



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:26 PM UTC

PDB ID : 4KYA / pdb_00004kya
Title : Crystal structure of non-classical TS inhibitor 3 in complex with Toxoplasma gondii TS-DHFR
Authors : Sharma, H.; Anderson, K.S.
Deposited on : 2013-05-28
Resolution : 3.26 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

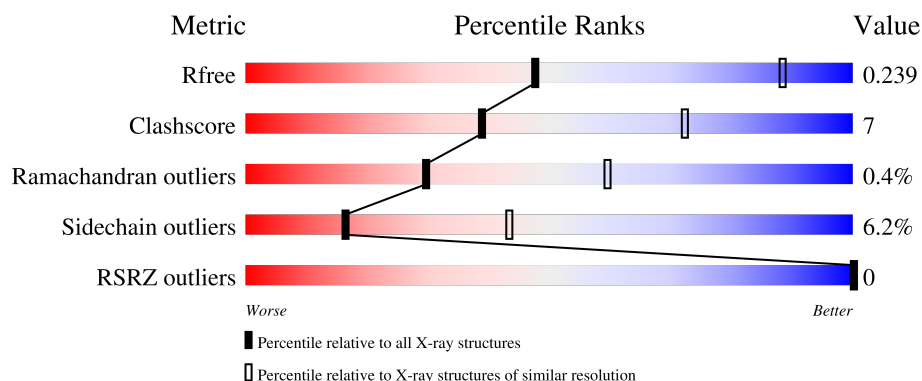
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

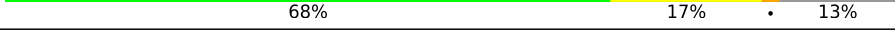
The reported resolution of this entry is 3.26 Å.

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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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

Mol	Chain	Length	Quality of chain
1	A	566	
1	B	566	
1	C	566	
1	D	566	
1	E	566	

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Mol	Chain	Length	Quality of chain
1	F	566	 68%17%•13%
1	G	566	 72%17%•10%
1	H	566	 69%16%•13%

2 Entry composition

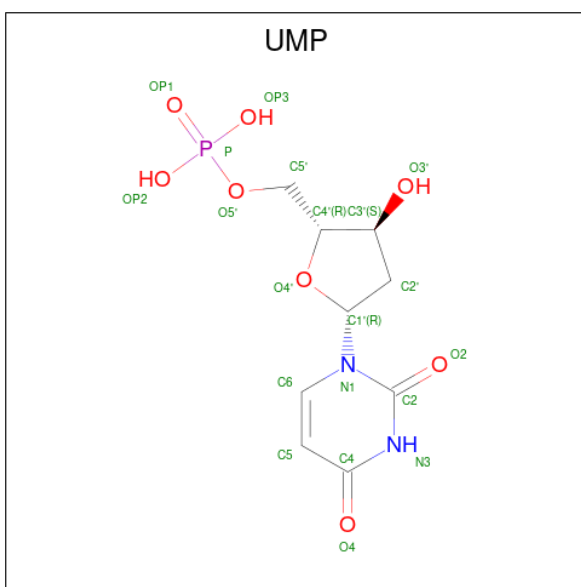
There are 5 unique types of molecules in this entry. The entry contains 33184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	B	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	C	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	D	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	E	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	F	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	G	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	H	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			

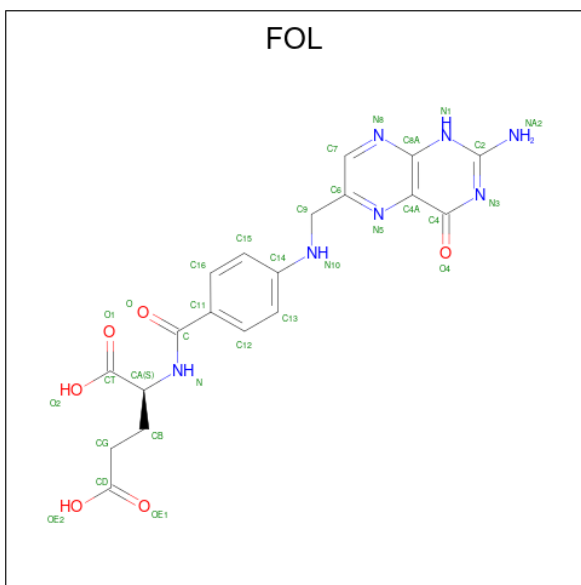
- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: C₉H₁₃N₂O₈P).



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

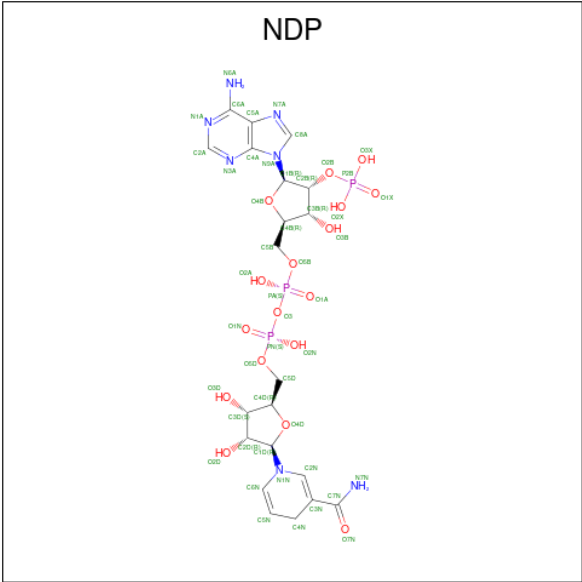
- Molecule 3 is 2-Amino-5-(1-naphthylsulfanyl)-3,9-dihydro-4H-pyrimido[4,5-b]indol-4-one (CCD ID: 1UG) (formula: C₂₀H₁₄N₄OS).





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

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).

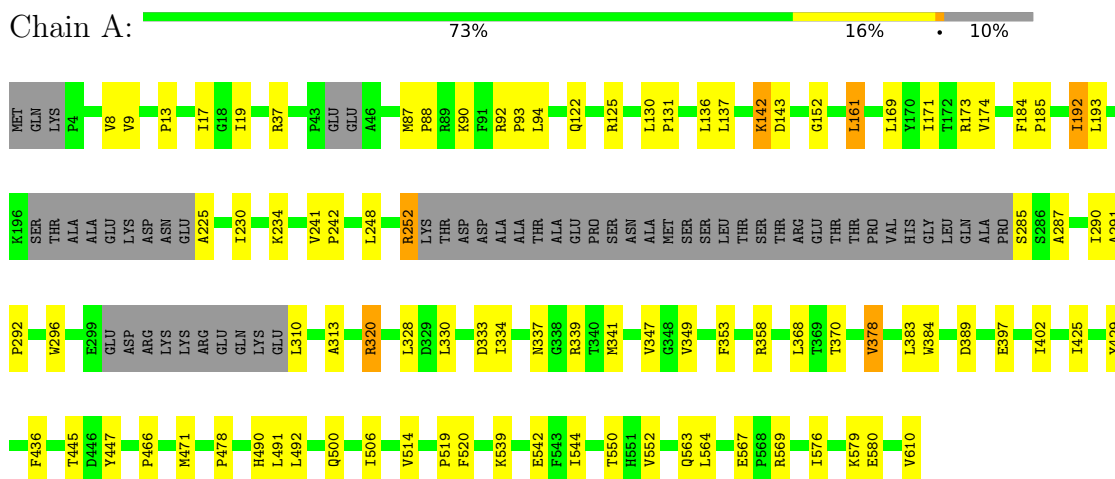


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	G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

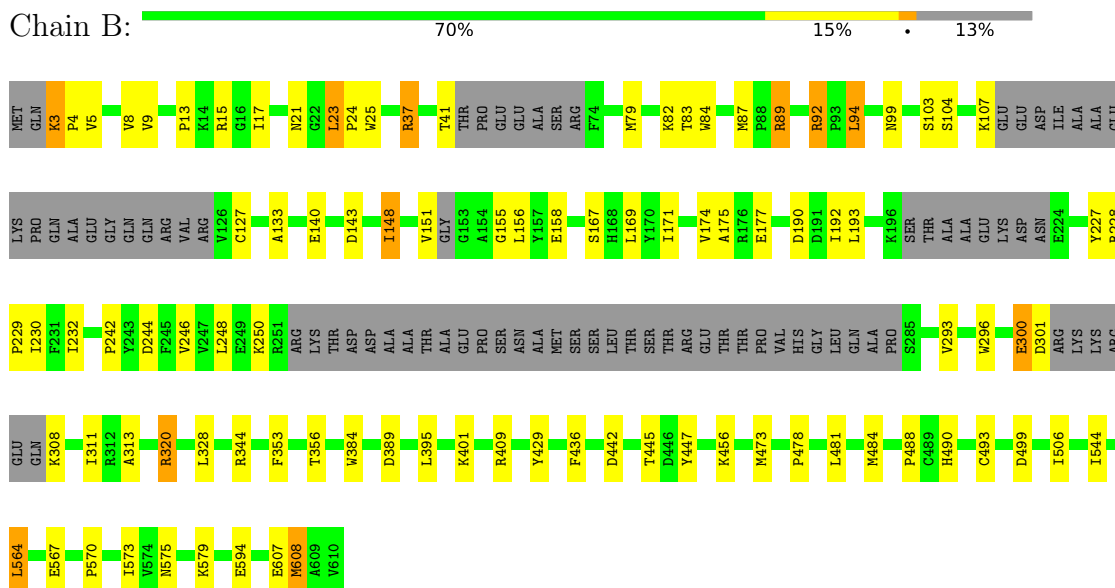
3 Residue-property plots

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

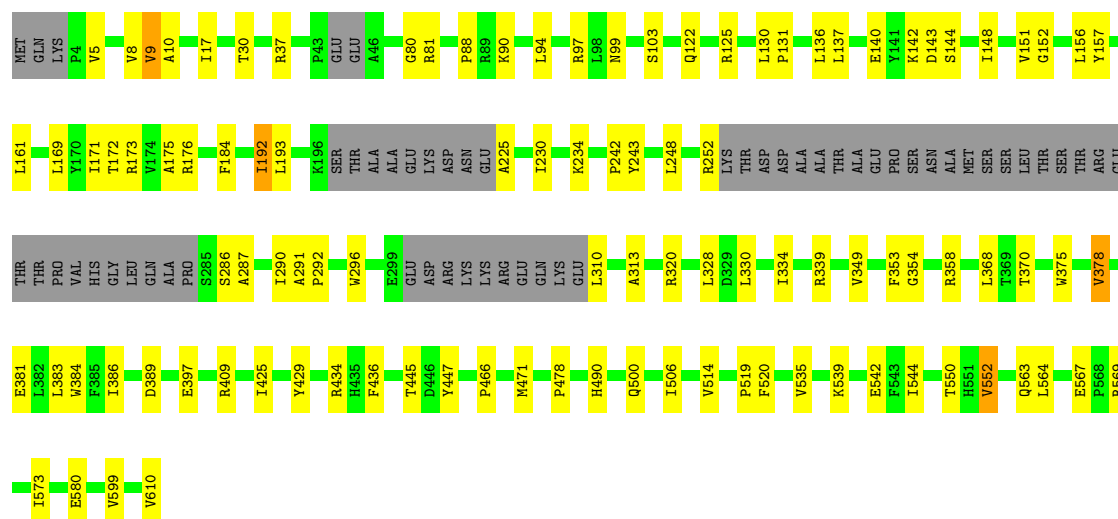


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



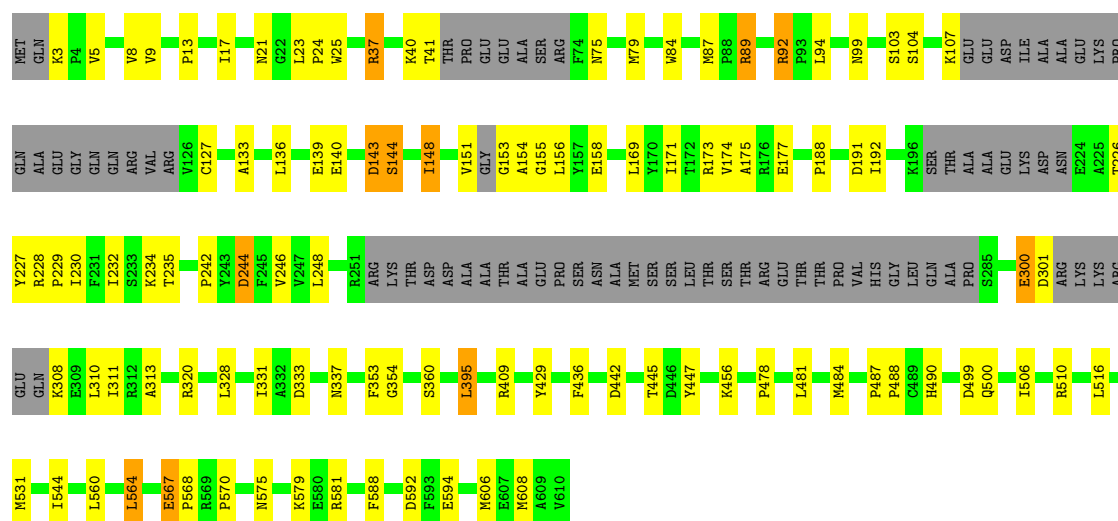
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain C:



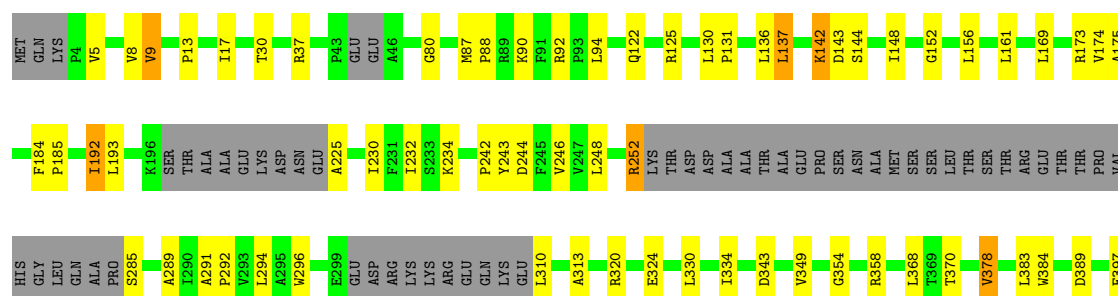
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain D:



- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

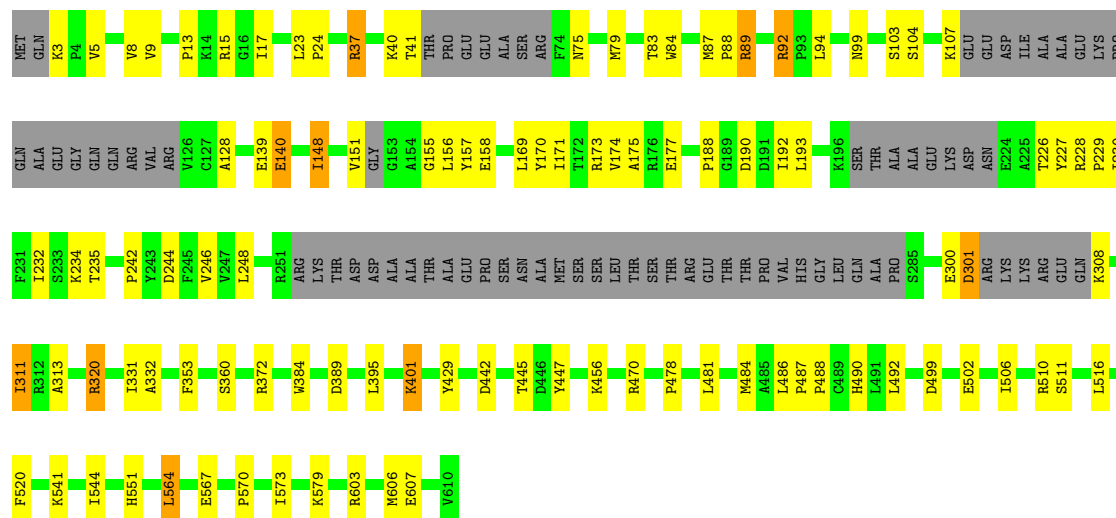
Chain E:





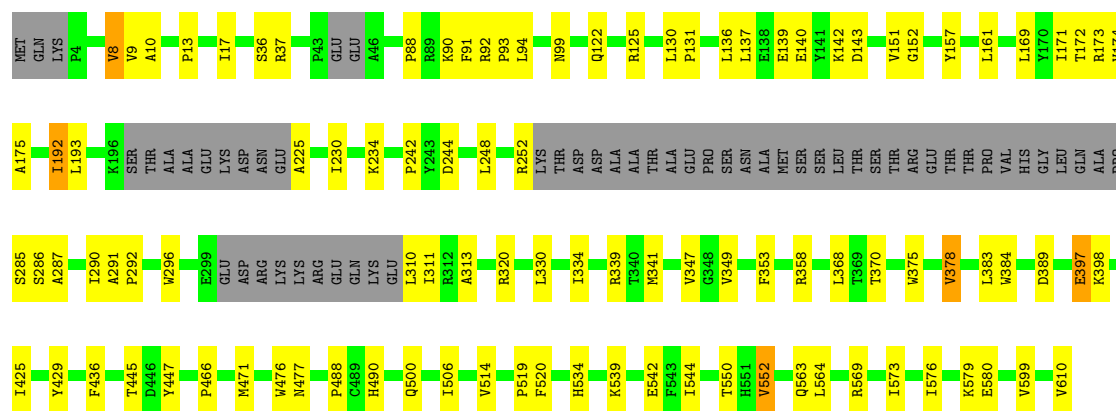
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain F: 68% 17% 13%



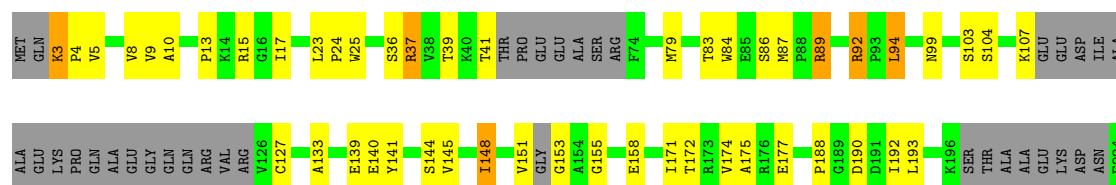
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

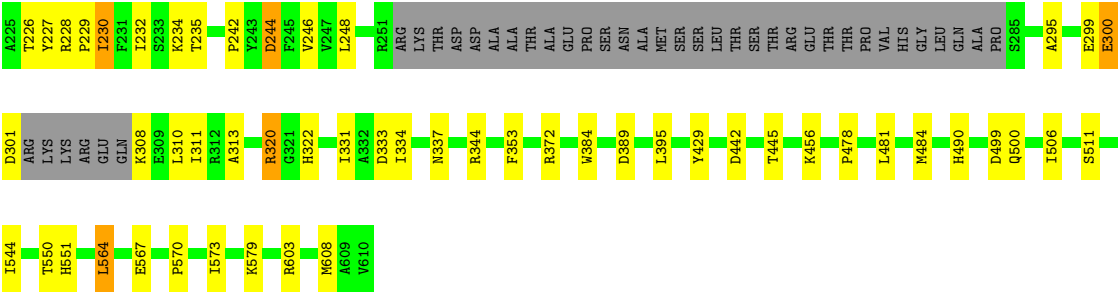
Chain G: 72% 17% 10%



- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain H: 69% 16% 13%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.53Å 145.08Å 176.61Å 90.07° 89.96° 90.07°	Depositor
Resolution (Å)	46.66 – 3.26 46.66 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.66-3.26) 98.5 (46.66-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.9_1692, REFMAC 5.7.0029	Depositor
R, R_{free}	0.182 , 0.241 0.182 , 0.239	Depositor DCC
R_{free} test set	4073 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 3.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l 0.448 for -h,k,-l 0.448 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33184	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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, FOL, 1UG

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	0.30	0/4196	0.74	0/5683
1	B	0.29	0/4043	0.75	4/5473 (0.1%)
1	C	0.30	0/4196	0.73	0/5683
1	D	0.29	0/4043	0.74	2/5473 (0.0%)
1	E	0.30	0/4196	0.73	0/5683
1	F	0.30	0/4043	0.75	2/5473 (0.0%)
1	G	0.30	0/4196	0.74	2/5683 (0.0%)
1	H	0.30	0/4043	0.75	2/5473 (0.0%)
All	All	0.30	0/32956	0.74	12/44624 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	477	ASN	CA-C-N	5.54	125.89	119.47
1	G	477	ASN	C-N-CA	5.54	125.89	119.47
1	B	23	LEU	CA-C-N	5.48	124.83	118.85
1	B	23	LEU	C-N-CA	5.48	124.83	118.85
1	D	92	ARG	CA-C-N	-5.47	113.00	119.84
1	D	92	ARG	C-N-CA	-5.47	113.00	119.84
1	B	92	ARG	CA-C-N	-5.37	113.12	119.84
1	B	92	ARG	C-N-CA	-5.37	113.12	119.84
1	H	92	ARG	CA-C-N	-5.30	113.21	119.84
1	H	92	ARG	C-N-CA	-5.30	113.21	119.84
1	F	92	ARG	CA-C-N	-5.14	113.41	119.84
1	F	92	ARG	C-N-CA	-5.14	113.41	119.84

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	4096	0	4058	49	0
1	B	3948	0	3910	53	0
1	C	4096	0	4058	59	0
1	D	3948	0	3910	63	0
1	E	4096	0	4058	55	0
1	F	3948	0	3910	61	0
1	G	4096	0	4058	59	0
1	H	3948	0	3910	53	0
2	A	20	0	11	0	0
2	B	20	0	11	0	0
2	C	20	0	11	0	0
2	D	20	0	11	0	0
2	E	20	0	11	0	0
2	F	20	0	11	0	0
2	G	20	0	11	0	0
2	H	20	0	11	0	0
3	A	26	0	14	2	0
3	B	26	0	14	2	0
3	C	26	0	14	4	0
3	D	26	0	14	2	0
3	E	26	0	14	5	0
3	F	26	0	14	4	0
3	G	26	0	14	3	0
3	H	26	0	14	2	0
4	A	32	0	17	1	0
4	B	32	0	17	4	0
4	C	32	0	17	1	0
4	D	32	0	17	4	0
4	E	32	0	17	1	0
4	F	32	0	17	4	0
4	G	32	0	17	5	0
4	H	32	0	17	4	0
5	A	48	0	26	3	0
5	B	48	0	26	4	0
5	C	48	0	26	3	0
5	D	48	0	26	4	0
5	E	48	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	48	0	26	5	0
5	G	48	0	26	3	0
5	H	48	0	26	4	0
All	All	33184	0	32416	447	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 7.

All (447) 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:H:608:MET:HE2	3:H:702:1UG:H6	1.60	0.82
1:H:481:LEU:HA	1:H:484:MET:HE2	1.64	0.79
1:E:313:ALA:O	1:E:320:ARG:NH2	2.14	0.79
1:F:481:LEU:HA	1:F:484:MET:HE2	1.65	0.78
1:D:481:LEU:HA	1:D:484:MET:HE2	1.66	0.77
1:A:313:ALA:O	1:A:320:ARG:NH2	2.16	0.77
1:F:244:ASP:HB2	1:F:570:PRO:HG3	1.66	0.76
1:B:481:LEU:HA	1:B:484:MET:HE2	1.66	0.76
1:G:313:ALA:O	1:G:320:ARG:NH2	2.17	0.76
1:B:313:ALA:O	1:B:320:ARG:NH1	2.19	0.74
1:D:175:ALA:HB3	1:D:242:PRO:HG2	1.69	0.74
1:F:175:ALA:HB3	1:F:242:PRO:HG2	1.70	0.74
1:A:370:THR:HG23	1:A:563:GLN:HE21	1.52	0.74
1:F:313:ALA:O	1:F:320:ARG:NH1	2.20	0.74
1:C:313:ALA:O	1:C:320:ARG:NH2	2.16	0.73
1:H:313:ALA:O	1:H:320:ARG:NH1	2.22	0.72
1:H:175:ALA:HB3	1:H:242:PRO:HG2	1.70	0.72
1:B:175:ALA:HB3	1:B:242:PRO:HG2	1.72	0.72
3:A:702:1UG:SAP	3:A:702:1UG:OAB	2.50	0.70
1:C:175:ALA:HB3	1:C:242:PRO:HG2	1.71	0.70
1:B:244:ASP:HB2	1:B:570:PRO:HG3	1.74	0.69
1:D:313:ALA:O	1:D:320:ARG:NH1	2.25	0.69
1:B:608:MET:HE2	3:B:702:1UG:H6	1.76	0.68
3:F:702:1UG:SAP	3:F:702:1UG:OAB	2.54	0.66
1:C:125:ARG:HG2	1:C:136:LEU:HD21	1.77	0.65
1:A:125:ARG:HG2	1:A:136:LEU:HD21	1.78	0.65
3:G:702:1UG:SAP	3:G:702:1UG:OAB	2.55	0.64
3:C:702:1UG:OAB	3:C:702:1UG:SAP	2.56	0.64
1:F:94:LEU:H	1:F:99:ASN:HD21	1.46	0.63
1:G:125:ARG:HG2	1:G:136:LEU:HD21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ASP:HB2	1:D:570:PRO:HG3	1.81	0.62
1:G:370:THR:HG23	1:G:563:GLN:HE21	1.64	0.62
1:C:313:ALA:HB2	1:C:564:LEU:HD22	1.81	0.62
1:G:296:TRP:HB3	1:H:37:ARG:HG2	1.80	0.62
1:G:313:ALA:HB2	1:G:564:LEU:HD22	1.80	0.62
3:E:702:1UG:SAP	3:E:702:1UG:OAB	2.58	0.61
1:E:125:ARG:HG2	1:E:136:LEU:HD21	1.82	0.60
1:A:313:ALA:HB2	1:A:564:LEU:HD22	1.83	0.60
4:A:703:FOL:C7	5:A:704:NDP:H42N	2.32	0.59
1:C:287:ALA:HA	1:C:290:ILE:HD12	1.84	0.59
1:A:152:GLY:HA3	5:A:704:NDP:H5N	1.83	0.59
1:G:506:ILE:HG12	1:G:544:ILE:HB	1.84	0.59
3:B:702:1UG:SAP	3:B:702:1UG:OAB	2.61	0.59
1:E:491:LEU:HD12	1:E:492:LEU:HB2	1.84	0.59
1:A:514:VAL:HB	1:A:552:VAL:HG12	1.85	0.58
1:E:175:ALA:HB3	1:E:242:PRO:HG2	1.84	0.58
1:C:370:THR:HG23	1:C:563:GLN:HE21	1.67	0.58
1:H:244:ASP:HB2	1:H:570:PRO:HG3	1.85	0.58
1:E:608:MET:HG3	3:E:702:1UG:H6	1.85	0.58
1:C:94:LEU:H	1:C:99:ASN:HD21	1.52	0.58
3:D:702:1UG:OAB	3:D:702:1UG:SAP	2.62	0.58
1:E:192:ILE:HD12	1:E:193:LEU:HG	1.85	0.58
1:A:192:ILE:HD12	1:A:193:LEU:HG	1.87	0.57
1:H:89:ARG:HA	1:H:92:ARG:HG3	1.86	0.57
1:H:506:ILE:HG12	1:H:544:ILE:HB	1.86	0.57
1:G:520:PHE:CE2	3:G:702:1UG:H2	2.39	0.57
1:H:8:VAL:HG12	4:H:703:FOL:HN1	1.70	0.57
4:C:703:FOL:C7	5:C:704:NDP:H42N	2.34	0.57
1:C:225:ALA:HA	1:C:252:ARG:HA	1.86	0.56
1:B:8:VAL:HG12	4:B:703:FOL:HN1	1.70	0.56
1:G:287:ALA:HA	1:G:290:ILE:HD12	1.87	0.56
1:C:520:PHE:CE2	3:C:702:1UG:H2	2.41	0.56
1:E:514:VAL:HB	1:E:552:VAL:HG12	1.86	0.56
1:D:608:MET:HE2	3:D:702:1UG:H6	1.87	0.56
1:C:88:PRO:HB2	1:C:90:LYS:HE3	1.88	0.56
1:G:152:GLY:HA3	5:G:704:NDP:H5N	1.86	0.56
1:E:313:ALA:HB2	1:E:564:LEU:HD22	1.88	0.56
1:G:242:PRO:HB3	1:G:573:ILE:HG13	1.88	0.56
1:G:225:ALA:HA	1:G:252:ARG:HA	1.88	0.56
4:D:703:FOL:C7	5:D:704:NDP:H42N	2.36	0.56
1:F:232:ILE:HG12	1:F:246:VAL:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:TRP:HA	1:C:378:VAL:HG13	1.87	0.56
1:D:8:VAL:HG12	4:D:703:FOL:HN1	1.71	0.55
1:E:370:THR:HG23	1:E:563:GLN:HE21	1.71	0.55
1:G:169:LEU:HD12	1:G:248:LEU:HD12	1.88	0.55
1:H:79:MET:HE2	1:H:84:TRP:HA	1.88	0.55
1:B:232:ILE:HG12	1:B:246:VAL:HG12	1.88	0.55
1:A:225:ALA:HA	1:A:252:ARG:HA	1.89	0.55
4:E:703:FOL:C7	5:E:704:NDP:H42N	2.36	0.55
4:G:703:FOL:C7	5:G:704:NDP:H42N	2.35	0.55
1:E:88:PRO:HB2	1:E:90:LYS:HE3	1.89	0.55
1:D:442:ASP:OD1	1:D:445:THR:OG1	2.24	0.55
1:G:94:LEU:H	1:G:99:ASN:HD21	1.55	0.55
1:A:506:ILE:HG12	1:A:544:ILE:HB	1.89	0.55
1:F:442:ASP:OD1	1:F:445:THR:OG1	2.23	0.55
1:C:192:ILE:HD12	1:C:193:LEU:HG	1.89	0.54
1:F:484:MET:HE1	1:F:488:PRO:HD3	1.90	0.54
1:F:520:PHE:CZ	3:F:702:1UG:H2	2.43	0.54
1:D:506:ILE:HG12	1:D:544:ILE:HB	1.88	0.54
1:E:506:ILE:HG12	1:E:544:ILE:HB	1.90	0.54
1:A:88:PRO:HB2	1:A:90:LYS:HE3	1.87	0.54
1:H:94:LEU:H	1:H:99:ASN:HD21	1.56	0.54
3:H:702:1UG:SAP	3:H:702:1UG:OAB	2.65	0.54
1:G:375:TRP:HA	1:G:378:VAL:HG13	1.89	0.54
1:F:8:VAL:HG12	4:F:703:FOL:HN1	1.73	0.54
1:D:94:LEU:H	1:D:99:ASN:HD21	1.55	0.53
4:B:703:FOL:C7	5:B:704:NDP:H42N	2.38	0.53
1:C:173:ARG:HH22	1:C:569:ARG:HA	1.74	0.53
1:D:232:ILE:HG12	1:D:246:VAL:HG12	1.91	0.53
1:B:5:VAL:HG13	1:B:148:ILE:HD11	1.90	0.53
1:C:339:ARG:HH12	1:D:500:GLN:HG2	1.74	0.53
1:B:575:ASN:HB2	1:B:594:GLU:HG2	1.90	0.53
1:G:192:ILE:HD12	1:G:193:LEU:HG	1.90	0.53
4:F:703:FOL:C7	5:F:704:NDP:H42N	2.39	0.53
1:E:289:ALA:O	1:F:170:TYR:OH	2.27	0.53
1:B:79:MET:HE2	1:B:84:TRP:HA	1.91	0.53
1:C:242:PRO:HB3	1:C:573:ILE:HG13	1.91	0.52
1:C:368:LEU:HD23	1:C:519:PRO:HB3	1.89	0.52
1:B:313:ALA:HB2	1:B:564:LEU:HD13	1.91	0.52
1:H:232:ILE:HG12	1:H:246:VAL:HG12	1.91	0.52
1:F:103:SER:OG	5:F:704:NDP:O1X	2.27	0.52
1:C:173:ARG:NH2	1:C:569:ARG:HA	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:TRP:HB3	1:D:37:ARG:HG2	1.92	0.52
1:D:484:MET:HE1	1:D:488:PRO:HD3	1.92	0.52
1:E:152:GLY:HA3	5:E:704:NDP:H5N	1.92	0.52
1:B:89:ARG:H	1:B:89:ARG:HE	1.57	0.52
1:H:499:ASP:OD1	1:H:499:ASP:N	2.43	0.52
1:A:296:TRP:HB3	1:B:37:ARG:HG2	1.91	0.52
1:B:94:LEU:H	1:B:99:ASN:HD21	1.56	0.52
1:E:80:GLY:N	1:E:152:GLY:O	2.42	0.52
1:E:466:PRO:HA	1:E:471:MET:HE1	1.92	0.52
1:G:175:ALA:HB3	1:G:242:PRO:HG2	1.92	0.52
1:A:173:ARG:HH22	1:A:569:ARG:HA	1.75	0.52
1:H:9:VAL:HG23	1:H:171:ILE:HA	1.92	0.52
1:A:173:ARG:NH2	1:A:569:ARG:HA	2.25	0.51
1:B:9:VAL:HG23	1:B:171:ILE:HA	1.91	0.51
1:H:192:ILE:HD12	1:H:248:LEU:HD21	1.92	0.51
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.92	0.51
1:E:17:ILE:O	5:E:704:NDP:H2N	2.11	0.51
1:F:40:LYS:HA	1:F:75:ASN:HD22	1.75	0.51
1:C:384:TRP:CD1	1:C:389:ASP:HB3	2.45	0.51
4:H:703:FOL:C7	5:H:704:NDP:H42N	2.40	0.51
1:E:520:PHE:CD2	3:E:702:1UG:H2	2.46	0.51
1:E:296:TRP:HB3	1:F:37:ARG:HG2	1.93	0.51
1:F:192:ILE:HD12	1:F:248:LEU:HD21	1.92	0.51
1:A:87:MET:O	1:A:92:ARG:NH2	2.44	0.51
1:C:152:GLY:HA3	5:C:704:NDP:H5N	1.92	0.51
1:F:313:ALA:HB2	1:F:564:LEU:HD13	1.92	0.51
1:A:402:ILE:HD12	3:A:702:1UG:H2	1.92	0.50
1:B:103:SER:OG	1:B:104:SER:N	2.43	0.50
1:H:313:ALA:HB2	1:H:564:LEU:HD13	1.92	0.50
1:H:84:TRP:CE2	1:H:92:ARG:HD2	2.47	0.50
1:A:287:ALA:HA	1:A:290:ILE:HD12	1.93	0.50
1:C:334:ILE:HD11	1:C:550:THR:HG22	1.93	0.50
1:D:313:ALA:HB3	1:D:320:ARG:HH12	1.76	0.50
1:E:384:TRP:CD1	1:E:389:ASP:HB3	2.47	0.50
1:H:83:THR:OG1	5:H:704:NDP:O2A	2.28	0.50
1:E:173:ARG:HH22	1:E:569:ARG:HA	1.77	0.50
1:B:17:ILE:O	5:B:704:NDP:H2N	2.11	0.50
1:C:339:ARG:NH1	1:D:499:ASP:OD1	2.44	0.50
1:H:372:ARG:HB3	1:H:603:ARG:HG2	1.94	0.50
1:H:151:VAL:HB	4:H:703:FOL:H7	1.94	0.50
1:H:384:TRP:CD1	1:H:389:ASP:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:SER:OG	5:D:704:NDP:O1X	2.25	0.49
1:E:173:ARG:NH2	1:E:569:ARG:HA	2.27	0.49
1:D:313:ALA:HB2	1:D:564:LEU:HD13	1.94	0.49
1:B:15:ARG:HG2	1:B:193:LEU:HD13	1.93	0.49
1:C:17:ILE:O	5:C:704:NDP:H2N	2.13	0.49
1:E:291:ALA:HA	1:E:294:LEU:HB2	1.94	0.49
1:D:192:ILE:HD12	1:D:248:LEU:HD21	1.93	0.49
1:G:368:LEU:HD23	1:G:519:PRO:HB3	1.93	0.49
1:E:225:ALA:HA	1:E:252:ARG:HA	1.95	0.49
1:F:9:VAL:HG12	1:F:157:TYR:CZ	2.47	0.49
1:C:445:THR:HB	1:C:447:TYR:CZ	2.48	0.49
1:D:300:GLU:HA	1:D:301:ASP:HA	1.57	0.49
1:B:384:TRP:CD1	1:B:389:ASP:HB3	2.48	0.49
1:C:514:VAL:HB	1:C:552:VAL:HG12	1.93	0.49
1:C:520:PHE:CD2	3:C:702:1UG:H2	2.47	0.49
1:C:436:PHE:CE2	1:D:478:PRO:HD2	2.48	0.48
1:F:89:ARG:HA	1:F:92:ARG:HG3	1.95	0.48
1:E:334:ILE:HD11	1:E:550:THR:HG22	1.94	0.48
4:F:703:FOL:C6	5:F:704:NDP:H42N	2.44	0.48
1:G:9:VAL:HG23	1:G:171:ILE:HA	1.96	0.48
1:B:84:TRP:CE2	1:B:92:ARG:HD2	2.48	0.48
1:C:370:THR:CG2	1:C:563:GLN:HE21	2.27	0.48
1:E:169:LEU:HD12	1:E:248:LEU:HD12	1.96	0.48
1:F:499:ASP:OD1	1:F:499:ASP:N	2.47	0.48
1:A:291:ALA:N	1:A:292:PRO:HD2	2.29	0.48
1:B:151:VAL:HB	4:B:703:FOL:H7	1.96	0.48
1:B:484:MET:HE1	1:B:488:PRO:HD3	1.94	0.48
1:A:17:ILE:O	5:A:704:NDP:H2N	2.14	0.47
1:C:506:ILE:HG12	1:C:544:ILE:HB	1.94	0.47
1:A:445:THR:HB	1:A:447:TYR:CZ	2.49	0.47
1:D:192:ILE:HD11	1:D:229:PRO:HD3	1.96	0.47
1:E:368:LEU:HD23	1:E:519:PRO:HB3	1.95	0.47
1:B:300:GLU:HA	1:B:301:ASP:HA	1.56	0.47
1:A:169:LEU:HD12	1:A:248:LEU:HD12	1.95	0.47
1:H:103:SER:OG	1:H:104:SER:N	2.48	0.47
4:H:703:FOL:C6	5:H:704:NDP:H42N	2.45	0.47
1:F:384:TRP:CD1	1:F:389:ASP:HB3	2.49	0.47
1:D:17:ILE:O	5:D:704:NDP:H2N	2.15	0.47
4:B:703:FOL:C6	5:B:704:NDP:H42N	2.45	0.47
1:E:520:PHE:CE2	3:E:702:1UG:H2	2.50	0.47
1:F:84:TRP:CE2	1:F:92:ARG:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:173:ARG:NH2	1:G:569:ARG:HA	2.29	0.47
1:G:291:ALA:N	1:G:292:PRO:HD2	2.30	0.47
1:C:81:ARG:HB2	1:C:103:SER:HB2	1.97	0.47
1:D:103:SER:OG	1:D:104:SER:N	2.44	0.47
1:G:173:ARG:HH22	1:G:569:ARG:HA	1.80	0.47
1:G:290:ILE:HD13	1:H:230:ILE:HG21	1.96	0.47
1:C:291:ALA:N	1:C:292:PRO:HD2	2.30	0.47
1:E:506:ILE:HG13	1:F:353:PHE:CE2	2.50	0.47
1:A:339:ARG:NH1	1:B:499:ASP:OD1	2.48	0.47
1:A:436:PHE:CE1	1:B:478:PRO:HD2	2.50	0.47
1:D:155:GLY:HA2	1:D:158:GLU:CD	2.39	0.47
1:H:227:TYR:HB3	1:H:248:LEU:HD23	1.98	0.46
1:H:442:ASP:OD1	1:H:445:THR:OG1	2.26	0.46
1:E:87:MET:HE1	1:E:94:LEU:HG	1.97	0.46
1:H:79:MET:HE1	1:H:87:MET:SD	2.56	0.46
4:D:703:FOL:C6	5:D:704:NDP:H42N	2.46	0.46
1:F:192:ILE:HD11	1:F:229:PRO:HD3	1.98	0.46
1:F:520:PHE:CE1	3:F:702:1UG:H2	2.50	0.46
1:A:87:MET:HE1	1:A:94:LEU:HG	1.96	0.46
1:A:368:LEU:HD23	1:A:519:PRO:HB3	1.96	0.46
1:E:436:PHE:CE2	1:F:478:PRO:HD2	2.51	0.46
1:G:384:TRP:HH2	1:G:425:ILE:HD13	1.81	0.46
1:D:151:VAL:HB	4:D:703:FOL:H7	1.98	0.46
1:E:370:THR:CG2	1:E:563:GLN:HE21	2.29	0.46
1:F:300:GLU:HA	1:F:301:ASP:HA	1.51	0.46
1:G:576:ILE:HB	1:G:579:LYS:HE2	1.98	0.46
1:G:370:THR:CG2	1:G:563:GLN:HE21	2.26	0.46
1:E:354:GLY:HA3	1:F:544:ILE:HD13	1.97	0.46
1:F:506:ILE:HG12	1:F:544:ILE:HB	1.97	0.46
1:H:141:TYR:O	1:H:145:VAL:HG12	2.16	0.46
1:B:89:ARG:HA	1:B:92:ARG:HG3	1.97	0.45
1:D:151:VAL:O	1:D:153:GLY:N	2.49	0.45
1:G:506:ILE:HG13	1:H:353:PHE:CE2	2.50	0.45
1:H:333:ASP:OD1	1:H:337:ASN:ND2	2.46	0.45
1:E:242:PRO:HB3	1:E:573:ILE:HG13	1.99	0.45
1:G:490:HIS:H	1:G:490:HIS:CD2	2.34	0.45
1:H:127:CYS:SG	1:H:133:ALA:HA	2.56	0.45
1:A:506:ILE:HG13	1:B:353:PHE:CE2	2.51	0.45
1:B:3:LYS:N	1:B:4:PRO:HD3	2.31	0.45
1:B:442:ASP:OD1	1:B:445:THR:OG1	2.30	0.45
1:C:169:LEU:HD12	1:C:248:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ILE:HD11	1:D:154:ALA:HB2	1.99	0.45
1:C:381:GLU:OE1	3:C:702:1UG:H13	2.16	0.45
1:A:466:PRO:HA	1:A:471:MET:HE1	1.99	0.45
1:B:79:MET:HE1	1:B:87:MET:SD	2.57	0.45
1:E:378:VAL:HG12	1:E:520:PHE:CE2	2.52	0.45
1:G:445:THR:HB	1:G:447:TYR:CZ	2.51	0.45
1:G:466:PRO:HA	1:G:471:MET:HE1	1.99	0.45
1:G:514:VAL:HB	1:G:552:VAL:HG12	1.97	0.45
1:A:370:THR:CG2	1:A:563:GLN:HE21	2.24	0.45
1:B:13:PRO:HD3	1:B:174:VAL:O	2.17	0.45
1:D:567:GLU:HA	1:D:568:PRO:HD3	1.83	0.45
1:E:445:THR:HB	1:E:447:TYR:CZ	2.52	0.45
1:D:490:HIS:H	1:D:490:HIS:CD2	2.35	0.45
1:G:151:VAL:HG13	4:G:703:FOL:H7	1.98	0.45
1:D:143:ASP:OD1	1:D:143:ASP:N	2.50	0.45
1:E:137:LEU:HD12	1:E:137:LEU:HA	1.85	0.45
1:B:167:SER:HA	1:B:250:LYS:HE2	1.99	0.44
1:F:169:LEU:HB2	1:F:248:LEU:HB2	1.98	0.44
1:F:490:HIS:CD2	1:F:490:HIS:H	2.35	0.44
1:H:13:PRO:HD3	1:H:174:VAL:O	2.17	0.44
1:H:17:ILE:O	5:H:704:NDP:H2N	2.18	0.44
1:B:445:THR:HB	1:B:447:TYR:CZ	2.52	0.44
1:C:378:VAL:HG12	1:C:520:PHE:CE2	2.52	0.44
1:F:79:MET:HE1	1:F:87:MET:SD	2.58	0.44
1:F:83:THR:OG1	5:F:704:NDP:O2A	2.28	0.44
1:G:88:PRO:HB2	1:G:90:LYS:HE3	1.99	0.44
1:D:79:MET:HE2	1:D:84:TRP:HA	1.98	0.44
1:D:328:LEU:HD22	1:D:564:LEU:HD22	1.99	0.44
1:F:5:VAL:HG13	1:F:148:ILE:HD11	1.98	0.44
1:F:103:SER:O	1:F:128:ALA:HA	2.17	0.44
1:G:17:ILE:O	5:G:704:NDP:H2N	2.17	0.44
1:G:334:ILE:HG21	1:G:552:VAL:HG13	1.98	0.44
1:E:291:ALA:N	1:E:292:PRO:HD2	2.33	0.44
1:F:188:PRO:HB2	1:F:226:THR:HA	1.99	0.44
1:G:173:ARG:HD3	1:G:244:ASP:OD1	2.18	0.44
1:F:151:VAL:HB	4:F:703:FOL:H7	2.00	0.44
1:H:232:ILE:HG22	1:H:322:HIS:HB2	1.99	0.44
1:C:30:THR:HB	1:C:243:TYR:OH	2.18	0.44
1:D:40:LYS:HA	1:D:75:ASN:HD22	1.82	0.44
1:F:487:PRO:O	1:F:510:ARG:NH1	2.39	0.44
1:G:8:VAL:HG22	4:G:703:FOL:HN1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:PRO:HG2	1:G:91:PHE:HB2	1.99	0.44
1:A:130:LEU:HB3	1:A:131:PRO:HD3	1.99	0.44
1:A:490:HIS:CD2	1:A:490:HIS:H	2.36	0.44
1:C:506:ILE:HG13	1:D:353:PHE:CE2	2.52	0.44
1:G:334:ILE:HD11	1:G:550:THR:HG22	1.99	0.44
1:G:520:PHE:CD2	3:G:702:1UG:H2	2.53	0.44
1:H:3:LYS:N	1:H:4:PRO:HD3	2.32	0.44
1:D:13:PRO:HD3	1:D:174:VAL:O	2.18	0.43
1:D:531:MET:HE3	1:D:588:PHE:CG	2.53	0.43
1:F:13:PRO:HD3	1:F:174:VAL:O	2.18	0.43
1:H:192:ILE:HD11	1:H:229:PRO:HD3	2.00	0.43
1:A:161:LEU:HD12	1:A:161:LEU:HA	1.77	0.43
1:A:333:ASP:OD1	1:A:337:ASN:ND2	2.51	0.43
1:B:490:HIS:H	1:B:490:HIS:CD2	2.35	0.43
1:C:9:VAL:HG23	1:C:171:ILE:HA	1.99	0.43
1:D:333:ASP:OD1	1:D:337:ASN:ND2	2.50	0.43
1:H:511:SER:OG	1:H:551:HIS:HE1	2.01	0.43
1:A:378:VAL:HG12	1:A:520:PHE:CE2	2.53	0.43
1:D:499:ASP:OD1	1:D:499:ASP:N	2.47	0.43
1:G:436:PHE:CE1	1:H:478:PRO:HD2	2.52	0.43
1:A:241:VAL:HA	1:A:242:PRO:HD3	1.85	0.43
1:A:384:TRP:CD1	1:A:389:ASP:HB3	2.53	0.43
1:D:89:ARG:HA	1:D:92:ARG:HG3	2.00	0.43
3:E:702:1UG:CAT	3:E:702:1UG:H7	2.47	0.43
1:H:5:VAL:HG13	1:H:148:ILE:HD11	1.99	0.43
1:H:15:ARG:HG2	1:H:193:LEU:HD13	1.99	0.43
1:D:23:LEU:HA	1:D:24:PRO:HD3	1.80	0.43
1:F:227:TYR:HB3	1:F:248:LEU:HD23	1.99	0.43
1:B:89:ARG:H	1:B:89:ARG:NE	2.16	0.43
1:B:127:CYS:SG	1:B:133:ALA:HA	2.58	0.43
1:B:192:ILE:HD12	1:B:248:LEU:HD21	2.00	0.43
1:D:9:VAL:HG23	1:D:171:ILE:HA	2.01	0.43
1:E:334:ILE:HG21	1:E:552:VAL:HG13	2.00	0.43
1:F:520:PHE:CE2	3:F:702:1UG:H2	2.54	0.43
1:G:384:TRP:CD1	1:G:389:ASP:HB3	2.54	0.43
1:B:143:ASP:N	1:B:143:ASP:OD1	2.50	0.43
1:B:23:LEU:HA	1:B:24:PRO:HD3	1.77	0.43
1:C:353:PHE:CE2	1:D:506:ILE:HG13	2.54	0.43
1:D:169:LEU:HB2	1:D:248:LEU:HB2	2.00	0.43
1:G:353:PHE:CE2	1:H:506:ILE:HG13	2.54	0.43
1:A:358:ARG:HD3	1:A:542:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:ILE:HD11	1:F:332:ALA:HA	2.00	0.43
1:A:384:TRP:HH2	1:A:425:ILE:HD13	1.83	0.42
1:F:15:ARG:HG2	1:F:193:LEU:HD13	2.00	0.42
1:G:36:SER:HB2	4:G:703:FOL:HB1	2.00	0.42
1:A:384:TRP:CH2	1:A:425:ILE:HD13	2.54	0.42
1:B:227:TYR:HB3	1:B:248:LEU:HD23	2.00	0.42
1:D:516:LEU:HD13	1:D:606:MET:HB2	2.00	0.42
1:G:358:ARG:NH1	1:G:542:GLU:OE2	2.52	0.42
1:A:328:LEU:HD21	1:A:370:THR:HG21	2.00	0.42
1:E:384:TRP:HH2	1:E:425:ILE:HD13	1.84	0.42
1:H:151:VAL:O	1:H:153:GLY:N	2.53	0.42
1:A:13:PRO:HD3	1:A:174:VAL:O	2.19	0.42
1:D:581:ARG:NH2	1:D:592:ASP:OD1	2.52	0.42
1:F:155:GLY:HA2	1:F:158:GLU:CD	2.43	0.42
1:G:339:ARG:NH1	1:H:499:ASP:OD1	2.51	0.42
1:A:576:ILE:HB	1:A:579:LYS:HE2	2.01	0.42
1:E:87:MET:O	1:E:92:ARG:NH2	2.53	0.42
1:G:10:ALA:HA	1:G:172:THR:HB	2.01	0.42
1:B:192:ILE:HD11	1:B:229:PRO:HD3	2.00	0.42
1:C:94:LEU:HB3	1:C:97:ARG:CZ	2.50	0.42
1:C:130:LEU:HB3	1:C:131:PRO:HD3	2.02	0.42
1:C:192:ILE:H	1:C:192:ILE:HG13	1.57	0.42
1:D:395:LEU:HD12	1:D:395:LEU:HA	1.88	0.42
1:F:156:LEU:HD12	1:F:156:LEU:HA	1.86	0.42
4:G:703:FOL:H13	4:G:703:FOL:C6	2.50	0.42
1:H:300:GLU:HA	1:H:301:ASP:HA	1.60	0.42
1:C:10:ALA:HA	1:C:172:THR:HB	2.02	0.42
1:D:156:LEU:HD12	1:D:156:LEU:HA	1.84	0.42
1:D:487:PRO:O	1:D:510:ARG:NH1	2.41	0.42
1:E:173:ARG:HD3	1:E:244:ASP:OD1	2.20	0.42
1:F:23:LEU:HA	1:F:24:PRO:HD3	1.79	0.42
1:G:151:VAL:O	1:G:157:TYR:OH	2.36	0.42
1:A:142:LYS:HD3	1:A:142:LYS:HA	1.84	0.42
1:C:328:LEU:HD21	1:C:370:THR:HG21	2.01	0.42
1:D:79:MET:HE1	1:D:87:MET:SD	2.60	0.42
1:D:188:PRO:HB2	1:D:226:THR:HA	2.01	0.42
1:D:234:LYS:HG2	1:D:235:THR:N	2.35	0.42
1:F:445:THR:HB	1:F:447:TYR:CZ	2.55	0.42
1:G:384:TRP:CH2	1:G:425:ILE:HD13	2.55	0.42
1:C:466:PRO:HA	1:C:471:MET:HE1	2.02	0.42
1:C:151:VAL:O	1:C:157:TYR:OH	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:HIS:CD2	1:C:490:HIS:H	2.38	0.42
1:G:142:LYS:HD3	1:G:142:LYS:HA	1.82	0.42
1:H:23:LEU:HA	1:H:24:PRO:HD3	1.81	0.42
1:C:334:ILE:HG21	1:C:552:VAL:HG13	2.01	0.41
1:D:94:LEU:HB2	1:D:99:ASN:HD21	1.85	0.41
1:E:130:LEU:HB3	1:E:131:PRO:HD3	2.02	0.41
1:F:234:LYS:HG2	1:F:235:THR:N	2.35	0.41
1:A:341:MET:HE3	1:A:341:MET:HB3	1.97	0.41
1:B:293:VAL:HA	1:B:296:TRP:CD1	2.55	0.41
1:C:5:VAL:HG23	1:C:148:ILE:HG22	2.02	0.41
1:C:384:TRP:CH2	1:C:425:ILE:HD13	2.55	0.41
1:D:227:TYR:HB3	1:D:248:LEU:HD23	2.02	0.41
1:F:79:MET:HE2	1:F:84:TRP:HA	2.02	0.41
1:B:83:THR:OG1	5:B:704:NDP:O2A	2.27	0.41
1:E:30:THR:HB	1:E:243:TYR:OH	2.20	0.41
1:E:358:ARG:HD3	1:E:542:GLU:OE1	2.20	0.41
1:D:5:VAL:HG13	1:D:148:ILE:HD11	2.02	0.41
1:F:516:LEU:HD13	1:F:606:MET:HB2	2.02	0.41
1:G:92:ARG:HA	1:G:93:PRO:C	2.46	0.41
1:G:341:MET:HE3	1:G:341:MET:HB3	1.93	0.41
1:A:491:LEU:HD12	1:A:492:LEU:HB2	2.03	0.41
1:C:176:ARG:HG3	1:C:242:PRO:HD2	2.02	0.41
1:E:384:TRP:CH2	1:E:425:ILE:HD13	2.55	0.41
1:F:103:SER:OG	1:F:104:SER:N	2.52	0.41
1:G:13:PRO:HD3	1:G:174:VAL:O	2.20	0.41
1:G:358:ARG:HD3	1:G:542:GLU:OE1	2.21	0.41
1:F:9:VAL:HG23	1:F:171:ILE:HA	2.03	0.41
1:F:372:ARG:HB3	1:F:603:ARG:HG2	2.03	0.41
1:F:486:LEU:HD23	1:F:486:LEU:HA	1.86	0.41
1:A:184:PHE:CG	1:A:185:PRO:HD2	2.56	0.41
1:A:353:PHE:CE2	1:B:506:ILE:HG13	2.56	0.41
1:B:169:LEU:HB2	1:B:248:LEU:HB2	2.03	0.41
1:D:445:THR:HB	1:D:447:TYR:CZ	2.55	0.41
1:E:13:PRO:HD3	1:E:174:VAL:O	2.21	0.41
1:F:502:GLU:HB3	1:F:541:LYS:HB2	2.03	0.41
1:G:476:TRP:HE3	1:G:488:PRO:HG2	1.86	0.41
1:H:234:LYS:HG2	1:H:235:THR:N	2.36	0.41
1:A:478:PRO:HD2	1:B:436:PHE:CE1	2.56	0.41
1:C:358:ARG:HD3	1:C:542:GLU:OE1	2.20	0.41
1:D:173:ARG:HD3	1:D:244:ASP:HB3	2.02	0.41
1:E:490:HIS:CD2	1:E:490:HIS:H	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:511:SER:OG	1:F:551:HIS:HE1	2.03	0.41
1:F:607:GLU:H	1:F:607:GLU:CD	2.27	0.41
1:G:130:LEU:HB3	1:G:131:PRO:HD3	2.02	0.41
1:A:334:ILE:HD11	1:A:550:THR:HG22	2.01	0.41
1:C:142:LYS:C	1:C:144:SER:H	2.29	0.41
1:C:358:ARG:NH2	1:D:354:GLY:O	2.54	0.41
1:D:331:ILE:HD13	1:D:560:LEU:HD22	2.03	0.41
1:E:9:VAL:HG11	1:E:184:PHE:CD1	2.56	0.41
1:E:142:LYS:C	1:E:144:SER:H	2.28	0.41
1:E:232:ILE:HG12	1:E:246:VAL:HG12	2.02	0.41
1:F:17:ILE:O	5:F:704:NDP:H2N	2.21	0.41
1:H:10:ALA:HA	1:H:172:THR:HB	2.03	0.41
1:H:295:ALA:O	1:H:299:GLU:HG3	2.21	0.41
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.86	0.40
1:B:607:GLU:H	1:B:607:GLU:CD	2.29	0.40
1:C:386:ILE:O	1:C:434:ARG:NH2	2.53	0.40
1:E:192:ILE:H	1:E:192:ILE:HG13	1.57	0.40
1:E:324:GLU:HG3	1:E:368:LEU:HD12	2.03	0.40
1:G:378:VAL:HG12	1:G:520:PHE:CE2	2.57	0.40
1:H:188:PRO:HB2	1:H:226:THR:HA	2.04	0.40
1:C:9:VAL:HG11	1:C:184:PHE:CD1	2.55	0.40
1:F:140:GLU:H	1:F:140:GLU:HG2	1.71	0.40
1:H:155:GLY:HA2	1:H:158:GLU:CD	2.47	0.40
1:H:490:HIS:CD2	1:H:490:HIS:H	2.38	0.40
1:B:21:ASN:OD1	1:B:82:LYS:HB3	2.21	0.40
1:B:155:GLY:HA2	1:B:158:GLU:HG2	2.03	0.40
1:C:80:GLY:N	1:C:152:GLY:O	2.52	0.40
1:C:142:LYS:O	1:C:143:ASP:HB3	2.20	0.40
1:D:127:CYS:SG	1:D:133:ALA:HA	2.60	0.40
1:F:87:MET:HA	1:F:88:PRO:HD2	1.88	0.40
1:G:534:HIS:CE1	1:G:579:LYS:HD3	2.56	0.40
1:A:92:ARG:HA	1:A:93:PRO:C	2.47	0.40
1:B:328:LEU:HD22	1:B:564:LEU:HD22	2.04	0.40
1:C:354:GLY:HA3	1:D:544:ILE:HD13	2.03	0.40
1:D:575:ASN:HB2	1:D:594:GLU:HG2	2.04	0.40
1:E:137:LEU:HD23	1:E:148:ILE:HD13	2.02	0.40
1:E:378:VAL:HG12	1:E:520:PHE:CD2	2.56	0.40
1:F:173:ARG:CZ	1:F:570:PRO:HD3	2.51	0.40
1:G:339:ARG:HH12	1:H:500:GLN:HG2	1.86	0.40
1:H:334:ILE:HD11	1:H:550:THR:HG22	2.03	0.40
1:H:484:MET:HE3	1:H:484:MET:HB2	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG23	1:A:171:ILE:HA	2.04	0.40
1:B:473:MET:HE2	1:B:493:CYS:SG	2.62	0.40
1:C:478:PRO:HD2	1:D:436:PHE:CE1	2.56	0.40
1:D:143:ASP:O	1:D:144:SER:HB2	2.22	0.40
1:E:184:PHE:CG	1:E:185:PRO:HD2	2.56	0.40
1:F:401:LYS:H	1:F:401:LYS:HG2	1.69	0.40
1:G:397:GLU:OE2	1:G:398:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	502/566 (89%)	482 (96%)	19 (4%)	1 (0%)	43 70
1	B	478/566 (84%)	447 (94%)	29 (6%)	2 (0%)	30 59
1	C	502/566 (89%)	485 (97%)	15 (3%)	2 (0%)	30 59
1	D	478/566 (84%)	448 (94%)	27 (6%)	3 (1%)	21 51
1	E	502/566 (89%)	486 (97%)	15 (3%)	1 (0%)	43 70
1	F	478/566 (84%)	448 (94%)	28 (6%)	2 (0%)	30 59
1	G	502/566 (89%)	485 (97%)	15 (3%)	2 (0%)	30 59
1	H	478/566 (84%)	449 (94%)	25 (5%)	4 (1%)	16 44
All	All	3920/4528 (87%)	3730 (95%)	173 (4%)	17 (0%)	30 59

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	429	TYR
1	H	429	TYR
1	E	429	TYR

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Mol	Chain	Res	Type
1	F	429	TYR
1	H	144	SER
1	A	429	TYR
1	B	429	TYR
1	C	429	TYR
1	D	144	SER
1	F	139	GLU
1	G	429	TYR
1	G	286	SER
1	B	94	LEU
1	C	286	SER
1	D	139	GLU
1	H	94	LEU
1	H	139	GLU

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	444/491 (90%)	418 (94%)	26 (6%)	18	45
1	B	431/491 (88%)	404 (94%)	27 (6%)	16	43
1	C	444/491 (90%)	418 (94%)	26 (6%)	18	45
1	D	431/491 (88%)	404 (94%)	27 (6%)	16	43
1	E	444/491 (90%)	415 (94%)	29 (6%)	15	42
1	F	431/491 (88%)	405 (94%)	26 (6%)	17	44
1	G	444/491 (90%)	418 (94%)	26 (6%)	18	45
1	H	431/491 (88%)	402 (93%)	29 (7%)	15	41
All	All	3500/3928 (89%)	3284 (94%)	216 (6%)	16	43

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL

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Mol	Chain	Res	Type
1	A	19	ILE
1	A	37	ARG
1	A	122	GLN
1	A	137	LEU
1	A	142	LYS
1	A	143	ASP
1	A	161	LEU
1	A	192	ILE
1	A	230	ILE
1	A	234	LYS
1	A	252	ARG
1	A	285	SER
1	A	310	LEU
1	A	320	ARG
1	A	330	LEU
1	A	347	VAL
1	A	349	VAL
1	A	378	VAL
1	A	383	LEU
1	A	397	GLU
1	A	500	GLN
1	A	539	LYS
1	A	567	GLU
1	A	580	GLU
1	A	610	VAL
1	B	3	LYS
1	B	25	TRP
1	B	37	ARG
1	B	41	THR
1	B	89	ARG
1	B	107	LYS
1	B	140	GLU
1	B	148	ILE
1	B	177	GLU
1	B	190	ASP
1	B	228	ARG
1	B	230	ILE
1	B	300	GLU
1	B	308	LYS
1	B	311	ILE
1	B	320	ARG
1	B	344	ARG

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Mol	Chain	Res	Type
1	B	356	THR
1	B	395	LEU
1	B	401	LYS
1	B	409	ARG
1	B	456	LYS
1	B	564	LEU
1	B	567	GLU
1	B	573	ILE
1	B	579	LYS
1	B	608	MET
1	C	8	VAL
1	C	9	VAL
1	C	37	ARG
1	C	122	GLN
1	C	137	LEU
1	C	140	GLU
1	C	156	LEU
1	C	161	LEU
1	C	192	ILE
1	C	230	ILE
1	C	234	LYS
1	C	310	LEU
1	C	330	LEU
1	C	349	VAL
1	C	378	VAL
1	C	383	LEU
1	C	397	GLU
1	C	409	ARG
1	C	500	GLN
1	C	535	VAL
1	C	539	LYS
1	C	552	VAL
1	C	567	GLU
1	C	580	GLU
1	C	599	VAL
1	C	610	VAL
1	D	3	LYS
1	D	21	ASN
1	D	25	TRP
1	D	37	ARG
1	D	41	THR
1	D	89	ARG

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Mol	Chain	Res	Type
1	D	107	LYS
1	D	136	LEU
1	D	140	GLU
1	D	143	ASP
1	D	148	ILE
1	D	177	GLU
1	D	191	ASP
1	D	228	ARG
1	D	230	ILE
1	D	244	ASP
1	D	300	GLU
1	D	308	LYS
1	D	310	LEU
1	D	311	ILE
1	D	360	SER
1	D	395	LEU
1	D	409	ARG
1	D	456	LYS
1	D	564	LEU
1	D	567	GLU
1	D	579	LYS
1	E	5	VAL
1	E	8	VAL
1	E	9	VAL
1	E	37	ARG
1	E	122	GLN
1	E	137	LEU
1	E	142	LYS
1	E	143	ASP
1	E	156	LEU
1	E	161	LEU
1	E	192	ILE
1	E	230	ILE
1	E	234	LYS
1	E	252	ARG
1	E	285	SER
1	E	310	LEU
1	E	330	LEU
1	E	343	ASP
1	E	349	VAL
1	E	378	VAL
1	E	383	LEU

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Mol	Chain	Res	Type
1	E	397	GLU
1	E	492	LEU
1	E	500	GLN
1	E	539	LYS
1	E	552	VAL
1	E	567	GLU
1	E	580	GLU
1	E	610	VAL
1	F	3	LYS
1	F	37	ARG
1	F	41	THR
1	F	89	ARG
1	F	107	LYS
1	F	140	GLU
1	F	148	ILE
1	F	177	GLU
1	F	190	ASP
1	F	228	ARG
1	F	230	ILE
1	F	301	ASP
1	F	308	LYS
1	F	311	ILE
1	F	320	ARG
1	F	331	ILE
1	F	360	SER
1	F	395	LEU
1	F	401	LYS
1	F	456	LYS
1	F	470	ARG
1	F	492	LEU
1	F	564	LEU
1	F	567	GLU
1	F	573	ILE
1	F	579	LYS
1	G	8	VAL
1	G	37	ARG
1	G	122	GLN
1	G	137	LEU
1	G	139	GLU
1	G	140	GLU
1	G	143	ASP
1	G	161	LEU

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Mol	Chain	Res	Type
1	G	192	ILE
1	G	230	ILE
1	G	234	LYS
1	G	285	SER
1	G	310	LEU
1	G	311	ILE
1	G	330	LEU
1	G	347	VAL
1	G	349	VAL
1	G	378	VAL
1	G	383	LEU
1	G	397	GLU
1	G	500	GLN
1	G	539	LYS
1	G	552	VAL
1	G	580	GLU
1	G	599	VAL
1	G	610	VAL
1	H	3	LYS
1	H	25	TRP
1	H	36	SER
1	H	37	ARG
1	H	39	THR
1	H	41	THR
1	H	86	SER
1	H	89	ARG
1	H	107	LYS
1	H	140	GLU
1	H	148	ILE
1	H	177	GLU
1	H	190	ASP
1	H	228	ARG
1	H	230	ILE
1	H	244	ASP
1	H	300	GLU
1	H	308	LYS
1	H	310	LEU
1	H	311	ILE
1	H	320	ARG
1	H	331	ILE
1	H	344	ARG
1	H	395	LEU

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Mol	Chain	Res	Type
1	H	456	LYS
1	H	564	LEU
1	H	567	GLU
1	H	573	ILE
1	H	579	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	99	ASN
1	A	117	GLN
1	A	168	HIS
1	A	406	ASN
1	A	432	GLN
1	A	435	HIS
1	A	450	GLN
1	A	534	HIS
1	A	545	HIS
1	A	549	ASN
1	A	563	GLN
1	A	575	ASN
1	B	444	HIS
1	B	450	GLN
1	C	99	ASN
1	C	117	GLN
1	C	435	HIS
1	C	450	GLN
1	C	549	ASN
1	C	563	GLN
1	C	575	ASN
1	D	99	ASN
1	D	435	HIS
1	D	500	GLN
1	E	99	ASN
1	E	117	GLN
1	E	406	ASN
1	E	432	GLN
1	E	435	HIS
1	E	450	GLN
1	E	563	GLN
1	E	575	ASN

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Mol	Chain	Res	Type
1	F	75	ASN
1	F	99	ASN
1	F	168	HIS
1	F	444	HIS
1	F	551	HIS
1	G	99	ASN
1	G	117	GLN
1	G	363	GLN
1	G	432	GLN
1	G	435	HIS
1	G	450	GLN
1	G	563	GLN
1	G	575	ASN
1	H	99	ASN
1	H	168	HIS
1	H	444	HIS
1	H	500	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](#)

32 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
2	UMP	E	701	-	21,21,21	1.60	3 (14%)	30,31,31	2.10	11 (36%)
2	UMP	D	701	-	21,21,21	1.59	3 (14%)	30,31,31	2.07	12 (40%)
3	1UG	D	702	-	30,30,30	2.04	10 (33%)	38,44,44	2.29	16 (42%)
5	NDP	C	704	-	51,52,52	1.34	5 (9%)	71,80,80	1.60	12 (16%)
5	NDP	B	704	-	51,52,52	1.37	6 (11%)	71,80,80	1.58	9 (12%)
2	UMP	C	701	-	21,21,21	1.59	3 (14%)	30,31,31	2.09	11 (36%)
3	1UG	A	702	-	30,30,30	2.12	11 (36%)	38,44,44	2.22	15 (39%)
2	UMP	B	701	-	21,21,21	1.59	3 (14%)	30,31,31	2.06	12 (40%)
5	NDP	H	704	-	51,52,52	1.37	6 (11%)	71,80,80	1.56	8 (11%)
4	FOL	F	703	-	34,34,34	1.18	3 (8%)	43,47,47	1.75	9 (20%)
5	NDP	A	704	-	51,52,52	1.35	6 (11%)	71,80,80	1.60	11 (15%)
2	UMP	A	701	-	21,21,21	1.59	3 (14%)	30,31,31	2.09	11 (36%)
4	FOL	G	703	-	34,34,34	1.21	3 (8%)	43,47,47	1.80	9 (20%)
5	NDP	D	704	-	51,52,52	1.39	6 (11%)	71,80,80	1.57	6 (8%)
4	FOL	A	703	-	34,34,34	1.20	3 (8%)	43,47,47	1.83	10 (23%)
4	FOL	D	703	-	34,34,34	1.18	3 (8%)	43,47,47	1.74	9 (20%)
4	FOL	B	703	-	34,34,34	1.18	3 (8%)	43,47,47	1.76	9 (20%)
3	1UG	H	702	-	30,30,30	2.02	10 (33%)	38,44,44	2.32	16 (42%)
2	UMP	F	701	-	21,21,21	1.59	3 (14%)	30,31,31	2.04	12 (40%)
3	1UG	E	702	-	30,30,30	2.04	10 (33%)	38,44,44	2.12	14 (36%)
3	1UG	C	702	-	30,30,30	2.08	10 (33%)	38,44,44	2.10	14 (36%)
3	1UG	F	702	-	30,30,30	2.06	10 (33%)	38,44,44	2.13	15 (39%)
4	FOL	H	703	-	34,34,34	1.18	3 (8%)	43,47,47	1.77	10 (23%)
5	NDP	G	704	-	51,52,52	1.34	5 (9%)	71,80,80	1.59	10 (14%)
2	UMP	G	701	-	21,21,21	1.60	3 (14%)	30,31,31	2.09	11 (36%)
3	1UG	G	702	-	30,30,30	2.06	10 (33%)	38,44,44	2.09	14 (36%)
3	1UG	B	702	-	30,30,30	2.02	10 (33%)	38,44,44	2.28	16 (42%)
2	UMP	H	701	-	21,21,21	1.59	3 (14%)	30,31,31	2.06	12 (40%)
4	FOL	E	703	-	34,34,34	1.20	4 (11%)	43,47,47	1.83	10 (23%)
4	FOL	C	703	-	34,34,34	1.19	4 (11%)	43,47,47	1.85	10 (23%)
5	NDP	E	704	-	51,52,52	1.36	6 (11%)	71,80,80	1.60	11 (15%)
5	NDP	F	704	-	51,52,52	1.38	7 (13%)	71,80,80	1.57	7 (9%)

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
2	UMP	E	701	-	-	4/10/22/22	0/2/2/2
2	UMP	D	701	-	-	4/10/22/22	0/2/2/2
3	1UG	D	702	-	-	1/4/4/4	0/5/5/5
5	NDP	C	704	-	-	3/34/77/77	0/5/5/5
5	NDP	B	704	-	-	7/34/77/77	0/5/5/5
2	UMP	C	701	-	-	3/10/22/22	0/2/2/2
3	1UG	A	702	-	-	0/4/4/4	0/5/5/5
2	UMP	B	701	-	-	4/10/22/22	0/2/2/2
5	NDP	H	704	-	-	9/34/77/77	0/5/5/5
4	FOL	F	703	-	-	1/22/22/22	0/3/3/3
5	NDP	A	704	-	-	2/34/77/77	0/5/5/5
2	UMP	A	701	-	-	4/10/22/22	0/2/2/2
4	FOL	G	703	-	-	5/22/22/22	0/3/3/3
5	NDP	D	704	-	-	10/34/77/77	0/5/5/5
4	FOL	A	703	-	-	5/22/22/22	0/3/3/3
4	FOL	D	703	-	-	1/22/22/22	0/3/3/3
4	FOL	B	703	-	-	0/22/22/22	0/3/3/3
3	1UG	H	702	-	-	2/4/4/4	0/5/5/5
2	UMP	F	701	-	-	1/10/22/22	0/2/2/2
3	1UG	E	702	-	-	0/4/4/4	0/5/5/5
3	1UG	C	702	-	-	0/4/4/4	0/5/5/5
3	1UG	F	702	-	-	0/4/4/4	0/5/5/5
4	FOL	H	703	-	-	0/22/22/22	0/3/3/3
5	NDP	G	704	-	-	3/34/77/77	0/5/5/5
2	UMP	G	701	-	-	3/10/22/22	0/2/2/2
3	1UG	G	702	-	-	0/4/4/4	0/5/5/5
3	1UG	B	702	-	-	1/4/4/4	0/5/5/5
2	UMP	H	701	-	-	1/10/22/22	0/2/2/2
4	FOL	E	703	-	-	5/22/22/22	0/3/3/3
4	FOL	C	703	-	-	5/22/22/22	0/3/3/3
5	NDP	E	704	-	-	3/34/77/77	0/5/5/5
5	NDP	F	704	-	-	7/34/77/77	0/5/5/5

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	1UG	CAS-SAP	5.27	1.86	1.78
3	D	702	1UG	CAS-SAP	5.24	1.86	1.78
3	H	702	1UG	CAS-SAP	5.16	1.85	1.78
3	B	702	1UG	CAS-SAP	5.14	1.85	1.78
3	C	702	1UG	CAS-SAP	5.12	1.85	1.78
3	E	702	1UG	CAS-SAP	4.99	1.85	1.78
3	F	702	1UG	CAS-SAP	4.92	1.85	1.78
3	G	702	1UG	CAS-SAP	4.88	1.85	1.78
5	D	704	NDP	C5A-C4A	4.54	1.47	1.39
5	E	704	NDP	C5A-C4A	4.51	1.47	1.39
5	F	704	NDP	C5A-C4A	4.50	1.47	1.39
5	G	704	NDP	C5A-C4A	4.48	1.47	1.39
5	B	704	NDP	C5A-C4A	4.46	1.47	1.39
5	A	704	NDP	C5A-C4A	4.46	1.47	1.39
5	H	704	NDP	C5A-C4A	4.44	1.47	1.39
5	C	704	NDP	C5A-C4A	4.39	1.46	1.39
3	A	702	1UG	CAY-CAZ	-4.37	1.36	1.46
3	G	702	1UG	CAY-CAZ	-4.31	1.36	1.46
3	F	702	1UG	CAY-CAZ	-4.31	1.36	1.46
3	C	702	1UG	CAY-CAZ	-4.28	1.36	1.46
3	A	702	1UG	CAZ-CAW	-4.26	1.35	1.45
3	E	702	1UG	CAZ-CAW	-4.25	1.35	1.45
3	C	702	1UG	CAZ-CAW	-4.24	1.35	1.45
3	F	702	1UG	CAZ-CAW	-4.23	1.35	1.45
3	G	702	1UG	CAZ-CAW	-4.22	1.35	1.45
3	E	702	1UG	CAY-CAZ	-4.19	1.36	1.46
3	D	702	1UG	CAZ-CAW	-4.19	1.35	1.45
3	B	702	1UG	CAZ-CAW	-4.18	1.35	1.45
3	H	702	1UG	CAZ-CAW	-4.17	1.35	1.45
3	B	702	1UG	CAY-CAZ	-4.11	1.37	1.46
3	D	702	1UG	CAY-CAZ	-4.11	1.37	1.46
3	H	702	1UG	CAY-CAZ	-4.10	1.37	1.46
5	D	704	NDP	PN-O3	3.99	1.63	1.59
5	F	704	NDP	PN-O3	3.86	1.63	1.59
5	B	704	NDP	PN-O3	3.82	1.63	1.59
5	H	704	NDP	PN-O3	3.79	1.63	1.59
5	A	704	NDP	PN-O3	3.72	1.63	1.59
5	E	704	NDP	PN-O3	3.67	1.63	1.59
5	C	704	NDP	PN-O3	3.58	1.63	1.59
5	G	704	NDP	PN-O3	3.53	1.63	1.59
3	F	702	1UG	CAY-CAV	-3.52	1.35	1.41
2	G	701	UMP	C2-N3	-3.50	1.31	1.38
3	G	702	1UG	CAY-CAV	-3.49	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	UMP	C2-N1	3.48	1.43	1.38
2	G	701	UMP	C2-N1	3.45	1.43	1.38
2	D	701	UMP	C2-N1	3.44	1.43	1.38
3	A	702	1UG	CAY-CAV	-3.43	1.36	1.41
2	C	701	UMP	C2-N1	3.43	1.43	1.38
2	A	701	UMP	C2-N3	-3.43	1.32	1.38
2	E	701	UMP	C2-N3	-3.42	1.32	1.38
4	G	703	FOL	C8A-N1	-3.41	1.33	1.38
2	B	701	UMP	C2-N1	3.41	1.43	1.38
3	C	702	1UG	CAY-CAV	-3.40	1.36	1.41
2	C	701	UMP	C2-N3	-3.37	1.32	1.38
2	A	701	UMP	C2-N1	3.37	1.43	1.38
2	F	701	UMP	C2-N1	3.37	1.43	1.38
2	H	701	UMP	C2-N1	3.36	1.43	1.38
4	A	703	FOL	C8A-N1	-3.36	1.33	1.38
4	E	703	FOL	C8A-N1	-3.34	1.33	1.38
2	B	701	UMP	C2-N3	-3.33	1.32	1.38
2	F	701	UMP	C2-N3	-3.31	1.32	1.38
3	E	702	1UG	CAY-CAV	-3.31	1.36	1.41
2	D	701	UMP	C2-N3	-3.29	1.32	1.38
4	C	703	FOL	C8A-N1	-3.27	1.33	1.38
2	H	701	UMP	C2-N3	-3.27	1.32	1.38
3	B	702	1UG	CAY-CAV	-3.21	1.36	1.41
3	D	702	1UG	CAY-CAV	-3.20	1.36	1.41
3	H	702	1UG	CAY-CAV	-3.16	1.36	1.41
3	F	702	1UG	CAZ-CAT	-3.14	1.36	1.43
3	A	702	1UG	CAZ-CAT	-3.12	1.36	1.43
4	F	703	FOL	C8A-N1	-3.11	1.34	1.38
4	D	703	FOL	C8A-N1	-3.11	1.34	1.38
2	A	701	UMP	C4-N3	-3.09	1.33	1.38
3	D	702	1UG	CAZ-CAT	-3.09	1.36	1.43
3	B	702	1UG	CAZ-CAT	-3.08	1.36	1.43
3	G	702	1UG	CAZ-CAT	-3.07	1.36	1.43
3	C	702	1UG	CAZ-CAT	-3.05	1.36	1.43
3	H	702	1UG	CAZ-CAT	-3.05	1.36	1.43
4	H	703	FOL	C8A-N1	-3.04	1.34	1.38
2	G	701	UMP	C4-N3	-3.04	1.33	1.38
3	E	702	1UG	CAZ-CAT	-3.03	1.36	1.43
4	B	703	FOL	C8A-N1	-3.02	1.34	1.38
2	C	701	UMP	C4-N3	-3.00	1.33	1.38
2	E	701	UMP	C4-N3	-2.99	1.33	1.38
2	B	701	UMP	C4-N3	-2.97	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	1UG	CAY-CAS	-2.96	1.36	1.41
2	F	701	UMP	C4-N3	-2.96	1.33	1.38
2	H	701	UMP	C4-N3	-2.95	1.33	1.38
2	D	701	UMP	C4-N3	-2.94	1.33	1.38
3	B	702	1UG	CAV-NAO	-2.90	1.33	1.38
3	G	702	1UG	CAY-CAS	-2.90	1.36	1.41
3	D	702	1UG	CAV-NAO	-2.88	1.33	1.38
3	C	702	1UG	CAV-NAO	-2.88	1.33	1.38
3	H	702	1UG	CAV-NAO	-2.87	1.33	1.38
3	A	702	1UG	CAV-NAO	-2.86	1.33	1.38
3	C	702	1UG	CAY-CAS	-2.84	1.36	1.41
3	F	702	1UG	CAV-NAO	-2.84	1.33	1.38
3	G	702	1UG	CAV-NAO	-2.83	1.33	1.38
3	F	702	1UG	CAY-CAS	-2.83	1.36	1.41
3	E	702	1UG	CAV-NAO	-2.80	1.33	1.38
3	E	702	1UG	CAY-CAS	-2.72	1.36	1.41
3	C	702	1UG	CAK-CAV	-2.71	1.35	1.39
3	D	702	1UG	CAK-CAV	-2.71	1.35	1.39
5	B	704	NDP	C5A-N7A	-2.69	1.34	1.39
5	H	704	NDP	C5A-N7A	-2.68	1.34	1.39
3	H	702	1UG	CAK-CAV	-2.68	1.35	1.39
3	A	702	1UG	CAK-CAV	-2.66	1.35	1.39
5	F	704	NDP	C5A-N7A	-2.65	1.34	1.39
3	G	702	1UG	CAK-CAV	-2.64	1.35	1.39
5	D	704	NDP	C5A-N7A	-2.63	1.34	1.39
5	E	704	NDP	C5A-N7A	-2.63	1.34	1.39
5	A	704	NDP	C5A-N7A	-2.61	1.34	1.39
3	E	702	1UG	CAK-CAV	-2.61	1.35	1.39
3	B	702	1UG	CAK-CAV	-2.59	1.35	1.39
5	C	704	NDP	C5A-N7A	-2.59	1.34	1.39
3	F	702	1UG	CAK-CAV	-2.57	1.35	1.39
5	G	704	NDP	C5A-N7A	-2.56	1.34	1.39
5	D	704	NDP	PA-O3	2.53	1.62	1.59
3	B	702	1UG	CAY-CAS	-2.43	1.37	1.41
5	F	704	NDP	PA-O3	2.42	1.62	1.59
4	A	703	FOL	C4A-C8A	2.39	1.49	1.42
3	H	702	1UG	CAY-CAS	-2.39	1.37	1.41
4	E	703	FOL	C4A-C8A	2.37	1.49	1.42
3	D	702	1UG	CAY-CAS	-2.35	1.37	1.41
4	C	703	FOL	C4A-C8A	2.35	1.49	1.42
5	B	704	NDP	PA-O3	2.35	1.62	1.59
4	G	703	FOL	C4A-C8A	2.34	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	703	FOL	C4A-C8A	2.33	1.48	1.42
5	H	704	NDP	PA-O3	2.32	1.62	1.59
5	E	704	NDP	C5A-C6A	2.30	1.47	1.41
5	D	704	NDP	C5A-C6A	2.30	1.47	1.41
4	D	703	FOL	C4A-C8A	2.30	1.48	1.42
4	F	703	FOL	C4-N3	-2.30	1.34	1.38
5	H	704	NDP	C5A-C6A	2.28	1.47	1.41
4	B	703	FOL	C4-N3	-2.28	1.34	1.38
3	A	702	1UG	CAJ-CAU	-2.28	1.37	1.42
4	F	703	FOL	C4A-C8A	2.27	1.48	1.42
4	D	703	FOL	C4-N3	-2.27	1.34	1.38
5	F	704	NDP	C5A-C6A	2.27	1.47	1.41
3	F	702	1UG	CAW-NAO	-2.26	1.32	1.36
4	B	703	FOL	C4A-C8A	2.26	1.48	1.42
5	B	704	NDP	C5A-C6A	2.26	1.47	1.41
4	H	703	FOL	C4-N3	-2.24	1.34	1.38
3	H	702	1UG	CAW-NAO	-2.24	1.32	1.36
4	G	703	FOL	C4-N3	-2.23	1.34	1.38
4	A	703	FOL	C4-N3	-2.23	1.34	1.38
5	C	704	NDP	C5A-C6A	2.22	1.47	1.41
3	B	702	1UG	CAJ-CAU	-2.22	1.37	1.42
4	E	703	FOL	C4-N3	-2.22	1.34	1.38
5	G	704	NDP	C5A-C6A	2.21	1.47	1.41
5	A	704	NDP	C5A-C6A	2.20	1.47	1.41
3	G	702	1UG	CAW-NAO	-2.19	1.33	1.36
3	D	702	1UG	CAJ-CAU	-2.18	1.37	1.42
3	D	702	1UG	CAW-NAO	-2.18	1.33	1.36
3	E	702	1UG	CAJ-CAU	-2.16	1.37	1.42
3	F	702	1UG	CAJ-CAU	-2.14	1.37	1.42
4	C	703	FOL	C4-N3	-2.14	1.34	1.38
3	E	702	1UG	CAW-NAO	-2.13	1.33	1.36
3	C	702	1UG	CAW-NAO	-2.12	1.33	1.36
3	B	702	1UG	CAW-NAO	-2.12	1.33	1.36
3	H	702	1UG	CAJ-CAU	-2.10	1.37	1.42
5	A	704	NDP	PA-O3	2.09	1.61	1.59
5	F	704	NDP	C4A-N9A	-2.09	1.33	1.37
3	C	702	1UG	CAJ-CAU	-2.09	1.37	1.42
5	B	704	NDP	C4A-N9A	-2.09	1.33	1.37
3	A	702	1UG	CAW-NAO	-2.08	1.33	1.36
5	E	704	NDP	PA-O3	2.06	1.61	1.59
5	H	704	NDP	C4A-N9A	-2.05	1.33	1.37
5	C	704	NDP	C4A-N9A	-2.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	702	1UG	CAJ-CAU	-2.03	1.37	1.42
4	C	703	FOL	C7-N8	2.03	1.38	1.34
5	E	704	NDP	C4A-N9A	-2.03	1.33	1.37
5	F	704	NDP	C8A-N7A	2.02	1.35	1.31
5	G	704	NDP	C4A-N9A	-2.02	1.33	1.37
4	E	703	FOL	C7-N8	2.01	1.38	1.34
5	A	704	NDP	C4A-N9A	-2.01	1.33	1.37
3	A	702	1UG	CAD-CAL	2.00	1.41	1.36
5	D	704	NDP	C4A-N9A	-2.00	1.33	1.37

All (362) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	704	NDP	C5A-C4A-N3A	-5.82	118.70	126.72
5	F	704	NDP	C5A-C4A-N3A	-5.77	118.77	126.72
5	D	704	NDP	C5A-C4A-N3A	-5.76	118.78	126.72
5	B	704	NDP	C5A-C4A-N3A	-5.75	118.79	126.72
5	A	704	NDP	C5A-C4A-N3A	-5.74	118.81	126.72
5	C	704	NDP	C5A-C4A-N3A	-5.72	118.83	126.72
5	G	704	NDP	C5A-C4A-N3A	-5.70	118.86	126.72
5	H	704	NDP	C5A-C4A-N3A	-5.67	118.91	126.72
4	H	703	FOL	N1-C8A-N8	5.47	124.54	116.38
4	B	703	FOL	N1-C8A-N8	5.41	124.46	116.38
4	F	703	FOL	N1-C8A-N8	5.35	124.37	116.38
4	D	703	FOL	N1-C8A-N8	5.34	124.36	116.38
3	A	702	1UG	CAI-CAU-CAX	5.28	125.94	119.12
4	C	703	FOL	C7-C6-N5	-5.08	117.58	120.87
4	G	703	FOL	N1-C8A-N8	4.97	123.80	116.38
3	D	702	1UG	CAI-CAU-CAX	4.94	125.50	119.12
3	H	702	1UG	CAI-CAU-CAX	4.94	125.50	119.12
4	C	703	FOL	N1-C8A-N8	4.93	123.75	116.38
3	F	702	1UG	CAI-CAU-CAX	4.93	125.49	119.12
4	E	703	FOL	N1-C8A-N8	4.89	123.69	116.38
4	A	703	FOL	N1-C8A-N8	4.89	123.69	116.38
5	E	704	NDP	N3A-C4A-N9A	4.89	135.49	127.17
4	A	703	FOL	C7-C6-N5	-4.89	117.70	120.87
3	B	702	1UG	CAI-CAU-CAX	4.88	125.42	119.12
4	E	703	FOL	C7-C6-N5	-4.88	117.70	120.87
5	A	704	NDP	N3A-C4A-N9A	4.86	135.43	127.17
5	G	704	NDP	N3A-C4A-N9A	4.83	135.38	127.17
5	C	704	NDP	N3A-C4A-N9A	4.82	135.37	127.17
3	G	702	1UG	CAI-CAU-CAX	4.81	125.33	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	704	NDP	N3A-C4A-N9A	4.79	135.31	127.17
4	G	703	FOL	C7-C6-N5	-4.76	117.78	120.87
3	E	702	1UG	CAI-CAU-CAX	4.73	125.22	119.12
5	H	704	NDP	N3A-C4A-N9A	4.72	135.20	127.17
3	C	702	1UG	CAI-CAU-CAX	4.72	125.22	119.12
5	D	704	NDP	N3A-C4A-N9A	4.72	135.19	127.17
3	C	702	1UG	CAQ-NAM-CAW	4.71	121.67	113.36
3	B	702	1UG	CAQ-NAM-CAW	4.69	121.64	113.36
5	F	704	NDP	N3A-C4A-N9A	4.69	135.14	127.17
3	E	702	1UG	CAQ-NAM-CAW	4.68	121.62	113.36
3	A	702	1UG	CAQ-NAM-CAW	4.67	121.59	113.36
3	D	702	1UG	CAQ-NAM-CAW	4.62	121.51	113.36
3	G	702	1UG	CAQ-NAM-CAW	4.60	121.48	113.36
3	H	702	1UG	CAQ-NAM-CAW	4.60	121.47	113.36
3	F	702	1UG	CAQ-NAM-CAW	4.57	121.42	113.36
3	H	702	1UG	CAX-CAR-SAP	4.51	132.47	120.23
5	A	704	NDP	N3A-C2A-N1A	-4.40	121.93	128.58
2	F	701	UMP	C4-N3-C2	-4.39	121.16	126.61
5	C	704	NDP	N3A-C2A-N1A	-4.39	121.94	128.58
5	G	704	NDP	N3A-C2A-N1A	-4.38	121.96	128.58
2	C	701	UMP	C4-N3-C2	-4.37	121.18	126.61
2	G	701	UMP	C5-C4-N3	4.36	120.91	114.80
2	D	701	UMP	C4-N3-C2	-4.36	121.20	126.61
2	H	701	UMP	C4-N3-C2	-4.35	121.21	126.61
2	G	701	UMP	C4-N3-C2	-4.35	121.22	126.61
2	B	701	UMP	C4-N3-C2	-4.32	121.25	126.61
2	A	701	UMP	C4-N3-C2	-4.31	121.26	126.61
2	C	701	UMP	C5-C4-N3	4.31	120.84	114.80
5	E	704	NDP	N3A-C2A-N1A	-4.31	122.06	128.58
2	E	701	UMP	C4-N3-C2	-4.31	121.26	126.61
4	A	703	FOL	C6-C7-N8	4.29	127.26	123.14
2	E	701	UMP	C5-C4-N3	4.29	120.81	114.80
3	D	702	1UG	CAX-CAR-SAP	4.26	131.82	120.23
2	A	701	UMP	C5-C4-N3	4.25	120.75	114.80
4	C	703	FOL	C6-C7-N8	4.25	127.21	123.14
5	B	704	NDP	N3A-C2A-N1A	-4.25	122.16	128.58
5	F	704	NDP	N3A-C2A-N1A	-4.23	122.18	128.58
5	H	704	NDP	N3A-C2A-N1A	-4.21	122.20	128.58
2	H	701	UMP	C5-C4-N3	4.21	120.70	114.80
4	E	703	FOL	C6-C7-N8	4.20	127.17	123.14
5	D	704	NDP	N3A-C2A-N1A	-4.19	122.25	128.58
2	B	701	UMP	C5-C4-N3	4.17	120.64	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	FOL	C7-C6-N5	-4.16	118.17	120.87
4	F	703	FOL	C7-C6-N5	-4.14	118.18	120.87
2	F	701	UMP	N3-C2-N1	4.13	120.27	114.89
3	B	702	1UG	CAC-CAD-CAL	4.11	125.91	120.40
2	D	701	UMP	C5-C4-N3	4.10	120.55	114.80
2	F	701	UMP	C5-C4-N3	4.08	120.51	114.80
3	D	702	1UG	CAC-CAD-CAL	4.05	125.82	120.40
3	B	702	1UG	CAX-CAR-SAP	4.05	131.23	120.23
3	H	702	1UG	CAC-CAD-CAL	4.04	125.81	120.40
5	A	704	NDP	C2A-N3A-C4A	4.03	121.67	111.83
5	E	704	NDP	C2A-N3A-C4A	4.03	121.67	111.83
2	D	701	UMP	N3-C2-N1	4.02	120.13	114.89
5	C	704	NDP	C2A-N3A-C4A	4.02	121.64	111.83
4	H	703	FOL	C7-C6-N5	-4.01	118.27	120.87
5	G	704	NDP	C2A-N3A-C4A	4.01	121.62	111.83
2	A	701	UMP	N3-C2-N1	4.00	120.10	114.89
5	B	704	NDP	C2A-N3A-C4A	3.99	121.56	111.83
3	A	702	1UG	CAC-CAD-CAL	3.98	125.73	120.40
5	F	704	NDP	C2A-N3A-C4A	3.97	121.54	111.83
2	E	701	UMP	N3-C2-N1	3.97	120.06	114.89
2	B	701	UMP	N3-C2-N1	3.97	120.06	114.89
5	D	704	NDP	C2A-N3A-C4A	3.96	121.50	111.83
2	H	701	UMP	N3-C2-N1	3.95	120.04	114.89
4	D	703	FOL	C7-C6-N5	-3.95	118.31	120.87
2	C	701	UMP	N3-C2-N1	3.95	120.03	114.89
5	H	704	NDP	C2A-N3A-C4A	3.95	121.47	111.83
4	G	703	FOL	C6-C7-N8	3.93	126.91	123.14
2	G	701	UMP	N3-C2-N1	3.91	119.99	114.89
3	E	702	1UG	CAC-CAD-CAL	3.86	125.57	120.40
3	F	702	1UG	CAC-CAD-CAL	3.74	125.41	120.40
3	G	702	1UG	CAC-CAD-CAL	3.67	125.31	120.40
4	H	703	FOL	O4-C4-N3	3.67	125.80	120.23
3	B	702	1UG	CAZ-CAT-NAN	3.65	120.88	116.41
3	E	702	1UG	CAZ-CAT-NAN	3.64	120.87	116.41
3	D	702	1UG	CAR-SAP-CAS	3.61	116.00	103.53
3	H	702	1UG	CAR-SAP-CAS	3.59	115.94	103.53
3	C	702	1UG	CAZ-CAT-NAN	3.59	120.81	116.41
4	B	703	FOL	O4-C4-N3	3.56	125.64	120.23
3	A	702	1UG	CAZ-CAT-NAN	3.55	120.76	116.41
3	H	702	1UG	CAZ-CAT-NAN	3.55	120.75	116.41
3	A	702	1UG	CAD-CAC-CAI	-3.54	115.67	120.40
4	D	703	FOL	O4-C4-N3	3.53	125.60	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	1UG	CAZ-CAT-NAN	3.52	120.73	116.41
3	C	702	1UG	CAC-CAD-CAL	3.51	125.10	120.40
3	F	702	1UG	CAZ-CAT-NAN	3.49	120.68	116.41
3	G	702	1UG	CAZ-CAT-NAN	3.48	120.67	116.41
4	F	703	FOL	O4-C4-N3	3.47	125.51	120.23
3	A	702	1UG	CAX-CAR-SAP	3.46	129.63	120.23
3	D	702	1UG	CAD-CAC-CAI	-3.37	115.89	120.40
3	H	702	1UG	CAI-CAU-CAJ	-3.37	115.33	123.01
3	F	702	1UG	CAD-CAC-CAI	-3.36	115.90	120.40
3	C	702	1UG	CAD-CAC-CAI	-3.35	115.92	120.40
3	E	702	1UG	CAQ-NAN-CAT	-3.35	119.04	125.11
3	B	702	1UG	CAD-CAC-CAI	-3.34	115.93	120.40
3	H	702	1UG	CAD-CAC-CAI	-3.33	115.94	120.40
4	G	703	FOL	O4-C4-N3	3.33	125.29	120.23
3	B	702	1UG	CAR-SAP-CAS	3.32	115.00	103.53
4	C	703	FOL	O4-C4-N3	3.31	125.27	120.23
3	D	702	1UG	CAI-CAU-CAJ	-3.31	115.46	123.01
3	B	702	1UG	CAQ-NAN-CAT	-3.30	119.13	125.11
3	F	702	1UG	CAX-CAR-SAP	3.30	129.19	120.23
4	A	703	FOL	O4-C4-N3	3.30	125.24	120.23
3	G	702	1UG	CAQ-NAN-CAT	-3.29	119.14	125.11
3	C	702	1UG	CAQ-NAN-CAT	-3.29	119.14	125.11
3	B	702	1UG	CAI-CAU-CAJ	-3.29	115.50	123.01
3	A	702	1UG	CAQ-NAN-CAT	-3.27	119.17	125.11
3	E	702	1UG	CAD-CAC-CAI	-3.27	116.02	120.40
4	H	703	FOL	C6-C7-N8	3.27	126.28	123.14
2	C	701	UMP	O5'-P-OP1	-3.27	97.61	106.44
3	G	702	1UG	CAD-CAC-CAI	-3.26	116.03	120.40
2	D	701	UMP	O5'-P-OP1	-3.26	97.63	106.44
3	F	702	1UG	CAQ-NAN-CAT	-3.26	119.20	125.11
4	E	703	FOL	O4-C4-N3	3.25	125.17	120.23
2	A	701	UMP	O5'-P-OP1	-3.25	97.66	106.44
4	B	703	FOL	C6-C7-N8	3.25	126.25	123.14
3	H	702	1UG	CAQ-NAN-CAT	-3.23	119.25	125.11
2	H	701	UMP	O5'-P-OP1	-3.22	97.75	106.44
3	A	702	1UG	CAI-CAU-CAJ	-3.22	115.68	123.01
3	D	702	1UG	CAQ-NAN-CAT	-3.21	119.29	125.11
2	B	701	UMP	O5'-P-OP1	-3.21	97.77	106.44
4	D	703	FOL	C6-C7-N8	3.20	126.21	123.14
4	F	703	FOL	C6-C7-N8	3.17	126.18	123.14
2	F	701	UMP	O5'-P-OP1	-3.12	98.00	106.44
2	G	701	UMP	O5'-P-OP1	-3.12	98.00	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	702	1UG	CAX-CAR-SAP	3.09	128.63	120.23
2	E	701	UMP	O5'-P-OP1	-3.09	98.08	106.44
3	C	702	1UG	CAX-CAR-SAP	3.08	128.60	120.23
2	E	701	UMP	O4-C4-C5	-3.08	119.85	125.16
3	C	702	1UG	CAI-CAU-CAJ	-3.06	116.03	123.01
4	E	703	FOL	C8A-C4A-C4	-3.05	117.58	119.56
2	H	701	UMP	O4-C4-C5	-3.05	119.91	125.16
2	G	701	UMP	O4-C4-C5	-3.04	119.92	125.16
2	C	701	UMP	O4-C4-C5	-3.03	119.93	125.16
4	C	703	FOL	C8A-C4A-C4	-3.03	117.59	119.56
3	E	702	1UG	CAX-CAR-SAP	3.02	128.45	120.23
4	A	703	FOL	C8A-C4A-C4	-3.00	117.61	119.56
3	G	702	1UG	CAI-CAU-CAJ	-3.00	116.17	123.01
2	B	701	UMP	O4-C4-C5	-2.98	120.03	125.16
3	E	702	1UG	CAI-CAU-CAJ	-2.97	116.23	123.01
3	F	702	1UG	CAI-CAU-CAJ	-2.97	116.24	123.01
2	F	701	UMP	O4-C4-C5	-2.97	120.05	125.16
2	D	701	UMP	O4-C4-C5	-2.96	120.06	125.16
2	D	701	UMP	O2-C2-N3	-2.95	116.05	121.49
2	A	701	UMP	O2-C2-N3	-2.93	116.09	121.49
2	A	701	UMP	O4-C4-C5	-2.93	120.12	125.16
2	G	701	UMP	O2-C2-N3	-2.92	116.11	121.49
2	B	701	UMP	C1'-N1-C2	2.90	123.34	117.66
2	D	701	UMP	C1'-N1-C2	2.89	123.30	117.66
2	H	701	UMP	C1'-N1-C2	2.87	123.27	117.66
3	H	702	1UG	CAG-CAR-SAP	-2.86	109.48	117.74
2	B	701	UMP	O2-C2-N3	-2.86	116.22	121.49
2	E	701	UMP	O2-C2-N3	-2.86	116.22	121.49
3	F	702	1UG	NAO-CAW-NAM	2.86	129.45	125.80
2	C	701	UMP	O2-C2-N3	-2.85	116.23	121.49
2	H	701	UMP	O2-C2-N3	-2.85	116.23	121.49
3	A	702	1UG	NAO-CAW-NAM	2.85	129.44	125.80
2	F	701	UMP	O2-C2-N3	-2.83	116.26	121.49
3	A	702	1UG	CAL-CAX-CAU	-2.83	114.26	117.92
4	H	703	FOL	CG-CB-CA	2.77	118.28	113.16
3	G	702	1UG	NAO-CAW-NAM	2.77	129.34	125.80
3	D	702	1UG	NAN-CAQ-NAM	-2.77	118.25	123.32
3	B	702	1UG	NAN-CAQ-NAM	-2.76	118.28	123.32
4	B	703	FOL	NA2-C2-N3	-2.75	114.30	119.67
3	H	702	1UG	NAN-CAQ-NAM	-2.74	118.30	123.32
4	H	703	FOL	NA2-C2-N3	-2.74	114.32	119.67
3	C	702	1UG	NAN-CAQ-NAM	-2.73	118.33	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	701	UMP	C1'-N1-C2	2.72	122.99	117.66
3	D	702	1UG	CAL-CAX-CAU	-2.72	114.40	117.92
3	C	702	1UG	NAO-CAW-NAM	2.72	129.28	125.80
3	A	702	1UG	NAN-CAQ-NAM	-2.71	118.37	123.32
4	G	703	FOL	CA-N-C	2.70	128.04	121.56
2	A	701	UMP	C1'-N1-C2	2.70	122.94	117.66
3	F	702	1UG	CAL-CAX-CAU	-2.69	114.44	117.92
3	E	702	1UG	NAN-CAQ-NAM	-2.69	118.40	123.32
3	E	702	1UG	NAO-CAW-NAM	2.68	129.23	125.80
4	D	703	FOL	CG-CB-CA	2.68	118.11	113.16
3	H	702	1UG	CAL-CAX-CAU	-2.68	114.45	117.92
4	F	703	FOL	NA2-C2-N3	-2.68	114.44	119.67
4	G	703	FOL	C8A-C4A-C4	-2.68	117.82	119.56
4	F	703	FOL	CG-CB-CA	2.66	118.07	113.16
4	E	703	FOL	NA2-C2-N3	-2.66	114.48	119.67
4	G	703	FOL	NA2-C2-N3	-2.65	114.50	119.67
4	D	703	FOL	NA2-C2-N3	-2.65	114.50	119.67
2	F	701	UMP	C1'-N1-C2	2.64	122.82	117.66
3	F	702	1UG	NAN-CAQ-NAM	-2.64	118.50	123.32
3	B	702	1UG	NAO-CAW-NAM	2.62	129.15	125.80
3	H	702	1UG	CAY-CAZ-CAT	2.62	134.94	130.67
3	D	702	1UG	CAG-CAR-SAP	-2.62	110.19	117.74
2	G	701	UMP	C1'-N1-C2	2.62	122.78	117.66
3	C	702	1UG	CAY-CAZ-CAT	2.61	134.93	130.67
3	G	702	1UG	NAN-CAQ-NAM	-2.61	118.54	123.32
4	A	703	FOL	CA-N-C	2.61	127.83	121.56
3	B	702	1UG	CAY-CAZ-CAT	2.60	134.90	130.67
4	C	703	FOL	NA2-C2-N3	-2.60	114.60	119.67
3	C	702	1UG	CAL-CAX-CAU	-2.60	114.56	117.92
3	D	702	1UG	CAY-CAZ-CAT	2.59	134.89	130.67
3	E	702	1UG	CAY-CAZ-CAT	2.57	134.86	130.67
3	B	702	1UG	CAL-CAX-CAU	-2.55	114.62	117.92
5	C	704	NDP	C2A-N1A-C6A	2.54	122.89	118.73
4	A	703	FOL	NA2-C2-N3	-2.52	114.76	119.67
2	C	701	UMP	C1'-N1-C2	2.51	122.57	117.66
5	G	704	NDP	C2A-N1A-C6A	2.51	122.86	118.73
3	A	702	1UG	CAY-CAZ-CAT	2.50	134.73	130.67
2	C	701	UMP	O4'-C4'-C5'	2.49	117.32	109.33
4	B	703	FOL	CG-CB-CA	2.49	117.75	113.16
5	A	704	NDP	C2A-N1A-C6A	2.49	122.82	118.73
3	D	702	1UG	NAO-CAW-NAM	2.48	128.98	125.80
5	F	704	NDP	C2A-N1A-C6A	2.48	122.81	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	701	UMP	O4'-C4'-C5'	2.48	117.28	109.33
3	G	702	1UG	CAY-CAZ-CAT	2.47	134.70	130.67
5	D	704	NDP	C2A-N1A-C6A	2.47	122.78	118.73
5	E	704	NDP	C2A-N1A-C6A	2.46	122.77	118.73
5	H	704	NDP	C2A-N1A-C6A	2.45	122.76	118.73
2	G	701	UMP	O4'-C4'-C5'	2.45	117.19	109.33
4	H	703	FOL	NA2-C2-N1	2.45	121.92	116.77
4	F	703	FOL	NA2-C2-N1	2.45	121.92	116.77
5	B	704	NDP	C2A-N1A-C6A	2.45	122.75	118.73
4	E	703	FOL	NA2-C2-N1	2.44	121.91	116.77
4	B	703	FOL	NA2-C2-N1	2.44	121.91	116.77
5	D	704	NDP	C4A-C5A-N7A	-2.42	107.81	110.58
3	G	702	1UG	CAL-CAX-CAU	-2.42	114.80	117.92
2	B	701	UMP	C1'-N1-C6	-2.41	116.78	121.53
2	D	701	UMP	C1'-N1-C6	-2.41	116.79	121.53
2	H	701	UMP	C1'-N1-C6	-2.41	116.80	121.53
4	D	703	FOL	O2-CT-CA	2.40	121.62	113.51
3	B	702	1UG	CAG-CAR-SAP	-2.39	110.83	117.74
3	H	702	1UG	NAO-CAW-NAM	2.39	128.86	125.80
4	B	703	FOL	O2-CT-CA	2.39	121.59	113.51
2	A	701	UMP	O4'-C4'-C5'	2.39	116.98	109.33
4	C	703	FOL	NA2-C2-N1	2.38	121.78	116.77
4	H	703	FOL	O2-CT-CA	2.38	121.56	113.51
2	B	701	UMP	OP3-P-O5'	2.37	112.86	106.67
5	F	704	NDP	C4A-C5A-N7A	-2.37	107.87	110.58
2	H	701	UMP	OP3-P-O5'	2.37	112.85	106.67
2	D	701	UMP	OP3-P-O5'	2.36	112.83	106.67
2	H	701	UMP	O4'-C4'-C5'	2.36	116.90	109.33
4	F	703	FOL	O2-CT-CA	2.36	121.50	113.51
4	D	703	FOL	NA2-C2-N1	2.36	121.74	116.77
3	F	702	1UG	CAY-CAZ-CAT	2.36	134.51	130.67
3	E	702	1UG	OAB-CAT-NAN	-2.36	115.68	120.11
4	G	703	FOL	NA2-C2-N1	2.35	121.71	116.77
5	E	704	NDP	C4A-C5A-N7A	-2.34	107.90	110.58
3	A	702	1UG	CAG-CAR-SAP	-2.34	110.98	117.74
2	C	701	UMP	OP3-P-O5'	2.34	112.76	106.67
4	C	703	FOL	CA-N-C	2.34	127.17	121.56
2	F	701	UMP	OP3-P-O5'	2.33	112.75	106.67
3	B	702	1UG	OAB-CAT-NAN	-2.32	115.76	120.11
5	B	704	NDP	C4A-C5A-N7A	-2.32	107.93	110.58
3	G	702	1UG	OAB-CAT-NAN	-2.31	115.77	120.11
3	A	702	1UG	OAB-CAT-NAN	-2.31	115.77	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	703	FOL	CA-N-C	2.31	127.10	121.56
3	C	702	1UG	OAB-CAT-NAN	-2.30	115.78	120.11
3	E	702	1UG	CAL-CAX-CAU	-2.30	114.94	117.92
3	D	702	1UG	OAB-CAT-NAN	-2.30	115.79	120.11
5	G	704	NDP	C4A-C5A-N7A	-2.30	107.95	110.58
5	C	704	NDP	C4A-C5A-N7A	-2.30	107.96	110.58
2	F	701	UMP	O4'-C4'-C5'	2.29	116.68	109.33
2	A	701	UMP	OP3-P-O5'	2.29	112.64	106.67
2	D	701	UMP	O4'-C4'-C5'	2.29	116.66	109.33
4	A	703	FOL	NA2-C2-N1	2.28	121.56	116.77
5	A	704	NDP	C4A-C5A-N7A	-2.27	107.98	110.58
3	H	702	1UG	OAB-CAT-NAN	-2.27	115.84	120.11
5	H	704	NDP	C4A-C5A-N7A	-2.27	107.99	110.58
4	F	703	FOL	C8A-C4A-C4	-2.26	118.09	119.56
3	E	702	1UG	CAH-CAF-CAK	-2.25	117.35	120.24
2	B	701	UMP	O4'-C4'-C5'	2.24	116.50	109.33
2	G	701	UMP	OP3-P-O5'	2.23	112.49	106.67
4	E	703	FOL	O2-CT-CA	2.22	121.01	113.51
5	A	704	NDP	C1D-N1N-C2N	-2.21	117.49	121.14
5	C	704	NDP	O2B-C2B-C1B	-2.20	102.32	110.05
2	F	701	UMP	O3'-C3'-C4'	-2.19	101.75	110.07
3	H	702	1UG	CAH-CAF-CAK	-2.19	117.42	120.24
2	E	701	UMP	OP3-P-O5'	2.19	112.38	106.67
4	G	703	FOL	O2-CT-CA	2.19	120.92	113.51
5	G	704	NDP	C4A-N9A-C8A	2.19	108.04	105.74
5	E	704	NDP	O2B-C2B-C1B	-2.19	102.36	110.05
3	F	702	1UG	OAB-CAT-NAN	-2.18	116.01	120.11
5	C	704	NDP	C4A-N9A-C8A	2.17	108.02	105.74
5	C	704	NDP	O2N-PN-O1N	2.17	122.54	112.44
3	G	702	1UG	CAH-CAF-CAK	-2.17	117.46	120.24
2	A	701	UMP	C1'-N1-C6	-2.16	117.27	121.53
3	C	702	1UG	CAH-CAF-CAK	-2.16	117.47	120.24
5	E	704	NDP	O2B-P2B-O1X	-2.16	101.65	109.33
4	C	703	FOL	O2-CT-CA	2.15	120.80	113.51
5	C	704	NDP	O2B-P2B-O1X	-2.15	101.67	109.33
5	G	704	NDP	O2N-PN-O1N	2.14	122.42	112.44
2	E	701	UMP	C1'-N1-C6	-2.14	117.32	121.53
2	H	701	UMP	O3'-C3'-C4'	-2.14	101.97	110.07
5	E	704	NDP	C4A-N9A-C8A	2.13	107.98	105.74
4	A	703	FOL	O2-CT-CA	2.13	120.73	113.51
5	B	704	NDP	O3B-C3B-C2B	2.13	117.15	111.19
2	G	701	UMP	C1'-N1-C6	-2.13	117.34	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	704	NDP	O2B-P2B-O1X	-2.13	101.75	109.33
3	A	702	1UG	CAH-CAF-CAK	-2.13	117.51	120.24
3	F	702	1UG	CAG-CAR-SAP	-2.13	111.60	117.74
5	A	704	NDP	C4A-N9A-C8A	2.12	107.96	105.74
2	F	701	UMP	C1'-N1-C6	-2.12	117.37	121.53
2	H	701	UMP	O5'-C5'-C4'	2.11	116.19	108.99
5	C	704	NDP	C1D-N1N-C2N	-2.11	117.66	121.14
5	A	704	NDP	O2N-PN-O1N	2.11	122.26	112.44
3	B	702	1UG	CAH-CAF-CAK	-2.11	117.53	120.24
4	D	703	FOL	C8A-C4A-C4	-2.11	118.19	119.56
2	G	701	UMP	O3'-C3'-C4'	-2.11	102.08	110.07
5	G	704	NDP	O2B-P2B-O1X	-2.10	101.83	109.33
4	C	703	FOL	C6-C9-N10	2.10	117.74	113.13
2	F	701	UMP	O5'-C5'-C4'	2.10	116.13	108.99
4	H	703	FOL	C8A-C4A-C4	-2.10	118.20	119.56
3	D	702	1UG	CAH-CAF-CAK	-2.09	117.56	120.24
5	E	704	NDP	O2N-PN-O1N	2.09	122.16	112.44
5	H	704	NDP	O2X-P2B-O1X	2.08	118.94	110.83
2	B	701	UMP	O5'-C5'-C4'	2.08	116.07	108.99
3	F	702	1UG	CAH-CAF-CAK	-2.08	117.57	120.24
2	C	701	UMP	O4'-C1'-N1	2.08	111.55	107.86
4	B	703	FOL	C8A-C4A-C4	-2.07	118.21	119.56
5	B	704	NDP	O2X-P2B-O1X	2.06	118.88	110.83
2	A	701	UMP	O3'-C3'-C4'	-2.06	102.25	110.07
5	A	704	NDP	O2B-C2B-C1B	-2.05	102.83	110.05
2	B	701	UMP	O3'-C3'-C4'	-2.05	102.32	110.07
5	H	704	NDP	O3B-C3B-C2B	2.04	116.91	111.19
4	E	703	FOL	C6-C9-N10	2.03	117.59	113.13
2	E	701	UMP	O3'-C3'-C4'	-2.03	102.37	110.07
2	D	701	UMP	O3'-C3'-C4'	-2.03	102.38	110.07
4	A	703	FOL	C6-C9-N10	2.03	117.58	113.13
4	H	703	FOL	O4-C4-C4A	-2.03	116.86	120.42
5	F	704	NDP	O2X-P2B-O1X	2.03	118.73	110.83
2	C	701	UMP	C1'-N1-C6	-2.03	117.55	121.53
5	E	704	NDP	C1D-N1N-C2N	-2.02	117.81	121.14
2	D	701	UMP	O5'-C5'-C4'	2.02	115.86	108.99
5	C	704	NDP	N6A-C6A-N1A	2.02	122.87	118.38
5	G	704	NDP	O2B-C2B-C1B	-2.00	103.01	110.05
5	B	704	NDP	O2B-P2B-O1X	-2.00	102.20	109.33

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	UMP	C5'-O5'-P-OP2
2	A	701	UMP	C5'-O5'-P-OP3
2	C	701	UMP	C5'-O5'-P-OP2
2	C	701	UMP	C5'-O5'-P-OP3
2	E	701	UMP	C5'-O5'-P-OP2
2	E	701	UMP	C5'-O5'-P-OP3
2	G	701	UMP	C5'-O5'-P-OP2
2	G	701	UMP	C5'-O5'-P-OP3
3	H	702	1UG	CAG-CAR-SAP-CAS
3	H	702	1UG	CAX-CAR-SAP-CAS
5	B	704	NDP	C5B-O5B-PA-O1A
5	F	704	NDP	C5B-O5B-PA-O1A
5	F	704	NDP	C5B-O5B-PA-O3
4	A	703	FOL	N-CA-CB-CG
4	C	703	FOL	N-CA-CB-CG
4	E	703	FOL	N-CA-CB-CG
4	G	703	FOL	N-CA-CB-CG
4	A	703	FOL	CT-CA-CB-CG
4	C	703	FOL	CT-CA-CB-CG
4	E	703	FOL	CT-CA-CB-CG
4	G	703	FOL	CT-CA-CB-CG
2	B	701	UMP	O4'-C4'-C5'-O5'
2	D	701	UMP	O4'-C4'-C5'-O5'
2	F	701	UMP	O4'-C4'-C5'-O5'
2	H	701	UMP	O4'-C4'-C5'-O5'
2	A	701	UMP	C5'-O5'-P-OP1
2	C	701	UMP	C5'-O5'-P-OP1
2	E	701	UMP	C5'-O5'-P-OP1
2	G	701	UMP	C5'-O5'-P-OP1
5	D	704	NDP	C3B-C4B-C5B-O5B
5	B	704	NDP	PA-O3-PN-O5D
5	D	704	NDP	PA-O3-PN-O5D
5	F	704	NDP	PA-O3-PN-O5D
5	H	704	NDP	PA-O3-PN-O5D
4	C	703	FOL	CA-CB-CG-CD
4	G	703	FOL	CA-CB-CG-CD
5	H	704	NDP	C3B-C4B-C5B-O5B
3	D	702	1UG	CAX-CAR-SAP-CAS
4	E	703	FOL	CA-CB-CG-CD
4	A	703	FOL	CA-CB-CG-CD
5	B	704	NDP	C5B-O5B-PA-O2A
5	B	704	NDP	C5B-O5B-PA-O3
5	D	704	NDP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	D	704	NDP	C5B-O5B-PA-O2A
5	D	704	NDP	C5B-O5B-PA-O3
5	F	704	NDP	C5B-O5B-PA-O2A
5	H	704	NDP	C5B-O5B-PA-O1A
5	H	704	NDP	C5B-O5B-PA-O2A
5	H	704	NDP	C5B-O5B-PA-O3
2	B	701	UMP	C5'-O5'-P-OP1
2	D	701	UMP	C5'-O5'-P-OP1
3	B	702	1UG	CAX-CAR-SAP-CAS
2	B	701	UMP	C3'-C4'-C5'-O5'
5	A	704	NDP	O4D-C1D-N1N-C2N
4	F	703	FOL	CT-CA-CB-CG
2	E	701	UMP	C2'-C1'-N1-C2
5	B	704	NDP	O4D-C1D-N1N-C2N
5	C	704	NDP	O4D-C1D-N1N-C2N
5	D	704	NDP	O4D-C1D-N1N-C2N
5	F	704	NDP	O4D-C1D-N1N-C2N
5	G	704	NDP	O4D-C1D-N1N-C2N
5	H	704	NDP	O4D-C1D-N1N-C2N
5	B	704	NDP	C4D-C5D-O5D-PN
5	D	704	NDP	C4D-C5D-O5D-PN
5	H	704	NDP	C4D-C5D-O5D-PN
4	A	703	FOL	OE2-CD-CG-CB
5	E	704	NDP	O4D-C1D-N1N-C2N
2	B	701	UMP	C2'-C1'-N1-C2
5	F	704	NDP	C4D-C5D-O5D-PN
4	A	703	FOL	OE1-CD-CG-CB
5	F	704	NDP	C2D-C1D-N1N-C2N
4	C	703	FOL	OE2-CD-CG-CB
4	G	703	FOL	OE2-CD-CG-CB
2	D	701	UMP	C2'-C1'-N1-C2
4	E	703	FOL	OE2-CD-CG-CB
4	G	703	FOL	OE1-CD-CG-CB
4	D	703	FOL	CT-CA-CB-CG
5	B	704	NDP	C2D-C1D-N1N-C2N
5	C	704	NDP	C2D-C1D-N1N-C2N
5	G	704	NDP	C2D-C1D-N1N-C2N
4	C	703	FOL	OE1-CD-CG-CB
4	E	703	FOL	OE1-CD-CG-CB
5	G	704	NDP	C4D-C5D-O5D-PN
5	D	704	NDP	O4B-C4B-C5B-O5B
5	D	704	NDP	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
5	E	704	NDP	C2D-C1D-N1N-C2N
5	H	704	NDP	C2D-C1D-N1N-C2N
5	A	704	NDP	C4D-C5D-O5D-PN
2	D	701	UMP	C3'-C4'-C5'-O5'
5	H	704	NDP	O4B-C4B-C5B-O5B
5	C	704	NDP	C4D-C5D-O5D-PN
5	E	704	NDP	C4D-C5D-O5D-PN
2	A	701	UMP	C4'-C5'-O5'-P
5	D	704	NDP	PA-O3-PN-O2N

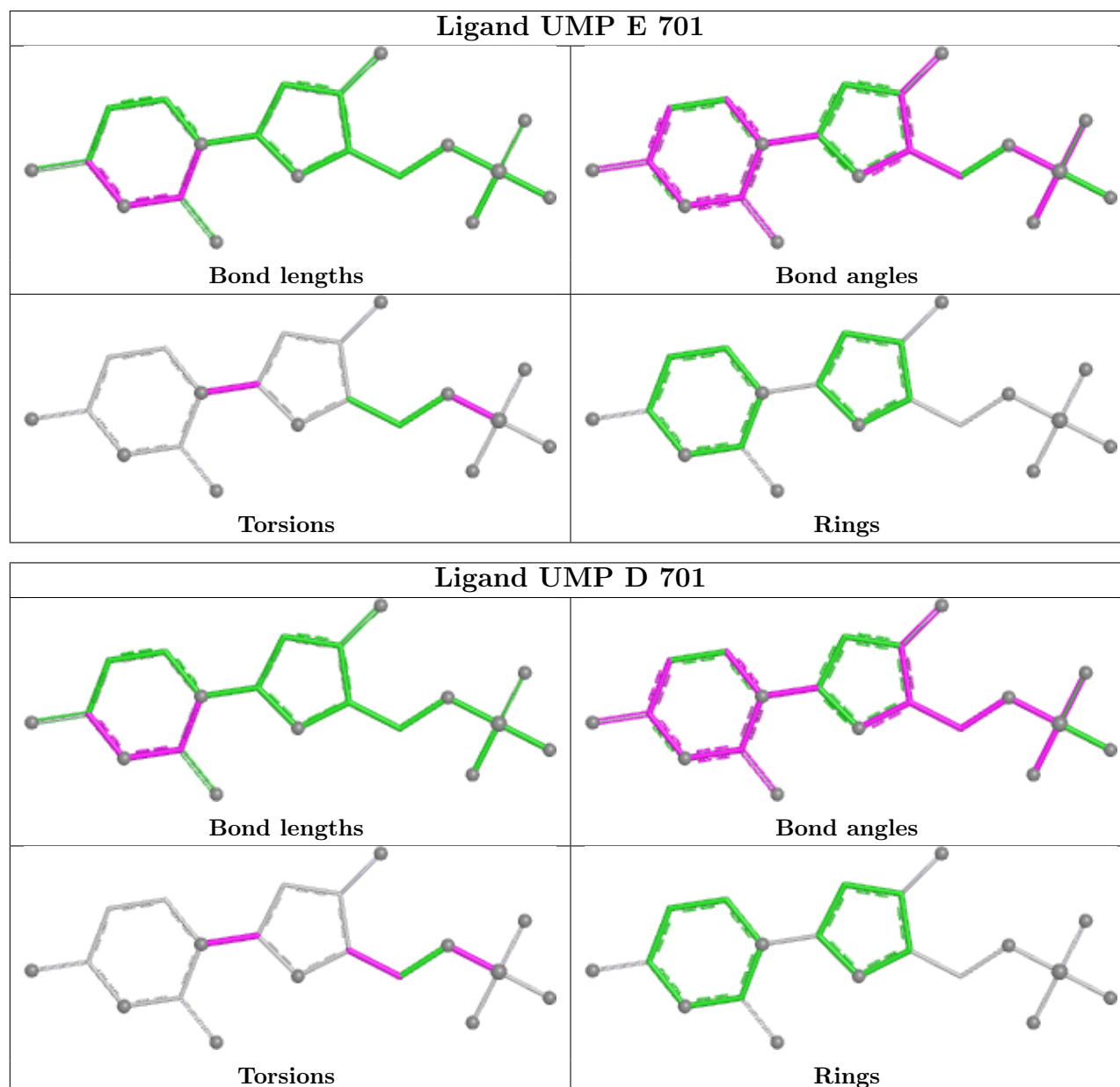
There are no ring outliers.

24 monomers are involved in 65 short contacts:

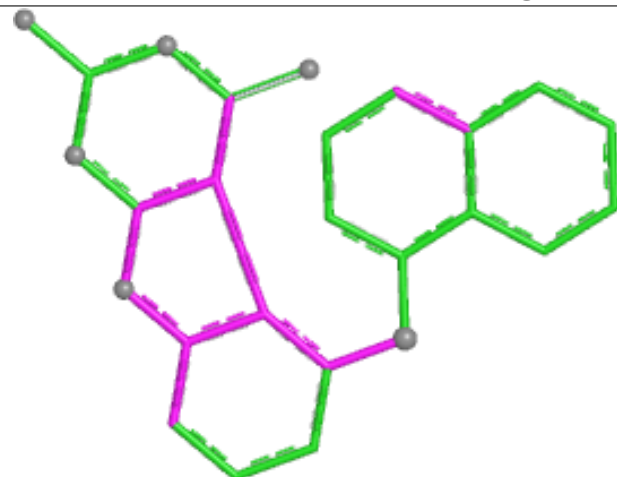
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	702	1UG	2	0
5	C	704	NDP	3	0
5	B	704	NDP	4	0
3	A	702	1UG	2	0
5	H	704	NDP	4	0
4	F	703	FOL	4	0
5	A	704	NDP	3	0
4	G	703	FOL	5	0
5	D	704	NDP	4	0
4	A	703	FOL	1	0
4	D	703	FOL	4	0
4	B	703	FOL	4	0
3	H	702	1UG	2	0
3	E	702	1UG	5	0
3	C	702	1UG	4	0
3	F	702	1UG	4	0
4	H	703	FOL	4	0
5	G	704	NDP	3	0
3	G	702	1UG	3	0
3	B	702	1UG	2	0
4	E	703	FOL	1	0
4	C	703	FOL	1	0
5	E	704	NDP	3	0
5	F	704	NDP	5	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

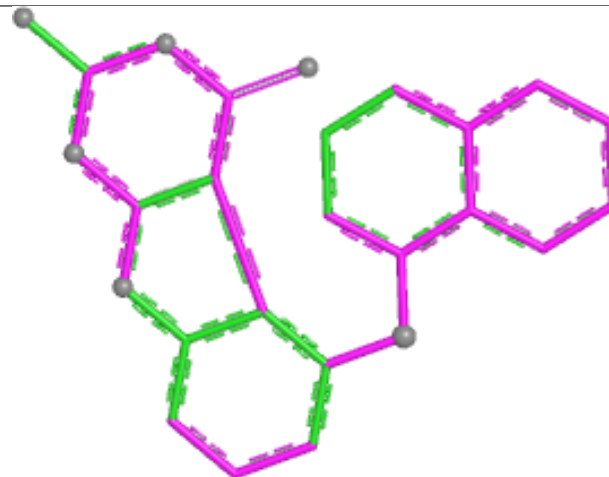
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



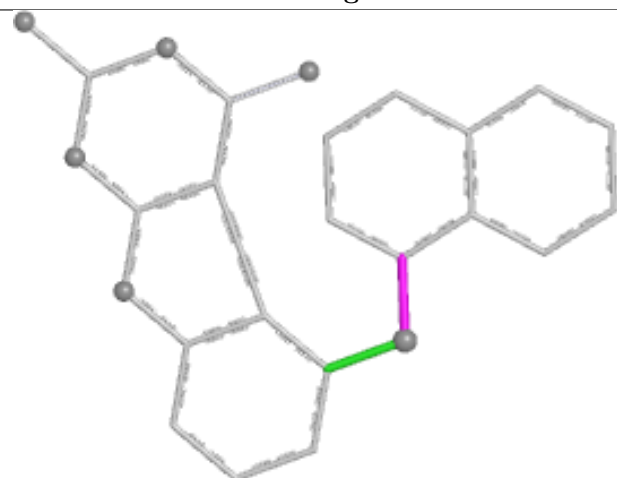
Ligand 1UG D 702



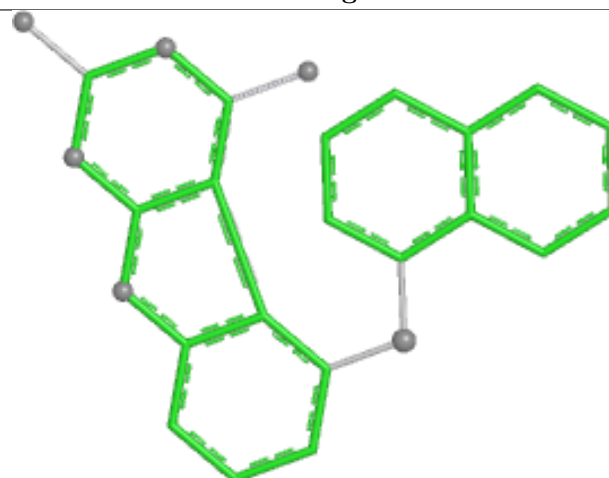
Bond lengths



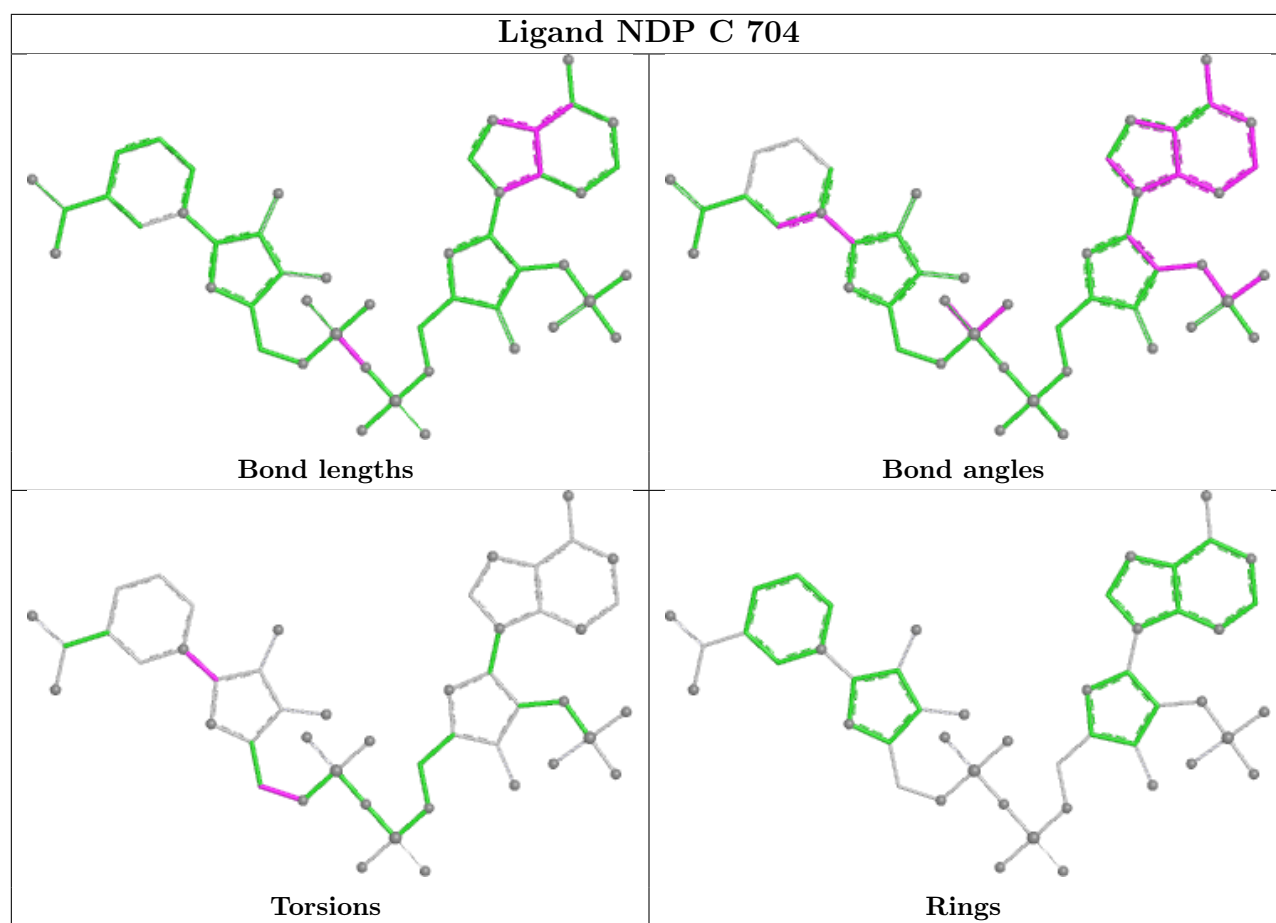
Bond angles

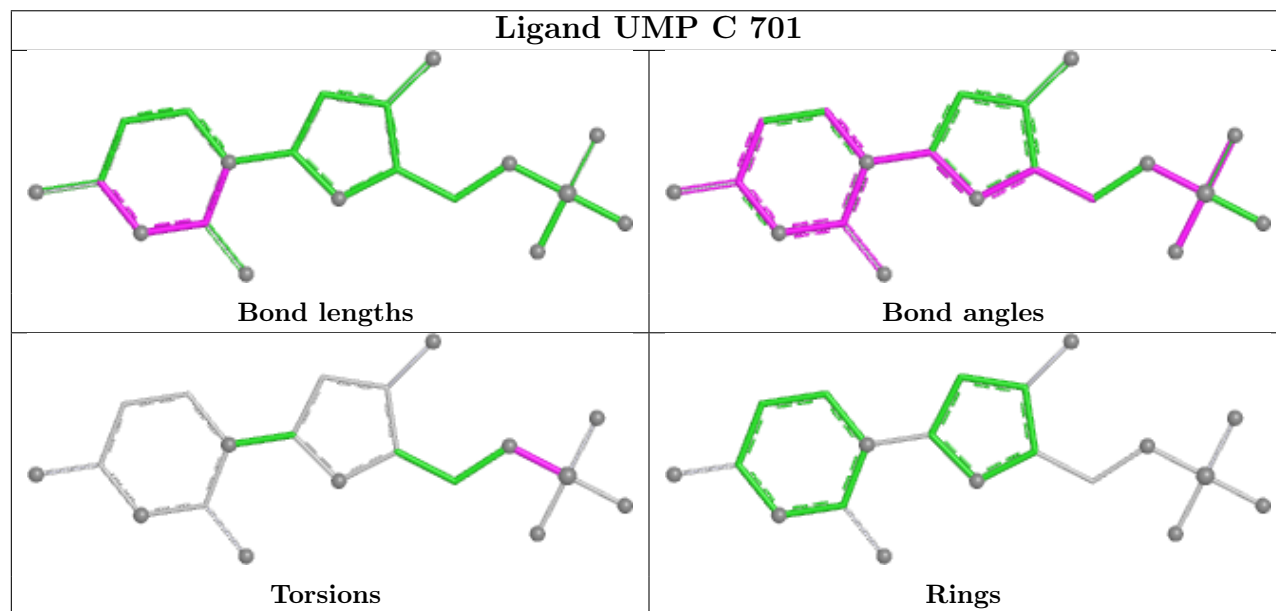
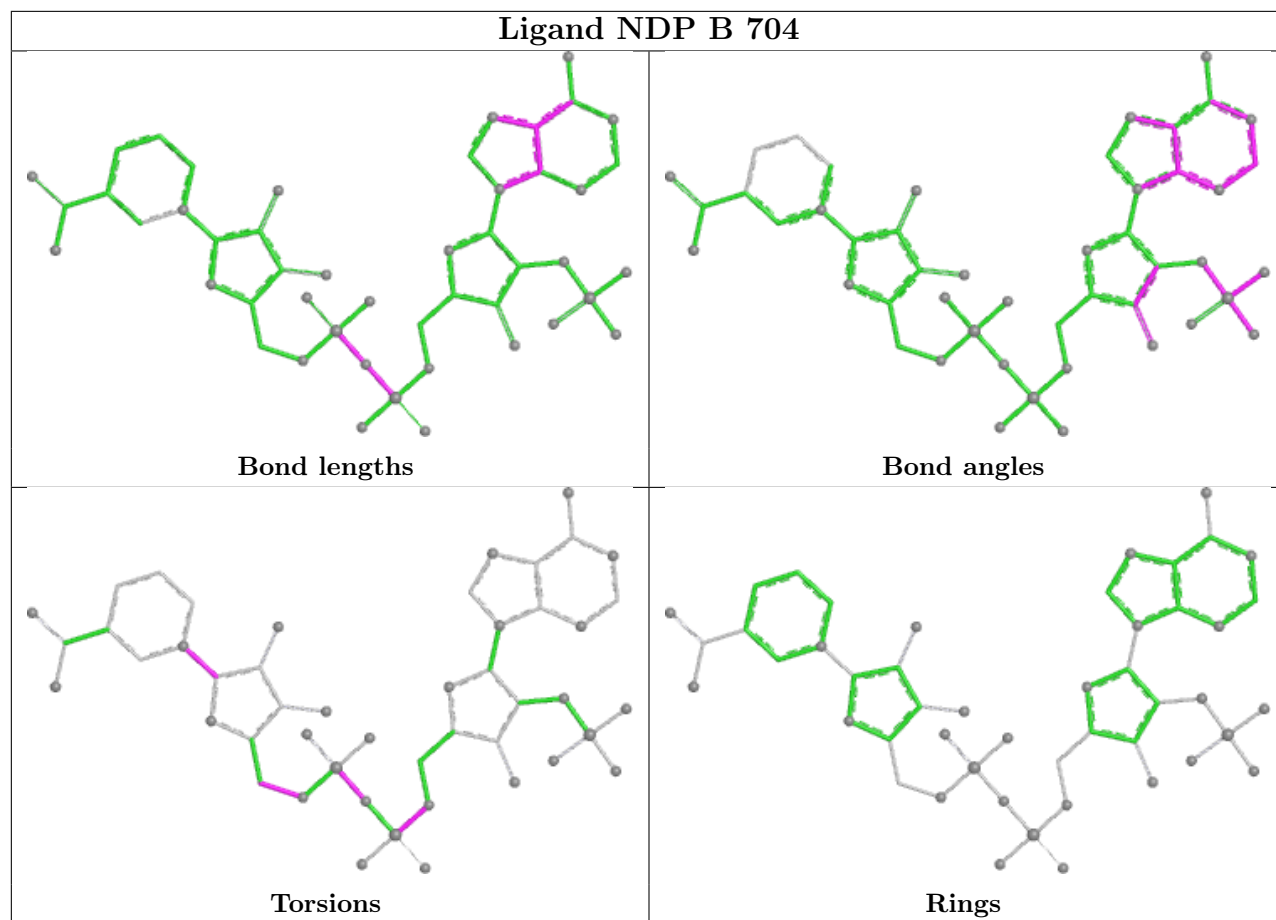


Torsions

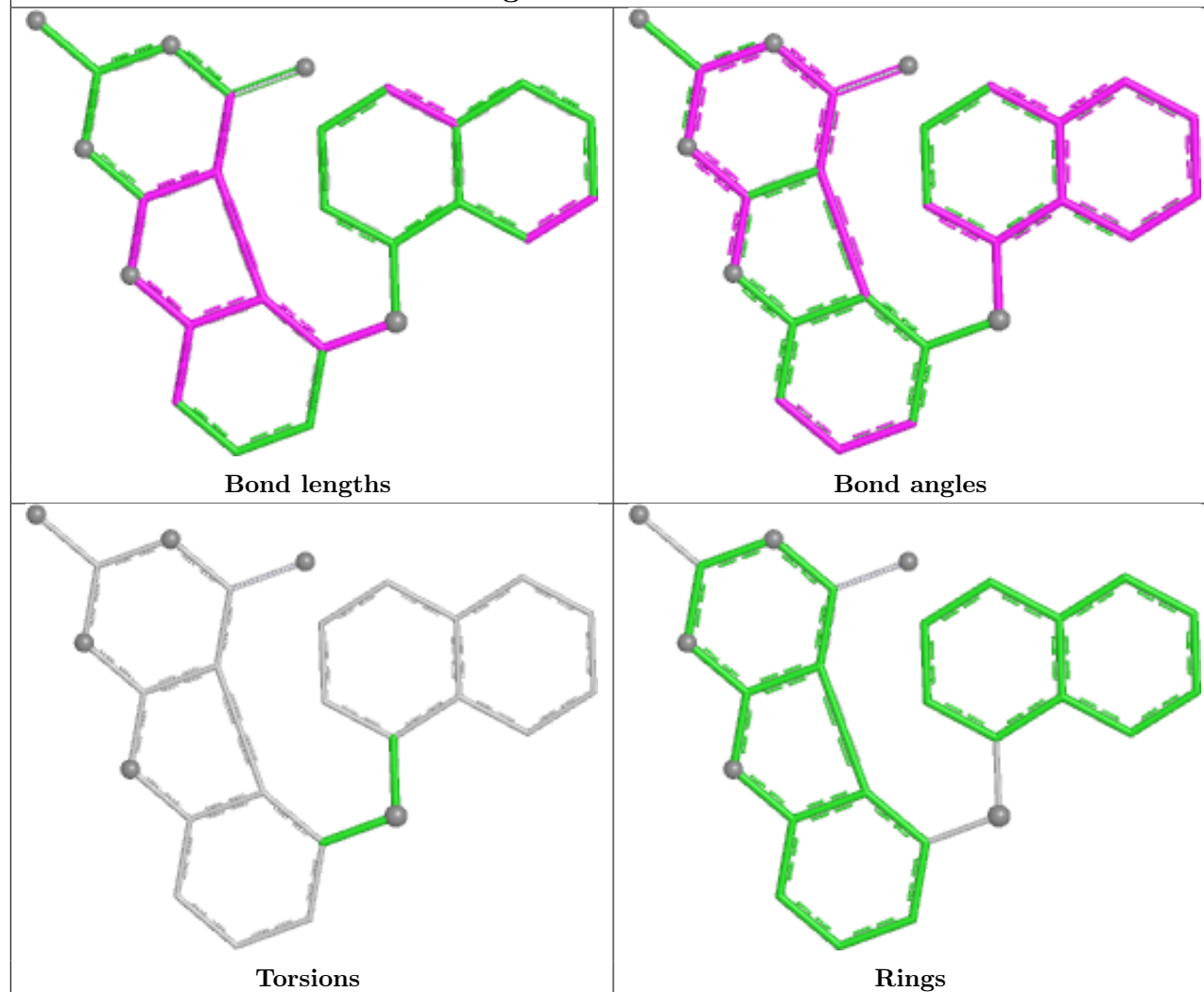


Rings

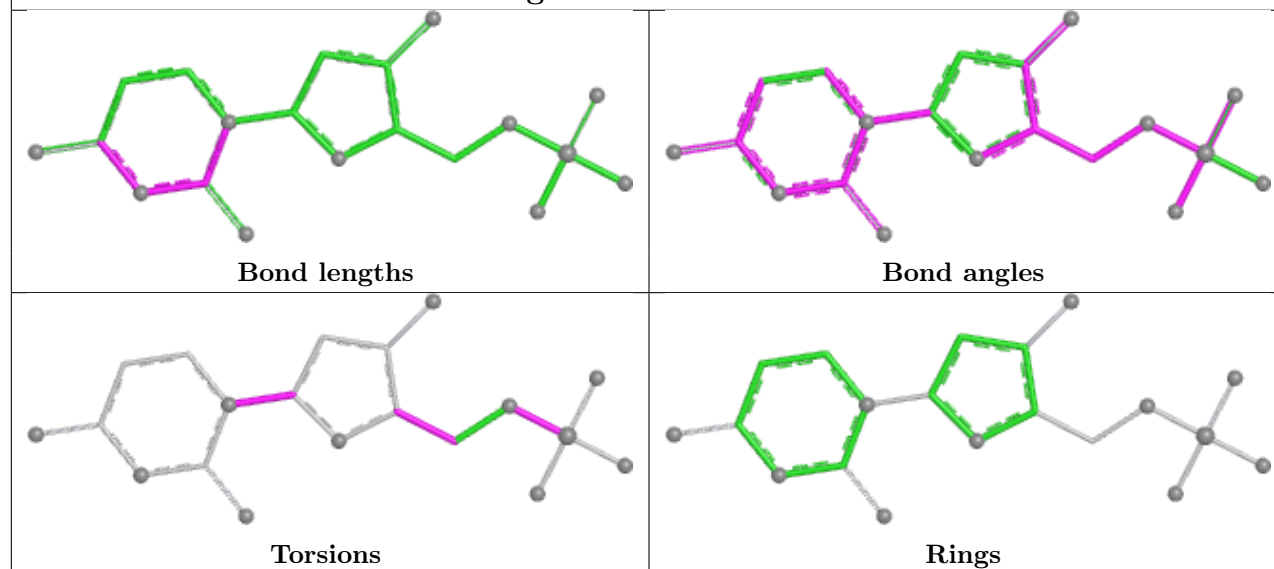


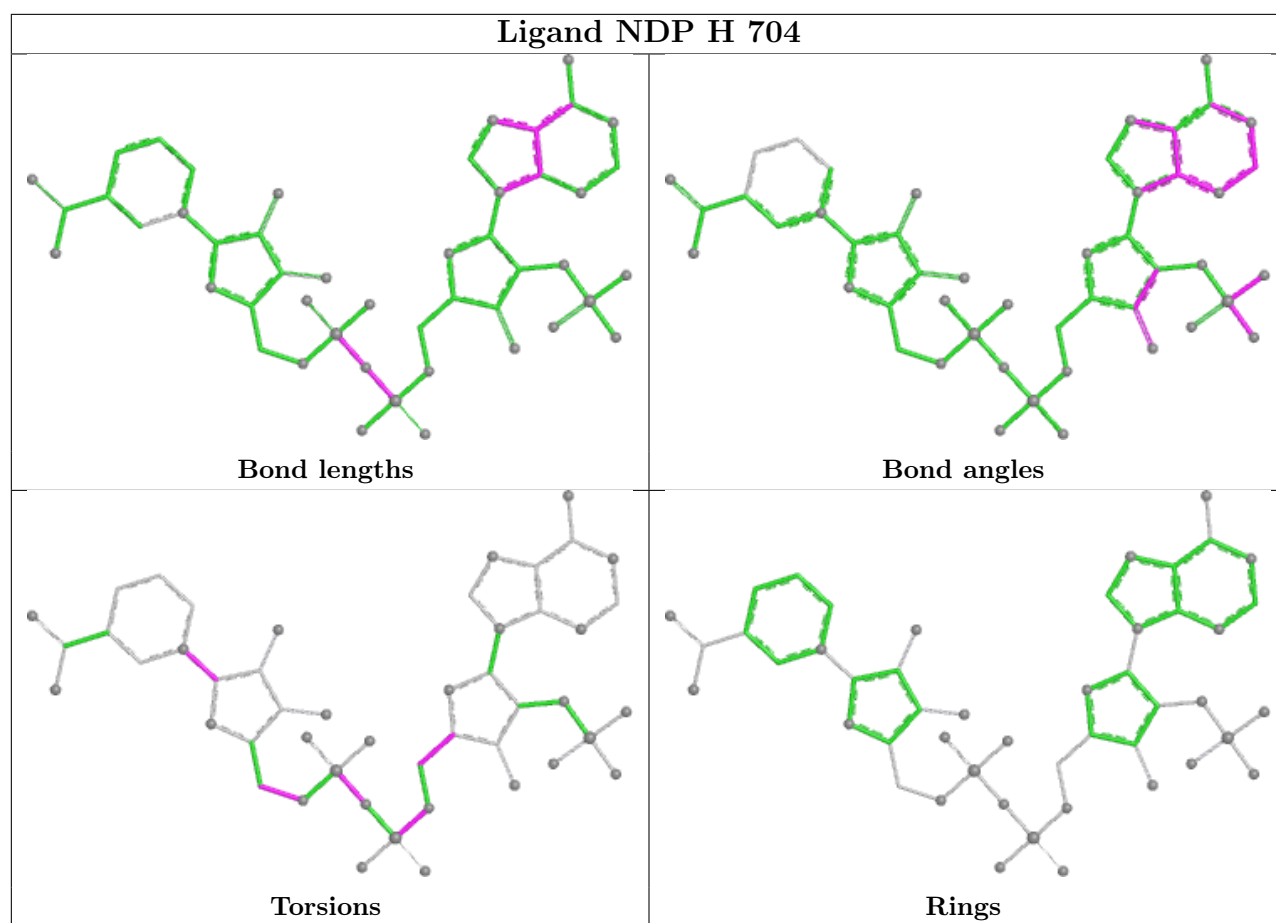


Ligand 1UG A 702

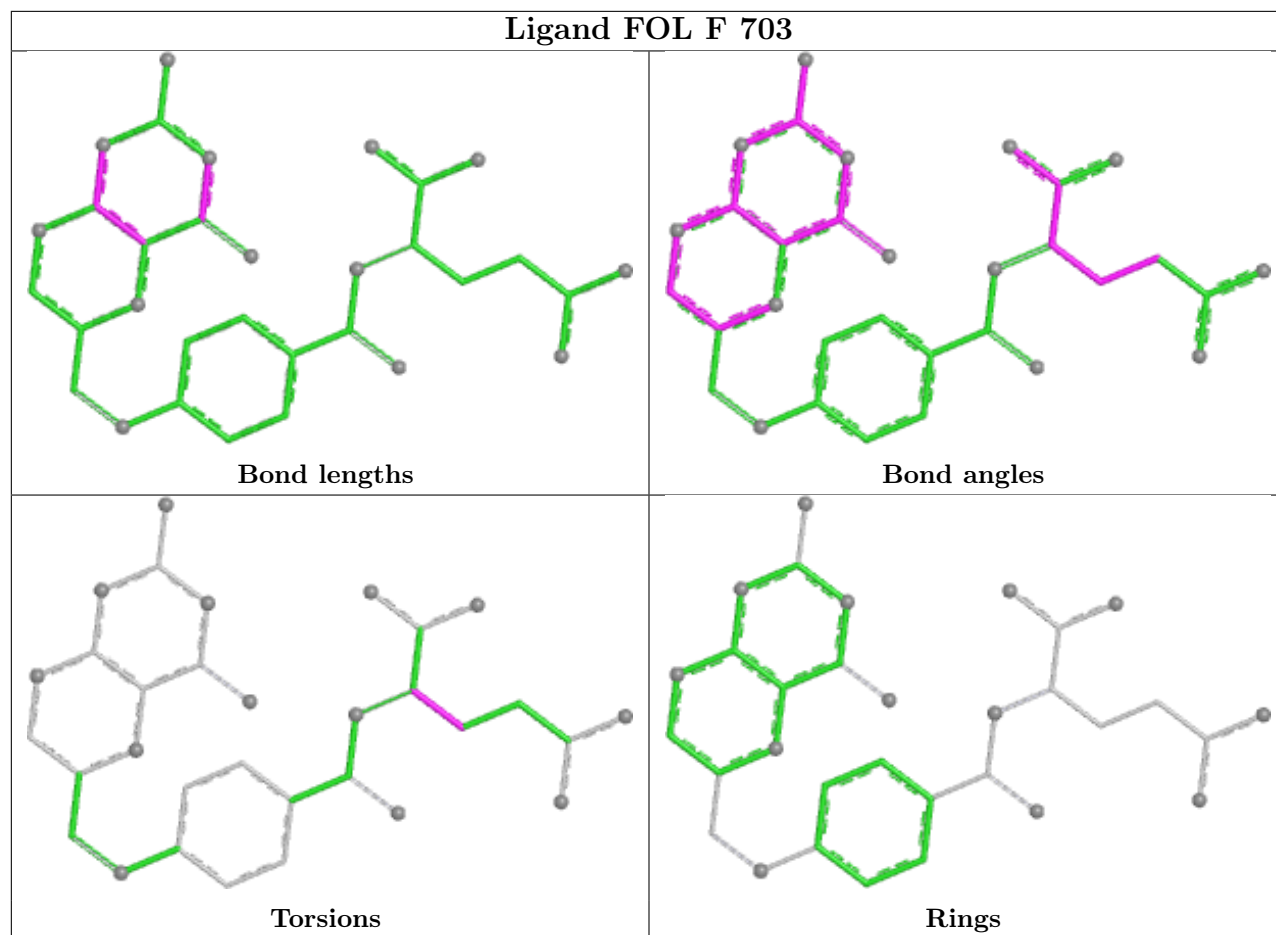


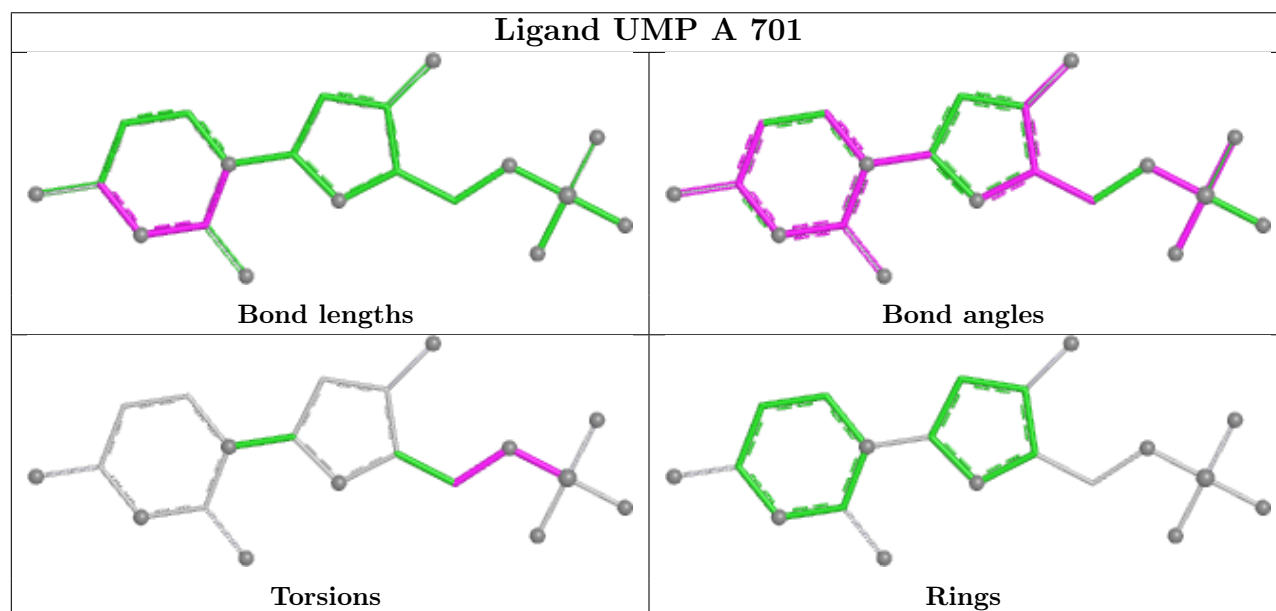
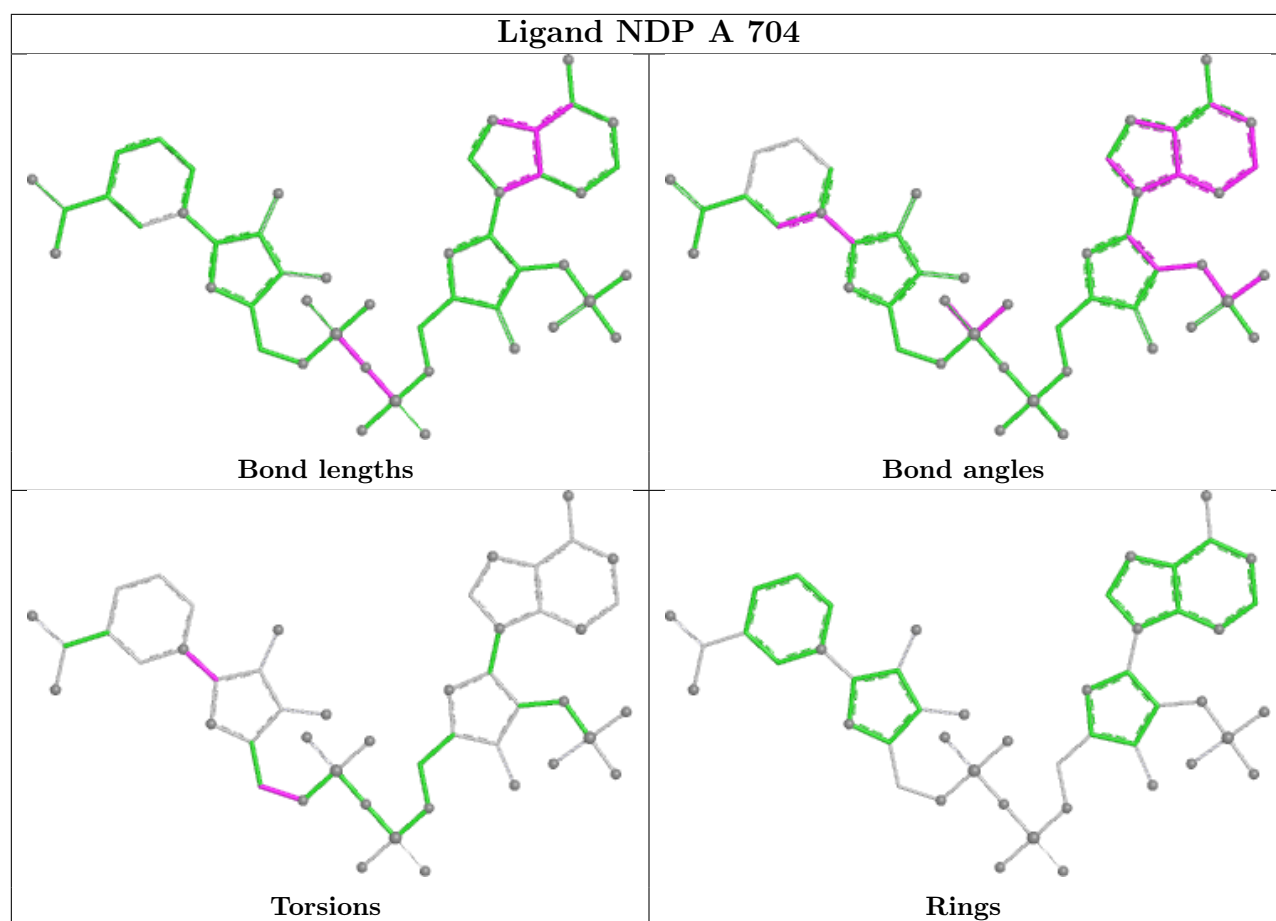
Ligand UMP B 701



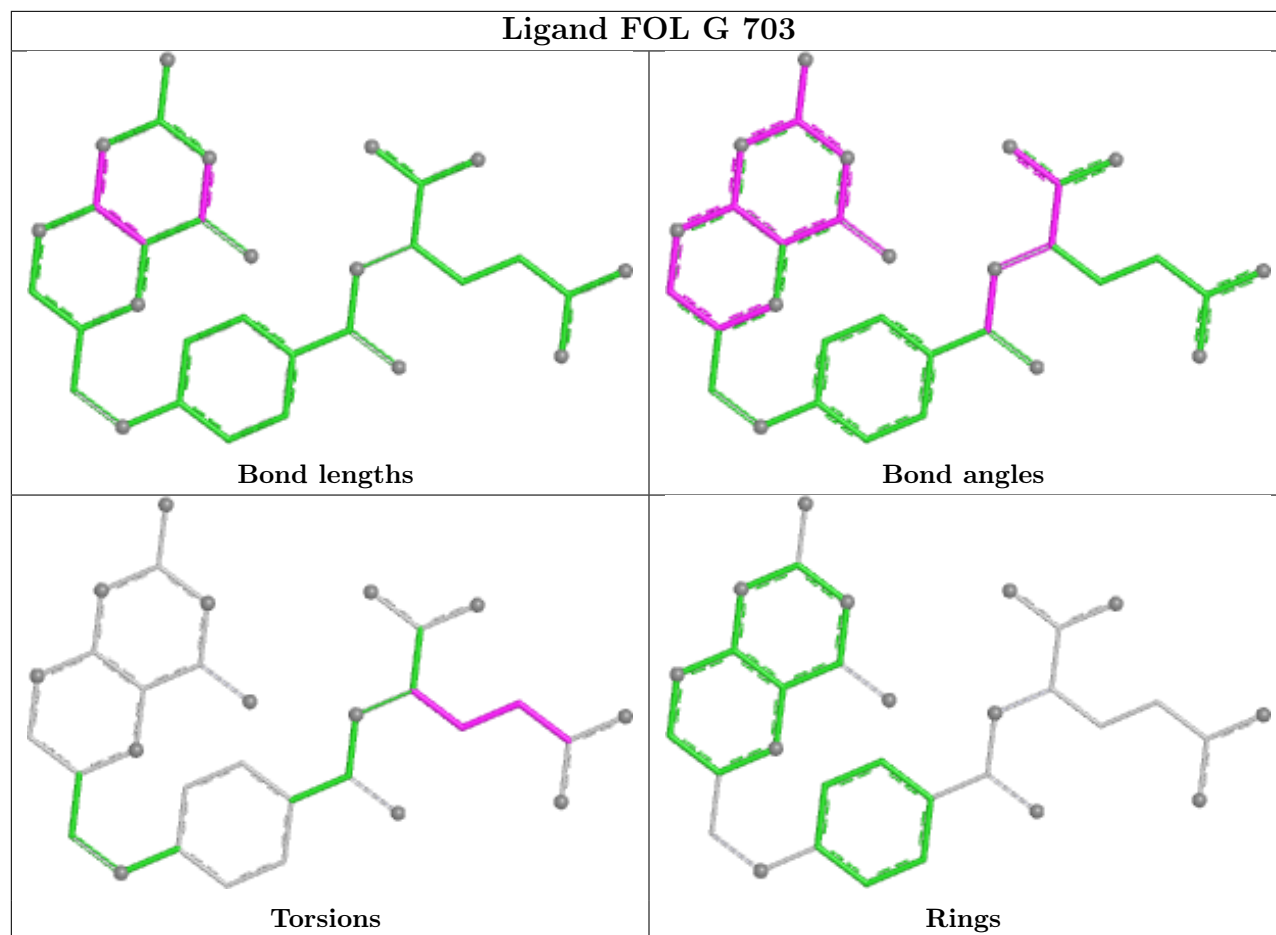


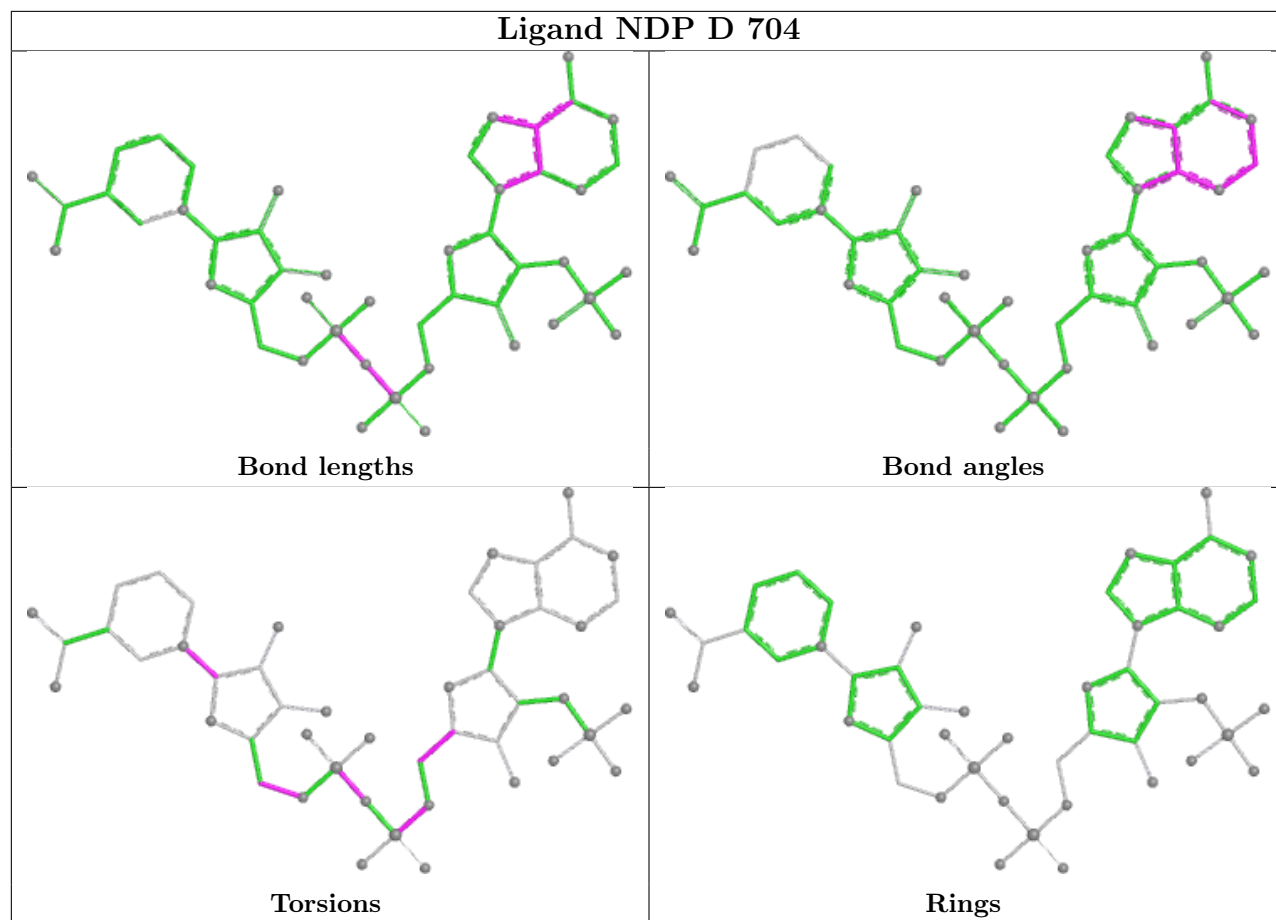
Ligand FOL F 703

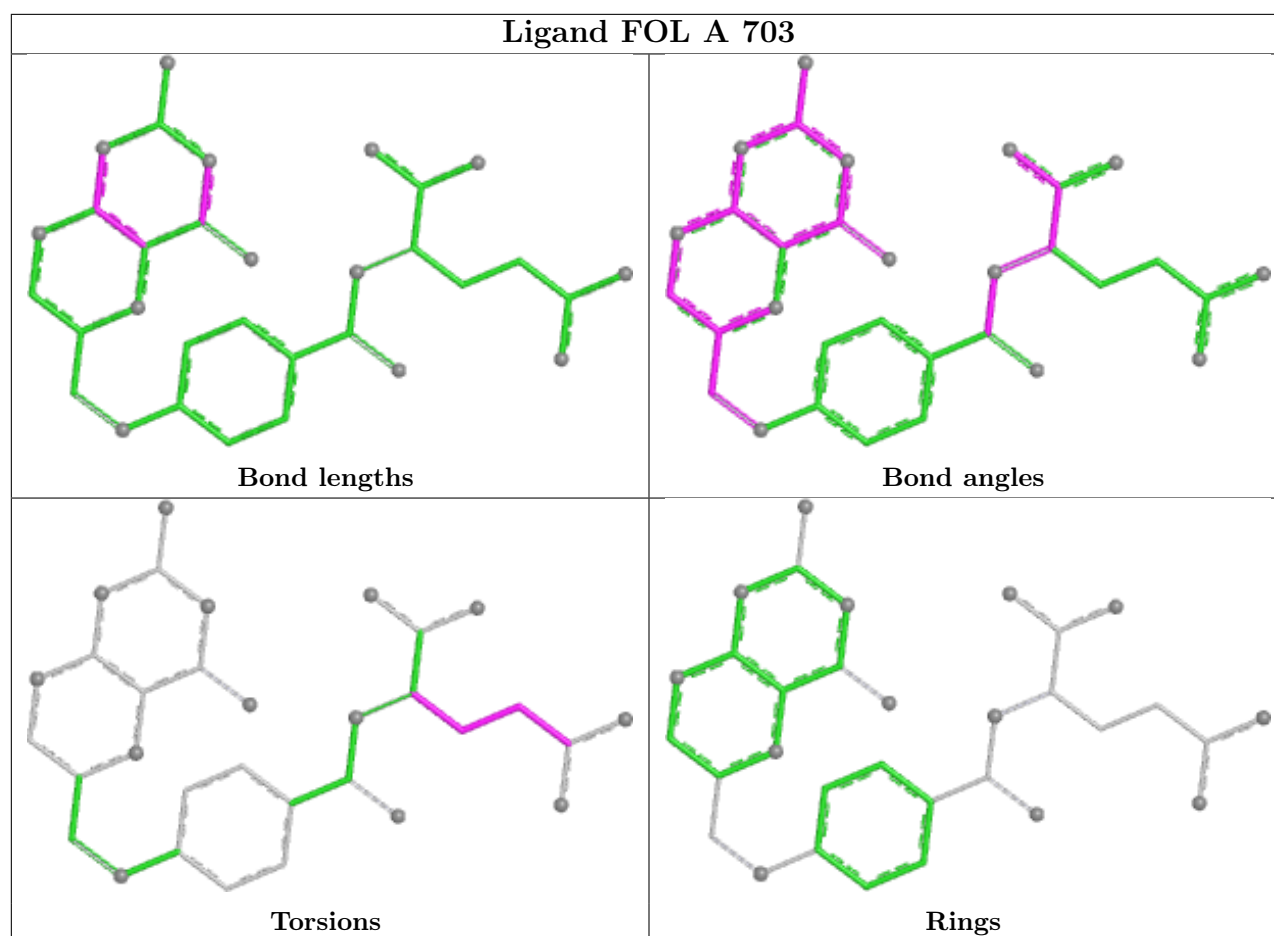




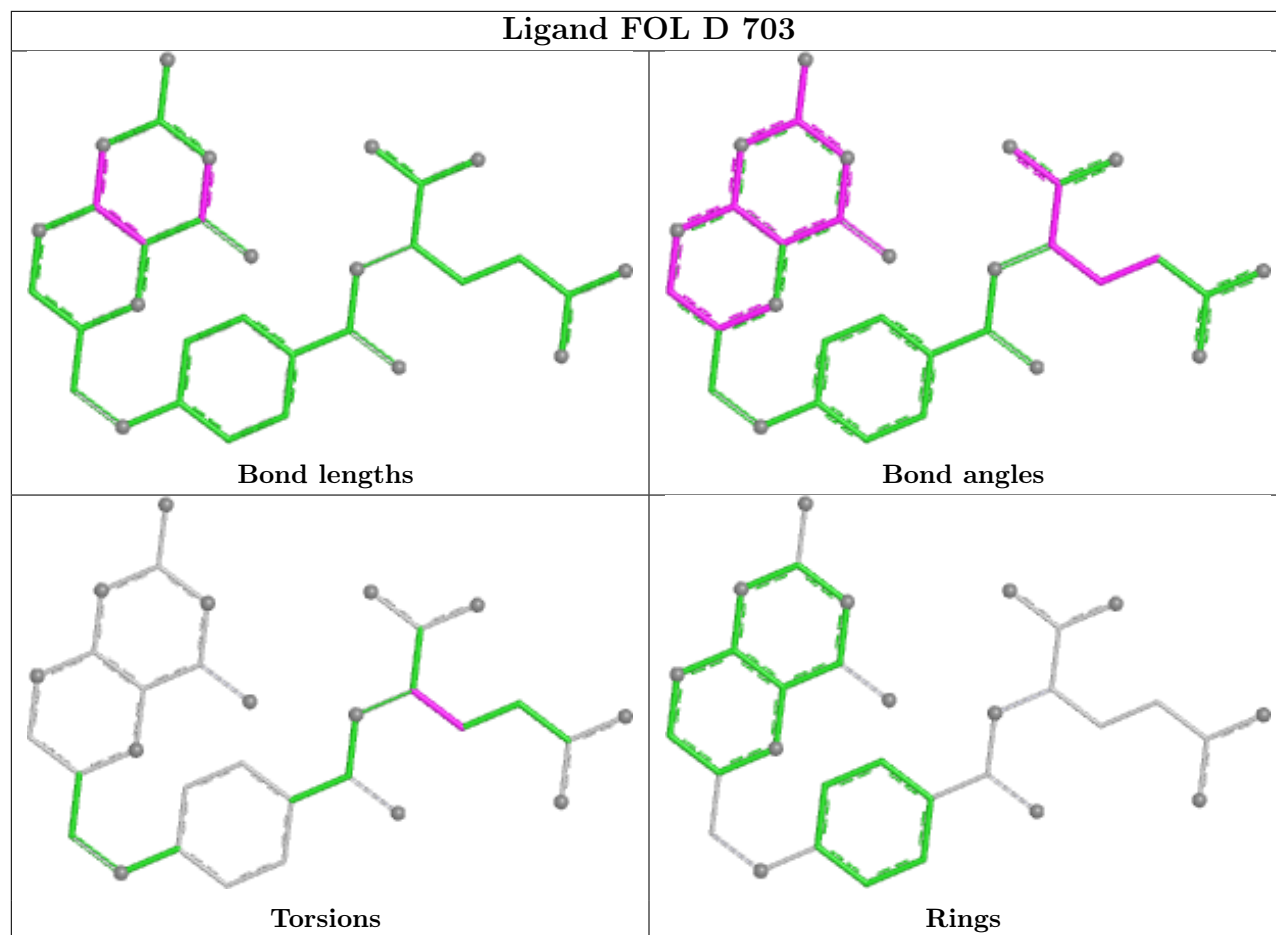
Ligand FOL G 703



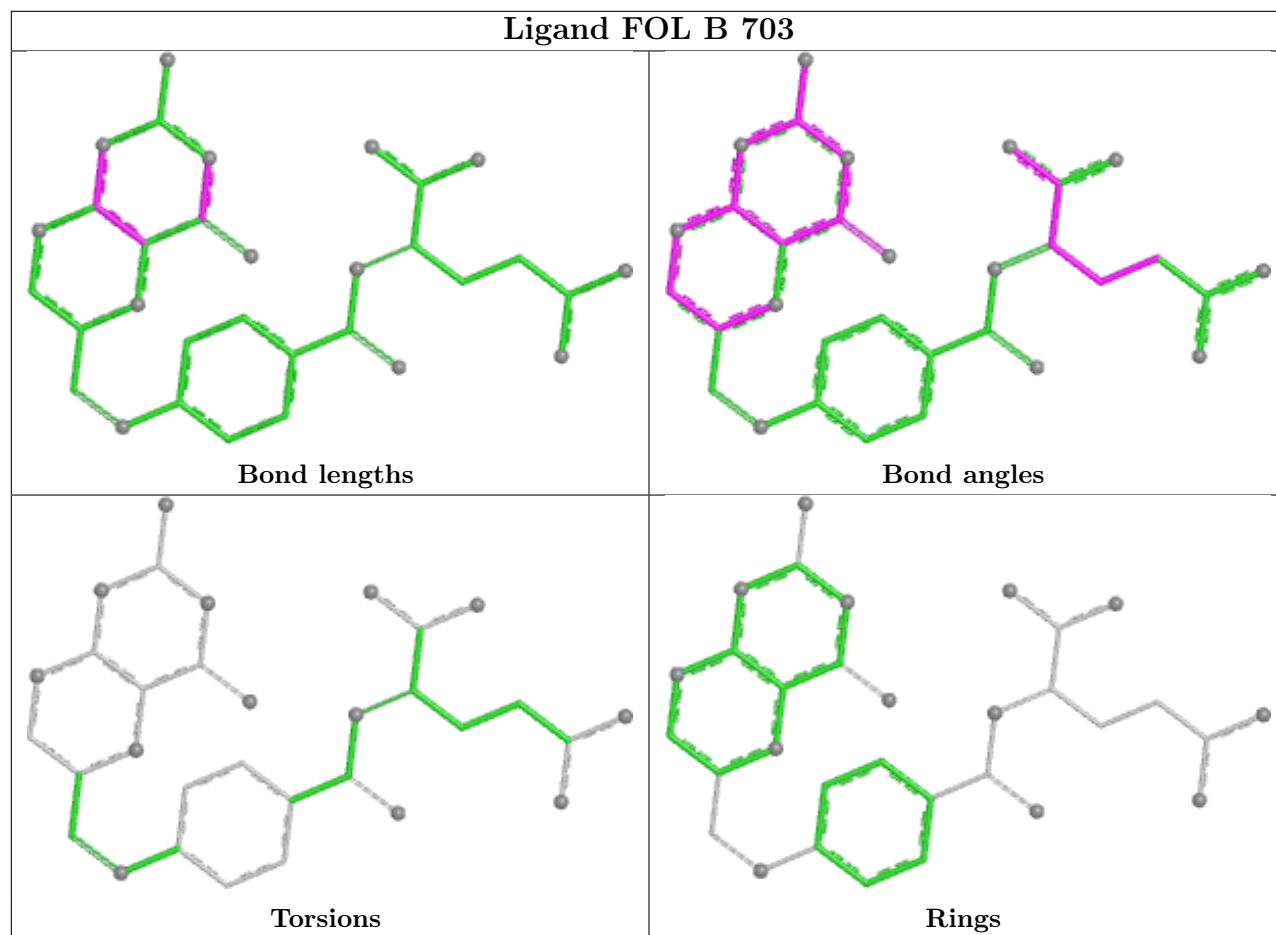




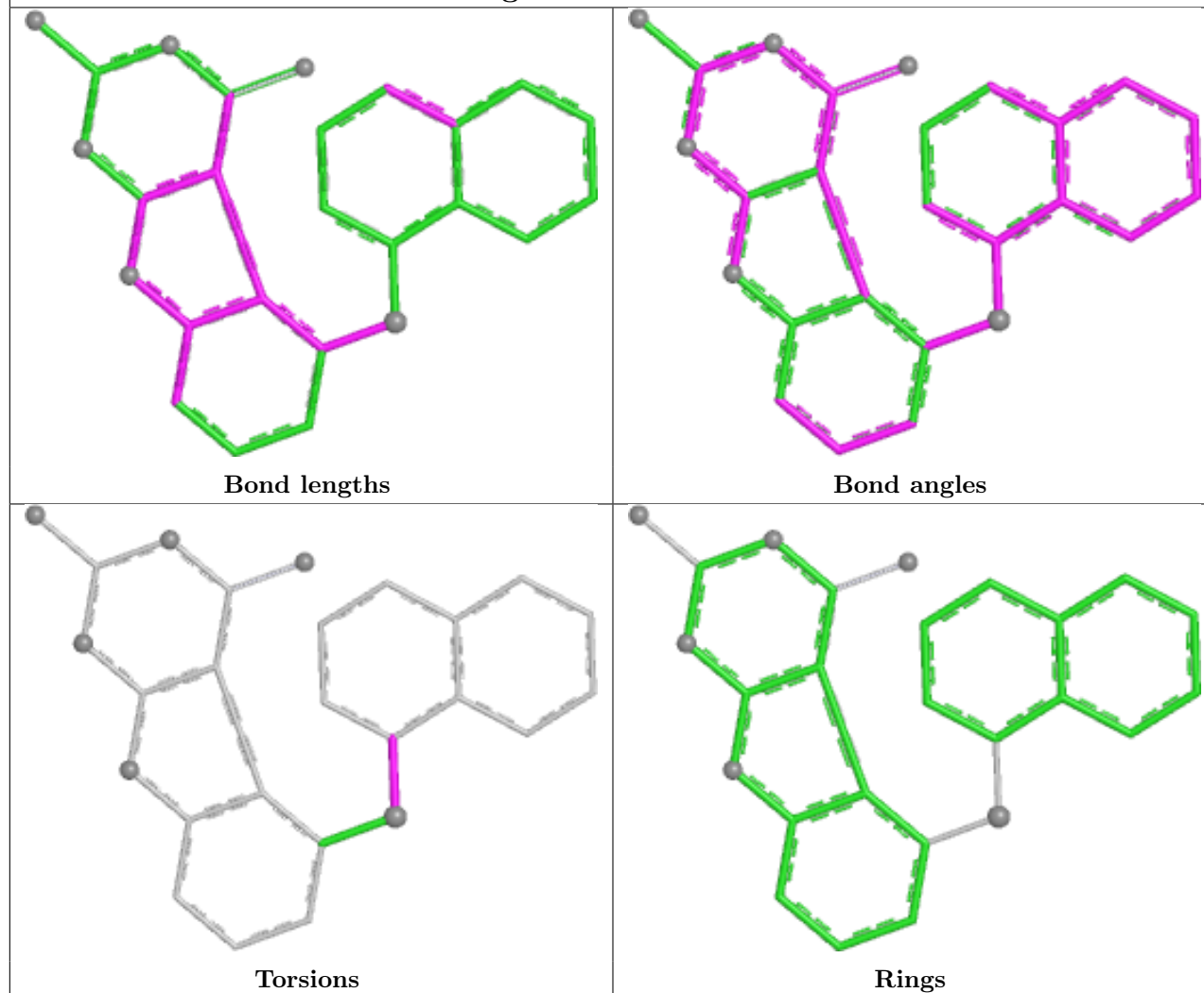
Ligand FOL D 703



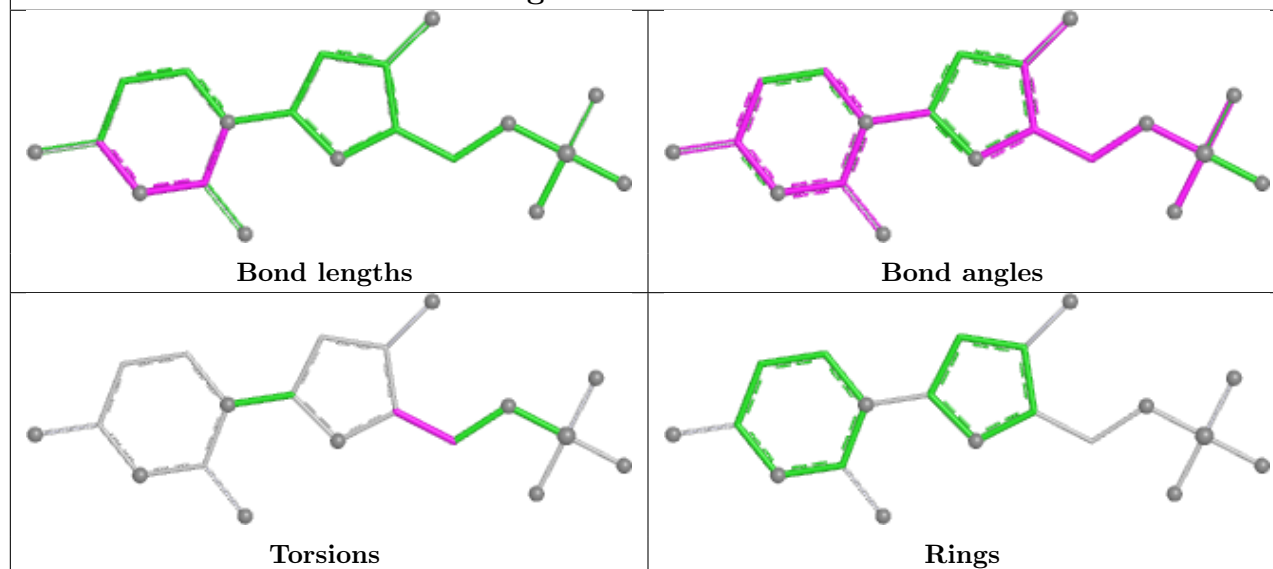
Ligand FOL B 703



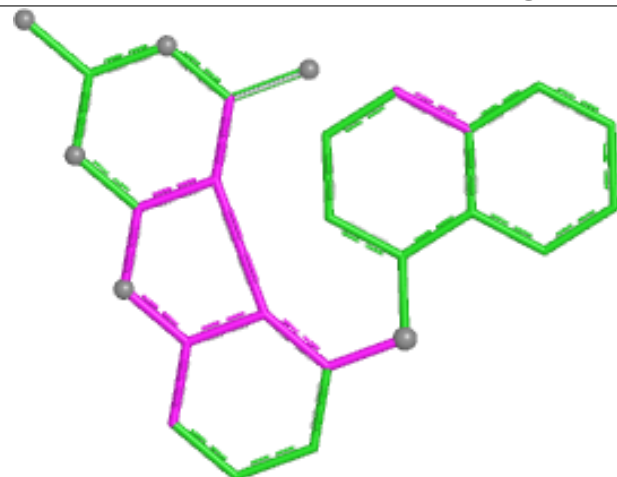
Ligand 1UG H 702



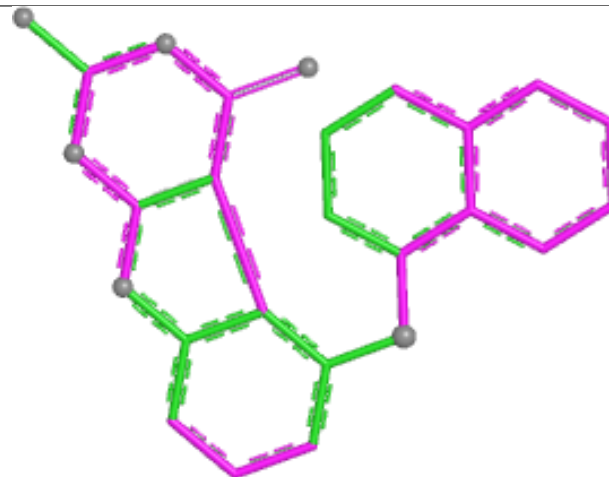
Ligand UMP F 701



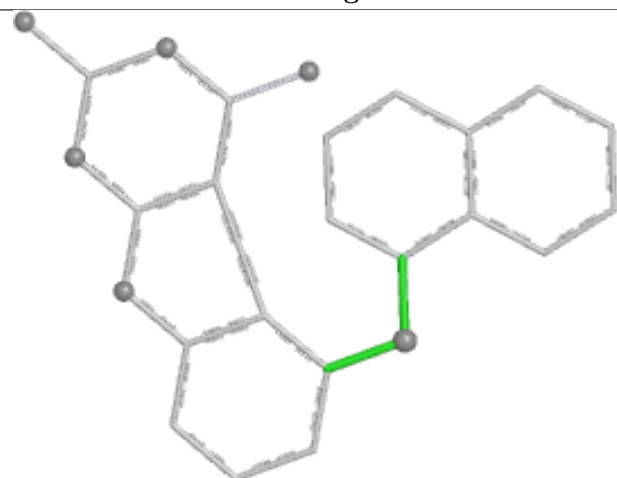
Ligand 1UG E 702



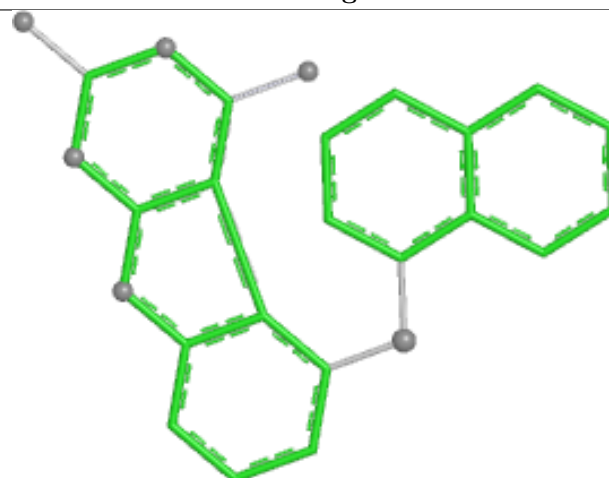
Bond lengths



Bond angles

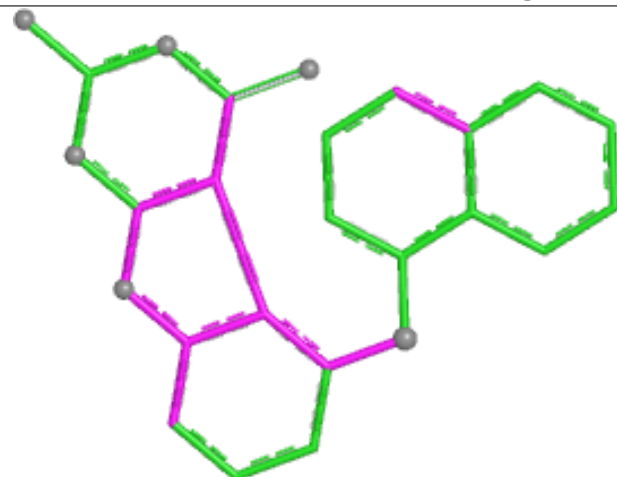


Torsions

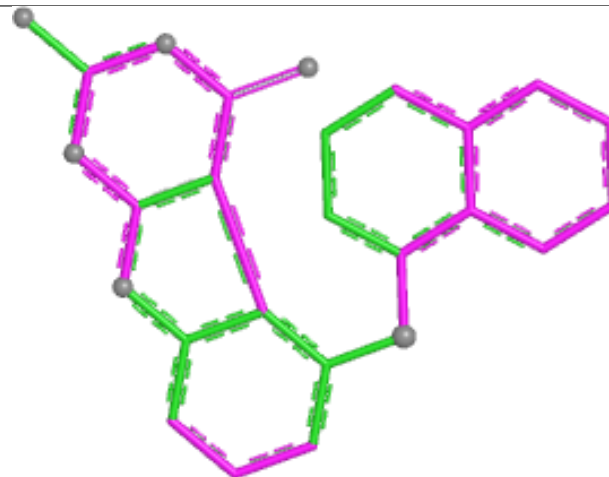


Rings

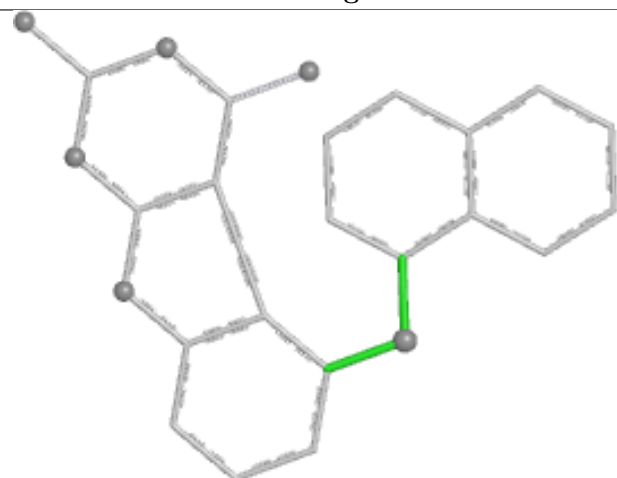
Ligand 1UG C 702



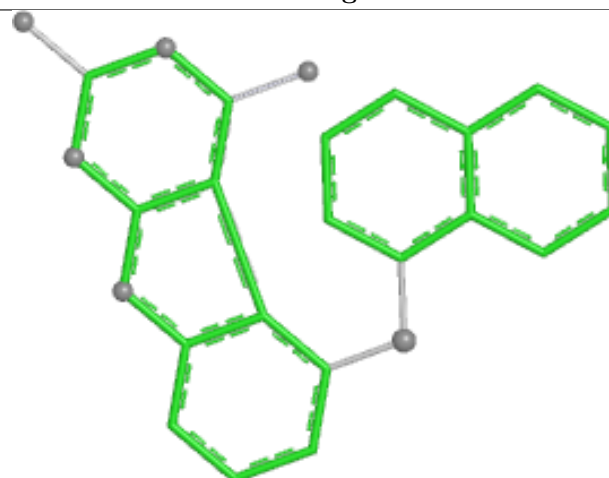
Bond lengths



Bond angles

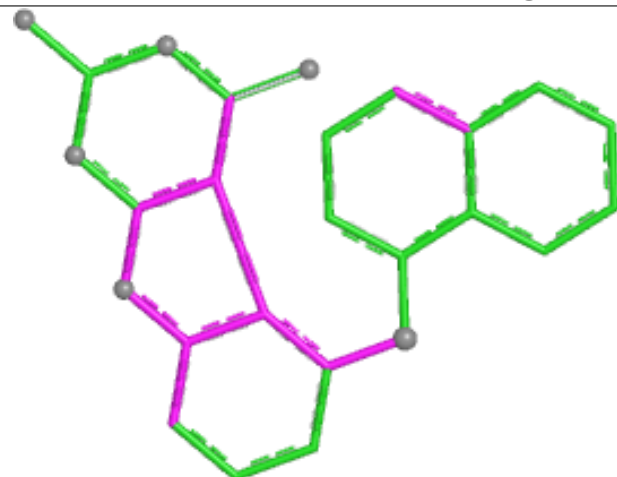


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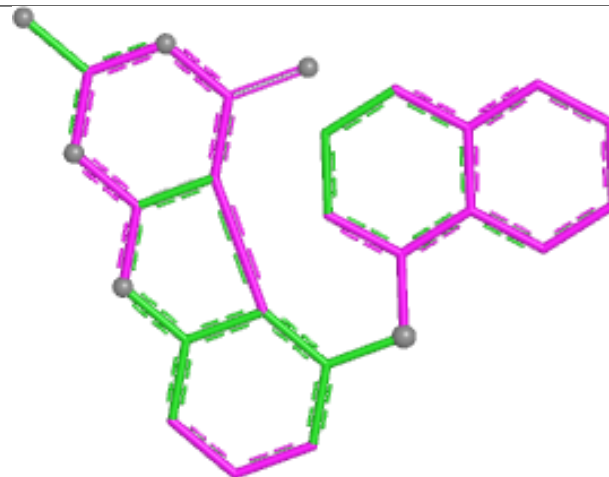


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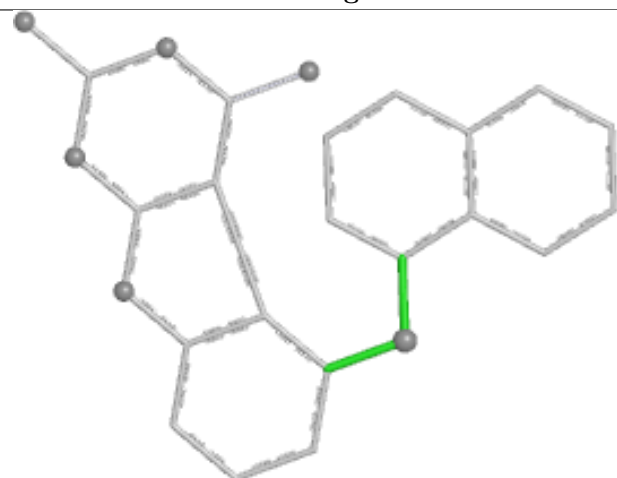
Ligand 1UG F 702



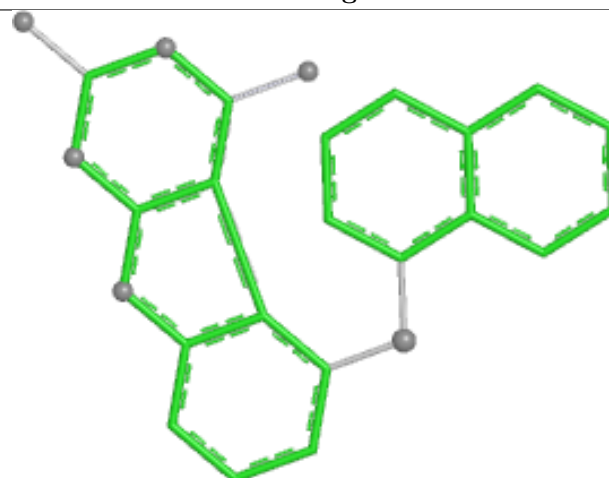
Bond lengths



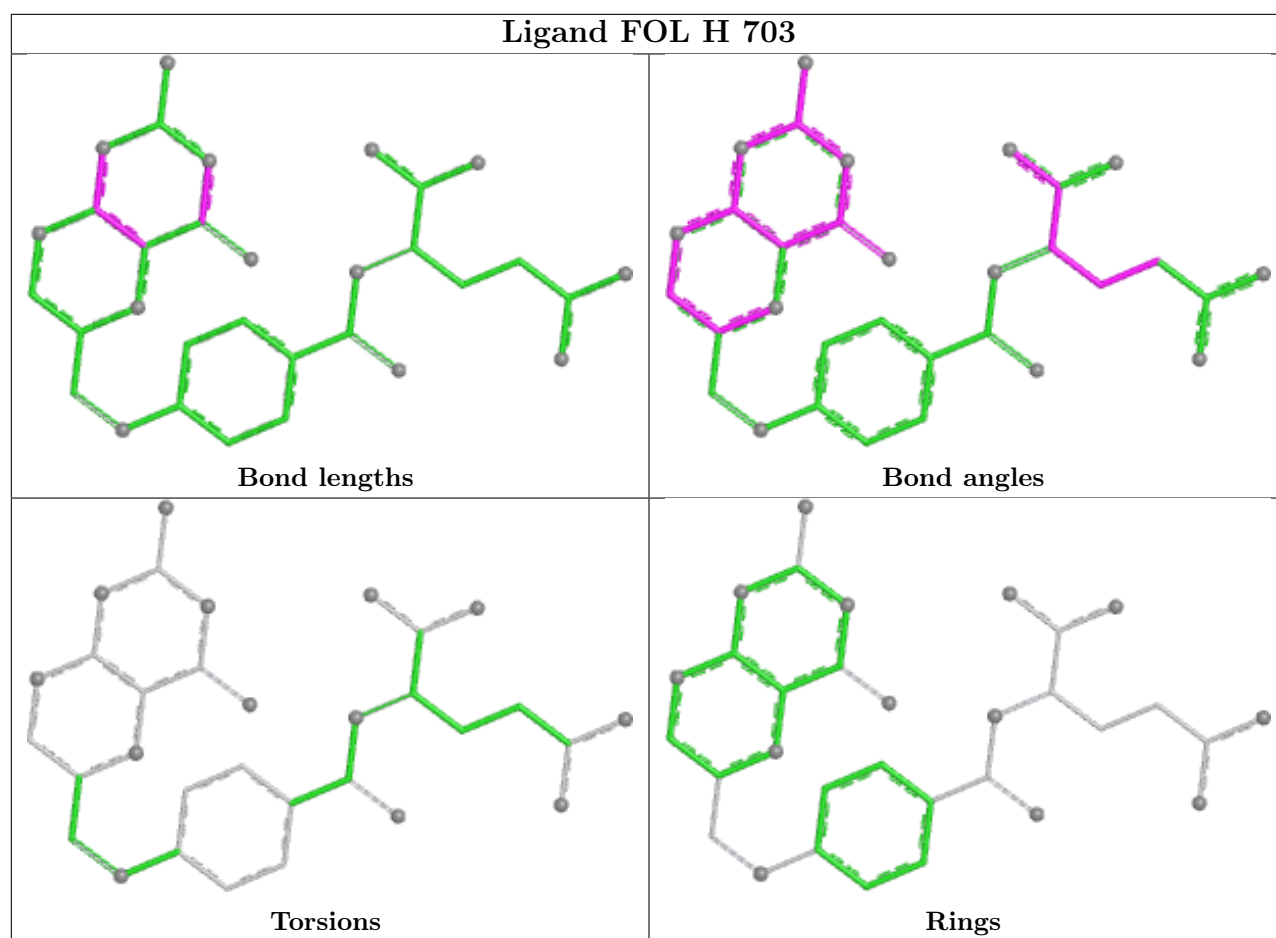
Bond angles

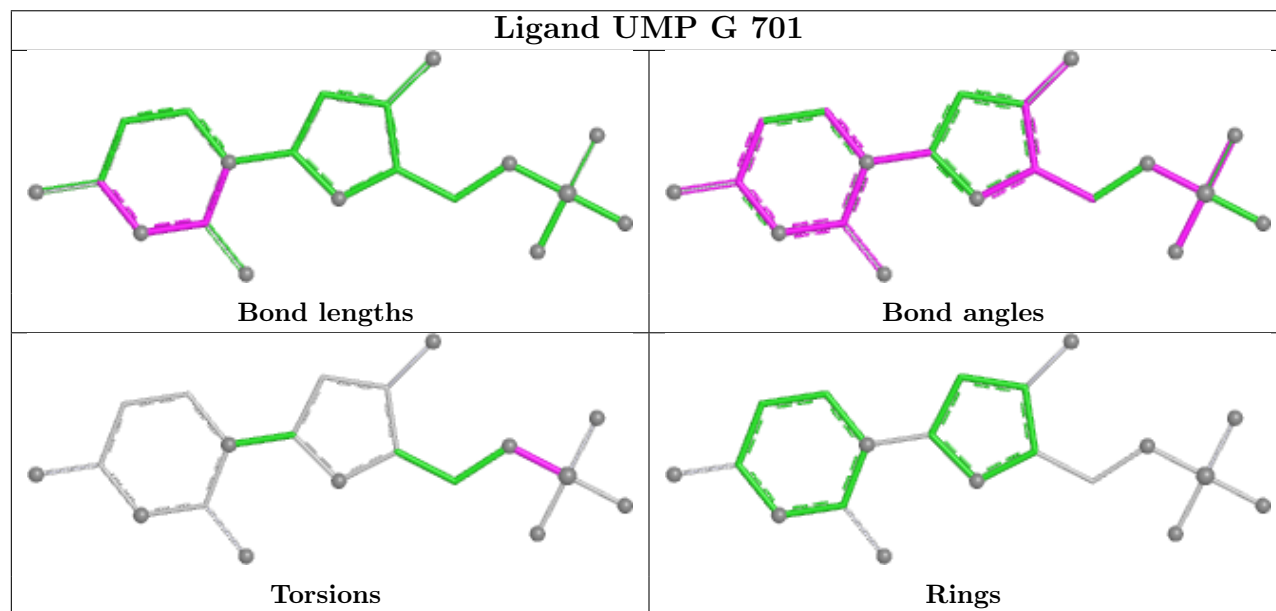
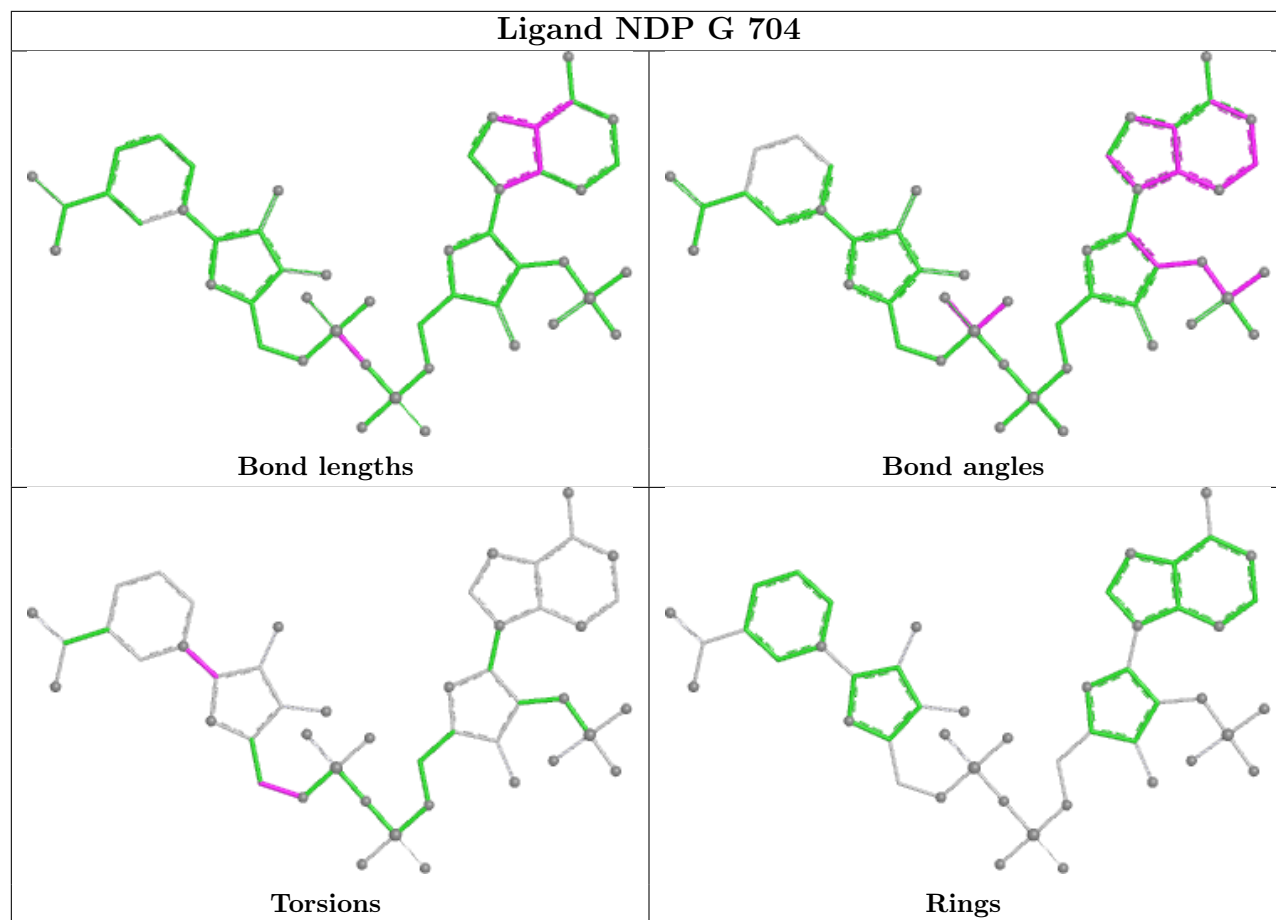


Torsions

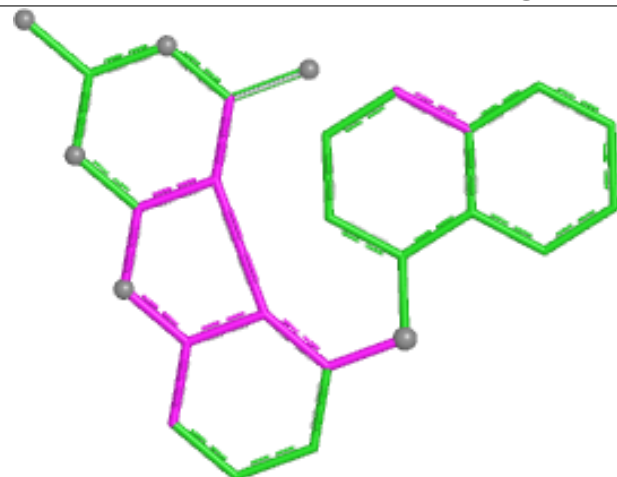


Rings

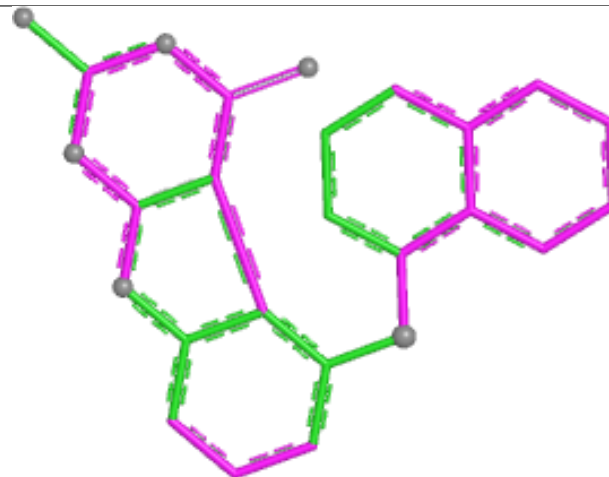




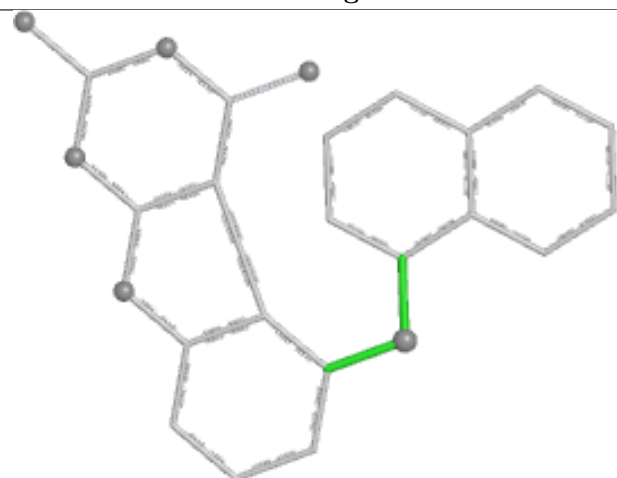
Ligand 1UG G 702



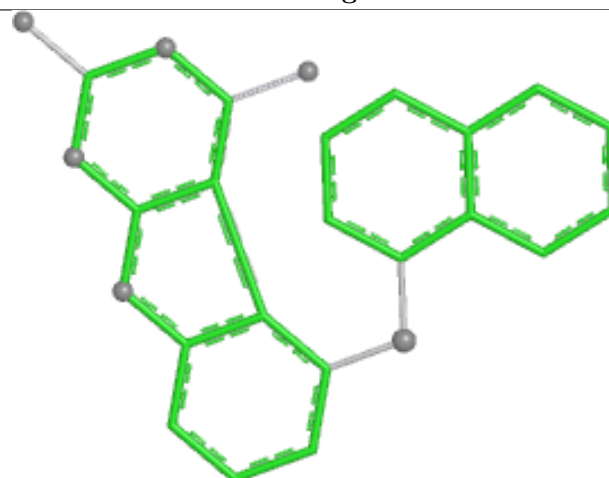
Bond lengths



Bond angles

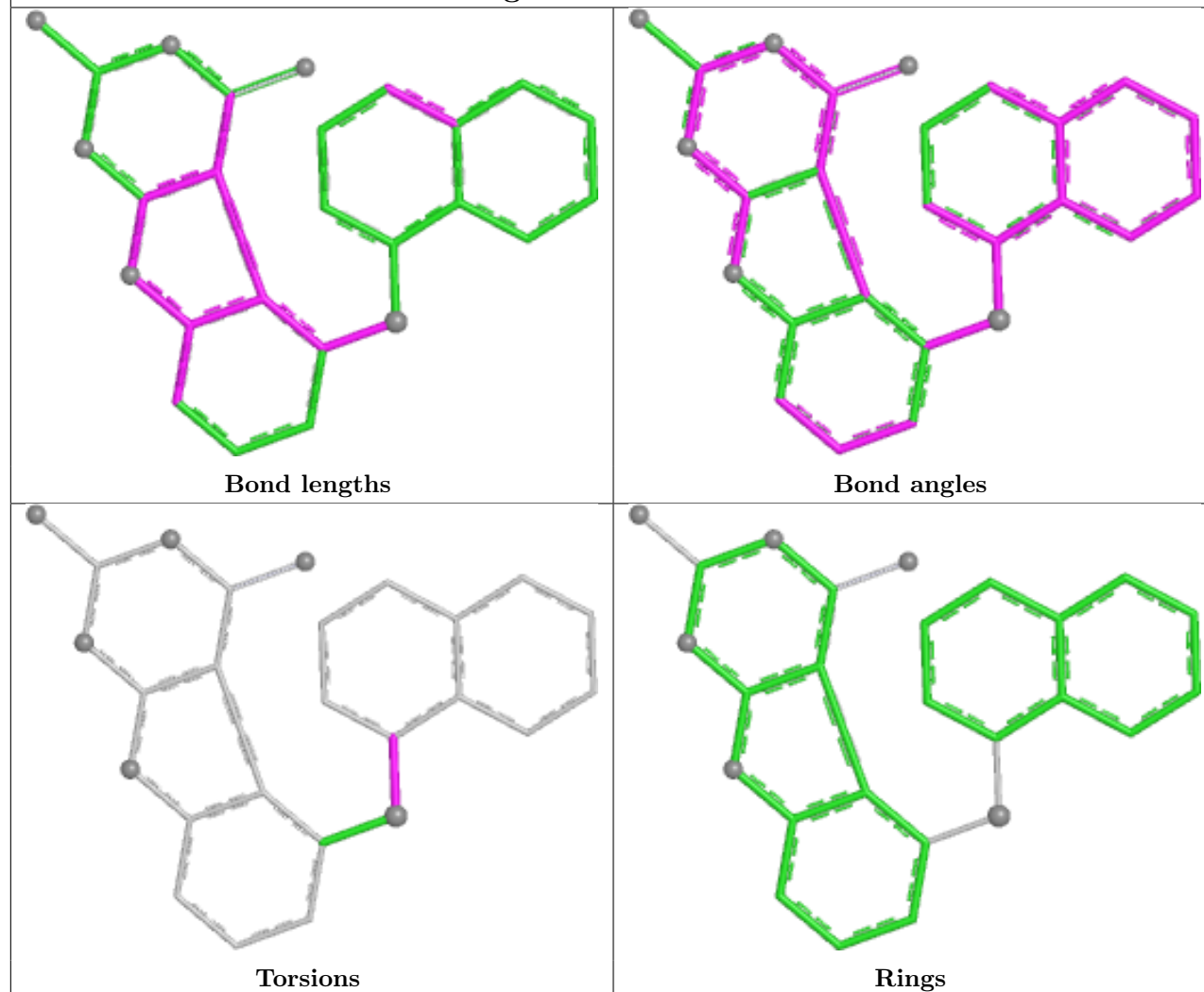


Torsions

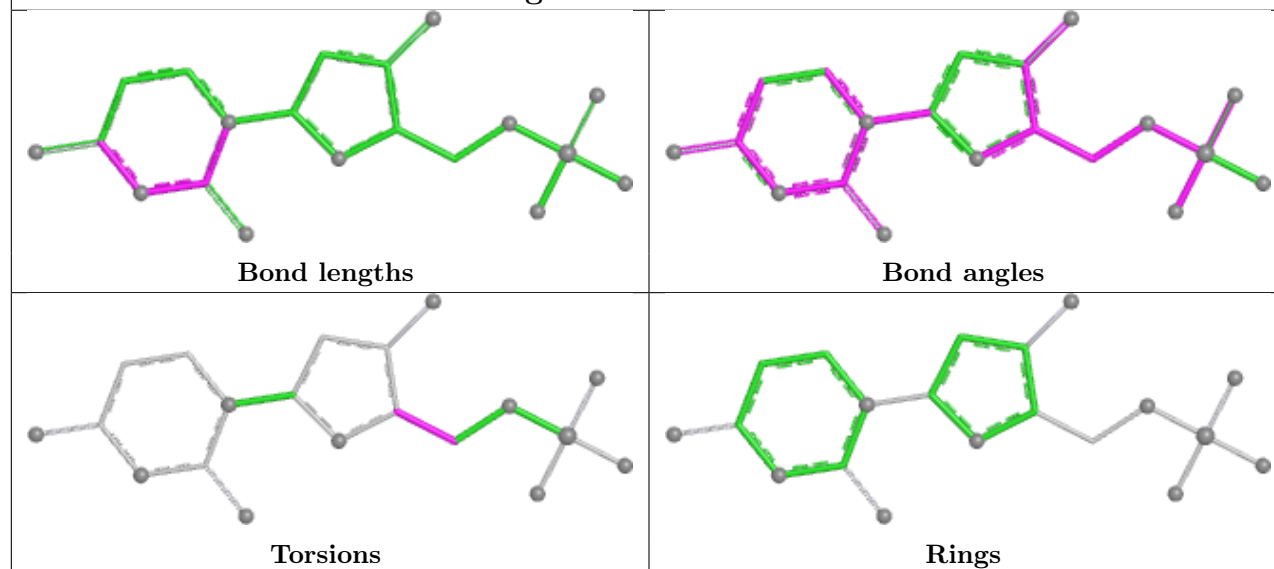


Rings

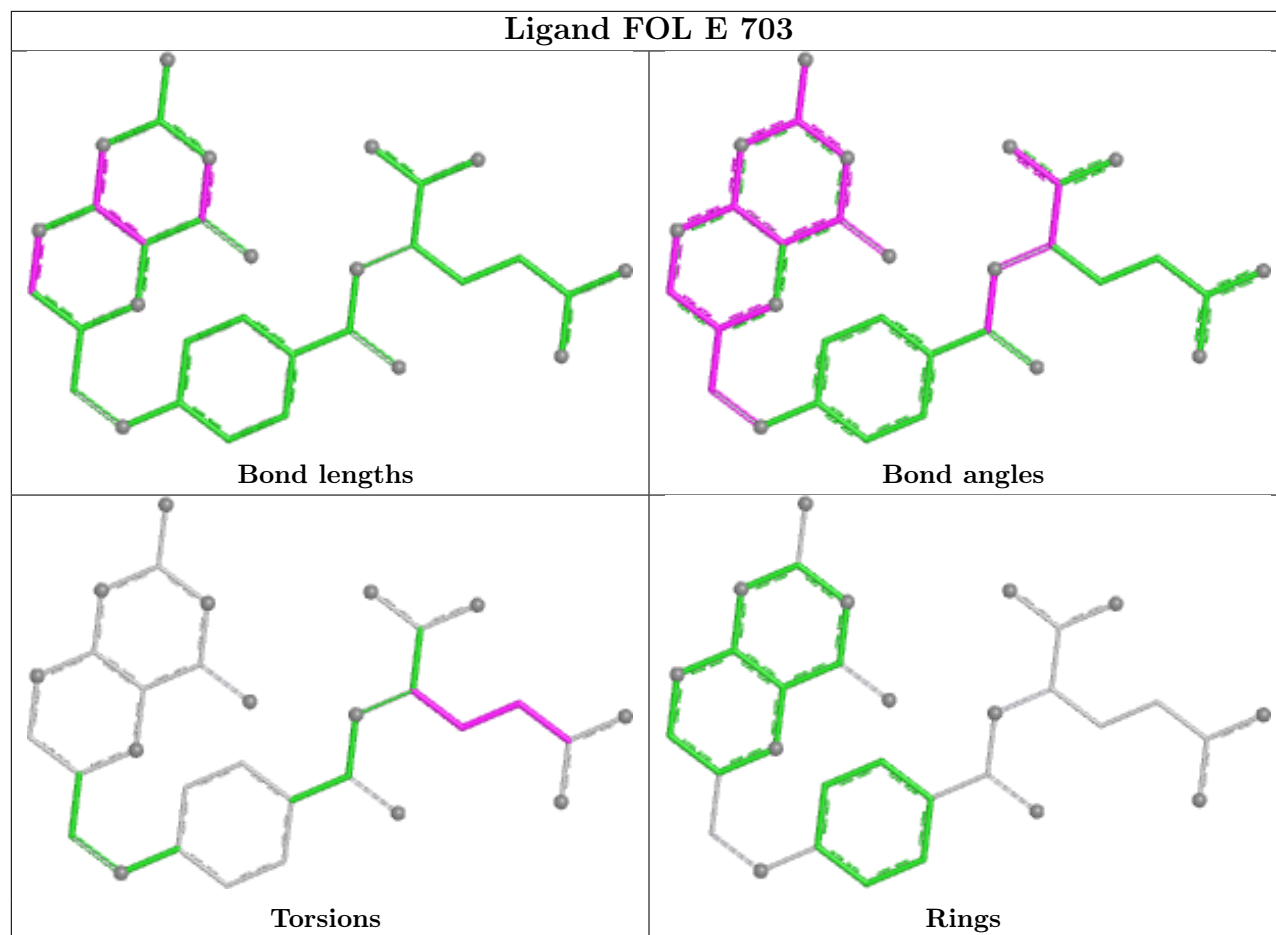
Ligand 1UG B 702



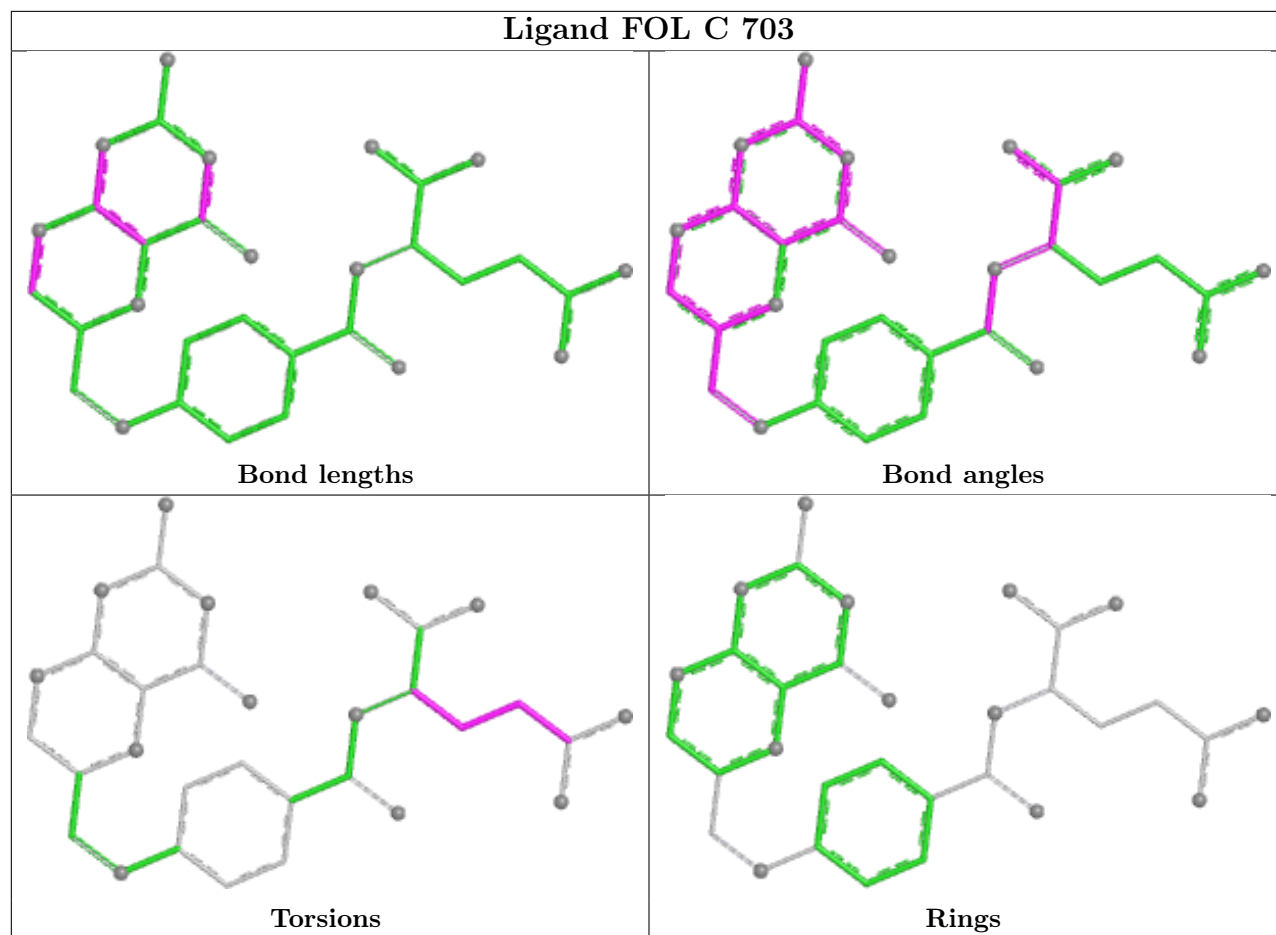
Ligand UMP H 701

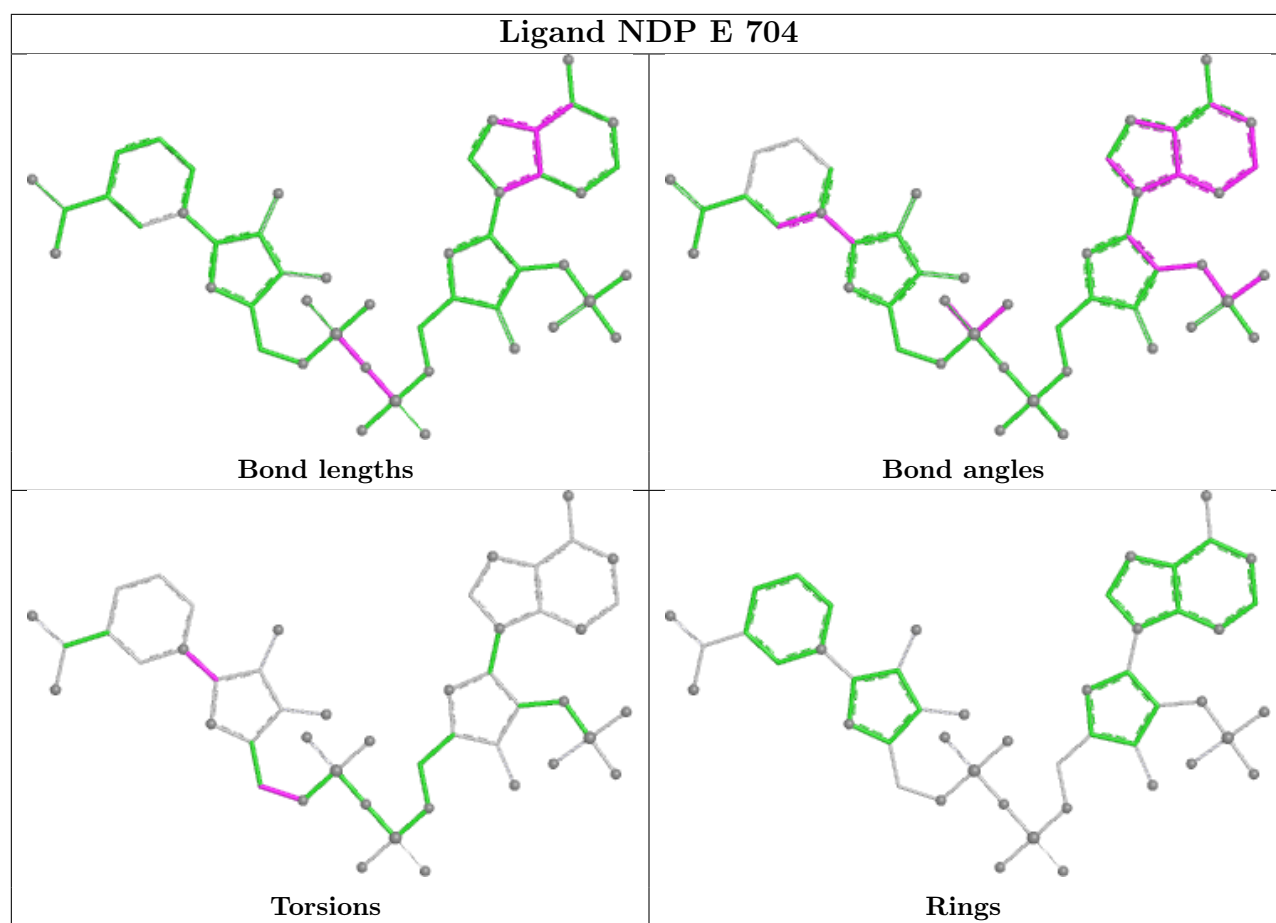


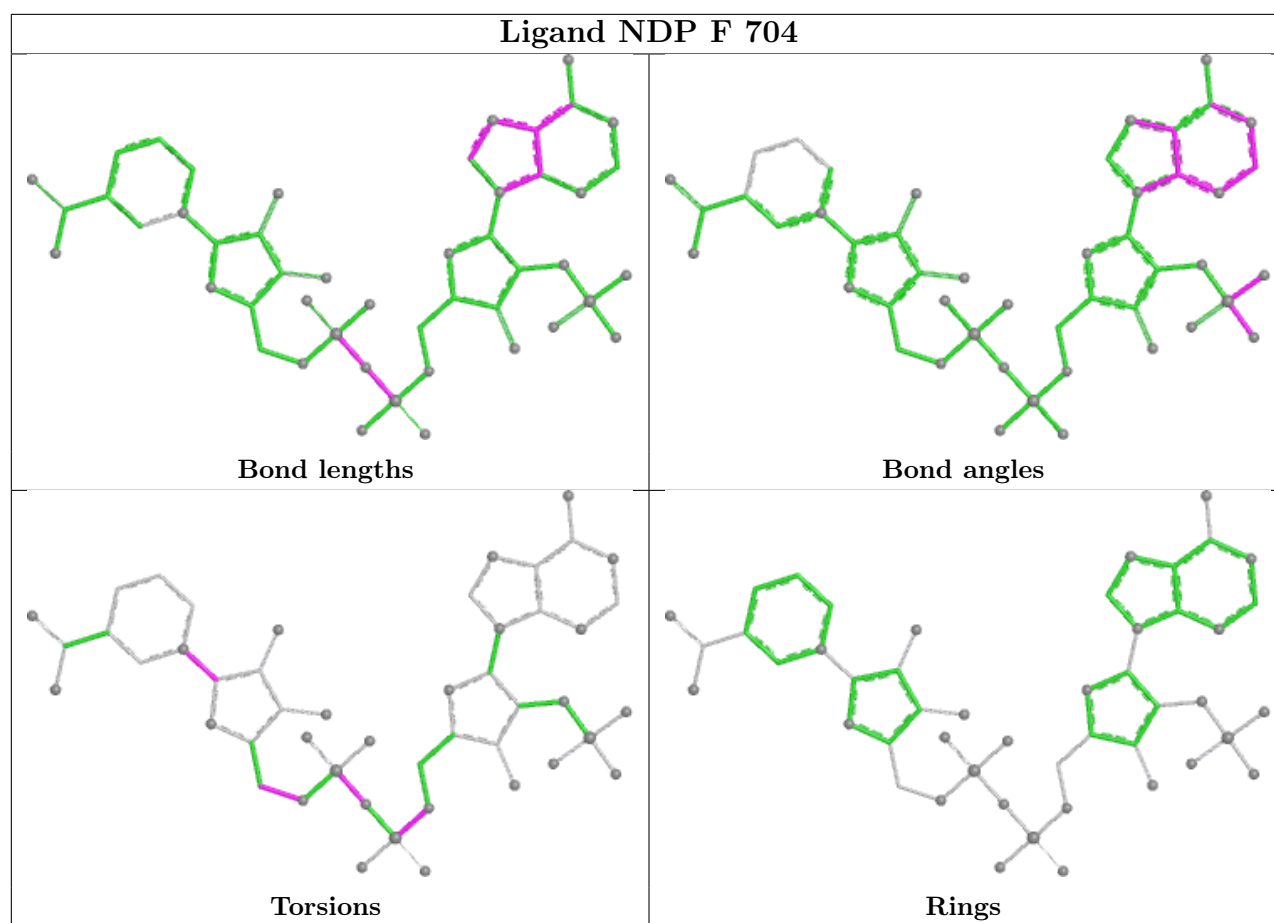
Ligand FOL E 703



Ligand FOL C 703







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	510/566 (90%)	-1.63	0 100 100	13, 30, 69, 99	2 (0%)
1	B	491/566 (86%)	-1.64	0 100 100	14, 32, 77, 93	1 (0%)
1	C	510/566 (90%)	-1.64	0 100 100	11, 31, 70, 100	2 (0%)
1	D	491/566 (86%)	-1.62	0 100 100	13, 32, 77, 96	1 (0%)
1	E	510/566 (90%)	-1.63	0 100 100	12, 30, 68, 98	2 (0%)
1	F	491/566 (86%)	-1.61	0 100 100	13, 32, 76, 98	1 (0%)
1	G	510/566 (90%)	-1.65	0 100 100	14, 30, 71, 104	2 (0%)
1	H	491/566 (86%)	-1.62	0 100 100	14, 33, 76, 96	1 (0%)
All	All	4004/4528 (88%)	-1.63	0 100 100	11, 31, 74, 104	12 (0%)

There are no RSRZ outliers to report.

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](#)

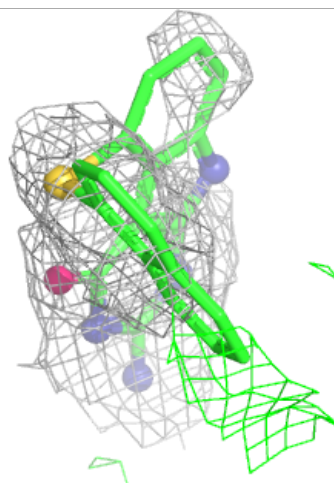
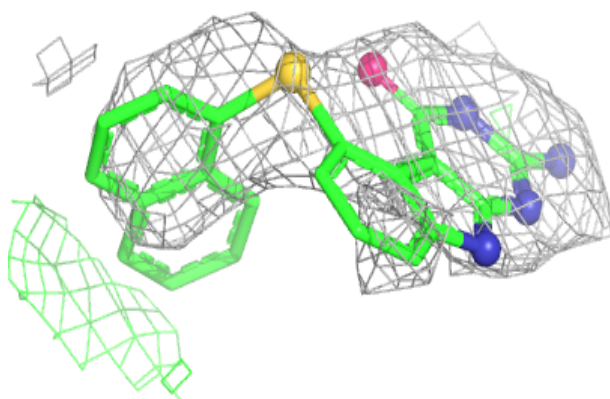
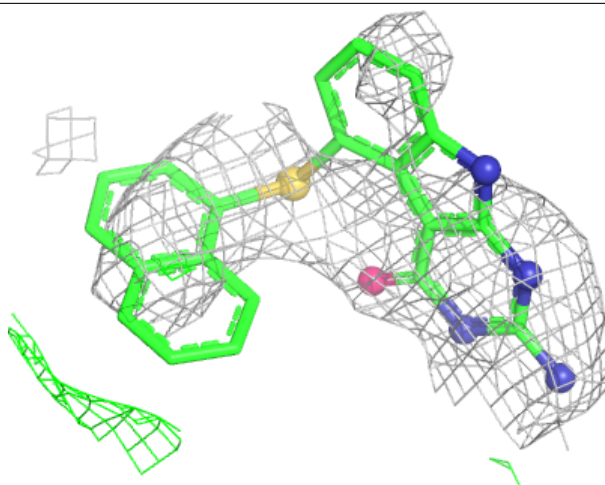
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	1UG	G	702	26/26	0.98	0.07	69,105,114,116	0
2	UMP	D	701	20/20	0.99	0.03	25,46,67,73	0
2	UMP	F	701	20/20	0.99	0.03	26,43,68,70	0
2	UMP	G	701	20/20	0.99	0.03	35,56,72,72	0
2	UMP	H	701	20/20	0.99	0.03	24,46,68,70	0
3	1UG	A	702	26/26	0.99	0.06	72,99,113,115	0
3	1UG	B	702	26/26	0.99	0.05	64,89,110,111	0
3	1UG	C	702	26/26	0.99	0.07	96,114,132,133	0
3	1UG	D	702	26/26	0.99	0.05	66,83,105,106	0
3	1UG	E	702	26/26	0.99	0.05	75,101,115,117	0
3	1UG	F	702	26/26	0.99	0.05	71,86,107,110	0
2	UMP	B	701	20/20	0.99	0.03	26,47,70,71	0
3	1UG	H	702	26/26	0.99	0.05	65,82,104,105	0
4	FOL	A	703	32/32	0.99	0.04	24,45,67,89	0
4	FOL	B	703	32/32	0.99	0.04	33,60,87,93	0
4	FOL	C	703	32/32	0.99	0.03	26,48,68,95	0
4	FOL	D	703	32/32	0.99	0.04	34,59,86,91	0
4	FOL	E	703	32/32	0.99	0.03	24,45,71,90	0
4	FOL	F	703	32/32	0.99	0.04	36,63,87,91	0
4	FOL	G	703	32/32	0.99	0.04	26,41,68,86	0
4	FOL	H	703	32/32	0.99	0.04	33,60,88,93	0
5	NDP	B	704	48/48	0.99	0.03	35,69,105,110	0
5	NDP	D	704	48/48	0.99	0.03	34,65,100,106	0
5	NDP	F	704	48/48	0.99	0.03	30,65,105,108	0
5	NDP	H	704	48/48	0.99	0.03	35,63,99,108	0
2	UMP	A	701	20/20	1.00	0.03	30,57,70,70	0
5	NDP	C	704	48/48	1.00	0.02	21,32,43,51	0
2	UMP	E	701	20/20	1.00	0.03	34,57,75,78	0
5	NDP	E	704	48/48	1.00	0.03	20,33,42,48	0
2	UMP	C	701	20/20	1.00	0.03	32,62,81,82	0
5	NDP	G	704	48/48	1.00	0.03	21,32,44,56	0
5	NDP	A	704	48/48	1.00	0.03	21,34,40,56	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.

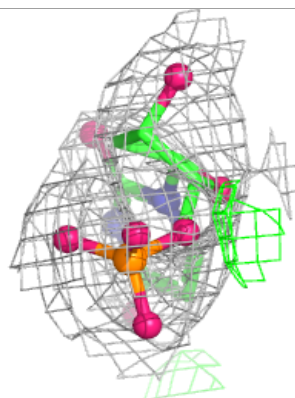
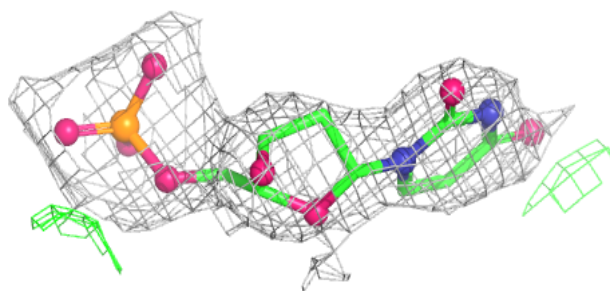
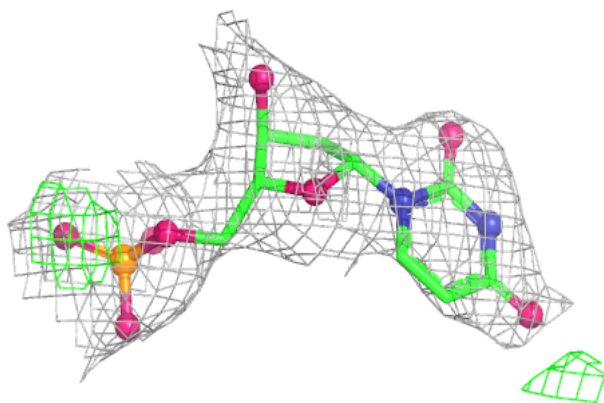
Electron density around 1UG G 702:

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

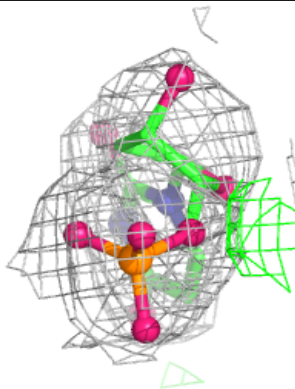
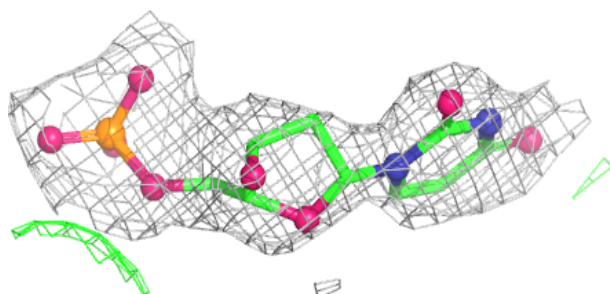
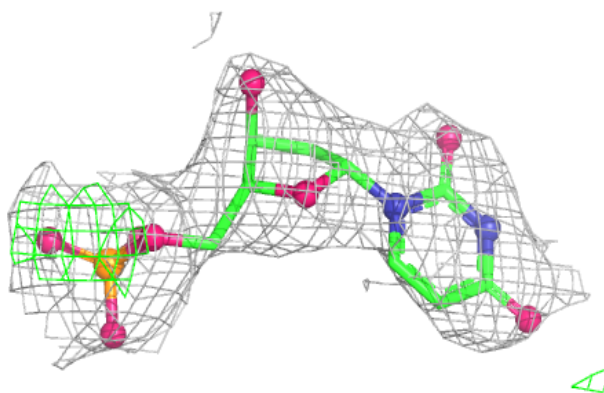


Electron density around UMP D 701:

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

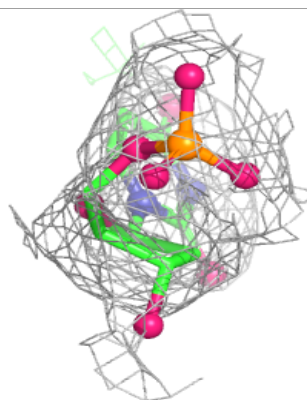
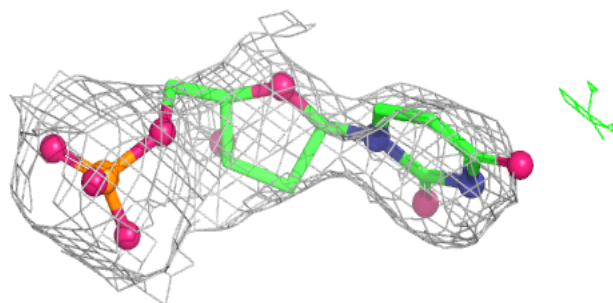
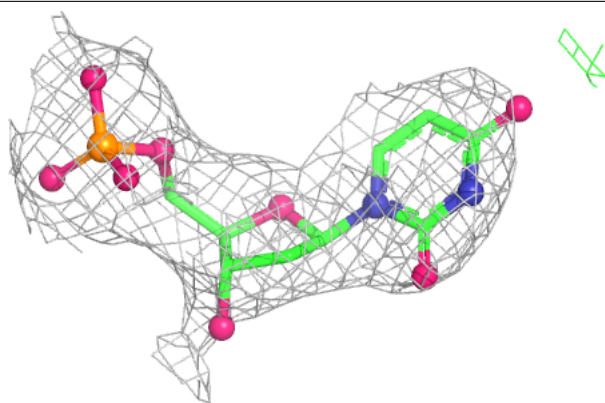
**Electron density around UMP F 701:**

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and green (positive)

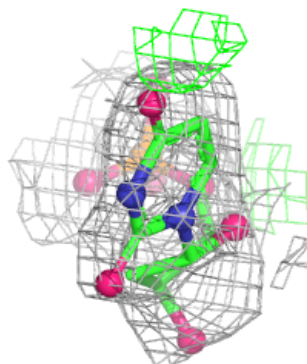
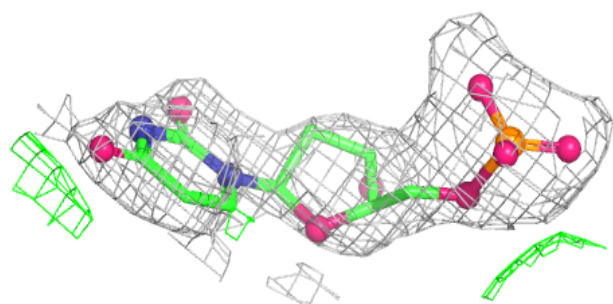
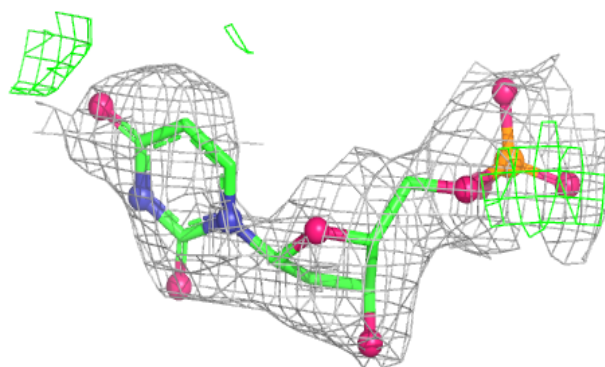


Electron density around UMP G 701:

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and green (positive)

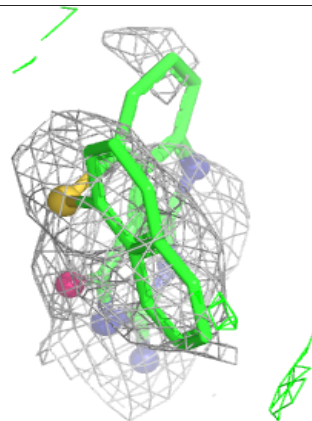
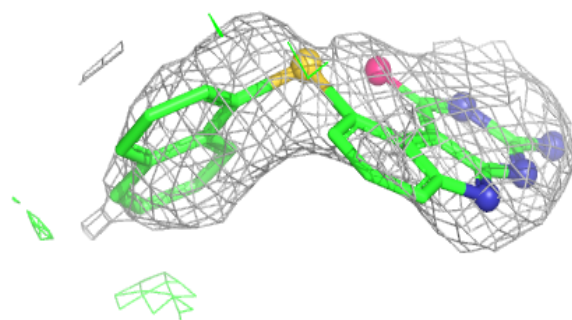
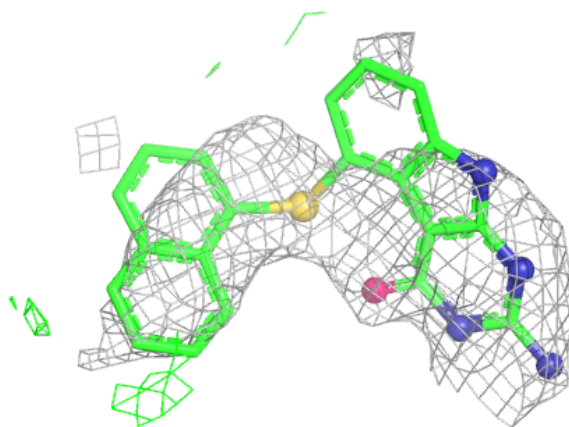
**Electron density around UMP H 701:**

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



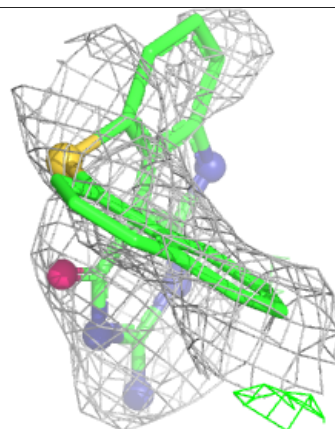
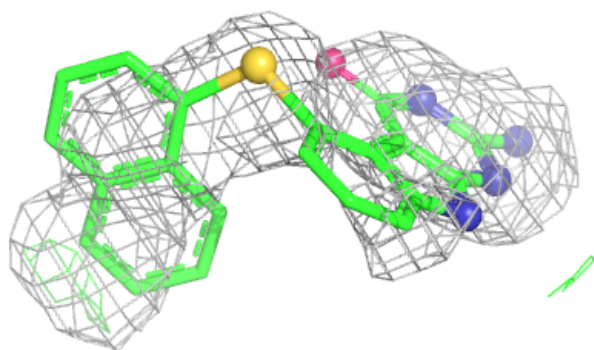
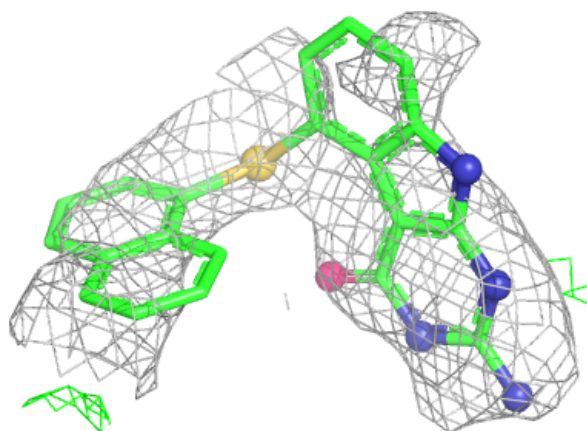
Electron density around 1UG A 702:

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



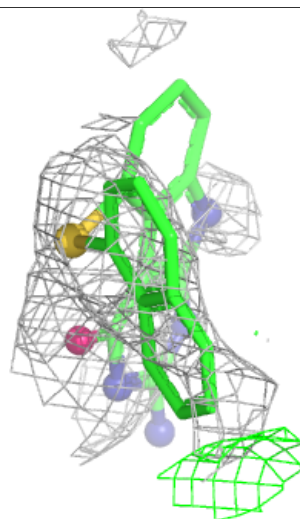
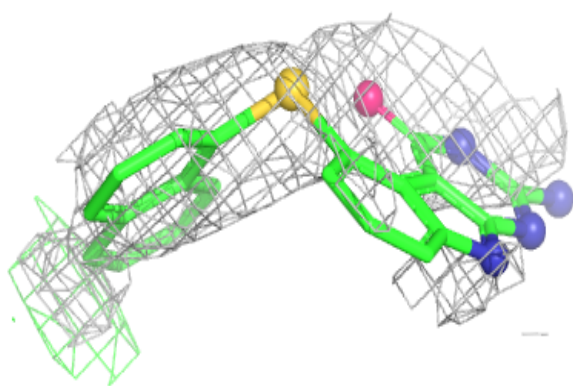
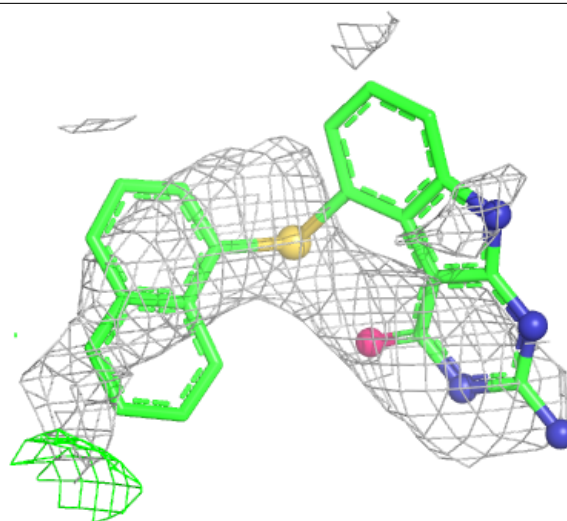
Electron density around 1UG B 702:

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



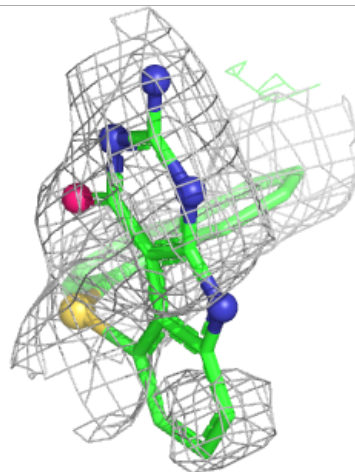
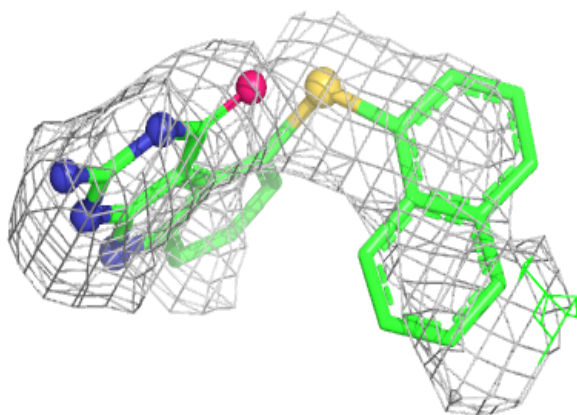
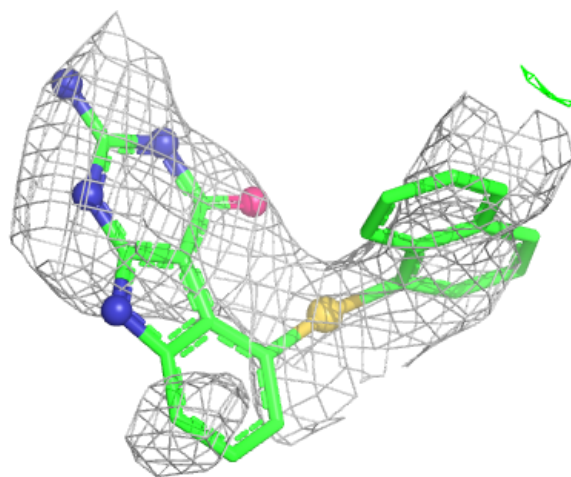
Electron density around 1UG C 702:

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



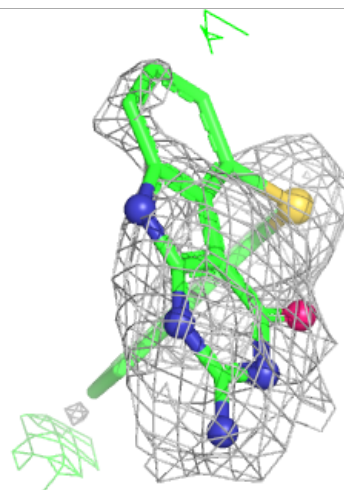
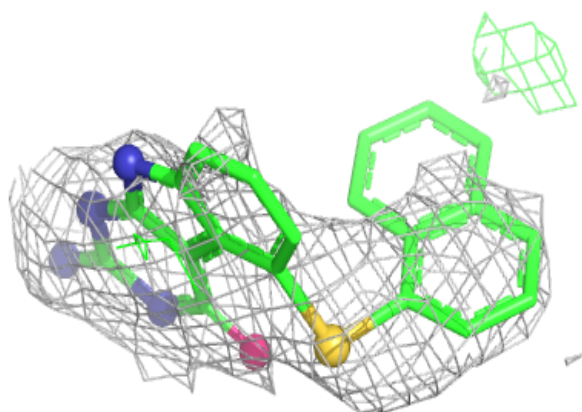
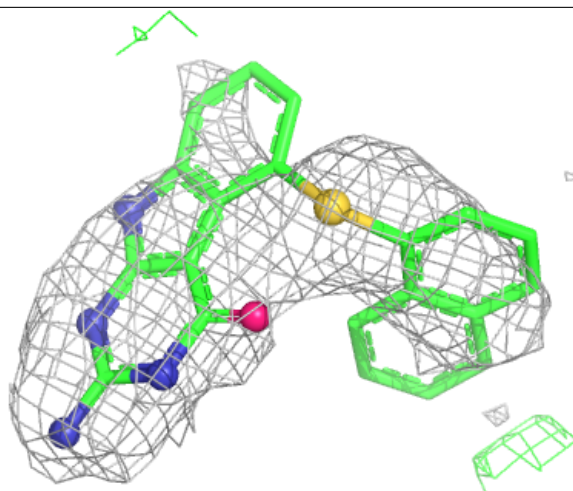
Electron density around 1UG D 702:

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



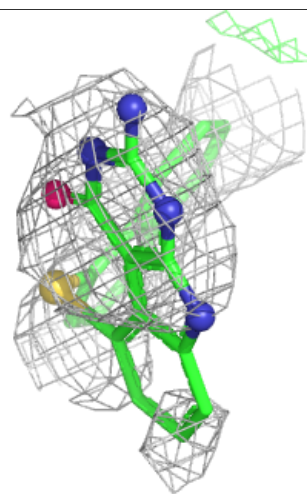
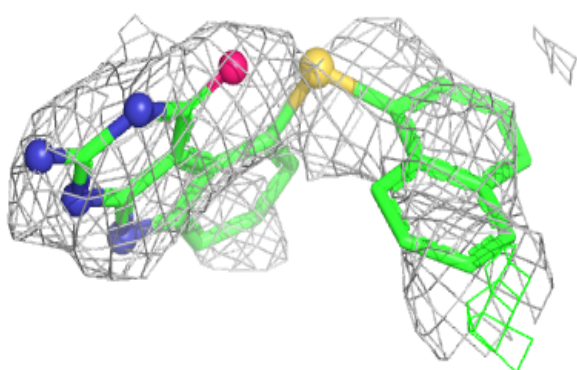
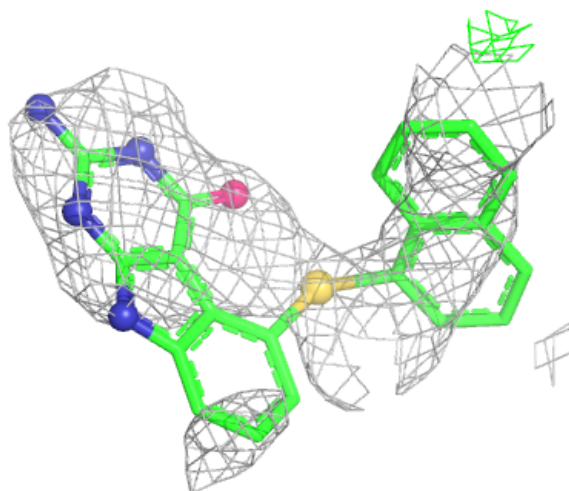
Electron density around 1UG E 702:

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



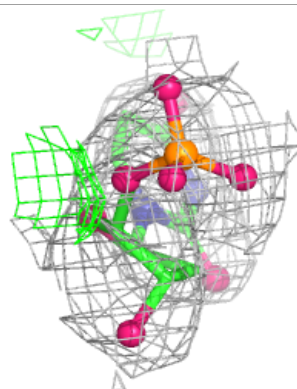
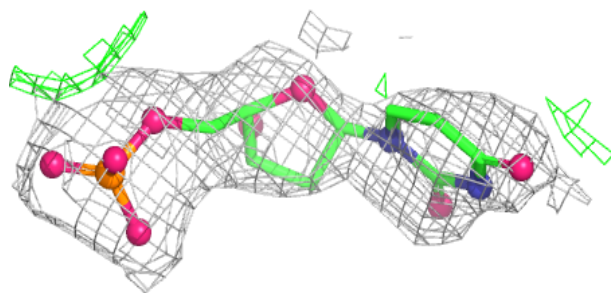
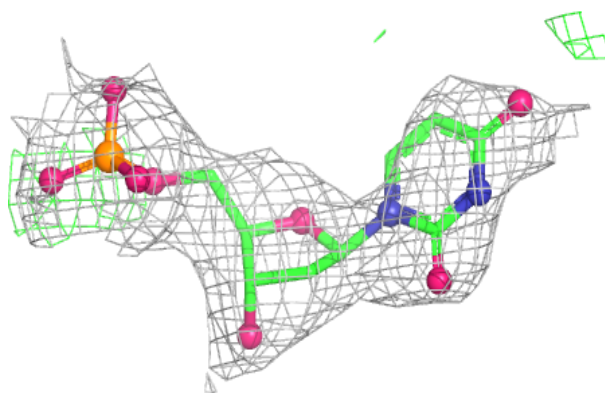
Electron density around 1UG F 702:

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



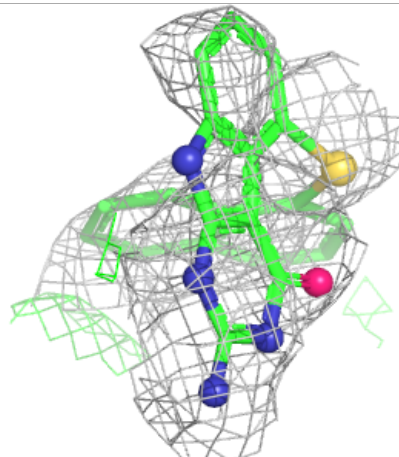
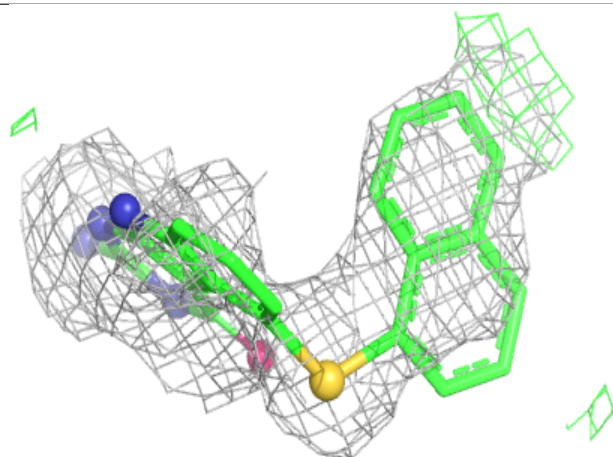
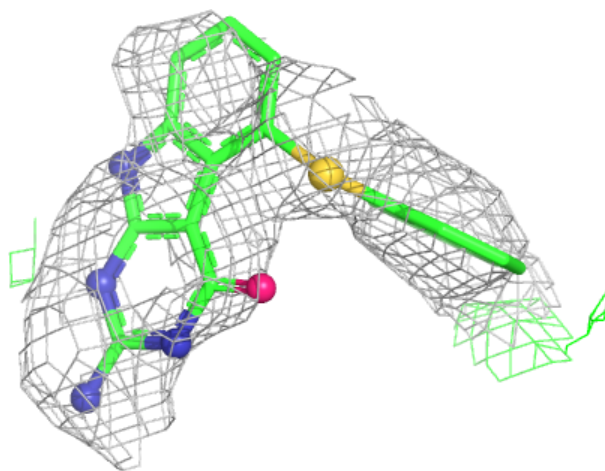
Electron density around UMP B 701:

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



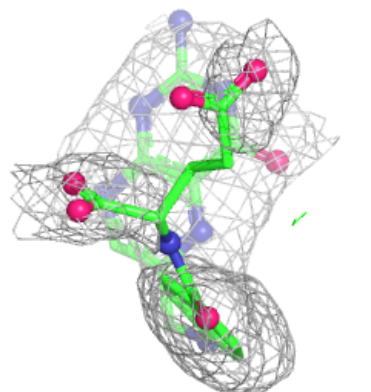
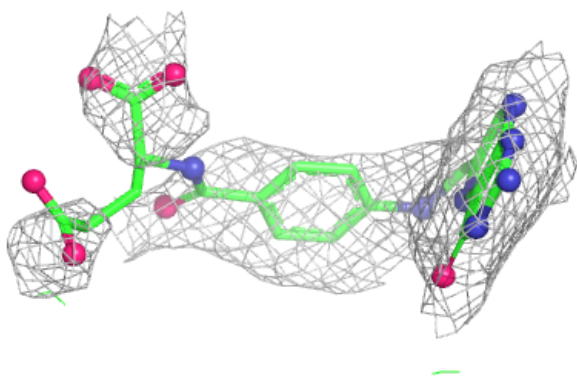
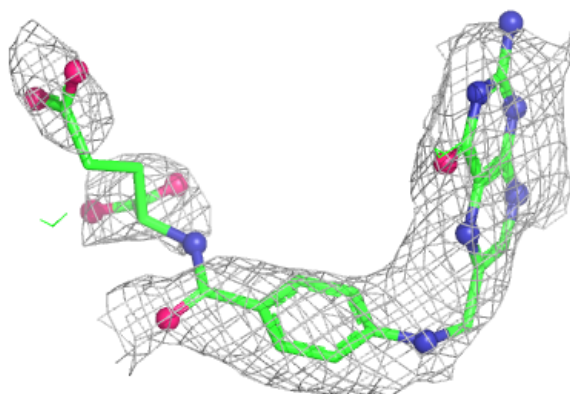
Electron density around 1UG H 702:

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

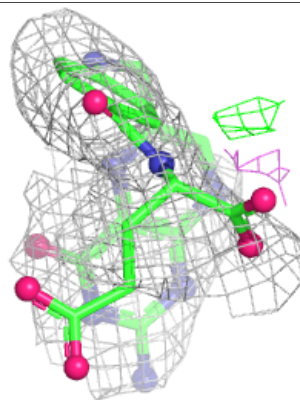
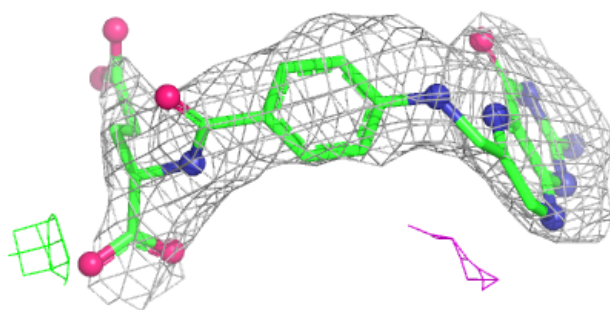
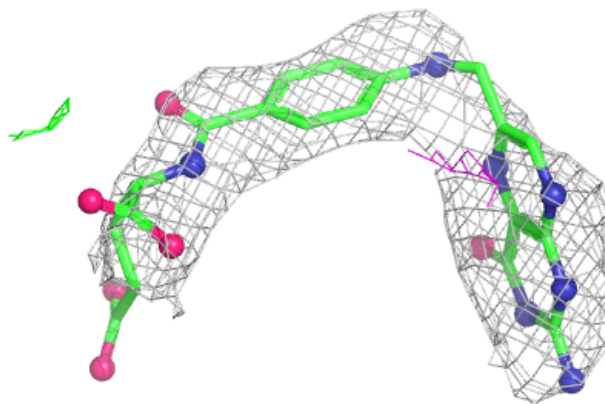


Electron density around FOL A 703:

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

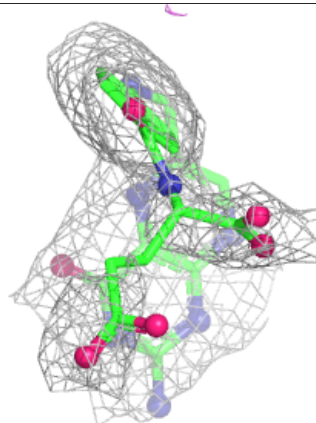
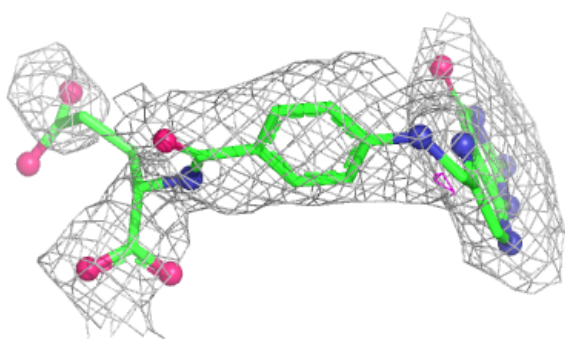
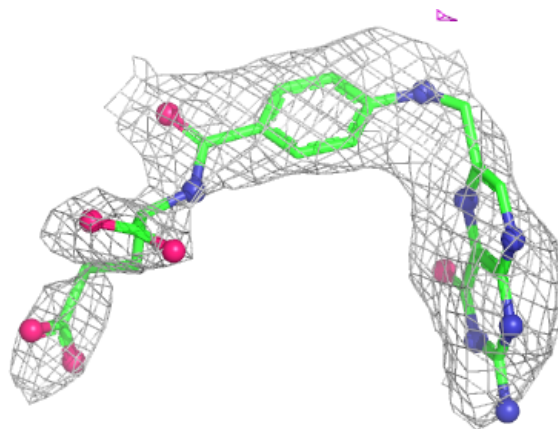
**Electron density around FOL B 703:**

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



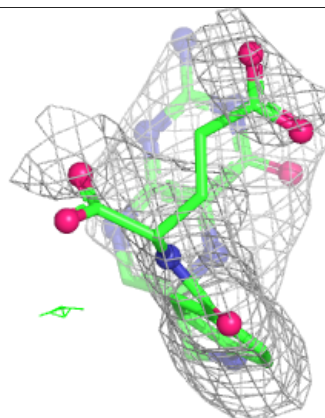
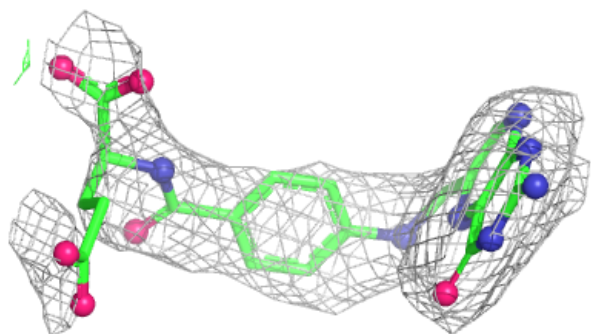
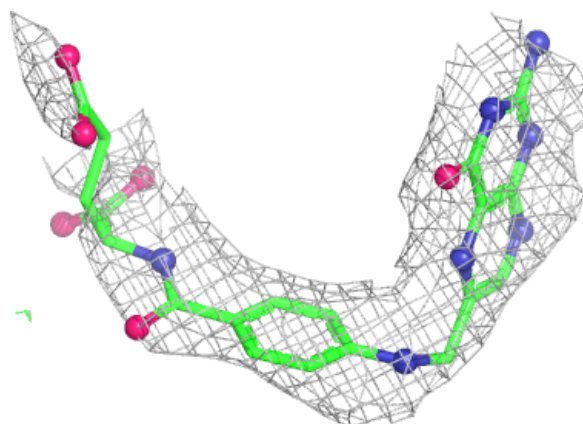
Electron density around FOL C 703:

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

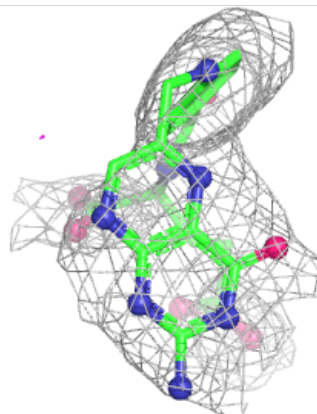
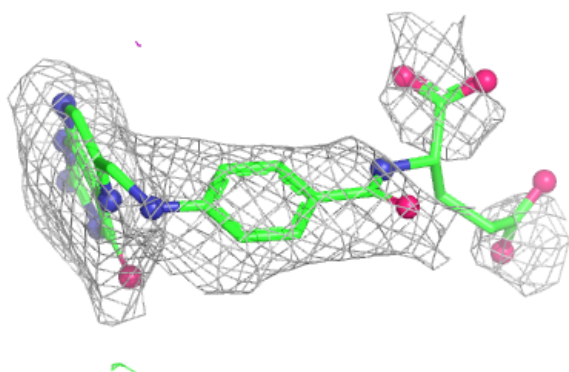
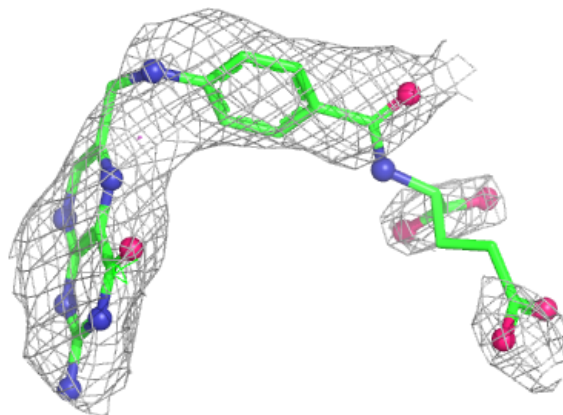


Electron density around FOL D 703:

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

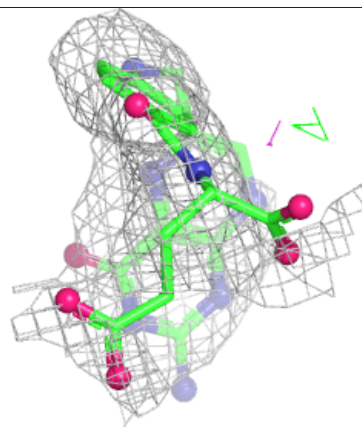
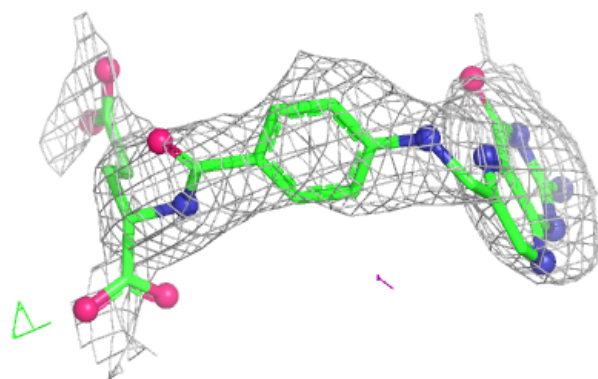
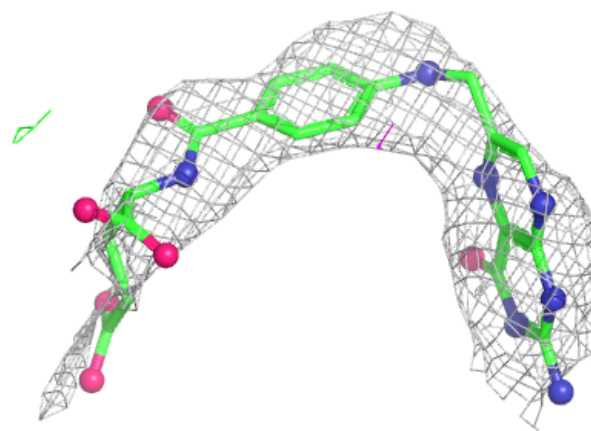
**Electron density around FOL E 703:**

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

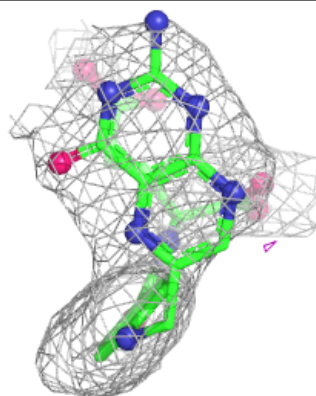
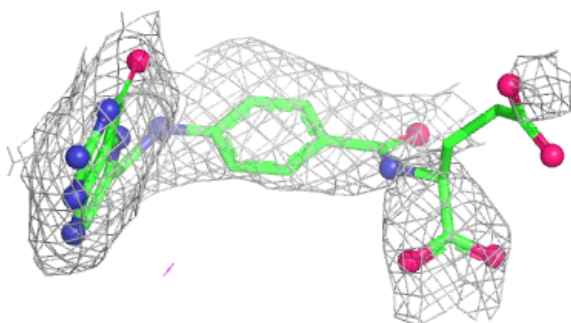
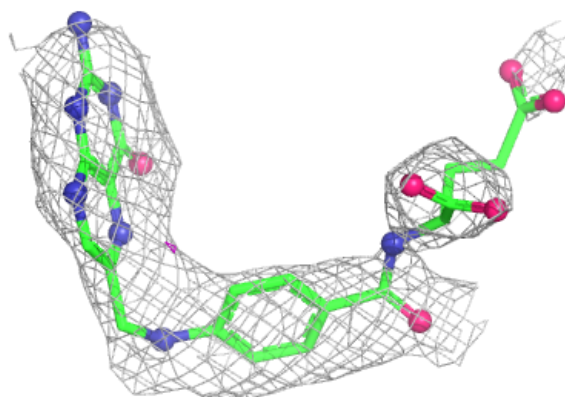


Electron density around FOL F 703:

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

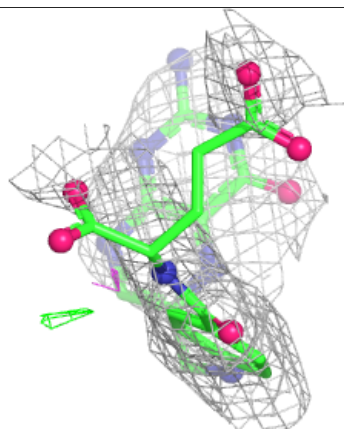
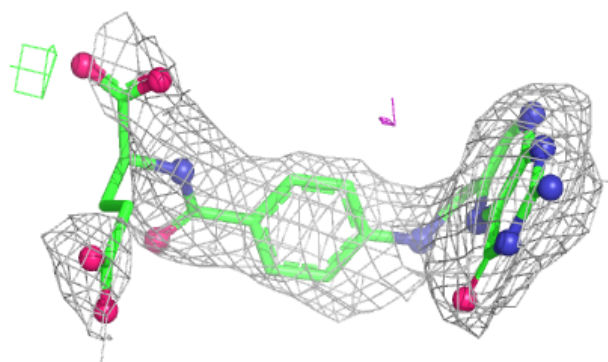
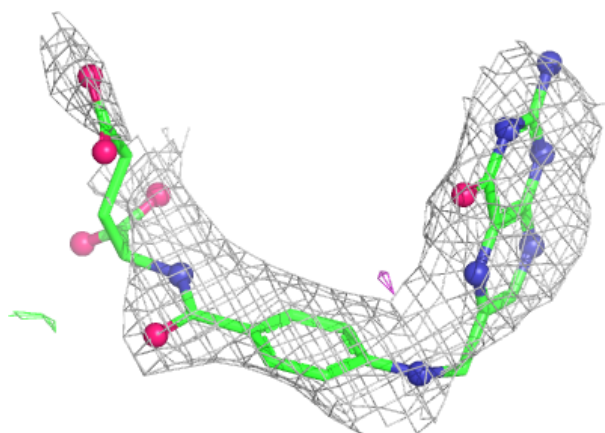
**Electron density around FOL G 703:**

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

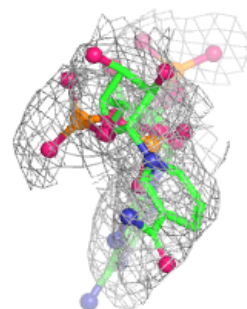
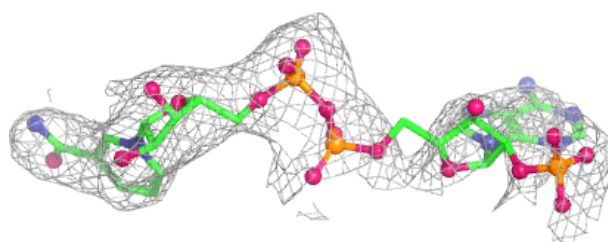
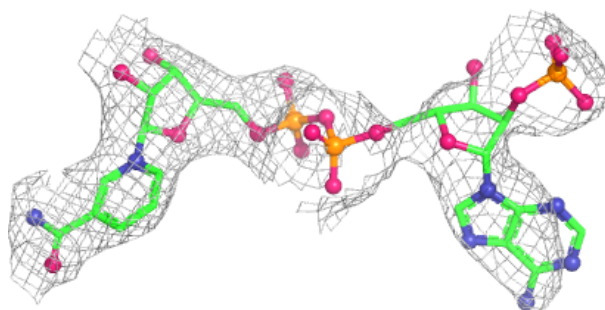


Electron density around FOL H 703:

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

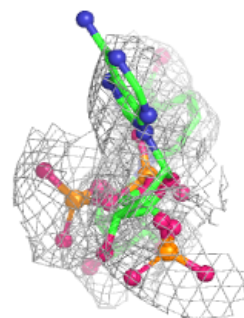
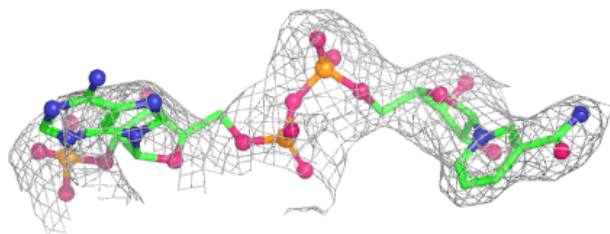
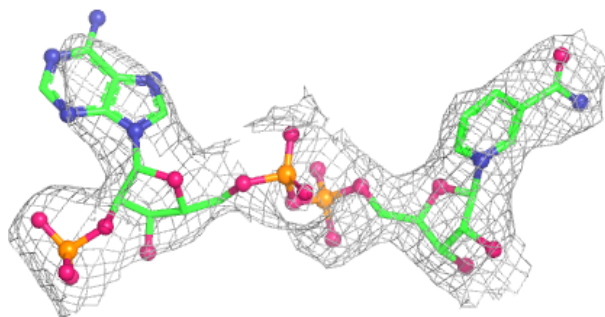
**Electron density around NDP B 704:**

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

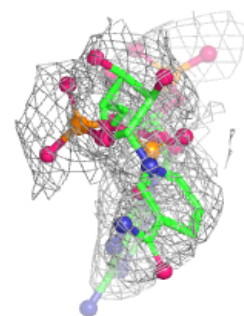
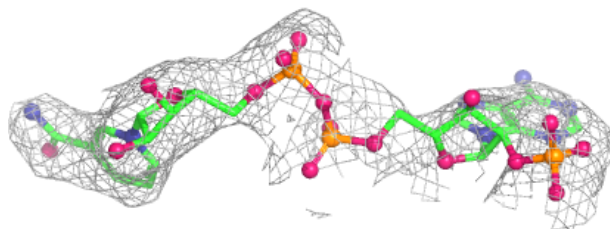
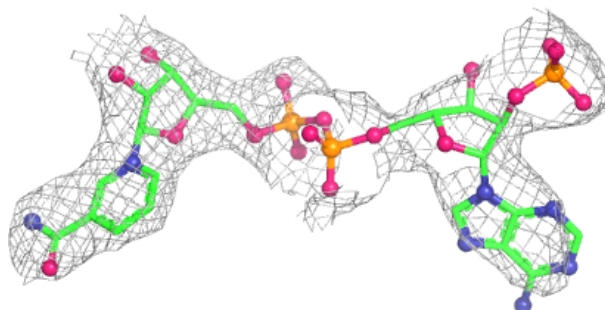


Electron density around NDP D 704:

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

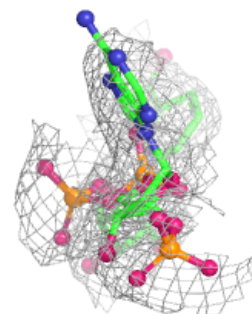
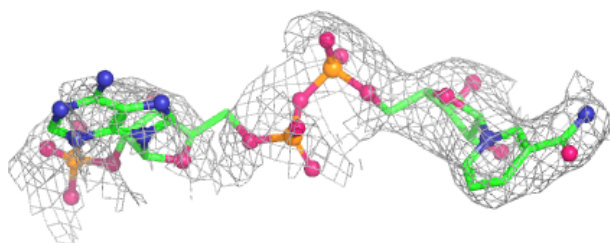
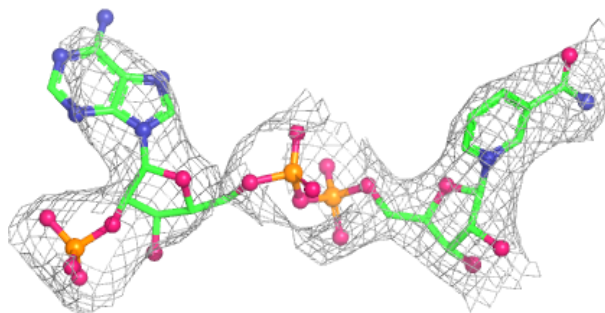
**Electron density around NDP F 704:**

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

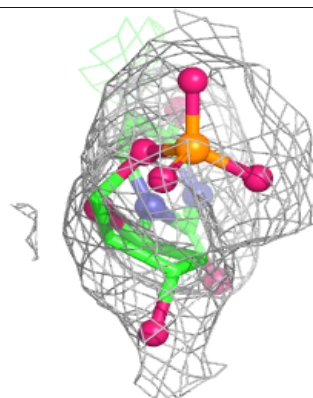
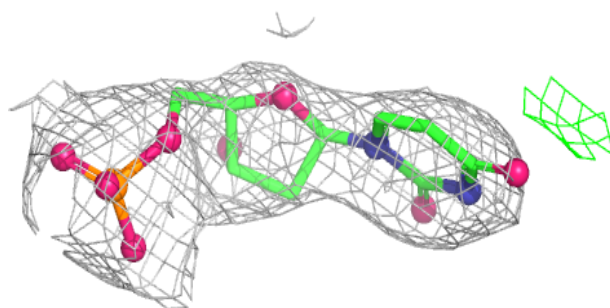
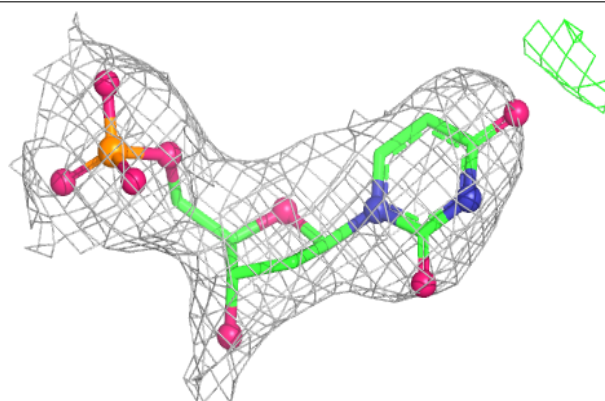


Electron density around NDP H 704:

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

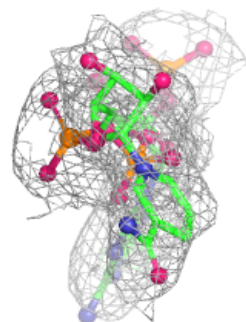
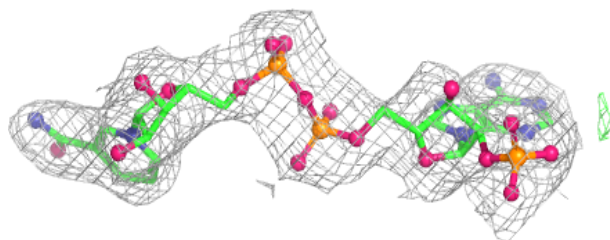
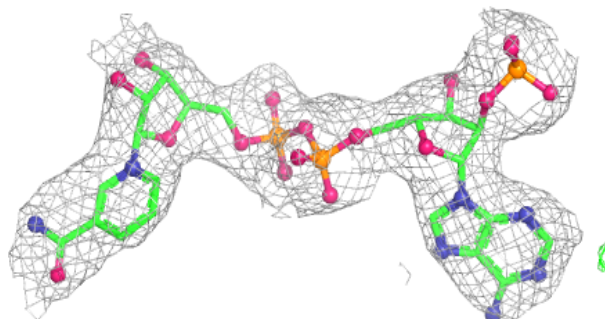
**Electron density around UMP A 701:**

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

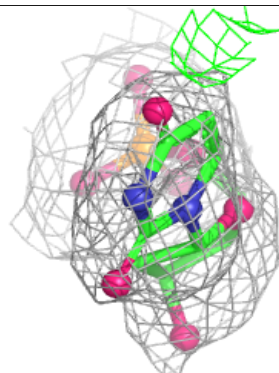
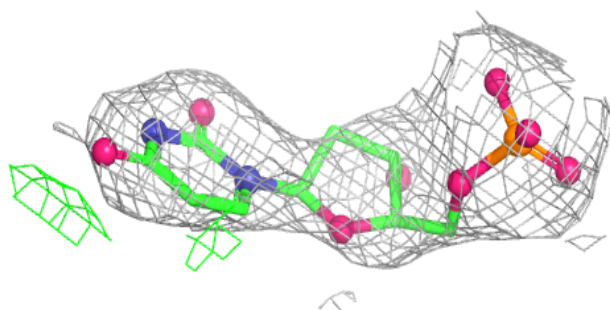
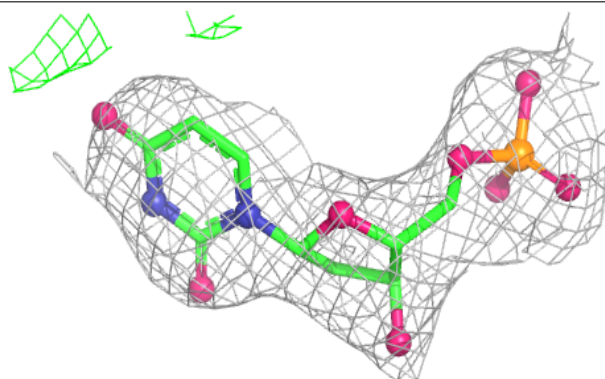


Electron density around NDP C 704:

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

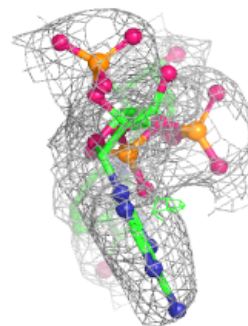
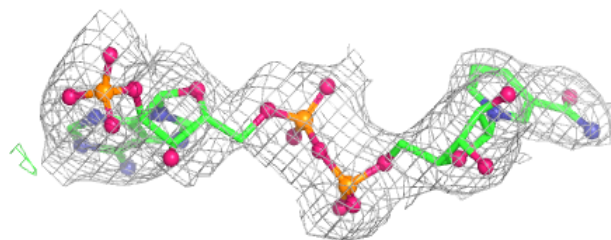
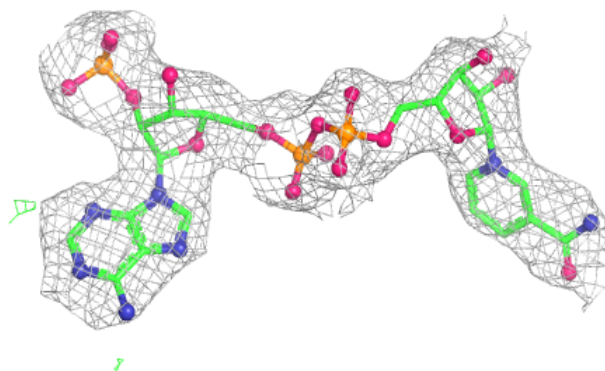
**Electron density around UMP E 701:**

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

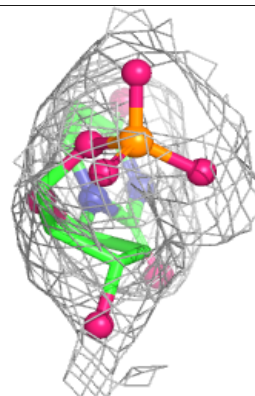
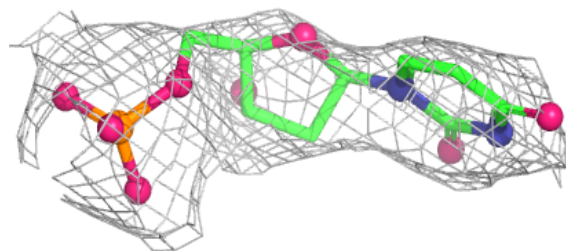
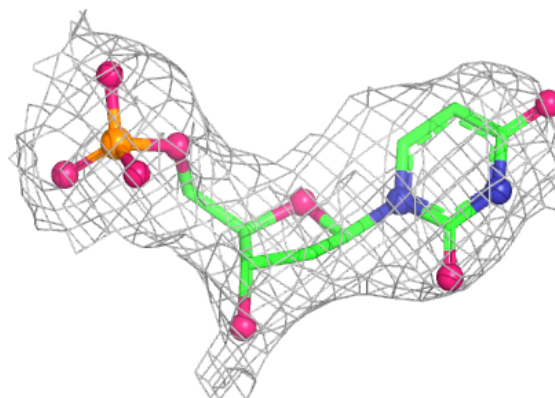


Electron density around NDP E 704:

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

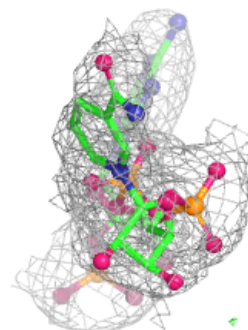
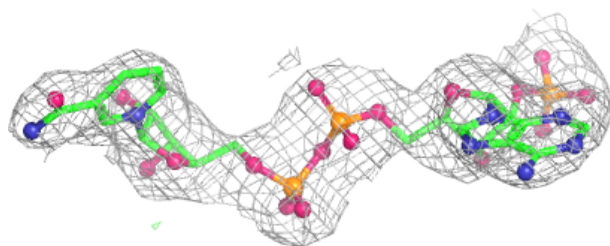
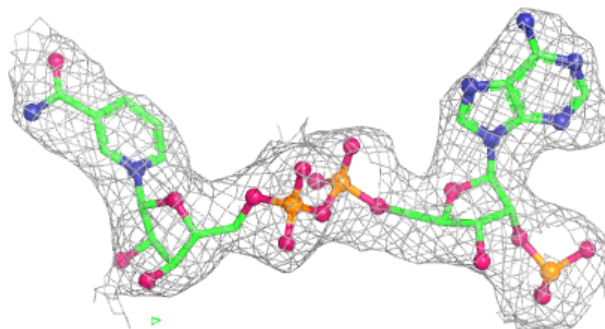
**Electron density around UMP C 701:**

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

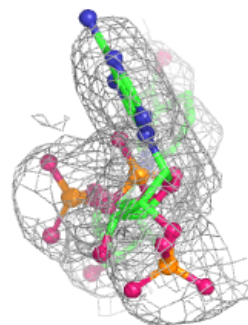
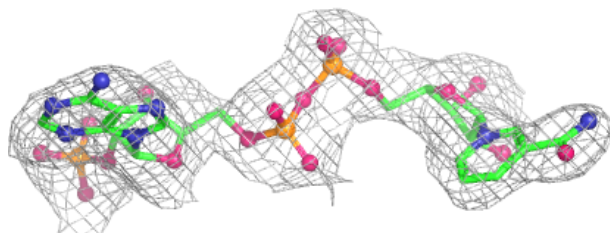
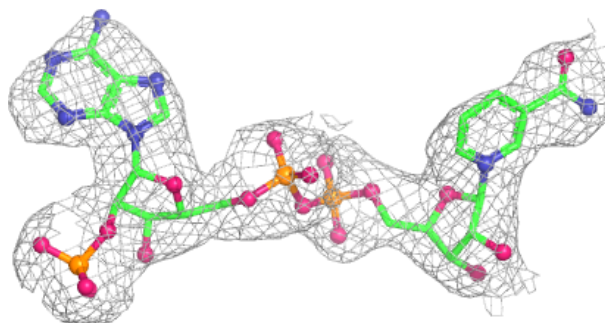


Electron density around NDP G 704:

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

**Electron density around NDP A 704:**

$2mF_o-DF_c$ (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.