Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 04:28 AM JST

PDB ID	:	6KP7
Title	:	Quadruple mutant (N51I+C59R+S108N+I164L) plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with B12154
Authors	:	Vanichtanankul, J.; Vitsupakorn, D.
Deposited on	:	2019-08-14
Resolution	:	1.97 Å(reported)

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

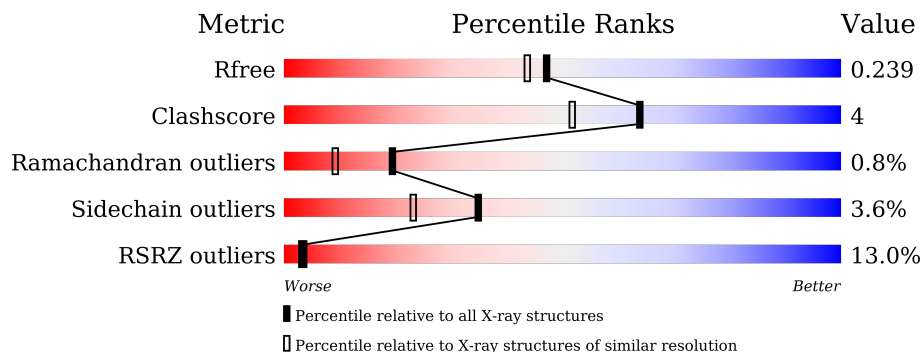|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.97 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	Percentile Ranks	Value
Rfree		0.239
Clashscore		4
Ramachandran outliers		0.8%
Sidechain outliers		3.6%
RSRZ outliers		13.0%

Worse ... *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 <=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	6% / 78% / 6% · 14%
1	B	608	17% / 74% / 12% · 12%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9391 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.
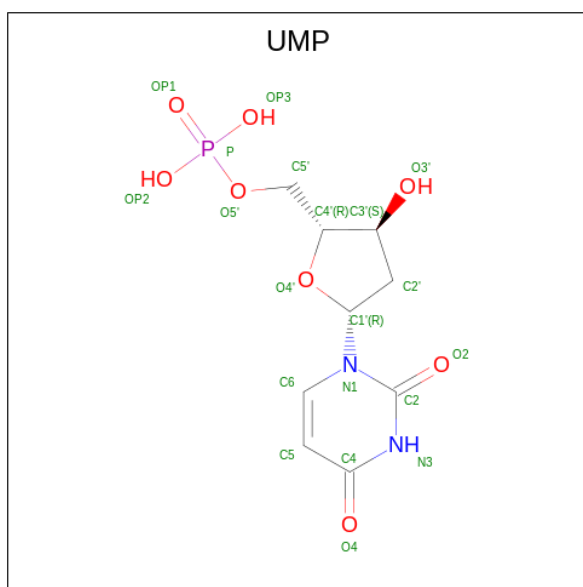
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4331	2811	715	781	24			
1	B	533	Total	C	N	O	S	0	0	0
			4436	2869	735	808	24			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).
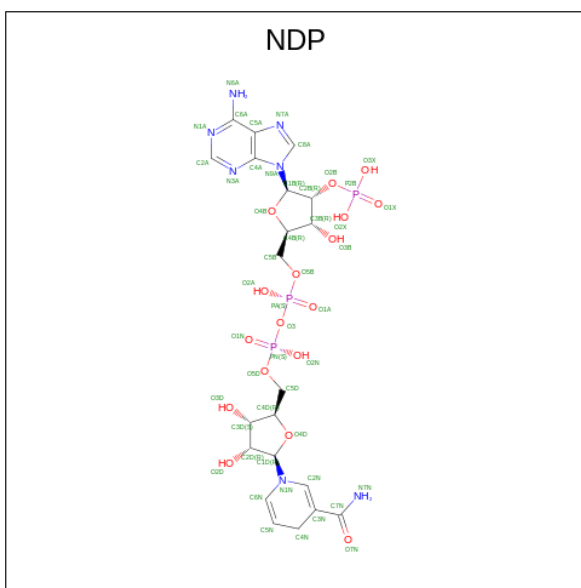
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).

UMP

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 2-[3-[3-[2,6-bis(azanyl)-5-(3-chlorophenyl)pyrimidin-4-yl]propoxy]phenox y]ethanoic acid (three-letter code: DQ9) (formula: $C_{21}H_{21}ClN_4O_4$) (labeled as "Ligand of Interest" by depositor).

DQ9
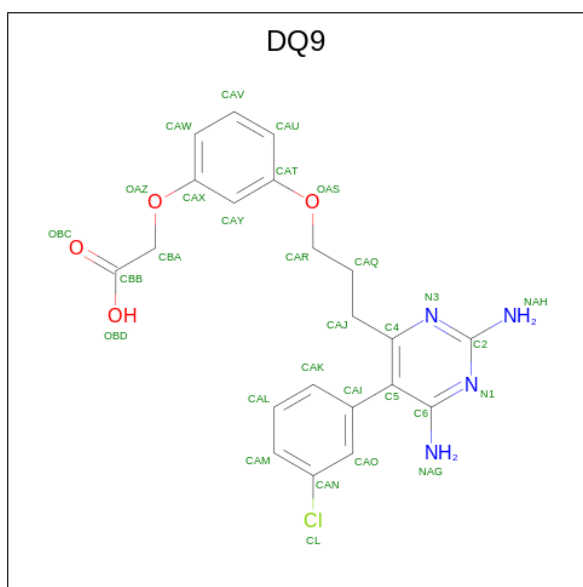
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	21	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	B	1	30	21	1	4	4	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	234	234	234	0	0
6	B	188	Total 188	O 188	0	0

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
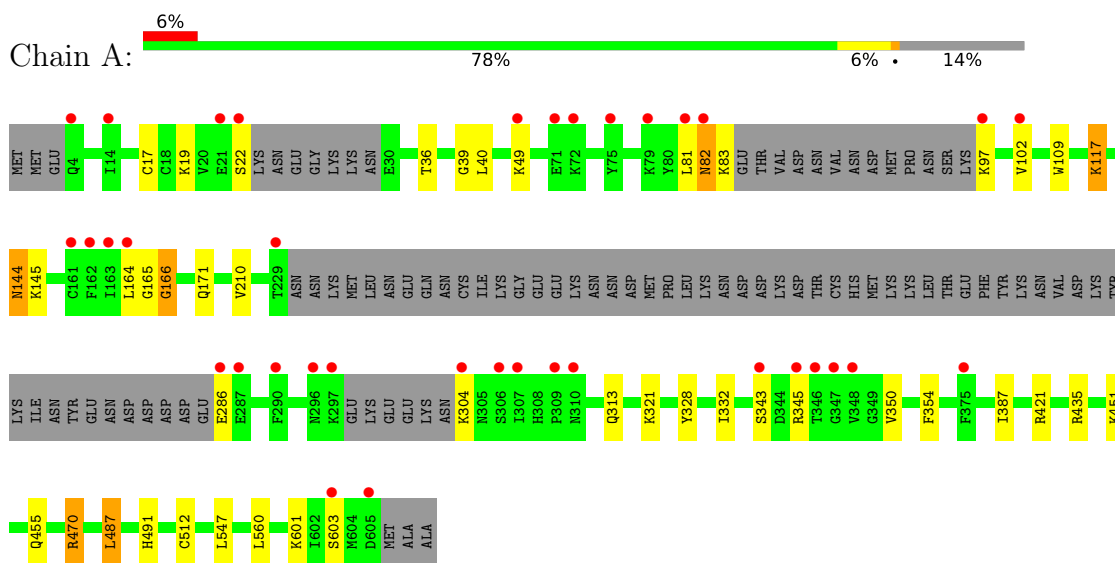
Chain A:

• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain B:
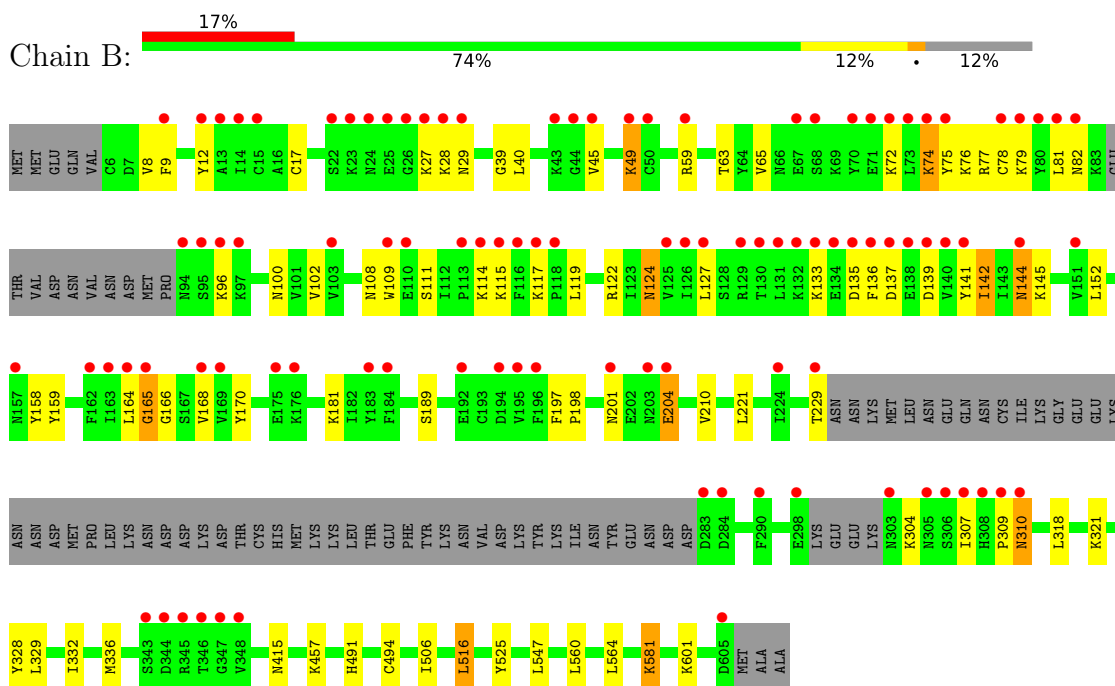
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.88Å 156.29Å 165.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.11 – 1.97 26.10 – 1.97	Depositor EDS
% Data completeness (in resolution range)	95.4 (26.11-1.97) 95.5 (26.10-1.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.194 , 0.233 0.202 , 0.239	Depositor DCC
R_{free} test set	5111 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.4	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9391	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: DQ9, UMP, GOL, NDP

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	0.76	0/4434	0.90	4/5989 (0.1%)
1	B	0.75	0/4540	0.87	0/6129
All	All	0.76	0/8974	0.89	4/12118 (0.0%)

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	4
1	B	0	1
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	470	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	117	LYS	CB-CA-C	-5.56	99.29	110.40
1	A	421	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	455	GLN	CB-CA-C	-5.02	100.35	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
1	A	350	VAL	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	4331	0	4301	29	0
1	B	4436	0	4395	47	0
2	A	48	0	26	4	0
2	B	48	0	26	4	0
3	A	20	0	11	1	0
3	B	20	0	11	1	0
4	A	30	0	0	0	0
4	B	30	0	0	1	0
5	B	6	0	8	0	0
6	A	234	0	0	8	0
6	B	188	0	0	3	0
All	All	9391	0	8778	75	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 4.

All (75) 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:415:ASN:HB2	6:B:969:HOH:O	1.65	0.96
1:A:166:GLY:HA3	2:A:701:NDP:O1A	1.68	0.93
1:A:166:GLY:HA3	2:A:701:NDP:PA	2.21	0.81
1:B:210:VAL:HB	6:B:910:HOH:O	1.90	0.72
1:B:328:TYR:CZ	1:B:332:ILE:HD11	2.26	0.70
1:A:328:TYR:CZ	1:A:332:ILE:HD11	2.31	0.66
1:B:59:ARG:O	1:B:63:THR:HG23	1.96	0.66
1:A:451:LYS:HE3	6:A:809:HOH:O	1.96	0.64
1:A:210:VAL:HB	6:A:984:HOH:O	2.00	0.62
1:B:165:GLY:HA3	1:B:170:TYR:CZ	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:O	1:B:124:ASN:ND2	2.34	0.60
1:A:109:TRP:CZ2	1:A:117:LYS:HD2	2.37	0.58
1:B:581:LYS:O	1:B:581:LYS:HD3	2.06	0.55
1:B:124:ASN:N	1:B:124:ASN:HD22	2.05	0.54
1:B:102:VAL:HB	1:B:164:LEU:HD11	1.90	0.53
1:B:136:PHE:CD2	1:B:142:ILE:HD11	2.44	0.53
1:A:109:TRP:CE2	1:A:117:LYS:HD2	2.45	0.52
1:A:491:HIS:CE1	3:A:702:UMP:O4	2.62	0.52
1:A:81:LEU:HB3	1:A:83:LYS:HE2	1.92	0.51
1:A:387:ILE:O	1:A:435:ARG:NH1	2.43	0.51
1:B:197:PHE:CD1	1:B:198:PRO:HD2	2.46	0.51
1:B:77:ARG:O	1:B:81:LEU:HB2	2.12	0.50
1:B:144:ASN:O	2:B:701:NDP:H2A	2.12	0.49
1:B:197:PHE:CG	1:B:198:PRO:HD2	2.48	0.49
1:B:109:TRP:CE2	1:B:117:LYS:HD2	2.48	0.49
1:B:65:VAL:HG22	1:B:159:TYR:CB	2.43	0.49
1:B:166:GLY:HA3	2:B:701:NDP:PA	2.52	0.48
1:B:336:MET:HE1	1:B:560:LEU:HB2	1.95	0.48
1:B:141:TYR:CD1	1:B:152:LEU:HD11	2.49	0.48
1:A:102:VAL:HB	1:A:164:LEU:HD11	1.96	0.48
1:A:40:LEU:O	2:A:701:NDP:H2N	2.13	0.48
1:B:201:ASN:HB3	1:B:204:GLU:HB2	1.96	0.47
1:A:487:LEU:N	1:A:487:LEU:CD2	2.78	0.47
1:B:108:ASN:O	1:B:111:SER:OG	2.33	0.46
1:A:166:GLY:CA	2:A:701:NDP:PA	3.00	0.46
1:A:451:LYS:CE	6:A:809:HOH:O	2.60	0.46
1:B:8:VAL:HA	1:B:76:LYS:CD	2.46	0.46
1:B:78:CYS:O	1:B:82:ASN:N	2.49	0.46
1:B:119:LEU:N	1:B:124:ASN:OD1	2.46	0.46
1:B:318:LEU:HB2	1:B:321:LYS:HD3	1.98	0.46
1:A:19:LYS:HG2	1:A:36:THR:HG22	1.98	0.46
1:A:601:LYS:CE	6:A:1012:HOH:O	2.64	0.46
1:B:165:GLY:HA3	1:B:170:TYR:CE2	2.50	0.45
1:A:332:ILE:HD13	1:A:560:LEU:HD22	1.98	0.45
1:B:109:TRP:CZ2	1:B:117:LYS:HD2	2.51	0.45
1:B:547:LEU:HD12	1:B:547:LEU:N	2.32	0.45
1:B:8:VAL:HA	1:B:76:LYS:HD3	1.98	0.45
1:B:329:LEU:HD22	1:B:564:LEU:HD12	1.98	0.44
1:A:470:ARG:HD3	6:B:903:HOH:O	2.18	0.44
1:B:336:MET:CE	1:B:560:LEU:HB2	2.47	0.44
1:B:59:ARG:NH1	4:B:703:DQ9:OBD	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ASN:OD1	1:B:159:TYR:HB3	2.18	0.43
1:B:491:HIS:CE1	3:B:702:UMP:O4	2.70	0.43
1:B:40:LEU:O	2:B:701:NDP:H2N	2.19	0.43
1:A:81:LEU:O	1:A:82:ASN:HB2	2.18	0.43
1:A:144:ASN:C	1:A:144:ASN:HD22	2.21	0.43
1:B:310:ASN:N	1:B:310:ASN:OD1	2.52	0.43
1:B:221:LEU:N	1:B:221:LEU:HD23	2.32	0.43
1:A:343:SER:HA	6:A:831:HOH:O	2.19	0.42
1:B:168:VAL:HG23	2:B:701:NDP:O2N	2.20	0.42
1:A:17:CYS:HA	1:A:39:GLY:O	2.20	0.42
1:A:321:LYS:CE	6:A:956:HOH:O	2.68	0.42
1:B:74:LYS:HD3	1:B:75:TYR:N	2.35	0.42
1:A:512:CYS:SG	1:A:547:LEU:HD22	2.60	0.41
1:B:17:CYS:HA	1:B:39:GLY:O	2.20	0.41
1:B:9:PHE:HA	1:B:158:TYR:OH	2.21	0.41
1:A:321:LYS:HE3	6:A:956:HOH:O	2.21	0.41
1:B:494:CYS:SG	1:B:525:TYR:CE2	3.14	0.41
1:A:354:PHE:CE2	1:B:506:ILE:HG13	2.56	0.40
1:A:601:LYS:HE2	6:A:1012:HOH:O	2.20	0.40
1:B:75:TYR:CE2	1:B:79:LYS:HD2	2.56	0.40
1:B:457:LYS:HB2	1:B:457:LYS:HE2	1.89	0.40
1:B:516:LEU:HD23	1:B:516:LEU:HA	1.89	0.40
1:A:487:LEU:N	1:A:487:LEU:HD23	2.36	0.40
1:B:12:TYR:CD1	1:B:181:LYS:HB2	2.56	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	510/608 (84%)	488 (96%)	19 (4%)	3 (1%)	25	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	525/608 (86%)	493 (94%)	27 (5%)	5 (1%)	15	6
All	All	1035/1216 (85%)	981 (95%)	46 (4%)	8 (1%)	19	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	166	GLY
1	A	345	ARG
1	B	96	LYS
1	B	49	LYS
1	B	27	LYS
1	B	114	LYS
1	B	309	PRO

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	486/570 (85%)	476 (98%)	10 (2%)	53	47
1	B	498/570 (87%)	473 (95%)	25 (5%)	24	12
All	All	984/1140 (86%)	949 (96%)	35 (4%)	35	23

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	49	LYS
1	A	97	LYS
1	A	144	ASN
1	A	145	LYS
1	A	171	GLN
1	A	286	GLU
1	A	313	GLN

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Mol	Chain	Res	Type
1	A	487	LEU
1	A	603	SER
1	B	28	LYS
1	B	29	ASN
1	B	45	VAL
1	B	49	LYS
1	B	72	LYS
1	B	74	LYS
1	B	115	LYS
1	B	124	ASN
1	B	127	LEU
1	B	133	LYS
1	B	135	ASP
1	B	137	ASP
1	B	139	ASP
1	B	142	ILE
1	B	144	ASN
1	B	145	LYS
1	B	189	SER
1	B	204	GLU
1	B	229	THR
1	B	304	LYS
1	B	307	ILE
1	B	310	ASN
1	B	516	LEU
1	B	581	LYS
1	B	601	LYS

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	144	ASN
1	A	171	GLN
1	A	394	ASN
1	A	407	ASN
1	A	415	ASN
1	A	424	ASN
1	B	29	ASN
1	B	94	ASN
1	B	99	GLN
1	B	144	ASN

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Mol	Chain	Res	Type
1	B	394	ASN
1	B	424	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	#$|Z| > 2$
5	GOL	B	704	-	5,5,5	0.24	0	5,5,5	0.42	0
3	UMP	B	702	-	21,21,21	0.82	0	31,31,31	1.05	3 (9%)
2	NDP	A	701	-	45,52,52	2.28	13 (28%)	53,80,80	1.49	8 (15%)
2	NDP	B	701	-	45,52,52	1.85	14 (31%)	53,80,80	1.55	9 (16%)
3	UMP	A	702	-	21,21,21	0.72	0	31,31,31	1.00	2 (6%)
4	DQ9	A	703	-	32,32,32	1.45	4 (12%)	43,43,43	2.46	12 (27%)
4	DQ9	B	703	-	32,32,32	1.30	3 (9%)	43,43,43	2.34	15 (34%)

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
5	GOL	B	704	-	-	2/4/4/4	-
3	UMP	B	702	-	-	2/10/22/22	0/2/2/2
2	NDP	A	701	-	-	4/30/77/77	0/5/5/5
2	NDP	B	701	-	-	8/30/77/77	0/5/5/5
3	UMP	A	702	-	-	2/10/22/22	0/2/2/2
4	DQ9	A	703	-	-	3/16/16/16	0/3/3/3
4	DQ9	B	703	-	-	8/16/16/16	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NDP	O4B-C1B	7.99	1.52	1.41
4	A	703	DQ9	C5-CAI	-4.57	1.41	1.50
2	A	701	NDP	C2A-N3A	4.39	1.39	1.32
4	B	703	DQ9	C5-CAI	-4.22	1.42	1.50
2	B	701	NDP	C2A-N3A	4.18	1.38	1.32
2	B	701	NDP	C2A-N1A	3.99	1.41	1.33
2	B	701	NDP	C6N-C5N	3.98	1.40	1.33
2	A	701	NDP	C2A-N1A	3.95	1.41	1.33
2	A	701	NDP	C6N-C5N	3.91	1.40	1.33
2	B	701	NDP	O4B-C1B	3.73	1.46	1.41
2	A	701	NDP	P2B-O2B	3.65	1.66	1.59
2	B	701	NDP	C4N-C3N	-3.59	1.42	1.49
2	A	701	NDP	O4D-C1D	3.47	1.50	1.42
4	A	703	DQ9	C4-N3	2.98	1.39	1.34
4	B	703	DQ9	CAJ-C4	-2.93	1.43	1.51
2	A	701	NDP	O3D-C3D	2.83	1.49	1.43
2	A	701	NDP	C2N-C3N	2.79	1.42	1.34
2	A	701	NDP	O3B-C3B	2.73	1.49	1.43
4	A	703	DQ9	C6-N1	2.73	1.38	1.35
2	B	701	NDP	PN-O5D	2.72	1.70	1.59
2	A	701	NDP	C2D-C1D	-2.65	1.45	1.53
2	B	701	NDP	C2N-C3N	2.58	1.42	1.34
2	A	701	NDP	O4B-C4B	-2.54	1.39	1.45
2	B	701	NDP	C6A-C5A	-2.51	1.34	1.43
2	B	701	NDP	C5A-C4A	-2.50	1.34	1.40
2	A	701	NDP	P2B-O2X	-2.45	1.45	1.54
2	B	701	NDP	O3D-C3D	2.39	1.48	1.43
2	B	701	NDP	C4N-C5N	-2.28	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	NDP	P2B-O2B	2.27	1.63	1.59
2	B	701	NDP	C7N-C3N	-2.19	1.44	1.48
2	B	701	NDP	O4D-C1D	2.15	1.47	1.42
4	B	703	DQ9	C4-N3	2.13	1.38	1.34
2	A	701	NDP	C3B-C2B	-2.12	1.48	1.52
4	A	703	DQ9	CAO-CAN	2.07	1.41	1.38

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	703	DQ9	C2-N3-C4	11.19	125.57	116.24
4	B	703	DQ9	C2-N3-C4	8.25	123.11	116.24
2	B	701	NDP	N3A-C2A-N1A	-6.24	118.93	128.68
4	A	703	DQ9	C5-C4-N3	-5.52	116.81	123.61
4	B	703	DQ9	C2-N1-C6	5.32	122.87	116.99
4	B	703	DQ9	N3-C2-N1	-5.07	117.47	125.42
2	A	701	NDP	O2N-PN-O1N	4.26	133.31	112.24
4	A	703	DQ9	N3-C2-N1	-4.25	118.75	125.42
2	A	701	NDP	N3A-C2A-N1A	-3.95	122.51	128.68
4	B	703	DQ9	C5-C4-N3	-3.53	119.27	123.61
2	A	701	NDP	C4A-C5A-N7A	-3.51	105.74	109.40
4	B	703	DQ9	NAH-C2-N3	3.09	122.06	117.25
4	B	703	DQ9	CAK-CAI-C5	3.00	125.77	120.79
2	B	701	NDP	C1B-N9A-C4A	-2.94	121.47	126.64
4	B	703	DQ9	CAR-OAS-CAT	-2.90	110.35	117.93
4	A	703	DQ9	CAQ-CAJ-C4	-2.88	105.88	112.79
4	B	703	DQ9	NAG-C6-N1	2.81	121.01	117.03
2	B	701	NDP	O2A-PA-O1A	2.69	125.56	112.24
2	A	701	NDP	O3X-P2B-O2X	2.68	117.89	107.64
4	B	703	DQ9	C5-C6-N1	-2.67	121.02	122.52
4	A	703	DQ9	NAH-C2-N3	2.62	121.33	117.25
2	B	701	NDP	O2N-PN-O5D	2.59	119.80	107.75
4	B	703	DQ9	CAI-CAO-CAN	2.59	122.81	119.24
4	B	703	DQ9	CAM-CAN-CL	2.56	123.36	119.35
3	A	702	UMP	O2-C2-N1	2.55	126.17	122.79
4	A	703	DQ9	C2-N1-C6	2.55	119.80	116.99
4	A	703	DQ9	CAW-CAX-CAY	-2.52	117.06	120.53
2	B	701	NDP	O4D-C1D-N1N	-2.46	103.24	108.06
2	B	701	NDP	O3X-P2B-O2X	2.41	116.87	107.64
4	A	703	DQ9	CAJ-CAQ-CAR	-2.39	105.29	113.34
4	B	703	DQ9	CAO-CAN-CL	-2.34	116.23	119.15
4	B	703	DQ9	OAZ-CBA-CBB	-2.31	103.36	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	703	DQ9	CAO-CAN-CL	-2.28	116.31	119.15
2	B	701	NDP	O2B-P2B-O1X	-2.26	100.66	109.39
2	A	701	NDP	O4B-C4B-C5B	2.24	116.73	109.37
2	B	701	NDP	O2N-PN-O1N	2.21	123.18	112.24
2	B	701	NDP	C5A-C6A-N6A	-2.20	117.00	120.35
2	A	701	NDP	O2A-PA-O5B	-2.19	97.58	107.75
3	B	702	UMP	O2-C2-N1	2.19	125.69	122.79
4	A	703	DQ9	CAV-CAW-CAX	2.16	122.42	118.96
4	B	703	DQ9	C5-C6-NAG	-2.09	117.93	120.86
4	B	703	DQ9	NAH-C2-N1	2.07	120.47	117.25
3	A	702	UMP	OP3-P-OP2	2.06	115.51	107.64
3	B	702	UMP	C1'-N1-C6	-2.04	117.51	121.55
4	A	703	DQ9	CAK-CAI-C5	2.03	124.16	120.79
4	A	703	DQ9	CAT-CAY-CAX	2.02	121.52	118.48
2	A	701	NDP	C2D-C1D-N1N	2.02	118.36	113.30
3	B	702	UMP	OP2-P-O5'	-2.01	101.37	106.73
2	A	701	NDP	C1D-N1N-C2N	-2.01	117.76	121.11

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	NDP	C5D-O5D-PN-O1N
2	B	701	NDP	C5D-O5D-PN-O1N
4	A	703	DQ9	C4-CAJ-CAQ-CAR
5	B	704	GOL	C1-C2-C3-O3
4	B	703	DQ9	CAW-CAX-OAZ-CBA
4	B	703	DQ9	CAY-CAX-OAZ-CBA
4	B	703	DQ9	CAJ-CAQ-CAR-OAS
4	B	703	DQ9	OAZ-CBA-CBB-OBC
4	B	703	DQ9	CAY-CAT-OAS-CAR
5	B	704	GOL	O2-C2-C3-O3
3	A	702	UMP	O4'-C4'-C5'-O5'
4	B	703	DQ9	CAU-CAT-OAS-CAR
4	B	703	DQ9	OAZ-CBA-CBB-OBD
3	A	702	UMP	C3'-C4'-C5'-O5'
3	B	702	UMP	O4'-C4'-C5'-O5'
2	B	701	NDP	C4D-C5D-O5D-PN
4	B	703	DQ9	C4-CAJ-CAQ-CAR
2	B	701	NDP	C5B-O5B-PA-O1A
4	A	703	DQ9	CAY-CAX-OAZ-CBA
2	A	701	NDP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	B	701	NDP	O4D-C1D-N1N-C2N
4	A	703	DQ9	CAW-CAX-OAZ-CBA
2	A	701	NDP	C2D-C1D-N1N-C2N
2	B	701	NDP	C2D-C1D-N1N-C2N
2	B	701	NDP	C3B-C4B-C5B-O5B
3	B	702	UMP	C3'-C4'-C5'-O5'
2	A	701	NDP	C4D-C5D-O5D-PN
2	B	701	NDP	C5B-O5B-PA-O3
2	B	701	NDP	C2N-C3N-C7N-N7N

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	UMP	1	0
2	A	701	NDP	4	0
2	B	701	NDP	4	0
3	A	702	UMP	1	0
4	B	703	DQ9	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 then 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

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP A 701

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand UMP A 702

Bond lengths

Bond angles

Torsions

Rings

Ligand DQ9 A 703

Bond lengths

Bond angles

Torsions

Rings

Ligand DQ9 B 703

Bond lengths

Bond angles

Torsions

Rings
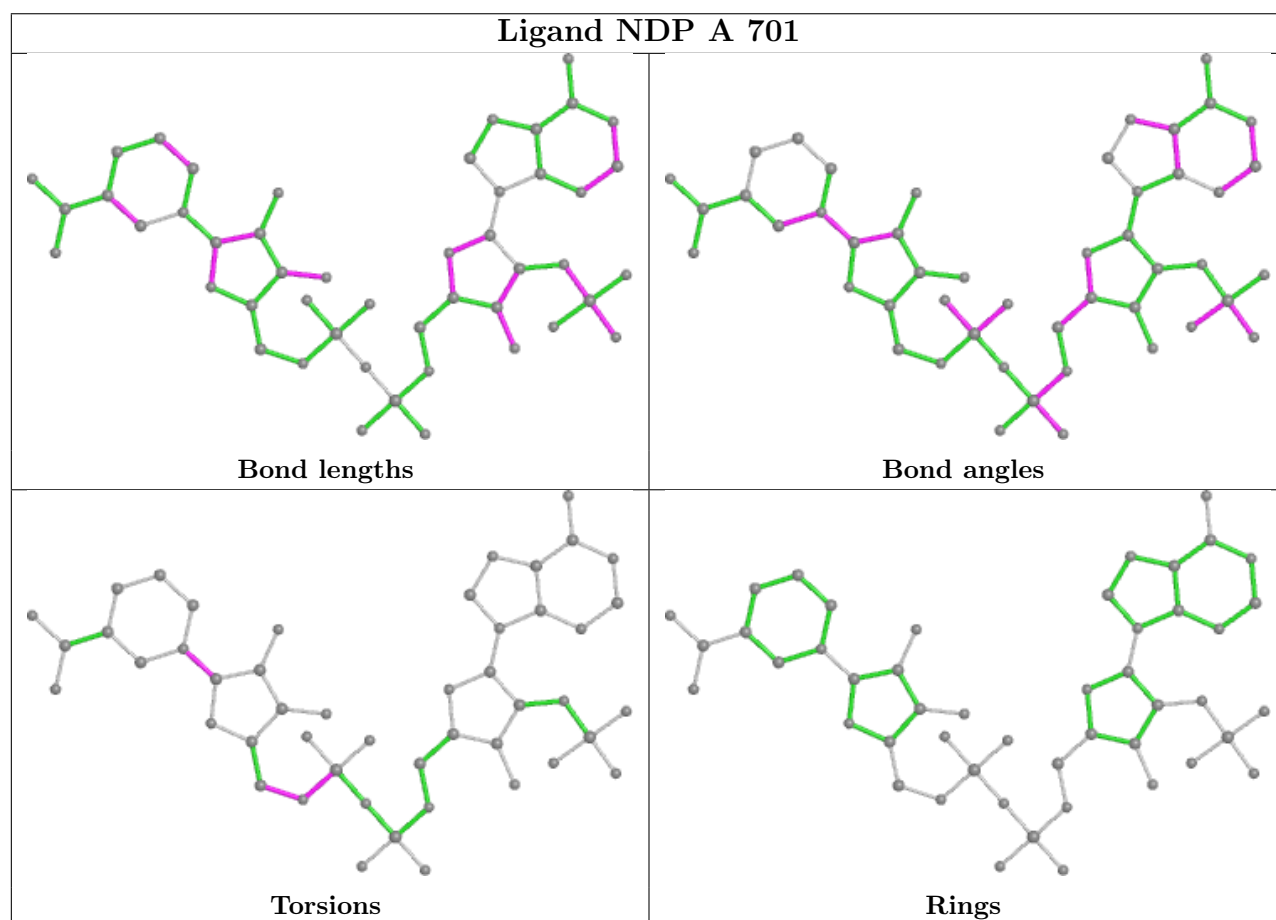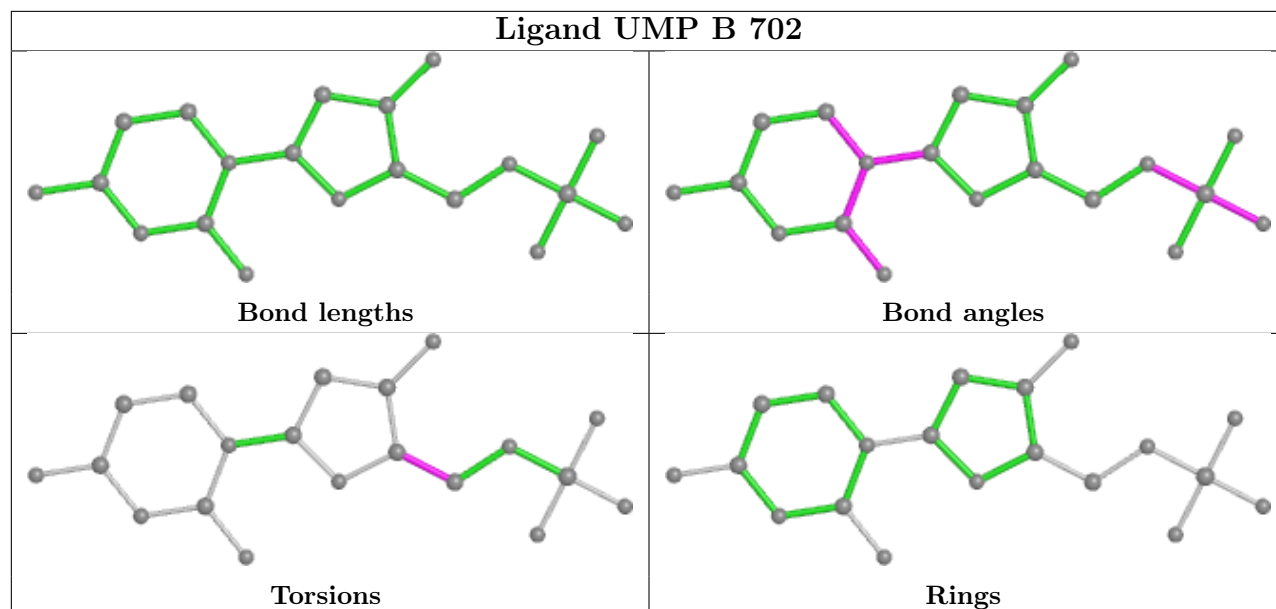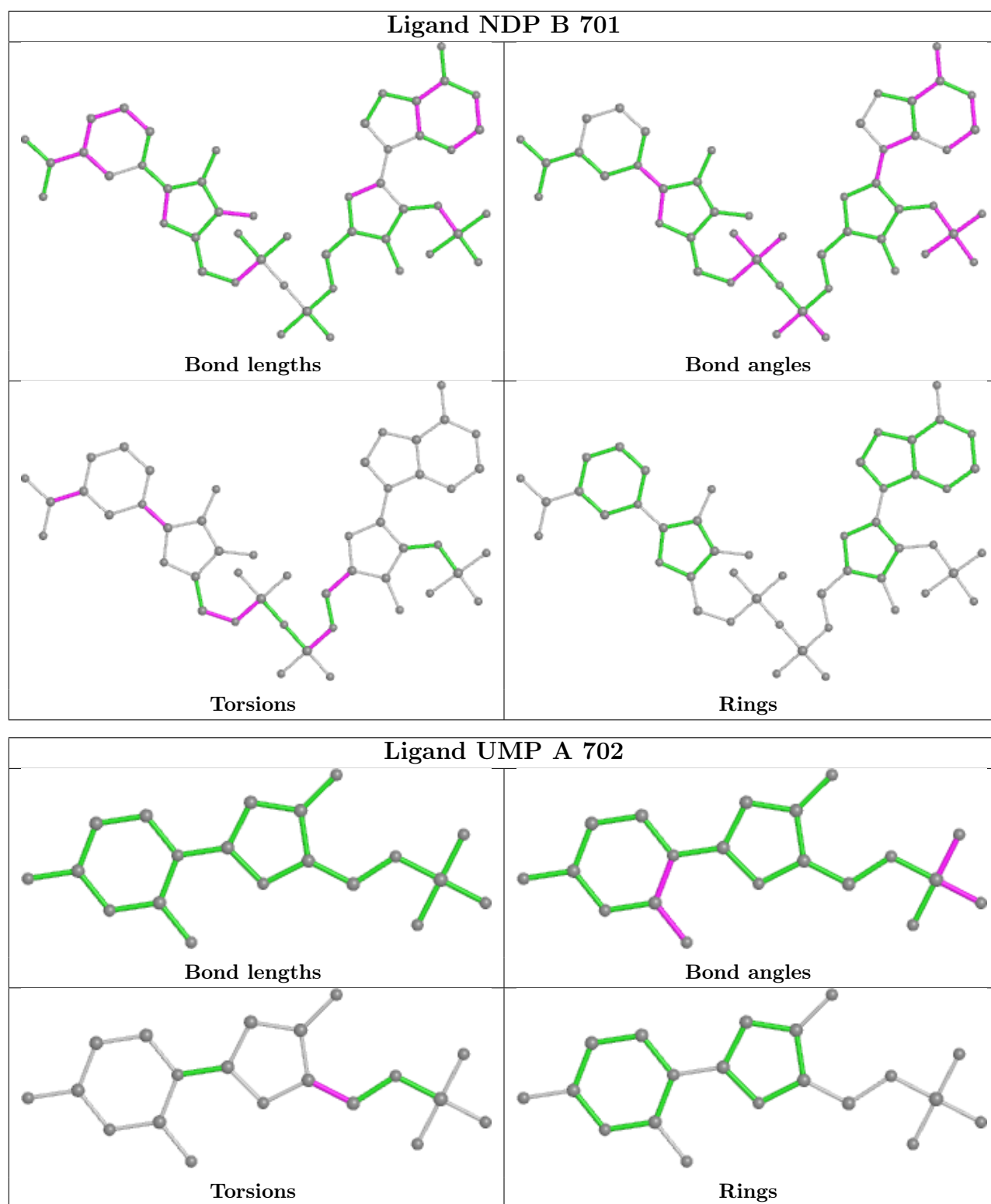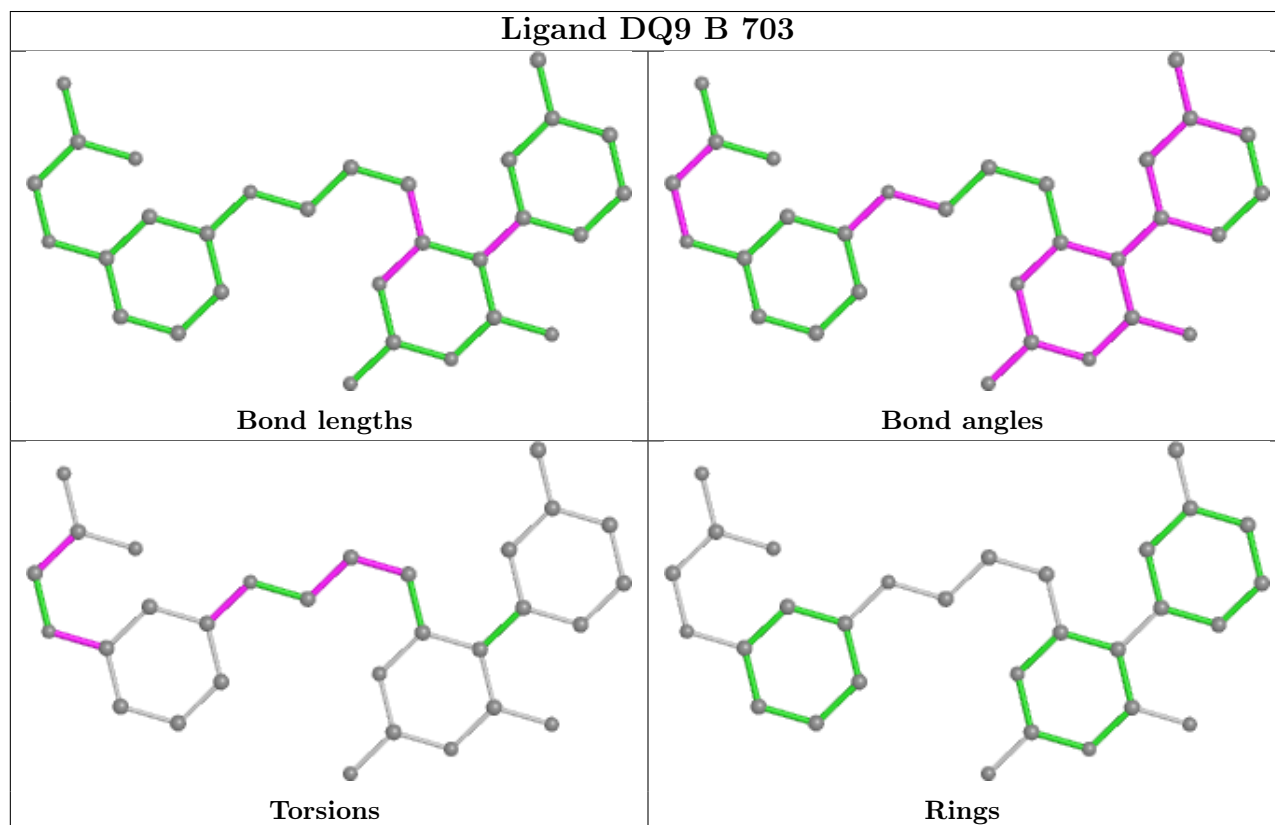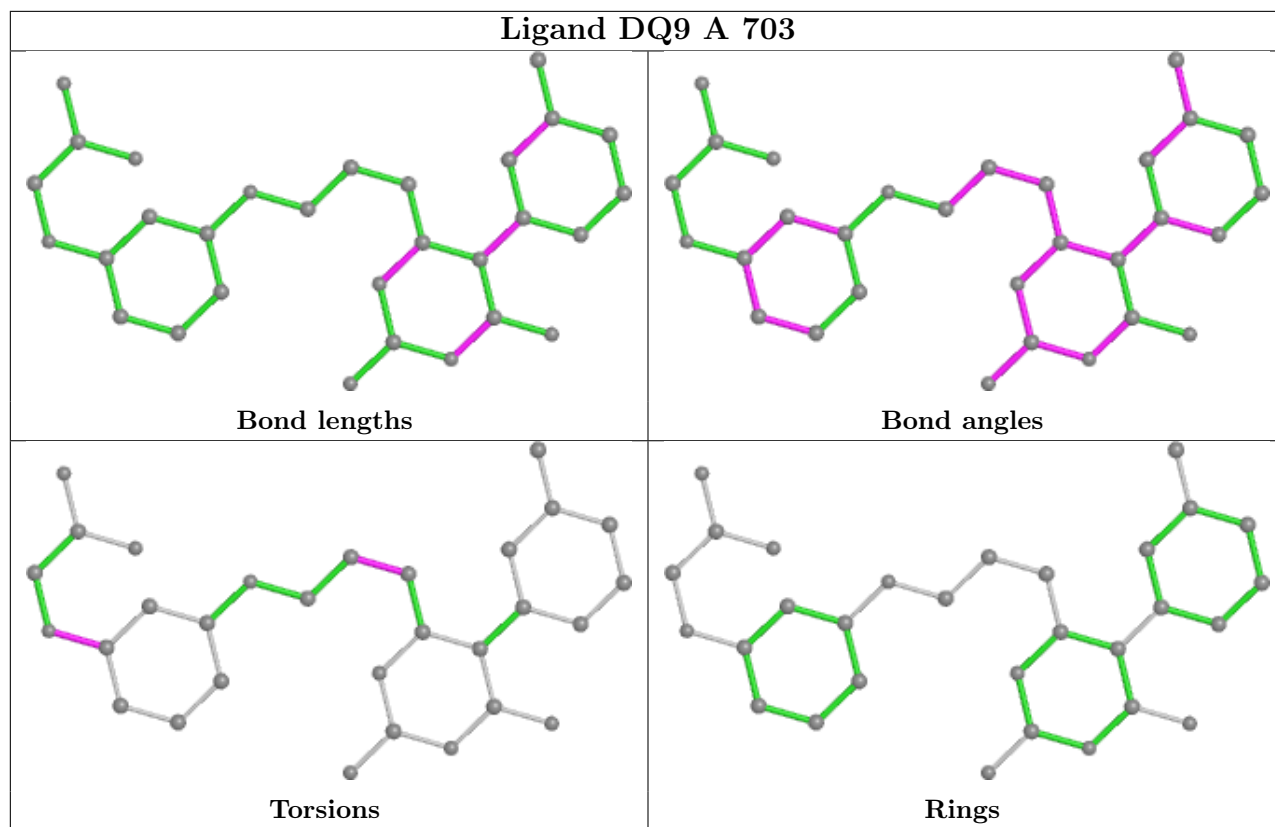
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	520/608 (85%)	0.29	36 (6%)	16	18	14, 26, 59, 90	0
1	B	533/608 (87%)	0.93	101 (18%)	1	1	13, 32, 91, 140	0
All	All	1053/1216 (86%)	0.61	137 (13%)	3	3	13, 28, 80, 140	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	LYS	10.8
1	B	26	GLY	9.4
1	B	116	PHE	7.9
1	B	138	GLU	7.9
1	B	96	LYS	7.8
1	B	136	PHE	7.7
1	B	134	GLU	7.1
1	B	23	LYS	7.0
1	B	94	ASN	6.8
1	B	24	ASN	6.5
1	B	28	LYS	6.1
1	B	75	TYR	6.1
1	B	114	LYS	6.0
1	B	14	ILE	5.7
1	B	9	PHE	5.6
1	B	346	THR	5.6
1	B	163	ILE	5.5
1	B	81	LEU	5.4
1	B	80	TYR	5.3
1	B	309	PRO	5.3
1	A	75	TYR	5.2
1	B	95	SER	5.2
1	B	25	GLU	5.2
1	B	22	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	135	ASP	4.9
1	B	144	ASN	4.7
1	B	131	LEU	4.5
1	B	298	GLU	4.5
1	B	151	VAL	4.4
1	B	29	ASN	4.2
1	B	307	ILE	4.2
1	B	113	PRO	4.2
1	B	73	LEU	4.2
1	B	97	LYS	4.1
1	B	78	CYS	4.1
1	B	118	PRO	4.1
1	B	130	THR	4.0
1	A	605	ASP	4.0
1	B	310	ASN	3.9
1	B	110	GLU	3.8
1	A	346	THR	3.8
1	A	297	LYS	3.8
1	A	307	ILE	3.7
1	B	127	LEU	3.7
1	B	283	ASP	3.7
1	B	162	PHE	3.6
1	B	204	GLU	3.6
1	B	164	LEU	3.6
1	B	348	VAL	3.6
1	B	157	ASN	3.6
1	A	287	GLU	3.5
1	B	13	ALA	3.5
1	A	345	ARG	3.5
1	B	229	THR	3.4
1	A	286	GLU	3.4
1	B	115	LYS	3.4
1	B	49	LYS	3.4
1	A	162	PHE	3.4
1	B	605	ASP	3.3
1	A	14	ILE	3.3
1	A	71	GLU	3.3
1	B	82	ASN	3.3
1	B	70	TYR	3.3
1	A	22	SER	3.3
1	B	303	ASN	3.2
1	B	117	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	165	GLY	3.2
1	B	184	PHE	3.2
1	B	284	ASP	3.1
1	B	109	TRP	3.1
1	B	305	ASN	3.1
1	B	345	ARG	3.1
1	B	196	PHE	3.1
1	A	306	SER	3.1
1	B	175	GLU	3.0
1	B	74	LYS	3.0
1	A	375	PHE	3.0
1	B	139	ASP	2.9
1	B	203	ASN	2.9
1	B	15	CYS	2.8
1	B	43	LYS	2.8
1	B	133	LYS	2.8
1	B	137	ASP	2.8
1	B	126	ILE	2.7
1	A	161	CYS	2.7
1	A	164	LEU	2.7
1	A	310	ASN	2.7
1	A	309	PRO	2.7
1	B	129	ARG	2.7
1	B	71	GLU	2.7
1	A	102	VAL	2.6
1	A	82	ASN	2.6
1	B	50	CYS	2.6
1	A	4	GLN	2.6
1	B	67	GLU	2.6
1	B	306	SER	2.6
1	A	304	LYS	2.6
1	A	79	LYS	2.5
1	B	141	TYR	2.5
1	B	72	LYS	2.5
1	A	296	ASN	2.5
1	A	97	LYS	2.4
1	B	176	LYS	2.4
1	A	348	VAL	2.4
1	B	125	VAL	2.4
1	A	21	GLU	2.4
1	B	308	HIS	2.4
1	B	192	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	81	LEU	2.4
1	B	344	ASP	2.4
1	A	49	LYS	2.3
1	B	201	ASN	2.3
1	B	45	VAL	2.3
1	B	168	VAL	2.3
1	B	12	TYR	2.3
1	A	72	LYS	2.3
1	B	79	LYS	2.3
1	B	132	LYS	2.3
1	B	343	SER	2.2
1	B	290	PHE	2.2
1	A	343	SER	2.2
1	B	103	VAL	2.2
1	B	169	VAL	2.2
1	B	59	ARG	2.1
1	B	194	ASP	2.1
1	B	68	SER	2.1
1	B	224	ILE	2.1
1	A	347	GLY	2.1
1	B	140	VAL	2.1
1	B	347	GLY	2.1
1	B	183	TYR	2.1
1	B	195	VAL	2.1
1	A	603	SER	2.1
1	A	163	ILE	2.1
1	A	229	THR	2.0
1	B	44	GLY	2.0
1	A	290	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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
4	DQ9	B	703	30/30	0.79	0.22	36,51,94,96	0
5	GOL	B	704	6/6	0.85	0.14	27,33,36,38	0
2	NDP	B	701	48/48	0.86	0.17	39,70,94,98	0
4	DQ9	A	703	30/30	0.90	0.16	16,22,49,54	0
2	NDP	A	701	48/48	0.96	0.09	21,30,37,41	0
3	UMP	A	702	20/20	0.96	0.12	22,36,43,45	0
3	UMP	B	702	20/20	0.96	0.15	26,40,50,54	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
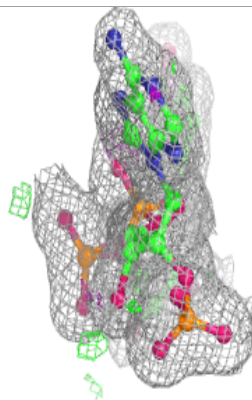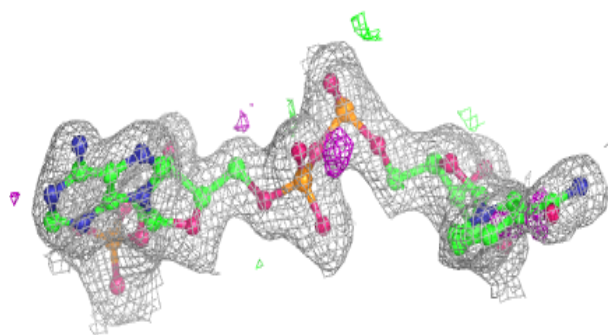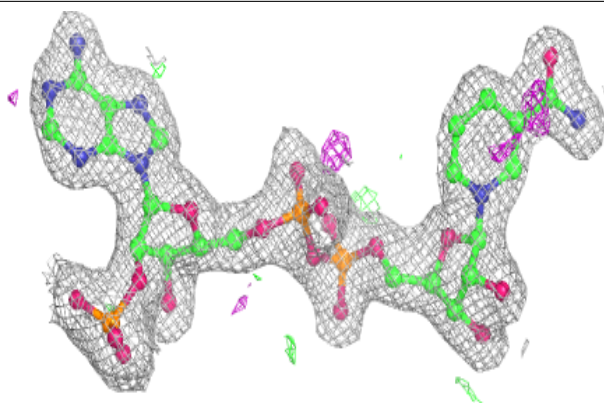

Electron density around DQ9 B 703:

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

Electron density around NDP B 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
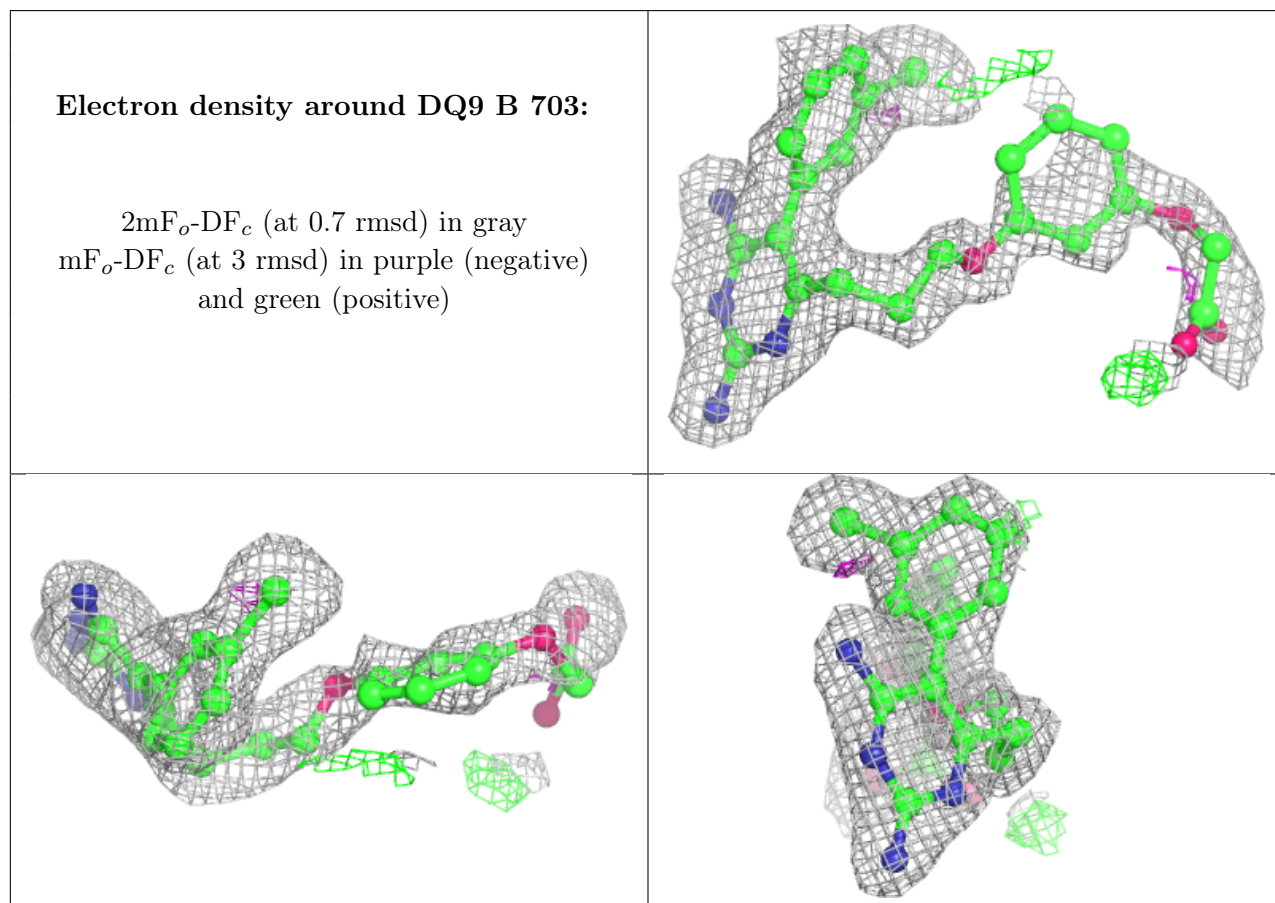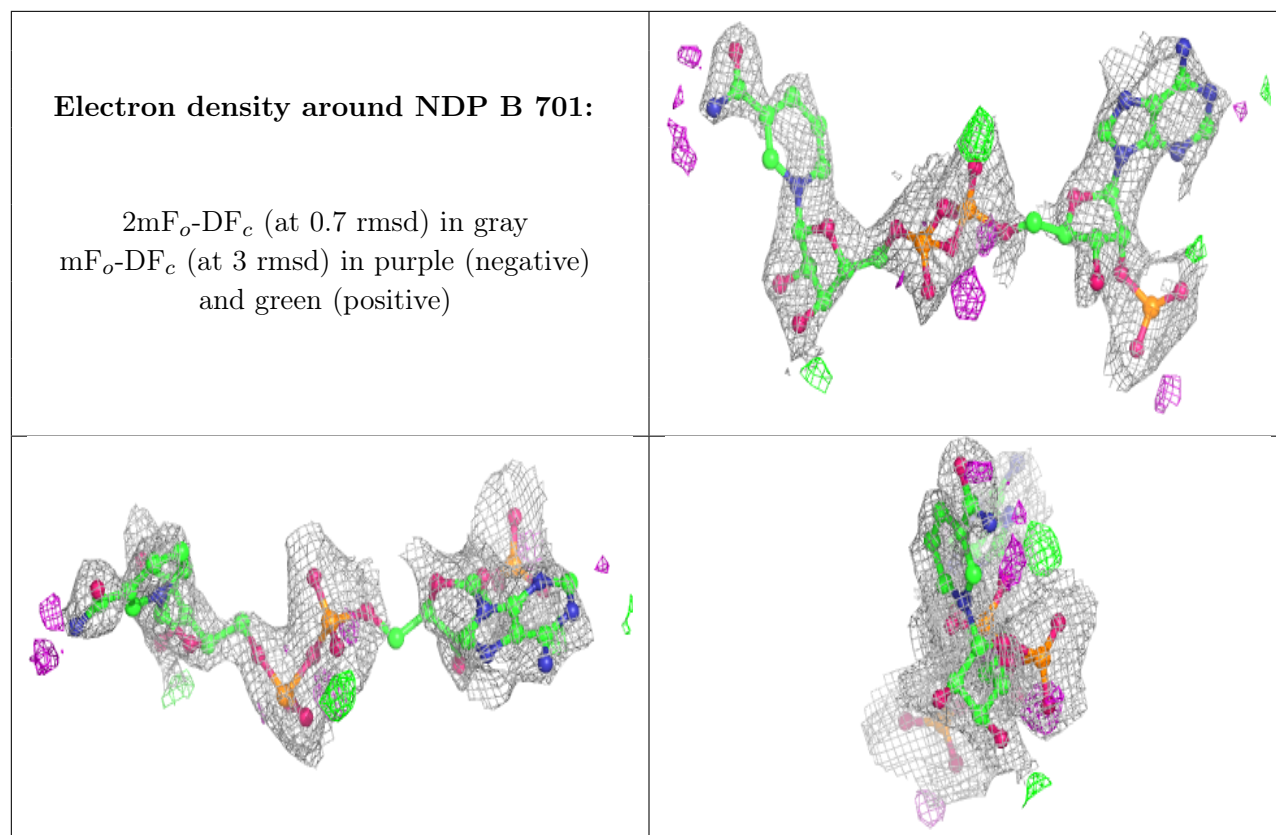
Electron density around DQ9 A 703:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
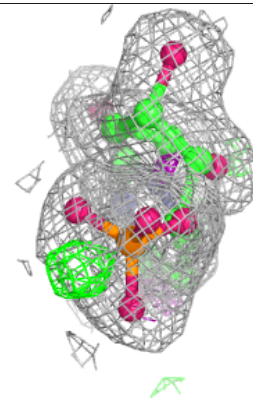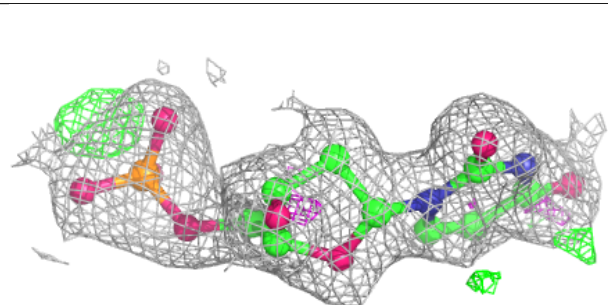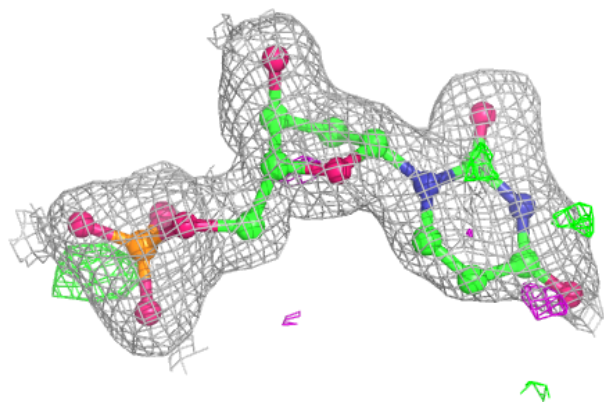$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
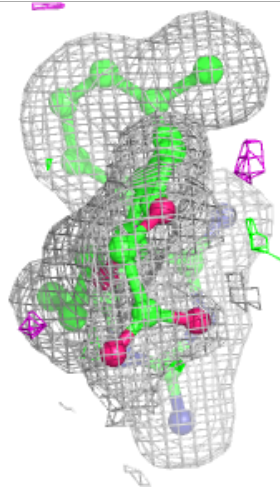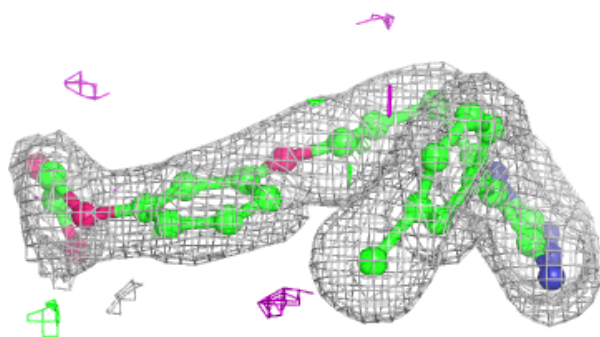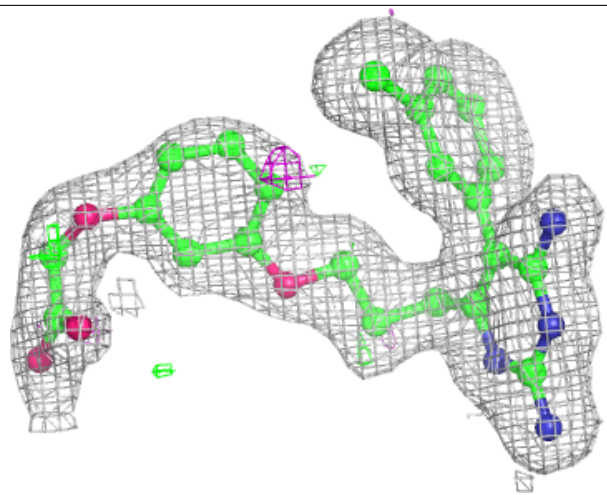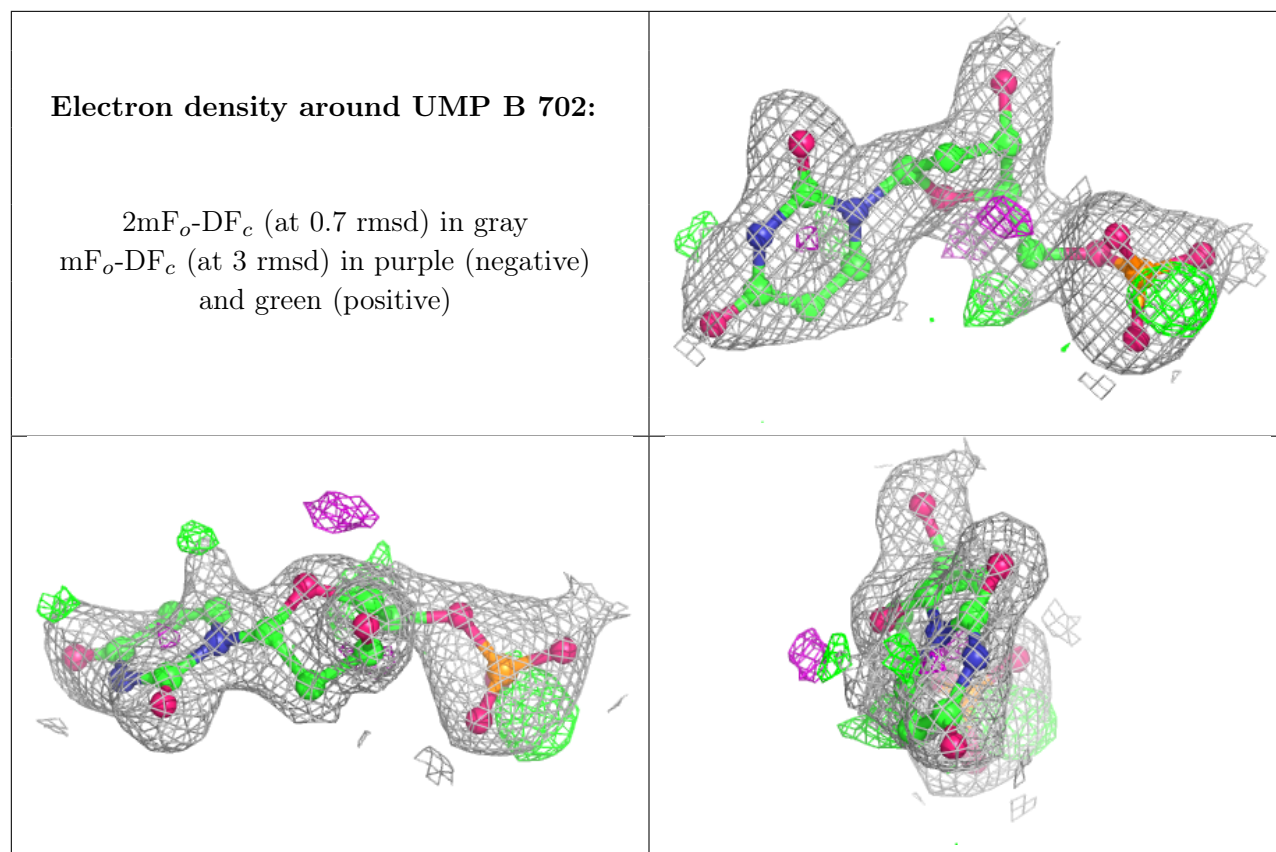
Electron density around NDP A 701:

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 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)

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)

6.5 Other polymers ⓘ

There are no such residues in this entry.