Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 12:05 PM EDT

PDB ID	:	3DOG
Title	:	Structure of Thr 160 phosphorylated CDK2/cyclin A in complex with the inhibitor N-&-N1
Authors	:	Echalier, A.; Endicott, J.
Deposited on	:	2008-07-04
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 ⓘ 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:

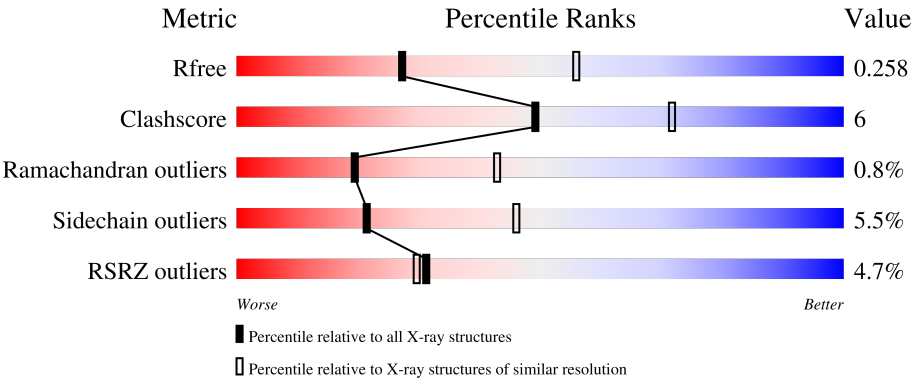
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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% 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	299	3% 82% 15%
1	C	299	4% 75% 12% 10%
2	B	264	3% 82% 15%
2	D	264	8% 86% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9088 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 Cell division protein kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	P	S	0	1	0
			2408	1564	410	425	1	8			
1	C	268	Total	C	N	O	P	S	0	0	0
			2152	1393	369	382	1	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

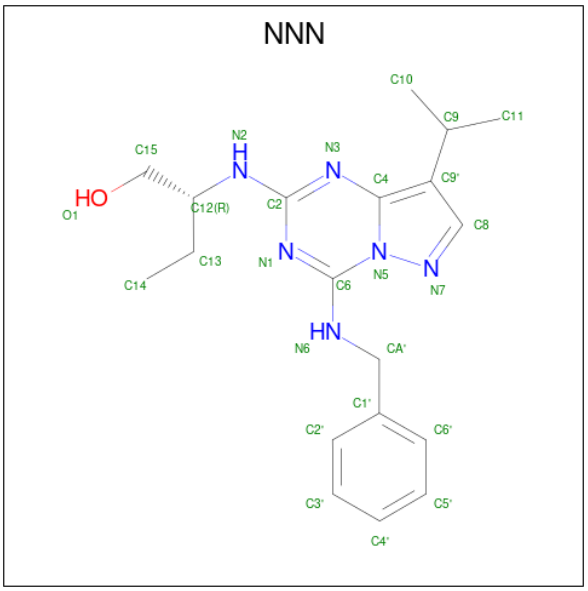
- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	0	0
			2112	1367	344	391	10			
2	D	264	Total	C	N	O	S	0	0	0
			2131	1378	348	395	10			

There are 4 discrepancies between the modelled and reference sequences:

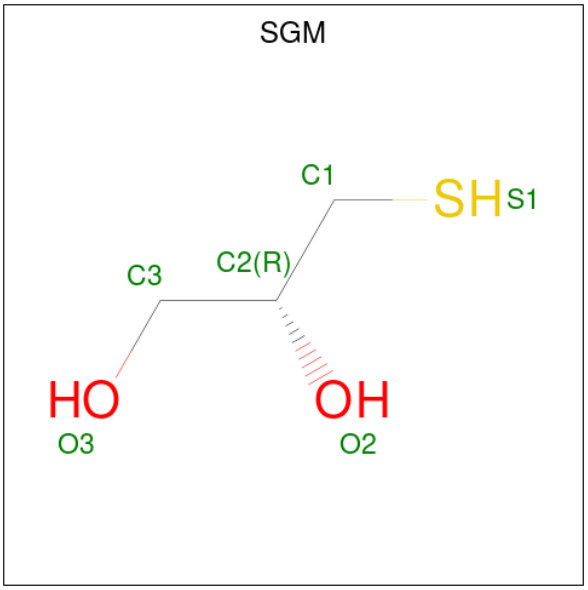
Chain	Residue	Modelled	Actual	Comment	Reference
B	433	GLU	-	expression tag	UNP P30274
B	434	HIS	-	expression tag	UNP P30274
D	433	GLU	-	expression tag	UNP P30274
D	434	HIS	-	expression tag	UNP P30274

- Molecule 3 is (2R)-2-{[4-(benzylamino)-8-(1-methylethyl)pyrazolo[1,5-a][1,3,5]triazin-2-yl]amino}butan-1-ol (three-letter code: NNN) (formula: $C_{19}H_{26}N_6O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	19	6	1		
3	C	1	Total	C	N	O	0	0
			26	19	6	1		

- Molecule 4 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: $C_3H_8O_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			6	3	2	1		
4	B	1	Total	C	O	S	0	0
			6	3	2	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O S 6 3 2 1	0	0

- Molecule 5 is water.

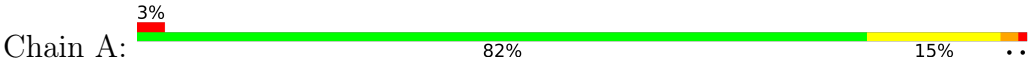
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	73	Total O 73 73	0	0
5	B	59	Total O 59 59	0	0
5	C	45	Total O 45 45	0	0
5	D	38	Total O 38 38	0	0

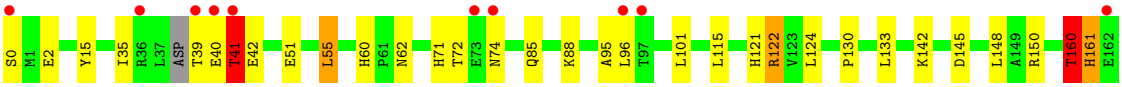
3 Residue-property plots (i)

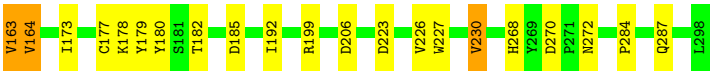
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cell division protein kinase 2

Chain A:

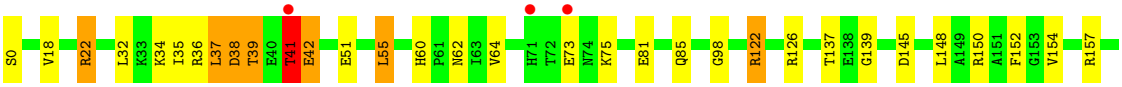


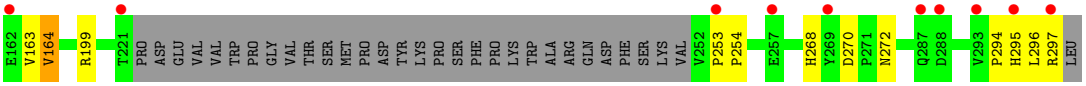




• Molecule 1: Cell division protein kinase 2

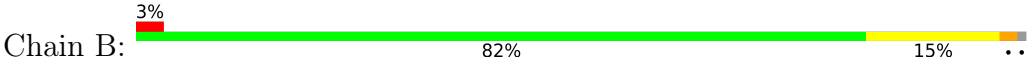
Chain C:

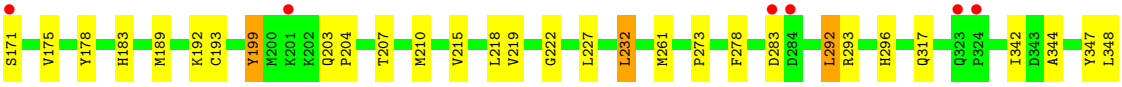




• Molecule 2: Cyclin-A2

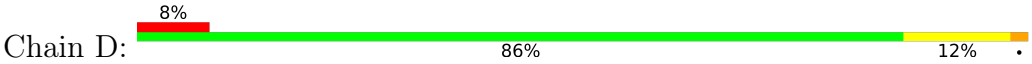
Chain B:

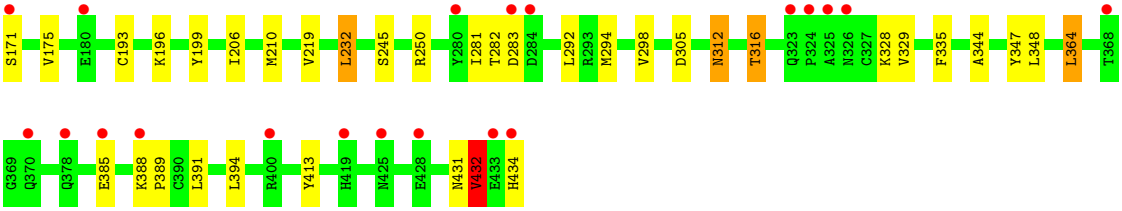




• Molecule 2: Cyclin-A2

Chain D:




S171
V175
E180
C193
K196
Y199
I206
M210
V219
L232
S245
R250
Y280
I281
T282
D283
D284
L292
R293
M294
V298
D305
N312
T316
Q323
P324
A325
N326
C327
K328
V329
F335
A344
Y347
L348
L364
T368
G369
Q370
Q378
E385
K388
P389
C390
L391
L394
R400
Y413
H419
M425
E428
N431
V432
E433
H434

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.42Å 133.49Å 148.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.91 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.70) 98.7 (19.91-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.248 0.212 , 0.258	Depositor DCC
R_{free} test set	2037 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 21.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9088	wwPDB-VP
Average B, all atoms (Å^2)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, NNN, SGM

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	0.41	0/2457	0.56	1/3331 (0.0%)
1	C	0.47	1/2189 (0.0%)	0.63	3/2963 (0.1%)
2	B	0.39	0/2162	0.58	1/2940 (0.0%)
2	D	0.38	0/2182	0.55	0/2967
All	All	0.41	1/8990 (0.0%)	0.58	5/12201 (0.0%)

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	1	1
1	C	0	1
All	All	1	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	39	THR	CA-CB	-5.13	1.40	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	41	THR	N-CA-C	-6.87	92.45	111.00
1	C	41	THR	C-N-CA	6.73	138.52	121.70
1	C	41	THR	O-C-N	-5.81	113.41	122.70
1	A	161	HIS	N-CA-C	5.55	126.00	111.00
2	B	428	GLU	C-N-CA	5.43	135.27	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	161	HIS	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	TPO	Peptide
1	C	41	THR	Peptide

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	2408	0	2462	30	0
1	C	2152	0	2207	31	0
2	B	2112	0	2129	32	0
2	D	2131	0	2143	18	0
3	A	26	0	26	1	0
3	C	26	0	26	3	0
4	B	12	0	15	2	0
4	D	6	0	8	2	0
5	A	73	0	0	2	0
5	B	59	0	0	3	0
5	C	45	0	0	4	0
5	D	38	0	0	1	0
All	All	9088	0	9016	106	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 (106) 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:C:37:LEU:HA	1:C:38:ASP:HB2	1.35	1.04
2:D:193:CYS:SG	4:D:1:SGM:S1	2.54	0.96
1:C:39:THR:HG22	1:C:39:THR:O	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:CYS:SG	4:B:1:SGM:S1	2.60	0.86
1:C:37:LEU:HA	1:C:38:ASP:CB	2.05	0.86
1:A:227:TRP:O	1:A:230:VAL:HG22	1.78	0.82
1:A:0:SER:N	1:A:2:GLU:OE1	2.11	0.82
1:A:60:HIS:HD2	1:A:62:ASN:H	1.32	0.76
1:A:60:HIS:CD2	1:A:62:ASN:H	2.07	0.72
1:C:154:VAL:O	2:D:316:THR:HG23	1.91	0.70
1:A:272:ASN:OD1	2:B:171:SER:HB3	1.91	0.70
2:B:415:ASN:HD22	2:B:417:LYS:H	1.40	0.69
1:C:39:THR:O	1:C:39:THR:CG2	2.38	0.69
1:C:37:LEU:CA	1:C:38:ASP:HB2	2.20	0.69
2:B:192:LYS:HB3	4:B:1:SGM:H31	1.77	0.67
2:D:312:ASN:HB3	5:D:488:HOH:O	1.94	0.66
1:C:295:HIS:O	1:C:296:LEU:HB2	1.93	0.66
1:C:85:GLN:HA	3:C:299:NNN:HA'A	1.77	0.66
1:A:85:GLN:HA	3:A:299:NNN:HA'A	1.83	0.61
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.36	0.60
1:C:295:HIS:CD2	1:C:296:LEU:HD13	2.37	0.59
1:C:60:HIS:CD2	1:C:62:ASN:H	2.20	0.59
1:C:272:ASN:OD1	2:D:171:SER:HB3	2.02	0.59
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.84	0.58
2:D:305:ASP:HB3	4:D:1:SGM:H12	1.86	0.57
1:A:121:HIS:O	1:A:122:ARG:HG3	2.04	0.57
2:D:210:MET:CE	2:D:250:ARG:HG3	2.35	0.57
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.87	0.57
1:C:64:VAL:HG21	3:C:299:NNN:H11A	1.86	0.57
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.88	0.56
1:A:148:LEU:HB3	5:A:360:HOH:O	2.06	0.56
1:C:22:ARG:HD2	5:C:317:HOH:O	2.05	0.56
1:A:88:LYS:HB2	1:A:130:PRO:HB2	1.87	0.56
1:C:60:HIS:HD2	1:C:62:ASN:H	1.53	0.55
2:D:210:MET:HE1	2:D:250:ARG:HG3	1.87	0.55
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.88	0.55
2:D:206:ILE:HG22	2:D:210:MET:CE	2.37	0.54
2:D:175:VAL:O	2:D:175:VAL:HG13	2.07	0.54
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.72	0.54
2:B:207:THR:OG1	2:B:210:MET:HG3	2.07	0.54
2:B:407:GLN:O	2:B:411:GLU:HG2	2.07	0.54
1:C:37:LEU:CA	1:C:38:ASP:CB	2.83	0.54
1:C:268:HIS:HD2	1:C:270:ASP:H	1.57	0.53
2:D:329:VAL:HG11	2:D:364:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:O	1:A:41:THR:N	2.41	0.52
2:B:171:SER:CB	5:B:453:HOH:O	2.57	0.52
1:A:160:TPO:O	1:A:180:TYR:OH	2.12	0.52
2:B:175:VAL:HG12	2:B:178:TYR:HB2	1.91	0.52
1:C:51:GLU:O	1:C:55:LEU:HB2	2.09	0.52
2:D:206:ILE:HG22	2:D:210:MET:HE1	1.93	0.51
1:C:126:ARG:HD2	1:C:163:VAL:HG21	1.92	0.51
2:B:171:SER:HB2	5:B:453:HOH:O	2.10	0.51
2:B:347:TYR:OH	2:B:394:LEU:HA	2.11	0.50
1:A:268:HIS:HD2	1:A:270:ASP:H	1.59	0.50
2:B:175:VAL:CG1	2:B:178:TYR:HB2	2.42	0.50
1:A:115:LEU:HD21	1:A:185:ASP:HB3	1.94	0.49
2:B:215:VAL:HG12	2:B:342:ILE:HD13	1.94	0.49
2:D:432:VAL:O	2:D:432:VAL:CG2	2.61	0.48
2:B:428:GLU:HB3	2:B:429:THR:OG1	2.14	0.48
1:C:122:ARG:HA	1:C:152:PHE:CZ	2.49	0.48
1:C:35:ILE:HG23	5:C:333:HOH:O	2.13	0.48
2:B:407:GLN:OE1	2:B:410:ARG:HD3	2.15	0.47
2:B:199:TYR:CE2	2:B:348:LEU:HD21	2.49	0.47
1:A:133:LEU:HD11	1:A:192:ILE:HD13	1.97	0.47
1:A:124:LEU:HD21	1:A:182:THR:HA	1.97	0.47
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.96	0.47
1:A:121:HIS:C	1:A:122:ARG:HG3	2.35	0.46
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.98	0.46
1:C:296:LEU:HA	5:C:331:HOH:O	2.16	0.46
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.98	0.46
2:B:273:PRO:HG2	2:B:278:PHE:CE2	2.51	0.46
1:A:39:THR:HB	2:B:292:LEU:HD23	1.98	0.45
1:C:126:ARG:O	1:C:164:VAL:HB	2.17	0.45
1:A:178:LYS:HE2	1:A:179:TYR:CZ	2.51	0.45
2:B:215:VAL:O	2:B:219:VAL:HG23	2.17	0.45
2:B:415:ASN:ND2	2:B:417:LYS:H	2.11	0.45
1:A:15:TYR:HE2	1:A:35:ILE:HD11	1.81	0.45
1:A:95:ALA:HA	1:A:199:ARG:NH1	2.31	0.45
1:A:124:LEU:CD2	1:A:182:THR:HA	2.46	0.45
1:A:163:VAL:HG12	1:A:173:ILE:HD13	2.00	0.44
2:D:347:TYR:OH	2:D:394:LEU:HA	2.18	0.43
2:B:218:LEU:HB3	2:B:261:MET:HE2	2.01	0.43
1:A:284:PRO:O	1:A:287:GLN:HG2	2.19	0.43
1:A:223:ASP:H	1:A:226:VAL:HG12	1.83	0.43
2:B:415:ASN:HD22	2:B:417:LYS:CB	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.92	0.43
1:C:18:VAL:HA	1:C:32:LEU:O	2.19	0.42
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.55	0.42
2:B:376:LEU:HD23	2:B:376:LEU:HA	1.88	0.42
2:B:203:GLN:HA	2:B:204:PRO:HD3	1.92	0.42
2:B:222:GLY:HA2	2:B:227:LEU:HD12	2.00	0.42
1:A:2:GLU:H	1:A:2:GLU:CD	2.23	0.42
1:A:41:THR:HB	1:A:42:GLU:H	1.51	0.41
1:C:253:PRO:HD2	1:C:254:PRO:HD3	2.01	0.41
2:B:361:HIS:HB2	2:B:372:TRP:HB2	2.03	0.41
1:A:51:GLU:O	1:A:55:LEU:HB2	2.21	0.41
1:A:62:ASN:HA	1:A:142:LYS:HG2	2.03	0.41
2:D:294:MET:O	2:D:298:VAL:HG23	2.21	0.41
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.89	0.41
1:C:81:GLU:O	3:C:299:NNN:H8	2.20	0.40
1:C:98:GLY:HA2	1:C:199:ARG:HD3	2.03	0.40
1:C:163:VAL:HG13	1:C:164:VAL:HG12	2.03	0.40
5:A:328:HOH:O	2:B:189:MET:CE	2.70	0.40
2:B:171:SER:HB3	5:B:453:HOH:O	2.21	0.40
1:C:41:THR:HB	1:C:42:GLU:HB2	2.03	0.40
1:C:164:VAL:HG23	5:C:338:HOH: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	294/299 (98%)	283 (96%)	7 (2%)	4 (1%)	11	28
1	C	263/299 (88%)	250 (95%)	11 (4%)	2 (1%)	19	43
2	B	260/264 (98%)	256 (98%)	3 (1%)	1 (0%)	34	60
2	D	262/264 (99%)	256 (98%)	4 (2%)	2 (1%)	19	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1079/1126 (96%)	1045 (97%)	25 (2%)	9 (1%)	19 43

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	41	THR
2	D	432	VAL
1	A	164	VAL
1	C	38	ASP
1	C	145	ASP
1	A	145	ASP
2	B	429	THR
2	D	431	ASN

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	263/263 (100%)	250 (95%)	13 (5%)	25 52
1	C	234/263 (89%)	218 (93%)	16 (7%)	16 36
2	B	235/237 (99%)	227 (97%)	8 (3%)	37 66
2	D	237/237 (100%)	221 (93%)	16 (7%)	16 36
All	All	969/1000 (97%)	916 (94%)	53 (6%)	21 46

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	55	LEU
1	A	72	THR
1	A	74	ASN
1	A	96	LEU
1	A	101	LEU

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Mol	Chain	Res	Type
1	A	122	ARG
1	A	150	ARG
1	A	161	HIS
1	A	163	VAL
1	A	177	CYS
1	A	206	ASP
1	A	230	VAL
2	B	199	TYR
2	B	232	LEU
2	B	283	ASP
2	B	292	LEU
2	B	293	ARG
2	B	384	LEU
2	B	398	TYR
2	B	432	VAL
1	C	0	SER
1	C	22	ARG
1	C	34	LYS
1	C	36	ARG
1	C	37	LEU
1	C	42	GLU
1	C	55	LEU
1	C	73	GLU
1	C	75	LYS
1	C	122	ARG
1	C	137	THR
1	C	148	LEU
1	C	150	ARG
1	C	157	ARG
1	C	164	VAL
1	C	297	ARG
2	D	196	LYS
2	D	199	TYR
2	D	232	LEU
2	D	245	SER
2	D	281	ILE
2	D	282	THR
2	D	283	ASP
2	D	292	LEU
2	D	312	ASN
2	D	316	THR
2	D	328	LYS

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Mol	Chain	Res	Type
2	D	364	LEU
2	D	385	GLU
2	D	391	LEU
2	D	432	VAL
2	D	434	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	268	HIS
2	B	254	GLN
2	B	296	HIS
2	B	317	GLN
2	B	370	GLN
2	B	403	GLN
2	B	415	ASN
1	C	60	HIS
1	C	71	HIS
1	C	119	HIS
1	C	268	HIS
1	C	287	GLN
1	C	295	HIS
2	D	183	HIS
2	D	254	GLN
2	D	403	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TPO	C	160	1	8,10,11	0.79	0	10,14,16	1.08	0
1	TPO	A	160	1	8,10,11	0.78	0	10,14,16	1.39	1 (10%)

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	C	160	1	-	1/9/11/13	-
1	TPO	A	160	1	-	2/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	160	TPO	O-C-CA	-2.79	117.45	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	C-CA-CB-CG2
1	A	160	TPO	O-C-CA-CB
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	160	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	NNN	C	299	-	22,28,28	0.59	0	25,38,38	1.78	6 (24%)
4	SGM	B	1	-	5,5,5	0.42	0	5,5,5	0.65	0
4	SGM	D	1	-	5,5,5	0.72	0	5,5,5	0.52	0
3	NNN	A	299	-	22,28,28	0.56	0	25,38,38	1.71	4 (16%)
4	SGM	B	435	-	5,5,5	1.15	1 (20%)	5,5,5	0.64	0

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	NNN	C	299	-	-	5/15/17/17	0/3/3/3
4	SGM	B	1	-	-	2/4/4/4	-
4	SGM	D	1	-	-	4/4/4/4	-
3	NNN	A	299	-	-	5/15/17/17	0/3/3/3
4	SGM	B	435	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	435	SGM	C1-S1	2.31	1.86	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	299	NNN	C6-N1-C2	4.82	121.62	115.14
3	A	299	NNN	C2-N2-C12	-4.20	117.22	124.31
3	C	299	NNN	N3-C2-N1	-4.04	119.85	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	299	NNN	C6-N1-C2	3.87	120.34	115.14
3	A	299	NNN	N3-C2-N1	-3.56	120.60	126.23
3	C	299	NNN	C2-N2-C12	-2.80	119.59	124.31
3	C	299	NNN	N6-C6-N1	2.23	120.96	118.28
3	C	299	NNN	N2-C2-N3	2.22	120.51	117.18
3	C	299	NNN	C1'-CA'-N6	-2.20	108.04	113.77
3	A	299	NNN	C1'-CA'-N6	-2.08	108.36	113.77

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	299	NNN	C13-C12-C15-O1
3	A	299	NNN	N2-C12-C15-O1
3	A	299	NNN	C15-C12-C13-C14
3	A	299	NNN	N2-C12-C13-C14
3	C	299	NNN	C13-C12-C15-O1
3	C	299	NNN	N2-C12-C15-O1
3	C	299	NNN	C15-C12-C13-C14
3	C	299	NNN	N2-C12-C13-C14
4	B	1	SGM	S1-C1-C2-O2
4	B	1	SGM	S1-C1-C2-C3
4	D	1	SGM	S1-C1-C2-O2
4	D	1	SGM	S1-C1-C2-C3
3	C	299	NNN	C10-C9-C9'-C8
3	A	299	NNN	C11-C9-C9'-C8
4	D	1	SGM	O2-C2-C3-O3
4	B	435	SGM	C1-C2-C3-O3
4	D	1	SGM	C1-C2-C3-O3
4	B	435	SGM	O2-C2-C3-O3

There are no ring outliers.

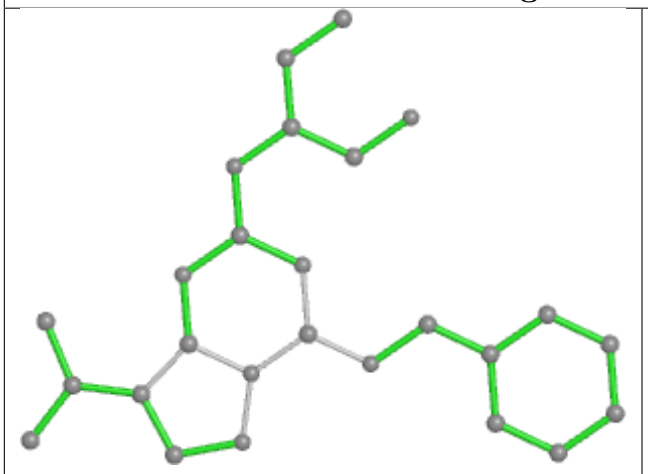
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	299	NNN	3	0
4	B	1	SGM	2	0
4	D	1	SGM	2	0
3	A	299	NNN	1	0

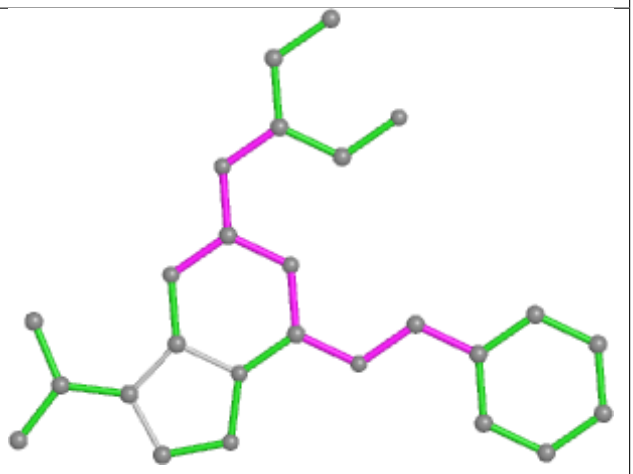
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

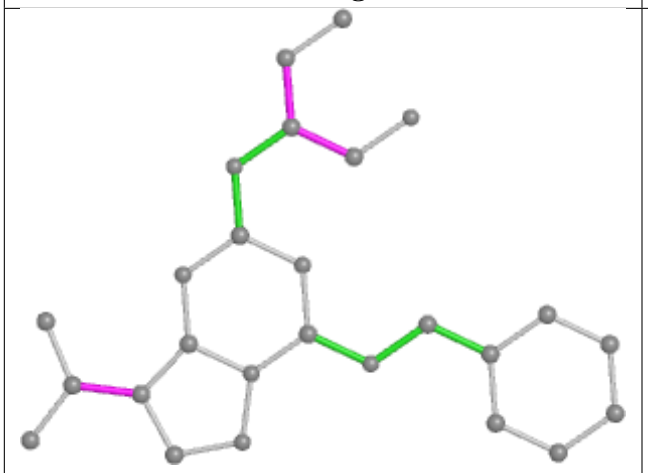
Ligand NNN C 299



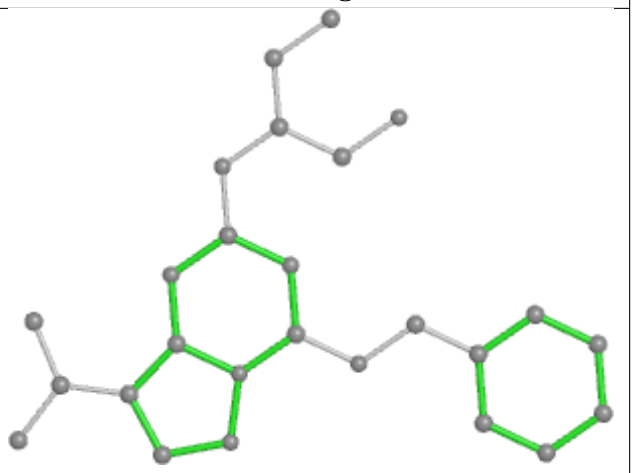
Bond lengths



Bond angles

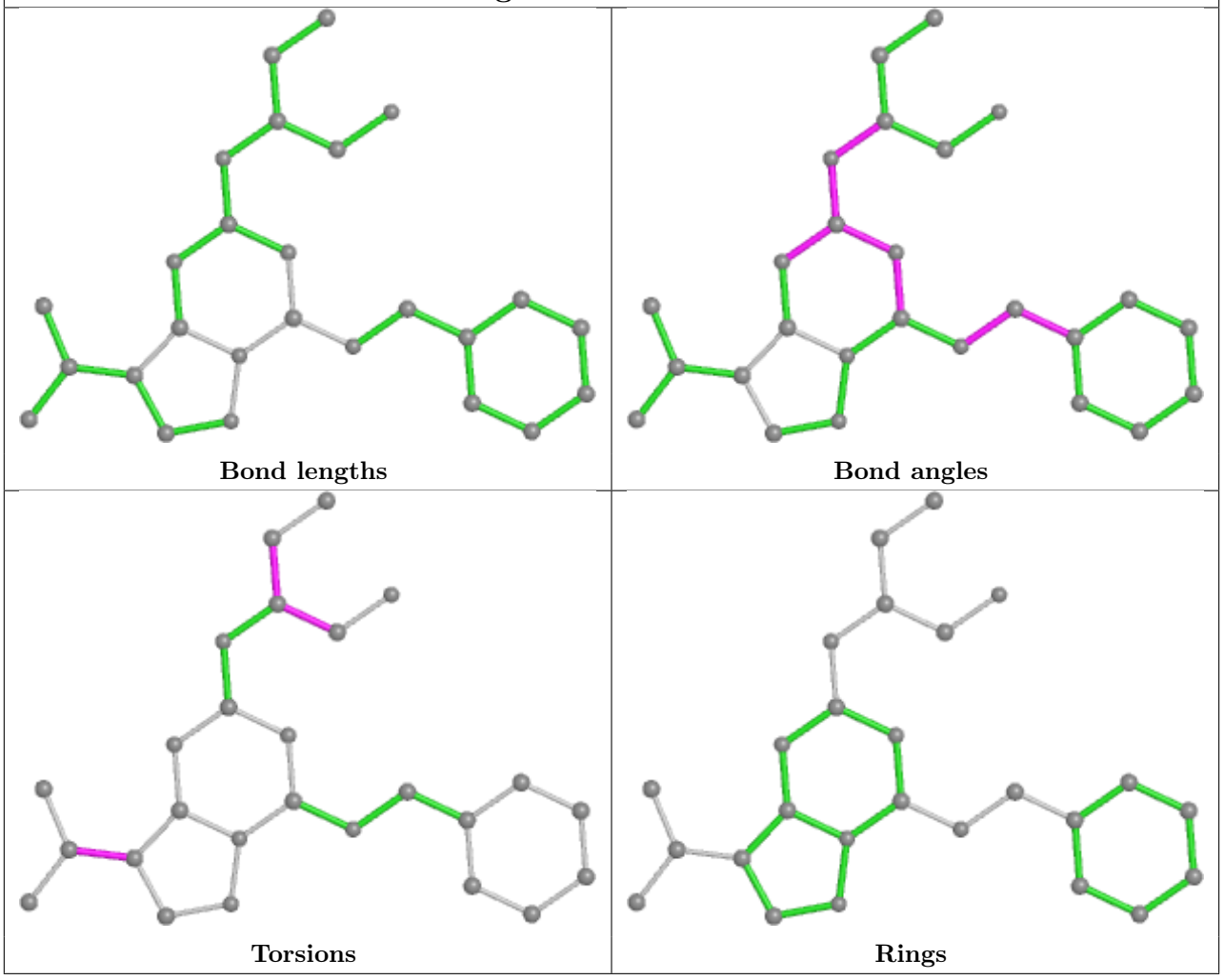


Torsions



Rings

Ligand NNN A 299



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	297/299 (99%)	-0.01	10 (3%)	45	45	2, 5, 19, 26	0
1	C	267/299 (89%)	-0.00	13 (4%)	29	28	2, 6, 20, 43	0
2	B	262/264 (99%)	-0.14	8 (3%)	49	49	2, 4, 14, 28	0
2	D	264/264 (100%)	0.20	20 (7%)	13	12	2, 6, 17, 54	0
All	All	1090/1126 (96%)	0.01	51 (4%)	31	30	2, 5, 18, 54	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	THR	5.9
2	D	434	HIS	5.1
1	A	73	GLU	5.0
1	C	221	THR	4.9
2	D	323	GLN	4.7
1	A	40	GLU	4.6
2	D	433	GLU	4.5
2	D	171	SER	4.2
1	C	253	PRO	3.9
1	A	162	GLU	3.7
1	A	96	LEU	3.7
2	B	171	SER	3.7
1	C	295	HIS	3.6
2	D	419	HIS	3.5
2	B	323	GLN	3.5
2	D	324	PRO	3.4
1	C	297	ARG	3.4
1	C	73	GLU	3.3
2	D	325	ALA	3.3
1	C	269	TYR	3.2
2	B	283	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	428	GLU	3.1
2	D	385	GLU	3.1
1	C	287	GLN	3.1
1	C	162	GLU	3.1
1	A	74	ASN	3.0
2	B	201	LYS	2.9
1	C	288	ASP	2.9
2	B	284	ASP	2.8
2	D	284	ASP	2.8
1	C	41	THR	2.8
2	D	378	GLN	2.8
1	A	36	ARG	2.8
1	A	0	SER	2.7
2	B	428	GLU	2.7
2	D	326	ASN	2.6
2	D	180	GLU	2.6
2	D	425	ASN	2.5
1	C	293	VAL	2.5
2	D	388	LYS	2.5
2	B	429	THR	2.4
1	A	41	THR	2.3
2	D	368	THR	2.3
1	A	97	THR	2.2
2	D	370	GLN	2.2
2	B	324	PRO	2.2
1	C	71	HIS	2.2
2	D	283	ASP	2.2
2	D	280	TYR	2.1
2	D	400	ARG	2.1
1	C	257	GLU	2.0

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, 95^{th} 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	160	11/12	0.95	0.17	4,7,9,10	0
1	TPO	C	160	11/12	0.98	0.10	4,8,11,11	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

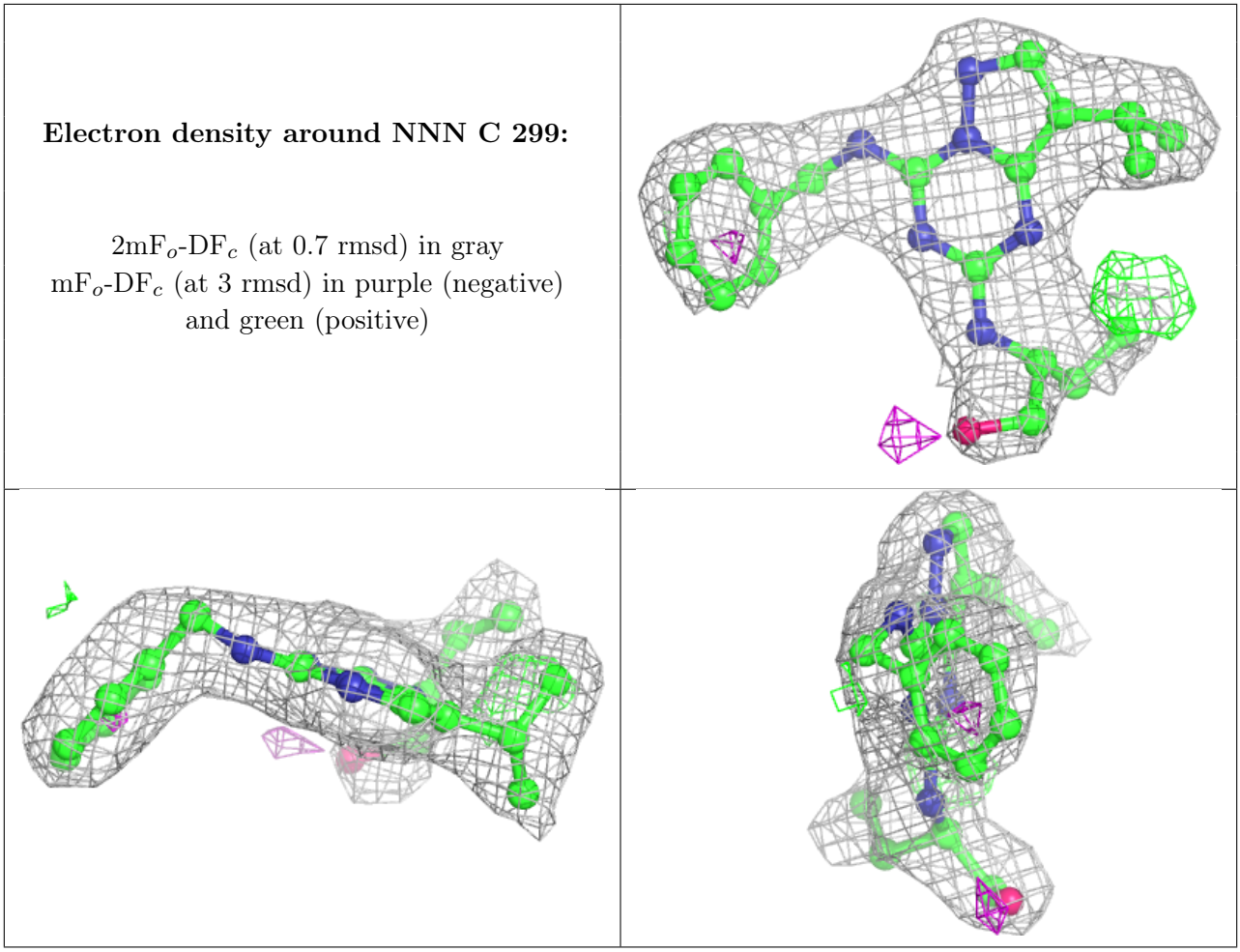
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	SGM	B	1	6/6	0.63	0.38	53,53,54,54	0
4	SGM	B	435	6/6	0.73	0.36	65,66,66,66	0
4	SGM	D	1	6/6	0.77	0.30	39,40,40,40	0
3	NNN	C	299	26/26	0.90	0.20	2,5,8,10	0
3	NNN	A	299	26/26	0.91	0.17	2,2,3,5	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.

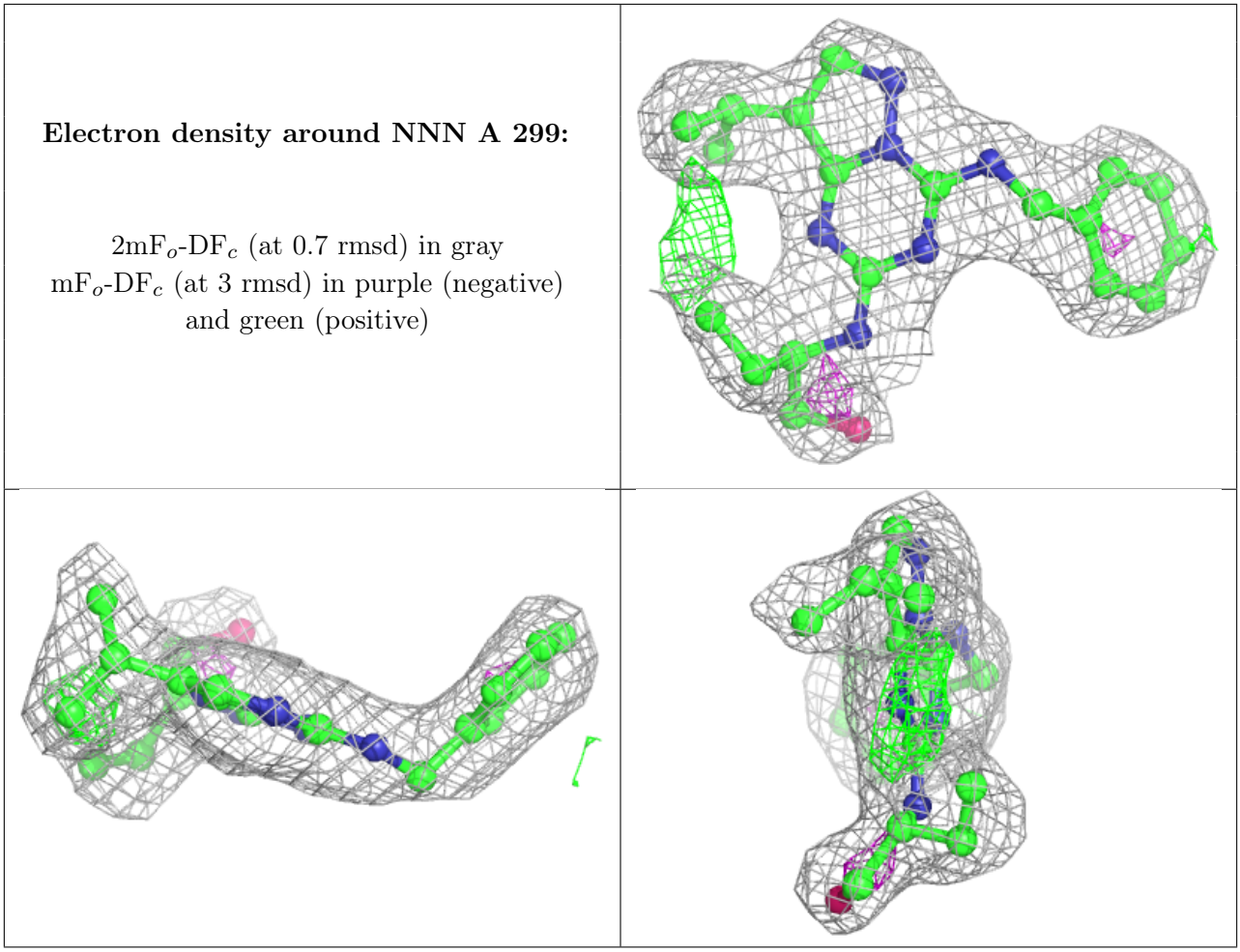
Electron density around NNN C 299:

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



Electron density around NNN A 299:

$2mF_o$-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.