Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 12:53 AM EST

PDB ID	:	1TKA
Title	:	SPECIFICITY OF COENZYME BINDING IN THIAMIN DIPHOSPHATE DEPENDENT ENZYMES: CRYSTAL STRUCTURES OF YEAST TRANSKETOLASE IN COMPLEX WITH ANALOGS OF THIAMIN DIPHOSPHATE
Authors	:	Schneider, G.; Koenig, S.
Deposited on	:	1994-02-07
Resolution	:	2.70 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:

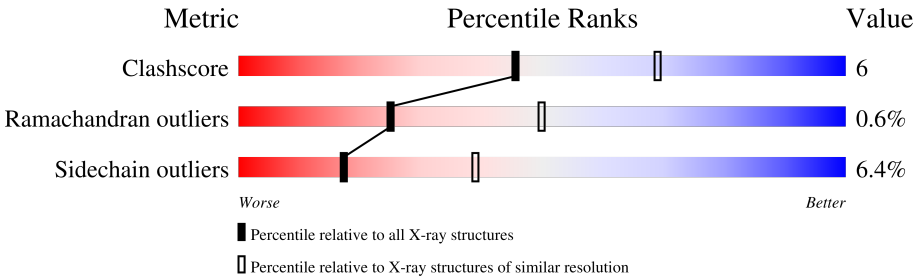
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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	678	76% 20% .
1	B	678	76% 20% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10450 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.

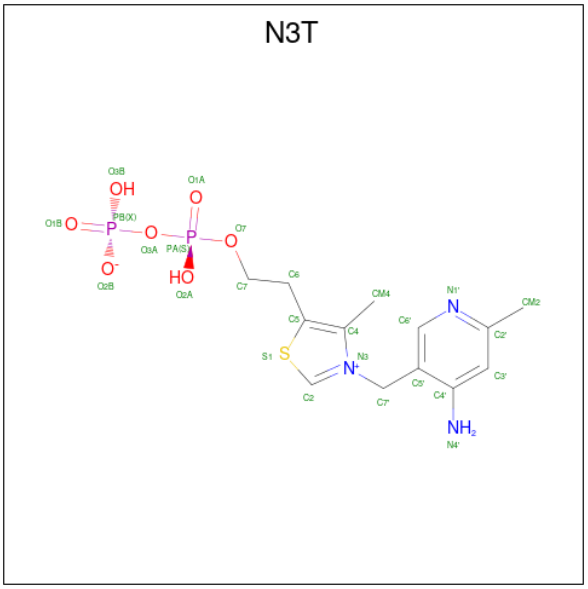
- Molecule 1 is a protein called TRANSKETOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	678	Total	C	N	O	S	0	0	0
			5198	3312	884	990	12			
1	B	678	Total	C	N	O	S	0	0	0
			5198	3312	884	990	12			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 3'-DEAZO-THIAMIN DIPHOSPHATE (three-letter code: N3T) (formula: $C_{13}H_{19}N_3O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		

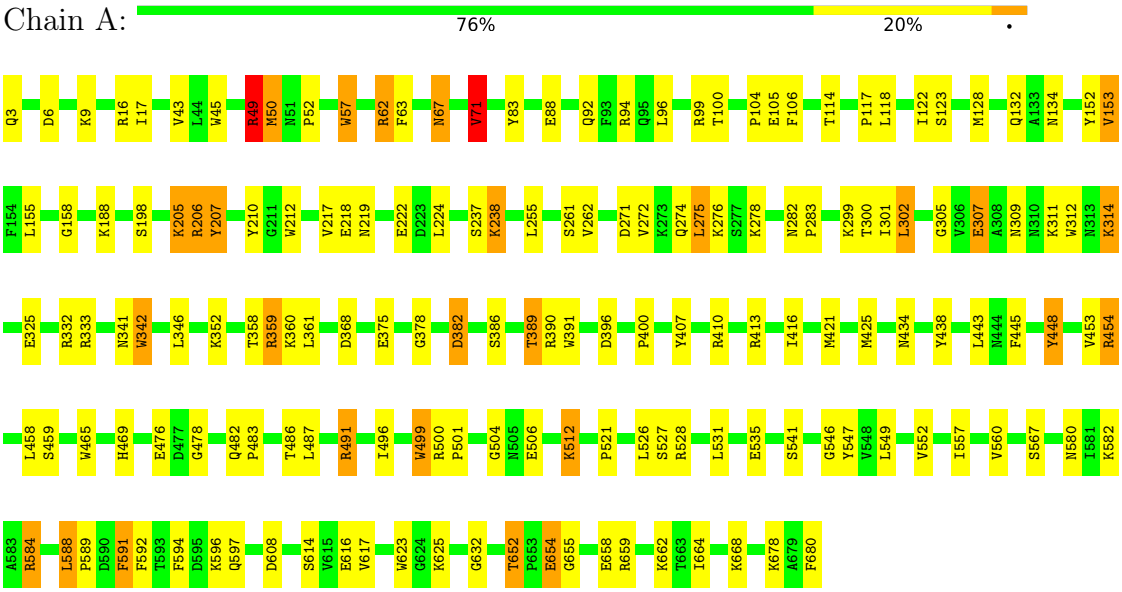
3 Residue-property plots (i)

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.

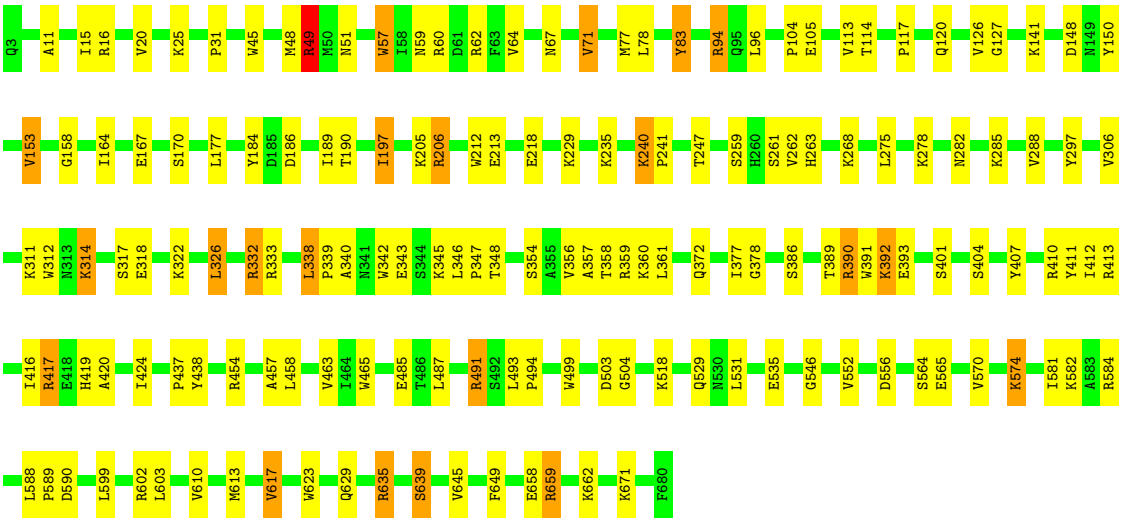
• Molecule 1: TRANSKETOLASE

Chain A:



• Molecule 1: TRANSKETOLASE

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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.30Å 113.30Å 160.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.158 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10450	wwPDB-VP
Average B, all atoms (Å^2)	10.0	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: CA, N3T

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	0.85	1/5324 (0.0%)	1.60	74/7230 (1.0%)
1	B	0.86	0/5324	1.57	69/7230 (1.0%)
All	All	0.85	1/10648 (0.0%)	1.58	143/14460 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	GLU	CD-OE2	7.96	1.34	1.25

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	417	ARG	NE-CZ-NH1	12.69	126.65	120.30
1	B	49	ARG	NE-CZ-NH2	-12.13	114.23	120.30
1	A	94	ARG	NE-CZ-NH1	11.67	126.14	120.30
1	A	333	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	A	49	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	B	602	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	A	448	TYR	CB-CG-CD2	-9.72	115.17	121.00
1	A	465	TRP	CD1-CG-CD2	9.71	114.07	106.30
1	A	623	TRP	CD1-CG-CD2	9.53	113.93	106.30
1	B	407	TYR	CB-CG-CD2	-9.41	115.36	121.00
1	B	465	TRP	CD1-CG-CD2	9.38	113.80	106.30
1	A	491	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	A	94	ARG	NE-CZ-NH2	-9.09	115.76	120.30
1	B	645	VAL	CG1-CB-CG2	-8.94	96.60	110.90
1	B	491	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	A	83	TYR	CB-CG-CD2	-8.71	115.77	121.00
1	B	342	TRP	CD1-CG-CD2	8.46	113.07	106.30
1	A	312	TRP	CD1-CG-CD2	8.42	113.03	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	206	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	184	TYR	CB-CG-CD2	-8.23	116.06	121.00
1	A	359	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	659	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	465	TRP	CG-CD2-CE3	8.18	141.26	133.90
1	A	465	TRP	CE2-CD2-CG	-8.06	100.85	107.30
1	B	410	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	62	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	A	500	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	A	659	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	499	TRP	CD1-CG-CD2	7.91	112.63	106.30
1	A	391	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	B	20	VAL	CG1-CB-CG2	-7.85	98.34	110.90
1	A	57	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	B	465	TRP	CE2-CD2-CG	-7.71	101.14	107.30
1	B	499	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A	623	TRP	CE2-CD2-CG	-7.63	101.19	107.30
1	A	389	THR	N-CA-CB	-7.49	96.07	110.30
1	B	57	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	A	57	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	B	206	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	312	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	A	391	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	B	45	TRP	CD1-CG-CD2	7.28	112.12	106.30
1	A	499	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	B	342	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	A	71	VAL	CB-CA-C	-7.16	97.80	111.40
1	B	391	TRP	CE2-CD2-CG	-7.16	101.58	107.30
1	A	342	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	A	342	TRP	CD1-CG-CD2	7.10	111.98	106.30
1	A	454	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	57	TRP	CE2-CD2-CG	-7.03	101.67	107.30
1	A	45	TRP	CE2-CD2-CG	-7.02	101.69	107.30
1	A	212	TRP	CD1-CG-CD2	6.98	111.88	106.30
1	A	623	TRP	CG-CD1-NE1	-6.89	103.21	110.10
1	B	16	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	B	94	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	391	TRP	CD1-CG-CD2	6.79	111.74	106.30
1	B	312	TRP	CE2-CD2-CG	-6.77	101.88	107.30
1	A	45	TRP	CD1-CG-CD2	6.76	111.71	106.30
1	A	332	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	A	413	ARG	NE-CZ-NH2	-6.67	116.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	212	TRP	CE2-CD2-CG	-6.58	102.04	107.30
1	B	499	TRP	CE2-CD2-CG	-6.56	102.05	107.30
1	B	454	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	465	TRP	CG-CD1-NE1	-6.53	103.57	110.10
1	B	45	TRP	CE2-CD2-CG	-6.52	102.08	107.30
1	A	49	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	B	83	TYR	CB-CG-CD1	-6.48	117.11	121.00
1	B	407	TYR	CB-CG-CD1	6.48	124.89	121.00
1	B	623	TRP	CE2-CD2-CG	-6.48	102.12	107.30
1	A	307	GLU	CA-CB-CG	6.45	127.59	113.40
1	B	333	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	B	465	TRP	CG-CD1-NE1	-6.41	103.69	110.10
1	A	465	TRP	CB-CG-CD1	-6.40	118.68	127.00
1	B	212	TRP	CE2-CD2-CG	-6.35	102.22	107.30
1	B	413	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	49	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	B	410	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	212	TRP	CD1-CG-CD2	6.29	111.33	106.30
1	A	454	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	312	TRP	CD1-CG-CD2	6.26	111.31	106.30
1	B	623	TRP	CD1-CG-CD2	6.18	111.25	106.30
1	B	584	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	659	ARG	CA-CB-CG	-6.17	99.84	113.40
1	A	584	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	332	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	94	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	417	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	105	GLU	CA-CB-CG	5.95	126.50	113.40
1	B	465	TRP	CG-CD2-CE3	5.95	139.25	133.90
1	A	207	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	B	390	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	B	48	MET	CG-SD-CE	-5.85	90.84	100.20
1	A	99	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	299	LYS	CA-CB-CG	5.84	126.24	113.40
1	B	413	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	654	GLU	CA-CB-CG	5.74	126.03	113.40
1	B	340	ALA	CA-C-N	-5.73	104.60	117.20
1	A	382	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	453	VAL	CG1-CB-CG2	-5.68	101.81	110.90
1	B	197	ILE	CA-CB-CG1	-5.66	100.25	111.00
1	A	57	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	B	235	LYS	CA-CB-CG	-5.63	101.01	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	312	TRP	CB-CG-CD1	-5.63	119.68	127.00
1	A	94	ARG	CA-CB-CG	-5.63	101.02	113.40
1	B	610	VAL	CG1-CB-CG2	-5.63	101.90	110.90
1	A	128	MET	CA-CB-CG	5.62	122.86	113.30
1	A	391	TRP	CB-CG-CD1	-5.53	119.82	127.00
1	B	659	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	391	TRP	CG-CD2-CE3	5.50	138.84	133.90
1	A	499	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	B	491	ARG	CB-CG-CD	5.49	125.87	111.60
1	B	150	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	B	342	TRP	CG-CD1-NE1	-5.44	104.66	110.10
1	A	312	TRP	CG-CD1-NE1	-5.43	104.67	110.10
1	A	255	LEU	CA-CB-CG	5.42	127.77	115.30
1	B	25	LYS	CA-CB-CG	5.40	125.29	113.40
1	B	391	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	B	503	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	16	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	391	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	A	123	SER	N-CA-CB	-5.30	102.54	110.50
1	B	333	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	342	TRP	CG-CD1-NE1	-5.28	104.82	110.10
1	B	126	VAL	CA-CB-CG2	-5.27	102.99	110.90
1	B	332	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	297	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	B	49	ARG	CB-CG-CD	-5.22	98.04	111.60
1	A	535	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	A	391	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	B	62	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	531	LEU	CA-CB-CG	5.14	127.13	115.30
1	B	312	TRP	CG-CD2-CE3	5.13	138.52	133.90
1	A	333	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	590	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	189	ILE	CA-C-N	-5.09	106.00	117.20
1	B	499	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	A	238	LYS	CA-CB-CG	5.08	124.57	113.40
1	A	499	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	A	591	PHE	CB-CG-CD2	-5.07	117.25	120.80
1	A	368	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	217	VAL	N-CA-C	-5.06	97.34	111.00
1	A	410	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	608	ASP	CA-C-N	-5.04	106.11	117.20

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	5198	0	5139	76	0
1	B	5198	0	5139	68	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	17	1	0
3	B	26	0	17	4	0
All	All	10450	0	10312	133	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 (133) 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:106:PHE:H	1:A:114:THR:HG22	1.36	0.90
1:A:652:THR:HG22	1:A:655:GLY:H	1.49	0.78
1:A:117:PRO:HA	3:A:681:N3T:H3'	1.66	0.77
1:A:118:LEU:HD12	1:B:416:ILE:HG21	1.67	0.76
1:B:105:GLU:HA	1:B:114:THR:HG23	1.72	0.72
1:A:342:TRP:HH2	1:A:512:LYS:HA	1.57	0.69
1:A:71:VAL:HG13	1:A:104:PRO:HD3	1.77	0.67
1:B:49:ARG:HH22	1:B:59:ASN:ND2	1.93	0.66
1:B:487:LEU:O	1:B:491:ARG:HG3	1.96	0.64
1:A:652:THR:HG22	1:A:655:GLY:N	2.12	0.64
1:B:635:ARG:HD2	1:B:649:PHE:HE1	1.63	0.64
1:B:117:PRO:HA	3:B:681:N3T:H3'	1.81	0.63
1:A:206:ARG:HG3	1:B:206:ARG:HG3	1.80	0.61
1:A:361:LEU:HD13	1:A:504:GLY:HA2	1.82	0.61
1:A:375:GLU:HG3	1:A:434:ASN:O	2.00	0.61
1:A:67:ASN:H	1:A:67:ASN:HD22	1.49	0.61
1:A:311:LYS:O	1:A:314:LYS:HG3	2.02	0.59
1:A:67:ASN:H	1:A:67:ASN:ND2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:THR:HG22	1:A:526:LEU:HD23	1.85	0.58
1:B:358:THR:HA	1:B:361:LEU:HD12	1.86	0.58
1:B:377:ILE:HD11	1:B:412:ILE:HD11	1.86	0.57
1:B:658:GLU:O	1:B:662:LYS:HG2	2.04	0.57
1:A:680:PHE:CG	1:B:659:ARG:HG2	2.41	0.56
1:A:478:GLY:O	1:A:482:GLN:HG3	2.05	0.56
1:A:358:THR:HB	1:A:527:SER:H	1.71	0.56
1:A:358:THR:HG21	1:A:501:PRO:HG2	1.89	0.55
1:B:259:SER:O	1:B:262:VAL:HG22	2.07	0.55
1:A:592:PHE:CE2	1:A:596:LYS:HD2	2.42	0.55
1:A:219:ASN:HD21	1:A:222:GLU:HB2	1.72	0.55
1:B:57:TRP:O	1:B:60:ARG:HD3	2.08	0.54
1:B:11:ALA:O	1:B:15:ILE:HG13	2.08	0.54
1:B:51:ASN:ND2	1:B:306:VAL:HG22	2.22	0.54
1:B:613:MET:HA	1:B:629:GLN:O	2.08	0.53
1:B:71:VAL:HB	1:B:104:PRO:HD3	1.90	0.53
1:A:421:MET:O	1:A:425:MET:HG3	2.09	0.52
1:B:117:PRO:HB2	1:B:120:GLN:HG3	1.90	0.52
1:B:570:VAL:O	1:B:574:LYS:HD2	2.09	0.52
1:A:158:GLY:HA2	1:B:416:ILE:HD13	1.91	0.52
1:B:392:LYS:HA	1:B:392:LYS:NZ	2.25	0.52
1:B:378:GLY:HA3	1:B:438:TYR:CZ	2.45	0.51
1:A:106:PHE:N	1:A:114:THR:HG22	2.16	0.51
1:A:359:ARG:HD2	1:A:386:SER:O	2.11	0.50
1:B:49:ARG:NH2	1:B:59:ASN:ND2	2.59	0.50
1:A:52:PRO:HD2	1:A:302:LEU:HD13	1.93	0.50
1:B:282:ASN:ND2	1:B:285:LYS:HD3	2.26	0.50
1:A:300:THR:HG22	1:A:301:ILE:HG13	1.93	0.50
1:A:382:ASP:OD2	3:B:681:N3T:H62	2.12	0.50
1:B:314:LYS:O	1:B:318:GLU:HG2	2.11	0.50
1:A:50:MET:O	1:A:305:GLY:HA3	2.12	0.50
1:A:114:THR:HG23	1:A:459:SER:OG	2.11	0.50
1:B:556:ASP:HB2	1:B:581:ILE:HG23	1.93	0.50
1:A:96:LEU:HA	1:B:639:SER:O	2.12	0.49
1:A:476:GLU:HB3	1:B:94:ARG:HD3	1.94	0.49
1:B:357:ALA:HA	1:B:529:GLN:O	2.13	0.49
1:B:186:ASP:HB3	1:B:247:THR:HA	1.93	0.49
1:B:599:LEU:HG	1:B:603:LEU:HD12	1.94	0.48
1:B:15:ILE:HD13	1:B:77:MET:SD	2.53	0.48
1:A:271:ASP:O	1:A:274:GLN:HG3	2.13	0.48
1:A:541:SER:HB3	1:A:547:TYR:CG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:LEU:HD13	1:B:504:GLY:HA2	1.95	0.48
1:A:552:VAL:HG21	1:A:582:LYS:HB3	1.95	0.48
1:A:483:PRO:HB3	1:A:486:THR:OG1	2.13	0.48
1:A:358:THR:HG22	1:A:526:LEU:CD2	2.43	0.48
1:B:437:PRO:HG2	1:B:463:VAL:HG12	1.95	0.48
1:A:546:GLY:HA2	1:A:588:LEU:HA	1.97	0.47
1:B:164:ILE:HD12	1:B:419:HIS:CD2	2.49	0.47
1:A:62:ARG:HH11	1:A:62:ARG:HG3	1.80	0.47
1:A:496:ILE:HG13	1:A:521:PRO:HG2	1.96	0.47
1:A:198:SER:HB2	1:B:417:ARG:HH21	1.79	0.46
1:A:49:ARG:HD3	1:A:57:TRP:CH2	2.50	0.46
1:A:378:GLY:HA3	1:A:438:TYR:CE1	2.50	0.46
1:A:487:LEU:O	1:A:491:ARG:HG3	2.16	0.46
1:A:352:LYS:HE2	1:A:352:LYS:HB2	1.78	0.45
1:B:356:VAL:HG12	1:B:360:LYS:HB3	1.99	0.45
1:A:658:GLU:O	1:A:662:LYS:HG2	2.17	0.45
1:A:560:VAL:O	1:A:614:SER:HA	2.17	0.45
1:B:275:LEU:O	1:B:278:LYS:HB3	2.17	0.45
1:B:332:ARG:NH1	1:B:339:PRO:HD3	2.32	0.45
1:A:346:LEU:HD11	1:A:512:LYS:HB3	1.99	0.45
1:B:493:LEU:HD12	1:B:494:PRO:HD2	1.99	0.45
1:A:17:ILE:HG21	1:A:276:LYS:HG2	1.99	0.44
1:A:205:LYS:HD3	1:B:205:LYS:HG2	1.97	0.44
1:A:476:GLU:HG2	1:B:94:ARG:O	2.16	0.44
1:B:190:THR:HA	3:B:681:N3T:H71	1.99	0.44
1:A:616:GLU:O	1:A:632:GLY:HA2	2.17	0.44
1:B:346:LEU:HA	1:B:347:PRO:HD3	1.68	0.44
1:A:469:HIS:CD2	1:A:528:ARG:HD3	2.52	0.44
1:B:167:GLU:HB3	1:B:420:ALA:HB2	1.99	0.44
1:B:345:LYS:NZ	1:B:372:GLN:HB2	2.32	0.44
1:B:78:LEU:O	1:B:83:TYR:HB2	2.18	0.44
1:A:207:TYR:HA	1:A:210:TYR:CD2	2.52	0.44
1:A:594:PHE:O	1:A:597:GLN:HG2	2.18	0.44
1:B:177:LEU:O	1:B:241:PRO:HB3	2.17	0.44
1:B:378:GLY:HA3	1:B:438:TYR:CE2	2.54	0.43
1:A:361:LEU:HD13	1:A:504:GLY:CA	2.46	0.43
1:B:64:VAL:HB	1:B:153:VAL:HG13	1.99	0.43
1:B:213:GLU:HB2	1:B:240:LYS:HD3	1.99	0.43
1:A:342:TRP:CH2	1:A:512:LYS:HA	2.45	0.43
1:A:445:PHE:O	1:A:448:TYR:HB2	2.18	0.43
1:B:552:VAL:HG21	1:B:582:LYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASN:ND2	1:A:222:GLU:HB2	2.33	0.43
1:B:546:GLY:HA3	1:B:588:LEU:HD12	2.00	0.43
1:A:282:ASN:HA	1:A:283:PRO:HD2	1.71	0.43
1:A:454:ARG:NH1	1:B:485:GLU:OE1	2.52	0.42
1:B:263:HIS:ND1	3:B:681:N3T:O3B	2.50	0.42
1:B:114:THR:HG21	1:B:458:LEU:HD22	2.02	0.42
1:B:390:ARG:HG2	1:B:411:TYR:CZ	2.54	0.42
1:A:416:ILE:HD13	1:B:158:GLY:HA2	2.01	0.42
1:A:664:ILE:HG21	1:A:664:ILE:HD13	1.79	0.42
1:B:546:GLY:HA2	1:B:589:PRO:HD2	2.01	0.42
1:B:51:ASN:HD21	1:B:306:VAL:HG22	1.85	0.42
1:A:118:LEU:HD13	1:A:158:GLY:HA3	2.01	0.41
1:A:443:LEU:HD23	1:A:483:PRO:HG2	2.02	0.41
1:A:63:PHE:HA	1:A:152:TYR:O	2.20	0.41
1:A:67:ASN:HD22	1:A:67:ASN:N	2.15	0.41
1:A:275:LEU:HA	1:A:278:LYS:HB3	2.02	0.41
1:B:531:LEU:HD21	1:B:564:SER:HB3	2.03	0.41
1:A:43:VAL:HG23	1:A:224:LEU:HD22	2.03	0.41
1:A:6:ASP:HA	1:A:9:LYS:HE3	2.01	0.41
1:A:272:VAL:O	1:A:275:LEU:HD23	2.20	0.41
1:B:127:GLY:HA2	1:B:424:ILE:HG23	2.02	0.41
1:A:122:ILE:HA	1:A:153:VAL:HG11	2.03	0.41
1:A:307:GLU:O	1:A:311:LYS:HG2	2.20	0.41
1:A:390:ARG:NH1	1:A:396:ASP:OD1	2.54	0.41
1:B:565:GLU:OE1	1:B:617:VAL:HG22	2.21	0.41
1:B:285:LYS:HB3	1:B:288:VAL:HG21	2.03	0.41
1:A:491:ARG:HD2	1:A:591:PHE:CD2	2.56	0.40
1:B:457:ALA:HB1	1:B:494:PRO:O	2.20	0.40
1:A:134:ASN:HA	1:A:407:TYR:O	2.21	0.40
1:A:499:TRP:CE3	1:A:589:PRO:HB2	2.57	0.40
1:B:326:LEU:HD12	1:B:326:LEU:HA	1.91	0.40
1:B:338:LEU:HD12	1:B:338:LEU:HA	1.90	0.40
1:B:359:ARG:HD2	1:B:386:SER:O	2.21	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	676/678 (100%)	637 (94%)	35 (5%)	4 (1%)	25	50
1	B	676/678 (100%)	633 (94%)	39 (6%)	4 (1%)	25	50
All	All	1352/1356 (100%)	1270 (94%)	74 (6%)	8 (1%)	25	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	SER
1	A	400	PRO
1	A	188	LYS
1	B	148	ASP
1	B	617	VAL
1	B	71	VAL
1	A	617	VAL
1	B	31	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	552/552 (100%)	514 (93%)	38 (7%)	15	35
1	B	552/552 (100%)	519 (94%)	33 (6%)	19	42
All	All	1104/1104 (100%)	1033 (94%)	71 (6%)	17	39

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	49	ARG
1	A	50	MET
1	A	67	ASN
1	A	71	VAL
1	A	88	GLU
1	A	92	GLN
1	A	100	THR
1	A	132	GLN
1	A	153	VAL
1	A	155	LEU
1	A	205	LYS
1	A	218	GLU
1	A	238	LYS
1	A	261	SER
1	A	262	VAL
1	A	275	LEU
1	A	302	LEU
1	A	309	ASN
1	A	314	LYS
1	A	325	GLU
1	A	341	ASN
1	A	360	LYS
1	A	389	THR
1	A	458	LEU
1	A	506	GLU
1	A	512	LYS
1	A	549	LEU
1	A	557	ILE
1	A	567	SER
1	A	580	ASN
1	A	584	ARG
1	A	588	LEU
1	A	625	LYS
1	A	652	THR
1	A	654	GLU
1	A	668	LYS
1	A	678	LYS
1	B	49	ARG
1	B	67	ASN
1	B	96	LEU
1	B	113	VAL
1	B	141	LYS

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Mol	Chain	Res	Type
1	B	153	VAL
1	B	170	SER
1	B	197	ILE
1	B	218	GLU
1	B	229	LYS
1	B	240	LYS
1	B	261	SER
1	B	268	LYS
1	B	311	LYS
1	B	314	LYS
1	B	317	SER
1	B	322	LYS
1	B	326	LEU
1	B	338	LEU
1	B	343	GLU
1	B	348	THR
1	B	354	SER
1	B	389	THR
1	B	392	LYS
1	B	393	GLU
1	B	401	SER
1	B	404	SER
1	B	518	LYS
1	B	535	GLU
1	B	574	LYS
1	B	635	ARG
1	B	639	SER
1	B	671	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	54	ASN
1	A	120	GLN
1	A	219	ASN
1	A	260	HIS
1	A	341	ASN
1	A	387	ASN
1	A	489	HIS
1	B	51	ASN
1	B	54	ASN

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Mol	Chain	Res	Type
1	B	59	ASN
1	B	67	ASN
1	B	120	GLN
1	B	309	ASN
1	B	313	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)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	N3T	B	681	2	22,27,27	2.13	4 (18%)	26,40,40	1.46	5 (19%)
3	N3T	A	681	2	22,27,27	2.00	4 (18%)	26,40,40	1.42	6 (23%)

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	N3T	B	681	2	-	3/16/17/17	0/2/2/2
3	N3T	A	681	2	-	3/16/17/17	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	681	N3T	C4-N3	-7.74	1.33	1.39
3	B	681	N3T	C4-N3	-7.62	1.33	1.39
3	B	681	N3T	C7'-N3	3.41	1.54	1.48
3	B	681	N3T	C4'-N4'	-2.52	1.29	1.37
3	A	681	N3T	C7'-N3	2.35	1.53	1.48
3	A	681	N3T	PB-O3B	-2.26	1.46	1.54
3	B	681	N3T	PB-O3B	-2.22	1.46	1.54
3	A	681	N3T	C4'-N4'	-2.11	1.30	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	681	N3T	C6'-N1'-C2'	3.78	121.83	117.45
3	B	681	N3T	C6'-N1'-C2'	2.82	120.71	117.45
3	B	681	N3T	C6-C5-C4	-2.53	125.40	127.43
3	A	681	N3T	C5-C4-N3	2.52	112.61	107.57
3	B	681	N3T	C5-C4-N3	2.43	112.43	107.57
3	B	681	N3T	C3'-C2'-N1'	-2.23	119.50	121.66
3	A	681	N3T	C3'-C2'-N1'	-2.15	119.58	121.66
3	A	681	N3T	O3A-PB-O1B	-2.11	99.48	111.19
3	B	681	N3T	C5'-C6'-N1'	-2.10	120.32	123.82
3	A	681	N3T	CM4-C4-N3	-2.07	119.89	122.53
3	A	681	N3T	C7'-C5'-C4'	2.07	121.99	120.55

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	681	N3T	C4-C5-C6-C7
3	A	681	N3T	C7-O7-PA-O3A
3	A	681	N3T	PB-O3A-PA-O2A
3	B	681	N3T	C6'-C5'-C7'-N3
3	A	681	N3T	C4-C5-C6-C7
3	B	681	N3T	PB-O3A-PA-O2A

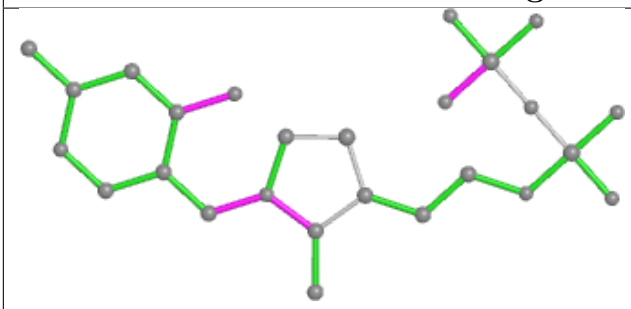
There are no ring outliers.

2 monomers are involved in 5 short contacts:

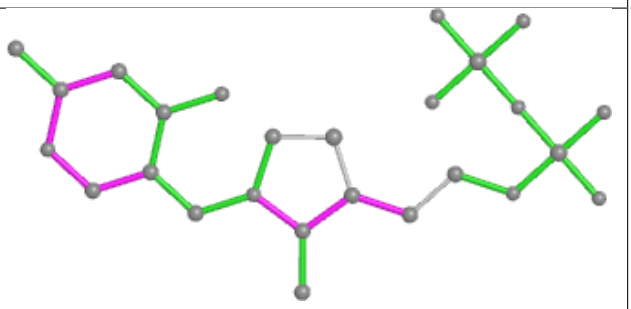
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	681	N3T	4	0
3	A	681	N3T	1	0

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.

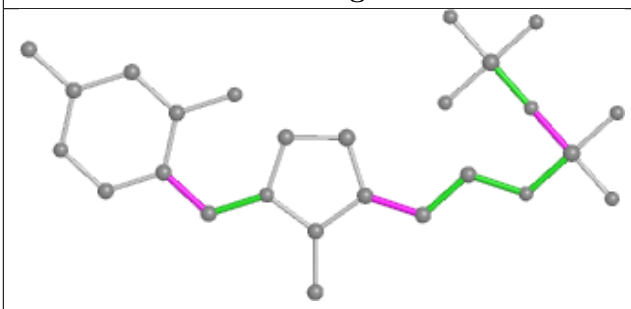
Ligand N3T B 681



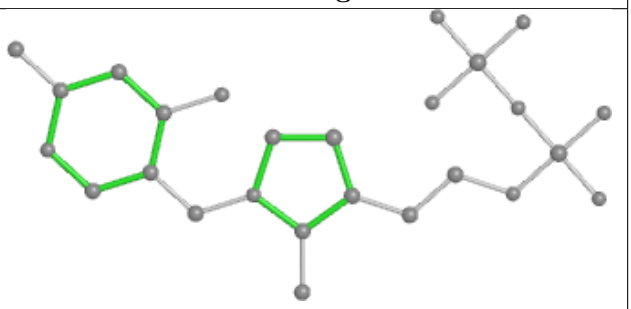
Bond lengths



Bond angles

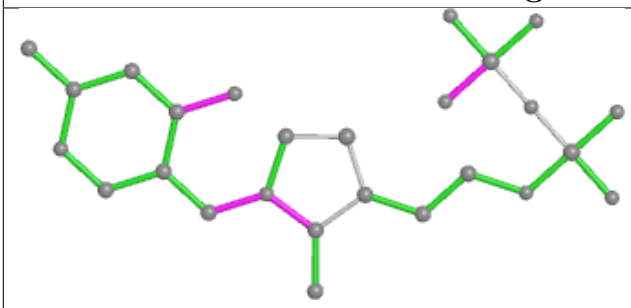


Torsions

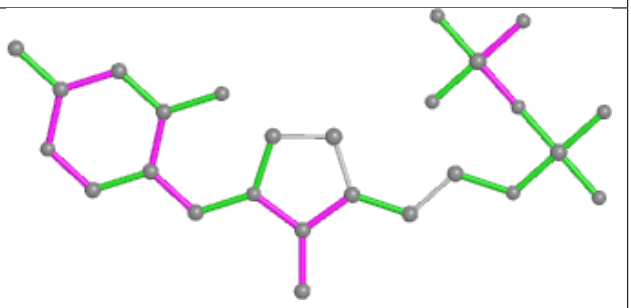


Rings

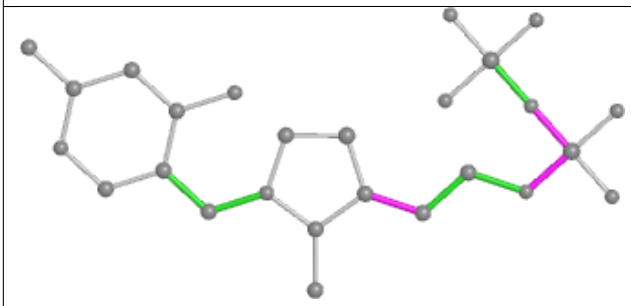
Ligand N3T A 681



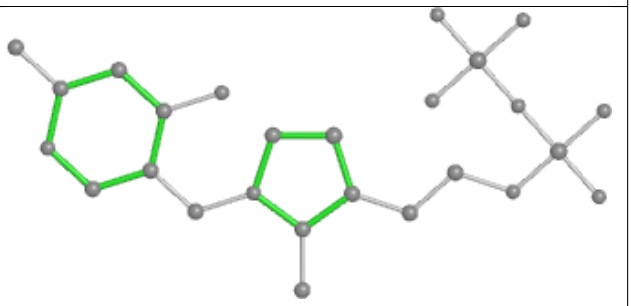
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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.