



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:27 am BST

PDB ID : 3CSE  
Title : Candida glabrata Dihydrofolate Reductase complexed with NADPH and 2, 4-diamino-5-(3-(2,5-dimethoxyphenyl)prop-1-ynyl)-6-ethylpyrimidine (UCP120B)  
Authors : Liu, J.; Anderson, A.C.  
Deposited on : 2008-04-09  
Resolution : 1.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

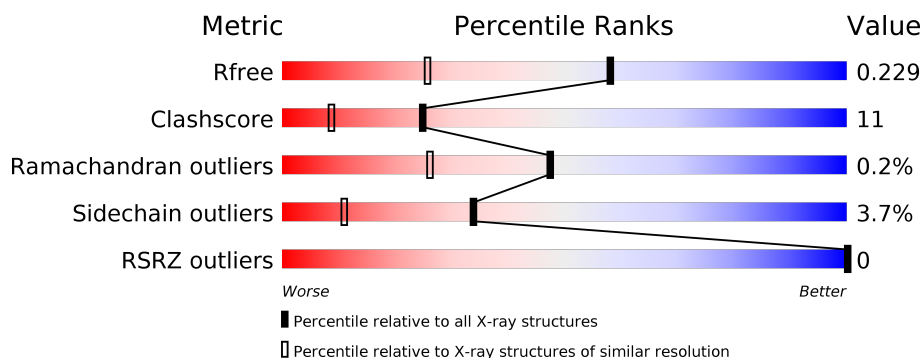
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	227	
1	B	227	

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
3	N22	A	302	-	X	-	-
3	N22	B	302	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4222 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.

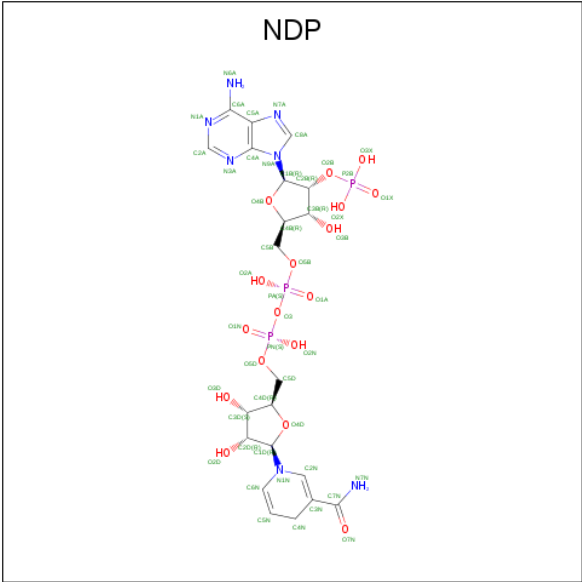
- Molecule 1 is a protein called Dihydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1846	1180	325	334	7			
1	B	225	Total	C	N	O	S	0	0	0
			1846	1180	325	334	7			

There are 20 discrepancies between the modelled and reference sequences:

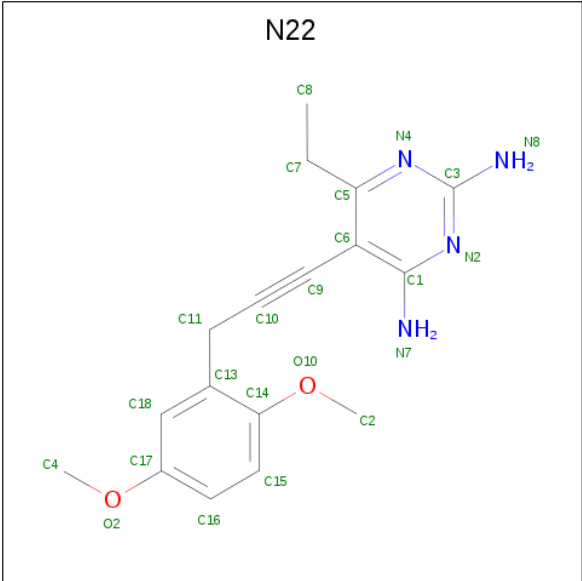
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	LEU	-	EXPRESSION TAG	UNP Q6FPH0
A	219	GLU	-	EXPRESSION TAG	UNP Q6FPH0
A	220	HIS	-	EXPRESSION TAG	UNP Q6FPH0
A	221	HIS	-	EXPRESSION TAG	UNP Q6FPH0
A	222	HIS	-	EXPRESSION TAG	UNP Q6FPH0
A	223	HIS	-	EXPRESSION TAG	UNP Q6FPH0
A	224	HIS	-	EXPRESSION TAG	UNP Q6FPH0
A	225	HIS	-	EXPRESSION TAG	UNP Q6FPH0
A	226	HIS	-	EXPRESSION TAG	UNP Q6FPH0
A	227	HIS	-	EXPRESSION TAG	UNP Q6FPH0
B	218	LEU	-	EXPRESSION TAG	UNP Q6FPH0
B	219	GLU	-	EXPRESSION TAG	UNP Q6FPH0
B	220	HIS	-	EXPRESSION TAG	UNP Q6FPH0
B	221	HIS	-	EXPRESSION TAG	UNP Q6FPH0
B	222	HIS	-	EXPRESSION TAG	UNP Q6FPH0
B	223	HIS	-	EXPRESSION TAG	UNP Q6FPH0
B	224	HIS	-	EXPRESSION TAG	UNP Q6FPH0
B	225	HIS	-	EXPRESSION TAG	UNP Q6FPH0
B	226	HIS	-	EXPRESSION TAG	UNP Q6FPH0
B	227	HIS	-	EXPRESSION TAG	UNP Q6FPH0

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 5-[3-(2,5-dimethoxyphenyl)prop-1-yn-1-yl]-6-ethylpyrimidine-2,4-diamine (three-letter code: N22) (formula: C<sub>17</sub>H<sub>20</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	17	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			23	17	4	2		

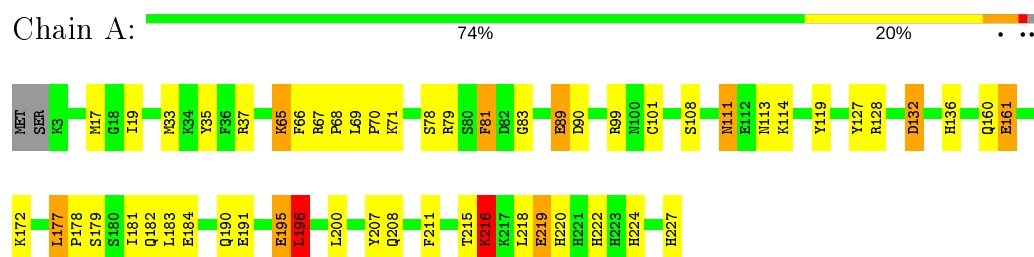
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	194	Total	O	0	0
			194	194		
4	B	194	Total	O	0	0
			194	194		

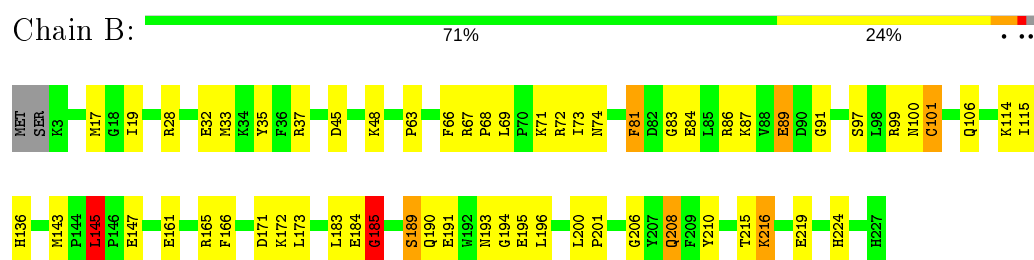
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.69 Å 42.69 Å 230.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.03 – 1.60 40.03 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.2 (40.03-1.60) 93.2 (40.03-1.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.60 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.181 , 0.232 0.179 , 0.229	Depositor DCC
$R_{free}$ test set	2558 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4222	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, N22

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	1.63	17/1891 (0.9%)	1.57	21/2556 (0.8%)
1	B	1.65	14/1891 (0.7%)	1.51	22/2556 (0.9%)
All	All	1.64	31/3782 (0.8%)	1.54	43/5112 (0.8%)

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	3
All	All	0	4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	191	GLU	CD-OE1	8.18	1.34	1.25
1	A	89	GLU	CD-OE2	7.36	1.33	1.25
1	A	127	TYR	CD1-CE1	6.91	1.49	1.39
1	B	89	GLU	CG-CD	6.76	1.62	1.51
1	A	207	TYR	CG-CD1	6.58	1.47	1.39
1	B	89	GLU	CD-OE1	6.58	1.32	1.25
1	B	208	GLN	CG-CD	6.56	1.66	1.51
1	A	128	ARG	CZ-NH2	6.55	1.41	1.33
1	B	185	GLY	N-CA	6.54	1.55	1.46
1	A	195	GLU	CG-CD	6.35	1.61	1.51
1	A	219	GLU	CD-OE1	6.20	1.32	1.25
1	B	191	GLU	CG-CD	6.15	1.61	1.51
1	B	127	TYR	CD1-CE1	6.05	1.48	1.39
1	B	91	GLY	N-CA	6.03	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	GLU	CD-OE1	5.92	1.32	1.25
1	A	161	GLU	CG-CD	-5.86	1.43	1.51
1	B	189	SER	CB-OG	5.78	1.49	1.42
1	A	167	TYR	CG-CD1	5.62	1.46	1.39
1	A	119	TYR	CE2-CZ	5.53	1.45	1.38
1	A	165	ARG	CG-CD	5.50	1.65	1.51
1	B	17	MET	CB-CG	5.44	1.68	1.51
1	A	191	GLU	CG-CD	5.29	1.59	1.51
1	A	208	GLN	CB-CG	5.15	1.66	1.52
1	B	195	GLU	CG-CD	5.15	1.59	1.51
1	A	218	LEU	N-CA	5.14	1.56	1.46
1	A	66	PHE	CD1-CE1	5.14	1.49	1.39
1	B	35	TYR	CE2-CZ	5.12	1.45	1.38
1	B	66	PHE	CD1-CE1	5.11	1.49	1.39
1	A	211	PHE	CD1-CE1	5.09	1.49	1.39
1	B	161	GLU	CD-OE2	5.03	1.31	1.25
1	A	119	TYR	CD2-CE2	5.00	1.46	1.39

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ARG	NE-CZ-NH2	15.88	128.24	120.30
1	A	37	ARG	NE-CZ-NH1	14.56	127.58	120.30
1	A	37	ARG	NE-CZ-NH2	-13.44	113.58	120.30
1	A	128	ARG	NE-CZ-NH1	-13.03	113.78	120.30
1	A	99	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	B	37	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	B	132	ASP	CB-CG-OD2	-9.47	109.78	118.30
1	B	37	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	A	196	LEU	CB-CG-CD2	9.18	126.60	111.00
1	A	99	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	A	132	ASP	CB-CG-OD2	-8.49	110.65	118.30
1	B	99	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	A	35	TYR	CB-CG-CD2	8.17	125.90	121.00
1	B	99	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	B	194	GLY	N-CA-C	-8.05	92.98	113.10
1	B	72	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	A	79	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	B	145	LEU	CB-CG-CD1	7.30	123.41	111.00
1	A	65	LYS	CD-CE-NZ	7.14	128.12	111.70
1	A	37	ARG	CD-NE-CZ	6.58	132.81	123.60
1	B	33	MET	CG-SD-CE	-6.41	89.94	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	ASP	CB-CG-OD1	6.35	124.01	118.30
1	B	101	CYS	CB-CA-C	6.27	122.94	110.40
1	A	216	LYS	CD-CE-NZ	6.04	125.58	111.70
1	B	35	TYR	CB-CG-CD2	5.94	124.56	121.00
1	B	210	TYR	CB-CG-CD1	-5.73	117.56	121.00
1	B	171	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	B	81	PHE	CB-CG-CD1	5.61	124.73	120.80
1	B	35	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	A	81	PHE	CB-CG-CD1	5.51	124.66	120.80
1	A	132	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	45	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	33	MET	CG-SD-CE	-5.46	91.47	100.20
1	A	90	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	B	17	MET	CB-CG-SD	-5.37	96.28	112.40
1	B	193	ASN	C-N-CA	5.37	133.57	122.30
1	A	35	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	A	17	MET	CB-CG-SD	-5.21	96.77	112.40
1	B	86	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	32	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	B	193	ASN	N-CA-C	5.15	124.90	111.00
1	A	128	ARG	CD-NE-CZ	5.05	130.68	123.60
1	A	177	LEU	CB-CG-CD1	5.02	119.53	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	GLY	Peptide
1	B	185	GLY	Peptide
1	B	81	PHE	Peptide
1	B	83	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	1846	0	1846	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1846	0	1846	35	3
2	A	48	0	26	1	0
2	B	48	0	26	1	0
3	A	23	0	20	2	0
3	B	23	0	20	2	0
4	A	194	0	0	21	5
4	B	194	0	0	18	1
All	All	4222	0	3784	82	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLN:HG2	4:A:529:HOH:O	1.17	1.25
1:A:183:LEU:HD12	1:A:200:LEU:CD1	1.84	1.07
1:B:224:HIS:HE1	4:B:447:HOH:O	1.36	1.07
1:A:224:HIS:HE1	4:A:485:HOH:O	1.39	1.03
1:A:219:GLU:OE1	4:A:542:HOH:O	1.80	0.99
1:A:161:GLU:HG3	4:A:583:HOH:O	1.63	0.98
1:A:132:ASP:OD2	1:B:132:ASP:OD2	1.83	0.97
1:B:184:GLU:OE1	4:B:560:HOH:O	1.83	0.95
1:A:179:SER:HB3	4:A:579:HOH:O	1.67	0.94
1:B:190:GLN:HG2	4:B:534:HOH:O	1.68	0.91
1:A:71:LYS:HE3	4:A:532:HOH:O	1.73	0.88
1:A:184:GLU:HG3	4:A:571:HOH:O	1.74	0.86
1:A:183:LEU:CD1	1:A:200:LEU:CD1	2.53	0.85
1:A:183:LEU:HD12	1:A:200:LEU:HD13	1.58	0.84
3:A:302:N22:H2A	4:A:433:HOH:O	1.80	0.81
1:A:183:LEU:CD1	1:A:200:LEU:HD13	2.13	0.79
1:B:69:LEU:H	1:B:74:ASN:HD21	1.30	0.79
1:B:114:LYS:NZ	4:B:520:HOH:O	2.18	0.77
1:B:132:ASP:HB2	4:B:530:HOH:O	1.87	0.75
1:A:195:GLU:CD	4:A:471:HOH:O	2.25	0.75
1:B:84:GLU:OE2	4:B:523:HOH:O	2.06	0.74
1:B:145:LEU:HD22	1:B:206:GLY:C	2.09	0.72
1:B:183:LEU:HD23	4:B:572:HOH:O	1.89	0.71
1:A:220:HIS:HD2	4:A:500:HOH:O	1.76	0.69
1:A:183:LEU:CD1	1:A:200:LEU:HD12	2.23	0.68
1:A:111:ASN:HD22	1:A:113:ASN:H	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:302:N22:C2	4:A:433:HOH:O	2.38	0.67
1:A:165:ARG:NH1	4:A:583:HOH:O	2.07	0.66
3:B:302:N22:H2A	4:B:463:HOH:O	1.95	0.66
1:A:111:ASN:ND2	1:A:113:ASN:H	1.93	0.66
1:A:216:LYS:HE3	4:A:546:HOH:O	1.96	0.65
1:A:111:ASN:C	1:A:111:ASN:HD22	2.00	0.65
1:A:132:ASP:HB2	4:A:528:HOH:O	1.99	0.63
1:B:183:LEU:CD2	4:B:572:HOH:O	2.44	0.61
1:B:173:LEU:HD23	1:B:200:LEU:HD12	1.82	0.60
1:B:73:ILE:HD12	1:B:115:ILE:HD11	1.85	0.58
3:B:302:N22:C2	4:B:463:HOH:O	2.50	0.56
1:A:19:ILE:O	2:A:301:NDP:H2N	2.07	0.55
1:A:224:HIS:CE1	4:A:485:HOH:O	2.26	0.55
1:A:183:LEU:HD12	1:A:200:LEU:HD12	1.76	0.54
1:B:224:HIS:CE1	4:B:447:HOH:O	2.26	0.54
1:B:67:ARG:HA	1:B:68:PRO:C	2.31	0.52
1:A:114:LYS:HB2	4:A:452:HOH:O	2.11	0.51
1:A:178:PRO:HD2	1:A:181:ILE:HD11	1.92	0.51
1:A:67:ARG:HA	1:A:68:PRO:C	2.32	0.50
1:A:222:HIS:HE1	4:B:501:HOH:O	1.94	0.50
1:B:185:GLY:CA	1:B:201:PRO:HD2	2.42	0.50
1:A:227:HIS:HD2	4:A:570:HOH:O	1.95	0.49
1:B:19:ILE:O	2:B:301:NDP:H2N	2.13	0.49
1:B:143:MET:HB2	1:B:208:GLN:CG	2.42	0.49
1:B:97:SER:HB3	1:B:100:ASN:HB2	1.95	0.48
1:B:172:LYS:NZ	4:B:580:HOH:O	2.47	0.48
1:A:136:HIS:HD2	1:A:215:THR:OG1	1.96	0.47
1:B:216:LYS:HE2	4:B:537:HOH:O	2.14	0.47
1:A:71:LYS:HB3	4:A:517:HOH:O	2.14	0.47
1:B:183:LEU:HG	1:B:200:LEU:HD13	1.97	0.47
1:B:166:PHE:CZ	1:B:216:LYS:HE3	2.49	0.47
1:B:136:HIS:HD2	1:B:215:THR:OG1	1.98	0.46
1:B:189:SER:HB3	1:B:196:LEU:HD11	1.99	0.45
1:A:160:GLN:O	1:A:164:GLN:HG3	2.17	0.44
1:A:160:GLN:HG3	1:A:164:GLN:HE21	1.81	0.44
1:A:108:SER:HA	1:A:111:ASN:ND2	2.33	0.44
1:B:48:LYS:HG2	1:B:114:LYS:HA	1.99	0.44
1:A:161:GLU:HB3	1:A:165:ARG:NH1	2.32	0.44
1:A:65:LYS:HE3	1:A:65:LYS:HB2	1.27	0.43
1:B:132:ASP:CB	4:B:530:HOH:O	2.55	0.42
1:B:173:LEU:CD2	1:B:200:LEU:HD12	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLN:CB	4:A:529:HOH:O	2.54	0.42
1:A:179:SER:CB	4:A:579:HOH:O	2.44	0.42
1:B:106:GLN:O	4:B:545:HOH:O	2.22	0.42
1:B:190:GLN:CG	4:B:534:HOH:O	2.45	0.42
1:B:165:ARG:HG3	1:B:165:ARG:HH11	1.84	0.41
1:B:185:GLY:HA3	1:B:201:PRO:HD2	2.03	0.41
1:A:132:ASP:OD2	1:B:132:ASP:CG	2.56	0.41
1:B:143:MET:HB2	1:B:208:GLN:HG3	2.00	0.41
1:B:190:GLN:CB	4:B:534:HOH:O	2.68	0.41
1:A:183:LEU:HD13	1:A:200:LEU:CD1	2.44	0.41
1:A:71:LYS:HA	1:A:71:LYS:HD3	1.81	0.41
1:A:78:SER:HB3	1:A:81:PHE:CD2	2.56	0.41
1:A:196:LEU:CD1	4:A:589:HOH:O	2.69	0.41
1:A:69:LEU:HA	1:A:70:PRO:HD3	1.92	0.40
1:A:178:PRO:HD2	1:A:181:ILE:CD1	2.51	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LYS:NZ	4:A:490:HOH:O[1_565]	1.87	0.33
1:B:219:GLU:OE1	4:A:527:HOH:O[1_655]	1.95	0.25
4:B:476:HOH:O	4:B:527:HOH:O[1_545]	2.03	0.17
4:A:460:HOH:O	4:A:478:HOH:O[1_655]	2.10	0.10
1:B:87:LYS:NZ	4:A:542:HOH:O[1_565]	2.16	0.04
4:A:478:HOH:O	4:A:495:HOH:O[1_455]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	223/227 (98%)	218 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	223/227 (98%)	217 (97%)	5 (2%)	1 (0%)	34	15
All	All	446/454 (98%)	435 (98%)	10 (2%)	1 (0%)	47	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	185	GLY

### 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	205/207 (99%)	197 (96%)	8 (4%)	32	10
1	B	205/207 (99%)	198 (97%)	7 (3%)	37	13
All	All	410/414 (99%)	395 (96%)	15 (4%)	34	11

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	101	CYS
1	A	111	ASN
1	A	172	LYS
1	A	177	LEU
1	A	182	GLN
1	A	196	LEU
1	A	216	LYS
1	B	28	ARG
1	B	63	PRO
1	B	89	GLU
1	B	101	CYS
1	B	145	LEU
1	B	147	GLU
1	B	216	LYS

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	111	ASN
1	A	136	HIS
1	A	158	GLN
1	A	164	GLN
1	A	193	ASN
1	A	203	GLN
1	A	208	GLN
1	A	220	HIS
1	A	222	HIS
1	A	224	HIS
1	B	74	ASN
1	B	113	ASN
1	B	136	HIS
1	B	221	HIS
1	B	224	HIS

### 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](#)

4 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	N22	B	302	-	24,24,24	2.97	16 (66%)	25,32,32	4.72	17 (68%)
2	NDP	A	301	-	45,52,52	1.65	8 (17%)	53,80,80	1.96	9 (16%)
2	NDP	B	301	-	45,52,52	1.55	6 (13%)	53,80,80	1.78	4 (7%)
3	N22	A	302	-	24,24,24	2.79	12 (50%)	25,32,32	4.70	15 (60%)

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	N22	B	302	-	-	4/11/12/12	0/2/2/2
2	NDP	A	301	-	-	2/30/77/77	0/5/5/5
2	NDP	B	301	-	-	2/30/77/77	0/5/5/5
3	N22	A	302	-	-	5/11/12/12	0/2/2/2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	N22	C18-C17	6.66	1.50	1.38
3	B	302	N22	C11-C10	-6.03	1.42	1.47
2	B	301	NDP	O4B-C1B	5.85	1.49	1.41
3	A	302	N22	C7-C5	5.49	1.60	1.51
3	B	302	N22	C11-C13	5.30	1.61	1.52
2	A	301	NDP	O4B-C1B	4.85	1.47	1.41
3	B	302	N22	C18-C17	4.57	1.46	1.38
3	B	302	N22	O10-C14	-4.54	1.29	1.37
3	A	302	N22	O10-C14	-4.29	1.30	1.37
3	B	302	N22	C6-C1	4.28	1.47	1.42
3	A	302	N22	C11-C10	-3.70	1.44	1.47
2	A	301	NDP	O7N-C7N	3.62	1.33	1.24
3	A	302	N22	C18-C13	3.45	1.45	1.39
3	B	302	N22	C3-N8	-3.37	1.27	1.33
3	A	302	N22	O10-C2	3.34	1.52	1.42
2	B	301	NDP	C6N-N1N	3.34	1.45	1.37
2	A	301	NDP	O3D-C3D	3.22	1.50	1.43
2	A	301	NDP	C6N-N1N	3.13	1.45	1.37
3	B	302	N22	C18-C13	3.09	1.44	1.39
3	B	302	N22	C15-C16	3.07	1.44	1.38
3	A	302	N22	C6-C1	2.99	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	N22	C6-C5	2.96	1.44	1.40
2	A	301	NDP	C2A-N3A	2.95	1.36	1.32
3	A	302	N22	C9-C10	-2.93	1.15	1.19
2	B	301	NDP	C2A-N3A	2.91	1.36	1.32
3	A	302	N22	C11-C13	2.79	1.56	1.52
3	B	302	N22	O2-C4	2.75	1.51	1.42
2	B	301	NDP	C7N-N7N	2.71	1.40	1.33
3	B	302	N22	C7-C5	2.68	1.55	1.51
2	A	301	NDP	P2B-O2B	2.60	1.64	1.59
3	B	302	N22	C6-C9	-2.58	1.39	1.43
2	A	301	NDP	C8A-N7A	2.52	1.39	1.34
2	B	301	NDP	O7N-C7N	2.41	1.30	1.24
3	B	302	N22	C9-C10	-2.33	1.16	1.19
3	A	302	N22	O2-C17	2.28	1.42	1.37
3	B	302	N22	C3-N4	2.26	1.39	1.35
3	B	302	N22	C1-N2	-2.14	1.32	1.35
3	B	302	N22	C1-N7	2.13	1.39	1.34
2	A	301	NDP	C3D-C4D	2.05	1.58	1.53
3	A	302	N22	C3-N4	2.02	1.39	1.35
2	B	301	NDP	C4N-C3N	-2.02	1.46	1.49
3	A	302	N22	C3-N8	-2.00	1.29	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	N22	C18-C13-C14	10.73	129.53	118.26
3	A	302	N22	C3-N4-C5	9.39	124.07	116.24
3	B	302	N22	C17-C18-C13	-9.02	107.97	120.47
3	A	302	N22	C3-N2-C1	8.72	126.61	116.99
2	A	301	NDP	N3A-C2A-N1A	-8.69	115.09	128.68
3	A	302	N22	C15-C16-C17	8.62	130.27	119.73
2	B	301	NDP	N3A-C2A-N1A	-8.56	115.29	128.68
3	B	302	N22	C3-N2-C1	8.27	126.12	116.99
3	A	302	N22	C18-C13-C14	8.22	126.89	118.26
3	B	302	N22	C3-N4-C5	7.44	122.44	116.24
3	B	302	N22	C15-C16-C17	6.94	128.22	119.73
3	A	302	N22	N2-C3-N4	-6.59	115.08	125.42
3	A	302	N22	C17-C18-C13	-6.36	111.65	120.47
3	A	302	N22	C2-O10-C14	6.35	127.11	117.53
3	A	302	N22	C8-C7-C5	-6.08	99.89	114.88
3	B	302	N22	N2-C3-N4	-5.28	117.13	125.42
3	B	302	N22	C8-C7-C5	-5.23	101.98	114.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NDP	C2A-N1A-C6A	5.23	127.69	118.75
3	B	302	N22	C16-C15-C14	-5.20	110.15	120.06
2	A	301	NDP	C2A-N1A-C6A	5.17	127.59	118.75
3	B	302	N22	C2-O10-C14	4.82	124.81	117.53
3	B	302	N22	N7-C1-N2	4.80	123.82	117.03
2	A	301	NDP	C3N-C2N-N1N	-4.38	116.84	123.10
3	A	302	N22	N8-C3-N2	4.37	124.05	117.25
3	A	302	N22	N7-C1-N2	4.32	123.14	117.03
3	B	302	N22	C7-C5-C6	3.60	125.22	122.66
2	A	301	NDP	C1D-N1N-C2N	-3.55	115.20	121.11
3	A	302	N22	C16-C15-C14	-3.37	113.64	120.06
3	B	302	N22	N8-C3-N4	3.11	122.08	117.25
3	B	302	N22	C6-C1-N2	-3.01	117.37	121.63
3	A	302	N22	C16-C17-C18	-2.96	116.47	120.53
2	A	301	NDP	C5A-C6A-N6A	2.78	124.58	120.35
2	A	301	NDP	O4D-C1D-N1N	2.77	113.46	108.06
3	A	302	N22	C6-C1-N2	-2.61	117.94	121.63
3	A	302	N22	C6-C1-N7	-2.45	118.80	121.62
3	B	302	N22	C6-C1-N7	-2.44	118.81	121.62
3	B	302	N22	C4-O2-C17	-2.42	112.26	117.51
2	A	301	NDP	O7N-C7N-N7N	-2.35	117.39	122.88
3	A	302	N22	N8-C3-N4	2.25	120.75	117.25
3	B	302	N22	O10-C14-C13	-2.14	113.00	115.97
2	B	301	NDP	O2B-C2B-C1B	-2.13	102.44	110.10
3	B	302	N22	N8-C3-N2	2.08	120.49	117.25
2	A	301	NDP	O2B-C2B-C1B	-2.08	102.61	110.10
2	A	301	NDP	C2D-C3D-C4D	-2.08	98.60	102.64
2	B	301	NDP	C5A-C6A-N1A	-2.04	115.73	120.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	N22	C9-C10-C11-C13
2	A	301	NDP	PA-O3-PN-O5D
2	B	301	NDP	PA-O3-PN-O5D
3	A	302	N22	C11-C10-C9-C6
3	A	302	N22	C9-C10-C11-C13
3	B	302	N22	C11-C10-C9-C6
2	A	301	NDP	O4D-C1D-N1N-C2N
2	B	301	NDP	O4D-C1D-N1N-C2N
3	A	302	N22	C5-C6-C9-C10

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Mol	Chain	Res	Type	Atoms
3	A	302	N22	N4-C5-C7-C8
3	B	302	N22	N4-C5-C7-C8
3	B	302	N22	C10-C11-C13-C18
3	A	302	N22	C6-C5-C7-C8

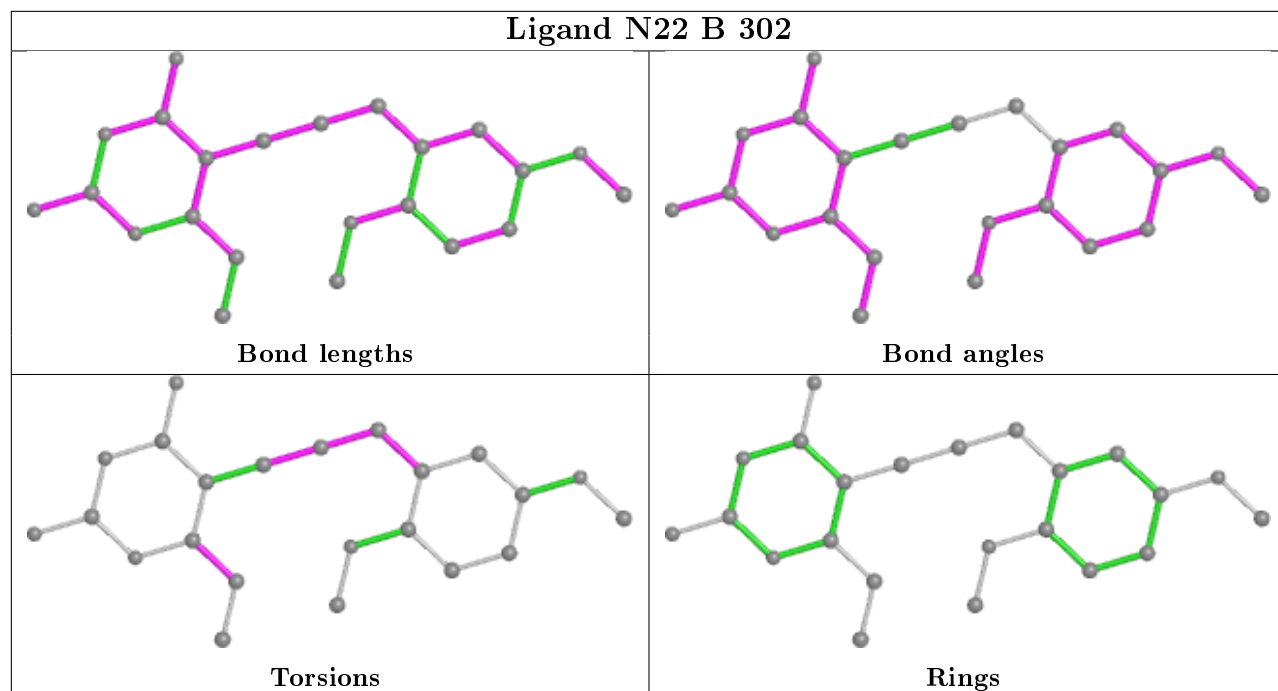
There are no ring outliers.

4 monomers are involved in 6 short contacts:

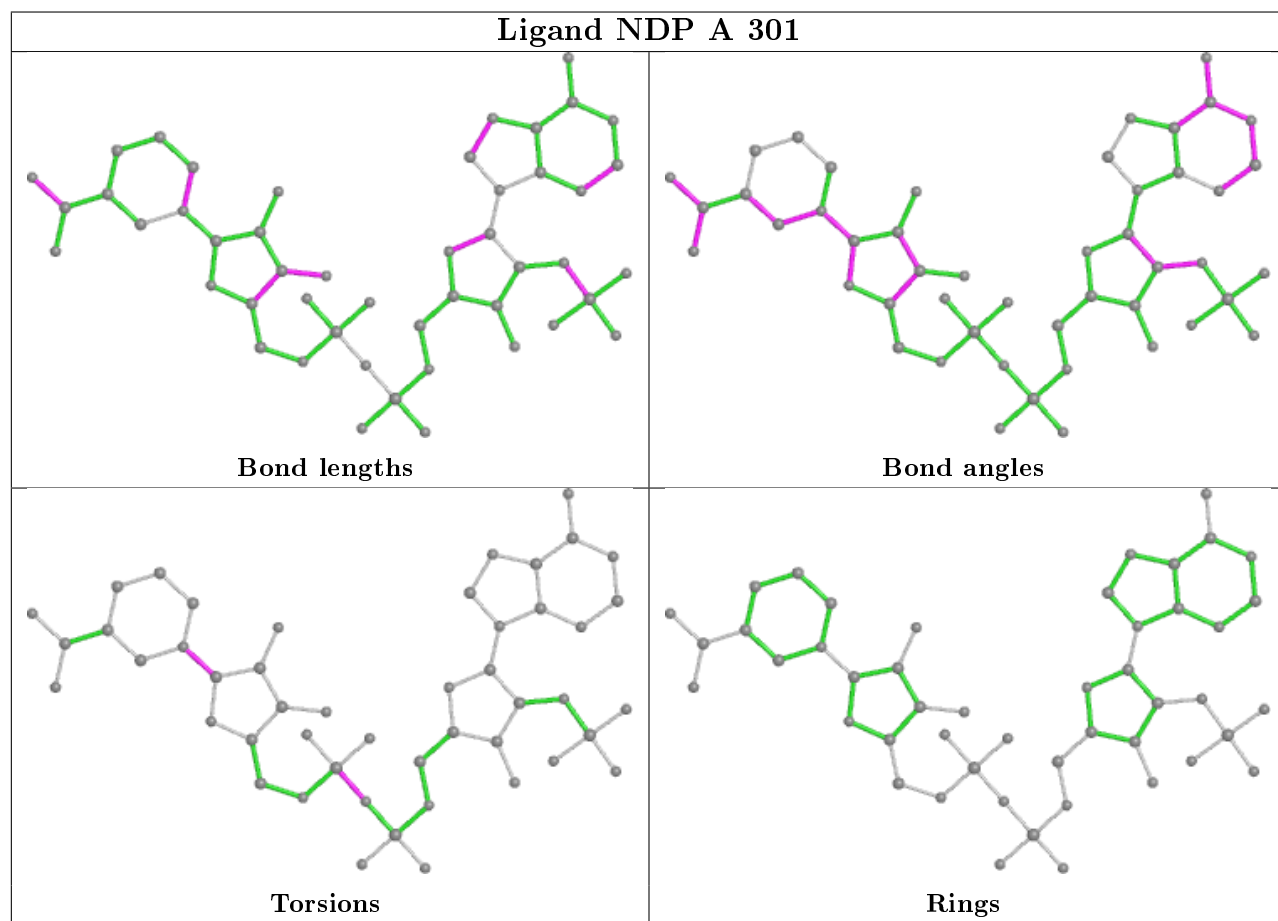
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	N22	2	0
2	A	301	NDP	1	0
2	B	301	NDP	1	0
3	A	302	N22	2	0

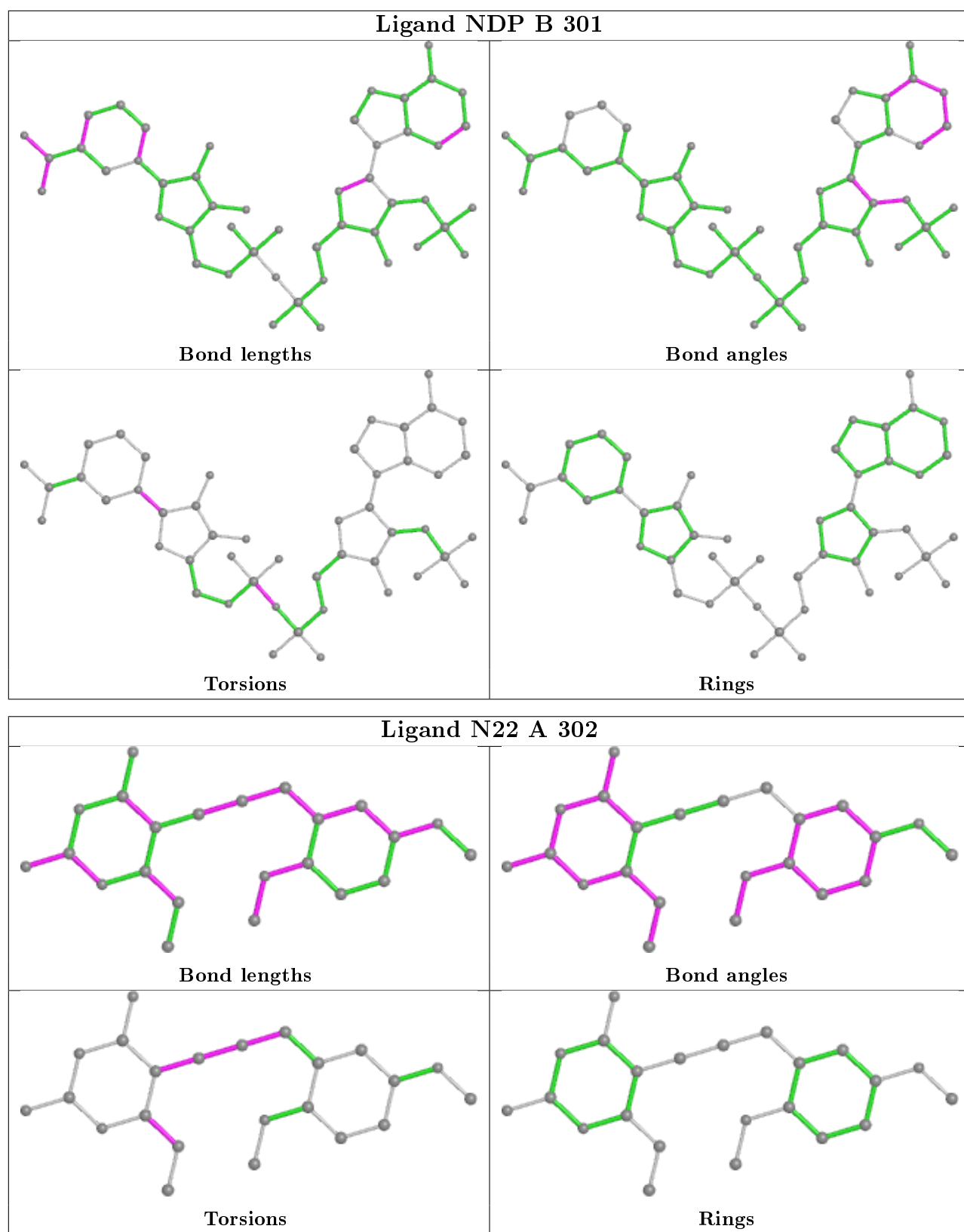
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand N22 B 302



## Ligand NDP A 301





## 5.7 Other polymers ⓘ

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 [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	225/227 (99%)	-0.53	0 100 100	15, 23, 37, 46	0
1	B	225/227 (99%)	-0.50	0 100 100	15, 23, 37, 46	1 (0%)
All	All	450/454 (99%)	-0.52	0 100 100	15, 23, 37, 46	1 (0%)

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	N22	B	302	23/23	0.95	0.08	15,22,32,38	0
3	N22	A	302	23/23	0.95	0.09	14,21,33,40	0
2	NDP	B	301	48/48	0.98	0.06	15,18,23,26	0
2	NDP	A	301	48/48	0.98	0.06	14,18,23,25	0

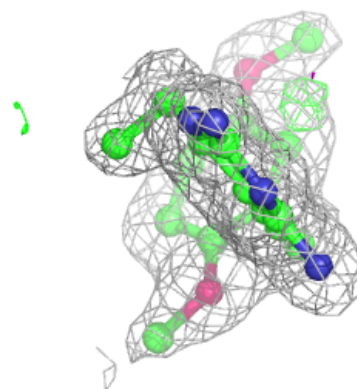
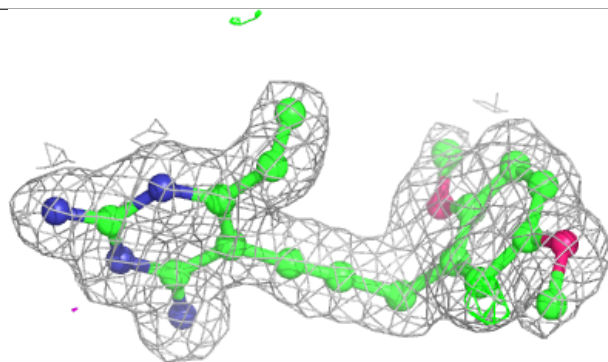
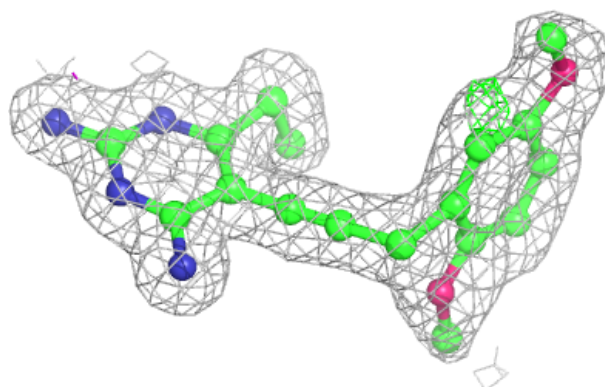
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers



as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

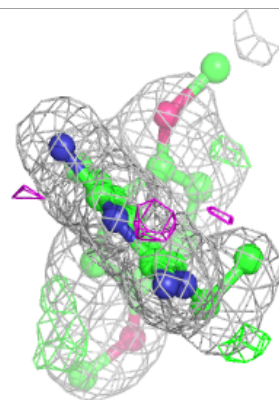
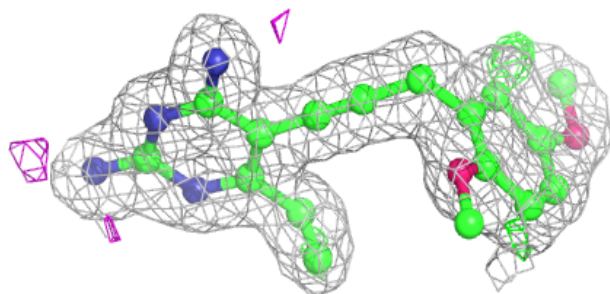
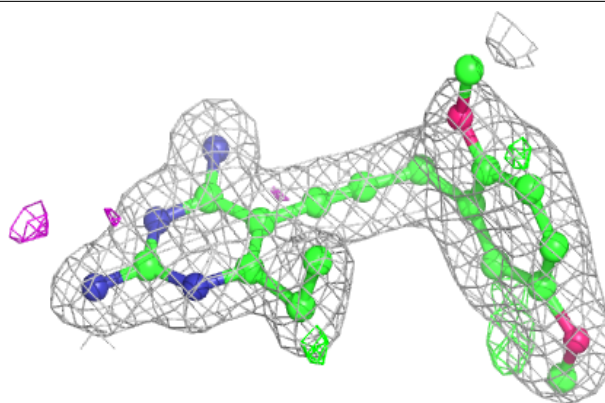
**Electron density around N22 B 302:**

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

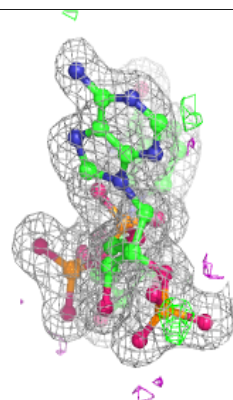
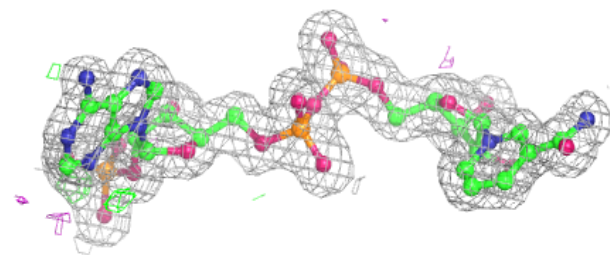
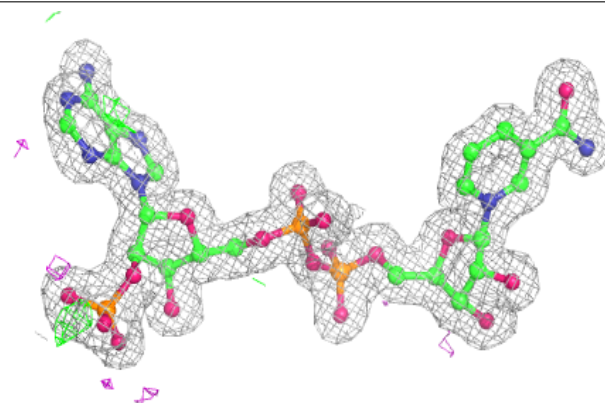


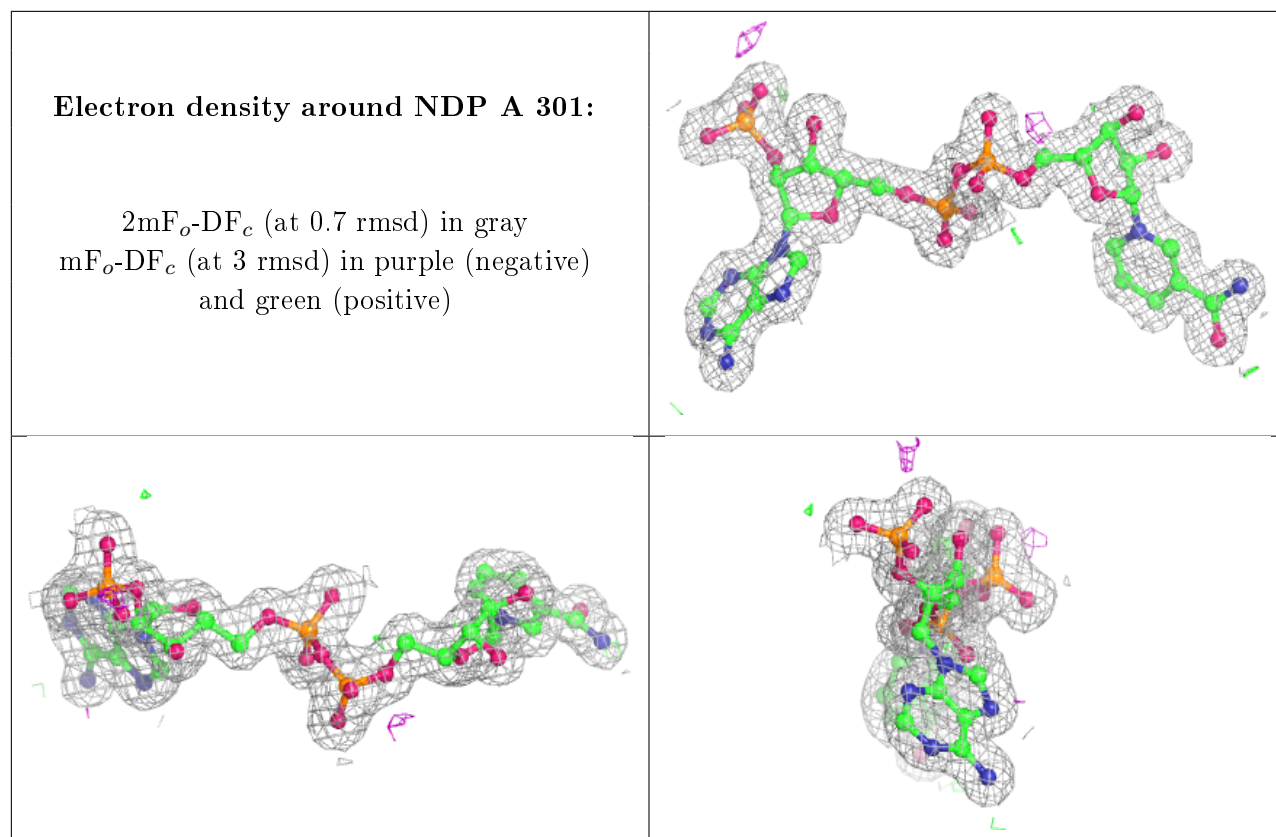
**Electron density around N22 A 302:**

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

**Electron density around NDP B 301:**

$2mF_o-DF_c$  (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.