



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2026 – 02:35 pm BST

PDB ID : 4BCJ / pdb_00004bcj
Title : Structure of CDK9 in complex with cyclin T and a 2-amino-4-heteroaryl-pyrimidine inhibitor
Authors : Hole, A.J.; Baumli, S.; Wang, S.; Endicott, J.A.; Noble, M.E.M.
Deposited on : 2012-10-02
Resolution : 3.16 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	:	1.8.4, CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

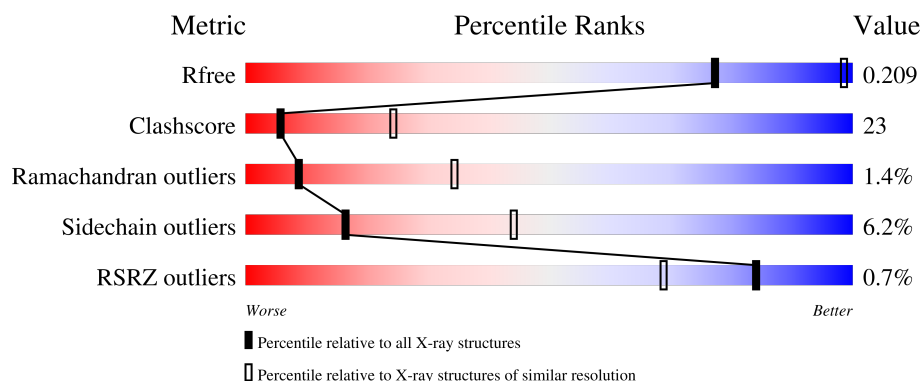
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	331	% 58% 30% 5% 6%
2	B	260	63% 28% 5%

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	T9N	A	1327	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4598 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 CYCLIN-DEPENDENT KINASE 9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	310	2507	1608	432	452	1	14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P50750
A	1	PRO	-	expression tag	UNP P50750

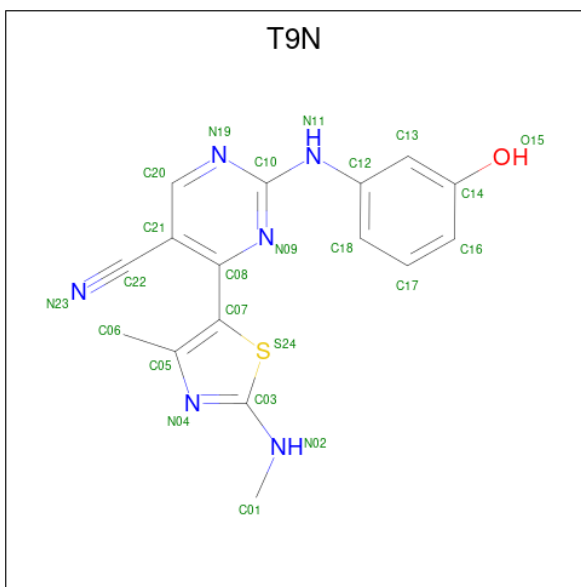
- Molecule 2 is a protein called CYCLIN-T1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	252	2061	1318	360	374	9	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP O60563
B	1	PRO	-	expression tag	UNP O60563
B	77	ARG	GLN	engineered mutation	UNP O60563
B	96	GLY	GLU	engineered mutation	UNP O60563
B	241	LEU	PHE	engineered mutation	UNP O60563

- Molecule 3 is 2-[(3-hydroxyphenyl)amino]-4-[4-methyl-2-(methylamino)-1,3-thiazol-5-yl]pyrimidine-5-carbonitrile (CCD ID: T9N) (formula: C₁₆H₁₄N₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	16	6	1	1		

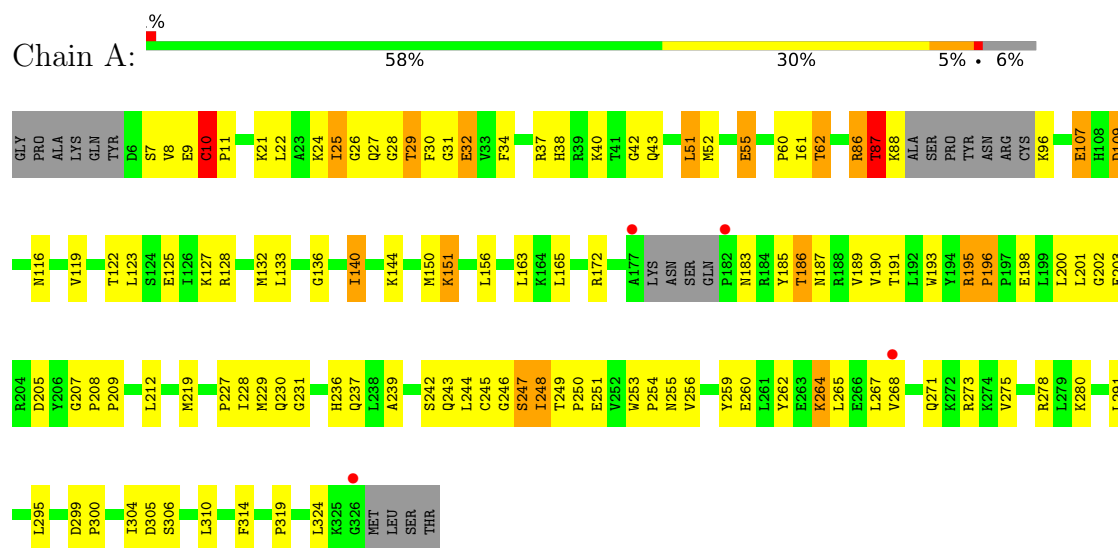
- Molecule 4 is water.

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

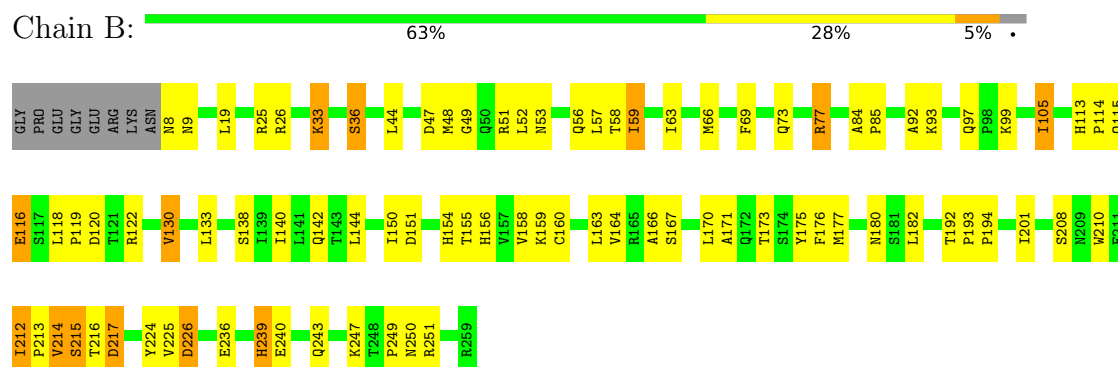
3 Residue-property plots

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: CYCLIN-DEPENDENT KINASE 9



• Molecule 2: CYCLIN-T1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	174.59Å 174.59Å 99.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.67 – 3.16 38.67 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.67-3.16) 99.5 (38.67-3.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.159 , 0.207 0.159 , 0.209	Depositor DCC
R_{free} test set	973 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	97.7	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4598	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: TPO, T9N

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	0.60	0/2545	0.96	10/3431 (0.3%)
2	B	0.75	0/2114	1.05	4/2879 (0.1%)
All	All	0.67	0/4659	1.00	14/6310 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	LYS	N-CA-C	-7.07	102.77	111.40
1	A	10	CYS	CA-C-N	6.54	126.47	119.28
1	A	10	CYS	C-N-CA	6.54	126.47	119.28
1	A	62	THR	CB-CA-C	-6.51	99.78	110.85
1	A	324	LEU	N-CA-C	5.81	117.99	108.52
1	A	196	PRO	CA-C-N	5.70	125.17	119.24
1	A	196	PRO	C-N-CA	5.70	125.17	119.24
2	B	53	ASN	CB-CA-C	-5.63	103.74	111.73
1	A	7	SER	N-CA-C	5.55	117.07	110.19
2	B	239	HIS	N-CA-C	-5.48	105.21	111.07
2	B	130	VAL	N-CA-C	-5.35	105.39	110.42
1	A	195	ARG	CA-C-N	5.20	125.73	120.38
1	A	195	ARG	C-N-CA	5.20	125.73	120.38
1	A	87	THR	N-CA-C	-5.13	106.97	113.43

There are no chirality outliers.

There are no planarity outliers.

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	2507	0	2558	119	0
2	B	2061	0	2049	87	0
3	A	24	0	14	11	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
All	All	4598	0	4621	214	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 23.

All (214) 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)
2:B:164:VAL:CG1	2:B:212:ILE:HD13	1.69	1.22
3:A:1327:T9N:N23	3:A:1327:T9N:H062	1.59	1.15
2:B:164:VAL:HG11	2:B:212:ILE:HD13	1.22	1.06
1:A:55:GLU:HG2	1:A:60:PRO:HG3	1.39	1.04
1:A:193:TRP:CD1	1:A:230:GLN:HA	1.93	1.04
2:B:118:LEU:HD12	2:B:119:PRO:HD2	1.41	0.99
3:A:1327:T9N:C22	3:A:1327:T9N:C06	2.43	0.96
3:A:1327:T9N:H062	3:A:1327:T9N:C22	1.96	0.96
2:B:160:CYS:SG	2:B:201:ILE:HD13	2.10	0.92
1:A:196:PRO:HB2	1:A:198:GLU:OE1	1.69	0.92
1:A:133:LEU:C	1:A:133:LEU:HD23	1.95	0.92
1:A:123:LEU:HD23	1:A:319:PRO:HD2	1.52	0.90
2:B:138:SER:O	2:B:142:GLN:HG3	1.73	0.89
2:B:77:ARG:HH11	2:B:77:ARG:CG	1.86	0.88
2:B:164:VAL:HG11	2:B:212:ILE:CD1	2.04	0.88
1:A:107:GLU:HA	1:A:107:GLU:OE1	1.72	0.87
2:B:164:VAL:HG13	2:B:212:ILE:HD13	1.56	0.87
2:B:77:ARG:HH11	2:B:77:ARG:HG2	1.40	0.87
2:B:113:HIS:HB3	2:B:116:GLU:HB2	1.56	0.86
1:A:249:THR:HG22	1:A:251:GLU:H	1.41	0.85
2:B:164:VAL:HG13	2:B:212:ILE:HG21	1.59	0.83
1:A:55:GLU:N	1:A:55:GLU:OE1	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:ALA:HB1	2:B:170:LEU:HD23	1.60	0.81
3:A:1327:T9N:N23	3:A:1327:T9N:C06	2.43	0.80
1:A:183:ASN:HB2	1:A:205:ASP:OD1	1.82	0.80
2:B:159:LYS:O	2:B:163:LEU:HD12	1.84	0.78
1:A:248:ILE:CG2	1:A:256:VAL:HG21	2.13	0.78
1:A:267:LEU:HG	1:A:268:VAL:N	1.99	0.76
2:B:171:ALA:O	2:B:175:TYR:CD1	2.42	0.73
1:A:51:LEU:O	1:A:52:MET:HG2	1.88	0.73
2:B:84:ALA:HB3	2:B:85:PRO:HD3	1.70	0.73
2:B:239:HIS:CE1	2:B:243:GLN:HE21	2.07	0.72
1:A:8:VAL:HG22	1:A:9:GLU:H	1.57	0.69
2:B:118:LEU:HD12	2:B:119:PRO:CD	2.22	0.69
2:B:150:ILE:HG22	2:B:151:ASP:N	2.06	0.69
3:A:1327:T9N:N09	3:A:1327:T9N:H18	2.08	0.68
2:B:192:THR:C	2:B:194:PRO:HD2	2.19	0.68
1:A:109:ASP:HB2	1:A:156:LEU:CD2	2.24	0.68
1:A:248:ILE:HG22	1:A:256:VAL:HG21	1.74	0.68
1:A:219:MET:HE1	1:A:291:LEU:HD23	1.75	0.68
2:B:217:ASP:OD2	2:B:224:TYR:OH	2.13	0.67
1:A:8:VAL:HG22	1:A:9:GLU:N	2.10	0.67
1:A:228:ILE:HG13	1:A:229:MET:HG3	1.77	0.66
2:B:239:HIS:CE1	2:B:243:GLN:NE2	2.63	0.66
1:A:30:PHE:CD1	1:A:30:PHE:O	2.48	0.66
1:A:267:LEU:HG	1:A:268:VAL:H	1.59	0.66
1:A:87:THR:O	1:A:88:LYS:HB2	1.96	0.65
1:A:239:ALA:HA	1:A:267:LEU:CD2	2.27	0.64
1:A:248:ILE:HG21	1:A:256:VAL:HG21	1.79	0.64
1:A:38:HIS:HE1	1:A:40:LYS:HB2	1.64	0.63
2:B:171:ALA:O	2:B:175:TYR:HD1	1.81	0.63
1:A:133:LEU:C	1:A:133:LEU:CD2	2.70	0.62
1:A:27:GLN:O	1:A:30:PHE:CD2	2.53	0.62
2:B:150:ILE:CG2	2:B:151:ASP:N	2.62	0.62
1:A:24:LYS:HG2	1:A:34:PHE:CE1	2.34	0.62
1:A:55:GLU:HG2	1:A:60:PRO:CG	2.22	0.62
1:A:193:TRP:NE1	1:A:230:GLN:HA	2.15	0.62
1:A:227:PRO:HB2	1:A:230:GLN:HE21	1.64	0.61
1:A:195:ARG:HD2	1:A:200:LEU:CD2	2.31	0.60
1:A:87:THR:O	1:A:88:LYS:CB	2.49	0.60
1:A:133:LEU:HD23	1:A:133:LEU:O	2.01	0.60
1:A:207:GLY:C	1:A:209:PRO:HD2	2.27	0.59
1:A:30:PHE:HE1	3:A:1327:T9N:C01	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:ARG:CG	2:B:77:ARG:NH1	2.56	0.59
1:A:245:CYS:HA	1:A:273:ARG:HG3	1.85	0.58
2:B:193:PRO:N	2:B:194:PRO:CD	2.65	0.58
2:B:173:THR:O	2:B:177:MET:HG2	2.03	0.58
1:A:195:ARG:HG3	1:A:196:PRO:HD2	1.85	0.58
1:A:172:ARG:HH21	1:A:185:TYR:HE1	1.52	0.57
1:A:249:THR:C	1:A:251:GLU:N	2.61	0.57
1:A:295:LEU:HD23	1:A:304:ILE:CG2	2.34	0.57
1:A:52:MET:HB2	1:A:55:GLU:HB2	1.86	0.57
1:A:254:PRO:O	1:A:255:ASN:HB2	2.05	0.57
1:A:187:ASN:ND2	1:A:202:GLY:HA2	2.19	0.57
2:B:193:PRO:HB2	2:B:194:PRO:HD3	1.87	0.57
1:A:123:LEU:HD23	1:A:319:PRO:CD	2.31	0.56
1:A:38:HIS:CE1	1:A:40:LYS:HB2	2.41	0.56
1:A:30:PHE:CE1	3:A:1327:T9N:C01	2.89	0.55
1:A:87:THR:CG2	1:A:88:LYS:N	2.68	0.55
1:A:187:ASN:C	1:A:187:ASN:OD1	2.49	0.55
1:A:242:SER:HA	1:A:246:GLY:O	2.07	0.55
1:A:244:LEU:HD13	1:A:278:ARG:NH1	2.21	0.55
1:A:239:ALA:HA	1:A:267:LEU:HD21	1.88	0.55
1:A:128:ARG:O	1:A:132:MET:HG3	2.06	0.55
1:A:239:ALA:HA	1:A:267:LEU:HD22	1.89	0.55
2:B:180:ASN:OD1	2:B:251:ARG:HD2	2.06	0.55
1:A:212:LEU:HD13	1:A:305:ASP:HA	1.89	0.55
2:B:44:LEU:HG	2:B:48:MET:HE2	1.89	0.55
2:B:105:ILE:HD11	2:B:130:VAL:HA	1.87	0.55
1:A:21:LYS:O	1:A:22:LEU:HD23	2.06	0.55
3:A:1327:T9N:C22	3:A:1327:T9N:H061	2.32	0.55
1:A:198:GLU:HG2	1:A:300:PRO:HG3	1.89	0.54
2:B:164:VAL:HG12	2:B:164:VAL:O	2.06	0.54
1:A:244:LEU:HD13	1:A:278:ARG:HH11	1.72	0.53
2:B:59:ILE:O	2:B:63:ILE:HG13	2.08	0.53
1:A:193:TRP:NE1	1:A:230:GLN:CA	2.72	0.53
1:A:55:GLU:OE1	1:A:55:GLU:CA	2.53	0.53
2:B:158:VAL:HG22	2:B:175:TYR:OH	2.08	0.53
2:B:192:THR:C	2:B:194:PRO:CD	2.81	0.53
1:A:122:THR:HG23	1:A:125:GLU:OE1	2.08	0.53
2:B:105:ILE:CD1	2:B:130:VAL:HA	2.39	0.53
2:B:170:LEU:HD22	2:B:210:TRP:CE3	2.44	0.53
1:A:201:LEU:O	1:A:259:TYR:HD2	1.91	0.53
1:A:87:THR:HG22	1:A:88:LYS:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TPO:O2P	1:A:186:TPO:HG22	2.09	0.52
1:A:30:PHE:O	1:A:30:PHE:HD1	1.94	0.51
1:A:116:ASN:HB3	1:A:119:VAL:HG23	1.90	0.51
3:A:1327:T9N:N09	3:A:1327:T9N:C18	2.73	0.51
1:A:239:ALA:O	1:A:243:GLN:HG3	2.11	0.51
2:B:225:VAL:O	2:B:226:ASP:HB2	2.09	0.51
2:B:214:VAL:O	2:B:215:SER:O	2.28	0.51
1:A:248:ILE:HD13	1:A:248:ILE:N	2.26	0.51
2:B:249:PRO:O	2:B:250:ASN:HB2	2.10	0.51
1:A:30:PHE:HE1	3:A:1327:T9N:H012	1.76	0.50
2:B:193:PRO:CB	2:B:194:PRO:HD3	2.41	0.50
2:B:69:PHE:CZ	2:B:73:GLN:HG3	2.45	0.50
2:B:225:VAL:O	2:B:225:VAL:HG12	2.11	0.50
1:A:109:ASP:HB2	1:A:156:LEU:HD22	1.92	0.50
2:B:192:THR:HB	2:B:194:PRO:HD2	1.93	0.49
2:B:154:HIS:O	2:B:155:THR:C	2.55	0.49
2:B:236:GLU:O	2:B:240:GLU:HG3	2.12	0.49
1:A:10:CYS:N	1:A:11:PRO:HD3	2.27	0.49
1:A:212:LEU:HD13	1:A:304:ILE:O	2.13	0.49
2:B:113:HIS:C	2:B:115:GLN:N	2.69	0.49
1:A:107:GLU:OE1	1:A:107:GLU:CA	2.47	0.49
2:B:133:LEU:HD23	2:B:133:LEU:C	2.38	0.48
2:B:33:LYS:O	2:B:36:SER:HB2	2.13	0.48
1:A:136:GLY:O	1:A:140:ILE:HG23	2.13	0.48
1:A:150:MET:HE1	1:A:165:LEU:HD22	1.95	0.48
1:A:267:LEU:CG	1:A:268:VAL:N	2.75	0.48
1:A:150:MET:O	1:A:151:LYS:HG2	2.13	0.48
1:A:195:ARG:HD2	1:A:200:LEU:HD21	1.95	0.48
1:A:264:LYS:O	1:A:264:LYS:HG3	2.14	0.48
1:A:127:LYS:HG2	1:A:314:PHE:CZ	2.49	0.48
1:A:193:TRP:CD1	1:A:230:GLN:CA	2.82	0.47
1:A:253:TRP:CD1	1:A:253:TRP:C	2.92	0.47
1:A:31:GLY:O	1:A:32:GLU:HB2	2.15	0.47
1:A:37:ARG:HH11	1:A:37:ARG:HG2	1.80	0.47
2:B:113:HIS:HB3	2:B:116:GLU:CB	2.36	0.47
2:B:166:ALA:CB	2:B:170:LEU:HD23	2.40	0.47
2:B:56:GLN:O	2:B:56:GLN:HG3	2.13	0.47
2:B:73:GLN:HA	2:B:73:GLN:OE1	2.14	0.47
1:A:109:ASP:CB	1:A:156:LEU:HD22	2.45	0.46
2:B:113:HIS:O	2:B:115:GLN:N	2.48	0.46
1:A:231:GLY:H	1:A:237:GLN:HE22	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:MET:C	1:A:151:LYS:CG	2.89	0.46
2:B:239:HIS:HE1	2:B:243:GLN:NE2	2.14	0.46
1:A:151:LYS:HD3	1:A:191:THR:OG1	2.16	0.46
1:A:249:THR:O	1:A:251:GLU:N	2.49	0.46
2:B:120:ASP:O	2:B:122:ARG:N	2.49	0.46
2:B:140:ILE:O	2:B:144:LEU:HG	2.15	0.46
1:A:24:LYS:CG	1:A:34:PHE:CE1	2.99	0.46
2:B:47:ASP:O	2:B:51:ARG:HG3	2.16	0.46
2:B:225:VAL:O	2:B:225:VAL:CG1	2.64	0.46
1:A:249:THR:C	1:A:251:GLU:H	2.23	0.46
2:B:19:LEU:HD23	2:B:19:LEU:HA	1.68	0.45
2:B:77:ARG:HH11	2:B:77:ARG:HG3	1.76	0.45
1:A:295:LEU:HD23	1:A:304:ILE:HG22	1.98	0.45
2:B:156:HIS:CD2	2:B:156:HIS:H	2.33	0.45
2:B:113:HIS:O	2:B:114:PRO:C	2.59	0.45
1:A:8:VAL:CG2	1:A:9:GLU:N	2.79	0.45
1:A:8:VAL:CG2	1:A:9:GLU:H	2.27	0.45
3:A:1327:T9N:C22	3:A:1327:T9N:C05	2.90	0.45
1:A:208:PRO:N	1:A:209:PRO:CD	2.80	0.45
1:A:260:GLU:C	1:A:262:TYR:H	2.24	0.45
1:A:249:THR:O	1:A:250:PRO:C	2.59	0.45
1:A:28:GLY:O	1:A:30:PHE:N	2.50	0.44
2:B:77:ARG:HG2	2:B:77:ARG:NH1	2.19	0.44
1:A:28:GLY:C	1:A:30:PHE:N	2.74	0.44
2:B:52:LEU:O	2:B:99:LYS:HE3	2.17	0.44
1:A:299:ASP:HA	1:A:300:PRO:HD2	1.84	0.44
2:B:25:ARG:CZ	2:B:25:ARG:HB2	2.47	0.44
1:A:109:ASP:HB2	1:A:156:LEU:HD23	1.97	0.44
2:B:171:ALA:O	2:B:175:TYR:CE1	2.70	0.44
2:B:192:THR:O	2:B:193:PRO:C	2.60	0.44
2:B:120:ASP:C	2:B:122:ARG:N	2.75	0.44
1:A:29:THR:O	1:A:29:THR:HG22	2.18	0.43
1:A:247:SER:OG	1:A:271:GLN:HB2	2.17	0.43
2:B:170:LEU:HD22	2:B:210:TRP:CD2	2.54	0.43
1:A:163:LEU:HD23	1:A:163:LEU:C	2.44	0.43
1:A:25:ILE:H	1:A:25:ILE:HG12	1.70	0.43
1:A:195:ARG:CG	1:A:196:PRO:HD2	2.48	0.43
1:A:24:LYS:HG2	1:A:34:PHE:CD1	2.54	0.43
2:B:49:GLY:HA3	2:B:59:ILE:HD11	2.01	0.43
2:B:164:VAL:CG1	2:B:212:ILE:HG21	2.41	0.43
1:A:195:ARG:HD2	1:A:200:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:LEU:HD12	2:B:57:LEU:HA	1.85	0.42
2:B:182:LEU:HA	2:B:182:LEU:HD23	1.87	0.42
1:A:52:MET:O	1:A:52:MET:HG3	2.20	0.42
2:B:92:ALA:HB1	2:B:97:GLN:O	2.20	0.42
2:B:120:ASP:C	2:B:122:ARG:H	2.28	0.42
1:A:236:HIS:O	1:A:239:ALA:HB3	2.20	0.42
2:B:58:THR:O	2:B:59:ILE:C	2.62	0.42
2:B:192:THR:CB	2:B:194:PRO:HD2	2.50	0.42
1:A:273:ARG:HG2	1:A:275:VAL:H	1.84	0.42
1:A:203:GLU:OE2	1:A:205:ASP:HB3	2.20	0.42
2:B:113:HIS:C	2:B:115:GLN:H	2.28	0.41
2:B:8:ASN:HB3	2:B:9:ASN:H	1.71	0.41
1:A:144:LYS:HD3	1:A:144:LYS:HA	1.80	0.41
2:B:173:THR:O	2:B:176:PHE:HB3	2.21	0.41
2:B:52:LEU:O	2:B:99:LYS:CE	2.69	0.41
1:A:187:ASN:HD21	1:A:202:GLY:HA2	1.84	0.41
1:A:248:ILE:HG23	1:A:253:TRP:HE3	1.86	0.41
2:B:247:LYS:O	2:B:249:PRO:HD3	2.19	0.41
1:A:86:ARG:HG3	1:A:87:THR:N	2.35	0.41
2:B:214:VAL:O	2:B:215:SER:C	2.64	0.41
1:A:116:ASN:HB3	1:A:119:VAL:CG2	2.51	0.41
1:A:310:LEU:HA	1:A:310:LEU:HD23	1.85	0.40
2:B:214:VAL:C	2:B:215:SER:O	2.64	0.40
1:A:51:LEU:O	1:A:52:MET:CG	2.65	0.40
2:B:66:MET:HE3	2:B:66:MET:HB3	2.01	0.40
2:B:164:VAL:CG1	2:B:164:VAL:O	2.70	0.40
1:A:42:GLY:O	1:A:43:GLN:C	2.65	0.40
2:B:212:ILE:HA	2:B:213:PRO:HD3	1.83	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	303/331 (92%)	269 (89%)	29 (10%)	5 (2%)	7	30
2	B	250/260 (96%)	232 (93%)	15 (6%)	3 (1%)	10	37
All	All	553/591 (94%)	501 (91%)	44 (8%)	8 (1%)	9	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	THR
2	B	215	SER
1	A	26	GLY
1	A	190	VAL
2	B	226	ASP
1	A	265	LEU
2	B	167	SER
1	A	51	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/291 (94%)	254 (93%)	19 (7%)	14	40
2	B	230/236 (98%)	218 (95%)	12 (5%)	21	49
All	All	503/527 (95%)	472 (94%)	31 (6%)	16	44

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	CYS
1	A	25	ILE
1	A	32	GLU
1	A	55	GLU
1	A	61	ILE
1	A	62	THR
1	A	86	ARG
1	A	87	THR

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Mol	Chain	Res	Type
1	A	96	LYS
1	A	107	GLU
1	A	109	ASP
1	A	140	ILE
1	A	151	LYS
1	A	189	VAL
1	A	247	SER
1	A	248	ILE
1	A	264	LYS
1	A	280	LYS
1	A	306	SER
2	B	26	ARG
2	B	33	LYS
2	B	36	SER
2	B	59	ILE
2	B	77	ARG
2	B	105	ILE
2	B	116	GLU
2	B	208	SER
2	B	212	ILE
2	B	214	VAL
2	B	216	THR
2	B	217	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	230	GLN
1	A	232	ASN
1	A	237	GLN
1	A	302	GLN
2	B	109	HIS
2	B	113	HIS
2	B	156	HIS
2	B	239	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	TPO	A	186	1	8,10,11	0.88	0	10,14,16	1.37	2 (20%)

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
1	TPO	A	186	1	-	6/9/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	TPO	P-OG1-CB	2.36	130.34	123.21
1	A	186	TPO	O-C-CA	-2.15	119.16	124.78

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	186	TPO	N-CA-CB-CG2
1	A	186	TPO	N-CA-CB-OG1
1	A	186	TPO	C-CA-CB-CG2
1	A	186	TPO	O-C-CA-CB
1	A	186	TPO	CG2-CB-OG1-P
1	A	186	TPO	CA-CB-OG1-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	186	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	T9N	A	1327	-	25,26,26	2.62	12 (48%)	30,36,36	4.51	12 (40%)

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	T9N	A	1327	-	-	5/10/12/12	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1327	T9N	C21-C22	5.59	1.52	1.44
3	A	1327	T9N	C10-N11	4.51	1.45	1.36
3	A	1327	T9N	C03-N04	4.49	1.37	1.31
3	A	1327	T9N	C03-N02	4.15	1.40	1.34
3	A	1327	T9N	C03-S24	-3.85	1.67	1.73
3	A	1327	T9N	C07-S24	-3.26	1.66	1.74
3	A	1327	T9N	C08-C07	3.20	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1327	T9N	C07-C05	3.12	1.41	1.36
3	A	1327	T9N	C12-N11	3.03	1.47	1.40
3	A	1327	T9N	C16-C14	2.95	1.44	1.38
3	A	1327	T9N	C10-N19	2.81	1.38	1.34
3	A	1327	T9N	C17-C18	2.19	1.43	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1327	T9N	C03-S24-C07	17.49	99.82	88.32
3	A	1327	T9N	S24-C03-N04	-9.73	106.86	115.85
3	A	1327	T9N	C05-C07-S24	-9.44	103.84	109.89
3	A	1327	T9N	C08-C07-S24	5.19	127.21	118.04
3	A	1327	T9N	C03-N04-C05	4.68	113.24	110.36
3	A	1327	T9N	C07-C08-N09	4.37	121.04	114.35
3	A	1327	T9N	C21-C20-N19	-3.03	118.88	123.42
3	A	1327	T9N	C01-N02-C03	-2.98	118.91	123.36
3	A	1327	T9N	N19-C10-N09	-2.64	124.05	126.55
3	A	1327	T9N	C12-N11-C10	-2.53	121.88	129.23
3	A	1327	T9N	C20-N19-C10	2.38	119.46	115.88
3	A	1327	T9N	C06-C05-C07	-2.27	122.82	127.15

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1327	T9N	N04-C03-N02-C01
3	A	1327	T9N	S24-C03-N02-C01
3	A	1327	T9N	C20-C21-C22-N23
3	A	1327	T9N	N09-C10-N11-C12
3	A	1327	T9N	N19-C10-N11-C12

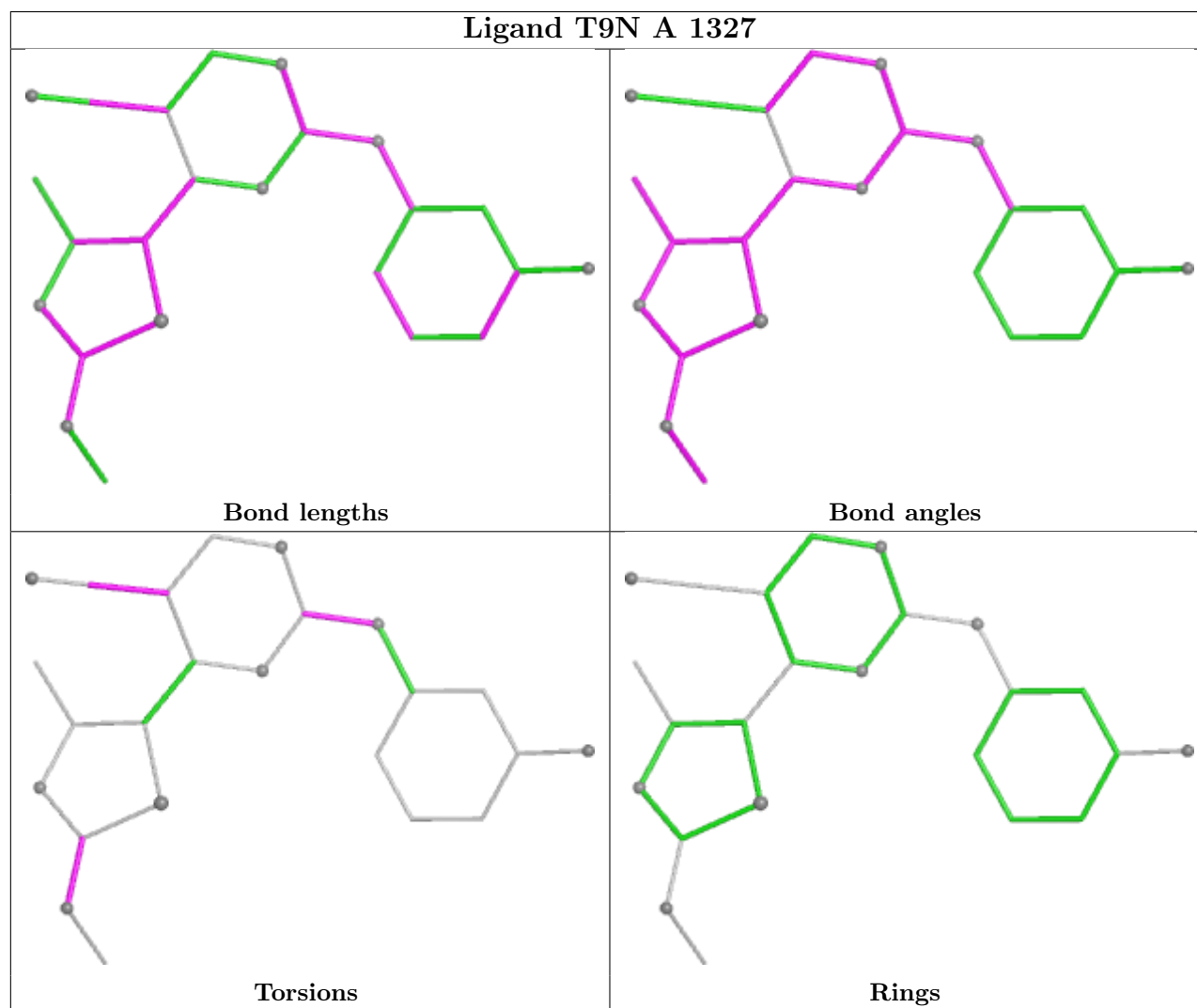
There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1327	T9N	11	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.



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	309/331 (93%)	-0.58	4 (1%) 75 55	60, 103, 164, 214	0
2	B	252/260 (96%)	-0.82	0 100 100	56, 86, 145, 195	0
All	All	561/591 (94%)	-0.69	4 (0%) 84 69	56, 95, 157, 214	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	VAL	3.6
1	A	182	PRO	3.2
1	A	326	GLY	2.4
1	A	177	ALA	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	A	186	11/12	0.98	0.05	88,96,103,104	0

6.3 Carbohydrates [i](#)

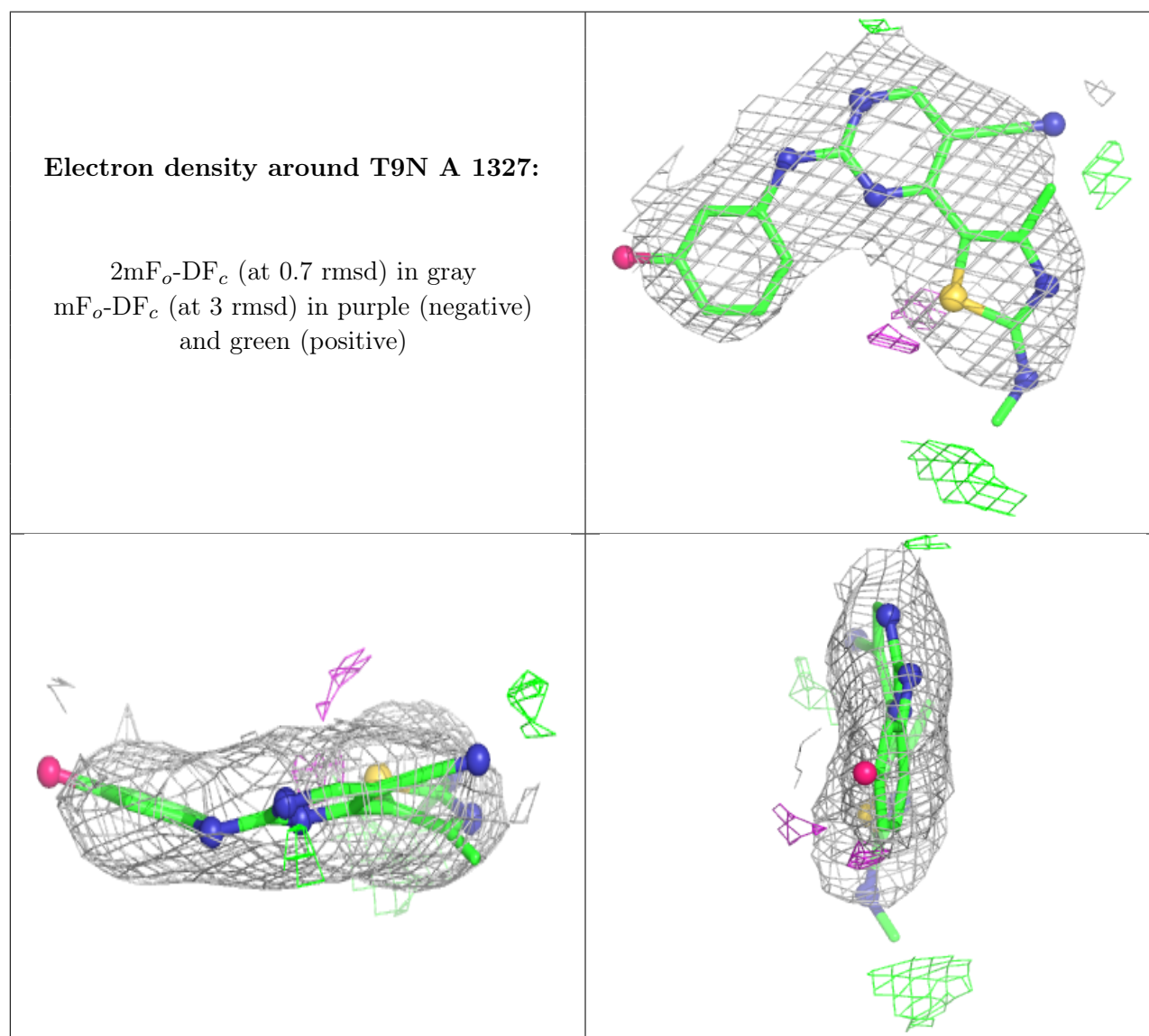
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	T9N	A	1327	24/24	0.97	0.07	72,87,103,124	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.