



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:34 PM UTC

PDB ID : 4Q0E / pdb_00004q0e
Title : Crystal structure of TS-DHFR from *Cryptosporidium hominis* in complex with NADPH, FdUMP and 2-amino-4-oxo-4,7-dihydro-pyrrolo[2,3-d]pyrimidine-methyl-phenyl-L-glutamic acid.
Authors : Kumar, V.P.; Anderson, K.S.
Deposited on : 2014-04-01
Resolution : 2.78 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:

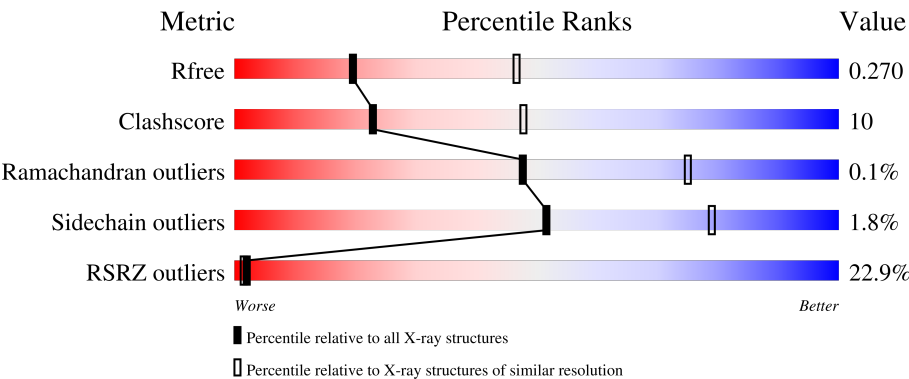
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	14% 73% 22% ..
1	B	521	20% 77% 19% ..
1	C	521	23% 73% 23% ..
1	D	521	21% 76% 19% ..

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Mol	Chain	Length	Quality of chain
1	E	521	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	2XB	A	604	X	-	-	-
4	2XB	B	604	X	-	-	-
4	2XB	C	604	X	-	-	-
4	2XB	D	604	X	-	-	-
4	2XB	E	604	X	-	-	-

2 Entry composition ⓘ

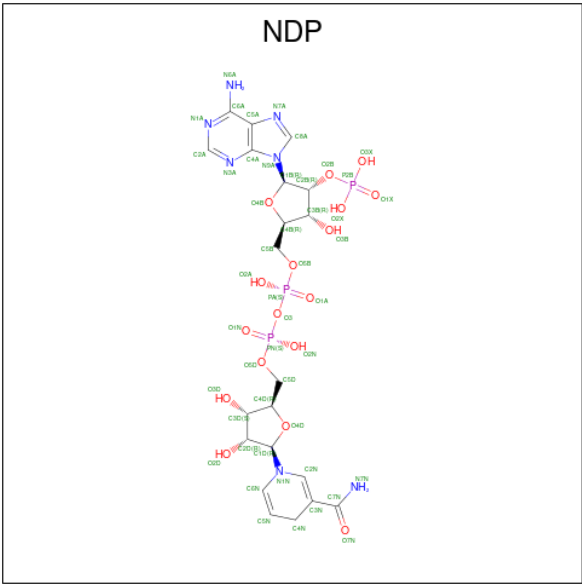
There are 5 unique types of molecules in this entry. The entry contains 21154 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	505	Total	C	N	O	S	0	0	0
			4099	2621	689	767	22			
1	B	505	Total	C	N	O	S	0	0	0
			4095	2619	689	765	22			
1	C	505	Total	C	N	O	S	0	0	0
			4099	2621	689	767	22			
1	D	505	Total	C	N	O	S	0	0	0
			4099	2621	689	767	22			
1	E	505	Total	C	N	O	S	0	0	0
			4099	2621	689	767	22			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



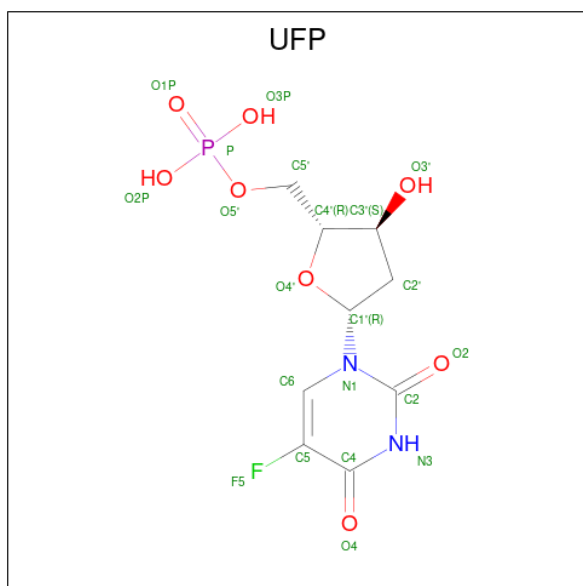
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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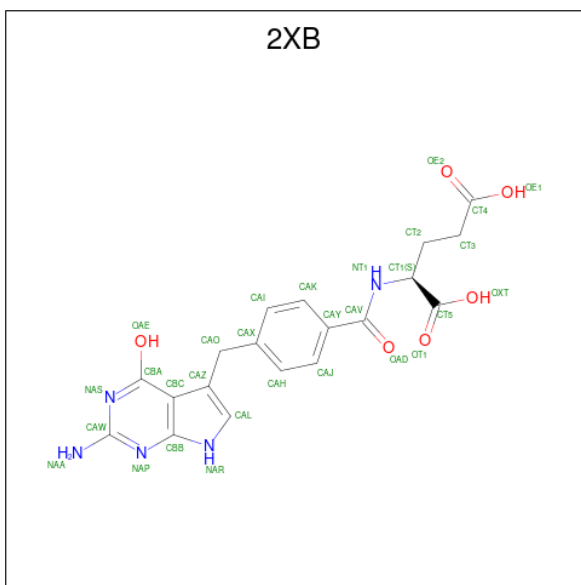
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (CCD ID: UFP) (formula: C₉H₁₂FN₂O₈P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	B	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	C	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	D	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	E	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0

- Molecule 4 is N-{4-[(2-amino-4-hydroxy-7H-pyrrolo[2,3-d]pyrimidin-5-yl)methyl]benzoyl}-L-glutamic acid (CCD ID: 2XB) (formula: C₁₉H₁₉N₅O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 30	C 19	N 5	O 6	0	0
4	A	1	Total 30	C 19	N 5	O 6	0	0
4	B	1	Total 30	C 19	N 5	O 6	0	0
4	B	1	Total 30	C 19	N 5	O 6	0	0
4	C	1	Total 30	C 19	N 5	O 6	0	0
4	C	1	Total 30	C 19	N 5	O 6	0	0
4	D	1	Total 30	C 19	N 5	O 6	0	0
4	D	1	Total 30	C 19	N 5	O 6	0	0
4	E	1	Total 30	C 19	N 5	O 6	0	0
4	E	1	Total 30	C 19	N 5	O 6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	8	Total O 8 8	0	0
5	B	2	Total O 2 2	0	0

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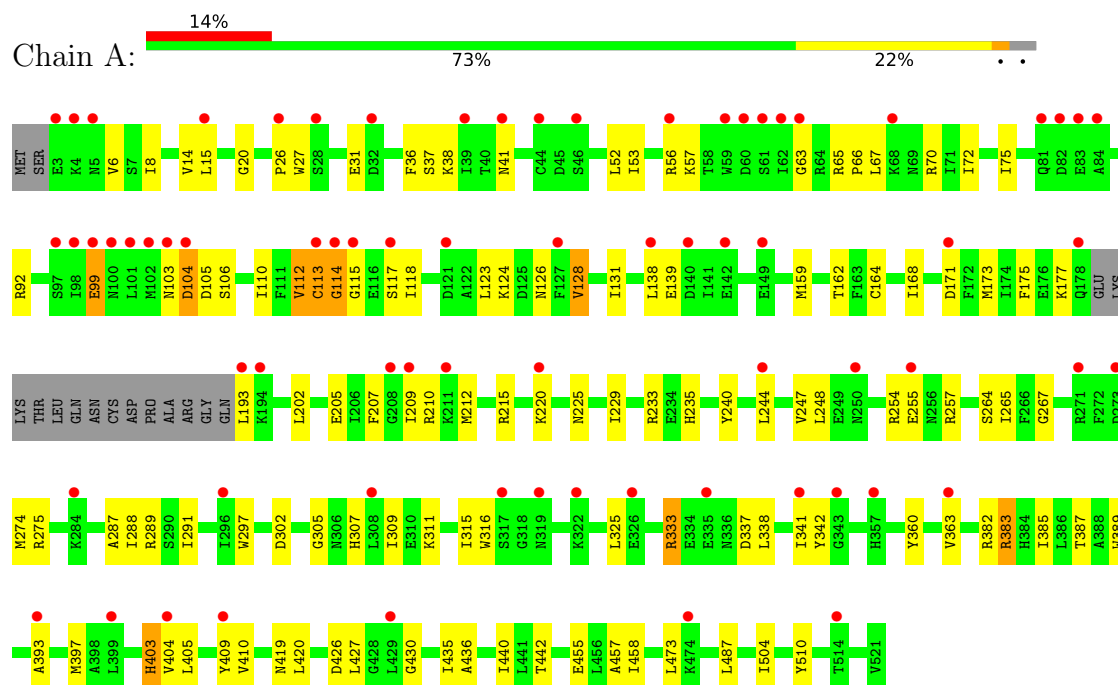
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	6	Total 6	O 6	0	0
5	D	1	Total 1	O 1	0	0
5	E	1	Total 1	O 1	0	0

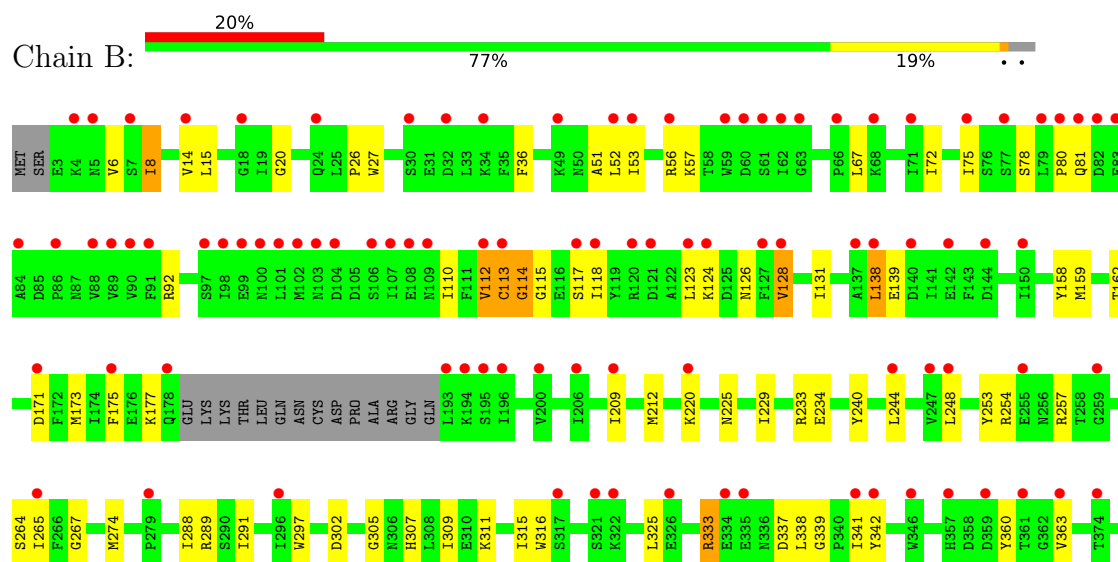
3 Residue-property plots [i](#)

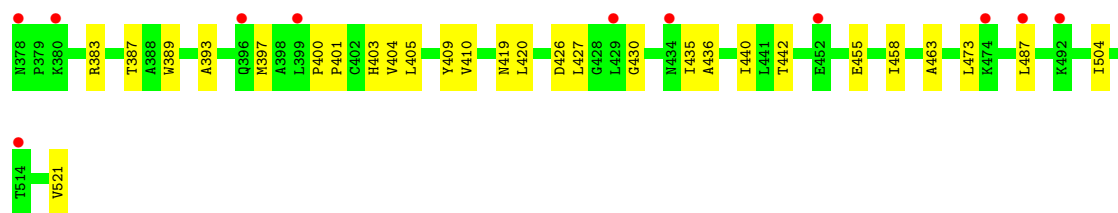
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

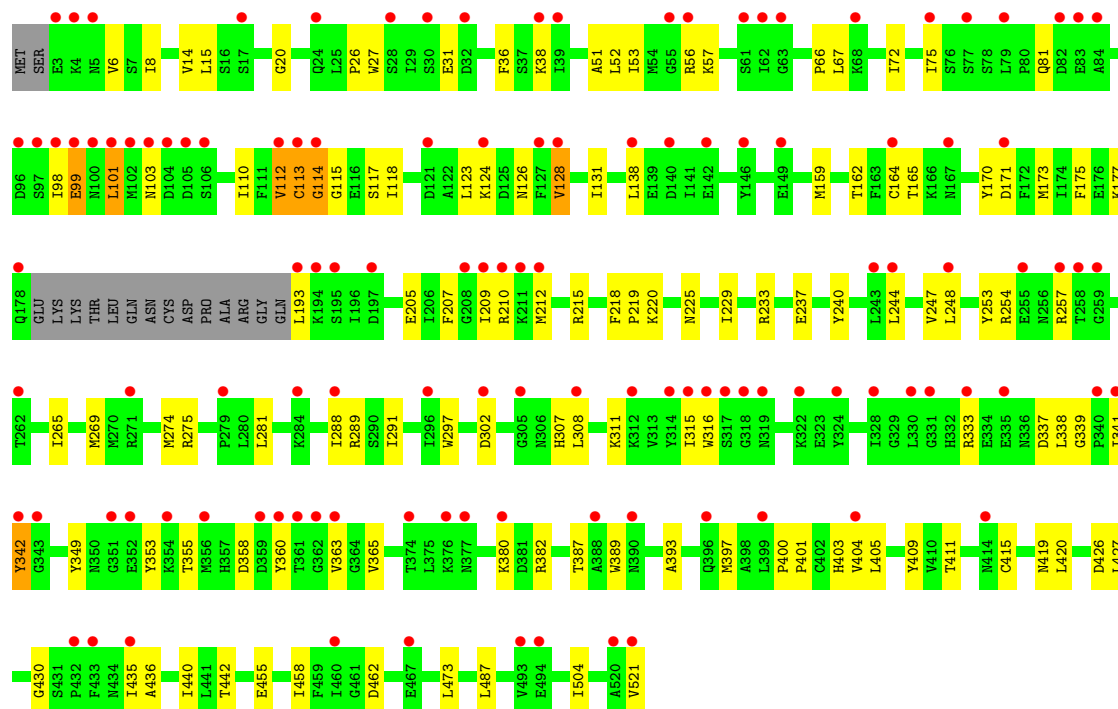
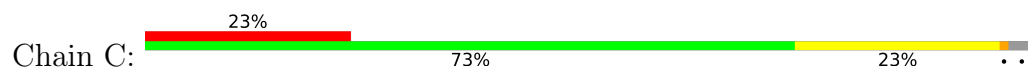


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

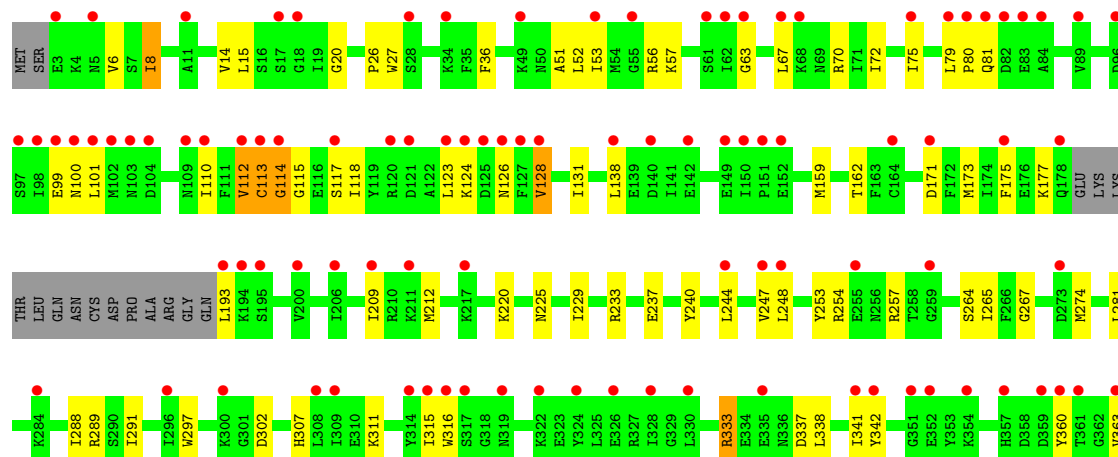
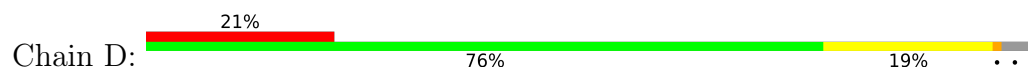


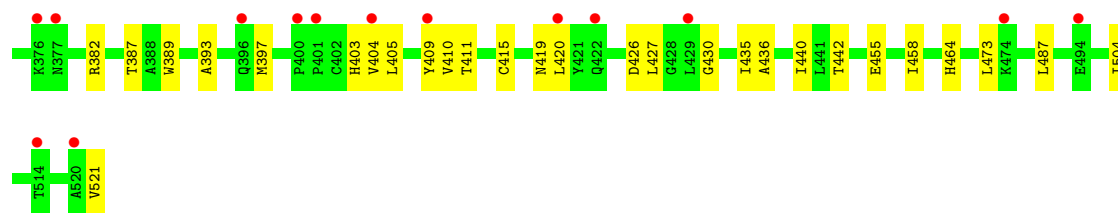


• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

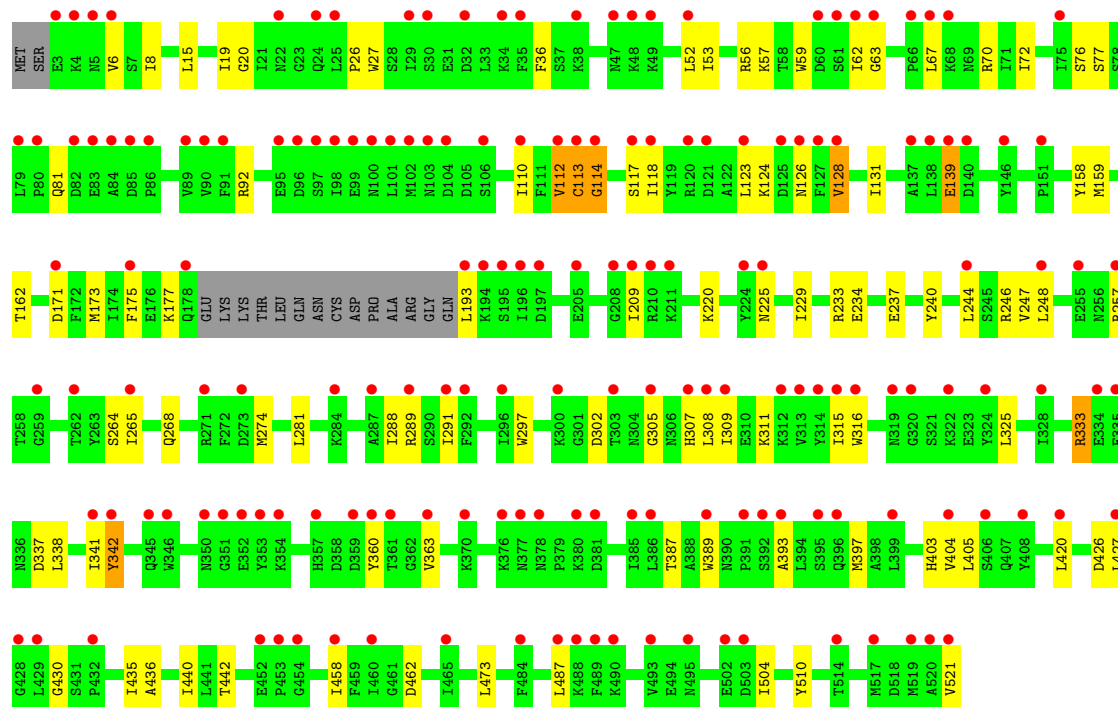
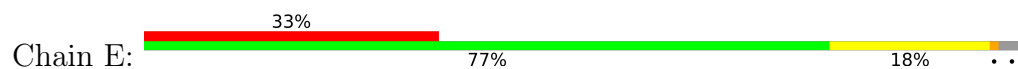


• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase





● 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	213.63Å 115.54Å 217.97Å 90.00° 94.56° 90.00°	Depositor
Resolution (Å)	48.05 – 2.78 48.05 – 2.78	Depositor EDS
% Data completeness (in resolution range)	93.2 (48.05-2.78) 89.0 (48.05-2.78)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.255 , 0.270 0.258 , 0.270	Depositor DCC
R_{free} test set	2017 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21154	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UFP, NDP, 2XB

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	0.42	3/4194 (0.1%)	0.78	8/5671 (0.1%)
1	B	0.37	3/4190 (0.1%)	0.78	10/5666 (0.2%)
1	C	0.38	1/4194 (0.0%)	0.76	7/5671 (0.1%)
1	D	0.35	1/4194 (0.0%)	0.75	6/5671 (0.1%)
1	E	0.32	1/4194 (0.0%)	0.76	6/5671 (0.1%)
All	All	0.37	9/20966 (0.0%)	0.76	37/28350 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	409	TYR	C-N	-6.45	1.25	1.33
1	D	114	GLY	C-N	6.23	1.42	1.33
1	A	114	GLY	C-N	6.22	1.42	1.33
1	E	114	GLY	C-N	6.22	1.42	1.33
1	C	114	GLY	C-N	6.21	1.42	1.33
1	B	114	GLY	C-N	6.17	1.42	1.33
1	A	403	HIS	CG-ND1	-5.70	1.31	1.38
1	B	410	VAL	C-N	-5.59	1.26	1.33
1	A	403	HIS	CA-C	-5.20	1.46	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	ARG	N-CA-C	8.31	123.60	112.88
1	B	410	VAL	O-C-N	-7.44	113.55	122.77
1	C	114	GLY	CA-C-N	-6.54	108.58	121.41
1	C	114	GLY	C-N-CA	-6.54	108.58	121.41
1	E	114	GLY	CA-C-N	-6.53	108.61	121.41
1	E	114	GLY	C-N-CA	-6.53	108.61	121.41
1	A	114	GLY	CA-C-N	-6.51	108.66	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	GLY	C-N-CA	-6.51	108.66	121.41
1	E	114	GLY	O-C-N	6.50	131.21	123.67
1	B	114	GLY	CA-C-N	-6.49	108.69	121.41
1	B	114	GLY	C-N-CA	-6.49	108.69	121.41
1	D	114	GLY	CA-C-N	-6.48	108.72	121.41
1	D	114	GLY	C-N-CA	-6.48	108.72	121.41
1	B	114	GLY	O-C-N	6.47	131.17	123.67
1	C	114	GLY	O-C-N	6.45	131.15	123.67
1	D	114	GLY	O-C-N	6.43	131.13	123.67
1	A	114	GLY	O-C-N	6.39	131.08	123.67
1	C	101	LEU	N-CA-C	6.11	118.02	111.36
1	B	409	TYR	O-C-N	-5.76	115.65	123.14
1	A	112	VAL	O-C-N	5.46	129.54	122.77
1	E	112	VAL	O-C-N	5.43	129.50	122.77
1	B	112	VAL	O-C-N	5.42	129.50	122.77
1	D	112	VAL	O-C-N	5.39	129.46	122.77
1	C	112	VAL	O-C-N	5.35	129.41	122.77
1	E	113	CYS	CA-C-N	-5.31	113.01	121.03
1	E	113	CYS	C-N-CA	-5.31	113.01	121.03
1	A	113	CYS	CA-C-N	-5.27	113.08	121.03
1	A	113	CYS	C-N-CA	-5.27	113.08	121.03
1	C	113	CYS	CA-C-N	-5.26	113.09	121.03
1	C	113	CYS	C-N-CA	-5.26	113.09	121.03
1	D	113	CYS	CA-C-N	-5.24	113.12	121.03
1	D	113	CYS	C-N-CA	-5.24	113.12	121.03
1	B	113	CYS	CA-C-N	-5.23	113.14	121.03
1	B	113	CYS	C-N-CA	-5.23	113.14	121.03
1	B	410	VAL	CA-C-N	5.18	130.80	121.06
1	B	410	VAL	C-N-CA	5.18	130.80	121.06
1	A	104	ASP	N-CA-C	5.06	118.60	111.52

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	4099	0	4021	104	0
1	B	4095	0	4017	82	0
1	C	4099	0	4021	100	0
1	D	4099	0	4021	86	0
1	E	4099	0	4021	82	0
2	A	48	0	26	12	0
2	B	48	0	26	12	0
2	C	48	0	26	12	0
2	D	48	0	26	12	0
2	E	48	0	26	9	0
3	A	21	0	10	3	0
3	B	21	0	10	3	0
3	C	21	0	10	3	0
3	D	21	0	10	3	0
3	E	21	0	10	2	0
4	A	60	0	34	6	0
4	B	60	0	34	6	0
4	C	60	0	34	6	0
4	D	60	0	34	6	0
4	E	60	0	34	5	0
5	A	8	0	0	2	0
5	B	2	0	0	0	0
5	C	6	0	0	2	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
All	All	21154	0	20451	431	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 10.

All (431) 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:E:139:GLU:HB2	1:E:510:TYR:CE1	1.44	1.51
1:E:139:GLU:HB2	1:E:510:TYR:CZ	1.68	1.29
1:B:254:ARG:CZ	1:D:409:TYR:OH	1.93	1.15
1:E:139:GLU:CB	1:E:510:TYR:CE1	2.28	1.15
1:B:254:ARG:NE	1:D:409:TYR:OH	1.95	0.98
1:B:254:ARG:HD2	1:B:264:SER:HB3	1.49	0.92
1:C:162:THR:HA	1:C:171:ASP:OD1	1.70	0.90
1:A:56:ARG:H	2:A:601:NDP:H4B	1.39	0.87
1:E:15:LEU:HD12	1:E:139:GLU:HG3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ARG:H	2:B:601:NDP:H4B	1.39	0.86
1:D:333:ARG:HH11	1:D:333:ARG:HG2	1.38	0.86
1:D:56:ARG:H	2:D:601:NDP:H4B	1.40	0.85
1:B:254:ARG:CZ	1:D:409:TYR:CZ	2.59	0.84
1:D:52:LEU:HD11	1:D:70:ARG:HD2	1.58	0.83
1:E:15:LEU:HB2	1:E:139:GLU:OE2	1.80	0.81
1:B:36:PHE:CE2	4:B:604:2XB:H9	2.17	0.80
1:E:36:PHE:CE2	4:E:604:2XB:H9	2.17	0.80
1:E:247:VAL:HA	1:E:265:ILE:HD12	1.64	0.78
1:B:254:ARG:HD2	1:B:264:SER:CB	2.13	0.78
1:A:36:PHE:CE2	4:A:604:2XB:H9	2.18	0.78
1:A:14:VAL:HG13	1:A:15:LEU:HG	1.65	0.78
1:A:15:LEU:HD11	1:A:510:TYR:HB3	1.65	0.77
1:E:113:CYS:O	4:E:604:2XB:H17	1.84	0.77
1:C:36:PHE:CE2	4:C:604:2XB:H9	2.19	0.77
1:B:113:CYS:O	4:B:604:2XB:H17	1.85	0.77
1:C:56:ARG:H	2:C:601:NDP:H4B	1.50	0.77
1:D:36:PHE:CE2	4:D:604:2XB:H9	2.20	0.76
1:A:409:TYR:OH	1:C:254:ARG:CZ	2.34	0.76
1:D:113:CYS:O	4:D:604:2XB:H17	1.87	0.75
1:A:56:ARG:N	2:A:601:NDP:H4B	2.02	0.74
1:C:113:CYS:O	4:C:604:2XB:H17	1.87	0.74
1:A:113:CYS:O	4:A:604:2XB:H17	1.88	0.74
1:C:56:ARG:N	2:C:601:NDP:H4B	2.03	0.73
1:B:56:ARG:N	2:B:601:NDP:H4B	2.02	0.73
1:B:57:LYS:HG3	2:B:601:NDP:H51A	1.72	0.71
1:D:56:ARG:N	2:D:601:NDP:H4B	2.03	0.71
1:D:57:LYS:HG3	2:D:601:NDP:H51A	1.72	0.71
1:A:57:LYS:HG3	2:A:601:NDP:H51A	1.72	0.71
1:C:57:LYS:HG3	2:C:601:NDP:H51A	1.71	0.70
1:D:333:ARG:HG2	1:D:333:ARG:NH1	1.99	0.70
1:E:8:ILE:HG12	1:E:112:VAL:HB	1.76	0.68
1:A:455:GLU:CD	1:C:212:MET:HE3	2.18	0.68
1:B:8:ILE:HG12	1:B:112:VAL:HB	1.76	0.68
1:B:56:ARG:HB3	2:B:601:NDP:O3B	1.94	0.68
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.75	0.68
1:C:8:ILE:HG12	1:C:112:VAL:HB	1.76	0.68
1:A:56:ARG:HB3	2:A:601:NDP:O3B	1.94	0.67
1:D:51:ALA:C	1:D:52:LEU:HD23	2.19	0.67
1:E:139:GLU:CB	1:E:510:TYR:CZ	2.63	0.67
1:D:411:THR:OG1	1:D:415:CYS:HB2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ARG:HB3	2:C:601:NDP:O3B	1.95	0.67
2:C:601:NDP:H42N	4:C:604:2XB:CAL	2.24	0.67
1:A:8:ILE:HG12	1:A:112:VAL:HB	1.76	0.67
1:B:162:THR:HA	1:B:171:ASP:OD1	1.95	0.67
1:D:247:VAL:HG22	1:D:265:ILE:HG12	1.75	0.67
1:D:8:ILE:HG12	1:D:112:VAL:HB	1.76	0.67
1:E:59:TRP:CE3	1:E:62:ILE:HD11	2.29	0.67
1:A:52:LEU:HD11	1:A:70:ARG:HD2	1.77	0.67
1:D:162:THR:HA	1:D:171:ASP:OD1	1.95	0.67
2:D:601:NDP:H42N	4:D:604:2XB:CAL	2.24	0.66
1:D:56:ARG:HB3	2:D:601:NDP:O3B	1.95	0.66
2:A:601:NDP:H42N	4:A:604:2XB:CAL	2.25	0.66
1:A:104:ASP:C	1:A:106:SER:H	2.03	0.66
1:A:205:GLU:OE1	1:C:38:LYS:NZ	2.29	0.66
2:D:601:NDP:H42N	4:D:604:2XB:CAZ	2.26	0.65
1:E:247:VAL:HA	1:E:265:ILE:CD1	2.26	0.65
1:D:253:TYR:HB3	1:E:63:GLY:HA2	1.78	0.65
1:C:253:TYR:HB3	1:D:63:GLY:HA2	1.76	0.65
2:C:601:NDP:H42N	4:C:604:2XB:CAZ	2.26	0.65
1:E:162:THR:HA	1:E:171:ASP:OD1	1.95	0.65
1:A:63:GLY:HA2	1:B:253:TYR:HB3	1.77	0.65
1:E:257:ARG:NE	3:E:602:UFP:O2P	2.28	0.65
2:A:601:NDP:H42N	4:A:604:2XB:CAZ	2.27	0.65
1:C:99:GLU:CD	1:C:103:ASN:HD21	2.05	0.65
1:D:244:LEU:HD11	1:D:473:LEU:HD13	1.79	0.65
1:D:333:ARG:HH11	1:D:333:ARG:CG	2.08	0.65
1:A:244:LEU:HD11	1:A:473:LEU:HD13	1.79	0.65
1:B:244:LEU:HD11	1:B:473:LEU:HD13	1.79	0.65
2:B:601:NDP:H42N	4:B:604:2XB:CAL	2.27	0.64
1:C:289:ARG:NH2	1:C:311:LYS:O	2.31	0.64
1:A:289:ARG:NH2	1:A:311:LYS:O	2.31	0.64
1:C:229:ILE:HG22	1:C:233:ARG:HG2	1.80	0.64
1:D:289:ARG:NH2	1:D:311:LYS:O	2.31	0.64
1:B:289:ARG:NH2	1:B:311:LYS:O	2.31	0.64
1:B:333:ARG:HH11	1:B:333:ARG:HG2	1.63	0.64
1:E:289:ARG:NH2	1:E:311:LYS:O	2.31	0.64
1:C:269:MET:HE3	5:C:702:HOH:O	1.97	0.64
1:E:229:ILE:HG22	1:E:233:ARG:HG2	1.80	0.64
1:E:333:ARG:NH1	1:E:333:ARG:HG2	2.10	0.64
1:E:244:LEU:HD11	1:E:473:LEU:HD13	1.79	0.64
1:B:333:ARG:HG2	1:B:333:ARG:NH1	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:NDP:H42N	4:B:604:2XB:CAZ	2.28	0.63
1:C:244:LEU:HD11	1:C:473:LEU:HD13	1.79	0.63
1:D:53:ILE:O	1:D:113:CYS:HB2	1.99	0.63
1:D:229:ILE:HG22	1:D:233:ARG:HG2	1.80	0.63
1:A:410:VAL:O	1:C:254:ARG:NH2	2.25	0.63
1:C:257:ARG:NE	3:C:602:UFP:O2P	2.30	0.62
1:C:247:VAL:HG22	1:C:265:ILE:HG12	1.79	0.62
1:B:229:ILE:HG22	1:B:233:ARG:HG2	1.80	0.62
1:A:275:ARG:HD2	1:C:215:ARG:NH1	2.14	0.62
1:B:225:ASN:O	1:B:233:ARG:NH2	2.33	0.62
1:A:225:ASN:O	1:A:233:ARG:NH2	2.33	0.62
1:A:409:TYR:OH	1:C:254:ARG:NE	2.33	0.62
1:C:225:ASN:O	1:C:233:ARG:NH2	2.33	0.62
1:A:53:ILE:O	1:A:113:CYS:HB2	1.99	0.62
1:B:254:ARG:NH1	1:D:409:TYR:CE1	2.68	0.62
1:B:53:ILE:O	1:B:113:CYS:HB2	2.00	0.62
1:A:229:ILE:HG22	1:A:233:ARG:HG2	1.80	0.61
3:B:602:UFP:O1P	1:D:382:ARG:NE	2.32	0.61
1:E:53:ILE:O	1:E:113:CYS:HB2	2.00	0.61
1:D:225:ASN:O	1:D:233:ARG:NH2	2.33	0.61
1:B:333:ARG:HH11	1:B:333:ARG:CG	2.12	0.61
1:E:225:ASN:O	1:E:233:ARG:NH2	2.33	0.61
1:C:53:ILE:O	1:C:113:CYS:HB2	1.99	0.61
1:E:139:GLU:N	1:E:510:TYR:OH	2.33	0.61
1:A:56:ARG:H	2:A:601:NDP:C4B	2.12	0.61
1:E:15:LEU:CD1	1:E:139:GLU:HG3	2.29	0.60
1:A:409:TYR:CZ	1:C:254:ARG:CZ	2.84	0.60
1:B:56:ARG:H	2:B:601:NDP:C4B	2.12	0.60
1:B:341:ILE:HA	1:B:397:MET:HE3	1.84	0.60
1:A:104:ASP:O	1:A:106:SER:N	2.35	0.59
1:E:341:ILE:HA	1:E:397:MET:HE3	1.84	0.59
3:A:602:UFP:O1P	1:C:382:ARG:NE	2.35	0.59
1:B:254:ARG:NH1	1:D:409:TYR:CZ	2.71	0.59
1:D:56:ARG:H	2:D:601:NDP:C4B	2.13	0.59
1:E:15:LEU:HD12	1:E:139:GLU:CG	2.31	0.59
1:A:403:HIS:HB2	1:A:420:LEU:HD11	1.85	0.58
1:C:341:ILE:HA	1:C:397:MET:HE3	1.84	0.58
1:D:117:SER:OG	2:D:601:NDP:O1A	2.21	0.58
1:D:341:ILE:HA	1:D:397:MET:HE3	1.84	0.58
1:E:333:ARG:HG2	1:E:333:ARG:HH11	1.68	0.58
1:A:341:ILE:HA	1:A:397:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ASN:OD1	1:C:177:LYS:NZ	2.36	0.58
1:C:98:ILE:HG22	1:C:101:LEU:HD13	1.86	0.58
1:A:212:MET:HE3	1:C:455:GLU:CD	2.28	0.58
1:C:409:TYR:HA	5:C:706:HOH:O	2.02	0.58
1:A:75:ILE:O	2:A:601:NDP:H1B	2.04	0.57
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.85	0.57
1:E:333:ARG:HG3	1:E:337:ASP:HB3	1.86	0.57
1:C:117:SER:OG	2:C:601:NDP:O1A	2.21	0.57
1:E:333:ARG:HH11	1:E:333:ARG:CG	2.17	0.57
1:A:117:SER:OG	2:A:601:NDP:O1A	2.22	0.57
1:B:75:ILE:O	2:B:601:NDP:H1B	2.04	0.57
1:E:126:ASN:OD1	1:E:177:LYS:NZ	2.36	0.57
1:A:126:ASN:OD1	1:A:177:LYS:NZ	2.36	0.57
1:D:114:GLY:O	1:D:118:ILE:HB	2.05	0.57
1:C:56:ARG:HB3	2:C:601:NDP:H4B	1.87	0.56
1:C:114:GLY:O	1:C:118:ILE:HB	2.06	0.56
1:D:75:ILE:O	2:D:601:NDP:H1B	2.05	0.56
1:C:98:ILE:CG2	1:C:101:LEU:HD13	2.35	0.56
1:D:56:ARG:HB3	2:D:601:NDP:H4B	1.87	0.56
1:C:75:ILE:O	2:C:601:NDP:H1B	2.05	0.56
1:A:56:ARG:HB3	2:A:601:NDP:H4B	1.88	0.56
1:A:382:ARG:NE	3:C:602:UFP:O1P	2.39	0.56
1:B:114:GLY:O	1:B:118:ILE:HB	2.06	0.56
1:B:288:ILE:HD11	1:B:440:ILE:HD11	1.88	0.55
1:A:114:GLY:O	1:A:118:ILE:HB	2.06	0.55
1:E:288:ILE:HD11	1:E:440:ILE:HD11	1.89	0.55
1:C:247:VAL:HG22	1:C:265:ILE:CD1	2.37	0.55
1:D:288:ILE:HD11	1:D:440:ILE:HD11	1.88	0.55
1:B:56:ARG:HB3	2:B:601:NDP:H4B	1.87	0.55
1:A:274:MET:HE1	1:A:442:THR:HG21	1.89	0.55
1:C:288:ILE:HD11	1:C:440:ILE:HD11	1.88	0.54
1:C:240:TYR:OH	1:C:427:LEU:O	2.25	0.54
1:D:126:ASN:OD1	1:D:177:LYS:NZ	2.36	0.54
1:A:267:GLY:HA2	1:C:419:ASN:HD21	1.72	0.54
1:E:114:GLY:O	1:E:118:ILE:HB	2.06	0.54
1:A:288:ILE:HD11	1:A:440:ILE:HD11	1.89	0.54
1:B:419:ASN:HD21	1:D:267:GLY:HA2	1.73	0.54
1:D:302:ASP:OD2	1:D:307:HIS:ND1	2.40	0.54
1:C:274:MET:HE1	1:C:442:THR:HG21	1.89	0.54
1:E:274:MET:HE1	1:E:442:THR:HG21	1.89	0.54
1:B:389:TRP:HB2	1:B:404:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:MET:HE1	1:D:442:THR:HG21	1.89	0.53
1:B:274:MET:HE1	1:B:442:THR:HG21	1.89	0.53
1:A:99:GLU:O	1:A:103:ASN:OD1	2.26	0.53
1:B:56:ARG:CB	2:B:601:NDP:H4B	2.39	0.53
1:B:240:TYR:OH	1:B:427:LEU:O	2.25	0.53
1:B:267:GLY:HA2	1:D:419:ASN:HD21	1.74	0.53
1:A:240:TYR:OH	1:A:427:LEU:O	2.25	0.53
1:E:302:ASP:OD2	1:E:307:HIS:ND1	2.40	0.53
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.90	0.53
1:A:257:ARG:NE	3:A:602:UFP:O2P	2.41	0.53
1:A:302:ASP:OD2	1:A:307:HIS:ND1	2.41	0.53
1:D:389:TRP:HB2	1:D:404:VAL:HG13	1.90	0.53
1:C:56:ARG:CB	2:C:601:NDP:H4B	2.39	0.53
1:D:56:ARG:CB	2:D:601:NDP:H4B	2.39	0.53
1:B:126:ASN:OD1	1:B:177:LYS:NZ	2.36	0.53
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.90	0.52
1:A:56:ARG:CB	2:A:601:NDP:H4B	2.39	0.52
1:A:104:ASP:C	1:A:106:SER:N	2.67	0.52
1:A:409:TYR:CE1	1:C:254:ARG:NH1	2.78	0.52
1:B:455:GLU:CD	1:D:212:MET:HE3	2.34	0.52
1:D:247:VAL:HG22	1:D:265:ILE:CD1	2.39	0.52
1:A:207:PHE:CE1	1:C:31:GLU:HG2	2.45	0.52
1:C:389:TRP:HB2	1:C:404:VAL:HG13	1.90	0.52
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.92	0.52
1:E:240:TYR:OH	1:E:427:LEU:O	2.25	0.52
1:A:382:ARG:HG2	1:C:462:ASP:OD2	2.10	0.52
1:C:56:ARG:H	2:C:601:NDP:C4B	2.21	0.52
1:D:99:GLU:O	1:D:101:LEU:N	2.43	0.52
1:A:210:ARG:NH2	1:C:164:CYS:O	2.43	0.51
1:A:275:ARG:HD2	1:C:215:ARG:CZ	2.40	0.51
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.92	0.51
1:E:77:SER:HB3	2:E:601:NDP:H2A	1.92	0.51
1:B:257:ARG:HH11	3:B:602:UFP:H5'2	1.76	0.51
1:C:302:ASP:OD2	1:C:307:HIS:ND1	2.41	0.51
4:D:604:2XB:OXT	4:D:604:2XB:H2	2.10	0.51
1:C:411:THR:OG1	1:C:415:CYS:HB2	2.11	0.51
1:B:26:PRO:HG2	1:B:27:TRP:CE3	2.46	0.51
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.46	0.51
1:D:123:LEU:HD23	1:D:128:VAL:HG11	1.93	0.51
4:E:604:2XB:OXT	4:E:604:2XB:H2	2.10	0.51
1:B:123:LEU:HD23	1:B:128:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ILE:HB	1:C:175:PHE:HB2	1.92	0.51
1:E:26:PRO:HG2	1:E:27:TRP:CE3	2.46	0.50
4:B:604:2XB:OXT	4:B:604:2XB:H2	2.10	0.50
1:E:257:ARG:HH11	3:E:602:UFP:H5'2	1.75	0.50
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.92	0.50
1:A:342:TYR:CD2	1:A:403:HIS:CE1	2.99	0.50
1:C:26:PRO:HG2	1:C:27:TRP:CE3	2.46	0.50
1:A:215:ARG:NH1	1:C:275:ARG:HD2	2.26	0.50
4:C:604:2XB:OXT	4:C:604:2XB:H2	2.10	0.50
4:A:604:2XB:OXT	4:A:604:2XB:H2	2.10	0.50
1:C:165:THR:OG1	1:C:170:TYR:OH	2.22	0.50
1:B:138:LEU:O	1:B:139:GLU:HG2	2.12	0.50
1:D:240:TYR:OH	1:D:427:LEU:O	2.25	0.50
1:E:56:ARG:HB3	2:E:601:NDP:H4B	1.94	0.50
1:E:123:LEU:HD23	1:E:128:VAL:HG11	1.93	0.50
1:A:342:TYR:CE2	1:A:403:HIS:CE1	3.00	0.50
1:B:302:ASP:OD2	1:B:307:HIS:ND1	2.40	0.50
1:A:341:ILE:O	1:A:342:TYR:C	2.54	0.50
1:A:123:LEU:HD23	1:A:128:VAL:HG11	1.93	0.50
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.92	0.50
1:C:341:ILE:O	1:C:342:TYR:C	2.53	0.50
1:D:247:VAL:HG22	1:D:265:ILE:CG1	2.41	0.49
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.94	0.49
1:A:138:LEU:O	1:A:139:GLU:HG2	2.12	0.49
1:B:212:MET:HE3	1:D:455:GLU:CD	2.38	0.49
1:A:31:GLU:HG2	1:C:207:PHE:CE1	2.48	0.49
1:A:409:TYR:CZ	1:C:254:ARG:NH1	2.80	0.49
1:E:6:VAL:HG22	1:E:110:ILE:HB	1.95	0.49
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.46	0.49
1:A:419:ASN:ND2	1:A:457:ALA:HB3	2.28	0.49
1:E:342:TYR:CD2	1:E:403:HIS:CE1	3.00	0.49
1:A:247:VAL:HG22	1:A:265:ILE:HG12	1.95	0.48
1:B:36:PHE:CE2	4:B:604:2XB:CAK	2.94	0.48
1:C:247:VAL:HG22	1:C:265:ILE:CG1	2.42	0.48
1:E:333:ARG:HA	1:E:333:ARG:HD3	1.66	0.48
1:A:6:VAL:HG22	1:A:110:ILE:HB	1.96	0.48
1:D:6:VAL:HG22	1:D:110:ILE:HB	1.95	0.48
1:D:257:ARG:NE	3:D:602:UFP:O2P	2.45	0.48
1:E:297:TRP:HH2	1:E:338:LEU:HD12	1.79	0.48
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.79	0.48
1:D:257:ARG:NH2	1:D:521:VAL:OXT	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:HB2	1:A:103:ASN:HD21	1.78	0.48
1:A:247:VAL:HG22	1:A:265:ILE:CD1	2.44	0.48
1:B:297:TRP:HH2	1:B:338:LEU:HD12	1.79	0.48
1:C:6:VAL:HG22	1:C:110:ILE:HB	1.95	0.48
1:C:123:LEU:HD23	1:C:128:VAL:HG11	1.93	0.48
1:E:36:PHE:CE2	4:E:604:2XB:CAK	2.94	0.48
1:E:56:ARG:NH1	2:E:601:NDP:O1X	2.47	0.48
1:C:115:GLY:HA2	2:C:601:NDP:O2A	2.14	0.48
1:D:297:TRP:HH2	1:D:338:LEU:HD12	1.79	0.47
1:A:115:GLY:HA2	2:A:601:NDP:O2A	2.14	0.47
1:B:117:SER:OG	2:B:601:NDP:O1A	2.24	0.47
1:B:6:VAL:HG22	1:B:110:ILE:HB	1.95	0.47
1:B:51:ALA:C	1:B:52:LEU:HD23	2.39	0.47
1:B:403:HIS:HB2	1:B:420:LEU:HD11	1.97	0.47
1:D:403:HIS:HB2	1:D:420:LEU:HD11	1.97	0.47
1:E:67:LEU:HG	1:E:72:ILE:HD11	1.97	0.47
1:B:257:ARG:NE	3:B:602:UFP:O2P	2.47	0.47
1:C:337:ASP:OD1	1:C:353:TYR:OH	2.24	0.47
1:C:355:THR:OG1	1:C:358:ASP:OD2	2.32	0.47
1:A:255:GLU:HG2	1:C:380:LYS:HD2	1.97	0.47
1:C:339:GLY:O	1:C:341:ILE:N	2.44	0.46
1:E:52:LEU:HD11	1:E:70:ARG:HD2	1.97	0.46
1:A:67:LEU:HG	1:A:72:ILE:HD11	1.97	0.46
1:D:115:GLY:HA2	2:D:601:NDP:O2A	2.15	0.46
1:E:20:GLY:HA2	1:E:26:PRO:HD3	1.97	0.46
1:A:37:SER:O	1:A:41:ASN:ND2	2.48	0.46
1:B:115:GLY:HA2	2:B:601:NDP:O2A	2.14	0.46
1:C:67:LEU:HG	1:C:72:ILE:HD11	1.97	0.46
1:D:387:THR:HB	1:D:405:LEU:HD12	1.98	0.46
1:E:325:LEU:HD13	1:E:333:ARG:HB3	1.97	0.46
1:A:455:GLU:OE1	1:C:212:MET:HE3	2.15	0.46
1:C:297:TRP:CH2	1:C:341:ILE:HD11	2.51	0.46
1:E:92:ARG:HD3	1:E:92:ARG:HA	1.64	0.46
1:E:291:ILE:HD13	1:E:436:ALA:HB3	1.98	0.46
1:A:20:GLY:HA2	1:A:26:PRO:HD3	1.98	0.46
1:E:257:ARG:NH2	1:E:521:VAL:OXT	2.42	0.46
1:A:164:CYS:O	1:C:210:ARG:NH2	2.49	0.46
1:B:67:LEU:HG	1:B:72:ILE:HD11	1.97	0.46
1:C:403:HIS:HB2	1:C:420:LEU:HD11	1.97	0.46
1:D:341:ILE:O	1:D:342:TYR:C	2.57	0.46
1:B:387:THR:HB	1:B:405:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ILE:HD13	1:D:436:ALA:HB3	1.98	0.46
1:A:215:ARG:CZ	1:C:275:ARG:HD2	2.46	0.46
1:D:14:VAL:HG13	1:D:15:LEU:HG	1.98	0.46
1:D:67:LEU:HG	1:D:72:ILE:HD11	1.97	0.46
1:B:14:VAL:HG13	1:B:15:LEU:HG	1.99	0.45
1:C:291:ILE:HD13	1:C:436:ALA:HB3	1.98	0.45
1:A:325:LEU:HD13	1:A:333:ARG:HB3	1.99	0.45
1:A:387:THR:HB	1:A:405:LEU:HD12	1.98	0.45
1:C:387:THR:HB	1:C:405:LEU:HD12	1.98	0.45
1:A:162:THR:HA	1:A:171:ASP:OD1	2.17	0.45
1:A:291:ILE:HD13	1:A:436:ALA:HB3	1.98	0.45
1:B:291:ILE:HD13	1:B:436:ALA:HB3	1.98	0.45
1:B:297:TRP:CH2	1:B:341:ILE:HD11	2.51	0.45
1:D:333:ARG:HA	1:D:333:ARG:HD3	1.68	0.45
1:D:52:LEU:HD23	1:D:52:LEU:N	2.30	0.45
1:B:257:ARG:NH2	1:B:521:VAL:OXT	2.42	0.45
1:C:14:VAL:HG13	1:C:15:LEU:HG	1.99	0.45
1:C:20:GLY:HA2	1:C:26:PRO:HD3	1.98	0.45
1:C:36:PHE:CE2	4:C:604:2XB:CAK	2.98	0.45
1:D:342:TYR:CD2	1:D:403:HIS:CE1	3.05	0.45
1:E:403:HIS:HB2	1:E:420:LEU:HD11	1.97	0.45
1:E:387:THR:HB	1:E:405:LEU:HD12	1.98	0.45
1:B:265:ILE:HG13	1:B:463:ALA:HB3	1.98	0.45
1:D:20:GLY:HA2	1:D:26:PRO:HD3	1.98	0.45
1:E:159:MET:HA	1:E:173:MET:HG2	2.00	0.44
1:B:20:GLY:HA2	1:B:26:PRO:HD3	1.98	0.44
1:B:254:ARG:NH2	1:D:410:VAL:O	2.42	0.44
1:C:257:ARG:HH11	3:C:602:UFP:H5'2	1.82	0.44
1:B:159:MET:HA	1:B:173:MET:HG2	2.00	0.44
1:A:63:GLY:O	1:A:65:ARG:HG3	2.17	0.44
1:A:92:ARG:HA	1:A:92:ARG:HD3	1.64	0.44
1:B:325:LEU:HD13	1:B:333:ARG:HB3	1.99	0.44
2:E:601:NDP:H52N	2:E:601:NDP:H6N	1.99	0.44
1:B:487:LEU:HD11	1:B:504:ILE:HG23	2.00	0.44
1:A:159:MET:HA	1:A:173:MET:HG2	2.00	0.44
1:A:487:LEU:HD11	1:A:504:ILE:HG23	2.00	0.44
1:C:51:ALA:C	1:C:52:LEU:HD23	2.43	0.44
1:C:257:ARG:NH2	1:C:521:VAL:OXT	2.42	0.43
1:E:487:LEU:HD11	1:E:504:ILE:HG23	2.00	0.43
1:C:487:LEU:HD11	1:C:504:ILE:HG23	2.00	0.43
1:D:159:MET:HA	1:D:173:MET:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:O	1:A:248:LEU:HB2	2.19	0.43
1:B:254:ARG:NH2	1:D:409:TYR:CZ	2.86	0.43
1:C:338:LEU:N	1:C:338:LEU:CD1	2.82	0.43
1:E:57:LYS:HB2	2:E:601:NDP:O3	2.19	0.43
1:B:244:LEU:O	1:B:248:LEU:HB2	2.19	0.43
1:B:341:ILE:O	1:B:342:TYR:C	2.62	0.43
1:C:159:MET:HA	1:C:173:MET:HG2	2.00	0.43
1:D:487:LEU:HD11	1:D:504:ILE:HG23	2.00	0.43
1:E:76:SER:HA	2:E:601:NDP:H1B	2.00	0.43
1:E:81:GLN:OE1	1:E:92:ARG:NH2	2.51	0.43
1:A:36:PHE:CE2	4:A:604:2XB:CAK	2.96	0.43
1:D:257:ARG:HH11	3:D:602:UFP:H5'2	1.84	0.43
1:E:19:ILE:HB	2:E:601:NDP:N7N	2.34	0.43
1:E:246:ARG:NH1	1:E:268:GLN:OE1	2.38	0.43
1:A:287:ALA:HB1	5:A:706:HOH:O	2.19	0.43
1:E:117:SER:OG	2:E:601:NDP:O1A	2.34	0.43
1:C:393:ALA:O	1:C:397:MET:HG3	2.19	0.42
1:E:308:LEU:HD12	1:E:308:LEU:HA	1.91	0.42
1:C:435:ILE:HG12	1:C:458:ILE:HD12	2.02	0.42
1:D:244:LEU:O	1:D:248:LEU:HB2	2.19	0.42
1:D:435:ILE:HG12	1:D:458:ILE:HD12	2.01	0.42
1:A:305:GLY:CA	5:A:708:HOH:O	2.66	0.42
1:D:36:PHE:CE2	4:D:604:2XB:CAK	2.98	0.42
1:B:333:ARG:HA	1:B:333:ARG:HD3	1.71	0.42
1:A:297:TRP:CH2	1:A:341:ILE:HD11	2.55	0.42
1:E:244:LEU:O	1:E:248:LEU:HB2	2.19	0.42
1:B:78:SER:O	1:B:80:PRO:HD3	2.19	0.42
1:B:393:ALA:O	1:B:397:MET:HG3	2.19	0.42
1:D:99:GLU:C	1:D:101:LEU:N	2.78	0.42
1:D:254:ARG:HD2	1:D:264:SER:HB3	2.02	0.42
1:D:393:ALA:O	1:D:397:MET:HG3	2.19	0.42
1:E:15:LEU:CB	1:E:139:GLU:OE2	2.61	0.42
1:B:81:GLN:NE2	1:B:92:ARG:HH21	2.17	0.42
1:B:339:GLY:O	1:B:341:ILE:N	2.43	0.42
1:E:139:GLU:CB	1:E:510:TYR:CD1	2.98	0.42
1:E:393:ALA:O	1:E:397:MET:HG3	2.19	0.42
1:A:257:ARG:HH11	3:A:602:UFP:H5'2	1.84	0.42
1:A:393:ALA:O	1:A:397:MET:HG3	2.19	0.42
1:E:297:TRP:CH2	1:E:341:ILE:HD11	2.55	0.42
1:E:341:ILE:O	1:E:342:TYR:C	2.62	0.42
1:A:333:ARG:HA	1:A:333:ARG:HD3	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:HG3	1:A:337:ASP:HB3	2.01	0.41
1:C:244:LEU:O	1:C:248:LEU:HB2	2.19	0.41
1:E:435:ILE:HG12	1:E:458:ILE:HD12	2.01	0.41
1:A:435:ILE:HG12	1:A:458:ILE:HD12	2.02	0.41
1:B:360:TYR:O	1:B:363:VAL:HG22	2.20	0.41
1:C:400:PRO:HA	1:C:401:PRO:HD3	1.92	0.41
1:E:360:TYR:O	1:E:363:VAL:HG22	2.20	0.41
1:E:426:ASP:HB3	1:E:430:GLY:H	1.85	0.41
1:D:360:TYR:O	1:D:363:VAL:HG22	2.20	0.41
1:A:426:ASP:HB3	1:A:430:GLY:H	1.85	0.41
1:B:315:ILE:HG13	1:B:316:TRP:CD1	2.56	0.41
1:B:400:PRO:HA	1:B:401:PRO:HD3	1.92	0.41
1:A:138:LEU:HD11	1:A:168:ILE:HD13	2.03	0.41
1:A:171:ASP:OD2	1:A:235:HIS:HD2	2.03	0.41
1:B:158:TYR:OH	1:B:234:GLU:OE2	2.33	0.41
1:D:297:TRP:CH2	1:D:341:ILE:HD11	2.55	0.41
1:D:426:ASP:HB3	1:D:430:GLY:H	1.85	0.41
1:E:315:ILE:HG13	1:E:316:TRP:CD1	2.56	0.41
1:C:315:ILE:HG13	1:C:316:TRP:CD1	2.56	0.41
1:A:383:ARG:O	1:A:385:ILE:N	2.54	0.41
1:C:360:TYR:O	1:C:363:VAL:HG22	2.20	0.41
1:D:79:LEU:HA	1:D:80:PRO:HD3	1.85	0.41
1:D:315:ILE:HG13	1:D:316:TRP:CD1	2.56	0.41
2:E:601:NDP:H42N	4:E:604:2XB:CAO	2.51	0.41
1:A:254:ARG:HD2	1:A:264:SER:HB3	2.03	0.41
1:B:426:ASP:HB3	1:B:430:GLY:H	1.86	0.41
1:B:435:ILE:HG12	1:B:458:ILE:HD12	2.01	0.41
1:C:338:LEU:HD23	1:C:341:ILE:HD13	2.03	0.41
1:C:426:ASP:HB3	1:C:430:GLY:H	1.85	0.41
1:E:139:GLU:N	1:E:510:TYR:CZ	2.89	0.41
1:A:38:LYS:NZ	1:C:205:GLU:OE1	2.54	0.41
1:A:315:ILE:HG13	1:A:316:TRP:CD1	2.56	0.41
1:A:360:TYR:O	1:A:363:VAL:HG22	2.20	0.41
1:E:158:TYR:OH	1:E:234:GLU:OE2	2.33	0.41
1:C:66:PRO:HA	1:C:72:ILE:HD12	2.04	0.40
1:C:237:GLU:HG3	1:C:281:LEU:HD22	2.03	0.40
1:A:305:GLY:O	1:A:309:ILE:HG13	2.22	0.40
1:A:341:ILE:O	1:A:342:TYR:O	2.40	0.40
1:B:305:GLY:O	1:B:309:ILE:HG13	2.22	0.40
1:A:66:PRO:HA	1:A:72:ILE:HD12	2.04	0.40
1:E:264:SER:OG	1:E:462:ASP:OD1	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:GLY:O	1:E:309:ILE:HG13	2.22	0.40
1:C:218:PHE:HA	1:C:219:PRO:HD3	1.95	0.40
1:C:349:TYR:HB3	1:C:365:VAL:HB	2.04	0.40
1:D:237:GLU:HG3	1:D:281:LEU:HD22	2.03	0.40
1:D:464:HIS:CE1	3:D:602:UFP:O3'	2.74	0.40
1:E:126:ASN:HD21	1:E:177:LYS:HE3	1.86	0.40
1:E:237:GLU:HG3	1:E:281:LEU:HD22	2.03	0.40
1:A:202:LEU:HD13	1:C:38:LYS:HB3	2.03	0.40
1:B:254:ARG:CD	1:D:409:TYR:OH	2.68	0.40
1:C:126:ASN:HD21	1:C:177:LYS:HE3	1.86	0.40
1:C:308:LEU:HD12	1:C:308:LEU:HA	1.91	0.40
1:E:139:GLU:CG	1:E:510:TYR:CD1	3.05	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	501/521 (96%)	473 (94%)	27 (5%)	1 (0%)	43	70
1	B	501/521 (96%)	472 (94%)	29 (6%)	0	100	100
1	C	501/521 (96%)	473 (94%)	28 (6%)	0	100	100
1	D	501/521 (96%)	469 (94%)	31 (6%)	1 (0%)	43	70
1	E	501/521 (96%)	474 (95%)	27 (5%)	0	100	100
All	All	2505/2605 (96%)	2361 (94%)	142 (6%)	2 (0%)	48	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	ASP
1	D	100	ASN

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	452/470 (96%)	445 (98%)	7 (2%)	57	81
1	B	451/470 (96%)	443 (98%)	8 (2%)	51	79
1	C	452/470 (96%)	443 (98%)	9 (2%)	48	77
1	D	452/470 (96%)	443 (98%)	9 (2%)	48	77
1	E	452/470 (96%)	444 (98%)	8 (2%)	51	79
All	All	2259/2350 (96%)	2218 (98%)	41 (2%)	51	79

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	GLU
1	A	124	LYS
1	A	128	VAL
1	A	193	LEU
1	A	209	ILE
1	A	220	LYS
1	A	333	ARG
1	B	8	ILE
1	B	124	LYS
1	B	128	VAL
1	B	138	LEU
1	B	209	ILE
1	B	220	LYS
1	B	333	ARG
1	B	383	ARG
1	C	81	GLN
1	C	99	GLU
1	C	124	LYS
1	C	128	VAL
1	C	138	LEU
1	C	193	LEU
1	C	209	ILE
1	C	220	LYS

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Mol	Chain	Res	Type
1	C	342	TYR
1	D	8	ILE
1	D	81	GLN
1	D	124	LYS
1	D	128	VAL
1	D	138	LEU
1	D	193	LEU
1	D	209	ILE
1	D	220	LYS
1	D	333	ARG
1	E	124	LYS
1	E	128	VAL
1	E	139	GLU
1	E	193	LEU
1	E	209	ILE
1	E	220	LYS
1	E	333	ARG
1	E	342	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	24	GLN
1	A	486	GLN
1	B	5	ASN
1	B	24	GLN
1	B	486	GLN
1	C	5	ASN
1	C	486	GLN
1	D	5	ASN
1	D	24	GLN
1	D	486	GLN
1	E	5	ASN
1	E	24	GLN
1	E	486	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	2XB	D	603	-	32,32,32	2.01	5 (15%)	40,45,45	2.45	13 (32%)
4	2XB	C	603	-	32,32,32	2.02	5 (15%)	40,45,45	2.46	13 (32%)
3	UFP	C	602	-	22,22,22	1.09	0	32,33,33	2.52	9 (28%)
4	2XB	B	604	-	32,32,32	2.04	6 (18%)	40,45,45	2.52	13 (32%)
2	NDP	C	601	-	51,52,52	1.93	12 (23%)	71,80,80	1.62	13 (18%)
4	2XB	E	604	-	32,32,32	2.05	6 (18%)	40,45,45	2.51	13 (32%)
4	2XB	C	604	-	32,32,32	2.05	6 (18%)	40,45,45	2.52	13 (32%)
2	NDP	B	601	-	51,52,52	1.93	12 (23%)	71,80,80	1.62	13 (18%)
4	2XB	D	604	-	32,32,32	2.04	6 (18%)	40,45,45	2.52	13 (32%)
2	NDP	E	601	-	51,52,52	1.94	12 (23%)	71,80,80	1.56	12 (16%)
4	2XB	A	604	-	32,32,32	2.04	6 (18%)	40,45,45	2.52	13 (32%)
4	2XB	E	603	-	32,32,32	2.02	5 (15%)	40,45,45	2.46	14 (35%)
4	2XB	A	603	-	32,32,32	2.02	5 (15%)	40,45,45	2.46	13 (32%)
3	UFP	E	602	-	22,22,22	1.10	1 (4%)	32,33,33	2.55	9 (28%)
3	UFP	B	602	-	22,22,22	1.08	0	32,33,33	2.57	9 (28%)
4	2XB	B	603	-	32,32,32	2.01	5 (15%)	40,45,45	2.46	13 (32%)
2	NDP	A	601	-	51,52,52	1.93	12 (23%)	71,80,80	1.61	13 (18%)
3	UFP	D	602	-	22,22,22	1.09	1 (4%)	32,33,33	2.52	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	D	601	-	51,52,52	1.93	12 (23%)	71,80,80	1.61	13 (18%)
3	UFP	A	602	-	22,22,22	1.08	1 (4%)	32,33,33	2.51	9 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2XB	D	603	-	-	6/21/21/21	0/3/3/3
4	2XB	C	603	-	-	6/21/21/21	0/3/3/3
3	UFP	C	602	-	-	4/10/22/22	0/2/2/2
4	2XB	B	604	-	1/1/4/5	11/21/21/21	0/3/3/3
2	NDP	C	601	-	-	6/34/77/77	0/5/5/5
4	2XB	E	604	-	1/1/4/5	11/21/21/21	0/3/3/3
4	2XB	C	604	-	1/1/4/5	11/21/21/21	0/3/3/3
2	NDP	B	601	-	-	6/34/77/77	0/5/5/5
4	2XB	D	604	-	1/1/4/5	11/21/21/21	0/3/3/3
2	NDP	E	601	-	-	5/34/77/77	0/5/5/5
4	2XB	A	604	-	1/1/4/5	11/21/21/21	0/3/3/3
4	2XB	E	603	-	-	6/21/21/21	0/3/3/3
4	2XB	A	603	-	-	6/21/21/21	0/3/3/3
3	UFP	E	602	-	-	4/10/22/22	0/2/2/2
3	UFP	B	602	-	-	4/10/22/22	0/2/2/2
4	2XB	B	603	-	-	6/21/21/21	0/3/3/3
2	NDP	A	601	-	-	6/34/77/77	0/5/5/5
3	UFP	D	602	-	-	4/10/22/22	0/2/2/2
2	NDP	D	601	-	-	6/34/77/77	0/5/5/5
3	UFP	A	602	-	-	4/10/22/22	0/2/2/2

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	2XB	CAW-NAS	6.15	1.46	1.35
4	C	604	2XB	CAW-NAS	6.14	1.46	1.35
4	E	604	2XB	CAW-NAS	6.12	1.46	1.35
4	B	604	2XB	CAW-NAS	6.11	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	604	2XB	CAW-NAS	6.09	1.45	1.35
4	C	603	2XB	CAW-NAS	6.05	1.45	1.35
4	A	603	2XB	CAW-NAS	6.05	1.45	1.35
4	E	603	2XB	CAW-NAS	6.04	1.45	1.35
4	B	603	2XB	CAW-NAS	6.04	1.45	1.35
4	D	603	2XB	CAW-NAS	6.01	1.45	1.35
2	D	601	NDP	C6A-N6A	5.82	1.49	1.34
2	B	601	NDP	C6A-N6A	5.80	1.49	1.34
2	A	601	NDP	C6A-N6A	5.78	1.49	1.34
2	C	601	NDP	C6A-N6A	5.76	1.48	1.34
2	E	601	NDP	C6A-N6A	5.72	1.48	1.34
4	C	604	2XB	CAW-NAA	4.82	1.43	1.33
4	D	604	2XB	CAW-NAA	4.80	1.43	1.33
4	A	604	2XB	CAW-NAA	4.80	1.43	1.33
4	B	604	2XB	CAW-NAA	4.79	1.43	1.33
4	E	604	2XB	CAW-NAA	4.77	1.43	1.33
4	C	603	2XB	CAW-NAA	4.73	1.43	1.33
4	E	603	2XB	CAW-NAA	4.73	1.43	1.33
4	A	603	2XB	CAW-NAA	4.71	1.43	1.33
4	B	603	2XB	CAW-NAA	4.71	1.43	1.33
4	D	603	2XB	CAW-NAA	4.68	1.43	1.33
2	B	601	NDP	C4N-C3N	-4.62	1.41	1.50
2	C	601	NDP	C4N-C3N	-4.62	1.41	1.50
2	A	601	NDP	C4N-C3N	-4.61	1.41	1.50
2	D	601	NDP	C4N-C3N	-4.60	1.41	1.50
2	E	601	NDP	C4N-C3N	-4.50	1.41	1.50
4	C	603	2XB	CAV-NT1	4.01	1.43	1.34
4	D	604	2XB	CAV-NT1	4.01	1.43	1.34
4	C	604	2XB	CAV-NT1	4.01	1.43	1.34
4	E	604	2XB	CAV-NT1	4.00	1.43	1.34
4	A	604	2XB	CAV-NT1	4.00	1.43	1.34
4	B	604	2XB	CAV-NT1	3.99	1.43	1.34
4	A	603	2XB	CAV-NT1	3.98	1.43	1.34
4	E	603	2XB	CAV-NT1	3.98	1.43	1.34
4	D	603	2XB	CAV-NT1	3.97	1.43	1.34
4	B	603	2XB	CAV-NT1	3.96	1.43	1.34
2	E	601	NDP	C2D-C3D	-3.86	1.42	1.53
2	E	601	NDP	C7N-N7N	3.75	1.44	1.33
2	C	601	NDP	C7N-N7N	3.74	1.44	1.33
2	D	601	NDP	C7N-N7N	3.74	1.44	1.33
2	A	601	NDP	C7N-N7N	3.73	1.44	1.33
2	B	601	NDP	C7N-N7N	3.72	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	NDP	C3B-C2B	-3.69	1.44	1.53
2	A	601	NDP	C2D-C3D	-3.64	1.43	1.53
2	B	601	NDP	C2D-C3D	-3.63	1.43	1.53
2	C	601	NDP	C2D-C3D	-3.62	1.43	1.53
2	D	601	NDP	C2D-C3D	-3.62	1.43	1.53
2	A	601	NDP	C3B-C2B	-3.57	1.45	1.53
2	C	601	NDP	C3B-C2B	-3.56	1.45	1.53
2	B	601	NDP	C3B-C2B	-3.55	1.45	1.53
2	D	601	NDP	C3B-C2B	-3.55	1.45	1.53
4	E	604	2XB	CBB-NAR	3.31	1.41	1.36
4	A	604	2XB	CBB-NAR	3.31	1.41	1.36
4	C	603	2XB	CBB-NAR	3.30	1.41	1.36
2	E	601	NDP	C4N-C5N	-3.30	1.40	1.49
4	B	604	2XB	CBB-NAR	3.29	1.41	1.36
4	A	603	2XB	CBB-NAR	3.27	1.41	1.36
4	C	604	2XB	CBB-NAR	3.27	1.41	1.36
4	E	603	2XB	CBB-NAR	3.27	1.41	1.36
4	D	604	2XB	CBB-NAR	3.26	1.41	1.36
4	B	603	2XB	CBB-NAR	3.24	1.41	1.36
4	D	603	2XB	CBB-NAR	3.23	1.41	1.36
4	B	604	2XB	CAW-NAP	3.23	1.41	1.35
2	D	601	NDP	C4N-C5N	-3.23	1.40	1.49
2	B	601	NDP	C4N-C5N	-3.22	1.40	1.49
4	D	604	2XB	CAW-NAP	3.20	1.40	1.35
4	A	604	2XB	CAW-NAP	3.20	1.40	1.35
4	C	604	2XB	CAW-NAP	3.20	1.40	1.35
2	A	601	NDP	C4N-C5N	-3.20	1.40	1.49
4	E	604	2XB	CAW-NAP	3.20	1.40	1.35
2	C	601	NDP	C4N-C5N	-3.18	1.40	1.49
4	A	603	2XB	CAW-NAP	3.14	1.40	1.35
4	D	603	2XB	CAW-NAP	3.13	1.40	1.35
4	C	603	2XB	CAW-NAP	3.12	1.40	1.35
4	E	603	2XB	CAW-NAP	3.11	1.40	1.35
4	B	603	2XB	CAW-NAP	3.11	1.40	1.35
2	E	601	NDP	C2B-C1B	-2.90	1.46	1.53
2	A	601	NDP	C2B-C1B	-2.86	1.46	1.53
2	D	601	NDP	C2B-C1B	-2.86	1.46	1.53
2	C	601	NDP	C2B-C1B	-2.85	1.46	1.53
2	B	601	NDP	C2B-C1B	-2.84	1.46	1.53
2	C	601	NDP	C4A-N3A	2.53	1.39	1.34
2	B	601	NDP	C4A-N3A	2.51	1.39	1.34
2	D	601	NDP	C4A-N3A	2.51	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NDP	C4A-N3A	2.50	1.39	1.34
2	E	601	NDP	C3B-C4B	-2.47	1.46	1.53
2	E	601	NDP	C4A-N3A	2.44	1.39	1.34
2	D	601	NDP	C3B-C4B	-2.42	1.46	1.53
2	B	601	NDP	C3B-C4B	-2.39	1.46	1.53
2	A	601	NDP	C3B-C4B	-2.38	1.46	1.53
2	C	601	NDP	C3B-C4B	-2.38	1.46	1.53
2	E	601	NDP	C3D-C4D	-2.33	1.47	1.53
2	C	601	NDP	C3D-C4D	-2.24	1.47	1.53
2	A	601	NDP	C3D-C4D	-2.21	1.47	1.53
2	B	601	NDP	C3D-C4D	-2.20	1.47	1.53
2	C	601	NDP	C6N-C5N	2.19	1.39	1.33
2	B	601	NDP	C6N-C5N	2.19	1.39	1.33
2	D	601	NDP	C3D-C4D	-2.19	1.47	1.53
2	D	601	NDP	C6N-C5N	2.18	1.39	1.33
2	A	601	NDP	C6N-C5N	2.18	1.39	1.33
2	E	601	NDP	C6N-C5N	2.17	1.39	1.33
4	D	604	2XB	CBB-NAP	2.13	1.38	1.34
4	C	604	2XB	CBB-NAP	2.11	1.38	1.34
4	E	604	2XB	CBB-NAP	2.11	1.38	1.34
2	D	601	NDP	C2N-C3N	2.10	1.41	1.35
2	A	601	NDP	C2N-C3N	2.09	1.40	1.35
2	B	601	NDP	C2N-C3N	2.09	1.40	1.35
2	C	601	NDP	C2N-C3N	2.08	1.40	1.35
4	B	604	2XB	CBB-NAP	2.07	1.38	1.34
2	E	601	NDP	C2N-C3N	2.06	1.40	1.35
3	D	602	UFP	C4-C5	-2.06	1.41	1.44
3	E	602	UFP	C4-N3	-2.05	1.35	1.38
4	A	604	2XB	CBB-NAP	2.04	1.38	1.34
3	A	602	UFP	C4-C5	-2.01	1.41	1.44

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	604	2XB	CBB-CBC-CBA	8.03	119.62	114.94
4	E	604	2XB	CBB-CBC-CBA	7.95	119.57	114.94
4	A	604	2XB	CBB-CBC-CBA	7.92	119.56	114.94
4	D	604	2XB	CBB-CBC-CBA	7.91	119.55	114.94
4	B	604	2XB	CBB-CBC-CBA	7.88	119.53	114.94
4	C	603	2XB	CBB-CBC-CBA	7.82	119.50	114.94
4	E	603	2XB	CBB-CBC-CBA	7.81	119.49	114.94
4	A	603	2XB	CBB-CBC-CBA	7.78	119.47	114.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	603	2XB	CBB-CBC-CBA	7.77	119.47	114.94
4	B	603	2XB	CBB-CBC-CBA	7.77	119.47	114.94
3	E	602	UFP	C5-C4-N3	7.05	119.08	112.64
3	B	602	UFP	C5-C4-N3	7.05	119.08	112.64
3	C	602	UFP	C5-C4-N3	7.04	119.08	112.64
3	D	602	UFP	C5-C4-N3	7.00	119.04	112.64
3	A	602	UFP	C5-C4-N3	6.95	119.00	112.64
3	E	602	UFP	O4-C4-C5	-6.24	120.38	125.69
3	D	602	UFP	O4-C4-C5	-6.18	120.43	125.69
3	B	602	UFP	O4-C4-C5	-6.14	120.47	125.69
3	C	602	UFP	O4-C4-C5	-5.95	120.62	125.69
3	A	602	UFP	O4-C4-C5	-5.91	120.66	125.69
2	C	601	NDP	C5A-C4A-N3A	-5.46	119.20	126.72
2	E	601	NDP	C5A-C4A-N3A	-5.45	119.22	126.72
2	A	601	NDP	C5A-C4A-N3A	-5.43	119.24	126.72
2	D	601	NDP	C5A-C4A-N3A	-5.43	119.24	126.72
2	B	601	NDP	C5A-C4A-N3A	-5.43	119.25	126.72
3	B	602	UFP	C4-N3-C2	-4.88	120.94	127.34
3	C	602	UFP	C4-N3-C2	-4.83	121.00	127.34
3	D	602	UFP	C4-N3-C2	-4.81	121.03	127.34
3	A	602	UFP	C4-N3-C2	-4.80	121.05	127.34
3	B	602	UFP	F5-C5-C4	4.77	120.65	116.47
3	E	602	UFP	C4-N3-C2	-4.74	121.12	127.34
4	A	604	2XB	CBC-CAZ-CAL	4.69	110.04	105.93
4	E	603	2XB	CBC-CAZ-CAL	4.69	110.04	105.93
4	B	603	2XB	CBC-CAZ-CAL	4.67	110.02	105.93
4	B	604	2XB	CBC-CAZ-CAL	4.67	110.02	105.93
4	C	603	2XB	CBC-CAZ-CAL	4.67	110.02	105.93
4	D	604	2XB	CBC-CAZ-CAL	4.66	110.02	105.93
3	E	602	UFP	F5-C5-C4	4.66	120.55	116.47
4	A	603	2XB	CBC-CAZ-CAL	4.66	110.01	105.93
3	C	602	UFP	F5-C5-C4	4.65	120.55	116.47
4	D	603	2XB	CBC-CAZ-CAL	4.64	110.00	105.93
4	B	604	2XB	NAP-CAW-NAS	-4.64	118.37	125.48
4	A	604	2XB	NAP-CAW-NAS	-4.62	118.41	125.48
4	E	604	2XB	CBC-CAZ-CAL	4.62	109.97	105.93
4	E	604	2XB	NAP-CAW-NAS	-4.61	118.42	125.48
4	C	604	2XB	NAP-CAW-NAS	-4.61	118.42	125.48
4	C	604	2XB	CBC-CAZ-CAL	4.59	109.95	105.93
4	D	604	2XB	NAP-CAW-NAS	-4.59	118.45	125.48
4	E	603	2XB	NAP-CAW-NAS	-4.55	118.50	125.48
4	A	603	2XB	NAP-CAW-NAS	-4.55	118.50	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	2XB	NAP-CAW-NAS	-4.55	118.50	125.48
3	A	602	UFP	F5-C5-C4	4.55	120.46	116.47
4	C	603	2XB	NAP-CAW-NAS	-4.52	118.56	125.48
4	D	603	2XB	NAP-CAW-NAS	-4.51	118.56	125.48
3	B	602	UFP	N3-C2-N1	4.46	120.69	114.89
3	D	602	UFP	F5-C5-C4	4.44	120.36	116.47
3	E	602	UFP	N3-C2-N1	4.42	120.64	114.89
3	C	602	UFP	N3-C2-N1	4.41	120.64	114.89
3	D	602	UFP	N3-C2-N1	4.40	120.62	114.89
3	A	602	UFP	N3-C2-N1	4.40	120.61	114.89
4	A	604	2XB	CT2-CT1-NT1	4.35	119.52	110.91
4	E	604	2XB	CT2-CT1-NT1	4.33	119.48	110.91
4	C	604	2XB	CT2-CT1-NT1	4.33	119.48	110.91
4	D	604	2XB	CT2-CT1-NT1	4.33	119.47	110.91
4	B	604	2XB	CT2-CT1-NT1	4.31	119.43	110.91
2	E	601	NDP	N3A-C2A-N1A	-4.20	122.23	128.58
2	C	601	NDP	N3A-C2A-N1A	-4.14	122.31	128.58
2	B	601	NDP	N3A-C2A-N1A	-4.13	122.33	128.58
2	D	601	NDP	N3A-C2A-N1A	-4.11	122.36	128.58
2	A	601	NDP	N3A-C2A-N1A	-4.10	122.37	128.58
4	C	603	2XB	CT2-CT1-NT1	4.07	118.97	110.91
4	B	603	2XB	CT2-CT1-NT1	4.06	118.95	110.91
4	A	603	2XB	CT2-CT1-NT1	4.04	118.91	110.91
4	E	603	2XB	CT2-CT1-NT1	4.04	118.91	110.91
4	D	603	2XB	CT2-CT1-NT1	4.03	118.89	110.91
3	E	602	UFP	C6-C5-C4	-3.99	118.93	122.57
3	B	602	UFP	C6-C5-C4	-3.94	118.98	122.57
3	C	602	UFP	C6-C5-C4	-3.92	119.00	122.57
3	D	602	UFP	C6-C5-C4	-3.85	119.06	122.57
4	E	604	2XB	CT2-CT1-CT5	3.84	119.47	110.35
2	E	601	NDP	N3A-C4A-N9A	3.84	133.69	127.17
4	D	604	2XB	CT2-CT1-CT5	3.84	119.46	110.35
4	C	604	2XB	CT5-CT1-NT1	3.84	119.47	110.57
4	D	604	2XB	CT5-CT1-NT1	3.83	119.46	110.57
4	B	604	2XB	CT2-CT1-CT5	3.83	119.44	110.35
4	A	604	2XB	CT2-CT1-CT5	3.83	119.44	110.35
4	A	604	2XB	CT5-CT1-NT1	3.82	119.44	110.57
4	B	604	2XB	CT5-CT1-NT1	3.82	119.44	110.57
4	E	604	2XB	CT5-CT1-NT1	3.82	119.44	110.57
4	C	604	2XB	CT2-CT1-CT5	3.81	119.40	110.35
2	C	601	NDP	N3A-C4A-N9A	3.78	133.60	127.17
2	A	601	NDP	N3A-C4A-N9A	3.77	133.58	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	603	2XB	CT2-CT1-CT5	3.77	119.29	110.35
2	B	601	NDP	N3A-C4A-N9A	3.76	133.57	127.17
4	D	603	2XB	CT2-CT1-CT5	3.76	119.28	110.35
4	A	603	2XB	CT2-CT1-CT5	3.76	119.28	110.35
2	D	601	NDP	N3A-C4A-N9A	3.76	133.56	127.17
4	B	603	2XB	CT2-CT1-CT5	3.75	119.27	110.35
4	C	603	2XB	CT2-CT1-CT5	3.74	119.24	110.35
3	A	602	UFP	C6-C5-C4	-3.73	119.17	122.57
2	E	601	NDP	C2A-N3A-C4A	3.58	120.56	111.83
4	D	603	2XB	CT5-CT1-NT1	3.54	118.77	110.57
4	A	603	2XB	CT5-CT1-NT1	3.54	118.77	110.57
4	E	603	2XB	CT5-CT1-NT1	3.53	118.76	110.57
4	B	603	2XB	CT5-CT1-NT1	3.53	118.75	110.57
4	C	603	2XB	CT5-CT1-NT1	3.52	118.75	110.57
2	C	601	NDP	C2A-N3A-C4A	3.52	120.42	111.83
2	B	601	NDP	C2A-N3A-C4A	3.50	120.38	111.83
2	D	601	NDP	C2A-N3A-C4A	3.50	120.38	111.83
2	A	601	NDP	C2A-N3A-C4A	3.50	120.38	111.83
3	A	602	UFP	C1'-N1-C2	3.47	124.44	117.66
4	A	604	2XB	CT3-CT2-CT1	3.44	119.50	113.16
4	C	604	2XB	CT3-CT2-CT1	3.44	119.50	113.16
4	D	604	2XB	CT3-CT2-CT1	3.43	119.49	113.16
4	B	604	2XB	CT3-CT2-CT1	3.42	119.47	113.16
4	E	604	2XB	CT3-CT2-CT1	3.42	119.46	113.16
4	A	603	2XB	CT3-CT2-CT1	3.38	119.39	113.16
4	C	603	2XB	CT3-CT2-CT1	3.36	119.36	113.16
4	D	603	2XB	CT3-CT2-CT1	3.36	119.35	113.16
4	E	603	2XB	CT3-CT2-CT1	3.36	119.35	113.16
4	B	603	2XB	CT3-CT2-CT1	3.35	119.33	113.16
3	B	602	UFP	C1'-N1-C2	3.34	124.20	117.66
3	E	602	UFP	C1'-N1-C2	3.34	124.19	117.66
3	C	602	UFP	C1'-N1-C2	3.29	124.10	117.66
2	D	601	NDP	N9A-C8A-N7A	-3.27	109.30	113.94
3	D	602	UFP	C1'-N1-C2	3.27	124.05	117.66
2	B	601	NDP	N9A-C8A-N7A	-3.26	109.31	113.94
2	C	601	NDP	N9A-C8A-N7A	-3.26	109.31	113.94
2	A	601	NDP	N9A-C8A-N7A	-3.25	109.32	113.94
2	E	601	NDP	N9A-C8A-N7A	-3.22	109.37	113.94
2	C	601	NDP	C4A-C5A-N7A	-3.20	106.93	110.58
2	A	601	NDP	C4A-C5A-N7A	-3.18	106.94	110.58
4	C	604	2XB	CBC-CBB-NAP	-3.18	121.54	126.54
2	B	601	NDP	C4A-C5A-N7A	-3.18	106.95	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	2XB	CBC-CBB-NAP	-3.17	121.55	126.54
2	D	601	NDP	C4A-C5A-N7A	-3.17	106.96	110.58
4	D	604	2XB	CBC-CBB-NAP	-3.17	121.56	126.54
4	B	604	2XB	CBC-CBB-NAP	-3.16	121.57	126.54
2	E	601	NDP	C4A-C5A-N7A	-3.16	106.97	110.58
4	E	604	2XB	CBC-CBB-NAP	-3.16	121.57	126.54
2	E	601	NDP	C5A-N7A-C8A	3.15	108.40	103.45
2	C	601	NDP	C5A-N7A-C8A	3.14	108.39	103.45
2	A	601	NDP	C5A-N7A-C8A	3.14	108.38	103.45
2	D	601	NDP	C5A-N7A-C8A	3.13	108.37	103.45
2	B	601	NDP	C5A-N7A-C8A	3.13	108.37	103.45
4	A	604	2XB	CAZ-CAL-NAR	-3.12	106.88	110.31
4	B	604	2XB	CAZ-CAL-NAR	-3.10	106.90	110.31
4	B	603	2XB	CBC-CBB-NAP	-3.09	121.67	126.54
4	E	604	2XB	CAZ-CAL-NAR	-3.09	106.91	110.31
4	D	604	2XB	CAZ-CAL-NAR	-3.09	106.92	110.31
4	E	603	2XB	CBC-CBB-NAP	-3.08	121.69	126.54
4	C	603	2XB	CAZ-CAL-NAR	-3.06	106.94	110.31
4	C	604	2XB	CAZ-CAL-NAR	-3.06	106.95	110.31
4	A	603	2XB	CAZ-CAL-NAR	-3.06	106.95	110.31
4	D	603	2XB	CBC-CBB-NAP	-3.06	121.73	126.54
4	C	603	2XB	CBC-CBB-NAP	-3.04	121.75	126.54
4	E	603	2XB	CAZ-CAL-NAR	-3.04	106.97	110.31
4	A	603	2XB	CBC-CBB-NAP	-3.04	121.75	126.54
4	D	603	2XB	CAZ-CAL-NAR	-3.04	106.97	110.31
4	B	603	2XB	CAZ-CAL-NAR	-3.03	106.98	110.31
3	A	602	UFP	C1'-N1-C6	-2.83	115.99	120.74
3	B	602	UFP	C1'-N1-C6	-2.71	116.19	120.74
4	A	604	2XB	CAW-NAP-CBB	2.69	120.98	114.59
4	B	604	2XB	CAW-NAP-CBB	2.68	120.97	114.59
4	C	604	2XB	CAW-NAP-CBB	2.68	120.95	114.59
4	D	604	2XB	CAW-NAP-CBB	2.67	120.94	114.59
4	E	604	2XB	CAW-NAP-CBB	2.67	120.94	114.59
3	C	602	UFP	C1'-N1-C6	-2.64	116.31	120.74
4	B	603	2XB	CAW-NAP-CBB	2.63	120.84	114.59
4	E	603	2XB	CAW-NAP-CBB	2.63	120.84	114.59
4	C	604	2XB	CT2-CT3-CT4	2.62	119.49	112.49
4	A	603	2XB	CT2-CT3-CT4	2.62	119.48	112.49
4	A	604	2XB	CT2-CT3-CT4	2.62	119.48	112.49
4	B	604	2XB	CT2-CT3-CT4	2.62	119.47	112.49
4	C	603	2XB	CT2-CT3-CT4	2.61	119.45	112.49
4	D	604	2XB	CT2-CT3-CT4	2.60	119.43	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	603	2XB	CT2-CT3-CT4	2.60	119.43	112.49
4	E	604	2XB	CT2-CT3-CT4	2.60	119.43	112.49
4	A	603	2XB	CAW-NAP-CBB	2.60	120.77	114.59
4	C	603	2XB	CAW-NAP-CBB	2.60	120.77	114.59
3	E	602	UFP	C1'-N1-C6	-2.60	116.38	120.74
4	D	603	2XB	CAW-NAP-CBB	2.60	120.76	114.59
4	D	603	2XB	CT2-CT3-CT4	2.60	119.42	112.49
4	B	603	2XB	CT2-CT3-CT4	2.59	119.41	112.49
3	D	602	UFP	C1'-N1-C6	-2.58	116.42	120.74
2	C	601	NDP	O5D-C5D-C4D	2.51	117.55	108.99
2	B	601	NDP	O5D-C5D-C4D	2.50	117.52	108.99
2	A	601	NDP	O5D-C5D-C4D	2.50	117.52	108.99
2	D	601	NDP	O5D-C5D-C4D	2.50	117.50	108.99
2	E	601	NDP	O5D-C5D-C4D	2.47	117.42	108.99
3	A	602	UFP	O2-C2-N3	-2.45	116.98	121.49
3	B	602	UFP	O2-C2-N3	-2.43	117.01	121.49
3	D	602	UFP	O2-C2-N3	-2.42	117.03	121.49
4	B	604	2XB	NAA-CAW-NAS	2.41	120.83	117.22
2	D	601	NDP	O5B-C5B-C4B	2.40	117.17	108.99
2	B	601	NDP	O5B-C5B-C4B	2.40	117.15	108.99
4	C	604	2XB	NAA-CAW-NAP	2.39	120.81	117.22
4	A	604	2XB	NAA-CAW-NAP	2.39	120.81	117.22
2	A	601	NDP	O5B-C5B-C4B	2.39	117.13	108.99
4	B	604	2XB	NAA-CAW-NAP	2.39	120.80	117.22
4	E	604	2XB	NAA-CAW-NAP	2.39	120.80	117.22
2	C	601	NDP	O5B-C5B-C4B	2.38	117.10	108.99
4	D	604	2XB	NAA-CAW-NAS	2.38	120.78	117.22
4	E	604	2XB	NAA-CAW-NAS	2.38	120.78	117.22
4	A	604	2XB	NAA-CAW-NAS	2.37	120.78	117.22
4	B	603	2XB	NAA-CAW-NAP	2.37	120.77	117.22
4	C	604	2XB	NAA-CAW-NAS	2.36	120.77	117.22
4	D	604	2XB	NAA-CAW-NAP	2.36	120.77	117.22
4	E	603	2XB	NAA-CAW-NAP	2.36	120.77	117.22
4	A	603	2XB	NAA-CAW-NAP	2.36	120.76	117.22
3	E	602	UFP	O2-C2-N3	-2.35	117.16	121.49
4	A	603	2XB	NAA-CAW-NAS	2.34	120.74	117.22
4	E	603	2XB	NAA-CAW-NAS	2.34	120.73	117.22
4	C	603	2XB	NAA-CAW-NAS	2.34	120.73	117.22
3	C	602	UFP	O2-C2-N3	-2.34	117.18	121.49
4	B	603	2XB	NAA-CAW-NAS	2.33	120.72	117.22
4	D	603	2XB	NAA-CAW-NAP	2.33	120.72	117.22
4	D	603	2XB	NAA-CAW-NAS	2.33	120.72	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NDP	C4A-N9A-C8A	2.33	108.18	105.74
4	C	603	2XB	NAA-CAW-NAP	2.33	120.71	117.22
2	C	601	NDP	C4A-N9A-C8A	2.32	108.18	105.74
2	E	601	NDP	C3N-C7N-N7N	2.32	121.79	117.67
2	B	601	NDP	C2B-C1B-N9A	-2.32	109.93	113.75
2	B	601	NDP	C3N-C7N-N7N	2.32	121.79	117.67
2	A	601	NDP	C4A-N9A-C8A	2.32	108.17	105.74
2	A	601	NDP	C3N-C7N-N7N	2.32	121.78	117.67
2	E	601	NDP	C4A-N9A-C8A	2.32	108.17	105.74
2	D	601	NDP	C4A-N9A-C8A	2.31	108.17	105.74
2	E	601	NDP	O5B-C5B-C4B	2.31	116.87	108.99
2	D	601	NDP	C3N-C7N-N7N	2.31	121.77	117.67
2	C	601	NDP	C3N-C7N-N7N	2.31	121.77	117.67
2	D	601	NDP	C2B-C1B-N9A	-2.30	109.97	113.75
2	A	601	NDP	C2B-C1B-N9A	-2.30	109.97	113.75
2	C	601	NDP	C2B-C1B-N9A	-2.30	109.97	113.75
2	D	601	NDP	C3D-C2D-C1D	2.23	105.67	101.46
2	B	601	NDP	C3D-C2D-C1D	2.22	105.66	101.46
2	A	601	NDP	C3D-C2D-C1D	2.21	105.65	101.46
2	C	601	NDP	C3D-C2D-C1D	2.20	105.63	101.46
2	E	601	NDP	C2B-C1B-N9A	-2.04	110.40	113.75
4	E	603	2XB	CAX-CAO-CAZ	-2.00	109.12	115.86

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	604	2XB	CT1
4	B	604	2XB	CT1
4	C	604	2XB	CT1
4	D	604	2XB	CT1
4	E	604	2XB	CT1

All (134) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NDP	C5B-O5B-PA-O1A
2	A	601	NDP	O4D-C4D-C5D-O5D
2	B	601	NDP	C5B-O5B-PA-O1A
2	B	601	NDP	O4D-C4D-C5D-O5D
2	C	601	NDP	C5B-O5B-PA-O1A
2	C	601	NDP	O4D-C4D-C5D-O5D
2	D	601	NDP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	D	601	NDP	O4D-C4D-C5D-O5D
3	A	602	UFP	C5'-O5'-P-O2P
3	A	602	UFP	C5'-O5'-P-O3P
3	B	602	UFP	C5'-O5'-P-O2P
3	B	602	UFP	C5'-O5'-P-O3P
3	C	602	UFP	C5'-O5'-P-O2P
3	C	602	UFP	C5'-O5'-P-O3P
3	D	602	UFP	C5'-O5'-P-O2P
3	D	602	UFP	C5'-O5'-P-O3P
3	E	602	UFP	C5'-O5'-P-O3P
4	A	604	2XB	NT1-CT1-CT2-CT3
4	B	604	2XB	NT1-CT1-CT2-CT3
4	C	604	2XB	NT1-CT1-CT2-CT3
4	D	604	2XB	NT1-CT1-CT2-CT3
4	E	604	2XB	NT1-CT1-CT2-CT3
2	A	601	NDP	C3D-C4D-C5D-O5D
2	B	601	NDP	C3D-C4D-C5D-O5D
2	C	601	NDP	C3D-C4D-C5D-O5D
2	D	601	NDP	C3D-C4D-C5D-O5D
2	E	601	NDP	C3B-C4B-C5B-O5B
4	A	604	2XB	CT5-CT1-CT2-CT3
4	B	604	2XB	CT5-CT1-CT2-CT3
4	C	604	2XB	CT5-CT1-CT2-CT3
4	D	604	2XB	CT5-CT1-CT2-CT3
4	E	604	2XB	CT5-CT1-CT2-CT3
2	E	601	NDP	O4B-C4B-C5B-O5B
4	A	603	2XB	NT1-CT1-CT5-OT1
4	A	603	2XB	NT1-CT1-CT5-OXT
4	B	603	2XB	NT1-CT1-CT5-OT1
4	B	603	2XB	NT1-CT1-CT5-OXT
4	C	603	2XB	NT1-CT1-CT5-OT1
4	C	603	2XB	NT1-CT1-CT5-OXT
4	D	603	2XB	NT1-CT1-CT5-OT1
4	D	603	2XB	NT1-CT1-CT5-OXT
4	E	603	2XB	NT1-CT1-CT5-OT1
4	E	603	2XB	NT1-CT1-CT5-OXT
4	A	603	2XB	CT5-CT1-CT2-CT3
4	B	603	2XB	CT5-CT1-CT2-CT3
4	C	603	2XB	CT5-CT1-CT2-CT3
4	D	603	2XB	CT5-CT1-CT2-CT3
4	E	603	2XB	CT5-CT1-CT2-CT3
4	A	604	2XB	CT1-CT2-CT3-CT4

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Mol	Chain	Res	Type	Atoms
4	B	604	2XB	CT1-CT2-CT3-CT4
4	C	604	2XB	CT1-CT2-CT3-CT4
4	D	604	2XB	CT1-CT2-CT3-CT4
4	E	604	2XB	CT1-CT2-CT3-CT4
3	A	602	UFP	C5'-O5'-P-O1P
3	B	602	UFP	C5'-O5'-P-O1P
3	C	602	UFP	C5'-O5'-P-O1P
3	D	602	UFP	C5'-O5'-P-O1P
3	E	602	UFP	C5'-O5'-P-O1P
2	A	601	NDP	O4D-C1D-N1N-C2N
2	B	601	NDP	O4D-C1D-N1N-C2N
2	C	601	NDP	O4D-C1D-N1N-C2N
2	D	601	NDP	O4D-C1D-N1N-C2N
3	E	602	UFP	C5'-O5'-P-O2P
4	A	604	2XB	CT2-CT1-CT5-OT1
4	D	604	2XB	CT2-CT1-CT5-OT1
4	B	604	2XB	CT2-CT1-CT5-OT1
4	C	604	2XB	CT2-CT1-CT5-OT1
4	E	604	2XB	CT2-CT1-CT5-OT1
4	B	603	2XB	CT2-CT1-NT1-CAV
4	A	603	2XB	CT2-CT1-NT1-CAV
4	C	603	2XB	CT2-CT1-NT1-CAV
4	E	603	2XB	CT2-CT1-NT1-CAV
4	D	603	2XB	CT2-CT1-NT1-CAV
4	B	604	2XB	CT2-CT1-CT5-OXT
4	C	604	2XB	CT2-CT1-CT5-OXT
4	E	604	2XB	CT2-CT1-CT5-OXT
3	A	602	UFP	C2'-C1'-N1-C2
3	E	602	UFP	C2'-C1'-N1-C2
2	A	601	NDP	C5D-O5D-PN-O3
2	A	601	NDP	C5D-O5D-PN-O2N
2	B	601	NDP	C5D-O5D-PN-O3
2	B	601	NDP	C5D-O5D-PN-O2N
2	C	601	NDP	C5D-O5D-PN-O3
2	C	601	NDP	C5D-O5D-PN-O2N
2	D	601	NDP	C5D-O5D-PN-O3
2	D	601	NDP	C5D-O5D-PN-O2N
4	A	604	2XB	CT2-CT1-CT5-OXT
4	D	604	2XB	CT2-CT1-CT5-OXT
2	E	601	NDP	C4D-C5D-O5D-PN
3	D	602	UFP	C2'-C1'-N1-C2
4	A	604	2XB	OAD-CAV-CAY-CAJ

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Mol	Chain	Res	Type	Atoms
4	D	604	2XB	OAD-CAV-CAY-CAJ
4	C	604	2XB	OAD-CAV-CAY-CAJ
3	B	602	UFP	C2'-C1'-N1-C2
4	B	604	2XB	OAD-CAV-CAY-CAJ
4	E	604	2XB	OAD-CAV-CAY-CAJ
4	C	604	2XB	NT1-CAV-CAY-CAJ
4	A	604	2XB	NT1-CAV-CAY-CAJ
4	D	604	2XB	NT1-CAV-CAY-CAJ
4	B	604	2XB	NT1-CAV-CAY-CAJ
4	E	604	2XB	NT1-CAV-CAY-CAJ
2	E	601	NDP	O4D-C1D-N1N-C2N
3	C	602	UFP	C2'-C1'-N1-C2
4	A	603	2XB	CT2-CT3-CT4-OE1
4	B	603	2XB	CT2-CT3-CT4-OE1
4	C	603	2XB	CT2-CT3-CT4-OE1
4	D	603	2XB	CT2-CT3-CT4-OE1
4	E	603	2XB	CT2-CT3-CT4-OE1
4	A	603	2XB	CT2-CT3-CT4-OE2
4	B	603	2XB	CT2-CT3-CT4-OE2
4	C	603	2XB	CT2-CT3-CT4-OE2
4	D	603	2XB	CT2-CT3-CT4-OE2
4	E	603	2XB	CT2-CT3-CT4-OE2
2	E	601	NDP	C2D-C1D-N1N-C2N
4	A	604	2XB	OAD-CAV-CAY-CAK
4	E	604	2XB	NT1-CAV-CAY-CAK
4	D	604	2XB	OAD-CAV-CAY-CAK
4	E	604	2XB	OAD-CAV-CAY-CAK
4	A	604	2XB	NT1-CAV-CAY-CAK
4	B	604	2XB	NT1-CAV-CAY-CAK
4	C	604	2XB	NT1-CAV-CAY-CAK
4	D	604	2XB	NT1-CAV-CAY-CAK
4	B	604	2XB	OAD-CAV-CAY-CAK
4	C	604	2XB	OAD-CAV-CAY-CAK
4	A	604	2XB	CT2-CT1-NT1-CAV
4	D	604	2XB	CT2-CT1-NT1-CAV
4	E	604	2XB	CT2-CT1-NT1-CAV
4	C	604	2XB	CT2-CT1-NT1-CAV
4	B	604	2XB	CT2-CT1-NT1-CAV
4	A	604	2XB	CT2-CT3-CT4-OE1
4	B	604	2XB	CT2-CT3-CT4-OE1
4	C	604	2XB	CT2-CT3-CT4-OE1
4	D	604	2XB	CT2-CT3-CT4-OE1

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Mol	Chain	Res	Type	Atoms
4	E	604	2XB	CT2-CT3-CT4-OE1

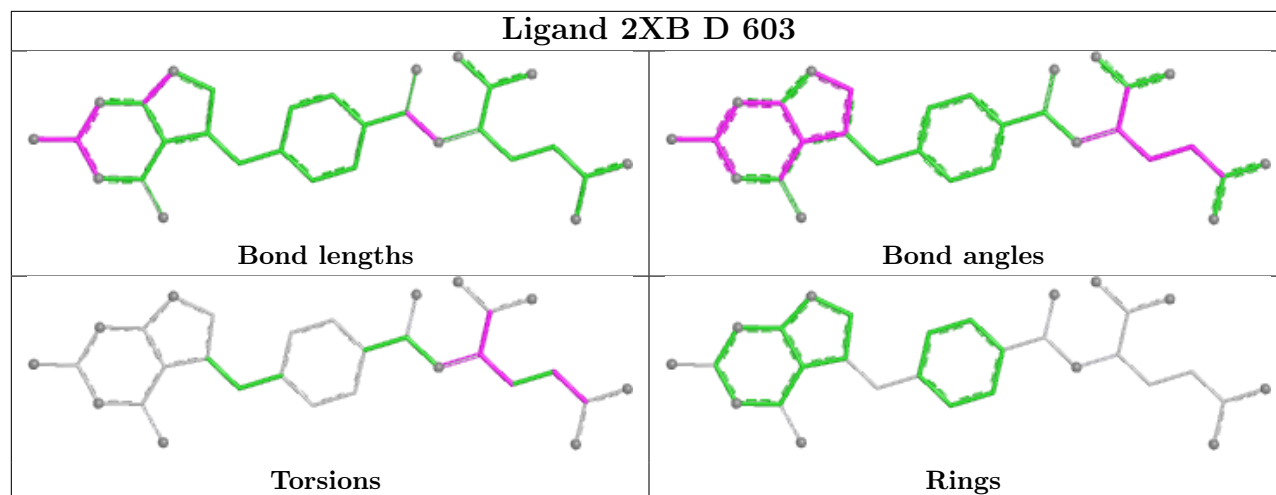
There are no ring outliers.

15 monomers are involved in 91 short contacts:

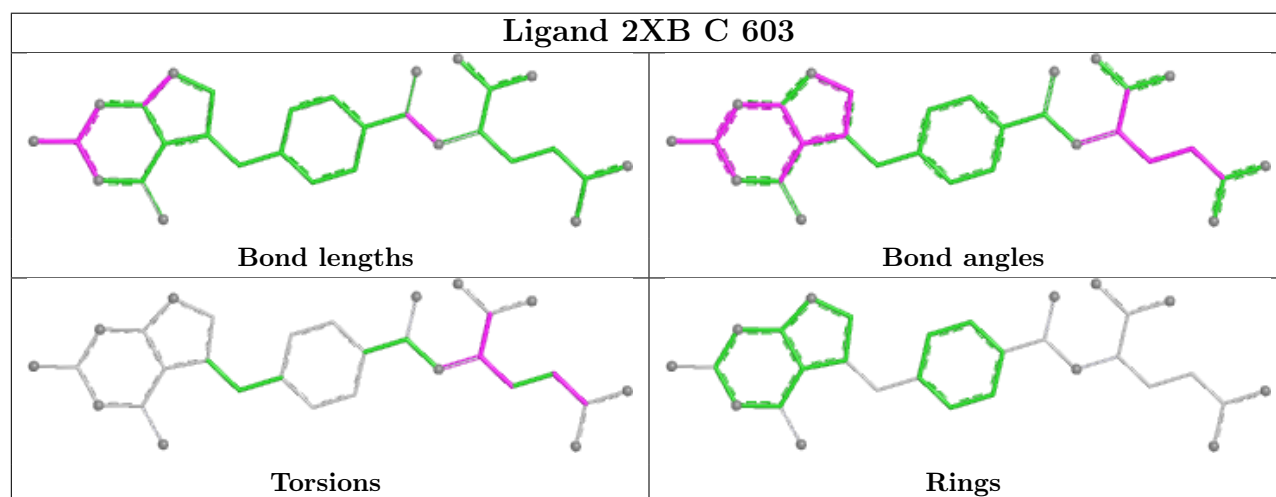
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	UFP	3	0
4	B	604	2XB	6	0
2	C	601	NDP	12	0
4	E	604	2XB	5	0
4	C	604	2XB	6	0
2	B	601	NDP	12	0
4	D	604	2XB	6	0
2	E	601	NDP	9	0
4	A	604	2XB	6	0
3	E	602	UFP	2	0
3	B	602	UFP	3	0
2	A	601	NDP	12	0
3	D	602	UFP	3	0
2	D	601	NDP	12	0
3	A	602	UFP	3	0

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

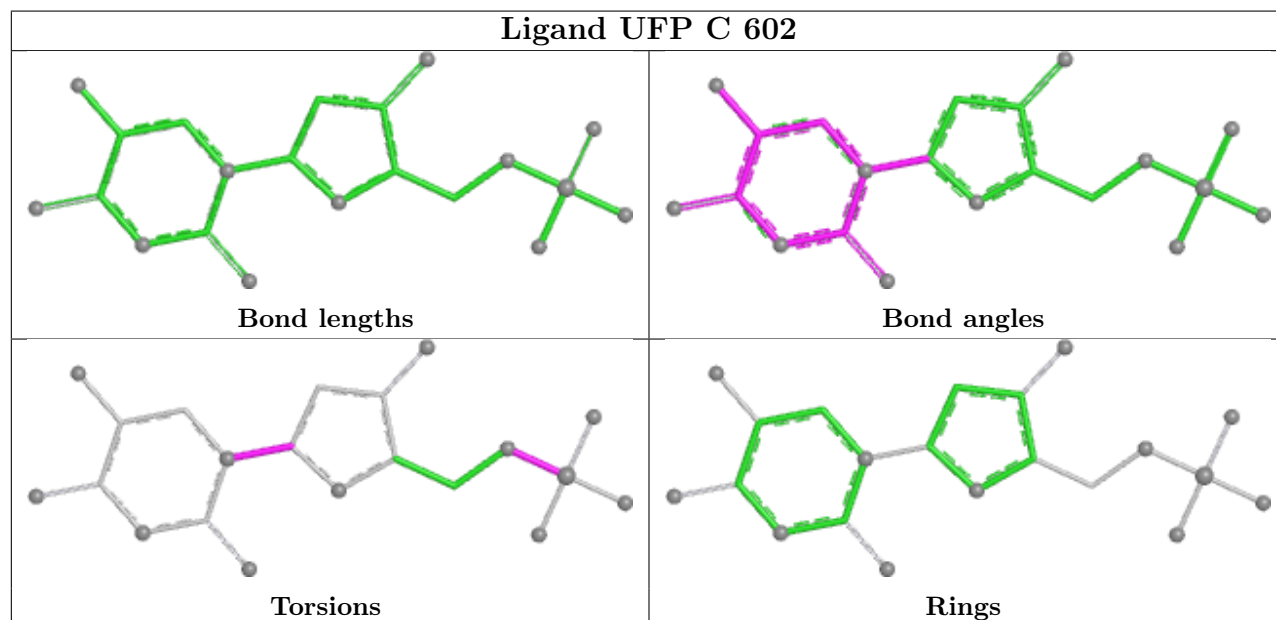
Ligand 2XB D 603



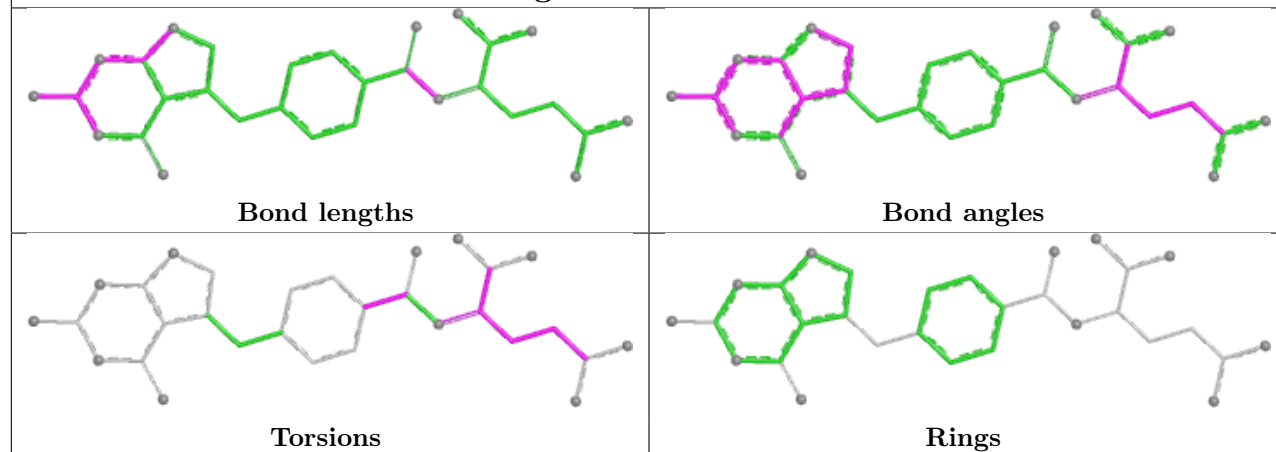
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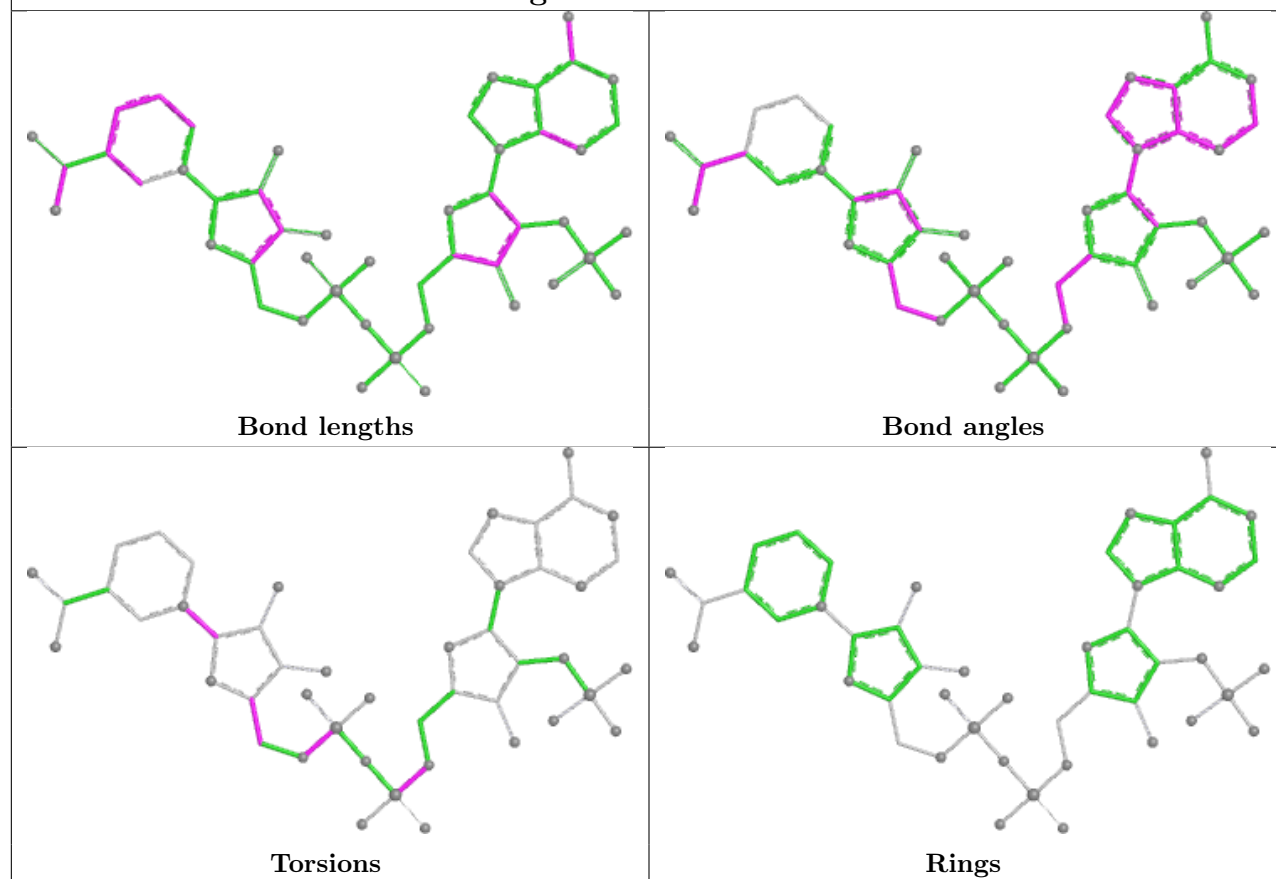
Ligand UFP C 602



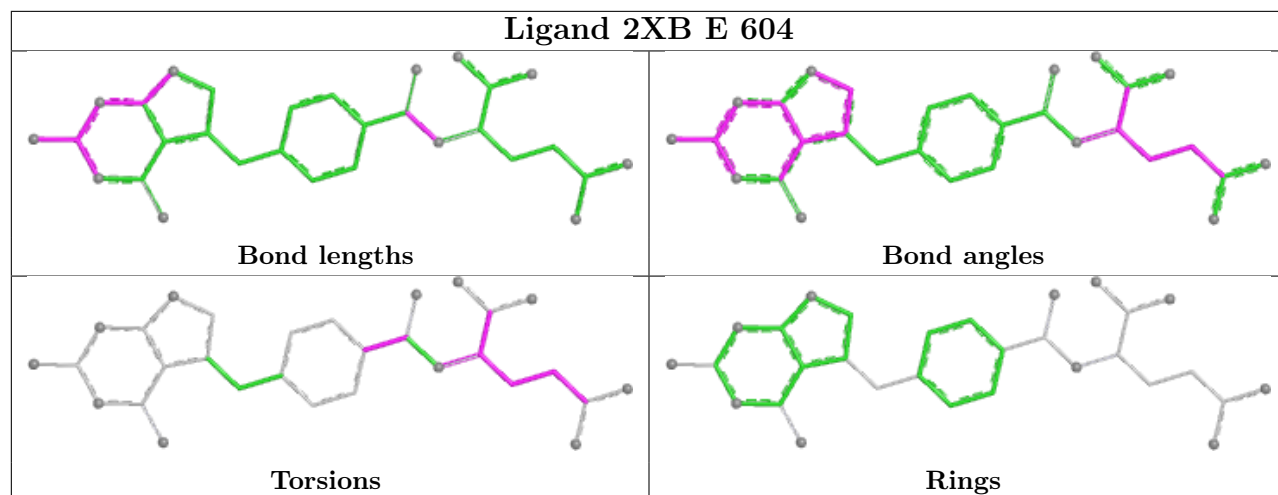
Ligand 2XB B 604



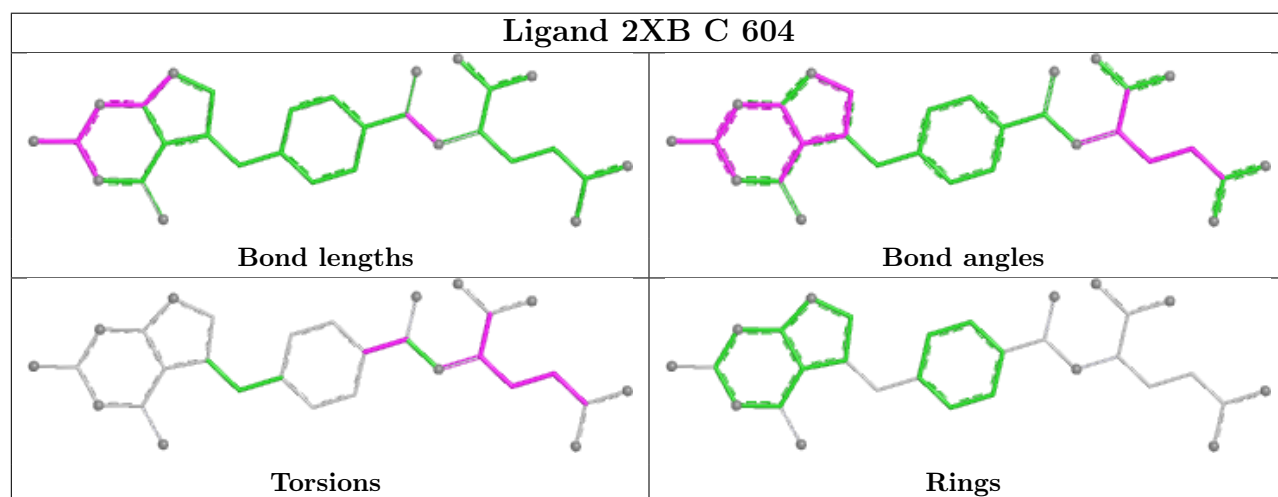
Ligand NDP C 601

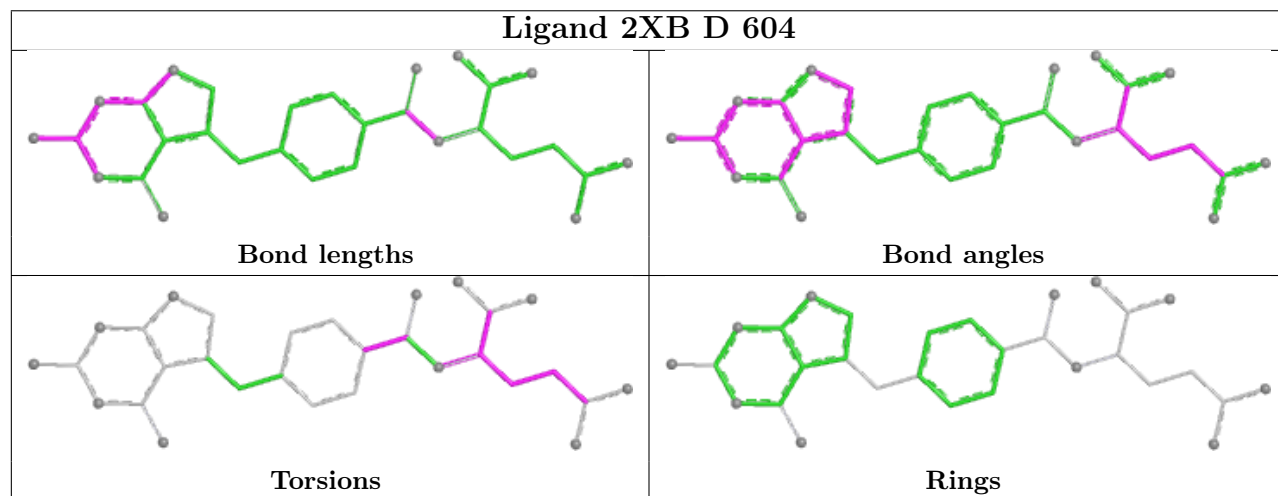
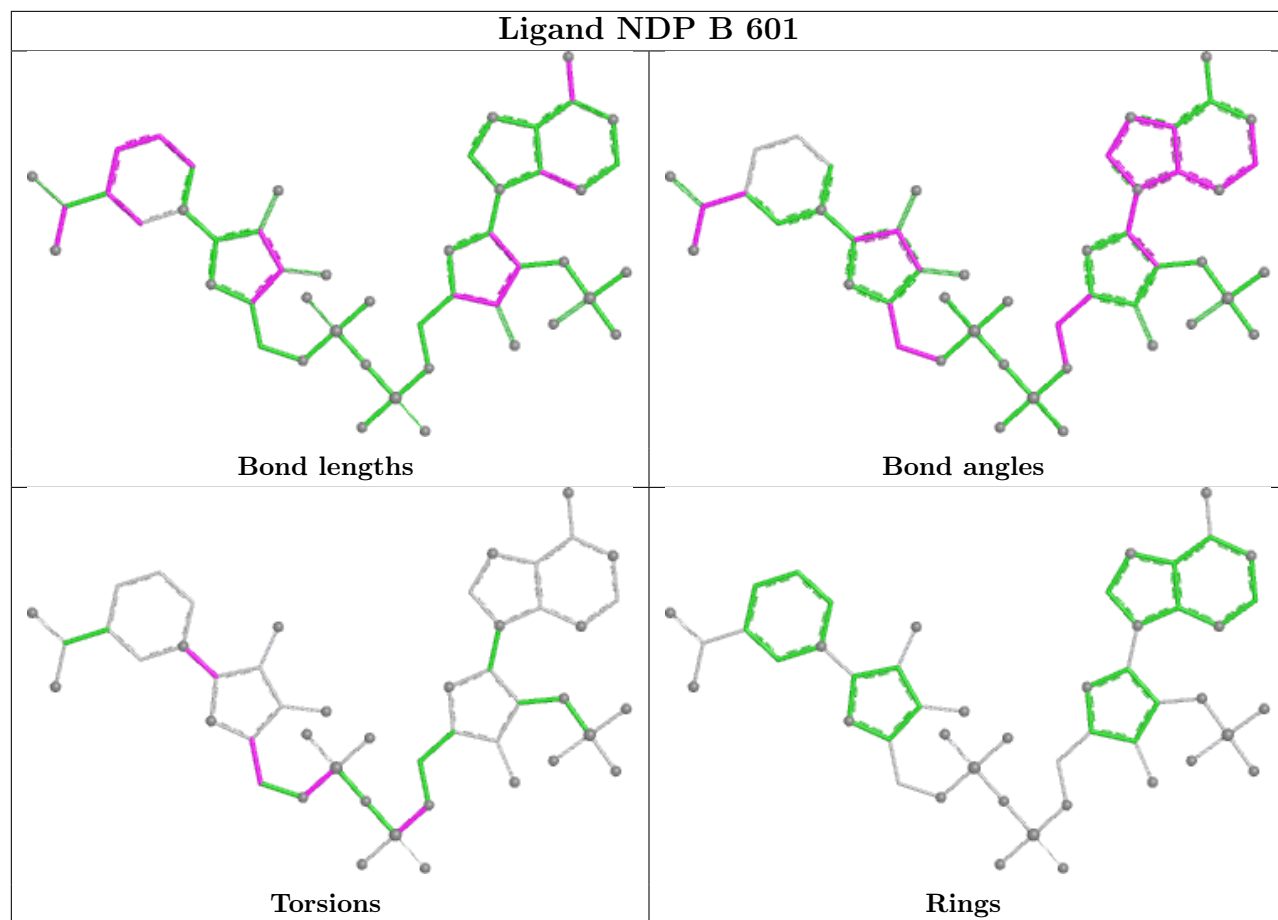


Ligand 2XB E 604

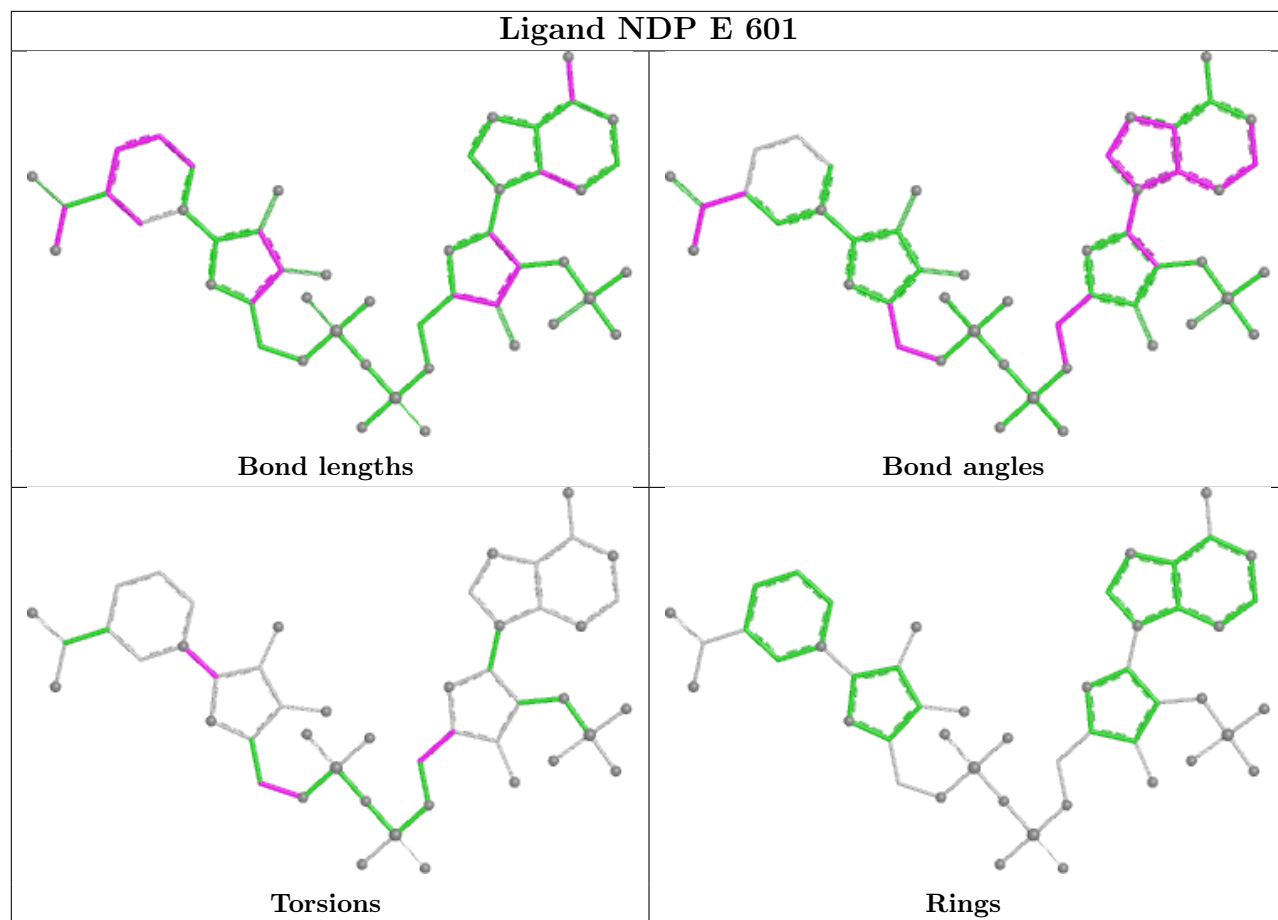


Ligand 2XB C 604

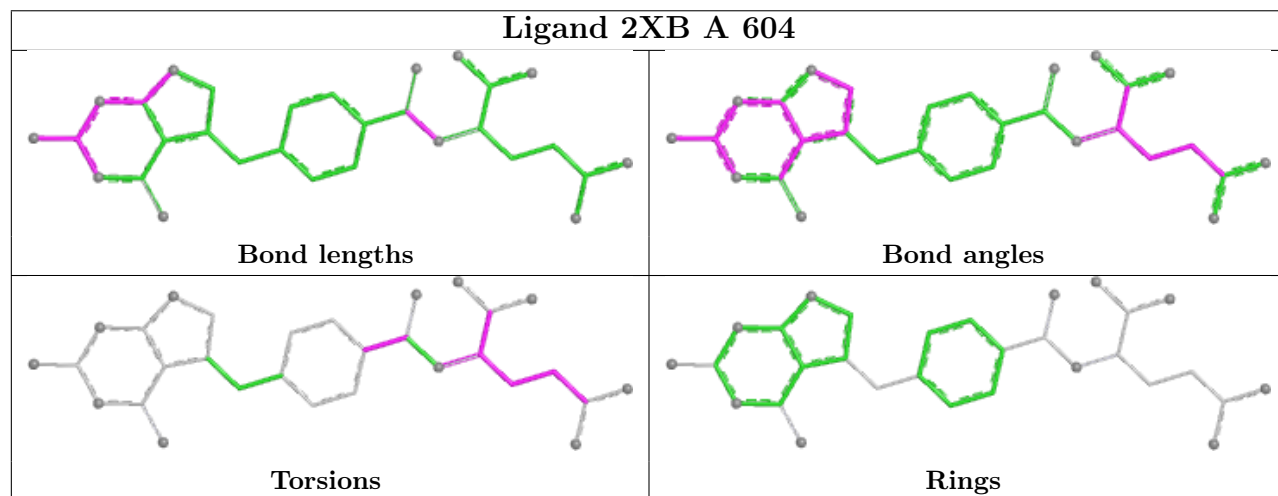




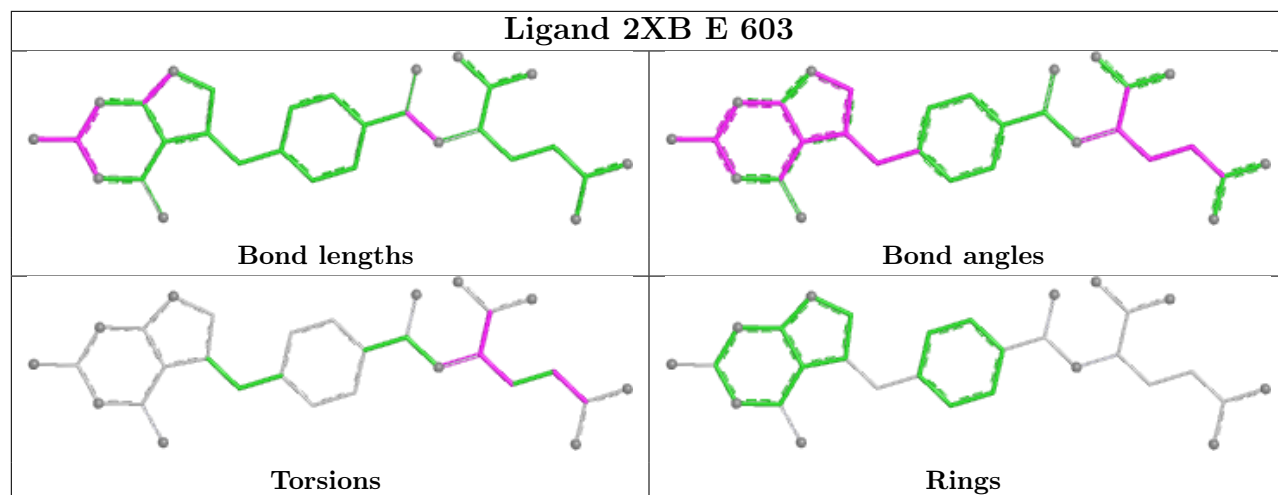
Ligand NDP E 601



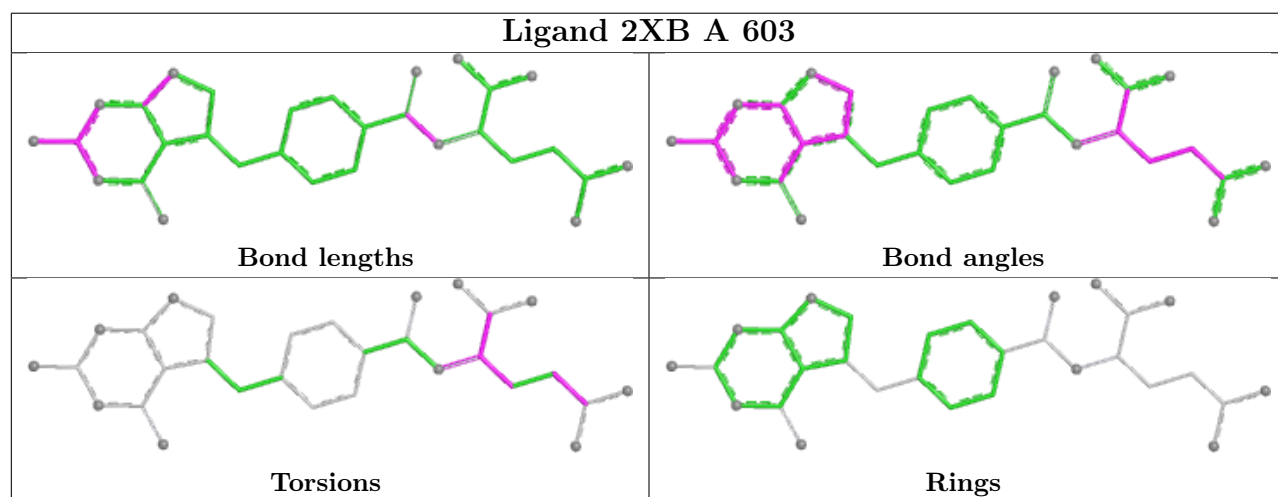
Ligand 2XB A 604



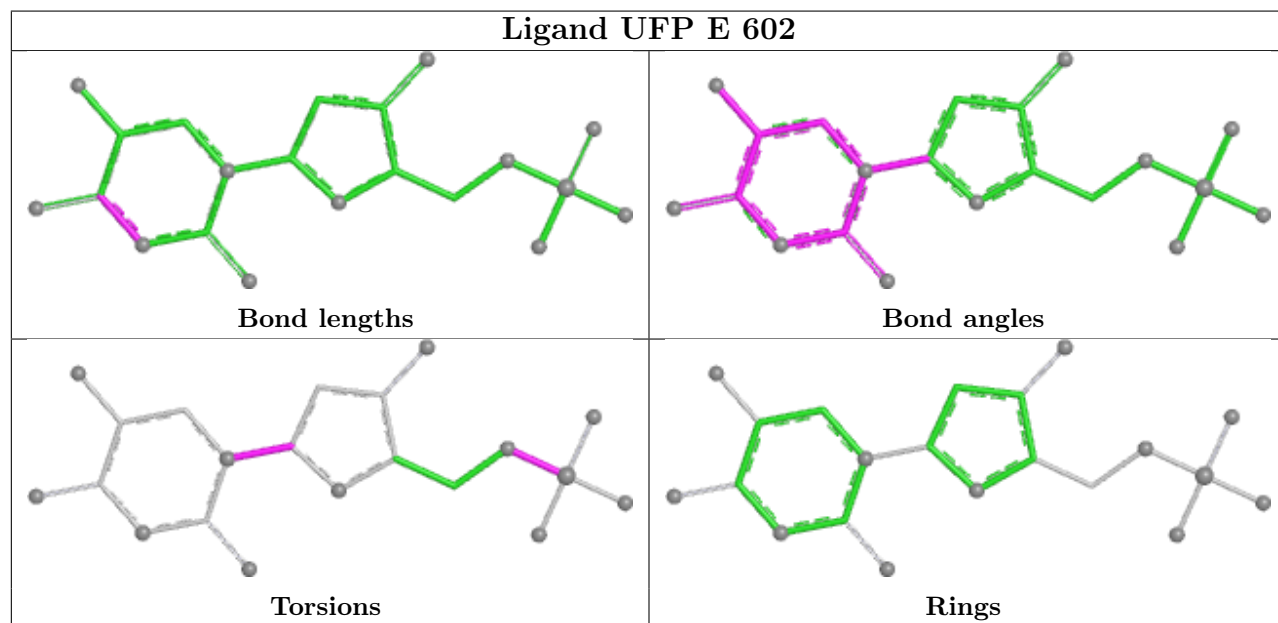
Ligand 2XB E 603



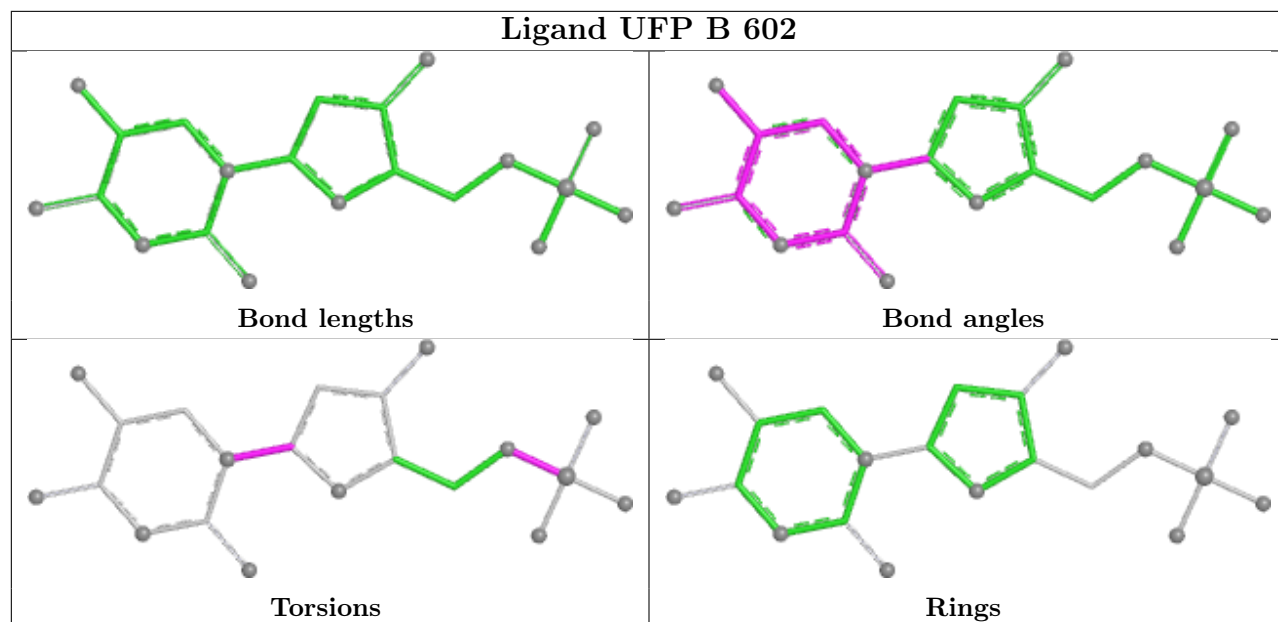
Ligand 2XB A 603



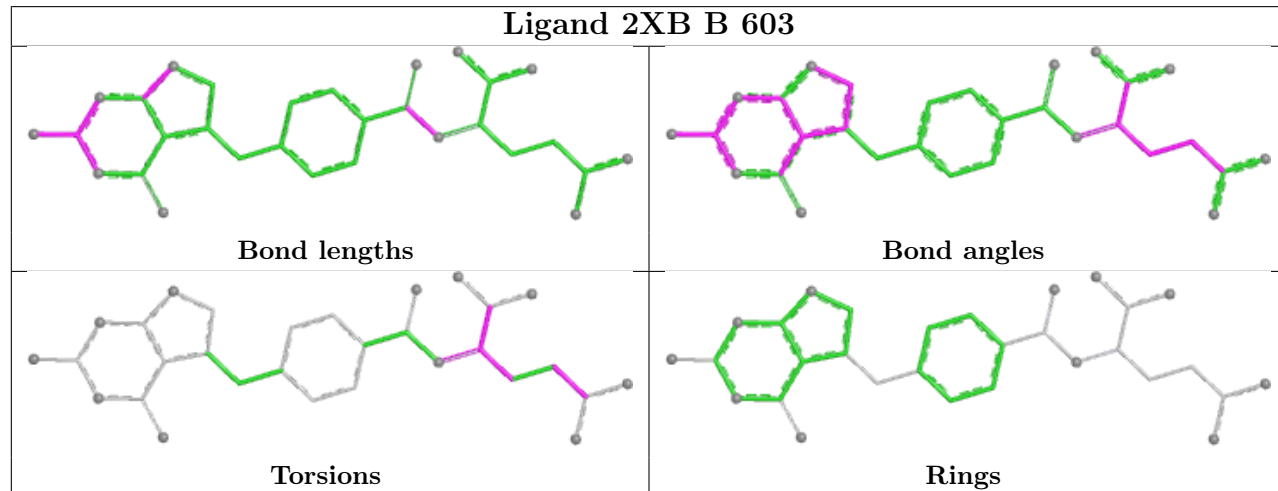
Ligand UFP E 602

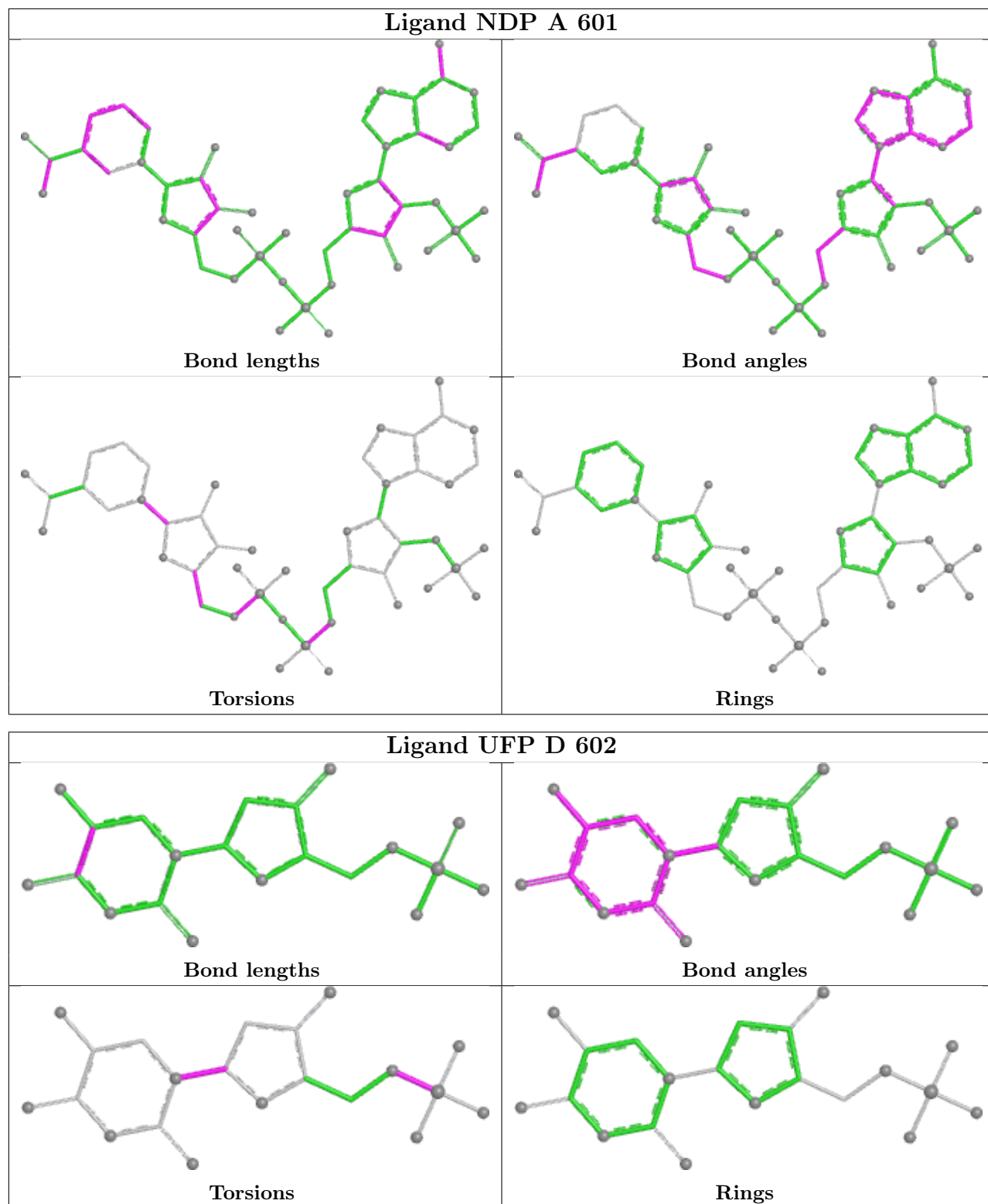


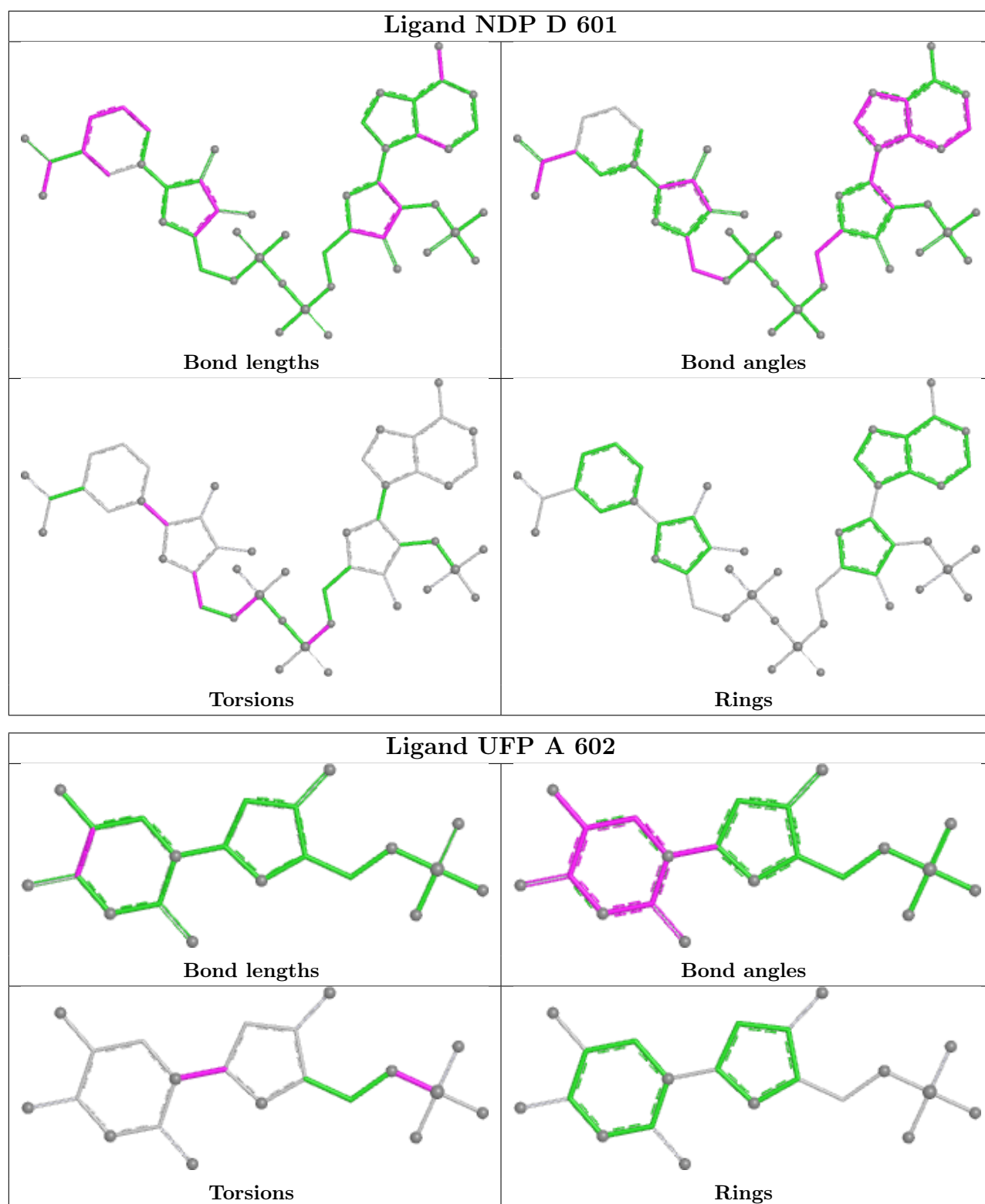
Ligand UFP B 602



Ligand 2XB B 603







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	505/521 (96%)	1.12	72 (14%) 6 5	31, 47, 79, 160	0
1	B	505/521 (96%)	1.34	106 (20%) 2 2	32, 57, 103, 166	0
1	C	505/521 (96%)	1.45	120 (23%) 2 1	32, 52, 91, 175	0
1	D	505/521 (96%)	1.40	111 (21%) 2 2	31, 61, 98, 198	0
1	E	505/521 (96%)	1.77	170 (33%) 1 1	47, 79, 122, 188	0
All	All	2525/2605 (96%)	1.42	579 (22%) 2 1	31, 59, 108, 198	0

All (579) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	LEU	11.9
1	A	193	LEU	9.1
1	B	171	ASP	8.6
1	E	139	GLU	8.2
1	C	193	LEU	7.9
1	A	82	ASP	7.7
1	B	84	ALA	7.7
1	A	171	ASP	7.5
1	D	82	ASP	7.5
1	E	82	ASP	7.5
1	D	193	LEU	7.3
1	C	82	ASP	7.2
1	D	171	ASP	7.2
1	C	171	ASP	7.1
1	B	61	SER	6.8
1	A	103	ASN	6.6
1	C	101	LEU	6.6
1	A	104	ASP	6.4
1	A	178	GLN	6.3
1	E	193	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	102	MET	6.1
1	B	82	ASP	6.0
1	D	102	MET	5.9
1	C	97	SER	5.8
1	B	62	ILE	5.8
1	B	117	SER	5.5
1	A	68	LYS	5.5
1	B	68	LYS	5.5
1	C	104	ASP	5.4
1	D	101	LEU	5.4
1	D	178	GLN	5.3
1	B	104	ASP	5.3
1	E	380	LYS	5.2
1	A	61	SER	5.2
1	E	171	ASP	5.2
1	B	178	GLN	5.1
1	C	341	ILE	5.1
1	E	61	SER	5.1
1	B	63	GLY	5.0
1	B	138	LEU	5.0
1	E	101	LEU	5.0
1	E	140	ASP	5.0
1	B	341	ILE	4.9
1	A	140	ASP	4.9
1	E	62	ILE	4.9
1	E	117	SER	4.9
1	B	101	LEU	4.8
1	D	61	SER	4.8
1	E	84	ALA	4.8
1	E	104	ASP	4.8
1	C	102	MET	4.8
1	E	316	TRP	4.8
1	A	62	ILE	4.7
1	D	62	ILE	4.7
1	D	68	LYS	4.7
1	C	100	ASN	4.7
1	B	99	GLU	4.7
1	E	24	GLN	4.6
1	C	324	TYR	4.6
1	B	100	ASN	4.6
1	C	114	GLY	4.5
1	E	341	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	361	THR	4.5
1	A	101	LEU	4.4
1	A	84	ALA	4.4
1	D	117	SER	4.3
1	D	194	LYS	4.3
1	C	121	ASP	4.3
1	E	342	TYR	4.3
1	A	194	LYS	4.2
1	C	178	GLN	4.2
1	C	61	SER	4.2
1	C	399	LEU	4.2
1	C	359	ASP	4.2
1	E	138	LEU	4.2
1	C	208	GLY	4.2
1	E	454	GLY	4.2
1	A	138	LEU	4.2
1	D	84	ALA	4.1
1	A	114	GLY	4.1
1	C	343	GLY	4.1
1	A	83	GLU	4.1
1	C	317	SER	4.1
1	C	521	VAL	4.1
1	A	63	GLY	4.1
1	E	97	SER	4.0
1	E	127	PHE	4.0
1	D	97	SER	4.0
1	C	149	GLU	4.0
1	B	140	ASP	3.9
1	D	104	ASP	3.9
1	C	140	ASP	3.9
1	D	121	ASP	3.9
1	C	103	ASN	3.9
1	B	363	VAL	3.9
1	E	194	LYS	3.8
1	E	102	MET	3.8
1	D	123	LEU	3.8
1	C	63	GLY	3.8
1	E	49	LYS	3.8
1	E	68	LYS	3.8
1	D	140	ASP	3.8
1	D	103	ASN	3.8
1	D	149	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	102	MET	3.7
1	E	514	THR	3.7
1	C	5	ASN	3.7
1	C	209	ILE	3.7
1	E	259	GLY	3.7
1	D	100	ASN	3.7
1	E	209	ILE	3.6
1	D	322	LYS	3.6
1	B	120	ARG	3.6
1	E	178	GLN	3.6
1	E	25	LEU	3.6
1	C	98	ILE	3.6
1	C	322	LYS	3.6
1	D	341	ILE	3.6
1	B	113	CYS	3.6
1	D	151	PRO	3.6
1	E	79	LEU	3.6
1	E	211	LYS	3.6
1	A	296	ILE	3.6
1	E	5	ASN	3.6
1	A	121	ASP	3.6
1	C	351	GLY	3.6
1	C	68	LYS	3.6
1	C	62	ILE	3.5
1	D	211	LYS	3.5
1	D	63	GLY	3.5
1	A	100	ASN	3.5
1	A	363	VAL	3.5
1	E	389	TRP	3.5
1	D	120	ARG	3.5
1	C	84	ALA	3.4
1	A	99	GLU	3.4
1	B	89	VAL	3.4
1	D	409	TYR	3.4
1	D	317	SER	3.4
1	E	361	THR	3.4
1	E	66	PRO	3.4
1	E	521	VAL	3.4
1	D	209	ILE	3.4
1	E	300	LYS	3.4
1	C	319	ASN	3.4
1	A	97	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	114	GLY	3.4
1	B	52	LEU	3.3
1	D	138	LEU	3.3
1	E	328	ILE	3.3
1	A	409	TYR	3.3
1	D	17	SER	3.3
1	B	79	LEU	3.3
1	B	127	PHE	3.3
1	E	100	ASN	3.3
1	E	271	ARG	3.3
1	B	80	PRO	3.3
1	D	79	LEU	3.3
1	B	103	ASN	3.3
1	E	284	LYS	3.2
1	E	322	LYS	3.2
1	C	128	VAL	3.2
1	E	319	ASN	3.2
1	E	121	ASP	3.2
1	E	429	LEU	3.2
1	D	324	TYR	3.2
1	B	144	ASP	3.2
1	E	32	ASP	3.2
1	C	194	LYS	3.2
1	D	124	LYS	3.2
1	E	308	LEU	3.2
1	C	296	ILE	3.2
1	D	127	PHE	3.2
1	D	128	VAL	3.2
1	C	354	LYS	3.2
1	E	123	LEU	3.2
1	B	91	PHE	3.2
1	C	333	ARG	3.1
1	B	81	GLN	3.1
1	E	314	TYR	3.1
1	D	314	TYR	3.1
1	B	5	ASN	3.1
1	D	255	GLU	3.1
1	B	514	THR	3.1
1	D	150	ILE	3.1
1	B	106	SER	3.1
1	B	121	ASP	3.1
1	E	359	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	453	PRO	3.1
1	C	28	SER	3.1
1	A	3	GLU	3.0
1	C	39	ILE	3.0
1	A	59	TRP	3.0
1	E	489	PHE	3.0
1	E	265	ILE	3.0
1	B	128	VAL	3.0
1	E	335	GLU	3.0
1	C	257	ARG	3.0
1	D	296	ILE	3.0
1	C	79	LEU	3.0
1	C	17	SER	3.0
1	D	99	GLU	3.0
1	A	60	ASP	3.0
1	B	60	ASP	3.0
1	A	326	GLU	2.9
1	E	255	GLU	2.9
1	E	360	TYR	2.9
1	C	259	GLY	2.9
1	E	208	GLY	2.9
1	E	363	VAL	2.9
1	D	83	GLU	2.9
1	C	314	TYR	2.9
1	C	75	ILE	2.9
1	E	428	GLY	2.9
1	E	262	THR	2.9
1	E	520	ALA	2.9
1	C	99	GLU	2.9
1	C	352	GLU	2.9
1	C	376	LYS	2.9
1	E	312	LYS	2.9
1	A	317	SER	2.9
1	D	195	SER	2.9
1	B	342	TYR	2.9
1	C	342	TYR	2.9
1	D	474	LYS	2.9
1	E	248	LEU	2.9
1	D	359	ASP	2.9
1	B	474	LYS	2.9
1	E	89	VAL	2.9
1	D	494	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	395	SER	2.8
1	E	296	ILE	2.8
1	B	259	GLY	2.8
1	B	322	LYS	2.8
1	E	113	CYS	2.8
1	E	52	LEU	2.8
1	B	200	VAL	2.8
1	A	209	ILE	2.8
1	B	34	LYS	2.8
1	C	330	LEU	2.8
1	E	67	LEU	2.8
1	E	313	VAL	2.8
1	E	289	ARG	2.8
1	A	341	ILE	2.8
1	B	195	SER	2.8
1	D	284	LYS	2.8
1	B	32	ASP	2.8
1	C	138	LEU	2.8
1	A	357	HIS	2.8
1	C	83	GLU	2.8
1	C	494	GLU	2.8
1	B	71	ILE	2.8
1	A	117	SER	2.8
1	A	399	LEU	2.8
1	A	149	GLU	2.8
1	C	3	GLU	2.8
1	C	493	VAL	2.8
1	E	315	ILE	2.7
1	E	303	THR	2.7
1	A	113	CYS	2.7
1	E	291	ILE	2.7
1	E	195	SER	2.7
1	A	273	ASP	2.7
1	B	53	ILE	2.7
1	D	244	LEU	2.7
1	E	120	ARG	2.7
1	A	404	VAL	2.7
1	D	96	ASP	2.7
1	D	164	CYS	2.7
1	B	123	LEU	2.7
1	C	356	MET	2.7
1	D	308	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	429	LEU	2.7
1	B	255	GLU	2.7
1	E	6	VAL	2.7
1	C	340	PRO	2.7
1	E	432	PRO	2.7
1	D	309	ILE	2.6
1	E	75	ILE	2.6
1	A	44	CYS	2.6
1	A	343	GLY	2.6
1	E	351	GLY	2.6
1	B	220	LYS	2.6
1	E	406	SER	2.6
1	B	24	GLN	2.6
1	B	265	ILE	2.6
1	D	75	ILE	2.6
1	B	326	GLU	2.6
1	B	492	LYS	2.6
1	C	255	GLU	2.6
1	C	331	GLY	2.6
1	A	5	ASN	2.6
1	D	5	ASN	2.6
1	D	89	VAL	2.6
1	E	103	ASN	2.6
1	E	128	VAL	2.6
1	C	262	THR	2.6
1	E	484	PHE	2.6
1	B	279	PRO	2.6
1	B	378	ASN	2.6
1	D	175	PHE	2.6
1	D	377	ASN	2.6
1	E	112	VAL	2.6
1	B	30	SER	2.6
1	B	97	SER	2.6
1	C	195	SER	2.6
1	C	248	LEU	2.6
1	C	210	ARG	2.6
1	C	284	LYS	2.6
1	E	370	LYS	2.6
1	E	99	GLU	2.6
1	E	352	GLU	2.6
1	C	362	GLY	2.6
1	D	113	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	391	PRO	2.6
1	B	317	SER	2.5
1	E	197	ASP	2.5
1	E	146	TYR	2.5
1	E	83	GLU	2.5
1	C	318	GLY	2.5
1	E	91	PHE	2.5
1	E	175	PHE	2.5
1	E	126	ASN	2.5
1	A	211	LYS	2.5
1	E	488	LYS	2.5
1	B	334	GLU	2.5
1	D	342	TYR	2.5
1	E	324	TYR	2.5
1	B	396	GLN	2.5
1	D	514	THR	2.5
1	C	4	LYS	2.5
1	E	29	ILE	2.5
1	E	273	ASP	2.5
1	E	354	LYS	2.5
1	B	83	GLU	2.5
1	D	114	GLY	2.5
1	B	175	PHE	2.5
1	E	519	MET	2.5
1	A	322	LYS	2.5
1	D	300	LYS	2.5
1	E	378	ASN	2.5
1	A	46	SER	2.5
1	B	118	ILE	2.5
1	C	243	LEU	2.5
1	C	55	GLY	2.5
1	D	351	GLY	2.5
1	E	305	GLY	2.5
1	B	112	VAL	2.5
1	E	345	GLN	2.5
1	E	225	ASN	2.4
1	B	209	ILE	2.4
1	C	315	ILE	2.4
1	E	399	LEU	2.4
1	B	357	HIS	2.4
1	E	357	HIS	2.4
1	E	381	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	255	GLU	2.4
1	B	108	GLU	2.4
1	B	452	GLU	2.4
1	C	142	GLU	2.4
1	E	95	GLU	2.4
1	B	66	PRO	2.4
1	B	4	LYS	2.4
1	B	247	VAL	2.4
1	C	396	GLN	2.4
1	D	354	LYS	2.4
1	D	363	VAL	2.4
1	B	137	ALA	2.4
1	B	98	ILE	2.4
1	D	206	ILE	2.4
1	E	385	ILE	2.4
1	E	386	LEU	2.4
1	E	460	ILE	2.4
1	B	59	TRP	2.4
1	C	197	ASP	2.4
1	E	3	GLU	2.4
1	E	80	PRO	2.4
1	C	360	TYR	2.4
1	E	257	ARG	2.4
1	D	273	ASP	2.4
1	E	96	ASP	2.4
1	E	125	ASP	2.4
1	B	380	LYS	2.4
1	D	80	PRO	2.4
1	E	4	LYS	2.4
1	E	490	LYS	2.4
1	D	360	TYR	2.4
1	B	361	THR	2.4
1	D	315	ILE	2.4
1	D	109	ASN	2.4
1	E	377	ASN	2.4
1	C	335	GLU	2.4
1	D	152	GLU	2.4
1	C	96	ASP	2.4
1	C	312	LYS	2.4
1	C	432	PRO	2.4
1	A	271	ARG	2.4
1	A	514	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	335	GLU	2.3
1	D	352	GLU	2.3
1	A	474	LYS	2.3
1	E	48	LYS	2.3
1	E	503	ASP	2.3
1	D	18	GLY	2.3
1	E	63	GLY	2.3
1	C	404	VAL	2.3
1	D	404	VAL	2.3
1	A	98	ILE	2.3
1	B	150	ILE	2.3
1	C	258	THR	2.3
1	E	307	HIS	2.3
1	D	319	ASN	2.3
1	E	495	ASN	2.3
1	B	49	LYS	2.3
1	B	194	LYS	2.3
1	C	467	GLU	2.3
1	A	32	ASP	2.3
1	A	81	GLN	2.3
1	B	244	LEU	2.3
1	B	399	LEU	2.3
1	E	292	PHE	2.3
1	E	393	ALA	2.3
1	E	487	LEU	2.3
1	B	75	ILE	2.3
1	E	458	ILE	2.3
1	D	361	THR	2.3
1	D	49	LYS	2.3
1	A	250	ASN	2.3
1	E	205	GLU	2.3
1	E	334	GLU	2.3
1	B	77	SER	2.3
1	C	30	SER	2.3
1	E	392	SER	2.3
1	C	279	PRO	2.3
1	C	363	VAL	2.3
1	D	247	VAL	2.3
1	A	244	LEU	2.3
1	D	67	LEU	2.3
1	E	137	ALA	2.3
1	C	380	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	32	ASP	2.3
1	C	105	ASP	2.3
1	D	401	PRO	2.3
1	E	106	SER	2.3
1	B	346	TRP	2.3
1	D	55	GLY	2.3
1	B	429	LEU	2.3
1	E	90	VAL	2.3
1	A	39	ILE	2.2
1	C	520	ALA	2.2
1	D	328	ILE	2.2
1	E	196	ILE	2.2
1	E	287	ALA	2.2
1	E	465	ILE	2.2
1	B	374	THR	2.2
1	D	142	GLU	2.2
1	E	452	GLU	2.2
1	C	414	ASN	2.2
1	A	56	ARG	2.2
1	A	28	SER	2.2
1	B	7	SER	2.2
1	B	18	GLY	2.2
1	B	14	VAL	2.2
1	B	487	LEU	2.2
1	D	248	LEU	2.2
1	E	346	TRP	2.2
1	E	420	LEU	2.2
1	C	328	ILE	2.2
1	D	217	LYS	2.2
1	E	35	PHE	2.2
1	D	520	ALA	2.2
1	E	98	ILE	2.2
1	E	309	ILE	2.2
1	E	517	MET	2.2
1	C	113	CYS	2.2
1	D	126	ASN	2.2
1	A	26	PRO	2.2
1	D	396	GLN	2.2
1	D	259	GLY	2.2
1	E	30	SER	2.2
1	B	88	VAL	2.2
1	B	90	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	316	TRP	2.2
1	A	393	ALA	2.2
1	B	142	GLU	2.2
1	E	408	TYR	2.2
1	A	15	LEU	2.2
1	C	106	SER	2.2
1	D	330	LEU	2.2
1	E	244	LEU	2.2
1	D	316	TRP	2.2
1	D	11	ALA	2.2
1	C	374	THR	2.2
1	B	56	ARG	2.2
1	E	210	ARG	2.2
1	C	377	ASN	2.2
1	D	400	PRO	2.2
1	B	124	LYS	2.2
1	E	376	LYS	2.2
1	E	320	GLY	2.2
1	D	28	SER	2.2
1	C	435	ILE	2.2
1	D	110	ILE	2.2
1	D	112	VAL	2.2
1	C	127	PHE	2.2
1	A	4	LYS	2.1
1	A	284	LYS	2.1
1	C	146	TYR	2.1
1	C	211	LYS	2.1
1	E	22	ASN	2.1
1	E	396	GLN	2.1
1	A	308	LEU	2.1
1	C	244	LEU	2.1
1	C	302	ASP	2.1
1	C	460	ILE	2.1
1	E	118	ILE	2.1
1	B	335	GLU	2.1
1	E	86	PRO	2.1
1	A	41	ASN	2.1
1	C	24	GLN	2.1
1	E	47	ASN	2.1
1	D	357	HIS	2.1
1	C	112	VAL	2.1
1	D	125	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	60	ASP	2.1
1	A	127	PHE	2.1
1	E	502	GLU	2.1
1	A	220	LYS	2.1
1	C	212	MET	2.1
1	B	248	LEU	2.1
1	C	308	LEU	2.1
1	D	420	LEU	2.1
1	C	390	ASN	2.1
1	A	115	GLY	2.1
1	E	224	TYR	2.1
1	E	85	ASP	2.1
1	C	77	SER	2.1
1	A	142	GLU	2.1
1	C	38	LYS	2.1
1	C	124	LYS	2.1
1	D	34	LYS	2.1
1	B	86	PRO	2.1
1	A	319	ASN	2.1
1	B	434	ASN	2.1
1	A	208	GLY	2.1
1	C	164	CYS	2.1
1	D	53	ILE	2.1
1	D	98	ILE	2.1
1	E	353	TYR	2.1
1	B	359	ASP	2.0
1	C	433	PHE	2.1
1	C	56	ARG	2.0
1	B	321	SER	2.0
1	C	388	ALA	2.0
1	D	3	GLU	2.0
1	E	38	LYS	2.0
1	E	151	PRO	2.0
1	A	429	LEU	2.0
1	D	81	GLN	2.0
1	E	427	LEU	2.0
1	B	109	ASN	2.0
1	C	167	ASN	2.0
1	B	107	ILE	2.0
1	B	196	ILE	2.0
1	C	288	ILE	2.0
1	E	110	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	404	VAL	2.0
1	E	493	VAL	2.0
1	D	326	GLU	2.0
1	D	335	GLU	2.0
1	D	376	LYS	2.0
1	E	34	LYS	2.0
1	D	422	GLN	2.0
1	B	206	ILE	2.0
1	B	296	ILE	2.0
1	C	305	GLY	2.0
1	E	350	ASN	2.0
1	C	271	ARG	2.0
1	D	200	VAL	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
4	2XB	B	604	30/30	0.81	0.21	60,66,87,89	0
2	NDP	B	601	48/48	0.82	0.18	79,90,94,99	0
4	2XB	C	603	30/30	0.84	0.18	61,69,83,89	0
4	2XB	E	603	30/30	0.84	0.19	87,95,109,115	0
2	NDP	D	601	48/48	0.85	0.17	62,73,77,82	0
4	2XB	E	604	30/30	0.85	0.17	65,72,93,95	0
4	2XB	D	604	30/30	0.86	0.18	51,57,78,80	0
4	2XB	A	603	30/30	0.86	0.17	47,55,69,75	0
4	2XB	C	604	30/30	0.86	0.17	44,50,71,73	0
4	2XB	B	603	30/30	0.87	0.19	61,69,83,89	0

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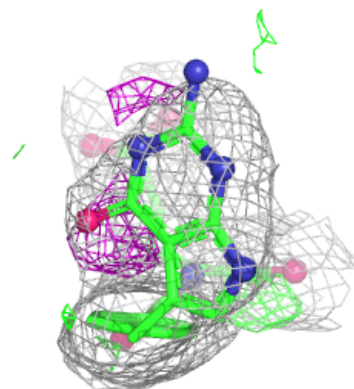
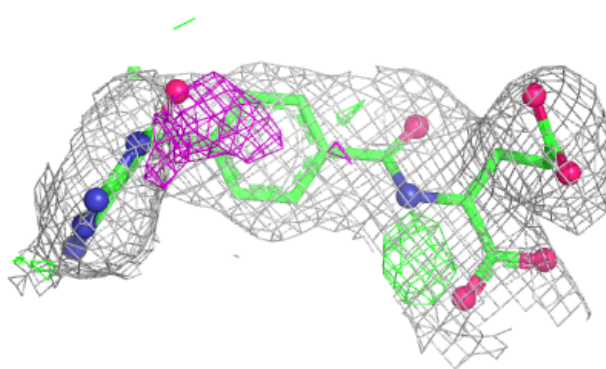
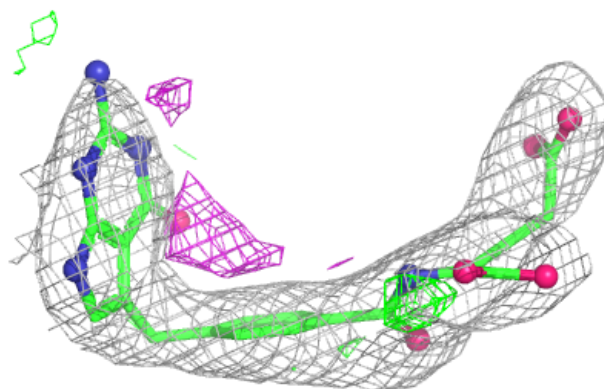
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UFP	E	602	21/21	0.88	0.14	80,89,97,115	0
4	2XB	A	604	30/30	0.88	0.15	37,44,64,67	0
4	2XB	D	603	30/30	0.88	0.19	71,79,93,99	0
3	UFP	C	602	21/21	0.89	0.15	57,66,74,92	0
2	NDP	C	601	48/48	0.89	0.15	45,56,60,65	0
2	NDP	A	601	48/48	0.90	0.14	47,58,62,68	0
2	NDP	E	601	48/48	0.90	0.13	69,80,84,90	0
3	UFP	A	602	21/21	0.90	0.14	41,50,58,76	0
3	UFP	B	602	21/21	0.93	0.14	54,64,71,90	0
3	UFP	D	602	21/21	0.95	0.10	60,70,78,96	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.

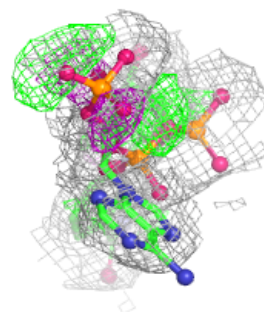
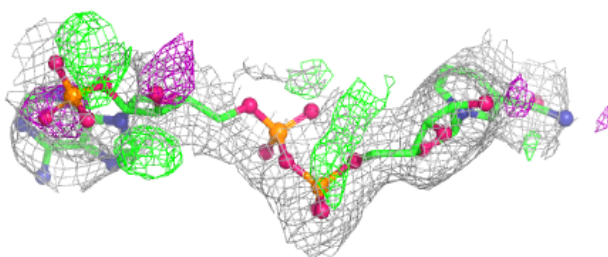
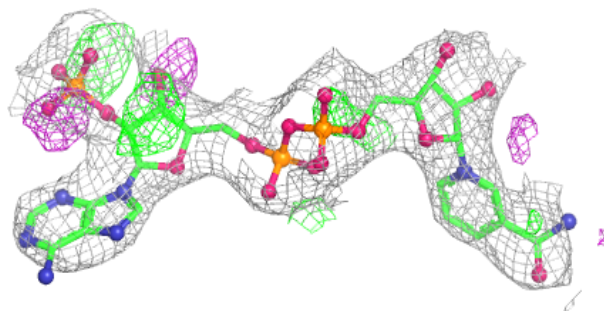
Electron density around 2XB B 604:

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

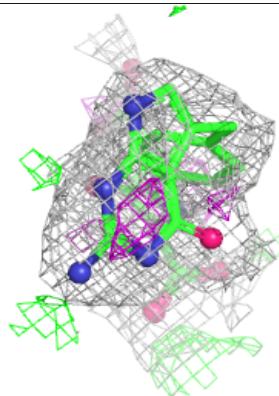
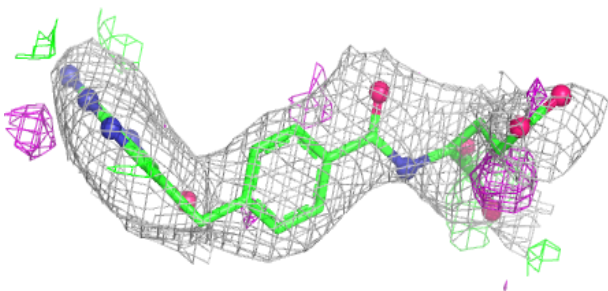
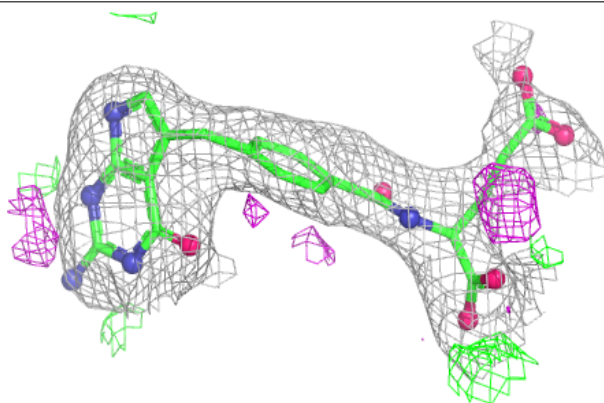


Electron density around NDP B 601:

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

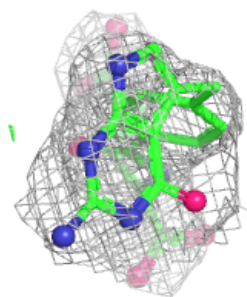
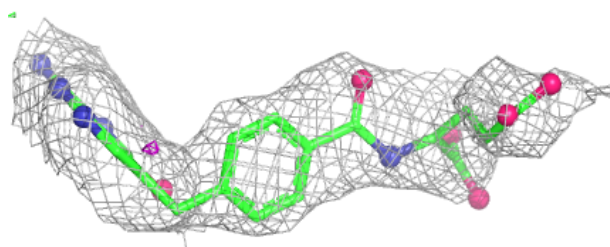
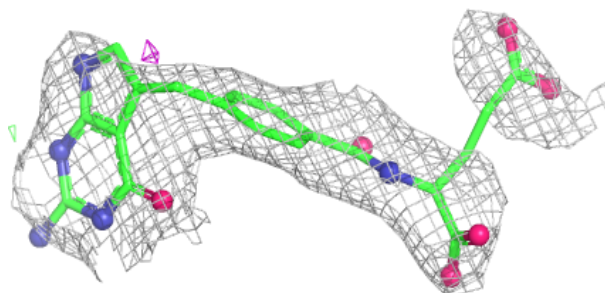
**Electron density around 2XB C 603:**

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

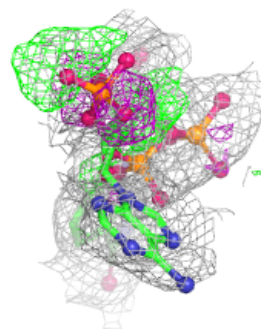
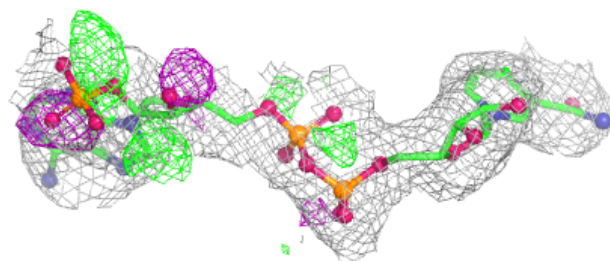
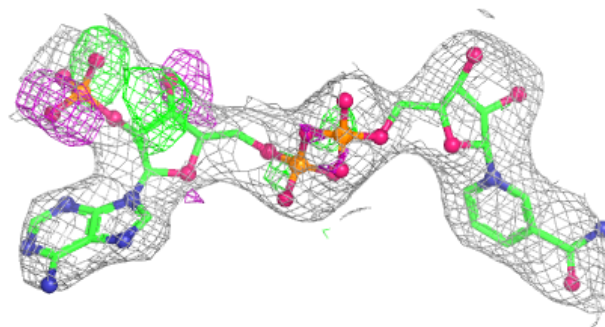


Electron density around 2XB E 603:

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

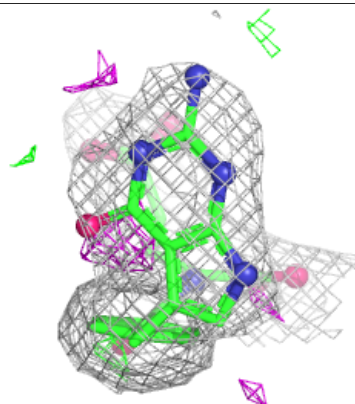
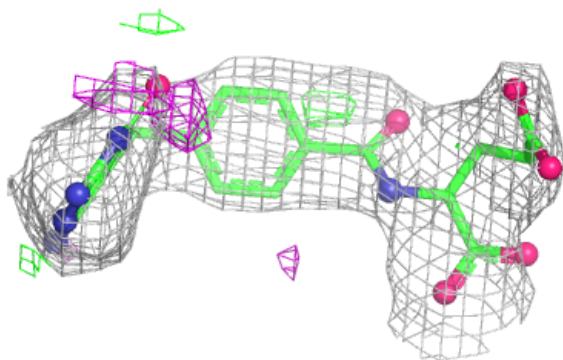
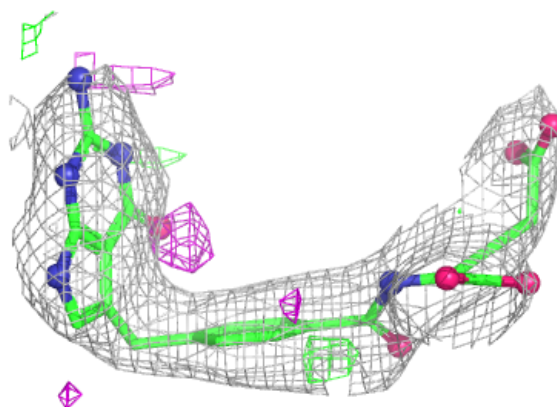
**Electron density around NDP D 601:**

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

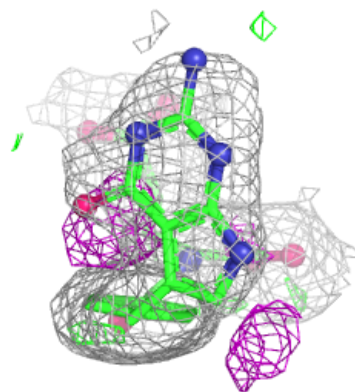
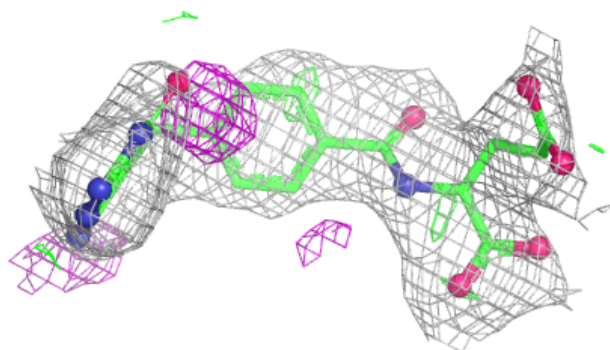
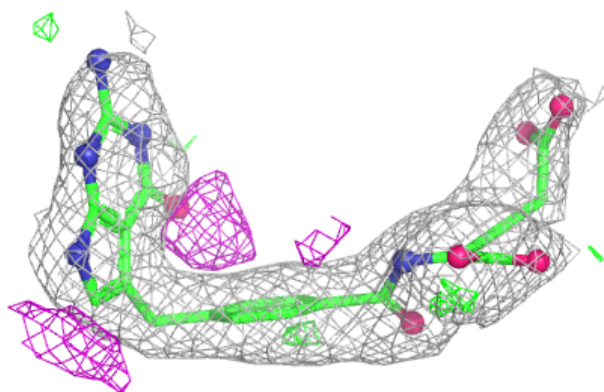


Electron density around 2XB E 604:

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

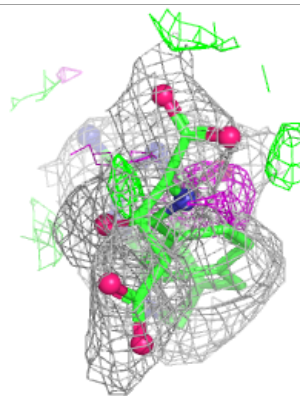
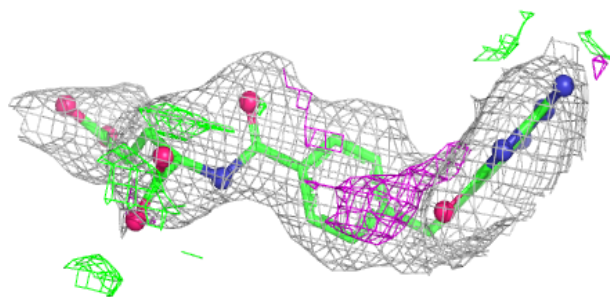
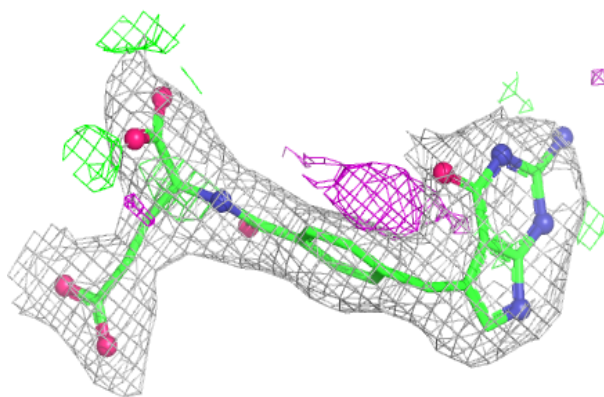
**Electron density around 2XB D 604:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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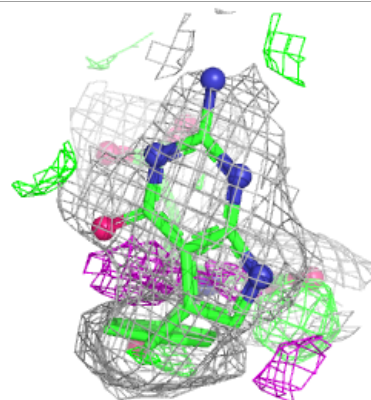
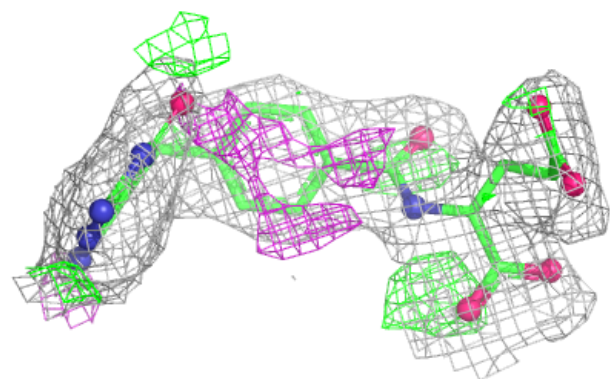
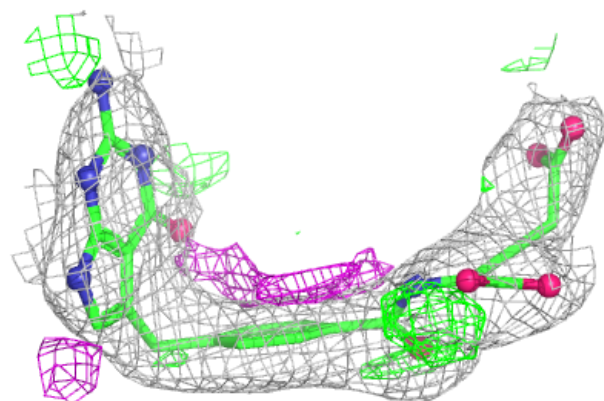


Electron density around 2XB A 603:

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and green (positive)

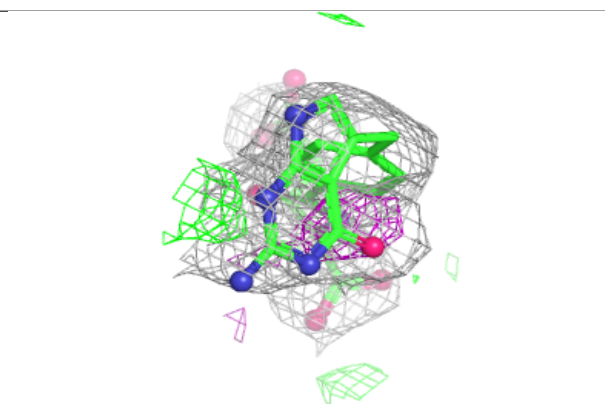
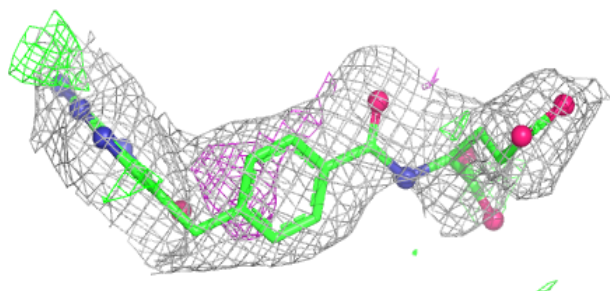
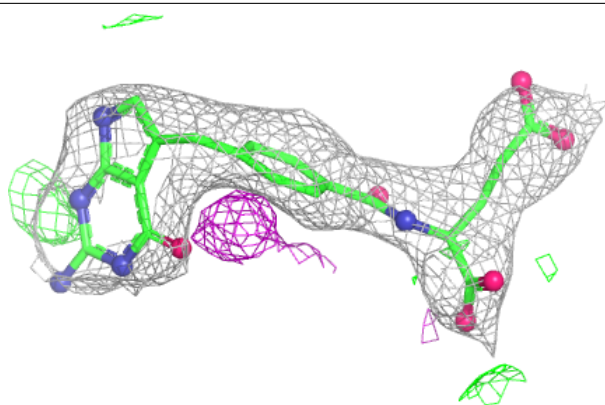
**Electron density around 2XB C 604:**

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and green (positive)

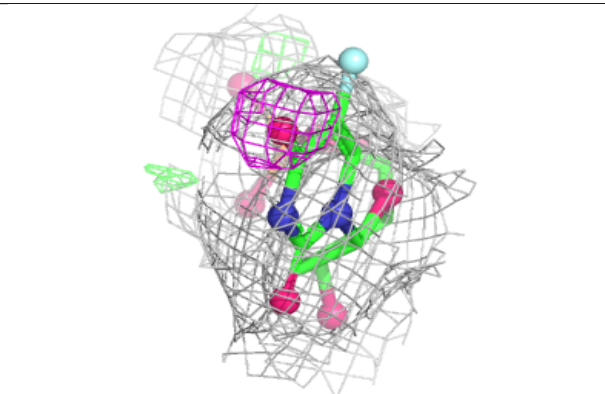
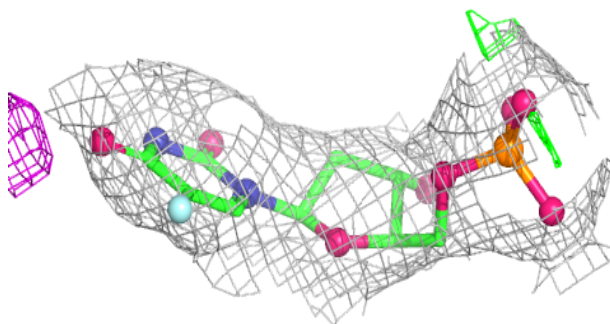
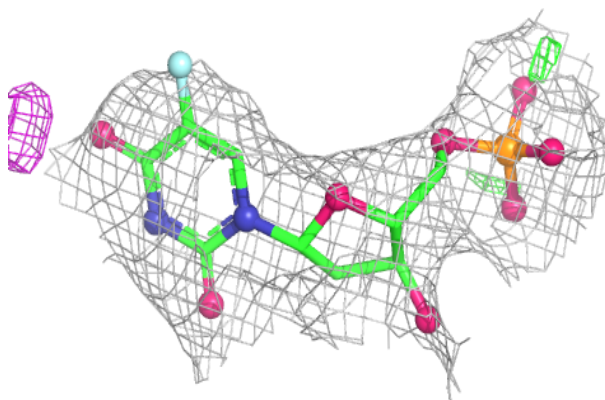


Electron density around 2XB B 603:

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and green (positive)

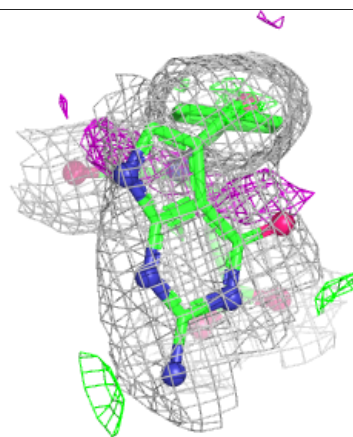
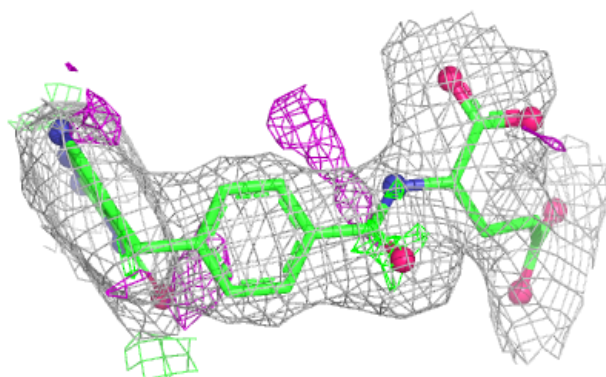
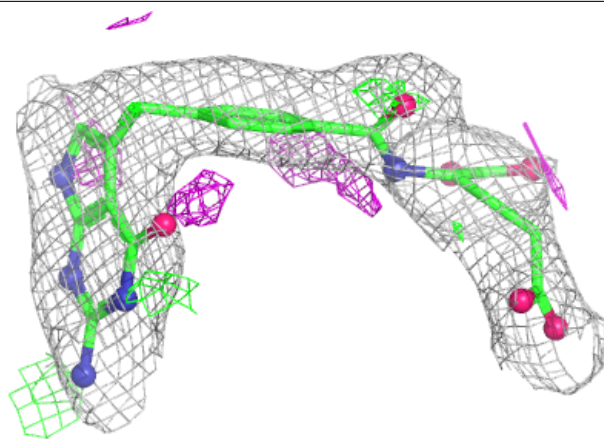
**Electron density around UFP E 602:**

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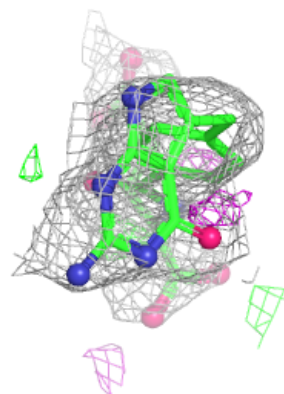
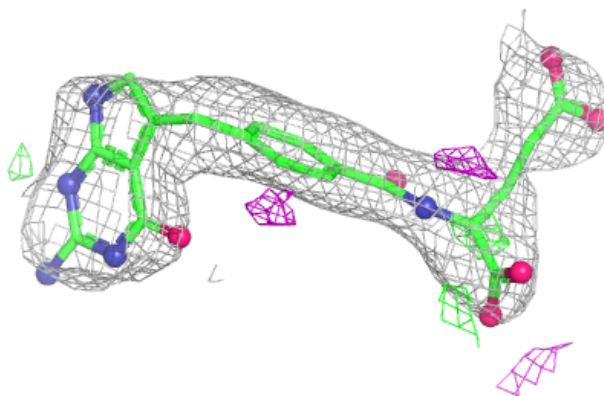


Electron density around 2XB A 604:

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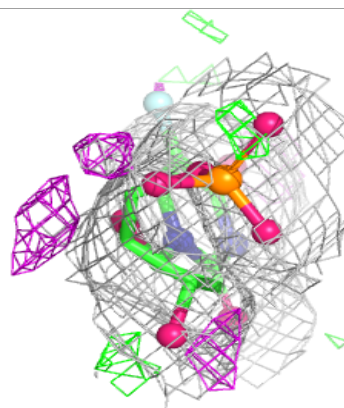
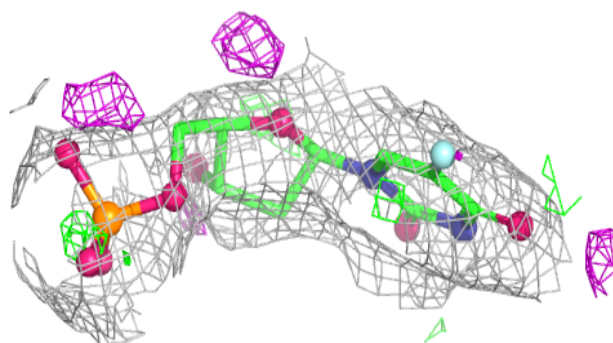
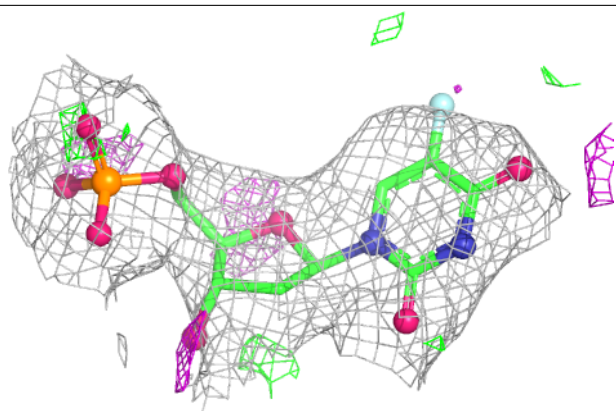
**Electron density around 2XB D 603:**

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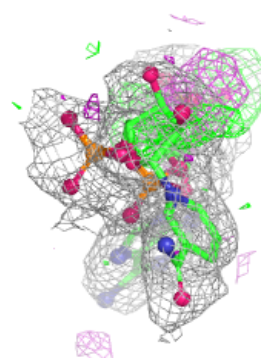
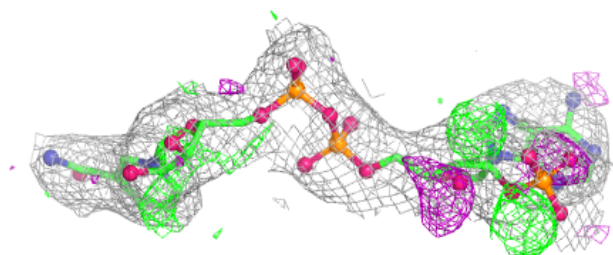
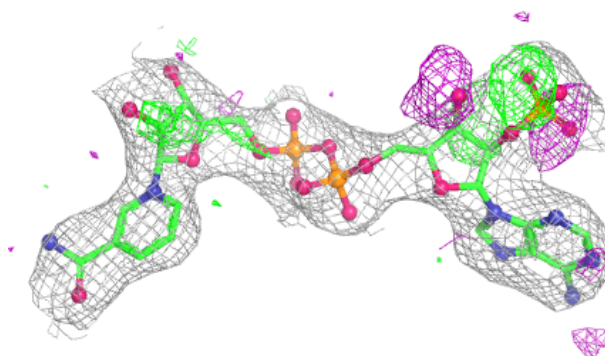


Electron density around UFP C 602:

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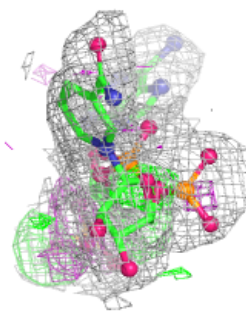
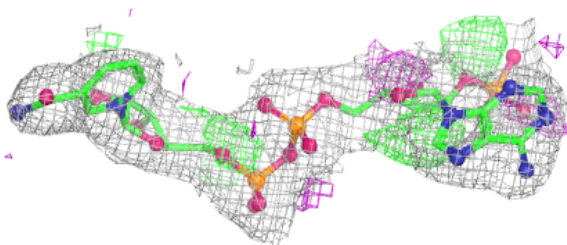
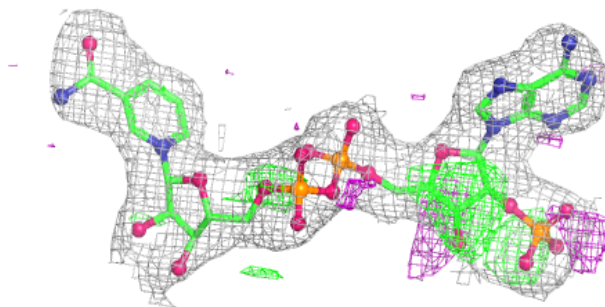
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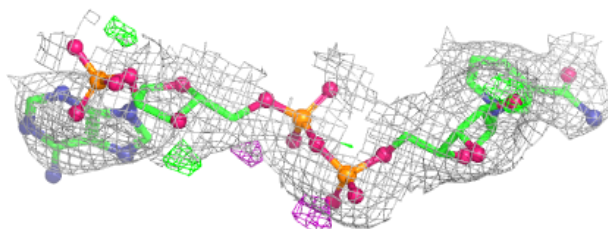
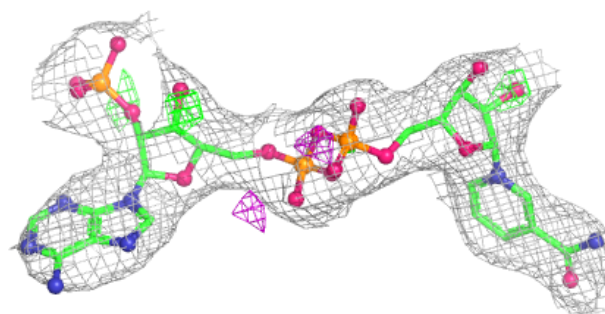


Electron density around NDP A 601:

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and green (positive)

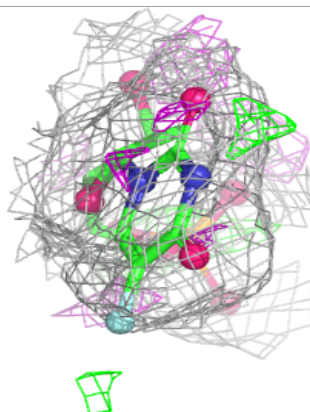
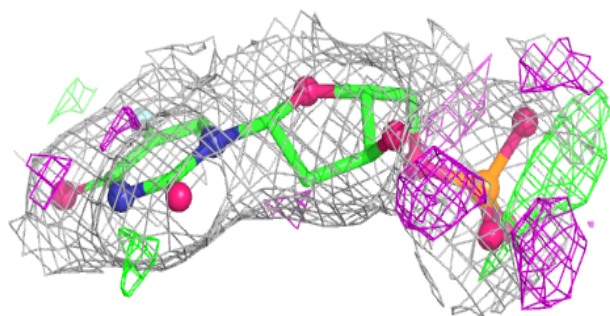
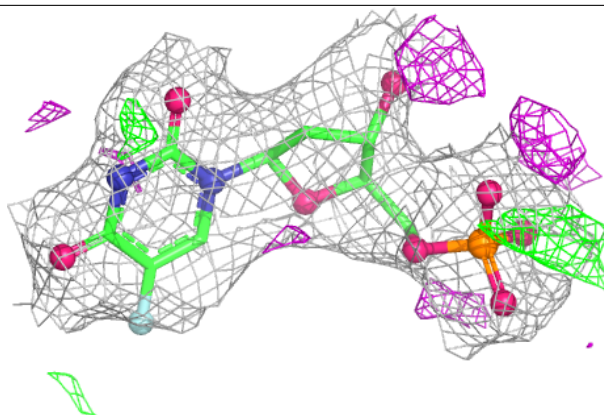
**Electron density around NDP E 601:**

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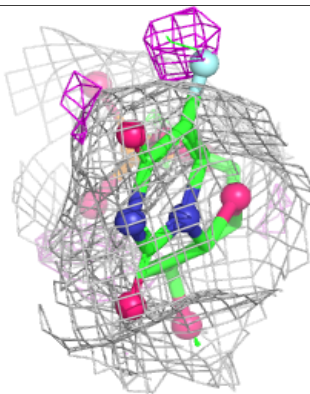
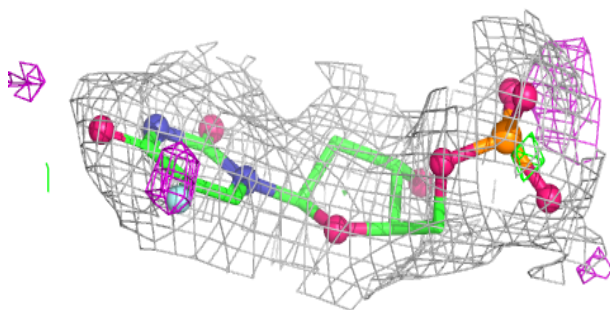
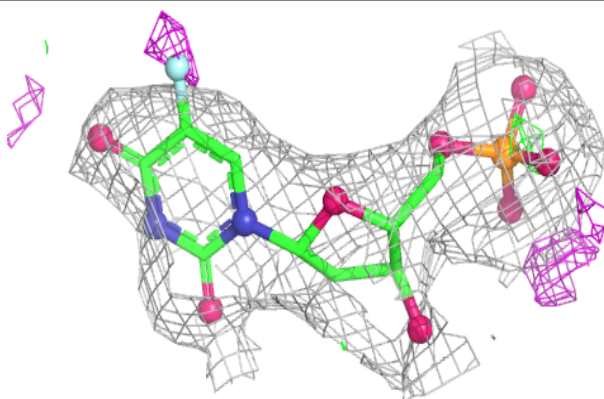


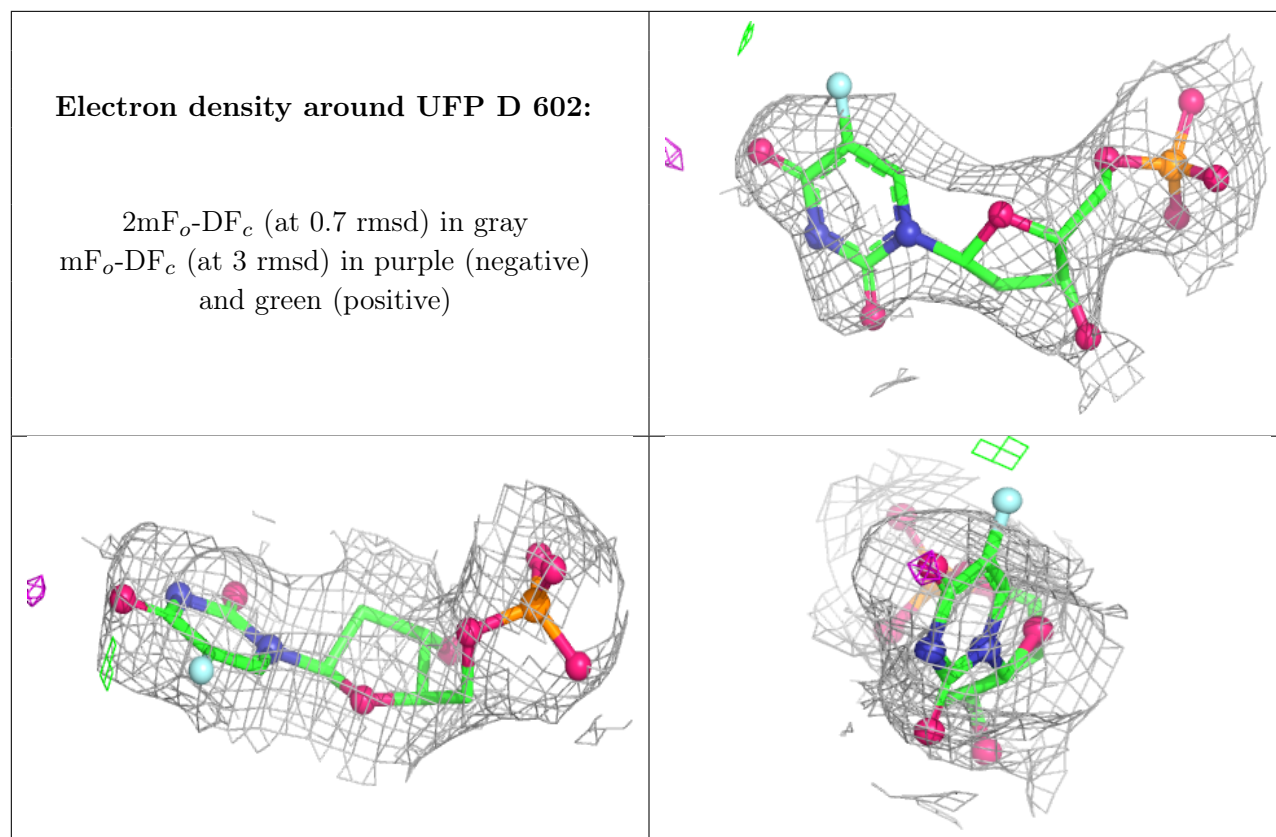
Electron density around UFP A 602:

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

**Electron density around UFP B 602:**

$2mF_o-DF_c$ (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.