Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 06:11 pm BST

PDB ID	:	4DPH
Title	:	Quadruple mutant (N51I+C59R+S108N+I164L) Plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with P65 and NADPH
Authors	:	Yuthavong, Y.; Vilaivan, T.; Kamchonwongpaisan, S.; Charman, S.A.; McLennan, D.N.; White, K.L.; Vivas, L.; Bongard, E.; Chitnumsub, P.; Tarnchompoo, B.; Thongphanchang, C.; Taweechai, S.; Vanichtanakul, J.; Arwon, U.; Fantauzzi, P.; Yuvaniyama, J.; Charman, W.N.; Matthews, D.
Deposited on	:	2012-02-13
Resolution	:	2.38 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

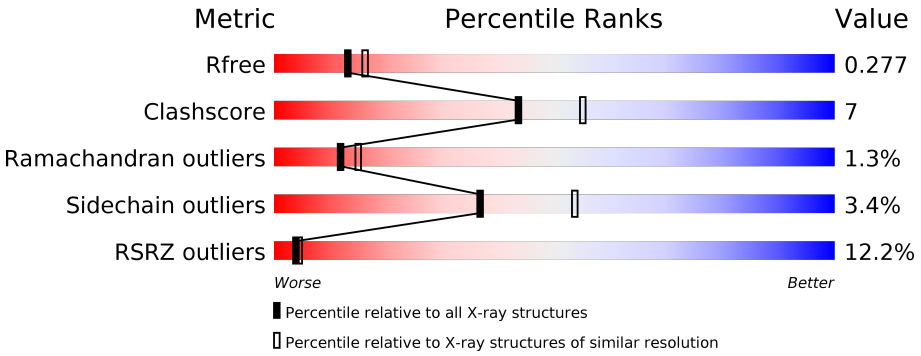
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 <=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	8% 74% 13% • 12%
1	B	608	13% 71% 14% • 13%

2 Entry composition

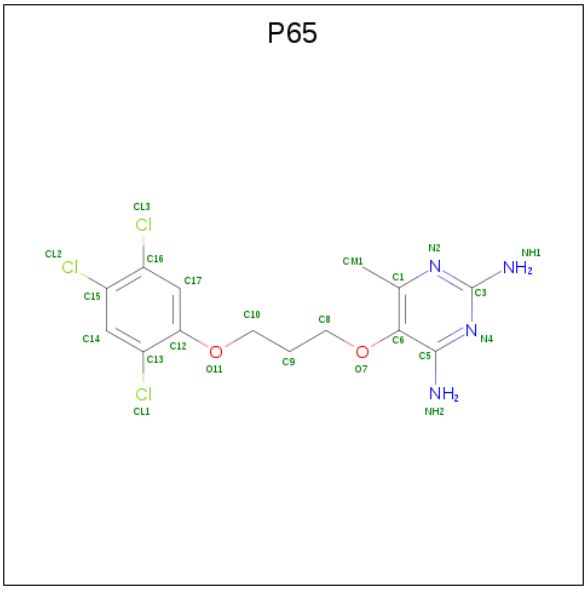
There are 6 unique types of molecules in this entry. The entry contains 9473 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

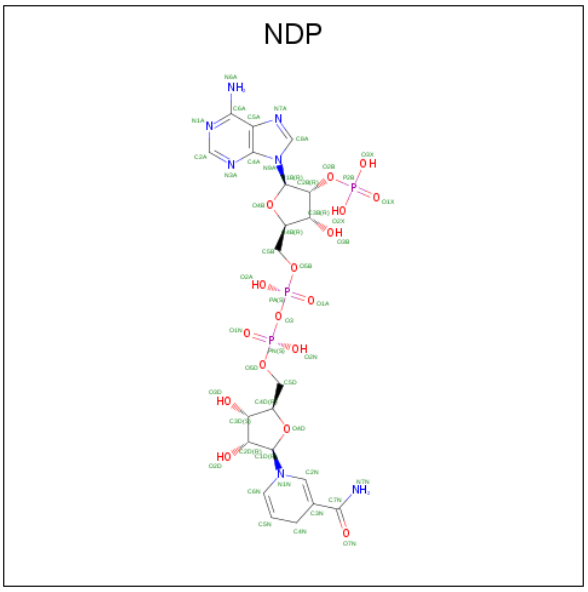
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4472	2890	740	817	25			
1	B	529	Total	C	N	O	S	0	0	0
			4395	2845	725	800	25			

- Molecule 2 is 2,4-diamino-6-methyl-5-[3-(2,4,5-trichlorophenoxy)propyloxy]pyrimidine (three-letter code: P65) (formula: $C_{14}H_{15}Cl_3N_4O_2$).



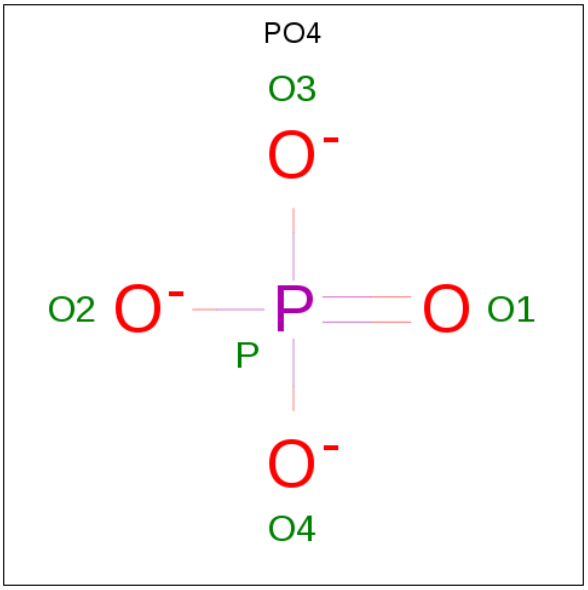
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			23	14	3	4	2		
2	B	1	Total	C	Cl	N	O	0	0
			23	14	3	4	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



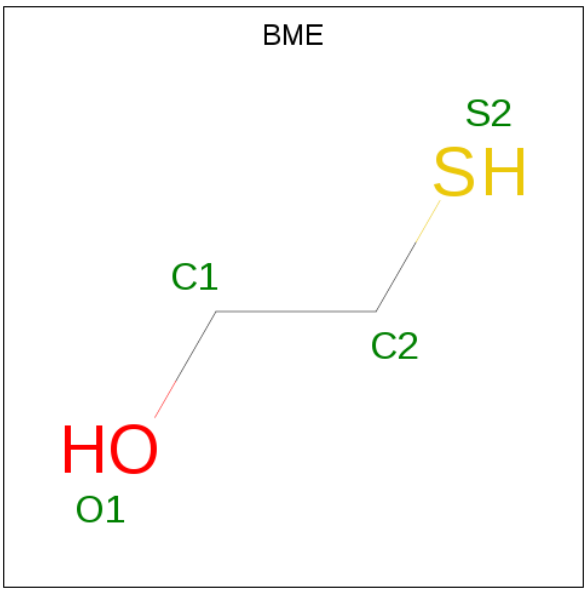
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is water.

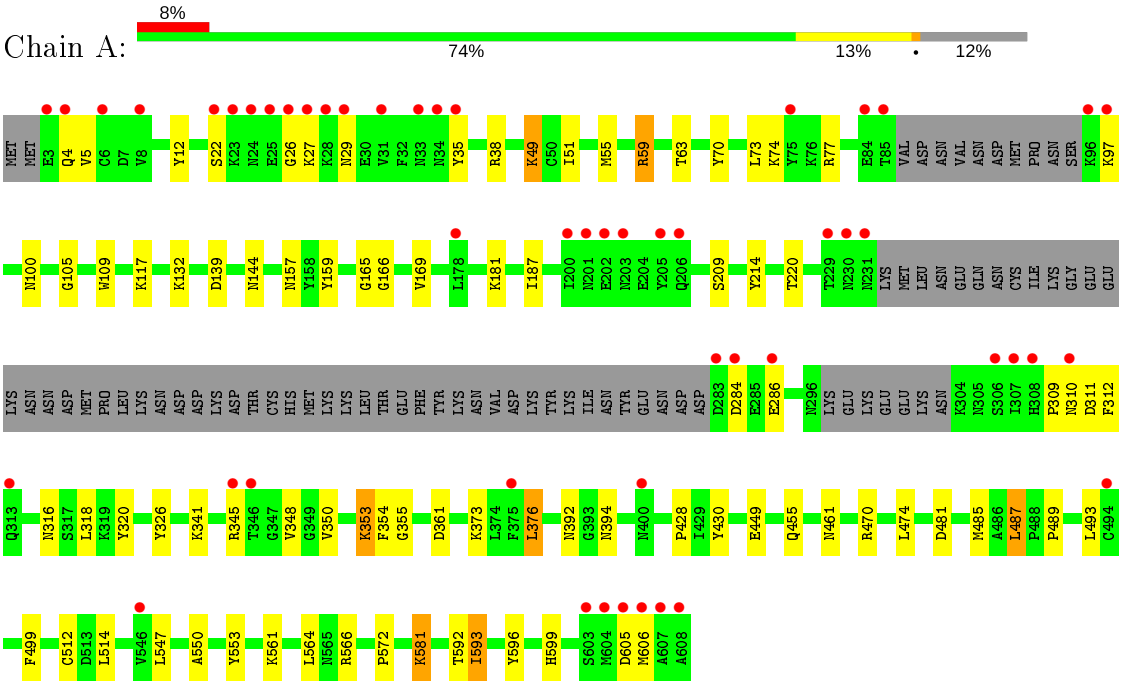
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	229	Total	O	0	0
			229	229		
6	B	209	Total	O	0	0
			209	209		

3 Residue-property plots (i)

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.

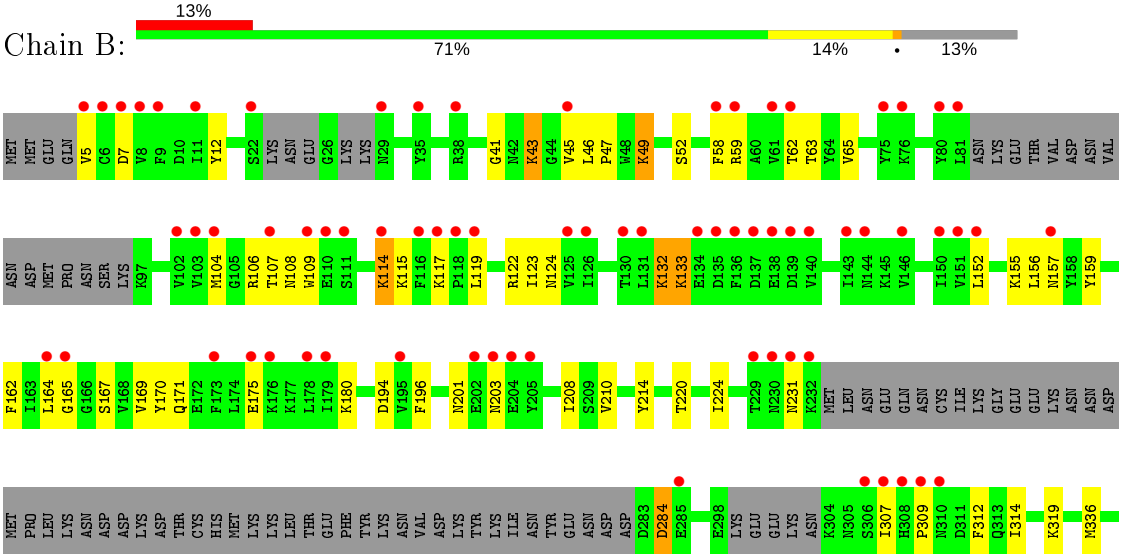
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

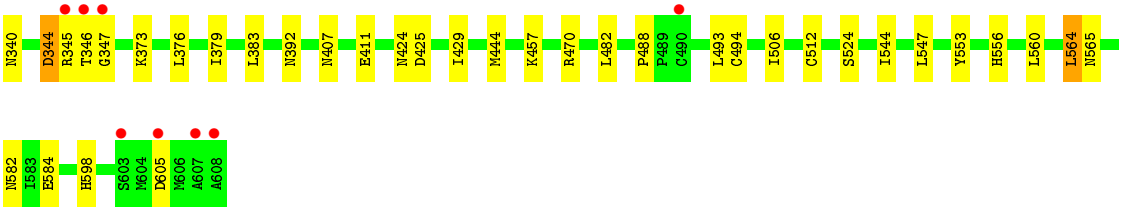
Chain A:



- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain B:




N340
D344
R345
T346
G347
K373
L376
I379
L383
N392
N407
E411
N424
D425
I429
M444
K457
R470
L482
P488
P489
C490
L493
C494
I506
C512
S524
I544
L547
Y553
H556
L560
L564
N565
N582
I583
E584
H598
S603
M604
D605
M606
A607
A608

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.95Å 156.45Å 164.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.66 – 2.38 51.79 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.1 (54.66-2.38) 99.1 (51.79-2.38)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.219 , 0.286 0.213 , 0.277	Depositor DCC
R_{free} test set	3072 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9473	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NDP, PO4, P65, BME

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.71	0/4576	0.74	4/6178 (0.1%)
1	B	0.67	1/4497 (0.0%)	0.71	1/6071 (0.0%)
All	All	0.69	1/9073 (0.0%)	0.73	5/12249 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	494	CYS	CB-SG	-5.35	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	470	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	487	LEU	CA-CB-CG	5.42	127.78	115.30
1	A	361	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	383	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	59	ARG	NE-CZ-NH1	5.11	122.85	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	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	4472	0	4426	49	0
1	B	4395	0	4346	73	0
2	A	23	0	15	1	0
2	B	23	0	15	0	0
3	A	48	0	26	2	0
3	B	48	0	26	5	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
5	A	12	0	18	0	0
5	B	4	0	6	0	0
6	A	229	0	0	6	0
6	B	209	0	0	12	0
All	All	9473	0	8878	120	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 (120) 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:425:ASP:HA	1:B:444:MET:CE	1.76	1.13
1:B:425:ASP:HA	1:B:444:MET:HE3	1.21	1.11
1:B:392:ASN:HA	1:B:444:MET:HE2	1.40	1.03
1:B:376:LEU:HD22	1:B:379:ILE:HD11	1.43	0.98
1:B:547:LEU:HG	6:B:957:HOH:O	1.61	0.97
1:B:584:GLU:HG3	6:B:803:HOH:O	1.66	0.94
1:A:461:ASN:HB3	6:A:973:HOH:O	1.70	0.90
1:B:425:ASP:CA	1:B:444:MET:HE3	2.03	0.89
1:B:392:ASN:HA	1:B:444:MET:CE	2.07	0.85
1:B:307:ILE:HG12	6:B:996:HOH:O	1.77	0.83
1:B:524:SER:HB2	6:B:915:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:VAL:HG23	3:B:702:NDP:O1A	1.81	0.79
1:B:425:ASP:HA	1:B:444:MET:HE1	1.67	0.74
1:B:171:GLN:HE21	1:B:175:GLU:HG3	1.53	0.73
1:B:210:VAL:HB	6:B:948:HOH:O	1.90	0.72
1:A:12:TYR:HD1	1:A:181:LYS:HB2	1.54	0.71
1:A:512:CYS:SG	1:A:547:LEU:HD22	2.31	0.70
1:B:512:CYS:SG	1:B:547:LEU:HD22	2.33	0.69
1:A:4:GLN:HB2	6:A:847:HOH:O	1.94	0.68
1:A:59:ARG:O	1:A:63:THR:HG23	1.94	0.67
1:B:7:ASP:HA	1:B:180:LYS:HE3	1.76	0.66
1:B:165:GLY:HA3	1:B:170:TYR:CZ	2.32	0.64
1:A:493:LEU:HD12	1:A:493:LEU:C	2.18	0.64
1:A:109:TRP:CZ2	1:A:117:LYS:HD2	2.34	0.63
1:A:312:PHE:CE1	1:A:564:LEU:HD23	2.34	0.63
1:B:210:VAL:O	1:B:210:VAL:HG23	1.97	0.62
1:B:425:ASP:CA	1:B:444:MET:CE	2.65	0.62
1:B:424:ASN:O	1:B:444:MET:HE1	2.00	0.61
1:A:74:LYS:C	6:A:959:HOH:O	2.39	0.60
1:B:43:LYS:N	1:B:194:ASP:OD2	2.29	0.60
1:B:167:SER:HB3	3:B:702:NDP:O2N	2.02	0.59
1:B:392:ASN:CA	1:B:444:MET:HE2	2.26	0.58
1:B:132:LYS:HD2	1:B:133:LYS:HD2	1.85	0.57
1:A:100:ASN:OD1	1:A:159:TYR:HB3	2.03	0.57
1:A:166:GLY:HA3	3:A:702:NDP:O1A	2.05	0.57
1:B:336:MET:HE1	1:B:560:LEU:HB2	1.87	0.56
1:B:45:VAL:HG12	1:B:46:LEU:H	1.71	0.56
1:A:12:TYR:CD1	1:A:181:LYS:HB2	2.39	0.56
1:A:572:PRO:HB3	1:A:596:TYR:HA	1.87	0.56
1:B:373:LYS:HG3	1:B:598:HIS:CE1	2.41	0.55
1:B:493:LEU:HD12	1:B:493:LEU:C	2.26	0.55
1:B:407:ASN:ND2	6:B:991:HOH:O	2.39	0.55
1:B:425:ASP:CB	1:B:444:MET:HE3	2.38	0.54
1:B:171:GLN:NE2	1:B:175:GLU:HG3	2.22	0.53
1:A:312:PHE:HE1	1:A:564:LEU:HD23	1.74	0.53
1:B:109:TRP:CZ2	1:B:117:LYS:HD2	2.45	0.51
1:A:499:PHE:CE1	1:B:340:ASN:HB3	2.44	0.51
1:A:350:VAL:HG12	1:A:553:TYR:CD1	2.46	0.51
1:B:482:LEU:HD22	1:B:488:PRO:HB3	1.93	0.51
1:B:307:ILE:HG23	6:B:958:HOH:O	2.11	0.51
1:B:307:ILE:CG2	1:B:312:PHE:HE2	2.23	0.51
1:B:41:GLY:HA2	1:B:47:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:TYR:OH	1:A:157:ASN:OD1	2.28	0.50
1:A:428:PRO:HG2	1:A:481:ASP:HB3	1.93	0.50
1:B:65:VAL:HG22	1:B:159:TYR:CB	2.41	0.50
1:A:214:TYR:O	1:A:220:THR:HA	2.11	0.50
1:B:122:ARG:O	1:B:124:ASN:ND2	2.42	0.49
1:B:201:ASN:HD21	1:B:203:ASN:HB2	1.77	0.49
1:B:5:VAL:N	6:B:967:HOH:O	2.46	0.49
1:A:27:LYS:HG2	1:A:27:LYS:O	2.13	0.49
1:A:514:LEU:HD21	1:A:550:ALA:HB1	1.95	0.49
1:B:376:LEU:HD22	1:B:379:ILE:CD1	2.31	0.49
1:A:581:LYS:HA	1:A:581:LYS:HE3	1.94	0.49
1:A:51:ILE:HD13	1:A:187:ILE:HD12	1.94	0.48
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.94	0.48
1:A:376:LEU:HD12	1:A:593:ILE:HD11	1.95	0.48
1:B:12:TYR:HE1	1:B:180:LYS:HD2	1.78	0.48
1:B:59:ARG:O	1:B:63:THR:HG23	2.12	0.48
1:A:55:MET:HE1	2:A:701:P65:CL1	2.51	0.48
1:A:311:ASP:OD2	1:A:561:LYS:NZ	2.42	0.48
1:B:152:LEU:O	1:B:156:LEU:HD12	2.13	0.48
1:A:166:GLY:HA3	3:A:702:NDP:PA	2.54	0.47
1:B:336:MET:CE	1:B:560:LEU:HB2	2.43	0.47
1:B:210:VAL:HG12	1:B:224:ILE:HG22	1.95	0.47
1:B:108:ASN:ND2	3:B:702:NDP:H5N	2.30	0.46
1:B:344:ASP:O	1:B:346:THR:N	2.48	0.46
1:B:553:TYR:O	1:B:556:HIS:HB2	2.15	0.46
1:A:512:CYS:SG	1:A:547:LEU:CD2	3.04	0.46
1:A:105:GLY:CA	1:A:169:VAL:HG21	2.46	0.45
1:B:411:GLU:HB2	6:B:869:HOH:O	2.15	0.45
1:B:171:GLN:HG3	1:B:175:GLU:OE2	2.16	0.45
1:B:582:ASN:HB3	6:B:803:HOH:O	2.15	0.45
1:B:43:LYS:HE3	1:B:43:LYS:HB2	1.58	0.45
1:A:354:PHE:CE2	1:B:506:ILE:HG13	2.51	0.45
1:A:355:GLY:HA2	1:A:547:LEU:O	2.16	0.45
1:B:214:TYR:O	1:B:220:THR:HA	2.17	0.45
1:A:318:LEU:HD11	1:A:326:TYR:OH	2.16	0.44
1:A:35:TYR:CZ	1:A:38:ARG:HD2	2.53	0.44
1:B:114:LYS:HD2	1:B:115:LYS:N	2.33	0.44
1:B:106:ARG:HE	3:B:702:NDP:P2B	2.40	0.44
1:B:312:PHE:CE1	1:B:564:LEU:HD23	2.52	0.44
1:B:109:TRP:CE2	1:B:117:LYS:HD2	2.53	0.44
1:A:105:GLY:N	1:A:169:VAL:HG21	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLY:HA3	1:B:170:TYR:CE2	2.53	0.43
1:A:29:ASN:OD1	1:A:373:LYS:NZ	2.51	0.43
1:A:312:PHE:HB2	1:A:316:ASN:ND2	2.34	0.43
1:B:344:ASP:O	1:B:347:GLY:N	2.52	0.43
1:A:392:ASN:OD1	1:A:394:ASN:HB2	2.19	0.43
1:B:210:VAL:O	1:B:210:VAL:CG2	2.67	0.43
1:A:312:PHE:HB2	1:A:316:ASN:HD22	1.84	0.43
1:B:470:ARG:NE	6:B:974:HOH:O	2.52	0.42
1:A:109:TRP:CH2	1:A:117:LYS:HD2	2.54	0.42
1:B:58:PHE:HE1	1:B:164:LEU:HD22	1.84	0.42
1:B:314:ILE:HB	1:B:565:ASN:HB3	2.02	0.42
1:A:77:ARG:N	6:A:959:HOH:O	2.53	0.41
1:A:353:LYS:HE2	1:A:353:LYS:HB3	1.65	0.41
1:A:70:TYR:HA	1:A:73:LEU:HD12	2.01	0.41
1:A:485:MET:SD	1:A:489:PRO:HD3	2.61	0.41
1:B:62:THR:HA	1:B:162:PHE:CE2	2.56	0.41
1:A:209:SER:OG	1:A:320:TYR:HD2	2.04	0.41
1:A:455:GLN:HB3	1:A:474:LEU:HD12	2.02	0.41
1:A:566:ARG:HD3	1:A:599:HIS:CG	2.56	0.41
1:A:77:ARG:HG3	6:A:995:HOH:O	2.21	0.41
1:A:493:LEU:CD1	1:A:493:LEU:C	2.89	0.40
1:B:157:ASN:HB3	6:B:904:HOH:O	2.21	0.40
1:B:133:LYS:HD2	1:B:133:LYS:H	1.87	0.40
1:A:286:GLU:HG2	1:B:319:LYS:HD3	2.02	0.40
4:A:703:PO4:O1	6:A:999:HOH:O	2.22	0.40
1:B:284:ASP:OD1	1:B:284:ASP:N	2.47	0.40
1:B:108:ASN:HD21	3:B:702:NDP:H5N	1.87	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	530/608 (87%)	491 (93%)	31 (6%)	8 (2%)	10	12
1	B	518/608 (85%)	474 (92%)	38 (7%)	6 (1%)	13	17
All	All	1048/1216 (86%)	965 (92%)	69 (7%)	14 (1%)	12	15

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	49	LYS
1	B	345	ARG
1	A	139	ASP
1	A	49	LYS
1	A	284	ASP
1	A	430	TYR
1	A	22	SER
1	A	26	GLY
1	A	310	ASN
1	B	119	LEU
1	A	309	PRO
1	B	309	PRO
1	B	123	ILE
1	B	429	ILE

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	501/570 (88%)	484 (97%)	17 (3%)	37	53
1	B	492/570 (86%)	475 (96%)	17 (4%)	36	52
All	All	993/1140 (87%)	959 (97%)	34 (3%)	37	53

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	49	LYS

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Mol	Chain	Res	Type
1	A	97	LYS
1	A	132	LYS
1	A	144	ASN
1	A	341	LYS
1	A	345	ARG
1	A	348	VAL
1	A	353	LYS
1	A	376	LEU
1	A	449	GLU
1	A	487	LEU
1	A	581	LYS
1	A	592	THR
1	A	593	ILE
1	A	605	ASP
1	A	606	MET
1	B	43	LYS
1	B	49	LYS
1	B	52	SER
1	B	104	MET
1	B	107	THR
1	B	114	LYS
1	B	132	LYS
1	B	133	LYS
1	B	155	LYS
1	B	196	PHE
1	B	208	ILE
1	B	231	ASN
1	B	284	ASP
1	B	344	ASP
1	B	457	LYS
1	B	564	LEU
1	B	605	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	144	ASN
1	A	294	ASN
1	A	316	ASN
1	A	394	ASN
1	A	424	ASN

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Mol	Chain	Res	Type
1	A	554	ASN
1	B	99	GLN
1	B	171	GLN
1	B	201	ASN
1	B	203	ASN
1	B	305	ASN
1	B	316	ASN
1	B	394	ASN
1	B	424	ASN

5.3.3 RNA (i)

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)

10 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	BME	B	704	-	3,3,3	0.43	0	1,2,2	0.27	0
2	P65	A	701	-	23,24,24	3.24	4 (17%)	29,33,33	2.18	10 (34%)
4	PO4	B	703	-	4,4,4	0.69	0	6,6,6	0.69	0
4	PO4	A	703	-	4,4,4	0.90	0	6,6,6	1.07	0
5	BME	A	705	-	3,3,3	0.48	0	1,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NDP	A	702	-	45,52,52	1.61	5 (11%)	53,80,80	1.31	7 (13%)
3	NDP	B	702	-	45,52,52	1.56	4 (8%)	53,80,80	1.08	2 (3%)
2	P65	B	701	-	23,24,24	3.53	3 (13%)	29,33,33	1.59	5 (17%)
5	BME	A	704	-	3,3,3	0.37	0	1,2,2	0.41	0
5	BME	A	706	-	3,3,3	0.33	0	1,2,2	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BME	B	704	-	-	0/1/1/1	-
2	P65	A	701	-	-	0/8/8/8	0/2/2/2
3	NDP	B	702	-	-	9/30/77/77	0/5/5/5
5	BME	A	705	-	-	1/1/1/1	-
3	NDP	A	702	-	-	3/30/77/77	0/5/5/5
5	BME	A	706	-	-	1/1/1/1	-
2	P65	B	701	-	-	0/8/8/8	0/2/2/2
5	BME	A	704	-	-	1/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	P65	C15-CL2	-10.09	1.49	1.73
2	B	701	P65	C13-CL1	-9.92	1.50	1.73
2	A	701	P65	C15-CL2	-9.27	1.51	1.73
2	B	701	P65	C16-CL3	-9.00	1.52	1.73
2	A	701	P65	C16-CL3	-8.46	1.53	1.73
2	A	701	P65	C13-CL1	-8.11	1.54	1.73
3	A	702	NDP	O7N-C7N	7.11	1.41	1.24
3	B	702	NDP	O7N-C7N	7.03	1.41	1.24
3	A	702	NDP	C6N-C5N	3.97	1.40	1.33
3	B	702	NDP	C2A-N3A	3.94	1.38	1.32
3	A	702	NDP	C2A-N3A	3.87	1.38	1.32
3	B	702	NDP	C6N-C5N	3.49	1.39	1.33
3	B	702	NDP	C2A-N1A	2.72	1.39	1.33
3	A	702	NDP	C2A-N1A	2.58	1.38	1.33
2	A	701	P65	C1-N2	2.19	1.37	1.34
3	A	702	NDP	C2N-C3N	2.11	1.40	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	NDP	N3A-C2A-N1A	-5.47	120.12	128.68
2	A	701	P65	C3-N2-C1	4.67	120.60	116.79
3	A	702	NDP	N3A-C2A-N1A	-4.64	121.43	128.68
2	B	701	P65	C3-N2-C1	4.53	120.48	116.79
2	A	701	P65	C3-N4-C5	4.26	121.69	116.99
2	A	701	P65	C17-C16-CL3	3.83	124.67	118.49
2	A	701	P65	N2-C3-N4	-3.52	119.90	125.42
2	B	701	P65	C3-N4-C5	3.45	120.80	116.99
2	A	701	P65	NH1-C3-N2	3.26	122.32	117.25
2	A	701	P65	C14-C15-CL2	3.25	123.74	118.49
2	A	701	P65	CM1-C1-N2	2.89	120.97	116.49
2	B	701	P65	N2-C3-N4	-2.87	120.92	125.42
3	A	702	NDP	C4A-C5A-N7A	-2.78	106.50	109.40
3	A	702	NDP	O2B-C2B-C1B	-2.73	100.28	110.10
2	A	701	P65	C16-C15-CL2	-2.67	114.34	120.85
2	A	701	P65	C14-C13-C12	-2.53	117.64	121.02
3	A	702	NDP	C1D-N1N-C2N	-2.53	116.91	121.11
2	B	701	P65	C10-O11-C12	2.38	123.50	117.69
3	A	702	NDP	O4D-C1D-N1N	2.33	112.62	108.06
3	A	702	NDP	O2N-PN-O1N	2.33	123.74	112.24
2	A	701	P65	C14-C13-CL1	2.17	122.00	118.49
3	B	702	NDP	PN-O3-PA	-2.13	125.51	132.83
3	A	702	NDP	N6A-C6A-N1A	-2.11	114.20	118.57
2	B	701	P65	NH1-C3-N4	2.06	120.45	117.25

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	NDP	C3B-C4B-C5B-O5B
3	B	702	NDP	C5D-O5D-PN-O1N
5	A	706	BME	O1-C1-C2-S2
3	B	702	NDP	O4B-C4B-C5B-O5B
3	B	702	NDP	C5D-O5D-PN-O3
3	B	702	NDP	O4D-C1D-N1N-C2N
5	A	705	BME	O1-C1-C2-S2
3	A	702	NDP	O4D-C1D-N1N-C2N
3	B	702	NDP	C2D-C1D-N1N-C2N
3	B	702	NDP	C2B-O2B-P2B-O1X
3	A	702	NDP	C2B-O2B-P2B-O2X
3	B	702	NDP	C2B-O2B-P2B-O3X

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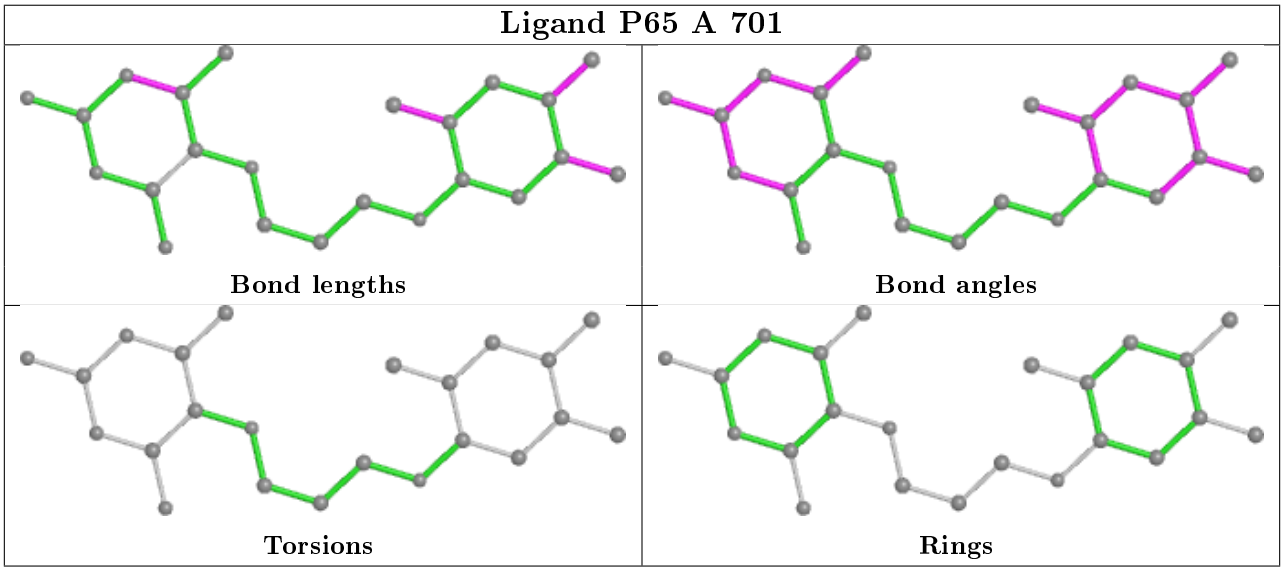
Mol	Chain	Res	Type	Atoms
3	B	702	NDP	C5D-O5D-PN-O2N
5	A	704	BME	O1-C1-C2-S2
3	A	702	NDP	C2D-C1D-N1N-C2N

There are no ring outliers.

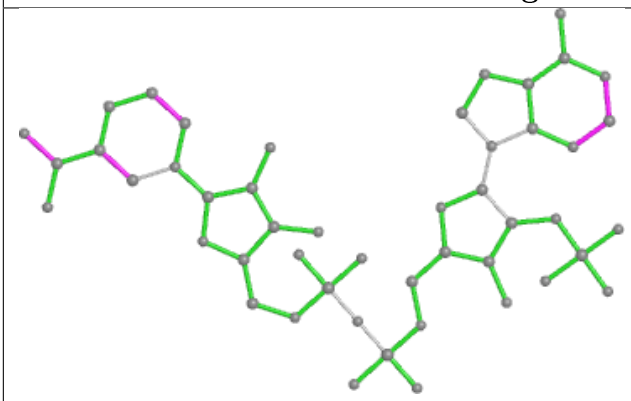
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	P65	1	0
4	A	703	PO4	1	0
3	A	702	NDP	2	0
3	B	702	NDP	5	0

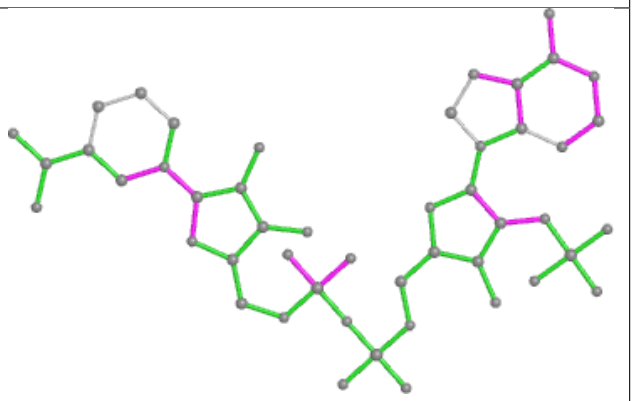
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



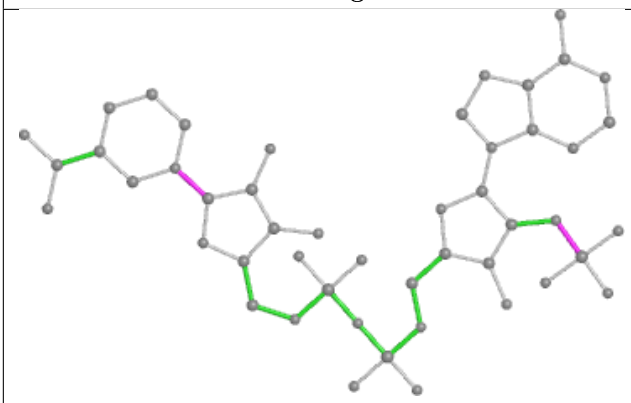
Ligand NDP A 702



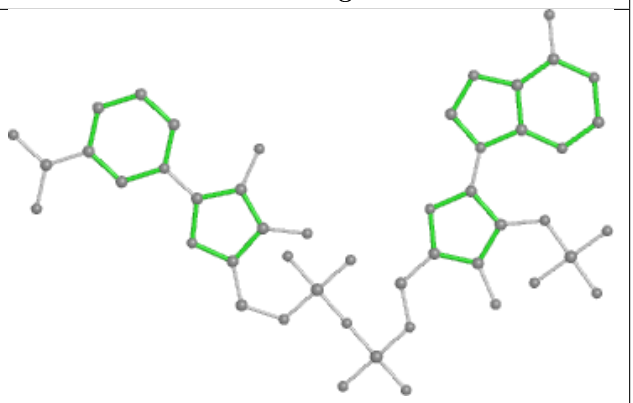
Bond lengths



Bond angles

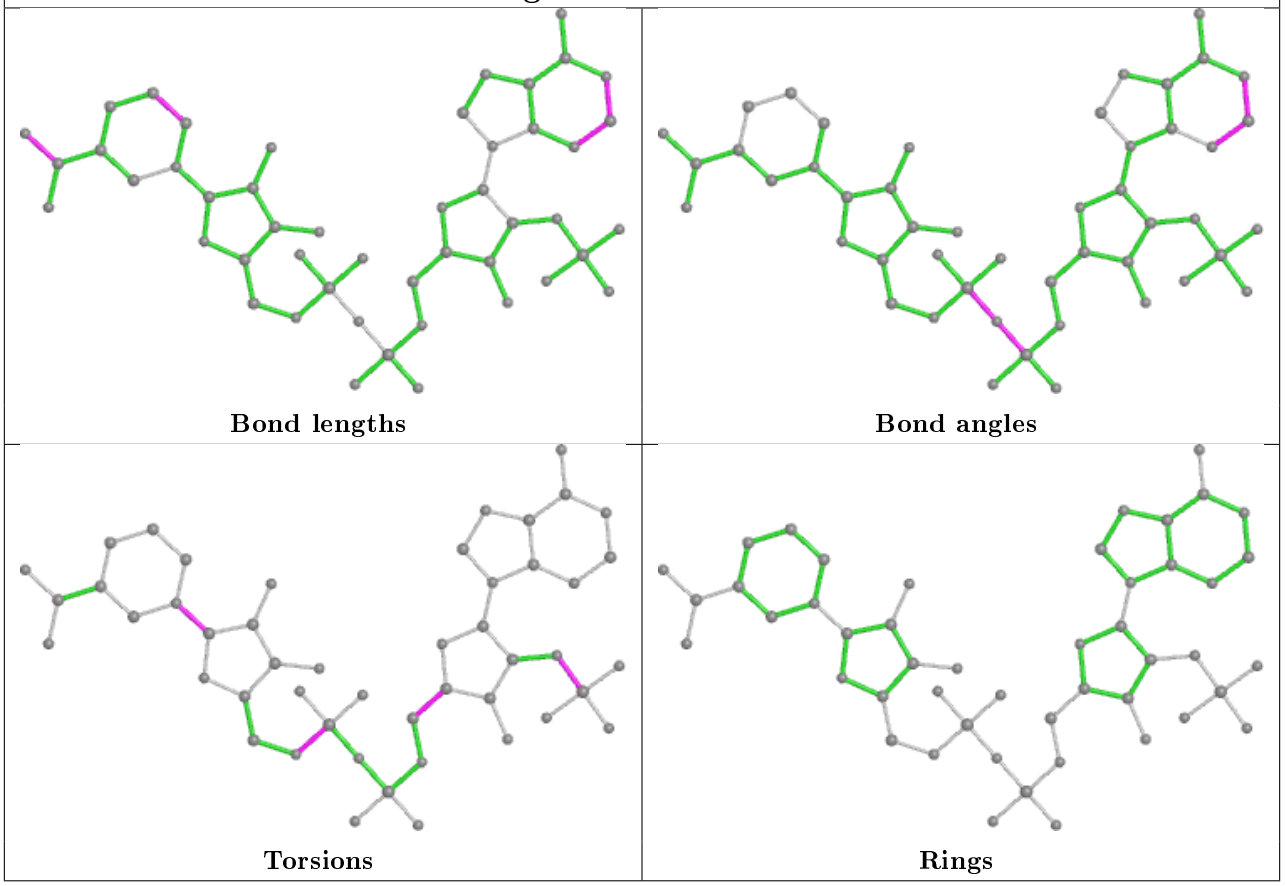


Torsions

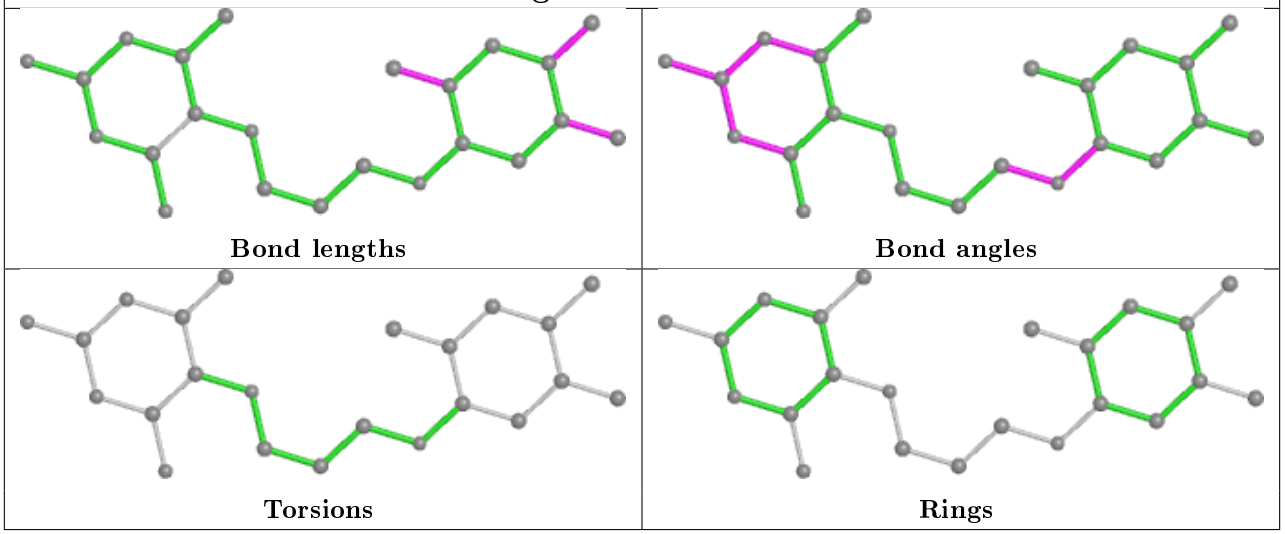


Rings

Ligand NDP B 702



Ligand P65 B 701



5.7 Other polymers (i)

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, 95^{th} 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	538/608 (88%)	0.60	51 (9%) 8 9	26, 39, 81, 98	0
1	B	529/608 (87%)	0.83	79 (14%) 2 2	24, 43, 96, 116	0
All	All	1067/1216 (87%)	0.71	130 (12%) 4 4	24, 41, 91, 116	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	THR	10.9
1	B	138	GLU	8.6
1	A	26	GLY	7.9
1	B	232	LYS	7.4
1	B	136	PHE	7.3
1	B	151	VAL	7.3
1	A	25	GLU	7.1
1	A	24	ASN	7.0
1	B	231	ASN	6.8
1	A	31	VAL	6.8
1	B	306	SER	6.2
1	B	346	THR	6.0
1	B	130	THR	5.9
1	B	607	ALA	5.7
1	A	29	ASN	5.4
1	B	345	ARG	5.4
1	B	118	PRO	5.4
1	A	231	ASN	5.3
1	A	608	ALA	5.2
1	B	75	TYR	5.1
1	A	230	ASN	5.0
1	B	9	PHE	5.0
1	A	607	ALA	4.7
1	B	80	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	178	LEU	4.5
1	B	307	ILE	4.3
1	B	310	ASN	4.3
1	A	283	ASP	4.2
1	B	135	ASP	4.2
1	A	606	MET	4.2
1	B	62	THR	4.2
1	A	28	LYS	4.2
1	B	608	ALA	4.1
1	A	27	LYS	4.1
1	B	7	ASP	4.1
1	A	200	ILE	4.0
1	B	8	VAL	4.0
1	B	116	PHE	4.0
1	B	309	PRO	3.9
1	A	310	ASN	3.8
1	B	230	ASN	3.8
1	A	345	ARG	3.8
1	B	204	GLU	3.8
1	B	131	LEU	3.7
1	B	109	TRP	3.7
1	B	29	ASN	3.6
1	B	126	ILE	3.6
1	A	306	SER	3.5
1	A	35	TYR	3.5
1	B	152	LEU	3.5
1	B	134	GLU	3.5
1	A	23	LYS	3.4
1	B	229	THR	3.3
1	B	110	GLU	3.3
1	A	22	SER	3.2
1	B	140	VAL	3.2
1	B	111	SER	3.2
1	B	347	GLY	3.2
1	B	102	VAL	3.2
1	B	103	VAL	3.1
1	B	285	GLU	3.1
1	B	11	ILE	3.1
1	A	3	GLU	3.0
1	A	203	ASN	3.0
1	A	202	GLU	3.0
1	B	22	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	313	GLN	3.0
1	A	346	THR	3.0
1	A	33	ASN	3.0
1	B	104	MET	2.9
1	A	604	MET	2.9
1	B	58	PHE	2.8
1	B	146	VAL	2.8
1	A	8	VAL	2.8
1	B	157	ASN	2.8
1	B	45	VAL	2.7
1	A	97	LYS	2.7
1	A	201	ASN	2.7
1	A	34	ASN	2.6
1	B	173	PHE	2.6
1	B	38	ARG	2.6
1	A	546	VAL	2.6
1	B	195	VAL	2.6
1	B	107	THR	2.6
1	B	61	VAL	2.5
1	B	35	TYR	2.5
1	B	164	LEU	2.5
1	A	4	GLN	2.5
1	A	206	GLN	2.5
1	B	59	ARG	2.4
1	A	375	PHE	2.4
1	B	308	HIS	2.4
1	A	286	GLU	2.4
1	B	137	ASP	2.4
1	B	203	ASN	2.4
1	B	139	ASP	2.4
1	A	307	ILE	2.4
1	B	202	GLU	2.4
1	B	205	TYR	2.4
1	B	165	GLY	2.4
1	B	81	LEU	2.4
1	B	119	LEU	2.3
1	A	6	CYS	2.3
1	A	605	ASP	2.3
1	A	75	TYR	2.3
1	B	179	ILE	2.3
1	A	494	CYS	2.2
1	B	150	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	175	GLU	2.2
1	B	144	ASN	2.2
1	B	605	ASP	2.2
1	B	117	LYS	2.2
1	A	84	GLU	2.2
1	B	5	VAL	2.2
1	B	603	SER	2.2
1	B	143	ILE	2.2
1	A	205	TYR	2.2
1	A	96	LYS	2.2
1	A	178	LEU	2.2
1	A	603	SER	2.2
1	B	6	CYS	2.1
1	A	308	HIS	2.1
1	B	125	VAL	2.1
1	A	284	ASP	2.1
1	B	76	LYS	2.1
1	B	176	LYS	2.1
1	A	400	ASN	2.1
1	B	490	CYS	2.1
1	A	229	THR	2.1
1	B	114	LYS	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BME	A	705	4/4	0.66	0.30	89,90,90,91	0

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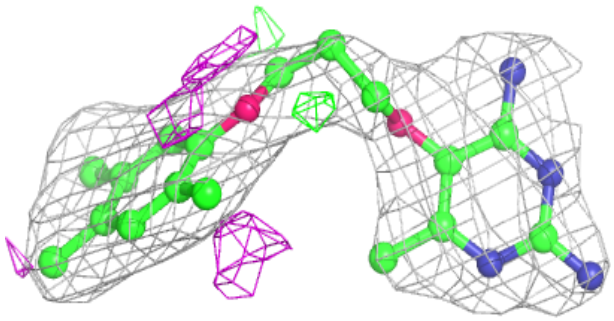
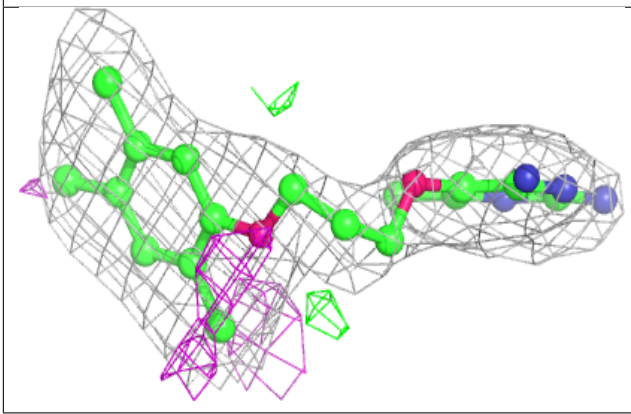
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BME	A	704	4/4	0.78	0.17	90,92,93,94	0
5	BME	B	704	4/4	0.86	0.16	65,67,68,71	0
2	P65	B	701	23/23	0.88	0.17	59,66,77,79	0
3	NDP	B	702	48/48	0.88	0.22	83,88,102,104	0
2	P65	A	701	23/23	0.92	0.14	26,31,53,58	0
5	BME	A	706	4/4	0.94	0.32	77,77,77,78	0
4	PO4	A	703	5/5	0.96	0.15	61,62,62,62	0
3	NDP	A	702	48/48	0.96	0.14	43,50,53,54	0
4	PO4	B	703	5/5	0.97	0.14	48,48,50,51	0

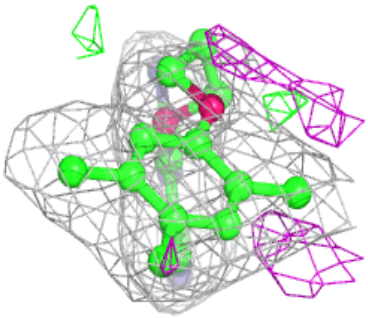
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P65 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)

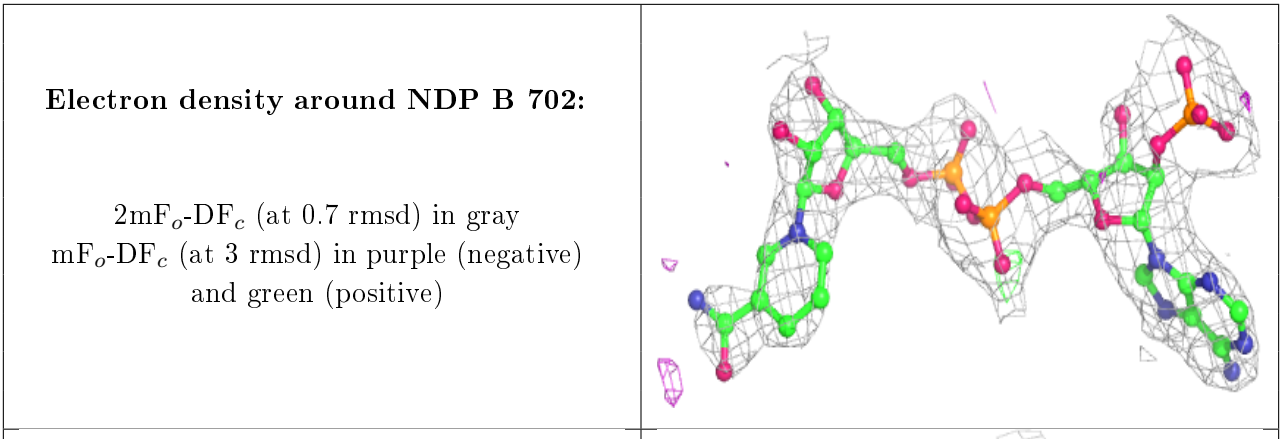






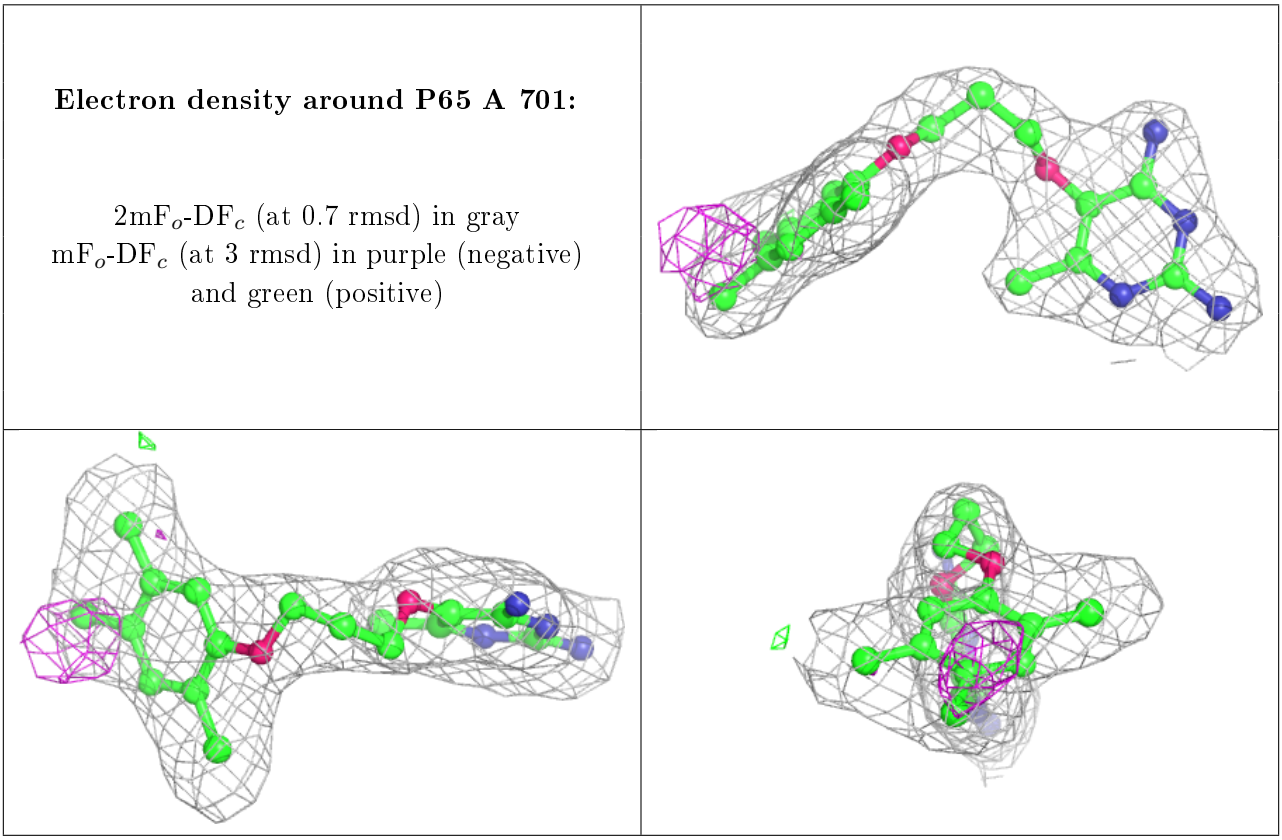
Electron density around NDP B 702:

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



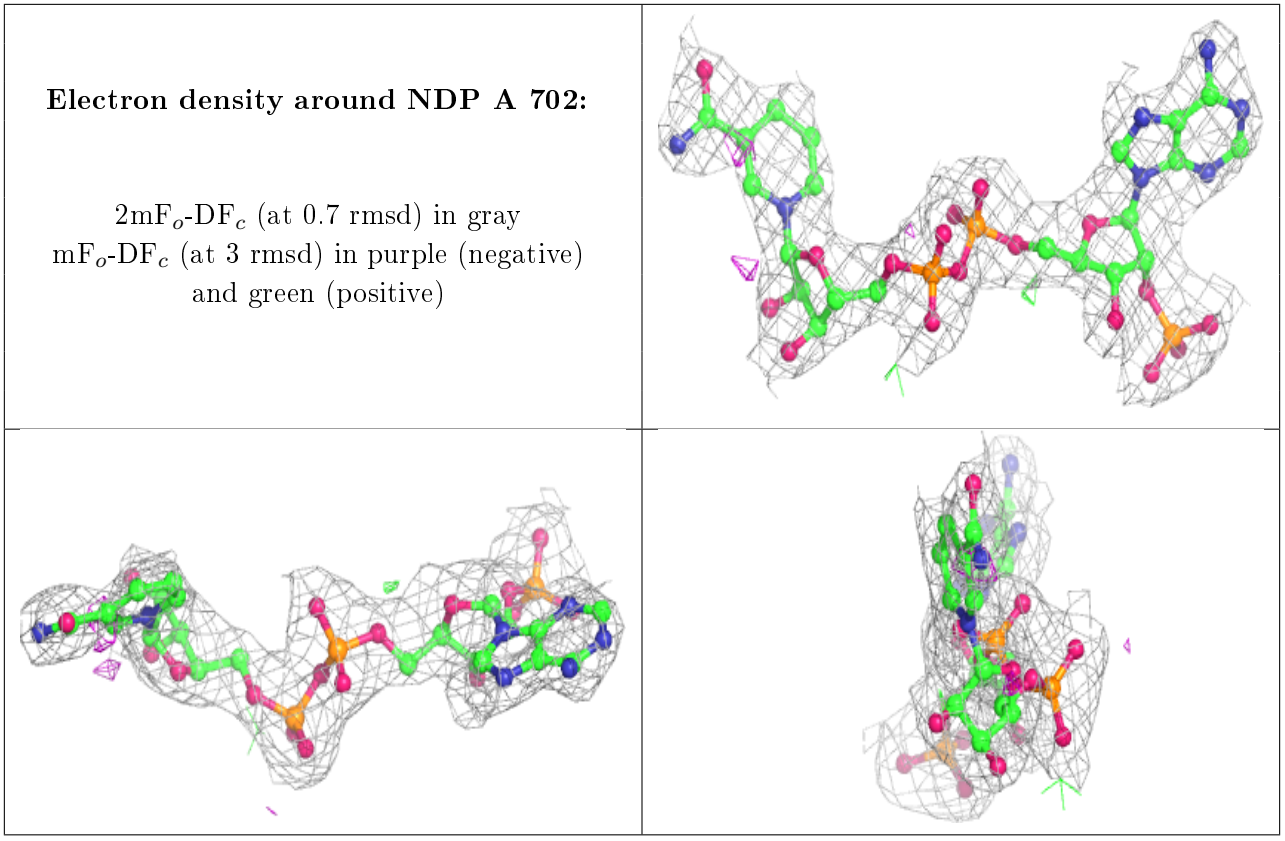
Electron density around P65 A 701:

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



Electron density around NDP A 702:

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



6.5 Other polymers (i)

There are no such residues in this entry.