



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:47 AM EDT

PDB ID : 1S3W / pdb_00001s3w
Title : Structure Determination of Tetrahydroquinazoline Antifoaltes in Complex with Human and Pneumocystis carinii Dihydrofolate Reductase: Correlations of Enzyme Selectivity and Stereochemistry
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Deposited on : 2004-01-14
Resolution : 1.90 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

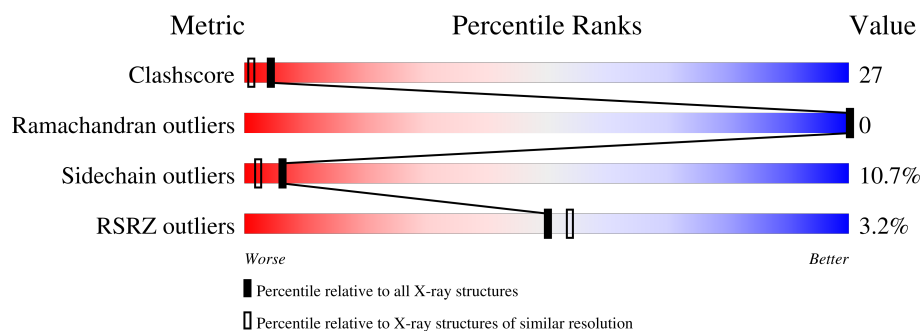
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	186	

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	TQT	A	188[A]	X	-	-	-
3	TQT	A	188[B]	X	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1671 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.

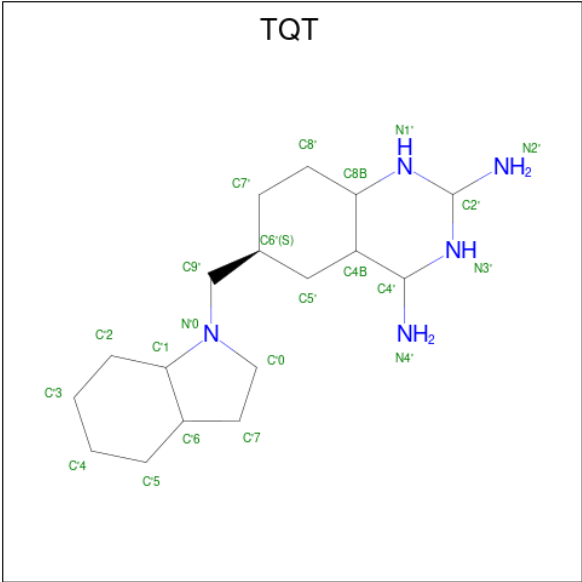
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1509	970	253	279	7	0	1	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 3 is 6-(OCTAHYDRO-1H-INDOL-1-YLMETHYL)DECAHYDROQUINAZOLIN E-2,4-DIAMINE (CCD ID: TQT) (formula: $C_{17}H_{33}N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	1
			32	26	6		

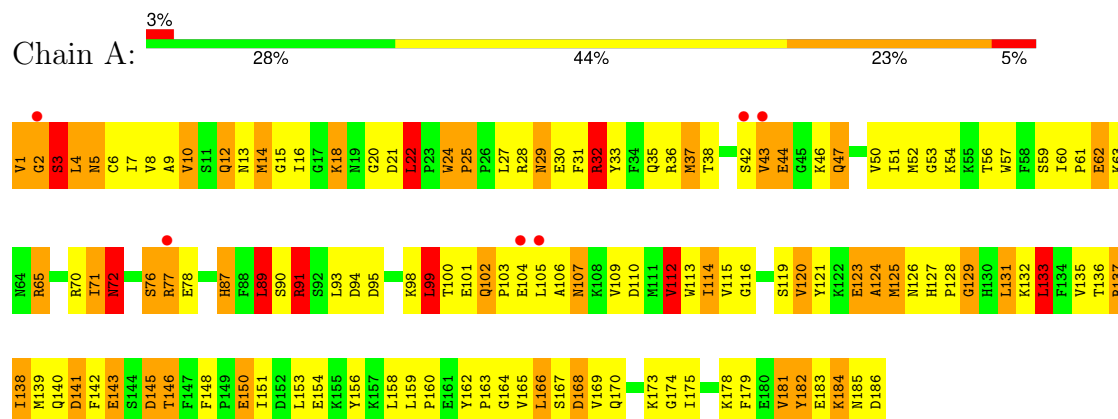
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total	O	0	0
			82	82		

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 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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	86.98Å 86.98Å 76.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.90) 64.5 (50.00-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 1.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.177 , 0.216 0.164 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1671	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.51	9/1549 (0.6%)	2.83	151/2089 (7.2%)

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	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	VAL	C-N	9.79	1.46	1.33
1	A	107	ASN	C-N	-8.57	1.21	1.33
1	A	114	ILE	C-O	6.08	1.30	1.24
1	A	175	ILE	N-CA	5.84	1.53	1.46
1	A	136	THR	C-O	5.62	1.31	1.24
1	A	38	THR	CA-CB	5.61	1.62	1.53
1	A	51	ILE	CA-CB	5.54	1.60	1.54
1	A	14	MET	C-N	-5.34	1.27	1.33
1	A	113	TRP	N-CA	5.16	1.52	1.46

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	CD-NE-CZ	19.39	151.55	124.40
1	A	65	ARG	NE-CZ-NH2	13.31	131.18	119.20
1	A	35	GLN	OE1-CD-NE2	-12.90	109.70	122.60
1	A	123	GLU	CB-CG-CD	12.48	133.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ASN	OD1-CG-ND2	-11.87	110.73	122.60
1	A	150	GLU	CB-CG-CD	11.30	131.81	112.60
1	A	91	ARG	NE-CZ-NH2	-11.18	109.13	119.20
1	A	116	GLY	CA-C-O	-10.05	114.19	122.33
1	A	72	ASN	CA-CB-CG	9.88	122.47	112.60
1	A	154	GLU	N-CA-CB	9.77	126.33	110.40
1	A	138	ILE	CA-CB-CG1	9.70	126.88	110.40
1	A	78	GLU	CA-CB-CG	9.56	133.21	114.10
1	A	181	VAL	CB-CA-C	9.44	124.10	110.33
1	A	126	ASN	OD1-CG-ND2	-9.34	113.26	122.60
1	A	24	TRP	O-C-N	9.28	127.82	121.14
1	A	91	ARG	CD-NE-CZ	-8.82	112.04	124.40
1	A	137	ARG	NE-CZ-NH2	8.77	127.09	119.20
1	A	146	THR	CB-CA-C	8.49	124.51	109.65
1	A	101	GLU	CB-CG-CD	8.32	126.74	112.60
1	A	174	GLY	CA-C-N	-8.15	113.09	123.19
1	A	174	GLY	C-N-CA	-8.15	113.09	123.19
1	A	140	GLN	N-CA-CB	8.04	123.84	111.46
1	A	25	PRO	N-CA-C	-7.81	102.97	110.47
1	A	13	ASN	CA-CB-CG	7.78	120.38	112.60
1	A	137	ARG	NE-CZ-NH1	-7.74	113.76	121.50
1	A	8	VAL	CA-C-O	-7.70	114.49	120.96
1	A	10	VAL	CA-CB-CG1	7.69	123.48	110.40
1	A	94	ASP	CA-CB-CG	-7.69	104.91	112.60
1	A	32	ARG	CA-C-N	7.64	130.38	120.44
1	A	32	ARG	C-N-CA	7.64	130.38	120.44
1	A	25	PRO	O-C-N	7.56	124.79	121.31
1	A	42	SER	CA-C-N	7.53	133.67	122.75
1	A	42	SER	C-N-CA	7.53	133.67	122.75
1	A	62	GLU	CB-CG-CD	7.51	125.37	112.60
1	A	60	ILE	CA-C-O	-7.40	113.40	119.47
1	A	138	ILE	CB-CG1-CD1	7.29	129.12	113.80
1	A	70	ARG	NE-CZ-NH2	-7.20	112.72	119.20
1	A	129	GLY	O-C-N	7.19	129.09	122.90
1	A	145	ASP	CA-C-O	7.14	127.10	119.03
1	A	154	GLU	N-CA-C	-7.12	104.07	112.89
1	A	166	LEU	N-CA-CB	-7.12	99.09	109.83
1	A	143	GLU	CB-CG-CD	7.08	124.63	112.60
1	A	112	VAL	CA-C-N	-7.07	113.25	123.00
1	A	112	VAL	C-N-CA	-7.07	113.25	123.00
1	A	179	PHE	CA-C-O	-7.00	112.80	120.43
1	A	126	ASN	CB-CA-C	6.99	121.82	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	CA-C-O	-6.99	112.56	119.69
1	A	44	GLU	N-CA-CB	6.88	120.08	109.97
1	A	148	PHE	CA-C-O	-6.85	113.25	120.23
1	A	65	ARG	CB-CA-C	-6.83	100.20	109.42
1	A	101	GLU	CA-CB-CG	6.79	127.68	114.10
1	A	3	SER	O-C-N	6.79	130.87	122.86
1	A	120	VAL	O-C-N	6.78	128.45	121.87
1	A	90	SER	O-C-N	6.67	131.83	123.15
1	A	13	ASN	CA-C-N	6.67	133.67	123.47
1	A	13	ASN	C-N-CA	6.67	133.67	123.47
1	A	32	ARG	O-C-N	-6.67	115.05	122.12
1	A	47	GLN	OE1-CD-NE2	6.63	129.24	122.60
1	A	65	ARG	NH1-CZ-NH2	-6.62	110.70	119.30
1	A	142	PHE	CA-CB-CG	6.59	120.39	113.80
1	A	47	GLN	CA-C-O	-6.52	113.48	121.11
1	A	50	VAL	N-CA-CB	6.50	120.08	111.25
1	A	153	LEU	CA-C-O	-6.49	110.62	119.12
1	A	163	PRO	CB-CA-C	-6.38	103.41	111.71
1	A	35	GLN	CA-C-O	6.37	127.51	120.82
1	A	158	LEU	CA-C-O	-6.33	113.53	120.81
1	A	132	LYS	CA-C-O	-6.32	114.01	120.71
1	A	32	ARG	NE-CZ-NH2	6.27	124.84	119.20
1	A	135	VAL	CA-C-O	-6.18	113.92	120.53
1	A	100	THR	O-C-N	6.17	129.86	122.27
1	A	1	VAL	CA-CB-CG1	6.15	120.86	110.40
1	A	91	ARG	NH1-CZ-NH2	6.13	127.27	119.30
1	A	137	ARG	CA-C-O	-6.09	113.72	120.60
1	A	60	ILE	O-C-N	6.05	128.53	121.57
1	A	70	ARG	CD-NE-CZ	6.04	132.86	124.40
1	A	27	LEU	CA-C-O	-6.02	114.02	120.46
1	A	146	THR	CA-CB-CG2	6.01	120.72	110.50
1	A	29	ASN	CA-CB-CG	-5.97	106.63	112.60
1	A	139	MET	CA-C-N	5.97	132.02	121.80
1	A	139	MET	C-N-CA	5.97	132.02	121.80
1	A	53	GLY	N-CA-C	-5.97	103.23	112.85
1	A	56	THR	CA-CB-OG1	-5.94	100.69	109.60
1	A	123	GLU	N-CA-CB	-5.92	101.40	110.16
1	A	25	PRO	CA-C-O	-5.87	116.67	120.90
1	A	124	ALA	N-CA-CB	5.86	118.73	110.12
1	A	113	TRP	CA-C-O	-5.80	114.06	120.38
1	A	77	ARG	CA-CB-CG	-5.80	102.50	114.10
1	A	6	CYS	O-C-N	5.80	130.73	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	MET	O-C-N	-5.79	114.89	122.59
1	A	90	SER	CA-C-O	-5.75	114.72	121.44
1	A	168	ASP	O-C-N	5.74	129.44	122.96
1	A	30	GLU	N-CA-C	-5.72	104.94	111.07
1	A	54	LYS	N-CA-C	5.72	117.60	111.36
1	A	15	GLY	N-CA-C	5.72	119.32	111.54
1	A	126	ASN	CB-CG-OD1	5.67	132.14	120.80
1	A	37	MET	N-CA-CB	5.66	118.22	110.01
1	A	98	LYS	N-CA-CB	5.66	118.43	110.12
1	A	90	SER	N-CA-CB	5.65	121.38	111.55
1	A	36	ARG	CD-NE-CZ	-5.63	116.51	124.40
1	A	12	GLN	CA-C-O	-5.63	114.58	120.55
1	A	71	ILE	N-CA-CB	5.63	117.25	110.95
1	A	184	LYS	CA-C-O	-5.59	114.57	121.11
1	A	141	ASP	O-C-N	5.59	129.65	123.16
1	A	21	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	164	GLY	CA-C-O	5.55	125.15	119.10
1	A	87	HIS	CB-CG-CD2	5.54	138.41	131.20
1	A	181	VAL	CA-CB-CG1	5.54	119.81	110.40
1	A	76	SER	CA-CB-OG	5.50	122.09	111.10
1	A	145	ASP	O-C-N	-5.46	116.28	122.23
1	A	151	ILE	CA-C-N	-5.46	115.16	122.42
1	A	151	ILE	C-N-CA	-5.46	115.16	122.42
1	A	61	PRO	CA-C-N	5.45	127.85	120.38
1	A	61	PRO	C-N-CA	5.45	127.85	120.38
1	A	183	GLU	CA-C-O	5.42	126.90	120.66
1	A	9	ALA	CA-C-O	-5.41	114.36	120.32
1	A	89	LEU	O-C-N	-5.41	116.98	123.31
1	A	113	TRP	N-CA-CB	-5.41	102.08	110.57
1	A	3	SER	CA-C-O	-5.40	115.67	121.56
1	A	115	VAL	CA-C-O	-5.35	114.06	119.89
1	A	38	THR	O-C-N	5.35	128.85	122.27
1	A	99	LEU	N-CA-CB	-5.32	102.03	110.22
1	A	143	GLU	CA-CB-CG	5.31	124.72	114.10
1	A	2	GLY	CA-C-N	5.29	129.25	120.94
1	A	2	GLY	C-N-CA	5.29	129.25	120.94
1	A	87	HIS	ND1-CE1-NE2	-5.29	103.11	108.40
1	A	22	LEU	N-CA-CB	-5.23	102.98	110.04
1	A	182	TYR	CA-C-O	-5.21	115.07	120.70
1	A	38	THR	OG1-CB-CG2	5.21	119.72	109.30
1	A	43	VAL	N-CA-CB	-5.21	103.15	111.58
1	A	136	THR	CA-CB-CG2	5.20	119.34	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	LEU	CA-CB-CG	5.20	134.49	116.30
1	A	136	THR	OG1-CB-CG2	5.16	119.62	109.30
1	A	9	ALA	N-CA-CB	5.13	118.61	110.55
1	A	102	GLN	N-CA-C	-5.12	101.97	109.50
1	A	44	GLU	CA-CB-CG	5.11	124.31	114.10
1	A	70	ARG	CA-C-N	5.10	128.94	121.80
1	A	70	ARG	C-N-CA	5.10	128.94	121.80
1	A	95	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	52	MET	CA-CB-CG	-5.08	103.93	114.10
1	A	7	ILE	CA-C-N	5.08	128.77	121.96
1	A	7	ILE	C-N-CA	5.08	128.77	121.96
1	A	4	LEU	O-C-N	-5.07	117.28	123.27
1	A	36	ARG	CB-CA-C	5.07	118.91	110.90
1	A	77	ARG	NE-CZ-NH1	5.05	126.55	121.50
1	A	166	LEU	CA-C-O	-5.04	115.64	121.19
1	A	167	SER	CA-CB-OG	5.04	121.19	111.10
1	A	169	VAL	CA-CB-CG2	5.04	118.97	110.40
1	A	162	TYR	CA-C-N	5.03	125.81	119.98
1	A	162	TYR	C-N-CA	5.03	125.81	119.98
1	A	5	ASN	CA-C-O	-5.02	115.23	121.11
1	A	131	LEU	N-CA-CB	-5.01	102.06	111.13

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	VAL	Mainchain
1	A	32	ARG	Sidechain
1	A	91	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1509	0	1516	83	0
2	A	48	0	25	6	0
3	A	32	0	41	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	82	0	0	1	0
All	All	1671	0	1582	85	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 27.

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:99:LEU:CD2	1:A:105:LEU:HD12	1.79	1.12
1:A:99:LEU:HD21	1:A:105:LEU:HD12	1.28	1.08
1:A:89:LEU:HD21	1:A:91:ARG:HH22	1.15	1.07
1:A:102:GLN:HB2	1:A:104:GLU:HG2	1.51	0.92
1:A:72:ASN:H	1:A:87:HIS:HD2	1.17	0.89
1:A:37:MET:HE1	1:A:165:VAL:HG22	1.56	0.87
1:A:43:VAL:HG13	1:A:46:LYS:HB2	1.58	0.86
1:A:33:TYR:CE2	1:A:37:MET:HE2	2.10	0.86
1:A:77:ARG:NH2	2:A:187:NAP:N1A	2.25	0.84
1:A:77:ARG:HA	1:A:91:ARG:HD2	1.57	0.84
1:A:22:LEU:HD13	3:A:188[A]:TQT:H'31	1.59	0.84
1:A:33:TYR:HE2	1:A:37:MET:HE2	1.43	0.82
1:A:37:MET:CE	1:A:165:VAL:HG22	2.11	0.80
1:A:76:SER:O	1:A:91:ARG:HD3	1.82	0.79
1:A:114:ILE:HD13	1:A:124:ALA:HB2	1.67	0.76
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.69	0.75
1:A:99:LEU:HD21	1:A:105:LEU:CD1	2.13	0.74
1:A:77:ARG:HH21	2:A:187:NAP:C6A	2.00	0.74
1:A:16:ILE:O	2:A:187:NAP:H2N	1.87	0.73
1:A:62:GLU:HG3	1:A:65:ARG:NH1	2.02	0.72
1:A:43:VAL:HG11	1:A:110:ASP:HB2	1.72	0.71
1:A:102:GLN:CB	1:A:104:GLU:HG2	2.21	0.71
1:A:2:GLY:N	1:A:110:ASP:O	2.22	0.71
1:A:47:GLN:O	1:A:109:VAL:HA	1.92	0.69
1:A:114:ILE:HD13	1:A:124:ALA:CB	2.23	0.69
1:A:145:ASP:OD1	1:A:146:THR:HG22	1.93	0.69
1:A:77:ARG:NH2	2:A:187:NAP:C6A	2.56	0.69
1:A:71:ILE:HD12	1:A:109:VAL:HG22	1.75	0.68
1:A:72:ASN:H	1:A:87:HIS:CD2	2.07	0.66
1:A:37:MET:HE1	1:A:165:VAL:CG2	2.25	0.66
1:A:77:ARG:HA	1:A:91:ARG:CD	2.27	0.65
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:HIS:CG	1:A:128:PRO:HD2	2.34	0.63
1:A:12:GLN:HB3	1:A:141:ASP:OD1	2.00	0.62
1:A:137:ARG:HB2	1:A:178:LYS:HG2	1.80	0.62
1:A:103:PRO:HA	1:A:106:ALA:HB3	1.81	0.61
1:A:33:TYR:CE2	1:A:37:MET:CE	2.83	0.61
1:A:43:VAL:CG1	1:A:110:ASP:HB2	2.32	0.59
1:A:43:VAL:HG11	1:A:46:LYS:HD2	1.84	0.59
1:A:121:TYR:O	1:A:125:MET:HB2	2.02	0.59
1:A:62:GLU:HG3	1:A:65:ARG:HH12	1.68	0.58
1:A:131:LEU:HD23	1:A:156:TYR:OH	2.03	0.57
1:A:71:ILE:HD12	1:A:109:VAL:CG2	2.35	0.57
1:A:43:VAL:CG1	1:A:46:LYS:HB2	2.32	0.56
1:A:18:LYS:NZ	1:A:143:GLU:OE2	2.37	0.56
1:A:43:VAL:HG13	1:A:43:VAL:O	2.04	0.56
1:A:31[A]:PHE:CE1	3:A:188[A]:TQT:H'01	2.41	0.55
1:A:57:TRP:CZ2	1:A:65:ARG:HD2	2.41	0.55
1:A:57:TRP:CE2	1:A:65:ARG:HD2	2.42	0.55
3:A:188[A]:TQT:H'01	3:A:188[A]:TQT:H7'2	1.90	0.53
1:A:89:LEU:HD21	1:A:91:ARG:NH2	2.00	0.51
1:A:99:LEU:O	1:A:99:LEU:HD23	2.09	0.51
1:A:129:GLY:O	1:A:184:LYS:NZ	2.35	0.51
1:A:99:LEU:HA	1:A:102:GLN:HG2	1.93	0.51
1:A:168:ASP:O	1:A:170:GLN:NE2	2.30	0.51
1:A:184:LYS:NZ	1:A:186:ASP:OD1	2.44	0.50
1:A:20:GLY:O	1:A:59:SER:HB2	2.11	0.50
1:A:22:LEU:HD13	3:A:188[A]:TQT:C'3	2.37	0.50
1:A:29:ASN:HA	1:A:32:ARG:HG3	1.94	0.50
1:A:99:LEU:HD23	1:A:99:LEU:C	2.36	0.50
1:A:102:GLN:C	1:A:104:GLU:H	2.21	0.49
1:A:28:ARG:O	1:A:32:ARG:HG3	2.13	0.48
2:A:187:NAP:H52A	2:A:187:NAP:H8A	1.95	0.48
1:A:102:GLN:C	1:A:104:GLU:N	2.70	0.48
1:A:127:HIS:CD2	1:A:128:PRO:HD2	2.49	0.48
1:A:105:LEU:HA	1:A:105:LEU:HD23	1.54	0.46
1:A:46:LYS:HE2	1:A:107:ASN:HA	1.98	0.46
1:A:43:VAL:HG11	1:A:46:LYS:CD	2.45	0.45
1:A:110:ASP:OD2	1:A:110:ASP:C	2.57	0.45
1:A:24:TRP:CB	1:A:25:PRO:HD2	2.44	0.45
1:A:43:VAL:HG21	1:A:46:LYS:HD2	1.98	0.45
1:A:159:LEU:HA	1:A:160:PRO:HD3	1.77	0.45
1:A:114:ILE:HG23	1:A:120:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HG22	1:A:14:MET:HA	1.99	0.44
1:A:33:TYR:OH	1:A:37:MET:HE3	2.18	0.43
1:A:133:LEU:HB2	1:A:182:TYR:HB2	2.00	0.43
1:A:93:LEU:HD23	1:A:123:GLU:HG3	2.00	0.43
1:A:99:LEU:CD2	1:A:99:LEU:C	2.91	0.43
1:A:156:TYR:CZ	1:A:184:LYS:HD3	2.54	0.43
1:A:77:ARG:HH21	2:A:187:NAP:C2A	2.24	0.42
1:A:72:ASN:N	1:A:87:HIS:HD2	1.99	0.42
1:A:2:GLY:CA	1:A:110:ASP:O	2.67	0.42
1:A:173:LYS:HD3	4:A:240:HOH:O	2.19	0.41
1:A:3:SER:HB3	1:A:5:ASN:HD21	1.84	0.41
1:A:102:GLN:O	1:A:104:GLU:N	2.53	0.41

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	185/186 (100%)	179 (97%)	6 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	169/168 (101%)	151 (89%)	18 (11%)	6 2

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

Mol	Chain	Res	Type
1	A	1	VAL
1	A	3	SER
1	A	18	LYS
1	A	22	LEU
1	A	44	GLU
1	A	63	LYS
1	A	72	ASN
1	A	89	LEU
1	A	99	LEU
1	A	112	VAL
1	A	119	SER
1	A	125	MET
1	A	133	LEU
1	A	138	ILE
1	A	150	GLU
1	A	166	LEU
1	A	181	VAL
1	A	185	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	87	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	TQT	A	188[A]	-	22,25,25	5.36	12 (54%)	26,36,36	5.41	18 (69%)
3	TQT	A	188[B]	-	22,15,25	5.35	12 (54%)	26,18,36	5.45	18 (69%)
2	NAP	A	187	-	50,52,52	3.77	23 (46%)	71,80,80	2.56	27 (38%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TQT	A	188[A]	-	6/6/8/10	2/4/49/49	0/4/4/4
3	TQT	A	188[B]	-	6/6/3/10	2/4/23/49	0/4/2/4
2	NAP	A	187	-	-	4/35/67/67	0/5/5/5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	188[A]	TQT	C'6-C'1	-11.69	1.33	1.53
3	A	188[A]	TQT	C8B-N1'	-10.81	1.33	1.47
3	A	188[B]	TQT	C8B-N1'	-10.81	1.33	1.47
3	A	188[B]	TQT	C'6-C'1	-10.71	1.35	1.53
2	A	187	NAP	C4N-C3N	10.43	1.55	1.39
2	A	187	NAP	C2N-N1N	9.96	1.45	1.35
2	A	187	NAP	P2B-O2B	9.80	1.76	1.59
3	A	188[A]	TQT	C4B-C8B	-8.75	1.33	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	188[B]	TQT	C4B-C8B	-8.75	1.33	1.54
3	A	188[B]	TQT	C'5-C'6	-8.46	1.33	1.53
2	A	187	NAP	O4B-C4B	-8.33	1.26	1.45
2	A	187	NAP	C5N-C4N	8.24	1.53	1.38
3	A	188[B]	TQT	C'2-C'1	-8.11	1.34	1.52
3	A	188[A]	TQT	C'4-C'5	-7.88	1.33	1.53
3	A	188[A]	TQT	C'2-C'1	-7.87	1.35	1.52
3	A	188[A]	TQT	C'5-C'6	-7.81	1.34	1.53
3	A	188[B]	TQT	C'4-C'5	-7.80	1.33	1.53
2	A	187	NAP	O4D-C1D	7.44	1.50	1.40
3	A	188[B]	TQT	C'3-C'2	-7.12	1.35	1.53
3	A	188[A]	TQT	C'3-C'2	-6.81	1.36	1.53
2	A	187	NAP	C5A-C6A	4.96	1.54	1.41
3	A	188[B]	TQT	C'4-C'3	-4.84	1.34	1.51
3	A	188[A]	TQT	C'4-C'3	-4.51	1.35	1.51
2	A	187	NAP	PN-O3	4.45	1.64	1.59
2	A	187	NAP	C5A-C4A	-4.12	1.31	1.39
2	A	187	NAP	C2N-C3N	-3.89	1.32	1.39
3	A	188[A]	TQT	C2'-N1'	-3.79	1.25	1.42
3	A	188[B]	TQT	C2'-N1'	-3.79	1.25	1.42
2	A	187	NAP	O3B-C3B	3.66	1.52	1.43
2	A	187	NAP	C4A-N9A	-3.45	1.30	1.37
2	A	187	NAP	C3B-C4B	3.22	1.61	1.53
2	A	187	NAP	O7N-C7N	-3.11	1.18	1.24
3	A	188[A]	TQT	C2'-N3'	-2.94	1.29	1.42
3	A	188[B]	TQT	C2'-N3'	-2.94	1.29	1.42
2	A	187	NAP	C5B-C4B	2.85	1.60	1.51
2	A	187	NAP	PN-O1N	-2.80	1.41	1.50
2	A	187	NAP	PA-O2A	-2.69	1.42	1.55
2	A	187	NAP	PN-O2N	-2.53	1.43	1.55
2	A	187	NAP	C6N-N1N	2.45	1.40	1.35
3	A	188[B]	TQT	C'1-N'0	-2.39	1.44	1.47
2	A	187	NAP	C6N-C5N	-2.36	1.33	1.38
3	A	188[A]	TQT	C8'-C7'	2.35	1.58	1.52
3	A	188[B]	TQT	C8'-C7'	2.35	1.58	1.52
2	A	187	NAP	PA-O5B	2.33	1.68	1.59
3	A	188[A]	TQT	C'7-C'0	2.21	1.56	1.52
2	A	187	NAP	C8A-N9A	-2.19	1.33	1.37
2	A	187	NAP	P2B-O3X	-2.14	1.46	1.54

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188[A]	TQT	C8'-C8B-C4B	17.17	126.45	111.12
3	A	188[B]	TQT	C8'-C8B-C4B	17.17	126.45	111.12
3	A	188[B]	TQT	C'2-C'1-N'0	12.08	134.35	117.16
3	A	188[A]	TQT	C'2-C'1-N'0	10.56	132.19	117.16
2	A	187	NAP	C5N-C4N-C3N	-10.07	110.47	120.36
3	A	188[A]	TQT	C5'-C4B-C8B	8.23	121.23	109.62
3	A	188[B]	TQT	C5'-C4B-C8B	8.23	121.23	109.62
2	A	187	NAP	O7N-C7N-C3N	-7.42	110.53	119.60
3	A	188[A]	TQT	C8B-N1'-C2'	6.42	122.74	113.24
3	A	188[B]	TQT	C8B-N1'-C2'	6.42	122.74	113.24
3	A	188[A]	TQT	C'7-C'6-C'1	6.27	114.50	103.93
2	A	187	NAP	C2N-C3N-C4N	6.08	125.33	118.26
3	A	188[A]	TQT	C'2-C'1-C'6	6.05	120.62	113.09
3	A	188[B]	TQT	C'7-C'6-C'1	5.63	113.42	103.93
2	A	187	NAP	O7N-C7N-N7N	4.99	129.82	122.62
3	A	188[A]	TQT	C'3-C'4-C'5	4.80	121.29	111.42
3	A	188[B]	TQT	C'3-C'4-C'5	4.60	120.88	111.42
3	A	188[B]	TQT	C'2-C'1-C'6	4.54	118.74	113.09
3	A	188[A]	TQT	C'0-N'0-C'1	4.32	111.70	104.94
3	A	188[B]	TQT	C'0-N'0-C'1	4.21	111.52	104.94
3	A	188[B]	TQT	C'4-C'3-C'2	4.20	120.06	111.42
3	A	188[A]	TQT	C'4-C'3-C'2	3.99	119.62	111.42
2	A	187	NAP	O4D-C4D-C5D	3.93	121.93	109.33
3	A	188[B]	TQT	C'4-C'5-C'6	3.88	118.81	111.89
3	A	188[A]	TQT	C'4-C'5-C'6	3.87	118.79	111.89
2	A	187	NAP	O5D-C5D-C4D	-3.82	96.00	108.99
3	A	188[A]	TQT	C8'-C8B-N1'	3.78	116.60	111.38
3	A	188[B]	TQT	C8'-C8B-N1'	3.78	116.60	111.38
3	A	188[B]	TQT	C'3-C'2-C'1	3.70	119.65	109.67
3	A	188[B]	TQT	C'7-C'6-C'5	3.65	124.76	114.52
3	A	188[B]	TQT	C'5-C'6-C'1	3.65	121.82	113.72
3	A	188[A]	TQT	C'0-N'0-C9'	3.62	129.87	112.37
3	A	188[A]	TQT	C'7-C'6-C'5	3.54	124.46	114.52
3	A	188[A]	TQT	C4'-C4B-C8B	3.51	117.98	111.50
3	A	188[B]	TQT	C4'-C4B-C8B	3.51	117.98	111.50
3	A	188[A]	TQT	C'3-C'2-C'1	3.35	118.68	109.67
2	A	187	NAP	C5D-C4D-C3D	-3.33	103.22	115.21
3	A	188[A]	TQT	C'5-C'6-C'1	3.23	120.89	113.72
3	A	188[A]	TQT	C4B-C5'-C6'	3.18	112.44	109.52
3	A	188[B]	TQT	C4B-C5'-C6'	3.18	112.44	109.52
2	A	187	NAP	O4B-C1B-C2B	-3.17	101.14	106.59
2	A	187	NAP	O2X-P2B-O1X	3.15	123.10	110.83
2	A	187	NAP	C6N-C5N-C4N	3.14	123.97	119.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	187	NAP	C2B-C3B-C4B	-3.13	95.26	101.99
2	A	187	NAP	O2D-C2D-C3D	-3.05	102.05	111.82
2	A	187	NAP	O2A-PA-O1A	3.01	126.46	112.44
2	A	187	NAP	C4B-O4B-C1B	2.98	116.05	109.47
2	A	187	NAP	O5B-C5B-C4B	-2.95	98.94	108.99
2	A	187	NAP	O2B-C2B-C1B	-2.95	99.68	110.05
3	A	188[B]	TQT	C'0-N'0-C9'	2.95	126.60	112.37
2	A	187	NAP	O2N-PN-O3	-2.79	99.74	107.27
2	A	187	NAP	C5B-C4B-C3B	-2.78	105.19	115.21
2	A	187	NAP	O3D-C3D-C2D	-2.54	103.68	111.82
2	A	187	NAP	O4B-C4B-C5B	-2.47	101.41	109.33
2	A	187	NAP	C4D-O4D-C1D	-2.47	107.66	109.92
2	A	187	NAP	O3B-C3B-C4B	-2.40	104.17	111.08
2	A	187	NAP	N6A-C6A-N1A	2.35	123.61	118.38
2	A	187	NAP	PN-O5D-C5D	2.23	134.15	121.35
2	A	187	NAP	C6N-N1N-C2N	2.22	123.77	121.88
3	A	188[A]	TQT	C'6-C'1-N'0	2.20	107.18	103.10
2	A	187	NAP	O3-PA-O1A	-2.16	104.19	110.70
2	A	187	NAP	O2X-P2B-O2B	-2.13	97.54	105.85
3	A	188[B]	TQT	C'6-C'1-N'0	2.05	106.90	103.10

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	188[A]	TQT	C'1
3	A	188[A]	TQT	C4'
3	A	188[A]	TQT	C8B
3	A	188[A]	TQT	C2'
3	A	188[A]	TQT	C4B
3	A	188[A]	TQT	C'6
3	A	188[B]	TQT	C'1
3	A	188[B]	TQT	C4'
3	A	188[B]	TQT	C8B
3	A	188[B]	TQT	C2'
3	A	188[B]	TQT	C4B
3	A	188[B]	TQT	C'6

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	187	NAP	O4D-C1D-N1N-C2N
2	A	187	NAP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	A	187	NAP	C2D-C1D-N1N-C2N
3	A	188[B]	TQT	C6'-C9'-N'0-C'0
3	A	188[A]	TQT	C7'-C6'-C9'-N'0
3	A	188[A]	TQT	C5'-C6'-C9'-N'0
2	A	187	NAP	PN-O3-PA-O1A
3	A	188[B]	TQT	C7'-C6'-C9'-N'0

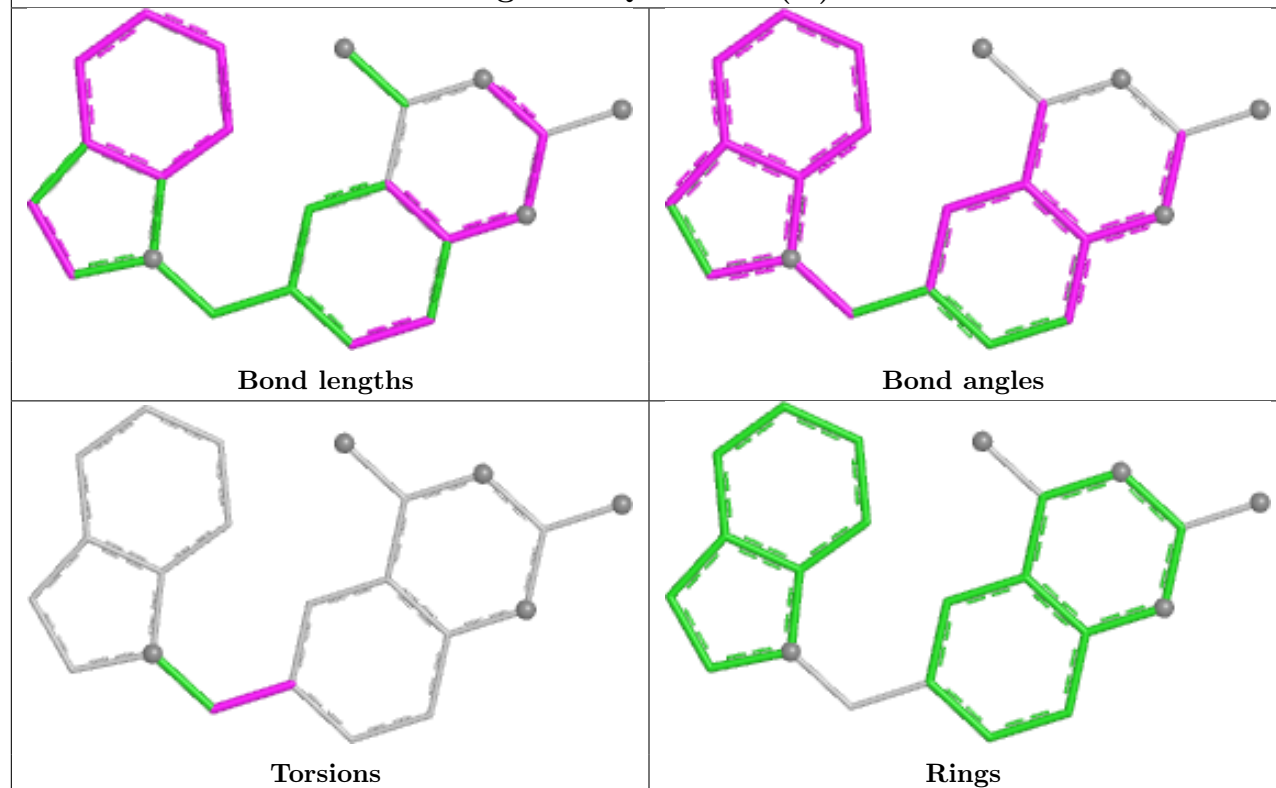
There are no ring outliers.

2 monomers are involved in 10 short contacts:

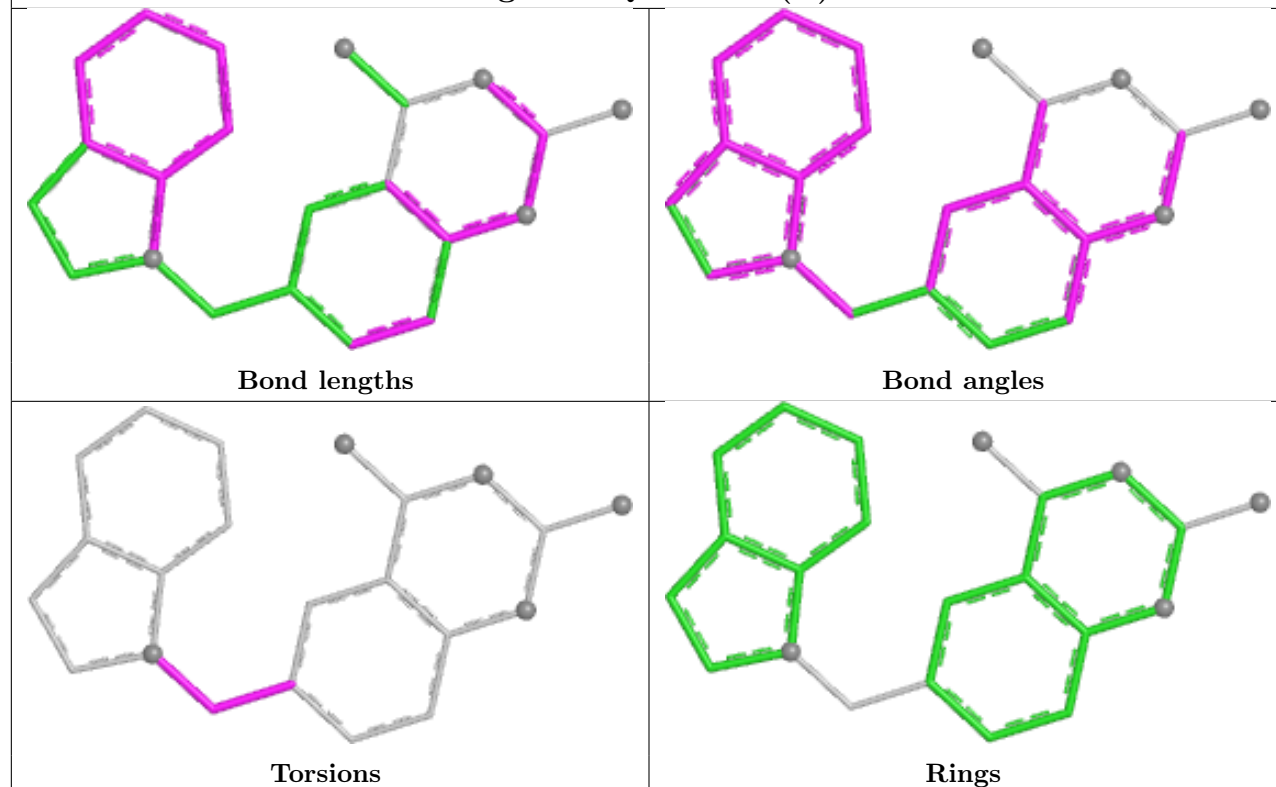
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	188[A]	TQT	4	0
2	A	187	NAP	6	0

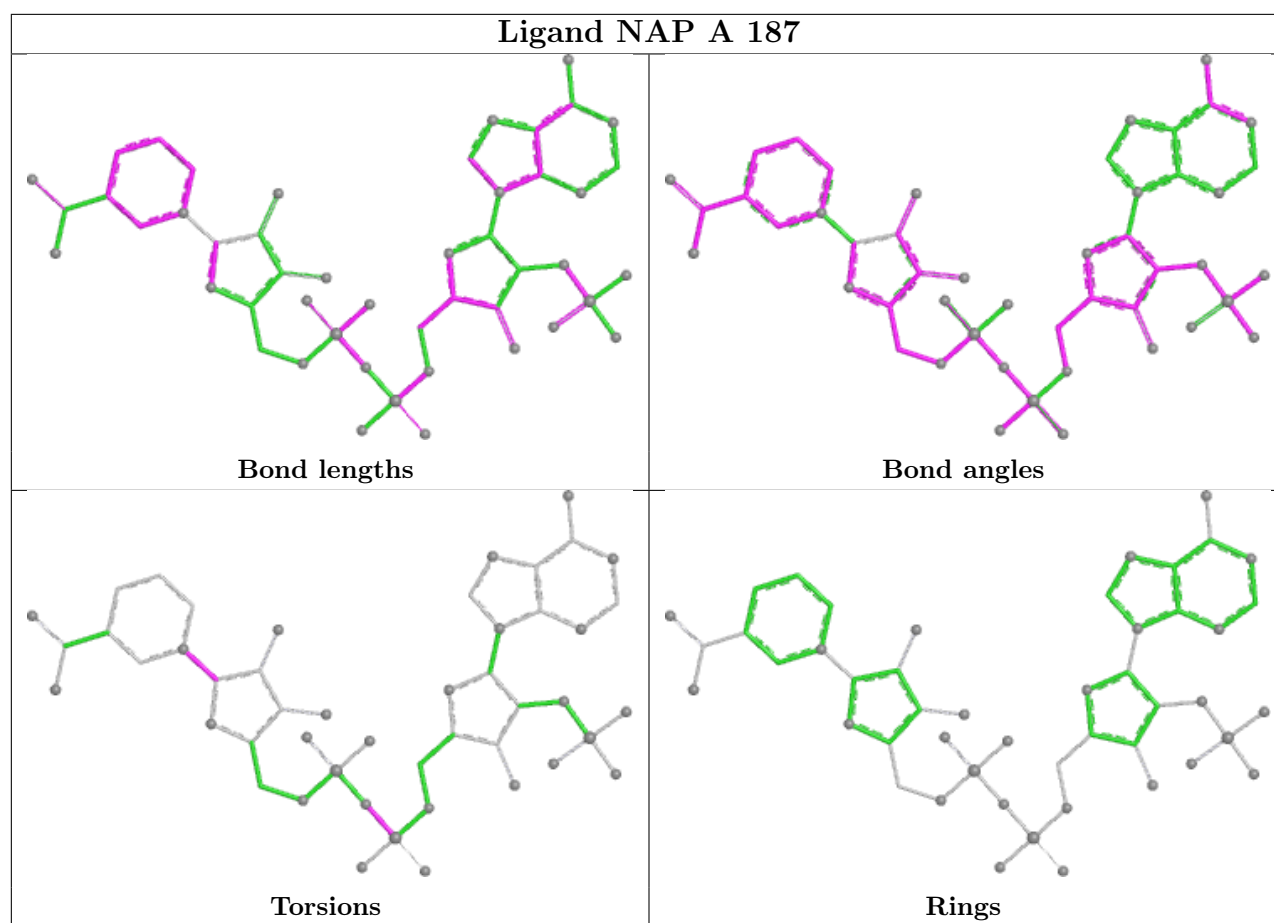
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 TQT A 188 (A)



Ligand TQT A 188 (B)





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](#)

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, 95th 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	186/186 (100%)	0.07	6 (3%) 50 54	17, 32, 54, 74	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	VAL	4.0
1	A	105	LEU	3.2
1	A	2	GLY	2.7
1	A	42	SER	2.7
1	A	77	ARG	2.5
1	A	104	GLU	2.4

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 oligosaccharides 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, 95th 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	TQT	A	188[A]	22/22	0.94	0.10	21,29,33,34	10

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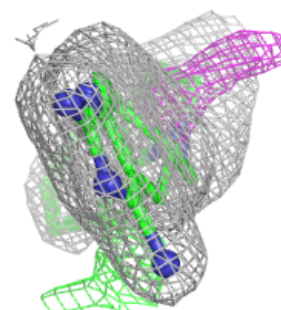
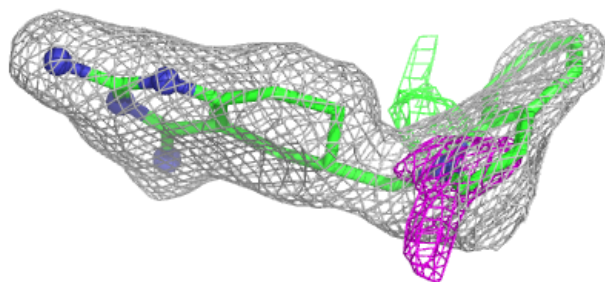
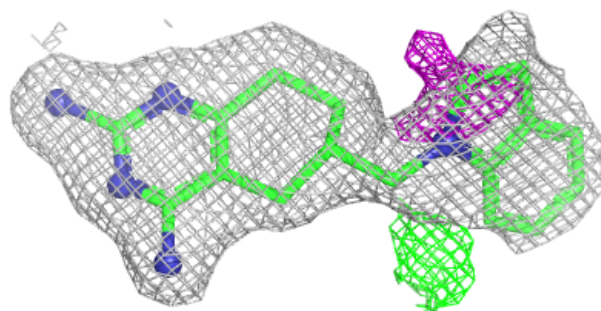
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TQT	A	188[B]	16/22	0.94	0.10	23,30,31,32	10
2	NAP	A	187	48/48	0.97	0.05	24,28,41,45	0

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.

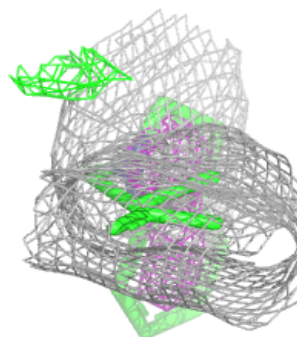
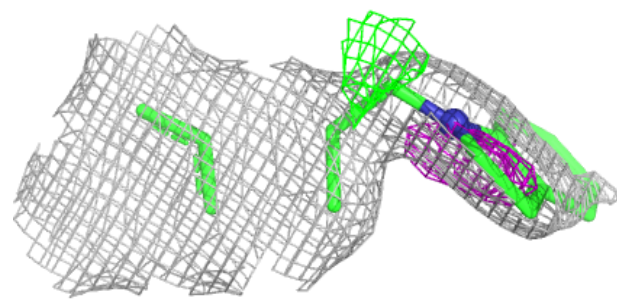
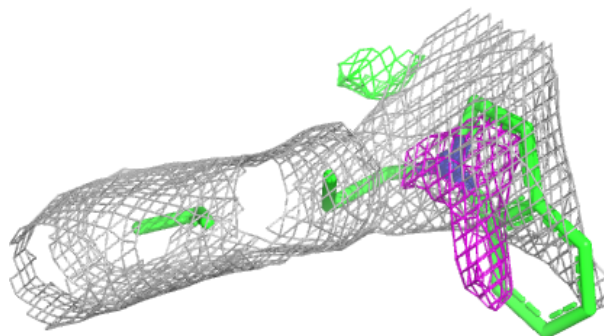
Electron density around TQT A 188 (A):

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

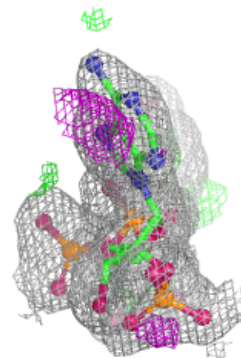
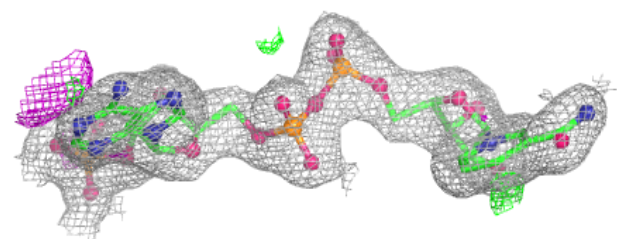
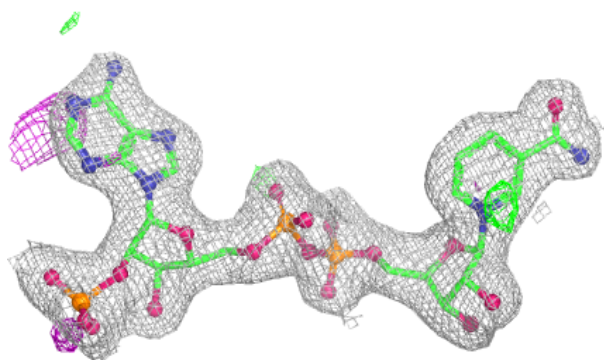


Electron density around TQT A 188 (B):

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

**Electron density around NAP A 187:**

$2mF_o-DF_c$ (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.