



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:04 AM BST

PDB ID : 2G9X
Title : Structure of Thr 160 phosphorylated CDK2/cyclin A in complex with the inhibitor NU6271
Authors : Echalier, A.; Endicott, J.A.; Noble, M.E.
Deposited on : 2006-03-07
Resolution : 2.50 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 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 : 2.13.1
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) : 2.13.1

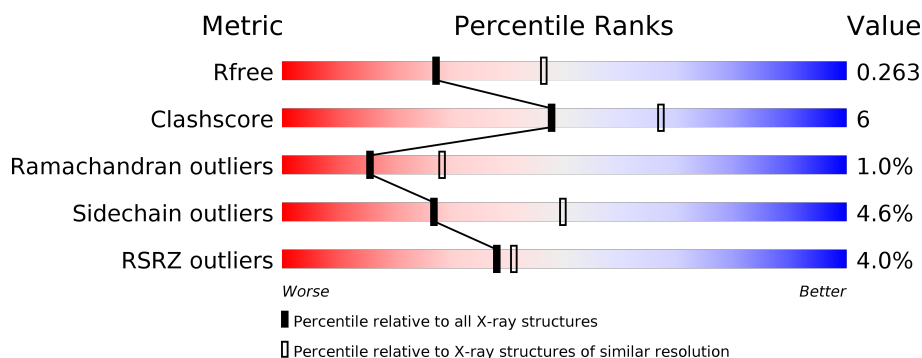
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	299	
1	C	299	
2	B	262	
2	D	262	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9066 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	299	Total	C	N	O	P	S	0	0	0
			2407	1562	409	427	1	8			
1	C	275	Total	C	N	O	P	S	0	0	0
			2208	1431	377	392	1	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	CLONING ARTIFACT	UNP P24941
A	160	TPO	THR	MODIFIED RESIDUE	UNP P24941
C	0	SER	-	CLONING ARTIFACT	UNP P24941
C	160	TPO	THR	MODIFIED RESIDUE	UNP P24941

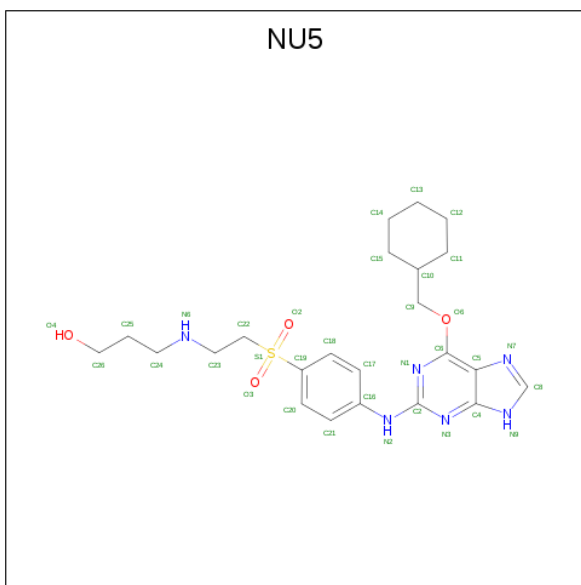
- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S		0	0	0
			2111	1367	344	390	10				
2	D	262	Total	C	N	O	S		0	0	0
			2111	1367	344	390	10				

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	171	GLY	-	CLONING ARTIFACT	UNP P30274
B	432	LEU	VAL	see remark 999	UNP P30274
D	171	GLY	-	CLONING ARTIFACT	UNP P30274
D	432	LEU	VAL	see remark 999	UNP P30274

- Molecule 3 is 3-({2-[(4-{[6-(CYCLOHEXYLMETHOXY)-9H-PURIN-2-YL]AMINO}PH ENYL)SULFONYL]ETHYL}AMINO)PROPAN-1-OL (three-letter code: NU5) (formula: C₂₃H₃₂N₆O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 34	C 23	N 6	O 4	S 1	0	0
3	C	1	Total 34	C 23	N 6	O 4	S 1	0	0

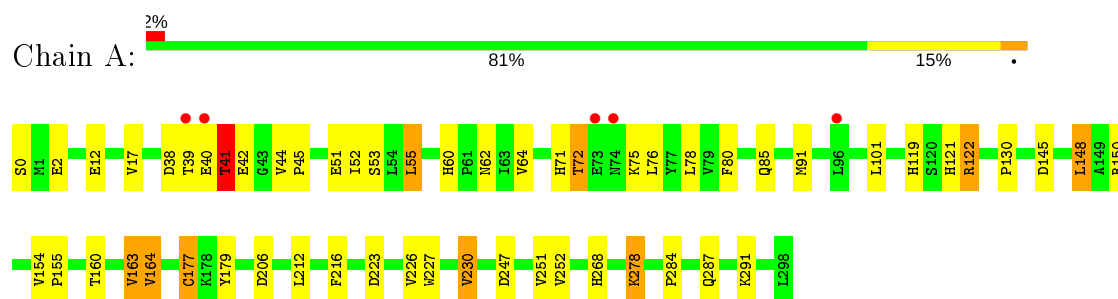
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	61	Total O 61 61	0	0
4	B	48	Total O 48 48	0	0
4	C	30	Total O 30 30	0	0
4	D	22	Total O 22 22	0	0

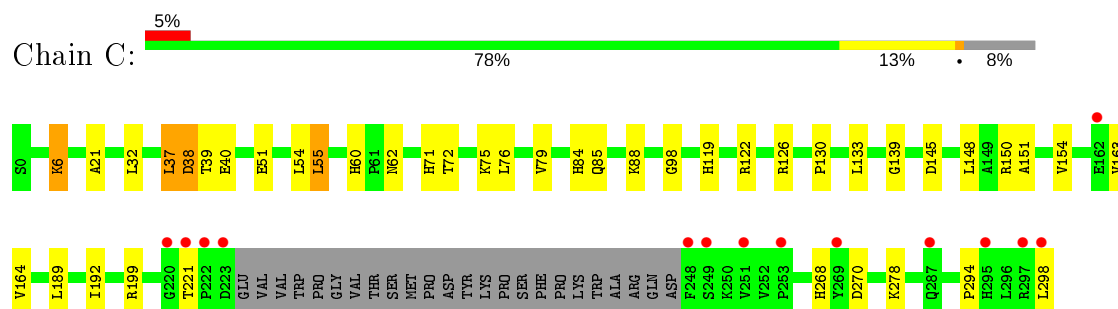
3 Residue-property plots

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

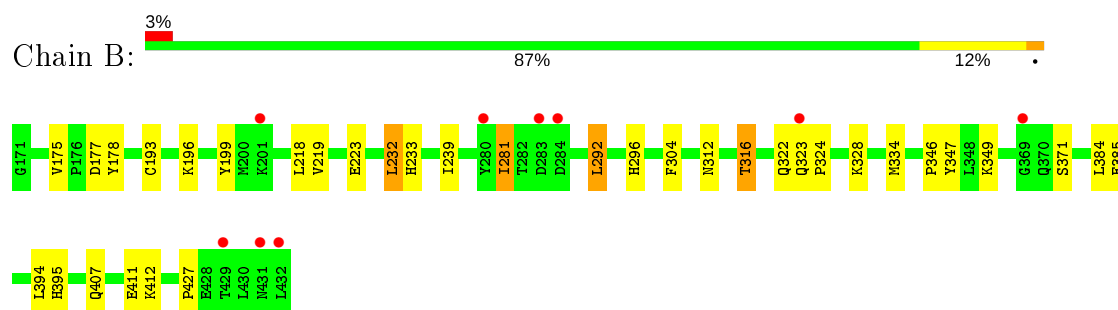
- Molecule 1: Cell division protein kinase 2



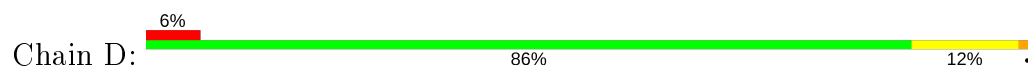
- Molecule 1: Cell division protein kinase 2

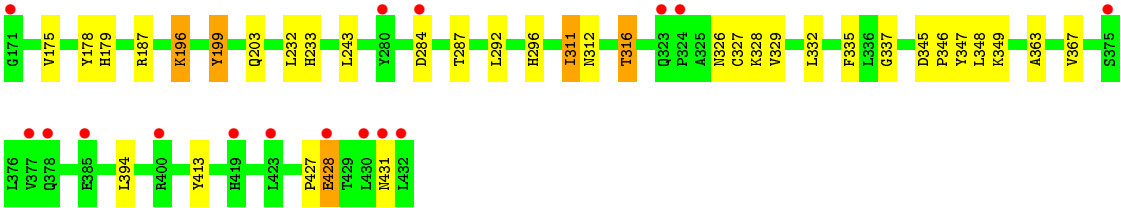


- Molecule 2: Cyclin-A2



- Molecule 2: Cyclin-A2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.58Å 134.99Å 148.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.20 – 2.50 34.20 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.5 (43.20-2.50) 92.6 (34.20-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.265 0.217 , 0.263	Depositor DCC
R_{free} test set	2346 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9066	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 3.64% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, NU5

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	0.47	0/2457	0.60	0/3333
1	C	0.42	0/2247	0.56	0/3042
2	B	0.44	0/2161	0.58	0/2938
2	D	0.39	0/2161	0.55	0/2938
All	All	0.43	0/9026	0.58	0/12251

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2407	0	2454	43	0
1	C	2208	0	2265	27	0
2	B	2111	0	2130	26	0
2	D	2111	0	2130	21	0
3	A	34	0	32	5	0
3	C	34	0	32	2	0
4	A	61	0	0	7	0
4	B	48	0	0	4	0
4	C	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	22	0	0	3	0
All	All	9066	0	9043	110	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 (110) 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	1.57	0.86
3:C:299:NU5:N1	3:C:299:NU5:H21	1.98	0.78
2:B:175:VAL:HG12	2:B:175:VAL:O	1.82	0.78
1:C:37:LEU:HA	1:C:38:ASP:CB	2.14	0.78
1:A:85:GLN:HA	3:A:299:NU5:C18	2.14	0.77
1:A:154:VAL:O	2:B:316:THR:CG2	2.36	0.73
2:B:312:ASN:ND2	2:B:334:MET:HE3	2.03	0.73
1:C:119:HIS:HD2	4:D:15:HOH:O	1.71	0.73
2:D:287:THR:HB	4:D:55:HOH:O	1.91	0.71
1:A:227:TRP:O	1:A:230:VAL:HG22	1.93	0.69
3:A:299:NU5:H21	3:A:299:NU5:N1	2.06	0.68
1:A:119:HIS:HD2	4:B:155:HOH:O	1.77	0.66
1:A:154:VAL:O	2:B:316:THR:HG22	1.95	0.64
2:B:407:GLN:O	2:B:411:GLU:HG2	1.98	0.64
2:B:175:VAL:CG1	2:B:178:TYR:HB2	2.28	0.63
1:A:177:CYS:SG	1:A:179:TYR:O	2.56	0.62
2:B:175:VAL:CG1	2:B:175:VAL:O	2.48	0.60
1:C:60:HIS:HD2	1:C:62:ASN:H	1.51	0.58
1:A:51:GLU:O	1:A:55:LEU:HB2	2.03	0.58
1:C:133:LEU:HD11	1:C:192:ILE:HD13	1.86	0.58
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.39	0.57
2:D:346:PRO:O	2:D:349:LYS:HG2	2.05	0.57
2:D:326:ASN:ND2	2:D:329:VAL:HG23	2.20	0.57
1:A:278:LYS:HE2	2:B:177:ASP:O	2.05	0.56
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.41	0.56
1:A:268:HIS:CD2	4:A:357:HOH:O	2.57	0.56
1:A:72:THR:HG22	4:A:311:HOH:O	2.05	0.56
2:D:196:LYS:HB3	2:D:199:TYR:HB3	1.88	0.56
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.41	0.55
1:A:60:HIS:HD2	1:A:62:ASN:H	1.52	0.55
1:C:268:HIS:HD2	1:C:270:ASP:H	1.54	0.54
1:C:60:HIS:CD2	1:C:62:ASN:H	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:HIS:CD2	1:A:62:ASN:H	2.26	0.54
1:A:39:THR:HG23	2:B:292:LEU:HD23	1.89	0.54
1:A:91:MET:HE1	1:A:130:PRO:HB3	1.91	0.53
1:C:51:GLU:O	1:C:55:LEU:HB2	2.09	0.53
1:A:121:HIS:O	1:A:122:ARG:HG3	2.09	0.53
1:A:60:HIS:HE1	4:A:327:HOH:O	1.92	0.52
2:B:193:CYS:SG	4:B:105:HOH:O	2.12	0.52
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.77	0.52
3:A:299:NU5:C21	3:A:299:NU5:N1	2.73	0.52
1:C:154:VAL:O	2:D:316:THR:HG23	2.09	0.52
1:A:291:LYS:HE3	4:A:319:HOH:O	2.09	0.51
1:A:268:HIS:HD2	4:A:357:HOH:O	1.91	0.51
1:C:88:LYS:HB2	1:C:130:PRO:HB2	1.92	0.51
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.93	0.51
1:C:84:HIS:HB3	1:C:298:LEU:CD1	2.40	0.50
1:A:212:LEU:HD22	1:A:216:PHE:CZ	2.46	0.50
2:B:233:HIS:HD2	4:B:36:HOH:O	1.94	0.50
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.46	0.49
1:C:85:GLN:HA	3:C:299:NU5:C18	2.42	0.49
2:B:347:TYR:OH	2:B:394:LEU:HA	2.13	0.48
1:C:39:THR:HG22	1:C:40:GLU:H	1.79	0.48
1:A:0:SER:C	1:A:2:GLU:H	2.15	0.48
2:D:326:ASN:HD22	2:D:329:VAL:HG23	1.77	0.48
2:B:312:ASN:O	2:B:316:THR:HB	2.13	0.48
1:A:80:PHE:CB	3:A:299:NU5:H8	2.44	0.48
1:C:71:HIS:NE2	2:D:296:HIS:CE1	2.82	0.47
1:A:154:VAL:O	2:B:316:THR:HG23	2.13	0.47
2:B:312:ASN:ND2	2:B:334:MET:CE	2.76	0.47
2:D:311:ILE:CD1	2:D:337:GLY:HA3	2.45	0.47
2:D:326:ASN:HD21	2:D:367:VAL:HG11	1.79	0.47
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.97	0.47
2:D:345:ASP:HA	2:D:346:PRO:HA	1.76	0.46
2:B:312:ASN:HD21	2:B:334:MET:CE	2.28	0.46
1:A:72:THR:HG23	4:A:334:HOH:O	2.16	0.46
1:C:71:HIS:HD2	1:C:76:LEU:HD13	1.81	0.46
2:D:175:VAL:CG1	2:D:178:TYR:HB2	2.46	0.45
1:C:37:LEU:CA	1:C:38:ASP:CB	2.91	0.45
1:A:227:TRP:CE3	1:A:230:VAL:CG1	3.00	0.45
1:C:6:LYS:HG3	1:C:21:ALA:HB2	1.99	0.45
1:A:121:HIS:C	1:A:122:ARG:HG3	2.37	0.45
1:A:223:ASP:OD1	1:A:226:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD23	4:A:318:HOH:O	2.17	0.45
1:A:284:PRO:O	1:A:287:GLN:HG2	2.16	0.44
2:B:223:GLU:HG2	2:B:412:LYS:HD2	1.98	0.44
1:C:84:HIS:HB3	1:C:298:LEU:HD13	1.99	0.44
2:D:311:ILE:HG13	2:D:312:ASN:N	2.31	0.44
1:C:126:ARG:HB3	1:C:163:VAL:HG22	1.99	0.43
1:A:12:GLU:HG2	1:A:17:VAL:HG13	2.00	0.43
2:B:281:ILE:H	2:B:281:ILE:HG13	1.63	0.43
1:C:189:LEU:HA	1:C:189:LEU:HD23	1.86	0.43
2:D:347:TYR:OH	2:D:394:LEU:HA	2.18	0.43
2:D:332:LEU:HD23	2:D:363:ALA:HA	2.00	0.43
1:A:53:SER:HB3	2:B:304:PHE:O	2.19	0.43
1:A:251:VAL:HG12	1:A:252:VAL:HG23	2.00	0.43
1:C:54:LEU:HD21	1:C:151:ALA:HB2	2.01	0.43
2:D:233:HIS:NE2	2:D:311:ILE:HG12	2.34	0.43
1:C:32:LEU:HD21	1:C:79:VAL:HG22	2.01	0.42
1:A:119:HIS:CD2	4:B:155:HOH:O	2.60	0.42
1:A:80:PHE:CG	3:A:299:NU5:H8	2.54	0.42
1:A:52:ILE:HD11	1:A:78:LEU:HD21	2.01	0.42
1:C:139:GLY:HA2	1:C:294:PRO:HD3	2.02	0.42
2:B:395:HIS:HE1	2:B:427:PRO:O	2.03	0.41
1:A:41:THR:HB	1:A:42:GLU:H	1.56	0.41
2:B:346:PRO:O	2:B:349:LYS:HG2	2.20	0.41
1:A:291:LYS:HG2	1:A:291:LYS:O	2.21	0.41
2:D:427:PRO:O	2:D:428:GLU:C	2.58	0.41
2:D:175:VAL:O	2:D:179:HIS:HB3	2.21	0.41
1:C:268:HIS:CD2	1:C:270:ASP:H	2.35	0.41
1:A:163:VAL:HG13	1:A:164:VAL:HG23	2.03	0.41
1:A:51:GLU:HG3	1:A:55:LEU:HD22	2.02	0.41
2:B:218:LEU:HD11	2:B:239:ILE:HD11	2.03	0.41
1:C:189:LEU:HD23	1:C:192:ILE:HD12	2.03	0.41
2:D:187:ARG:HD3	4:D:54:HOH:O	2.21	0.41
2:B:323:GLN:HA	2:B:324:PRO:HA	1.90	0.40
1:A:44:VAL:HA	1:A:45:PRO:HD3	1.84	0.40
2:D:203:GLN:NE2	2:D:243:LEU:O	2.53	0.40
1:C:98:GLY:HA2	1:C:199:ARG:HD3	2.04	0.40
2:D:199:TYR:CD1	2:D:199:TYR:C	2.94	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	296/299 (99%)	279 (94%)	11 (4%)	6 (2%)	7	12
1	C	270/299 (90%)	254 (94%)	13 (5%)	3 (1%)	14	26
2	B	260/262 (99%)	257 (99%)	3 (1%)	0	100	100
2	D	260/262 (99%)	251 (96%)	7 (3%)	2 (1%)	19	35
All	All	1086/1122 (97%)	1041 (96%)	34 (3%)	11 (1%)	15	28

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
2	D	428	GLU
1	A	164	VAL
1	C	145	ASP
1	C	38	ASP
1	C	164	VAL
2	D	431	ASN
1	A	40	GLU
1	A	72	THR
1	A	145	ASP
1	A	247	ASP

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	263/263 (100%)	249 (95%)	14 (5%)	22	43
1	C	241/263 (92%)	231 (96%)	10 (4%)	30	55
2	B	234/234 (100%)	223 (95%)	11 (5%)	26	49
2	D	234/234 (100%)	224 (96%)	10 (4%)	29	53
All	All	972/994 (98%)	927 (95%)	45 (5%)	27	50

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	41	THR
1	A	55	LEU
1	A	64	VAL
1	A	75	LYS
1	A	101	LEU
1	A	122	ARG
1	A	148	LEU
1	A	150	ARG
1	A	163	VAL
1	A	177	CYS
1	A	206	ASP
1	A	230	VAL
1	A	278	LYS
2	B	196	LYS
2	B	199	TYR
2	B	232	LEU
2	B	281	ILE
2	B	292	LEU
2	B	316	THR
2	B	322	GLN
2	B	328	LYS
2	B	371	SER
2	B	384	LEU
2	B	385	GLU
1	C	6	LYS
1	C	37	LEU
1	C	55	LEU
1	C	72	THR
1	C	75	LYS
1	C	122	ARG
1	C	148	LEU
1	C	150	ARG

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Mol	Chain	Res	Type
1	C	221	THR
1	C	278	LYS
2	D	196	LYS
2	D	199	TYR
2	D	232	LEU
2	D	284	ASP
2	D	292	LEU
2	D	311	ILE
2	D	316	THR
2	D	327	CYS
2	D	328	LYS
2	D	348	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	84	HIS
1	A	119	HIS
1	A	268	HIS
2	B	183	HIS
2	B	233	HIS
2	B	254	GLN
2	B	312	ASN
2	B	317	GLN
2	B	370	GLN
2	B	378	GLN
2	B	403	GLN
2	B	431	ASN
1	C	60	HIS
1	C	84	HIS
1	C	119	HIS
1	C	268	HIS
2	D	183	HIS
2	D	317	GLN
2	D	370	GLN
2	D	378	GLN
2	D	396	GLN
2	D	403	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	0.74	0	10,14,16	1.09	0
1	TPO	A	160	1	8,10,11	0.69	0	10,14,16	1.29	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	-	0/9/11/13	-
1	TPO	A	160	1	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	160	TPO	OG1-P-O1P	-2.78	98.65	109.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	NU5	C	299	-	34,37,37	2.03	4 (11%)	41,50,50	2.56	11 (26%)
3	NU5	A	299	-	34,37,37	2.08	4 (11%)	41,50,50	2.50	12 (29%)

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	NU5	C	299	-	-	10/23/31/31	0/4/4/4
3	NU5	A	299	-	-	14/23/31/31	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	299	NU5	C19-S1	-9.64	1.60	1.76
3	C	299	NU5	C19-S1	-9.35	1.61	1.76
3	A	299	NU5	C22-S1	-5.28	1.67	1.77
3	C	299	NU5	C22-S1	-5.17	1.67	1.77
3	C	299	NU5	C6-N1	2.63	1.36	1.31
3	A	299	NU5	C5-C4	2.48	1.47	1.40
3	C	299	NU5	C5-C4	2.31	1.47	1.40
3	A	299	NU5	C16-N2	-2.03	1.36	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	299	NU5	O3-S1-O2	-10.12	106.61	118.44
3	A	299	NU5	O3-S1-O2	-9.95	106.81	118.44
3	C	299	NU5	C2-N3-C4	5.54	121.57	115.28
3	A	299	NU5	C2-N3-C4	5.45	121.46	115.28
3	A	299	NU5	C2-N1-C6	4.28	122.72	115.18
3	C	299	NU5	C11-C10-C15	4.20	119.60	109.33
3	C	299	NU5	O6-C6-N1	4.00	123.58	120.12
3	C	299	NU5	C9-O6-C6	3.99	121.32	117.50
3	A	299	NU5	C11-C10-C15	3.86	118.76	109.33
3	A	299	NU5	C22-S1-C19	3.83	110.26	105.03
3	C	299	NU5	C2-N1-C6	3.77	121.83	115.18
3	C	299	NU5	C22-S1-C19	3.76	110.17	105.03
3	A	299	NU5	C9-O6-C6	3.53	120.88	117.50
3	A	299	NU5	C14-C15-C10	3.49	118.75	112.15
3	C	299	NU5	C14-C15-C10	2.89	117.62	112.15
3	C	299	NU5	N3-C2-N1	-2.84	121.74	126.23
3	A	299	NU5	N3-C2-N1	-2.81	121.78	126.23
3	A	299	NU5	C5-C6-N1	-2.69	118.15	123.26
3	A	299	NU5	O3-S1-C22	2.53	112.74	108.20
3	C	299	NU5	O2-S1-C19	2.47	110.88	108.36
3	A	299	NU5	C20-C19-S1	2.28	121.98	119.49
3	A	299	NU5	O2-S1-C19	2.26	110.66	108.36
3	C	299	NU5	C5-C6-N1	-2.22	119.04	123.26

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	299	NU5	C23-C22-S1-O2
3	C	299	NU5	C23-C22-S1-O3
3	C	299	NU5	C23-C22-S1-C19
3	C	299	NU5	C24-C25-C26-O4
3	C	299	NU5	C5-C6-O6-C9
3	A	299	NU5	C23-C22-S1-O2
3	A	299	NU5	C23-C22-S1-O3
3	A	299	NU5	C23-C22-S1-C19
3	A	299	NU5	C18-C19-S1-O3
3	A	299	NU5	C20-C19-S1-O3
3	C	299	NU5	N1-C6-O6-C9
3	A	299	NU5	C25-C24-N6-C23
3	A	299	NU5	C22-C23-N6-C24
3	A	299	NU5	N1-C6-O6-C9
3	A	299	NU5	C20-C19-S1-C22

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Mol	Chain	Res	Type	Atoms
3	A	299	NU5	C10-C9-O6-C6
3	C	299	NU5	C10-C9-O6-C6
3	A	299	NU5	C18-C19-S1-C22
3	C	299	NU5	C18-C19-S1-O3
3	C	299	NU5	C20-C19-S1-O3
3	C	299	NU5	C25-C24-N6-C23
3	A	299	NU5	C5-C6-O6-C9
3	A	299	NU5	S1-C22-C23-N6
3	A	299	NU5	C15-C10-C9-O6

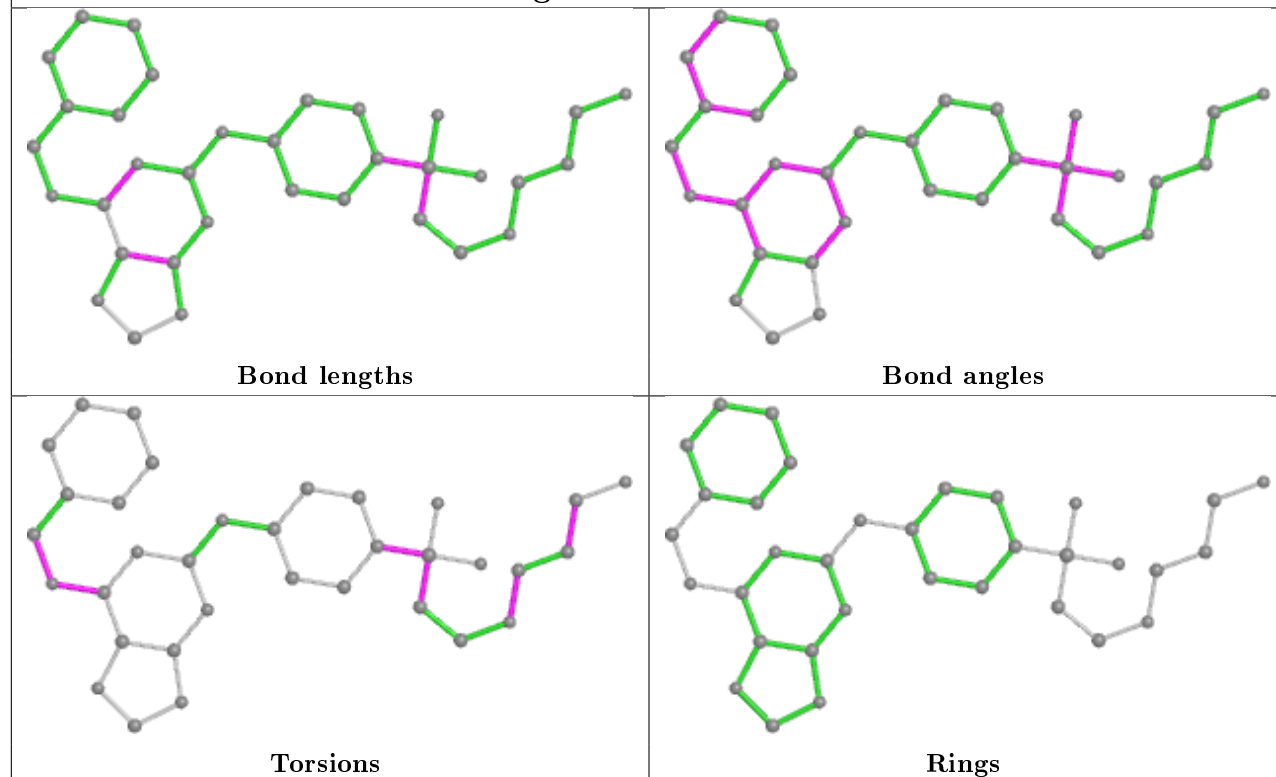
There are no ring outliers.

2 monomers are involved in 7 short contacts:

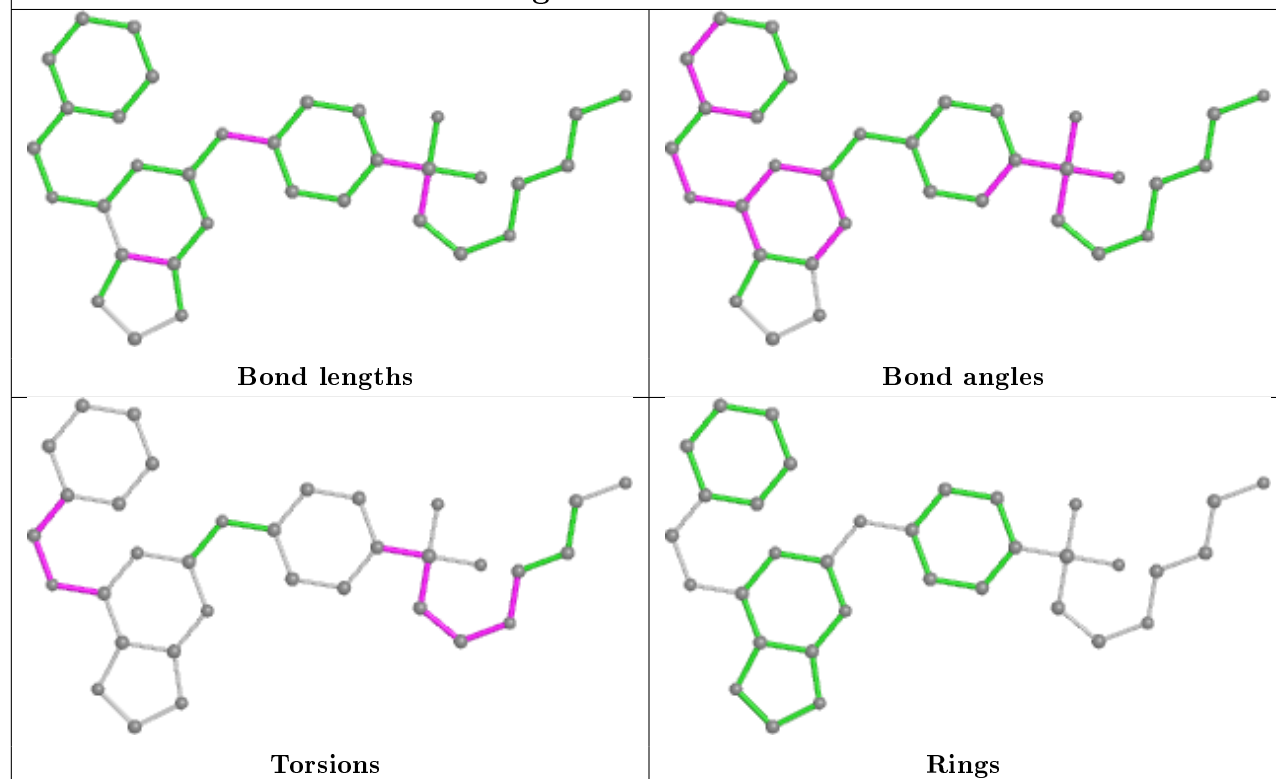
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	299	NU5	2	0
3	A	299	NU5	5	0

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 NU5 C 299



Ligand NU5 A 299



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	298/299 (99%)	-0.12	5 (1%) 70 72	2, 6, 18, 24	0
1	C	274/299 (91%)	0.01	14 (5%) 28 29	2, 5, 26, 40	0
2	B	262/262 (100%)	-0.11	9 (3%) 45 48	2, 6, 15, 32	0
2	D	262/262 (100%)	0.33	16 (6%) 21 22	2, 7, 21, 49	0
All	All	1096/1122 (97%)	0.02	44 (4%) 38 41	2, 6, 19, 49	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	221	THR	8.5
1	C	222	PRO	6.7
1	C	298	LEU	6.1
1	C	223	ASP	5.2
1	A	96	LEU	4.5
1	C	295	HIS	4.3
2	D	428	GLU	4.2
1	C	297	ARG	4.1
1	C	251	VAL	4.0
2	D	171	GLY	3.9
2	B	323	GLN	3.5
2	B	432	LEU	3.4
2	B	284	ASP	3.4
2	D	378	GLN	3.3
2	D	432	LEU	3.3
1	C	248	PHE	3.2
1	A	40	GLU	3.0
1	C	220	GLY	2.9
2	D	400	ARG	2.9
1	C	249	SER	2.8
1	A	39	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	269	TYR	2.7
2	D	423	LEU	2.7
1	A	74	ASN	2.6
2	B	429	THR	2.6
2	B	280	TYR	2.6
1	C	253	PRO	2.6
2	D	430	LEU	2.5
1	C	287	GLN	2.5
2	D	419	HIS	2.5
1	A	73	GLU	2.5
2	D	377	VAL	2.4
2	B	201	LYS	2.4
2	D	431	ASN	2.4
2	D	284	ASP	2.3
2	D	385	GLU	2.2
2	B	283	ASP	2.2
2	D	323	GLN	2.2
2	B	369	GLY	2.1
2	B	431	ASN	2.1
1	C	162	GLU	2.1
2	D	375	SER	2.1
2	D	324	PRO	2.0
2	D	280	TYR	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, 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(\AA^2)	Q<0.9
1	TPO	C	160	11/12	0.98	0.10	4,5,7,7	0
1	TPO	A	160	11/12	0.99	0.12	3,4,6,6	0

6.3 Carbohydrates [i](#)

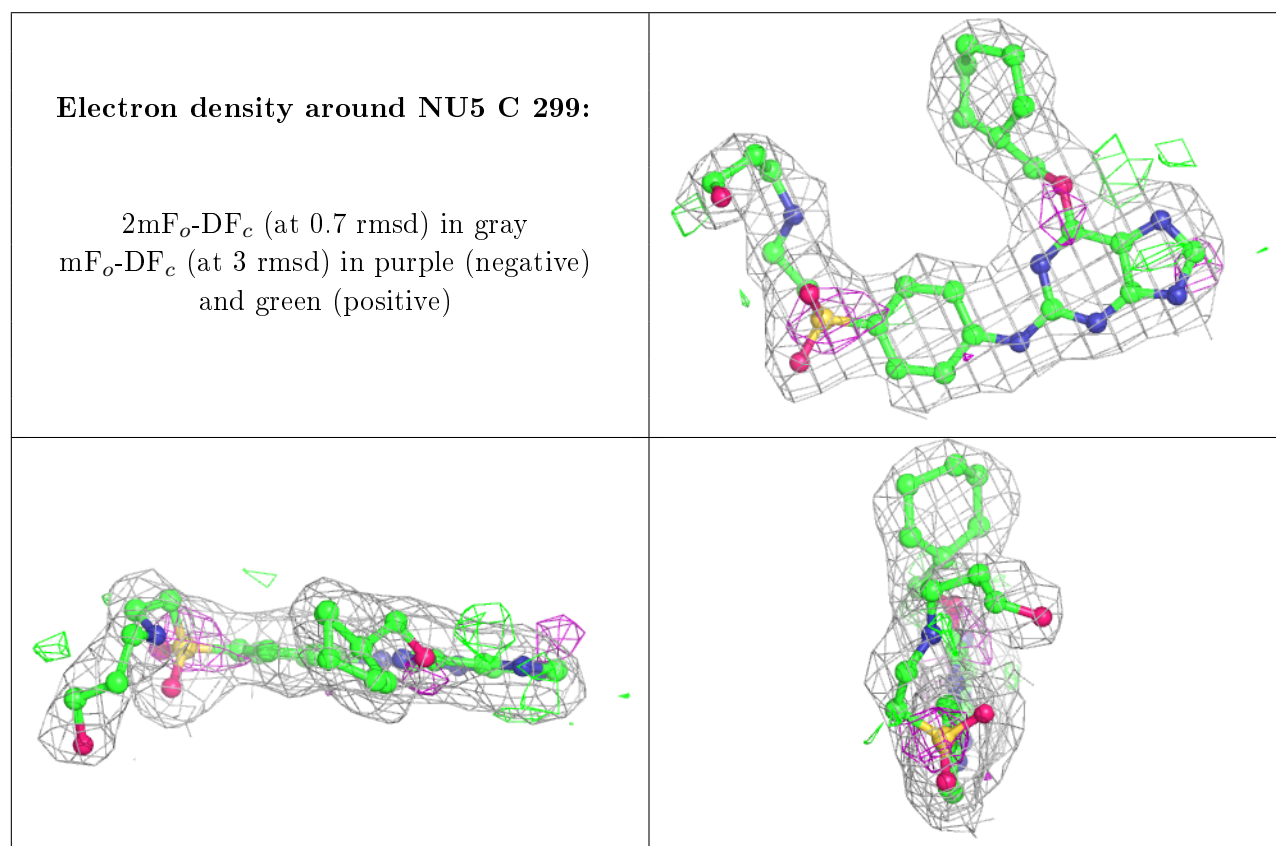
There are no monosaccharides in this entry.

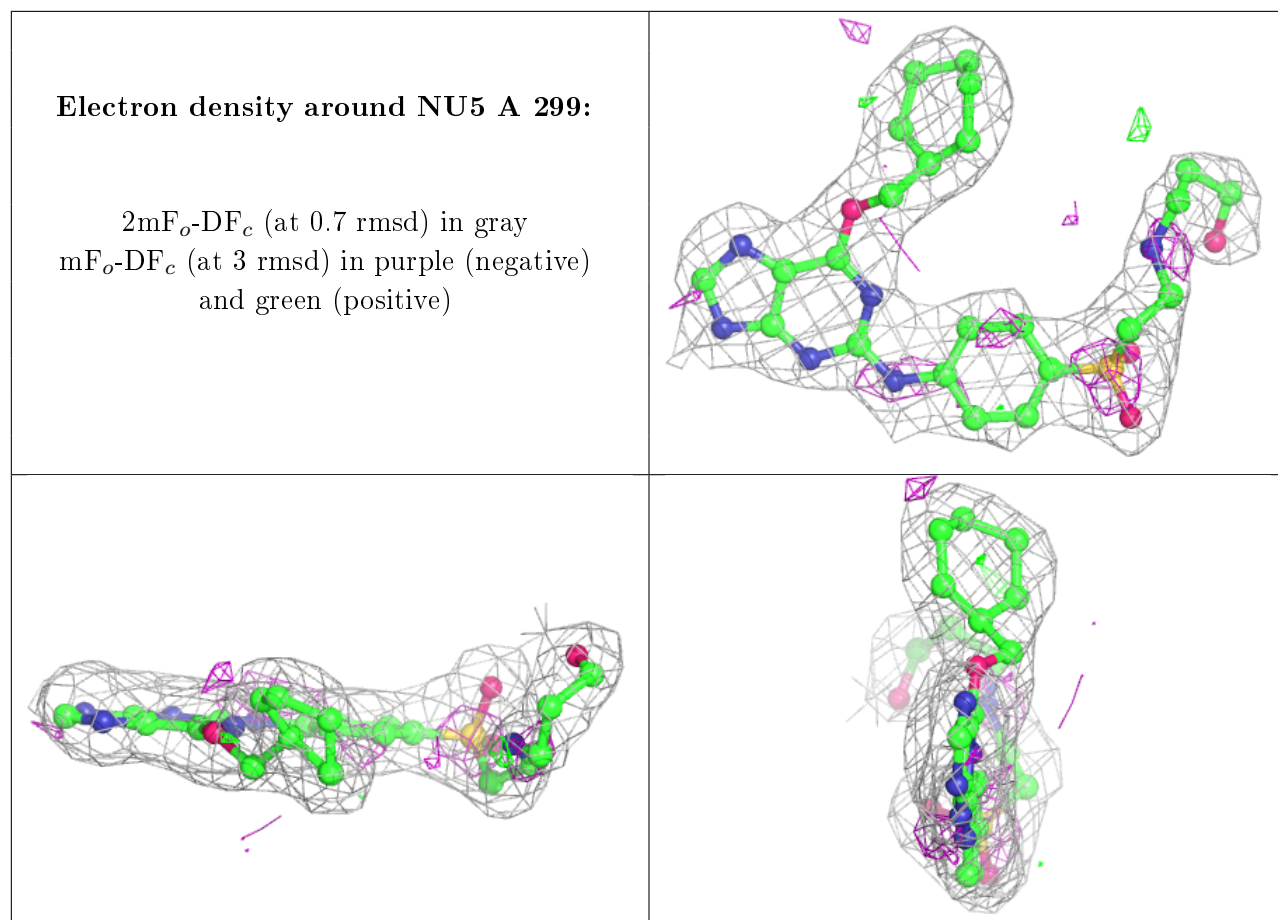
6.4 Ligands ⓘ

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	NU5	C	299	34/34	0.95	0.13	4,7,16,17	0
3	NU5	A	299	34/34	0.96	0.13	2,6,15,15	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 ⓘ

There are no such residues in this entry.