



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:46 AM UTC

PDB ID : 4DPD / pdb_00004dpd
Title : WILD TYPE PLASMODIUM FALCIPARUM DIHYDROFOLATE REDUCTASE-THYMIDYLATE SYNTHASE (PfDHFR-TS), DHF COMPLEX, NADP⁺, dUMP
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Deposited on : 2012-02-13
Resolution : 2.50 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

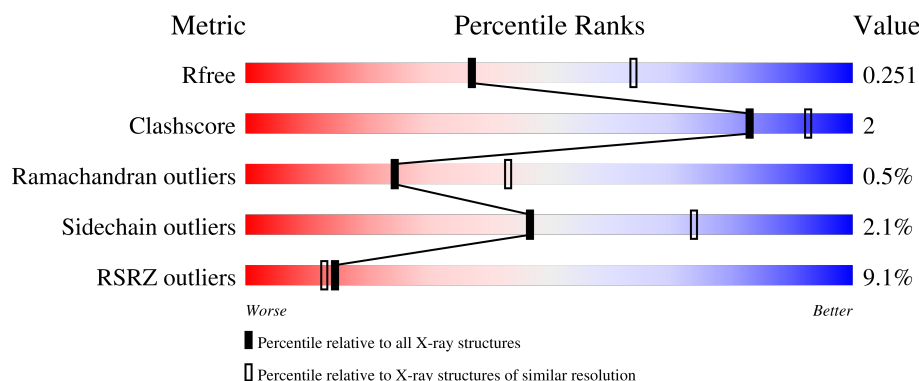
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	
1	B	608	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.49

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DHF	A	701	-	-	-	X

2 Entry composition [i](#)

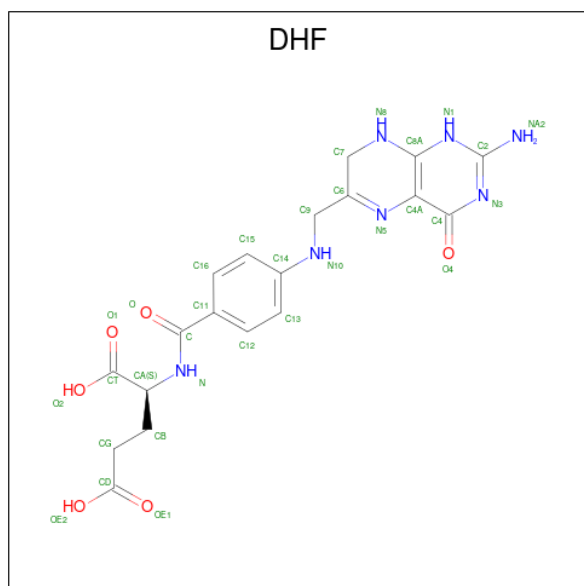
There are 5 unique types of molecules in this entry. The entry contains 9454 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	530	Total	C	N	O	S	0	0	0
			4413	2857	725	804	27			
1	B	543	Total	C	N	O	S	0	0	0
			4514	2914	745	829	26			

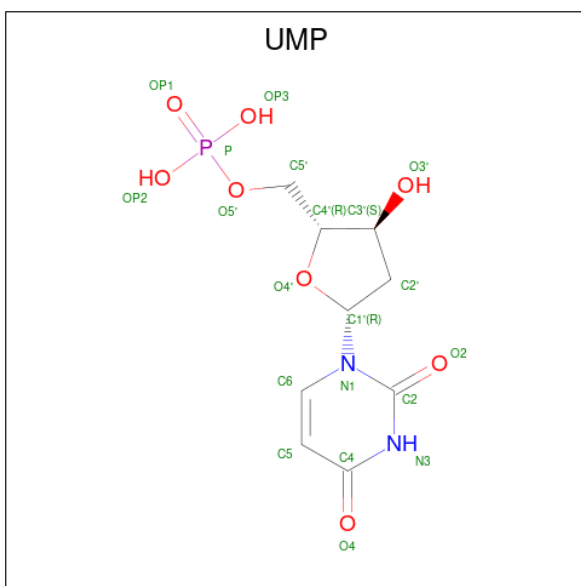
- Molecule 2 is DIHYDROFOLIC ACID (CCD ID: DHF) (formula: $C_{19}H_{21}N_7O_6$).





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

- Molecule 4 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: $C_9H_{13}N_2O_8P$).



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

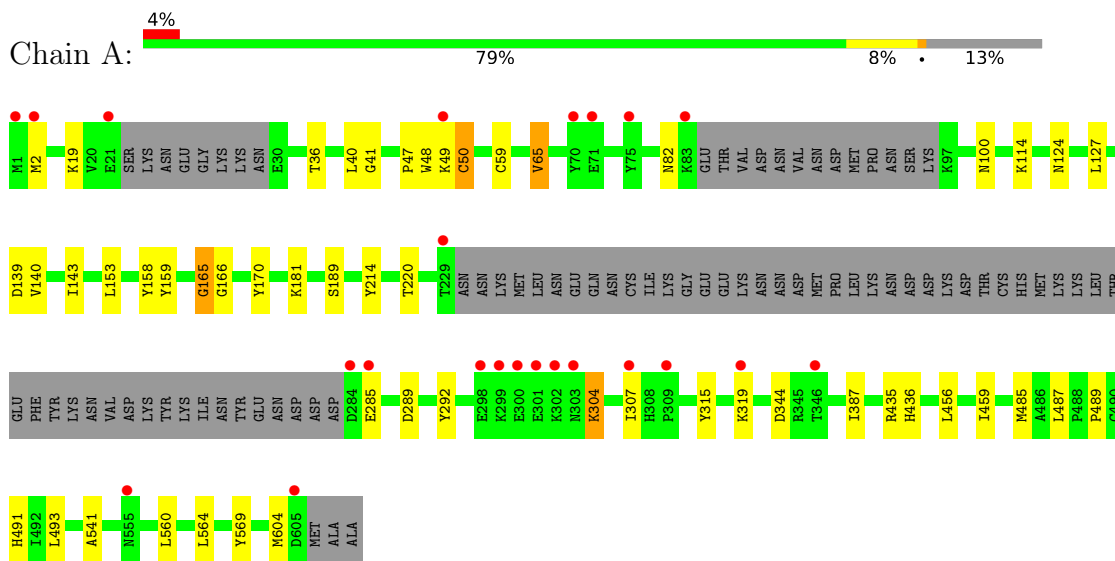
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	222	Total 222	O 222	0	0
5	B	185	Total 185	O 185	0	0

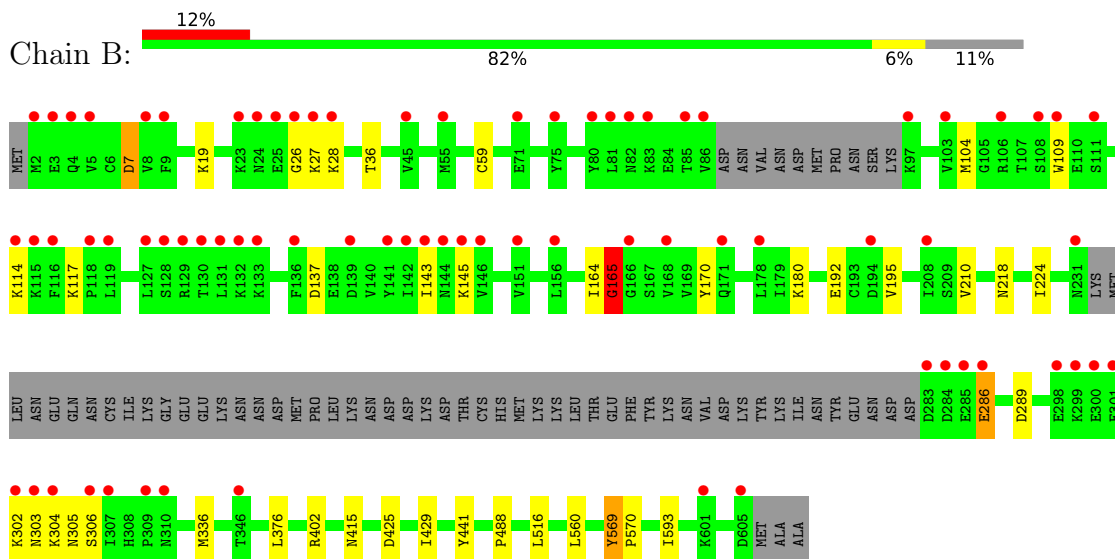
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.06Å 156.78Å 165.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.82 – 2.50 49.82 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.82-2.50) 99.7 (49.82-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.48Å)	Xtriage
Refinement program	CNS, REFMAC 5.6.0117	Depositor
R, R_{free}	0.212 , 0.266 0.205 , 0.251	Depositor DCC
R_{free} test set	2112 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9454	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, DHF, NAP

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	0.73	1/4517 (0.0%)	0.83	3/6099 (0.0%)
1	B	0.71	1/4619 (0.0%)	0.79	4/6237 (0.1%)
All	All	0.72	2/9136 (0.0%)	0.81	7/12336 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	488	PRO	CA-C	6.96	1.56	1.52
1	A	541	ALA	CA-C	5.53	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	286	GLU	N-CA-C	-6.81	105.53	114.31
1	B	165	GLY	N-CA-C	6.38	122.92	112.84
1	A	304	LYS	N-CA-C	6.18	118.99	108.67
1	B	569	TYR	CA-C-N	-5.58	114.03	119.78
1	B	569	TYR	C-N-CA	-5.58	114.03	119.78
1	A	569	TYR	CA-C-N	-5.27	114.33	119.76
1	A	569	TYR	C-N-CA	-5.27	114.33	119.76

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	GLY	Peptide
1	A	304	LYS	Peptide
1	B	165	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4413	0	4370	26	0
1	B	4514	0	4462	18	0
2	A	32	0	19	1	0
3	A	48	0	25	4	0
4	A	20	0	11	1	0
4	B	20	0	11	0	0
5	A	222	0	0	2	0
5	B	185	0	0	3	0
All	All	9454	0	8898	43	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 2.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:CYS:SG	5:A:975:HOH:O	2.30	0.88
1:B:59:CYS:SG	5:B:984:HOH:O	2.34	0.85
1:A:59:CYS:SG	5:A:931:HOH:O	2.16	0.66
1:B:210:VAL:HG12	1:B:224:ILE:HG22	1.80	0.64
1:A:40:LEU:O	3:A:702:NAP:H2N	2.03	0.58
1:A:166:GLY:HA3	3:A:702:NAP:PA	2.44	0.57
1:A:127:LEU:HD23	1:A:143:ILE:HG13	1.88	0.54
1:A:19:LYS:HG2	1:A:36:THR:HG22	1.94	0.50
1:A:181:LYS:NZ	1:B:289:ASP:OD2	2.46	0.47
1:B:303:ASN:O	1:B:305:ASN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:LEU:HG	1:A:604:MET:HE1	1.97	0.47
1:B:19:LYS:HG2	1:B:36:THR:HG22	1.96	0.46
1:B:336:MET:HE1	1:B:560:LEU:HB2	1.98	0.46
1:B:104:MET:HE2	1:B:164:ILE:HD11	1.98	0.46
1:A:315:TYR:HB2	1:A:564:LEU:O	2.16	0.45
1:A:319:LYS:HD3	1:B:286:GLU:HG3	1.98	0.45
1:A:456:LEU:O	1:A:459:ILE:HG13	2.17	0.45
1:B:192:GLU:O	5:B:850:HOH:O	2.21	0.44
1:B:109:TRP:CE2	1:B:117:LYS:HD2	2.53	0.44
1:B:415:ASN:ND2	5:B:829:HOH:O	2.51	0.43
1:B:114:LYS:HA	1:B:117:LYS:HB3	2.00	0.43
1:A:214:TYR:O	1:A:220:THR:HA	2.19	0.42
1:A:100:ASN:OD1	1:A:159:TYR:HB3	2.20	0.42
1:A:153:LEU:HD22	1:A:158:TYR:CZ	2.55	0.42
2:A:701:DHF:H72	3:A:702:NAP:C5N	2.50	0.42
1:B:165:GLY:HA3	1:B:170:TYR:CZ	2.55	0.42
1:A:166:GLY:HA3	3:A:702:NAP:O1A	2.20	0.42
1:A:41:GLY:HA2	1:A:47:PRO:HD3	2.02	0.41
1:B:569:TYR:HB3	1:B:570:PRO:HD2	2.01	0.41
1:A:491:HIS:CE1	4:A:703:UMP:O4	2.73	0.41
1:A:165:GLY:HA3	1:A:170:TYR:CZ	2.55	0.41
1:A:435:ARG:HB2	1:A:436:HIS:CD2	2.56	0.41
1:B:425:ASP:OD1	1:B:441:TYR:OH	2.39	0.41
1:A:65:VAL:HG22	1:A:159:TYR:CB	2.51	0.41
1:A:124:ASN:HB2	1:A:140:VAL:HG12	2.02	0.41
1:A:387:ILE:O	1:A:435:ARG:NH1	2.50	0.41
1:B:165:GLY:CA	1:B:170:TYR:CZ	3.04	0.41
1:B:376:LEU:HD12	1:B:593:ILE:HG13	2.03	0.40
1:A:48:TRP:O	1:A:49:LYS:HB2	2.22	0.40
1:A:485:MET:SD	1:A:489:PRO:HD3	2.62	0.40
1:A:493:LEU:HD12	1:A:493:LEU:C	2.46	0.40
1:B:7:ASP:HA	1:B:180:LYS:HE2	2.03	0.40
1:A:289:ASP:HA	1:A:292:TYR:CD2	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	522/608 (86%)	495 (95%)	25 (5%)	2 (0%)	30	49
1	B	537/608 (88%)	506 (94%)	28 (5%)	3 (1%)	21	38
All	All	1059/1216 (87%)	1001 (94%)	53 (5%)	5 (0%)	24	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	304	LYS
1	A	139	ASP
1	B	26	GLY
1	A	82	ASN
1	B	429	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	496/570 (87%)	487 (98%)	9 (2%)	51	77
1	B	508/570 (89%)	496 (98%)	12 (2%)	43	70
All	All	1004/1140 (88%)	983 (98%)	21 (2%)	47	74

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET

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Mol	Chain	Res	Type
1	A	50	CYS
1	A	65	VAL
1	A	114	LYS
1	A	189	SER
1	A	285	GLU
1	A	307	ILE
1	A	344	ASP
1	A	487	LEU
1	B	7	ASP
1	B	27	LYS
1	B	28	LYS
1	B	137	ASP
1	B	143	ILE
1	B	145	LYS
1	B	195	VAL
1	B	218	ASN
1	B	302	LYS
1	B	306	SER
1	B	402	ARG
1	B	516	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	157	ASN
1	A	308	HIS
1	A	340	ASN
1	A	394	ASN
1	A	424	ASN
1	A	450	ASN
1	B	42	ASN
1	B	206	GLN
1	B	316	ASN
1	B	400	ASN
1	B	563	GLN
1	B	582	ASN

5.3.3 RNA ⓘ

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	UMP	A	703	-	21,21,21	1.34	4 (19%)	30,31,31	1.96	9 (30%)
4	UMP	B	701	-	21,21,21	1.35	2 (9%)	30,31,31	1.96	9 (30%)
3	NAP	A	702	-	50,52,52	1.25	4 (8%)	71,80,80	1.55	11 (15%)
2	DHF	A	701	-	32,34,34	1.13	2 (6%)	38,47,47	1.06	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UMP	A	703	-	-	3/10/22/22	0/2/2/2
4	UMP	B	701	-	-	4/10/22/22	0/2/2/2
3	NAP	A	702	-	-	3/35/67/67	0/5/5/5
2	DHF	A	701	-	-	2/20/31/31	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NAP	C5A-C4A	5.14	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	UMP	C2-N1	3.40	1.43	1.38
2	A	701	DHF	C4A-C8A	3.18	1.48	1.43
4	B	701	UMP	C2-N1	3.06	1.43	1.38
3	A	702	NAP	C5A-N7A	-2.88	1.33	1.39
3	A	702	NAP	C5A-C6A	2.76	1.48	1.41
4	A	703	UMP	C2-N3	-2.35	1.33	1.38
3	A	702	NAP	C8A-N7A	2.27	1.36	1.31
4	A	703	UMP	C5-C4	-2.16	1.39	1.43
4	B	701	UMP	C4-N3	-2.15	1.34	1.38
2	A	701	DHF	C7-C6	2.09	1.52	1.49
4	A	703	UMP	C4-N3	-2.09	1.35	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NAP	C5A-C4A-N3A	-5.42	119.25	126.72
4	A	703	UMP	C5-C4-N3	4.37	120.92	114.80
3	A	702	NAP	N3A-C4A-N9A	4.21	134.33	127.17
4	A	703	UMP	O4-C4-C5	-3.82	118.57	125.16
4	B	701	UMP	C4-N3-C2	-3.73	121.98	126.61
4	A	703	UMP	C4-N3-C2	-3.58	122.17	126.61
4	B	701	UMP	N3-C2-N1	3.58	119.55	114.89
4	B	701	UMP	O4-C4-C5	-3.54	119.06	125.16
4	B	701	UMP	C1'-N1-C2	3.51	124.52	117.66
3	A	702	NAP	C3N-C7N-N7N	3.48	122.02	117.74
4	B	701	UMP	C5-C4-N3	3.43	119.60	114.80
3	A	702	NAP	C2A-N3A-C4A	3.34	119.98	111.83
3	A	702	NAP	C4A-C5A-N7A	-3.30	106.80	110.58
4	A	703	UMP	C1'-N1-C2	3.26	124.03	117.66
4	A	703	UMP	N3-C2-N1	2.95	118.74	114.89
3	A	702	NAP	N3A-C2A-N1A	-2.78	124.38	128.58
3	A	702	NAP	C2B-C1B-N9A	-2.69	109.32	113.75
4	B	701	UMP	C2'-C1'-N1	2.63	120.39	113.81
4	A	703	UMP	O2-C2-N3	-2.63	116.64	121.49
3	A	702	NAP	O2A-PA-O1A	2.55	124.31	112.44
4	B	701	UMP	O2-C2-N3	-2.54	116.81	121.49
4	A	703	UMP	C2'-C1'-N1	2.47	119.98	113.81
4	B	701	UMP	C1'-N1-C6	-2.42	116.77	121.53
3	A	702	NAP	O7N-C7N-N7N	-2.38	119.18	122.62
4	A	703	UMP	C1'-N1-C6	-2.28	117.06	121.53
4	A	703	UMP	OP3-P-OP2	2.27	116.31	107.80
4	B	701	UMP	O4'-C4'-C3'	-2.24	100.54	105.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NAP	C5A-N7A-C8A	2.18	106.88	103.45
2	A	701	DHF	C4A-C8A-N8	2.11	120.22	115.89
2	A	701	DHF	C4A-N5-C6	2.10	120.40	116.24
3	A	702	NAP	C2A-N1A-C6A	2.09	122.17	118.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

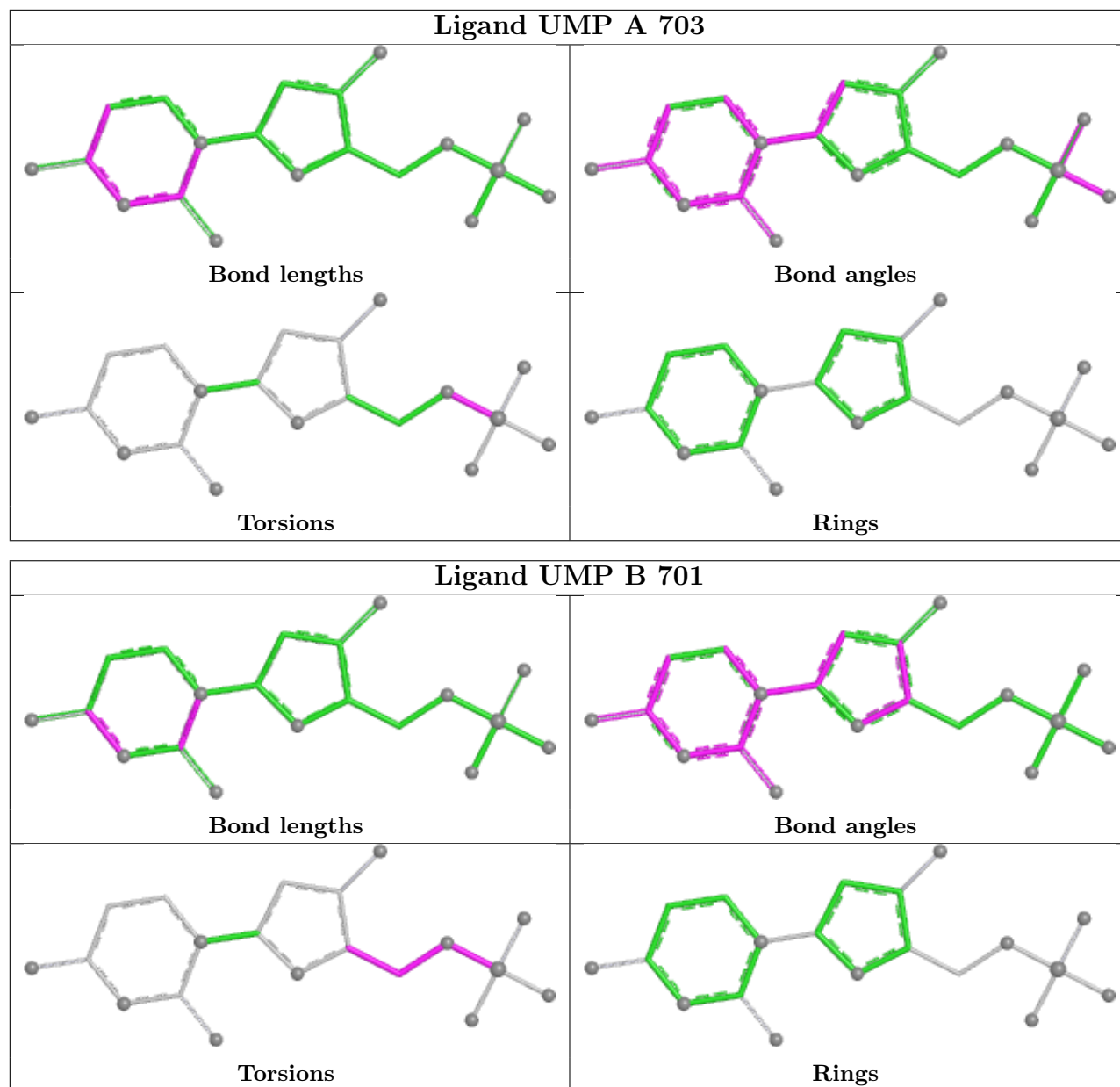
Mol	Chain	Res	Type	Atoms
2	A	701	DHF	CT-CA-CB-CG
3	A	702	NAP	O4D-C1D-N1N-C6N
4	A	703	UMP	C5'-O5'-P-OP2
4	A	703	UMP	C5'-O5'-P-OP3
2	A	701	DHF	N-CA-CB-CG
4	B	701	UMP	C3'-C4'-C5'-O5'
4	B	701	UMP	O4'-C4'-C5'-O5'
4	A	703	UMP	C5'-O5'-P-OP1
4	B	701	UMP	C5'-O5'-P-OP1
3	A	702	NAP	C2B-O2B-P2B-O2X
4	B	701	UMP	C4'-C5'-O5'-P
3	A	702	NAP	O4D-C1D-N1N-C2N

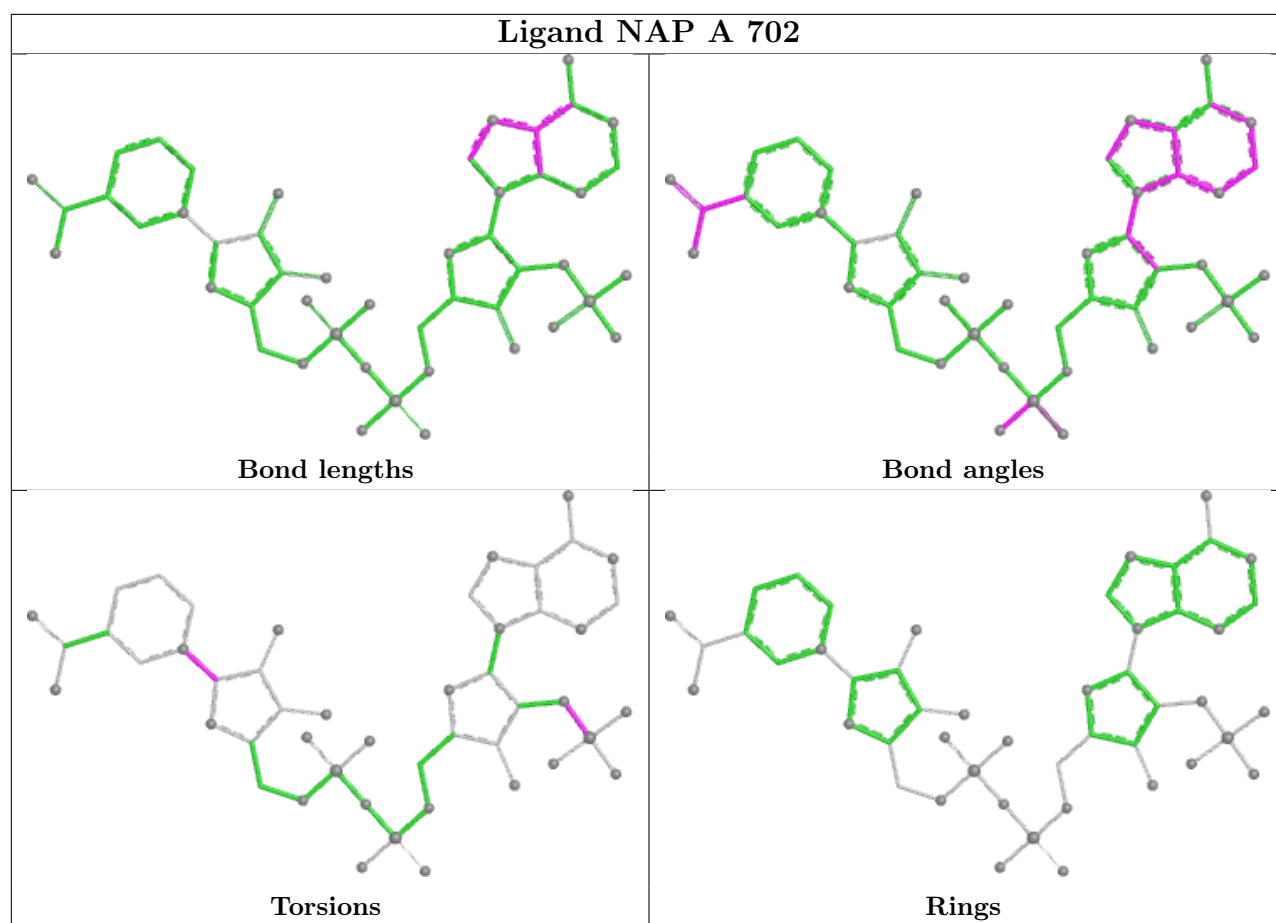
There are no ring outliers.

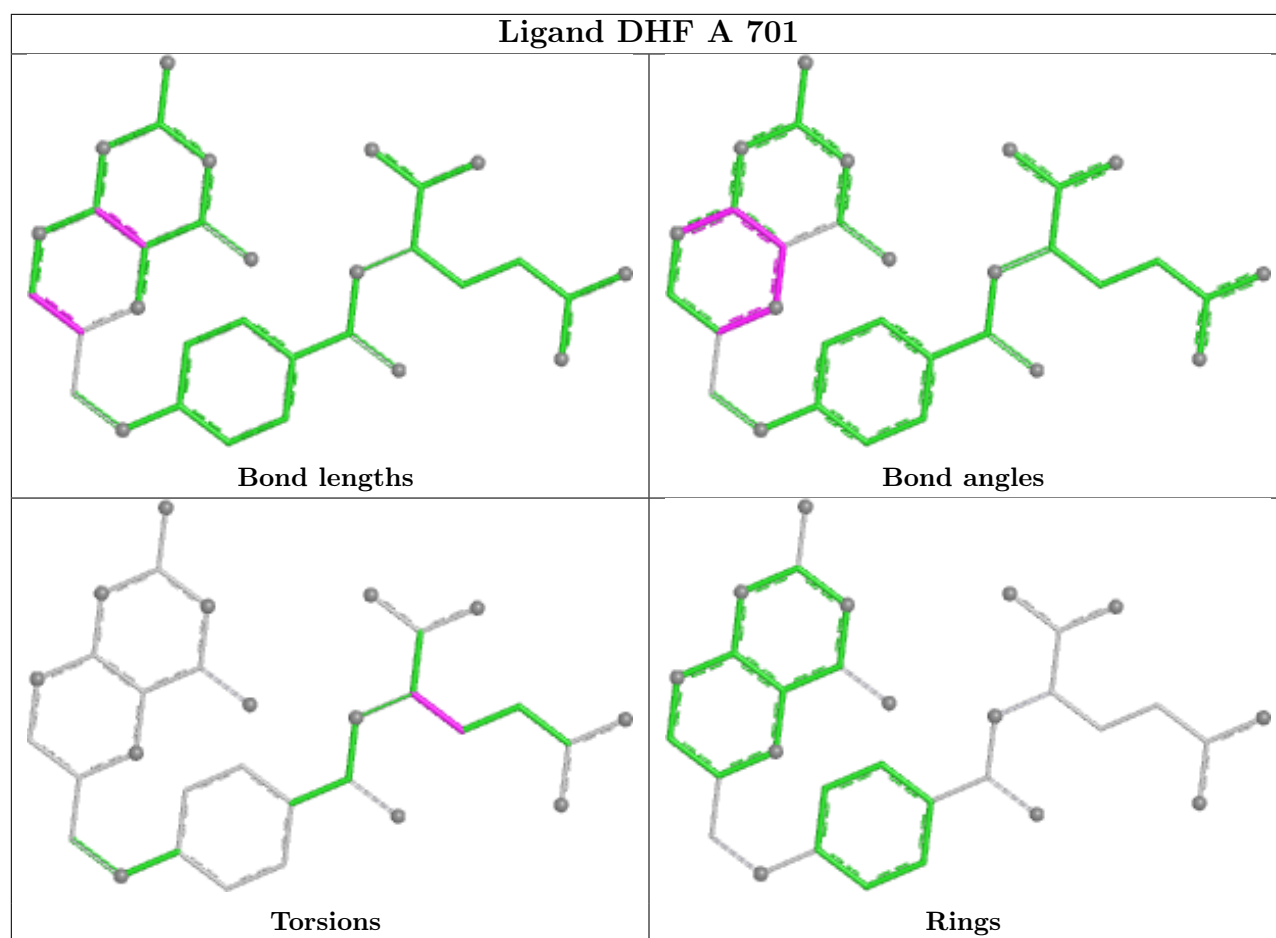
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	UMP	1	0
3	A	702	NAP	4	0
2	A	701	DHF	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.







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	530/608 (87%)	0.03	23 (4%) 40 35	20, 31, 72, 90	0
1	B	543/608 (89%)	0.54	75 (13%) 6 5	20, 38, 90, 90	0
All	All	1073/1216 (88%)	0.29	98 (9%) 15 13	20, 34, 89, 90	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	THR	7.7
1	B	75	TYR	5.1
1	B	86	VAL	4.9
1	B	26	GLY	4.7
1	B	285	GLU	4.4
1	A	307	ILE	4.3
1	B	605	ASP	4.3
1	B	136	PHE	4.3
1	B	302	LYS	4.1
1	A	605	ASP	3.9
1	A	83	LYS	3.9
1	B	2	MET	3.9
1	B	309	PRO	3.9
1	B	303	ASN	3.9
1	B	27	LYS	3.6
1	B	118	PRO	3.6
1	A	2	MET	3.6
1	B	24	ASN	3.6
1	B	82	ASN	3.6
1	B	307	ILE	3.6
1	A	309	PRO	3.5
1	A	302	LYS	3.5
1	A	299	LYS	3.5
1	A	303	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	168	VAL	3.4
1	A	301	GLU	3.4
1	B	116	PHE	3.3
1	B	284	ASP	3.3
1	B	310	ASN	3.3
1	B	129	ARG	3.2
1	B	304	LYS	3.2
1	A	75	TYR	3.2
1	B	55	MET	3.2
1	B	5	VAL	3.2
1	B	109	TRP	3.1
1	B	231	ASN	3.0
1	B	166	GLY	2.9
1	B	142	ILE	2.9
1	B	28	LYS	2.9
1	B	286	GLU	2.9
1	B	299	LYS	2.9
1	A	285	GLU	2.9
1	B	127	LEU	2.9
1	A	284	ASP	2.9
1	B	25	GLU	2.9
1	B	346	THR	2.8
1	A	300	GLU	2.8
1	B	143	ILE	2.8
1	B	115	LYS	2.8
1	B	119	LEU	2.8
1	B	146	VAL	2.7
1	A	49	LYS	2.7
1	A	346	THR	2.7
1	B	132	LYS	2.7
1	B	133	LYS	2.7
1	B	144	ASN	2.7
1	A	1	MET	2.6
1	B	151	VAL	2.6
1	B	156	LEU	2.6
1	A	21	GLU	2.6
1	A	319	LYS	2.6
1	B	23	LYS	2.6
1	A	298	GLU	2.5
1	B	9	PHE	2.5
1	B	8	VAL	2.5
1	B	106	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	108	SER	2.5
1	B	128	SER	2.5
1	B	81	LEU	2.4
1	B	103	VAL	2.4
1	B	131	LEU	2.4
1	B	4	GLN	2.4
1	A	229	THR	2.4
1	B	83	LYS	2.4
1	B	601	LYS	2.3
1	B	71	GLU	2.3
1	B	301	GLU	2.3
1	B	283	ASP	2.3
1	B	97	LYS	2.2
1	B	141	TYR	2.2
1	B	208	ILE	2.2
1	A	70	TYR	2.1
1	A	71	GLU	2.1
1	B	45	VAL	2.1
1	B	178	LEU	2.1
1	B	3	GLU	2.1
1	B	80	TYR	2.1
1	B	298	GLU	2.1
1	B	300	GLU	2.1
1	B	111	SER	2.1
1	B	194	ASP	2.1
1	B	130	THR	2.1
1	B	171	GLN	2.0
1	A	555	ASN	2.0
1	B	114	LYS	2.0
1	B	145	LYS	2.0
1	B	139	ASP	2.0
1	B	306	SER	2.0

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

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

6.3 Carbohydrates [i](#)

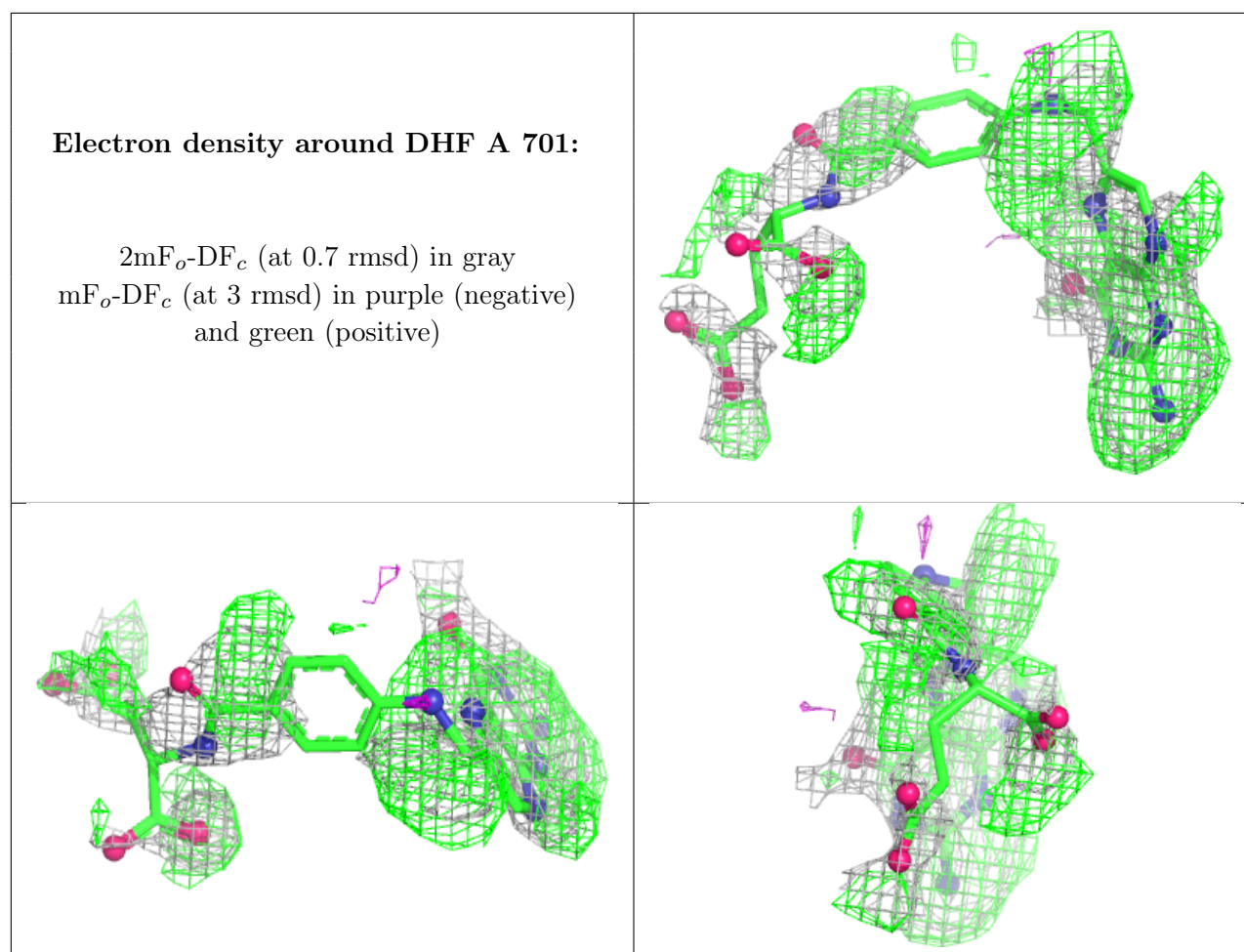
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

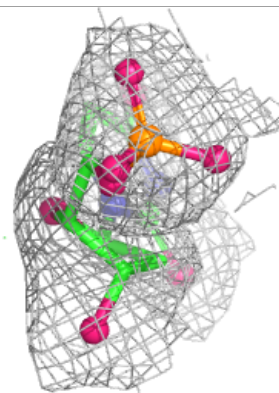
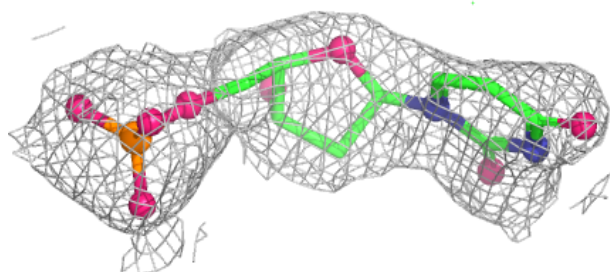
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DHF	A	701	32/32	0.67	0.50	25,34,36,37	32
4	UMP	A	703	20/20	0.95	0.08	29,36,41,42	0
4	UMP	B	701	20/20	0.95	0.09	28,39,50,51	0
3	NAP	A	702	48/48	0.97	0.06	24,33,41,45	0

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.

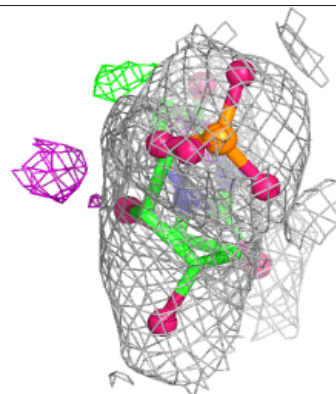
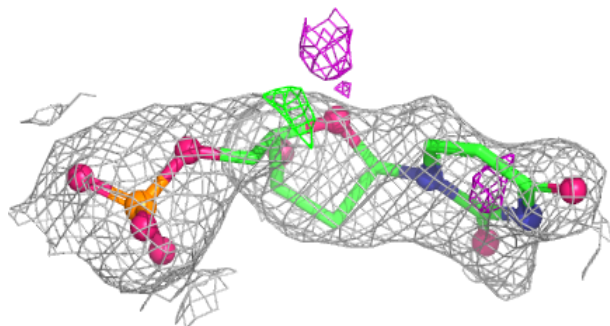
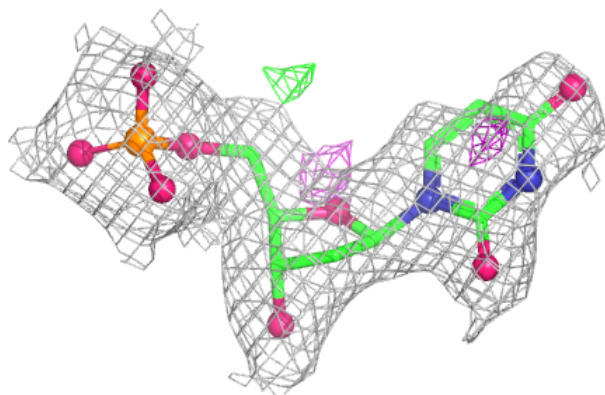


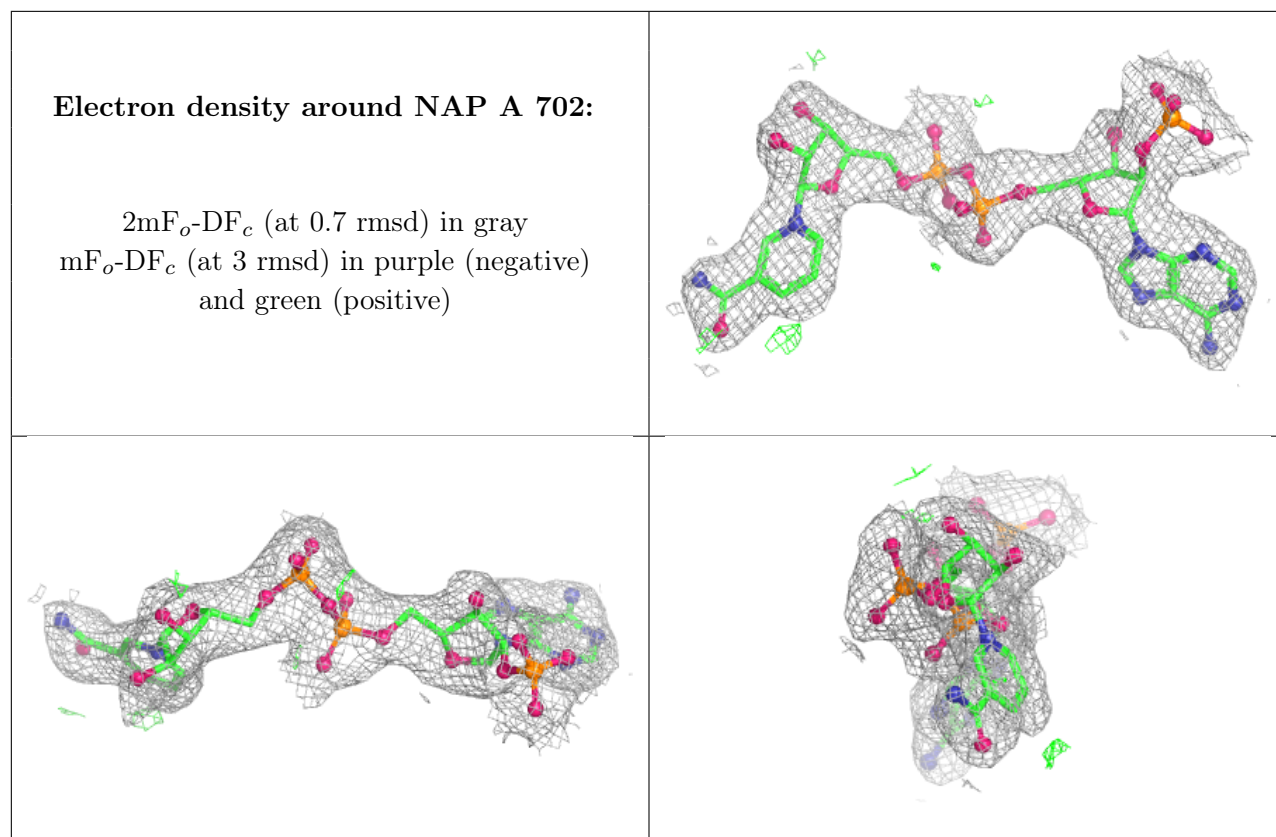
Electron density around UMP A 703:

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

**Electron density around UMP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.