	ALA	N-CA-C	6.40	119.57	110.68
1	E	257	ARG	CD-NE-CZ	6.39	133.35	124.40
1	D	226	THR	CA-C-N	6.37	126.86	119.47
1	D	226	THR	C-N-CA	6.37	126.86	119.47
1	E	137	ALA	N-CA-C	6.37	119.53	110.68
1	B	14	VAL	N-CA-C	6.37	117.11	110.62
1	A	207	PHE	N-CA-C	-6.33	101.15	110.52
1	C	470	LEU	N-CA-C	6.31	117.82	111.07
1	D	257	ARG	NE-CZ-NH1	-6.29	115.21	121.50
1	B	264	SER	N-CA-C	6.28	118.72	109.24
1	B	257	ARG	CD-NE-CZ	6.24	133.14	124.40
1	C	14	VAL	N-CA-C	6.23	116.97	110.62
1	C	79	LEU	CA-C-N	6.23	126.18	119.76
1	C	79	LEU	C-N-CA	6.23	126.18	119.76
1	B	470	LEU	N-CA-C	6.22	117.72	111.07
1	D	137	ALA	N-CA-C	6.20	119.30	110.68
1	E	14	VAL	N-CA-C	6.19	116.93	110.62
1	D	264	SER	N-CA-C	6.17	118.56	109.24
1	E	5	ASN	N-CA-C	6.14	119.16	110.50
1	A	99	GLU	N-CA-C	-6.14	97.72	110.80
1	A	137	ALA	N-CA-C	6.14	119.21	110.68
1	E	470	LEU	N-CA-C	6.13	117.63	111.07
1	C	5	ASN	N-CA-C	6.13	119.55	110.48
1	B	5	ASN	N-CA-C	6.11	119.11	110.50
1	C	99	GLU	N-CA-C	-6.09	97.83	110.80
1	E	105	ASP	N-CA-C	-6.07	105.58	112.87
1	E	264	SER	N-CA-C	6.05	118.37	109.24
1	E	99	GLU	N-CA-C	-6.01	97.99	110.80
1	B	99	GLU	N-CA-C	-6.01	98.00	110.80
1	A	257	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	C	257	ARG	NE-CZ-NH2	5.97	124.58	119.20
1	B	137	ALA	N-CA-C	5.97	118.98	110.68
1	D	99	GLU	N-CA-C	-5.95	98.13	110.80
1	A	470	LEU	N-CA-C	5.95	117.44	111.07
1	E	257	ARG	NE-CZ-NH1	5.93	127.44	121.50
1	D	5	ASN	N-CA-C	5.92	119.24	110.48
1	A	5	ASN	N-CA-C	5.90	119.22	110.48
1	A	257	ARG	NE-CZ-NH1	-5.89	115.61	121.50
1	D	414	ASN	N-CA-C	5.89	119.55	111.54
1	B	79	LEU	CA-C-N	5.87	125.81	119.76
1	B	79	LEU	C-N-CA	5.87	125.81	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	470	LEU	N-CA-C	5.86	117.34	111.07
1	A	79	LEU	CA-C-N	5.85	125.78	119.76
1	A	79	LEU	C-N-CA	5.85	125.78	119.76
1	A	264	SER	N-CA-C	5.85	118.58	109.52
1	A	14	VAL	N-CA-C	5.84	116.57	110.62
1	C	257	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	C	264	SER	N-CA-C	5.78	118.48	109.52
1	A	414	ASN	N-CA-C	5.77	119.39	111.54
1	B	257	ARG	NE-CZ-NH1	5.77	127.27	121.50
1	D	14	VAL	N-CA-C	5.76	116.50	110.62
1	C	105	ASP	N-CA-C	-5.69	106.04	112.87
1	C	414	ASN	N-CA-C	5.68	119.27	111.54
1	D	344	PHE	N-CA-C	-5.67	105.10	111.28
1	B	161	GLN	N-CA-C	-5.67	103.44	110.41
1	C	344	PHE	N-CA-C	-5.66	105.11	111.28
1	B	414	ASN	N-CA-C	5.64	119.36	111.74
1	E	474	LYS	N-CA-C	-5.63	105.22	111.36
1	E	344	PHE	N-CA-C	-5.58	105.19	111.28
1	E	161	GLN	N-CA-C	-5.55	103.58	110.41
1	D	474	LYS	N-CA-C	-5.47	105.40	111.36
1	C	474	LYS	N-CA-C	-5.47	105.40	111.36
1	C	33	LEU	N-CA-C	-5.43	105.45	111.36
1	E	414	ASN	N-CA-C	5.39	119.02	111.74
1	C	161	GLN	N-CA-C	-5.38	103.79	110.41
1	D	79	LEU	CA-C-N	5.38	125.30	119.76
1	D	79	LEU	C-N-CA	5.38	125.30	119.76
1	E	79	LEU	CA-C-N	5.37	125.30	119.76
1	E	79	LEU	C-N-CA	5.37	125.30	119.76
1	A	474	LYS	N-CA-C	-5.37	105.50	111.36
1	A	243	LEU	N-CA-C	-5.36	105.54	111.71
1	D	161	GLN	N-CA-C	-5.35	103.55	110.19
1	D	65	ARG	CA-C-N	5.35	125.34	119.89
1	D	65	ARG	C-N-CA	5.35	125.34	119.89
1	B	344	PHE	N-CA-C	-5.34	105.45	111.28
1	A	344	PHE	N-CA-C	-5.33	105.55	111.36
1	D	106	SER	N-CA-C	-5.29	105.69	111.82
1	E	512	TYR	N-CA-C	-5.27	102.48	110.39
1	A	161	GLN	N-CA-C	-5.24	103.97	110.41
1	C	507	ILE	N-CA-C	5.22	116.22	108.23
1	E	243	LEU	N-CA-C	-5.15	105.79	111.71
1	B	474	LYS	N-CA-C	-5.15	105.75	111.36
1	D	243	LEU	N-CA-C	-5.14	105.80	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	507	ILE	N-CA-C	5.13	116.08	108.23
1	A	504	ILE	N-CA-C	5.12	116.33	108.71
1	C	512	TYR	N-CA-C	-5.11	102.73	110.39
1	D	263	TYR	N-CA-C	-5.09	100.11	108.41
1	E	504	ILE	N-CA-C	5.09	116.30	108.71
1	E	507	ILE	N-CA-C	5.08	116.01	108.23
1	A	33	LEU	N-CA-C	-5.02	105.89	111.36
1	B	512	TYR	N-CA-C	-5.00	102.88	110.39
1	C	243	LEU	N-CA-C	-5.00	105.96	111.71

There are no chirality outliers.

There are no planarity outliers.

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	4223	0	4159	257	0
1	B	4223	0	4159	245	0
1	C	4223	0	4159	255	0
1	D	4223	0	4159	253	0
1	E	4223	0	4159	237	0
2	A	20	0	11	7	0
2	B	20	0	11	8	0
2	C	20	0	11	7	0
2	D	20	0	11	3	0
2	E	20	0	11	6	0
3	A	35	0	21	3	0
3	B	35	0	21	3	0
3	C	35	0	21	3	0
3	D	35	0	21	3	0
3	E	35	0	21	4	0
4	A	32	0	17	9	0
4	B	32	0	17	8	0
4	C	32	0	17	8	0
4	D	32	0	17	9	0
4	E	32	0	17	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	48	0	26	10	0
5	B	48	0	26	7	0
5	C	48	0	26	9	0
5	D	48	0	26	10	0
5	E	48	0	26	10	0
6	A	101	0	0	7	0
6	B	116	0	0	3	0
6	C	83	0	0	1	0
6	D	71	0	0	6	0
6	E	35	0	0	2	0
All	All	22196	0	21170	1244	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (1244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:MET:HE2	1:B:269:MET:HE2	1.09	1.07
1:C:269:MET:HE2	1:D:269:MET:HE2	1.11	1.04
1:A:434:ASN:HD21	2:A:603:UMP:HN3	0.98	0.97
4:D:617:FOL:C7	5:D:618:NDP:H42N	1.94	0.96
4:E:621:FOL:N5	4:E:621:FOL:H13	1.81	0.96
4:D:617:FOL:H13	4:D:617:FOL:N5	1.83	0.94
1:A:269:MET:HE2	1:B:269:MET:CE	1.98	0.93
1:A:209:ILE:HD12	1:A:209:ILE:H	1.34	0.93
4:B:609:FOL:H13	4:B:609:FOL:N5	1.83	0.93
4:A:605:FOL:H13	4:A:605:FOL:N5	1.81	0.93
1:B:3:GLU:HG3	1:B:4:LYS:H	1.33	0.92
1:A:269:MET:CE	1:B:269:MET:HE2	1.99	0.92
1:E:3:GLU:HG3	1:E:4:LYS:H	1.34	0.92
1:A:3:GLU:HG3	1:A:4:LYS:H	1.34	0.92
4:C:613:FOL:H13	4:C:613:FOL:N5	1.82	0.92
1:E:102:MET:HE3	1:E:102:MET:HA	1.50	0.92
1:C:102:MET:HE3	1:C:102:MET:HA	1.51	0.92
1:B:102:MET:HE3	1:B:102:MET:HA	1.50	0.91
1:D:102:MET:HE3	1:D:102:MET:HA	1.52	0.90
1:C:3:GLU:HG3	1:C:4:LYS:H	1.33	0.90
1:D:434:ASN:ND2	6:D:621:HOH:O	2.05	0.90
4:E:621:FOL:C7	5:E:622:NDP:H42N	2.02	0.90
1:A:102:MET:HA	1:A:102:MET:HE3	1.51	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:MET:CE	1:D:269:MET:HE2	2.02	0.88
1:E:4:LYS:HB3	1:E:101:LEU:CD2	2.04	0.88
1:C:269:MET:HE2	1:D:269:MET:CE	2.02	0.87
1:C:209:ILE:H	1:C:209:ILE:HD12	1.39	0.87
1:D:3:GLU:HG3	1:D:4:LYS:H	1.36	0.87
1:E:209:ILE:H	1:E:209:ILE:HD12	1.39	0.86
1:D:4:LYS:HB3	1:D:101:LEU:CD2	2.05	0.86
1:C:4:LYS:HB3	1:C:101:LEU:CD2	2.05	0.86
1:B:4:LYS:HB3	1:B:101:LEU:CD2	2.06	0.86
1:B:209:ILE:HD12	1:B:209:ILE:H	1.40	0.85
1:D:209:ILE:HD12	1:D:209:ILE:H	1.38	0.85
1:D:360:TYR:O	1:D:363:VAL:HG12	1.78	0.84
1:E:360:TYR:O	1:E:363:VAL:HG12	1.78	0.84
4:C:613:FOL:C7	5:C:614:NDP:H42N	2.08	0.83
1:A:4:LYS:HB3	1:A:101:LEU:CD2	2.08	0.83
1:C:3:GLU:CG	1:C:4:LYS:H	1.92	0.82
1:C:402:CYS:SG	2:C:611:UMP:C6	2.73	0.82
1:B:304:ASN:C	1:B:304:ASN:HD22	1.86	0.82
1:C:304:ASN:C	1:C:304:ASN:HD22	1.88	0.81
1:D:293:GLU:HA	1:D:296:ILE:HD11	1.61	0.81
1:B:3:GLU:CG	1:B:4:LYS:H	1.93	0.81
1:A:3:GLU:CG	1:A:4:LYS:H	1.94	0.81
1:A:217:LYS:H	1:A:250:ASN:HD21	1.25	0.81
1:E:3:GLU:CG	1:E:4:LYS:H	1.93	0.81
1:E:293:GLU:HA	1:E:296:ILE:HD11	1.64	0.80
1:B:293:GLU:HA	1:B:296:ILE:HD11	1.63	0.80
1:B:217:LYS:H	1:B:250:ASN:HD21	1.28	0.80
1:B:360:TYR:O	1:B:363:VAL:HG12	1.82	0.79
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.17	0.79
1:C:360:TYR:O	1:C:363:VAL:HG12	1.82	0.79
1:C:56:ARG:HD3	5:C:614:NDP:O2X	1.82	0.79
1:C:293:GLU:HA	1:C:296:ILE:HD11	1.64	0.79
1:A:293:GLU:HA	1:A:296:ILE:HD11	1.63	0.79
1:A:360:TYR:O	1:A:363:VAL:HG12	1.82	0.79
4:A:605:FOL:C7	5:A:606:NDP:H42N	2.12	0.79
1:A:304:ASN:HD22	1:A:304:ASN:C	1.89	0.79
1:C:349:TYR:CE2	1:D:391:PRO:HD2	2.18	0.79
1:E:26:PRO:HG2	1:E:27:TRP:CE3	2.18	0.79
1:B:26:PRO:HG2	1:B:27:TRP:CE3	2.18	0.78
1:D:217:LYS:H	1:D:250:ASN:HD21	1.29	0.78
1:C:4:LYS:HB3	1:C:101:LEU:HD22	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:LYS:H	1:C:250:ASN:HD21	1.32	0.78
1:D:3:GLU:CG	1:D:4:LYS:H	1.96	0.78
1:D:304:ASN:C	1:D:304:ASN:HD22	1.91	0.78
1:C:391:PRO:HD2	1:D:349:TYR:CE2	2.20	0.77
1:E:341:ILE:HA	1:E:397:MET:HE3	1.67	0.77
4:B:609:FOL:C7	5:B:610:NDP:H42N	2.14	0.77
1:E:217:LYS:H	1:E:250:ASN:HD21	1.29	0.77
1:A:349:TYR:CE2	1:B:391:PRO:HD2	2.20	0.77
1:B:402:CYS:SG	2:B:607:UMP:C6	2.78	0.77
1:E:4:LYS:HB3	1:E:101:LEU:HD22	1.66	0.77
1:C:26:PRO:HG2	1:C:27:TRP:CE3	2.19	0.77
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.19	0.76
1:A:217:LYS:N	1:A:250:ASN:HD21	1.84	0.76
1:E:304:ASN:C	1:E:304:ASN:HD22	1.92	0.76
1:D:4:LYS:HB3	1:D:101:LEU:HD22	1.68	0.76
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.21	0.76
1:B:193:LEU:HD21	1:B:196:ILE:HD12	1.68	0.75
1:A:341:ILE:HA	1:A:397:MET:HE3	1.68	0.75
1:B:4:LYS:HB3	1:B:101:LEU:HD22	1.67	0.75
2:E:619:UMP:H1'	3:E:620:CB3:C4	2.17	0.75
1:C:193:LEU:HD21	1:C:196:ILE:HD12	1.67	0.75
1:D:193:LEU:HD21	1:D:196:ILE:HD12	1.70	0.74
1:E:397:MET:HE1	1:E:401:PRO:HG3	1.69	0.74
1:D:26:PRO:HG2	1:D:27:TRP:CZ3	2.22	0.74
1:E:26:PRO:HG2	1:E:27:TRP:CZ3	2.23	0.74
2:C:611:UMP:H1'	3:C:612:CB3:C4	2.16	0.74
1:D:341:ILE:HA	1:D:397:MET:HE3	1.69	0.74
1:B:341:ILE:HA	1:B:397:MET:HE3	1.68	0.74
1:A:4:LYS:HB3	1:A:101:LEU:HD22	1.69	0.74
1:A:304:ASN:ND2	1:A:306:ASN:H	1.86	0.74
2:B:607:UMP:H1'	3:B:608:CB3:C4	2.17	0.74
1:D:4:LYS:HB3	1:D:101:LEU:HD23	1.70	0.74
1:E:56:ARG:HD3	5:E:622:NDP:O2X	1.87	0.74
1:C:304:ASN:ND2	1:C:306:ASN:H	1.85	0.73
1:E:4:LYS:HB3	1:E:101:LEU:HD23	1.69	0.73
1:B:304:ASN:ND2	1:B:306:ASN:H	1.86	0.73
1:B:217:LYS:N	1:B:250:ASN:HD21	1.87	0.73
1:E:193:LEU:HD21	1:E:196:ILE:HD12	1.71	0.73
1:A:209:ILE:HD12	1:A:209:ILE:N	2.02	0.72
1:E:217:LYS:N	1:E:250:ASN:HD21	1.86	0.72
1:C:267:GLY:O	1:D:271:ARG:NH2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:ILE:HA	1:C:397:MET:HE3	1.70	0.72
1:D:151:PRO:HG2	1:D:154:PHE:HD2	1.54	0.72
1:D:217:LYS:N	1:D:250:ASN:HD21	1.86	0.72
1:A:26:PRO:HG2	1:A:27:TRP:CZ3	2.23	0.72
1:B:26:PRO:HG2	1:B:27:TRP:CZ3	2.23	0.72
1:E:297:TRP:CD1	1:E:302:ASP:HB3	2.24	0.72
1:A:271:ARG:NH2	1:B:267:GLY:O	2.22	0.72
1:A:297:TRP:CD1	1:A:302:ASP:HB3	2.25	0.72
1:C:79:LEU:HD23	1:C:80:PRO:HD2	1.70	0.72
1:D:209:ILE:HD12	1:D:209:ILE:N	2.05	0.72
1:C:26:PRO:HG2	1:C:27:TRP:CZ3	2.25	0.72
1:A:193:LEU:HD21	1:A:196:ILE:HD12	1.72	0.71
1:C:397:MET:HE1	1:C:401:PRO:HG3	1.72	0.71
1:D:297:TRP:CD1	1:D:302:ASP:HB3	2.25	0.71
1:C:217:LYS:N	1:C:250:ASN:HD21	1.88	0.71
1:E:79:LEU:HD23	1:E:80:PRO:HD2	1.72	0.71
1:E:183:LEU:HD21	6:E:644:HOH:O	1.89	0.71
1:B:4:LYS:HB3	1:B:101:LEU:HD23	1.72	0.71
1:D:304:ASN:ND2	1:D:306:ASN:H	1.89	0.71
1:A:192:GLN:HG3	1:B:231:PHE:CD2	2.26	0.71
1:D:397:MET:HE1	1:D:401:PRO:HG3	1.71	0.71
1:A:397:MET:HE1	1:A:401:PRO:HG3	1.73	0.70
1:A:402:CYS:SG	2:A:603:UMP:C6	2.84	0.70
1:C:192:GLN:HG3	1:D:231:PHE:CD2	2.26	0.70
1:B:79:LEU:HD23	1:B:80:PRO:HD2	1.71	0.70
1:E:209:ILE:HD12	1:E:209:ILE:N	2.06	0.70
1:C:4:LYS:HB3	1:C:101:LEU:HD23	1.73	0.70
1:E:4:LYS:HE3	1:E:101:LEU:HA	1.74	0.70
1:C:136:VAL:HG12	1:C:138:LEU:HD22	1.74	0.70
1:C:209:ILE:HD12	1:C:209:ILE:N	2.06	0.70
1:D:317:SER:HA	6:D:650:HOH:O	1.91	0.70
1:A:217:LYS:H	1:A:250:ASN:ND2	1.90	0.69
2:A:603:UMP:H1'	3:A:604:CB3:C4	2.21	0.69
1:E:151:PRO:HG2	1:E:154:PHE:HD2	1.56	0.69
1:B:136:VAL:HG12	1:B:138:LEU:HD22	1.74	0.69
1:E:304:ASN:ND2	1:E:306:ASN:H	1.89	0.69
1:A:4:LYS:HB3	1:A:101:LEU:HD23	1.73	0.69
1:C:4:LYS:HE3	1:C:101:LEU:HA	1.74	0.69
1:E:136:VAL:HG12	1:E:138:LEU:HD22	1.74	0.69
1:A:231:PHE:CD2	1:B:192:GLN:HG3	2.27	0.69
1:A:79:LEU:HD23	1:A:80:PRO:HD2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:PRO:HG2	1:C:154:PHE:HD2	1.56	0.69
1:B:209:ILE:HD12	1:B:209:ILE:N	2.07	0.69
1:D:56:ARG:HD3	5:D:618:NDP:O2X	1.93	0.69
1:A:151:PRO:HG2	1:A:154:PHE:HD2	1.58	0.69
1:B:99:GLU:OE2	1:B:99:GLU:C	2.36	0.69
1:E:257:ARG:HD3	2:E:619:UMP:OP1	1.92	0.68
1:B:4:LYS:HE3	1:B:101:LEU:HA	1.75	0.68
1:D:114:GLY:HA2	1:D:119:TYR:CZ	2.28	0.68
1:C:297:TRP:CD1	1:C:302:ASP:HB3	2.28	0.68
1:A:99:GLU:OE2	1:A:99:GLU:C	2.37	0.68
1:E:114:GLY:HA2	1:E:119:TYR:CZ	2.28	0.67
1:A:114:GLY:HA2	1:A:119:TYR:CZ	2.29	0.67
1:B:397:MET:HE1	1:B:401:PRO:HG3	1.74	0.67
1:D:136:VAL:HG12	1:D:138:LEU:HD22	1.75	0.67
1:D:257:ARG:NE	2:D:615:UMP:OP1	2.27	0.67
4:E:621:FOL:N5	4:E:621:FOL:C13	2.56	0.67
1:C:114:GLY:HA2	1:C:119:TYR:CZ	2.30	0.67
1:B:297:TRP:CD1	1:B:302:ASP:HB3	2.30	0.67
1:B:103:ASN:O	1:B:104:ASP:C	2.37	0.67
1:B:114:GLY:HA2	1:B:119:TYR:CZ	2.30	0.67
1:D:209:ILE:H	1:D:209:ILE:CD1	2.08	0.67
1:C:231:PHE:CD2	1:D:192:GLN:HG3	2.29	0.67
1:A:4:LYS:HE3	1:A:101:LEU:HA	1.77	0.67
1:D:180:LYS:HG3	1:D:181:LYS:H	1.60	0.67
1:E:217:LYS:H	1:E:250:ASN:ND2	1.93	0.67
1:A:180:LYS:HG3	1:A:181:LYS:H	1.59	0.66
4:A:605:FOL:N5	4:A:605:FOL:C13	2.57	0.66
1:B:102:MET:O	1:B:103:ASN:HB3	1.95	0.66
4:C:613:FOL:N5	4:C:613:FOL:C13	2.58	0.66
4:B:609:FOL:N5	4:B:609:FOL:C13	2.58	0.66
1:C:103:ASN:O	1:C:104:ASP:C	2.38	0.66
1:C:256:ASN:HD22	1:C:258:THR:H	1.44	0.66
1:D:103:ASN:O	1:D:104:ASP:C	2.38	0.66
1:E:103:ASN:O	1:E:104:ASP:C	2.38	0.66
1:A:56:ARG:HD3	5:A:606:NDP:O1X	1.94	0.66
1:A:136:VAL:HG12	1:A:138:LEU:HD22	1.77	0.66
1:A:256:ASN:HD22	1:A:258:THR:H	1.44	0.66
1:B:56:ARG:HD3	5:B:610:NDP:O1X	1.96	0.66
1:C:113:CYS:O	4:C:613:FOL:H7	1.95	0.66
1:E:308:LEU:HD12	1:E:313:VAL:HG11	1.78	0.66
1:A:103:ASN:O	1:A:104:ASP:C	2.37	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:PRO:HG2	1:B:154:PHE:HD2	1.60	0.66
1:B:180:LYS:HG3	1:B:181:LYS:H	1.60	0.66
1:D:217:LYS:H	1:D:250:ASN:ND2	1.92	0.66
1:D:260:ILE:HD12	1:D:260:ILE:N	2.11	0.66
1:E:83:GLU:OE2	1:E:83:GLU:HA	1.95	0.66
1:C:257:ARG:NE	2:C:611:UMP:OP1	2.28	0.66
1:B:83:GLU:OE2	1:B:83:GLU:HA	1.96	0.66
1:D:402:CYS:SG	2:D:615:UMP:C6	2.89	0.66
1:E:99:GLU:C	1:E:99:GLU:OE2	2.39	0.66
1:A:297:TRP:CG	1:A:308:LEU:HD21	2.31	0.65
1:B:297:TRP:CG	1:B:308:LEU:HD21	2.31	0.65
1:D:83:GLU:HA	1:D:83:GLU:OE2	1.96	0.65
1:D:99:GLU:OE2	1:D:99:GLU:C	2.38	0.65
1:A:434:ASN:ND2	2:A:603:UMP:HN3	1.83	0.65
1:B:217:LYS:H	1:B:250:ASN:ND2	1.93	0.65
1:B:223:ILE:O	1:B:245:SER:HB3	1.97	0.65
1:E:297:TRP:CG	1:E:308:LEU:HD21	2.31	0.65
1:A:38:LYS:HB3	1:B:202:LEU:HG	1.78	0.65
1:B:419:ASN:ND2	1:B:457:ALA:HB3	2.10	0.65
1:B:509:TYR:HA	6:B:624:HOH:O	1.97	0.65
1:C:4:LYS:CE	1:C:101:LEU:HA	2.27	0.65
1:C:209:ILE:H	1:C:209:ILE:CD1	2.10	0.65
1:C:419:ASN:ND2	1:C:457:ALA:HB3	2.11	0.65
4:E:621:FOL:C6	5:E:622:NDP:H42N	2.26	0.65
1:A:83:GLU:HA	1:A:83:GLU:OE2	1.96	0.65
1:B:256:ASN:HD22	1:B:258:THR:H	1.44	0.65
1:A:209:ILE:H	1:A:209:ILE:CD1	2.05	0.65
1:A:267:GLY:O	1:B:271:ARG:NH2	2.30	0.65
1:C:271:ARG:NH2	1:D:267:GLY:O	2.30	0.65
1:C:297:TRP:CG	1:C:308:LEU:HD21	2.31	0.65
1:C:102:MET:O	1:C:103:ASN:HB3	1.95	0.64
1:D:79:LEU:HD23	1:D:80:PRO:HD2	1.79	0.64
1:E:209:ILE:H	1:E:209:ILE:CD1	2.09	0.64
1:E:260:ILE:N	1:E:260:ILE:HD12	2.13	0.64
1:B:209:ILE:H	1:B:209:ILE:CD1	2.10	0.64
1:E:180:LYS:HG3	1:E:181:LYS:H	1.61	0.64
1:D:4:LYS:HE3	1:D:101:LEU:HA	1.78	0.64
1:D:308:LEU:HD12	1:D:313:VAL:HG11	1.78	0.64
1:E:223:ILE:O	1:E:245:SER:HB3	1.97	0.64
1:C:260:ILE:N	1:C:260:ILE:HD12	2.13	0.64
1:B:3:GLU:HG3	1:B:4:LYS:N	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:GLU:C	1:C:99:GLU:OE2	2.40	0.64
4:D:617:FOL:N5	4:D:617:FOL:C13	2.58	0.64
1:A:102:MET:O	1:A:103:ASN:HB3	1.98	0.64
1:B:104:ASP:C	1:B:106:SER:H	2.04	0.64
1:D:52:LEU:HB3	1:D:113:CYS:SG	2.38	0.64
1:E:52:LEU:HB3	1:E:113:CYS:SG	2.38	0.64
1:B:4:LYS:CE	1:B:101:LEU:HA	2.28	0.64
1:C:3:GLU:HG3	1:C:4:LYS:N	2.11	0.64
1:C:223:ILE:O	1:C:245:SER:HB3	1.98	0.64
1:D:223:ILE:O	1:D:245:SER:HB3	1.98	0.64
1:E:4:LYS:CE	1:E:101:LEU:HA	2.28	0.63
1:A:260:ILE:N	1:A:260:ILE:HD12	2.13	0.63
1:C:180:LYS:HG3	1:C:181:LYS:H	1.62	0.63
1:C:217:LYS:H	1:C:250:ASN:ND2	1.96	0.63
1:E:102:MET:O	1:E:103:ASN:HB3	1.97	0.63
1:A:102:MET:HA	1:A:102:MET:CE	2.27	0.63
1:D:297:TRP:CG	1:D:308:LEU:HD21	2.33	0.63
1:C:502:GLU:CD	1:C:502:GLU:H	2.07	0.63
1:E:19:ILE:HB	5:E:622:NDP:N7N	2.14	0.63
1:E:419:ASN:ND2	1:E:457:ALA:HB3	2.14	0.63
1:E:19:ILE:O	5:E:622:NDP:H2N	1.98	0.63
1:D:102:MET:HA	1:D:102:MET:CE	2.27	0.63
1:A:223:ILE:O	1:A:245:SER:HB3	1.99	0.62
1:C:63:GLY:O	1:C:65:ARG:HG3	1.98	0.62
1:A:52:LEU:HB3	1:A:113:CYS:SG	2.40	0.62
1:B:260:ILE:HD12	1:B:260:ILE:N	2.14	0.62
1:D:256:ASN:HD22	1:D:258:THR:H	1.47	0.62
1:A:3:GLU:HG3	1:A:4:LYS:N	2.12	0.62
1:B:257:ARG:HD3	2:B:607:UMP:OP1	2.00	0.62
1:C:93:ASN:HD21	1:C:95:GLU:HB3	1.64	0.62
1:B:502:GLU:H	1:B:502:GLU:CD	2.08	0.62
1:A:126:ASN:HA	6:A:703:HOH:O	2.00	0.62
1:A:202:LEU:HG	1:B:38:LYS:HB3	1.81	0.62
1:E:3:GLU:HG3	1:E:4:LYS:N	2.11	0.62
1:E:102:MET:HA	1:E:102:MET:CE	2.27	0.62
1:A:104:ASP:C	1:A:106:SER:H	2.05	0.61
1:D:104:ASP:C	1:D:106:SER:H	2.08	0.61
1:C:225:ASN:O	1:C:233:ARG:NH2	2.33	0.61
1:D:4:LYS:CE	1:D:101:LEU:HA	2.31	0.61
1:A:308:LEU:HD12	1:A:313:VAL:HG11	1.82	0.61
1:A:419:ASN:ND2	1:A:457:ALA:HB3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ASP:C	1:C:106:SER:H	2.08	0.61
1:B:308:LEU:HD12	1:B:313:VAL:HG11	1.82	0.61
1:D:102:MET:O	1:D:103:ASN:HB3	1.99	0.61
1:D:304:ASN:C	1:D:304:ASN:ND2	2.59	0.61
1:E:341:ILE:HA	1:E:397:MET:CE	2.30	0.61
1:E:63:GLY:O	1:E:65:ARG:HG3	2.00	0.61
1:E:62:ILE:HD13	4:E:621:FOL:C16	2.31	0.61
1:E:113:CYS:O	4:E:621:FOL:H7	2.01	0.61
1:E:3:GLU:OE2	1:E:3:GLU:HA	2.01	0.61
1:E:93:ASN:HD21	1:E:95:GLU:HB3	1.66	0.61
1:A:104:ASP:C	1:A:106:SER:N	2.58	0.60
1:B:304:ASN:C	1:B:304:ASN:ND2	2.56	0.60
1:C:341:ILE:HA	1:C:397:MET:CE	2.31	0.60
1:A:4:LYS:CE	1:A:101:LEU:HA	2.30	0.60
1:A:505:GLU:HB3	1:A:507:ILE:HD11	1.84	0.60
1:C:296:ILE:HD12	1:C:297:TRP:H	1.67	0.60
1:C:468:ASN:N	1:C:468:ASN:HD22	1.99	0.60
1:A:225:ASN:O	1:A:233:ARG:NH2	2.34	0.60
1:E:3:GLU:CG	1:E:4:LYS:N	2.65	0.60
1:A:304:ASN:HD22	1:A:306:ASN:H	1.48	0.60
1:D:502:GLU:CD	1:D:502:GLU:H	2.09	0.60
1:E:104:ASP:C	1:E:106:SER:H	2.09	0.60
1:B:341:ILE:HA	1:B:397:MET:CE	2.30	0.59
1:C:304:ASN:C	1:C:304:ASN:ND2	2.58	0.59
1:C:308:LEU:HD12	1:C:313:VAL:HG11	1.84	0.59
1:D:225:ASN:O	1:D:233:ARG:NH2	2.35	0.59
1:D:468:ASN:N	1:D:468:ASN:HD22	2.00	0.59
1:A:502:GLU:CD	1:A:502:GLU:H	2.09	0.59
1:B:3:GLU:OE2	1:B:3:GLU:HA	2.01	0.59
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.84	0.59
1:D:3:GLU:HG3	1:D:4:LYS:N	2.15	0.59
1:E:225:ASN:O	1:E:233:ARG:NH2	2.35	0.59
1:E:256:ASN:HD22	1:E:258:THR:H	1.49	0.59
1:B:63:GLY:O	1:B:65:ARG:HG3	2.03	0.59
1:A:41:ASN:HD21	1:A:69:ASN:HB2	1.67	0.59
1:C:304:ASN:HD22	1:C:306:ASN:H	1.48	0.59
1:B:468:ASN:N	1:B:468:ASN:HD22	1.99	0.59
1:C:468:ASN:HD22	1:C:468:ASN:H	1.50	0.59
1:E:512:TYR:HB3	1:E:513:PRO:HD2	1.83	0.59
1:C:102:MET:HA	1:C:102:MET:CE	2.28	0.59
1:A:180:LYS:HG3	1:A:181:LYS:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:ILE:HD12	1:D:297:TRP:H	1.68	0.59
1:D:419:ASN:ND2	1:D:457:ALA:HB3	2.18	0.59
1:E:151:PRO:HG2	1:E:154:PHE:CD2	2.38	0.59
1:E:502:GLU:CD	1:E:502:GLU:H	2.10	0.59
1:A:304:ASN:C	1:A:304:ASN:ND2	2.59	0.59
1:C:173:MET:HE2	1:C:175:PHE:CZ	2.38	0.59
1:E:183:LEU:HD23	1:E:184:GLN:N	2.18	0.59
1:E:468:ASN:HD22	1:E:468:ASN:N	2.00	0.59
1:A:296:ILE:HD12	1:A:297:TRP:H	1.68	0.58
1:B:102:MET:HA	1:B:102:MET:CE	2.27	0.58
1:B:173:MET:HE2	1:B:175:PHE:CZ	2.38	0.58
1:D:151:PRO:HG2	1:D:154:PHE:CD2	2.36	0.58
1:A:173:MET:HE2	1:A:175:PHE:CZ	2.38	0.58
1:D:359:ASP:OD2	1:D:361:THR:HG22	2.03	0.58
1:C:83:GLU:OE2	1:C:83:GLU:HA	2.02	0.58
1:A:104:ASP:CG	1:A:107:ILE:HD13	2.28	0.58
1:A:468:ASN:N	1:A:468:ASN:HD22	2.01	0.58
1:D:341:ILE:HA	1:D:397:MET:CE	2.32	0.58
1:E:41:ASN:HD21	1:E:69:ASN:HB2	1.69	0.58
1:D:41:ASN:HD21	1:D:69:ASN:HB2	1.67	0.58
1:E:173:MET:HE2	1:E:175:PHE:CZ	2.38	0.58
1:B:113:CYS:O	4:B:609:FOL:H7	2.03	0.58
1:C:104:ASP:C	1:C:106:SER:N	2.60	0.58
1:B:41:ASN:HD21	1:B:69:ASN:HB2	1.69	0.58
1:B:183:LEU:HD23	1:B:184:GLN:N	2.18	0.58
1:D:37:SER:HB2	4:D:617:FOL:HG1	1.86	0.58
1:D:93:ASN:HD21	1:D:95:GLU:HB3	1.68	0.58
1:D:512:TYR:HB3	1:D:513:PRO:HD2	1.86	0.58
1:E:467:GLU:HA	1:E:470:LEU:HD13	1.86	0.58
1:B:104:ASP:C	1:B:106:SER:N	2.58	0.58
1:B:512:TYR:HB3	1:B:513:PRO:HD2	1.86	0.58
1:C:41:ASN:HD21	1:C:69:ASN:HB2	1.69	0.58
1:E:388:ALA:O	1:E:401:PRO:HG2	2.04	0.58
1:B:225:ASN:O	1:B:233:ARG:NH2	2.37	0.58
4:C:613:FOL:C6	5:C:614:NDP:H42N	2.33	0.58
1:D:467:GLU:HA	1:D:470:LEU:HD13	1.86	0.58
1:C:297:TRP:CD2	1:C:308:LEU:HD21	2.39	0.58
1:E:75:ILE:O	5:E:622:NDP:H1B	2.04	0.58
1:B:468:ASN:HD22	1:B:468:ASN:H	1.49	0.57
1:C:183:LEU:HD23	1:C:184:GLN:N	2.19	0.57
1:A:93:ASN:HD21	1:A:95:GLU:HB3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:LYS:HG3	1:D:181:LYS:N	2.19	0.57
2:D:615:UMP:H1'	3:D:616:CB3:C4	2.34	0.57
1:A:341:ILE:HA	1:A:397:MET:CE	2.32	0.57
1:E:104:ASP:CG	1:E:107:ILE:HD13	2.29	0.57
1:B:505:GLU:HB3	1:B:507:ILE:HD11	1.87	0.57
1:E:359:ASP:OD2	1:E:361:THR:HG22	2.04	0.57
1:B:180:LYS:HG3	1:B:181:LYS:N	2.19	0.57
1:A:63:GLY:O	1:A:65:ARG:HG3	2.05	0.57
1:A:183:LEU:HD23	1:A:184:GLN:N	2.18	0.57
1:B:247:VAL:HG21	1:B:465:ILE:HG13	1.87	0.57
1:D:104:ASP:C	1:D:106:SER:N	2.60	0.57
1:D:183:LEU:HD23	1:D:184:GLN:N	2.19	0.57
1:D:260:ILE:HD12	1:D:260:ILE:H	1.67	0.57
1:A:247:VAL:HG21	1:A:465:ILE:HG13	1.85	0.57
1:C:3:GLU:HA	1:C:3:GLU:OE2	2.05	0.57
1:E:116:GLU:HB2	1:E:145:THR:HG23	1.87	0.57
1:A:512:TYR:HB3	1:A:513:PRO:HD2	1.87	0.57
1:B:296:ILE:HD12	1:B:297:TRP:H	1.70	0.57
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.86	0.57
1:B:434:ASN:OD1	2:B:607:UMP:N3	2.36	0.57
1:C:405:LEU:C	1:C:405:LEU:HD23	2.30	0.57
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.85	0.57
1:B:304:ASN:HD22	1:B:306:ASN:H	1.52	0.56
1:C:151:PRO:HG2	1:C:154:PHE:CD2	2.38	0.56
1:D:63:GLY:O	1:D:65:ARG:HG3	2.05	0.56
1:E:296:ILE:HD12	1:E:297:TRP:H	1.70	0.56
1:A:158:TYR:HB3	1:A:174:ILE:HG12	1.87	0.56
1:A:467:GLU:HA	1:A:470:LEU:HD13	1.87	0.56
1:B:126:ASN:CG	1:B:177:LYS:HZ1	2.12	0.56
1:D:405:LEU:C	1:D:405:LEU:HD23	2.30	0.56
1:E:468:ASN:HD22	1:E:468:ASN:H	1.52	0.56
1:A:3:GLU:HA	1:A:3:GLU:OE2	2.05	0.56
1:A:16:SER:OG	1:A:139:GLU:OE2	2.18	0.56
1:A:468:ASN:HD22	1:A:468:ASN:H	1.53	0.56
1:C:206:ILE:HD11	1:D:35:PHE:HA	1.86	0.56
1:C:400:PRO:HG2	1:D:383:ARG:CZ	2.36	0.56
1:A:333:ARG:HG3	1:A:337:ASP:HB3	1.87	0.56
1:C:43:LYS:NZ	1:C:48:LYS:O	2.34	0.56
1:D:3:GLU:OE2	1:D:3:GLU:HA	2.05	0.56
1:E:104:ASP:C	1:E:106:SER:N	2.60	0.56
1:E:405:LEU:HD23	1:E:405:LEU:C	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:PRO:HG2	1:A:154:PHE:CD2	2.40	0.56
1:D:359:ASP:CG	1:D:361:THR:HG22	2.30	0.56
2:C:611:UMP:OP2	1:D:382:ARG:NE	2.38	0.56
1:E:308:LEU:HD12	1:E:313:VAL:CG1	2.35	0.56
1:D:505:GLU:HB3	1:D:507:ILE:HD11	1.87	0.56
1:B:151:PRO:HG2	1:B:154:PHE:CD2	2.41	0.56
1:C:180:LYS:HG3	1:C:181:LYS:N	2.20	0.56
1:C:512:TYR:HB3	1:C:513:PRO:HD2	1.87	0.56
1:C:104:ASP:CG	1:C:107:ILE:HD13	2.30	0.55
1:C:247:VAL:HG21	1:C:465:ILE:HG13	1.87	0.55
1:A:297:TRP:CD2	1:A:308:LEU:HD21	2.41	0.55
1:C:52:LEU:HB3	1:C:113:CYS:SG	2.47	0.55
1:C:431:SER:HB3	1:C:432:PRO:HD3	1.88	0.55
4:E:621:FOL:C7	5:E:622:NDP:C4N	2.82	0.55
1:B:104:ASP:CG	1:B:107:ILE:HD13	2.32	0.55
1:B:467:GLU:HA	1:B:470:LEU:HD13	1.88	0.55
1:E:180:LYS:HG3	1:E:181:LYS:N	2.21	0.55
1:C:202:LEU:HG	1:D:38:LYS:HB3	1.89	0.55
1:C:505:GLU:HB3	1:C:507:ILE:HD11	1.88	0.55
1:D:308:LEU:HD12	1:D:313:VAL:CG1	2.35	0.55
1:D:468:ASN:HD22	1:D:468:ASN:H	1.53	0.55
1:E:158:TYR:HB3	1:E:174:ILE:HG12	1.88	0.55
1:A:19:ILE:O	5:A:606:NDP:H2N	2.06	0.55
1:D:104:ASP:CG	1:D:107:ILE:HD13	2.30	0.55
1:E:333:ARG:HG3	1:E:337:ASP:HB3	1.88	0.55
1:A:431:SER:HB3	1:A:432:PRO:HD3	1.89	0.55
1:D:15:LEU:HB2	1:D:139:GLU:HG2	1.89	0.55
1:D:247:VAL:HG12	1:D:265:ILE:CD1	2.37	0.55
1:B:3:GLU:O	1:B:4:LYS:HB2	2.07	0.55
1:C:467:GLU:HA	1:C:470:LEU:HD13	1.88	0.55
2:C:611:UMP:OP2	1:D:382:ARG:NH2	2.40	0.55
1:E:260:ILE:HD12	1:E:260:ILE:H	1.70	0.55
1:A:35:PHE:HA	1:B:206:ILE:HD11	1.88	0.55
1:B:19:ILE:O	5:B:610:NDP:H2N	2.07	0.55
1:B:405:LEU:C	1:B:405:LEU:HD23	2.31	0.55
1:D:296:ILE:O	1:D:300:LYS:HG2	2.07	0.55
1:B:297:TRP:CD2	1:B:308:LEU:HD21	2.41	0.55
1:D:75:ILE:O	5:D:618:NDP:H1B	2.07	0.55
1:A:388:ALA:O	1:A:401:PRO:HG2	2.06	0.54
1:B:388:ALA:O	1:B:401:PRO:HG2	2.07	0.54
1:E:340:PRO:HG3	1:E:353:TYR:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:CYS:O	4:A:605:FOL:H7	2.07	0.54
1:D:388:ALA:O	1:D:401:PRO:HG2	2.08	0.54
1:C:158:TYR:HB3	1:C:174:ILE:HG12	1.88	0.54
1:E:297:TRP:CD2	1:E:308:LEU:HD21	2.43	0.54
1:B:79:LEU:HD23	1:B:80:PRO:CD	2.37	0.54
1:D:116:GLU:HB2	1:D:145:THR:HG23	1.89	0.54
1:A:289:ARG:NH1	6:A:633:HOH:O	2.41	0.54
1:C:116:GLU:HB2	1:C:145:THR:HG23	1.89	0.54
1:B:93:ASN:HD21	1:B:95:GLU:HB3	1.73	0.54
1:C:114:GLY:HA3	5:C:614:NDP:H5N	1.89	0.54
1:C:509:TYR:HA	6:C:673:HOH:O	2.08	0.54
1:D:3:GLU:O	1:D:4:LYS:HB2	2.07	0.54
1:D:16:SER:OG	1:D:139:GLU:OE2	2.21	0.54
1:E:505:GLU:HB3	1:E:507:ILE:HD11	1.90	0.54
1:C:3:GLU:O	1:C:4:LYS:HB2	2.08	0.54
1:D:114:GLY:HA3	5:D:618:NDP:H5N	1.88	0.54
1:D:154:PHE:CE1	1:D:177:LYS:HB2	2.43	0.54
1:A:101:LEU:O	1:A:103:ASN:N	2.39	0.54
1:C:62:ILE:HD13	4:C:613:FOL:C16	2.38	0.54
1:C:388:ALA:O	1:C:401:PRO:HG2	2.07	0.54
1:D:297:TRP:CD2	1:D:308:LEU:HD21	2.43	0.54
4:D:617:FOL:C7	5:D:618:NDP:C4N	2.80	0.54
1:B:158:TYR:HB3	1:B:174:ILE:HG12	1.90	0.54
1:B:434:ASN:ND2	2:B:607:UMP:O4	2.36	0.54
1:E:296:ILE:O	1:E:300:LYS:HG2	2.07	0.54
1:A:260:ILE:HD12	1:A:260:ILE:H	1.71	0.54
1:A:359:ASP:OD2	1:A:361:THR:HG22	2.07	0.54
1:A:494:GLU:HG3	1:A:495:ASN:N	2.23	0.54
1:C:154:PHE:CE1	1:C:177:LYS:HB2	2.43	0.54
1:D:113:CYS:O	4:D:617:FOL:H7	2.08	0.54
1:D:431:SER:HB3	1:D:432:PRO:HD3	1.89	0.54
1:E:43:LYS:NZ	1:E:48:LYS:O	2.32	0.54
1:B:103:ASN:C	1:B:103:ASN:ND2	2.66	0.53
1:C:260:ILE:HD12	1:C:260:ILE:H	1.72	0.53
1:E:101:LEU:O	1:E:103:ASN:N	2.40	0.53
1:E:304:ASN:HD22	1:E:306:ASN:H	1.53	0.53
1:A:374:THR:HG22	1:A:384:HIS:CE1	2.43	0.53
1:A:405:LEU:C	1:A:405:LEU:HD23	2.33	0.53
1:D:304:ASN:HD22	1:D:306:ASN:H	1.56	0.53
1:A:19:ILE:HB	5:A:606:NDP:N7N	2.23	0.53
1:A:79:LEU:HD23	1:A:80:PRO:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HB2	1:A:139:GLU:HG2	1.90	0.53
1:B:243:LEU:O	1:B:247:VAL:HG13	2.09	0.53
1:E:93:ASN:OD1	1:E:96:ASP:HB2	2.09	0.53
1:A:3:GLU:O	1:A:4:LYS:HB2	2.08	0.53
1:C:289:ARG:HG3	1:C:501:TRP:CE2	2.43	0.53
1:C:296:ILE:HD12	1:C:297:TRP:N	2.23	0.53
1:C:374:THR:HG22	1:C:384:HIS:CE1	2.44	0.53
1:D:56:ARG:O	1:D:59:TRP:HB3	2.08	0.53
1:E:289:ARG:HG3	1:E:501:TRP:CE2	2.43	0.53
1:A:340:PRO:HG3	1:A:353:TYR:CB	2.39	0.53
1:B:380:LYS:HE3	1:B:412:ASN:ND2	2.24	0.53
1:A:383:ARG:CZ	1:B:400:PRO:HG2	2.38	0.53
1:B:296:ILE:O	1:B:300:LYS:HG2	2.07	0.53
1:D:103:ASN:CG	1:D:104:ASP:N	2.65	0.53
1:D:171:ASP:OD1	6:D:675:HOH:O	2.19	0.53
1:D:291:ILE:HD13	1:D:436:ALA:HB3	1.90	0.53
1:B:225:ASN:O	1:B:226:THR:C	2.52	0.53
1:E:247:VAL:HG21	1:E:465:ILE:HG13	1.89	0.53
1:A:359:ASP:CG	1:A:361:THR:HG22	2.34	0.52
1:B:260:ILE:HD12	1:B:260:ILE:H	1.73	0.52
1:C:3:GLU:CG	1:C:4:LYS:N	2.64	0.52
1:D:158:TYR:HB3	1:D:174:ILE:HG12	1.90	0.52
1:E:397:MET:HE1	1:E:401:PRO:CG	2.39	0.52
1:D:247:VAL:HG21	1:D:465:ILE:HG13	1.90	0.52
1:A:247:VAL:HG12	1:A:265:ILE:CD1	2.40	0.52
1:A:257:ARG:NE	2:A:603:UMP:OP1	2.41	0.52
1:B:402:CYS:SG	2:B:607:UMP:H6	2.30	0.52
1:E:56:ARG:O	1:E:59:TRP:HB3	2.08	0.52
1:A:289:ARG:HG3	1:A:501:TRP:CE2	2.45	0.52
1:D:173:MET:HE2	1:D:175:PHE:CZ	2.45	0.52
1:E:101:LEU:C	1:E:103:ASN:H	2.17	0.52
1:A:116:GLU:HB2	1:A:145:THR:HG23	1.91	0.52
1:D:494:GLU:HG3	1:D:495:ASN:N	2.25	0.52
1:E:429:LEU:HD11	1:E:517:MET:HB2	1.92	0.52
1:E:431:SER:HB3	1:E:432:PRO:HD3	1.91	0.52
1:A:93:ASN:OD1	1:A:96:ASP:HB2	2.09	0.52
1:C:296:ILE:O	1:C:300:LYS:HG2	2.09	0.52
1:E:247:VAL:HG12	1:E:265:ILE:CD1	2.39	0.52
3:E:620:CB3:CP2	3:E:620:CB3:H13	2.40	0.52
1:D:101:LEU:C	1:D:103:ASN:H	2.18	0.52
1:D:429:LEU:HD11	1:D:517:MET:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ALA:C	1:A:52:LEU:HD23	2.35	0.52
1:A:291:ILE:HD13	1:A:436:ALA:HB3	1.91	0.52
1:A:308:LEU:HD12	1:A:313:VAL:CG1	2.38	0.52
1:C:38:LYS:HB3	1:D:202:LEU:HG	1.91	0.52
3:C:612:CB3:H13	3:C:612:CB3:CP2	2.40	0.52
1:E:79:LEU:HD23	1:E:80:PRO:CD	2.39	0.52
1:E:154:PHE:CE1	1:E:177:LYS:HB2	2.44	0.52
1:E:291:ILE:HD13	1:E:436:ALA:HB3	1.91	0.52
1:E:381:ASP:HB3	1:E:384:HIS:CE1	2.45	0.52
1:B:101:LEU:C	1:B:103:ASN:H	2.18	0.52
1:C:19:ILE:HB	5:C:614:NDP:N7N	2.25	0.52
1:C:359:ASP:OD2	1:C:361:THR:HG22	2.10	0.52
1:A:237:GLU:OE2	1:A:283:THR:HG23	2.11	0.52
1:B:99:GLU:C	1:B:101:LEU:N	2.63	0.52
1:B:233:ARG:NH1	1:B:242:ASP:OD1	2.38	0.52
1:B:359:ASP:CG	1:B:361:THR:HG22	2.34	0.52
1:B:494:GLU:HG3	1:B:495:ASN:N	2.24	0.52
1:C:99:GLU:C	1:C:101:LEU:N	2.65	0.52
1:D:19:ILE:HB	5:D:618:NDP:N7N	2.25	0.52
1:A:397:MET:HE1	1:A:401:PRO:CG	2.40	0.51
1:D:93:ASN:OD1	1:D:96:ASP:HB2	2.09	0.51
1:B:116:GLU:HB2	1:B:145:THR:HG23	1.93	0.51
1:C:93:ASN:OD1	1:C:96:ASP:HB2	2.09	0.51
1:C:103:ASN:CG	1:C:104:ASP:N	2.65	0.51
1:D:340:PRO:HG3	1:D:353:TYR:CB	2.40	0.51
1:A:99:GLU:C	1:A:101:LEU:N	2.64	0.51
1:A:223:ILE:HD11	1:A:249:GLU:OE1	2.09	0.51
1:B:101:LEU:O	1:B:103:ASN:N	2.41	0.51
1:B:103:ASN:CG	1:B:104:ASP:N	2.66	0.51
1:B:359:ASP:OD2	1:B:361:THR:HG22	2.10	0.51
3:B:608:CB3:CP2	3:B:608:CB3:H13	2.40	0.51
1:C:51:ALA:C	1:C:52:LEU:HD23	2.36	0.51
1:C:502:GLU:CD	1:C:502:GLU:N	2.68	0.51
1:E:92:ARG:O	5:E:622:NDP:H2A	2.10	0.51
1:A:296:ILE:O	1:A:300:LYS:HG2	2.10	0.51
1:B:193:LEU:HD21	1:B:196:ILE:CD1	2.38	0.51
1:C:79:LEU:HD23	1:C:80:PRO:CD	2.37	0.51
1:A:284:LYS:HD2	6:A:637:HOH:O	2.09	0.51
1:B:154:PHE:CE1	1:B:177:LYS:HB2	2.46	0.51
1:C:246:ARG:HE	1:C:268:GLN:HE22	1.57	0.51
1:E:3:GLU:O	1:E:4:LYS:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:ASP:CG	1:E:361:THR:HG22	2.34	0.51
1:A:233:ARG:NH1	1:A:242:ASP:OD1	2.38	0.51
4:B:609:FOL:C6	5:B:610:NDP:H42N	2.40	0.51
1:C:101:LEU:O	1:C:103:ASN:N	2.43	0.51
1:C:291:ILE:HD13	1:C:436:ALA:HB3	1.92	0.51
1:D:123:LEU:HD13	1:D:128:VAL:CG1	2.40	0.51
1:D:397:MET:HE1	1:D:401:PRO:CG	2.39	0.51
1:C:56:ARG:O	1:C:59:TRP:HB3	2.11	0.51
1:D:99:GLU:C	1:D:101:LEU:N	2.64	0.51
1:D:223:ILE:HD11	1:D:249:GLU:OE1	2.11	0.51
1:D:296:ILE:HD12	1:D:297:TRP:N	2.25	0.51
1:B:378:ASN:O	1:B:381:ASP:HB2	2.11	0.51
1:C:243:LEU:O	1:C:247:VAL:HG13	2.10	0.51
1:D:8:ILE:HG12	1:D:112:VAL:HB	1.92	0.51
1:D:289:ARG:HG3	1:D:501:TRP:CE2	2.46	0.51
1:E:193:LEU:HD21	1:E:196:ILE:CD1	2.39	0.51
2:E:619:UMP:H1'	3:E:620:CB3:C4A	2.40	0.51
1:B:103:ASN:C	1:B:103:ASN:HD22	2.19	0.51
1:E:99:GLU:C	1:E:101:LEU:N	2.64	0.51
1:A:43:LYS:NZ	1:A:48:LYS:O	2.29	0.51
1:A:101:LEU:C	1:A:103:ASN:H	2.18	0.51
1:A:114:GLY:HA3	5:A:606:NDP:H5N	1.93	0.51
1:B:247:VAL:HG12	1:B:265:ILE:CD1	2.41	0.51
1:C:308:LEU:HD12	1:C:313:VAL:CG1	2.41	0.51
1:D:193:LEU:HD21	1:D:196:ILE:CD1	2.40	0.51
1:E:15:LEU:HB2	1:E:139:GLU:HG2	1.93	0.51
1:E:378:ASN:O	1:E:381:ASP:HB2	2.11	0.51
1:E:380:LYS:HE3	1:E:412:ASN:ND2	2.26	0.51
1:B:15:LEU:HB2	1:B:139:GLU:HG2	1.92	0.50
1:C:133:LEU:HD22	1:C:134:THR:N	2.26	0.50
1:C:359:ASP:CG	1:C:361:THR:HG22	2.36	0.50
4:C:613:FOL:H13	4:C:613:FOL:C6	2.41	0.50
1:E:8:ILE:HG12	1:E:112:VAL:HB	1.93	0.50
4:E:621:FOL:H13	4:E:621:FOL:C6	2.41	0.50
1:B:308:LEU:HD12	1:B:313:VAL:CG1	2.41	0.50
1:B:431:SER:HB3	1:B:432:PRO:HD3	1.91	0.50
1:C:494:GLU:HG3	1:C:495:ASN:N	2.26	0.50
3:D:616:CB3:CP2	3:D:616:CB3:H13	2.41	0.50
1:A:296:ILE:HD12	1:A:297:TRP:N	2.25	0.50
1:B:296:ILE:HD12	1:B:297:TRP:N	2.25	0.50
1:D:103:ASN:C	1:D:103:ASN:ND2	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:O	1:A:226:THR:C	2.53	0.50
1:A:246:ARG:HH11	1:A:268:GLN:HE21	1.60	0.50
1:B:56:ARG:O	1:B:59:TRP:HB3	2.12	0.50
1:C:334:GLU:OE2	1:C:357:HIS:HE1	1.94	0.50
1:D:246:ARG:HE	1:D:268:GLN:HE22	1.60	0.50
1:A:378:ASN:O	1:A:381:ASP:HB2	2.12	0.50
1:C:378:ASN:ND2	1:C:381:ASP:HB2	2.26	0.50
1:C:397:MET:HE1	1:C:401:PRO:CG	2.40	0.50
1:E:296:ILE:HD12	1:E:297:TRP:N	2.25	0.50
1:A:115:GLY:HA3	5:A:606:NDP:O1A	2.11	0.50
1:A:154:PHE:CE1	1:A:177:LYS:HB2	2.46	0.50
1:B:429:LEU:HD11	1:B:517:MET:HB2	1.93	0.50
1:C:402:CYS:SG	2:C:611:UMP:H6	2.33	0.50
4:D:617:FOL:H13	4:D:617:FOL:C6	2.42	0.50
4:D:617:FOL:C6	5:D:618:NDP:H42N	2.39	0.50
4:B:609:FOL:H13	4:B:609:FOL:C6	2.42	0.50
1:C:8:ILE:HG12	1:C:112:VAL:HB	1.94	0.50
1:C:19:ILE:O	5:C:614:NDP:H2N	2.11	0.50
1:D:79:LEU:HD23	1:D:80:PRO:CD	2.42	0.50
1:D:101:LEU:O	1:D:103:ASN:N	2.41	0.50
1:D:225:ASN:O	1:D:226:THR:C	2.54	0.50
1:D:381:ASP:HB3	1:D:384:HIS:CE1	2.47	0.50
1:A:103:ASN:CG	1:A:104:ASP:N	2.67	0.50
1:C:103:ASN:C	1:C:103:ASN:ND2	2.69	0.50
1:D:502:GLU:CD	1:D:502:GLU:N	2.70	0.50
1:E:225:ASN:O	1:E:226:THR:C	2.54	0.50
1:E:494:GLU:HG3	1:E:495:ASN:N	2.25	0.50
3:A:604:CB3:CP2	3:A:604:CB3:H13	2.41	0.50
1:B:340:PRO:HG3	1:B:353:TYR:CB	2.42	0.50
1:C:67:LEU:HG	1:C:72:ILE:HD11	1.94	0.50
1:C:101:LEU:C	1:C:103:ASN:H	2.19	0.50
1:C:115:GLY:HA3	5:C:614:NDP:O1A	2.11	0.50
1:C:247:VAL:HG12	1:C:265:ILE:CD1	2.41	0.50
1:C:381:ASP:HB3	1:C:384:HIS:CE1	2.46	0.50
1:E:402:CYS:SG	2:E:619:UMP:C6	3.04	0.50
1:A:8:ILE:HG12	1:A:112:VAL:HB	1.94	0.49
1:B:12:ALA:HB1	1:B:17:SER:HA	1.94	0.49
1:B:381:ASP:HB3	1:B:384:HIS:CE1	2.47	0.49
1:C:163:PHE:HA	1:C:276:GLU:HB3	1.93	0.49
1:A:56:ARG:O	1:A:59:TRP:HB3	2.12	0.49
1:A:103:ASN:C	1:A:103:ASN:ND2	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HD22	1:A:134:THR:N	2.27	0.49
1:B:52:LEU:HB3	1:B:113:CYS:SG	2.52	0.49
1:B:246:ARG:HH11	1:B:268:GLN:HE21	1.60	0.49
1:B:291:ILE:HD13	1:B:436:ALA:HB3	1.94	0.49
1:C:15:LEU:HB2	1:C:139:GLU:HG2	1.94	0.49
1:C:246:ARG:HE	1:C:268:GLN:NE2	2.10	0.49
1:C:429:LEU:HD11	1:C:517:MET:HB2	1.93	0.49
1:E:378:ASN:ND2	1:E:381:ASP:HB2	2.27	0.49
1:B:468:ASN:H	1:B:468:ASN:ND2	2.11	0.49
1:E:104:ASP:HB3	1:E:107:ILE:HD13	1.94	0.49
1:E:163:PHE:HA	1:E:276:GLU:HB3	1.93	0.49
1:E:220:LYS:HB2	1:E:220:LYS:NZ	2.27	0.49
1:E:422:GLN:HE21	1:E:425:CYS:HB2	1.76	0.49
1:A:429:LEU:HD11	1:A:517:MET:HB2	1.93	0.49
1:B:8:ILE:HG12	1:B:112:VAL:HB	1.94	0.49
1:D:126:ASN:CG	1:D:177:LYS:HZ1	2.21	0.49
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.95	0.49
1:C:12:ALA:HB1	1:C:17:SER:HA	1.93	0.49
1:C:378:ASN:O	1:C:381:ASP:HB2	2.12	0.49
1:D:320:GLY:O	1:D:335:GLU:O	2.30	0.49
1:E:51:ALA:C	1:E:52:LEU:HD23	2.38	0.49
1:B:183:LEU:O	1:B:184:GLN:HB3	2.12	0.49
1:C:340:PRO:HG3	1:C:353:TYR:CB	2.42	0.49
1:E:126:ASN:HD21	1:E:177:LYS:HE3	1.77	0.49
1:E:133:LEU:HD22	1:E:134:THR:N	2.28	0.49
1:E:246:ARG:HE	1:E:268:GLN:HE22	1.60	0.49
1:E:293:GLU:O	1:E:296:ILE:HD12	2.12	0.49
1:E:372:ILE:O	1:E:376:LYS:HG2	2.12	0.49
1:A:243:LEU:O	1:A:247:VAL:HG13	2.13	0.49
1:A:293:GLU:O	1:A:296:ILE:HD12	2.12	0.49
1:E:179:GLU:HG2	1:E:180:LYS:N	2.27	0.49
1:E:321:SER:O	1:E:325:LEU:HD13	2.13	0.49
1:E:383:ARG:O	1:E:385:ILE:N	2.46	0.49
1:B:43:LYS:NZ	1:B:48:LYS:O	2.33	0.49
1:B:374:THR:HG22	1:B:384:HIS:CE1	2.48	0.49
1:B:502:GLU:CD	1:B:502:GLU:N	2.70	0.49
1:C:123:LEU:HD13	1:C:128:VAL:CG1	2.42	0.49
1:E:103:ASN:C	1:E:103:ASN:ND2	2.71	0.49
1:E:123:LEU:HD13	1:E:128:VAL:CG1	2.43	0.49
1:A:321:SER:O	1:A:325:LEU:HD13	2.13	0.49
1:C:48:LYS:HB3	1:C:106:SER:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:ARG:HH11	1:D:268:GLN:HE21	1.61	0.49
1:D:422:GLN:NE2	1:D:425:CYS:SG	2.85	0.49
1:E:103:ASN:CG	1:E:104:ASP:N	2.68	0.49
1:E:246:ARG:HH11	1:E:268:GLN:NE2	2.10	0.49
1:A:163:PHE:HA	1:A:276:GLU:HB3	1.94	0.49
4:A:605:FOL:H13	4:A:605:FOL:C6	2.42	0.49
1:B:93:ASN:OD1	1:B:96:ASP:HB2	2.13	0.49
1:B:163:PHE:HA	1:B:276:GLU:HB3	1.94	0.49
1:E:212:MET:HG3	1:E:215:ARG:NH2	2.28	0.49
1:E:246:ARG:HH11	1:E:268:GLN:HE21	1.60	0.49
1:A:422:GLN:HE22	1:A:434:ASN:ND2	2.10	0.48
1:B:114:GLY:HA3	5:B:610:NDP:H5N	1.94	0.48
1:B:237:GLU:OE2	1:B:283:THR:HG23	2.12	0.48
1:B:334:GLU:OE2	1:B:357:HIS:HE1	1.96	0.48
1:C:75:ILE:O	5:C:614:NDP:H1B	2.12	0.48
1:D:233:ARG:NH1	1:D:242:ASP:OD1	2.42	0.48
1:C:193:LEU:HD21	1:C:196:ILE:CD1	2.38	0.48
1:D:163:PHE:HA	1:D:276:GLU:HB3	1.95	0.48
1:A:246:ARG:HH11	1:A:268:GLN:NE2	2.11	0.48
1:A:320:GLY:O	1:A:335:GLU:O	2.30	0.48
1:B:378:ASN:ND2	1:B:381:ASP:HB2	2.28	0.48
1:B:397:MET:HE1	1:B:401:PRO:CG	2.41	0.48
1:C:179:GLU:HG2	1:C:180:LYS:N	2.28	0.48
1:C:223:ILE:HD11	1:C:249:GLU:OE1	2.13	0.48
1:E:183:LEU:O	1:E:184:GLN:HB3	2.13	0.48
1:E:239:GLN:HG3	1:E:271:ARG:O	2.13	0.48
1:A:305:GLY:O	1:A:309:ILE:HG13	2.13	0.48
1:B:212:MET:HG3	1:B:215:ARG:NH2	2.27	0.48
1:C:405:LEU:HD11	1:D:404:VAL:HG11	1.94	0.48
1:D:51:ALA:C	1:D:52:LEU:HD23	2.39	0.48
1:A:15:LEU:HB2	1:A:139:GLU:CD	2.38	0.48
1:A:381:ASP:HB3	1:A:384:HIS:CE1	2.47	0.48
1:D:389:TRP:HB2	1:D:404:VAL:HG13	1.96	0.48
1:C:15:LEU:HB2	1:C:139:GLU:CD	2.38	0.48
1:C:225:ASN:O	1:C:226:THR:C	2.56	0.48
1:E:11:ALA:HB2	4:E:621:FOL:NA2	2.29	0.48
1:E:12:ALA:HB1	1:E:17:SER:HA	1.95	0.48
1:A:502:GLU:CD	1:A:502:GLU:N	2.71	0.48
1:D:293:GLU:O	1:D:296:ILE:HD12	2.13	0.48
1:D:378:ASN:O	1:D:381:ASP:HB2	2.14	0.48
1:E:340:PRO:HG3	1:E:353:TYR:CG	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:HB1	1:A:17:SER:HA	1.95	0.48
1:A:405:LEU:HD11	1:B:404:VAL:HG11	1.95	0.48
1:B:15:LEU:HB2	1:B:139:GLU:CD	2.39	0.48
1:B:289:ARG:HG3	1:B:501:TRP:CE2	2.49	0.48
1:D:220:LYS:HB2	1:D:220:LYS:NZ	2.29	0.48
1:D:246:ARG:HH11	1:D:268:GLN:NE2	2.12	0.48
1:E:67:LEU:HG	1:E:72:ILE:HD11	1.95	0.48
1:B:223:ILE:HD11	1:B:249:GLU:OE1	2.14	0.48
1:B:293:GLU:O	1:B:296:ILE:HD12	2.14	0.48
1:D:380:LYS:HE3	1:D:412:ASN:ND2	2.28	0.48
1:E:27:TRP:CZ2	1:E:136:VAL:HG21	2.49	0.48
1:A:183:LEU:O	1:A:184:GLN:HB3	2.13	0.48
1:A:487:LEU:C	1:A:487:LEU:HD23	2.39	0.48
1:B:10:VAL:HG22	1:B:11:ALA:N	2.29	0.48
1:B:133:LEU:CD1	1:B:135:ARG:HG2	2.44	0.48
1:B:246:ARG:HH11	1:B:268:GLN:NE2	2.12	0.48
1:C:133:LEU:CD1	1:C:135:ARG:HG2	2.43	0.48
1:C:246:ARG:HH11	1:C:268:GLN:HE21	1.62	0.48
1:C:405:LEU:CD1	1:D:404:VAL:HG11	2.44	0.48
1:D:67:LEU:HG	1:D:72:ILE:HD11	1.96	0.48
1:E:10:VAL:HG22	1:E:11:ALA:N	2.28	0.48
1:A:133:LEU:HD13	1:A:135:ARG:HG2	1.95	0.47
1:B:62:ILE:HD13	4:B:609:FOL:C16	2.43	0.47
1:B:320:GLY:O	1:B:335:GLU:O	2.32	0.47
1:C:212:MET:HG3	1:C:215:ARG:NH2	2.29	0.47
1:D:12:ALA:HB1	1:D:17:SER:HA	1.95	0.47
1:D:27:TRP:CZ2	1:D:136:VAL:HG21	2.48	0.47
1:E:243:LEU:O	1:E:247:VAL:HG13	2.13	0.47
1:A:239:GLN:HG3	1:A:271:ARG:O	2.13	0.47
1:A:400:PRO:HG2	1:B:383:ARG:CZ	2.45	0.47
1:B:126:ASN:CG	1:B:177:LYS:NZ	2.73	0.47
1:D:212:MET:HG3	1:D:215:ARG:NH2	2.30	0.47
1:D:422:GLN:HE21	1:D:425:CYS:CB	2.28	0.47
1:E:115:GLY:O	1:E:116:GLU:C	2.57	0.47
1:E:166:LYS:O	1:E:167:ASN:HB2	2.13	0.47
1:A:67:LEU:HG	1:A:72:ILE:HD11	1.96	0.47
1:B:123:LEU:HD13	1:B:128:VAL:CG1	2.45	0.47
1:C:53:ILE:HG23	1:C:75:ILE:HD13	1.95	0.47
1:D:179:GLU:HG2	1:D:180:LYS:N	2.30	0.47
1:D:305:GLY:O	1:D:309:ILE:HG13	2.14	0.47
1:D:374:THR:HG22	1:D:384:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:ILE:HD11	1:E:249:GLU:OE1	2.14	0.47
1:E:305:GLY:O	1:E:309:ILE:HG13	2.13	0.47
1:E:422:GLN:HE21	1:E:425:CYS:CB	2.27	0.47
1:B:178:GLN:NE2	6:B:721:HOH:O	2.46	0.47
1:C:116:GLU:HB2	1:C:145:THR:CG2	2.44	0.47
1:E:48:LYS:HB3	1:E:106:SER:O	2.14	0.47
1:A:83:GLU:OE2	1:A:83:GLU:CA	2.62	0.47
1:B:115:GLY:HA3	5:B:610:NDP:O1A	2.14	0.47
1:B:246:ARG:HE	1:B:268:GLN:NE2	2.12	0.47
1:E:502:GLU:CD	1:E:502:GLU:N	2.71	0.47
1:A:123:LEU:HD13	1:A:128:VAL:CG1	2.45	0.47
1:A:380:LYS:HE3	1:A:412:ASN:ND2	2.30	0.47
1:B:67:LEU:HG	1:B:72:ILE:HD11	1.96	0.47
1:B:179:GLU:HG2	1:B:180:LYS:N	2.29	0.47
1:C:115:GLY:O	1:C:116:GLU:C	2.58	0.47
1:C:233:ARG:NH1	1:C:242:ASP:OD1	2.40	0.47
1:A:10:VAL:HG22	1:A:11:ALA:N	2.29	0.47
1:A:69:ASN:ND2	6:A:699:HOH:O	2.48	0.47
1:A:115:GLY:O	1:A:116:GLU:C	2.57	0.47
1:A:193:LEU:HD21	1:A:196:ILE:CD1	2.40	0.47
1:A:264:SER:HB3	1:A:464:HIS:HB3	1.96	0.47
1:B:53:ILE:HG23	1:B:75:ILE:HD13	1.97	0.47
1:B:133:LEU:HD13	1:B:135:ARG:HG2	1.97	0.47
1:B:246:ARG:HE	1:B:268:GLN:HE22	1.63	0.47
1:B:264:SER:HB3	1:B:464:HIS:HB3	1.96	0.47
1:C:468:ASN:H	1:C:468:ASN:ND2	2.11	0.47
2:C:611:UMP:P	1:D:382:ARG:HE	2.38	0.47
1:D:133:LEU:HD22	1:D:134:THR:N	2.30	0.47
1:D:183:LEU:O	1:D:184:GLN:HB3	2.15	0.47
1:E:53:ILE:HG23	1:E:75:ILE:HD13	1.97	0.47
1:E:116:GLU:HB2	1:E:145:THR:CG2	2.44	0.47
1:C:97:SER:O	1:C:99:GLU:HG3	2.15	0.47
1:C:383:ARG:CZ	1:D:400:PRO:HG2	2.45	0.47
1:D:116:GLU:HB2	1:D:145:THR:CG2	2.45	0.47
1:A:404:VAL:HG11	1:B:405:LEU:HD11	1.97	0.47
1:A:507:ILE:HG22	6:A:707:HOH:O	2.15	0.47
1:C:246:ARG:HH11	1:C:268:GLN:NE2	2.11	0.47
1:D:343:GLY:HA2	1:D:346:TRP:HB2	1.97	0.47
1:E:126:ASN:CG	1:E:177:LYS:HZ1	2.22	0.47
1:A:100:ASN:HB2	1:A:110:ILE:HD11	1.97	0.47
1:A:104:ASP:HB3	1:A:107:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ILE:CD1	1:D:35:PHE:HA	2.45	0.47
1:C:209:ILE:N	1:C:209:ILE:CD1	2.74	0.47
1:C:380:LYS:HE3	1:C:412:ASN:ND2	2.29	0.47
1:D:15:LEU:HB2	1:D:139:GLU:CD	2.40	0.47
1:D:36:PHE:CD1	1:D:36:PHE:C	2.93	0.47
1:D:104:ASP:HB3	1:D:107:ILE:HD13	1.95	0.47
1:D:115:GLY:O	1:D:116:GLU:C	2.58	0.47
1:E:133:LEU:CD1	1:E:135:ARG:HG2	2.45	0.47
1:E:237:GLU:OE2	1:E:283:THR:HG23	2.14	0.47
1:E:320:GLY:O	1:E:335:GLU:O	2.33	0.47
1:C:264:SER:HB3	1:C:464:HIS:HB3	1.97	0.46
1:A:97:SER:O	1:A:99:GLU:HG3	2.15	0.46
1:A:133:LEU:CD1	1:A:135:ARG:HG2	2.44	0.46
1:C:103:ASN:C	1:C:103:ASN:HD22	2.23	0.46
1:D:239:GLN:HG3	1:D:271:ARG:O	2.14	0.46
1:C:343:GLY:HA2	1:C:346:TRP:HB2	1.98	0.46
1:E:16:SER:OG	1:E:139:GLU:OE2	2.16	0.46
1:E:200:VAL:HG13	1:E:211:LYS:HE2	1.96	0.46
1:E:339:GLY:HA2	1:E:353:TYR:CE2	2.50	0.46
1:B:19:ILE:HB	5:B:610:NDP:N7N	2.30	0.46
1:B:220:LYS:NZ	1:B:220:LYS:HB2	2.30	0.46
1:C:487:LEU:C	1:C:487:LEU:HD23	2.41	0.46
1:D:246:ARG:HE	1:D:268:GLN:NE2	2.12	0.46
1:E:15:LEU:HB2	1:E:139:GLU:CD	2.41	0.46
1:E:257:ARG:HD3	2:E:619:UMP:P	2.54	0.46
1:E:334:GLU:OE2	1:E:357:HIS:HE1	1.98	0.46
1:A:334:GLU:OE2	1:A:357:HIS:HE1	1.98	0.46
1:A:403:HIS:HB2	1:A:420:LEU:HD11	1.97	0.46
1:C:10:VAL:HG22	1:C:11:ALA:N	2.30	0.46
1:C:389:TRP:HB2	1:C:404:VAL:HG13	1.98	0.46
1:C:404:VAL:HG11	1:D:405:LEU:HD11	1.96	0.46
1:D:83:GLU:OE2	1:D:83:GLU:CA	2.62	0.46
1:E:487:LEU:C	1:E:487:LEU:HD23	2.41	0.46
1:A:410:VAL:O	1:B:254:ARG:NH2	2.39	0.46
1:B:27:TRP:CZ2	1:B:136:VAL:HG21	2.51	0.46
1:C:237:GLU:OE2	1:C:283:THR:HG23	2.16	0.46
1:C:320:GLY:O	1:C:335:GLU:O	2.33	0.46
1:E:246:ARG:HE	1:E:268:GLN:NE2	2.13	0.46
1:E:468:ASN:H	1:E:468:ASN:ND2	2.13	0.46
1:A:126:ASN:CG	1:A:177:LYS:NZ	2.74	0.46
1:A:220:LYS:HB2	1:A:220:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:VAL:HG11	1:B:405:LEU:CD1	2.45	0.46
1:B:133:LEU:HD22	1:B:134:THR:N	2.31	0.46
1:D:200:VAL:HG13	1:D:211:LYS:HE2	1.98	0.46
1:D:439:ALA:O	1:D:443:MET:HG3	2.16	0.46
1:E:411:THR:OG1	1:E:415:CYS:HB2	2.16	0.46
1:A:53:ILE:HG23	1:A:75:ILE:HD13	1.96	0.46
1:B:100:ASN:HB2	1:B:110:ILE:HD11	1.98	0.46
1:B:248:LEU:HD13	1:B:465:ILE:HD12	1.98	0.46
1:C:422:GLN:HE21	1:C:425:CYS:HB2	1.80	0.46
1:D:133:LEU:CD1	1:D:135:ARG:HG2	2.46	0.46
1:D:334:GLU:OE2	1:D:357:HIS:HE1	1.98	0.46
1:A:62:ILE:HD13	4:A:605:FOL:C16	2.45	0.46
1:B:51:ALA:C	1:B:52:LEU:HD23	2.41	0.46
1:B:166:LYS:O	1:B:167:ASN:HB2	2.15	0.46
1:B:403:HIS:HB2	1:B:420:LEU:HD11	1.98	0.46
1:C:383:ARG:O	1:C:385:ILE:N	2.49	0.46
1:D:19:ILE:O	5:D:618:NDP:H2N	2.16	0.46
1:D:237:GLU:OE2	1:D:283:THR:HG23	2.15	0.46
1:E:100:ASN:HB2	1:E:110:ILE:HD11	1.98	0.46
1:A:340:PRO:HG3	1:A:353:TYR:CG	2.51	0.46
1:B:48:LYS:HB3	1:B:106:SER:O	2.16	0.46
1:C:104:ASP:HB3	1:C:107:ILE:HD13	1.98	0.46
1:D:224:TYR:O	1:D:227:PRO:HG3	2.16	0.46
1:D:264:SER:HB3	1:D:464:HIS:HB3	1.97	0.46
1:D:372:ILE:O	1:D:376:LYS:HG2	2.16	0.46
1:A:248:LEU:HD13	1:A:465:ILE:HD12	1.98	0.45
1:B:389:TRP:HB2	1:B:404:VAL:HG13	1.98	0.45
1:C:183:LEU:O	1:C:184:GLN:HB3	2.15	0.45
1:A:27:TRP:CE3	1:A:138:LEU:HD21	2.51	0.45
1:A:36:PHE:CD1	1:A:36:PHE:C	2.94	0.45
1:A:49:LYS:NZ	6:A:700:HOH:O	2.48	0.45
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.99	0.45
1:D:243:LEU:O	1:D:247:VAL:HG13	2.15	0.45
1:E:343:GLY:HA2	1:E:346:TRP:HB2	1.98	0.45
1:C:35:PHE:HA	1:D:206:ILE:HD11	1.98	0.45
1:C:79:LEU:HA	1:C:80:PRO:HD3	1.73	0.45
1:C:200:VAL:HG13	1:C:211:LYS:HE2	1.98	0.45
1:C:248:LEU:HD13	1:C:465:ILE:HD12	1.98	0.45
1:E:75:ILE:HG22	5:E:622:NDP:C4A	2.47	0.45
1:E:104:ASP:CB	1:E:107:ILE:HD13	2.46	0.45
1:B:36:PHE:CD1	1:B:36:PHE:C	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LEU:HD22	1:C:133:LEU:C	2.42	0.45
1:D:103:ASN:C	1:D:103:ASN:HD22	2.23	0.45
1:D:422:GLN:HE21	1:D:425:CYS:HB2	1.80	0.45
1:D:448:VAL:HG13	6:D:636:HOH:O	2.16	0.45
1:E:77:SER:O	1:E:92:ARG:NH1	2.49	0.45
1:E:304:ASN:C	1:E:304:ASN:ND2	2.60	0.45
1:A:172:PHE:CD2	1:B:203:LEU:HD11	2.52	0.45
1:A:247:VAL:HG12	1:A:265:ILE:HD11	1.99	0.45
1:B:116:GLU:HB2	1:B:145:THR:CG2	2.46	0.45
1:B:200:VAL:HG13	1:B:211:LYS:HE2	1.99	0.45
1:C:32:ASP:OD2	4:C:613:FOL:N3	2.49	0.45
1:D:487:LEU:C	1:D:487:LEU:HD23	2.41	0.45
1:E:10:VAL:HG11	1:E:147:PHE:CE2	2.52	0.45
1:E:115:GLY:HA3	5:E:622:NDP:O1A	2.16	0.45
1:E:374:THR:HG22	1:E:384:HIS:CE1	2.51	0.45
1:A:116:GLU:HB2	1:A:145:THR:CG2	2.46	0.45
1:A:439:ALA:O	1:A:443:MET:HG3	2.17	0.45
1:B:115:GLY:O	1:B:116:GLU:C	2.60	0.45
1:B:340:PRO:HG3	1:B:353:TYR:CG	2.52	0.45
1:C:133:LEU:HD13	1:C:135:ARG:HG2	1.98	0.45
1:E:133:LEU:HD13	1:E:135:ARG:HG2	1.98	0.45
1:A:75:ILE:O	5:A:606:NDP:H1B	2.17	0.45
1:C:404:VAL:HG11	1:D:405:LEU:CD1	2.47	0.45
1:D:53:ILE:HG23	1:D:75:ILE:HD13	1.98	0.45
1:B:158:TYR:O	1:B:173:MET:HB2	2.17	0.45
1:B:487:LEU:O	1:B:488:LYS:HD3	2.17	0.45
1:C:239:GLN:HG3	1:C:271:ARG:O	2.17	0.45
1:D:339:GLY:HA2	1:D:353:TYR:CE2	2.52	0.45
1:D:403:HIS:HB2	1:D:420:LEU:HD11	1.99	0.45
1:E:233:ARG:NH1	1:E:242:ASP:OD1	2.42	0.45
1:A:179:GLU:HG2	1:A:180:LYS:N	2.31	0.45
1:A:246:ARG:HE	1:A:268:GLN:NE2	2.14	0.45
1:C:44:CYS:N	1:C:108:GLU:OE1	2.45	0.45
1:C:166:LYS:O	1:C:167:ASN:HB2	2.16	0.45
1:C:372:ILE:O	1:C:376:LYS:HG2	2.17	0.45
1:D:169:SER:OG	1:D:486:GLN:HG2	2.17	0.45
1:D:321:SER:O	1:D:325:LEU:HD13	2.16	0.45
1:E:97:SER:O	1:E:99:GLU:HG3	2.17	0.45
1:E:126:ASN:CG	1:E:177:LYS:NZ	2.75	0.45
1:A:27:TRP:CZ2	1:A:136:VAL:HG21	2.51	0.45
1:B:304:ASN:HD22	1:B:305:GLY:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:TRP:CZ2	1:C:136:VAL:HG21	2.52	0.45
1:C:36:PHE:CD1	1:C:36:PHE:C	2.95	0.45
1:D:104:ASP:CB	1:D:107:ILE:HD13	2.47	0.45
1:A:246:ARG:HE	1:A:268:GLN:HE22	1.64	0.44
1:B:439:ALA:O	1:B:443:MET:HG3	2.17	0.44
1:C:293:GLU:O	1:C:296:ILE:HD12	2.17	0.44
1:D:92:ARG:O	5:D:618:NDP:H2A	2.16	0.44
1:D:247:VAL:HG12	1:D:265:ILE:HD11	1.98	0.44
1:E:104:ASP:OD2	1:E:106:SER:OG	2.35	0.44
1:A:126:ASN:HA	1:A:126:ASN:HD22	1.65	0.44
1:A:405:LEU:CD1	1:B:404:VAL:HG11	2.47	0.44
1:B:321:SER:O	1:B:325:LEU:HD13	2.17	0.44
1:D:10:VAL:HG22	1:D:11:ALA:N	2.32	0.44
1:D:27:TRP:CE3	1:D:138:LEU:HD21	2.52	0.44
1:D:48:LYS:HB3	1:D:106:SER:O	2.17	0.44
1:E:403:HIS:HB2	1:E:420:LEU:HD11	1.98	0.44
1:E:439:ALA:O	1:E:443:MET:HG3	2.17	0.44
1:C:77:SER:O	1:C:92:ARG:NH1	2.50	0.44
1:C:126:ASN:CG	1:C:177:LYS:HZ1	2.25	0.44
1:D:383:ARG:O	1:D:385:ILE:N	2.51	0.44
1:A:104:ASP:CB	1:A:107:ILE:HD13	2.48	0.44
1:C:104:ASP:OD2	1:C:106:SER:OG	2.36	0.44
1:D:10:VAL:HG11	1:D:147:PHE:CE2	2.52	0.44
1:E:27:TRP:CE3	1:E:138:LEU:HD21	2.52	0.44
1:E:169:SER:OG	1:E:486:GLN:HG2	2.17	0.44
1:A:468:ASN:H	1:A:468:ASN:ND2	2.14	0.44
1:B:16:SER:OG	1:B:139:GLU:OE2	2.20	0.44
1:B:32:ASP:OD2	4:B:609:FOL:N3	2.50	0.44
1:B:239:GLN:HG3	1:B:271:ARG:O	2.16	0.44
1:B:257:ARG:HD3	2:B:607:UMP:OP2	2.18	0.44
1:B:372:ILE:O	1:B:376:LYS:HG2	2.16	0.44
1:C:220:LYS:HB2	1:C:220:LYS:NZ	2.32	0.44
1:C:340:PRO:HG3	1:C:353:TYR:CG	2.52	0.44
1:C:422:GLN:HE21	1:C:425:CYS:CB	2.30	0.44
1:D:27:TRP:CD1	1:D:27:TRP:C	2.96	0.44
1:D:49:LYS:NZ	6:D:645:HOH:O	2.38	0.44
1:E:103:ASN:C	1:E:103:ASN:HD22	2.25	0.44
1:D:43:LYS:NZ	1:D:48:LYS:O	2.34	0.44
1:B:27:TRP:CE3	1:B:138:LEU:HD21	2.53	0.44
1:B:79:LEU:HA	1:B:80:PRO:HD3	1.75	0.44
1:C:27:TRP:CE3	1:C:138:LEU:HD21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:TRP:CD1	1:C:27:TRP:C	2.95	0.44
1:D:115:GLY:HA3	5:D:618:NDP:O1A	2.17	0.44
1:D:340:PRO:HG3	1:D:353:TYR:CG	2.52	0.44
1:E:36:PHE:CD1	1:E:36:PHE:C	2.94	0.44
1:E:264:SER:HB3	1:E:464:HIS:HB3	1.98	0.44
1:A:104:ASP:OD2	1:A:106:SER:OG	2.36	0.44
1:B:248:LEU:HD12	1:B:248:LEU:HA	1.87	0.44
1:B:468:ASN:N	1:B:468:ASN:ND2	2.66	0.44
1:D:133:LEU:HD13	1:D:135:ARG:HG2	1.99	0.44
1:D:294:GLU:O	1:D:297:TRP:HB3	2.18	0.44
1:E:292:PHE:CD1	1:E:504:ILE:HD11	2.53	0.44
1:A:497:GLU:H	1:A:497:GLU:HG2	1.53	0.44
1:B:305:GLY:O	1:B:309:ILE:HG13	2.17	0.44
1:D:97:SER:O	1:D:99:GLU:HG3	2.17	0.44
1:D:378:ASN:ND2	1:D:381:ASP:HB2	2.32	0.44
1:D:468:ASN:H	1:D:468:ASN:ND2	2.14	0.44
1:A:422:GLN:HE21	1:A:425:CYS:HB2	1.83	0.43
1:B:4:LYS:HE2	1:B:101:LEU:HA	2.00	0.43
1:E:224:TYR:O	1:E:227:PRO:HG3	2.17	0.43
1:E:269:MET:HA	1:E:458:ILE:O	2.18	0.43
1:E:422:GLN:NE2	1:E:425:CYS:SG	2.91	0.43
1:A:103:ASN:C	1:A:103:ASN:HD22	2.25	0.43
1:A:383:ARG:O	1:A:385:ILE:N	2.51	0.43
1:B:257:ARG:HD3	2:B:607:UMP:P	2.57	0.43
1:C:93:ASN:ND2	1:C:95:GLU:HB3	2.32	0.43
1:C:126:ASN:HD22	1:C:126:ASN:HA	1.69	0.43
1:C:304:ASN:HD21	1:C:306:ASN:HB2	1.83	0.43
1:C:411:THR:OG1	1:C:415:CYS:HB2	2.18	0.43
1:E:133:LEU:HD22	1:E:133:LEU:C	2.42	0.43
1:E:294:GLU:O	1:E:297:TRP:HB3	2.18	0.43
1:B:298:PHE:CE1	1:B:342:TYR:HB2	2.53	0.43
1:B:381:ASP:HB3	1:B:384:HIS:NE2	2.33	0.43
1:D:337:ASP:HA	1:D:356:MET:SD	2.57	0.43
1:A:115:GLY:HA3	5:A:606:NDP:PA	2.58	0.43
1:B:104:ASP:HB3	1:B:107:ILE:HD13	2.00	0.43
1:B:182:THR:HG23	1:B:183:LEU:N	2.33	0.43
1:C:393:ALA:O	1:C:394:LEU:C	2.61	0.43
1:A:62:ILE:HD13	4:A:605:FOL:C15	2.49	0.43
1:A:393:ALA:O	1:A:394:LEU:C	2.62	0.43
1:A:505:GLU:HB3	1:A:507:ILE:CD1	2.47	0.43
1:B:343:GLY:HA2	1:B:346:TRP:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:SER:O	1:C:111:PHE:HA	2.19	0.43
1:C:10:VAL:HG11	1:C:147:PHE:CE2	2.54	0.43
1:C:133:LEU:HD13	1:C:135:ARG:CG	2.48	0.43
1:C:288:ILE:HA	1:C:291:ILE:HD12	2.01	0.43
1:E:133:LEU:HD13	1:E:135:ARG:CG	2.49	0.43
1:E:226:THR:N	1:E:227:PRO:HD3	2.33	0.43
1:E:393:ALA:O	1:E:394:LEU:C	2.61	0.43
1:A:133:LEU:HD13	1:A:135:ARG:CG	2.48	0.43
1:A:273:ASP:HB2	1:B:212:MET:SD	2.58	0.43
1:B:133:LEU:HD13	1:B:135:ARG:CG	2.49	0.43
1:C:468:ASN:N	1:C:468:ASN:ND2	2.66	0.43
1:D:34:LYS:NZ	6:D:682:HOH:O	2.39	0.43
1:A:269:MET:HA	1:A:458:ILE:O	2.19	0.43
1:C:247:VAL:HG12	1:C:265:ILE:HD11	2.01	0.43
1:C:381:ASP:HB3	1:C:384:HIS:NE2	2.33	0.43
1:C:403:HIS:HB2	1:C:420:LEU:HD11	1.99	0.43
1:D:158:TYR:O	1:D:173:MET:HB2	2.19	0.43
1:B:83:GLU:OE2	1:B:83:GLU:CA	2.63	0.43
1:C:4:LYS:HE2	1:C:101:LEU:HA	1.98	0.43
1:C:337:ASP:OD2	1:C:353:TYR:OH	2.37	0.43
1:E:182:THR:OG1	1:E:183:LEU:N	2.51	0.43
1:A:200:VAL:HG13	1:A:211:LYS:HE2	2.00	0.43
1:B:126:ASN:HD21	1:B:177:LYS:HE3	1.84	0.43
1:C:305:GLY:O	1:C:309:ILE:HG13	2.19	0.43
1:C:374:THR:HG22	1:C:384:HIS:HE1	1.84	0.43
1:D:133:LEU:HD22	1:D:133:LEU:C	2.43	0.43
1:D:393:ALA:O	1:D:394:LEU:C	2.62	0.43
1:A:52:LEU:HD23	1:A:52:LEU:N	2.34	0.43
1:A:206:ILE:HD11	1:B:35:PHE:HA	2.00	0.43
1:B:223:ILE:O	1:B:245:SER:CB	2.65	0.43
1:B:247:VAL:HG12	1:B:265:ILE:HD11	2.00	0.43
1:D:226:THR:N	1:D:227:PRO:HD3	2.34	0.43
1:E:182:THR:HG23	1:E:183:LEU:N	2.34	0.43
1:E:359:ASP:OD2	1:E:361:THR:CG2	2.66	0.43
1:A:10:VAL:HG11	1:A:147:PHE:CE2	2.53	0.42
1:A:27:TRP:CD1	1:A:27:TRP:C	2.97	0.42
1:A:293:GLU:O	1:A:296:ILE:CD1	2.67	0.42
1:A:479:ARG:HD3	1:A:512:TYR:CG	2.54	0.42
4:A:605:FOL:C6	5:A:606:NDP:H42N	2.48	0.42
1:C:203:LEU:HD11	1:D:172:PHE:CD2	2.53	0.42
1:D:126:ASN:CG	1:D:177:LYS:NZ	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:THR:OG1	1:D:183:LEU:N	2.52	0.42
1:D:304:ASN:HD22	1:D:305:GLY:N	2.15	0.42
1:D:306:ASN:ND2	1:D:336:ASN:HB2	2.34	0.42
1:E:27:TRP:CD1	1:E:27:TRP:C	2.97	0.42
1:E:93:ASN:ND2	1:E:95:GLU:HB3	2.33	0.42
1:E:139:GLU:O	1:E:139:GLU:HG3	2.18	0.42
1:A:422:GLN:NE2	1:A:425:CYS:SG	2.92	0.42
1:B:256:ASN:ND2	1:B:258:THR:H	2.13	0.42
1:D:359:ASP:OD2	1:D:361:THR:CG2	2.66	0.42
1:D:479:ARG:HD3	1:D:512:TYR:CG	2.54	0.42
1:A:48:LYS:HB3	1:A:106:SER:O	2.19	0.42
1:A:133:LEU:HD22	1:A:133:LEU:C	2.44	0.42
1:B:120:ARG:NH1	1:B:148:PRO:HB3	2.35	0.42
1:B:288:ILE:HA	1:B:291:ILE:HD12	2.01	0.42
1:B:479:ARG:HD3	1:B:512:TYR:CG	2.54	0.42
1:B:495:ASN:OD1	1:B:497:GLU:HG2	2.20	0.42
1:B:505:GLU:HB3	1:B:507:ILE:CD1	2.48	0.42
1:C:495:ASN:OD1	1:C:497:GLU:HG2	2.20	0.42
1:D:349:TYR:HB3	1:D:365:VAL:HB	2.00	0.42
1:A:391:PRO:HD2	1:B:349:TYR:CD2	2.55	0.42
1:A:431:SER:O	1:A:432:PRO:C	2.61	0.42
1:B:27:TRP:CD1	1:B:27:TRP:C	2.97	0.42
1:B:514:THR:HG21	6:B:713:HOH:O	2.19	0.42
1:C:16:SER:OG	1:C:139:GLU:OE2	2.16	0.42
1:D:385:ILE:CG2	1:D:386:LEU:N	2.83	0.42
1:E:26:PRO:HG3	1:E:143:PHE:HE1	1.84	0.42
1:A:158:TYR:O	1:A:173:MET:HB2	2.18	0.42
1:B:383:ARG:O	1:B:385:ILE:N	2.52	0.42
1:D:62:ILE:HD13	4:D:617:FOL:C16	2.50	0.42
1:E:4:LYS:HE2	1:E:101:LEU:HA	2.01	0.42
1:E:92:ARG:HA	1:E:92:ARG:HD3	1.90	0.42
1:E:495:ASN:OD1	1:E:497:GLU:HG2	2.20	0.42
1:A:402:CYS:SG	2:A:603:UMP:H6	2.40	0.42
1:C:100:ASN:HB2	1:C:110:ILE:HD11	2.02	0.42
1:C:158:TYR:O	1:C:173:MET:HB2	2.20	0.42
1:D:126:ASN:HD21	1:D:177:LYS:HE3	1.84	0.42
1:E:7:SER:O	1:E:111:PHE:HA	2.19	0.42
1:E:479:ARG:HD3	1:E:512:TYR:CG	2.54	0.42
1:A:304:ASN:HD22	1:A:305:GLY:N	2.17	0.42
1:C:21:ILE:HG23	1:C:21:ILE:O	2.20	0.42
1:D:100:ASN:HB2	1:D:110:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:CYS:N	1:E:108:GLU:OE1	2.45	0.42
1:A:32:ASP:OD2	4:A:605:FOL:N3	2.53	0.42
1:C:104:ASP:CB	1:C:107:ILE:HD13	2.49	0.42
1:C:229:ILE:HG22	1:C:233:ARG:HG2	2.01	0.42
1:C:321:SER:O	1:C:325:LEU:HD13	2.20	0.42
1:C:422:GLN:NE2	1:C:425:CYS:SG	2.93	0.42
1:C:439:ALA:O	1:C:443:MET:HG3	2.20	0.42
1:D:7:SER:O	1:D:111:PHE:HA	2.20	0.42
1:E:32:ASP:OD2	4:E:621:FOL:N3	2.52	0.42
1:E:288:ILE:HA	1:E:291:ILE:HD12	2.01	0.42
1:A:422:GLN:HE21	1:A:425:CYS:CB	2.33	0.42
1:B:180:LYS:CG	1:B:181:LYS:N	2.83	0.42
1:C:431:SER:O	1:C:432:PRO:C	2.63	0.42
1:D:288:ILE:HA	1:D:291:ILE:HD12	2.02	0.42
1:A:337:ASP:HA	1:A:356:MET:SD	2.60	0.42
1:C:52:LEU:HD23	1:C:52:LEU:N	2.35	0.42
1:C:256:ASN:ND2	1:C:258:THR:H	2.13	0.42
1:D:133:LEU:HD13	1:D:135:ARG:CG	2.50	0.42
1:D:235:HIS:CE1	1:D:237:GLU:HB2	2.55	0.42
1:D:487:LEU:O	1:D:488:LYS:HD3	2.20	0.42
1:A:306:ASN:ND2	1:A:336:ASN:HB2	2.33	0.41
1:D:411:THR:OG1	1:D:415:CYS:HB2	2.20	0.41
1:E:126:ASN:HD22	1:E:126:ASN:HA	1.70	0.41
1:E:247:VAL:O	1:E:251:GLY:N	2.45	0.41
1:A:223:ILE:O	1:A:245:SER:CB	2.67	0.41
1:A:507:ILE:N	1:A:507:ILE:HD12	2.36	0.41
1:C:298:PHE:CE1	1:C:342:TYR:HB2	2.55	0.41
1:E:211:LYS:HG2	6:E:650:HOH:O	2.20	0.41
1:E:223:ILE:O	1:E:245:SER:CB	2.66	0.41
1:E:247:VAL:HG12	1:E:265:ILE:HD11	2.00	0.41
1:E:248:LEU:HD13	1:E:465:ILE:HD12	2.02	0.41
1:A:224:TYR:O	1:A:227:PRO:HG3	2.20	0.41
1:B:487:LEU:HD23	1:B:487:LEU:C	2.44	0.41
1:D:114:GLY:HA2	1:D:119:TYR:CE2	2.55	0.41
1:E:423:ARG:NH1	2:E:619:UMP:OP3	2.46	0.41
1:E:430:GLY:O	1:E:431:SER:C	2.63	0.41
1:A:349:TYR:HB3	1:A:365:VAL:HB	2.02	0.41
1:B:349:TYR:HB3	1:B:365:VAL:HB	2.02	0.41
1:D:180:LYS:CG	1:D:181:LYS:N	2.82	0.41
1:D:292:PHE:CD1	1:D:504:ILE:HD11	2.54	0.41
1:E:85:ASP:OD1	1:E:86:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:ASN:ND2	1:E:336:ASN:HB2	2.35	0.41
1:E:431:SER:O	1:E:432:PRO:C	2.62	0.41
3:E:620:CB3:C6	3:E:620:CB3:H15	2.50	0.41
1:A:126:ASN:ND2	6:A:703:HOH:O	2.48	0.41
1:A:212:MET:HG3	1:A:215:ARG:NH2	2.36	0.41
1:C:226:THR:N	1:C:227:PRO:HD3	2.35	0.41
1:C:244:LEU:HD21	1:C:473:LEU:HD22	2.01	0.41
1:C:292:PHE:CD1	1:C:504:ILE:HD11	2.55	0.41
1:E:79:LEU:HA	1:E:80:PRO:HD3	1.74	0.41
1:A:325:LEU:HD23	1:A:333:ARG:HB3	2.03	0.41
1:A:339:GLY:HA2	1:A:353:TYR:CE2	2.55	0.41
1:B:21:ILE:O	1:B:21:ILE:HG23	2.20	0.41
1:C:103:ASN:CG	1:C:104:ASP:H	2.29	0.41
1:C:487:LEU:O	1:C:488:LYS:HD3	2.21	0.41
3:C:612:CB3:C6	3:C:612:CB3:H15	2.50	0.41
1:D:37:SER:O	1:D:41:ASN:HB2	2.20	0.41
1:D:247:VAL:O	1:D:251:GLY:N	2.46	0.41
1:E:229:ILE:HG22	1:E:233:ARG:HG2	2.02	0.41
1:E:337:ASP:OD2	1:E:353:TYR:OH	2.38	0.41
1:E:480:THR:HA	1:E:481:PRO:HD3	1.93	0.41
1:A:256:ASN:ND2	1:A:258:THR:H	2.14	0.41
1:B:3:GLU:CG	1:B:4:LYS:N	2.64	0.41
1:B:199:THR:O	1:B:203:LEU:HB2	2.20	0.41
1:C:114:GLY:HA2	1:C:119:TYR:CE2	2.55	0.41
1:C:169:SER:OG	1:C:486:GLN:HG2	2.21	0.41
1:C:429:LEU:HD12	1:C:429:LEU:HA	1.87	0.41
1:D:269:MET:HA	1:D:458:ILE:O	2.21	0.41
1:D:363:VAL:HG22	1:D:364:GLY:N	2.36	0.41
1:D:497:GLU:H	1:D:497:GLU:HG2	1.53	0.41
1:D:505:GLU:HB3	1:D:507:ILE:CD1	2.50	0.41
1:E:107:ILE:HD12	1:E:107:ILE:N	2.35	0.41
1:A:180:LYS:CG	1:A:181:LYS:N	2.82	0.41
1:A:343:GLY:HA2	1:A:346:TRP:HB2	2.02	0.41
1:A:372:ILE:O	1:A:376:LYS:HG2	2.20	0.41
1:B:7:SER:O	1:B:111:PHE:HA	2.20	0.41
1:D:298:PHE:CE1	1:D:342:TYR:HB2	2.55	0.41
1:E:468:ASN:N	1:E:468:ASN:ND2	2.68	0.41
1:A:4:LYS:HE2	1:A:101:LEU:HA	2.02	0.41
1:A:21:ILE:HG23	1:A:21:ILE:O	2.21	0.41
1:A:99:GLU:OE2	1:A:99:GLU:O	2.39	0.41
1:A:226:THR:N	1:A:227:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLU:O	1:A:297:TRP:HB3	2.20	0.41
1:A:304:ASN:HD21	1:A:306:ASN:HB2	1.85	0.41
1:A:381:ASP:HB3	1:A:384:HIS:NE2	2.36	0.41
1:A:434:ASN:OD1	2:A:603:UMP:O4	2.38	0.41
1:A:516:LYS:HE3	1:A:518:ASP:OD1	2.20	0.41
3:A:604:CB3:C6	3:A:604:CB3:H15	2.51	0.41
1:B:104:ASP:OD2	1:B:106:SER:OG	2.39	0.41
1:B:133:LEU:HD22	1:B:133:LEU:C	2.46	0.41
1:B:229:ILE:HG22	1:B:233:ARG:HG2	2.03	0.41
1:B:411:THR:OG1	1:B:415:CYS:HB2	2.21	0.41
1:B:466:TYR:HB3	1:B:468:ASN:ND2	2.36	0.41
3:B:608:CB3:H15	3:B:608:CB3:C6	2.50	0.41
1:C:102:MET:O	1:C:103:ASN:CB	2.66	0.41
1:C:233:ARG:HH12	1:C:242:ASP:CG	2.29	0.41
1:E:158:TYR:O	1:E:173:MET:HB2	2.21	0.41
1:E:180:LYS:CG	1:E:181:LYS:N	2.84	0.41
1:E:274:MET:HE1	1:E:442:THR:HG21	2.03	0.41
1:E:349:TYR:HB3	1:E:365:VAL:HB	2.02	0.41
1:E:429:LEU:HD12	1:E:429:LEU:HA	1.87	0.41
1:A:126:ASN:HD21	1:A:177:LYS:HE3	1.85	0.41
1:B:363:VAL:HG22	1:B:364:GLY:N	2.35	0.41
1:C:39:ILE:CG2	1:C:40:THR:N	2.84	0.41
1:C:285:LYS:HE2	1:C:514:THR:HG22	2.03	0.41
1:D:4:LYS:HE2	1:D:101:LEU:HA	2.02	0.41
1:E:114:GLY:HA2	1:E:119:TYR:CE2	2.55	0.41
1:A:244:LEU:HD21	1:A:473:LEU:HD22	2.03	0.40
1:C:107:ILE:HD12	1:C:107:ILE:N	2.36	0.40
1:D:123:LEU:HD13	1:D:128:VAL:HG11	2.02	0.40
1:E:363:VAL:HG22	1:E:364:GLY:N	2.36	0.40
1:A:15:LEU:HB2	1:A:139:GLU:CG	2.51	0.40
1:A:166:LYS:O	1:A:167:ASN:HB2	2.20	0.40
1:A:333:ARG:HH11	1:A:333:ARG:HG2	1.86	0.40
1:B:77:SER:O	1:B:92:ARG:NH1	2.54	0.40
1:B:422:GLN:NE2	1:B:425:CYS:SG	2.94	0.40
1:B:431:SER:O	1:B:432:PRO:C	2.63	0.40
1:C:132:TYR:CD2	1:C:174:ILE:CG2	3.05	0.40
1:C:199:THR:O	1:C:203:LEU:HB2	2.21	0.40
1:C:223:ILE:O	1:C:245:SER:CB	2.68	0.40
1:C:479:ARG:HD3	1:C:512:TYR:CG	2.56	0.40
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.86	0.40
1:B:224:TYR:O	1:B:227:PRO:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:HIS:CE1	1:B:237:GLU:HB2	2.57	0.40
1:B:269:MET:HA	1:B:458:ILE:O	2.22	0.40
1:B:293:GLU:O	1:B:296:ILE:CD1	2.69	0.40
1:B:393:ALA:O	1:B:394:LEU:C	2.64	0.40
1:C:26:PRO:HG3	1:C:143:PHE:HE1	1.86	0.40
1:D:26:PRO:HG3	1:D:143:PHE:HE1	1.86	0.40
1:D:99:GLU:OE2	1:D:99:GLU:O	2.39	0.40
1:D:132:TYR:CD2	1:D:174:ILE:CG2	3.05	0.40
1:D:430:GLY:O	1:D:431:SER:C	2.64	0.40
1:A:92:ARG:O	5:A:606:NDP:H2A	2.21	0.40
1:A:212:MET:SD	1:B:273:ASP:HB2	2.60	0.40
1:A:374:THR:HG22	1:A:384:HIS:HE1	1.84	0.40
1:A:385:ILE:CG2	1:A:386:LEU:N	2.84	0.40
1:B:92:ARG:HA	1:B:92:ARG:HD3	1.89	0.40
1:C:349:TYR:CD2	1:D:391:PRO:HD2	2.55	0.40
1:C:505:GLU:HB3	1:C:507:ILE:CD1	2.51	0.40
1:E:429:LEU:CD1	1:E:517:MET:HB2	2.52	0.40
1:A:199:THR:O	1:A:203:LEU:HB2	2.20	0.40
1:C:92:ARG:O	5:C:614:NDP:H2A	2.22	0.40
1:C:139:GLU:HG3	1:C:139:GLU:O	2.21	0.40
1:C:248:LEU:HD12	1:C:248:LEU:HA	1.87	0.40
1:C:323:GLU:H	1:C:323:GLU:CD	2.28	0.40
1:C:430:GLY:O	1:C:431:SER:C	2.65	0.40
1:C:472:GLN:O	1:C:475:GLU:HB3	2.21	0.40
1:D:132:TYR:HA	1:D:174:ILE:HG22	2.03	0.40
1:D:166:LYS:O	1:D:167:ASN:HB2	2.20	0.40
1:D:189:ALA:O	1:D:192:GLN:HG2	2.22	0.40
1:D:293:GLU:O	1:D:296:ILE:CD1	2.69	0.40
3:D:616:CB3:C6	3:D:616:CB3:H15	2.51	0.40
1:E:293:GLU:O	1:E:296:ILE:CD1	2.69	0.40
1:E:297:TRP:HH2	1:E:338:LEU:HD12	1.87	0.40
1:E:381:ASP:HB3	1:E:384:HIS:NE2	2.36	0.40

There are no symmetry-related clashes.

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	517/521 (99%)	468 (90%)	40 (8%)	9 (2%)	7	25
1	B	517/521 (99%)	466 (90%)	43 (8%)	8 (2%)	8	28
1	C	517/521 (99%)	466 (90%)	42 (8%)	9 (2%)	7	25
1	D	517/521 (99%)	466 (90%)	42 (8%)	9 (2%)	7	25
1	E	517/521 (99%)	468 (90%)	40 (8%)	9 (2%)	7	25
All	All	2585/2605 (99%)	2334 (90%)	207 (8%)	44 (2%)	7	25

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ALA
1	A	102	MET
1	A	103	ASN
1	B	84	ALA
1	B	102	MET
1	B	103	ASN
1	C	84	ALA
1	C	102	MET
1	C	103	ASN
1	D	84	ALA
1	D	102	MET
1	D	103	ASN
1	E	84	ALA
1	E	102	MET
1	E	103	ASN
1	A	4	LYS
1	A	99	GLU
1	A	182	THR
1	B	4	LYS
1	B	99	GLU
1	B	182	THR
1	B	335	GLU
1	C	4	LYS
1	C	99	GLU
1	C	182	THR
1	C	335	GLU
1	D	4	LYS

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Mol	Chain	Res	Type
1	D	99	GLU
1	D	182	THR
1	E	4	LYS
1	E	99	GLU
1	E	182	THR
1	A	335	GLU
1	D	335	GLU
1	E	335	GLU
1	E	384	HIS
1	A	281	LEU
1	D	384	HIS
1	C	384	HIS
1	A	341	ILE
1	C	341	ILE
1	D	341	ILE
1	E	341	ILE
1	B	341	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/470 (100%)	430 (92%)	38 (8%)	11	33
1	B	468/470 (100%)	432 (92%)	36 (8%)	12	36
1	C	468/470 (100%)	430 (92%)	38 (8%)	11	33
1	D	468/470 (100%)	432 (92%)	36 (8%)	12	36
1	E	468/470 (100%)	432 (92%)	36 (8%)	12	36
All	All	2340/2350 (100%)	2156 (92%)	184 (8%)	11	35

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	52	LEU

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Mol	Chain	Res	Type
1	A	79	LEU
1	A	96	ASP
1	A	99	GLU
1	A	102	MET
1	A	103	ASN
1	A	104	ASP
1	A	124	LYS
1	A	126	ASN
1	A	128	VAL
1	A	133	LEU
1	A	138	LEU
1	A	142	GLU
1	A	176	GLU
1	A	179	GLU
1	A	183	LEU
1	A	202	LEU
1	A	209	ILE
1	A	220	LYS
1	A	247	VAL
1	A	257	ARG
1	A	258	THR
1	A	295	LEU
1	A	296	ILE
1	A	304	ASN
1	A	371	LEU
1	A	373	GLU
1	A	383	ARG
1	A	427	LEU
1	A	429	LEU
1	A	431	SER
1	A	468	ASN
1	A	474	LYS
1	A	497	GLU
1	A	506	LEU
1	A	514	THR
1	A	516	LYS
1	B	41	ASN
1	B	79	LEU
1	B	96	ASP
1	B	99	GLU
1	B	102	MET
1	B	103	ASN

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Mol	Chain	Res	Type
1	B	104	ASP
1	B	124	LYS
1	B	126	ASN
1	B	128	VAL
1	B	133	LEU
1	B	138	LEU
1	B	142	GLU
1	B	176	GLU
1	B	179	GLU
1	B	183	LEU
1	B	202	LEU
1	B	209	ILE
1	B	220	LYS
1	B	247	VAL
1	B	258	THR
1	B	295	LEU
1	B	296	ILE
1	B	304	ASN
1	B	371	LEU
1	B	373	GLU
1	B	383	ARG
1	B	427	LEU
1	B	429	LEU
1	B	431	SER
1	B	468	ASN
1	B	474	LYS
1	B	497	GLU
1	B	506	LEU
1	B	514	THR
1	B	516	LYS
1	C	41	ASN
1	C	52	LEU
1	C	79	LEU
1	C	96	ASP
1	C	99	GLU
1	C	102	MET
1	C	103	ASN
1	C	104	ASP
1	C	124	LYS
1	C	126	ASN
1	C	128	VAL
1	C	133	LEU

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Mol	Chain	Res	Type
1	C	138	LEU
1	C	142	GLU
1	C	176	GLU
1	C	179	GLU
1	C	183	LEU
1	C	202	LEU
1	C	209	ILE
1	C	220	LYS
1	C	247	VAL
1	C	257	ARG
1	C	258	THR
1	C	295	LEU
1	C	296	ILE
1	C	304	ASN
1	C	371	LEU
1	C	373	GLU
1	C	383	ARG
1	C	427	LEU
1	C	429	LEU
1	C	431	SER
1	C	468	ASN
1	C	474	LYS
1	C	497	GLU
1	C	506	LEU
1	C	514	THR
1	C	516	LYS
1	D	41	ASN
1	D	52	LEU
1	D	79	LEU
1	D	96	ASP
1	D	99	GLU
1	D	102	MET
1	D	103	ASN
1	D	104	ASP
1	D	124	LYS
1	D	126	ASN
1	D	128	VAL
1	D	133	LEU
1	D	138	LEU
1	D	142	GLU
1	D	176	GLU
1	D	179	GLU

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Mol	Chain	Res	Type
1	D	183	LEU
1	D	202	LEU
1	D	209	ILE
1	D	220	LYS
1	D	247	VAL
1	D	257	ARG
1	D	295	LEU
1	D	296	ILE
1	D	304	ASN
1	D	371	LEU
1	D	373	GLU
1	D	383	ARG
1	D	427	LEU
1	D	429	LEU
1	D	468	ASN
1	D	474	LYS
1	D	497	GLU
1	D	506	LEU
1	D	514	THR
1	D	516	LYS
1	E	41	ASN
1	E	52	LEU
1	E	79	LEU
1	E	96	ASP
1	E	99	GLU
1	E	102	MET
1	E	103	ASN
1	E	104	ASP
1	E	124	LYS
1	E	126	ASN
1	E	128	VAL
1	E	133	LEU
1	E	138	LEU
1	E	142	GLU
1	E	176	GLU
1	E	179	GLU
1	E	183	LEU
1	E	202	LEU
1	E	209	ILE
1	E	220	LYS
1	E	247	VAL
1	E	258	THR

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Mol	Chain	Res	Type
1	E	295	LEU
1	E	296	ILE
1	E	304	ASN
1	E	371	LEU
1	E	373	GLU
1	E	383	ARG
1	E	427	LEU
1	E	429	LEU
1	E	468	ASN
1	E	474	LYS
1	E	497	GLU
1	E	506	LEU
1	E	514	THR
1	E	516	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	22	ASN
1	A	24	GLN
1	A	41	ASN
1	A	47	ASN
1	A	69	ASN
1	A	93	ASN
1	A	103	ASN
1	A	109	ASN
1	A	167	ASN
1	A	216	HIS
1	A	250	ASN
1	A	256	ASN
1	A	268	GLN
1	A	304	ASN
1	A	306	ASN
1	A	336	ASN
1	A	357	HIS
1	A	377	ASN
1	A	412	ASN
1	A	422	GLN
1	A	434	ASN
1	A	468	ASN
1	A	476	GLN

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Mol	Chain	Res	Type
1	B	5	ASN
1	B	22	ASN
1	B	24	GLN
1	B	41	ASN
1	B	47	ASN
1	B	93	ASN
1	B	103	ASN
1	B	167	ASN
1	B	192	GLN
1	B	216	HIS
1	B	250	ASN
1	B	256	ASN
1	B	268	GLN
1	B	304	ASN
1	B	306	ASN
1	B	357	HIS
1	B	377	ASN
1	B	378	ASN
1	B	412	ASN
1	B	419	ASN
1	B	422	GLN
1	B	468	ASN
1	B	476	GLN
1	C	5	ASN
1	C	22	ASN
1	C	24	GLN
1	C	41	ASN
1	C	47	ASN
1	C	93	ASN
1	C	103	ASN
1	C	109	ASN
1	C	167	ASN
1	C	192	GLN
1	C	216	HIS
1	C	250	ASN
1	C	256	ASN
1	C	268	GLN
1	C	304	ASN
1	C	306	ASN
1	C	357	HIS
1	C	377	ASN
1	C	378	ASN

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Mol	Chain	Res	Type
1	C	412	ASN
1	C	422	GLN
1	C	468	ASN
1	C	476	GLN
1	C	486	GLN
1	D	5	ASN
1	D	22	ASN
1	D	24	GLN
1	D	41	ASN
1	D	47	ASN
1	D	93	ASN
1	D	103	ASN
1	D	167	ASN
1	D	192	GLN
1	D	216	HIS
1	D	250	ASN
1	D	256	ASN
1	D	268	GLN
1	D	304	ASN
1	D	306	ASN
1	D	357	HIS
1	D	377	ASN
1	D	378	ASN
1	D	412	ASN
1	D	422	GLN
1	D	468	ASN
1	D	476	GLN
1	E	5	ASN
1	E	22	ASN
1	E	24	GLN
1	E	41	ASN
1	E	47	ASN
1	E	93	ASN
1	E	103	ASN
1	E	109	ASN
1	E	167	ASN
1	E	192	GLN
1	E	214	ASN
1	E	216	HIS
1	E	250	ASN
1	E	256	ASN
1	E	268	GLN

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Mol	Chain	Res	Type
1	E	304	ASN
1	E	306	ASN
1	E	319	ASN
1	E	357	HIS
1	E	377	ASN
1	E	378	ASN
1	E	412	ASN
1	E	419	ASN
1	E	422	GLN
1	E	468	ASN
1	E	476	GLN
1	E	486	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CB3	C	612	-	37,37,37	2.32	8 (21%)	50,51,51	1.05	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CB3	E	620	-	37,37,37	2.39	10 (27%)	50,51,51	1.03	3 (6%)
4	FOL	A	605	-	34,34,34	2.02	9 (26%)	43,47,47	1.87	10 (23%)
3	CB3	B	608	-	37,37,37	2.35	8 (21%)	50,51,51	1.04	2 (4%)
3	CB3	A	604	-	37,37,37	2.43	9 (24%)	50,51,51	0.98	1 (2%)
5	NDP	B	610	-	51,52,52	1.81	11 (21%)	71,80,80	1.93	22 (30%)
5	NDP	C	614	-	51,52,52	1.73	11 (21%)	71,80,80	1.88	21 (29%)
5	NDP	D	618	-	51,52,52	1.73	11 (21%)	71,80,80	1.90	22 (30%)
4	FOL	D	617	-	34,34,34	2.01	9 (26%)	43,47,47	1.89	10 (23%)
4	FOL	B	609	-	34,34,34	2.01	9 (26%)	43,47,47	1.86	10 (23%)
2	UMP	A	603	-	21,21,21	3.05	7 (33%)	30,31,31	2.29	9 (30%)
5	NDP	A	606	-	51,52,52	1.88	12 (23%)	71,80,80	1.92	23 (32%)
5	NDP	E	622	-	51,52,52	1.80	12 (23%)	71,80,80	1.95	24 (33%)
2	UMP	D	615	-	21,21,21	3.11	7 (33%)	30,31,31	2.29	9 (30%)
2	UMP	E	619	-	21,21,21	3.03	6 (28%)	30,31,31	2.33	9 (30%)
4	FOL	E	621	-	34,34,34	2.02	9 (26%)	43,47,47	1.85	10 (23%)
3	CB3	D	616	-	37,37,37	2.37	9 (24%)	50,51,51	1.03	3 (6%)
2	UMP	C	611	-	21,21,21	2.99	5 (23%)	30,31,31	2.30	9 (30%)
2	UMP	B	607	-	21,21,21	2.99	5 (23%)	30,31,31	2.33	9 (30%)
4	FOL	C	613	-	34,34,34	2.01	9 (26%)	43,47,47	1.86	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CB3	C	612	-	1/1/5/6	7/27/28/28	0/3/3/3
3	CB3	E	620	-	1/1/5/6	7/27/28/28	0/3/3/3
4	FOL	A	605	-	-	6/22/22/22	0/3/3/3
3	CB3	B	608	-	1/1/5/6	7/27/28/28	0/3/3/3
3	CB3	A	604	-	1/1/5/6	7/27/28/28	0/3/3/3
5	NDP	B	610	-	-	6/34/77/77	0/5/5/5
5	NDP	C	614	-	-	6/34/77/77	0/5/5/5
5	NDP	D	618	-	-	6/34/77/77	0/5/5/5
4	FOL	D	617	-	-	6/22/22/22	0/3/3/3
4	FOL	B	609	-	-	6/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UMP	A	603	-	-	2/10/22/22	0/2/2/2
5	NDP	A	606	-	-	6/34/77/77	0/5/5/5
5	NDP	E	622	-	-	5/34/77/77	0/5/5/5
2	UMP	D	615	-	-	3/10/22/22	0/2/2/2
2	UMP	E	619	-	-	3/10/22/22	0/2/2/2
4	FOL	E	621	-	-	6/22/22/22	0/3/3/3
3	CB3	D	616	-	1/1/5/6	7/27/28/28	0/3/3/3
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	FOL	C	613	-	-	6/22/22/22	0/3/3/3

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	615	UMP	C6-C5	8.66	1.55	1.35
2	E	619	UMP	C6-C5	8.49	1.54	1.35
2	A	603	UMP	C6-C5	8.46	1.54	1.35
2	C	611	UMP	C6-C5	8.46	1.54	1.35
2	B	607	UMP	C6-C5	8.44	1.54	1.35
3	E	620	CB3	O4-C4	8.27	1.37	1.23
3	A	604	CB3	O4-C4	8.25	1.37	1.23
3	D	616	CB3	O4-C4	8.23	1.37	1.23
3	B	608	CB3	O4-C4	8.07	1.37	1.23
3	C	612	CB3	O4-C4	7.94	1.36	1.23
2	D	615	UMP	C6-N1	6.03	1.52	1.38
2	A	603	UMP	C6-N1	5.79	1.51	1.38
2	B	607	UMP	C6-N1	5.77	1.51	1.38
2	C	611	UMP	C6-N1	5.75	1.51	1.38
2	E	619	UMP	C6-N1	5.73	1.51	1.38
2	D	615	UMP	C5-C4	5.69	1.56	1.43
2	C	611	UMP	C5-C4	5.68	1.56	1.43
2	B	607	UMP	C5-C4	5.59	1.55	1.43
2	A	603	UMP	C5-C4	5.50	1.55	1.43
2	E	619	UMP	C5-C4	5.46	1.55	1.43
4	A	605	FOL	C9-C6	-5.36	1.39	1.50
4	D	617	FOL	C9-C6	-5.28	1.39	1.50
4	E	621	FOL	C9-C6	-5.25	1.39	1.50
4	C	613	FOL	C9-C6	-5.22	1.39	1.50
4	B	609	FOL	C9-C6	-5.22	1.39	1.50
3	A	604	CB3	CP1-CP2	5.18	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	606	NDP	C4N-C3N	-4.97	1.40	1.50
5	A	606	NDP	PN-O3	4.96	1.64	1.59
3	A	604	CB3	CP1-N10	4.94	1.50	1.46
5	B	610	NDP	C4N-C3N	-4.93	1.40	1.50
3	E	620	CB3	CP1-CP2	4.89	1.54	1.46
3	B	608	CB3	CP1-CP2	4.88	1.54	1.46
3	D	616	CB3	CP1-CP2	4.87	1.54	1.46
5	C	614	NDP	C4N-C3N	-4.82	1.40	1.50
5	A	606	NDP	PA-O3	4.81	1.64	1.59
5	D	618	NDP	C4N-C3N	-4.80	1.40	1.50
5	E	622	NDP	C4N-C3N	-4.73	1.41	1.50
3	C	612	CB3	C4A-C4	-4.69	1.40	1.48
5	E	622	NDP	PA-O3	4.68	1.64	1.59
5	E	622	NDP	PN-O3	4.67	1.64	1.59
3	C	612	CB3	CP1-N10	4.64	1.50	1.46
5	B	610	NDP	PN-O3	4.62	1.64	1.59
3	B	608	CB3	C4A-C4	-4.51	1.40	1.48
5	C	614	NDP	PN-O3	4.45	1.64	1.59
3	E	620	CB3	CP1-N10	4.45	1.50	1.46
3	C	612	CB3	CP1-CP2	4.43	1.53	1.46
2	D	615	UMP	C2-N1	4.37	1.45	1.38
3	A	604	CB3	C4A-C4	-4.34	1.40	1.48
3	B	608	CB3	CP1-N10	4.33	1.50	1.46
3	E	620	CB3	C4A-C4	-4.30	1.40	1.48
3	D	616	CB3	CP1-N10	4.28	1.50	1.46
3	D	616	CB3	C4A-C4	-4.27	1.40	1.48
5	D	618	NDP	PA-O3	4.18	1.64	1.59
4	E	621	FOL	C4A-C4	-4.14	1.39	1.47
4	A	605	FOL	C4A-C4	-4.13	1.39	1.47
4	D	617	FOL	C4A-C4	-4.12	1.39	1.47
2	A	603	UMP	C2-N1	4.12	1.44	1.38
5	B	610	NDP	PA-O3	4.12	1.63	1.59
4	B	609	FOL	C4A-C4	-4.09	1.39	1.47
4	C	613	FOL	C4A-C4	-4.09	1.39	1.47
4	B	609	FOL	C9-N10	-3.99	1.32	1.45
4	C	613	FOL	C9-N10	-3.99	1.32	1.45
2	C	611	UMP	C2-N1	3.97	1.44	1.38
4	E	621	FOL	C9-N10	-3.96	1.32	1.45
5	D	618	NDP	PN-O3	3.95	1.63	1.59
5	A	606	NDP	P2B-O1X	3.95	1.62	1.50
4	D	617	FOL	C9-N10	-3.93	1.32	1.45
2	E	619	UMP	C2-N1	3.93	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	619	UMP	P-OP1	3.93	1.62	1.50
4	A	605	FOL	C9-N10	-3.92	1.33	1.45
5	B	610	NDP	P2B-O1X	3.90	1.62	1.50
5	C	614	NDP	PA-O3	3.89	1.63	1.59
2	B	607	UMP	C2-N1	3.86	1.44	1.38
2	D	615	UMP	P-OP1	3.72	1.62	1.50
4	B	609	FOL	C8A-N8	3.64	1.40	1.35
4	A	605	FOL	C8A-N8	3.63	1.40	1.35
4	D	617	FOL	C8A-N8	3.60	1.40	1.35
4	C	613	FOL	C8A-N8	3.59	1.40	1.35
4	E	621	FOL	C6-N5	3.59	1.40	1.34
4	A	605	FOL	C6-N5	3.58	1.40	1.34
4	E	621	FOL	C8A-N8	3.57	1.40	1.35
4	C	613	FOL	C6-N5	3.56	1.40	1.34
4	D	617	FOL	C6-N5	3.49	1.40	1.34
2	A	603	UMP	P-OP1	3.47	1.61	1.50
4	B	609	FOL	C6-N5	3.45	1.40	1.34
2	C	611	UMP	P-OP1	3.40	1.61	1.50
5	B	610	NDP	C5A-N7A	-3.36	1.32	1.39
5	A	606	NDP	C5A-N7A	-3.30	1.33	1.39
5	B	610	NDP	C4N-C5N	-3.28	1.40	1.49
5	D	618	NDP	C5A-N7A	-3.27	1.33	1.39
2	B	607	UMP	P-OP1	3.26	1.60	1.50
3	A	604	CB3	C9-N10	3.24	1.51	1.46
5	C	614	NDP	C4N-C5N	-3.21	1.40	1.49
5	E	622	NDP	O4B-C1B	3.19	1.49	1.42
5	A	606	NDP	C4N-C5N	-3.19	1.40	1.49
5	C	614	NDP	O4B-C1B	3.18	1.49	1.42
5	E	622	NDP	C4N-C5N	-3.15	1.40	1.49
4	D	617	FOL	C7-N8	3.11	1.40	1.34
4	E	621	FOL	C7-N8	3.10	1.40	1.34
5	D	618	NDP	C4N-C5N	-3.09	1.41	1.49
4	B	609	FOL	C7-N8	3.09	1.40	1.34
4	C	613	FOL	C7-N8	3.08	1.40	1.34
3	C	612	CB3	C9-N10	3.08	1.50	1.46
4	A	605	FOL	C7-N8	3.05	1.40	1.34
4	E	621	FOL	C2-N3	3.05	1.40	1.33
4	D	617	FOL	C4A-N5	3.04	1.40	1.34
4	B	609	FOL	C2-N3	3.03	1.40	1.33
4	E	621	FOL	C4A-N5	3.03	1.40	1.34
5	D	618	NDP	O4B-C1B	3.03	1.49	1.42
4	C	613	FOL	C2-N3	3.02	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	609	FOL	C4A-N5	3.02	1.40	1.34
4	C	613	FOL	C4A-N5	3.00	1.40	1.34
4	D	617	FOL	C2-N3	3.00	1.40	1.33
4	A	605	FOL	C2-N3	2.99	1.40	1.33
3	B	608	CB3	C9-N10	2.97	1.50	1.46
5	A	606	NDP	O4B-C1B	2.97	1.48	1.42
4	A	605	FOL	C4A-N5	2.96	1.40	1.34
5	E	622	NDP	C5A-N7A	-2.95	1.33	1.39
3	D	616	CB3	C9-N10	2.93	1.50	1.46
5	C	614	NDP	C5A-N7A	-2.92	1.33	1.39
3	E	620	CB3	C9-N10	2.87	1.50	1.46
5	B	610	NDP	O4B-C1B	2.78	1.48	1.42
5	E	622	NDP	C7N-C3N	2.70	1.54	1.48
5	E	622	NDP	O4D-C1D	2.63	1.48	1.42
2	E	619	UMP	O4'-C1'	2.62	1.48	1.42
5	D	618	NDP	C7N-C3N	2.60	1.54	1.48
5	C	614	NDP	O4D-C1D	2.60	1.48	1.42
3	D	616	CB3	C11-C	2.60	1.55	1.50
3	E	620	CB3	C15-C14	2.60	1.44	1.39
5	A	606	NDP	P2B-O2X	-2.57	1.45	1.54
3	B	608	CB3	C15-C14	2.56	1.44	1.39
3	E	620	CB3	C16-C15	2.53	1.42	1.38
3	C	612	CB3	C11-C	2.53	1.55	1.50
5	D	618	NDP	O4D-C1D	2.52	1.47	1.42
5	B	610	NDP	P2B-O2X	-2.51	1.45	1.54
5	C	614	NDP	C7N-C3N	2.51	1.54	1.48
3	C	612	CB3	C15-C14	2.49	1.44	1.39
3	A	604	CB3	C11-C	2.48	1.55	1.50
3	B	608	CB3	C11-C	2.48	1.55	1.50
5	E	622	NDP	P2B-O3X	-2.46	1.45	1.54
3	C	612	CB3	C16-C15	2.46	1.42	1.38
5	B	610	NDP	C7N-C3N	2.45	1.54	1.48
3	D	616	CB3	C16-C15	2.44	1.42	1.38
3	A	604	CB3	C16-C15	2.44	1.42	1.38
5	A	606	NDP	C7N-C3N	2.42	1.53	1.48
2	A	603	UMP	O4'-C1'	2.41	1.47	1.42
3	E	620	CB3	C11-C	2.41	1.55	1.50
5	E	622	NDP	P2B-O2X	2.38	1.63	1.54
5	E	622	NDP	C6N-N1N	2.38	1.43	1.37
3	D	616	CB3	C15-C14	2.34	1.43	1.39
5	D	618	NDP	C6N-N1N	2.34	1.42	1.37
5	C	614	NDP	P2B-O2X	2.34	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	CB3	C15-C14	2.33	1.43	1.39
5	E	622	NDP	C6N-C5N	2.32	1.40	1.33
3	B	608	CB3	C16-C15	2.31	1.42	1.38
5	D	618	NDP	C6N-C5N	2.31	1.40	1.33
5	D	618	NDP	P2B-O2X	2.31	1.63	1.54
2	A	603	UMP	O4'-C4'	2.28	1.50	1.45
5	B	610	NDP	O4D-C1D	2.28	1.47	1.42
5	C	614	NDP	C6N-C5N	2.26	1.40	1.33
5	A	606	NDP	C6N-C5N	2.24	1.39	1.33
2	D	615	UMP	O4'-C1'	2.23	1.47	1.42
5	B	610	NDP	C6N-C5N	2.23	1.39	1.33
5	C	614	NDP	C6N-N1N	2.22	1.42	1.37
4	D	617	FOL	C8A-N1	2.16	1.40	1.38
4	A	605	FOL	C8A-N1	2.11	1.40	1.38
5	A	606	NDP	O4D-C1D	2.11	1.46	1.42
4	C	613	FOL	C8A-N1	2.11	1.40	1.38
4	B	609	FOL	C8A-N1	2.10	1.40	1.38
3	E	620	CB3	CA-N	2.10	1.50	1.45
3	D	616	CB3	CG-CD	2.10	1.55	1.50
5	A	606	NDP	C6N-N1N	2.09	1.42	1.37
4	E	621	FOL	C8A-N1	2.08	1.40	1.38
2	D	615	UMP	O4'-C4'	2.08	1.49	1.45
3	A	604	CB3	CA-N	2.06	1.50	1.45
3	E	620	CB3	CG-CD	2.02	1.55	1.50

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	617	FOL	C6-C9-N10	7.46	129.50	113.13
4	B	609	FOL	C6-C9-N10	7.33	129.22	113.13
4	C	613	FOL	C6-C9-N10	7.32	129.21	113.13
4	A	605	FOL	C6-C9-N10	7.31	129.19	113.13
4	E	621	FOL	C6-C9-N10	7.24	129.02	113.13
2	E	619	UMP	C5-C6-N1	-5.85	112.33	121.84
2	B	607	UMP	C5-C6-N1	-5.84	112.35	121.84
2	E	619	UMP	C6-C5-C4	-5.83	112.09	119.53
2	D	615	UMP	C5-C6-N1	-5.76	112.47	121.84
2	A	603	UMP	C6-C5-C4	-5.76	112.18	119.53
2	C	611	UMP	C5-C6-N1	-5.76	112.48	121.84
2	D	615	UMP	C6-C5-C4	-5.72	112.22	119.53
2	A	603	UMP	C5-C6-N1	-5.70	112.57	121.84
2	B	607	UMP	C6-C5-C4	-5.66	112.30	119.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	611	UMP	C6-C5-C4	-5.61	112.36	119.53
5	B	610	NDP	N3A-C2A-N1A	-5.34	120.49	128.58
5	A	606	NDP	N3A-C2A-N1A	-5.33	120.52	128.58
5	D	618	NDP	N3A-C2A-N1A	-5.31	120.54	128.58
5	C	614	NDP	N3A-C2A-N1A	-5.22	120.69	128.58
5	E	622	NDP	N3A-C2A-N1A	-5.19	120.72	128.58
5	A	606	NDP	C5A-C4A-N3A	-4.99	119.84	126.72
5	E	622	NDP	C5A-C4A-N3A	-4.97	119.87	126.72
5	B	610	NDP	C5A-C4A-N3A	-4.96	119.88	126.72
5	D	618	NDP	C5A-C4A-N3A	-4.95	119.89	126.72
5	C	614	NDP	C5A-C4A-N3A	-4.94	119.92	126.72
2	B	607	UMP	N3-C2-N1	4.72	121.03	114.89
2	C	611	UMP	N3-C2-N1	4.62	120.91	114.89
2	E	619	UMP	N3-C2-N1	4.54	120.80	114.89
5	A	606	NDP	O3-PN-O1N	-4.53	97.06	110.70
5	B	610	NDP	O3-PN-O1N	-4.51	97.13	110.70
2	A	603	UMP	N3-C2-N1	4.50	120.75	114.89
2	D	615	UMP	N3-C2-N1	4.45	120.69	114.89
5	E	622	NDP	O3-PN-O1N	-4.44	97.35	110.70
5	D	618	NDP	O3-PN-O1N	-4.34	97.64	110.70
5	C	614	NDP	O3-PN-O1N	-4.28	97.83	110.70
2	D	615	UMP	C5-C4-N3	4.28	120.79	114.80
2	B	607	UMP	C5-C4-N3	4.25	120.75	114.80
4	D	617	FOL	C7-C6-N5	-4.24	118.12	120.87
2	C	611	UMP	C5-C4-N3	4.24	120.73	114.80
2	E	619	UMP	C5-C4-N3	4.18	120.65	114.80
2	A	603	UMP	C5-C4-N3	4.17	120.64	114.80
4	E	621	FOL	C7-C6-N5	-3.98	118.29	120.87
4	A	605	FOL	C7-C6-N5	-3.96	118.30	120.87
4	C	613	FOL	C7-C6-N5	-3.87	118.36	120.87
4	B	609	FOL	C7-C6-N5	-3.82	118.39	120.87
5	E	622	NDP	C2A-N3A-C4A	3.68	120.81	111.83
5	A	606	NDP	C2A-N3A-C4A	3.67	120.80	111.83
5	B	610	NDP	C2A-N3A-C4A	3.67	120.78	111.83
5	C	614	NDP	C2A-N3A-C4A	3.65	120.74	111.83
5	D	618	NDP	C2A-N3A-C4A	3.64	120.72	111.83
2	E	619	UMP	O4'-C1'-N1	3.60	114.25	107.86
5	C	614	NDP	O2N-PN-O3	-3.60	97.55	107.27
5	D	618	NDP	O2N-PN-O3	-3.55	97.68	107.27
5	E	622	NDP	N9A-C8A-N7A	-3.55	108.90	113.94
5	C	614	NDP	N9A-C8A-N7A	-3.49	108.98	113.94
4	D	617	FOL	C9-C6-N5	3.48	123.13	116.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	615	UMP	O4'-C1'-N1	3.46	114.00	107.86
5	D	618	NDP	N9A-C8A-N7A	-3.45	109.04	113.94
5	B	610	NDP	O2N-PN-O3	-3.45	97.96	107.27
4	A	605	FOL	C9-C6-N5	3.45	123.07	116.56
5	B	610	NDP	N9A-C8A-N7A	-3.44	109.05	113.94
4	C	613	FOL	C9-C6-N5	3.44	123.06	116.56
4	B	609	FOL	C9-C6-N5	3.43	123.05	116.56
5	E	622	NDP	O2N-PN-O3	-3.43	97.99	107.27
5	B	610	NDP	N3A-C4A-N9A	3.43	133.00	127.17
5	D	618	NDP	N3A-C4A-N9A	3.43	133.00	127.17
2	C	611	UMP	O4'-C1'-N1	3.43	113.95	107.86
5	A	606	NDP	N3A-C4A-N9A	3.42	132.99	127.17
5	E	622	NDP	N3A-C4A-N9A	3.42	132.98	127.17
4	A	605	FOL	C15-C14-N10	-3.41	113.25	120.96
2	A	603	UMP	O4'-C1'-N1	3.41	113.91	107.86
5	D	618	NDP	C2B-C1B-N9A	-3.41	108.15	113.75
5	A	606	NDP	N9A-C8A-N7A	-3.40	109.11	113.94
4	E	621	FOL	C9-C6-N5	3.40	122.98	116.56
5	C	614	NDP	N3A-C4A-N9A	3.38	132.91	127.17
2	B	607	UMP	O4'-C1'-N1	3.38	113.86	107.86
5	E	622	NDP	C2B-C1B-N9A	-3.35	108.24	113.75
5	B	610	NDP	C2B-C1B-N9A	-3.34	108.25	113.75
5	A	606	NDP	O2N-PN-O3	-3.32	98.31	107.27
5	A	606	NDP	C2B-C1B-N9A	-3.31	108.30	113.75
4	D	617	FOL	C15-C14-N10	-3.31	113.49	120.96
4	B	609	FOL	C15-C14-N10	-3.30	113.49	120.96
4	E	621	FOL	C15-C14-N10	-3.30	113.51	120.96
4	C	613	FOL	C15-C14-N10	-3.30	113.51	120.96
5	C	614	NDP	C2B-C1B-N9A	-3.26	108.39	113.75
5	B	610	NDP	O2X-P2B-O2B	3.14	118.09	105.85
5	A	606	NDP	O2X-P2B-O2B	3.11	117.97	105.85
5	E	622	NDP	O3X-P2B-O2B	3.07	117.81	105.85
2	B	607	UMP	O4-C4-C5	-3.07	119.88	125.16
2	E	619	UMP	O4-C4-C5	-3.06	119.89	125.16
5	B	610	NDP	O5B-PA-O1A	-3.05	96.86	108.94
2	D	615	UMP	O4-C4-C5	-3.03	119.94	125.16
2	C	611	UMP	O4-C4-C5	-3.00	119.99	125.16
5	C	614	NDP	O5B-PA-O1A	-2.98	97.14	108.94
5	A	606	NDP	O5B-PA-O1A	-2.98	97.14	108.94
2	A	603	UMP	O4-C4-C5	-2.95	120.08	125.16
5	E	622	NDP	O5B-PA-O1A	-2.92	97.36	108.94
5	D	618	NDP	O5B-PA-O1A	-2.91	97.40	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	618	NDP	C5A-N7A-C8A	2.90	108.01	103.45
5	E	622	NDP	C5A-N7A-C8A	2.88	107.97	103.45
5	E	622	NDP	O3X-P2B-O2X	2.88	118.59	107.80
3	C	612	CB3	CP2-CP1-N10	-2.86	110.81	113.45
2	A	603	UMP	OP3-P-OP2	2.86	118.51	107.80
2	B	607	UMP	OP3-P-OP2	2.84	118.44	107.80
5	A	606	NDP	C5A-N7A-C8A	2.82	107.89	103.45
2	C	611	UMP	OP3-P-OP2	2.81	118.36	107.80
5	B	610	NDP	C5A-N7A-C8A	2.81	107.86	103.45
5	C	614	NDP	C5A-N7A-C8A	2.80	107.84	103.45
2	D	615	UMP	OP3-P-OP2	2.79	118.28	107.80
4	C	613	FOL	C6-C7-N8	-2.77	120.49	123.14
5	D	618	NDP	O4D-C1D-N1N	2.75	113.33	108.08
2	E	619	UMP	OP3-P-OP2	2.74	118.09	107.80
4	B	609	FOL	C6-C7-N8	-2.74	120.51	123.14
4	E	621	FOL	C6-C7-N8	-2.74	120.51	123.14
5	E	622	NDP	O4D-C1D-N1N	2.72	113.27	108.08
3	D	616	CB3	CP2-CP1-N10	-2.72	110.94	113.45
5	B	610	NDP	O4D-C1D-N1N	2.71	113.25	108.08
5	D	618	NDP	O2N-PN-O1N	2.70	125.00	112.44
5	E	622	NDP	O2N-PN-O1N	2.70	124.99	112.44
5	C	614	NDP	O4D-C1D-N1N	2.69	113.22	108.08
5	C	614	NDP	O2N-PN-O1N	2.67	124.87	112.44
5	E	622	NDP	O2A-PA-O1A	2.67	124.85	112.44
5	D	618	NDP	O2A-PA-O1A	2.66	124.82	112.44
4	A	605	FOL	C6-C7-N8	-2.66	120.59	123.14
5	C	614	NDP	O2A-PA-O1A	2.66	124.81	112.44
5	E	622	NDP	O2B-P2B-O1X	-2.64	99.93	109.33
5	D	618	NDP	C3N-C2N-N1N	-2.63	119.34	123.20
5	B	610	NDP	O2A-PA-O1A	2.63	124.68	112.44
5	C	614	NDP	C3N-C2N-N1N	-2.62	119.35	123.20
5	B	610	NDP	O2N-PN-O1N	2.62	124.61	112.44
5	A	606	NDP	O2N-PN-O1N	2.61	124.61	112.44
3	E	620	CB3	CP2-CP1-N10	-2.61	111.04	113.45
5	E	622	NDP	C3N-C2N-N1N	-2.61	119.37	123.20
3	B	608	CB3	CP2-CP1-N10	-2.61	111.05	113.45
5	A	606	NDP	O2A-PA-O1A	2.60	124.52	112.44
5	A	606	NDP	O3X-P2B-O1X	-2.59	100.73	110.83
5	A	606	NDP	O4D-C1D-N1N	2.59	113.03	108.08
5	E	622	NDP	O2X-P2B-O1X	-2.58	100.77	110.83
4	D	617	FOL	C6-C7-N8	-2.58	120.66	123.14
4	D	617	FOL	N1-C8A-N8	2.56	120.20	116.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606	NDP	O3-PA-O1A	2.55	118.38	110.70
4	A	605	FOL	N1-C8A-N8	2.53	120.15	116.38
5	D	618	NDP	O2A-PA-O3	2.52	114.08	107.27
5	B	610	NDP	O3-PA-O1A	2.52	118.27	110.70
5	A	606	NDP	C3N-C2N-N1N	-2.49	119.55	123.20
5	C	614	NDP	O2A-PA-O3	2.49	114.00	107.27
5	C	614	NDP	O3-PA-O1A	2.49	118.18	110.70
5	B	610	NDP	C3N-C2N-N1N	-2.47	119.58	123.20
5	E	622	NDP	O2A-PA-O3	2.47	113.94	107.27
5	B	610	NDP	O2A-PA-O3	2.47	113.94	107.27
5	E	622	NDP	O3-PA-O1A	2.46	118.11	110.70
4	E	621	FOL	N1-C8A-N8	2.46	120.04	116.38
4	C	613	FOL	N1-C8A-N8	2.45	120.03	116.38
4	B	609	FOL	N1-C8A-N8	2.44	120.03	116.38
5	D	618	NDP	O3-PA-O1A	2.43	118.02	110.70
5	A	606	NDP	O2A-PA-O3	2.43	113.84	107.27
5	E	622	NDP	C4A-C5A-N7A	-2.43	107.81	110.58
2	B	607	UMP	O2-C2-N1	-2.42	119.64	122.80
2	B	607	UMP	C4-N3-C2	-2.41	123.62	126.61
4	E	621	FOL	C7-N8-C8A	2.40	120.90	116.19
5	D	618	NDP	O2B-P2B-O1X	2.40	117.89	109.33
5	C	614	NDP	O2B-P2B-O1X	2.40	117.89	109.33
5	D	618	NDP	C4A-C5A-N7A	-2.39	107.86	110.58
5	B	610	NDP	O3X-P2B-O1X	-2.38	101.56	110.83
4	D	617	FOL	C7-N8-C8A	2.37	120.84	116.19
4	A	605	FOL	C7-N8-C8A	2.36	120.82	116.19
4	A	605	FOL	N1-C2-N3	-2.36	119.00	123.32
3	C	612	CB3	CA-N-C	2.36	127.23	121.56
4	C	613	FOL	C7-N8-C8A	2.36	120.81	116.19
4	E	621	FOL	N1-C2-N3	-2.36	119.00	123.32
2	E	619	UMP	O2-C2-N1	-2.36	119.73	122.80
5	E	622	NDP	O2A-PA-O5B	-2.35	96.91	107.57
5	C	614	NDP	O2A-PA-O5B	-2.35	96.93	107.57
4	D	617	FOL	N1-C2-N3	-2.35	119.03	123.32
4	B	609	FOL	C7-N8-C8A	2.34	120.78	116.19
5	A	606	NDP	C4A-C5A-N7A	-2.34	107.91	110.58
2	C	611	UMP	C4-N3-C2	-2.33	123.72	126.61
5	D	618	NDP	O2A-PA-O5B	-2.33	97.00	107.57
4	B	609	FOL	N1-C2-N3	-2.33	119.06	123.32
5	E	622	NDP	C4A-N9A-C8A	2.32	108.17	105.74
4	B	609	FOL	C9-C6-C7	-2.29	117.25	121.38
2	C	611	UMP	O2-C2-N1	-2.29	119.82	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	610	NDP	O2A-PA-O5B	-2.28	97.22	107.57
5	A	606	NDP	O2A-PA-O5B	-2.27	97.26	107.57
5	C	614	NDP	C4A-C5A-N7A	-2.27	107.99	110.58
2	E	619	UMP	C4-N3-C2	-2.26	123.81	126.61
5	B	610	NDP	C4A-C5A-N7A	-2.24	108.02	110.58
4	C	613	FOL	N1-C2-N3	-2.24	119.23	123.32
4	A	605	FOL	C9-C6-C7	-2.24	117.36	121.38
4	C	613	FOL	C9-C6-C7	-2.23	117.36	121.38
3	B	608	CB3	CA-N-C	2.23	126.92	121.56
5	A	606	NDP	O2N-PN-O5D	2.22	117.63	107.57
2	A	603	UMP	C4-N3-C2	-2.19	123.89	126.61
5	B	610	NDP	O2N-PN-O5D	2.19	117.50	107.57
5	E	622	NDP	O2N-PN-O5D	2.19	117.50	107.57
4	D	617	FOL	C9-C6-C7	-2.19	117.44	121.38
5	C	614	NDP	O5D-PN-O1N	2.18	117.56	108.94
5	D	618	NDP	O5D-PN-O1N	2.17	117.52	108.94
5	C	614	NDP	C4A-N9A-C8A	2.17	108.01	105.74
3	D	616	CB3	CA-N-C	2.16	126.76	121.56
2	D	615	UMP	C4-N3-C2	-2.16	123.94	126.61
5	D	618	NDP	C4A-N9A-C8A	2.15	108.00	105.74
4	E	621	FOL	C9-C6-C7	-2.13	117.54	121.38
2	A	603	UMP	O2-C2-N1	-2.13	120.03	122.80
5	B	610	NDP	C4A-N9A-C8A	2.11	107.96	105.74
3	A	604	CB3	CA-N-C	2.09	126.58	121.56
5	A	606	NDP	C4A-N9A-C8A	2.08	107.93	105.74
2	D	615	UMP	O2-C2-N1	-2.08	120.09	122.80
3	E	620	CB3	CA-N-C	2.06	126.51	121.56
4	E	621	FOL	C9-N10-C14	2.05	128.45	121.87
4	B	609	FOL	C9-N10-C14	2.05	128.44	121.87
4	C	613	FOL	C9-N10-C14	2.04	128.42	121.87
4	D	617	FOL	C9-N10-C14	2.04	128.40	121.87
5	A	606	NDP	O2X-P2B-O1X	2.04	118.77	110.83
4	A	605	FOL	C9-N10-C14	2.03	128.38	121.87
5	D	618	NDP	O2X-P2B-O1X	2.02	118.69	110.83
3	E	620	CB3	C11-C-N	-2.01	113.32	117.04
3	C	612	CB3	C11-C-N	-2.00	113.33	117.04
3	D	616	CB3	OE1-CD-CG	-2.00	116.74	123.09

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	604	CB3	CA

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Mol	Chain	Res	Type	Atom
3	B	608	CB3	CA
3	C	612	CB3	CA
3	D	616	CB3	CA
3	E	620	CB3	CA

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	605	FOL	C6-C9-N10-C14
4	B	609	FOL	C6-C9-N10-C14
4	C	613	FOL	C6-C9-N10-C14
4	D	617	FOL	C6-C9-N10-C14
4	E	621	FOL	C6-C9-N10-C14
5	A	606	NDP	C5D-O5D-PN-O2N
5	B	610	NDP	C5D-O5D-PN-O2N
5	C	614	NDP	C5D-O5D-PN-O1N
5	D	618	NDP	C5D-O5D-PN-O1N
5	E	622	NDP	C5D-O5D-PN-O2N
3	A	604	CB3	CB-CA-N-C
3	B	608	CB3	CB-CA-N-C
3	C	612	CB3	CB-CA-N-C
3	D	616	CB3	CB-CA-N-C
3	E	620	CB3	CB-CA-N-C
2	A	603	UMP	C2'-C1'-N1-C2
2	B	607	UMP	C2'-C1'-N1-C2
2	C	611	UMP	C2'-C1'-N1-C2
2	D	615	UMP	C2'-C1'-N1-C2
2	E	619	UMP	C2'-C1'-N1-C2
3	B	608	CB3	N-CA-CT-O2
3	D	616	CB3	N-CA-CT-O2
3	A	604	CB3	N-CA-CT-O2
3	E	620	CB3	N-CA-CT-O2
3	C	612	CB3	N-CA-CT-O2
3	D	616	CB3	N-CA-CT-O1
5	A	606	NDP	PA-O3-PN-O5D
5	B	610	NDP	PA-O3-PN-O5D
5	C	614	NDP	PA-O3-PN-O5D
5	D	618	NDP	PA-O3-PN-O5D
5	E	622	NDP	PA-O3-PN-O5D
3	A	604	CB3	N-CA-CT-O1
3	B	608	CB3	N-CA-CT-O1
3	C	612	CB3	N-CA-CT-O1

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Mol	Chain	Res	Type	Atoms
3	E	620	CB3	N-CA-CT-O1
3	D	616	CB3	CB-CA-CT-O2
5	A	606	NDP	C4D-C5D-O5D-PN
5	B	610	NDP	C4D-C5D-O5D-PN
5	C	614	NDP	C4D-C5D-O5D-PN
5	D	618	NDP	C4D-C5D-O5D-PN
5	E	622	NDP	C4D-C5D-O5D-PN
3	A	604	CB3	CB-CA-CT-O2
3	B	608	CB3	CB-CA-CT-O2
3	C	612	CB3	CB-CA-CT-O2
3	E	620	CB3	CB-CA-CT-O2
4	B	609	FOL	CB-CA-CT-O1
4	C	613	FOL	CB-CA-CT-O1
4	A	605	FOL	CB-CA-CT-O1
4	D	617	FOL	CB-CA-CT-O1
4	E	621	FOL	CB-CA-CT-O1
4	A	605	FOL	CB-CA-CT-O2
4	B	609	FOL	CB-CA-CT-O2
4	C	613	FOL	CB-CA-CT-O2
4	D	617	FOL	CB-CA-CT-O2
4	E	621	FOL	CB-CA-CT-O2
5	A	606	NDP	C2B-O2B-P2B-O3X
5	B	610	NDP	C2B-O2B-P2B-O3X
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
3	C	612	CB3	CB-CA-CT-O1
3	D	616	CB3	CB-CA-CT-O1
5	C	614	NDP	O4D-C1D-N1N-C2N
5	D	618	NDP	O4D-C1D-N1N-C2N
5	E	622	NDP	O4D-C1D-N1N-C2N
4	B	609	FOL	C13-C14-N10-C9
4	B	609	FOL	OE2-CD-CG-CB
4	C	613	FOL	OE2-CD-CG-CB
4	E	621	FOL	OE2-CD-CG-CB
4	A	605	FOL	C13-C14-N10-C9
4	C	613	FOL	C13-C14-N10-C9
3	A	604	CB3	CB-CA-CT-O1
3	B	608	CB3	CB-CA-CT-O1
4	D	617	FOL	OE2-CD-CG-CB
4	A	605	FOL	OE2-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
5	A	606	NDP	C2N-C3N-C7N-N7N
5	B	610	NDP	C2N-C3N-C7N-N7N
5	C	614	NDP	C2N-C3N-C7N-N7N
5	D	618	NDP	C2N-C3N-C7N-N7N
5	E	622	NDP	C2N-C3N-C7N-N7N
4	E	621	FOL	C13-C14-N10-C9
3	E	620	CB3	CB-CA-CT-O1
4	A	605	FOL	OE1-CD-CG-CB
4	C	613	FOL	OE1-CD-CG-CB
4	B	609	FOL	OE1-CD-CG-CB
4	D	617	FOL	OE1-CD-CG-CB
4	E	621	FOL	OE1-CD-CG-CB
4	D	617	FOL	C13-C14-N10-C9
2	E	619	UMP	C2'-C1'-N1-C6
3	D	616	CB3	OE2-CD-CG-CB
3	C	612	CB3	OE1-CD-CG-CB
3	A	604	CB3	OE1-CD-CG-CB
3	B	608	CB3	OE1-CD-CG-CB
2	A	603	UMP	C2'-C1'-N1-C6
3	A	604	CB3	OE2-CD-CG-CB
3	D	616	CB3	OE1-CD-CG-CB
3	E	620	CB3	OE1-CD-CG-CB
3	E	620	CB3	OE2-CD-CG-CB
3	C	612	CB3	OE2-CD-CG-CB
2	B	607	UMP	C2'-C1'-N1-C6
2	C	611	UMP	C2'-C1'-N1-C6
3	B	608	CB3	OE2-CD-CG-CB
2	D	615	UMP	C2'-C1'-N1-C6
2	B	607	UMP	O4'-C4'-C5'-O5'
2	D	615	UMP	O4'-C4'-C5'-O5'
2	E	619	UMP	O4'-C4'-C5'-O5'

There are no ring outliers.

20 monomers are involved in 119 short contacts:

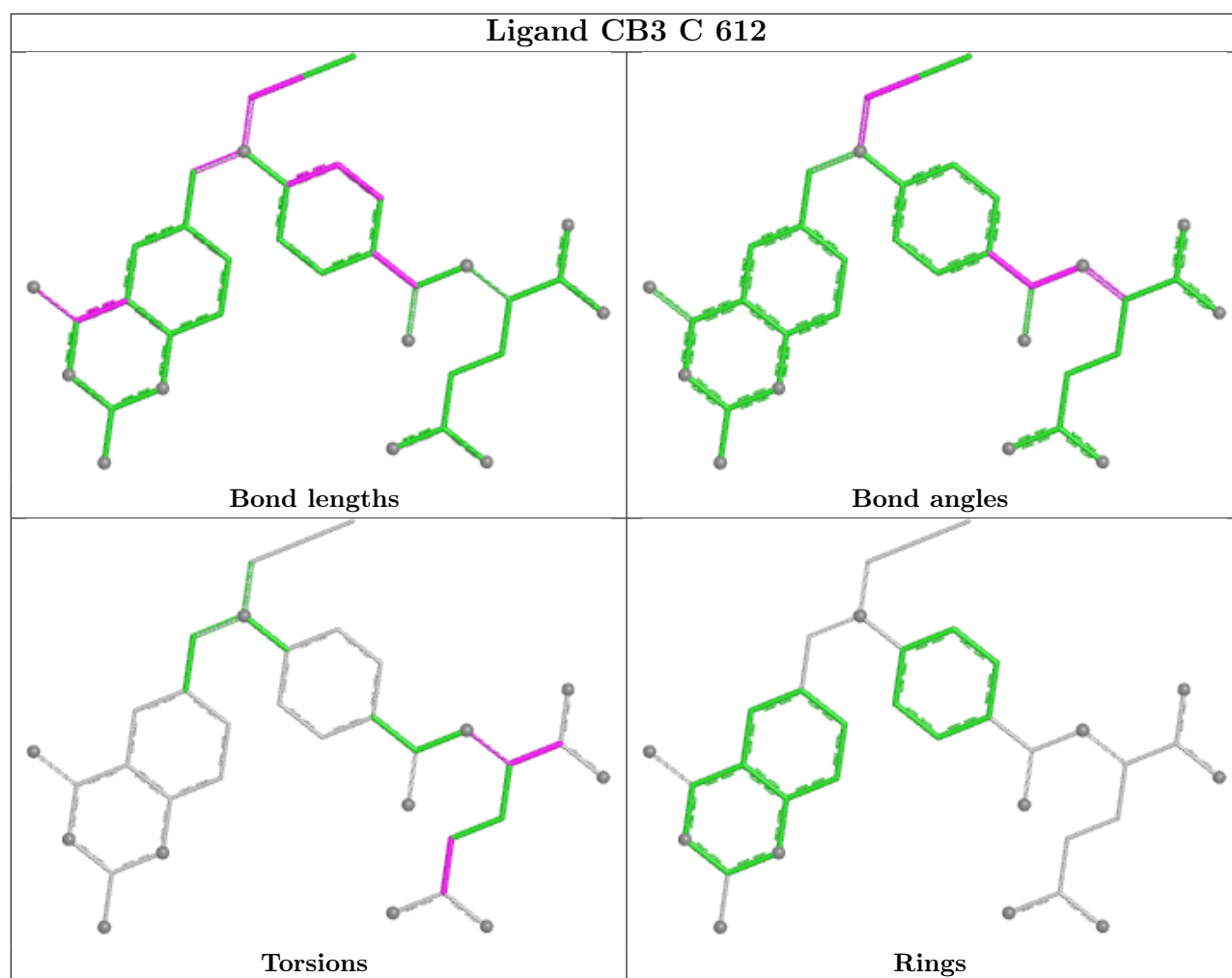
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	612	CB3	3	0
3	E	620	CB3	4	0
4	A	605	FOL	9	0
3	B	608	CB3	3	0
3	A	604	CB3	3	0
5	B	610	NDP	7	0

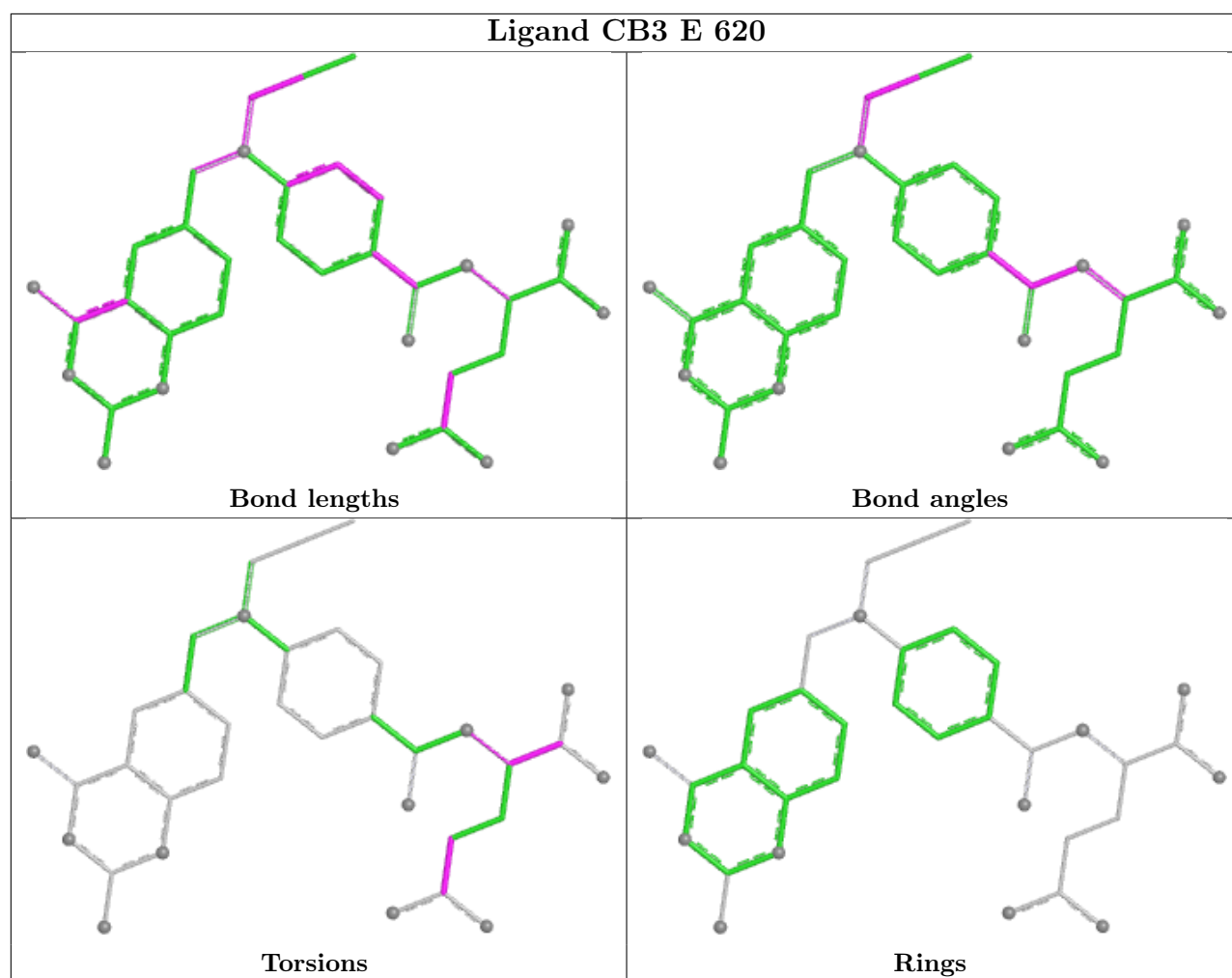
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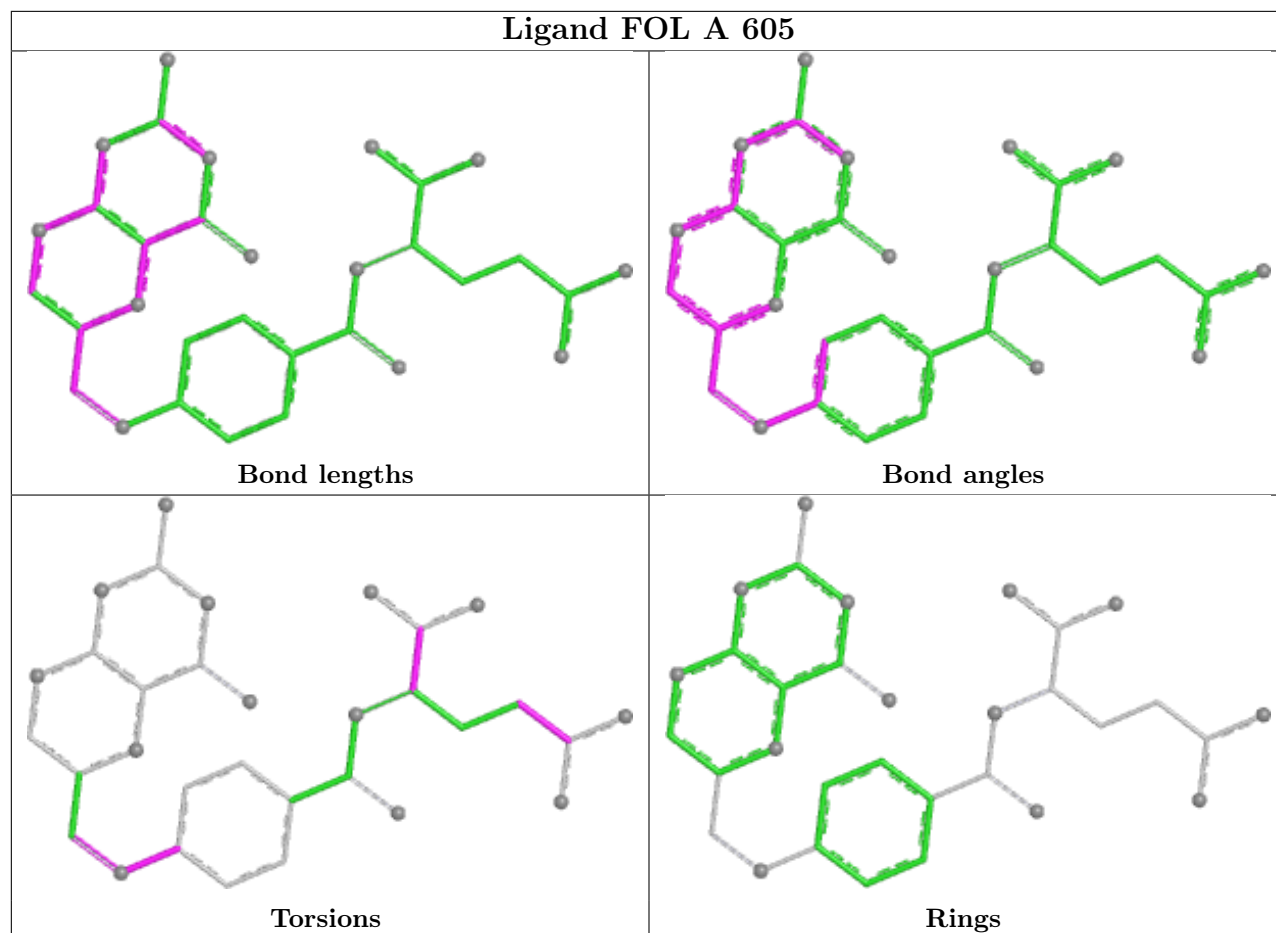
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	614	NDP	9	0
5	D	618	NDP	10	0
4	D	617	FOL	9	0
4	B	609	FOL	8	0
2	A	603	UMP	7	0
5	A	606	NDP	10	0
5	E	622	NDP	10	0
2	D	615	UMP	3	0
2	E	619	UMP	6	0
4	E	621	FOL	10	0
3	D	616	CB3	3	0
2	C	611	UMP	7	0
2	B	607	UMP	8	0
4	C	613	FOL	8	0

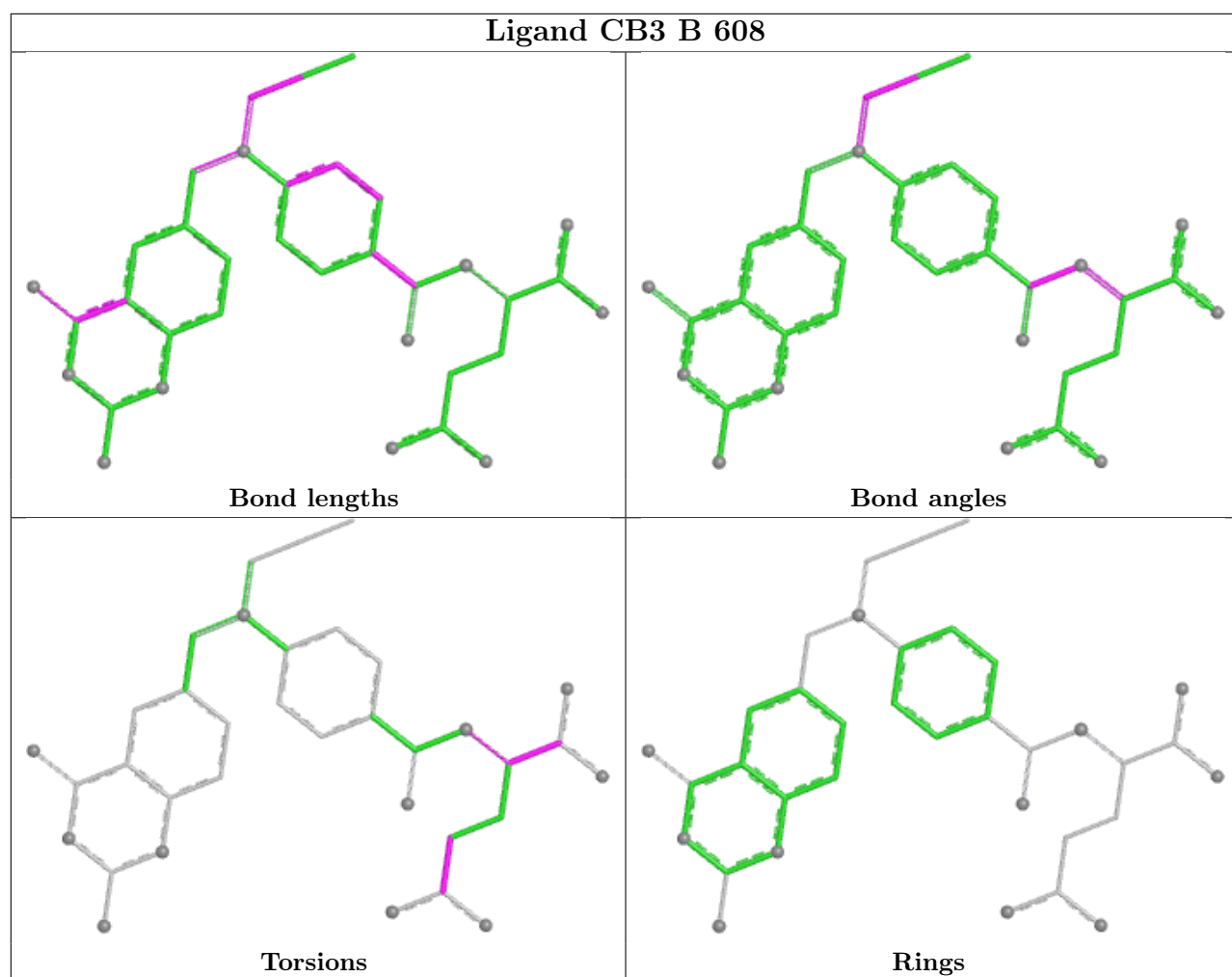
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

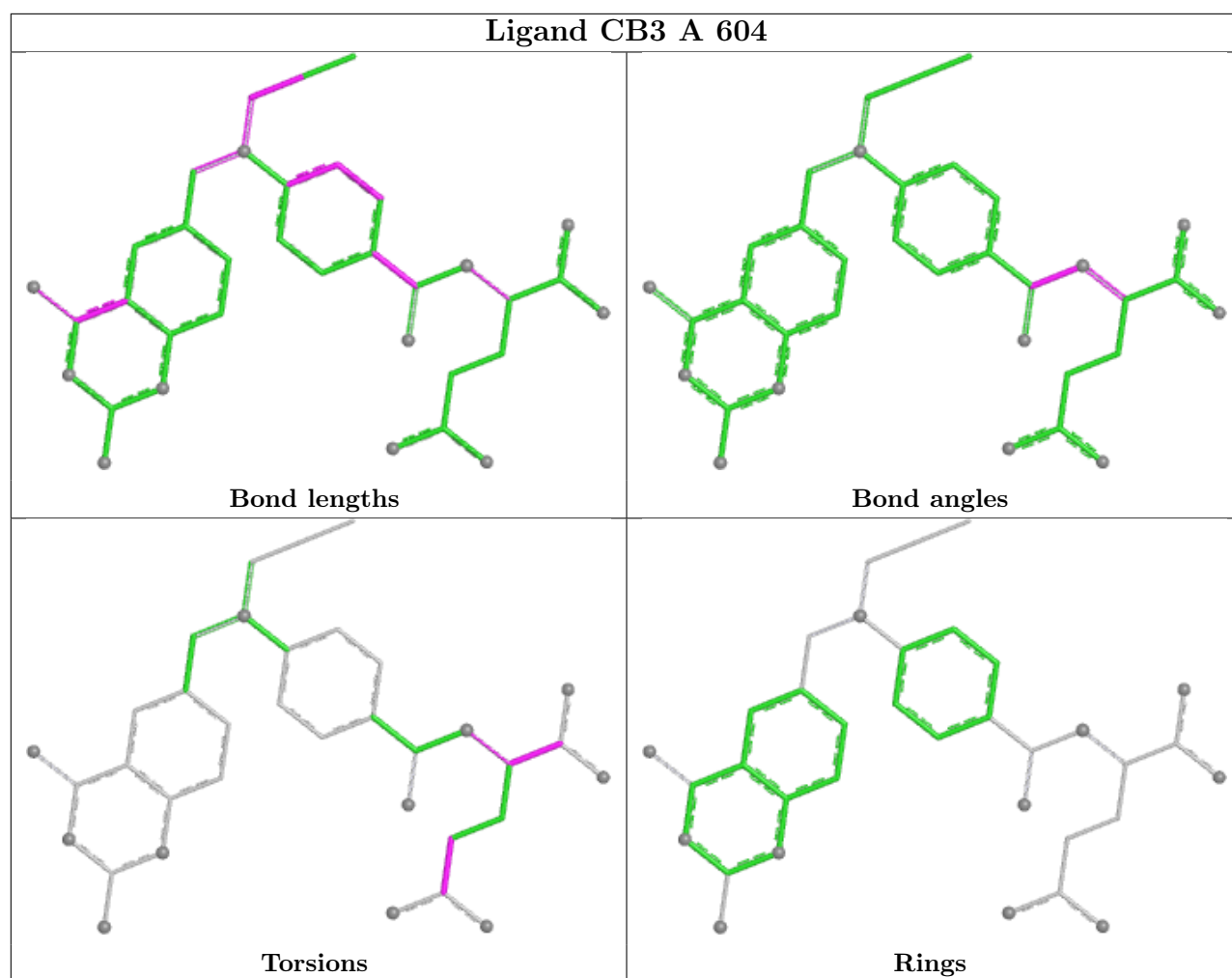


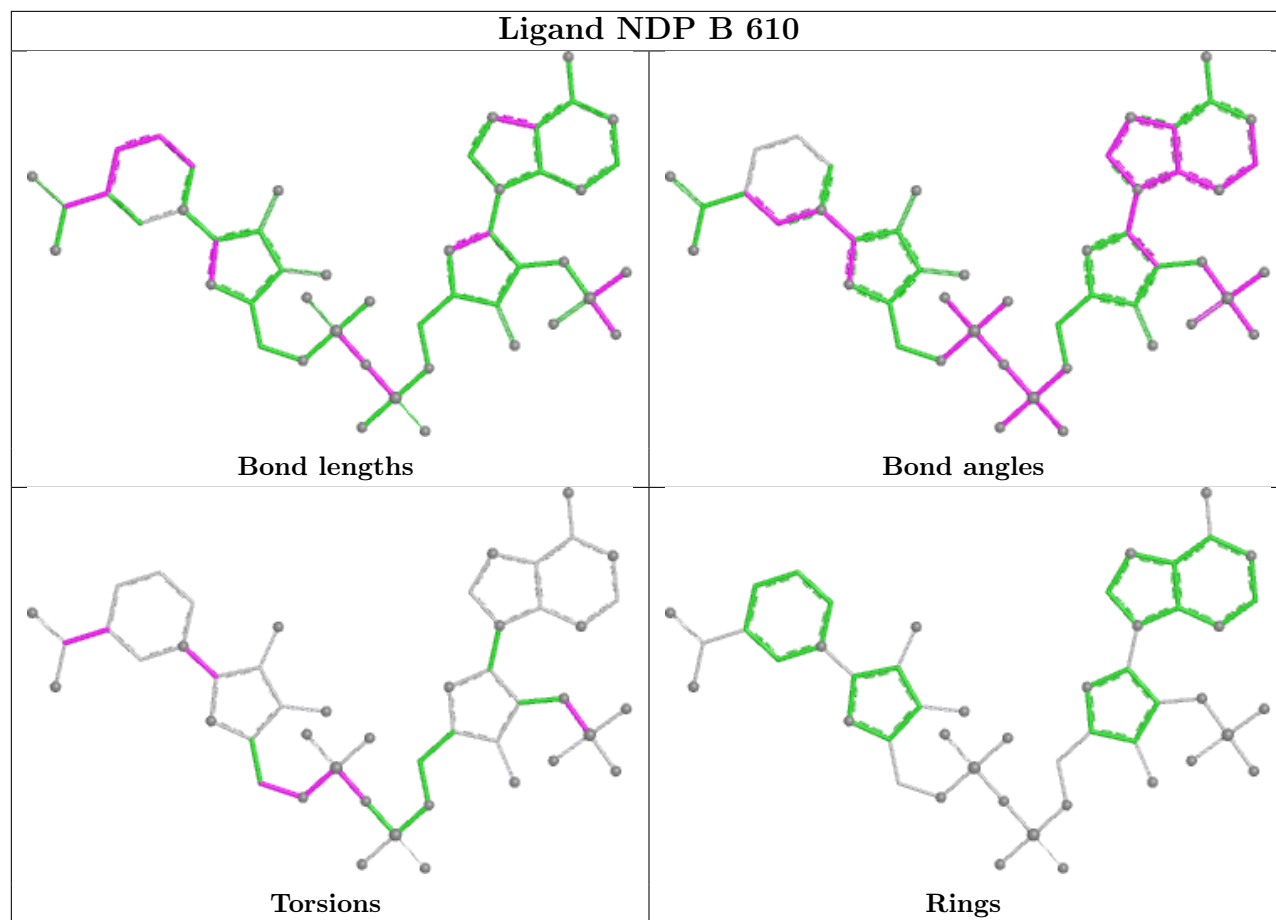


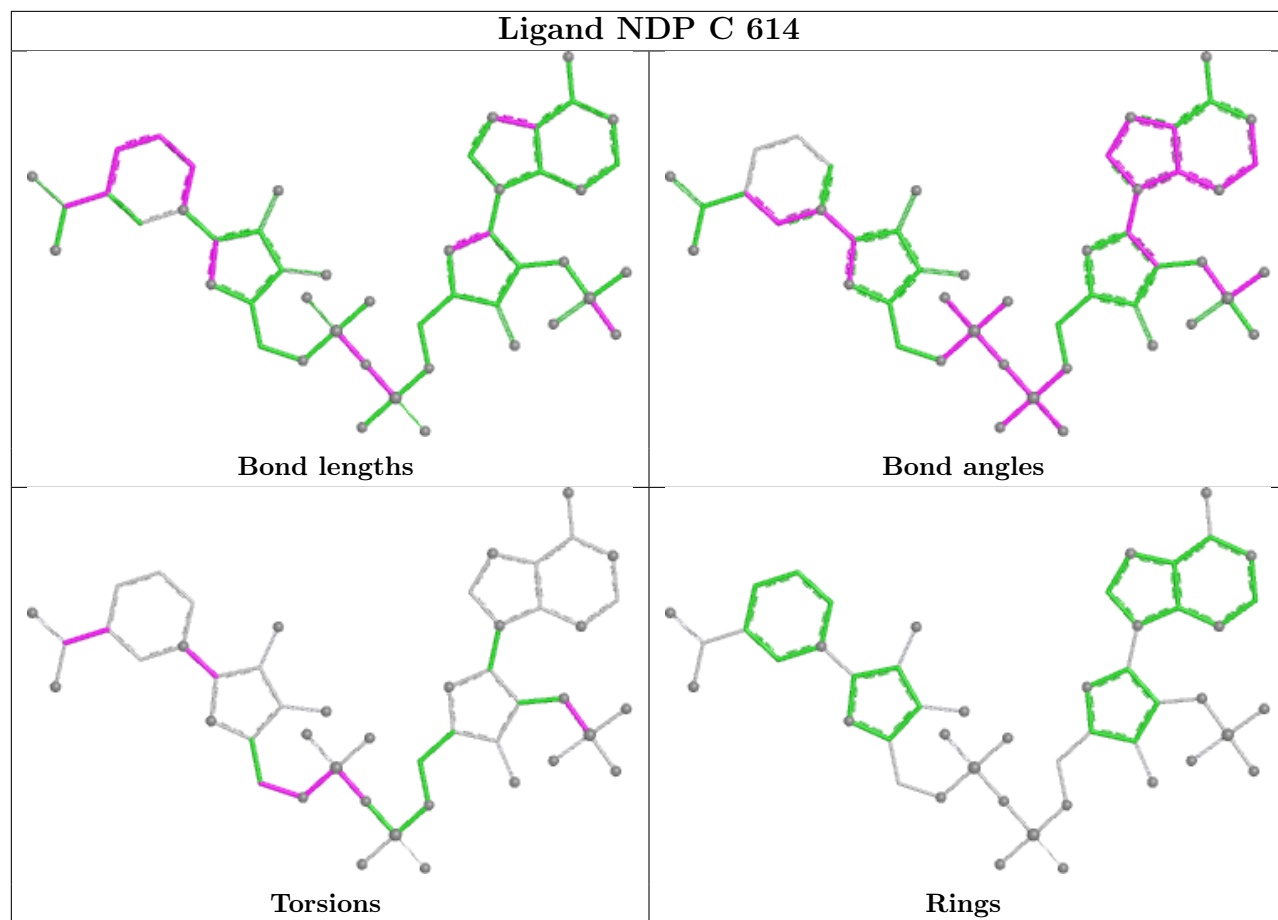
Ligand FOL A 605

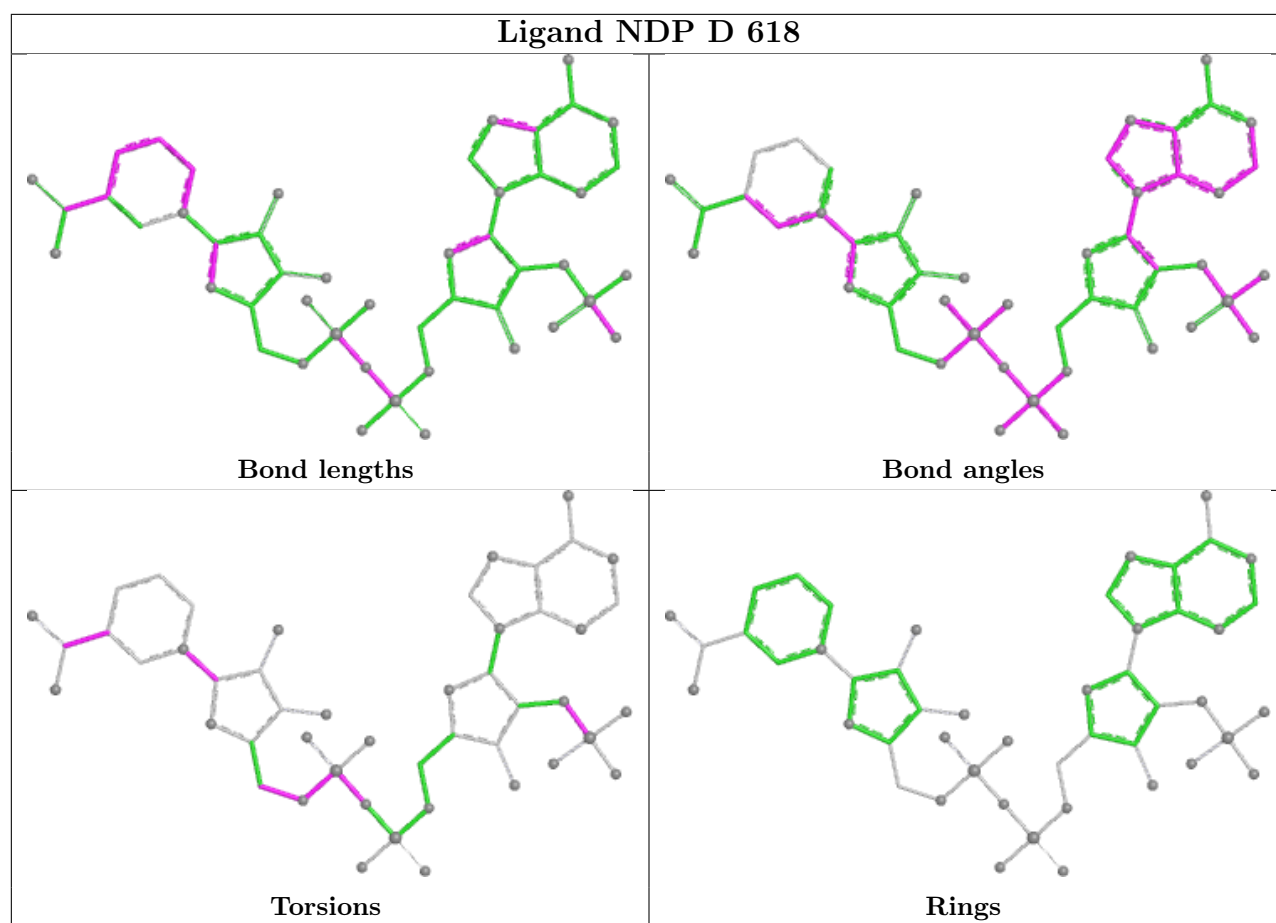




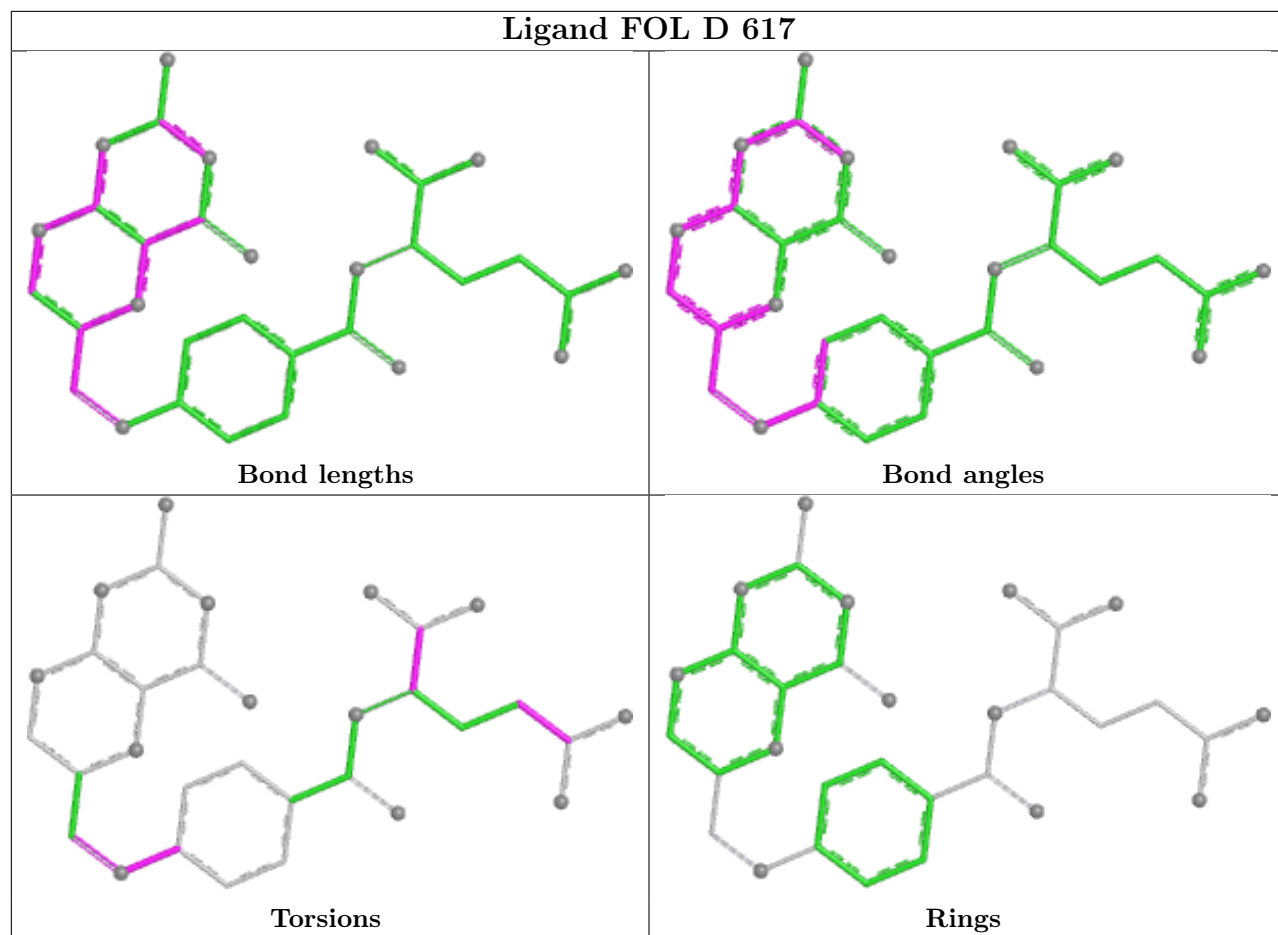




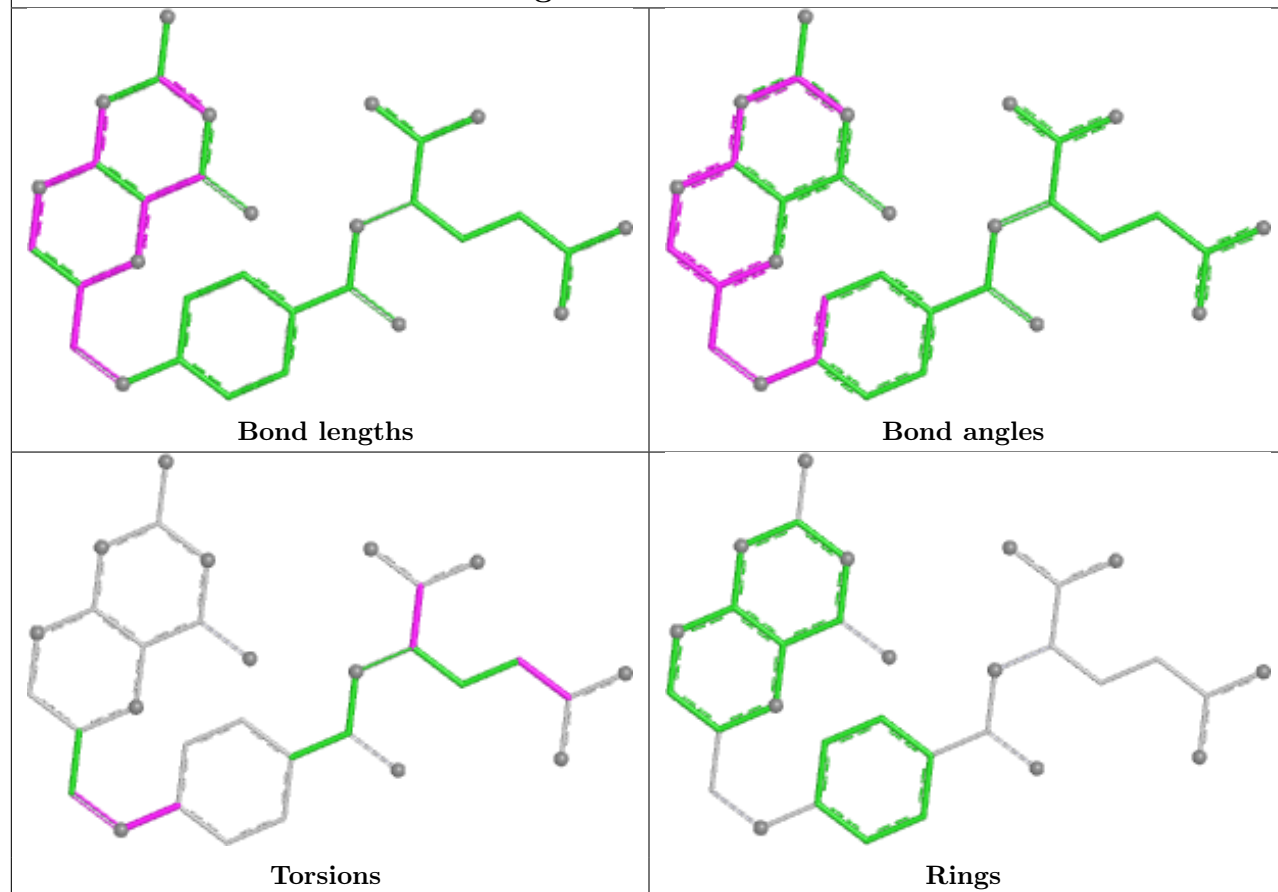




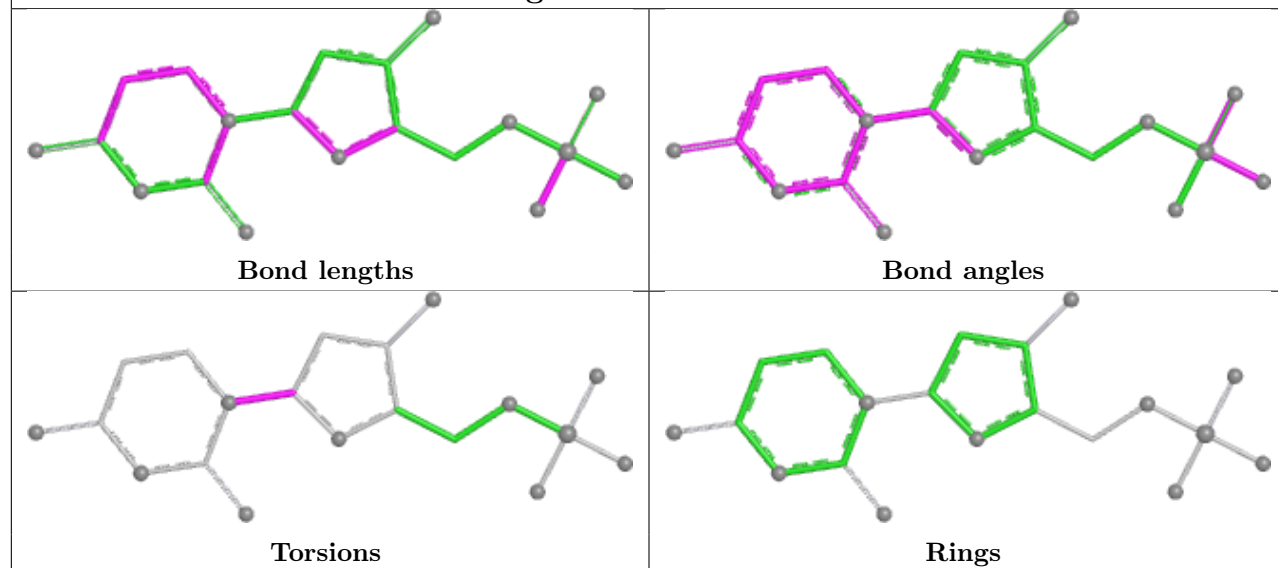
Ligand FOL D 617

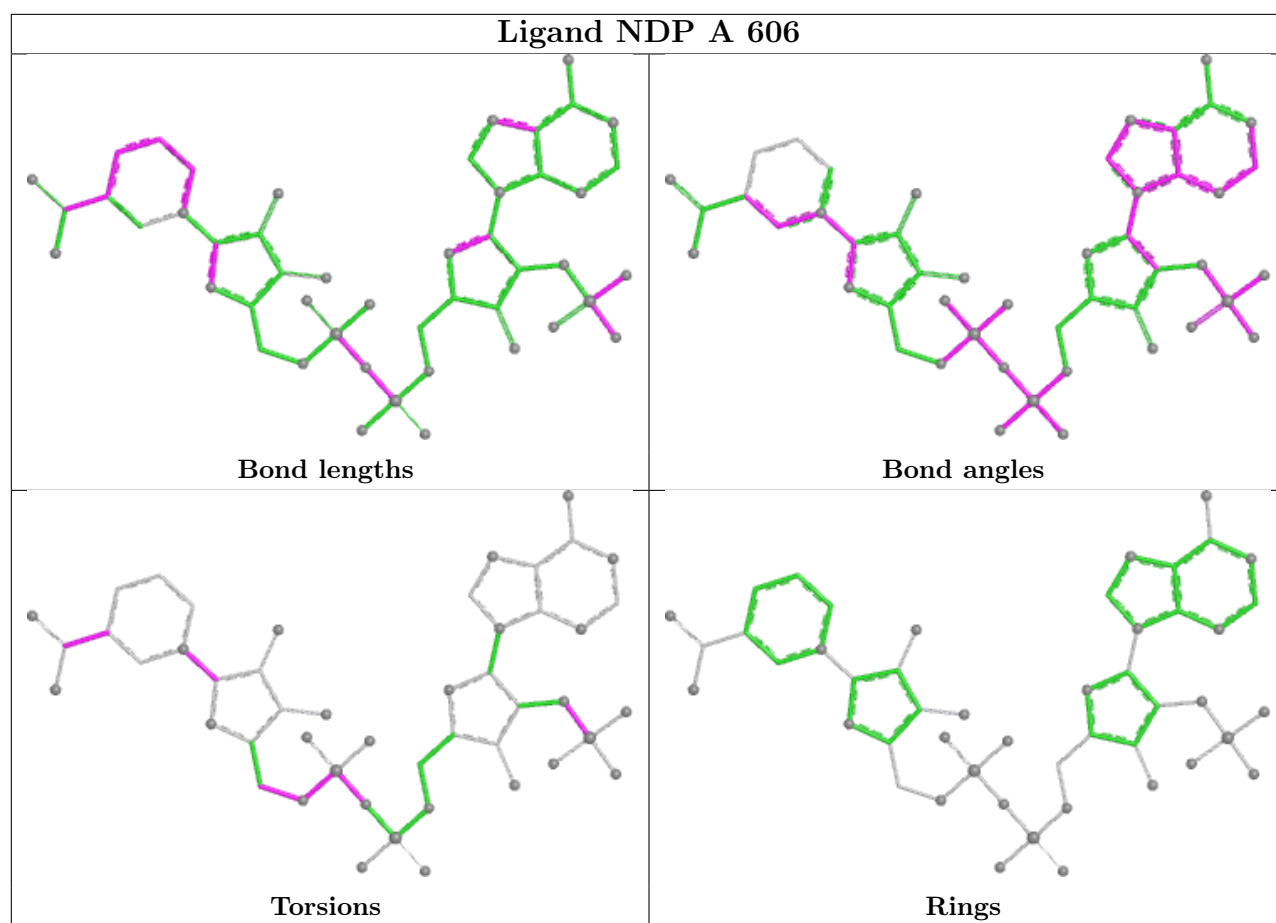


Ligand FOL B 609

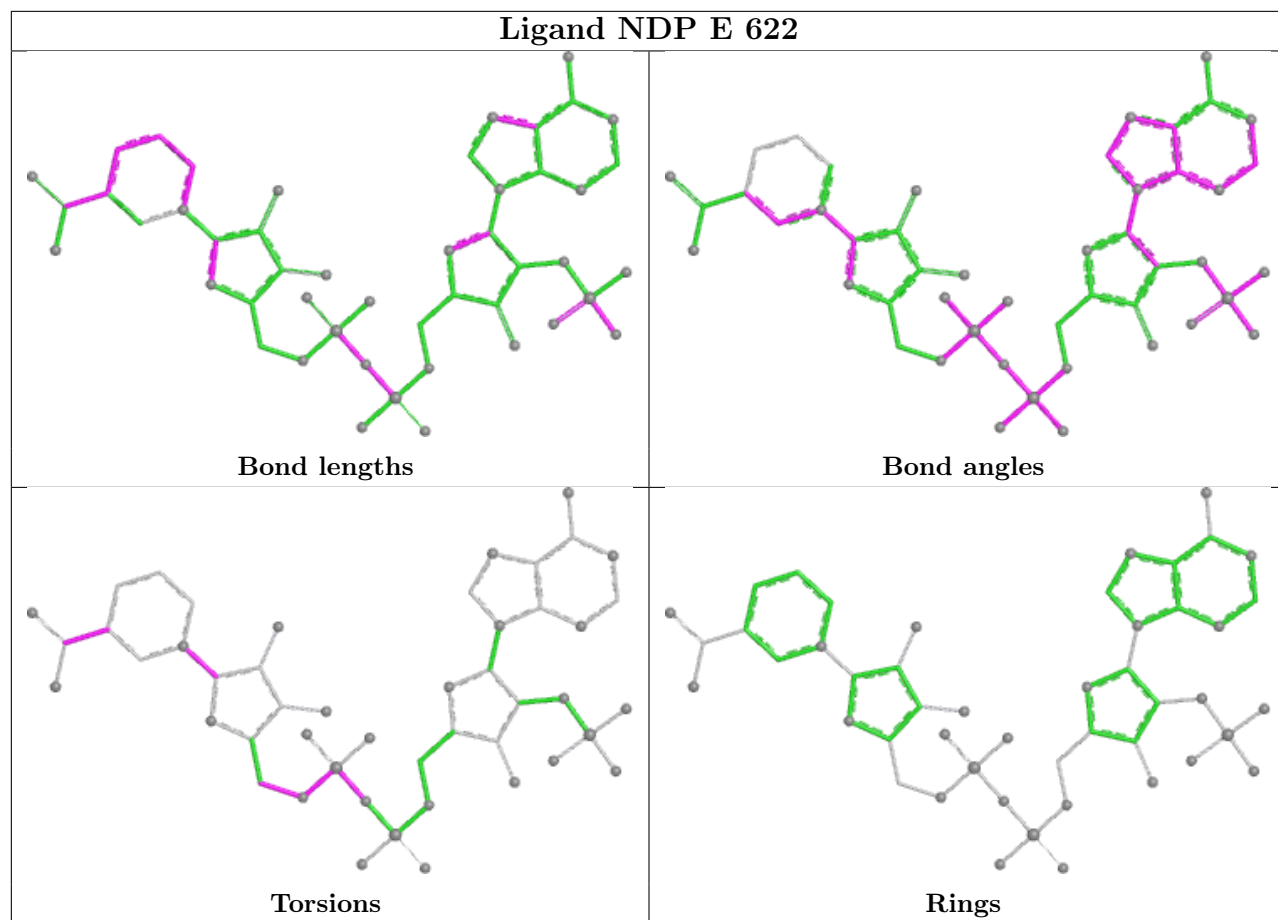


Ligand UMP A 603

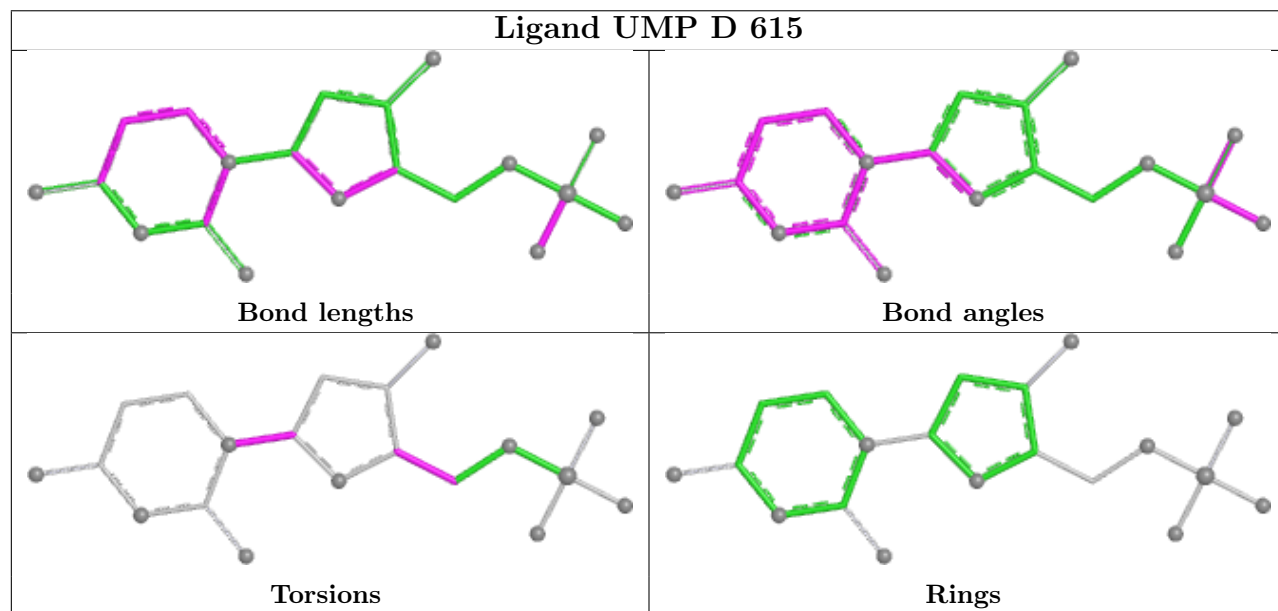


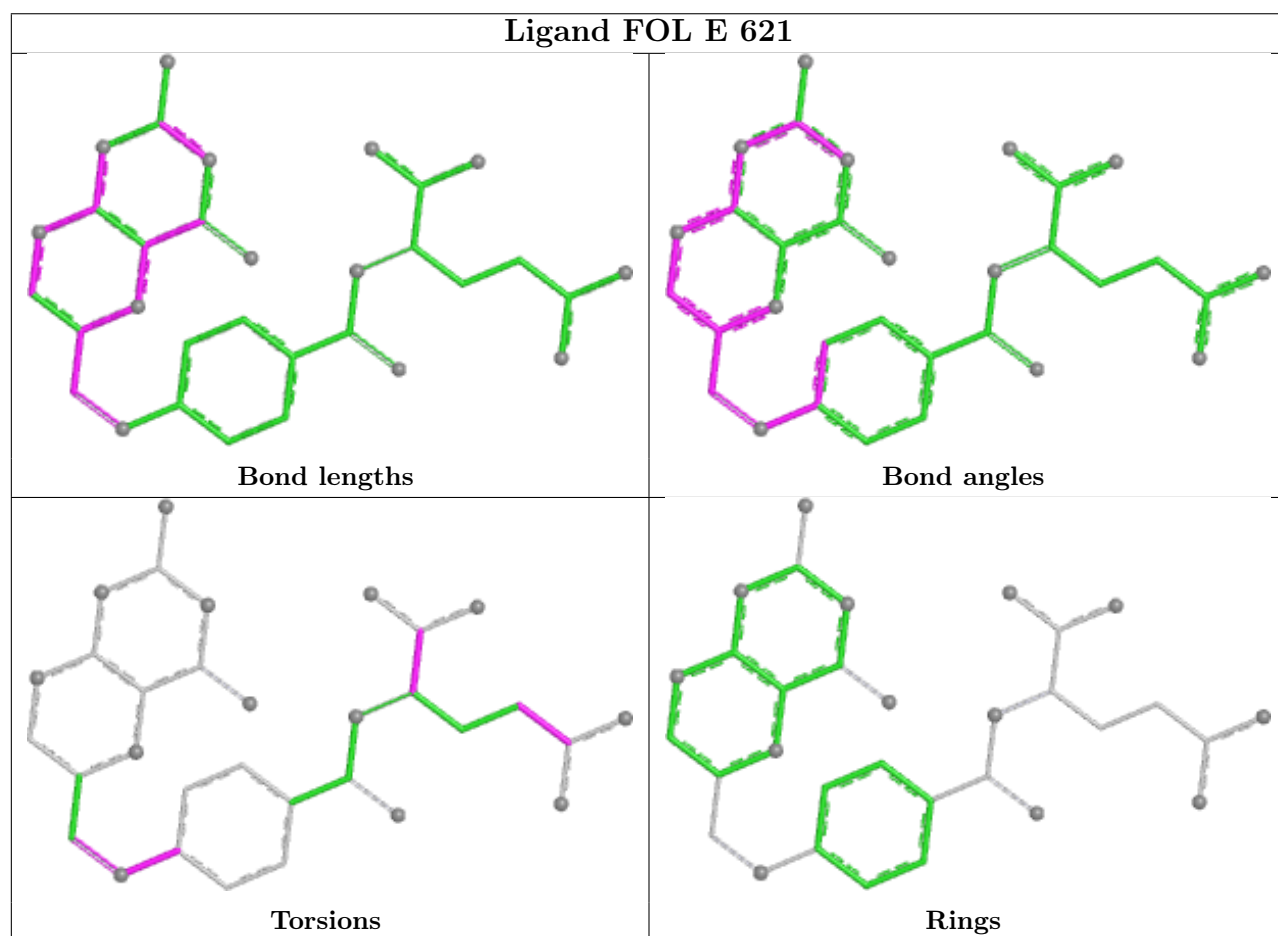
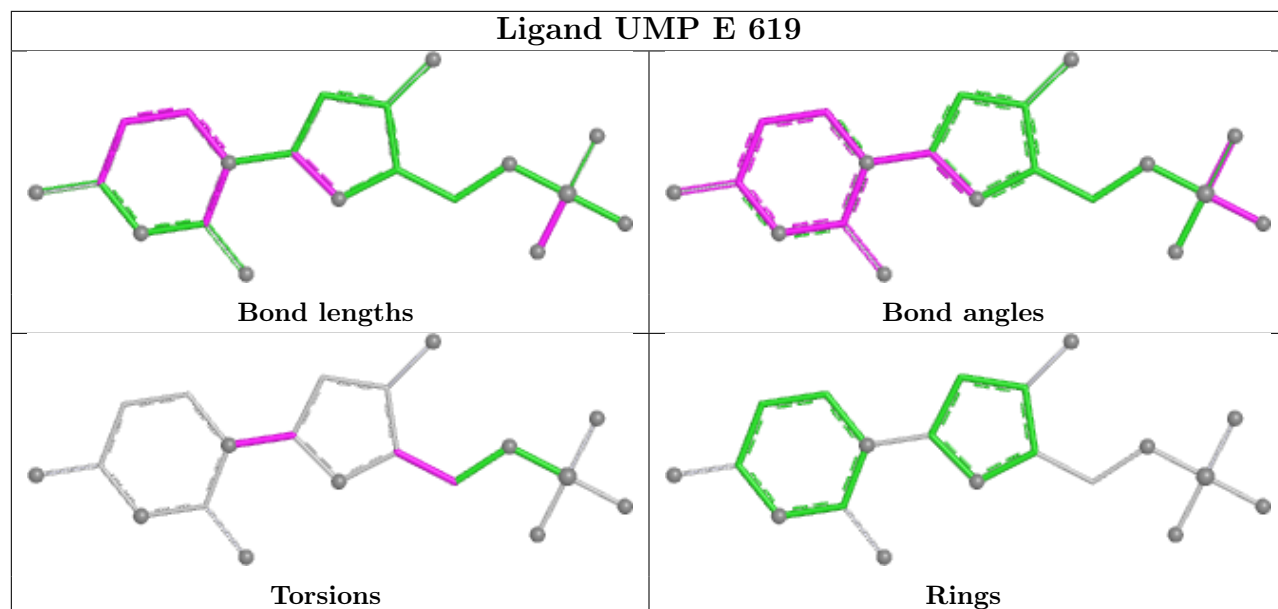


Ligand NDP E 622

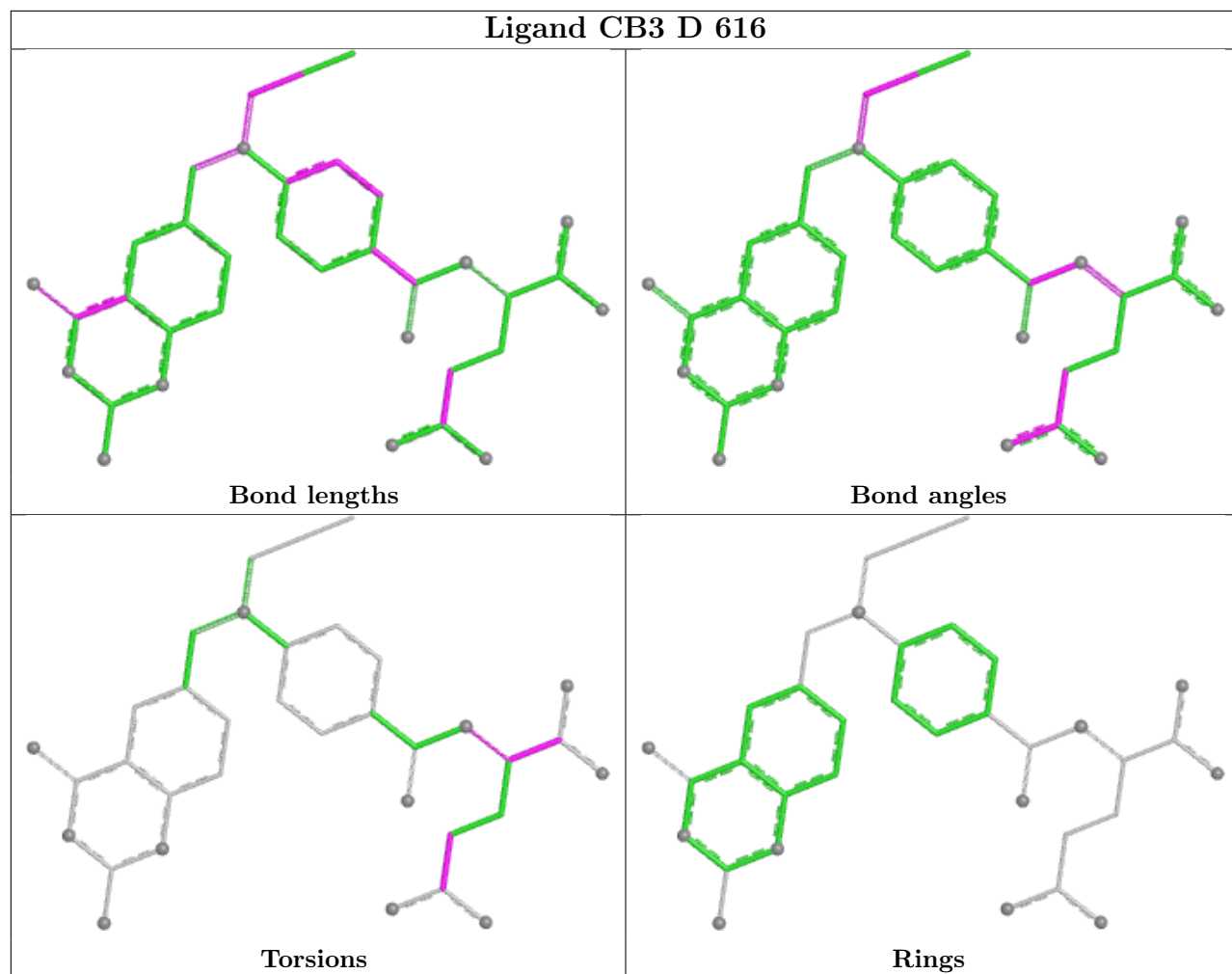


Ligand UMP D 615

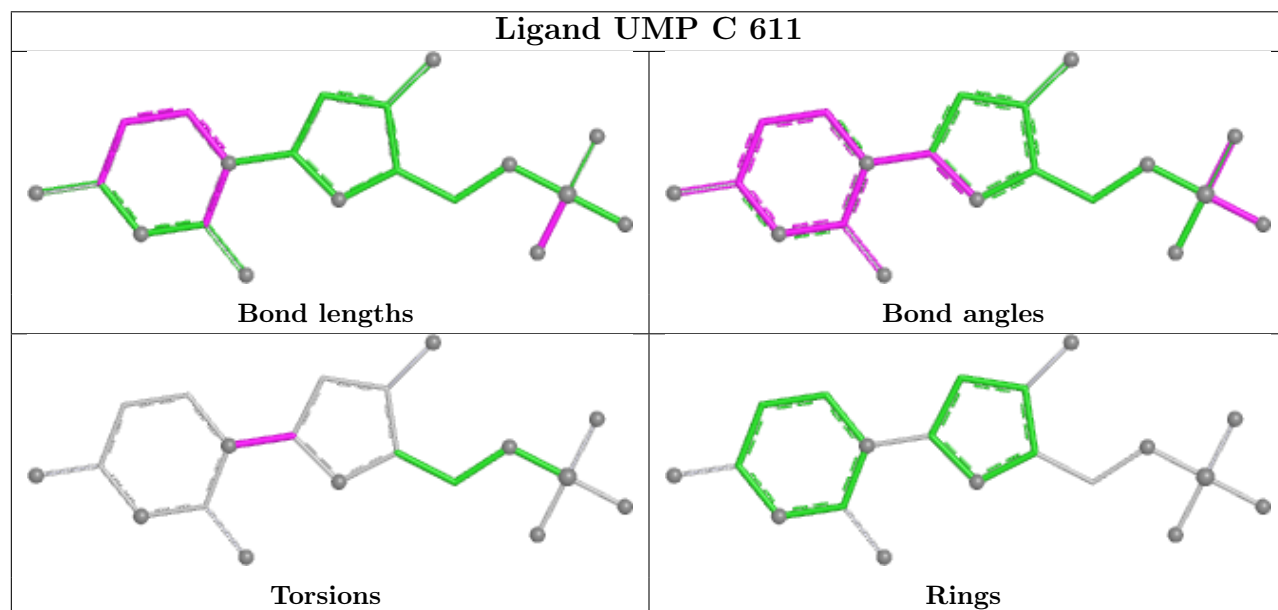


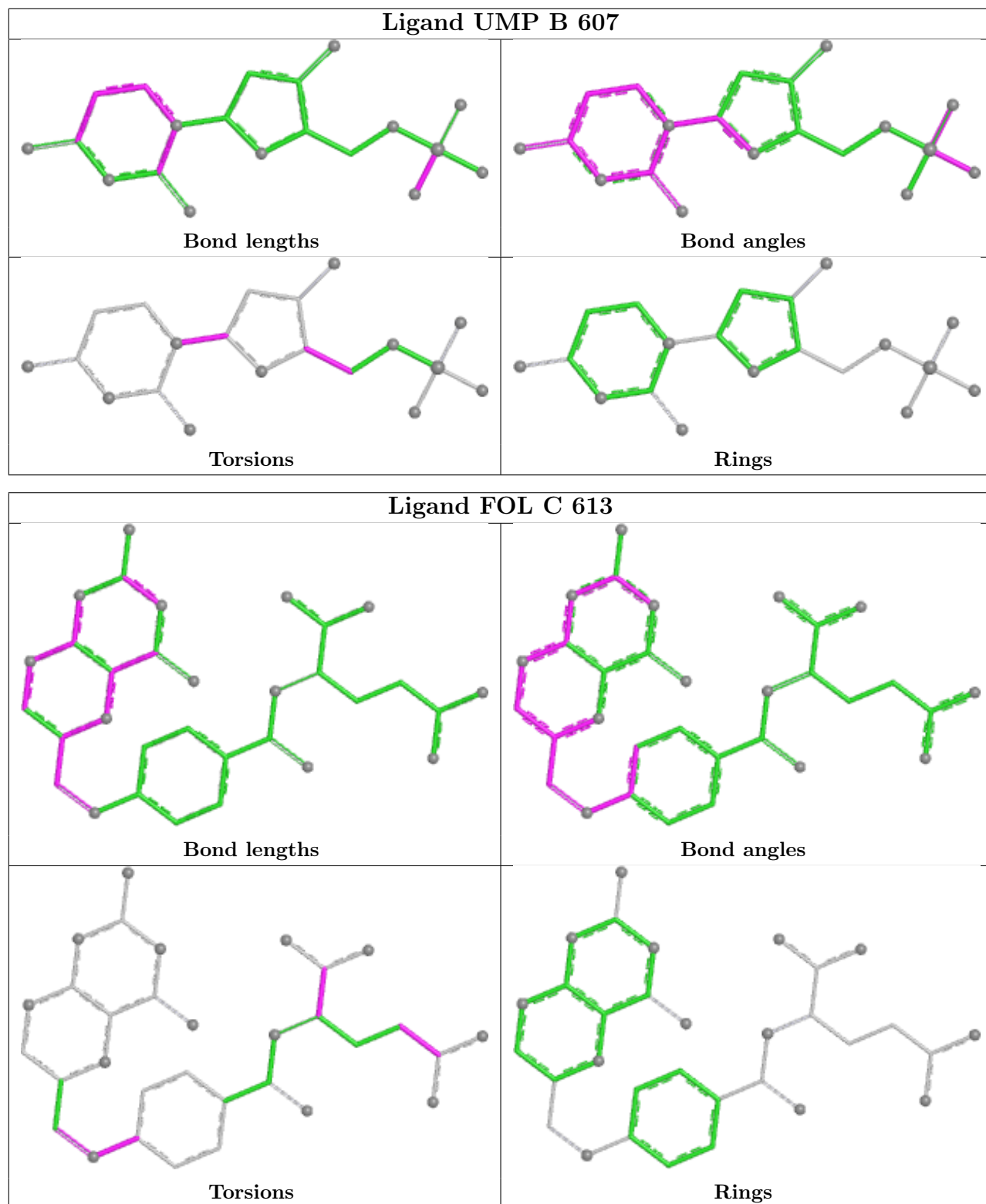


Ligand CB3 D 616



Ligand UMP C 611





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	519/521 (99%)	0.23	30 (5%)	29	22	21, 35, 59, 82	0
1	B	519/521 (99%)	0.29	27 (5%)	33	25	21, 34, 56, 81	0
1	C	519/521 (99%)	0.17	21 (4%)	42	33	22, 36, 57, 82	0
1	D	519/521 (99%)	0.17	24 (4%)	37	29	24, 36, 60, 82	0
1	E	519/521 (99%)	0.30	19 (3%)	45	36	25, 38, 60, 82	0
All	All	2595/2605 (99%)	0.23	121 (4%)	36	29	21, 36, 59, 82	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	182	THR	5.8
1	E	521	VAL	5.1
1	D	182	THR	4.8
1	A	331	GLY	4.7
1	B	82	ASP	4.6
1	E	182	THR	4.6
1	D	183	LEU	4.6
1	A	521	VAL	4.5
1	B	180	LYS	4.5
1	B	183	LEU	4.1
1	A	183	LEU	4.0
1	A	102	MET	4.0
1	B	322	LYS	4.0
1	B	434	ASN	3.9
1	D	521	VAL	3.8
1	C	183	LEU	3.8
1	D	102	MET	3.7
1	A	182	THR	3.7
1	B	182	THR	3.7
1	D	180	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	183	LEU	3.6
1	D	181	LYS	3.5
1	E	102	MET	3.5
1	A	180	LYS	3.5
1	B	103	ASN	3.5
1	D	331	GLY	3.5
1	C	3	GLU	3.4
1	D	82	ASP	3.4
1	E	180	LYS	3.4
1	B	179	GLU	3.4
1	D	179	GLU	3.4
1	A	434	ASN	3.4
1	A	305	GLY	3.4
1	C	434	ASN	3.3
1	B	3	GLU	3.2
1	C	82	ASP	3.2
1	E	181	LYS	3.2
1	D	434	ASN	3.2
1	C	180	LYS	3.2
1	A	82	ASP	3.1
1	A	336	ASN	3.1
1	A	335	GLU	3.0
1	B	101	LEU	2.9
1	B	323	GLU	2.9
1	C	102	MET	2.9
1	A	343	GLY	2.9
1	A	184	GLN	2.8
1	E	184	GLN	2.8
1	A	520	ALA	2.8
1	A	101	LEU	2.8
1	B	358	ASP	2.7
1	E	82	ASP	2.7
1	A	179	GLU	2.7
1	B	354	LYS	2.7
1	A	324	TYR	2.6
1	D	323	GLU	2.6
1	C	181	LYS	2.6
1	A	356	MET	2.6
1	B	102	MET	2.6
1	B	326	GLU	2.6
1	B	99	GLU	2.6
1	D	184	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	103	ASN	2.5
1	C	179	GLU	2.5
1	A	316	TRP	2.5
1	A	326	GLU	2.4
1	B	100	ASN	2.4
1	B	325	LEU	2.4
1	B	104	ASP	2.4
1	A	306	ASN	2.4
1	C	354	LYS	2.4
1	A	255	GLU	2.4
1	C	325	LEU	2.4
1	E	434	ASN	2.4
1	C	28	SER	2.4
1	A	330	LEU	2.4
1	A	3	GLU	2.3
1	C	322	LYS	2.3
1	A	317	SER	2.3
1	B	84	ALA	2.3
1	D	357	HIS	2.3
1	A	332	HIS	2.3
1	D	332	HIS	2.3
1	C	103	ASN	2.2
1	D	84	ALA	2.2
1	E	3	GLU	2.2
1	E	319	ASN	2.2
1	E	101	LEU	2.2
1	B	184	GLN	2.2
1	C	381	ASP	2.2
1	C	101	LEU	2.2
1	B	319	ASN	2.2
1	D	103	ASN	2.2
1	E	179	GLU	2.2
1	A	257	ARG	2.2
1	C	184	GLN	2.2
1	A	354	LYS	2.2
1	E	324	TYR	2.2
1	B	28	SER	2.2
1	B	494	GLU	2.2
1	E	326	GLU	2.2
1	B	495	ASN	2.1
1	E	306	ASN	2.1
1	D	305	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	3	GLU	2.1
1	D	255	GLU	2.1
1	E	336	ASN	2.1
1	D	520	ALA	2.1
1	C	99	GLU	2.1
1	D	342	TYR	2.1
1	E	316	TRP	2.1
1	B	317	SER	2.0
1	E	86	PRO	2.0
1	C	333	ARG	2.0
1	C	255	GLU	2.0
1	B	521	VAL	2.0
1	C	138	LEU	2.0
1	D	101	LEU	2.0
1	D	306	ASN	2.0
1	D	327	ARG	2.0
1	A	98	ILE	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	D	616	35/35	0.72	0.21	66,71,77,78	0
2	UMP	A	603	20/20	0.78	0.21	55,68,73,73	0
3	CB3	E	620	35/35	0.78	0.18	67,71,76,77	0
3	CB3	A	604	35/35	0.79	0.19	66,71,77,78	0
2	UMP	D	615	20/20	0.80	0.21	57,69,74,74	0
2	UMP	C	611	20/20	0.80	0.22	55,66,73,73	0

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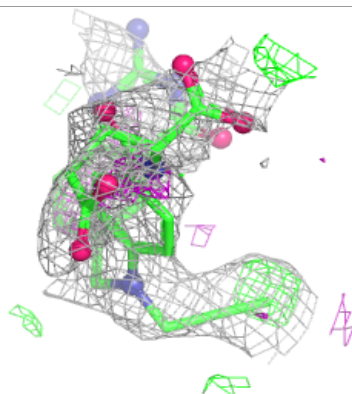
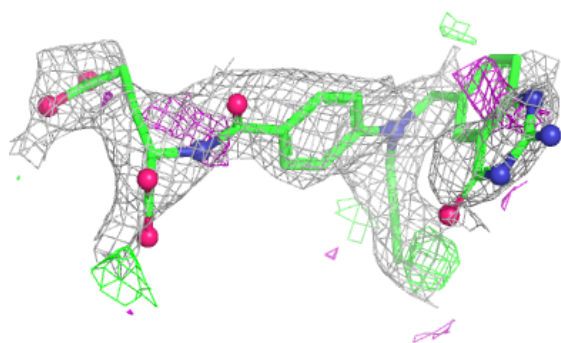
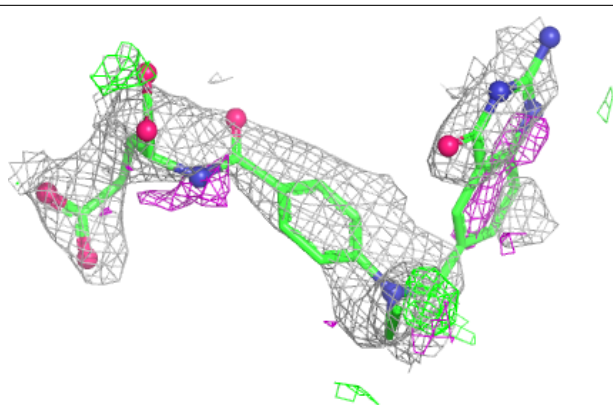
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UMP	E	619	20/20	0.82	0.18	60,70,74,74	0
3	CB3	C	612	35/35	0.83	0.20	65,69,76,76	0
2	UMP	B	607	20/20	0.85	0.23	52,66,72,72	0
4	FOL	E	621	32/32	0.85	0.15	40,45,47,47	0
3	CB3	B	608	35/35	0.86	0.20	63,69,76,76	0
4	FOL	C	613	32/32	0.87	0.15	37,44,47,47	0
4	FOL	D	617	32/32	0.88	0.14	37,43,47,48	0
4	FOL	B	609	32/32	0.91	0.15	36,43,44,45	0
4	FOL	A	605	32/32	0.91	0.14	34,43,44,44	0
5	NDP	E	622	48/48	0.93	0.12	40,48,57,58	0
5	NDP	C	614	48/48	0.94	0.10	39,48,57,58	0
5	NDP	D	618	48/48	0.95	0.10	40,48,56,57	0
5	NDP	B	610	48/48	0.96	0.10	37,43,53,55	0
5	NDP	A	606	48/48	0.96	0.10	36,43,52,54	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.

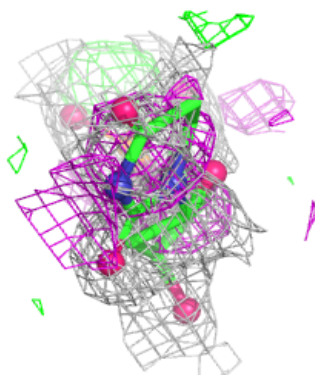
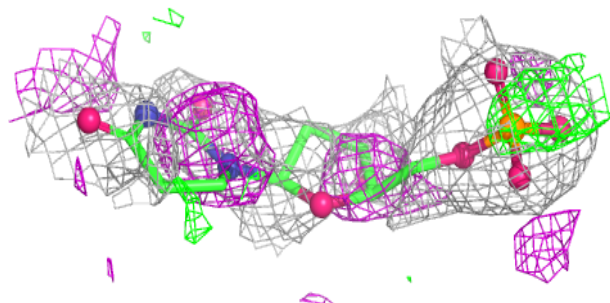
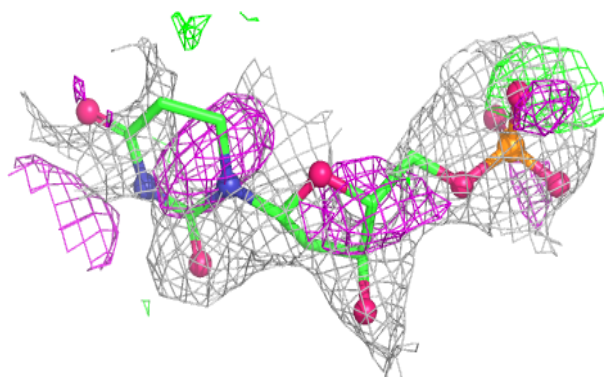
Electron density around CB3 D 616:

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

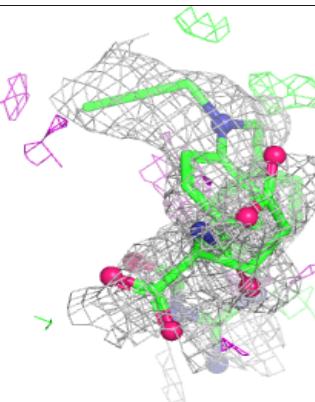
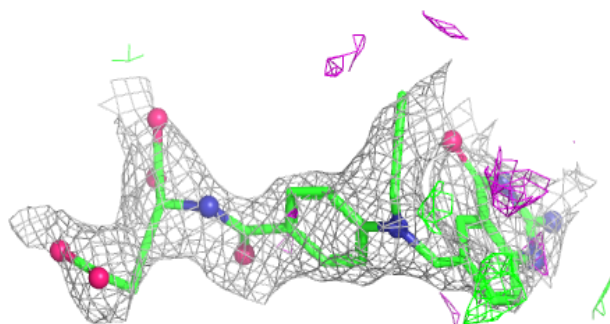
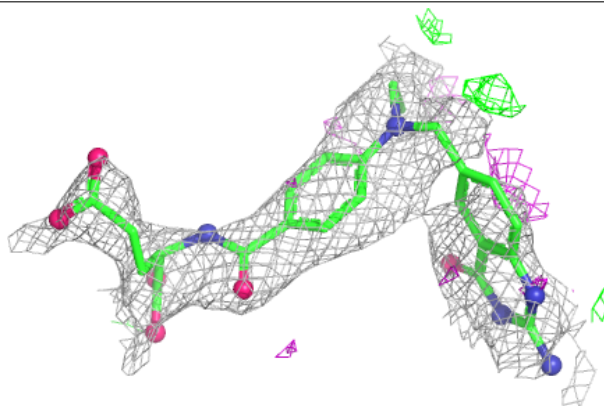


Electron density around UMP A 603:

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

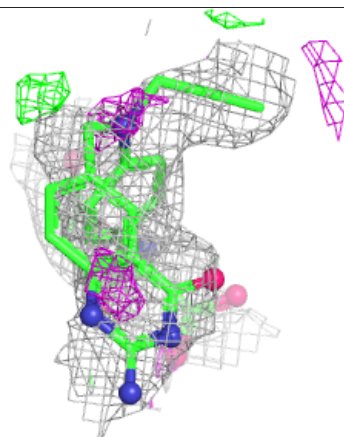
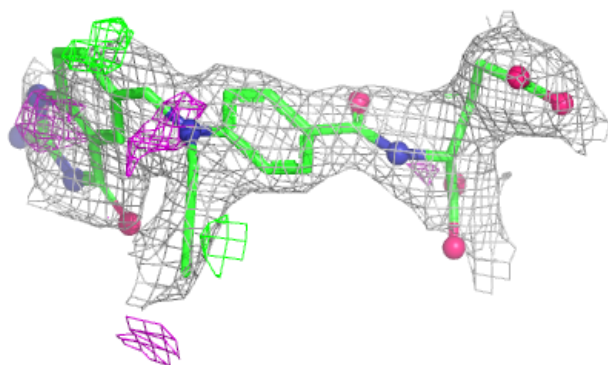
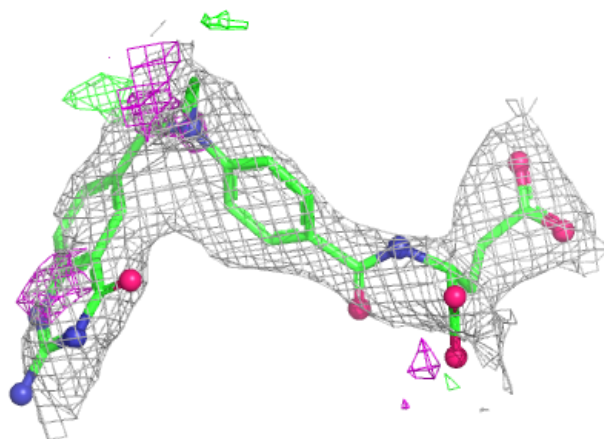
**Electron density around CB3 E 620:**

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and green (positive)

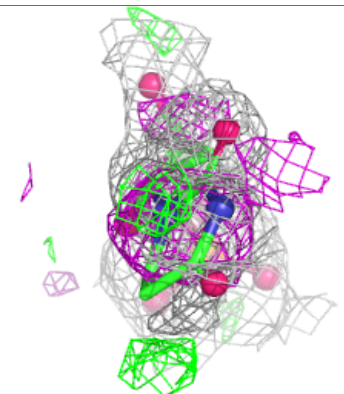
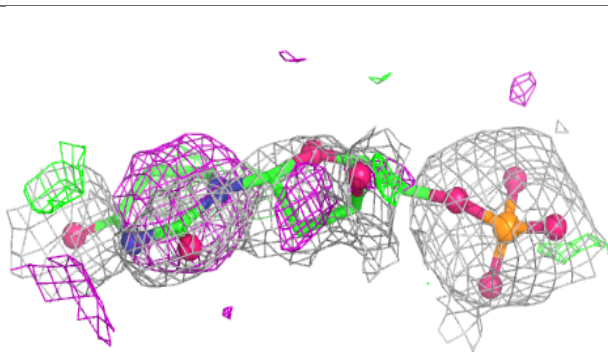
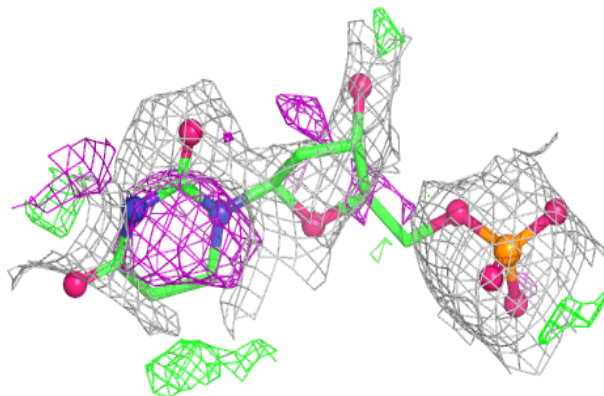


Electron density around CB3 A 604:

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

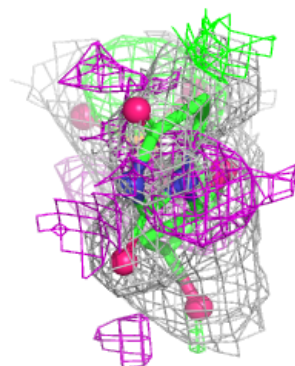
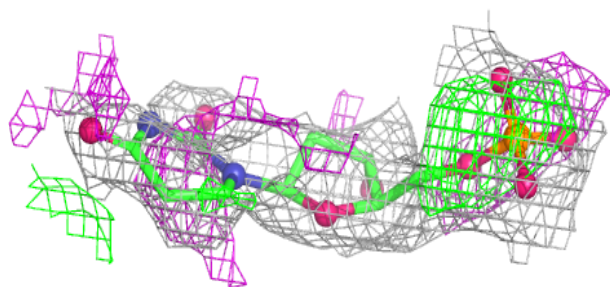
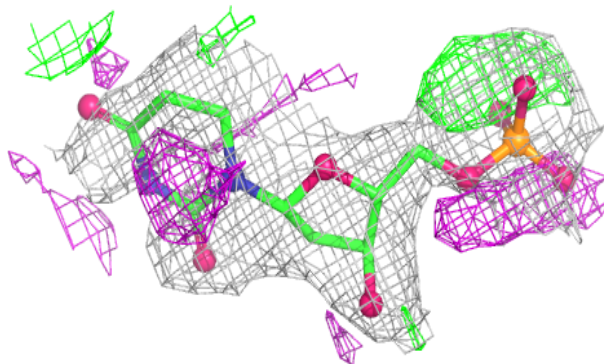
**Electron density around UMP D 615:**

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

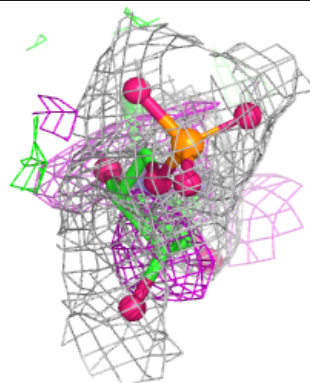
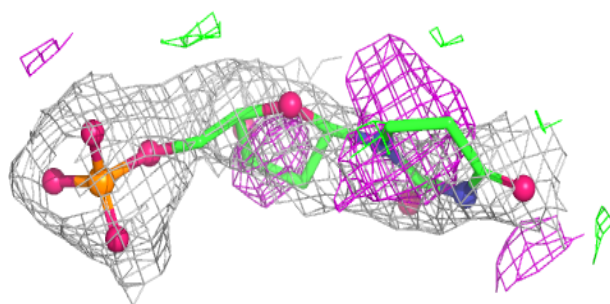
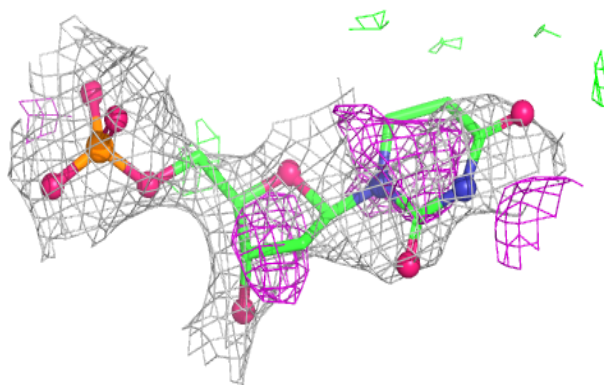


Electron density around UMP C 611:

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

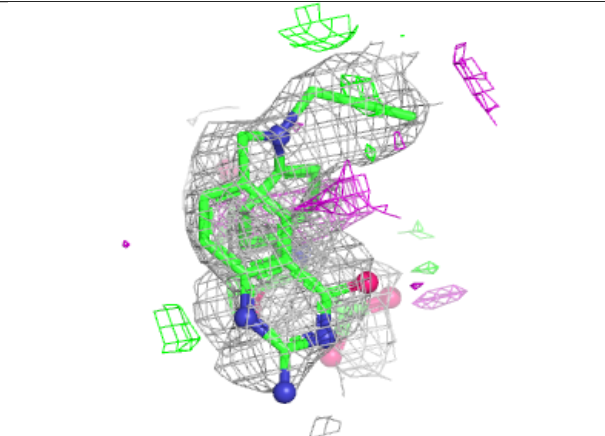
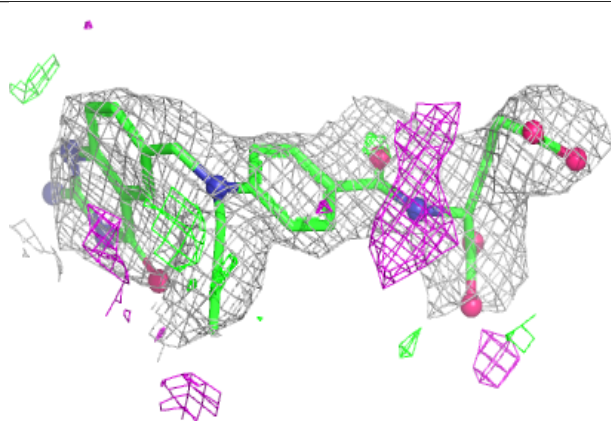
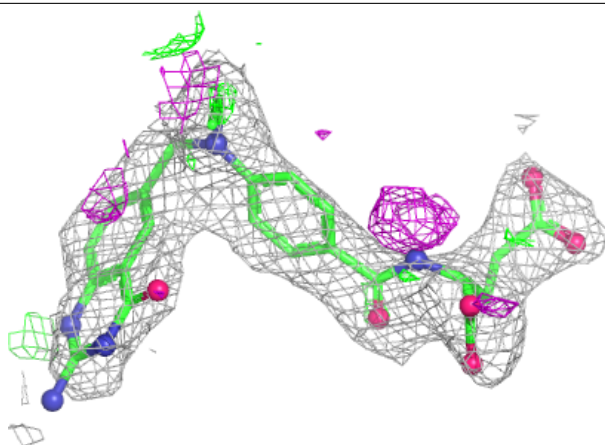
**Electron density around UMP E 619:**

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and green (positive)

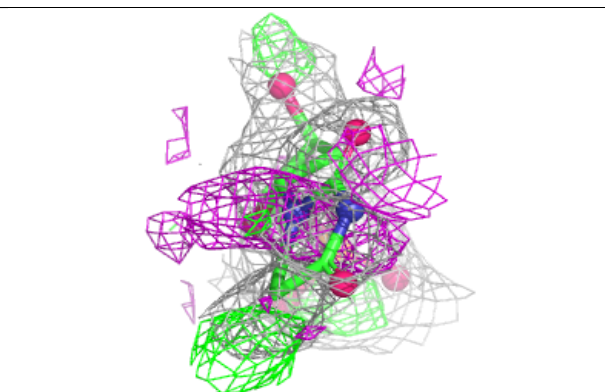
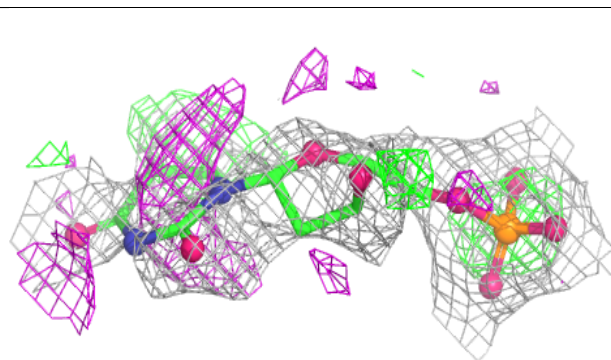
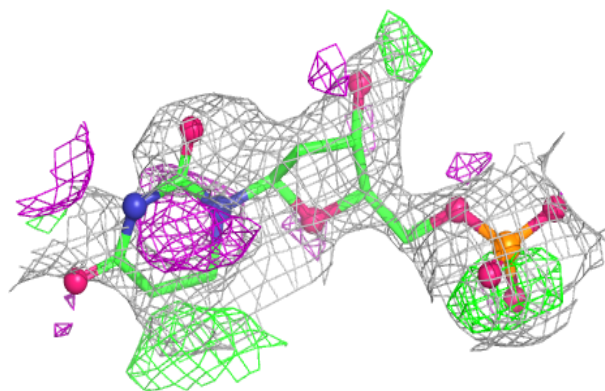


Electron density around CB3 C 612:

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and green (positive)

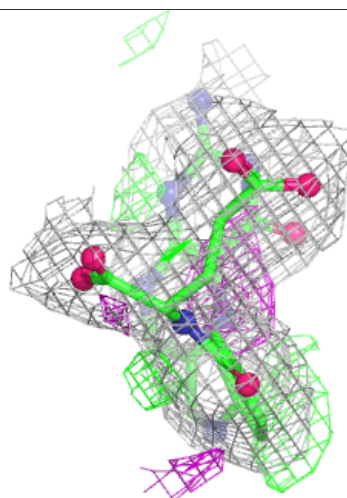
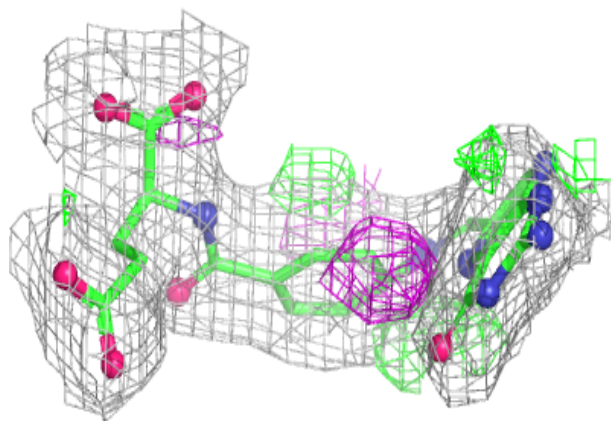
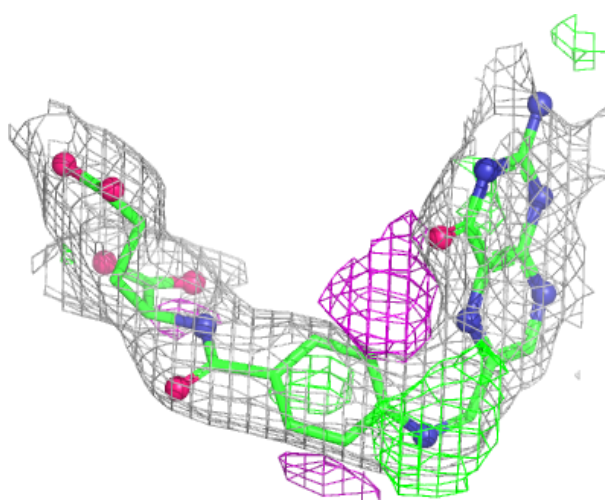
**Electron density around UMP B 607:**

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



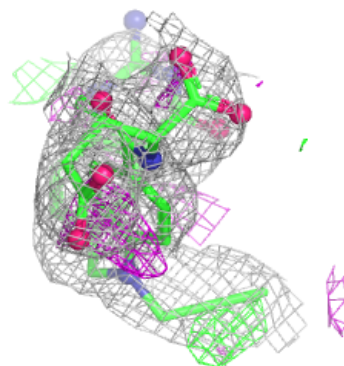
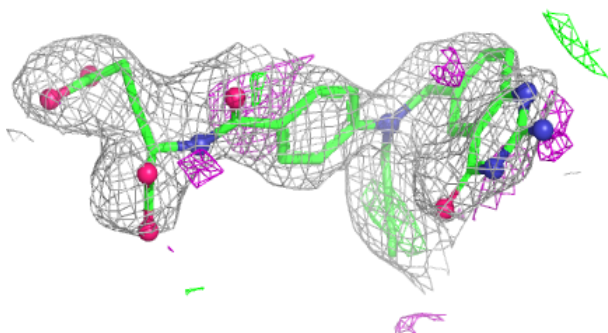
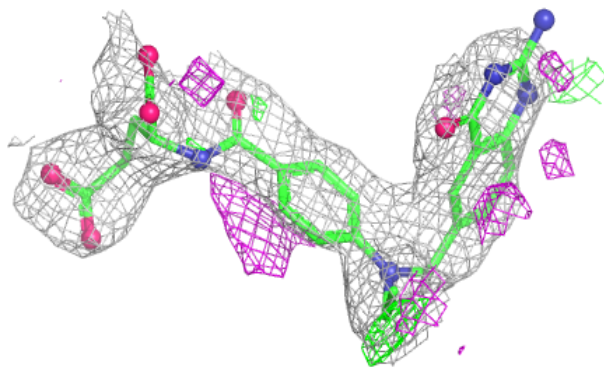
Electron density around FOL E 621:

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



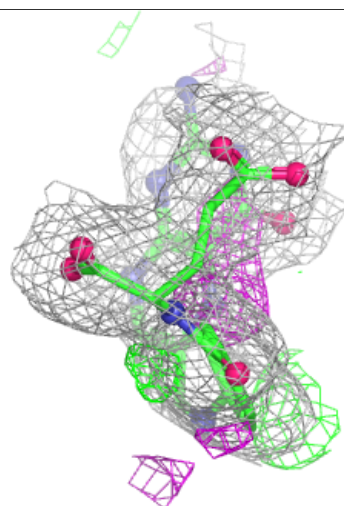
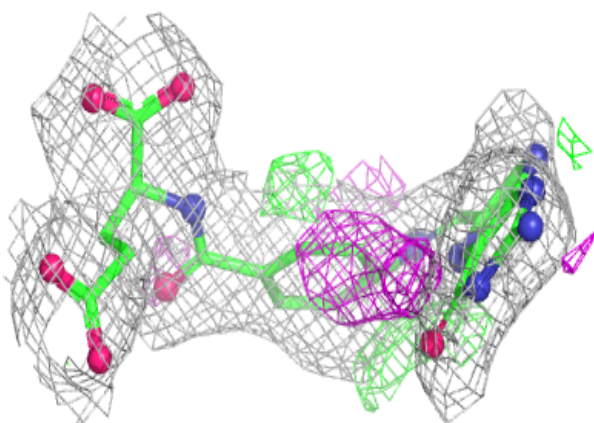
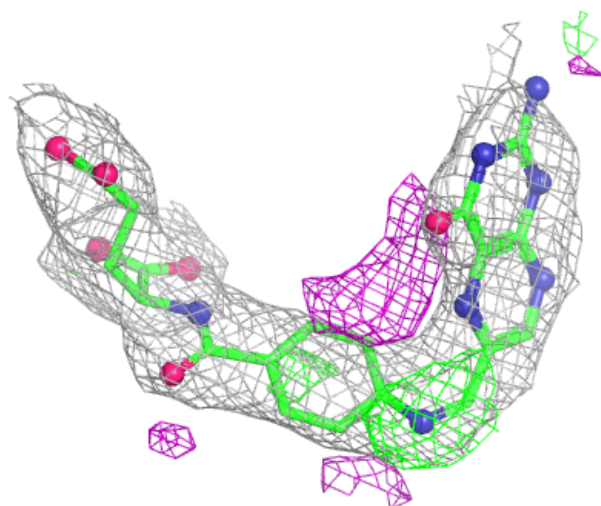
Electron density around CB3 B 608:

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



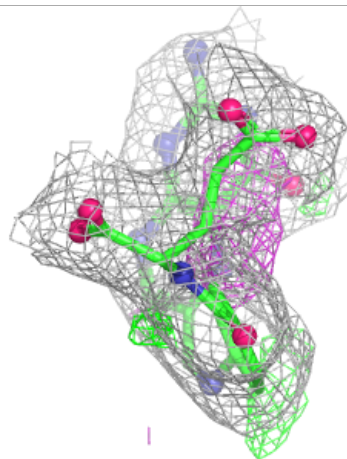
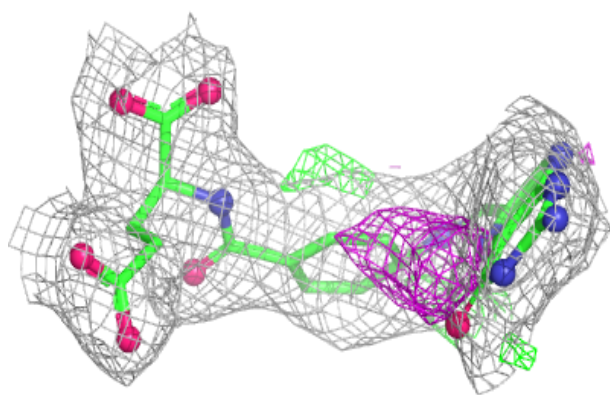
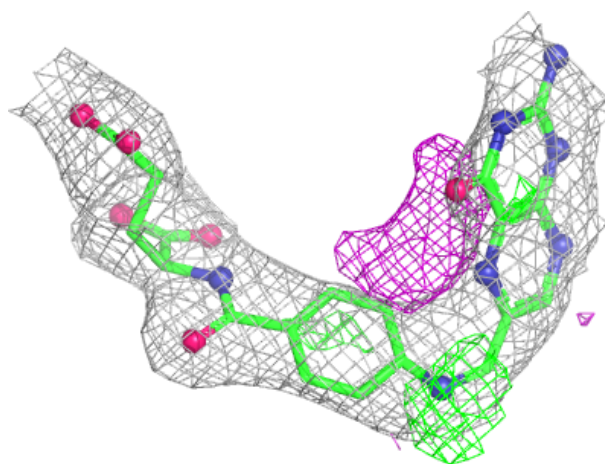
Electron density around FOL C 613:

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



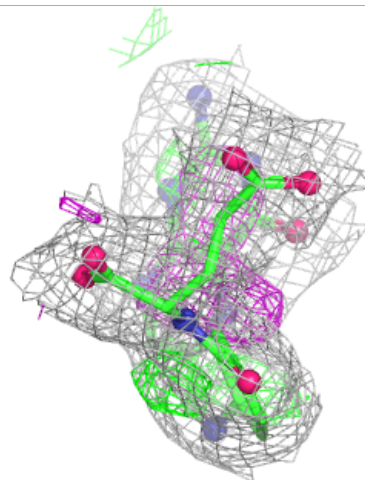
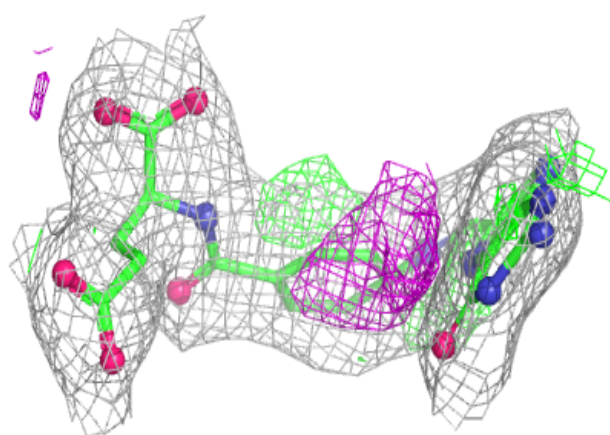
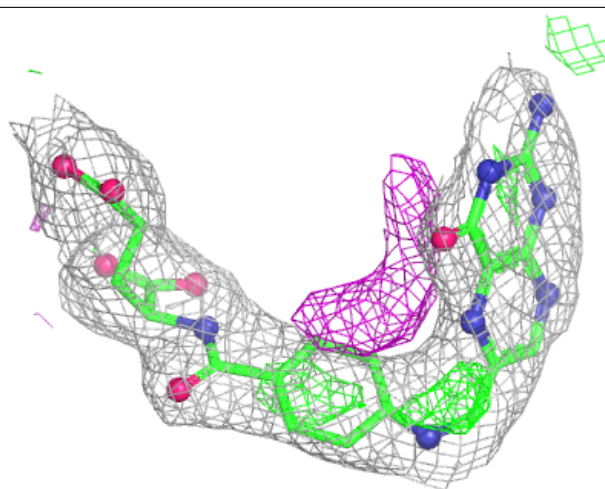
Electron density around FOL D 617:

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



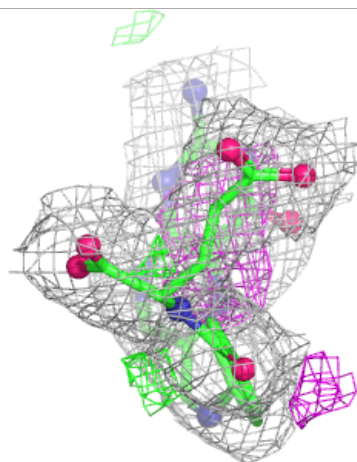
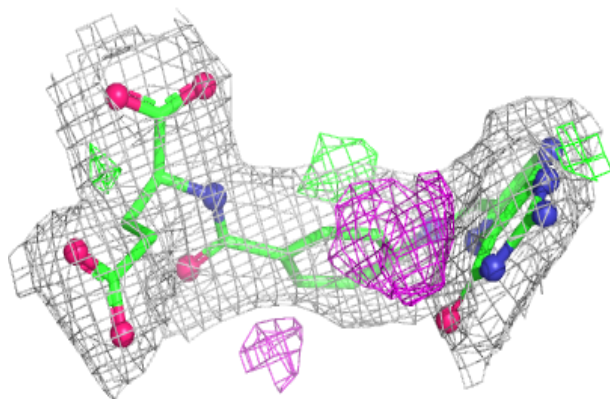
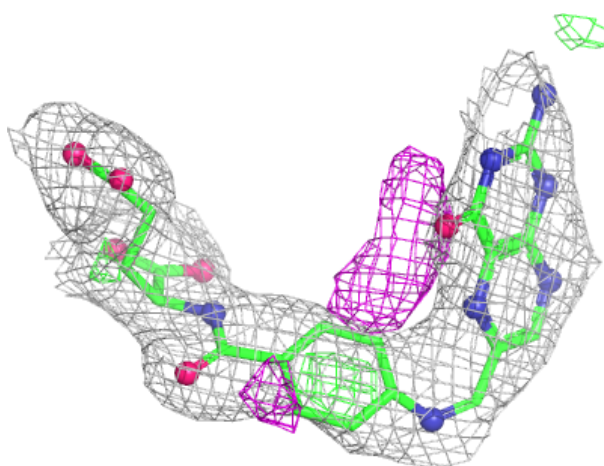
Electron density around FOL B 609:

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



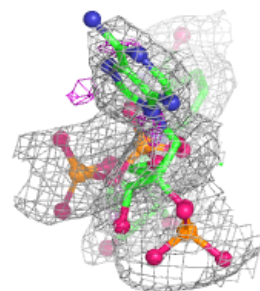
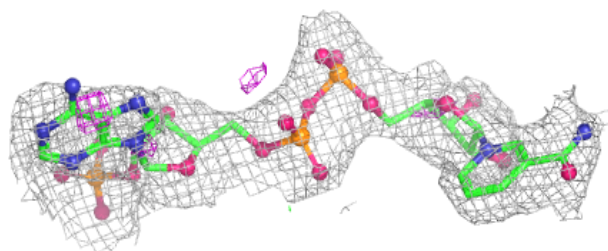
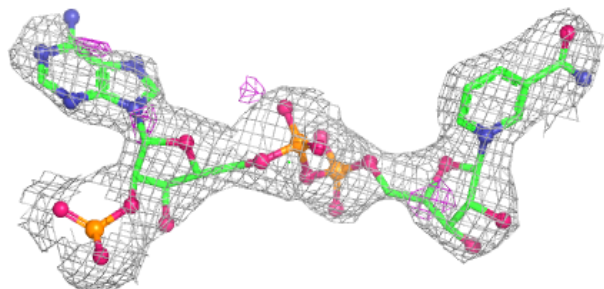
Electron density around FOL A 605:

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

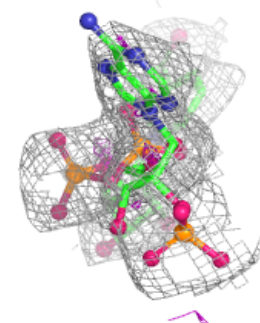
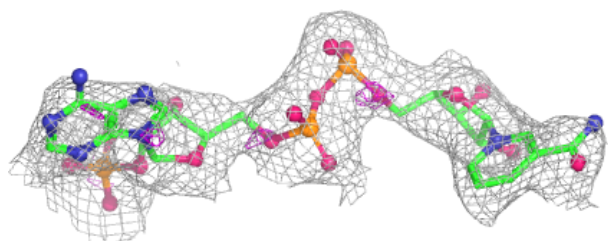
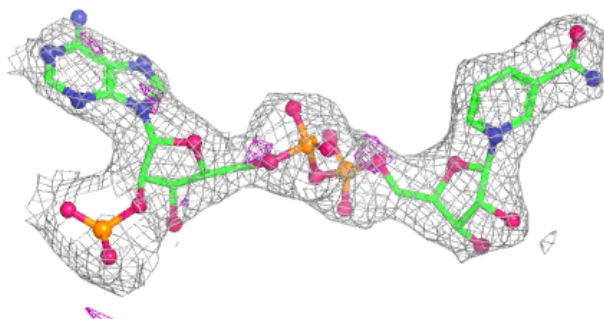


Electron density around NDP E 622:

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

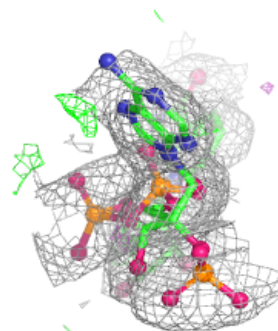
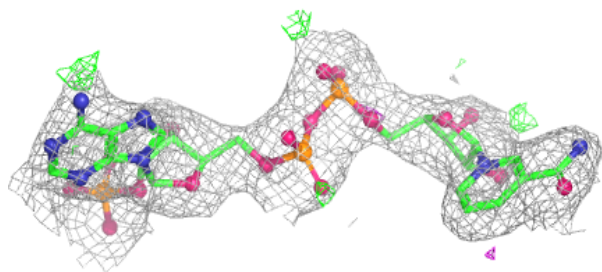
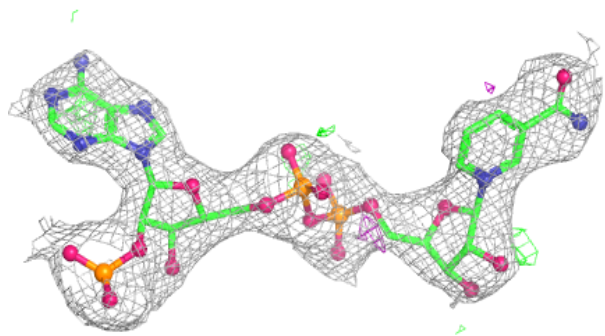
**Electron density around NDP C 614:**

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

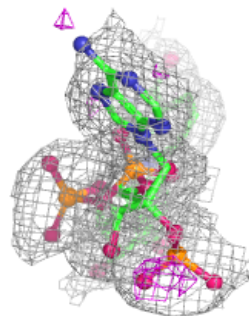
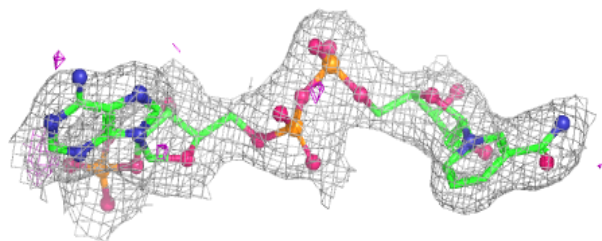
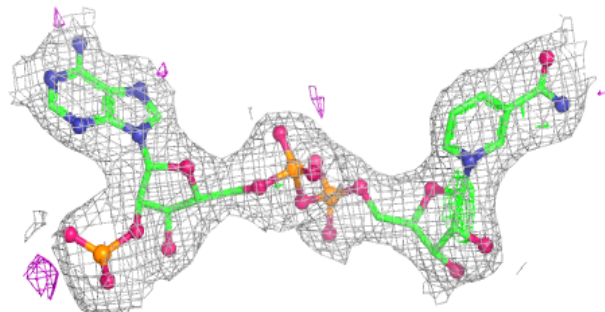


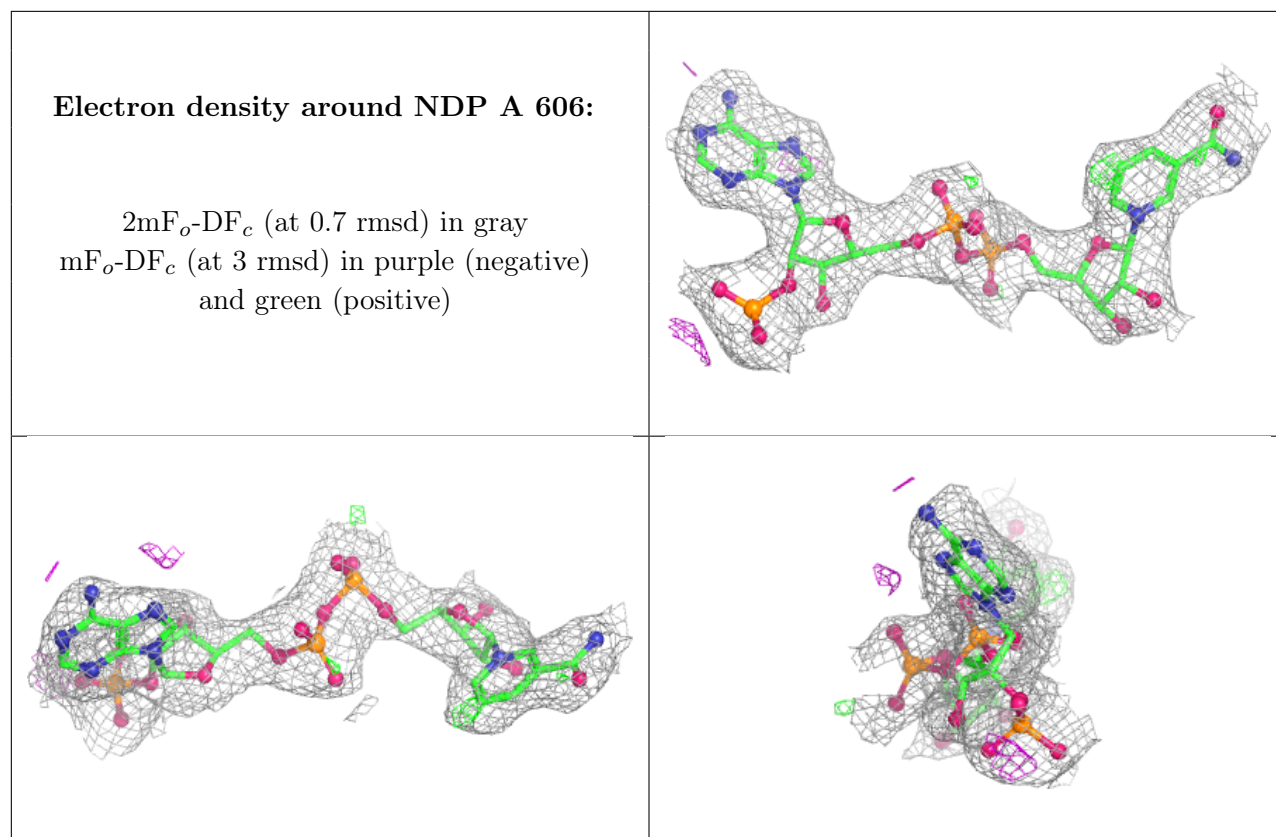
Electron density around NDP D 618:

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

**Electron density around NDP 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.