Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 09:49 AM JST

PDB ID	:	6LH9
Title	:	Quadruple mutant (N51I+C59R+S108N+I164L) plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with compound 46 and NADPH
Authors	:	Vanichtanankul, J.; Vitsupakorn, D.
Deposited on	:	2019-12-07
Resolution	:	2.64 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

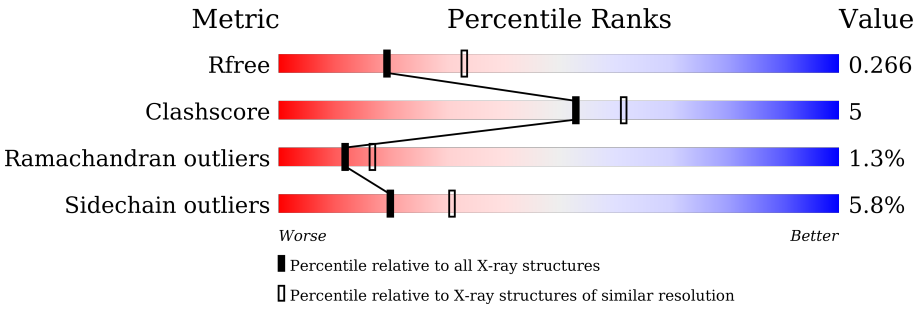
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	608	73% 14% 12%
1	B	608	68% 16% • 13%

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	NDP	B	902	X	-	-	-

2 Entry composition

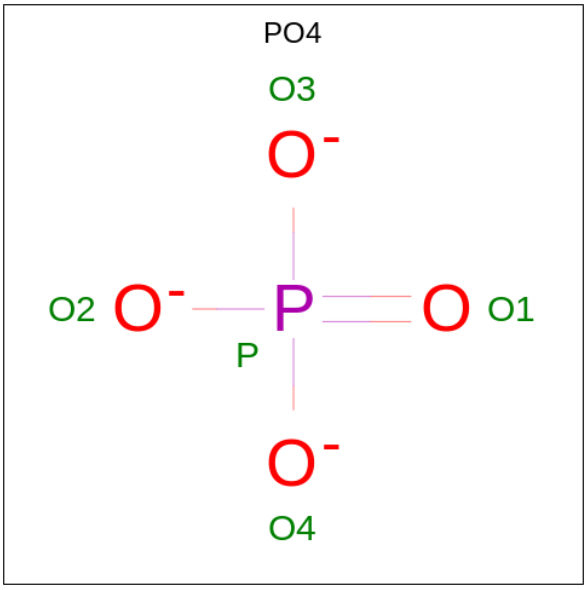
There are 5 unique types of molecules in this entry. The entry contains 17882 atoms, of which 8825 are hydrogens and 0 are deuteriums.

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.

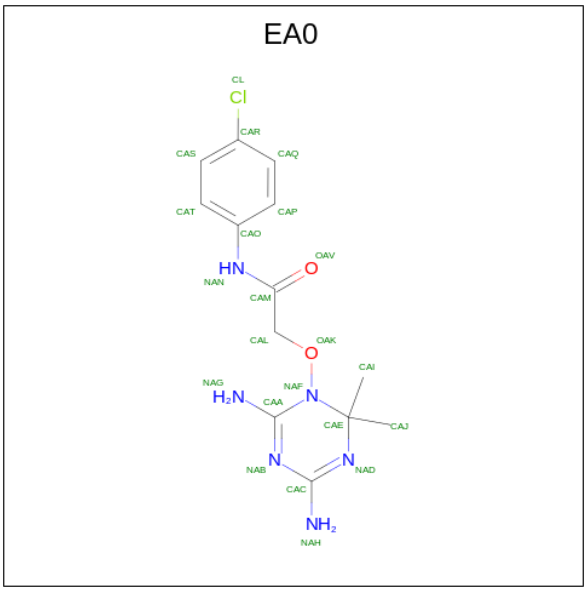
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	532	Total	C	H	N	O	S	256	0	0
			8832	2867	4399	733	809	24			
1	B	526	Total	C	H	N	O	S	251	0	0
			8730	2838	4345	723	800	24			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



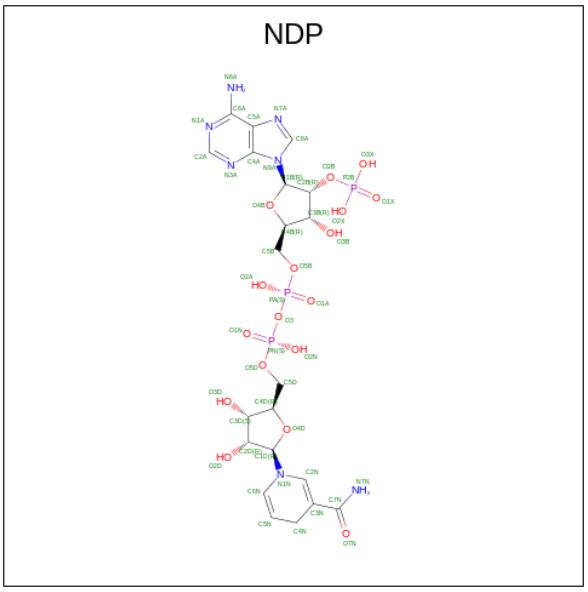
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 2-[[4,6-bis(azanyl)-2,2-dimethyl-1,3,5-triazin-1-yl]oxy]-N-(4-chlorophenyl)etha namide (three-letter code: EA0) (formula: $C_{13}H_{17}ClN_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	H	N	O	4	0
			39	13	1	17	6	2		
3	B	1	Total	C	Cl	H	N	O	4	0
			39	13	1	17	6	2		

- Molecule 4 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
4	A	1	Total	C	H	N	O	P	3	0
			72	21	24	7	17	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	P	3	0
			71	21	23	7	17	3		

- Molecule 5 is water.

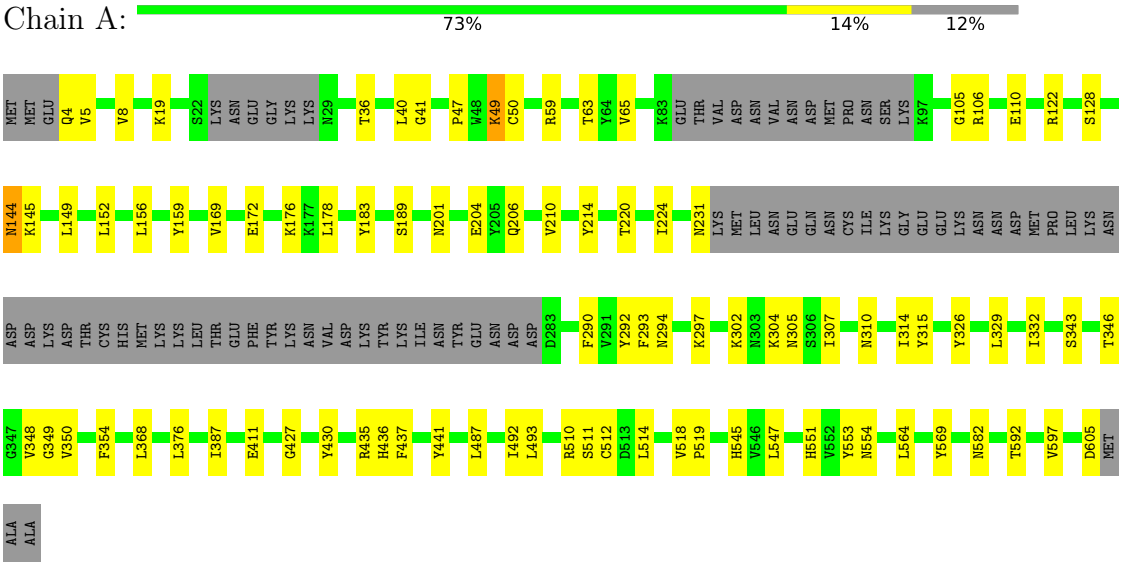
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total	O	0	0
			50	50		
5	B	39	Total	O	0	0
			39	39		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

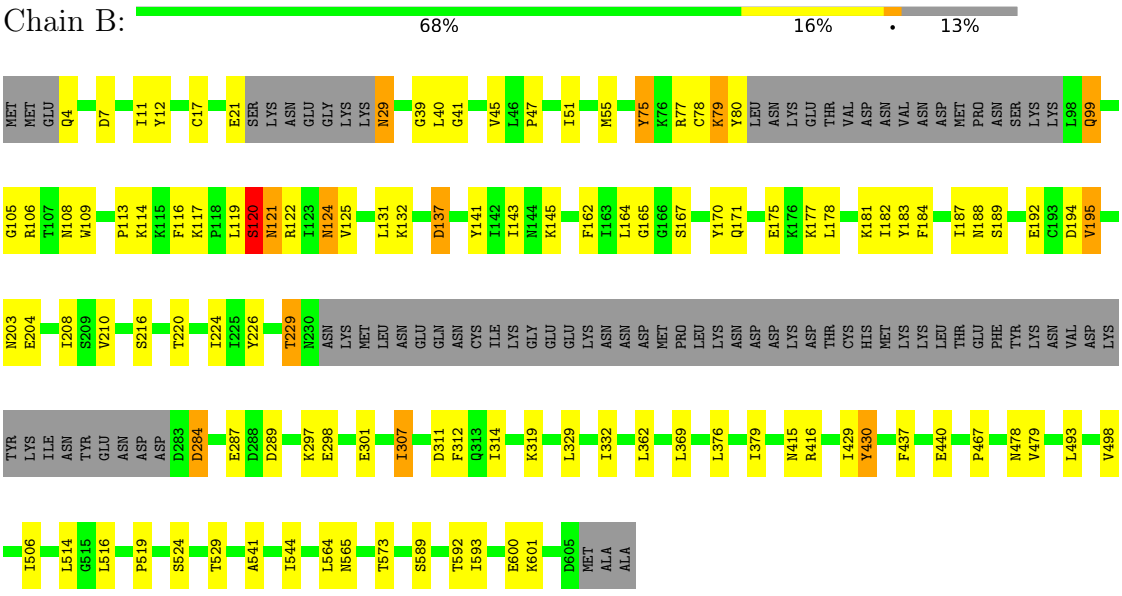
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain A:



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.70Å 155.88Å 164.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.95 – 2.64 43.95 – 2.64	Depositor EDS
% Data completeness (in resolution range)	89.7 (43.95-2.64) 82.7 (43.95-2.64)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.252 , 0.332 0.190 , 0.266	Depositor DCC
R_{free} test set	1980 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17882	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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, EA0

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	0.70	0/4537	0.85	0/6128
1	B	0.72	0/4489	0.88	1/6065 (0.0%)
All	All	0.71	0/9026	0.86	1/12193 (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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	529	THR	CA-CB-OG1	-5.15	98.19	109.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	284	ASP	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	4433	4399	4384	43	0
1	B	4385	4345	4330	55	0
2	A	10	0	0	1	0
3	A	22	17	0	0	0
3	B	22	17	0	0	0
4	A	48	24	26	2	0
4	B	48	23	26	2	0
5	A	50	0	0	0	0
5	B	39	0	0	0	0
All	All	9057	8825	8766	95	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 5.

All (95) 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:99:GLN:NE2	1:B:121:ASN:O	2.09	0.86
1:A:349:GLY:C	1:A:554:ASN:ND2	2.40	0.74
1:A:144:ASN:HD21	1:A:145:LYS:HE3	1.55	0.71
1:A:349:GLY:C	1:A:554:ASN:HD22	1.94	0.70
1:B:369:LEU:HD12	1:B:519:PRO:HB3	1.74	0.69
1:B:171:GLN:NE2	1:B:175:GLU:OE1	2.26	0.68
1:B:122:ARG:O	1:B:124:ASN:ND2	2.27	0.68
1:B:121:ASN:O	1:B:121:ASN:ND2	2.24	0.66
1:B:124:ASN:N	1:B:124:ASN:HD22	1.99	0.61
1:B:75:TYR:O	1:B:79:LYS:HD3	2.01	0.61
1:A:144:ASN:ND2	1:A:145:LYS:HE3	2.16	0.61
1:B:108:ASN:HD22	1:B:165:GLY:C	2.04	0.60
1:B:204:GLU:O	1:B:229:THR:OG1	2.20	0.58
1:A:290:PHE:CE2	1:A:294:ASN:ND2	2.72	0.57
1:A:387:ILE:O	1:A:435:ARG:NH1	2.37	0.57
1:A:41:GLY:HA2	1:A:47:PRO:HD3	1.85	0.56
1:A:427:GLY:HA2	1:A:441:TYR:CE2	2.43	0.54
1:A:214:TYR:O	1:A:220:THR:HA	2.09	0.53
1:B:493:LEU:HD12	1:B:493:LEU:C	2.27	0.53
1:A:201:ASN:HD22	1:A:204:GLU:HG3	1.74	0.53
1:B:78:CYS:O	1:B:80:TYR:N	2.42	0.53
1:B:78:CYS:C	1:B:80:TYR:H	2.12	0.53
1:B:105:GLY:O	1:B:108:ASN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:O	4:B:902:NDP:H41N	2.09	0.52
1:B:311:ASP:O	1:B:565:ASN:ND2	2.42	0.52
1:B:314:ILE:HD13	1:B:565:ASN:HB3	1.92	0.51
1:A:545:HIS:CD2	1:A:547:LEU:CD2	2.93	0.51
1:B:376:LEU:HD12	1:B:593:ILE:HG13	1.93	0.50
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.93	0.50
1:B:167:SER:HB3	4:B:902:NDP:O1N	2.10	0.49
1:A:292:TYR:C	1:A:294:ASN:H	2.16	0.49
1:A:332:ILE:CD1	1:A:514:LEU:HB3	2.43	0.48
1:B:329:LEU:HD22	1:B:564:LEU:HD12	1.94	0.48
1:A:511:SER:OG	1:A:551:HIS:HE1	1.96	0.48
1:A:210:VAL:HG12	1:A:224:ILE:HG22	1.96	0.48
1:A:492:ILE:HD11	1:A:510:ARG:HD3	1.95	0.48
1:B:194:ASP:OD1	1:B:195:VAL:HG22	2.13	0.48
1:A:40:LEU:O	4:A:803:NDP:H2N	2.15	0.47
1:B:51:ILE:HD13	1:B:187:ILE:HD12	1.97	0.47
1:B:75:TYR:O	1:B:79:LYS:CD	2.64	0.46
1:A:65:VAL:HG12	1:A:159:TYR:HB3	1.96	0.46
1:A:493:LEU:C	1:A:493:LEU:HD12	2.36	0.46
1:B:181:LYS:HD3	1:B:183:TYR:OH	2.16	0.46
1:A:547:LEU:HD23	1:A:547:LEU:N	2.31	0.46
1:A:19:LYS:HG2	1:A:36:THR:HG22	1.97	0.45
1:B:182:ILE:HB	1:B:226:TYR:HB2	1.97	0.45
1:A:4:GLN:O	1:A:8:VAL:HG23	2.17	0.45
1:B:429:ILE:O	1:B:430:TYR:C	2.55	0.45
1:B:379:ILE:HD12	1:B:379:ILE:C	2.37	0.45
1:B:284:ASP:HB2	1:B:287:GLU:HB2	1.98	0.44
1:A:128:SER:HA	4:A:803:NDP:H1B	2.00	0.44
1:B:188:ASN:HB3	1:B:220:THR:OG1	2.16	0.44
1:A:350:VAL:HG12	1:A:553:TYR:CD1	2.53	0.44
1:B:125:VAL:HA	1:B:141:TYR:O	2.18	0.44
1:A:518:VAL:N	1:A:519:PRO:CD	2.81	0.44
1:A:569:TYR:CD2	1:A:597:VAL:HG12	2.53	0.44
1:A:106:ARG:O	1:A:110:GLU:HG3	2.19	0.43
1:A:315:TYR:HB2	1:A:564:LEU:O	2.18	0.43
1:A:368:LEU:HD13	1:A:376:LEU:HD21	1.99	0.43
1:A:435:ARG:HB2	1:A:436:HIS:CD2	2.53	0.43
1:B:17:CYS:HA	1:B:39:GLY:O	2.18	0.43
1:A:144:ASN:C	1:A:144:ASN:HD22	2.22	0.43
1:A:437:PHE:CD1	1:B:479:VAL:HB	2.54	0.43
1:B:125:VAL:CG1	1:B:143:ILE:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:O	1:A:152:LEU:HB3	2.19	0.43
1:A:326:TYR:HA	1:A:329:LEU:HB2	1.99	0.43
1:B:17:CYS:SG	1:B:184:PHE:CZ	3.12	0.42
1:A:510:ARG:NH2	2:A:801:PO4:O3	2.44	0.42
1:B:105:GLY:O	1:B:106:ARG:C	2.57	0.42
1:A:411:GLU:H	1:A:411:GLU:CD	2.23	0.42
1:B:220:THR:HG23	1:B:573:THR:CG2	2.49	0.42
1:B:165:GLY:HA3	1:B:170:TYR:CZ	2.54	0.42
1:B:119:LEU:O	1:B:120:SER:C	2.58	0.42
1:B:467:PRO:HB2	1:B:498:VAL:HG11	2.01	0.42
1:A:63:THR:HG22	1:A:122:ARG:CD	2.49	0.42
1:A:354:PHE:CE2	1:B:506:ILE:HG13	2.55	0.42
1:B:362:LEU:HB2	1:B:541:ALA:O	2.20	0.42
1:B:516:LEU:HD23	1:B:516:LEU:HA	1.84	0.42
1:B:109:TRP:CZ2	1:B:117:LYS:HD2	2.55	0.42
1:B:307:ILE:HG22	1:B:312:PHE:CE2	2.55	0.42
1:B:29:ASN:HD22	1:B:29:ASN:N	2.18	0.41
1:B:210:VAL:HG12	1:B:224:ILE:HG22	2.02	0.41
1:B:332:ILE:CD1	1:B:514:LEU:HB3	2.50	0.41
1:B:437:PHE:CE2	1:B:478:ASN:HB2	2.54	0.41
1:B:12:TYR:O	1:B:162:PHE:HA	2.21	0.41
1:B:41:GLY:HA2	1:B:47:PRO:HD3	2.01	0.41
1:B:11:ILE:HB	1:B:178:LEU:O	2.18	0.41
1:A:176:LYS:O	1:A:178:LEU:HG	2.21	0.41
1:A:152:LEU:HD11	1:A:156:LEU:HD11	2.03	0.41
1:B:121:ASN:HD22	1:B:121:ASN:C	2.19	0.41
1:A:349:GLY:O	1:A:554:ASN:ND2	2.52	0.40
1:B:78:CYS:C	1:B:80:TYR:N	2.74	0.40
1:A:105:GLY:N	1:A:169:VAL:HG21	2.36	0.40
1:B:40:LEU:HD23	1:B:40:LEU:HA	1.95	0.40
1:A:183:TYR:OH	1:B:289:ASP:OD1	2.27	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	524/608 (86%)	476 (91%)	42 (8%)	6 (1%)	14 20
1	B	518/608 (85%)	463 (89%)	47 (9%)	8 (2%)	10 14
All	All	1042/1216 (86%)	939 (90%)	89 (8%)	14 (1%)	12 17

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	LYS
1	B	114	LYS
1	B	120	SER
1	A	49	LYS
1	A	310	ASN
1	A	293	PHE
1	A	348	VAL
1	B	177	LYS
1	B	301	GLU
1	B	430	TYR
1	A	304	LYS
1	B	137	ASP
1	A	430	TYR
1	B	113	PRO

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	498/570 (87%)	477 (96%)	21 (4%)	30 45
1	B	492/570 (86%)	456 (93%)	36 (7%)	14 21
All	All	990/1140 (87%)	933 (94%)	57 (6%)	20 31

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	49	LYS
1	A	50	CYS
1	A	59	ARG
1	A	144	ASN
1	A	172	GLU
1	A	189	SER
1	A	206	GLN
1	A	231	ASN
1	A	297	LYS
1	A	302	LYS
1	A	305	ASN
1	A	307	ILE
1	A	314	ILE
1	A	343	SER
1	A	346	THR
1	A	487	LEU
1	A	512	CYS
1	A	582	ASN
1	A	592	THR
1	A	605	ASP
1	B	4	GLN
1	B	7	ASP
1	B	21	GLU
1	B	29	ASN
1	B	45	VAL
1	B	55	MET
1	B	75	TYR
1	B	77	ARG
1	B	99	GLN
1	B	116	PHE
1	B	120	SER
1	B	121	ASN
1	B	124	ASN
1	B	131	LEU
1	B	132	LYS
1	B	137	ASP
1	B	145	LYS
1	B	189	SER
1	B	192	GLU
1	B	195	VAL
1	B	203	ASN
1	B	208	ILE

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Mol	Chain	Res	Type
1	B	216	SER
1	B	229	THR
1	B	297	LYS
1	B	298	GLU
1	B	307	ILE
1	B	319	LYS
1	B	415	ASN
1	B	416	ARG
1	B	440	GLU
1	B	524	SER
1	B	589	SER
1	B	592	THR
1	B	600	GLU
1	B	601	LYS

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

Mol	Chain	Res	Type
1	A	99	GLN
1	A	144	ASN
1	A	201	ASN
1	A	394	ASN
1	A	424	ASN
1	A	551	HIS
1	A	554	ASN
1	B	108	ASN
1	B	157	ASN
1	B	316	ASN
1	B	394	ASN
1	B	424	ASN
1	B	554	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	EA0	B	901	-	19,23,23	0.56	0	21,33,33	0.43	0
2	PO4	A	801	-	4,4,4	1.08	0	6,6,6	0.28	0
2	PO4	A	804	-	4,4,4	0.69	0	6,6,6	0.50	0
3	EA0	A	802	-	19,23,23	0.59	0	21,33,33	0.38	0
4	NDP	A	803	-	45,52,52	0.63	0	53,80,80	0.85	2 (3%)
4	NDP	B	902	-	45,52,52	0.66	1 (2%)	53,80,80	0.89	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EA0	B	901	-	-	6/9/28/28	0/2/2/2
3	EA0	A	802	-	-	4/9/28/28	0/2/2/2
4	NDP	B	902	-	1/1/17/17	11/30/77/77	0/5/5/5
4	NDP	A	803	-	-	3/30/77/77	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	NDP	P2B-O2B	2.02	1.63	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	902	NDP	C3N-C2N-N1N	-2.67	119.29	123.10
4	A	803	NDP	C5A-C6A-N6A	2.66	124.39	120.35
4	B	902	NDP	C5A-C6A-N6A	2.36	123.94	120.35
4	B	902	NDP	O2B-C2B-C1B	2.09	117.61	110.10
4	A	803	NDP	O2B-C2B-C1B	-2.06	102.70	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	902	NDP	C2B

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	EA0	OAK-CAL-CAM-NAN
3	A	802	EA0	CAL-CAM-NAN-CAO
3	A	802	EA0	OAV-CAM-NAN-CAO
3	B	901	EA0	OAK-CAL-CAM-NAN
3	B	901	EA0	CAL-CAM-NAN-CAO
3	B	901	EA0	OAV-CAM-NAN-CAO
4	B	902	NDP	C5D-O5D-PN-O3
4	B	902	NDP	C2D-C1D-N1N-C6N
4	B	902	NDP	C2D-C1D-N1N-C2N
3	A	802	EA0	OAK-CAL-CAM-OAV
3	B	901	EA0	OAK-CAL-CAM-OAV
4	B	902	NDP	C3D-C4D-C5D-O5D
4	A	803	NDP	PA-O3-PN-O5D
4	A	803	NDP	O4D-C1D-N1N-C2N
4	B	902	NDP	C2B-O2B-P2B-O2X
4	B	902	NDP	O4D-C1D-N1N-C6N
3	B	901	EA0	CAT-CAO-NAN-CAM
4	B	902	NDP	C3B-C4B-C5B-O5B
3	B	901	EA0	CAP-CAO-NAN-CAM
4	A	803	NDP	C2B-O2B-P2B-O3X
4	B	902	NDP	C2B-O2B-P2B-O3X
4	B	902	NDP	PN-O3-PA-O1A
4	B	902	NDP	PN-O3-PA-O2A
4	B	902	NDP	C5D-O5D-PN-O1N

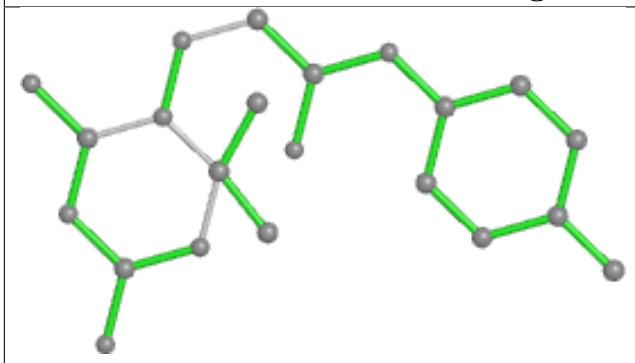
There are no ring outliers.

3 monomers are involved in 5 short contacts:

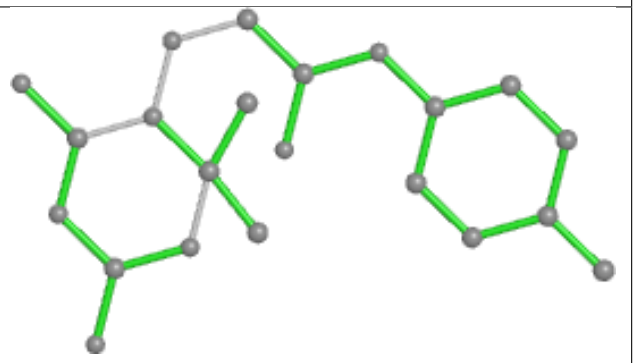
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PO4	1	0
4	A	803	NDP	2	0
4	B	902	NDP	2	0

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 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.

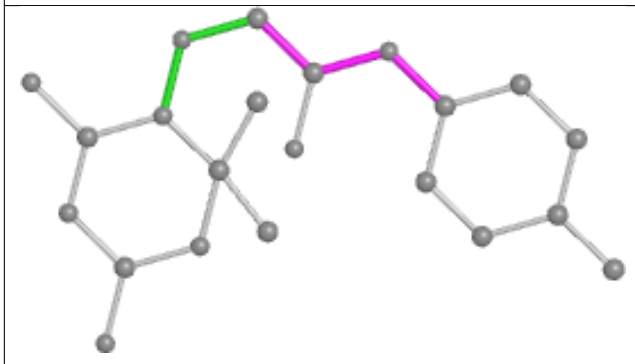
Ligand EA0 B 901



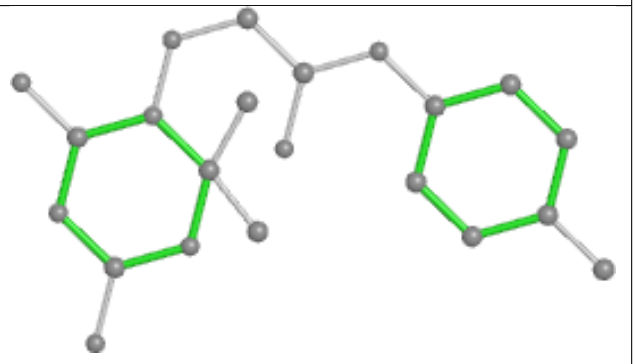
Bond lengths



Bond angles

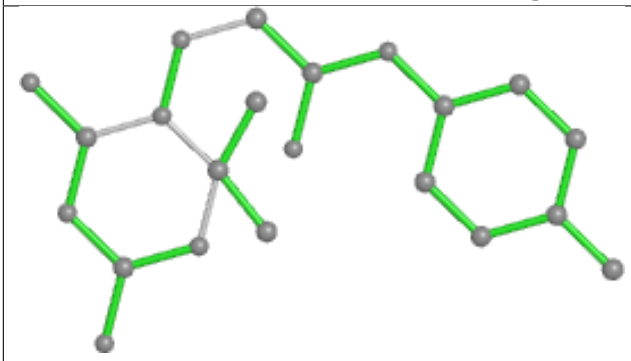


Torsions

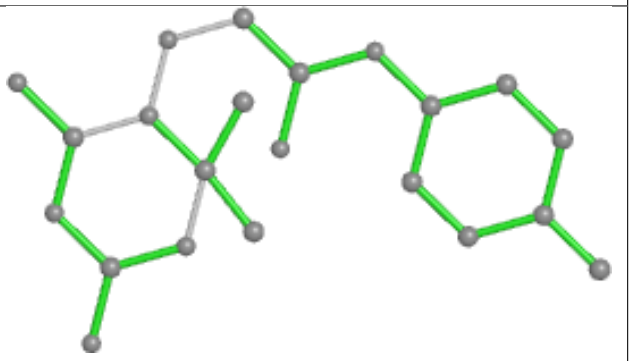


Rings

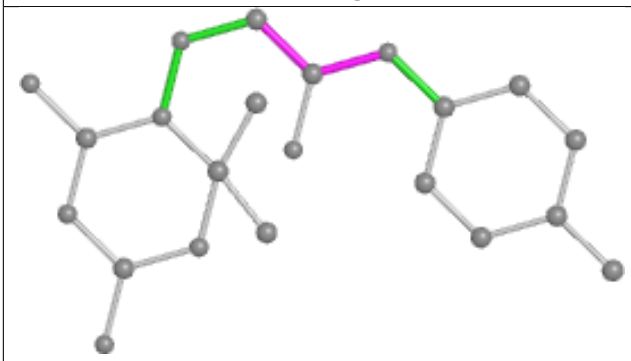
Ligand EA0 A 802



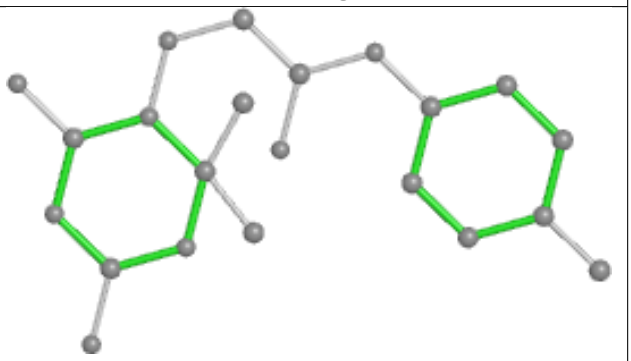
Bond lengths



Bond angles

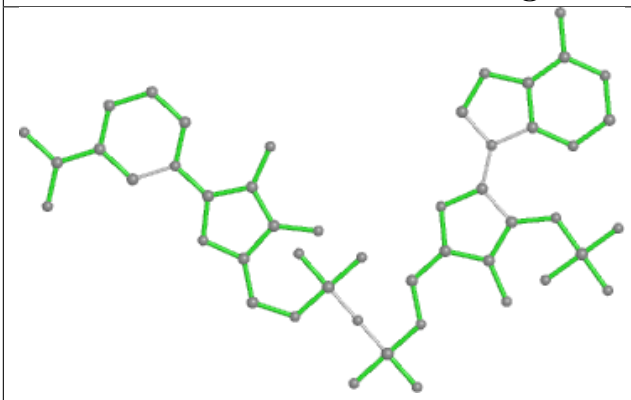


Torsions

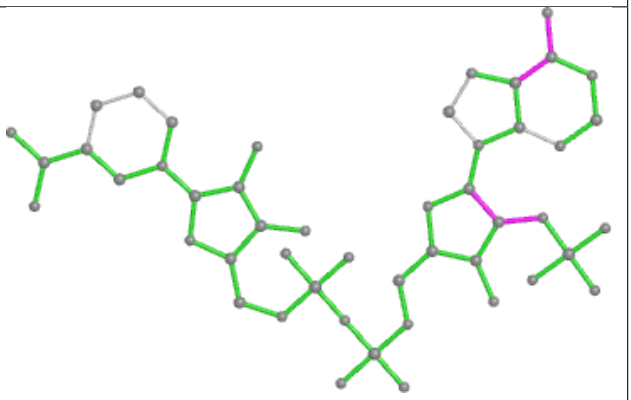


Rings

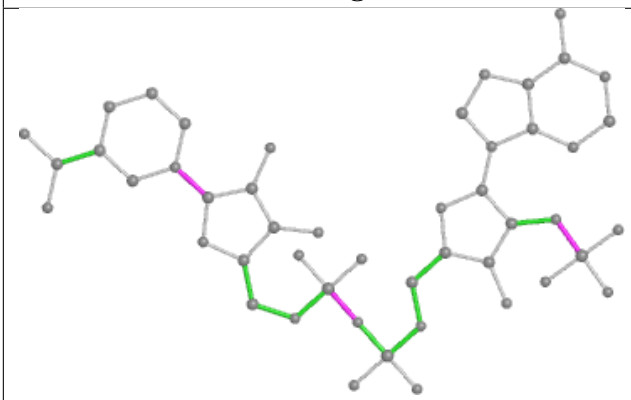
Ligand NDP A 803



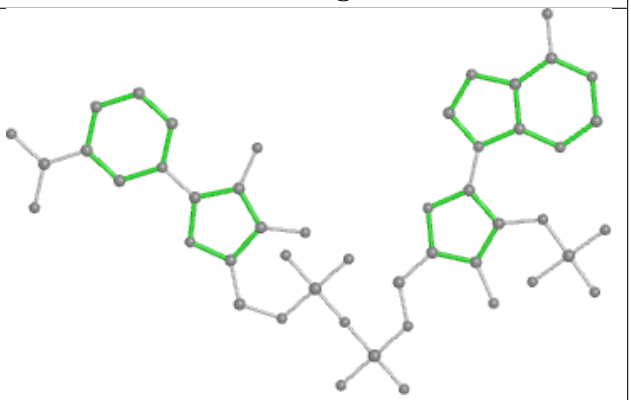
Bond lengths



Bond angles

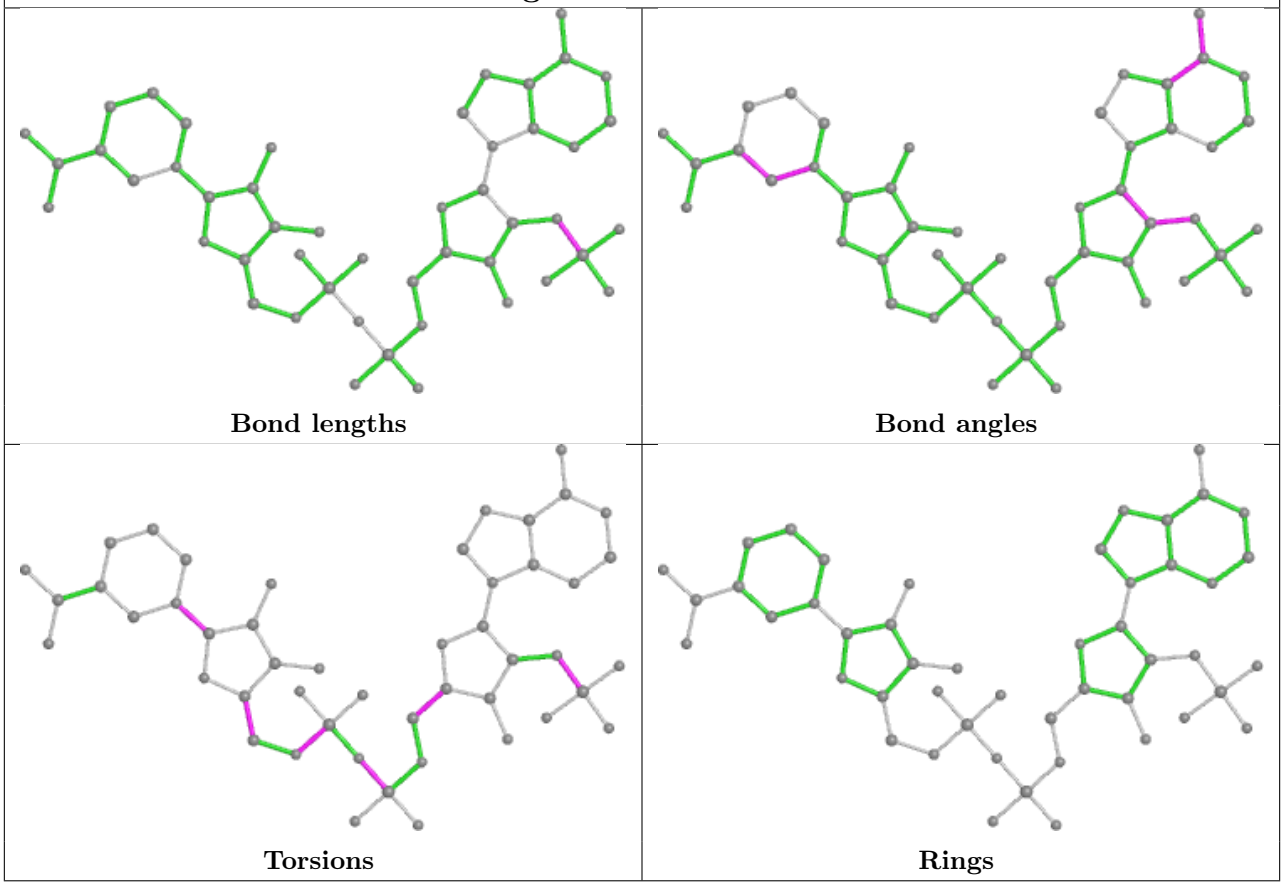


Torsions



Rings

Ligand NDP B 902



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

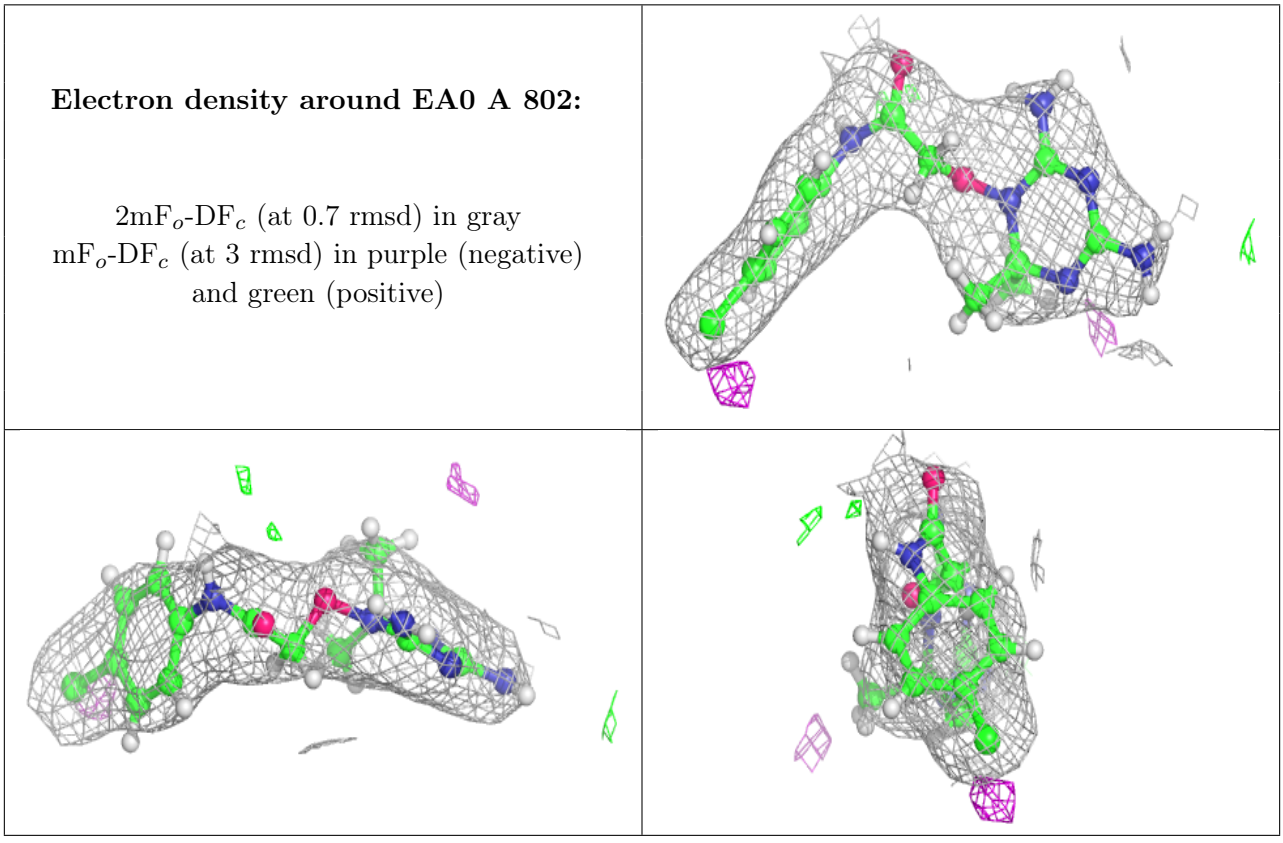
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

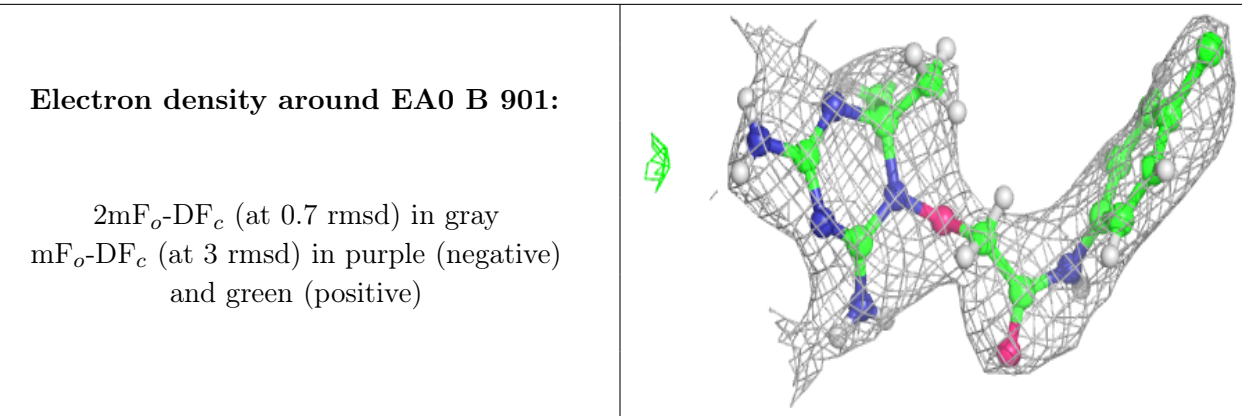
Electron density around EA0 A 802:

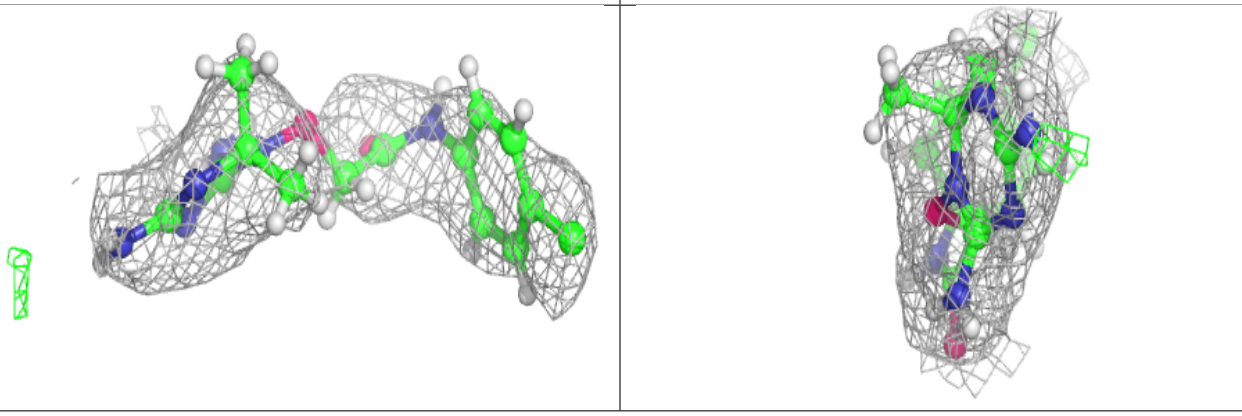
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around EA0 B 901:

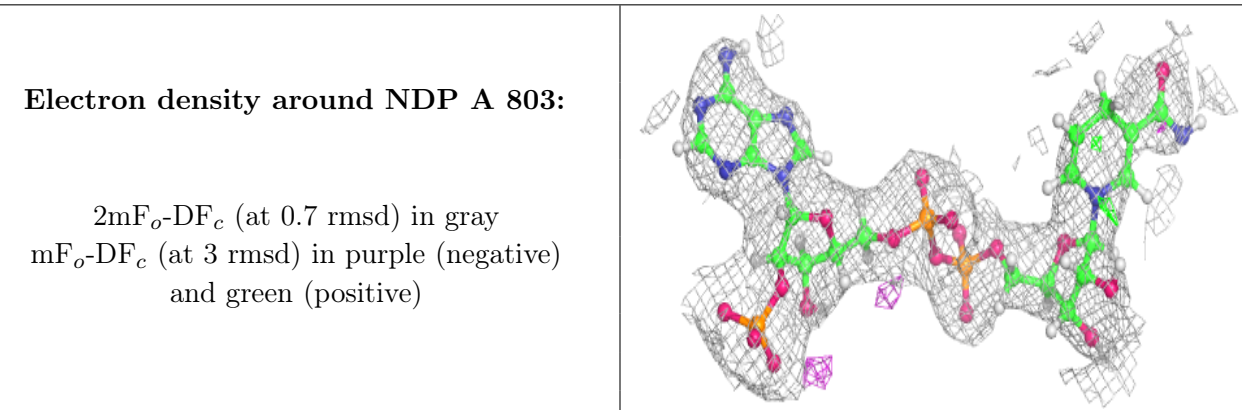
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

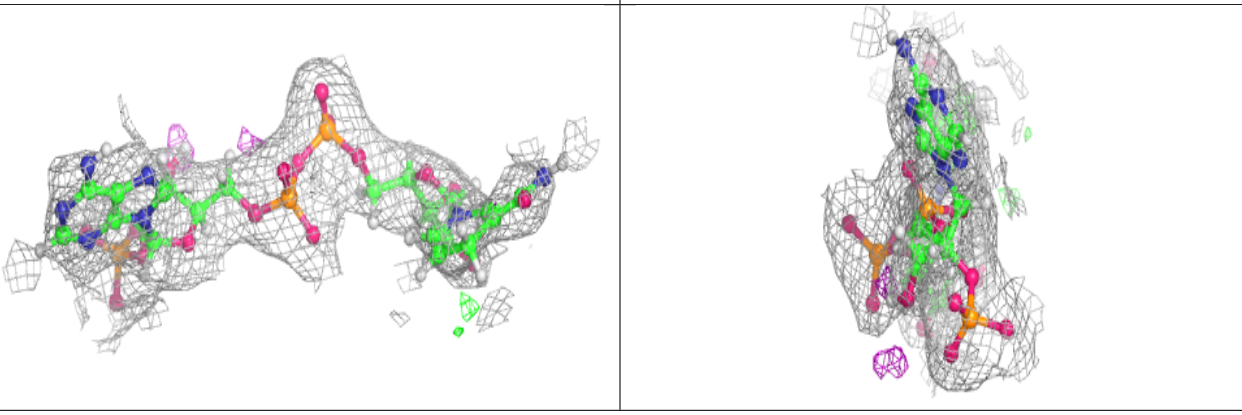




Electron density around NDP A 803:

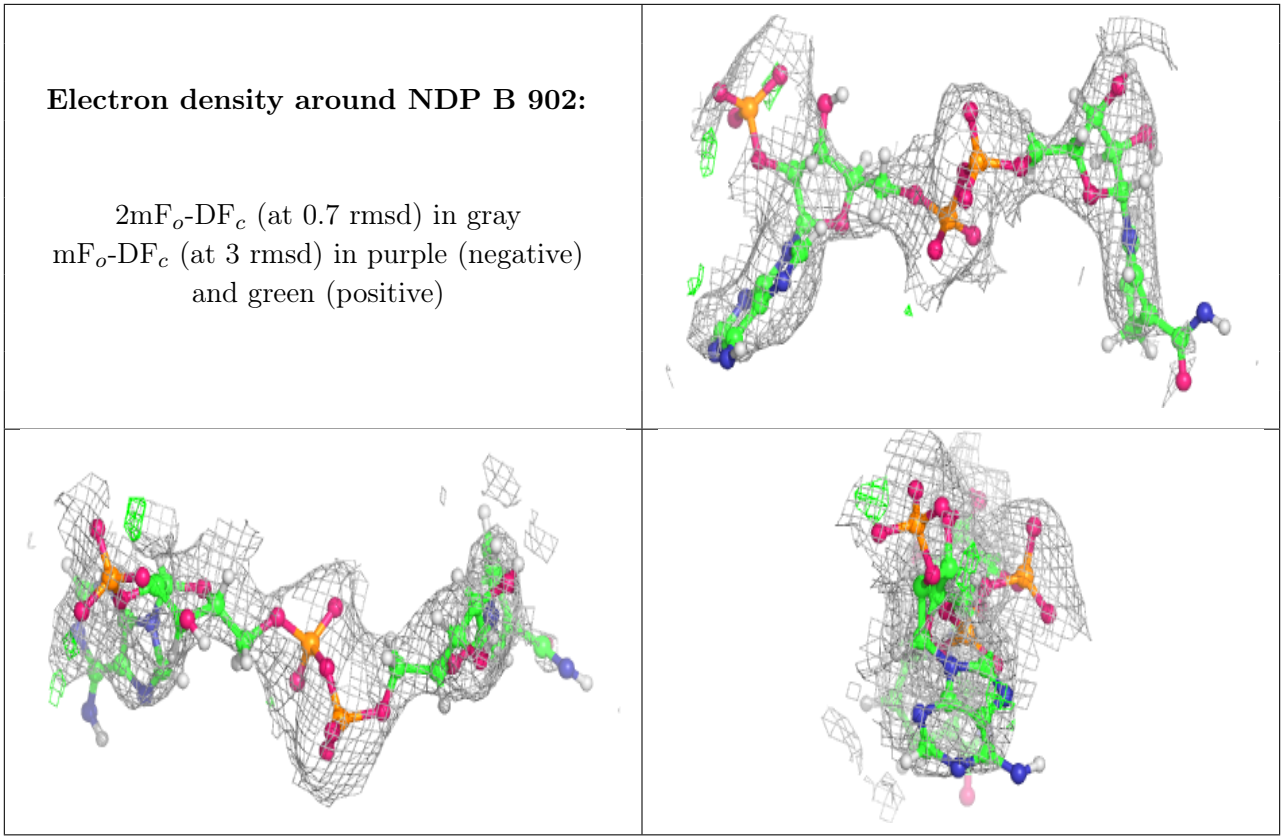
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around NDP B 902:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.