



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 08:27 PM EDT

PDB ID : 4BCN
Title : Structure of CDK2 in complex with cyclin A 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 : 2.10 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

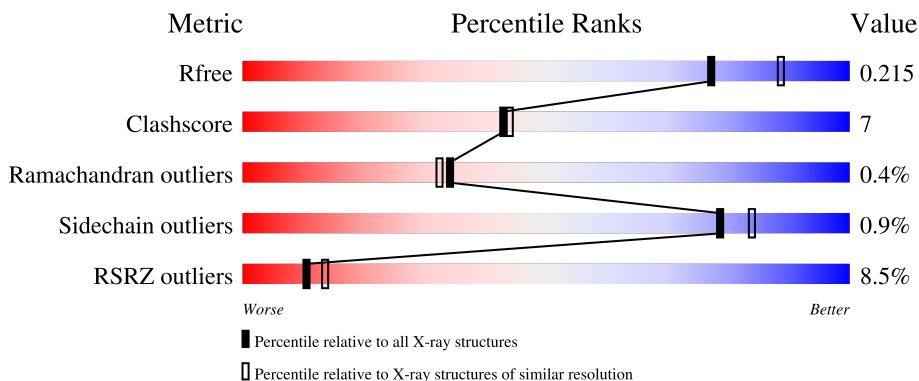
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	300	
1	C	300	
2	B	262	
3	D	262	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9678 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	297	Total	C	N	O	P	S	0	1	0
			2398	1558	409	422	1	8			
1	C	296	Total	C	N	O	P	S	0	0	0
			2374	1540	401	424	1	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-1	GLY	-	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
			Total	C	N	O	S			
2	B	257	Total	C	N	O	S	0	2	0
			2092	1357	344	381	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	357	ALA	GLY	conflict	UNP P20248
B	392	LEU	MET	conflict	UNP P20248
B	400	ARG	LYS	conflict	UNP P20248
B	403	LYS	GLN	conflict	UNP P20248

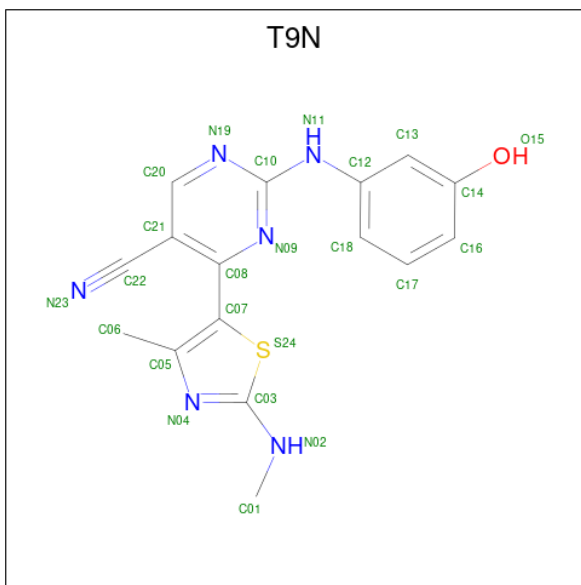
- Molecule 3 is a protein called CYCLIN-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	255	Total	C	N	O	S	0	1	0
			2069	1340	339	380	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	432	VAL	-	expression tag	UNP P20248
D	357	ALA	GLY	conflict	UNP P20248
D	392	LEU	MET	conflict	UNP P20248

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



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

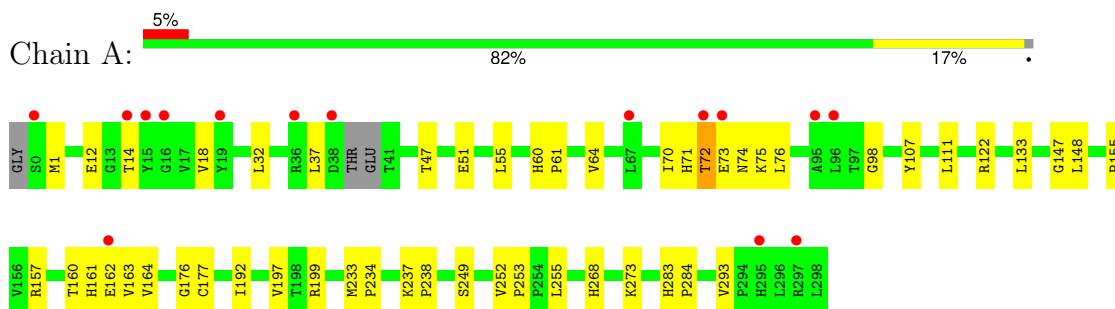
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	288	Total	O	0	0
			288	288		
6	B	199	Total	O	0	0
			199	199		
6	C	110	Total	O	0	0
			110	110		
6	D	90	Total	O	0	0
			90	90		

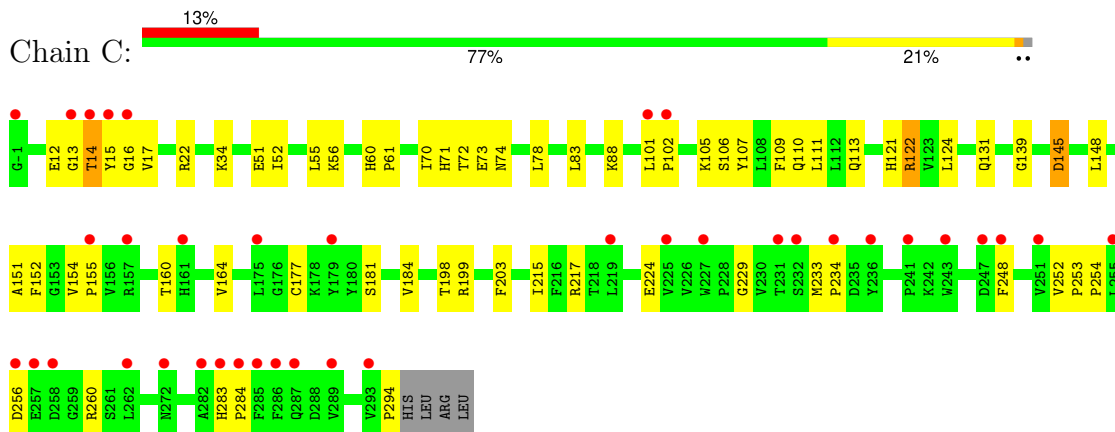
3 Residue-property plots [i](#)

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.

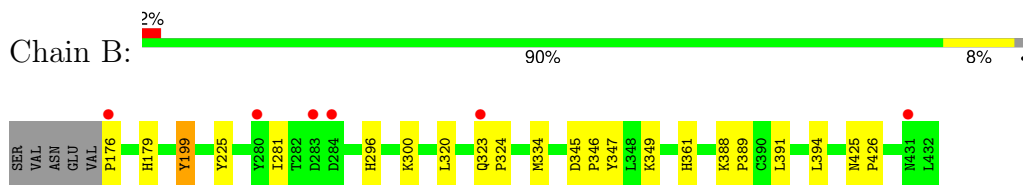
- Molecule 1: CYCLIN-DEPENDENT KINASE 2



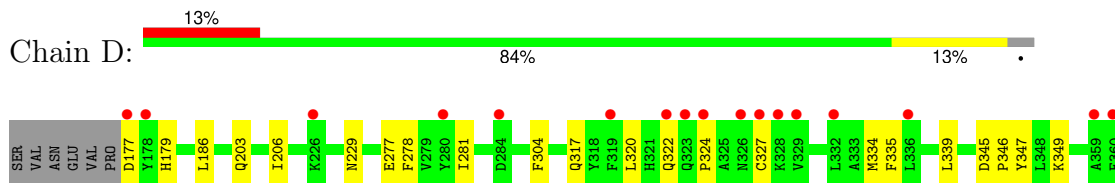
- Molecule 1: CYCLIN-DEPENDENT KINASE 2

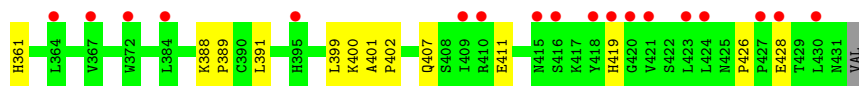


- Molecule 2: CYCLIN-A2



- Molecule 3: 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	74.05Å 135.08Å 148.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.91 – 2.10 49.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.91-2.10) 99.8 (49.91-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.184 , 0.219 0.178 , 0.215	Depositor DCC
R_{free} test set	4376 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtrriage
Anisotropy	0.190	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9678	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: T9N, SO4, TPO

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	0.27	0/2451	0.44	0/3323
1	C	0.23	0/2423	0.42	0/3287
2	B	0.26	0/2150	0.43	0/2919
3	D	0.23	0/2121	0.40	0/2879
All	All	0.25	0/9145	0.42	0/12408

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	2398	0	2447	41	0
1	C	2374	0	2415	42	0
2	B	2092	0	2118	19	0
3	D	2069	0	2093	27	0
4	A	24	0	14	2	0
4	C	24	0	14	4	0
5	B	5	0	0	0	0
5	D	5	0	0	0	0
6	A	288	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	199	0	0	2	0
6	C	110	0	0	2	0
6	D	90	0	0	2	0
All	All	9678	0	9101	123	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 7.

All (123) 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:155:PRO:HG3	3:D:320:LEU:HD21	1.59	0.83
1:A:72:THR:HG22	1:A:75:LYS:H	1.44	0.82
1:C:71:HIS:CE1	3:D:304:PHE:HE2	2.03	0.76
1:C:88:LYS:HD2	1:C:131:GLN:HG3	1.64	0.76
1:A:1:MET:SD	1:A:70:ILE:HD12	2.29	0.72
1:A:72:THR:HG23	1:A:73:GLU:N	2.08	0.69
1:A:268:HIS:CD2	1:A:273:LYS:HB2	2.28	0.69
2:B:346:PRO:O	2:B:349:LYS:HG2	1.94	0.67
3:D:346:PRO:O	3:D:349:LYS:HG2	1.96	0.66
3:D:203:GLN:O	6:D:2016:HOH:O	2.14	0.65
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.79	0.63
3:D:388:LYS:HB3	3:D:389:PRO:HD3	1.82	0.61
1:C:88:LYS:HD2	1:C:131:GLN:CG	2.31	0.61
1:A:161[B]:HIS:ND1	1:A:162:GLU:HG3	2.15	0.60
4:C:1296:T9N:H13	4:C:1296:T9N:N09	2.17	0.60
1:A:161[B]:HIS:CE1	1:A:162:GLU:HG3	2.38	0.59
1:C:154:VAL:HB	3:D:317:GLN:HG2	1.85	0.58
1:C:52:ILE:O	1:C:56:LYS:HG3	2.03	0.58
1:C:217:ARG:NH1	6:C:2103:HOH:O	2.37	0.58
1:C:13:GLY:O	1:C:14:THR:CB	2.53	0.57
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.85	0.57
1:A:72:THR:HG22	1:A:75:LYS:N	2.18	0.56
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.40	0.56
4:A:1299:T9N:H13	4:A:1299:T9N:N09	2.20	0.56
1:A:73:GLU:HG2	1:A:74:ASN:N	2.22	0.55
2:B:176:PRO:HB2	2:B:179[B]:HIS:CD2	2.42	0.55
1:C:177:CYS:HB3	1:C:233:MET:HE1	1.89	0.54
1:C:16:GLY:HA2	1:C:34:LYS:O	2.07	0.54
1:C:72:THR:HG22	1:C:74:ASN:H	1.73	0.54
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:428:GLU:HG2	6:D:2090:HOH:O	2.06	0.53
1:C:256:ASP:O	1:C:260:ARG:HG3	2.07	0.53
1:C:13:GLY:O	1:C:14:THR:HB	2.08	0.53
1:C:252:VAL:O	1:C:252:VAL:HG13	2.09	0.53
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.44	0.52
3:D:399:LEU:HD23	3:D:426:PRO:HB2	1.91	0.52
1:C:145:ASP:HB2	4:C:1296:T9N:H013	1.91	0.52
1:A:252:VAL:HG12	1:A:255:LEU:HB2	1.91	0.51
1:C:198:THR:O	1:C:199:ARG:HB2	2.08	0.51
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.45	0.51
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.92	0.51
3:D:407:GLN:O	3:D:411:GLU:HG2	2.11	0.51
2:B:300:LYS:NZ	6:B:2126:HOH:O	2.45	0.50
3:D:277:GLU:O	3:D:281:ILE:HG23	2.12	0.50
1:C:51:GLU:O	1:C:55:LEU:HB2	2.12	0.49
3:D:322:GLN:HB3	3:D:324:PRO:O	2.13	0.49
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.95	0.48
2:B:225:TYR:HE2	2:B:281:ILE:HG21	1.77	0.48
1:A:72:THR:CG2	1:A:73:GLU:N	2.76	0.48
1:A:47:THR:HG23	1:A:147:GLY:O	2.14	0.48
1:A:98:GLY:HA2	1:A:199:ARG:NH1	2.29	0.47
1:A:71:HIS:NE2	2:B:296[B]:HIS:ND1	2.60	0.47
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.45	0.47
1:C:177:CYS:HB3	1:C:233:MET:CE	2.43	0.47
3:D:346:PRO:HD2	3:D:347:TYR:CD2	2.50	0.47
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.50	0.47
2:B:334:MET:HE2	6:B:2085:HOH:O	2.14	0.46
1:C:203:PHE:CE1	1:C:215:ILE:HA	2.51	0.46
1:A:71:HIS:NE2	2:B:296[A]:HIS:CD2	2.84	0.46
1:C:124:LEU:HG	1:C:152:PHE:CD1	2.51	0.46
3:D:400:LYS:O	3:D:400:LYS:HG2	2.16	0.45
1:C:224:GLU:OE2	1:C:229:GLY:N	2.44	0.45
1:A:157:ARG:HD3	6:A:2155:HOH:O	2.15	0.45
1:C:106:SER:O	1:C:110:GLN:HG3	2.17	0.45
1:C:181:SER:O	1:C:184:VAL:HG22	2.16	0.45
3:D:177:ASP:C	3:D:179:HIS:H	2.20	0.45
3:D:335:PHE:CZ	3:D:339:LEU:HD11	2.52	0.45
1:C:109:PHE:O	1:C:113:GLN:HG3	2.17	0.45
1:A:293:VAL:HG23	1:A:293:VAL:O	2.17	0.44
2:B:199:TYR:C	2:B:199:TYR:CD1	2.90	0.44
1:A:18:VAL:HA	1:A:32:LEU:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLU:O	1:A:55:LEU:HB2	2.18	0.44
1:A:148:LEU:HB3	6:A:2127:HOH:O	2.17	0.44
2:B:323:GLN:HA	2:B:324:PRO:HA	1.77	0.44
1:C:22:ARG:HD2	6:C:2012:HOH:O	2.16	0.44
1:C:71:HIS:CE1	3:D:304:PHE:CE2	2.94	0.44
1:A:155:PRO:HG3	2:B:320:LEU:HD21	2.00	0.43
1:A:252:VAL:HG12	1:A:252:VAL:O	2.17	0.43
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.85	0.43
3:D:278:PHE:O	3:D:281:ILE:HG12	2.18	0.43
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.84	0.43
1:A:73:GLU:HG2	1:A:74:ASN:H	1.82	0.43
1:A:268:HIS:CD2	6:A:2220:HOH:O	2.72	0.43
1:C:121:HIS:C	1:C:122:ARG:HG3	2.39	0.43
1:A:64:VAL:HB	6:A:2072:HOH:O	2.18	0.43
1:A:199:ARG:HH11	1:A:199:ARG:HG3	1.83	0.42
2:B:425:ASN:HA	2:B:426:PRO:HD3	1.95	0.42
1:C:105:LYS:HE3	1:C:105:LYS:HB2	1.73	0.42
3:D:361:HIS:CD2	3:D:391:LEU:HD21	2.53	0.42
1:A:107:TYR:O	1:A:111:LEU:HG	2.19	0.42
4:C:1296:T9N:N09	4:C:1296:T9N:C13	2.83	0.42
3:D:361:HIS:HD2	3:D:391:LEU:HD21	1.84	0.42
1:A:133:LEU:HD11	1:A:192:ILE:HD13	2.01	0.42
1:C:83:LEU:O	4:C:1296:T9N:N11	2.53	0.42
3:D:345:ASP:HA	3:D:346:PRO:HA	1.80	0.42
2:B:345:ASP:HA	2:B:346:PRO:HA	1.84	0.42
3:D:203:GLN:HB3	3:D:206:ILE:HG12	2.01	0.42
3:D:327:CYS:HB3	3:D:419:HIS:CE1	2.55	0.42
1:A:233:MET:HA	1:A:234:PRO:HD3	1.93	0.42
1:C:72:THR:HG22	1:C:73:GLU:N	2.34	0.42
1:A:283:HIS:ND1	1:A:284:PRO:HD2	2.34	0.42
2:B:176:PRO:HD2	2:B:179[A]:HIS:CE1	2.55	0.42
2:B:347:TYR:OH	2:B:394:LEU:HA	2.20	0.41
3:D:186:LEU:HD12	3:D:317:GLN:HE22	1.85	0.41
1:C:71:HIS:HE1	3:D:304:PHE:CE2	2.37	0.41
1:A:177:CYS:HB2	6:A:2177:HOH:O	2.21	0.41
3:D:401:ALA:HB3	3:D:402:PRO:HD3	2.01	0.41
1:A:37:LEU:HD13	2:B:296[B]:HIS:CE1	2.56	0.41
1:A:249:SER:O	1:A:253:PRO:HA	2.19	0.41
1:C:12:GLU:HG2	1:C:17:VAL:HG22	2.02	0.41
1:C:107:TYR:O	1:C:111:LEU:HG	2.21	0.41
3:D:229:ASN:HD22	3:D:334:MET:CE	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:177:ASP:N	3:D:179:HIS:HD2	2.18	0.40
1:C:101:LEU:N	1:C:102:PRO:CD	2.84	0.40
1:A:176:GLY:O	1:A:234:PRO:HG2	2.22	0.40
4:A:1299:T9N:H013	6:A:2133:HOH:O	2.21	0.40
1:C:233:MET:HA	1:C:234:PRO:HD3	1.94	0.40
1:A:161[B]:HIS:ND1	1:A:162:GLU:N	2.70	0.40
1:A:163:VAL:HG12	6:A:2127:HOH:O	2.21	0.40
2:B:334:MET:HB3	2:B:334:MET:HE3	1.91	0.40
1:A:71:HIS:CE1	2:B:296[A]:HIS:CD2	3.10	0.40
1:A:237:LYS:HA	1:A:238:PRO:HD3	1.96	0.40
1:C:122:ARG:O	1:C:151:ALA:HA	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	293/300 (98%)	283 (97%)	9 (3%)	1 (0%)	41	41
1	C	293/300 (98%)	285 (97%)	5 (2%)	3 (1%)	15	11
2	B	257/262 (98%)	255 (99%)	2 (1%)	0	100	100
3	D	254/262 (97%)	249 (98%)	5 (2%)	0	100	100
All	All	1097/1124 (98%)	1072 (98%)	21 (2%)	4 (0%)	34	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	THR
1	C	164	VAL
1	A	164	VAL
1	C	145	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	262/263 (100%)	258 (98%)	4 (2%)	65	71
1	C	259/263 (98%)	255 (98%)	4 (2%)	65	71
2	B	233/236 (99%)	232 (100%)	1 (0%)	91	94
3	D	230/236 (98%)	230 (100%)	0	100	100
All	All	984/998 (99%)	975 (99%)	9 (1%)	78	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	14	THR
1	A	72	THR
1	A	122	ARG
2	B	199	TYR
1	C	15	TYR
1	C	70	ILE
1	C	122	ARG
1	C	248	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	179	HIS

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	1.11	0	10,14,16	1.92	1 (10%)
1	TPO	A	160	1	8,10,11	1.17	0	10,14,16	1.61	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	-	0/9/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	160	TPO	P-OG1-CB	-5.38	108.71	123.33
1	A	160	TPO	P-OG1-CB	-4.18	111.98	123.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

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

4 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
4	T9N	C	1296	-	19,26,26	3.23	6 (31%)	21,36,36	4.83	6 (28%)
4	T9N	A	1299	-	19,26,26	3.20	5 (26%)	21,36,36	4.81	8 (38%)
5	SO4	D	1432	-	4,4,4	0.37	0	6,6,6	0.10	0
5	SO4	B	1433	-	4,4,4	0.38	0	6,6,6	0.18	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
4	T9N	C	1296	-	-	2/6/12/12	0/3/3/3
4	T9N	A	1299	-	-	3/6/12/12	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1299	T9N	C13-C14	8.87	1.52	1.39
4	C	1296	T9N	C13-C14	8.65	1.52	1.39
4	C	1296	T9N	C18-C12	6.81	1.50	1.39
4	A	1299	T9N	C18-C12	6.67	1.50	1.39
4	C	1296	T9N	C17-C16	5.82	1.48	1.38
4	A	1299	T9N	C17-C16	5.47	1.48	1.38
4	C	1296	T9N	C10-N11	3.58	1.44	1.36
4	C	1296	T9N	C21-C22	3.49	1.49	1.44
4	A	1299	T9N	C10-N11	3.44	1.43	1.36
4	A	1299	T9N	C21-C22	3.39	1.49	1.44
4	C	1296	T9N	C13-C12	-2.04	1.36	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1296	T9N	N19-C10-N09	-15.23	111.70	126.42
4	A	1299	T9N	N19-C10-N09	-14.69	112.21	126.42
4	A	1299	T9N	C01-N02-C03	-13.79	110.06	122.85
4	C	1296	T9N	C01-N02-C03	-13.55	110.28	122.85
4	C	1296	T9N	C20-N19-C10	6.63	124.89	115.81
4	A	1299	T9N	C20-N19-C10	6.59	124.84	115.81
4	A	1299	T9N	C07-C08-N09	3.40	119.77	115.10
4	C	1296	T9N	C12-N11-C10	-3.23	120.68	129.38
4	C	1296	T9N	N11-C10-N19	2.85	124.37	116.29
4	A	1299	T9N	C12-N11-C10	-2.57	122.46	129.38
4	A	1299	T9N	N11-C10-N19	2.57	123.56	116.29
4	A	1299	T9N	C20-C21-C22	2.23	123.75	118.87
4	A	1299	T9N	N11-C10-N09	2.12	124.19	116.90
4	C	1296	T9N	N11-C10-N09	2.03	123.88	116.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1299	T9N	N19-C10-N11-C12
4	C	1296	T9N	N19-C10-N11-C12
4	A	1299	T9N	N09-C10-N11-C12
4	C	1296	T9N	N09-C10-N11-C12
4	A	1299	T9N	C20-C21-C22-N23

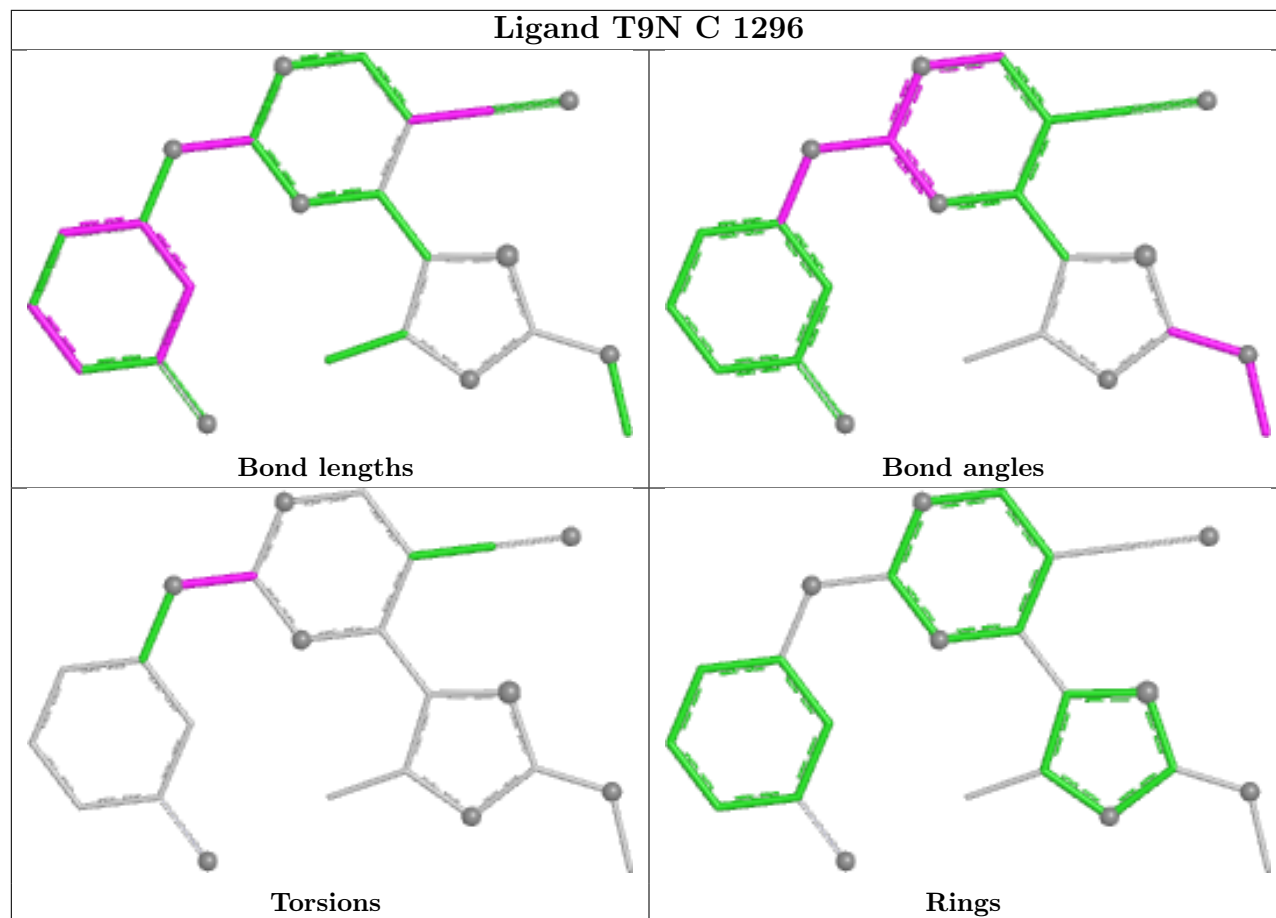
There are no ring outliers.

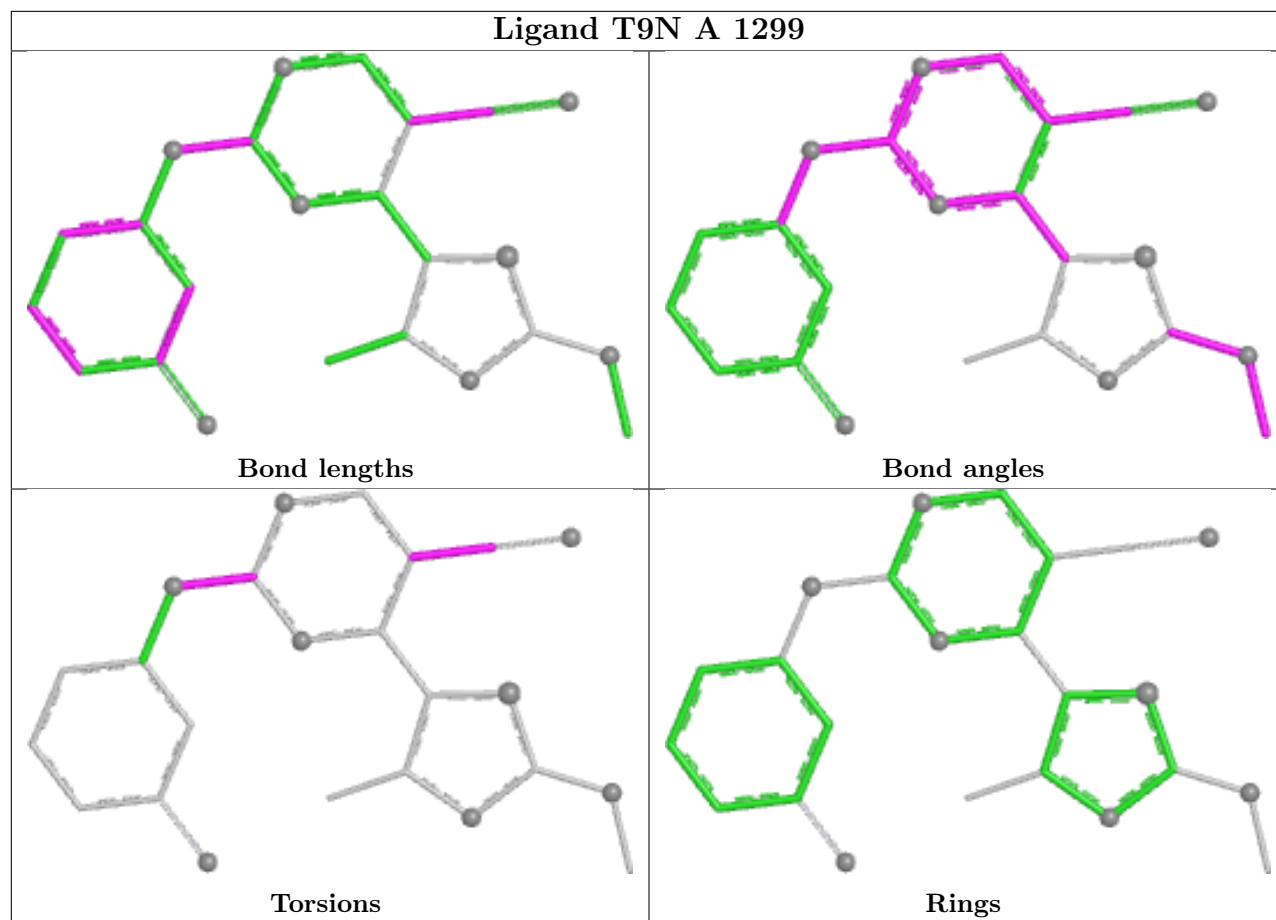
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1296	T9N	4	0
4	A	1299	T9N	2	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	296/300 (98%)	0.35	15 (5%) 28 33	14, 24, 71, 92	0
1	C	295/300 (98%)	0.77	38 (12%) 3 4	26, 50, 82, 109	0
2	B	257/262 (98%)	0.14	6 (2%) 60 65	16, 28, 52, 81	0
3	D	255/262 (97%)	0.77	35 (13%) 3 4	23, 45, 83, 112	0
All	All	1103/1124 (98%)	0.51	94 (8%) 10 13	14, 36, 78, 112	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	LEU	7.0
3	D	367	VAL	6.7
1	A	15	TYR	6.6
1	C	14	THR	5.9
3	D	329	VAL	5.0
1	C	15	TYR	5.0
1	A	14	THR	4.8
3	D	177	ASP	4.5
1	A	295	HIS	4.4
1	C	13	GLY	4.3
3	D	423	LEU	4.2
3	D	323	GLN	4.0
1	C	256	ASP	4.0
1	A	95	ALA	3.9
1	C	287	GLN	3.9
3	D	372	TRP	3.8
1	C	282	ALA	3.7
1	C	236	TYR	3.6
3	D	324	PRO	3.6
1	C	101	LEU	3.6
1	C	248	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	255	LEU	3.5
1	C	219	LEU	3.5
3	D	327	CYS	3.4
1	C	234	PRO	3.4
3	D	319	PHE	3.4
2	B	284	ASP	3.4
3	D	178	TYR	3.4
1	C	251	VAL	3.4
1	A	36	ARG	3.3
3	D	409	ILE	3.2
3	D	360	PHE	3.2
1	A	297	ARG	3.1
1	C	289	VAL	3.1
3	D	421	VAL	3.1
1	A	162	GLU	3.1
1	C	286	PHE	3.1
1	C	293	VAL	3.1
3	D	415	ASN	3.0
3	D	359	ALA	3.0
1	C	258	ASP	2.9
3	D	419	HIS	2.9
3	D	420	GLY	2.9
1	C	247	ASP	2.9
3	D	430	LEU	2.9
3	D	395	HIS	2.8
2	B	280	TYR	2.8
3	D	418	TYR	2.8
1	C	262	LEU	2.7
3	D	416	SER	2.7
1	C	231	THR	2.7
1	A	72	THR	2.6
1	C	16	GLY	2.6
1	A	73	GLU	2.6
3	D	384	LEU	2.6
1	C	161	HIS	2.5
1	C	157	ARG	2.5
2	B	283	ASP	2.5
3	D	328	LYS	2.5
3	D	336	LEU	2.4
1	C	155	PRO	2.4
2	B	431	ASN	2.4
3	D	280	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	323	GLN	2.4
3	D	428	GLU	2.4
1	A	0	SER	2.3
3	D	226	LYS	2.3
1	C	241	PRO	2.3
3	D	424	LEU	2.3
1	C	175	LEU	2.3
1	C	232	SER	2.3
1	C	243	TRP	2.2
1	A	19	TYR	2.2
1	C	257	GLU	2.2
3	D	326	ASN	2.2
3	D	322	GLN	2.2
1	C	225	VAL	2.2
1	C	284	PRO	2.2
3	D	427	PRO	2.2
2	B	176	PRO	2.2
1	C	179	TYR	2.2
1	C	285	PHE	2.1
3	D	332	LEU	2.1
1	C	-1	GLY	2.1
1	C	227	TRP	2.1
1	A	38	ASP	2.1
3	D	284	ASP	2.1
3	D	364	LEU	2.1
1	C	102	PRO	2.1
3	D	410[A]	ARG	2.1
1	A	16	GLY	2.1
1	C	272	ASN	2.0
1	C	283	HIS	2.0
1	A	67	LEU	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(Å ²)	Q < 0.9
1	TPO	C	160	11/12	0.94	0.17	34,41,47,50	0
1	TPO	A	160	11/12	0.99	0.11	18,22,24,26	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

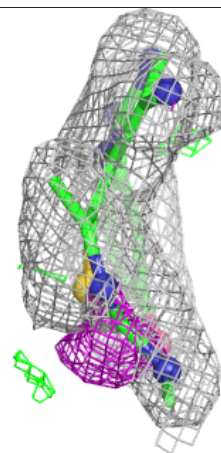
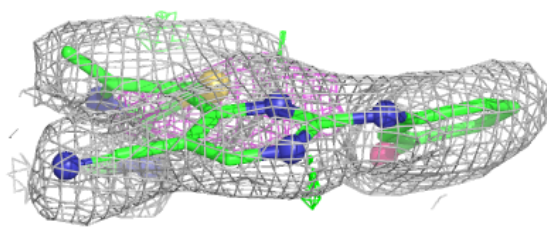
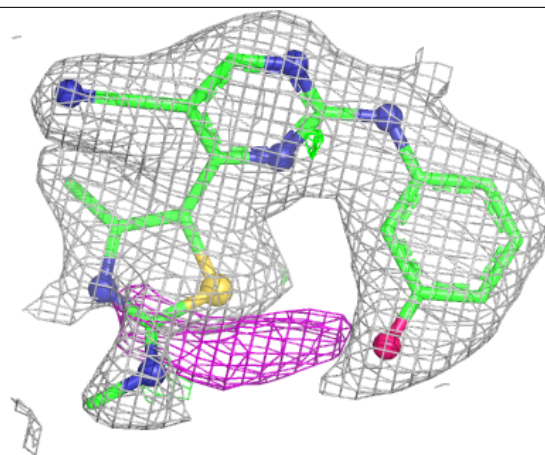
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

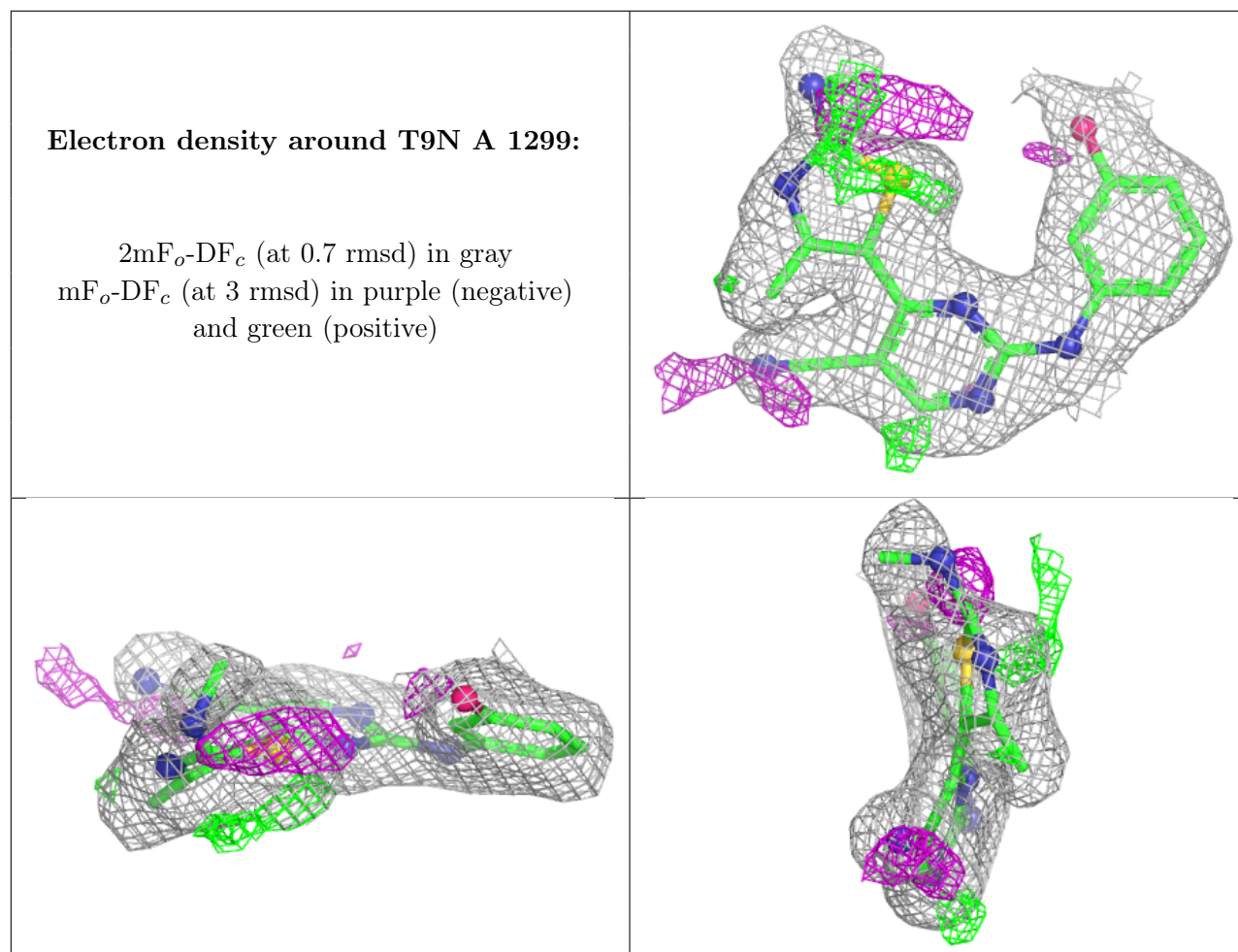
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	B	1433	5/5	0.90	0.21	68,72,76,81	0
4	T9N	C	1296	24/24	0.92	0.14	29,38,73,73	0
4	T9N	A	1299	24/24	0.92	0.16	20,31,60,62	0
5	SO4	D	1432	5/5	0.93	0.21	84,86,87,87	0

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 T9N C 1296:

$2mF_o-DF_c$ (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.