



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:11 pm BST

PDB ID : 5T0L
Title : Crystal structure of Toxoplasma gondii TS-DHFR complexed with NADPH, dUMP, PDDF and 5-(4-(3,4-dichlorophenyl)piperazin-1-yl)pyrimidine-2,4-diamine (TRC-15)
Authors : Thomas, S.B.; Chen, Z.; Lu, H.; Li, Y.
Deposited on : 2016-08-16
Resolution : 3.13 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 : 2.11
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) : 2.11

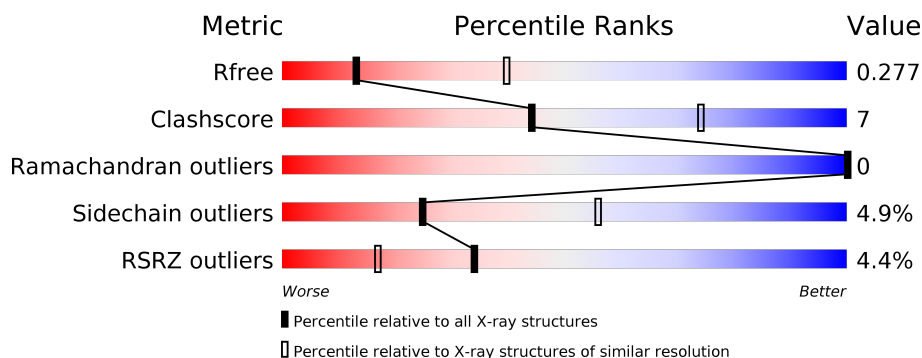
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	566	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>10%</div> </div> </div>
1	B	566	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>10%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CB3	B	703	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8410 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	508	Total	C	N	O	S	0	1	0
			4074	2606	713	730	25			
1	B	510	Total	C	N	O	S	0	1	0
			4086	2612	715	734	25			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	ASN	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	TRP	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	ARG	deletion	UNP Q07422
A	?	-	LYS	deletion	UNP Q07422
A	?	-	PHE	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	LYS	deletion	UNP Q07422
A	?	-	THR	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	ASP	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	VAL	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	LYS	deletion	UNP Q07422

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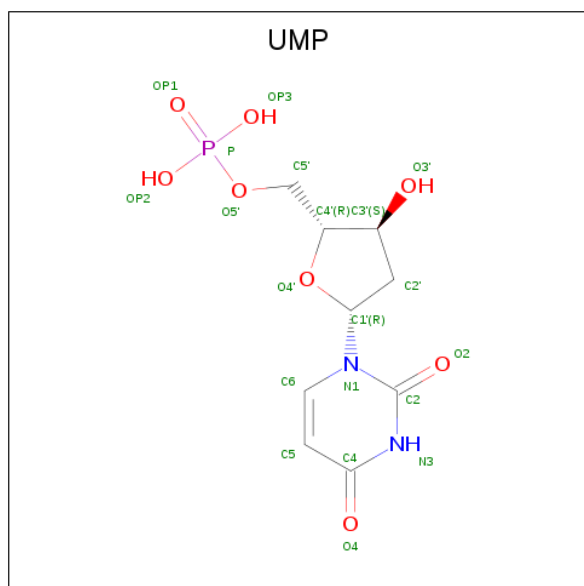
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	GLU	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	VAL	deletion	UNP Q07422
A	?	-	PHE	deletion	UNP Q07422
A	?	-	VAL	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	PHE	deletion	UNP Q07422
A	?	-	CYS	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	GLU	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	ARG	deletion	UNP Q07422
B	?	-	ARG	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	ASN	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	TRP	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	ARG	deletion	UNP Q07422
B	?	-	LYS	deletion	UNP Q07422
B	?	-	PHE	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	LYS	deletion	UNP Q07422
B	?	-	THR	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	ASP	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	VAL	deletion	UNP Q07422

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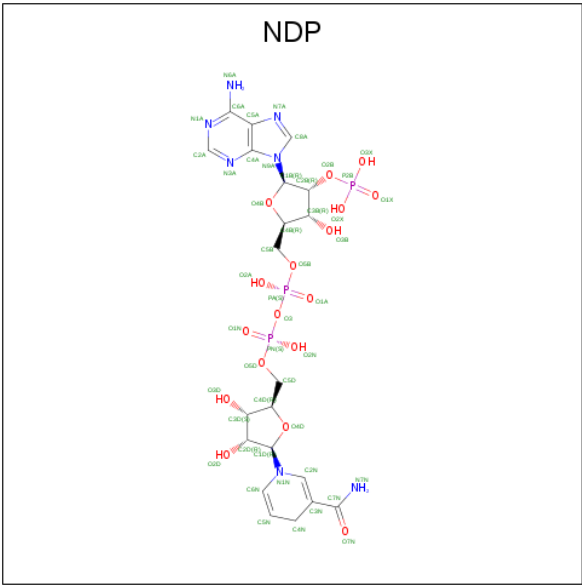
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP Q07422
B	?	-	LYS	deletion	UNP Q07422
B	?	-	GLN	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	GLU	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	VAL	deletion	UNP Q07422
B	?	-	PHE	deletion	UNP Q07422
B	?	-	VAL	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	PHE	deletion	UNP Q07422
B	?	-	CYS	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	GLU	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	ARG	deletion	UNP Q07422

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



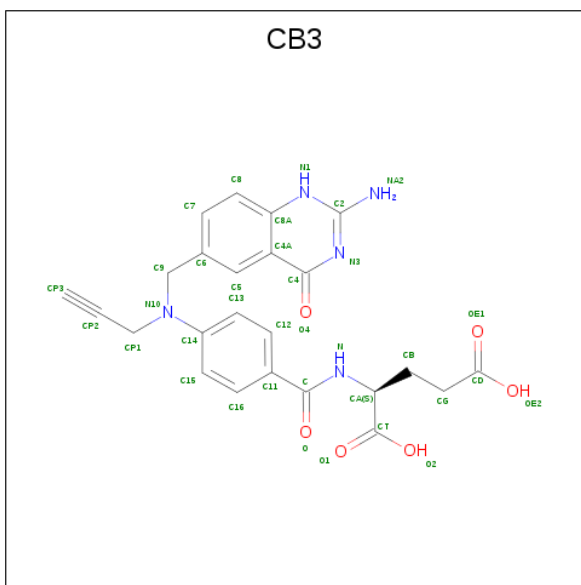
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



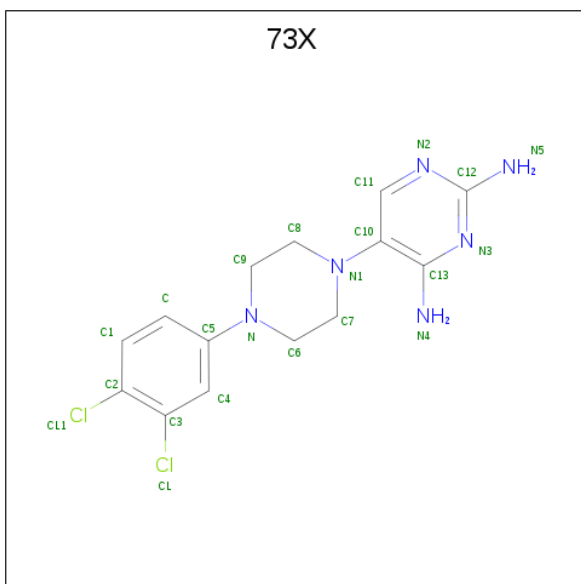
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: C₂₄H₂₃N₅O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	24	5	6		
4	B	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 5 is 5-[4-(3,4-dichlorophenyl)piperazin-1-yl]pyrimidine-2,4-diamine (three-letter code: 73X) (formula: C₁₄H₁₆Cl₂N₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	0	0
			22	14	2	6		

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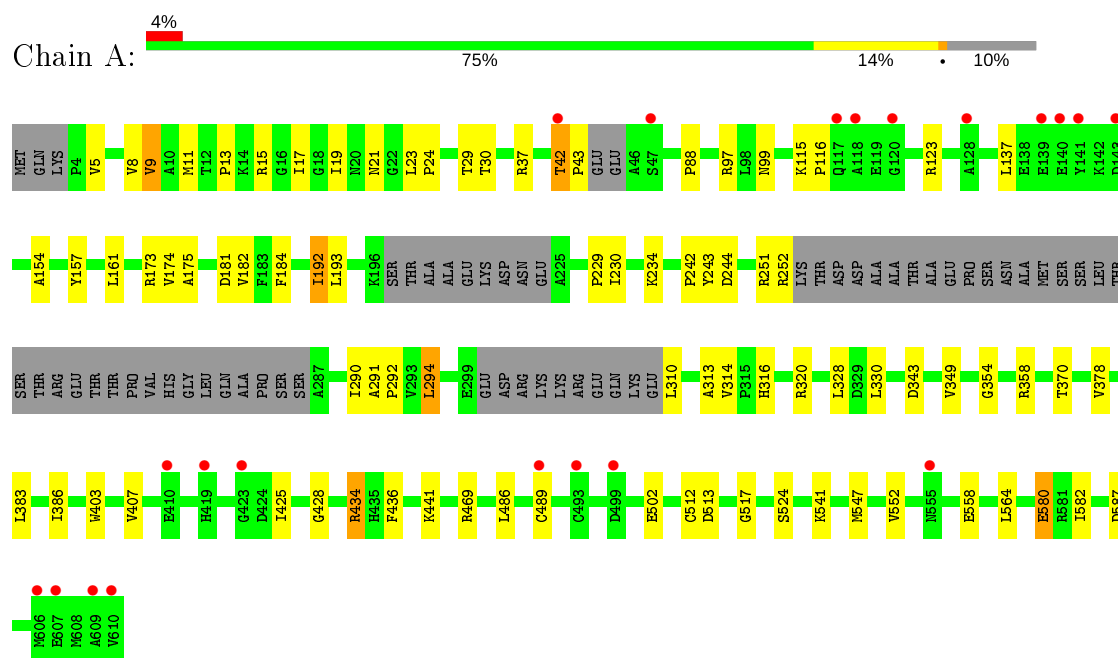
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	0	0
			22	14	2	6		

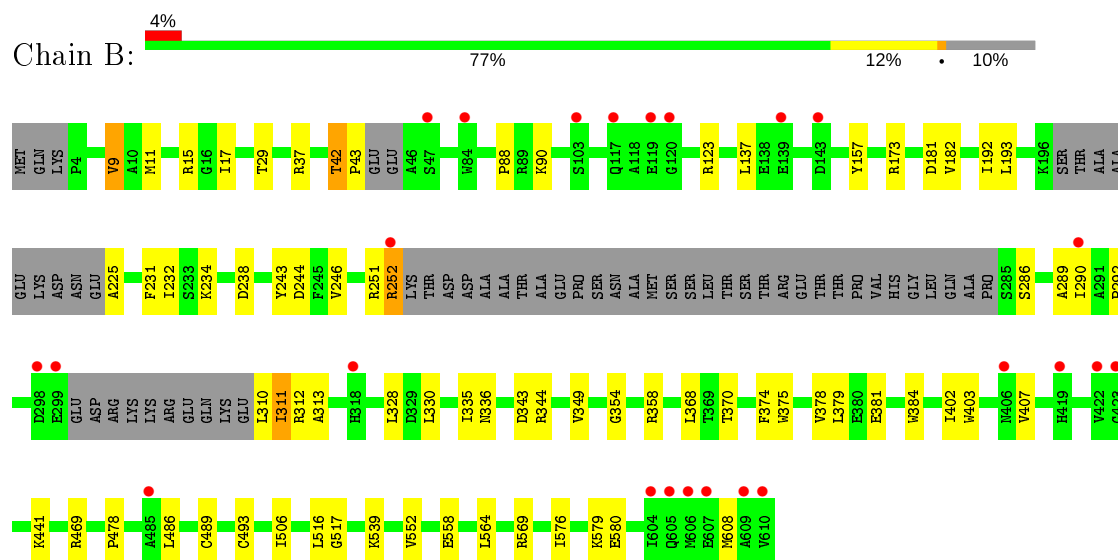
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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	51.28Å 143.98Å 170.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.93 – 3.13 37.49 – 3.13	Depositor EDS
% Data completeness (in resolution range)	92.3 (109.93-3.13) 92.4 (37.49-3.13)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.253 , 0.274 0.253 , 0.277	Depositor DCC
R_{free} test set	1101 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8410	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: CB3, UMP, NDP, 73X

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	0.29	0/4173	0.52	0/5652
1	B	0.30	0/4185	0.50	0/5668
All	All	0.29	0/8358	0.51	0/11320

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4074	0	4042	55	0
1	B	4086	0	4052	50	0
2	A	20	0	11	6	0
2	B	20	0	11	3	0
3	A	48	0	26	2	0
3	B	48	0	26	4	0
4	A	35	0	21	8	0
4	B	35	0	21	13	0
5	A	22	0	0	4	0
5	B	22	0	0	4	0
All	All	8410	0	8210	109	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (109) 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:469:ARG:NH1	2:B:701:UMP:OP1	2.07	0.87
3:B:702:NDP:H8A	3:B:702:NDP:H52A	1.59	0.81
1:A:313:ALA:O	1:A:320:ARG:NH2	2.16	0.79
2:A:701:UMP:P	1:B:469:ARG:HH12	2.07	0.77
3:B:702:NDP:H42N	5:B:704:73X:C8	2.14	0.77
1:A:290:ILE:HG23	1:B:231:PHE:HD2	1.51	0.76
1:A:88:PRO:CD	5:A:704:73X:CL	2.79	0.68
1:B:286:SER:O	1:B:290:ILE:HD13	1.93	0.68
1:A:88:PRO:HD2	5:A:704:73X:CL	2.31	0.67
2:A:701:UMP:P	1:B:469:ARG:NH1	2.68	0.67
1:B:313:ALA:HB2	1:B:564:LEU:HD22	1.76	0.66
1:A:154:ALA:N	3:A:702:NDP:O2N	2.26	0.66
1:A:290:ILE:HG23	1:B:231:PHE:CD2	2.31	0.65
1:A:489:CYS:SG	2:A:701:UMP:C6	2.90	0.64
1:A:192:ILE:HD12	1:A:193:LEU:HG	1.78	0.64
1:B:328:LEU:HD21	1:B:370:THR:HG21	1.80	0.64
1:B:88:PRO:HD2	5:B:704:73X:CL1	2.35	0.64
2:A:701:UMP:OP2	1:B:469:ARG:NH1	2.31	0.63
1:A:230:ILE:HG21	1:B:290:ILE:HD11	1.80	0.63
1:A:88:PRO:HD3	5:A:704:73X:CL	2.38	0.61
1:B:42:THR:HG22	1:B:43:PRO:HD2	1.82	0.61
1:B:403:TRP:CZ3	4:B:703:CB3:H7	2.36	0.60
1:B:88:PRO:CD	5:B:704:73X:CL1	2.87	0.60
1:B:289:ALA:O	1:B:292:PRO:HD2	2.02	0.59
1:A:313:ALA:HB2	1:A:564:LEU:HD22	1.82	0.59
1:A:21:ASN:HA	3:A:702:NDP:O3D	2.03	0.59
1:A:489:CYS:SG	2:A:701:UMP:C5	2.96	0.59
1:B:489:CYS:SG	2:B:701:UMP:C6	2.95	0.59
1:A:354:GLY:O	1:B:358:ARG:NH2	2.36	0.58
1:A:517:GLY:CA	4:A:703:CB3:HP3	2.35	0.57
1:A:469:ARG:NH2	1:B:343:ASP:OD1	2.37	0.57
1:B:516:LEU:HD11	4:B:703:CB3:HN	1.69	0.56
1:A:8:VAL:HG22	5:A:704:73X:N3	2.20	0.56
4:A:703:CB3:C6	4:A:703:CB3:H15	2.34	0.55
4:B:703:CB3:C6	4:B:703:CB3:H15	2.35	0.55
1:B:402:ILE:HB	4:B:703:CB3:C15	2.37	0.55
1:B:225:ALA:HA	1:B:252:ARG:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASP:OD1	1:B:469:ARG:NH2	2.39	0.54
1:A:513:ASP:HB2	2:A:701:UMP:H1'	1.89	0.54
1:A:328:LEU:HD21	1:A:370:THR:HG21	1.89	0.54
1:A:425:ILE:HD12	1:A:428:GLY:HA3	1.89	0.54
1:A:115:LYS:HG2	1:A:116:PRO:HD2	1.90	0.53
1:B:311:ILE:HD12	1:B:336:ASN:CG	2.29	0.53
1:A:517:GLY:HA2	4:A:703:CB3:HP3	1.91	0.52
1:A:582:ILE:HG23	1:A:587:ASP:HB2	1.91	0.52
1:A:358:ARG:NH2	1:B:354:GLY:O	2.43	0.52
1:B:17:ILE:O	3:B:702:NDP:H2N	2.09	0.52
1:B:192:ILE:HD12	1:B:193:LEU:HG	1.92	0.51
1:A:314:VAL:HG13	1:A:316:HIS:CE1	2.47	0.50
1:A:42:THR:HG22	1:A:43:PRO:HD2	1.93	0.50
1:A:229:PRO:O	1:A:316:HIS:HD2	1.94	0.50
4:B:703:CB3:C15	4:B:703:CB3:C6	2.90	0.49
4:A:703:CB3:C5	4:A:703:CB3:C15	2.90	0.49
1:A:517:GLY:HA2	4:A:703:CB3:CP3	2.43	0.49
3:B:702:NDP:C4N	5:B:704:73X:C8	2.90	0.49
1:A:290:ILE:HG22	1:A:294:LEU:HD12	1.95	0.49
4:B:703:CB3:H5	4:B:703:CB3:C14	2.42	0.49
4:B:703:CB3:C15	4:B:703:CB3:C5	2.91	0.49
1:A:354:GLY:HA2	1:A:547:MET:O	2.14	0.48
1:B:181:ASP:OD1	1:B:182:VAL:HG23	2.14	0.48
1:A:502:GLU:HB3	1:A:541:LYS:HB2	1.96	0.48
4:A:703:CB3:C14	4:A:703:CB3:C5	2.91	0.48
4:A:703:CB3:C6	4:A:703:CB3:C15	2.90	0.48
4:A:703:CB3:C14	4:A:703:CB3:H5	2.44	0.48
1:B:608:MET:HE2	4:B:703:CB3:H16	1.96	0.48
1:B:311:ILE:HD12	1:B:336:ASN:ND2	2.29	0.48
1:A:558[A]:GLU:CD	1:A:558[A]:GLU:H	2.18	0.47
1:B:608:MET:CE	4:B:703:CB3:H16	2.44	0.47
1:A:403:TRP:O	1:A:407:VAL:HG22	2.14	0.47
4:B:703:CB3:C5	4:B:703:CB3:C14	2.89	0.47
1:B:375:TRP:CH2	1:B:379:LEU:HD22	2.49	0.47
1:B:558[A]:GLU:H	1:B:558[A]:GLU:CD	2.18	0.46
1:B:403:TRP:O	1:B:407:VAL:HG22	2.15	0.46
1:B:11:MET:HG2	1:B:15:ARG:HA	1.98	0.46
1:B:344:ARG:NE	2:B:701:UMP:OP3	2.49	0.46
1:A:17:ILE:HG13	1:A:182:VAL:O	2.16	0.46
1:A:173:ARG:HD3	1:A:244:ASP:OD1	2.16	0.46
1:B:192:ILE:H	1:B:192:ILE:HG13	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASP:OD1	1:A:182:VAL:HG23	2.17	0.45
1:B:517:GLY:HA2	4:B:703:CB3:HP3	1.97	0.45
1:B:173:ARG:NH2	1:B:569:ARG:HA	2.32	0.45
1:A:9:VAL:HG13	1:A:157:TYR:CZ	2.51	0.45
1:B:238:ASP:OD2	1:B:243:TYR:OH	2.34	0.44
1:A:11:MET:HG2	1:A:15:ARG:HA	2.00	0.43
1:A:175:ALA:HB3	1:A:242:PRO:HG2	2.00	0.43
1:A:13:PRO:HD3	1:A:174:VAL:O	2.18	0.43
1:B:251:ARG:O	1:B:252:ARG:HB3	2.17	0.43
1:A:512:CYS:SG	1:A:547:MET:HG2	2.59	0.43
1:A:15:ARG:HD2	1:A:184:PHE:O	2.18	0.43
1:B:402:ILE:HB	4:B:703:CB3:C14	2.49	0.43
1:B:232:ILE:HG12	1:B:246:VAL:HG12	2.01	0.43
1:B:173:ARG:HD3	1:B:244:ASP:OD1	2.19	0.43
1:B:374:PHE:HB3	4:B:703:CB3:HG2	2.00	0.42
1:A:192:ILE:HG13	1:A:192:ILE:H	1.54	0.42
1:A:436:PHE:CE1	1:B:478:PRO:HD2	2.55	0.42
1:B:576:ILE:HB	1:B:579:LYS:HE2	2.02	0.42
1:A:251:ARG:O	1:A:252:ARG:HB3	2.19	0.41
1:A:291:ALA:N	1:A:292:PRO:HD2	2.35	0.41
1:B:381:GLU:O	1:B:384:TRP:HB3	2.20	0.41
1:A:19:ILE:HA	1:A:181:ASP:OD1	2.20	0.41
1:B:311:ILE:HD13	1:B:335:ILE:HB	2.02	0.41
1:A:23:LEU:HA	1:A:24:PRO:HD3	1.88	0.41
1:A:386:ILE:O	1:A:434:ARG:HD3	2.21	0.41
1:A:580:GLU:H	1:A:580:GLU:CD	2.23	0.41
1:B:493:CYS:HA	1:B:506:ILE:O	2.22	0.40
1:A:30:THR:HB	1:A:243:TYR:OH	2.22	0.40
1:B:9:VAL:HG13	1:B:157:TYR:CZ	2.56	0.40
1:A:97:ARG:O	1:A:99:ASN:ND2	2.55	0.40
1:A:354:GLY:CA	1:B:506:ILE:HD11	2.51	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	499/566 (88%)	480 (96%)	19 (4%)	0	100	100
1	B	501/566 (88%)	481 (96%)	20 (4%)	0	100	100
All	All	1000/1132 (88%)	961 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	441/491 (90%)	419 (95%)	22 (5%)	24	55
1	B	443/491 (90%)	422 (95%)	21 (5%)	26	57
All	All	884/982 (90%)	841 (95%)	43 (5%)	25	56

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	9	VAL
1	A	29	THR
1	A	37	ARG
1	A	42	THR
1	A	123	ARG
1	A	137	LEU
1	A	161	LEU
1	A	192	ILE
1	A	234	LYS
1	A	294	LEU
1	A	310	LEU
1	A	330	LEU
1	A	349	VAL
1	A	378	VAL

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Mol	Chain	Res	Type
1	A	383	LEU
1	A	434	ARG
1	A	441	LYS
1	A	486	LEU
1	A	524	SER
1	A	552	VAL
1	A	580	GLU
1	B	9	VAL
1	B	29	THR
1	B	37	ARG
1	B	42	THR
1	B	90	LYS
1	B	123	ARG
1	B	137	LEU
1	B	234	LYS
1	B	252	ARG
1	B	310	LEU
1	B	311	ILE
1	B	312	ARG
1	B	330	LEU
1	B	349	VAL
1	B	368	LEU
1	B	378	VAL
1	B	441	LYS
1	B	486	LEU
1	B	539	LYS
1	B	552	VAL
1	B	580	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	HIS
1	A	575	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 carbohydrates 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$
3	NDP	B	702	-	45,52,52	1.03	2 (4%)	53,80,80	1.04	3 (5%)
2	UMP	A	701	-	18,21,21	0.72	0	21,31,31	0.85	0
4	CB3	B	703	-	30,37,37	1.20	3 (10%)	38,51,51	2.43	8 (21%)
4	CB3	A	703	-	30,37,37	1.19	3 (10%)	38,51,51	2.50	8 (21%)
2	UMP	B	701	-	18,21,21	0.69	0	21,31,31	0.89	0
5	73X	A	704	-	24,24,24	0.96	2 (8%)	30,34,34	2.32	9 (30%)
5	73X	B	704	-	24,24,24	0.91	2 (8%)	30,34,34	1.99	8 (26%)
3	NDP	A	702	-	45,52,52	1.07	2 (4%)	53,80,80	1.10	4 (7%)

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
3	NDP	B	702	-	-	8/30/77/77	0/5/5/5
2	UMP	A	701	-	-	3/7/22/22	0/2/2/2
4	CB3	B	703	-	-	5/21/28/28	0/3/3/3
4	CB3	A	703	-	-	5/21/28/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UMP	B	701	-	-	6/7/22/22	0/2/2/2
5	73X	A	704	-	-	2/8/18/18	0/3/3/3
5	73X	B	704	-	-	1/8/18/18	0/3/3/3
3	NDP	A	702	-	-	6/30/77/77	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	CB3	C4A-C8A	3.77	1.48	1.41
3	A	702	NDP	C6N-C5N	3.64	1.39	1.33
4	B	703	CB3	C4A-C8A	3.61	1.48	1.41
3	B	702	NDP	C6N-C5N	3.51	1.39	1.33
4	B	703	CB3	CP2-CP3	3.40	1.28	1.18
4	A	703	CB3	CP2-CP3	3.29	1.28	1.18
5	B	704	73X	C3-CL	2.76	1.80	1.73
3	B	702	NDP	C5A-C4A	2.68	1.48	1.40
3	A	702	NDP	C5A-C4A	2.66	1.48	1.40
5	A	704	73X	C3-CL	2.44	1.79	1.73
5	A	704	73X	C2-CL1	2.41	1.79	1.73
5	B	704	73X	C2-CL1	2.36	1.79	1.73
4	B	703	CB3	C8A-N1	-2.16	1.34	1.37
4	A	703	CB3	C8A-N1	-2.11	1.34	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	CB3	C4A-C4-N3	-9.43	117.83	124.40
4	B	703	CB3	C4A-C4-N3	-9.00	118.13	124.40
4	A	703	CB3	C4A-C8A-N1	-8.35	119.07	123.60
4	B	703	CB3	C4A-C8A-N1	-8.04	119.23	123.60
5	A	704	73X	C7-C6-N	-6.44	98.18	110.70
5	A	704	73X	C7-N1-C8	6.28	125.37	111.52
5	B	704	73X	C7-N1-C8	5.85	124.43	111.52
5	A	704	73X	N2-C12-N3	-4.22	120.57	125.70
4	A	703	CB3	C4-N3-C2	3.98	122.25	115.93
5	B	704	73X	C7-C6-N	-3.94	103.04	110.70
5	B	704	73X	N2-C12-N3	-3.79	121.09	125.70
5	A	704	73X	C12-N3-C13	3.66	121.03	116.99
4	B	703	CB3	C4-N3-C2	3.66	121.74	115.93
4	A	703	CB3	N1-C2-N3	-3.42	122.66	127.22
5	B	704	73X	C6-N-C9	3.41	119.05	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NDP	N3A-C2A-N1A	-3.38	123.40	128.68
4	B	703	CB3	N1-C2-N3	-3.34	122.76	127.22
3	A	702	NDP	N3A-C2A-N1A	-3.27	123.57	128.68
4	B	703	CB3	C6-C9-N10	-3.10	109.20	114.18
4	A	703	CB3	C6-C9-N10	-3.03	109.31	114.18
5	B	704	73X	C12-N3-C13	2.93	120.22	116.99
4	B	703	CB3	C6-C5-C4A	-2.89	118.33	122.65
4	A	703	CB3	C6-C5-C4A	-2.76	118.52	122.65
5	A	704	73X	C8-C9-N	-2.75	105.35	110.70
5	B	704	73X	C4-C5-N	-2.56	118.58	121.33
3	A	702	NDP	C4A-C5A-N7A	-2.50	106.79	109.40
5	A	704	73X	C6-N-C9	2.43	116.89	111.52
4	B	703	CB3	C4-C4A-C8A	-2.40	116.50	118.59
4	A	703	CB3	C4-C4A-C8A	-2.37	116.52	118.59
3	A	702	NDP	PN-O3-PA	-2.36	124.72	132.83
5	A	704	73X	N5-C12-N3	2.36	120.92	117.25
5	B	704	73X	N5-C12-N2	2.33	119.80	117.44
5	A	704	73X	N4-C13-N3	2.25	120.22	117.03
5	A	704	73X	C11-N2-C12	2.22	120.56	116.44
5	B	704	73X	C11-N2-C12	2.21	120.54	116.44
4	A	703	CB3	C2-N1-C8A	2.16	121.67	116.33
3	A	702	NDP	O3X-P2B-O2X	2.15	115.83	107.64
4	B	703	CB3	C2-N1-C8A	2.14	121.63	116.33
3	B	702	NDP	C4A-C5A-N7A	-2.12	107.19	109.40
3	B	702	NDP	O3D-C3D-C4D	-2.09	105.01	111.05

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	NDP	C5B-O5B-PA-O2A
2	A	701	UMP	C5'-O5'-P-OP2
4	B	703	CB3	C11-C-N-CA
4	B	703	CB3	CT-CA-CB-CG
4	B	703	CB3	CA-CB-CG-CD
4	A	703	CB3	C11-C-N-CA
4	A	703	CB3	CT-CA-CB-CG
4	A	703	CB3	CA-CB-CG-CD
2	B	701	UMP	C3'-C4'-C5'-O5'
2	B	701	UMP	O4'-C4'-C5'-O5'
2	B	701	UMP	C5'-O5'-P-OP1
2	B	701	UMP	C5'-O5'-P-OP3

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Mol	Chain	Res	Type	Atoms
3	A	702	NDP	O4D-C4D-C5D-O5D
3	A	702	NDP	C3D-C4D-C5D-O5D
4	B	703	CB3	O-C-N-CA
4	A	703	CB3	O-C-N-CA
4	A	703	CB3	N-CA-CB-CG
5	A	704	73X	C11-C10-N1-C8
4	B	703	CB3	N-CA-CB-CG
5	B	704	73X	C11-C10-N1-C8
2	A	701	UMP	O4'-C4'-C5'-O5'
3	B	702	NDP	C5B-O5B-PA-O3
3	A	702	NDP	O4D-C1D-N1N-C2N
3	B	702	NDP	C5B-O5B-PA-O1A
3	B	702	NDP	O4D-C1D-N1N-C2N
5	A	704	73X	C13-C10-N1-C8
2	A	701	UMP	C3'-C4'-C5'-O5'
3	B	702	NDP	PA-O3-PN-O2N
3	A	702	NDP	PA-O3-PN-O1N
2	B	701	UMP	C5'-O5'-P-OP2
3	B	702	NDP	C2B-O2B-P2B-O2X
3	B	702	NDP	PN-O3-PA-O2A
3	A	702	NDP	PA-O3-PN-O2N
2	B	701	UMP	C4'-C5'-O5'-P
3	A	702	NDP	C2N-C3N-C7N-N7N
3	B	702	NDP	C4D-C5D-O5D-PN

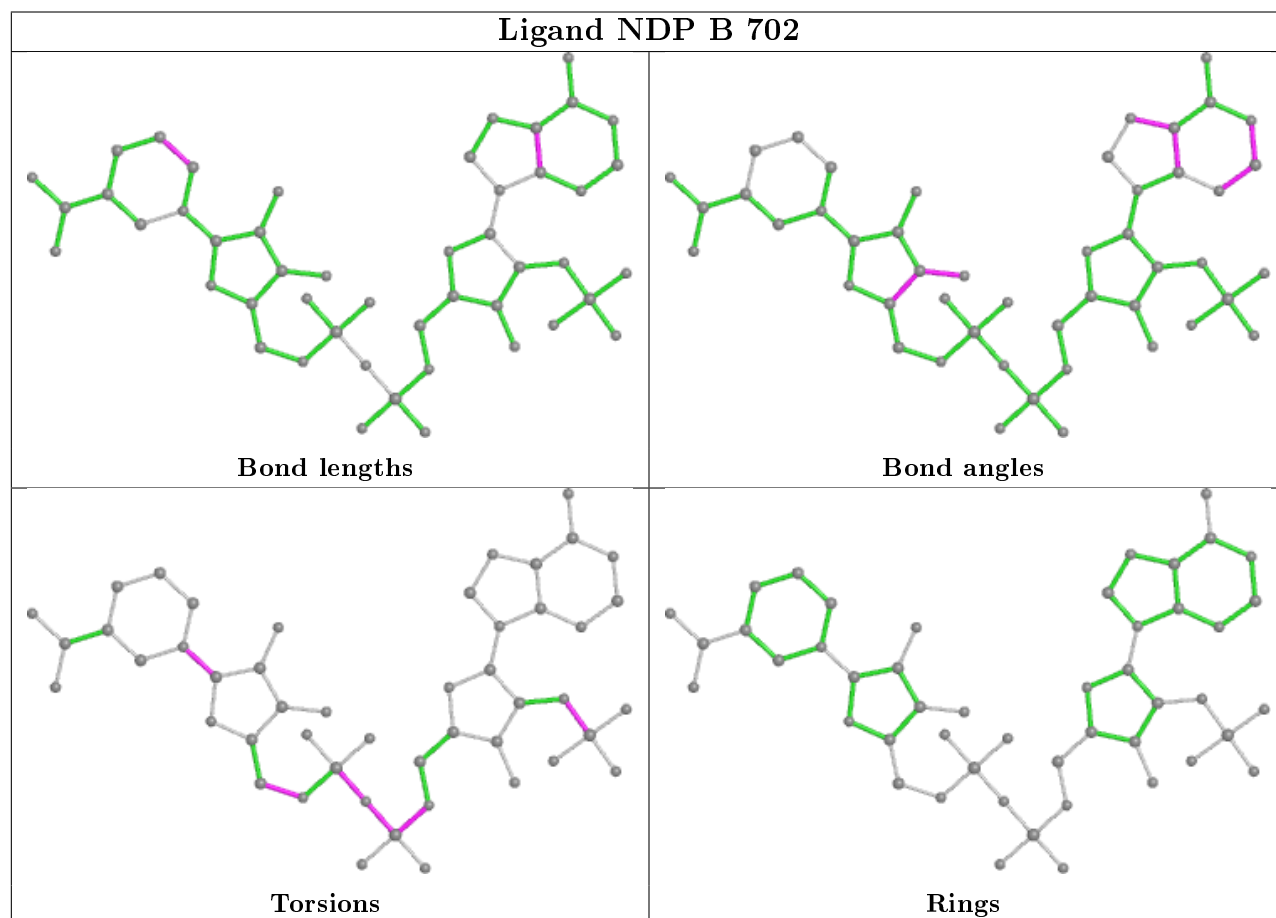
There are no ring outliers.

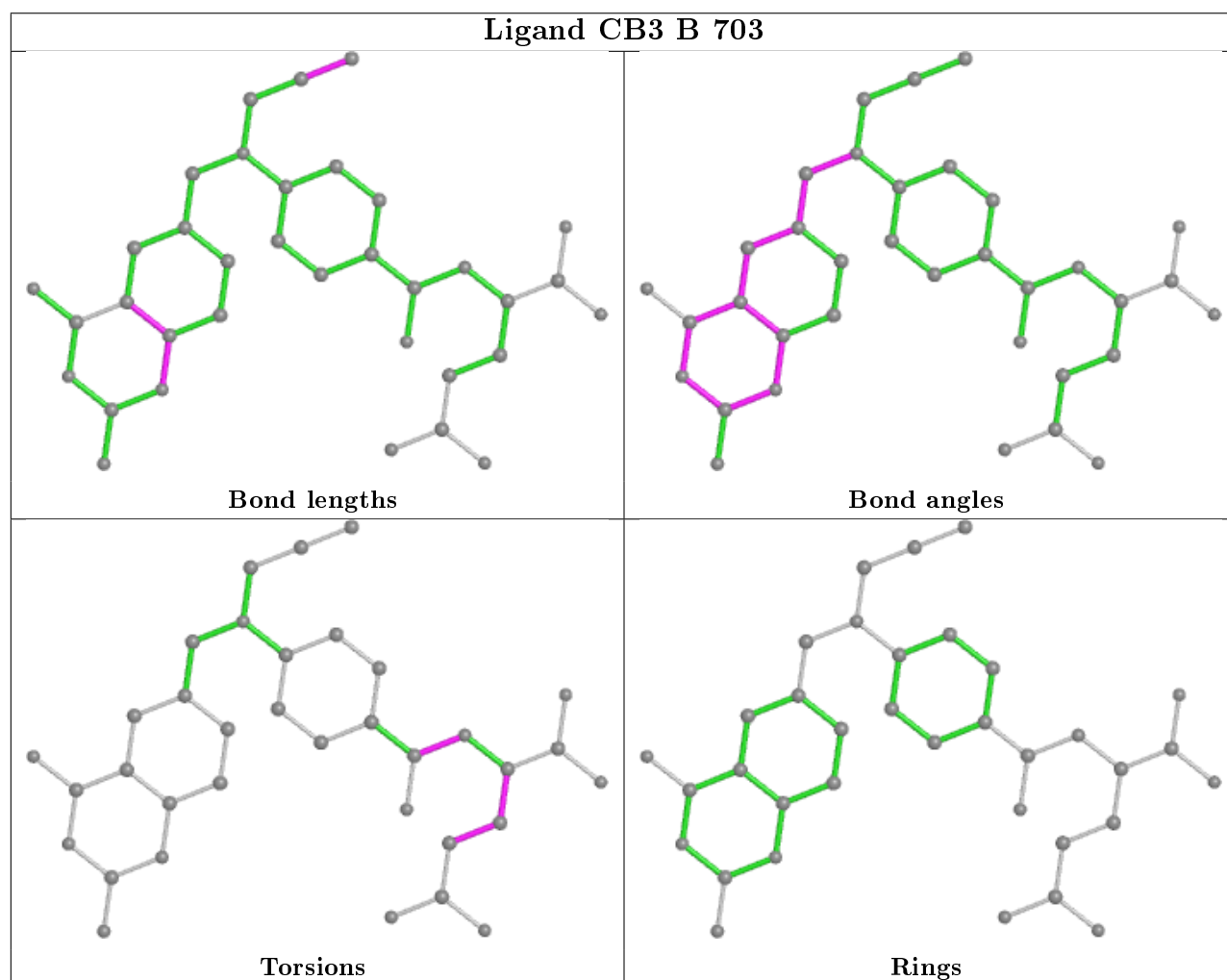
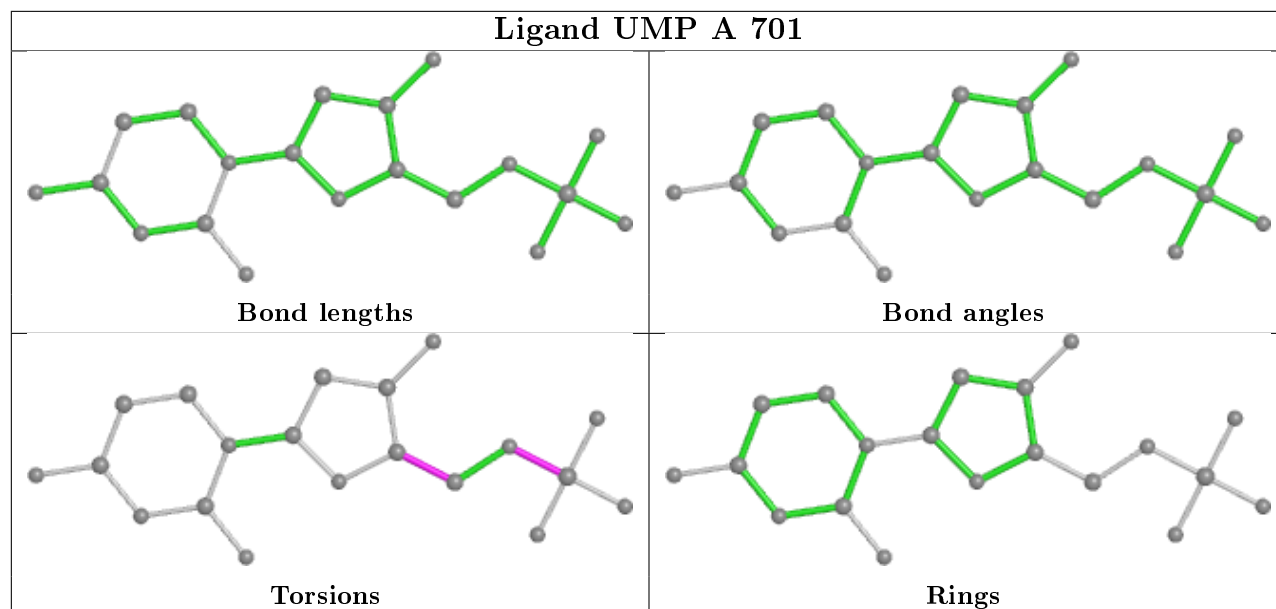
8 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	NDP	4	0
2	A	701	UMP	6	0
4	B	703	CB3	13	0
4	A	703	CB3	8	0
2	B	701	UMP	3	0
5	A	704	73X	4	0
5	B	704	73X	4	0
3	A	702	NDP	2	0

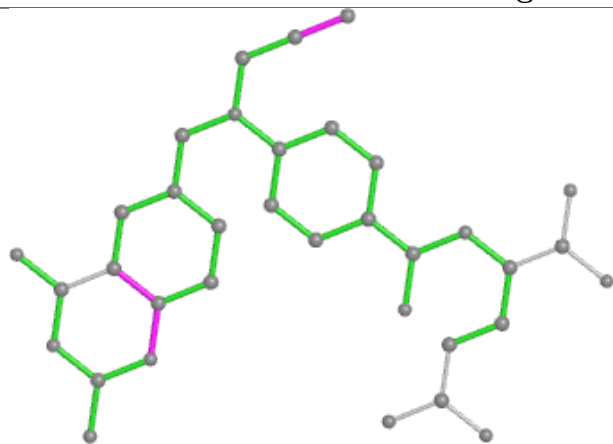
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

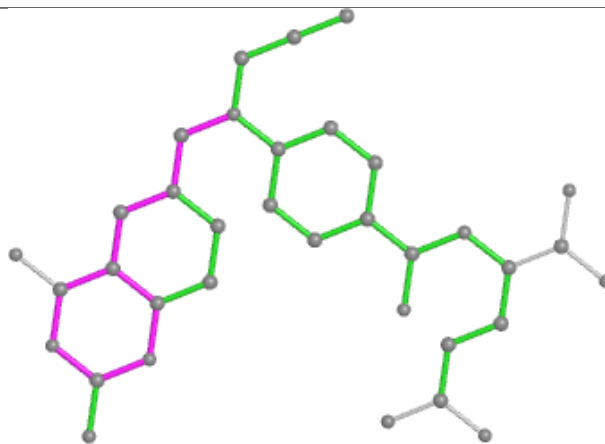




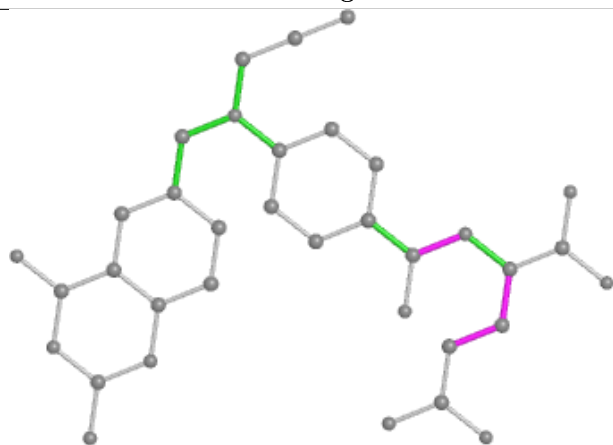
Ligand CB3 A 703



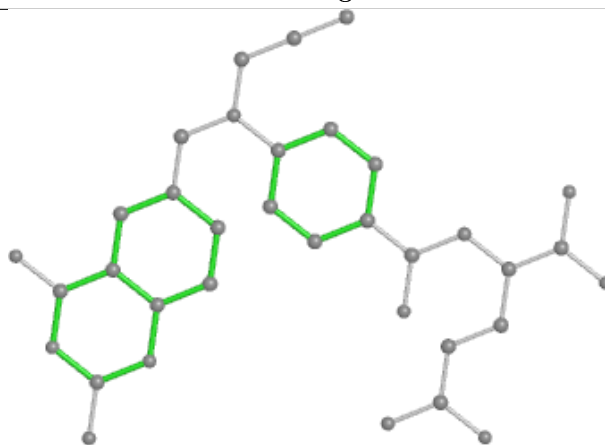
Bond lengths



Bond angles

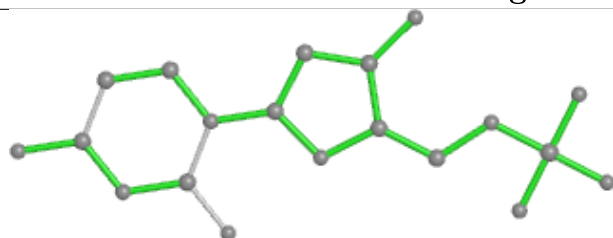


Torsions

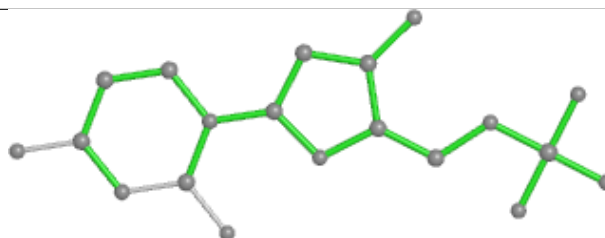


Rings

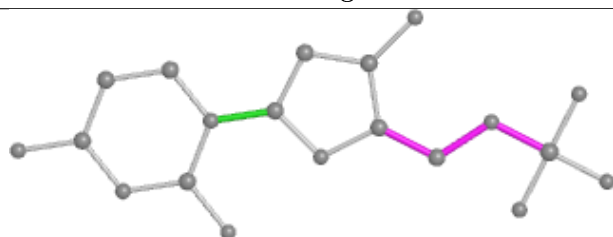
Ligand UMP B 701



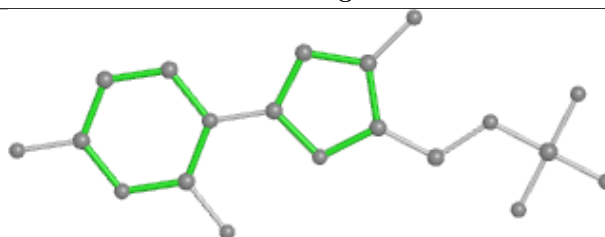
Bond lengths



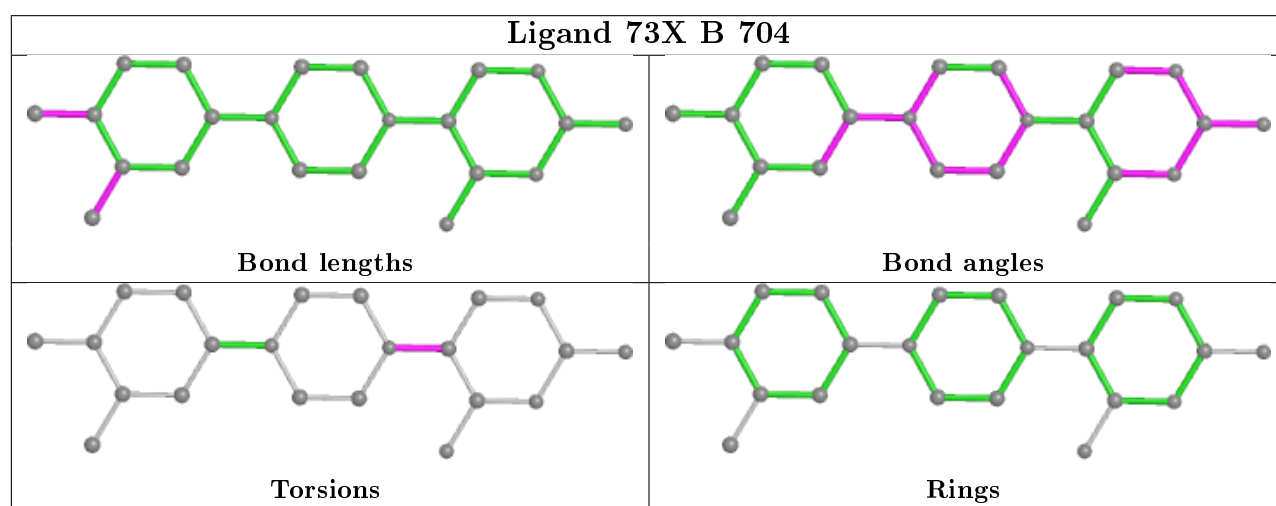
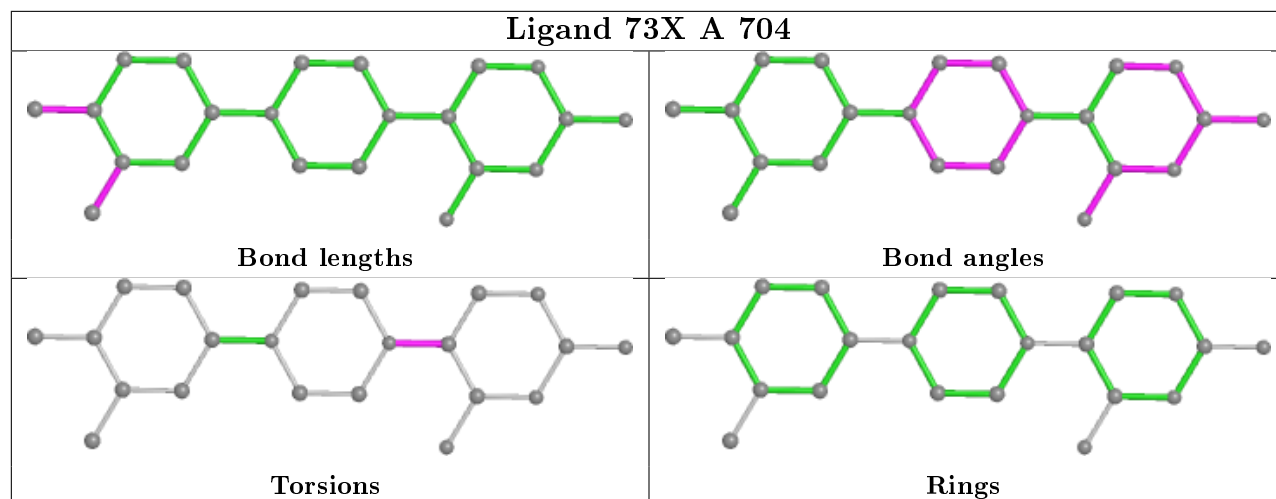
Bond angles

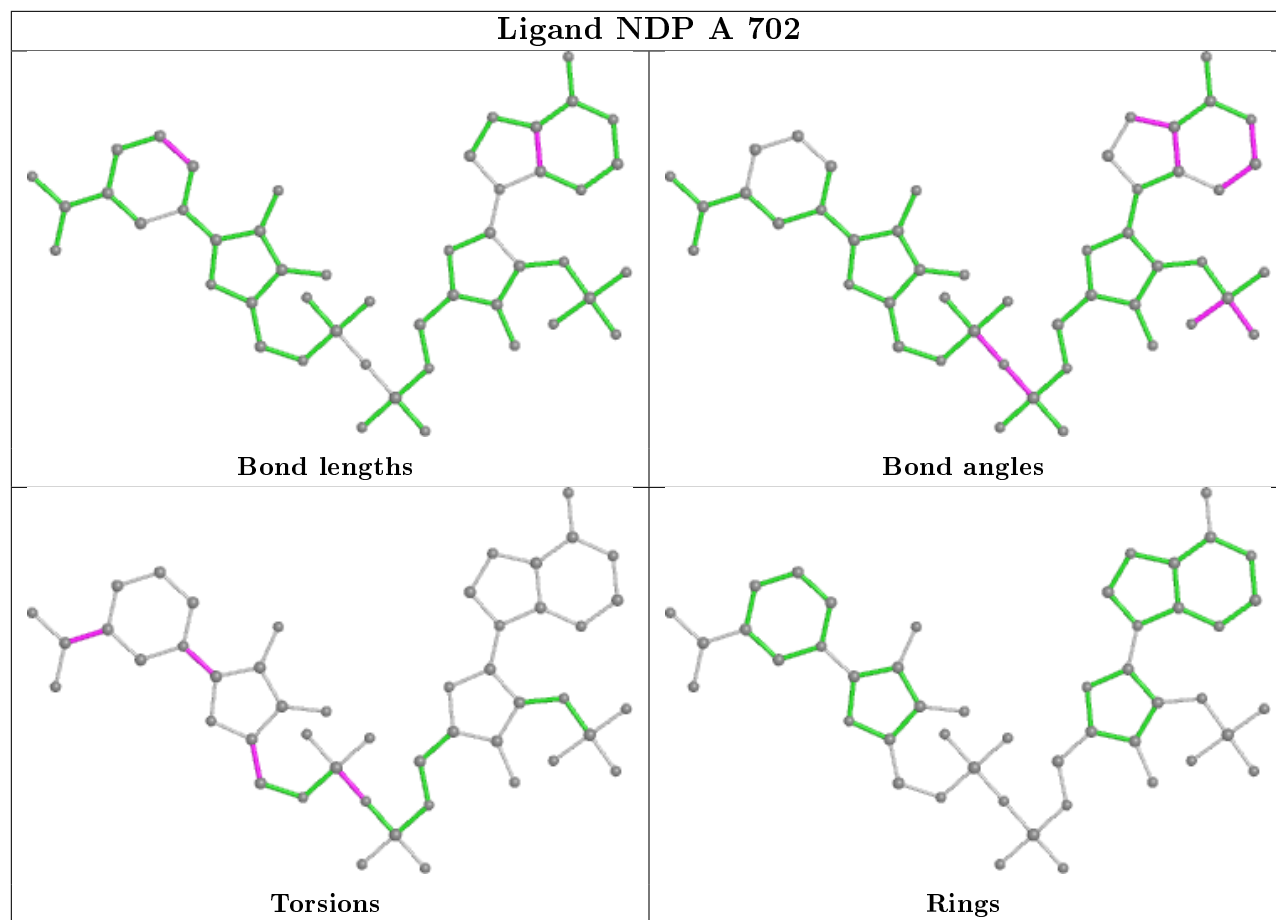


Torsions



Rings





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	508/566 (89%)	0.12	21 (4%)	37 19	48, 70, 109, 131	0
1	B	510/566 (90%)	0.17	24 (4%)	31 15	48, 74, 119, 138	0
All	All	1018/1132 (89%)	0.15	45 (4%)	34 17	48, 72, 114, 138	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	610	VAL	6.7
1	B	606	MET	4.8
1	B	423	GLY	4.4
1	B	117	GLN	4.0
1	A	609	ALA	3.8
1	A	607	GLU	3.7
1	B	47	SER	3.6
1	A	47	SER	3.5
1	B	422	VAL	3.5
1	A	606	MET	3.5
1	A	143	ASP	3.4
1	B	298	ASP	3.4
1	B	485	ALA	3.3
1	B	103	SER	3.2
1	A	423	GLY	3.2
1	A	555	ASN	3.1
1	A	410	GLU	3.1
1	B	604	ILE	3.1
1	A	139	GLU	3.0
1	A	499	ASP	2.9
1	B	318	HIS	2.9
1	A	141	TYR	2.8
1	A	117	GLN	2.8
1	B	119	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	406	ASN	2.7
1	B	605	GLN	2.7
1	B	607	GLU	2.7
1	B	419	HIS	2.7
1	B	290	ILE	2.7
1	B	610	VAL	2.6
1	A	120	GLY	2.6
1	A	128	ALA	2.6
1	A	419	HIS	2.4
1	A	489	CYS	2.4
1	A	493	CYS	2.3
1	B	84	TRP	2.3
1	B	120	GLY	2.2
1	B	252	ARG	2.2
1	B	143	ASP	2.2
1	A	140	GLU	2.2
1	B	139	GLU	2.2
1	A	42	THR	2.2
1	B	609	ALA	2.1
1	A	118	ALA	2.0
1	B	299	GLU	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 carbohydrates 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(\AA^2)	Q<0.9
5	73X	B	704	22/22	0.77	0.35	25,27,31,35	22
5	73X	A	704	22/22	0.78	0.37	25,27,31,35	22

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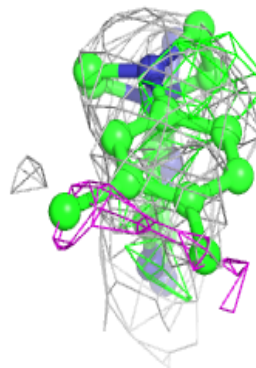
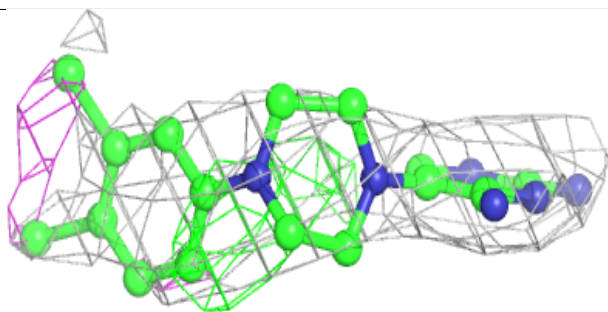
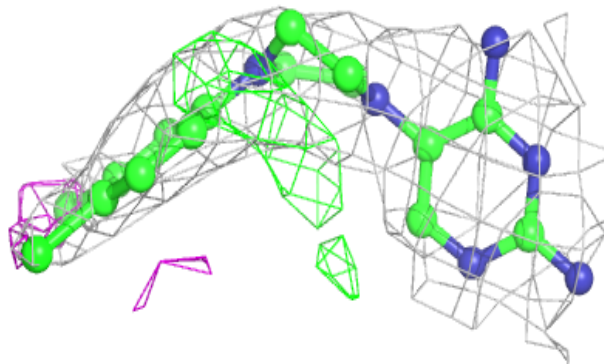
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CB3	B	703	35/35	0.80	0.36	21,22,23,23	35
4	CB3	A	703	35/35	0.81	0.35	20,22,28,29	35
3	NDP	B	702	48/48	0.92	0.19	70,78,94,95	0
2	UMP	B	701	20/20	0.93	0.19	78,83,85,85	0
2	UMP	A	701	20/20	0.94	0.20	72,75,77,77	0
3	NDP	A	702	48/48	0.94	0.15	69,78,92,93	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.

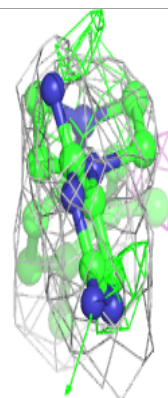
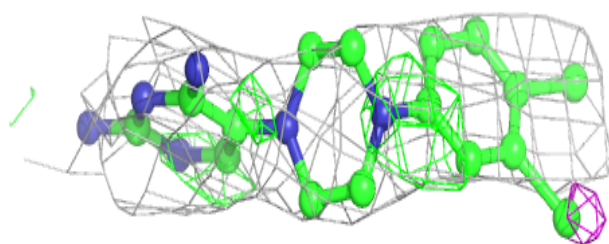
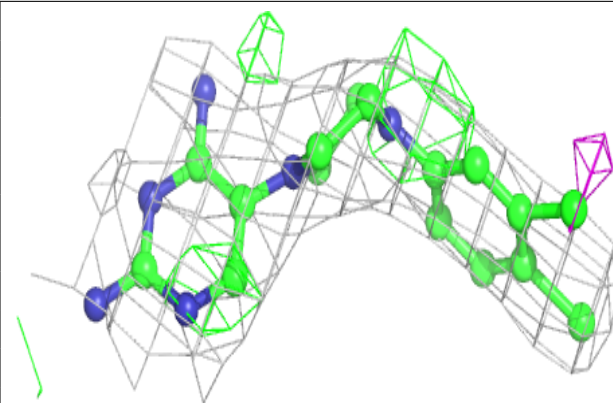
Electron density around 73X B 704:

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

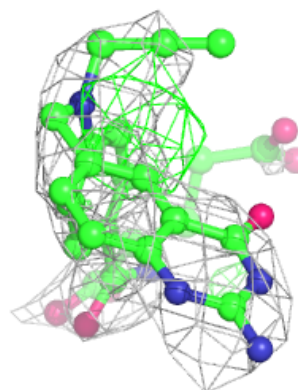
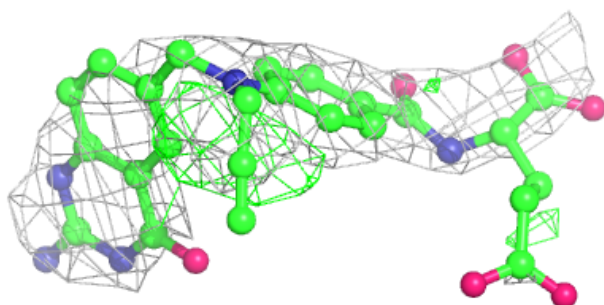
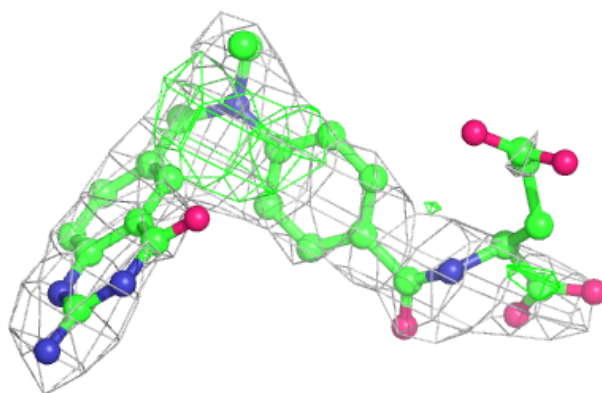


Electron density around 73X A 704:

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

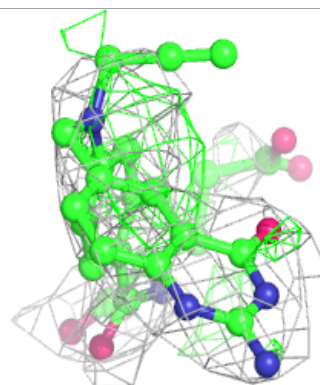
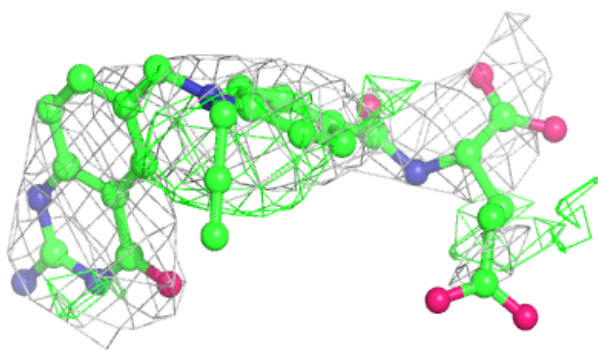
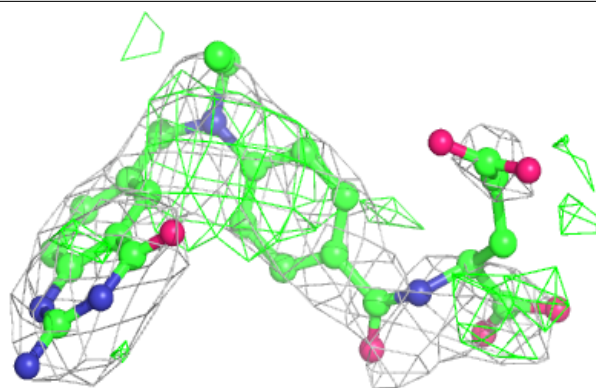
**Electron density around CB3 B 703:**

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

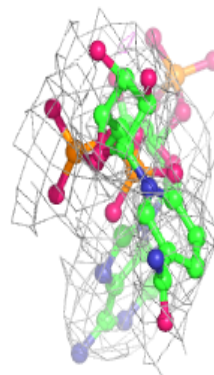
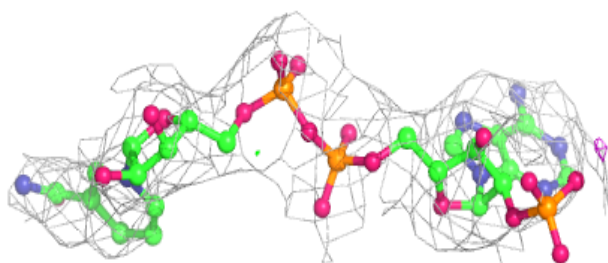
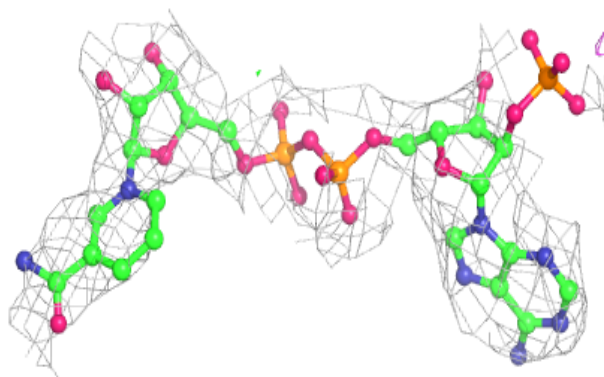


Electron density around CB3 A 703:

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

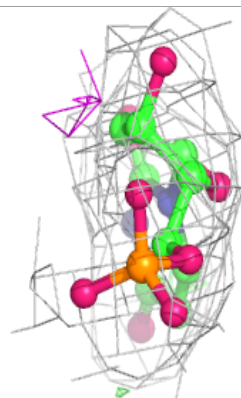
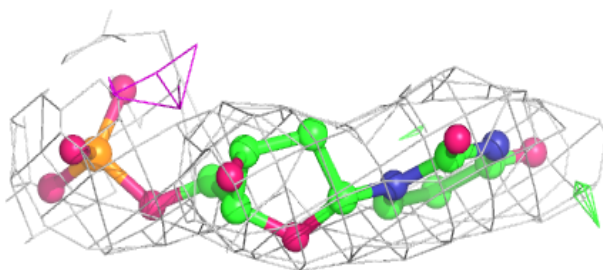
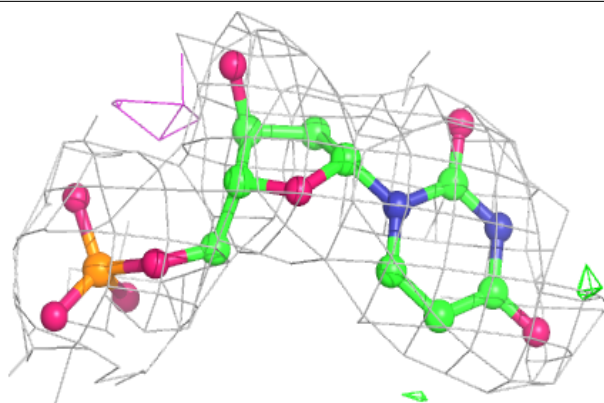
**Electron density around NDP B 702:**

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

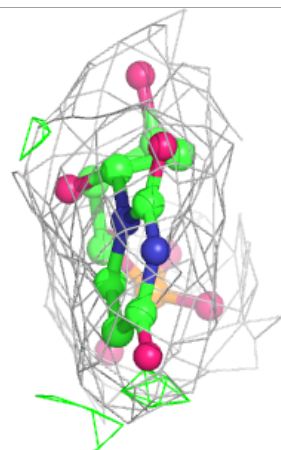
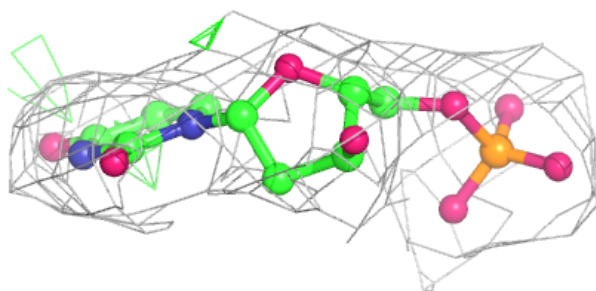
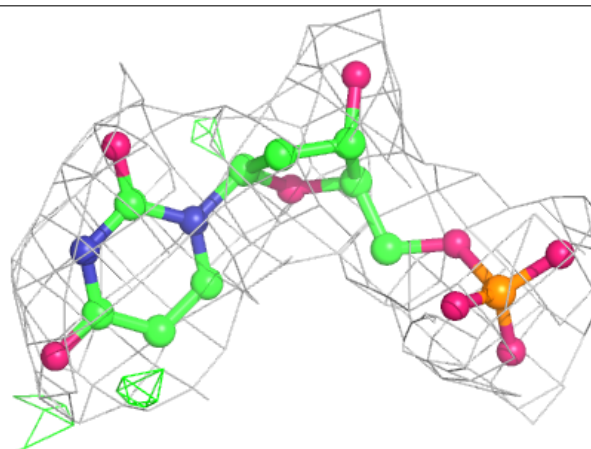


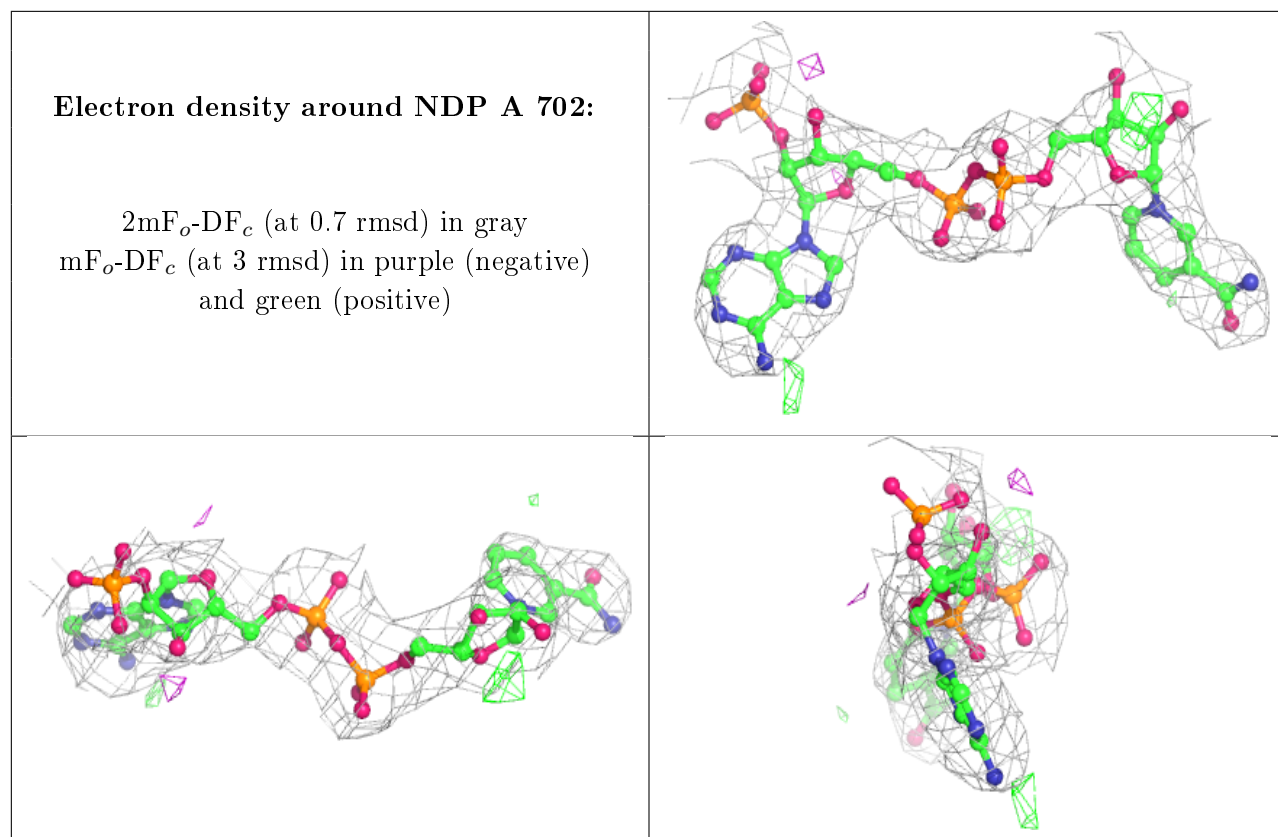
Electron density around UMP B 701:

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

**Electron density around UMP A 701:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.