



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:50 am BST

PDB ID : 3QG2  
Title : Plasmodium falciparum DHFR-TS quadruple mutant (N51I+C59R+S108N+I164L, V1/S) pyrimethamine complex  
Authors : Vanichtanankul, J.; Yuvaniyama, J.; Taweechai, S.; Chitnumsub, P.; Kamchonwongpaisan, S.; Yuthavong, Y.  
Deposited on : 2011-01-24  
Resolution : 2.30 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](mailto: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.

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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

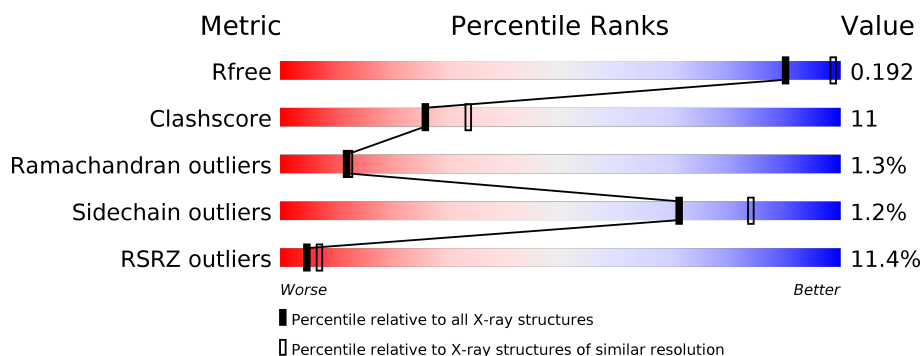
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	608	<div> <div>7%</div> <div>71%</div> <div>18%</div> <div>• 10%</div> </div>
1	B	608	<div> <div>13%</div> <div>68%</div> <div>21%</div> <div>• 11%</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
2	CP6	A	609	-	X	-	-
2	CP6	B	709	-	X	-	-

## 2 Entry composition [i](#)

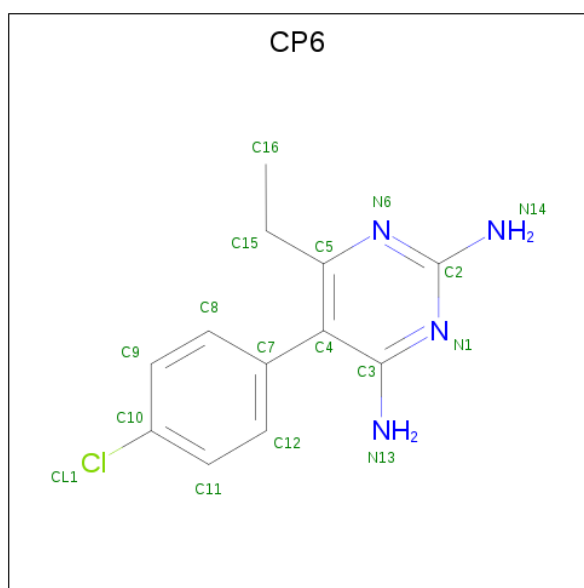
There are 5 unique types of molecules in this entry. The entry contains 9757 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	547	Total	C	N	O	S	0	0	0
			4550	2937	753	833	27			
1	B	542	Total	C	N	O	S	0	0	0
			4508	2912	745	824	27			

- Molecule 2 is 5-(4-CHLORO-PHENYL)-6-ETHYL-PYRIMIDINE-2,4-DIAMINE (three-letter code: CP6) (formula: C<sub>12</sub>H<sub>13</sub>ClN<sub>4</sub>).



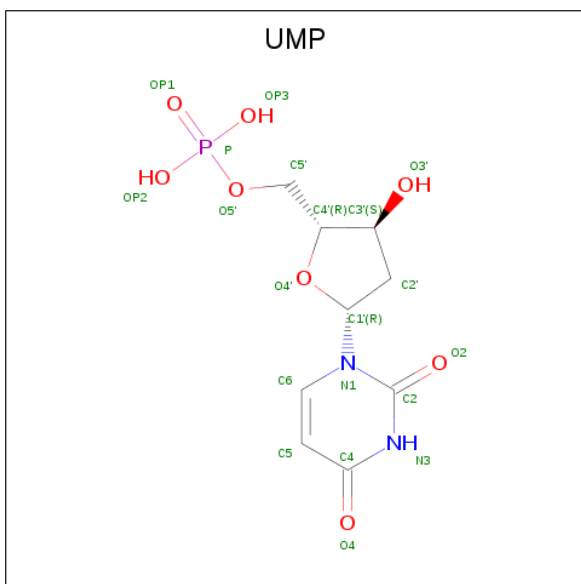
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			17	12	1	4		
2	B	1	Total	C	Cl	N	0	0
			17	12	1	4		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

- Molecule 4 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula:  $\text{C}_9\text{H}_{13}\text{N}_2\text{O}_8\text{P}$ ).



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

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

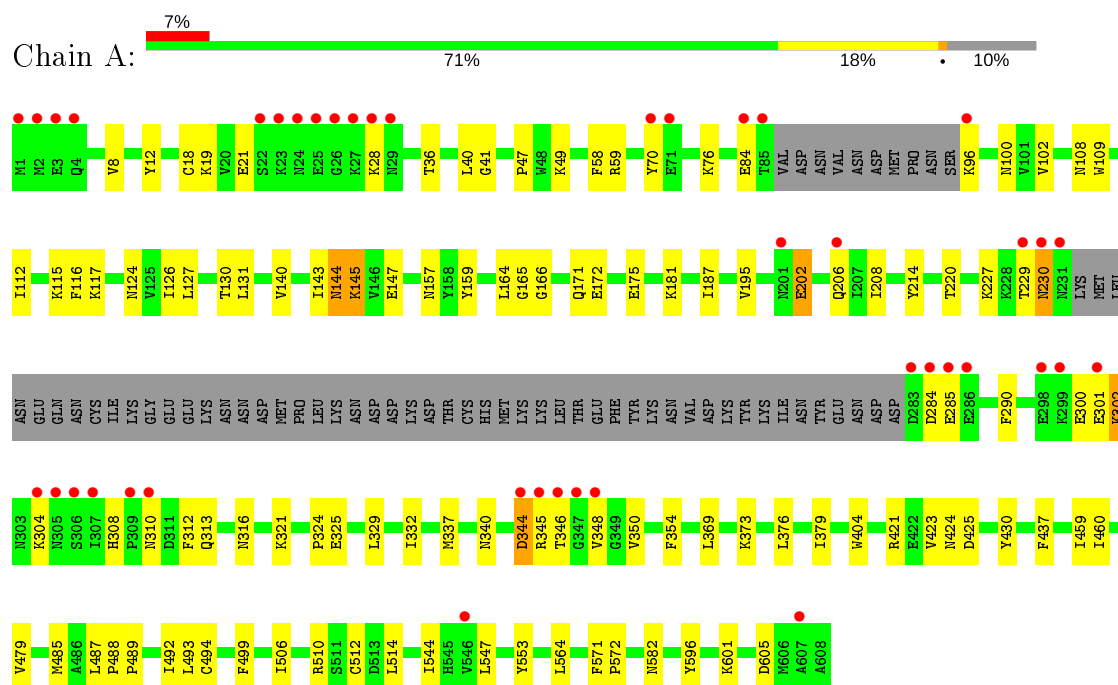
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	274	Total	O	0	0
			274	274		
5	B	255	Total	O	0	0
			255	255		

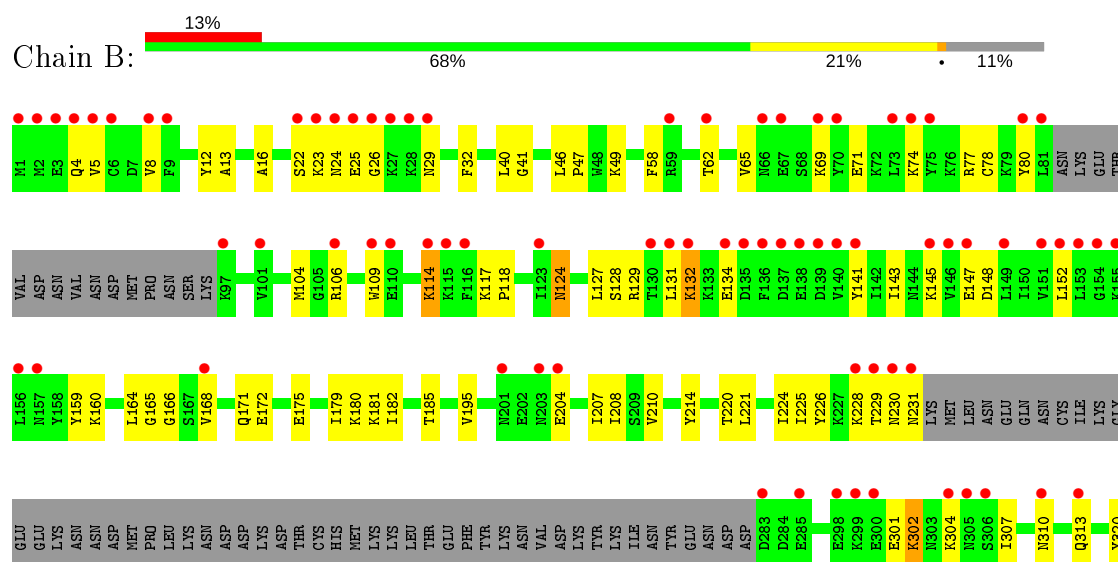
### 3 Residue-property plots

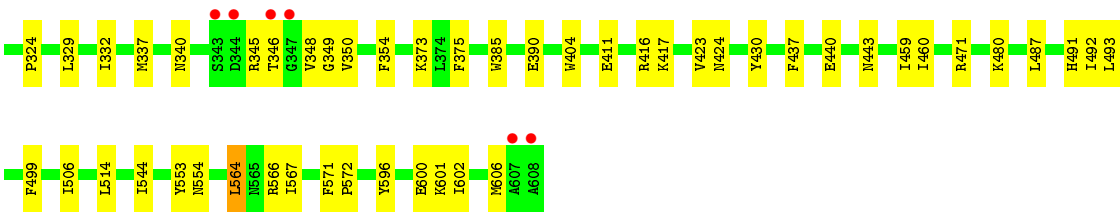
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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, $\alpha$ , $\beta$ , $\gamma$	56.49Å 155.27Å 165.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.30 49.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.39-2.30) 98.9 (49.38-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.20Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.198 , 0.233 0.192 , 0.192	Depositor DCC
$R_{free}$ test set	3712 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9757	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NDP, UMP, CP6

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	0.35	0/4655	0.60	0/6281
1	B	0.34	0/4613	0.59	0/6226
All	All	0.34	0/9268	0.59	0/12507

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	4550	0	4511	91	0
1	B	4508	0	4466	117	0
2	A	17	0	13	1	0
2	B	17	0	13	0	0
3	A	48	0	26	10	0
3	B	48	0	26	6	0
4	A	20	0	11	0	0
4	B	20	0	11	1	0
5	A	274	0	0	4	0
5	B	255	0	0	4	0
All	All	9757	0	9077	193	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 11.

All (193) 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:165:GLY:HA3	3:A:610:NDP:H5N	1.40	1.03
1:B:114:LYS:H	1:B:114:LYS:HD2	1.46	0.79
1:A:376:LEU:HD22	1:A:379:ILE:HD11	1.64	0.78
1:B:124:ASN:HD22	1:B:124:ASN:N	1.80	0.77
1:B:346:THR:HB	1:B:348:VAL:HG23	1.69	0.75
1:B:182:ILE:HB	1:B:226:TYR:HB2	1.71	0.72
1:A:344:ASP:CG	1:A:345:ARG:H	1.93	0.71
1:B:171:GLN:HE21	1:B:175:GLU:HG3	1.54	0.70
1:B:165:GLY:HA3	3:B:710:NDP:H5N	1.73	0.70
1:A:208:ILE:HD13	1:A:227:LYS:HB2	1.77	0.67
1:A:324:PRO:HB2	1:A:571:PHE:HE2	1.61	0.66
1:B:572:PRO:HB3	1:B:596:TYR:HA	1.79	0.64
1:A:171:GLN:O	1:A:175:GLU:HB2	1.97	0.64
1:A:145:LYS:HE3	5:A:1515:HOH:O	1.99	0.63
1:B:204:GLU:O	1:B:228:LYS:HD2	2.00	0.62
1:B:4:GLN:O	1:B:8:VAL:HG23	2.00	0.62
1:A:59:ARG:HH11	1:A:59:ARG:HG2	1.65	0.60
1:B:145:LYS:HB3	1:B:148:ASP:OD2	2.01	0.59
1:B:41:GLY:H	1:B:195:VAL:HG23	1.66	0.59
1:B:12:TYR:CD1	1:B:181:LYS:HB2	2.37	0.59
1:A:506:ILE:HG13	1:B:354:PHE:CE2	2.37	0.59
1:B:78:CYS:C	1:B:80:TYR:H	2.05	0.59
1:A:100:ASN:OD1	1:A:159:TYR:HB3	2.03	0.58
1:A:492:ILE:HD11	1:A:510:ARG:HD3	1.85	0.58
1:A:127:LEU:HD23	1:A:143:ILE:HG13	1.85	0.58
1:B:40:LEU:O	3:B:710:NDP:H2N	2.04	0.58
1:A:284:ASP:HB3	1:B:69:LYS:NZ	2.18	0.58
1:B:301:GLU:O	1:B:304:LYS:HG2	2.03	0.58
1:B:141:TYR:CD2	1:B:152:LEU:HD11	2.39	0.57
1:B:29:ASN:HB2	1:B:32:PHE:CZ	2.39	0.57
1:B:171:GLN:HE21	1:B:175:GLU:CG	2.16	0.57
1:B:349:GLY:HA3	1:B:554:ASN:ND2	2.20	0.57
1:B:41:GLY:N	1:B:195:VAL:HG23	2.20	0.57
1:B:302:LYS:HZ1	1:B:340:ASN:HA	1.70	0.56
1:A:202:GLU:CD	1:A:202:GLU:H	2.08	0.56
1:B:301:GLU:HB2	1:B:304:LYS:HG2	1.86	0.56
1:A:376:LEU:HD22	1:A:379:ILE:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:PHE:HE1	1:B:164:LEU:HD22	1.69	0.56
1:B:166:GLY:HA2	3:B:710:NDP:H5N	1.87	0.56
1:B:109:TRP:CZ2	1:B:117:LYS:HD3	2.40	0.56
1:B:208:ILE:HG22	1:B:225:ILE:O	2.05	0.55
1:B:65:VAL:HG13	1:B:159:TYR:HB2	1.88	0.55
1:A:166:GLY:HA2	3:A:610:NDP:C5N	2.36	0.55
1:A:302:LYS:HG3	5:A:1234:HOH:O	2.06	0.55
1:A:340:ASN:HB3	1:B:499:PHE:CE1	2.41	0.55
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.89	0.55
1:A:19:LYS:HG2	1:A:36:THR:HG22	1.89	0.55
1:B:166:GLY:HA2	3:B:710:NDP:C5N	2.37	0.54
1:B:145:LYS:HE3	1:B:147:GLU:HB2	1.89	0.54
1:A:350:VAL:HG12	1:A:553:TYR:CD1	2.43	0.53
1:A:290:PHE:HB2	1:B:320:TYR:OH	2.09	0.53
1:B:600:GLU:HG3	5:B:1517:HOH:O	2.07	0.53
1:B:77:ARG:O	1:B:80:TYR:HB3	2.08	0.53
1:B:302:LYS:NZ	1:B:340:ASN:HA	2.24	0.53
1:A:344:ASP:CG	1:A:345:ARG:N	2.62	0.53
1:A:166:GLY:HA2	3:A:610:NDP:C6N	2.38	0.52
1:A:572:PRO:HB3	1:A:596:TYR:HA	1.91	0.52
1:A:423:VAL:O	1:A:424:ASN:HB2	2.10	0.52
1:A:485:MET:SD	1:A:489:PRO:HD3	2.50	0.52
1:B:22:SER:C	1:B:24:ASN:H	2.12	0.52
1:B:423:VAL:O	1:B:424:ASN:HB2	2.08	0.52
1:B:141:TYR:H	1:B:141:TYR:HD1	1.56	0.52
1:B:310:ASN:O	1:B:313:GLN:HG3	2.09	0.52
1:A:488:PRO:HG2	1:B:471:ARG:HD3	1.92	0.52
1:B:58:PHE:CE1	1:B:164:LEU:HD22	2.45	0.52
1:B:307:ILE:HB	1:B:337:MET:CE	2.40	0.51
1:B:69:LYS:HZ2	1:B:69:LYS:HB3	1.74	0.51
1:A:166:GLY:HA2	3:A:610:NDP:H5N	1.93	0.51
1:A:373:LYS:HB3	1:A:601:LYS:HB3	1.92	0.51
1:B:229:THR:C	1:B:231:ASN:H	2.14	0.51
1:A:354:PHE:CE2	1:B:506:ILE:HG13	2.46	0.51
1:A:229:THR:HG22	1:A:230:ASN:ND2	2.27	0.50
1:A:512:CYS:SG	1:A:547:LEU:HD22	2.51	0.50
1:B:41:GLY:HA2	1:B:47:PRO:HD3	1.93	0.50
1:A:40:LEU:O	3:A:610:NDP:H2N	2.11	0.50
1:B:114:LYS:CD	1:B:114:LYS:H	2.13	0.50
1:B:127:LEU:HA	1:B:143:ILE:HG13	1.94	0.50
1:B:385:TRP:CD1	1:B:390:GLU:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ILE:HG12	1:A:544:ILE:HB	1.95	0.49
1:A:59:ARG:NH1	1:A:59:ARG:HG2	2.28	0.49
1:A:127:LEU:O	3:A:610:NDP:H1B	2.13	0.49
1:A:459:ILE:HG13	1:A:460:ILE:N	2.28	0.49
1:B:168:VAL:O	1:B:172:GLU:HG3	2.13	0.49
1:A:41:GLY:HA2	1:A:47:PRO:HD3	1.95	0.48
1:B:324:PRO:HB2	1:B:571:PHE:HE2	1.79	0.48
1:B:493:LEU:HD12	1:B:493:LEU:C	2.34	0.48
1:A:340:ASN:HB3	1:B:499:PHE:CZ	2.49	0.48
1:B:124:ASN:ND2	1:B:124:ASN:N	2.52	0.48
1:B:141:TYR:N	1:B:141:TYR:CD1	2.82	0.47
1:B:12:TYR:HD1	1:B:181:LYS:HB2	1.79	0.47
1:A:214:TYR:O	1:A:220:THR:HA	2.15	0.47
1:B:29:ASN:HB2	1:B:32:PHE:CE1	2.49	0.47
1:A:325:GLU:HG3	1:A:369:LEU:HD22	1.97	0.47
1:A:332:ILE:CD1	1:A:514:LEU:HB3	2.44	0.47
1:A:166:GLY:HA2	3:A:610:NDP:H6N	1.96	0.47
1:B:459:ILE:HG13	1:B:460:ILE:N	2.29	0.47
1:A:493:LEU:HD12	1:A:493:LEU:C	2.35	0.47
1:B:171:GLN:HG3	1:B:175:GLU:OE2	2.14	0.46
1:B:207:ILE:HB	1:B:567:ILE:HD13	1.96	0.46
1:A:285:GLU:HG3	1:B:180:LYS:HZ1	1.80	0.46
1:B:443:ASN:HB3	5:B:1434:HOH:O	2.14	0.46
1:B:109:TRP:CE2	1:B:117:LYS:HD3	2.51	0.46
1:B:104:MET:HA	1:B:165:GLY:O	2.14	0.46
1:B:350:VAL:HG12	1:B:553:TYR:CD1	2.51	0.46
1:A:112:ILE:O	1:A:117:LYS:HE3	2.15	0.46
1:A:115:LYS:HE3	1:A:116:PHE:CZ	2.50	0.46
1:A:404:TRP:CZ3	1:A:487:LEU:HD21	2.51	0.46
1:B:329:LEU:HD22	1:B:564:LEU:HD12	1.97	0.46
1:B:332:ILE:CD1	1:B:514:LEU:HB3	2.46	0.46
1:A:344:ASP:OD2	1:A:345:ARG:HG2	2.15	0.46
1:A:285:GLU:HG3	1:B:180:LYS:NZ	2.31	0.46
1:A:12:TYR:HD1	1:A:181:LYS:HB2	1.81	0.46
1:A:421:ARG:HD2	1:A:425:ASP:HB3	1.98	0.46
1:B:127:LEU:CD1	1:B:143:ILE:HG13	2.46	0.46
1:B:404:TRP:CZ3	1:B:487:LEU:HD21	2.51	0.46
1:A:172:GLU:OE2	3:A:610:NDP:N7A	2.49	0.45
1:B:106:ARG:HG2	1:B:106:ARG:HH11	1.81	0.45
1:A:493:LEU:CD2	1:B:492:ILE:HG21	2.46	0.45
1:B:349:GLY:C	1:B:554:ASN:ND2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASN:HB2	1:A:140:VAL:HG12	1.99	0.45
1:A:70:TYR:OH	1:A:157:ASN:HA	2.17	0.45
1:B:221:LEU:N	1:B:221:LEU:HD23	2.31	0.45
1:A:300:GLU:OE1	1:A:304:LYS:HD3	2.16	0.45
1:B:65:VAL:HG13	1:B:159:TYR:CG	2.52	0.45
1:B:480:LYS:HE2	5:B:1118:HOH:O	2.16	0.45
1:A:312:PHE:HB2	1:A:316:ASN:ND2	2.32	0.45
1:B:16:ALA:HA	1:B:185:THR:HB	1.98	0.45
1:A:582:ASN:HB3	5:A:1375:HOH:O	2.17	0.44
1:A:202:GLU:CD	1:A:202:GLU:N	2.69	0.44
1:B:118:PRO:HB2	1:B:124:ASN:OD1	2.18	0.44
1:A:284:ASP:CB	1:B:69:LYS:NZ	2.80	0.44
1:B:127:LEU:HD13	1:B:143:ILE:HG13	1.99	0.44
1:B:416:ARG:O	1:B:417:LYS:HB2	2.17	0.44
1:B:114:LYS:N	1:B:114:LYS:HD2	2.25	0.44
1:A:229:THR:HG22	1:A:230:ASN:HD22	1.82	0.44
1:B:65:VAL:HG13	1:B:159:TYR:CB	2.47	0.44
1:B:214:TYR:O	1:B:220:THR:HA	2.18	0.44
1:A:130:THR:O	1:A:131:LEU:HD23	2.17	0.44
1:A:202:GLU:O	1:A:206:GLN:NE2	2.51	0.44
1:A:8:VAL:HA	1:A:76:LYS:HD3	1.98	0.43
1:B:566:ARG:NH1	1:B:602:ILE:HD11	2.33	0.43
1:A:229:THR:HG22	1:A:230:ASN:N	2.33	0.43
1:B:78:CYS:C	1:B:80:TYR:N	2.70	0.43
1:A:321:LYS:HD2	5:A:1445:HOH:O	2.17	0.43
1:A:344:ASP:HB2	5:B:1246:HOH:O	2.19	0.43
1:A:109:TRP:CD2	1:A:126:ILE:HD11	2.54	0.43
1:A:144:ASN:C	1:A:144:ASN:HD22	2.20	0.43
1:B:128:SER:OG	1:B:129:ARG:N	2.52	0.43
1:B:12:TYR:CE2	1:B:160:LYS:HD3	2.54	0.43
1:B:307:ILE:HB	1:B:337:MET:HE3	2.00	0.43
1:B:71:GLU:HA	1:B:74:LYS:HB3	2.00	0.43
1:A:284:ASP:HB3	1:B:69:LYS:HZ3	1.83	0.43
1:B:12:TYR:HE2	1:B:160:LYS:HD3	1.84	0.43
1:B:129:ARG:HG3	3:B:710:NDP:H2A	2.01	0.43
1:A:109:TRP:CE3	1:A:126:ILE:HD11	2.54	0.42
1:A:84:GLU:CD	1:A:84:GLU:H	2.22	0.42
1:B:345:ARG:O	1:B:346:THR:CB	2.67	0.42
1:B:12:TYR:CE1	1:B:180:LYS:HD3	2.54	0.42
1:A:479:VAL:HB	1:B:437:PHE:CD1	2.54	0.42
1:B:207:ILE:HB	1:B:567:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:PHE:CE1	1:B:340:ASN:HB3	2.53	0.42
1:B:58:PHE:CE1	1:B:62:THR:HG21	2.54	0.42
1:A:41:GLY:H	1:A:195:VAL:HG13	1.84	0.42
1:A:499:PHE:CZ	1:B:340:ASN:HB3	2.55	0.42
1:B:349:GLY:CA	1:B:554:ASN:ND2	2.82	0.42
1:B:25:GLU:HG3	1:B:26:GLY:N	2.34	0.42
1:B:13:ALA:HB2	1:B:179:ILE:HD12	2.01	0.42
1:B:128:SER:OG	1:B:131:LEU:HG	2.20	0.42
1:A:18:CYS:HA	1:A:187:ILE:HB	2.02	0.42
1:B:491:HIS:CE1	4:B:711:UMP:O4	2.73	0.41
1:B:210:VAL:HG13	1:B:224:ILE:HG22	2.02	0.41
1:B:166:GLY:HA2	3:B:710:NDP:C6N	2.50	0.41
1:B:345:ARG:O	1:B:346:THR:HB	2.21	0.41
1:A:230:ASN:HD22	1:A:230:ASN:C	2.24	0.41
1:A:345:ARG:NE	1:A:348:VAL:HG21	2.36	0.41
1:B:411:GLU:CD	1:B:411:GLU:H	2.24	0.41
1:A:28:LYS:HA	1:A:28:LYS:HD2	1.77	0.41
1:B:229:THR:C	1:B:231:ASN:N	2.74	0.41
1:A:108:ASN:OD1	3:A:610:NDP:H6N	2.21	0.41
1:A:301:GLU:OE1	1:A:337:MET:HB3	2.20	0.40
1:A:102:VAL:HB	1:A:164:LEU:HD11	2.04	0.40
1:A:421:ARG:CD	1:A:425:ASP:HB3	2.52	0.40
1:A:437:PHE:C	1:A:437:PHE:CD1	2.94	0.40
1:A:108:ASN:OD1	3:A:610:NDP:C6N	2.70	0.40
1:B:46:LEU:HA	1:B:47:PRO:HD3	1.91	0.40
1:A:494:CYS:HA	1:A:506:ILE:O	2.22	0.40
1:A:329:LEU:HD22	1:A:564:LEU:HD12	2.03	0.40
1:B:22:SER:C	1:B:24:ASN:N	2.74	0.40
1:B:373:LYS:HE2	1:B:375:PHE:CE1	2.57	0.40
1:B:373:LYS:HB3	1:B:601:LYS:HB3	2.02	0.40
1:A:310:ASN:O	1:A:313:GLN:HG3	2.22	0.40
1:A:58:PHE:CZ	2:A:609:CP6:H12	2.56	0.40
1:B:132:LYS:C	1:B:134:GLU:H	2.23	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	541/608 (89%)	503 (93%)	31 (6%)	7 (1%)	12	12
1	B	536/608 (88%)	490 (91%)	39 (7%)	7 (1%)	12	12
All	All	1077/1216 (89%)	993 (92%)	70 (6%)	14 (1%)	12	12

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	ASP
1	A	346	THR
1	A	430	TYR
1	B	430	TYR
1	A	302	LYS
1	B	230	ASN
1	B	606	MET
1	A	21	GLU
1	B	302	LYS
1	A	49	LYS
1	A	308	HIS
1	B	5	VAL
1	B	23	LYS
1	B	132	LYS

### 5.3.2 Protein sidechains [i](#)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	510/570 (90%)	503 (99%)	7 (1%)	67	81
1	B	505/570 (89%)	500 (99%)	5 (1%)	76	87
All	All	1015/1140 (89%)	1003 (99%)	12 (1%)	71	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	144	ASN
1	A	145	LYS
1	A	147	GLU
1	A	202	GLU
1	A	230	ASN
1	A	605	ASP
1	B	49	LYS
1	B	114	LYS
1	B	124	ASN
1	B	440	GLU
1	B	564	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	99	GLN
1	A	144	ASN
1	A	230	ASN
1	A	294	ASN
1	A	316	ASN
1	A	394	ASN
1	A	424	ASN
1	A	450	ASN
1	A	554	ASN
1	B	99	GLN
1	B	171	GLN
1	B	316	ASN
1	B	394	ASN
1	B	407	ASN
1	B	424	ASN
1	B	554	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	710	-	45,52,52	1.41	6 (13%)	53,80,80	1.51	8 (15%)
2	CP6	B	709	-	18,18,18	3.76	15 (83%)	25,25,25	1.94	8 (32%)
4	UMP	A	611	-	18,21,21	1.90	3 (16%)	21,31,31	1.68	6 (28%)
3	NDP	A	610	-	45,52,52	1.42	6 (13%)	53,80,80	1.55	7 (13%)
4	UMP	B	711	-	18,21,21	1.96	3 (16%)	21,31,31	1.71	6 (28%)
2	CP6	A	609	-	18,18,18	3.55	14 (77%)	25,25,25	1.93	7 (28%)

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	710	-	-	2/30/77/77	0/5/5/5
2	CP6	B	709	-	-	0/6/6/6	0/2/2/2
4	UMP	A	611	-	-	1/7/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	A	610	-	-	2/30/77/77	0/5/5/5
4	UMP	B	711	-	-	2/7/22/22	0/2/2/2
2	CP6	A	609	-	-	0/6/6/6	0/2/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	709	CP6	C4-C5	6.57	1.55	1.40
2	A	609	CP6	C4-C5	6.28	1.54	1.40
2	B	709	CP6	C9-C10	6.16	1.49	1.38
4	B	711	UMP	C4-N3	5.59	1.42	1.33
4	A	611	UMP	C4-N3	5.55	1.42	1.33
2	A	609	CP6	C9-C10	5.23	1.47	1.38
2	B	709	CP6	C12-C7	5.17	1.50	1.39
2	A	609	CP6	C12-C7	5.10	1.50	1.39
3	B	710	NDP	C6N-N1N	4.70	1.49	1.37
3	A	610	NDP	C6N-N1N	4.48	1.48	1.37
2	B	709	CP6	C12-C11	4.25	1.46	1.38
2	B	709	CP6	C3-N1	4.19	1.41	1.35
2	A	609	CP6	C12-C11	4.07	1.46	1.38
2	A	609	CP6	C10-CL1	-4.04	1.65	1.74
2	B	709	CP6	C4-C3	4.04	1.52	1.43
2	A	609	CP6	C2-N6	3.91	1.42	1.35
2	B	709	CP6	C10-CL1	-3.80	1.66	1.74
2	B	709	CP6	C9-C8	3.80	1.45	1.38
2	A	609	CP6	C4-C3	3.77	1.51	1.43
2	B	709	CP6	C2-N1	3.72	1.42	1.35
4	B	711	UMP	O4'-C1'	3.69	1.50	1.42
4	A	611	UMP	O4'-C1'	3.67	1.50	1.42
2	A	609	CP6	C2-N1	3.57	1.41	1.35
2	B	709	CP6	C2-N14	3.54	1.41	1.33
2	B	709	CP6	C2-N6	3.50	1.41	1.35
2	A	609	CP6	C5-N6	3.36	1.40	1.34
2	A	609	CP6	C4-C7	-3.14	1.44	1.50
2	A	609	CP6	C11-C10	3.09	1.43	1.38
2	A	609	CP6	C2-N14	2.91	1.39	1.33
2	A	609	CP6	C9-C8	2.84	1.43	1.38
3	B	710	NDP	C4A-N3A	2.83	1.39	1.35
2	A	609	CP6	C3-N1	2.79	1.39	1.35
2	B	709	CP6	C11-C10	2.72	1.43	1.38
2	B	709	CP6	C5-N6	2.72	1.39	1.34
3	B	710	NDP	C7N-C3N	2.71	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	610	NDP	C4A-N3A	2.63	1.39	1.35
3	A	610	NDP	C7N-C3N	2.49	1.54	1.48
2	B	709	CP6	C8-C7	2.47	1.44	1.39
2	B	709	CP6	C4-C7	-2.26	1.45	1.50
4	A	611	UMP	P-OP3	-2.18	1.46	1.54
4	B	711	UMP	P-OP3	-2.15	1.46	1.54
3	A	610	NDP	C5D-C4D	2.14	1.58	1.51
3	B	710	NDP	C8A-N7A	2.14	1.38	1.34
3	B	710	NDP	O4D-C1D	2.12	1.47	1.42
3	A	610	NDP	C8A-N7A	2.11	1.38	1.34
3	B	710	NDP	C5D-C4D	2.02	1.57	1.51
3	A	610	NDP	O4D-C1D	2.00	1.46	1.42

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	710	NDP	N3A-C2A-N1A	-5.91	119.44	128.68
3	A	610	NDP	N3A-C2A-N1A	-5.65	119.85	128.68
2	A	609	CP6	C15-C5-C4	-4.36	119.54	122.57
3	A	610	NDP	C1B-N9A-C4A	-3.85	119.87	126.64
2	B	709	CP6	C15-C5-C4	-3.78	119.95	122.57
2	B	709	CP6	C2-N6-C5	3.74	119.36	116.24
3	A	610	NDP	O2B-C2B-C3B	-3.64	98.50	111.68
2	A	609	CP6	C11-C10-CL1	3.58	124.95	119.35
3	B	710	NDP	O4B-C1B-C2B	-3.56	100.41	106.59
4	A	611	UMP	C5-C4-N3	-3.39	115.84	123.31
2	B	709	CP6	C3-C4-C5	-3.33	113.17	115.91
4	B	711	UMP	C5-C4-N3	-3.31	116.03	123.31
2	A	609	CP6	C9-C10-CL1	-3.26	114.26	119.35
3	A	610	NDP	O4B-C1B-C2B	-3.20	101.03	106.59
2	A	609	CP6	C2-N6-C5	3.08	118.81	116.24
3	B	710	NDP	C1B-N9A-C4A	-3.07	121.24	126.64
4	B	711	UMP	O4'-C1'-C2'	-3.00	100.58	106.25
2	B	709	CP6	C11-C10-CL1	2.96	123.98	119.35
3	B	710	NDP	O2B-C2B-C3B	-2.94	101.01	111.68
2	A	609	CP6	C2-N1-C3	2.89	120.18	116.99
4	A	611	UMP	O4'-C1'-C2'	-2.87	100.82	106.25
2	B	709	CP6	C2-N1-C3	2.84	120.13	116.99
4	B	711	UMP	C2'-C1'-N1	2.84	120.81	114.27
4	B	711	UMP	C4'-O4'-C1'	2.83	116.29	109.45
3	A	610	NDP	C2A-N1A-C6A	2.77	123.49	118.75
2	A	609	CP6	C3-C4-C5	-2.75	113.65	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	611	UMP	C4'-O4'-C1'	2.71	116.00	109.45
4	A	611	UMP	C2'-C1'-N1	2.68	120.44	114.27
3	B	710	NDP	C2A-N1A-C6A	2.67	123.32	118.75
3	A	610	NDP	C3N-C2N-N1N	-2.57	119.43	123.10
4	B	711	UMP	O4'-C4'-C3'	-2.53	99.77	105.67
2	B	709	CP6	C9-C10-CL1	-2.51	115.44	119.35
4	A	611	UMP	O4'-C4'-C3'	-2.36	100.16	105.67
2	B	709	CP6	N13-C3-N1	2.35	120.36	117.03
4	A	611	UMP	C2'-C3'-C4'	2.30	107.56	102.76
4	B	711	UMP	C2'-C3'-C4'	2.16	107.26	102.76
3	B	710	NDP	C1D-N1N-C2N	-2.14	117.55	121.11
3	B	710	NDP	PN-O3-PA	-2.12	125.54	132.83
2	B	709	CP6	C8-C7-C4	2.12	124.31	120.79
2	A	609	CP6	N13-C3-N1	2.10	120.00	117.03
3	B	710	NDP	C3N-C2N-N1N	-2.01	120.22	123.10
3	A	610	NDP	O5B-C5B-C4B	-2.01	102.08	108.99

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	710	NDP	O4D-C1D-N1N-C2N
3	A	610	NDP	O4D-C1D-N1N-C2N
4	A	611	UMP	O4'-C4'-C5'-O5'
4	B	711	UMP	C3'-C4'-C5'-O5'
3	B	710	NDP	C2N-C3N-C7N-N7N
3	A	610	NDP	C2N-C3N-C7N-N7N
4	B	711	UMP	O4'-C4'-C5'-O5'

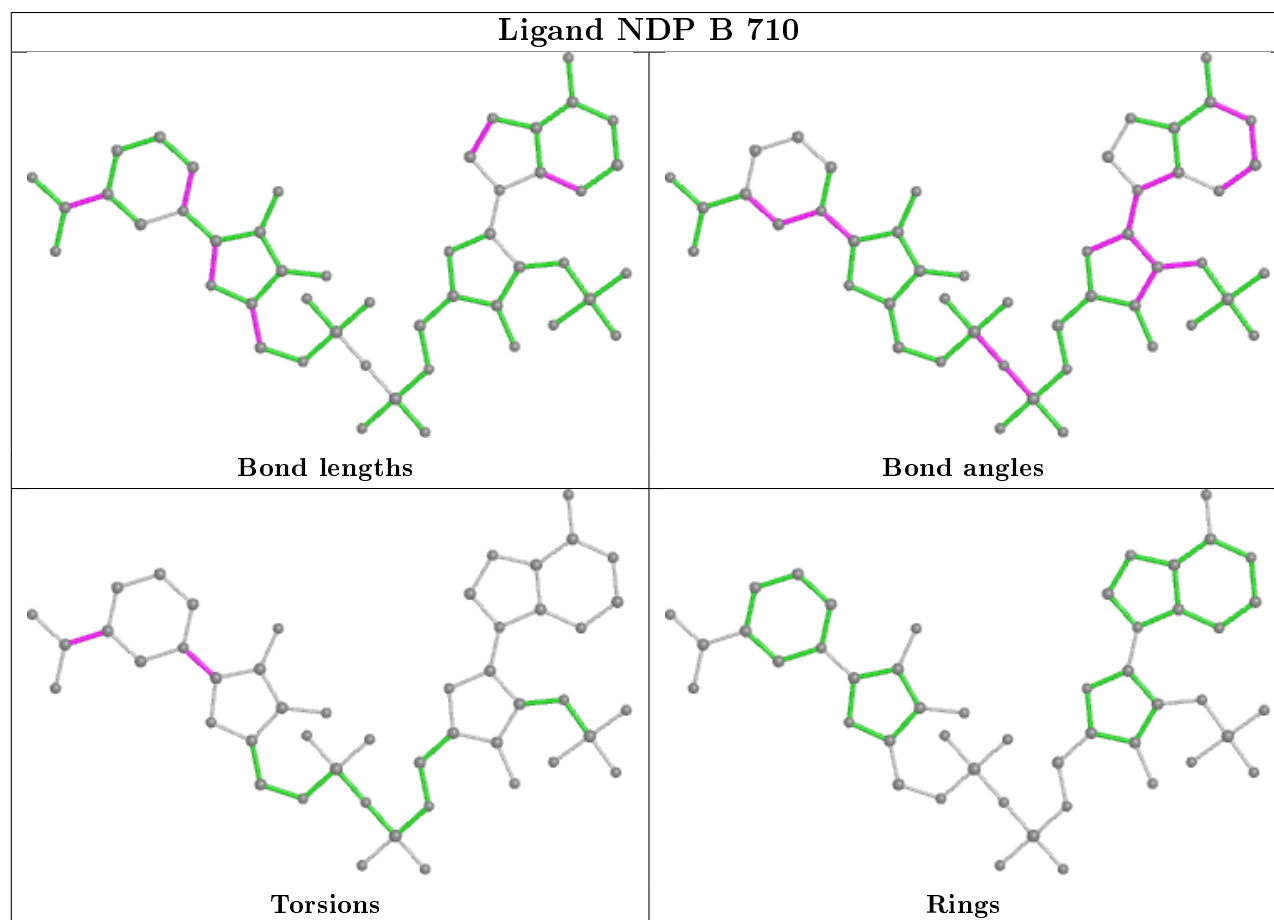
There are no ring outliers.

4 monomers are involved in 18 short contacts:

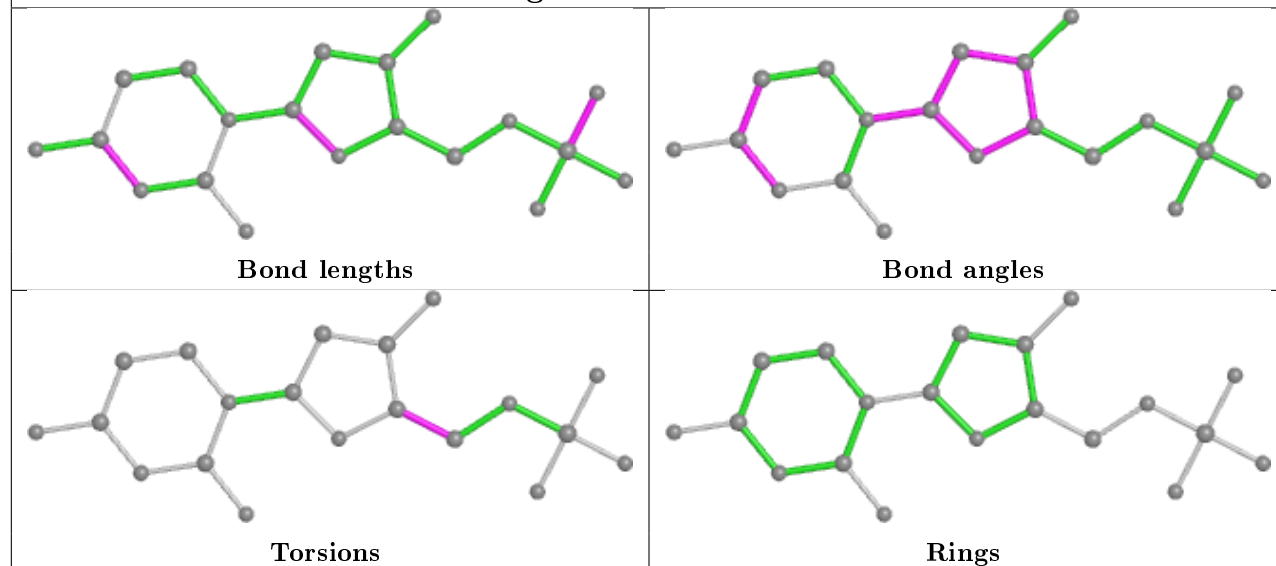
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	710	NDP	6	0
3	A	610	NDP	10	0
4	B	711	UMP	1	0
2	A	609	CP6	1	0

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

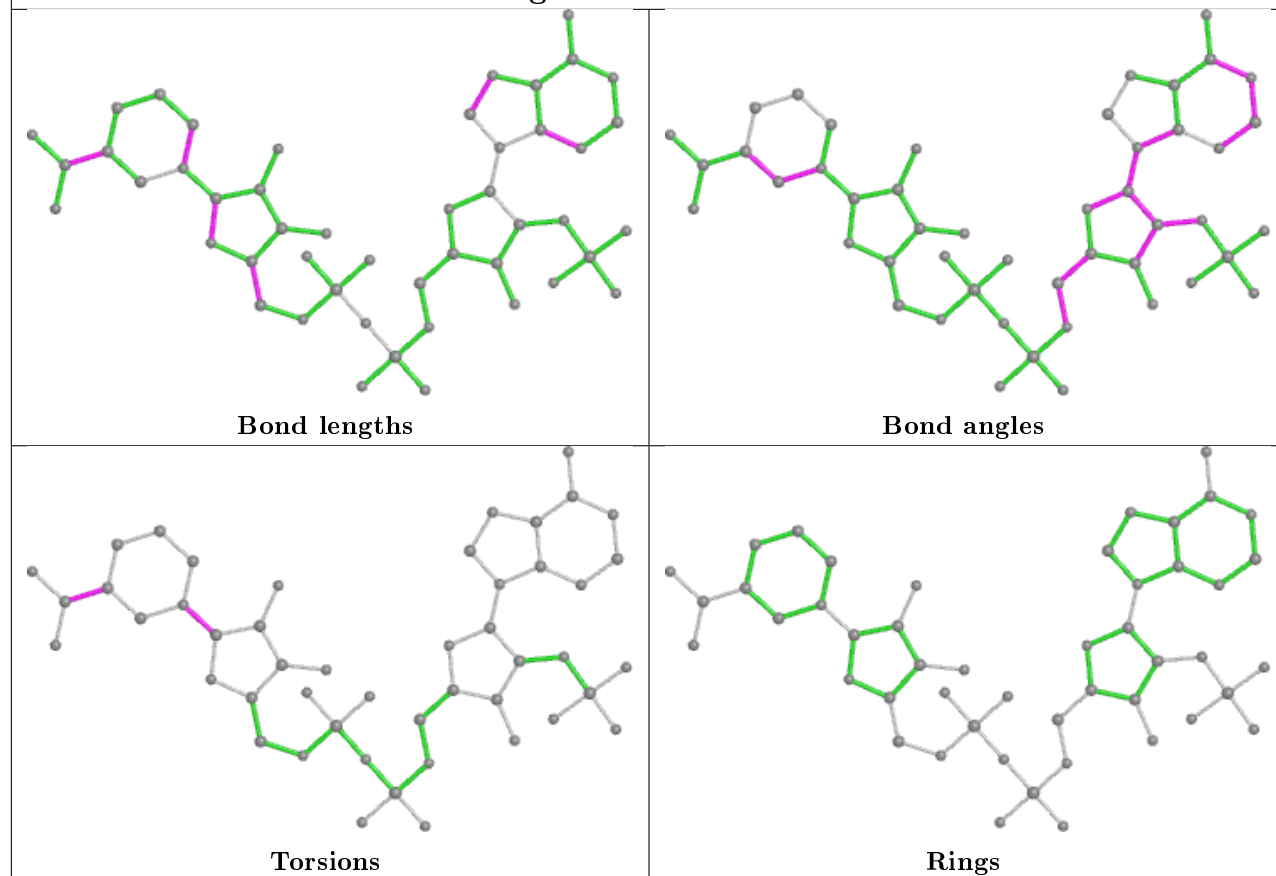
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

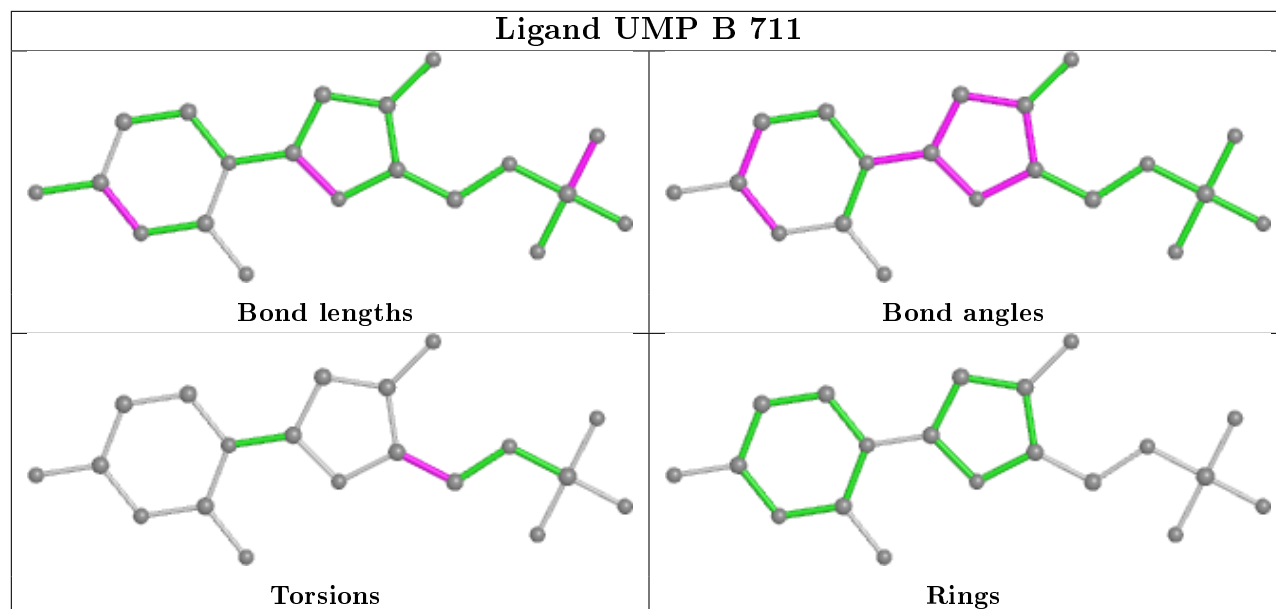


## Ligand UMP A 611



## Ligand NDP A 610





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	547/608 (89%)	0.17	42 (7%) 13 17	17, 30, 80, 90	0
1	B	542/608 (89%)	0.55	82 (15%) 2 3	16, 36, 89, 90	0
All	All	1089/1216 (89%)	0.36	124 (11%) 5 7	16, 32, 88, 90	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	GLY	12.5
1	A	1	MET	11.9
1	B	608	ALA	11.8
1	B	27	LYS	11.0
1	A	24	ASN	9.9
1	B	2	MET	9.7
1	B	28	LYS	9.4
1	A	346	THR	9.2
1	B	1	MET	8.3
1	A	25	GLU	8.3
1	A	231	ASN	8.3
1	A	299	LYS	8.1
1	A	230	ASN	7.7
1	A	2	MET	7.7
1	B	3	GLU	7.6
1	B	230	ASN	7.5
1	A	27	LYS	7.4
1	B	136	PHE	7.1
1	B	346	THR	7.1
1	B	23	LYS	7.0
1	B	344	ASP	6.6
1	B	135	ASP	6.5
1	A	26	GLY	6.3
1	B	4	GLN	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	75	TYR	5.8
1	A	85	THR	5.8
1	B	22	SER	5.5
1	B	138	GLU	5.4
1	B	25	GLU	5.4
1	A	284	ASP	5.3
1	B	81	LEU	5.3
1	B	151	VAL	5.1
1	B	231	ASN	5.1
1	B	305	ASN	5.0
1	B	141	TYR	4.9
1	B	134	GLU	4.6
1	B	139	ASP	4.6
1	A	345	ARG	4.6
1	A	285	GLU	4.3
1	B	299	LYS	4.3
1	A	306	SER	4.3
1	B	9	PHE	4.2
1	A	307	ILE	4.2
1	B	66	ASN	4.2
1	A	23	LYS	4.2
1	B	24	ASN	4.1
1	B	115	LYS	4.1
1	A	305	ASN	4.1
1	A	29	ASN	4.1
1	A	607	ALA	4.0
1	B	283	ASP	4.0
1	B	203	ASN	4.0
1	B	97	LYS	3.9
1	B	285	GLU	3.9
1	B	116	PHE	3.7
1	B	347	GLY	3.7
1	B	110	GLU	3.6
1	B	306	SER	3.5
1	B	130	THR	3.5
1	A	298	GLU	3.5
1	B	157	ASN	3.4
1	B	70	TYR	3.4
1	B	137	ASP	3.4
1	A	3	GLU	3.3
1	B	313	GLN	3.3
1	B	155	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	140	VAL	3.2
1	B	131	LEU	3.1
1	A	28	LYS	3.1
1	B	154	GLY	3.1
1	A	347	GLY	3.0
1	B	168	VAL	3.0
1	A	309	PRO	3.0
1	B	304	LYS	2.9
1	B	29	ASN	2.9
1	B	156	LEU	2.8
1	A	22	SER	2.7
1	B	201	ASN	2.7
1	B	73	LEU	2.7
1	B	6	CYS	2.6
1	B	74	LYS	2.6
1	B	101	VAL	2.6
1	A	286	GLU	2.6
1	B	109	TRP	2.6
1	A	84	GLU	2.6
1	A	96	LYS	2.6
1	A	344	ASP	2.5
1	B	607	ALA	2.5
1	B	147	GLU	2.5
1	B	69	LYS	2.5
1	B	343	SER	2.4
1	A	206	GLN	2.4
1	B	298	GLU	2.4
1	B	132	LYS	2.4
1	B	80	TYR	2.3
1	B	152	LEU	2.3
1	B	228	LYS	2.3
1	A	229	THR	2.3
1	B	146	VAL	2.3
1	B	8	VAL	2.3
1	A	301	GLU	2.3
1	B	229	THR	2.2
1	B	5	VAL	2.2
1	B	67	GLU	2.2
1	A	283	ASP	2.2
1	A	546	VAL	2.2
1	B	153	LEU	2.2
1	A	70	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	310	ASN	2.2
1	B	123	ILE	2.2
1	B	145	LYS	2.1
1	A	4	GLN	2.1
1	A	71	GLU	2.1
1	A	348	VAL	2.1
1	B	114	LYS	2.1
1	B	149	LEU	2.1
1	B	204	GLU	2.1
1	B	62	THR	2.1
1	B	300	GLU	2.0
1	B	106	ARG	2.0
1	A	304	LYS	2.0
1	A	201	ASN	2.0
1	B	59	ARG	2.0
1	A	310	ASN	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](#)

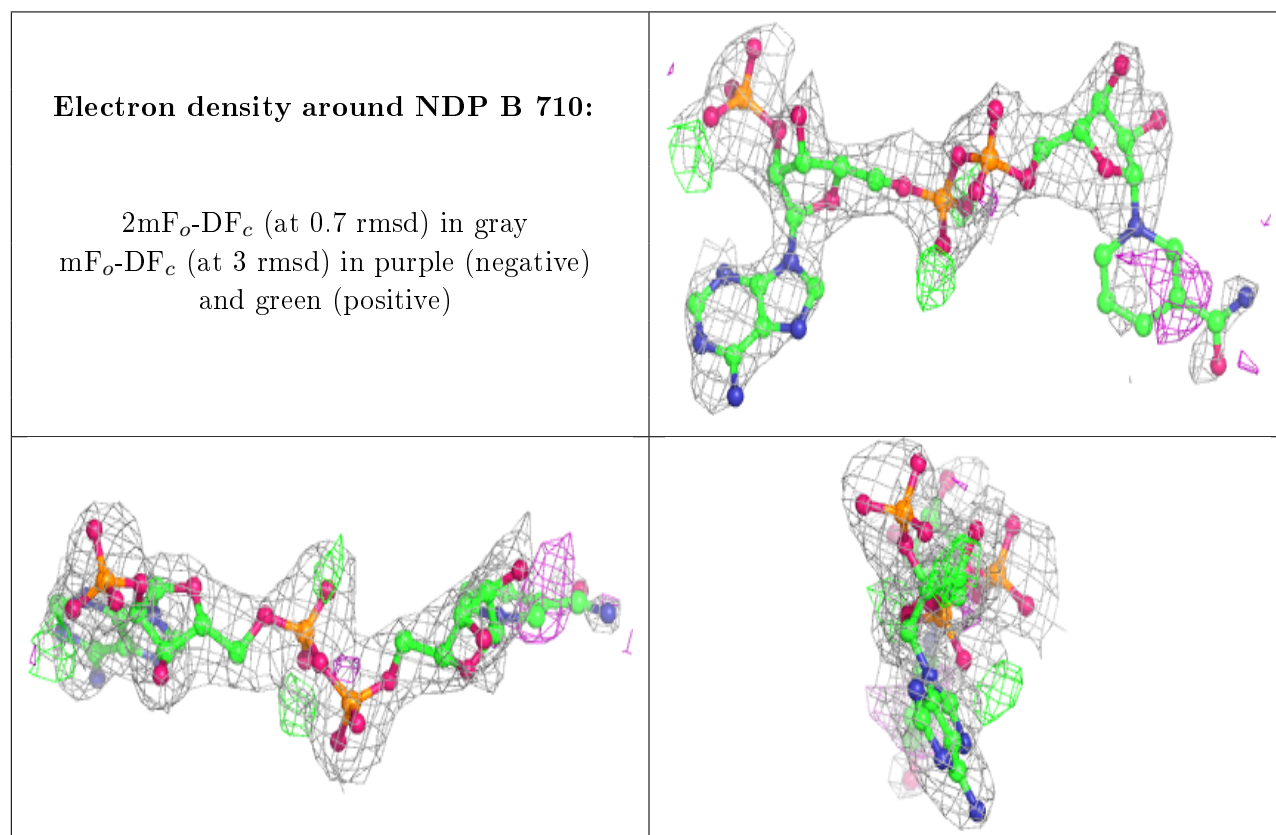
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

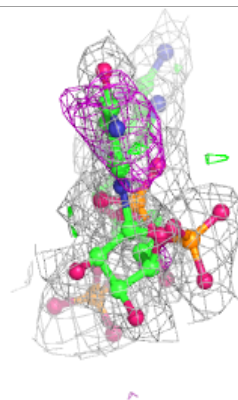
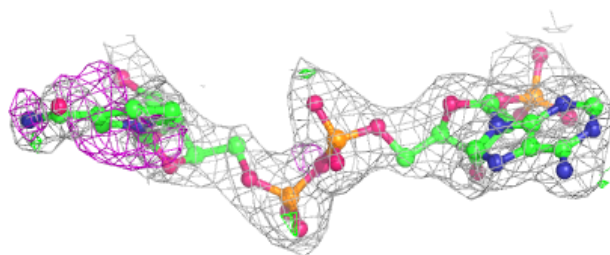
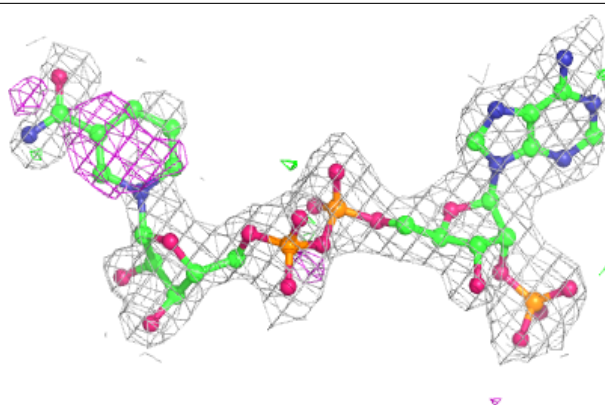
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NDP	B	710	48/48	0.76	0.27	84,89,90,90	0
3	NDP	A	610	48/48	0.90	0.19	37,45,54,55	0
2	CP6	B	709	17/17	0.92	0.13	47,49,57,57	0
2	CP6	A	609	17/17	0.95	0.13	18,21,31,35	0
4	UMP	B	711	20/20	0.96	0.12	30,34,36,37	0
4	UMP	A	611	20/20	0.97	0.12	27,34,39,40	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.

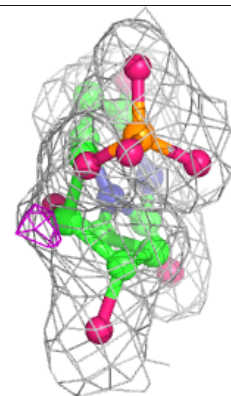
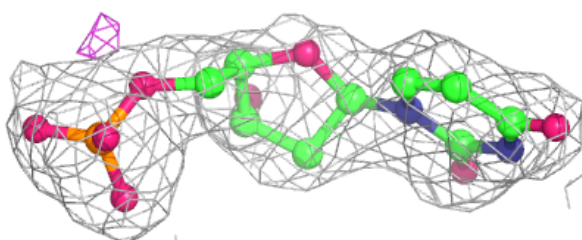
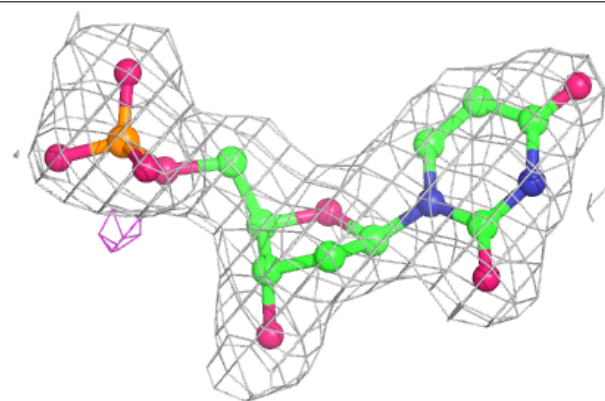


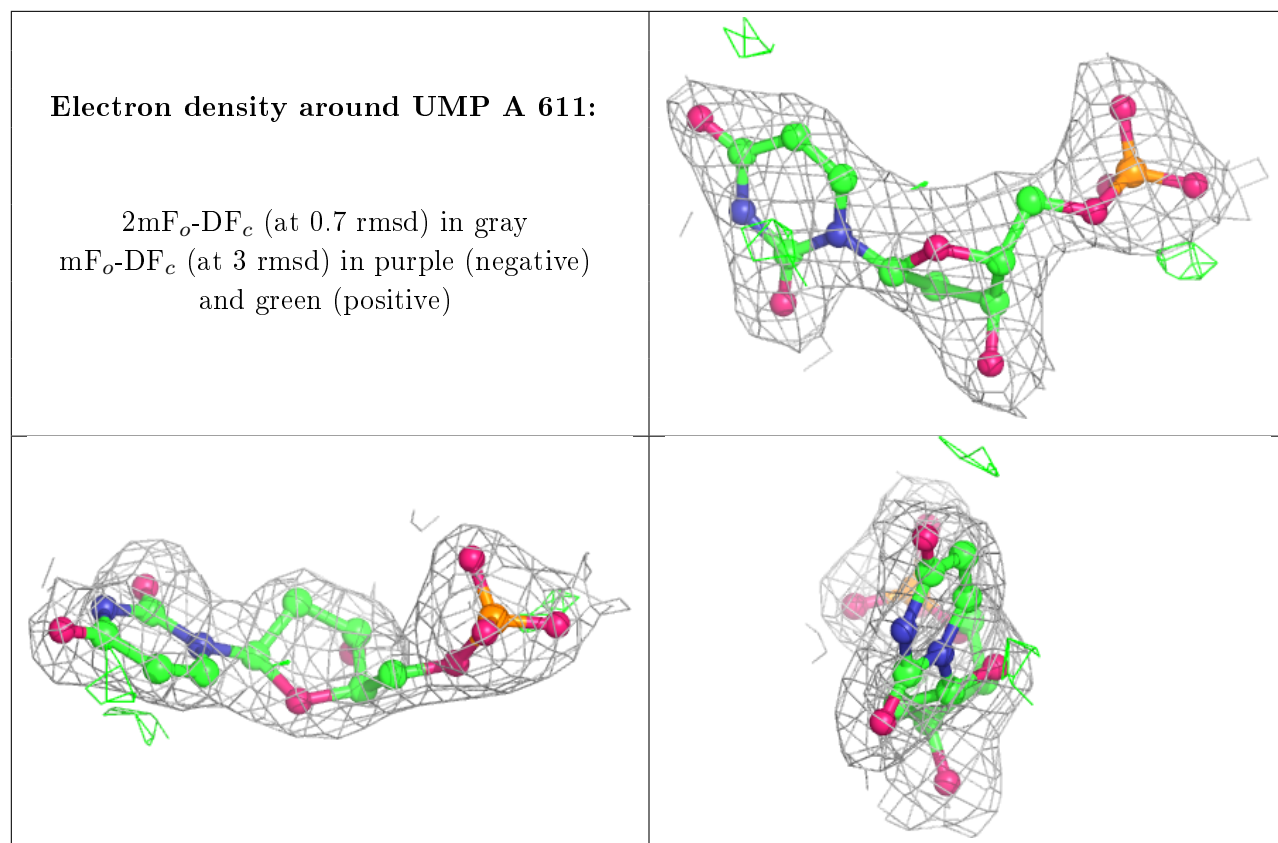
**Electron density around NDP A 610:**

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

**Electron density around UMP B 711:**

$2mF_o-DF_c$  (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.