



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 04:08 PM JST

PDB ID : 7F3Z
Title : Double mutant Plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS-K1, C59R+S108N) complexed with Trimethoprim (TOP), NADPH and dUMP
Authors : Vanichtanankul, J.; Tanramluk, D.; Chitnumsub, P.; Yuvaniyama, J.; Yuthavong, Y.
Deposited on : 2021-06-17
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

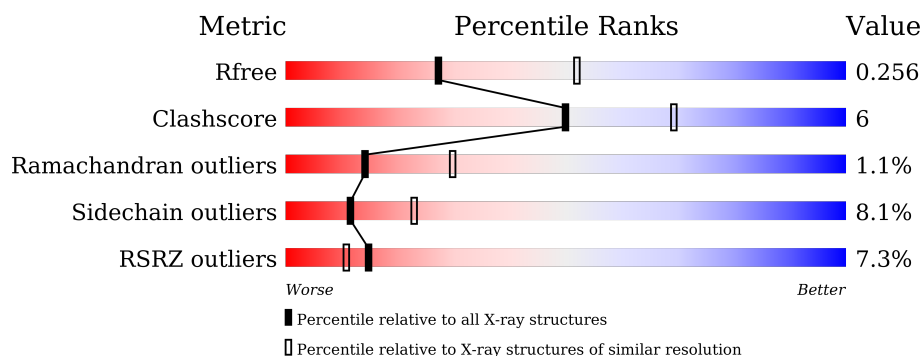
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	608	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>• 10%</div> </div> </div>
1	B	608	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>• 10%</div> </div> </div>

2 Entry composition [i](#)

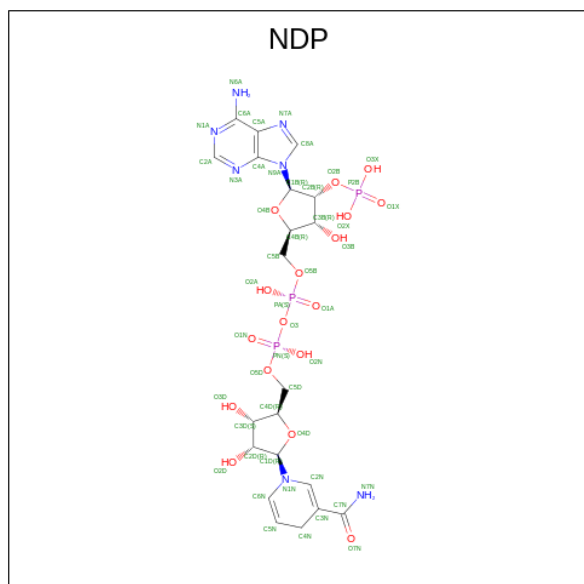
There are 6 unique types of molecules in this entry. The entry contains 9494 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

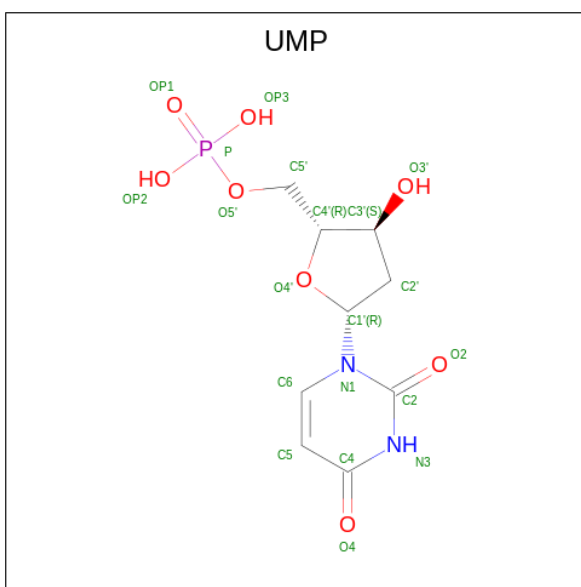
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4555	2938	755	835	27			
1	B	548	Total	C	N	O	S	0	0	0
			4555	2938	755	835	27			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



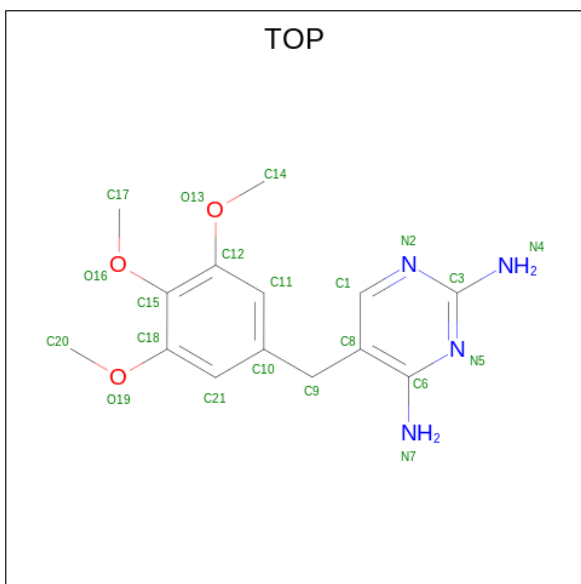
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is TRIMETHOPRIM (three-letter code: TOP) (formula: $C_{14}H_{18}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



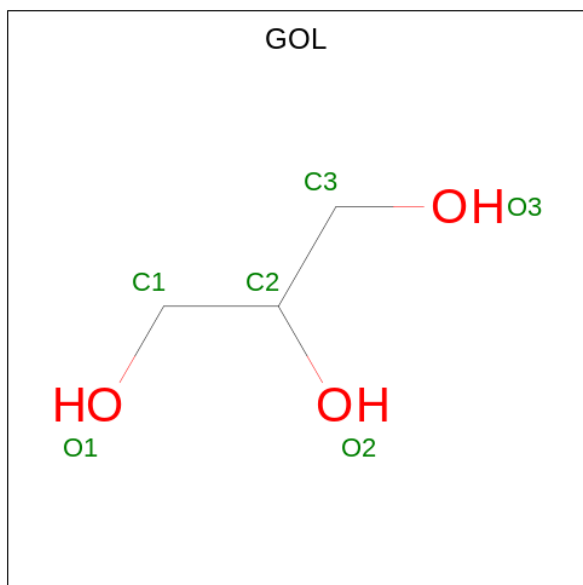
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	14	4	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			21	14	4	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).

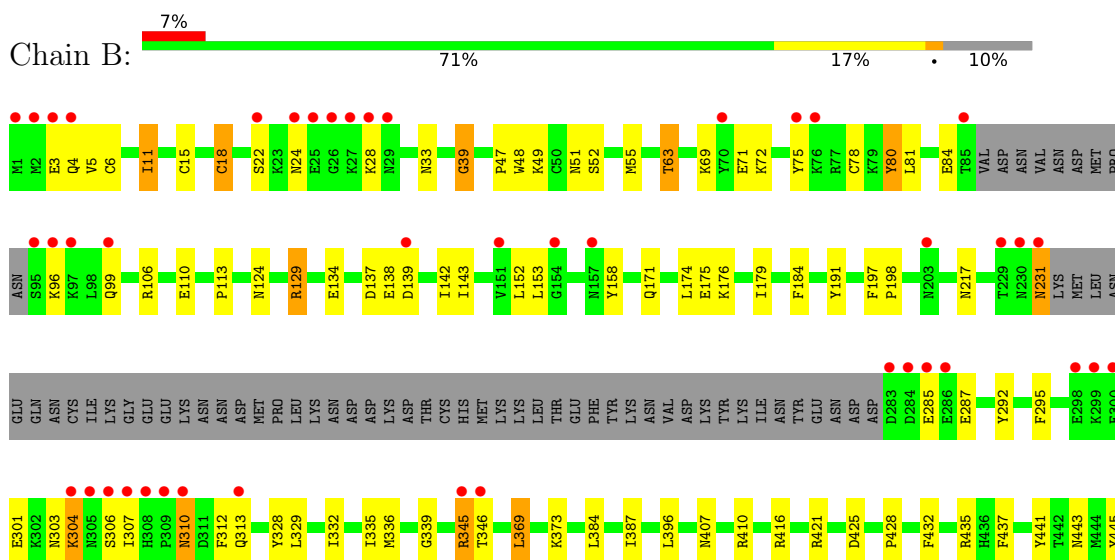


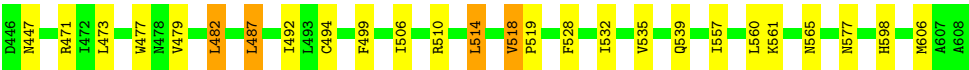
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	106	Total	O	0	0
			106	106		
6	B	88	Total	O	0	0
			88	88		

- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.33Å 153.74Å 164.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.78 – 2.60 39.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (39.78-2.60) 97.5 (39.75-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.198 , 0.253 0.207 , 0.256	Depositor DCC
R_{free} test set	2178 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9494	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.71	0/4660	0.87	0/6288
1	B	0.71	0/4660	0.89	2/6288 (0.0%)
All	All	0.71	0/9320	0.88	2/12576 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	CYS	CB-CA-C	-5.82	98.76	110.40
1	B	416	ARG	CG-CD-NE	-5.31	100.65	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4555	0	4508	50	0
1	B	4555	0	4508	64	0
2	A	48	0	26	1	0
2	B	48	0	26	1	0
3	A	20	0	11	0	0
3	B	20	0	11	0	0
4	A	21	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	21	0	18	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	106	0	0	7	0
6	B	88	0	0	2	0
All	All	9494	0	9142	107	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 6.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:PHE:HA	1:B:565:ASN:HD21	1.44	0.82
1:A:325:GLU:OE2	1:A:371:THR:HG22	1.81	0.80
1:A:174:LEU:HA	6:A:827:HOH:O	1.91	0.69
1:A:371:THR:HG23	1:A:563:GLN:HE21	1.59	0.68
1:A:177:LYS:HA	6:A:827:HOH:O	1.92	0.68
1:B:142:ILE:O	1:B:143:ILE:HG23	1.96	0.66
1:A:421:ARG:NH1	6:A:801:HOH:O	2.21	0.62
1:A:146:VAL:HG12	6:A:840:HOH:O	1.99	0.62
1:B:410:ARG:NH2	1:B:421:ARG:O	2.28	0.60
1:B:171:GLN:NE2	1:B:175:GLU:OE1	2.36	0.58
1:A:189:SER:HG	1:A:219:THR:HG1	1.49	0.58
1:A:189:SER:HB2	1:A:191:TYR:CE2	2.39	0.57
1:A:348:VAL:HG21	6:A:864:HOH:O	2.04	0.57
1:A:100:ASN:HD22	1:A:160:LYS:H	1.53	0.57
1:B:307:ILE:O	1:B:561:LYS:NZ	2.37	0.56
1:B:6:CYS:HA	1:B:11:ILE:HG23	1.88	0.56
1:A:416:ARG:HD3	1:A:486:ALA:O	2.06	0.55
1:B:55:MET:CE	6:B:823:HOH:O	2.54	0.55
1:B:312:PHE:CA	1:B:565:ASN:HD21	2.19	0.54
1:B:197:PHE:CD1	1:B:198:PRO:HD2	2.42	0.53
1:A:493:LEU:C	1:A:493:LEU:HD12	2.28	0.53
1:B:428:PRO:HB3	1:B:432:PHE:CD2	2.43	0.53
1:B:99:GLN:O	1:B:158:TYR:HA	2.09	0.52
1:A:479:VAL:HB	1:B:437:PHE:CD1	2.44	0.52
1:B:231:ASN:C	1:B:231:ASN:HD22	2.13	0.52
1:B:332:ILE:HD13	1:B:560:LEU:HD22	1.92	0.52
1:A:167:SER:HB2	1:A:195:VAL:CG1	2.40	0.51
1:B:310:ASN:N	1:B:310:ASN:ND2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:SER:OG	1:A:219:THR:OG1	2.22	0.51
1:A:284:ASP:N	1:A:284:ASP:OD1	2.44	0.51
1:B:479:VAL:HA	1:B:482:LEU:HD22	1.92	0.51
1:B:312:PHE:HA	1:B:565:ASN:ND2	2.22	0.51
1:B:310:ASN:ND2	1:B:310:ASN:H	2.07	0.51
1:A:284:ASP:O	1:B:69:LYS:NZ	2.44	0.50
1:B:47:PRO:HD2	1:B:48:TRP:CZ3	2.46	0.50
1:B:369:LEU:HD22	1:B:519:PRO:HB3	1.93	0.50
1:A:427:GLY:HA2	1:A:441:TYR:CE2	2.48	0.49
1:B:336:MET:CE	1:B:560:LEU:HB2	2.42	0.49
1:B:142:ILE:HG22	1:B:143:ILE:N	2.28	0.49
1:A:409:THR:HG22	1:A:411:GLU:N	2.28	0.49
1:A:416:ARG:CD	1:A:486:ALA:O	2.61	0.49
1:A:108:ASN:ND2	2:A:701:NDP:C6N	2.75	0.49
1:B:303:ASN:HB3	1:B:306:SER:HB3	1.96	0.48
1:B:336:MET:HE1	1:B:560:LEU:HB2	1.94	0.47
1:A:492:ILE:HD11	1:A:510:ARG:HD3	1.96	0.47
1:B:518:VAL:N	1:B:519:PRO:CD	2.78	0.47
1:B:494:CYS:HA	1:B:506:ILE:O	2.14	0.47
1:B:373:LYS:HG3	1:B:598:HIS:CE1	2.50	0.47
1:B:492:ILE:HD11	1:B:510:ARG:HD3	1.97	0.47
1:A:477:TRP:CZ2	1:A:482:LEU:HD21	2.50	0.46
1:A:493:LEU:CD2	1:B:492:ILE:HG21	2.45	0.46
1:B:477:TRP:CZ2	1:B:482:LEU:HD21	2.50	0.46
1:A:435:ARG:NH1	1:A:454:ASP:OD2	2.48	0.46
1:A:220:THR:HG23	1:A:573:THR:HG23	1.98	0.46
1:A:355:GLY:HA2	1:A:547:LEU:O	2.15	0.46
1:A:425:ASP:CG	1:A:444:MET:HG3	2.36	0.46
1:B:129:ARG:HG2	2:B:701:NDP:O3X	2.16	0.46
1:A:334:ASP:OD1	1:A:338:ASN:ND2	2.49	0.46
1:B:106:ARG:NH1	1:B:110:GLU:OE1	2.49	0.46
1:B:310:ASN:O	1:B:313:GLN:HG3	2.16	0.46
1:B:15:CYS:SG	1:B:184:PHE:CD2	3.09	0.46
1:A:340:ASN:HB3	1:B:499:PHE:CE1	2.51	0.45
1:B:18:CYS:SG	1:B:48:TRP:CE3	3.10	0.45
1:B:387:ILE:O	1:B:435:ARG:NH1	2.49	0.45
1:A:82:ASN:O	1:A:83:LYS:HG3	2.16	0.45
1:A:488:PRO:HG2	1:B:471:ARG:HD3	1.98	0.45
1:A:20:VAL:C	1:A:22:SER:H	2.21	0.44
1:A:460:ILE:O	1:A:464:LYS:HG2	2.17	0.44
1:B:63:THR:HG23	1:B:63:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:CYS:HA	1:A:39:GLY:O	2.17	0.44
1:B:55:MET:HE1	6:B:823:HOH:O	2.16	0.44
1:B:443:ASN:OD1	1:B:445:TYR:HB2	2.18	0.44
1:B:47:PRO:HD2	1:B:48:TRP:CE3	2.53	0.43
1:B:425:ASP:OD1	1:B:441:TYR:OH	2.30	0.43
1:A:390:GLU:OE1	1:A:395:THR:HG21	2.18	0.43
1:B:301:GLU:O	1:B:304:LYS:HB2	2.19	0.43
1:B:557:ILE:O	1:B:561:LYS:HG3	2.19	0.43
1:A:127:LEU:HD23	1:A:143:ILE:HG13	2.01	0.42
1:A:555:ASN:HB3	1:A:605:ASP:OD1	2.19	0.42
1:B:71:GLU:OE2	1:B:71:GLU:HA	2.18	0.42
1:B:335:ILE:O	1:B:339:GLY:N	2.49	0.42
1:A:332:ILE:CD1	1:A:514:LEU:HB3	2.50	0.42
1:B:335:ILE:CD1	1:B:514:LEU:HD13	2.49	0.42
1:A:479:VAL:HB	1:B:437:PHE:CE1	2.55	0.42
1:B:514:LEU:HA	1:B:518:VAL:HG13	2.02	0.42
1:A:133:LYS:HA	1:A:142:ILE:HG13	2.02	0.42
1:A:354:PHE:CZ	1:B:506:ILE:HD12	2.55	0.42
1:B:231:ASN:C	1:B:231:ASN:ND2	2.74	0.41
1:B:407:ASN:ND2	1:B:487:LEU:HD12	2.35	0.41
1:A:109:TRP:CH2	1:A:117:LYS:HB3	2.55	0.41
1:B:18:CYS:SG	1:B:191:TYR:HD1	2.43	0.41
1:B:307:ILE:HG13	1:B:336:MET:O	2.20	0.41
1:A:403:ILE:HG22	1:A:404:TRP:CD1	2.56	0.41
1:B:328:TYR:CZ	1:B:332:ILE:CD1	3.03	0.41
1:B:18:CYS:HB2	1:B:39:GLY:HA3	2.02	0.41
1:B:174:LEU:HD21	1:B:179:ILE:HD11	2.01	0.41
1:B:528:PHE:O	1:B:532:ILE:HG12	2.21	0.41
1:B:292:TYR:O	1:B:295:PHE:HB3	2.21	0.41
1:A:109:TRP:O	1:A:117:LYS:HD3	2.21	0.41
1:A:130:THR:HG21	6:A:881:HOH:O	2.19	0.41
1:A:372:LYS:NZ	6:A:809:HOH:O	2.45	0.40
1:A:19:LYS:HG2	1:A:36:THR:HG22	2.04	0.40
1:A:146:VAL:HG11	1:A:176:LYS:HE3	2.02	0.40
1:B:482:LEU:HD12	1:B:482:LEU:HA	1.89	0.40
1:B:80:TYR:CD1	1:B:80:TYR:C	2.95	0.40
1:B:577:ASN:OD1	1:B:577:ASN:C	2.59	0.40
1:A:35:TYR:CZ	1:A:38:ARG:HD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	542/608 (89%)	500 (92%)	36 (7%)	6 (1%)	14	30
1	B	542/608 (89%)	489 (90%)	47 (9%)	6 (1%)	14	30
All	All	1084/1216 (89%)	989 (91%)	83 (8%)	12 (1%)	14	30

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	ARG
1	B	49	LYS
1	A	49	LYS
1	B	113	PRO
1	B	134	GLU
1	A	82	ASN
1	A	308	HIS
1	B	345	ARG
1	A	21	GLU
1	B	75	TYR
1	A	79	LYS
1	B	39	GLY

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	510/570 (90%)	473 (93%)	37 (7%)	14	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	510/570 (90%)	464 (91%)	46 (9%)	9	18
All	All	1020/1140 (90%)	937 (92%)	83 (8%)	11	23

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	MET
1	A	19	LYS
1	A	23	LYS
1	A	31	VAL
1	A	49	LYS
1	A	52	SER
1	A	68	SER
1	A	71	GLU
1	A	85	THR
1	A	114	LYS
1	A	132	LYS
1	A	230	ASN
1	A	284	ASP
1	A	286	GLU
1	A	287	GLU
1	A	303	ASN
1	A	304	LYS
1	A	306	SER
1	A	329	LEU
1	A	343	SER
1	A	344	ASP
1	A	346	THR
1	A	348	VAL
1	A	373	LYS
1	A	376	LEU
1	A	384	LEU
1	A	411	GLU
1	A	447	ASN
1	A	451	LYS
1	A	462	LEU
1	A	464	LYS
1	A	487	LEU
1	A	507	MET
1	A	579	ASP
1	A	584	GLU

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Mol	Chain	Res	Type
1	A	592	THR
1	B	3	GLU
1	B	4	GLN
1	B	5	VAL
1	B	11	ILE
1	B	22	SER
1	B	24	ASN
1	B	28	LYS
1	B	33	ASN
1	B	51	ASN
1	B	52	SER
1	B	63	THR
1	B	72	LYS
1	B	78	CYS
1	B	80	TYR
1	B	81	LEU
1	B	84	GLU
1	B	96	LYS
1	B	124	ASN
1	B	129	ARG
1	B	137	ASP
1	B	138	GLU
1	B	139	ASP
1	B	152	LEU
1	B	153	LEU
1	B	176	LYS
1	B	217	ASN
1	B	231	ASN
1	B	285	GLU
1	B	287	GLU
1	B	304	LYS
1	B	310	ASN
1	B	329	LEU
1	B	345	ARG
1	B	346	THR
1	B	369	LEU
1	B	384	LEU
1	B	396	LEU
1	B	447	ASN
1	B	473	LEU
1	B	482	LEU
1	B	487	LEU

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Mol	Chain	Res	Type
1	B	514	LEU
1	B	518	VAL
1	B	535	VAL
1	B	539	GLN
1	B	606	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	29	ASN
1	A	100	ASN
1	A	108	ASN
1	A	217	ASN
1	A	230	ASN
1	A	327	GLN
1	A	424	ASN
1	A	563	GLN
1	B	33	ASN
1	B	51	ASN
1	B	171	GLN
1	B	217	ASN
1	B	231	ASN
1	B	310	ASN
1	B	327	GLN
1	B	394	ASN
1	B	407	ASN
1	B	424	ASN
1	B	554	ASN
1	B	565	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	NDP	A	701	-	45,52,52	0.65	0	53,80,80	0.89	1 (1%)
3	UMP	A	702	-	18,21,21	1.08	1 (5%)	21,31,31	1.13	1 (4%)
5	GOL	B	704	-	5,5,5	0.21	0	5,5,5	0.44	0
3	UMP	B	702	-	18,21,21	1.14	2 (11%)	21,31,31	1.16	1 (4%)
4	TOP	A	703	-	22,22,22	0.35	0	30,30,30	0.57	0
2	NDP	B	701	-	45,52,52	0.69	1 (2%)	53,80,80	0.90	2 (3%)
5	GOL	A	704	-	5,5,5	0.11	0	5,5,5	0.24	0
4	TOP	B	703	-	22,22,22	0.32	0	30,30,30	0.66	0

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	NDP	A	701	-	-	5/30/77/77	0/5/5/5
3	UMP	A	702	-	-	1/7/22/22	0/2/2/2
5	GOL	B	704	-	-	0/4/4/4	-
3	UMP	B	702	-	-	4/7/22/22	0/2/2/2
4	TOP	A	703	-	-	2/10/10/10	0/2/2/2
2	NDP	B	701	-	-	4/30/77/77	0/5/5/5
5	GOL	A	704	-	-	0/4/4/4	-
4	TOP	B	703	-	-	2/10/10/10	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	UMP	C4-N3	3.38	1.38	1.33
3	B	702	UMP	C4-N3	3.27	1.38	1.33
3	B	702	UMP	C6-N1	2.25	1.38	1.35
2	B	701	NDP	C2N-C3N	2.14	1.40	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	UMP	C5-C4-N3	-3.89	114.74	123.31
3	B	702	UMP	C5-C4-N3	-3.86	114.81	123.31
2	A	701	NDP	C5A-C6A-N6A	2.48	124.12	120.35
2	B	701	NDP	C3D-C2D-C1D	2.36	105.91	101.43
2	B	701	NDP	C5A-C6A-N6A	2.27	123.80	120.35

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	NDP	PA-O3-PN-O5D
2	B	701	NDP	O4D-C1D-N1N-C2N
3	B	702	UMP	C5'-O5'-P-OP1
3	B	702	UMP	C5'-O5'-P-OP3
3	B	702	UMP	C3'-C4'-C5'-O5'
3	B	702	UMP	O4'-C4'-C5'-O5'
4	B	703	TOP	C15-C12-O13-C14
4	A	703	TOP	C15-C12-O13-C14
4	B	703	TOP	C11-C12-O13-C14
4	A	703	TOP	C11-C12-O13-C14
2	A	701	NDP	O4D-C1D-N1N-C2N
3	A	702	UMP	O4'-C4'-C5'-O5'
2	A	701	NDP	C2B-O2B-P2B-O1X
2	A	701	NDP	C2B-O2B-P2B-O2X
2	A	701	NDP	C2B-O2B-P2B-O3X
2	B	701	NDP	C5D-O5D-PN-O3
2	A	701	NDP	C2N-C3N-C7N-N7N
2	B	701	NDP	C5B-O5B-PA-O1A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

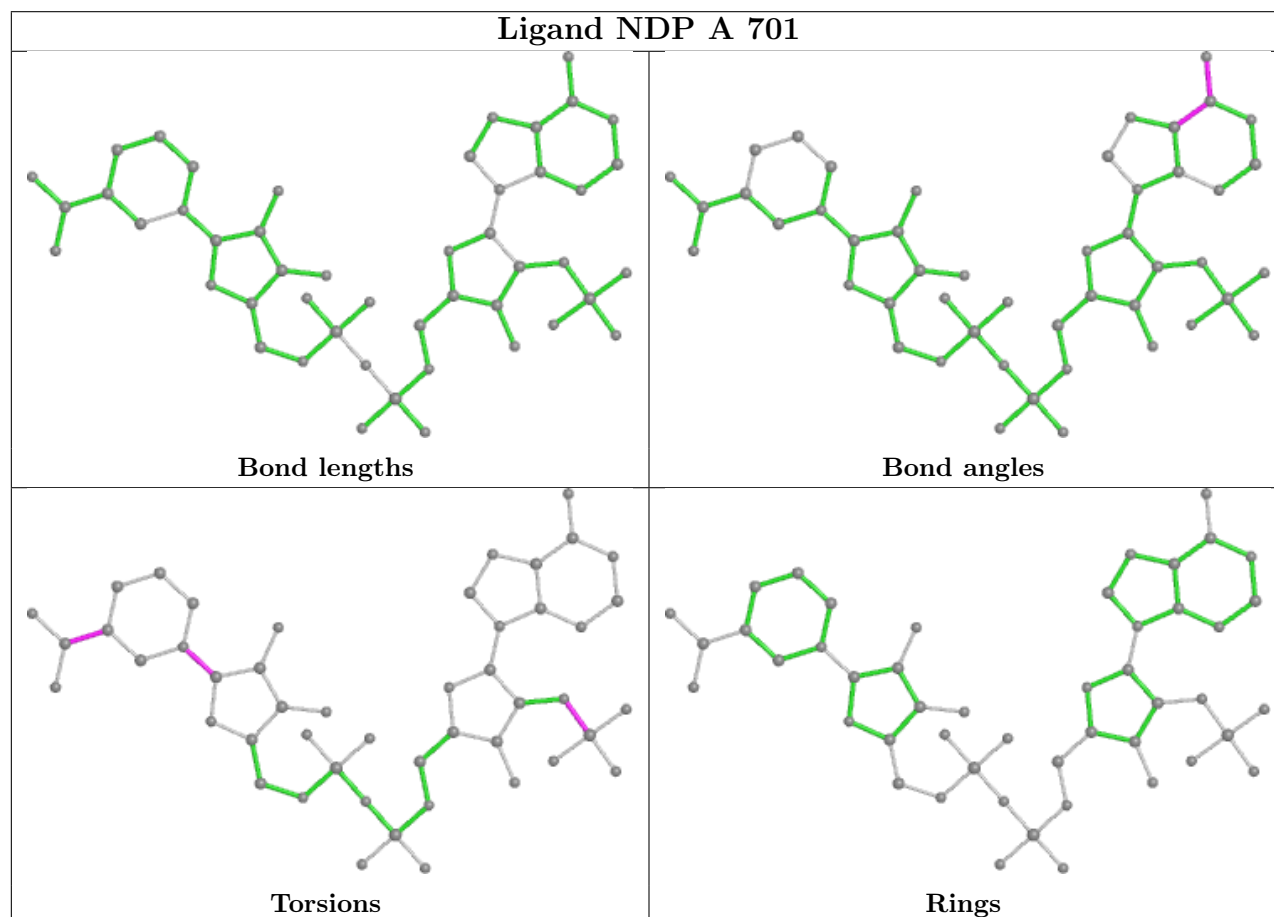
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	NDP	1	0

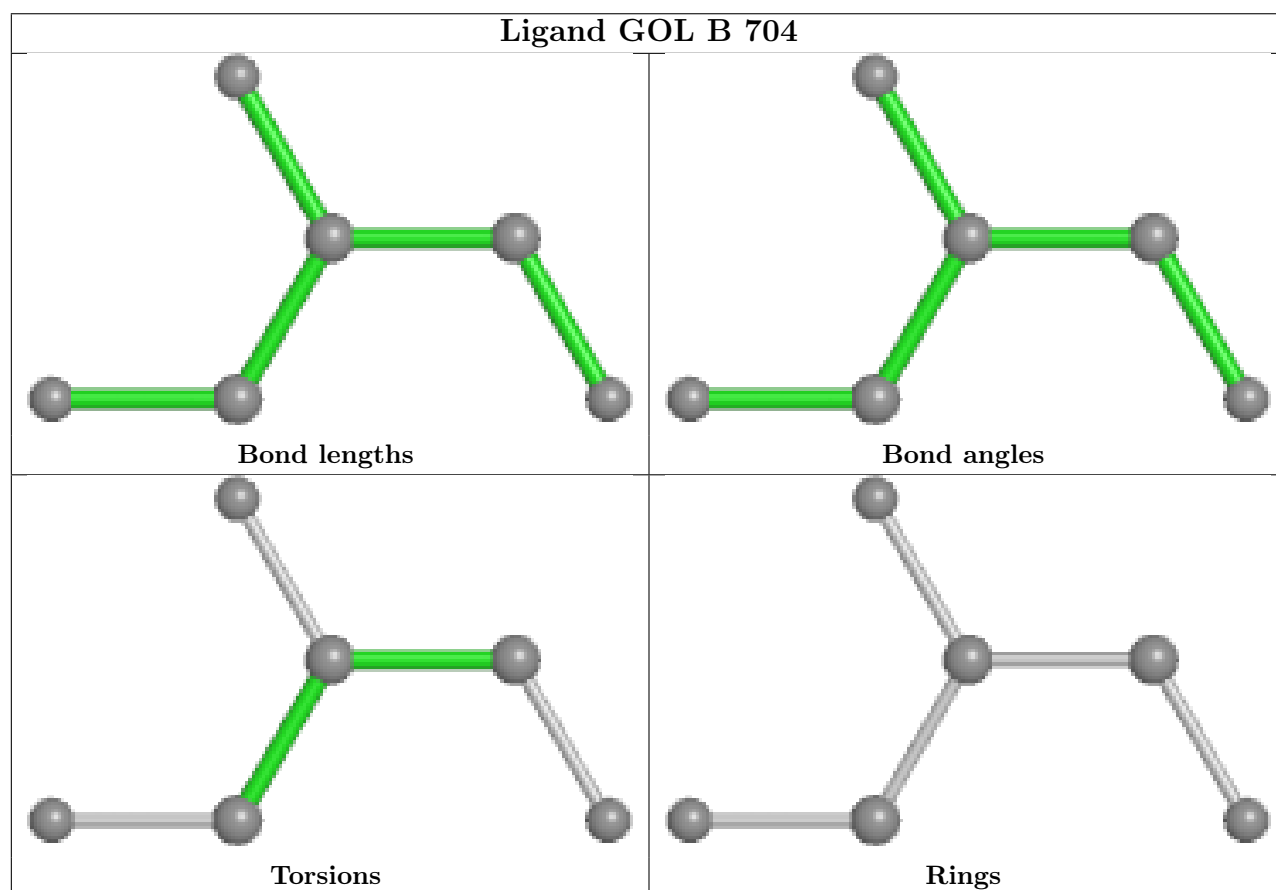
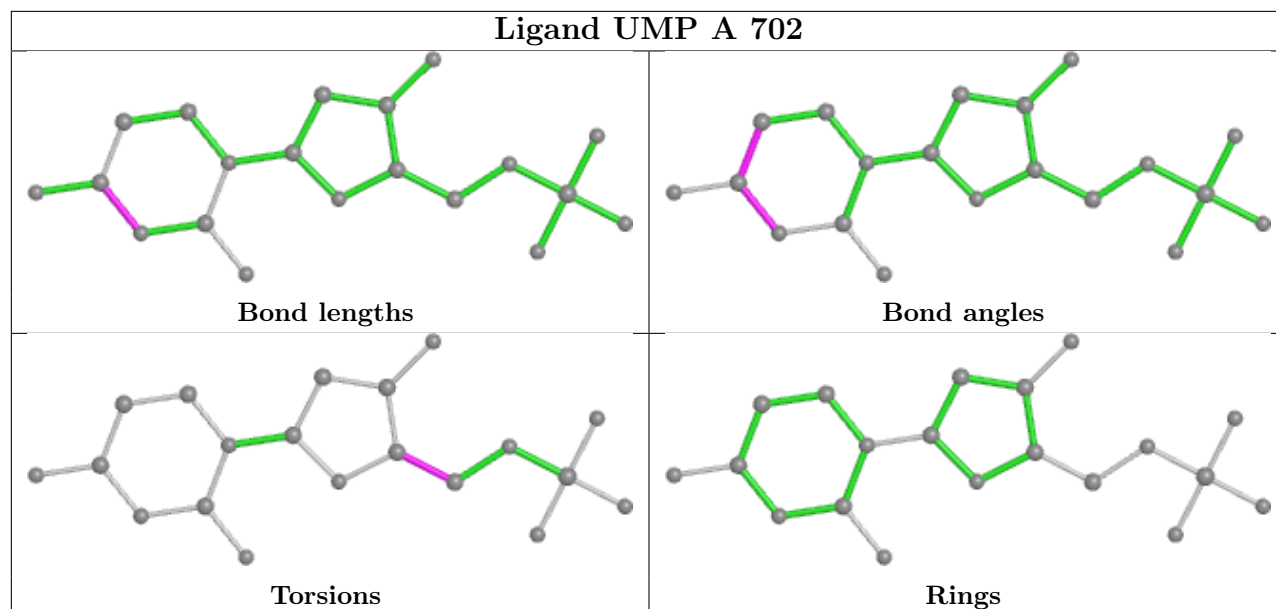
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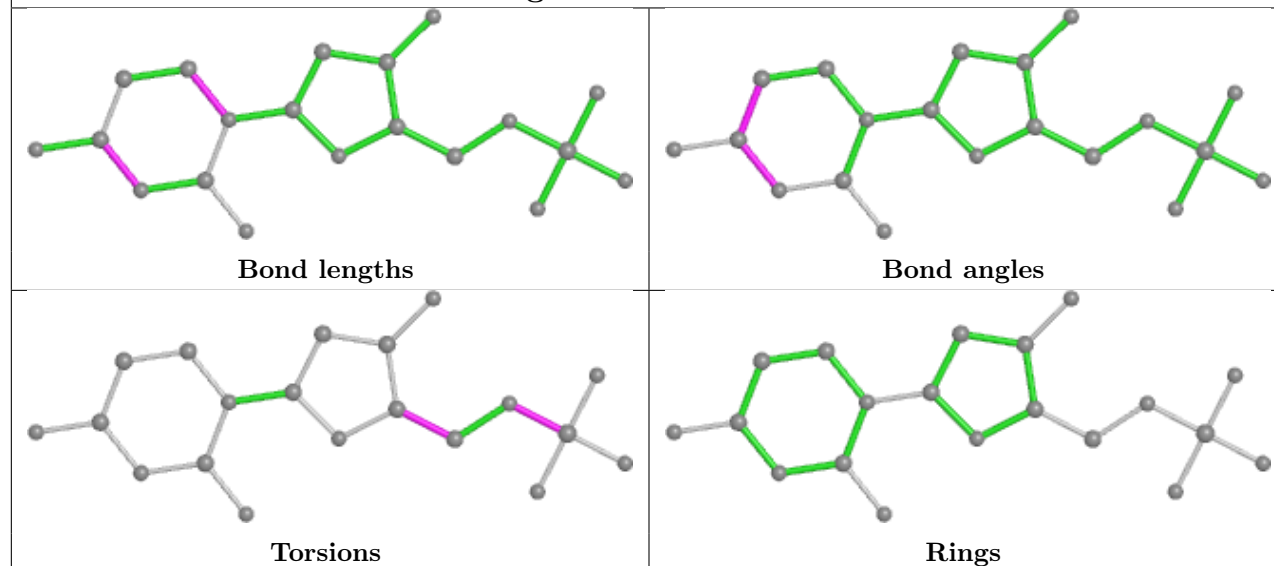
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	NDP	1	0

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.

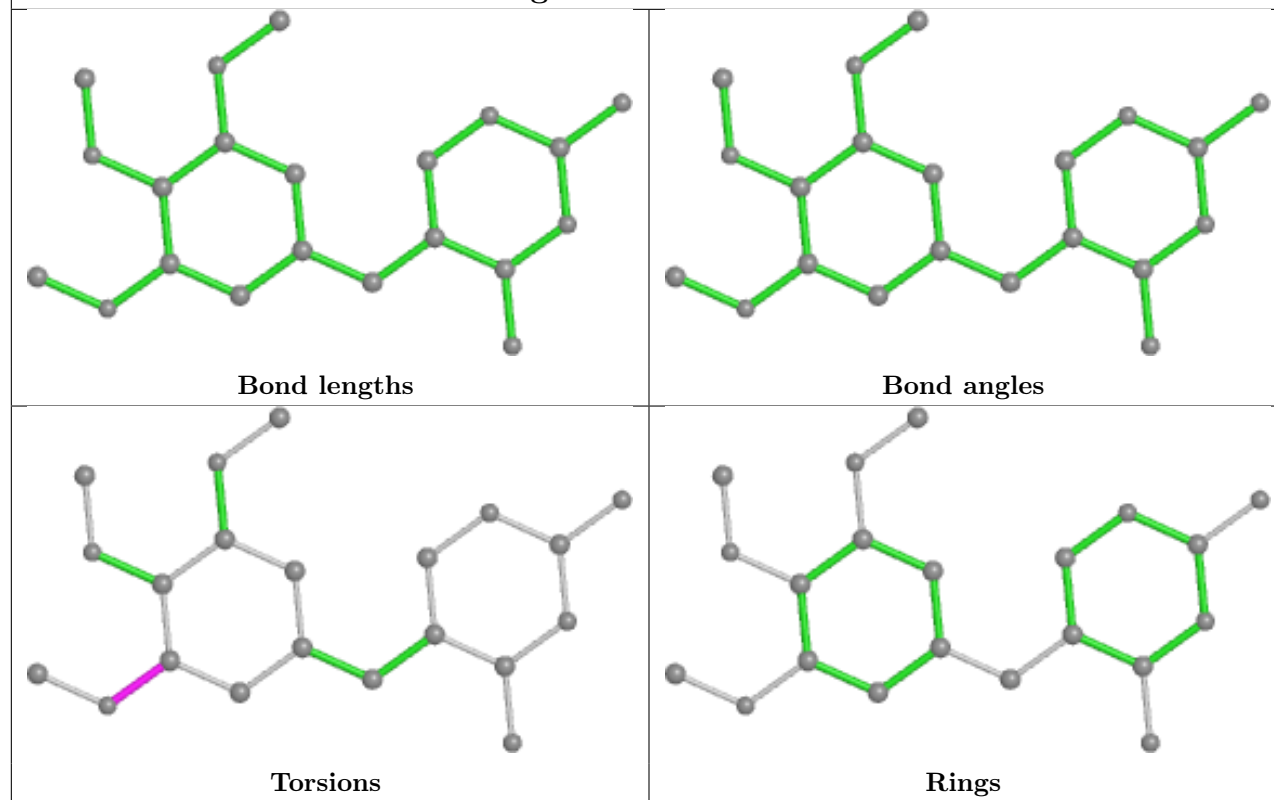


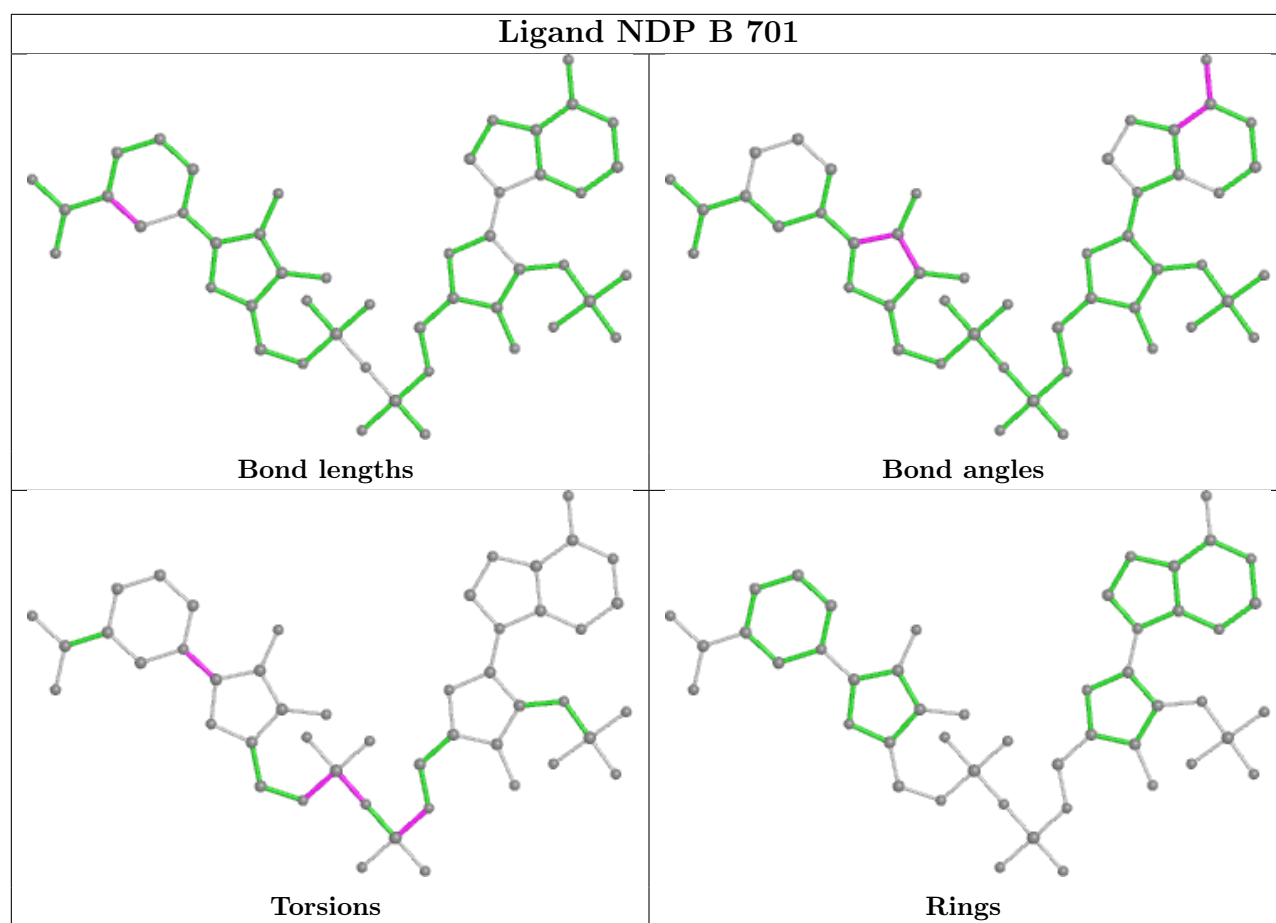


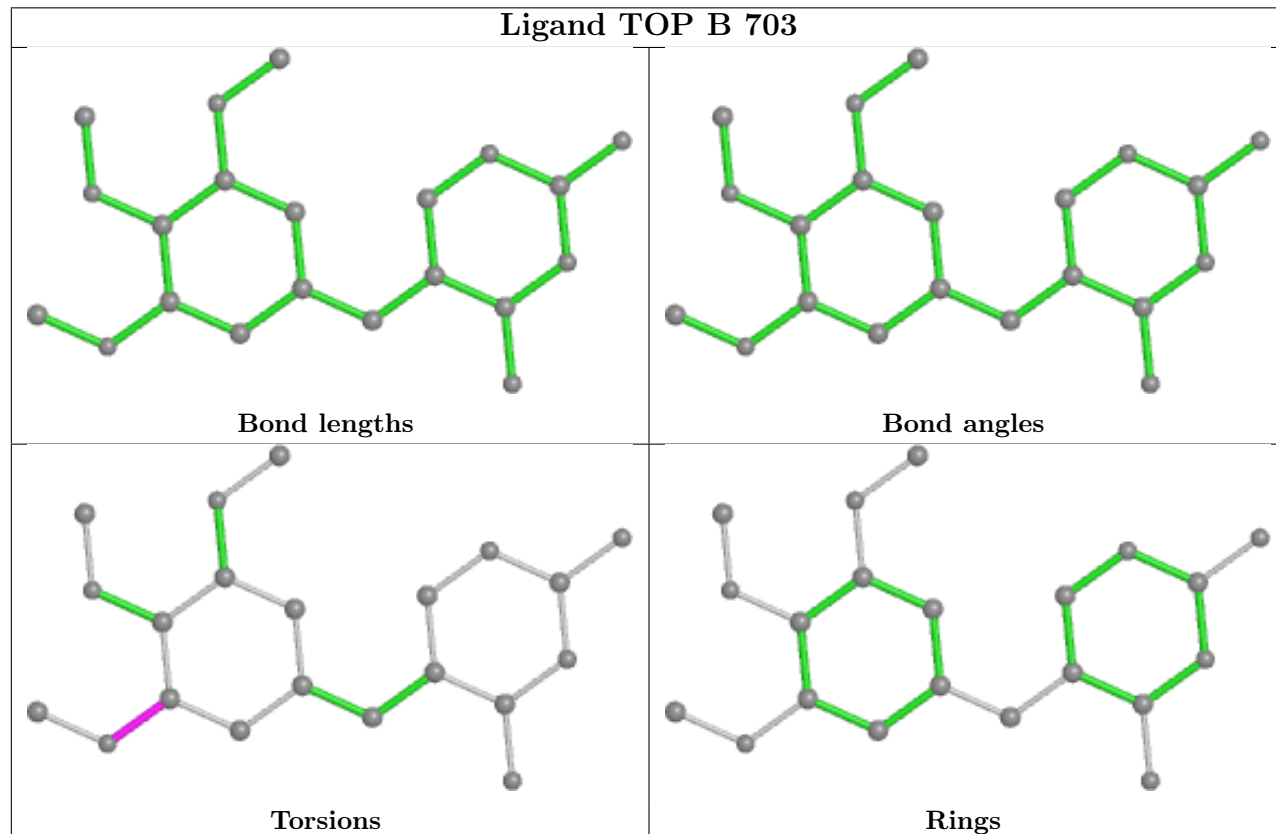
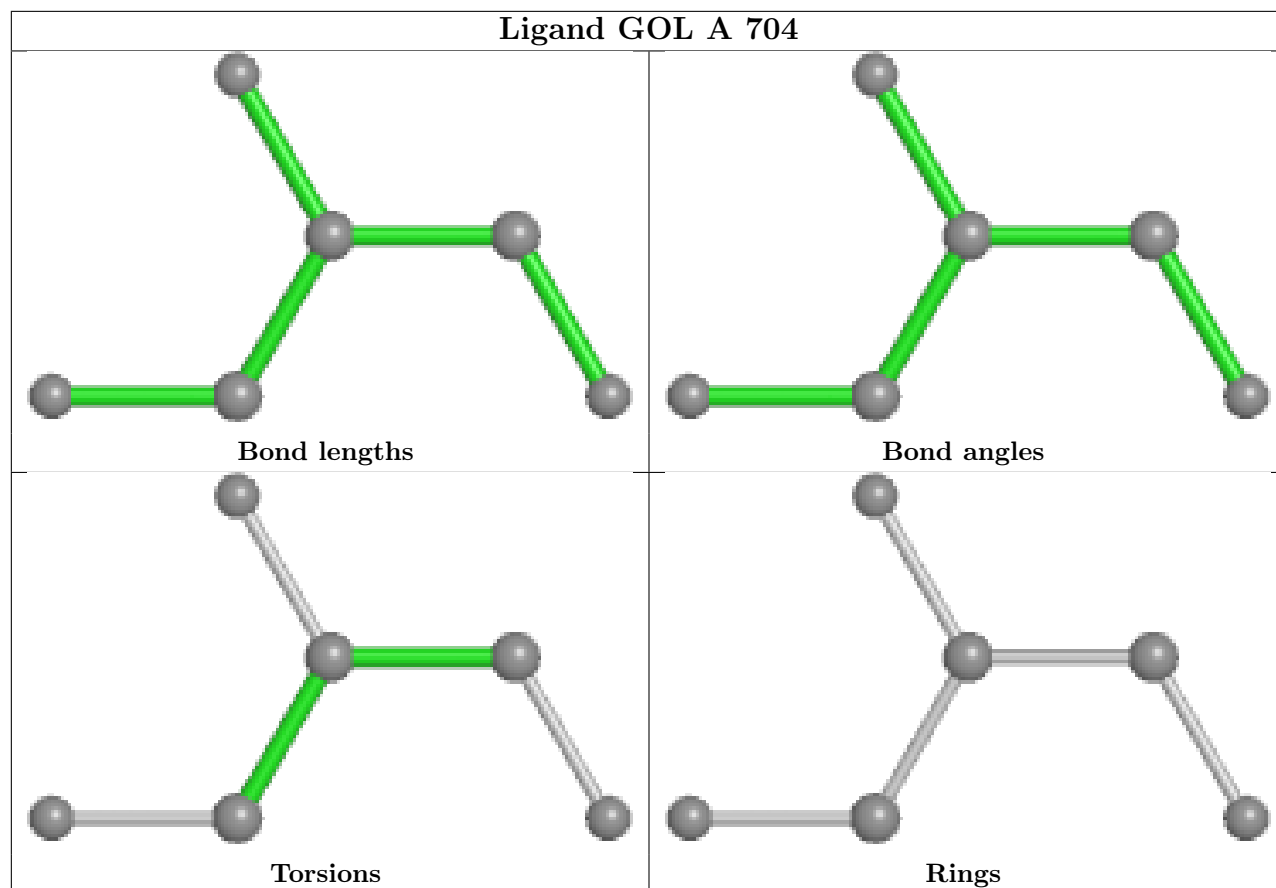
Ligand UMP B 702



Ligand TOP A 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	548/608 (90%)	0.18	36 (6%) 18 13	35, 52, 98, 99	0
1	B	548/608 (90%)	0.23	44 (8%) 12 9	37, 55, 99, 99	0
All	All	1096/1216 (90%)	0.21	80 (7%) 15 11	35, 53, 99, 99	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	THR	10.1
1	A	1	MET	9.9
1	B	26	GLY	8.8
1	B	1	MET	7.1
1	B	231	ASN	7.0
1	A	299	LYS	6.7
1	B	95	SER	6.5
1	A	24	ASN	6.5
1	A	26	GLY	6.3
1	A	284	ASP	6.0
1	A	85	THR	6.0
1	B	2	MET	5.7
1	B	25	GLU	5.6
1	A	2	MET	5.6
1	A	231	ASN	5.5
1	B	3	GLU	5.3
1	B	70	TYR	5.1
1	B	305	ASN	5.0
1	B	300	GLU	4.8
1	B	96	LYS	4.7
1	B	28	LYS	4.6
1	A	306	SER	4.6
1	B	306	SER	4.6
1	B	299	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	25	GLU	4.4
1	B	285	GLU	4.4
1	B	24	ASN	4.3
1	B	75	TYR	4.3
1	B	230	ASN	4.1
1	B	283	ASP	4.0
1	A	22	SER	3.9
1	A	27	LYS	3.8
1	B	76	LYS	3.7
1	A	29	ASN	3.7
1	A	84	GLU	3.7
1	B	309	PRO	3.6
1	A	346	THR	3.6
1	A	28	LYS	3.5
1	A	304	LYS	3.5
1	A	298	GLU	3.5
1	A	230	ASN	3.5
1	A	23	LYS	3.4
1	A	305	ASN	3.3
1	A	96	LYS	3.3
1	B	99	GLN	3.3
1	B	157	ASN	3.2
1	A	345	ARG	3.2
1	A	307	ILE	3.2
1	A	309	PRO	3.1
1	A	286	GLU	3.1
1	A	283	ASP	3.0
1	B	286	GLU	3.0
1	B	154	GLY	2.9
1	B	345	ARG	2.9
1	B	308	HIS	2.8
1	B	298	GLU	2.8
1	A	31	VAL	2.7
1	B	313	GLN	2.7
1	B	346	THR	2.7
1	B	284	ASP	2.7
1	B	151	VAL	2.5
1	A	83	LYS	2.4
1	A	522	ILE	2.4
1	B	307	ILE	2.4
1	B	27	LYS	2.3
1	B	97	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	139	ASP	2.3
1	B	4	GLN	2.2
1	B	229	THR	2.2
1	A	30	GLU	2.2
1	A	310	ASN	2.2
1	B	29	ASN	2.2
1	A	300	GLU	2.2
1	A	308	HIS	2.1
1	B	22	SER	2.1
1	B	203	ASN	2.1
1	B	304	LYS	2.1
1	A	285	GLU	2.1
1	A	523	ALA	2.1
1	B	310	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

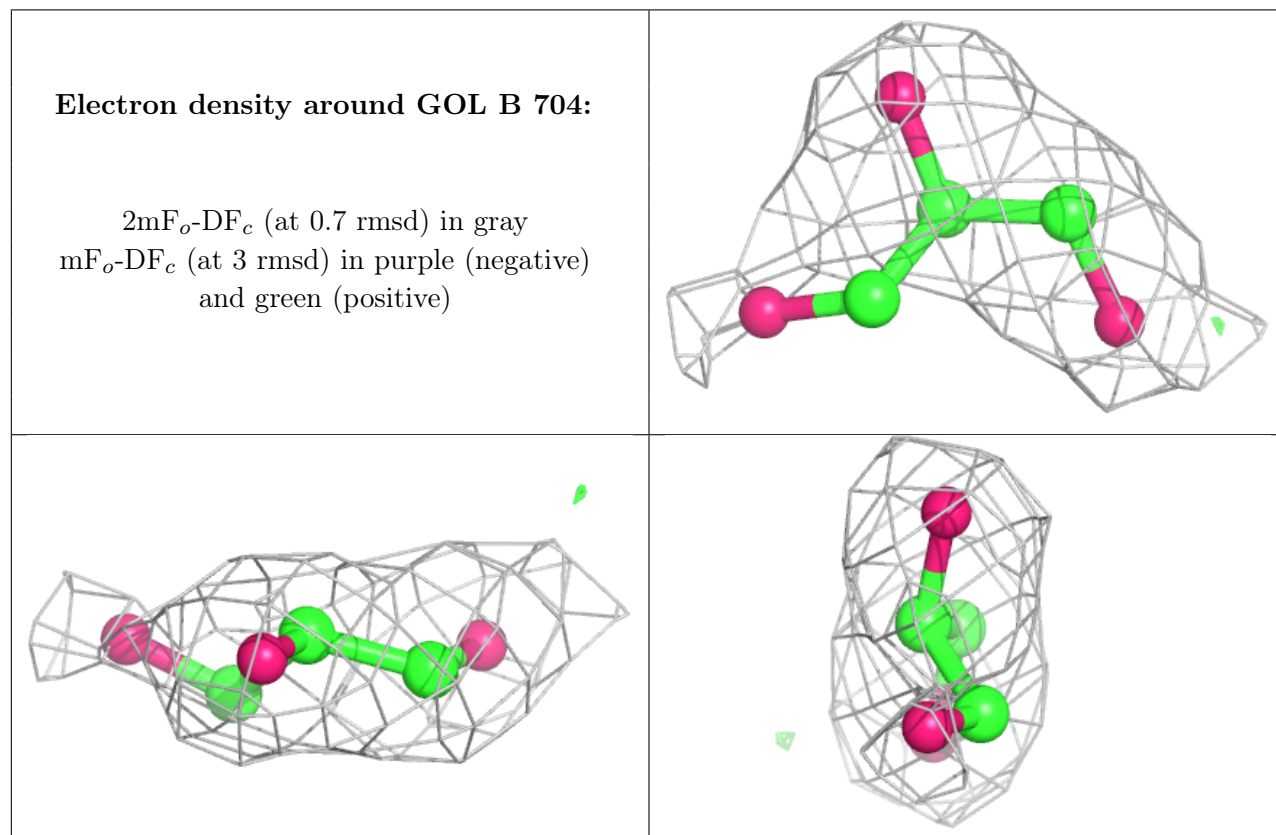
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

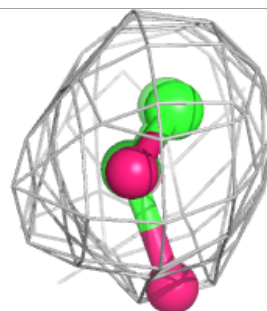
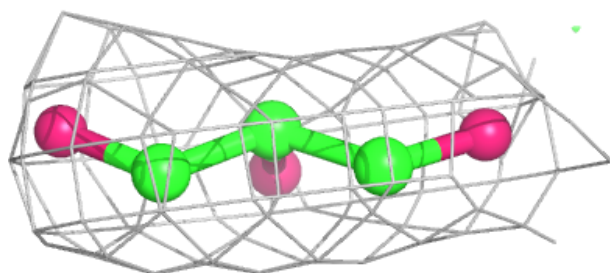
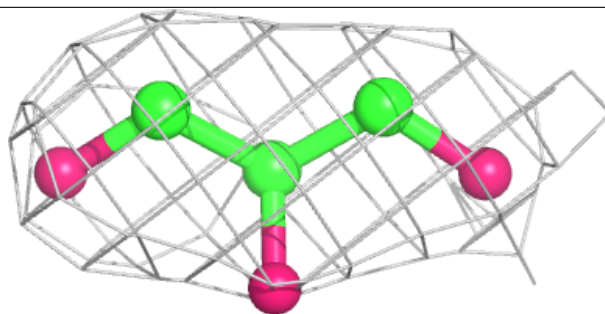
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	B	704	6/6	0.84	0.30	53,60,81,82	0
5	GOL	A	704	6/6	0.88	0.20	51,53,54,64	0
2	NDP	B	701	48/48	0.94	0.21	56,99,99,99	0
3	UMP	B	702	20/20	0.94	0.19	58,78,93,98	0
4	TOP	B	703	21/21	0.95	0.17	56,67,72,74	0
4	TOP	A	703	21/21	0.96	0.15	40,44,52,55	0
3	UMP	A	702	20/20	0.96	0.18	57,78,98,99	0
2	NDP	A	701	48/48	0.97	0.15	42,59,95,99	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.

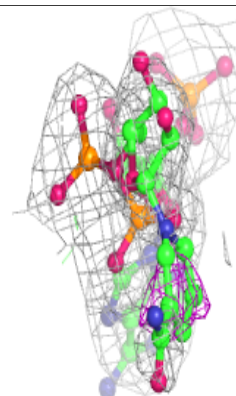
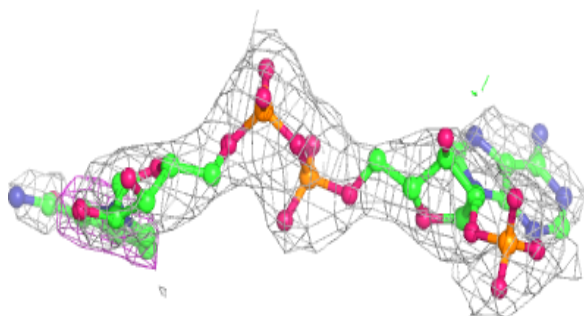
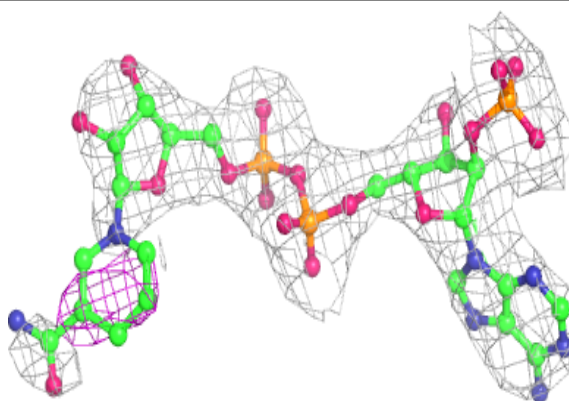


Electron density around GOL A 704:

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

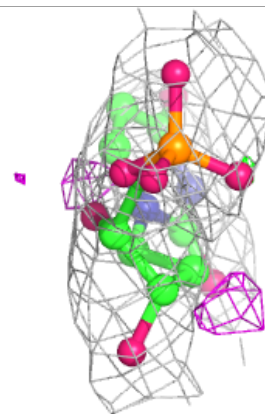
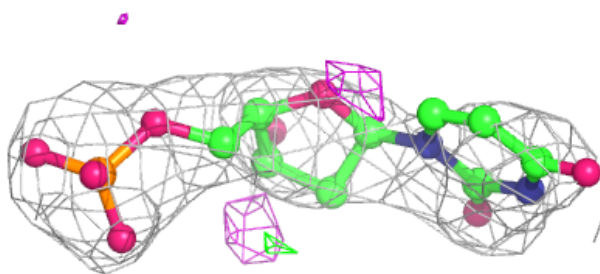
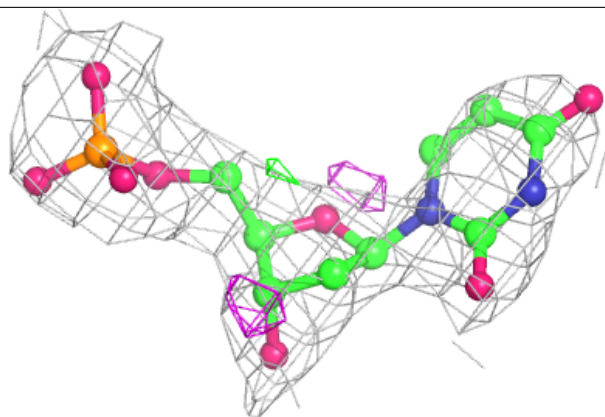
**Electron density around NDP B 701:**

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

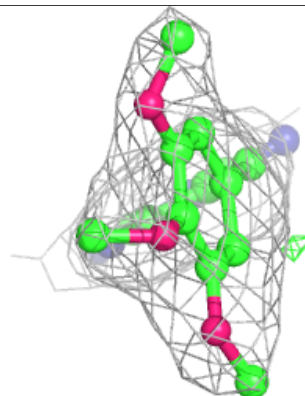
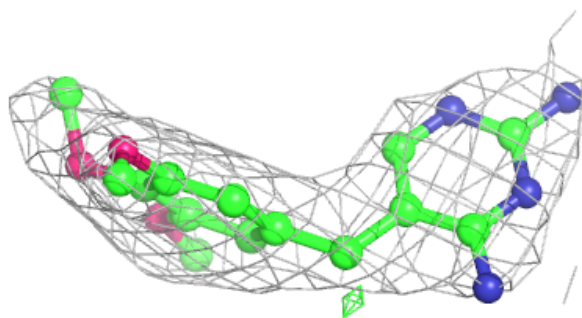
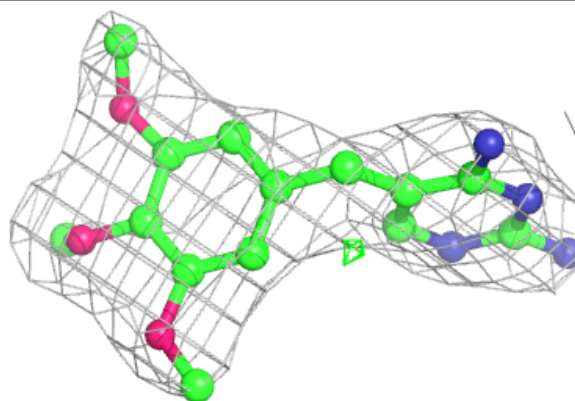


Electron density around UMP B 702:

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

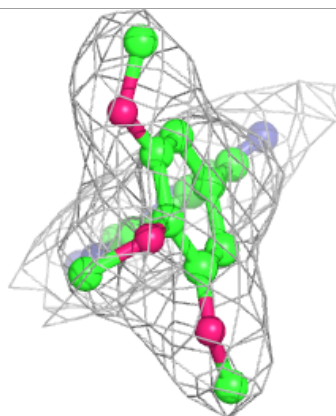
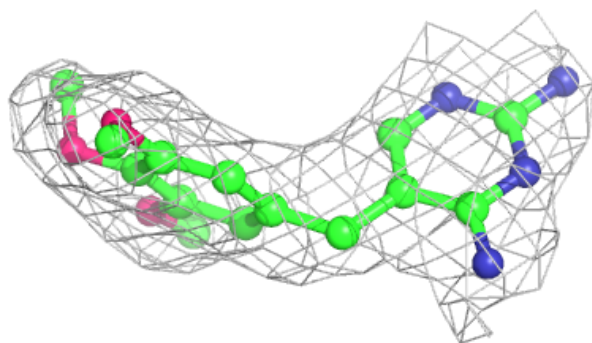
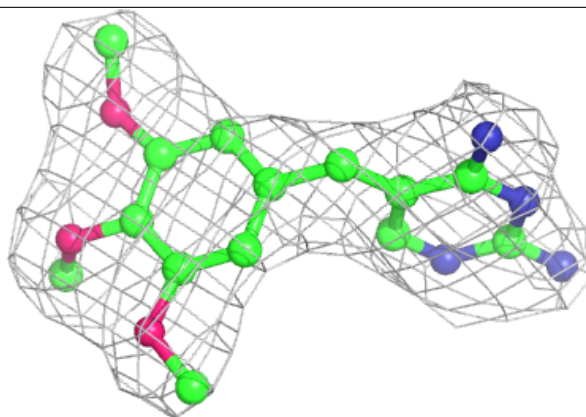
**Electron density around TOP B 703:**

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

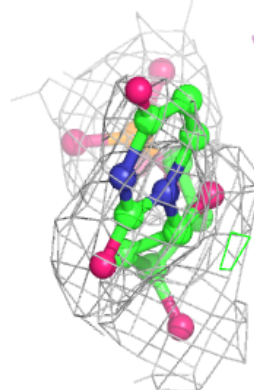
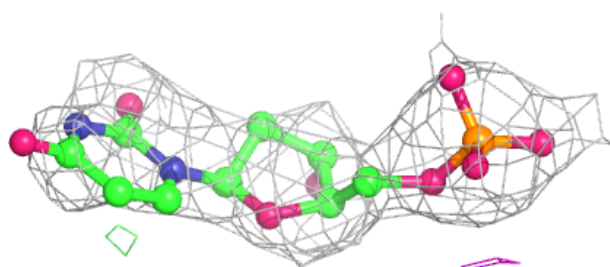
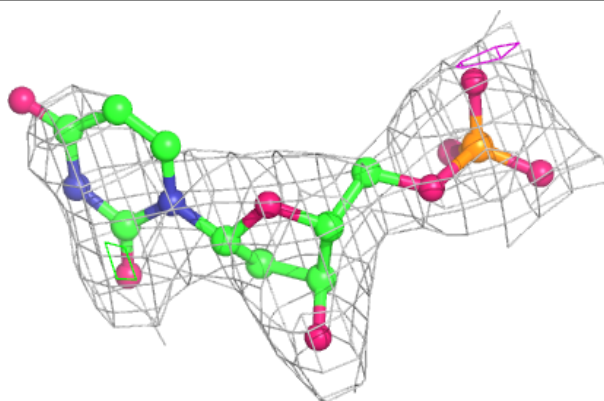


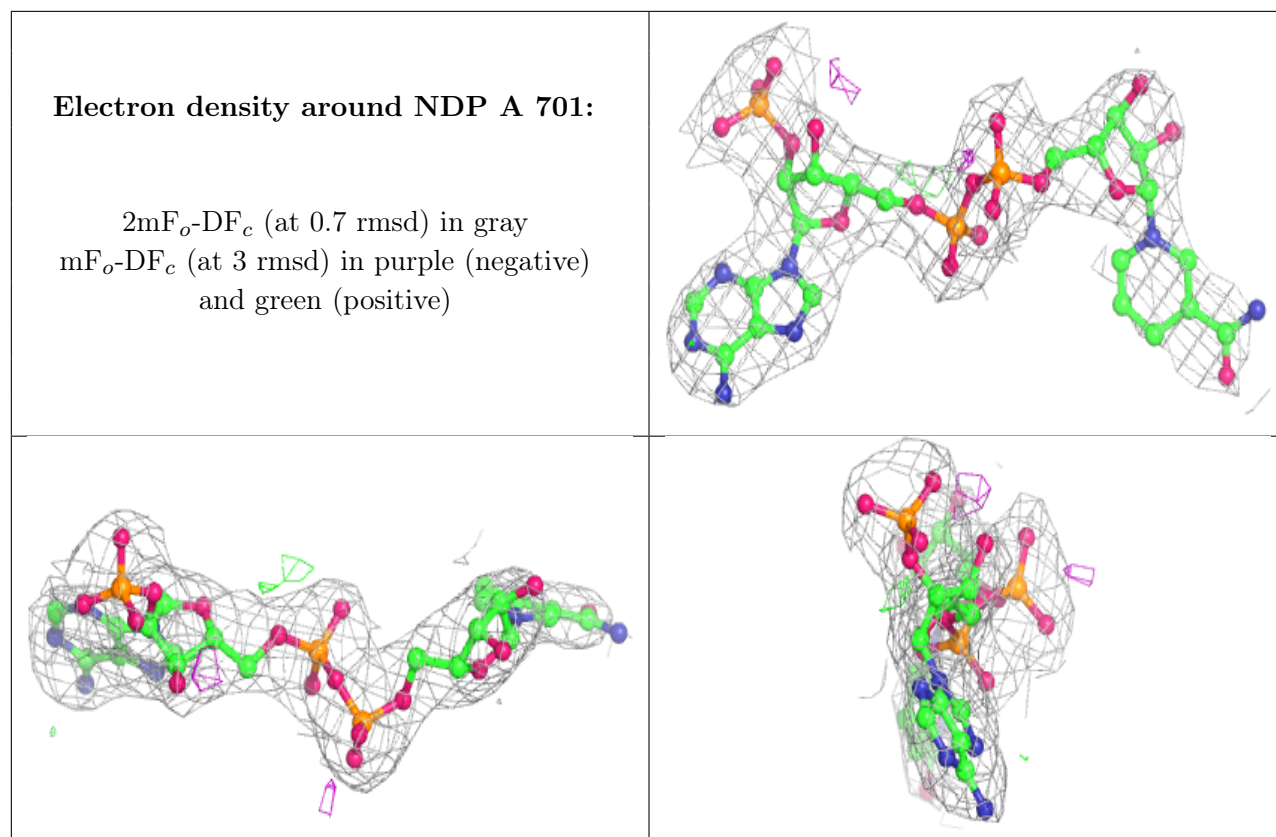
Electron density around TOP A 703:

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

**Electron density around UMP A 702:**

$2mF_o - DF_c$ (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.