Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2024 – 03:23 am GMT

PDB ID	:	8COP
Title	:	Mycobacterium tuberculosis dihydrofolate reductase in complex with N-(4-(2, 6-diamino-5-(cyclopropylethynyl)pyrimidin-4-yl)phenyl)methanesulfonamide
Authors	:	Kirkman, T.J.; Dias, M.V.B.
Deposited on	:	2023-02-28
Resolution	:	1.80 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:

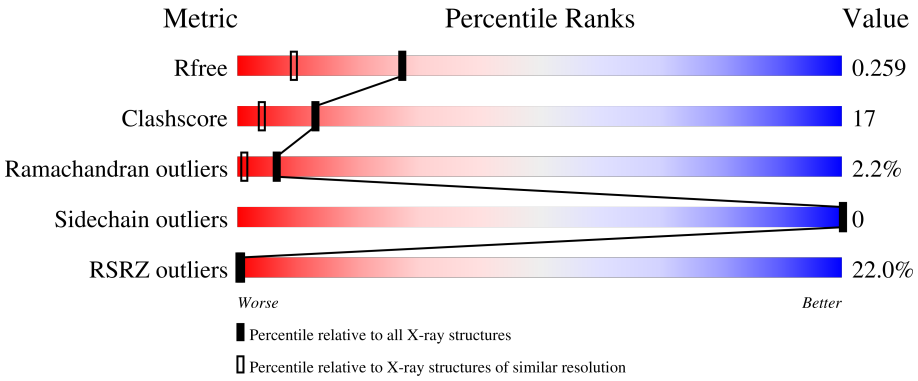
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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% 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	161	14% 65% 30%
1	B	161	29% 58% 37%

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	PO4	B	202	-	-	-	X

2 Entry composition

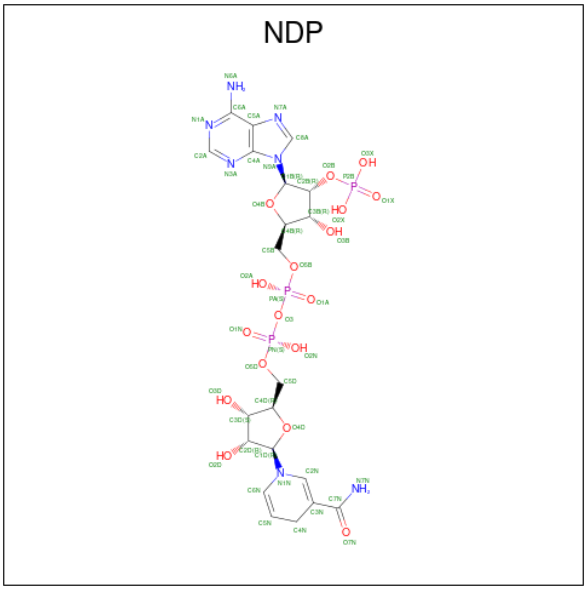
There are 6 unique types of molecules in this entry. The entry contains 2709 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

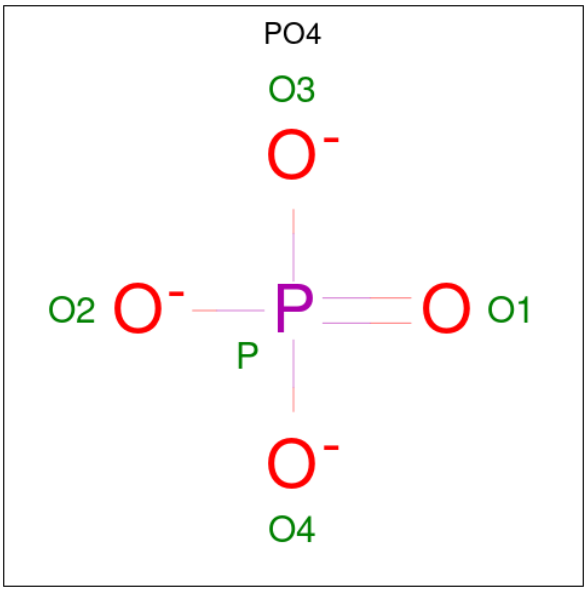
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	4	1	0
			1248	787	228	228	5			
1	B	159	Total	C	N	O	S	0	0	0
			1244	783	228	228	5			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



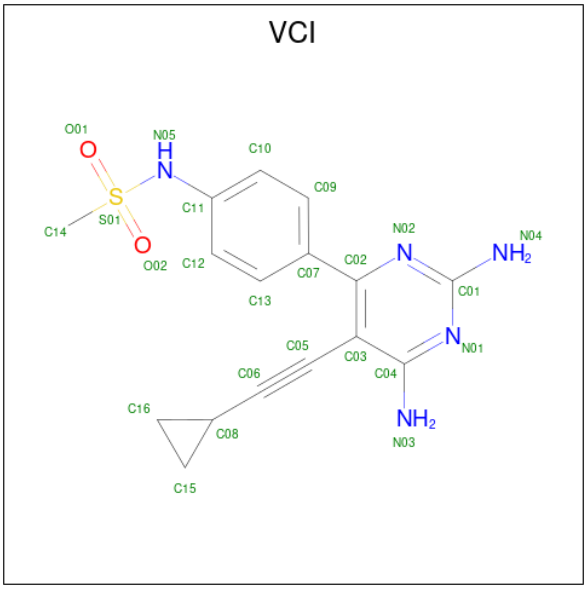
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is {N}-[4-[2,6-bis(azanyl)-5-(2-cyclopropylethynyl)pyrimidin-4-yl]phenyl]methanesulfonamide (three-letter code: VCI) (formula: $C_{16}H_{17}N_5O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			24	16	5	2	1		
4	B	1	Total	C	N	O	S	0	0
			24	16	5	2	1		

- Molecule 5 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Co	0	0
			1	1		
5	B	1	Total	Co	0	0
			1	1		

- Molecule 6 is water.

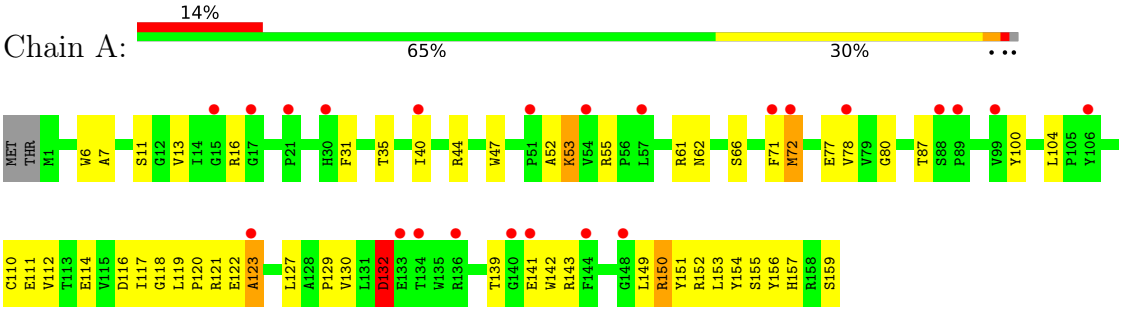
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	24	Total	O	0	0
			24	24		
6	B	32	Total	O	0	0
			32	32		

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

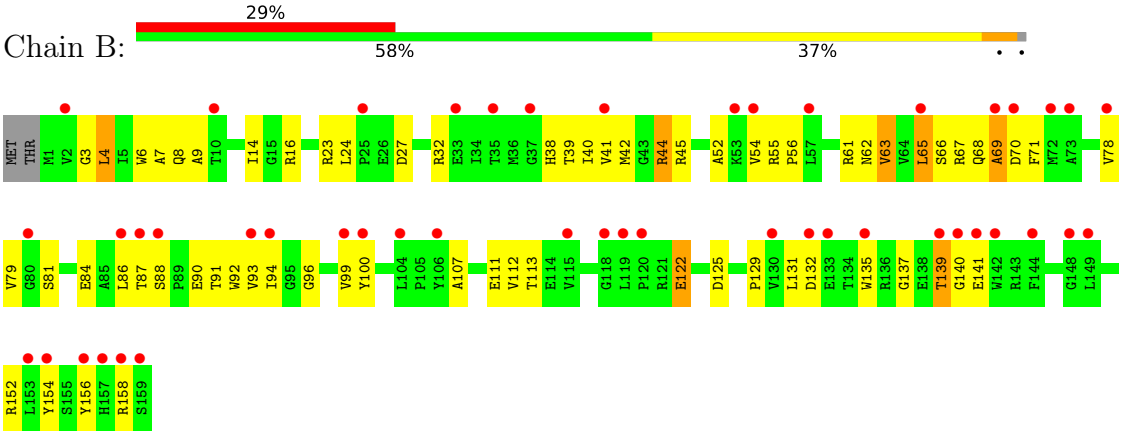
• Molecule 1: Dihydrofolate reductase

Chain A:



• Molecule 1: Dihydrofolate reductase

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	61.03Å 71.93Å 72.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.66 – 1.80 46.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.66-1.80) 98.2 (46.66-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.95 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.199 , 0.257 0.204 , 0.259	Depositor DCC
R_{free} test set	2003 reflections (6.64%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 35.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.397 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2709	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.57% 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: CO, NDP, PO4, VCI

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	0.69	2/1282 (0.2%)	1.80	8/1742 (0.5%)
1	B	0.48	1/1275 (0.1%)	0.85	5/1732 (0.3%)
All	All	0.60	3/2557 (0.1%)	1.41	13/3474 (0.4%)

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	2
1	B	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	LYS	C-N	-16.14	0.96	1.34
1	A	52	ALA	C-N	5.89	1.47	1.34
1	B	63	VAL	CB-CG2	-5.00	1.42	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	132	ASP	CB-CG-OD1	49.28	162.65	118.30
1	A	132	ASP	CB-CG-OD2	-38.66	83.51	118.30
1	A	132	ASP	OD1-CG-OD2	-17.58	89.89	123.30
1	A	53	LYS	O-C-N	-12.83	102.17	122.70
1	B	65	LEU	CB-CG-CD2	-7.90	97.56	111.00
1	A	72	MET	CG-SD-CE	-7.28	88.55	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	44	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	A	130	VAL	CG1-CB-CG2	5.90	120.35	110.90
1	B	4	LEU	CB-CG-CD2	-5.88	101.01	111.00
1	B	44	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	65	LEU	CA-CB-CG	5.70	128.42	115.30
1	A	150	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	150	ARG	CD-NE-CZ	5.05	130.68	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ASP	Sidechain
1	A	53	LYS	Mainchain
1	B	131	LEU	Peptide

5.2 Too-close contacts (i)

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	1248	0	1231	36	2
1	B	1244	0	1223	50	2
2	A	48	0	26	2	0
2	B	48	0	25	3	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
4	A	24	0	0	0	0
4	B	24	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	24	0	0	4	0
6	B	32	0	0	10	0
All	All	2709	0	2505	85	2

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 17.

All (85) 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:139:THR:HG23	1:A:154:TYR:CZ	1.97	0.99
1:B:7:ALA:H	2:B:201:NDP:H72N	1.12	0.96
1:B:96:GLY:O	6:B:301:HOH:O	1.81	0.96
1:A:139:THR:HG23	1:A:154:TYR:CE1	2.06	0.90
1:A:7:ALA:H	2:A:201:NDP:H72N	1.20	0.88
1:B:45:ARG:NH2	6:B:304:HOH:O	2.07	0.86
1:B:69:ALA:O	6:B:302:HOH:O	1.94	0.83
1:B:125:ASP:OD1	6:B:303:HOH:O	2.04	0.74
1:B:56:PRO:HB2	1:B:62:ASN:ND2	2.04	0.73
1:A:61:ARG:NH1	6:A:301:HOH:O	2.13	0.73
1:A:11:SER:O	1:A:121:ARG:NH1	2.20	0.72
1:B:111:GLU:OE1	6:B:305:HOH:O	2.12	0.68
1:B:99:VAL:N	6:B:301:HOH:O	2.27	0.68
1:B:4:LEU:HD13	1:B:107:ALA:HB2	1.76	0.67
1:A:129:PRO:O	6:A:302:HOH:O	2.14	0.65
1:B:8:GLN:HG2	1:B:9:ALA:O	1.97	0.65
1:A:112:VAL:HB	1:A:154:TYR:HB2	1.78	0.64
1:A:117:ILE:O	6:A:303:HOH:O	2.14	0.64
1:B:45:ARG:NH1	6:B:308:HOH:O	2.30	0.64
1:B:100:TYR:N	6:B:301:HOH:O	1.93	0.63
1:B:66:SER:OG	1:B:68:GLN:HG2	2.00	0.61
1:B:158:ARG:NH1	6:B:306:HOH:O	2.23	0.59
1:A:143:ARG:HH11	1:A:153:LEU:HG	1.68	0.58
1:A:142:TRP:CE3	1:A:152:ARG:HG2	2.38	0.58
1:A:132:ASP:OD2	1:A:132:ASP:N	2.30	0.55
1:B:24:LEU:HD23	1:B:27:ASP:H	1.72	0.55
1:A:117:ILE:HB	1:A:149:LEU:HD13	1.90	0.54
1:B:112:VAL:HB	1:B:154:TYR:HB2	1.89	0.54
1:A:40:ILE:HD11	1:A:62:ASN:OD1	2.09	0.53
1:A:141:GLU:OE1	1:B:141:GLU:HA	2.10	0.52
1:B:122:GLU:HB3	1:B:125:ASP:OD2	2.09	0.52
1:A:157:HIS:HE1	1:A:159:SER:HA	1.75	0.52
1:A:16:ARG:NH2	1:A:120:PRO:O	2.43	0.51
1:B:67:ARG:HG2	2:B:201:NDP:O2X	2.10	0.51
1:A:44:ARG:HD3	2:A:201:NDP:O2X	2.10	0.51
1:B:87:THR:O	1:B:88:SER:OG	2.25	0.50
1:B:44:ARG:HD2	1:B:44:ARG:C	2.32	0.50
1:A:143:ARG:NH1	1:A:153:LEU:HG	2.26	0.49
1:B:44:ARG:HH21	1:B:45:ARG:HE	1.59	0.49
1:B:86:LEU:HD23	1:B:91:THR:HG21	1.93	0.49
1:B:68:GLN:O	1:B:70:ASP:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:CYS:HB2	1:A:156:TYR:HB2	1.94	0.48
1:A:116:ASP:HB3	1:A:150:ARG:HB2	1.94	0.48
1:B:41:VAL:HG22	1:B:63:VAL:HG21	1.94	0.48
1:B:152:ARG:NE	1:B:154:TYR:OH	2.47	0.48
1:B:40:ILE:O	1:B:63:VAL:HG22	2.14	0.47
1:B:137:GLY:HA3	1:B:156:TYR:CD2	2.50	0.47
1:B:7:ALA:HA	1:B:113:THR:HB	1.96	0.47
1:A:47:TRP:CH2	1:A:55:ARG:HG2	2.51	0.46
1:B:41:VAL:HG22	1:B:63:VAL:CG2	2.46	0.46
1:B:139:THR:HG22	1:B:140:GLY:N	2.31	0.46
1:B:39:THR:HA	1:B:61:ARG:HB3	1.97	0.45
1:A:66:SER:O	1:A:80:GLY:HA2	2.17	0.45
1:A:142:TRP:CZ3	1:A:152:ARG:HG2	2.52	0.44
1:B:71:PHE:HB3	1:B:78:VAL:HG11	1.99	0.44
1:B:100:TYR:HB3	1:B:129:PRO:HG3	1.98	0.44
1:B:135:TRP:CZ2	1:B:158:ARG:HD3	2.52	0.44
1:B:4:LEU:HG	1:B:93:VAL:HB	1.99	0.44
1:B:14:ILE:O	2:B:201:NDP:H2N	2.18	0.44
1:A:71:PHE:N	6:A:304:HOH:O	2.50	0.44
1:B:6:TRP:CD1	1:B:8:GLN:HB2	2.53	0.44
1:B:3:GLY:HA3	1:B:92:TRP:CZ3	2.53	0.43
1:A:13:VAL:HA	1:A:127:LEU:HD23	2.01	0.43
1:A:72:MET:O	1:A:72:MET:HG3	2.18	0.43
1:A:139:THR:HG23	1:A:154:TYR:OH	2.14	0.43
1:B:23:ARG:HD3	1:B:23:ARG:HA	1.88	0.43
1:B:65:LEU:HD21	1:B:81:SER:C	2.39	0.43
1:B:52:ALA:HA	1:B:55:ARG:HG2	2.01	0.42
1:A:122:GLU:O	1:A:123:ALA:O	2.38	0.42
1:B:152:ARG:NH2	1:B:154:TYR:OH	2.52	0.42
1:A:114:GLU:O	1:A:151:TYR:HA	2.20	0.42
1:B:32:ARG:NH1	6:B:313:HOH:O	2.53	0.41
1:B:79:VAL:CG1	1:B:84:GLU:HB2	2.51	0.41
1:A:6:TRP:HB3	1:A:100:TYR:CZ	2.56	0.41
1:A:44:ARG:HG3	1:A:71:PHE:CD1	2.54	0.41
1:A:111:GLU:CD	1:A:155:SER:HG	2.24	0.41
1:B:41:VAL:HA	1:B:63:VAL:CG2	2.50	0.41
1:A:31:PHE:CE1	1:A:35:THR:HG21	2.56	0.41
1:B:6:TRP:HB3	1:B:100:TYR:CZ	2.56	0.41
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.84	0.41
1:B:42:MET:HE1	1:B:94:ILE:HD11	2.03	0.41
1:A:71:PHE:HB3	1:A:78:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:THR:O	1:B:87:THR:HG23	2.21	0.40
1:A:104:LEU:HD12	1:A:104:LEU:HA	1.93	0.40
1:B:38:HIS:HB3	1:B:90:GLU:O	2.22	0.40

All (2) 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:A:118:GLY:O	1:B:61:ARG:NH2[2_555]	2.10	0.10
1:A:77:GLU:OE2	1:B:16:ARG:NH2[3_655]	2.12	0.08

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	158/161 (98%)	149 (94%)	7 (4%)	2 (1%)	12 3
1	B	157/161 (98%)	142 (90%)	10 (6%)	5 (3%)	4 0
All	All	315/322 (98%)	291 (92%)	17 (5%)	7 (2%)	6 1

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ALA
1	B	132	ASP
1	B	54	VAL
1	B	122	GLU
1	B	139	THR
1	A	87	THR
1	B	69	ALA

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	128/129 (99%)	128 (100%)	0	100	100
1	B	127/129 (98%)	127 (100%)	0	100	100
All	All	255/258 (99%)	255 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	$\#\|Z\|>2$
2	NDP	B	201	-	45,52,52	2.15	6 (13%)	53,80,80	1.61	8 (15%)
4	VCI	A	204	-	26,26,26	2.77	11 (42%)	37,38,38	3.74	12 (32%)
4	VCI	B	203	-	26,26,26	2.99	11 (42%)	37,38,38	4.01	17 (45%)
2	NDP	A	201	-	45,52,52	2.25	6 (13%)	53,80,80	1.51	9 (16%)
3	PO4	A	202	-	4,4,4	0.94	0	6,6,6	0.56	0
3	PO4	A	203	-	4,4,4	0.80	0	6,6,6	0.57	0
3	PO4	B	202	-	4,4,4	0.93	0	6,6,6	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	VCI	B	203	-	-	5/11/16/16	0/3/3/3
2	NDP	A	201	-	-	4/30/77/77	0/5/5/5
2	NDP	B	201	-	-	8/30/77/77	0/5/5/5
4	VCI	A	204	-	-	3/11/16/16	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	NDP	P2B-O2B	12.16	1.82	1.59
2	B	201	NDP	P2B-O2B	11.37	1.80	1.59
4	B	203	VCI	S01-N05	7.20	1.72	1.63
4	A	204	VCI	C01-N04	6.56	1.47	1.33
4	B	203	VCI	C01-N04	6.39	1.46	1.33
4	B	203	VCI	C03-C05	6.03	1.53	1.43
4	A	204	VCI	C03-C05	5.84	1.52	1.43
4	A	204	VCI	S01-N05	5.27	1.70	1.63
4	B	203	VCI	C07-C02	5.22	1.55	1.49
4	B	203	VCI	C04-N03	4.80	1.46	1.34
4	A	204	VCI	C07-C02	4.77	1.54	1.49
4	A	204	VCI	C04-N03	4.53	1.45	1.34
2	B	201	NDP	PN-O5D	4.02	1.75	1.59
2	A	201	NDP	PN-O5D	3.39	1.73	1.59
2	B	201	NDP	O2B-C2B	-3.38	1.31	1.44
4	B	203	VCI	C14-S01	3.31	1.83	1.75
4	A	204	VCI	C03-C04	-3.25	1.38	1.42
2	A	201	NDP	O2B-C2B	-3.24	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	204	VCI	C14-S01	3.10	1.82	1.75
4	B	203	VCI	C03-C04	-2.89	1.38	1.42
2	A	201	NDP	O4B-C1B	2.77	1.45	1.41
2	B	201	NDP	O3B-C3B	-2.73	1.36	1.43
4	A	204	VCI	O01-S01	2.61	1.48	1.43
2	B	201	NDP	O4B-C4B	-2.51	1.39	1.45
4	B	203	VCI	C04-N01	-2.44	1.31	1.35
2	B	201	NDP	C7N-N7N	2.37	1.39	1.33
4	B	203	VCI	O01-S01	2.36	1.47	1.43
4	A	204	VCI	C08-C06	2.27	1.53	1.46
2	A	201	NDP	O3D-C3D	-2.26	1.37	1.43
4	A	204	VCI	O02-S01	2.16	1.47	1.43
4	A	204	VCI	C04-N01	-2.12	1.32	1.35
4	B	203	VCI	C08-C06	2.11	1.53	1.46
2	A	201	NDP	O4B-C4B	-2.03	1.40	1.45
4	B	203	VCI	C11-N05	2.02	1.46	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	203	VCI	C02-N02-C01	13.44	130.71	117.22
4	B	203	VCI	O02-S01-O01	-12.92	100.27	118.85
4	A	204	VCI	C02-N02-C01	12.36	129.63	117.22
4	A	204	VCI	O02-S01-O01	-10.45	103.82	118.85
4	B	203	VCI	N02-C01-N01	-7.09	114.31	125.42
4	A	204	VCI	N02-C01-N01	-6.57	115.11	125.42
4	A	204	VCI	C07-C02-N02	6.42	123.62	115.09
4	B	203	VCI	C03-C02-N02	-6.00	113.95	121.36
4	A	204	VCI	C03-C04-N03	-5.98	114.73	121.62
4	A	204	VCI	C03-C02-N02	-5.87	114.10	121.36
4	B	203	VCI	C07-C02-N02	5.74	122.71	115.09
2	B	201	NDP	PN-O3-PA	-5.32	114.57	132.83
2	A	201	NDP	PN-O3-PA	-4.97	115.76	132.83
4	A	204	VCI	C03-C04-N01	4.54	128.06	121.63
4	B	203	VCI	N04-C01-N01	3.84	123.22	117.25
4	B	203	VCI	C02-C03-C04	-3.63	115.00	119.09
4	A	204	VCI	C02-C03-C04	-3.57	115.07	119.09
4	A	204	VCI	N04-C01-N02	3.47	122.65	117.25
4	B	203	VCI	C03-C04-N01	3.44	126.50	121.63
4	B	203	VCI	C11-N05-S01	-3.41	113.52	123.83
2	B	201	NDP	O2B-P2B-O1X	-3.39	96.30	109.39
4	B	203	VCI	C03-C04-N03	-3.38	117.72	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	203	VCI	N04-C01-N02	3.36	122.47	117.25
2	A	201	NDP	O2B-P2B-O1X	-3.27	96.77	109.39
4	A	204	VCI	N04-C01-N01	3.21	122.24	117.25
4	A	204	VCI	C14-S01-N05	3.17	110.25	106.63
4	B	203	VCI	O01-S01-N05	2.88	112.98	107.10
2	A	201	NDP	PA-O5B-C5B	-2.78	105.36	121.68
4	B	203	VCI	O02-S01-C14	2.75	112.69	108.28
4	A	204	VCI	O02-S01-C14	2.74	112.68	108.28
4	B	203	VCI	C16-C08-C06	-2.57	112.08	119.06
2	B	201	NDP	O3X-P2B-O2X	2.56	117.44	107.64
2	A	201	NDP	PN-O5D-C5D	-2.45	107.32	121.68
2	B	201	NDP	PA-O5B-C5B	-2.45	107.32	121.68
2	A	201	NDP	O3X-P2B-O2X	2.45	116.98	107.64
2	B	201	NDP	PN-O5D-C5D	-2.37	107.80	121.68
2	B	201	NDP	C2A-N1A-C6A	-2.33	114.77	118.75
4	B	203	VCI	C04-C03-C05	2.27	122.51	118.57
4	B	203	VCI	C01-N01-C04	2.27	119.49	116.99
2	B	201	NDP	O2N-PN-O1N	2.22	123.23	112.24
2	A	201	NDP	O3X-P2B-O2B	-2.20	96.14	105.99
2	A	201	NDP	C2A-N1A-C6A	-2.17	115.05	118.75
2	B	201	NDP	C2D-C1D-N1N	-2.08	108.09	113.30
2	A	201	NDP	C3N-C2N-N1N	-2.07	120.14	123.10
2	A	201	NDP	O7N-C7N-C3N	2.03	124.73	120.90
4	B	203	VCI	O01-S01-C14	2.01	111.50	108.28

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	204	VCI	C03-C05-C06-C08
4	A	204	VCI	C11-N05-S01-C14
4	A	204	VCI	C11-N05-S01-O02
4	B	203	VCI	C11-N05-S01-C14
4	B	203	VCI	C11-N05-S01-O02
2	B	201	NDP	C3B-C4B-C5B-O5B
4	B	203	VCI	C11-N05-S01-O01
2	B	201	NDP	O4B-C4B-C5B-O5B
2	A	201	NDP	PA-O3-PN-O5D
2	B	201	NDP	PA-O3-PN-O5D
2	A	201	NDP	C3B-C4B-C5B-O5B
4	B	203	VCI	C03-C05-C06-C08
2	B	201	NDP	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	A	201	NDP	O4D-C1D-N1N-C2N
2	A	201	NDP	C2D-C1D-N1N-C2N
2	B	201	NDP	O4D-C1D-N1N-C2N
2	B	201	NDP	C2D-C1D-N1N-C2N
4	B	203	VCI	C02-C03-C05-C06
2	B	201	NDP	C5D-O5D-PN-O3
2	B	201	NDP	C5D-O5D-PN-O1N

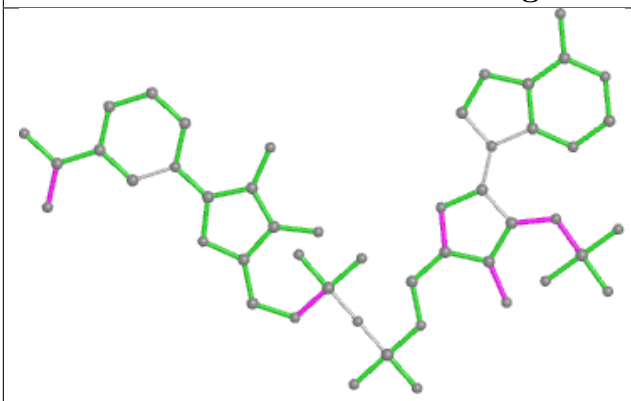
There are no ring outliers.

2 monomers are involved in 5 short contacts:

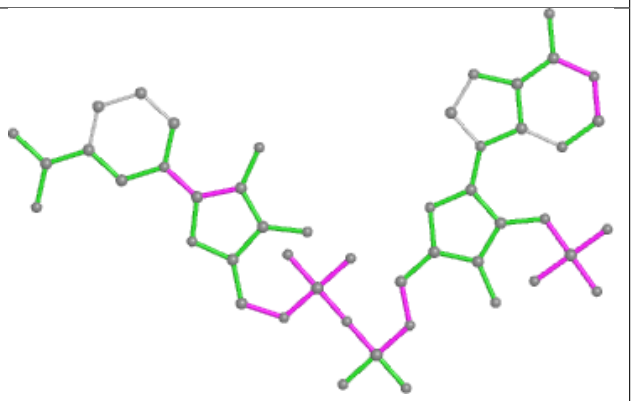
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	NDP	3	0
2	A	201	NDP	2	0

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.

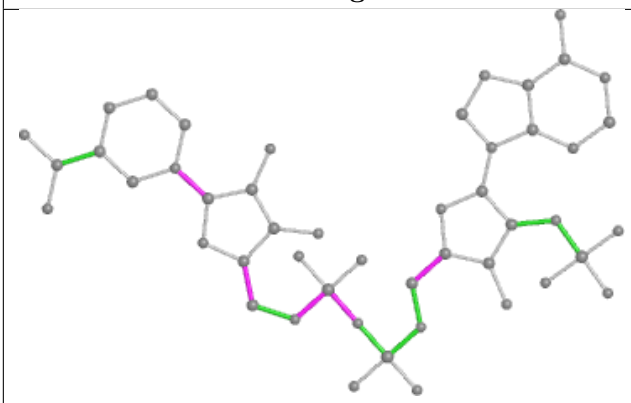
Ligand NDP B 201



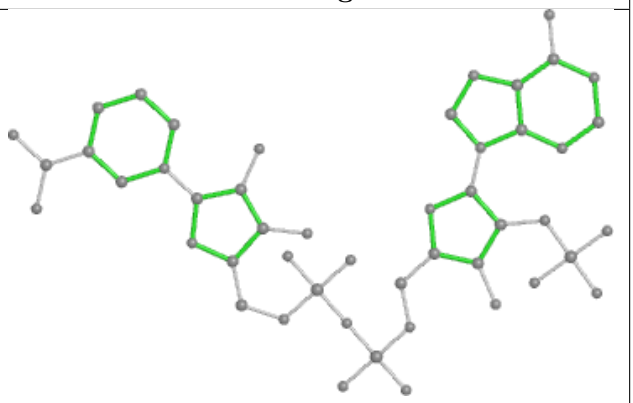
Bond lengths



Bond angles

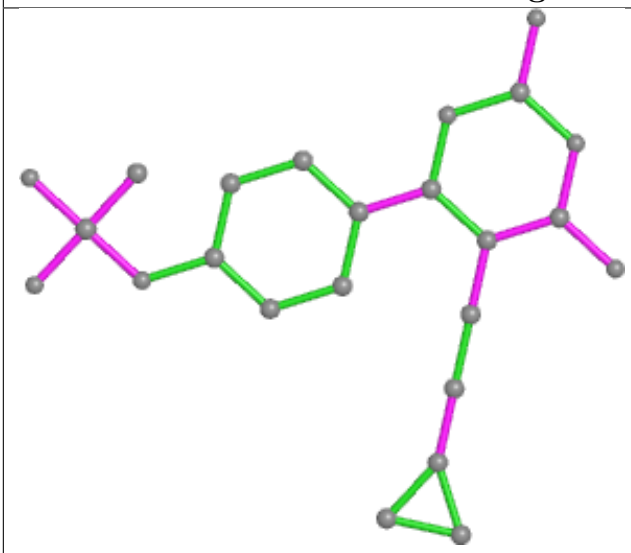


Torsions

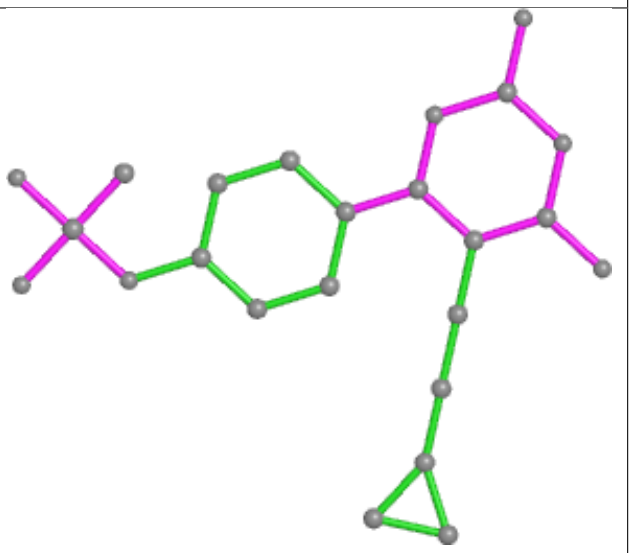


Rings

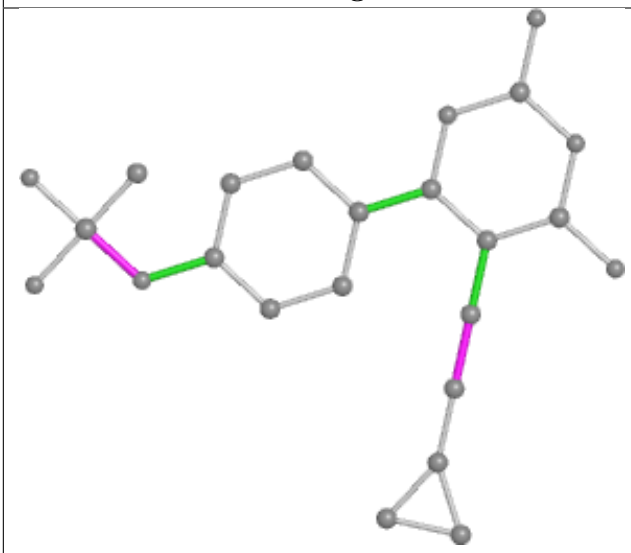
Ligand VCI A 204



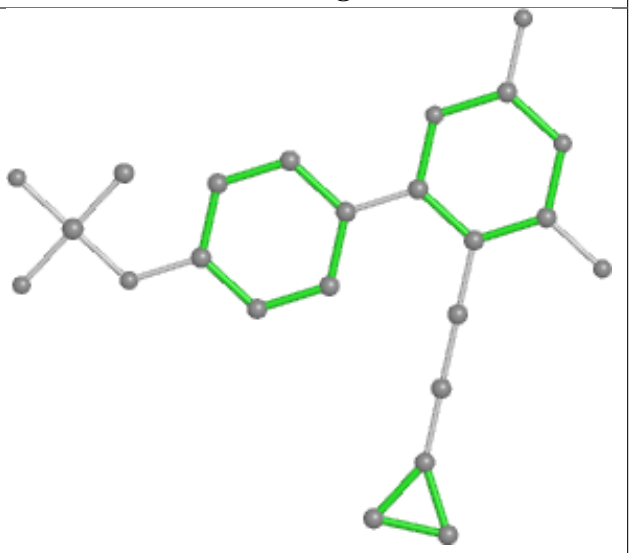
Bond lengths



Bond angles

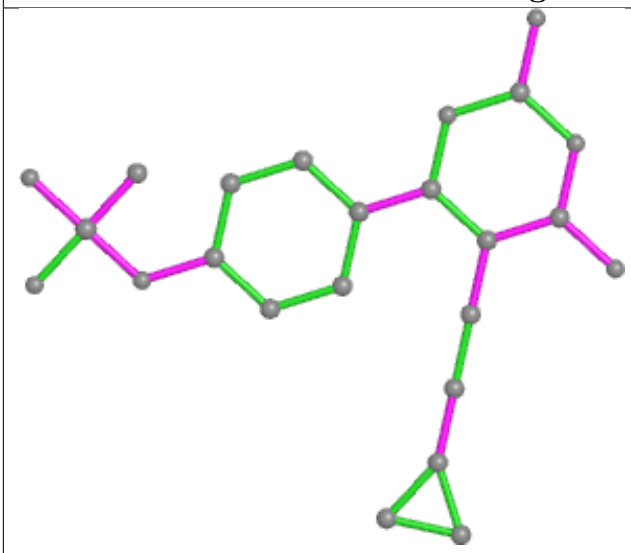


Torsions

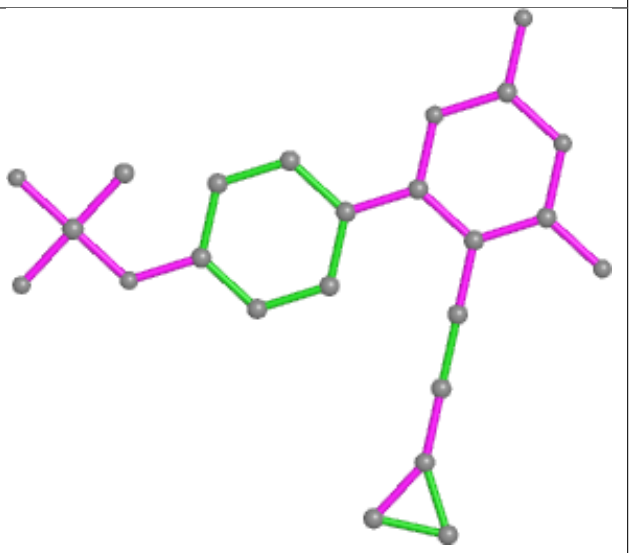


Rings

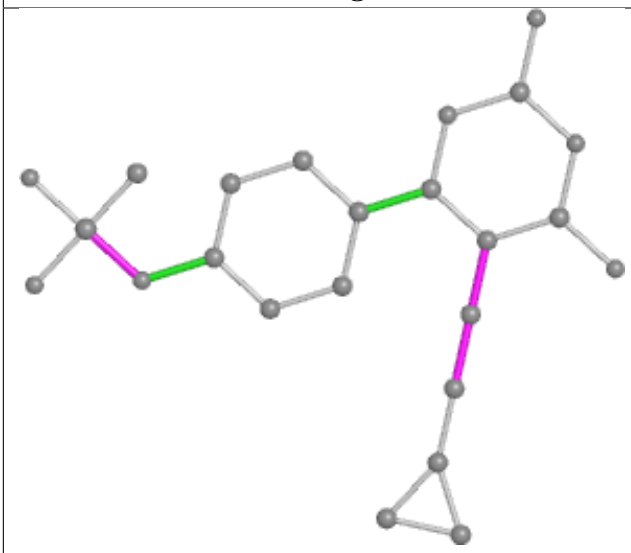
Ligand VCI B 203



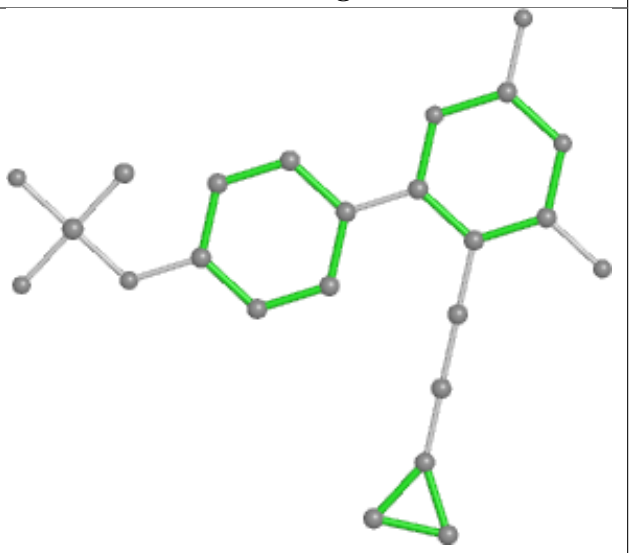
Bond lengths



Bond angles

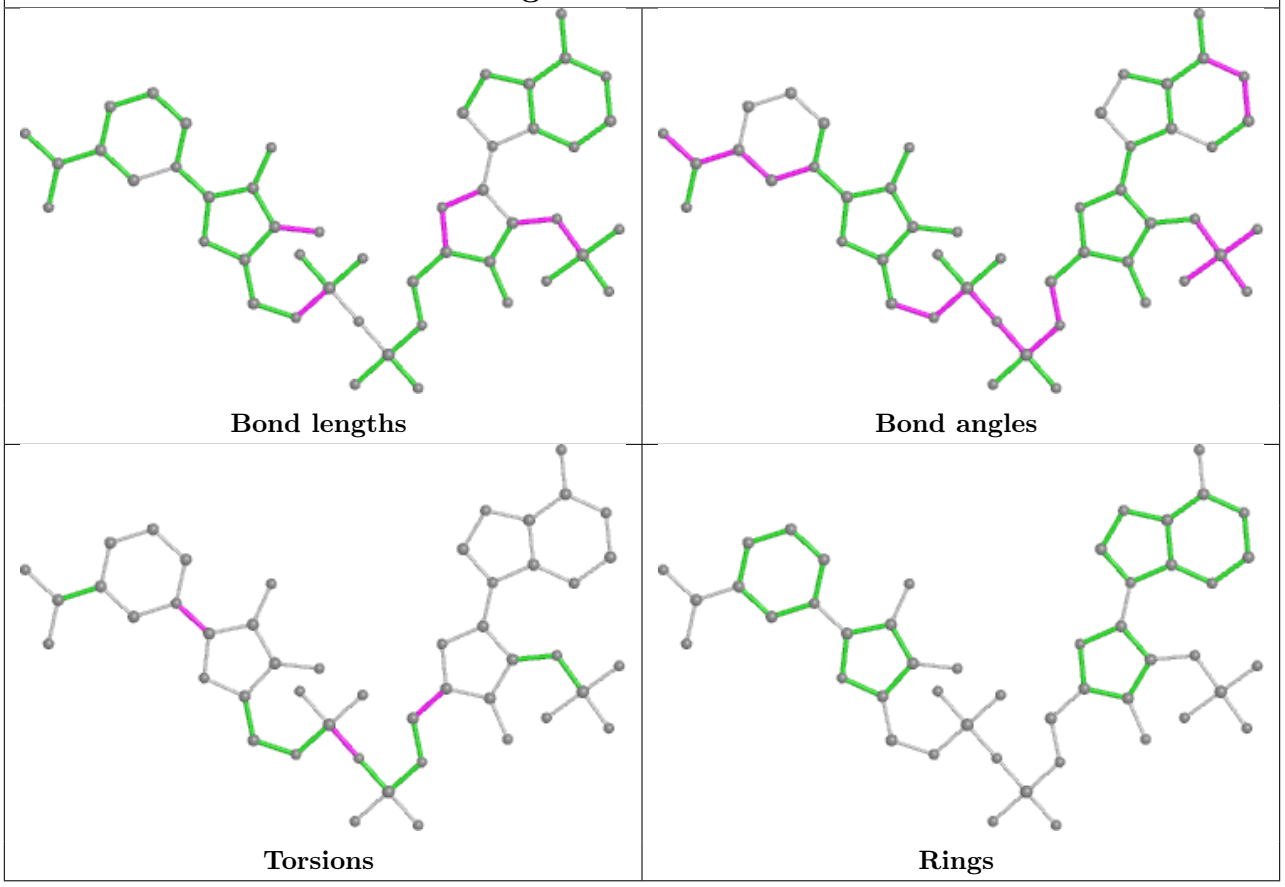


Torsions



Rings

Ligand NDP A 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	53:LYS	C	54:VAL	N	0.96

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	159/161 (98%)	1.15	23 (14%)	2	1	25, 34, 44, 59	0
1	B	159/161 (98%)	1.50	47 (29%)	0	0	25, 37, 51, 66	0
All	All	318/322 (98%)	1.33	70 (22%)	0	0	25, 35, 48, 66	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	132	ASP	5.2
1	B	139	THR	4.9
1	B	130	VAL	4.6
1	B	106	TYR	4.6
1	A	54	VAL	4.3
1	B	133	GLU	4.1
1	B	159	SER	3.9
1	B	65	LEU	3.7
1	B	53	LYS	3.6
1	A	72	MET	3.4
1	A	141	GLU	3.4
1	B	154	TYR	3.3
1	B	69	ALA	3.3
1	B	88	SER	3.2
1	B	153	LEU	3.2
1	A	123	ALA	3.2
1	B	41	VAL	3.1
1	B	70	ASP	3.1
1	B	72	MET	3.1
1	A	144	PHE	3.1
1	A	21	PRO	3.0
1	A	40	ILE	3.0
1	B	73	ALA	3.0
1	A	17	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	54	VAL	2.8
1	B	141	GLU	2.8
1	B	144	PHE	2.8
1	A	89	PRO	2.8
1	A	78	VAL	2.8
1	B	149	LEU	2.7
1	B	118	GLY	2.7
1	B	140	GLY	2.6
1	B	37	GLY	2.6
1	A	133	GLU	2.6
1	A	134	THR	2.6
1	B	25	PRO	2.5
1	B	80	GLY	2.5
1	B	57	LEU	2.5
1	B	100	TYR	2.5
1	B	93	VAL	2.5
1	B	156	TYR	2.5
1	B	158	ARG	2.5
1	A	148	GLY	2.4
1	B	148	GLY	2.4
1	B	10	THR	2.4
1	A	99	VAL	2.4
1	B	86	LEU	2.4
1	A	106	TYR	2.4
1	B	135	TRP	2.4
1	B	142	TRP	2.4
1	A	15	GLY	2.4
1	B	120	PRO	2.4
1	B	104	LEU	2.3
1	A	88	SER	2.3
1	A	140	GLY	2.3
1	B	2	VAL	2.3
1	B	99	VAL	2.3
1	A	57	LEU	2.3
1	B	119	LEU	2.3
1	A	30	HIS	2.2
1	B	115	VAL	2.2
1	B	78	VAL	2.1
1	A	136	ARG	2.1
1	B	157	HIS	2.1
1	A	51	PRO	2.1
1	A	71	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	94	ILE	2.0
1	B	87	THR	2.0
1	B	33	GLU	2.0
1	B	35	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

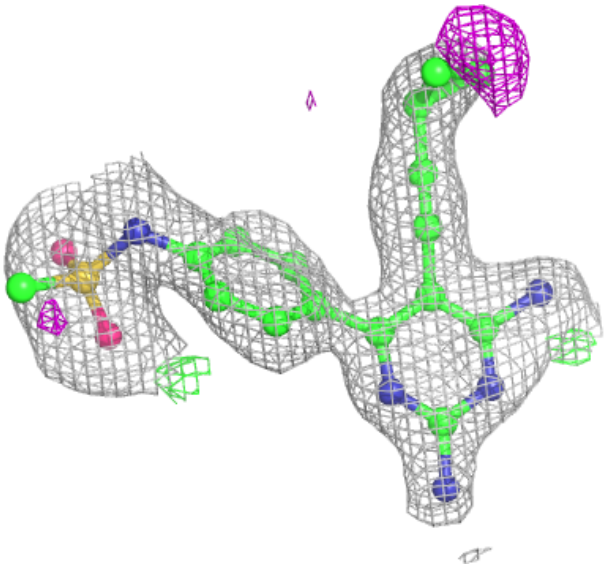
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

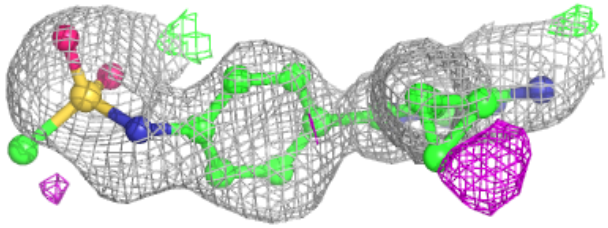
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	B	202	5/5	0.35	0.42	189,206,213,214	0
3	PO4	A	202	5/5	0.75	0.23	97,99,111,117	0
4	VCI	B	203	24/24	0.83	0.23	25,31,48,53	0
3	PO4	A	203	5/5	0.84	0.18	60,64,72,78	0
4	VCI	A	204	24/24	0.85	0.19	26,32,48,52	0
2	NDP	A	201	48/48	0.88	0.17	23,31,38,47	0
2	NDP	B	201	48/48	0.89	0.14	25,33,39,44	0
5	CO	A	205	1/1	0.97	0.14	37,37,37,37	0
5	CO	B	204	1/1	0.97	0.15	42,42,42,42	0

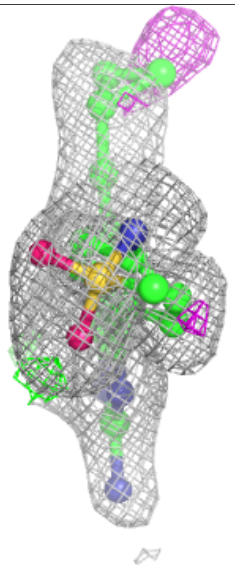
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VCI B 203:

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

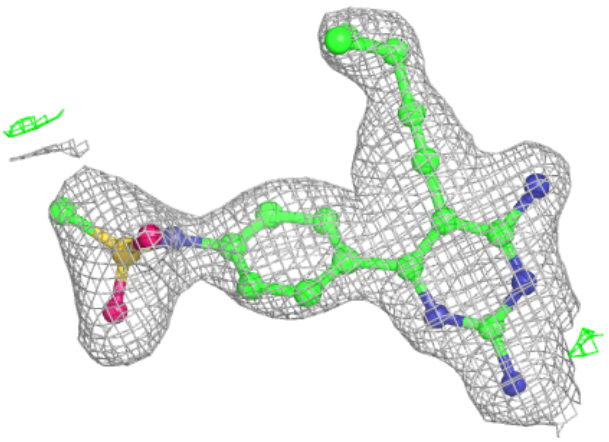


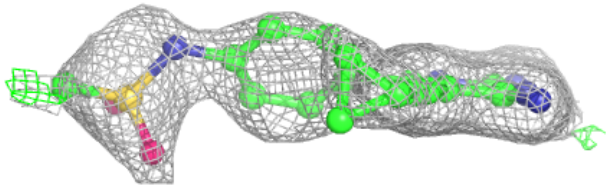


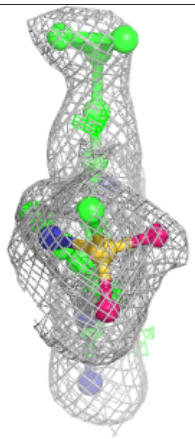


Electron density around VCI A 204:

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

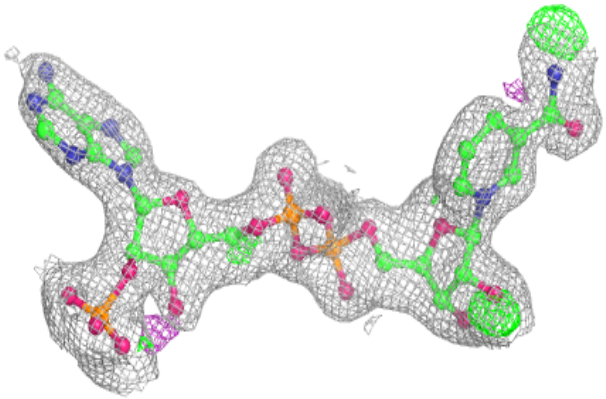


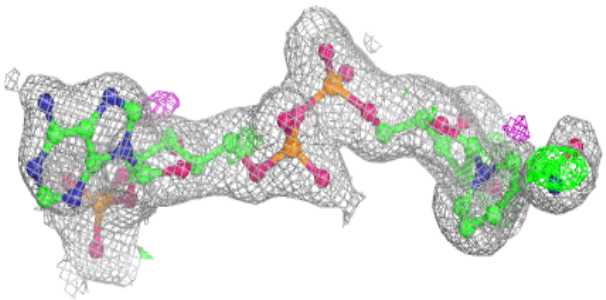


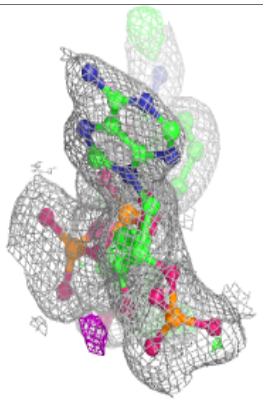


Electron density around NDP A 201:

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

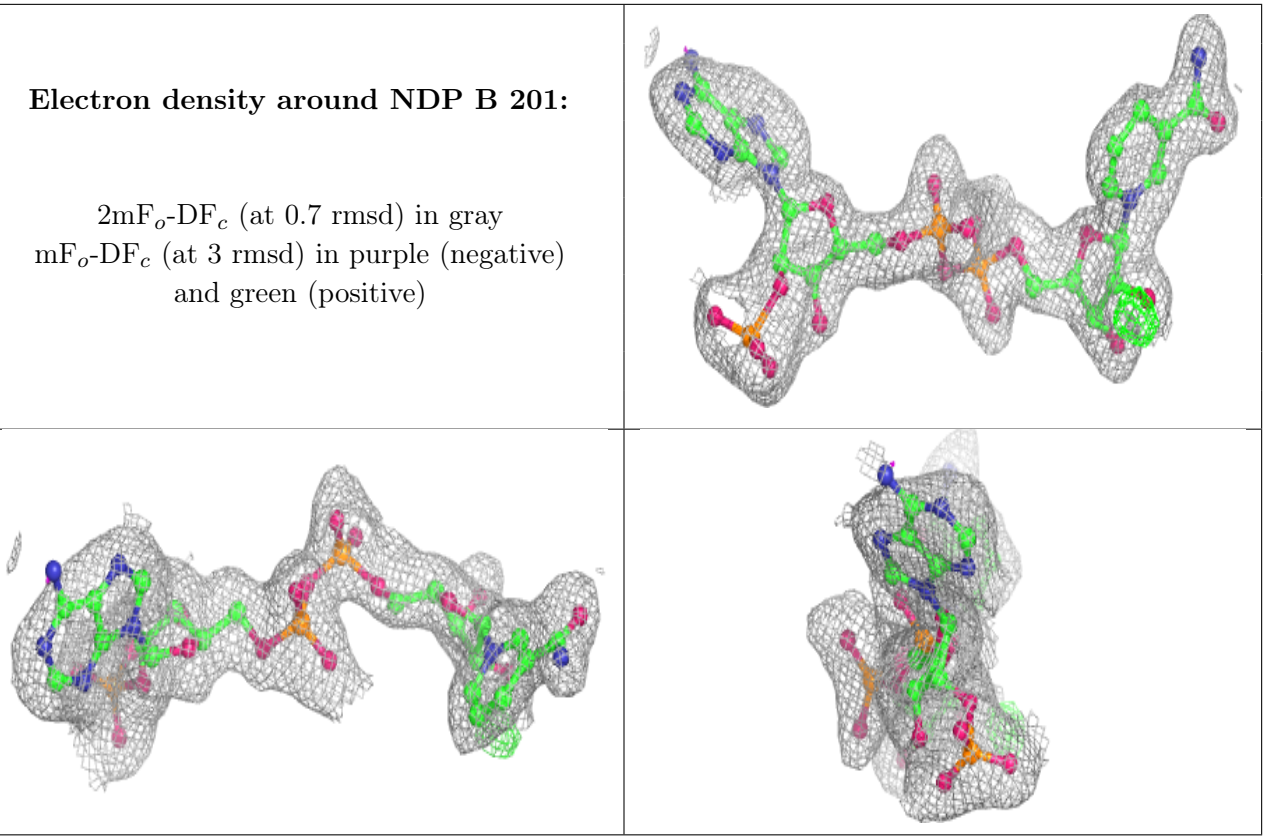






Electron density around NDP B 201:

$2mF_o$-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.