



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:55 PM UTC

PDB ID : 1VJ3 / pdb_00001vj3
Title : STRUCTURAL STUDIES ON BIO-ACTIVE COMPOUNDS. CRYSTAL
STRUCTURE AND MOLECULAR MODELING STUDIES ON THE
PNEUMOCYSTIS CARINII DIHYDROFOLATE REDUCTASE COFAC-
TOR COMPLEX WITH TAB, A HIGHLY SELECTIVE ANTIFOLATE.
Authors : Cody, V.; Galitsky, N.; Rak, D.; Luft, J.R.; Queener, S.F.; Laughton, C.A.;
Malcolm, F.G.
Deposited on : 2004-01-13
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

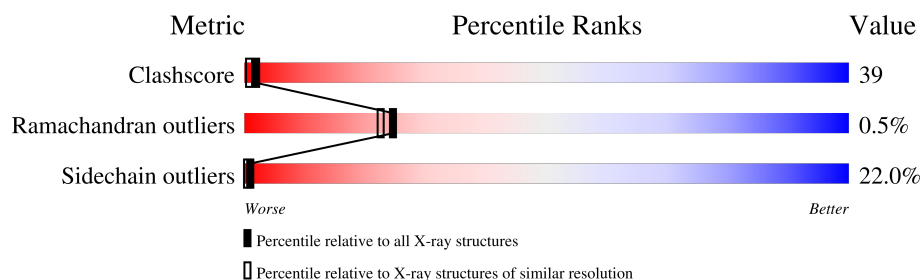
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	205	23% 45% 25% 7%

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	TAB	A	300[A]	-	-	X	-

2 Entry composition [i](#)

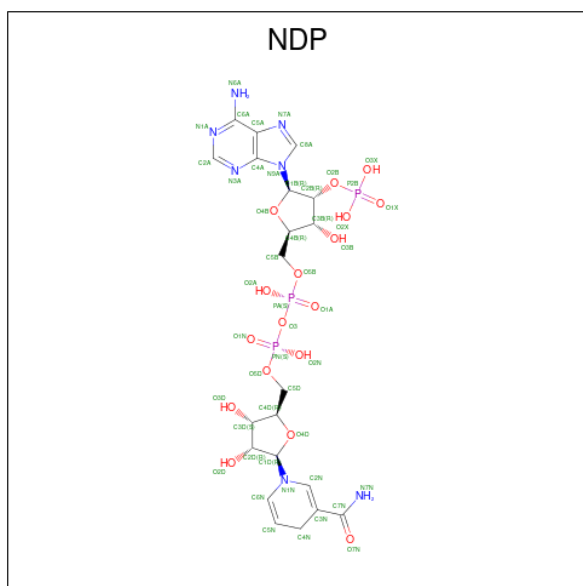
There are 4 unique types of molecules in this entry. The entry contains 1847 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

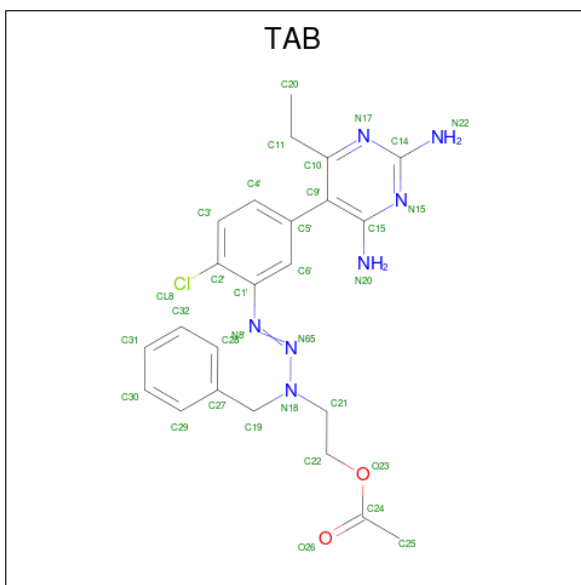
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	205	1678	1081	287	304	6	0	0	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: 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	48	21	7	17	3	0	0

- Molecule 3 is ACETIC ACID N-[2-CHLORO-5-[6-ETHYL-2,4-DIAMINO-PYRIMID-5-YL]-PHENYL]-[BENZYL-TRIAZEN-3-YL]ETHYL ESTER (CCD ID: TAB) (formula: $C_{23}H_{26}ClN_7O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	
			46	34	1	7	4	
								0
								1

- Molecule 4 is water.

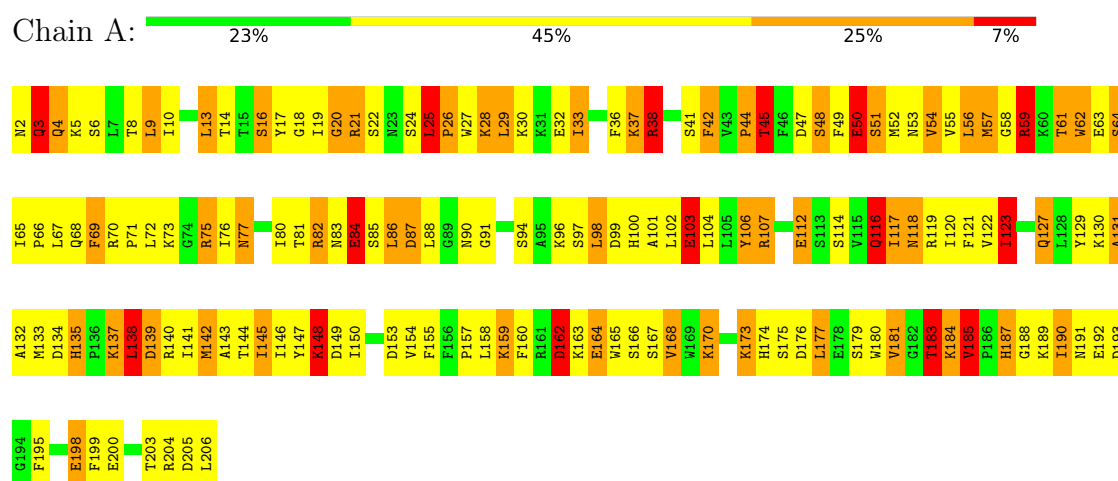
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O		
			75	75		
					0	0

3 Residue-property plots

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



4 Data and refinement statistics

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	37.48Å 43.14Å 61.29Å 90.00° 94.74° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	97.8 (8.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1847	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.33	6/1720 (0.3%)	3.08	198/2320 (8.5%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	ILE	CA-CB	7.13	1.62	1.54
1	A	19	ILE	N-CA	6.82	1.52	1.46
1	A	122	VAL	C-O	6.22	1.31	1.24
1	A	18	GLY	C-O	5.57	1.29	1.23
1	A	143	ALA	N-CA	5.50	1.52	1.45
1	A	36	PHE	N-CA	5.01	1.52	1.46

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ARG	CD-NE-CZ	39.44	179.61	124.40
1	A	176	ASP	CA-CB-CG	22.19	134.79	112.60
1	A	38	ARG	CD-NE-CZ	21.08	153.92	124.40
1	A	195	PHE	CA-CB-CG	16.21	130.01	113.80
1	A	63	GLU	CB-CG-CD	13.46	135.49	112.60
1	A	25	LEU	CB-CA-C	13.28	128.51	109.38
1	A	38	ARG	NE-CZ-NH2	13.00	130.90	119.20
1	A	38	ARG	CA-CB-CG	12.06	138.22	114.10
1	A	193	ASP	CA-CB-CG	11.65	124.25	112.60
1	A	50	GLU	CA-C-N	11.01	136.35	120.71
1	A	50	GLU	C-N-CA	11.01	136.35	120.71
1	A	103	GLU	CB-CG-CD	10.92	131.16	112.60
1	A	127	GLN	CA-C-O	-10.89	108.88	120.42
1	A	87	ASP	CA-CB-CG	10.15	122.75	112.60
1	A	132	ALA	CA-C-O	10.13	131.16	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	MET	CA-C-O	-9.80	110.73	120.92
1	A	59	ARG	CA-C-O	-9.77	109.06	120.10
1	A	138	LEU	CB-CA-C	9.74	126.27	110.29
1	A	63	GLU	CA-CB-CG	9.60	133.30	114.10
1	A	84	GLU	CB-CG-CD	9.50	128.75	112.60
1	A	130	LYS	CA-C-N	9.32	132.77	120.28
1	A	130	LYS	C-N-CA	9.32	132.77	120.28
1	A	25	LEU	N-CA-C	-9.26	96.37	109.24
1	A	3	GLN	CA-CB-CG	9.04	132.19	114.10
1	A	204	ARG	NE-CZ-NH2	9.00	127.30	119.20
1	A	83	ASN	CA-CB-CG	8.98	121.58	112.60
1	A	38	ARG	NH1-CZ-NH2	-8.96	107.65	119.30
1	A	69	PHE	N-CA-C	8.83	124.11	113.16
1	A	123	ILE	CB-CG1-CD1	8.82	132.31	113.80
1	A	135	HIS	CB-CA-C	8.77	121.23	108.87
1	A	27	TRP	CA-C-N	8.73	136.40	123.12
1	A	27	TRP	C-N-CA	8.73	136.40	123.12
1	A	149	ASP	CA-CB-CG	-8.67	103.93	112.60
1	A	62	TRP	CA-C-N	8.61	132.16	120.54
1	A	62	TRP	C-N-CA	8.61	132.16	120.54
1	A	157	PRO	N-CA-C	8.58	124.58	114.03
1	A	82	ARG	CD-NE-CZ	8.46	136.24	124.40
1	A	99	ASP	OD1-CG-OD2	8.38	143.02	122.90
1	A	106	TYR	CA-C-N	8.13	131.01	120.44
1	A	106	TYR	C-N-CA	8.13	131.01	120.44
1	A	2	ASN	CA-CB-CG	8.12	120.72	112.60
1	A	99	ASP	CA-CB-CG	-8.01	104.59	112.60
1	A	168	VAL	CB-CA-C	7.96	121.19	111.80
1	A	77	ASN	CA-CB-CG	7.94	120.54	112.60
1	A	130	LYS	O-C-N	-7.76	114.08	122.07
1	A	28	LYS	CB-CA-C	-7.71	99.78	111.73
1	A	44	PRO	CA-C-N	7.68	131.46	120.79
1	A	44	PRO	C-N-CA	7.68	131.46	120.79
1	A	13	LEU	CB-CG-CD1	7.65	133.64	110.70
1	A	185	VAL	CB-CA-C	7.63	116.81	109.33
1	A	132	ALA	CA-C-N	7.55	130.40	120.28
1	A	132	ALA	C-N-CA	7.55	130.40	120.28
1	A	107	ARG	CD-NE-CZ	-7.54	113.84	124.40
1	A	204	ARG	NH1-CZ-NH2	-7.50	109.55	119.30
1	A	107	ARG	NE-CZ-NH1	-7.48	114.02	121.50
1	A	139	ASP	O-C-N	7.47	130.37	122.23
1	A	57	MET	CA-C-N	7.47	128.15	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	MET	C-N-CA	7.47	128.15	120.60
1	A	127	GLN	OE1-CD-NE2	7.46	130.06	122.60
1	A	21	ARG	NE-CZ-NH2	-7.44	112.50	119.20
1	A	205	ASP	CA-CB-CG	7.44	120.04	112.60
1	A	61	THR	N-CA-C	-7.39	103.24	111.82
1	A	119	ARG	NE-CZ-NH2	-7.39	112.55	119.20
1	A	37	LYS	CA-CB-CG	7.36	128.81	114.10
1	A	127	GLN	O-C-N	7.35	130.53	122.15
1	A	168	VAL	CA-CB-CG2	7.33	122.86	110.40
1	A	56	LEU	O-C-N	-7.32	115.00	123.27
1	A	176	ASP	CA-C-O	-7.27	110.29	119.31
1	A	162	ASP	CA-CB-CG	7.23	119.83	112.60
1	A	123	ILE	N-CA-C	7.22	118.34	111.91
1	A	144	THR	N-CA-CB	7.22	121.89	110.55
1	A	167	SER	N-CA-C	-7.17	104.34	113.23
1	A	99	ASP	CB-CG-OD2	-7.14	101.98	118.40
1	A	69	PHE	CA-CB-CG	-7.13	106.67	113.80
1	A	64	SER	CA-C-O	-7.11	110.89	119.49
1	A	63	GLU	CA-C-N	7.10	131.96	120.60
1	A	63	GLU	C-N-CA	7.10	131.96	120.60
1	A	118	ASN	OD1-CG-ND2	-7.08	115.53	122.60
1	A	32	GLU	N-CA-C	-7.02	103.06	111.69
1	A	121	PHE	CA-C-O	-6.94	113.20	120.70
1	A	138	LEU	CA-C-O	6.92	128.52	120.49
1	A	190	ILE	CA-C-O	-6.91	112.59	120.67
1	A	99	ASP	O-C-N	6.89	130.75	122.27
1	A	73	LYS	N-CA-C	6.87	121.05	110.20
1	A	64	SER	O-C-N	6.84	131.28	122.39
1	A	176	ASP	CB-CA-C	6.76	124.12	109.99
1	A	132	ALA	N-CA-CB	-6.75	100.17	110.16
1	A	16	SER	N-CA-CB	-6.75	100.71	110.56
1	A	10	ILE	CB-CA-C	6.70	120.11	110.33
1	A	91	GLY	N-CA-C	-6.61	105.18	116.01
1	A	139	ASP	CA-CB-CG	-6.55	106.05	112.60
1	A	54	VAL	CB-CA-C	-6.55	100.86	110.62
1	A	170	LYS	CA-C-O	-6.53	113.74	121.11
1	A	59	ARG	CA-CB-CG	6.50	127.11	114.10
1	A	177	LEU	N-CA-C	-6.48	104.29	111.36
1	A	45	THR	N-CA-CB	-6.40	100.10	109.82
1	A	175	SER	CA-C-N	-6.39	109.95	121.14
1	A	175	SER	C-N-CA	-6.39	109.95	121.14
1	A	53	ASN	N-CA-CB	6.39	120.13	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ARG	CD-NE-CZ	-6.36	115.50	124.40
1	A	20	GLY	O-C-N	6.33	130.88	123.66
1	A	131	ALA	O-C-N	-6.28	115.46	122.12
1	A	192	GLU	CA-C-N	6.28	131.05	122.07
1	A	192	GLU	C-N-CA	6.28	131.05	122.07
1	A	37	LYS	CA-C-O	-6.27	114.23	120.82
1	A	200	GLU	CG-CD-OE1	6.26	132.79	118.40
1	A	63	GLU	CA-C-O	6.24	127.58	120.90
1	A	191	ASN	CA-C-O	6.24	126.98	120.30
1	A	185	VAL	O-C-N	6.15	125.57	121.69
1	A	3	GLN	CA-C-O	6.14	129.30	120.51
1	A	163	LYS	CA-C-O	-6.12	114.07	120.55
1	A	160	PHE	N-CA-C	6.10	119.82	112.38
1	A	101	ALA	CB-CA-C	6.03	120.35	110.88
1	A	26	PRO	N-CA-C	6.01	124.85	112.47
1	A	29	LEU	CA-C-N	5.99	128.31	120.28
1	A	29	LEU	C-N-CA	5.99	128.31	120.28
1	A	75	ARG	NE-CZ-NH2	-5.98	113.81	119.20
1	A	18	GLY	CA-C-N	-5.98	113.16	121.53
1	A	18	GLY	C-N-CA	-5.98	113.16	121.53
1	A	117	ILE	CA-C-O	-5.97	114.01	121.11
1	A	58	GLY	N-CA-C	-5.96	104.02	112.37
1	A	91	GLY	O-C-N	5.95	128.69	122.51
1	A	127	GLN	N-CA-CB	5.94	118.96	110.16
1	A	53	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	A	134	ASP	CA-C-O	-5.89	112.30	119.43
1	A	184	LYS	N-CA-C	-5.80	102.31	110.50
1	A	96	LYS	CA-CB-CG	5.77	125.63	114.10
1	A	100	HIS	N-CA-CB	5.75	118.66	110.16
1	A	139	ASP	CA-C-O	-5.75	112.54	119.03
1	A	112	GLU	CB-CG-CD	5.73	122.33	112.60
1	A	158	LEU	CB-CA-C	5.71	119.64	109.65
1	A	173	LYS	N-CA-CB	5.71	118.43	110.04
1	A	4	GLN	CA-C-N	5.71	133.12	122.74
1	A	4	GLN	C-N-CA	5.71	133.12	122.74
1	A	155	PHE	N-CA-CB	-5.69	101.35	111.08
1	A	51	SER	N-CA-C	5.69	118.48	110.23
1	A	114	SER	N-CA-C	-5.69	106.50	113.50
1	A	145	ILE	CA-C-O	-5.68	114.40	120.59
1	A	14	THR	CA-CB-CG2	5.68	120.15	110.50
1	A	42	PHE	CA-C-O	5.66	126.77	120.43
1	A	28	LYS	CA-C-O	-5.66	114.56	121.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	VAL	N-CA-C	5.65	116.62	108.48
1	A	183	THR	CB-CA-C	5.62	118.93	109.48
1	A	116	GLN	CB-CG-CD	5.62	122.14	112.60
1	A	94	SER	CA-CB-OG	5.61	122.32	111.10
1	A	9	LEU	CA-C-O	-5.58	114.61	120.80
1	A	63	GLU	OE1-CD-OE2	-5.55	109.58	122.90
1	A	140	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	A	167	SER	CA-C-N	-5.52	116.06	122.63
1	A	167	SER	C-N-CA	-5.52	116.06	122.63
1	A	192	GLU	CG-CD-OE2	-5.50	105.76	118.40
1	A	107	ARG	CA-CB-CG	5.48	125.07	114.10
1	A	77	ASN	CB-CG-ND2	5.47	124.61	116.40
1	A	87	ASP	CB-CG-OD1	5.47	130.98	118.40
1	A	168	VAL	CA-CB-CG1	5.47	119.69	110.40
1	A	190	ILE	O-C-N	5.46	129.08	123.18
1	A	158	LEU	O-C-N	5.46	130.02	123.36
1	A	90	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	146	ILE	CA-C-O	5.45	126.53	120.59
1	A	162	ASP	O-C-N	5.44	129.35	122.65
1	A	198	GLU	CB-CG-CD	5.41	121.79	112.60
1	A	187	HIS	CA-CB-CG	-5.39	108.41	113.80
1	A	8	THR	N-CA-CB	5.37	120.09	110.80
1	A	42	PHE	N-CA-C	5.37	117.50	108.96
1	A	132	ALA	O-C-N	-5.36	116.04	122.15
1	A	101	ALA	N-CA-CB	-5.35	102.25	110.01
1	A	142	MET	N-CA-CB	5.34	118.30	110.35
1	A	164	GLU	CB-CG-CD	5.33	121.66	112.60
1	A	203	THR	CA-CB-CG2	5.32	119.55	110.50
1	A	181	VAL	CA-CB-CG2	5.28	119.37	110.40
1	A	55	VAL	N-CA-CB	5.26	118.47	111.64
1	A	148	LYS	CA-CB-CG	5.24	124.58	114.10
1	A	26	PRO	O-C-N	-5.23	115.57	122.64
1	A	203	THR	CA-C-N	5.23	130.80	122.59
1	A	203	THR	C-N-CA	5.23	130.80	122.59
1	A	48	SER	O-C-N	5.22	129.66	122.46
1	A	64	SER	CA-CB-OG	-5.21	100.69	111.10
1	A	166	SER	N-CA-C	5.20	118.73	112.38
1	A	87	ASP	CA-C-N	-5.18	114.22	121.72
1	A	87	ASP	C-N-CA	-5.18	114.22	121.72
1	A	205	ASP	O-C-N	5.17	129.24	123.19
1	A	141	ILE	CA-CB-CG1	5.16	119.18	110.40
1	A	83	ASN	CB-CA-C	5.16	120.69	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ASN	CA-C-O	5.16	127.92	121.89
1	A	97	SER	O-C-N	5.14	128.39	123.04
1	A	141	ILE	CA-C-O	-5.13	114.83	120.48
1	A	75	ARG	CA-C-N	-5.11	115.98	122.37
1	A	75	ARG	C-N-CA	-5.11	115.98	122.37
1	A	135	HIS	CA-CB-CG	-5.09	108.70	113.80
1	A	82	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	A	51	SER	CA-C-N	5.07	130.95	122.73
1	A	51	SER	C-N-CA	5.07	130.95	122.73
1	A	58	GLY	CA-C-N	-5.07	112.98	120.28
1	A	58	GLY	C-N-CA	-5.07	112.98	120.28
1	A	148	LYS	CB-CA-C	5.06	120.48	110.42
1	A	154	VAL	CA-CB-CG2	5.06	119.00	110.40
1	A	199	PHE	CA-CB-CG	-5.05	108.75	113.80
1	A	142	MET	N-CA-C	-5.01	99.17	107.99

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	1678	0	1681	124	0
2	A	48	0	26	13	0
3	A	46	0	28	16	0
4	A	75	0	0	6	0
All	All	1847	0	1735	136	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 39.

All (136) 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:42:PHE:HB3	4:A:270:HOH:O	1.45	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:HH11	1:A:107:ARG:HG2	1.09	1.14
1:A:50:GLU:CD	1:A:116:GLN:HG3	1.82	1.05
1:A:170:LYS:HG2	4:A:222:HOH:O	1.67	0.94
1:A:107:ARG:HG2	1:A:107:ARG:NH1	1.82	0.94
1:A:98:LEU:HD12	1:A:98:LEU:H	1.30	0.92
1:A:50:GLU:HG3	1:A:116:GLN:HG2	1.54	0.89
1:A:20:GLY:HA2	1:A:26:PRO:HD3	1.56	0.87
1:A:50:GLU:HG3	1:A:116:GLN:CG	2.05	0.86
1:A:86:LEU:H	1:A:86:LEU:HD12	1.41	0.85
1:A:112:GLU:HG2	1:A:112:GLU:O	1.77	0.84
1:A:50:GLU:HG2	1:A:51:SER:N	1.96	0.81
1:A:3:GLN:HA	1:A:106:TYR:HE2	1.48	0.78
1:A:187:HIS:ND1	1:A:188:GLY:N	2.33	0.77
1:A:50:GLU:OE2	1:A:116:GLN:HG3	1.86	0.76
1:A:107:ARG:HH11	1:A:107:ARG:CG	1.79	0.74
1:A:54:VAL:HG12	1:A:56:LEU:HD12	1.68	0.73
1:A:33:ILE:HG13	3:A:300[A]:TAB:C32	2.19	0.73
1:A:50:GLU:CG	1:A:116:GLN:HG3	2.19	0.73
1:A:104:LEU:HD23	1:A:104:LEU:C	2.14	0.73
1:A:70:ARG:HA	1:A:71:PRO:C	2.14	0.72
1:A:33:ILE:HG13	3:A:300[A]:TAB:H321	1.72	0.71
3:A:300[A]:TAB:C29	3:A:300[A]:TAB:H211	2.20	0.70
1:A:54:VAL:CG1	1:A:56:LEU:HD12	2.21	0.70
1:A:80:ILE:O	2:A:207:NDP:H1B	1.92	0.70
1:A:38:ARG:NE	1:A:183:THR:HG21	2.07	0.69
1:A:135:HIS:HD2	1:A:137:LYS:H	1.38	0.69
1:A:44:PRO:O	1:A:48:SER:N	2.26	0.69
1:A:66:PRO:HG2	3:A:300[A]:TAB:H291	1.73	0.69
1:A:66:PRO:HG2	3:A:300[A]:TAB:C29	2.23	0.68
1:A:145:ILE:H	1:A:145:ILE:HD12	1.58	0.68
1:A:86:LEU:HD12	1:A:86:LEU:N	2.10	0.67
1:A:61:THR:O	1:A:65:ILE:HG13	1.95	0.67
1:A:98:LEU:HD12	4:A:236:HOH:O	1.95	0.67
1:A:37:LYS:HG3	3:A:300[B]:TAB:H311	1.77	0.66
1:A:21:ARG:HA	1:A:153:ASP:OD2	1.97	0.65
1:A:38:ARG:HD2	1:A:183:THR:HG21	1.77	0.65
1:A:107:ARG:NH1	1:A:107:ARG:CG	2.48	0.65
1:A:5:LYS:NZ	1:A:118:ASN:O	2.23	0.65
1:A:98:LEU:CD1	4:A:236:HOH:O	2.44	0.65
1:A:50:GLU:CG	1:A:116:GLN:CG	2.73	0.64
1:A:148:LYS:HG3	1:A:150:ILE:HG13	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HD12	1:A:145:ILE:N	2.13	0.63
1:A:68:GLN:HG2	1:A:69:PHE:CE1	2.33	0.63
1:A:82:ARG:HG3	2:A:207:NDP:H2A	1.81	0.63
1:A:25:LEU:HD12	1:A:25:LEU:O	2.00	0.61
1:A:56:LEU:CD1	1:A:120:ILE:CG2	2.78	0.61
1:A:147:TYR:CE2	1:A:189:LYS:HE3	2.36	0.61
1:A:148:LYS:HG3	1:A:150:ILE:CG1	2.31	0.60
1:A:38:ARG:CZ	1:A:183:THR:CG2	2.79	0.60
1:A:38:ARG:CD	1:A:183:THR:HG21	2.31	0.59
1:A:52:MET:HE3	1:A:76:ILE:CG1	2.32	0.59
1:A:162:ASP:OD2	4:A:212:HOH:O	2.17	0.59
1:A:9:LEU:HB2	1:A:138:LEU:HD21	1.85	0.59
1:A:69:PHE:CD1	3:A:300[A]:TAB:H301	2.38	0.59
1:A:66:PRO:CG	3:A:300[A]:TAB:H291	2.34	0.57
1:A:174:HIS:CE1	1:A:185:VAL:HG22	2.39	0.57
1:A:51:SER:HB3	1:A:118:ASN:HB2	1.87	0.56
1:A:52:MET:HE3	1:A:76:ILE:HG13	1.88	0.56
1:A:135:HIS:CD2	1:A:137:LYS:H	2.21	0.56
1:A:129:TYR:OH	2:A:207:NDP:H41N	2.06	0.55
1:A:66:PRO:HD3	3:A:300[A]:TAB:H192	1.88	0.55
1:A:84:GLU:OE2	1:A:84:GLU:O	2.25	0.55
1:A:38:ARG:CZ	1:A:183:THR:HG22	2.36	0.54
1:A:56:LEU:HD13	1:A:120:ILE:HG22	1.89	0.54
1:A:38:ARG:CZ	1:A:183:THR:HG21	2.38	0.54
1:A:66:PRO:CG	3:A:300[A]:TAB:C29	2.86	0.54
1:A:38:ARG:NE	1:A:183:THR:CG2	2.71	0.53
1:A:98:LEU:HD11	1:A:131:ALA:HB1	1.90	0.53
1:A:50:GLU:HG3	1:A:116:GLN:HG3	1.80	0.53
1:A:47:ASP:O	1:A:51:SER:HB2	2.09	0.53
1:A:3:GLN:HG2	1:A:137:LYS:HG3	1.91	0.51
1:A:69:PHE:CE1	3:A:300[A]:TAB:H301	2.47	0.50
1:A:164:GLU:HG3	1:A:165:TRP:CD1	2.46	0.50
1:A:68:GLN:HG2	1:A:69:PHE:CZ	2.47	0.50
1:A:82:ARG:HG3	2:A:207:NDP:C2A	2.41	0.50
1:A:174:HIS:CE1	1:A:185:VAL:CG2	2.94	0.50
3:A:300[A]:TAB:H211	3:A:300[A]:TAB:H291	1.93	0.49
1:A:57:MET:HB3	1:A:123:ILE:HD11	1.96	0.47
1:A:65:ILE:CG2	1:A:66:PRO:HD2	2.43	0.47
1:A:66:PRO:CD	3:A:300[A]:TAB:H291	2.44	0.47
1:A:98:LEU:HD12	1:A:98:LEU:N	2.10	0.47
1:A:103:GLU:O	1:A:107:ARG:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MET:HE2	1:A:180:TRP:CZ3	2.49	0.46
1:A:159:LYS:CE	1:A:162:ASP:OD2	2.64	0.46
1:A:56:LEU:HD11	1:A:120:ILE:CG2	2.44	0.46
1:A:47:ASP:C	1:A:49:PHE:H	2.19	0.46
1:A:45:THR:O	1:A:49:PHE:HD1	1.98	0.46
1:A:72:LEU:HB3	1:A:75:ARG:NH2	2.31	0.46
1:A:3:GLN:HG2	1:A:137:LYS:CG	2.46	0.45
1:A:86:LEU:N	1:A:86:LEU:CD1	2.71	0.45
1:A:159:LYS:HB3	1:A:159:LYS:HE3	1.70	0.45
1:A:70:ARG:HB2	1:A:71:PRO:HA	1.99	0.45
1:A:81:THR:O	1:A:81:THR:HG23	2.17	0.45
1:A:145:ILE:HD12	1:A:198:GLU:O	2.18	0.44
1:A:37:LYS:HG3	3:A:300[A]:TAB:H251	2.00	0.43
1:A:16:SER:O	1:A:17:TYR:HB2	2.17	0.43
1:A:56:LEU:CD1	1:A:120:ILE:HG23	2.49	0.43
1:A:159:LYS:HE3	1:A:162:ASP:OD2	2.18	0.43
1:A:66:PRO:CD	3:A:300[A]:TAB:H192	2.49	0.43
1:A:137:LYS:HB3	1:A:137:LYS:HE2	1.76	0.43
1:A:33:ILE:HD13	1:A:33:ILE:HA	1.89	0.43
1:A:25:LEU:O	1:A:25:LEU:CD1	2.67	0.43
1:A:59:ARG:O	1:A:62:TRP:HB3	2.19	0.43
1:A:3:GLN:HA	1:A:106:TYR:CE2	2.40	0.43
1:A:104:LEU:C	1:A:104:LEU:CD2	2.89	0.43
1:A:54:VAL:HG11	1:A:56:LEU:HD12	1.98	0.42
1:A:86:LEU:HD12	1:A:86:LEU:O	2.19	0.42
1:A:87:ASP:HA	4:A:265:HOH:O	2.19	0.42
1:A:54:VAL:HG11	1:A:56:LEU:CD1	2.50	0.42
1:A:3:GLN:HB3	1:A:102:LEU:HD13	2.02	0.42
1:A:65:ILE:HG23	1:A:66:PRO:HD2	2.01	0.42
1:A:56:LEU:HD13	1:A:120:ILE:CG2	2.46	0.42
1:A:38:ARG:O	1:A:42:PHE:HB2	2.20	0.41
1:A:47:ASP:C	1:A:49:PHE:N	2.76	0.41
1:A:139:ASP:HB3	1:A:206:LEU:HD11	2.03	0.41
1:A:129:TYR:O	1:A:133:MET:HG2	2.20	0.41
1:A:187:HIS:ND1	1:A:187:HIS:C	2.78	0.41
1:A:188:GLY:O	1:A:190:ILE:HD12	2.21	0.41
3:A:300[A]:TAB:C29	3:A:300[A]:TAB:C21	2.93	0.41
1:A:59:ARG:O	1:A:62:TRP:N	2.53	0.40
1:A:187:HIS:CG	1:A:188:GLY:N	2.90	0.40
1:A:21:ARG:HH21	1:A:21:ARG:HD3	1.50	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	203/205 (99%)	190 (94%)	12 (6%)	1 (0%)	24	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLN

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	186/186 (100%)	145 (78%)	41 (22%)	1	0

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	4	GLN
1	A	6	SER
1	A	13	LEU
1	A	22	SER
1	A	24	SER
1	A	25	LEU
1	A	28	LYS
1	A	29	LEU
1	A	30	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	33	ILE
1	A	38	ARG
1	A	41	SER
1	A	45	THR
1	A	50	GLU
1	A	59	ARG
1	A	67	LEU
1	A	77	ASN
1	A	84	GLU
1	A	85	SER
1	A	86	LEU
1	A	88	LEU
1	A	98	LEU
1	A	103	GLU
1	A	116	GLN
1	A	117	ILE
1	A	123	ILE
1	A	127	GLN
1	A	137	LYS
1	A	138	LEU
1	A	148	LYS
1	A	159	LYS
1	A	162	ASP
1	A	168	VAL
1	A	173	LYS
1	A	177	LEU
1	A	179	SER
1	A	181	VAL
1	A	183	THR
1	A	184	LYS
1	A	185	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	116	GLN
1	A	135	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	TAB	A	300[A]	-	35,35,35	2.02	5 (14%)	43,47,47	3.63	17 (39%)
2	NDP	A	207	-	51,52,52	2.58	18 (35%)	71,80,80	2.13	19 (26%)
3	TAB	A	300[B]	-	35,35,35	1.96	5 (14%)	43,47,47	3.53	15 (34%)

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	TAB	A	300[A]	-	-	1/21/21/21	0/3/3/3
2	NDP	A	207	-	-	3/34/77/77	0/5/5/5
3	TAB	A	300[B]	-	-	8/21/21/21	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	207	NDP	O4B-C4B	-9.70	1.23	1.45
2	A	207	NDP	P2B-O2B	7.26	1.72	1.59
3	A	300[A]	TAB	C9'-C5'	-5.95	1.39	1.50
3	A	300[B]	TAB	C9'-C5'	-5.95	1.39	1.50
2	A	207	NDP	C5A-C6A	5.66	1.56	1.41
3	A	300[A]	TAB	C21-N18	-5.07	1.41	1.46
3	A	300[A]	TAB	C1'-N8'	-4.66	1.32	1.42
3	A	300[B]	TAB	C1'-N8'	-4.66	1.32	1.42
2	A	207	NDP	C5A-C4A	-4.42	1.31	1.39
3	A	300[A]	TAB	N8'-N65	4.41	1.35	1.27
3	A	300[B]	TAB	N8'-N65	4.41	1.35	1.27
2	A	207	NDP	C3B-C4B	4.40	1.64	1.53
3	A	300[B]	TAB	C21-N18	-4.01	1.42	1.46
2	A	207	NDP	C6A-N1A	-2.91	1.27	1.35
2	A	207	NDP	C5A-N7A	2.88	1.44	1.39
2	A	207	NDP	C4A-N9A	-2.86	1.31	1.37
3	A	300[A]	TAB	N18-N65	2.82	1.44	1.34
3	A	300[B]	TAB	N18-N65	2.82	1.44	1.34
2	A	207	NDP	PN-O1N	-2.77	1.41	1.50
2	A	207	NDP	C1D-N1N	2.61	1.53	1.46
2	A	207	NDP	C4N-C3N	2.58	1.54	1.50
2	A	207	NDP	O3B-C3B	2.51	1.49	1.43
2	A	207	NDP	O4D-C1D	2.46	1.47	1.42
2	A	207	NDP	O4D-C4D	2.27	1.50	1.45
2	A	207	NDP	O2D-C2D	-2.26	1.37	1.43
2	A	207	NDP	PA-O2A	-2.19	1.45	1.55
2	A	207	NDP	C2A-N3A	-2.16	1.30	1.33
2	A	207	NDP	PN-O3	2.15	1.61	1.59

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300[A]	TAB	C9'-C15-N15	-10.38	116.53	122.55
3	A	300[B]	TAB	C9'-C15-N15	-10.38	116.53	122.55
3	A	300[A]	TAB	C1'-N8'-N65	9.33	123.89	112.17
3	A	300[B]	TAB	C1'-N8'-N65	9.33	123.89	112.17
3	A	300[A]	TAB	C3'-C2'-C1'	-8.51	114.16	121.48
3	A	300[B]	TAB	C3'-C2'-C1'	-8.51	114.16	121.48
2	A	207	NDP	O3B-C3B-C4B	-7.32	90.05	111.08
3	A	300[A]	TAB	C14-N15-C15	7.27	126.01	117.28
3	A	300[B]	TAB	C14-N15-C15	7.27	126.01	117.28
3	A	300[A]	TAB	C6'-C1'-C2'	5.74	124.05	117.99
3	A	300[B]	TAB	C6'-C1'-C2'	5.74	124.05	117.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300[A]	TAB	N20-C15-N15	5.40	124.31	117.03
3	A	300[B]	TAB	N20-C15-N15	5.40	124.31	117.03
2	A	207	NDP	C3N-C2N-N1N	-5.34	115.36	123.20
3	A	300[A]	TAB	N22-C14-N15	4.91	124.58	117.22
3	A	300[B]	TAB	N22-C14-N15	4.91	124.58	117.22
2	A	207	NDP	P2B-O2B-C2B	4.72	136.05	123.43
2	A	207	NDP	C6N-N1N-C2N	4.34	123.96	119.32
2	A	207	NDP	O3X-P2B-O1X	4.28	127.52	110.83
3	A	300[A]	TAB	O26-C24-C25	-4.25	109.73	124.77
3	A	300[B]	TAB	O26-C24-C25	-4.23	109.78	124.77
3	A	300[A]	TAB	C19-C27-C28	4.15	128.39	120.75
3	A	300[A]	TAB	C5'-C9'-C10	-4.13	118.32	123.30
3	A	300[B]	TAB	C5'-C9'-C10	-4.13	118.32	123.30
3	A	300[A]	TAB	N15-C14-N17	-3.93	119.46	125.48
3	A	300[B]	TAB	N15-C14-N17	-3.93	119.46	125.48
2	A	207	NDP	C1D-N1N-C6N	-3.80	112.74	120.77
3	A	300[A]	TAB	C19-C27-C29	-3.68	113.97	120.75
2	A	207	NDP	C3N-C7N-N7N	-3.67	111.16	117.67
2	A	207	NDP	C5B-C4B-C3B	-3.60	102.24	115.21
3	A	300[A]	TAB	C1'-C2'-CL8	3.48	123.61	119.70
3	A	300[B]	TAB	C1'-C2'-CL8	3.48	123.61	119.70
2	A	207	NDP	C2B-C3B-C4B	-3.15	95.21	101.99
2	A	207	NDP	N6A-C6A-N1A	3.14	125.37	118.38
2	A	207	NDP	C3B-C2B-C1B	-3.06	96.94	102.81
3	A	300[A]	TAB	C5'-C9'-C15	2.84	123.98	120.33
3	A	300[B]	TAB	C5'-C9'-C15	2.84	123.98	120.33
2	A	207	NDP	O7N-C7N-N7N	2.84	129.26	122.89
2	A	207	NDP	O2A-PA-O3	2.77	114.77	107.27
2	A	207	NDP	C5A-N7A-C8A	-2.34	99.77	103.45
2	A	207	NDP	O5D-PN-O1N	2.24	117.80	108.94
2	A	207	NDP	C4B-O4B-C1B	2.24	114.40	109.47
2	A	207	NDP	N3A-C2A-N1A	2.18	131.88	128.58
2	A	207	NDP	C4A-N9A-C8A	2.18	108.02	105.74
2	A	207	NDP	PN-O5D-C5D	2.13	133.56	121.35
3	A	300[A]	TAB	C20-C11-C10	-2.11	108.91	114.59
3	A	300[B]	TAB	C20-C11-C10	-2.11	108.91	114.59
3	A	300[A]	TAB	C30-C29-C27	2.08	123.54	120.61
3	A	300[A]	TAB	C15-C9'-C10	2.05	117.45	115.97
3	A	300[B]	TAB	C15-C9'-C10	2.05	117.45	115.97
3	A	300[B]	TAB	C30-C29-C27	2.05	123.50	120.61

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	300[A]	TAB	N18-N65-N8'-C1'
3	A	300[B]	TAB	N18-N65-N8'-C1'
3	A	300[B]	TAB	C22-C21-N18-C19
3	A	300[B]	TAB	C19-N18-N65-N8'
3	A	300[B]	TAB	C21-N18-N65-N8'
3	A	300[B]	TAB	N18-C21-C22-O23
3	A	300[B]	TAB	C25-C24-O23-C22
3	A	300[B]	TAB	O26-C24-O23-C22
2	A	207	NDP	C3B-C4B-C5B-O5B
2	A	207	NDP	O4D-C1D-N1N-C2N
3	A	300[B]	TAB	C27-C19-N18-C21
2	A	207	NDP	C2N-C3N-C7N-N7N

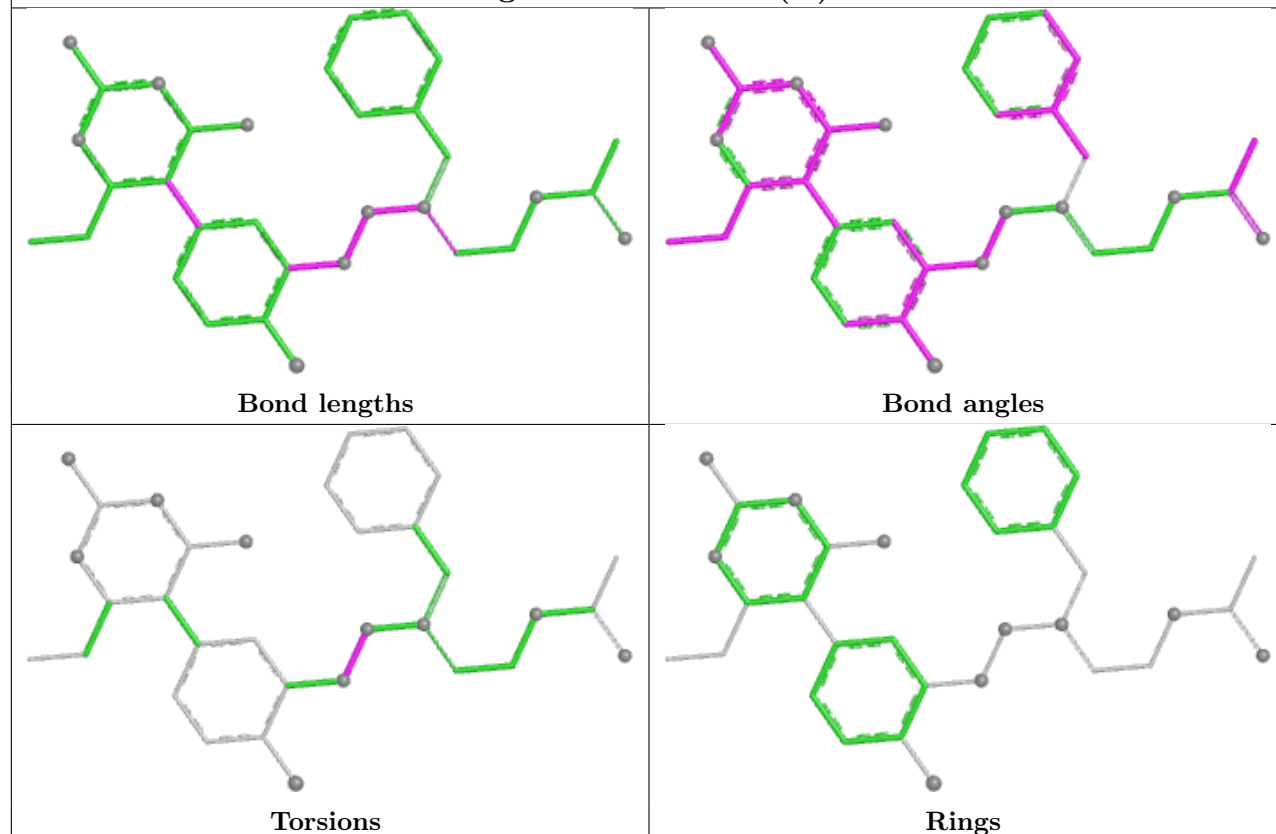
There are no ring outliers.

3 monomers are involved in 29 short contacts:

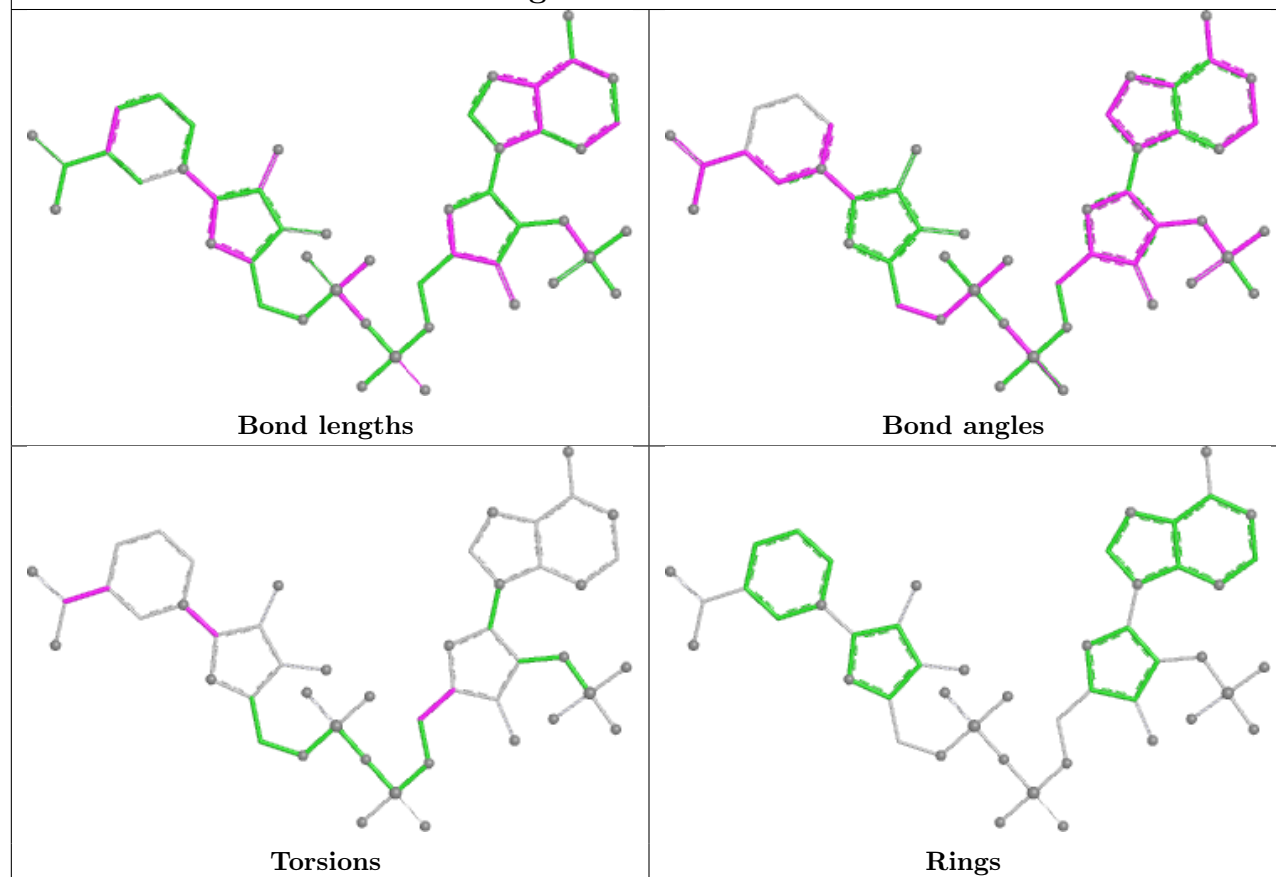
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	300[A]	TAB	15	0
2	A	207	NDP	13	0
3	A	300[B]	TAB	1	0

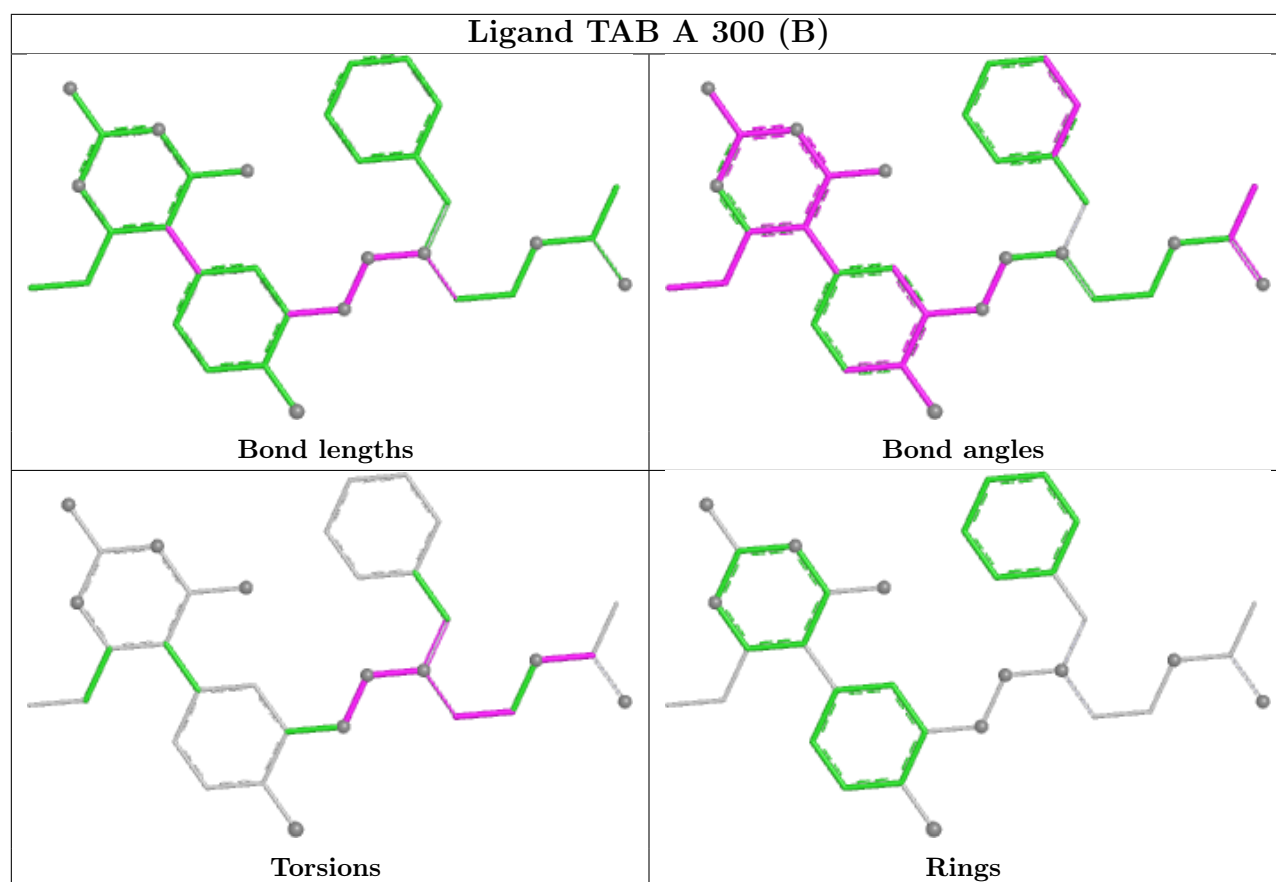
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 TAB A 300 (A)



Ligand NDP A 207





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.