Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 11:27 PM EDT

PDB ID	:	1IA3
Title	:	Candida albicans dihydrofolate reductase complex in which the dihydronicotinamide moiety of dihydro-nicotinamide-adenine-dinucleotide phosphate (NADPH) is displaced by 5-[(4-TERT-BUTYLPHENYL)SULFANYL]-2,4-QUINAZOLINEDIAMINE (GW995)
Authors	:	Whitlow, M.; Howard, A.J.; Kuyper, L.F.
Deposited on	:	2001-03-22
Resolution	:	1.78 Å(reported)

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

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

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

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

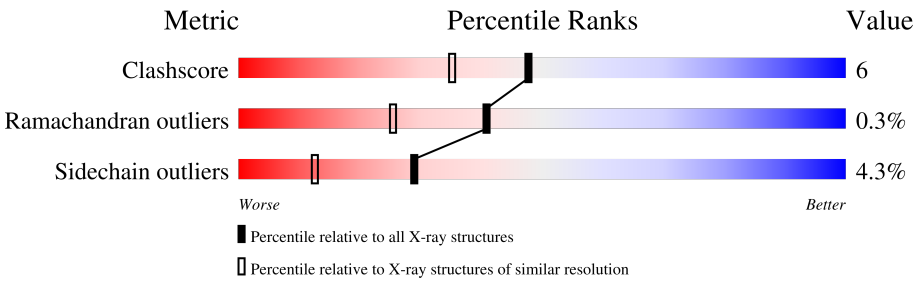
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.78 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))
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	192	77% 19% • •
1	B	192	76% 19% • •

2 Entry composition (i)

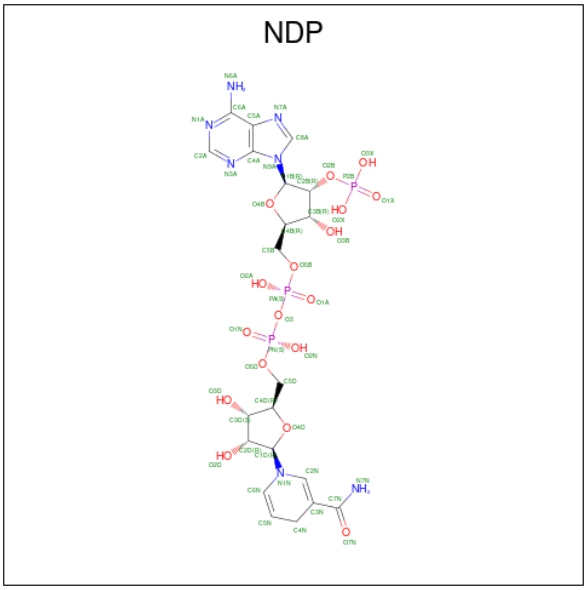
There are 5 unique types of molecules in this entry. The entry contains 3671 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

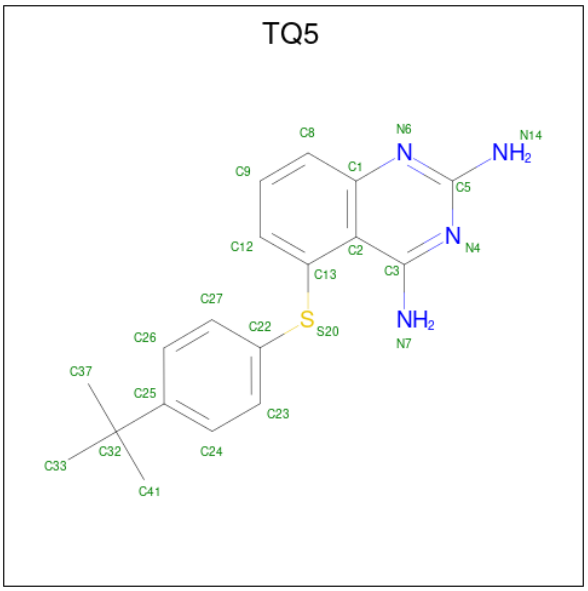
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	192	1590	1019	271	296	4	0	11	0
			Total	C	N	O	S			
1	B	192	1591	1021	265	301	4	0	11	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



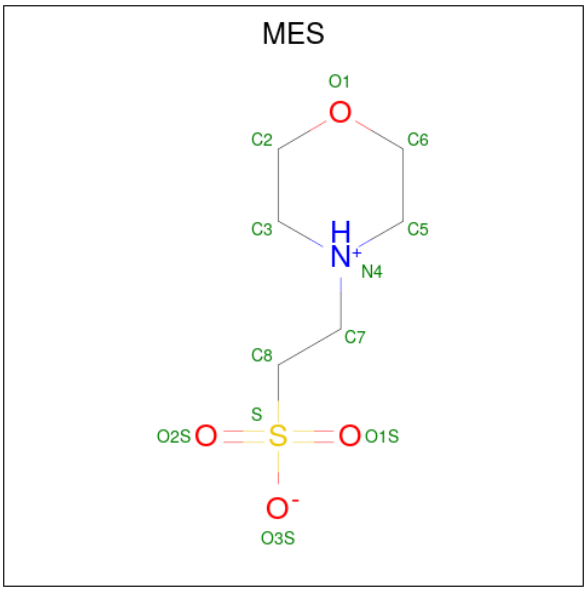
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	35	13	5	14	3	0	0
			Total	C	N	O	P		
2	B	1	35	13	5	14	3	0	0

- Molecule 3 is 5-[4-TERT-BUTYLPHENYLSULFANYL]-2,4-QUINAZOLINEDIAMINE (three-letter code: TQ5) (formula: $C_{18}H_{20}N_4S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
3	A	1	23	18	4	1	0	0
			Total	C	N	S		
3	B	1	23	18	4	1	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	12	6	1	4	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	12	6	1	4	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	156	163	163	0	7
			Total	O		
5	B	183	187	187	0	4

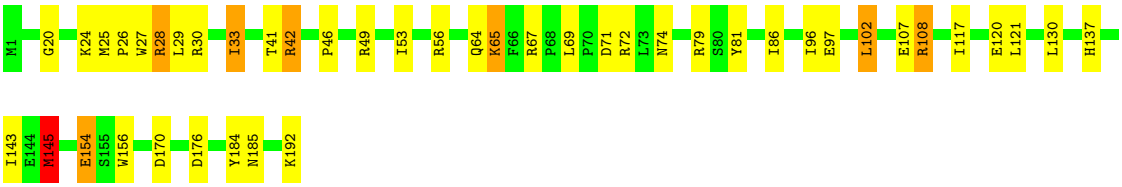
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: DIHYDROFOLATE REDUCTASE

Chain A:



• Molecule 1: DIHYDROFOLATE REDUCTASE

Chain B:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.91Å 67.28Å 38.49Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	10.00 – 1.78	Depositor
% Data completeness (in resolution range)	84.6 (10.00-1.78)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3671	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

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: MES, NDP, TQ5

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	1.20	1/1682 (0.1%)	1.91	41/2279 (1.8%)
1	B	1.19	1/1683 (0.1%)	1.63	32/2278 (1.4%)
All	All	1.20	2/3365 (0.1%)	1.77	73/4557 (1.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	GLU	CD-OE1	-7.51	1.17	1.25
1	B	179	GLU	CD-OE1	-6.43	1.18	1.25

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	49	ARG	NE-CZ-NH2	-19.61	110.50	120.30
1	A	30[A]	ARG	NE-CZ-NH1	19.29	129.94	120.30
1	A	30[B]	ARG	NE-CZ-NH1	19.29	129.94	120.30
1	A	108	ARG	NE-CZ-NH1	-14.75	112.92	120.30
1	B	108	ARG	NE-CZ-NH1	14.39	127.50	120.30
1	B	108	ARG	NE-CZ-NH2	-12.75	113.93	120.30
1	A	67	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	A	72	ARG	NE-CZ-NH1	10.51	125.56	120.30
1	A	67	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	A	28	ARG	CD-NE-CZ	10.11	137.75	123.60
1	B	49	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	154	GLU	CA-CB-CG	8.40	131.89	113.40
1	B	97	GLU	OE1-CD-OE2	-8.22	113.44	123.30
1	A	42[A]	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	A	42[B]	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	A	30[A]	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	30[B]	ARG	NE-CZ-NH2	-7.72	116.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	ARG	NH1-CZ-NH2	7.55	127.70	119.40
1	B	153	LEU	CB-CA-C	7.34	124.15	110.20
1	A	56	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	B	67	ARG	CD-NE-CZ	7.12	133.56	123.60
1	A	56	ARG	CD-NE-CZ	7.09	133.52	123.60
1	A	81	TYR	CB-CG-CD1	6.94	125.16	121.00
1	A	145	MET	CG-SD-CE	6.86	111.17	100.20
1	A	79[A]	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	79[B]	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	146	ASP	CB-CG-OD1	6.68	124.31	118.30
1	B	119	ASN	CB-CA-C	6.46	123.33	110.40
1	A	102	LEU	CA-CB-CG	6.40	130.03	115.30
1	B	56	ARG	CD-NE-CZ	6.40	132.56	123.60
1	A	42[A]	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	42[B]	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	145	MET	N-CA-CB	-6.33	99.21	110.60
1	A	192	LYS	CA-CB-CG	6.30	127.27	113.40
1	A	72	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	79[A]	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	79[B]	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	B	72	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	67	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	B	56	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	B	118	TYR	CB-CG-CD2	-5.96	117.42	121.00
1	A	71	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	118	TYR	CB-CG-CD1	5.83	124.50	121.00
1	B	147	THR	CA-CB-CG2	5.73	120.42	112.40
1	B	79	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	153	LEU	CB-CG-CD1	5.67	120.63	111.00
1	A	56	ARG	NH1-CZ-NH2	-5.61	113.23	119.40
1	B	34	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	175	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	B	144	GLU	OE1-CD-OE2	5.43	129.81	123.30
1	B	75	ILE	O-C-N	5.42	131.36	122.70
1	A	81	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	A	30[A]	ARG	CD-NE-CZ	5.36	131.10	123.60
1	A	30[B]	ARG	CD-NE-CZ	5.36	131.10	123.60
1	A	33[A]	ILE	CB-CG1-CD1	5.33	128.83	113.90
1	A	33[B]	ILE	CB-CG1-CD1	5.33	128.83	113.90
1	A	184	TYR	CG-CD2-CE2	5.30	125.54	121.30
1	A	30[A]	ARG	NH1-CZ-NH2	-5.26	113.61	119.40
1	A	30[B]	ARG	NH1-CZ-NH2	-5.26	113.61	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	149	LEU	O-C-N	5.25	131.10	122.70
1	B	67	ARG	CB-CA-C	5.21	120.81	110.40
1	B	61	SER	CB-CA-C	5.20	119.99	110.10
1	B	28	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	81	TYR	CB-CG-CD1	5.14	124.08	121.00
1	B	149	LEU	CA-CB-CG	5.12	127.06	115.30
1	B	105[A]	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	B	105[B]	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	108	ARG	NH1-CZ-NH2	5.09	125.00	119.40
1	B	79	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	30	ARG	CD-NE-CZ	5.04	130.66	123.60
1	A	42[A]	ARG	CD-NE-CZ	5.04	130.65	123.60
1	A	42[B]	ARG	CD-NE-CZ	5.04	130.65	123.60
1	A	97	GLU	CG-CD-OE2	-5.01	108.29	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1590	0	1613	20	0
1	B	1591	0	1615	21	0
2	A	35	0	14	0	0
2	B	35	0	14	0	0
3	A	23	0	20	1	0
3	B	23	0	20	0	0
4	A	12	0	13	1	0
4	B	12	0	13	1	0
5	A	163	0	0	4	0
5	B	187	0	0	2	0
All	All	3671	0	3322	41	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 6.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ARG:HH11	1:B:30:ARG:HG2	1.44	0.81
1:B:124:ASN:HD22	1:B:126:LEU:H	1.31	0.78
1:B:176:ASP:H	1:B:185:ASN:HD21	1.34	0.73
1:A:176:ASP:H	1:A:185:ASN:HD21	1.42	0.66
1:B:83:ASN:ND2	1:B:94:SER:H	1.95	0.64
1:B:137:HIS:HD2	1:B:139:SER:H	1.45	0.64
1:B:176:ASP:H	1:B:185:ASN:ND2	1.95	0.63
1:A:64:GLN:HG2	1:A:65:LYS:HE3	1.81	0.61
1:B:137:HIS:CD2	1:B:139:SER:H	2.21	0.59
1:B:83:ASN:HD21	1:B:94:SER:H	1.51	0.58
1:B:69:LEU:HD22	4:B:202:MES:H82	1.85	0.58
1:A:176:ASP:H	1:A:185:ASN:ND2	2.02	0.57
1:B:151:PHE:HB2	1:B:153:LEU:HD13	1.89	0.54
1:A:41[B]:THR:HG21	5:A:446:HOH:O	2.08	0.53
1:A:69:LEU:HD22	4:A:201:MES:H82	1.91	0.52
1:A:117:ILE:HG23	1:A:121[A]:LEU:HD12	1.92	0.51
1:A:20:GLY:HA2	1:A:26:PRO:HD3	1.93	0.49
1:A:65:LYS:H	1:A:65:LYS:CD	2.26	0.48
1:A:42[A]:ARG:NH1	1:A:170:ASP:H	2.13	0.47
1:A:137:HIS:CD2	1:A:143:ILE:HD11	2.49	0.47
1:A:25:MET:HE1	1:A:27:TRP:HE1	1.79	0.47
1:A:33[A]:ILE:HD12	3:A:194:TQ5:HC9	1.98	0.45
1:B:137:HIS:O	1:B:140:PRO:HD3	2.16	0.45
1:A:29:LEU:O	1:A:33[A]:ILE:HG12	2.17	0.45
1:A:53:ILE:HD13	1:A:96:ILE:HG13	1.98	0.44
1:B:67:ARG:HA	1:B:68:PRO:C	2.39	0.43
1:B:149:LEU:HD22	1:B:151:PHE:CZ	2.53	0.43
1:A:25:MET:HE1	5:A:232:HOH:O	2.19	0.43
1:B:144:GLU:HB2	5:B:384:HOH:O	2.19	0.42
1:B:164:LEU:HG	1:B:173[A]:LEU:HD21	2.01	0.42
1:B:65[B]:LYS:HE3	1:B:66:PHE:CE2	2.54	0.42
1:A:28:ARG:HH21	1:A:28:ARG:HB3	1.85	0.42
1:A:145:MET:HE1	5:A:260[B]:HOH:O	2.19	0.42
1:B:111[B]:ILE:HD13	1:B:121:LEU:HG	2.01	0.41
1:A:25:MET:HA	1:A:26:PRO:HD3	1.83	0.41
1:B:5[B]:ASN:ND2	5:B:387:HOH:O	2.53	0.41
1:A:130:LEU:HG	1:A:156:TRP:CZ3	2.56	0.41
1:B:64:GLN:HG2	1:B:65[A]:LYS:NZ	2.36	0.41
1:B:63:PRO:HB3	1:B:65[A]:LYS:HE2	2.03	0.40
1:A:108:ARG:HD2	5:A:485:HOH:O	2.20	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	201/192 (105%)	196 (98%)	4 (2%)	1 (0%)	29 14
1	B	201/192 (105%)	198 (98%)	3 (2%)	0	100 100
All	All	402/384 (105%)	394 (98%)	7 (2%)	1 (0%)	41 32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	185/177 (104%)	177 (96%)	8 (4%)	29 12
1	B	186/177 (105%)	176 (95%)	10 (5%)	22 8
All	All	371/354 (105%)	353 (95%)	18 (5%)	29 9

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	65	LYS

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Mol	Chain	Res	Type
1	A	74	ASN
1	A	86	ILE
1	A	102	LEU
1	A	120	GLU
1	A	145	MET
1	A	154	GLU
1	B	5[A]	ASN
1	B	5[B]	ASN
1	B	28	ARG
1	B	65[A]	LYS
1	B	65[B]	LYS
1	B	74	ASN
1	B	124	ASN
1	B	153	LEU
1	B	173[A]	LEU
1	B	173[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	159	GLN
1	A	185	ASN
1	B	83	ASN
1	B	89	ASN
1	B	101	ASN
1	B	123	ASN
1	B	124	ASN
1	B	137	HIS
1	B	185	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TQ5	A	194	-	25,25,25	1.74	5 (20%)	36,37,37	2.39	11 (30%)
4	MES	B	202	-	12,12,12	7.77	7 (58%)	14,16,16	2.91	5 (35%)
4	MES	A	201	-	12,12,12	7.37	6 (50%)	14,16,16	2.73	6 (42%)
2	NDP	B	195	-	30,37,52	1.49	6 (20%)	35,57,80	1.26	3 (8%)
2	NDP	A	193	-	30,37,52	1.40	5 (16%)	35,57,80	1.37	6 (17%)
3	TQ5	B	196	-	25,25,25	1.49	3 (12%)	36,37,37	2.28	13 (36%)

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	TQ5	A	194	-	-	0/10/10/10	0/3/3/3
4	MES	B	202	-	-	2/6/14/14	0/1/1/1
4	MES	A	201	-	-	2/6/14/14	0/1/1/1
2	NDP	B	195	-	-	0/23/43/77	0/3/3/5
2	NDP	A	193	-	-	3/23/43/77	0/3/3/5
3	TQ5	B	196	-	-	0/10/10/10	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	202	MES	C8-S	-25.94	1.40	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	MES	C8-S	-24.36	1.42	1.77
3	A	194	TQ5	C24-C25	4.80	1.46	1.39
3	B	196	TQ5	C1-N6	4.32	1.44	1.37
2	B	195	NDP	O4B-C1B	-4.15	1.35	1.41
4	A	201	MES	C5-N4	4.01	1.58	1.46
3	A	194	TQ5	C1-N6	3.75	1.43	1.37
4	A	201	MES	O1-C6	3.35	1.56	1.42
4	A	201	MES	O1-C2	3.27	1.55	1.42
3	A	194	TQ5	C3-N4	-3.27	1.27	1.33
2	A	193	NDP	P2B-O2B	3.14	1.65	1.59
4	B	202	MES	C3-N4	3.08	1.55	1.46
3	B	196	TQ5	C3-N4	-2.97	1.28	1.33
4	B	202	MES	C5-N4	2.96	1.55	1.46
3	B	196	TQ5	C5-N4	-2.91	1.30	1.35
4	B	202	MES	O1-C6	2.90	1.54	1.42
4	B	202	MES	O1-C2	2.80	1.54	1.42
2	A	193	NDP	PA-O1A	-2.73	1.41	1.50
2	B	195	NDP	P2B-O2B	2.69	1.64	1.59
2	A	193	NDP	P2B-O2X	-2.59	1.44	1.54
4	B	202	MES	O2S-S	2.48	1.52	1.45
4	B	202	MES	C7-N4	2.47	1.53	1.47
4	A	201	MES	C7-N4	2.46	1.53	1.47
2	B	195	NDP	PA-O2A	-2.33	1.44	1.55
3	A	194	TQ5	C41-C32	2.31	1.61	1.53
2	B	195	NDP	C5A-C4A	-2.30	1.34	1.40
2	A	193	NDP	C2A-N1A	2.29	1.38	1.33
2	B	195	NDP	PN-O2N	-2.23	1.44	1.55
4	A	201	MES	C3-N4	2.21	1.53	1.46
2	B	195	NDP	P2B-O3X	-2.13	1.46	1.54
3	A	194	TQ5	C22-S20	2.12	1.82	1.77
2	A	193	NDP	C5A-C4A	-2.02	1.35	1.40

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	202	MES	O1S-S-C8	8.50	117.15	106.92
3	B	196	TQ5	N6-C5-N4	-6.57	118.46	127.22
3	A	194	TQ5	C24-C23-C22	6.42	128.24	120.50
4	A	201	MES	O1S-S-C8	6.31	114.51	106.92
3	A	194	TQ5	N6-C5-N4	-5.80	119.48	127.22
3	B	196	TQ5	N14-C5-N4	5.69	126.10	117.25
3	A	194	TQ5	C27-C26-C25	4.80	127.63	121.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	201	MES	O3S-S-C8	4.72	113.40	105.77
4	B	202	MES	O3S-S-C8	4.22	112.59	105.77
3	A	194	TQ5	C27-C22-C23	-4.17	111.83	118.82
4	A	201	MES	C2-C3-N4	4.04	116.22	110.10
3	A	194	TQ5	C26-C25-C24	-3.98	112.05	117.97
3	B	196	TQ5	C27-C22-C23	-3.97	112.16	118.82
3	B	196	TQ5	C26-C25-C24	-3.81	112.31	117.97
3	A	194	TQ5	C33-C32-C25	3.74	119.32	110.36
2	A	193	NDP	C4A-C5A-N7A	3.67	113.23	109.40
3	A	194	TQ5	C26-C25-C32	3.34	128.14	121.58
4	B	202	MES	O2S-S-C8	-3.00	103.30	106.92
3	B	196	TQ5	C9-C8-C1	-2.95	115.84	120.08
3	A	194	TQ5	C23-C22-S20	2.85	129.07	120.34
3	B	196	TQ5	C5-N4-C3	2.80	124.72	116.72
3	A	194	TQ5	N14-C5-N4	2.74	121.51	117.25
3	B	196	TQ5	C26-C27-C22	2.72	123.78	120.50
4	B	202	MES	O3S-S-O2S	-2.65	104.79	111.27
3	B	196	TQ5	C23-C24-C25	2.60	124.69	121.22
4	A	201	MES	O3S-S-O2S	-2.57	105.00	111.27
3	A	194	TQ5	C41-C32-C33	-2.50	100.19	108.32
3	B	196	TQ5	C8-C1-C2	2.50	124.29	119.50
2	B	195	NDP	C5A-C6A-N6A	2.49	124.14	120.35
2	B	195	NDP	C5A-C6A-N1A	-2.47	114.75	120.35
2	A	193	NDP	O2B-P2B-O1X	-2.46	99.89	109.39
2	A	193	NDP	N6A-C6A-N1A	2.46	123.68	118.57
2	A	193	NDP	O2X-P2B-O1X	2.45	120.26	110.68
4	A	201	MES	C7-N4-C3	2.38	117.31	111.23
4	A	201	MES	O2S-S-C8	-2.32	104.13	106.92
2	A	193	NDP	C5A-C6A-N1A	-2.30	115.13	120.35
2	B	195	NDP	C3B-C2B-C1B	-2.28	98.60	102.89
3	B	196	TQ5	C27-C26-C25	2.24	124.21	121.22
2	A	193	NDP	O2B-C2B-C1B	-2.23	102.09	110.10
3	B	196	TQ5	C26-C25-C32	2.22	125.93	121.58
3	B	196	TQ5	C33-C32-C25	2.13	115.46	110.36
3	A	194	TQ5	C5-N4-C3	2.10	122.72	116.72
4	B	202	MES	O2S-S-O1S	-2.09	106.72	113.95
3	B	196	TQ5	N7-C3-N4	-2.07	111.45	117.07

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	193	NDP	C5D-O5D-PN-O1N
4	B	202	MES	C8-C7-N4-C3
4	B	202	MES	C8-C7-N4-C5
2	A	193	NDP	C5D-O5D-PN-O2N
4	A	201	MES	C8-C7-N4-C3
4	A	201	MES	C8-C7-N4-C5
2	A	193	NDP	C5D-O5D-PN-O3

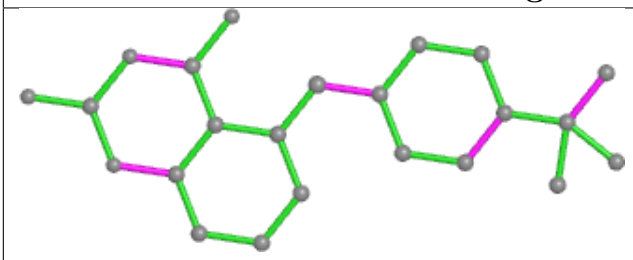
There are no ring outliers.

3 monomers are involved in 3 short contacts:

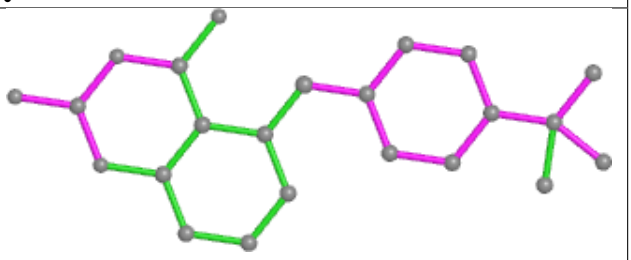
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	194	TQ5	1	0
4	B	202	MES	1	0
4	A	201	MES	1	0

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.

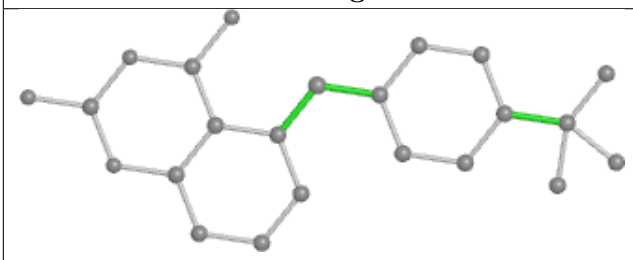
Ligand TQ5 A 194



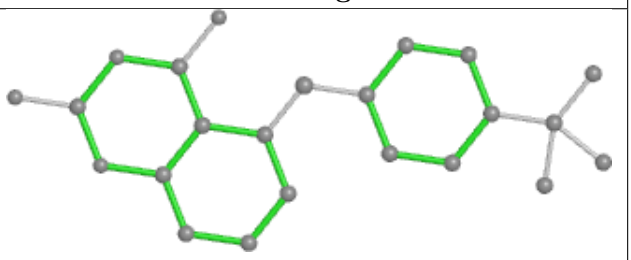
Bond lengths



Bond angles

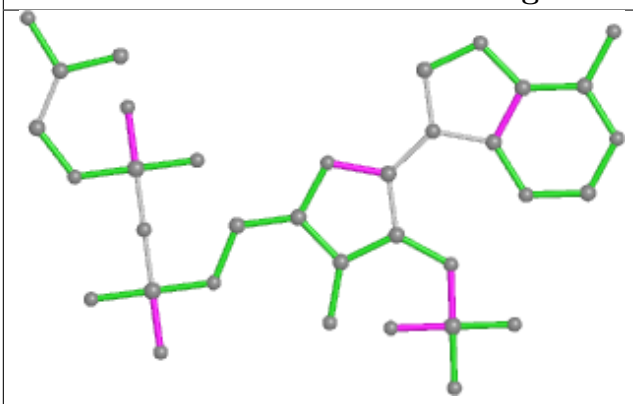


Torsions

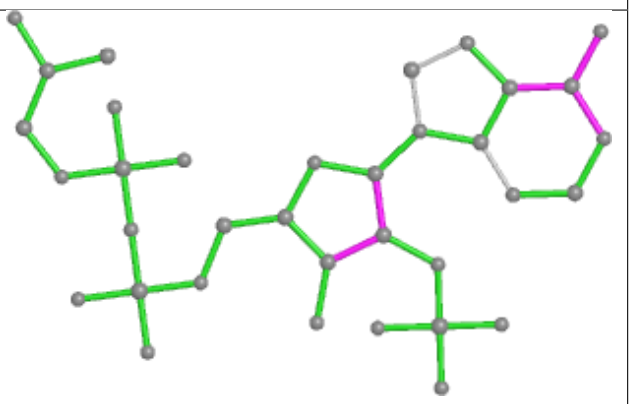


Rings

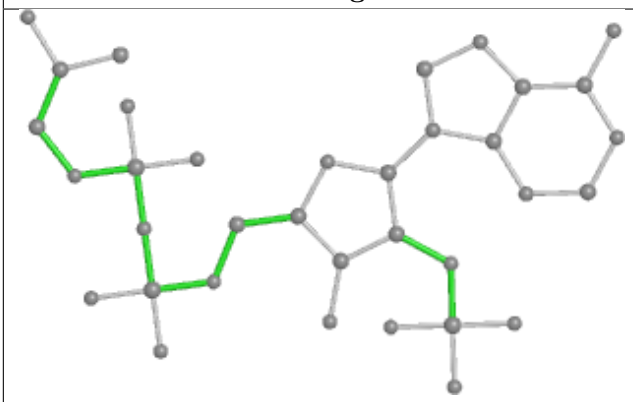
Ligand NDP B 195



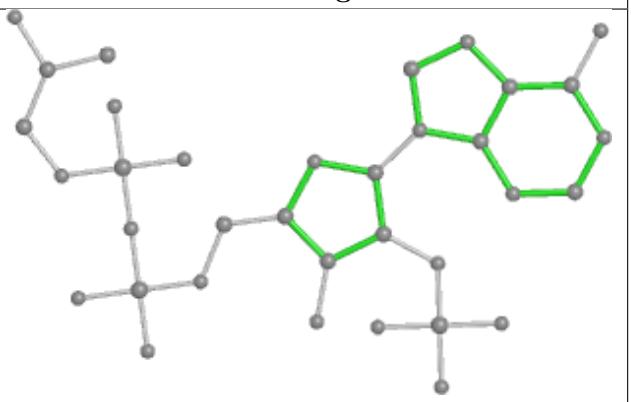
Bond lengths



Bond angles

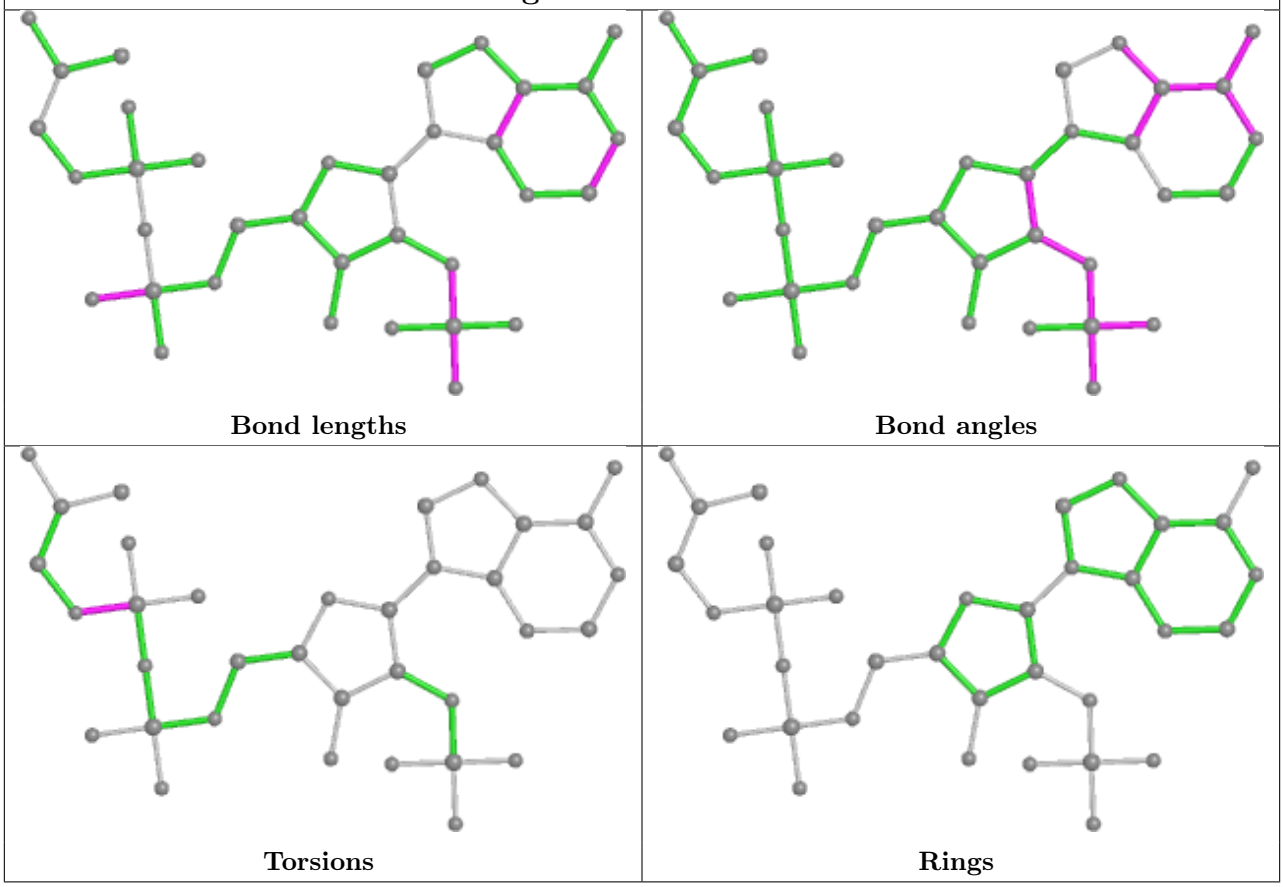


Torsions

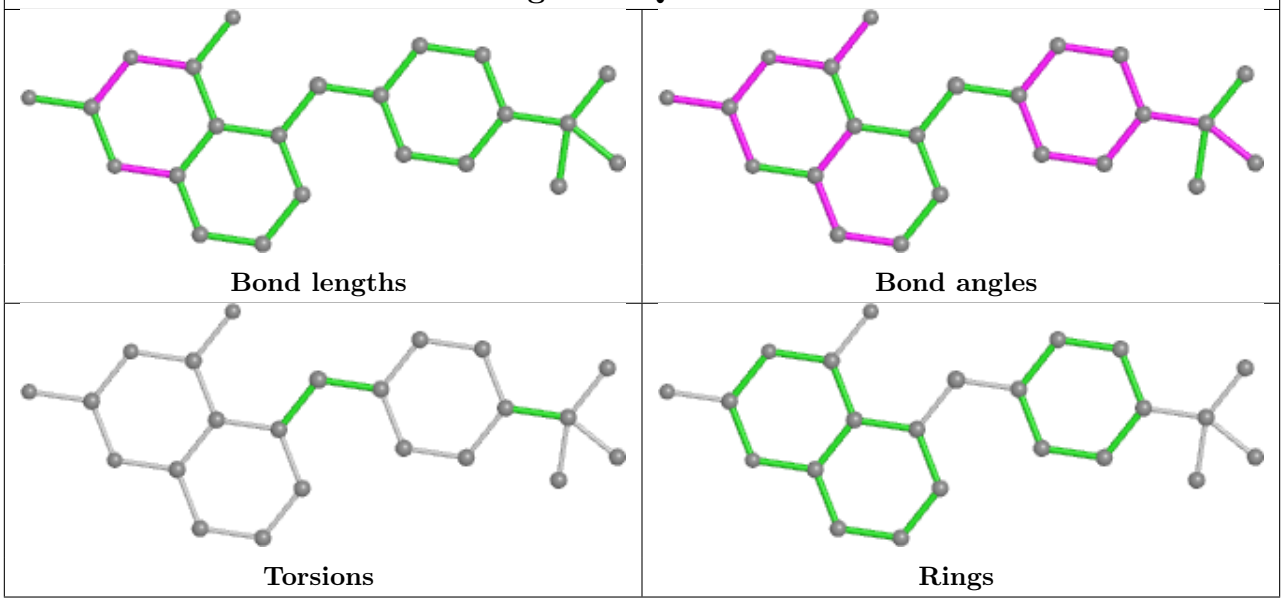


Rings

Ligand NDP A 193



Ligand TQ5 B 196



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.