



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:54 AM UTC

PDB ID : 6LEZ / pdb_00006lez
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 : 2019-11-27
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

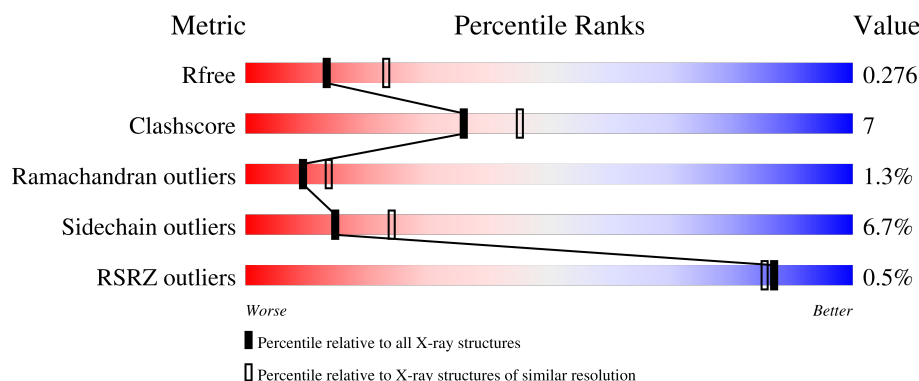
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (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 $\leq 5\%$. 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	
1	B	608	

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	EA0	B	701	-	-	X	-

2 Entry composition [i](#)

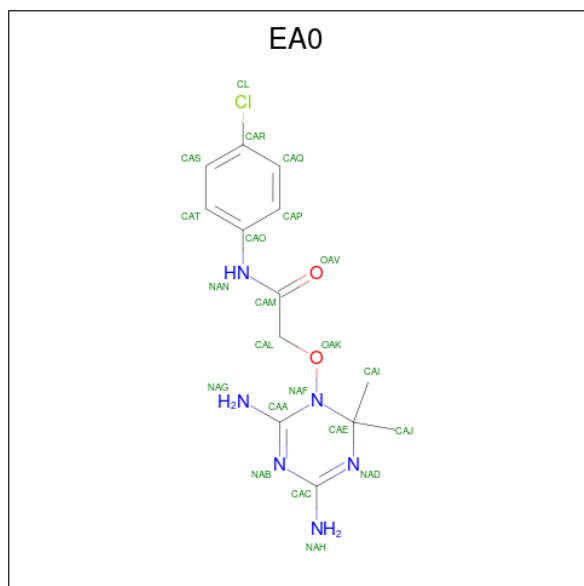
There are 5 unique types of molecules in this entry. The entry contains 8956 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

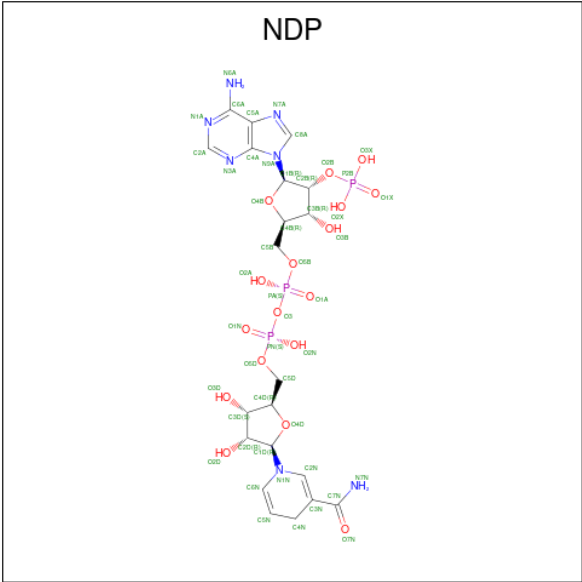
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	0	0
			4398	2847	727	800	24			
1	B	522	Total	C	N	O	S	0	0	0
			4349	2816	717	792	24			

- Molecule 2 is 2-[[4,6-bis(azanyl)-2,2-dimethyl-1,3,5-triazin-1-yl]oxy]-N-(4-chlorophenyl) ethanamide (CCD ID: EA0) (formula: C₁₃H₁₇ClN₆O₂) (labeled as "Ligand of Interest" by depositor).



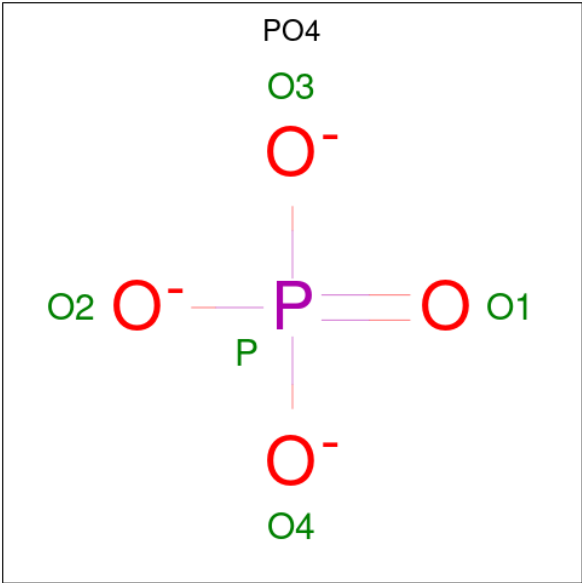
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			22	13	1	6	2		
2	B	1	Total	C	Cl	N	O	0	0
			22	13	1	6	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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 PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



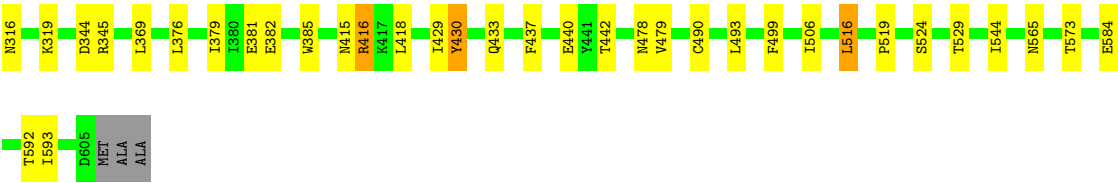
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total 32	O 32	0	0
5	B	27	Total 27	O 27	0	0

- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.70Å 155.88Å 164.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.64 10.00 – 2.64	Depositor EDS
% Data completeness (in resolution range)	87.8 (10.00-2.64) 87.8 (10.00-2.64)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.188 , 0.271 0.195 , 0.276	Depositor DCC
R_{free} test set	1915 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8956	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, EA0, NDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.04	0/4501	1.44	9/6079 (0.1%)
1	B	1.07	0/4452	1.43	9/6016 (0.1%)
All	All	1.06	0/8953	1.43	18/12095 (0.1%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529	THR	CA-CB-OG1	-7.10	98.95	109.60
1	A	517	GLY	CA-C-N	5.95	123.99	120.24
1	A	517	GLY	C-N-CA	5.95	123.99	120.24
1	A	344	ASP	CA-C-N	5.93	129.04	120.38
1	A	344	ASP	C-N-CA	5.93	129.04	120.38
1	B	116	PHE	CA-CB-CG	5.46	119.26	113.80
1	B	490	CYS	N-CA-C	-5.39	105.48	111.36
1	B	344	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	493	LEU	CA-C-N	5.28	130.43	122.99
1	A	493	LEU	C-N-CA	5.28	130.43	122.99
1	B	381	GLU	CB-CG-CD	5.24	121.51	112.60
1	B	75	TYR	CB-CA-C	5.22	120.26	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	LEU	CA-C-N	5.16	126.24	121.86
1	B	164	LEU	C-N-CA	5.16	126.24	121.86
1	B	442	THR	O-C-N	5.05	126.29	120.58
1	A	146	VAL	N-CA-C	-5.05	105.06	110.36
1	A	491	HIS	CA-C-N	5.00	127.52	120.42
1	A	491	HIS	C-N-CA	5.00	127.52	120.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	GLY	Peptide
1	B	165	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4398	0	4352	59	0
1	B	4349	0	4291	71	0
2	A	22	0	0	1	0
2	B	22	0	0	8	0
3	A	48	0	26	5	0
3	B	48	0	26	3	0
4	A	10	0	0	0	0
5	A	32	0	0	0	0
5	B	27	0	0	0	0
All	All	8956	0	8695	129	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 (129) 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)
2:B:701:EA0:OAK	2:B:701:EA0:NAF	1.60	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:GLN:NE2	1:B:121:ASN:O	2.06	0.88
1:B:122:ARG:O	1:B:124:ASN:ND2	2.14	0.81
1:A:349:GLY:C	1:A:554:ASN:ND2	2.39	0.80
1:B:121:ASN:O	1:B:121:ASN:ND2	2.15	0.80
1:A:349:GLY:C	1:A:554:ASN:HD22	1.93	0.76
2:B:701:EA0:OAK	2:B:701:EA0:CAA	2.36	0.74
1:A:144:ASN:HD21	1:A:145:LYS:HE3	1.54	0.71
1:B:165:GLY:HA3	1:B:170:TYR:CZ	2.29	0.68
1:B:171:GLN:NE2	1:B:175:GLU:OE1	2.28	0.66
1:B:78:CYS:O	1:B:80:TYR:N	2.29	0.65
1:B:99:GLN:HE22	1:B:121:ASN:C	2.05	0.63
1:A:108:ASN:OD1	2:A:701:EA0:OAV	2.16	0.63
1:B:125:VAL:CG1	1:B:143:ILE:HD11	2.30	0.62
1:B:314:ILE:HD13	1:B:565:ASN:HB3	1.80	0.62
1:A:144:ASN:ND2	1:A:145:LYS:HE3	2.15	0.60
1:A:166:GLY:HA3	3:A:702:NDP:PA	2.43	0.59
1:B:55:MET:CE	2:B:701:EA0:CAI	2.81	0.59
1:B:124:ASN:N	1:B:124:ASN:HD22	2.01	0.58
1:B:369:LEU:HD12	1:B:519:PRO:HB3	1.87	0.57
1:A:290:PHE:CE2	1:A:294:ASN:ND2	2.74	0.55
1:A:40:LEU:O	3:A:702:NDP:H2N	2.06	0.55
1:B:493:LEU:HD12	1:B:493:LEU:C	2.30	0.55
1:A:454:ASP:OD2	1:A:457:LYS:HG3	2.07	0.55
1:B:40:LEU:HD22	3:B:702:NDP:N7N	2.23	0.54
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.89	0.54
1:A:427:GLY:HA2	1:A:441:TYR:CE2	2.43	0.53
1:A:214:TYR:O	1:A:220:THR:HA	2.09	0.52
1:A:292:TYR:C	1:A:294:ASN:H	2.17	0.52
1:B:55:MET:HE2	1:B:55:MET:HA	1.91	0.52
1:B:141:TYR:CE1	1:B:156:LEU:HD11	2.44	0.52
1:B:108:ASN:ND2	1:B:165:GLY:C	2.68	0.51
1:B:204:GLU:O	1:B:229:THR:OG1	2.29	0.51
1:A:41:GLY:HA2	1:A:47:PRO:HD3	1.91	0.51
1:B:376:LEU:HD12	1:B:593:ILE:HG13	1.92	0.51
1:B:55:MET:HE3	2:B:701:EA0:CAI	2.41	0.50
1:B:108:ASN:HD22	1:B:165:GLY:C	2.18	0.50
1:A:144:ASN:C	1:A:144:ASN:HD22	2.20	0.50
1:A:493:LEU:C	1:A:493:LEU:HD12	2.36	0.50
1:A:545:HIS:CD2	1:A:547:LEU:CD2	2.95	0.50
1:A:166:GLY:HA3	3:A:702:NDP:O2A	2.12	0.50
1:B:141:TYR:HE1	1:B:156:LEU:HD11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ASP:OD1	1:B:195:VAL:HG22	2.11	0.49
1:A:65:VAL:HG12	1:A:159:TYR:HB3	1.93	0.49
1:B:165:GLY:HA3	1:B:170:TYR:CE1	2.47	0.49
2:B:701:EA0:OAK	2:B:701:EA0:CAE	2.57	0.49
1:A:492:ILE:HD11	1:A:510:ARG:HD3	1.93	0.49
1:B:108:ASN:ND2	1:B:165:GLY:O	2.45	0.49
1:A:109:TRP:CZ2	1:A:117:LYS:HD2	2.48	0.49
1:B:17:CYS:HA	1:B:39:GLY:O	2.13	0.49
1:B:51:ILE:HD13	1:B:187:ILE:HD12	1.94	0.49
1:B:125:VAL:HG11	1:B:143:ILE:HD11	1.95	0.48
1:A:332:ILE:CD1	1:A:514:LEU:HB3	2.43	0.48
1:A:285:GLU:OE2	1:B:12:TYR:OH	2.27	0.48
1:A:166:GLY:HA2	3:A:702:NDP:O5D	2.14	0.48
1:A:19:LYS:HG2	1:A:36:THR:HG22	1.95	0.47
1:B:437:PHE:CE2	1:B:478:ASN:HB2	2.48	0.47
1:B:304:LYS:HD2	1:B:304:LYS:H	1.78	0.47
1:B:121:ASN:C	1:B:121:ASN:HD22	2.14	0.47
1:B:141:TYR:CD1	1:B:152:LEU:HD11	2.50	0.47
1:A:152:LEU:HD11	1:A:156:LEU:HD11	1.97	0.47
2:B:701:EA0:OAK	2:B:701:EA0:CAI	2.64	0.46
1:B:210:VAL:HG12	1:B:224:ILE:HG22	1.97	0.46
1:A:4:GLN:O	1:A:8:VAL:HG23	2.15	0.46
1:B:137:ASP:HB2	1:B:140:VAL:HG23	1.96	0.46
1:A:201:ASN:HD22	1:A:204:GLU:HG3	1.81	0.46
1:A:569:TYR:CD2	1:A:597:VAL:HG12	2.51	0.46
1:B:63:THR:HG22	1:B:122:ARG:NE	2.31	0.46
1:A:319:LYS:HG2	1:B:286:GLU:HG2	1.97	0.46
1:B:429:ILE:O	1:B:430:TYR:C	2.59	0.45
1:B:516:LEU:HD23	1:B:516:LEU:HA	1.81	0.45
1:A:326:TYR:HA	1:A:329:LEU:HB2	1.98	0.45
1:A:80:TYR:CD2	1:A:80:TYR:C	2.95	0.45
1:A:40:LEU:HD22	3:A:702:NDP:C7N	2.47	0.45
1:A:511:SER:OG	1:A:551:HIS:HE1	2.00	0.45
1:B:119:LEU:O	1:B:120:SER:C	2.59	0.45
1:B:181:LYS:HD3	1:B:183:TYR:OH	2.18	0.44
1:A:105:GLY:N	1:A:169:VAL:HG21	2.32	0.44
1:A:173:PHE:O	1:A:178:LEU:HB2	2.17	0.44
1:B:6:CYS:HB3	1:B:178:LEU:O	2.18	0.44
1:B:14:ILE:O	2:B:701:EA0:NAG	2.51	0.44
1:B:379:ILE:HD12	1:B:379:ILE:C	2.43	0.44
1:B:182:ILE:HB	1:B:226:TYR:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLY:O	1:A:554:ASN:ND2	2.51	0.44
1:B:12:TYR:O	1:B:162:PHE:HA	2.18	0.43
1:A:59:ARG:O	1:A:63:THR:HG23	2.18	0.43
1:A:437:PHE:CD1	1:B:479:VAL:HB	2.53	0.43
1:B:41:GLY:HA2	1:B:47:PRO:HD3	2.01	0.43
1:B:176:LYS:O	1:B:177:LYS:C	2.61	0.43
1:A:576:LEU:O	1:A:577:ASN:C	2.61	0.43
1:A:354:PHE:CE2	1:B:506:ILE:HG13	2.53	0.43
1:B:307:ILE:HG22	1:B:312:PHE:CE2	2.53	0.43
1:B:382:GLU:O	1:B:385:TRP:HB3	2.18	0.43
1:A:42:ASN:HA	1:A:194:ASP:CG	2.45	0.42
1:B:173:PHE:O	1:B:178:LEU:HB2	2.19	0.42
1:B:433:GLN:O	1:B:437:PHE:HB2	2.19	0.42
1:A:435:ARG:HB2	1:A:436:HIS:CD2	2.54	0.42
1:A:285:GLU:CD	1:B:12:TYR:HH	2.23	0.42
1:A:340:ASN:HB3	1:B:499:PHE:CE1	2.55	0.42
1:A:358:MET:HE1	1:A:522:ILE:HD11	2.01	0.42
1:B:59:ARG:O	1:B:63:THR:HG23	2.19	0.42
1:A:63:THR:HG22	1:A:122:ARG:CD	2.50	0.42
1:A:518:VAL:N	1:A:519:PRO:CD	2.82	0.42
1:A:545:HIS:CD2	1:A:547:LEU:HD21	2.55	0.42
1:B:109:TRP:CZ2	1:B:117:LYS:HD2	2.55	0.42
1:B:311:ASP:O	1:B:565:ASN:ND2	2.51	0.42
1:B:220:THR:HG23	1:B:573:THR:CG2	2.49	0.42
1:B:312:PHE:HB2	1:B:316:ASN:ND2	2.35	0.42
3:B:702:NDP:O1A	3:B:702:NDP:O2N	2.37	0.41
1:A:183:TYR:CD1	1:A:225:ILE:HG12	2.54	0.41
1:A:221:LEU:HD23	1:A:221:LEU:N	2.34	0.41
1:B:55:MET:HE1	2:B:701:EA0:CAI	2.50	0.41
1:B:416:ARG:HB3	1:B:418:LEU:HG	2.02	0.41
1:A:144:ASN:HD22	1:A:145:LYS:N	2.17	0.41
1:A:514:LEU:HD21	1:A:550:ALA:HB1	2.03	0.41
1:B:181:LYS:HA	1:B:226:TYR:O	2.21	0.41
1:A:65:VAL:HG12	1:A:159:TYR:CB	2.50	0.41
1:A:312:PHE:HA	1:A:565:ASN:HD21	1.85	0.41
1:A:487:LEU:N	1:A:487:LEU:CD2	2.83	0.41
1:B:43:LYS:N	1:B:194:ASP:OD2	2.38	0.41
1:A:149:LEU:O	1:A:152:LEU:HB3	2.21	0.41
1:A:547:LEU:HD23	1:A:547:LEU:N	2.36	0.41
1:B:127:LEU:O	3:B:702:NDP:H1B	2.21	0.41
1:B:292:TYR:O	1:B:295:PHE:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ASN:O	1:B:36:THR:HB	2.21	0.40
1:A:518:VAL:O	1:A:519:PRO:C	2.64	0.40
1:A:411:GLU:CD	1:A:411:GLU:H	2.28	0.40
1:B:11:ILE:HB	1:B:178:LEU:O	2.20	0.40
1:B:48:TRP:CD1	1:B:51:ILE:HD12	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/608 (85%)	477 (92%)	35 (7%)	6 (1%)	10	15
1	B	512/608 (84%)	457 (89%)	48 (9%)	7 (1%)	9	12
All	All	1030/1216 (85%)	934 (91%)	83 (8%)	13 (1%)	9	14

All (13) 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	348	VAL
1	B	177	LYS
1	A	295	PHE
1	A	304	LYS
1	A	310	ASN
1	B	430	TYR
1	A	293	PHE
1	B	137	ASP
1	B	113	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	494/570 (87%)	470 (95%)	24 (5%)	22	37
1	B	488/570 (86%)	446 (91%)	42 (9%)	10	15
All	All	982/1140 (86%)	916 (93%)	66 (7%)	15	24

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	8	VAL
1	A	49	LYS
1	A	50	CYS
1	A	52	SER
1	A	59	ARG
1	A	107	THR
1	A	144	ASN
1	A	189	SER
1	A	206	GLN
1	A	284	ASP
1	A	297	LYS
1	A	302	LYS
1	A	307	ILE
1	A	314	ILE
1	A	341	LYS
1	A	343	SER
1	A	346	THR
1	A	487	LEU
1	A	512	CYS
1	A	555	ASN
1	A	582	ASN
1	A	592	THR
1	A	605	ASP
1	B	4	GLN
1	B	7	ASP
1	B	11	ILE

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Mol	Chain	Res	Type
1	B	21	GLU
1	B	29	ASN
1	B	36	THR
1	B	45	VAL
1	B	67	GLU
1	B	75	TYR
1	B	99	GLN
1	B	106	ARG
1	B	116	PHE
1	B	120	SER
1	B	121	ASN
1	B	124	ASN
1	B	127	LEU
1	B	132	LYS
1	B	134	GLU
1	B	142	ILE
1	B	145	LYS
1	B	147	GLU
1	B	155	LYS
1	B	189	SER
1	B	190	THR
1	B	192	GLU
1	B	195	VAL
1	B	203	ASN
1	B	208	ILE
1	B	216	SER
1	B	228	LYS
1	B	229	THR
1	B	297	LYS
1	B	307	ILE
1	B	319	LYS
1	B	345	ARG
1	B	415	ASN
1	B	416	ARG
1	B	440	GLU
1	B	516	LEU
1	B	524	SER
1	B	584	GLU
1	B	592	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) 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	407	ASN
1	A	415	ASN
1	A	424	ASN
1	A	551	HIS
1	A	554	ASN
1	A	556	HIS
1	B	29	ASN
1	B	42	ASN
1	B	108	ASN
1	B	171	GLN
1	B	201	ASN
1	B	316	ASN
1	B	394	ASN
1	B	407	ASN
1	B	424	ASN
1	B	554	ASN
1	B	582	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 oligosaccharides 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	NDP	B	702	-	51,52,52	2.45	12 (23%)	71,80,80	2.16	20 (28%)
4	PO4	A	703	-	4,4,4	0.81	0	6,6,6	0.59	0
4	PO4	A	704	-	4,4,4	0.36	0	6,6,6	0.57	0
2	EA0	B	701	-	20,23,23	3.91	5 (25%)	24,33,33	4.04	8 (33%)
2	EA0	A	701	-	20,23,23	3.35	6 (30%)	24,33,33	4.04	11 (45%)
3	NDP	A	702	-	51,52,52	1.93	16 (31%)	71,80,80	2.14	16 (22%)

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
2	EA0	A	701	-	-	4/9/28/28	0/1/2/2
3	NDP	A	702	-	-	9/34/77/77	0/5/5/5
3	NDP	B	702	-	-	5/34/77/77	0/5/5/5
2	EA0	B	701	-	-	5/9/28/28	0/1/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	EA0	OAK-NAF	16.01	1.60	1.40
2	A	701	EA0	OAK-NAF	11.94	1.55	1.40
3	B	702	NDP	PN-O3	9.11	1.69	1.59
3	B	702	NDP	PA-O3	8.79	1.69	1.59
2	A	701	EA0	CAO-NAN	-5.95	1.29	1.41
3	A	702	NDP	PN-O3	5.58	1.65	1.59
3	B	702	NDP	C4N-C3N	-4.92	1.40	1.50
2	B	701	EA0	CAO-NAN	-4.73	1.32	1.41
3	A	702	NDP	C2A-N1A	4.54	1.42	1.33
2	A	701	EA0	CAR-CL	-4.49	1.63	1.74
3	A	702	NDP	PA-O3	3.98	1.63	1.59
3	B	702	NDP	C2A-N3A	3.92	1.40	1.33
3	A	702	NDP	C4N-C3N	-3.59	1.43	1.50
3	B	702	NDP	C2A-N1A	3.56	1.40	1.33
3	B	702	NDP	C4N-C5N	-3.31	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NDP	C2A-N3A	3.22	1.39	1.33
3	B	702	NDP	C5A-N7A	-3.19	1.33	1.39
3	A	702	NDP	O4D-C1D	2.99	1.48	1.42
3	A	702	NDP	C4N-C5N	-2.97	1.41	1.49
3	A	702	NDP	C5A-N7A	-2.91	1.33	1.39
3	B	702	NDP	C5A-C4A	-2.83	1.34	1.39
3	B	702	NDP	C8A-N9A	-2.79	1.32	1.37
2	A	701	EA0	CAM-NAN	-2.70	1.29	1.35
3	A	702	NDP	C4A-N9A	-2.67	1.32	1.37
3	B	702	NDP	O4B-C1B	2.61	1.48	1.42
3	B	702	NDP	C7N-C3N	-2.43	1.43	1.48
3	A	702	NDP	C8A-N9A	-2.41	1.33	1.37
3	A	702	NDP	C2N-C3N	2.38	1.41	1.35
3	A	702	NDP	C6N-C5N	2.35	1.40	1.33
2	B	701	EA0	CAR-CL	-2.34	1.68	1.74
2	A	701	EA0	OAK-CAL	2.34	1.49	1.45
3	A	702	NDP	PN-O5D	2.33	1.68	1.59
3	A	702	NDP	C5A-C4A	-2.21	1.35	1.39
3	B	702	NDP	C5A-C6A	-2.20	1.34	1.41
3	A	702	NDP	C2B-C1B	-2.19	1.47	1.53
3	A	702	NDP	C7N-C3N	-2.12	1.44	1.48
2	B	701	EA0	CAC-NAD	2.09	1.40	1.34
2	B	701	EA0	CAC-NAB	-2.07	1.31	1.36
2	A	701	EA0	CAC-NAB	-2.01	1.31	1.36

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	EA0	CAL-OAK-NAF	17.45	128.51	110.00
2	A	701	EA0	CAL-OAK-NAF	14.67	125.56	110.00
3	A	702	NDP	O3-PN-O1N	-9.13	83.24	110.70
2	A	701	EA0	NAF-CAA-NAB	7.46	126.36	121.53
3	A	702	NDP	O2N-PN-O3	-6.94	88.51	107.27
3	B	702	NDP	O2N-PN-O3	-6.78	88.95	107.27
3	B	702	NDP	N3A-C2A-N1A	-6.65	118.52	128.58
3	B	702	NDP	O3-PN-O1N	-5.64	93.74	110.70
3	A	702	NDP	N3A-C2A-N1A	-5.34	120.51	128.58
3	B	702	NDP	C5A-C4A-N3A	-4.97	119.88	126.72
2	A	701	EA0	NAB-CAC-NAD	-4.90	118.39	126.48
3	A	702	NDP	N9A-C8A-N7A	-4.35	107.77	113.94
3	B	702	NDP	N9A-C8A-N7A	-4.30	107.83	113.94
2	A	701	EA0	CAL-CAM-NAN	-4.13	107.39	115.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	EA0	CAL-CAM-NAN	-4.00	107.63	115.62
3	B	702	NDP	C5A-N7A-C8A	3.64	109.16	103.45
2	A	701	EA0	NAH-CAC-NAD	3.63	122.71	117.09
3	A	702	NDP	C4A-C5A-N7A	-3.60	106.46	110.58
3	A	702	NDP	C5A-C4A-N3A	-3.54	121.84	126.72
3	B	702	NDP	O2N-PN-O5D	3.50	123.43	107.57
2	B	701	EA0	NAF-CAA-NAB	3.46	123.77	121.53
3	B	702	NDP	C2A-N3A-C4A	3.44	120.23	111.83
3	B	702	NDP	O4B-C1B-N9A	3.41	114.64	108.09
3	A	702	NDP	C5A-N7A-C8A	3.40	108.80	103.45
2	B	701	EA0	NAH-CAC-NAD	3.35	122.28	117.09
2	A	701	EA0	CAQ-CAR-CL	-3.30	114.48	119.36
3	B	702	NDP	C4A-C5A-N7A	-3.30	106.81	110.58
2	B	701	EA0	NAB-CAC-NAD	-3.16	121.26	126.48
2	B	701	EA0	CAJ-CAE-CAI	-3.04	105.64	110.68
3	B	702	NDP	C1D-N1N-C2N	-3.03	116.14	121.14
2	A	701	EA0	NAG-CAA-NAF	3.03	119.95	117.46
3	B	702	NDP	O4D-C1D-N1N	-2.99	102.39	108.08
3	A	702	NDP	O2N-PN-O1N	2.99	126.33	112.44
3	A	702	NDP	C6A-C5A-C4A	2.88	121.11	117.18
3	B	702	NDP	C6A-C5A-C4A	2.86	121.08	117.18
2	A	701	EA0	NAG-CAA-NAB	-2.82	113.33	119.75
2	B	701	EA0	OAV-CAM-NAN	2.80	128.67	123.64
2	A	701	EA0	CAS-CAR-CL	2.78	123.45	119.36
3	A	702	NDP	C5A-C4A-N9A	2.72	108.78	105.81
3	B	702	NDP	N3A-C4A-N9A	2.71	131.77	127.17
3	A	702	NDP	O2N-PN-O5D	2.69	119.78	107.57
2	A	701	EA0	OAV-CAM-NAN	2.69	128.46	123.64
3	B	702	NDP	C5A-C6A-N6A	-2.57	116.92	123.29
2	B	701	EA0	NAG-CAA-NAF	2.55	119.56	117.46
3	A	702	NDP	C4A-N9A-C1B	-2.54	120.69	126.63
3	A	702	NDP	O3X-P2B-O2X	2.52	117.27	107.80
3	B	702	NDP	C5A-C4A-N9A	2.33	108.36	105.81
3	A	702	NDP	C4A-N9A-C8A	2.33	108.18	105.74
3	A	702	NDP	C2A-N3A-C4A	2.31	117.48	111.83
3	B	702	NDP	O3X-P2B-O2X	2.30	116.43	107.80
3	A	702	NDP	C1D-N1N-C2N	-2.26	117.42	121.14
3	B	702	NDP	C4D-O4D-C1D	-2.14	104.74	109.47
3	B	702	NDP	O2N-PN-O1N	2.09	122.17	112.44
2	A	701	EA0	CAT-CAO-CAP	2.01	121.71	119.04
3	B	702	NDP	C4A-N9A-C8A	2.00	107.84	105.74

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	EA0	CAE-NAF-OAK-CAL
2	A	701	EA0	CAA-NAF-OAK-CAL
2	A	701	EA0	OAK-CAL-CAM-NAN
2	B	701	EA0	CAE-NAF-OAK-CAL
2	B	701	EA0	OAK-CAL-CAM-NAN
3	A	702	NDP	C5B-O5B-PA-O1A
3	A	702	NDP	C5D-O5D-PN-O1N
3	B	702	NDP	C5D-O5D-PN-O1N
3	B	702	NDP	C2D-C1D-N1N-C2N
2	B	701	EA0	CAM-CAL-OAK-NAF
2	A	701	EA0	OAK-CAL-CAM-OAV
2	B	701	EA0	OAK-CAL-CAM-OAV
3	A	702	NDP	PA-O3-PN-O5D
3	A	702	NDP	C3B-C4B-C5B-O5B
3	A	702	NDP	C4D-C5D-O5D-PN
3	B	702	NDP	O4D-C1D-N1N-C2N
2	B	701	EA0	CAT-CAO-NAN-CAM
3	A	702	NDP	O4D-C1D-N1N-C2N
3	A	702	NDP	C2N-C3N-C7N-N7N
3	B	702	NDP	C2N-C3N-C7N-N7N
3	A	702	NDP	C2D-C1D-N1N-C2N
3	B	702	NDP	C2D-C1D-N1N-C6N
3	A	702	NDP	C2B-O2B-P2B-O1X

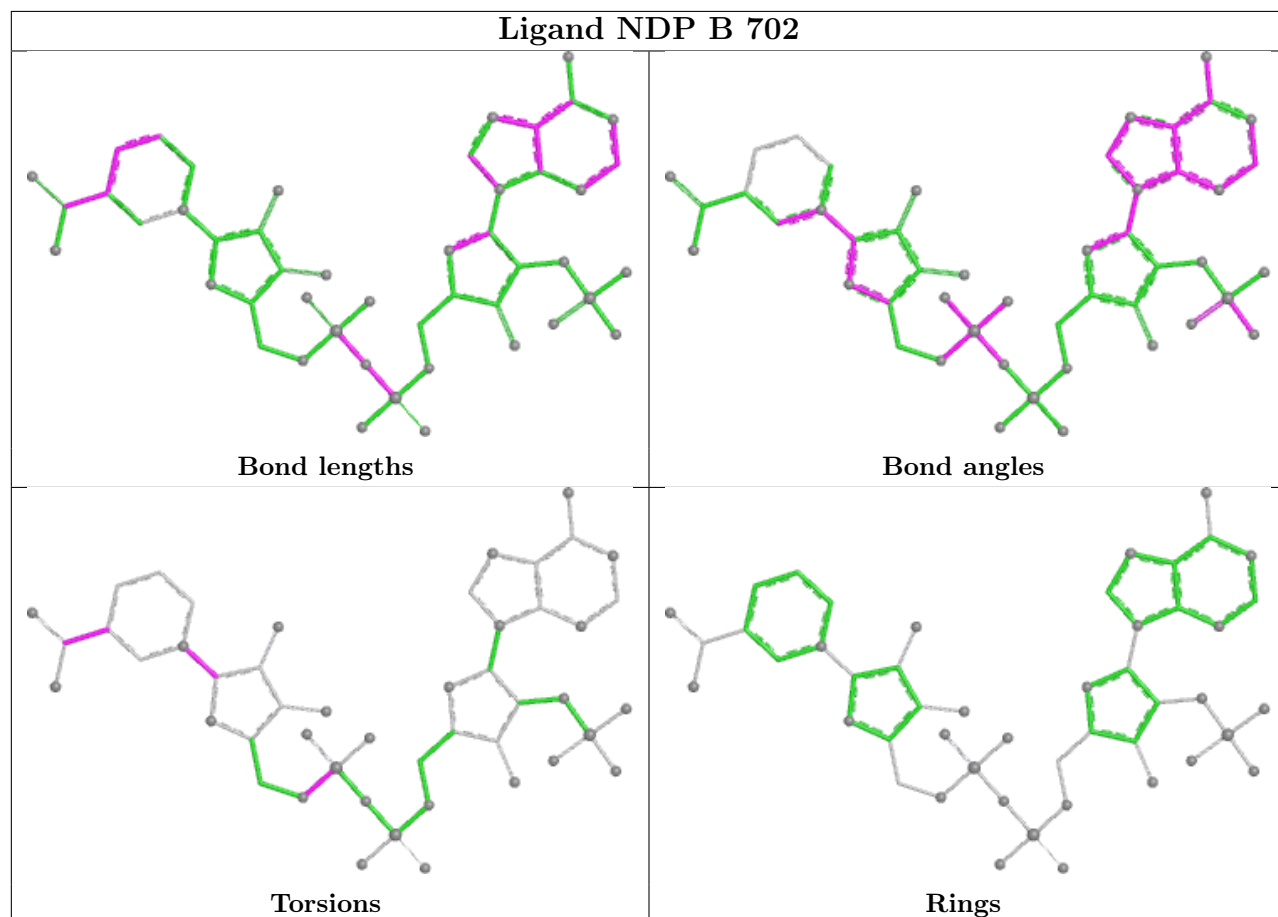
There are no ring outliers.

4 monomers are involved in 17 short contacts:

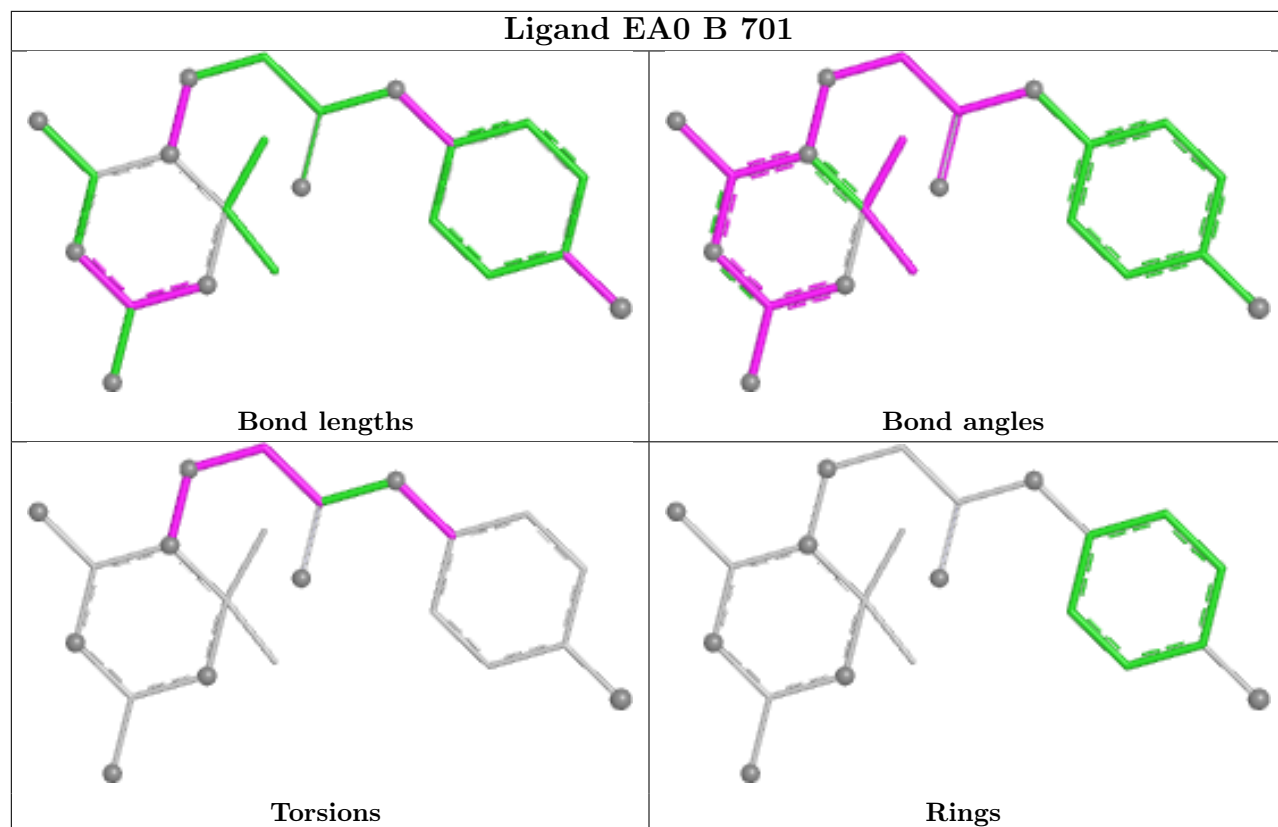
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	NDP	3	0
2	B	701	EA0	8	0
2	A	701	EA0	1	0
3	A	702	NDP	5	0

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 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

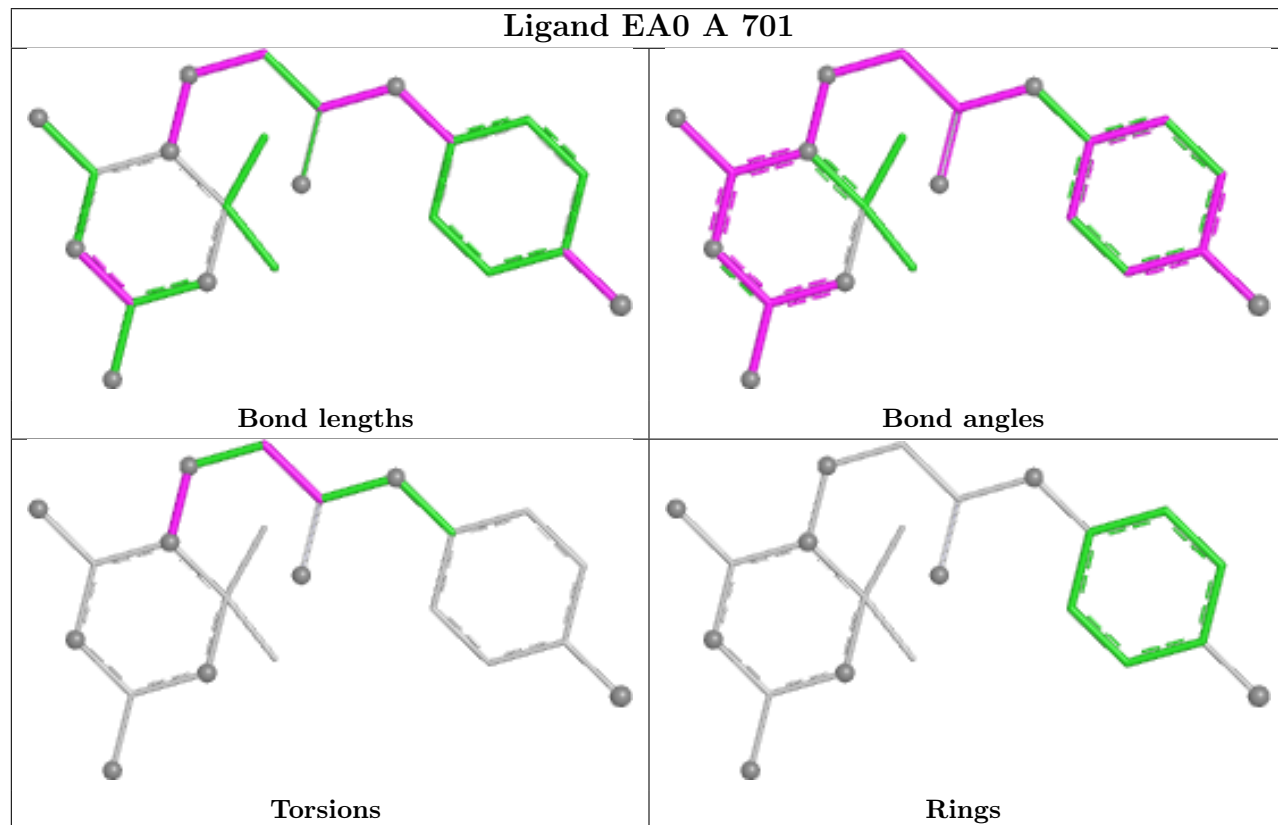
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

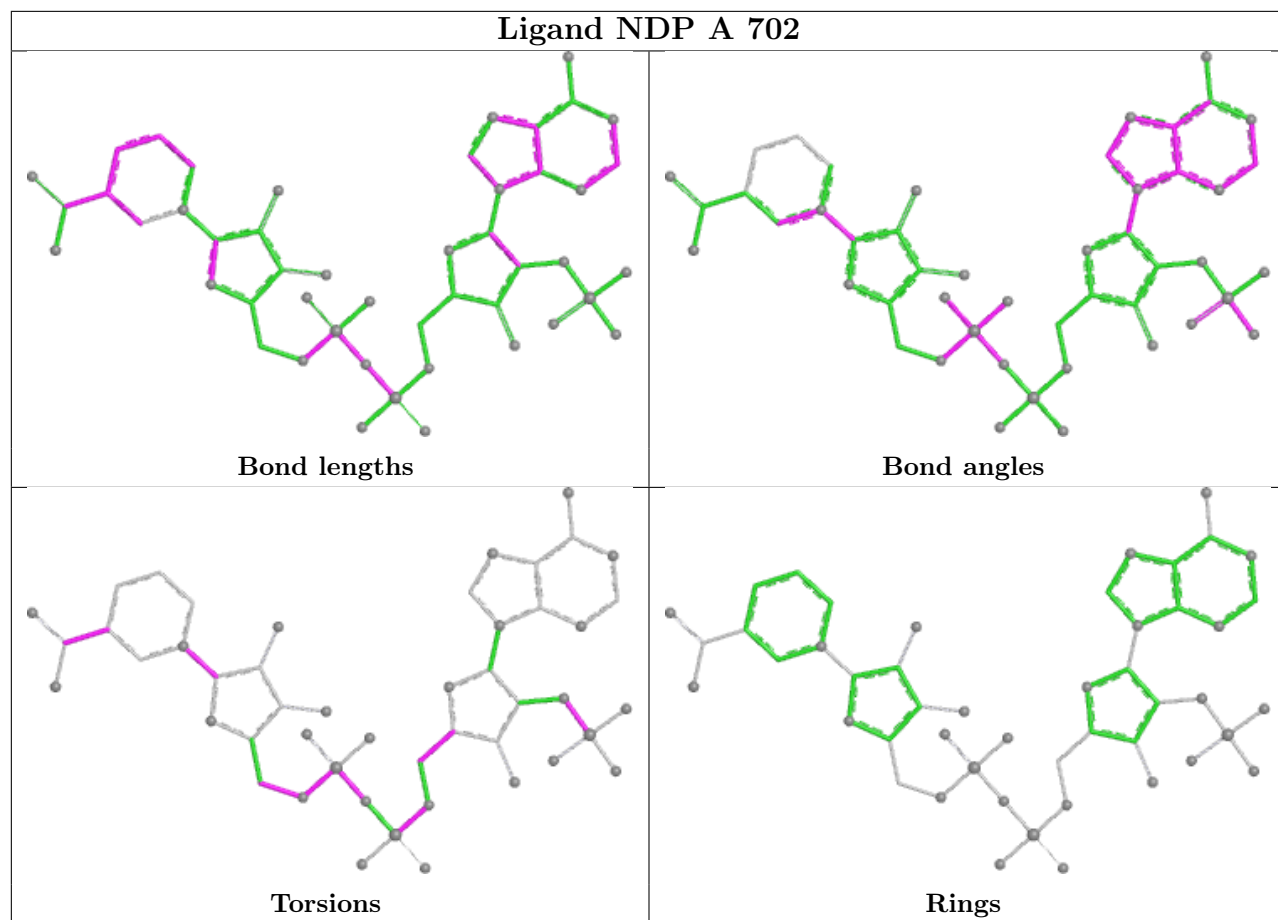


Ligand EA0 B 701



Ligand EA0 A 701





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	528/608 (86%)	-0.66	0	100 100	27, 42, 96, 145	0
1	B	522/608 (85%)	-0.47	5 (0%)	79 76	24, 47, 119, 147	0
All	All	1050/1216 (86%)	-0.57	5 (0%)	87 85	24, 44, 114, 147	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	VAL	4.3
1	B	303	ASN	3.4
1	B	6	CYS	2.9
1	B	116	PHE	2.3
1	B	113	PRO	2.1

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](#)

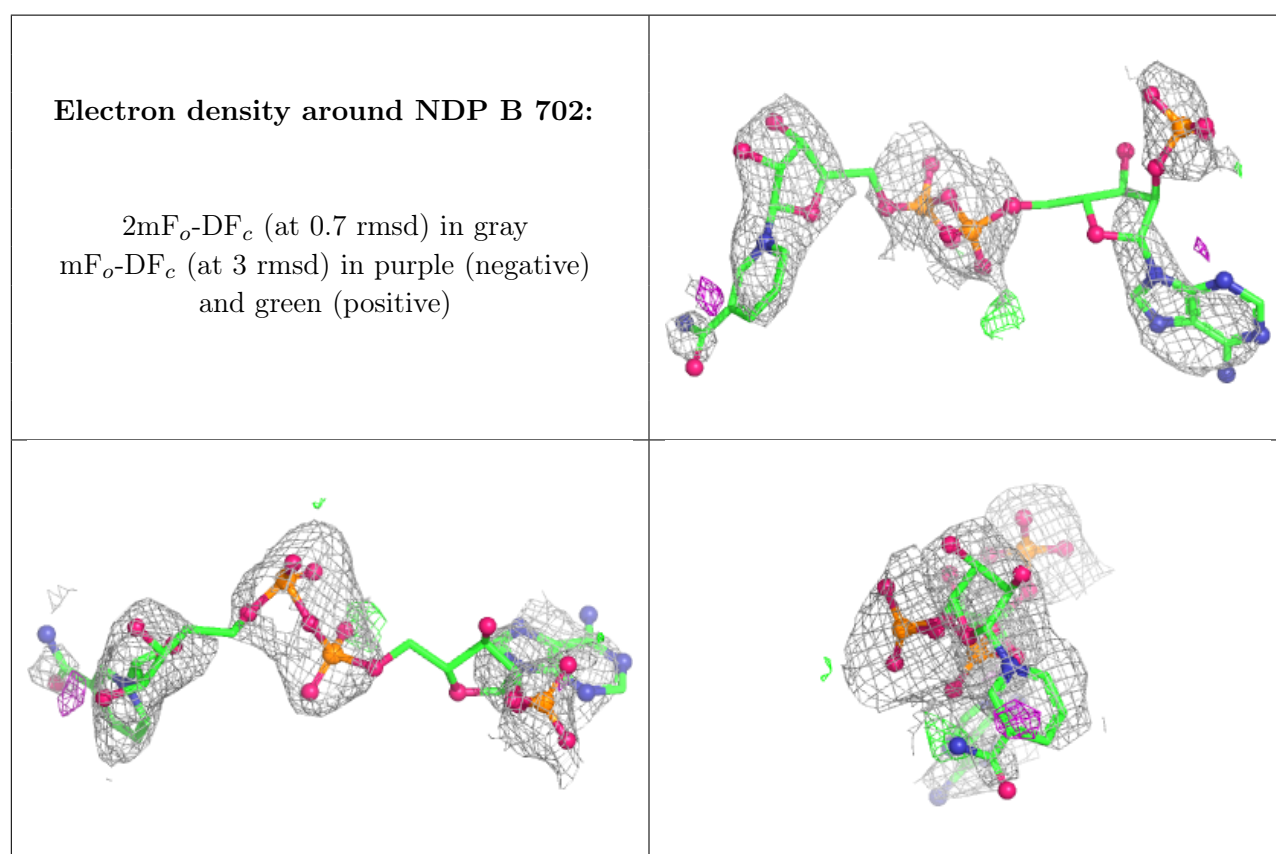
There are no oligosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

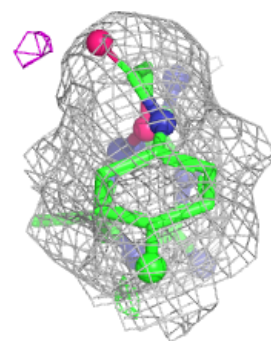
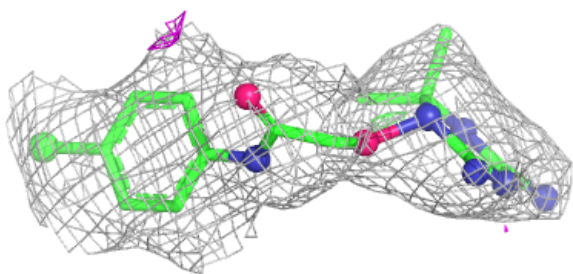
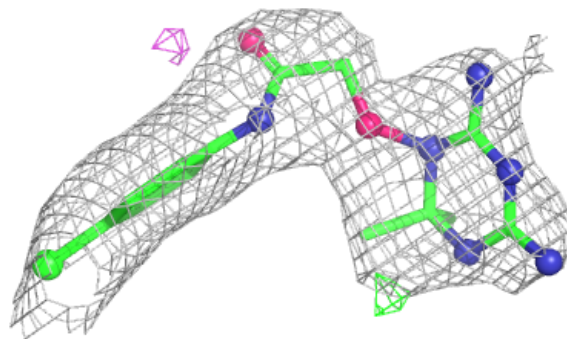
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NDP	B	702	48/48	0.84	0.11	77,108,144,158	0
2	EA0	B	701	22/22	0.86	0.09	58,95,109,124	0
2	EA0	A	701	22/22	0.94	0.06	36,53,67,73	0
3	NDP	A	702	48/48	0.95	0.07	45,60,66,69	0
4	PO4	A	703	5/5	0.99	0.06	32,35,38,42	0
4	PO4	A	704	5/5	0.99	0.07	37,39,43,47	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.

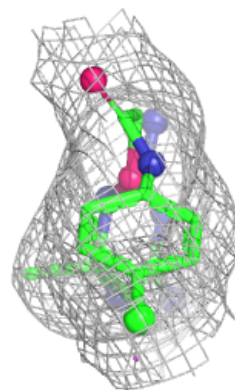
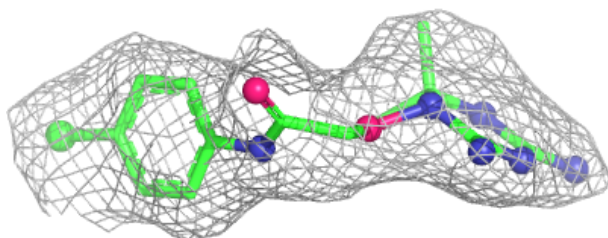
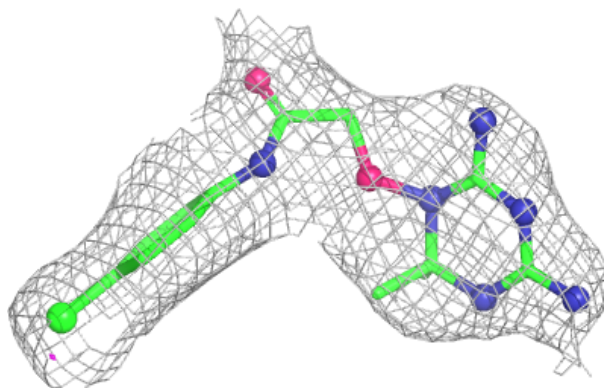


Electron density around EA0 B 701:

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

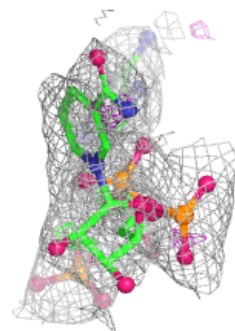
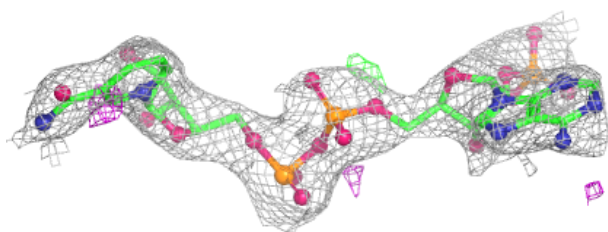
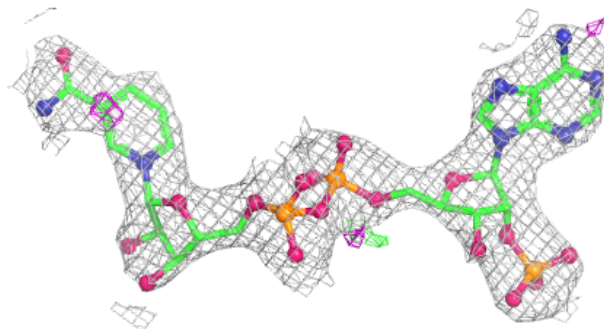
**Electron density around EA0 A 701:**

$2mF_o-DF_c$ (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.