



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:17 am BST

PDB ID : 4BCP  
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 : 2.26 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](mailto: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.

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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 : 2.11  
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) : 2.11

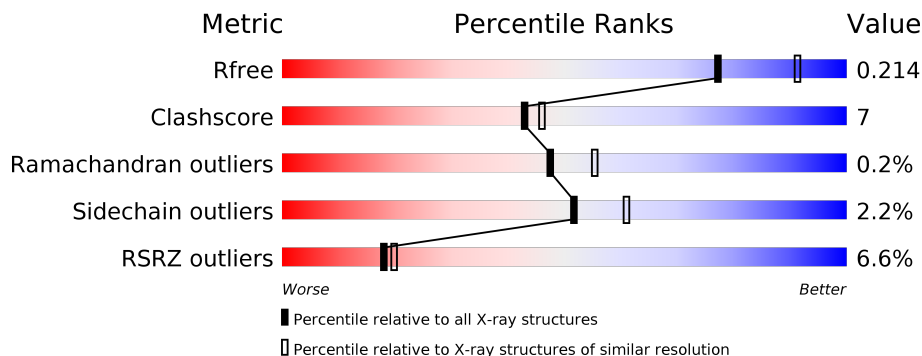
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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  $\geq 3$ , 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	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 30px;">3%      87%      12%      •</p>
1	C	300	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 30px;">9%      72%      16%      •      11%</p>
2	B	262	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 30px;">5%      89%      9%      •</p>
2	D	262	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 30px;">9%      84%      13%      •</p>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	T3C	A	1299[A]	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9233 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	299	2406	1562	409	426	1	8	0	0	0
1	C	268	2157	1400	369	380	1	7	0	1	0

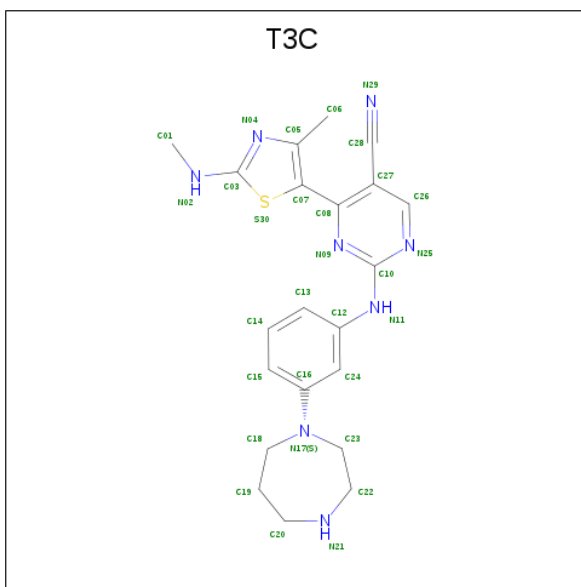
There are 4 discrepancies between the modelled and reference sequences:

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.

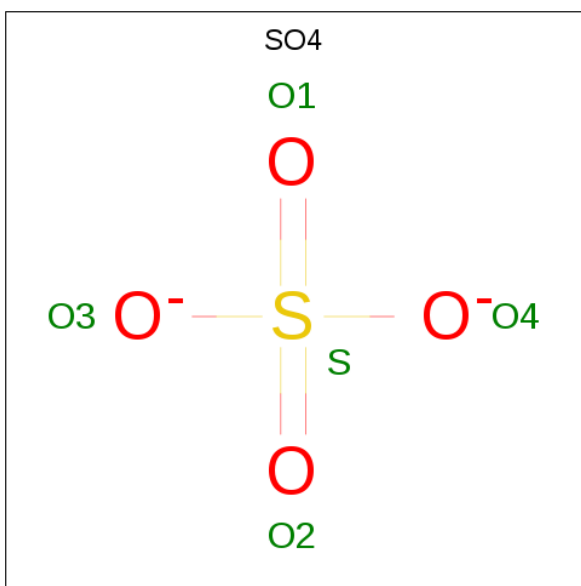
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	257	2083	1350	340	382	11	0	1	0
2	D	257	2076	1345	338	382	11	0	0	0

- Molecule 3 is 2-[[3-(1,4-diazepan-1-yl)phenyl]amino]-4-[4-methyl-2-(methylamino)-1,3-thiazol-5-yl]pyrimidine-5-carbonitrile (three-letter code: T3C) (formula: C<sub>21</sub>H<sub>24</sub>N<sub>8</sub>S).



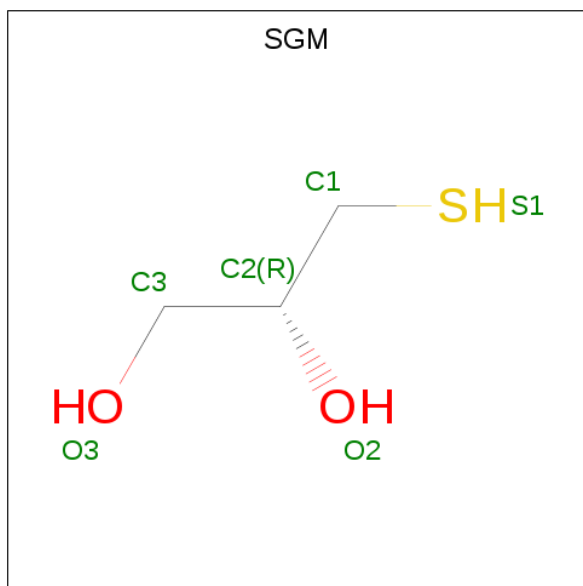
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			S
3	A	1	60	42	16	2	0	1
3	C	1	60	42	16	2	0	1

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>S).



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

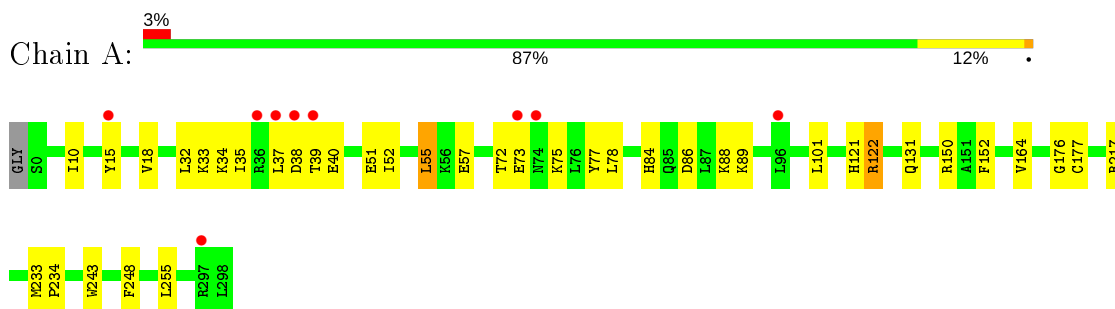
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	143	Total	O	0	0
			143	143		
6	B	105	Total	O	0	0
			105	105		
6	C	64	Total	O	0	0
			64	64		
6	D	51	Total	O	0	0
			51	51		

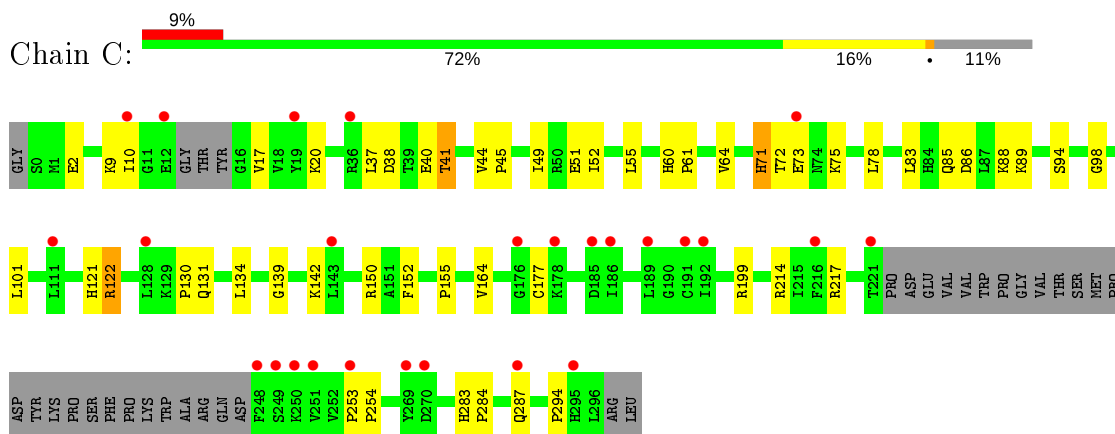
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

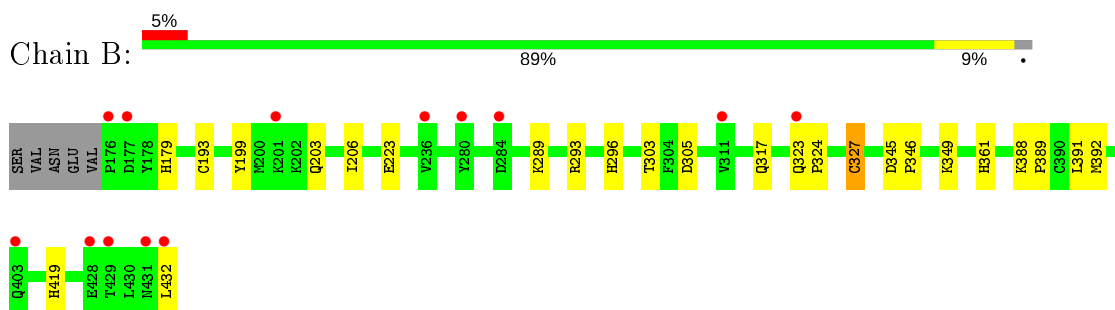
- Molecule 1: CYCLIN-DEPENDENT KINASE 2



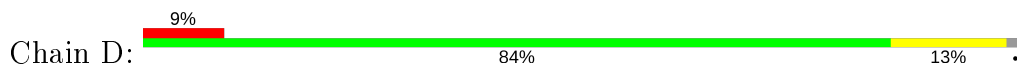
- Molecule 1: CYCLIN-DEPENDENT KINASE 2

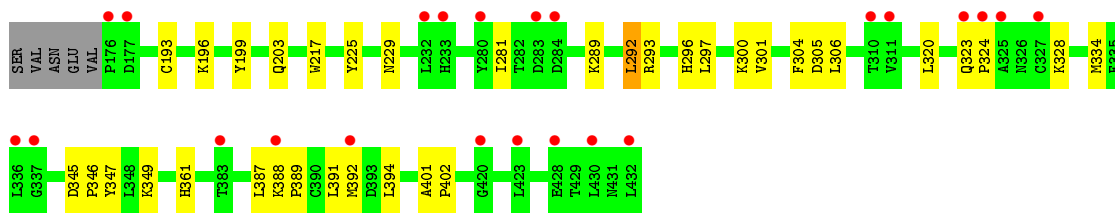


- Molecule 2: CYCLIN-A2



- Molecule 2: CYCLIN-A2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.81Å 134.55Å 149.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.68 – 2.26 29.68 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.68-2.26) 98.9 (29.68-2.26)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.26Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.181 , 0.217 0.179 , 0.214	Depositor DCC
$R_{free}$ test set	3512 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtrriage
Anisotropy	0.203	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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, SGM, SO4, T3C

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	0.24	0/2456	0.41	0/3332
1	C	0.22	0/2197	0.40	0/2972
2	B	0.23	0/2137	0.40	0/2901
2	D	0.22	0/2126	0.39	0/2886
All	All	0.23	0/8916	0.40	0/12091

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	2406	0	2451	34	0
1	C	2157	0	2214	42	0
2	B	2083	0	2106	16	0
2	D	2076	0	2099	32	0
3	A	60	0	48	18	0
3	C	60	0	48	5	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
5	B	12	0	16	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	6	0	8	2	0
6	A	143	0	0	4	0
6	B	105	0	0	0	0
6	C	64	0	0	1	0
6	D	51	0	0	1	0
All	All	9233	0	8990	122	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 (122) 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:38:ASP:HB3	1:C:41:THR:HG23	1.54	0.87
2:B:327:CYS:HG	5:B:1435:SGM:HO2	1.08	0.84
2:B:193:CYS:SG	5:B:1434:SGM:S1	2.52	0.81
1:A:89:LYS:NZ	3:A:1299[A]:T3C:H15	1.96	0.81
2:B:327:CYS:SG	5:B:1435:SGM:O2	2.31	0.80
2:D:193:CYS:SG	5:D:1434:SGM:S1	2.55	0.79
1:A:89:LYS:HZ1	3:A:1299[A]:T3C:H15	1.52	0.74
1:A:10:ILE:HG22	3:A:1299[A]:T3C:H181	1.69	0.73
3:C:1297[A]:T3C:H24	3:C:1297[A]:T3C:N09	2.05	0.72
1:C:155:PRO:HG3	2:D:320:LEU:HD21	1.71	0.72
2:B:327:CYS:SG	5:B:1435:SGM:S1	2.85	0.70
1:A:37:LEU:O	1:A:40:GLU:HB2	1.91	0.69
2:B:289:LYS:O	2:B:293:ARG:HG3	1.93	0.69
3:A:1299[A]:T3C:H24	3:A:1299[A]:T3C:N09	2.09	0.68
1:A:72:THR:HG22	1:A:75:LYS:HB2	1.75	0.67
1:A:86:ASP:OD2	3:A:1299[A]:T3C:H221	1.94	0.67
1:C:177:CYS:SG	6:C:2052:HOH:O	2.52	0.67
1:C:98:GLY:HA2	1:C:199:ARG:HD3	1.77	0.65
2:D:361:HIS:HD2	2:D:391:LEU:HD21	1.63	0.63
1:C:10:ILE:HG22	3:C:1297[A]:T3C:H181	1.80	0.62
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.33	0.62
2:D:388:LYS:HG2	2:D:392:MET:HE1	1.82	0.62
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.35	0.61
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.84	0.60
2:D:346:PRO:O	2:D:349:LYS:HG2	2.01	0.60
1:A:89:LYS:HZ1	3:A:1299[B]:T3C:H182	1.67	0.59
1:A:15:TYR:HE1	1:A:35:ILE:HD11	1.68	0.59
1:C:85:GLN:NE2	1:C:89:LYS:HB3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:GLN:HE21	1:C:89:LYS:HB3	1.68	0.58
1:C:64:VAL:HG21	3:C:1297[A]:T3C:N29	2.18	0.58
1:C:51:GLU:O	1:C:55:LEU:HB2	2.04	0.57
1:A:51:GLU:O	1:A:55:LEU:HB2	2.04	0.57
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.86	0.57
2:B:346:PRO:O	2:B:349:LYS:HG2	2.05	0.57
1:A:84:HIS:O	3:A:1299[B]:T3C:H222	2.05	0.56
1:A:88:LYS:NZ	6:A:2047:HOH:O	2.37	0.56
1:A:72:THR:HG23	1:A:73:GLU:N	2.20	0.55
1:C:131:GLN:O	3:C:1297[A]:T3C:H222	2.06	0.55
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.42	0.55
1:A:177:CYS:HB2	1:A:233:MET:CE	2.37	0.54
1:A:89:LYS:HZ1	3:A:1299[B]:T3C:H15	1.73	0.54
1:C:88:LYS:HB2	1:C:130:PRO:HB2	1.90	0.54
1:A:15:TYR:O	1:A:33:LYS:HE2	2.08	0.53
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.90	0.53
1:A:89:LYS:HZ3	3:A:1299[A]:T3C:H15	1.71	0.53
1:C:122:ARG:HA	1:C:152:PHE:CE2	2.44	0.52
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.92	0.52
2:D:289:LYS:HE2	2:D:293:ARG:NH1	2.25	0.52
1:C:71[A]:HIS:CE1	2:D:296:HIS:NE2	2.78	0.52
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.92	0.52
1:A:38:ASP:O	1:A:39:THR:OG1	2.16	0.51
1:C:86:ASP:OD2	1:C:89:LYS:HD3	2.10	0.51
1:C:9:LYS:HE3	1:C:17:VAL:HG13	1.93	0.51
1:A:34:LYS:HE2	1:A:77:TYR:OH	2.10	0.51
1:C:71[B]:HIS:HE2	2:D:304:PHE:HE2	1.57	0.51
1:C:71[A]:HIS:CD2	2:D:300:LYS:HG2	2.46	0.50
2:D:347:TYR:OH	2:D:394:LEU:HA	2.12	0.50
1:C:72:THR:HG22	1:C:73:GLU:N	2.27	0.49
1:C:214:ARG:O	1:C:217:ARG:HG2	2.12	0.49
1:C:83:LEU:HD22	1:C:134:LEU:HB2	1.95	0.49
1:C:72:THR:HB	1:C:75:LYS:O	2.12	0.48
1:A:18:VAL:HA	1:A:32:LEU:O	2.13	0.48
1:A:72:THR:CG2	1:A:75:LYS:HB2	2.43	0.48
2:D:229:ASN:HD22	2:D:334:MET:CE	2.27	0.48
2:B:303:THR:HG23	2:B:305:ASP:OD2	2.14	0.48
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.96	0.47
2:B:203:GLN:HB3	2:B:206:ILE:HG12	1.96	0.47
3:A:1299[A]:T3C:C24	3:A:1299[A]:T3C:N09	2.78	0.47
2:D:203:GLN:O	6:D:2007:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:305:ASP:HB3	5:D:1434:SGM:H31	1.97	0.46
1:A:217:ARG:HG2	1:A:243:TRP:CE2	2.50	0.46
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.50	0.46
1:C:214:ARG:HA	1:C:217:ARG:HD3	1.98	0.46
1:C:71[A]:HIS:CE1	2:D:296:HIS:HE2	2.34	0.46
2:B:305:ASP:HB3	5:B:1434:SGM:H31	1.96	0.46
2:D:387:LEU:O	2:D:391:LEU:HB2	2.17	0.46
1:A:121:HIS:C	1:A:122:ARG:HG3	2.37	0.45
1:A:176:GLY:O	1:A:234:PRO:HG2	2.16	0.45
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.98	0.45
1:C:71[A]:HIS:CG	2:D:296:HIS:HE2	2.35	0.45
3:A:1299[B]:T3C:H011	6:A:2008:HOH:O	2.17	0.45
1:C:71[B]:HIS:NE2	2:D:304:PHE:HE2	2.15	0.45
1:C:61:PRO:O	1:C:142:LYS:HE2	2.16	0.44
1:C:9:LYS:HE3	1:C:17:VAL:CG1	2.47	0.44
1:A:10:ILE:HG21	3:A:1299[A]:T3C:C24	2.48	0.44
3:A:1299[A]:T3C:C28	3:A:1299[A]:T3C:H061	2.47	0.44
2:B:345:ASP:HA	2:B:346:PRO:HA	1.76	0.44
2:D:225:TYR:HE2	2:D:281:ILE:HG21	1.82	0.44
2:B:179[B]:HIS:CD2	2:B:317:GLN:OE1	2.71	0.44
1:A:121:HIS:O	1:A:122:ARG:HG3	2.18	0.44
2:D:289:LYS:HE2	2:D:293:ARG:HH12	1.82	0.44
1:A:217:ARG:HG2	1:A:243:TRP:CD2	2.53	0.43
2:D:345:ASP:HA	2:D:346:PRO:HA	1.80	0.43
1:C:44:VAL:HA	1:C:45:PRO:HD3	1.91	0.43
1:C:71[A]:HIS:NE2	2:D:304:PHE:HE2	2.17	0.43
2:D:401:ALA:HB3	2:D:402:PRO:HD3	2.01	0.43
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.54	0.42
1:C:10:ILE:HD11	1:C:20:LYS:HB2	2.00	0.42
2:D:323:GLN:HA	2:D:324:PRO:HA	1.80	0.42
1:A:89:LYS:NZ	3:A:1299[B]:T3C:H15	2.33	0.42
1:C:10:ILE:HG21	3:C:1297[A]:T3C:C24	2.50	0.42
1:C:94:SER:O	1:C:199:ARG:HD2	2.20	0.42
2:D:217:TRP:CZ2	2:D:281:ILE:HD13	2.55	0.42
2:B:323:GLN:HA	2:B:324:PRO:HA	1.75	0.42
1:C:37:LEU:HD22	1:C:44:VAL:HG22	2.01	0.42
2:D:346:PRO:HB2	2:D:349:LYS:HE2	2.00	0.41
2:B:361:HIS:HD2	2:B:391:LEU:HD21	1.84	0.41
1:C:121:HIS:C	1:C:122:ARG:HG3	2.41	0.41
2:B:327:CYS:SG	2:B:419:HIS:CE1	3.13	0.41
1:A:131:GLN:O	3:A:1299[A]:T3C:H222	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:OE2	6:A:2031:HOH:O	2.21	0.41
1:C:88:LYS:HG2	1:C:131:GLN:NE2	2.36	0.41
1:C:284:PRO:O	1:C:287:GLN:HG2	2.20	0.41
2:D:292:LEU:HD12	2:D:292:LEU:HA	1.86	0.41
3:A:1299[A]:T3C:H011	6:A:2008:HOH:O	2.21	0.41
3:A:1299[A]:T3C:C28	3:A:1299[A]:T3C:C06	2.98	0.40
1:A:255:LEU:HD12	1:A:255:LEU:HA	1.90	0.40
2:D:388:LYS:CG	2:D:392:MET:HE1	2.50	0.40
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.86	0.40
2:D:199:TYR:CD1	2:D:199:TYR:C	2.95	0.40
1:A:86:ASP:HB3	3:A:1299[A]:T3C:H232	2.03	0.40
2:D:297:LEU:O	2:D:301:VAL:HG23	2.22	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	296/300 (99%)	289 (98%)	6 (2%)	1 (0%)	41	46
1	C	262/300 (87%)	254 (97%)	7 (3%)	1 (0%)	34	37
2	B	256/262 (98%)	255 (100%)	1 (0%)	0	100	100
2	D	255/262 (97%)	251 (98%)	4 (2%)	0	100	100
All	All	1069/1124 (95%)	1049 (98%)	18 (2%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	VAL
1	C	164	VAL

### 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%)	257 (98%)	5 (2%)	57	66
1	C	235/263 (89%)	227 (97%)	8 (3%)	37	45
2	B	232/236 (98%)	226 (97%)	6 (3%)	46	55
2	D	231/236 (98%)	228 (99%)	3 (1%)	69	79
All	All	960/998 (96%)	938 (98%)	22 (2%)	52	59

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	101	LEU
1	A	122	ARG
1	A	150	ARG
1	A	248	PHE
2	B	199	TYR
2	B	223	GLU
2	B	296	HIS
2	B	327	CYS
2	B	392	MET
2	B	432	LEU
1	C	2	GLU
1	C	40	GLU
1	C	41	THR
1	C	71[A]	HIS
1	C	71[B]	HIS
1	C	101	LEU
1	C	122	ARG
1	C	150	ARG
2	D	196	LYS
2	D	292	LEU
2	D	328	LYS

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

Mol	Chain	Res	Type
1	C	85	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	1.12	0
1	TPO	A	160	1	8,10,11	0.78	0	10,14,16	1.13	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
1	TPO	C	160	1	-	0/9/11/13	-
1	TPO	A	160	1	-	0/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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	SO4	D	1433	-	4,4,4	0.15	0	6,6,6	0.06	0
3	T3C	A	1299[B]	-	24,33,33	2.14	6 (25%)	27,45,45	2.18	8 (29%)
3	T3C	A	1299[A]	-	24,33,33	2.14	7 (29%)	27,45,45	2.07	8 (29%)
5	SGM	B	1434	-	5,5,5	0.62	0	5,5,5	0.50	0
5	SGM	D	1434	-	5,5,5	0.33	0	5,5,5	0.89	0
3	T3C	C	1297[B]	-	24,33,33	2.15	7 (29%)	27,45,45	2.13	9 (33%)
3	T3C	C	1297[A]	-	24,33,33	2.15	7 (29%)	27,45,45	2.08	8 (29%)
5	SGM	B	1435	-	5,5,5	0.35	0	5,5,5	0.46	0
4	SO4	B	1433	-	4,4,4	0.15	0	6,6,6	0.07	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	T3C	A	1299[B]	-	-	3/9/25/25	0/4/4/4
3	T3C	A	1299[A]	-	-	7/9/25/25	0/4/4/4
5	SGM	B	1434	-	-	1/4/4/4	-
5	SGM	D	1434	-	-	2/4/4/4	-
3	T3C	C	1297[B]	-	-	3/9/25/25	0/4/4/4
3	T3C	C	1297[A]	-	-	7/9/25/25	0/4/4/4
5	SGM	B	1435	-	-	4/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1299[A]	T3C	C10-N11	5.67	1.48	1.36
3	C	1297[A]	T3C	C10-N11	5.62	1.48	1.36
3	C	1297[B]	T3C	C10-N11	5.60	1.47	1.36
3	A	1299[B]	T3C	C10-N11	5.59	1.47	1.36
3	C	1297[B]	T3C	C08-C07	-4.11	1.39	1.49
3	C	1297[A]	T3C	C08-C07	-4.06	1.40	1.49
3	A	1299[B]	T3C	C08-C07	-4.04	1.40	1.49
3	A	1299[A]	T3C	C08-C07	-4.04	1.40	1.49
3	A	1299[A]	T3C	C16-N17	3.54	1.48	1.38
3	C	1297[A]	T3C	C16-N17	3.50	1.48	1.38
3	C	1297[B]	T3C	C16-N17	3.45	1.48	1.38
3	A	1299[B]	T3C	C16-N17	3.41	1.48	1.38
3	C	1297[B]	T3C	C27-C28	3.34	1.49	1.44
3	C	1297[A]	T3C	C27-C28	3.30	1.49	1.44
3	A	1299[B]	T3C	C27-C28	3.23	1.49	1.44
3	A	1299[A]	T3C	C27-C28	3.19	1.49	1.44
3	A	1299[B]	T3C	C13-C12	2.86	1.44	1.39
3	C	1297[B]	T3C	C13-C12	2.83	1.44	1.39
3	A	1299[A]	T3C	C13-C12	2.78	1.43	1.39
3	C	1297[A]	T3C	C13-C12	2.77	1.43	1.39
3	C	1297[A]	T3C	C06-C05	2.53	1.54	1.50
3	A	1299[A]	T3C	C06-C05	2.53	1.54	1.50
3	A	1299[B]	T3C	C06-C05	2.51	1.54	1.50
3	C	1297[B]	T3C	C06-C05	2.50	1.54	1.50
3	C	1297[A]	T3C	C23-N17	-2.07	1.44	1.46
3	C	1297[B]	T3C	C23-N17	-2.06	1.44	1.46
3	A	1299[A]	T3C	C23-N17	-2.05	1.44	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1297[A]	T3C	N25-C10-N09	-6.29	120.59	126.55
3	A	1299[A]	T3C	N25-C10-N09	-6.25	120.63	126.55
3	C	1297[B]	T3C	N25-C10-N09	-6.07	120.80	126.55
3	A	1299[B]	T3C	N25-C10-N09	-6.05	120.82	126.55
3	A	1299[B]	T3C	C01-N02-C03	-4.31	119.16	122.87
3	A	1299[A]	T3C	C01-N02-C03	-4.31	119.16	122.87
3	C	1297[B]	T3C	C23-N17-C16	-3.97	106.56	119.65
3	A	1299[B]	T3C	C23-N17-C16	-3.92	106.74	119.65
3	C	1297[A]	T3C	C01-N02-C03	-3.77	119.63	122.87
3	C	1297[B]	T3C	C01-N02-C03	-3.46	119.89	122.87
3	C	1297[A]	T3C	C26-N25-C10	3.28	120.83	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1299[B]	T3C	C07-C08-N09	3.24	119.00	115.03
3	C	1297[A]	T3C	C23-N17-C16	-3.22	109.02	119.65
3	A	1299[A]	T3C	C23-N17-C16	-3.22	109.03	119.65
3	C	1297[B]	T3C	C26-N25-C10	3.21	120.73	115.88
3	C	1297[B]	T3C	C07-C08-N09	3.21	118.97	115.03
3	A	1299[A]	T3C	C26-N25-C10	3.19	120.69	115.88
3	A	1299[B]	T3C	C26-N25-C10	3.15	120.64	115.88
3	C	1297[A]	T3C	C07-C08-N09	3.15	118.90	115.03
3	A	1299[B]	T3C	C23-N17-C18	-2.94	112.22	117.47
3	C	1297[B]	T3C	C23-N17-C18	-2.92	112.25	117.47
3	C	1297[A]	T3C	C27-C26-N25	-2.79	119.24	123.42
3	A	1299[B]	T3C	C27-C26-N25	-2.74	119.31	123.42
3	C	1297[B]	T3C	C27-C26-N25	-2.70	119.38	123.42
3	A	1299[A]	T3C	C27-C26-N25	-2.68	119.40	123.42
3	C	1297[A]	T3C	C18-N17-C16	2.68	128.50	119.65
3	A	1299[A]	T3C	C07-C08-N09	2.65	118.29	115.03
3	C	1297[B]	T3C	C18-N17-C16	2.54	128.03	119.65
3	A	1299[A]	T3C	C18-N17-C16	2.54	128.02	119.65
3	A	1299[B]	T3C	C18-N17-C16	2.42	127.64	119.65
3	C	1297[B]	T3C	C12-N11-C10	-2.34	122.45	129.23
3	C	1297[A]	T3C	C12-N11-C10	-2.22	122.78	129.23
3	A	1299[A]	T3C	C12-N11-C10	-2.10	123.15	129.23

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1299[B]	T3C	N09-C10-N11-C12
3	A	1299[A]	T3C	C15-C16-N17-C18
3	A	1299[A]	T3C	C15-C16-N17-C23
3	A	1299[A]	T3C	C24-C16-N17-C18
3	A	1299[A]	T3C	C24-C16-N17-C23
3	A	1299[A]	T3C	C26-C27-C28-N29
3	C	1297[A]	T3C	C15-C16-N17-C18
3	C	1297[A]	T3C	C15-C16-N17-C23
3	C	1297[A]	T3C	C24-C16-N17-C18
3	C	1297[A]	T3C	C24-C16-N17-C23
5	B	1435	SGM	S1-C1-C2-C3
5	B	1435	SGM	C1-C2-C3-O3
5	B	1435	SGM	O2-C2-C3-O3
3	A	1299[B]	T3C	N25-C10-N11-C12
3	C	1297[B]	T3C	N09-C10-N11-C12

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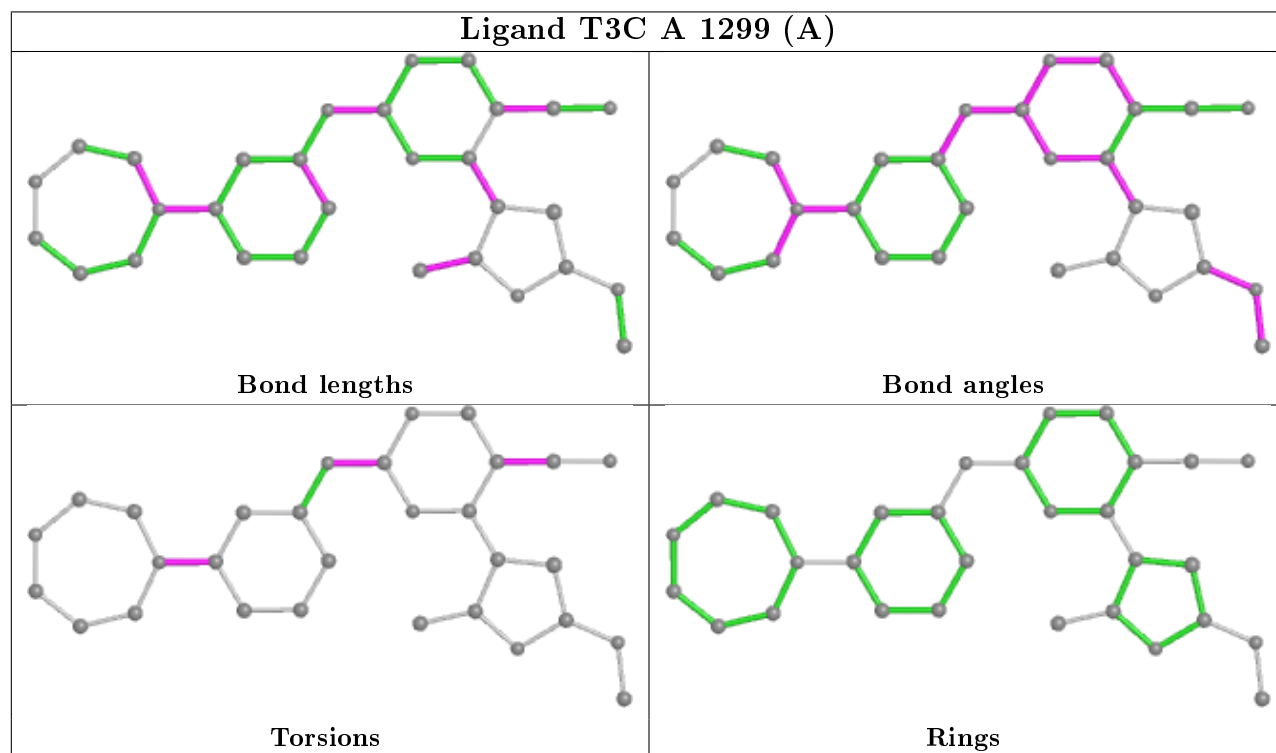
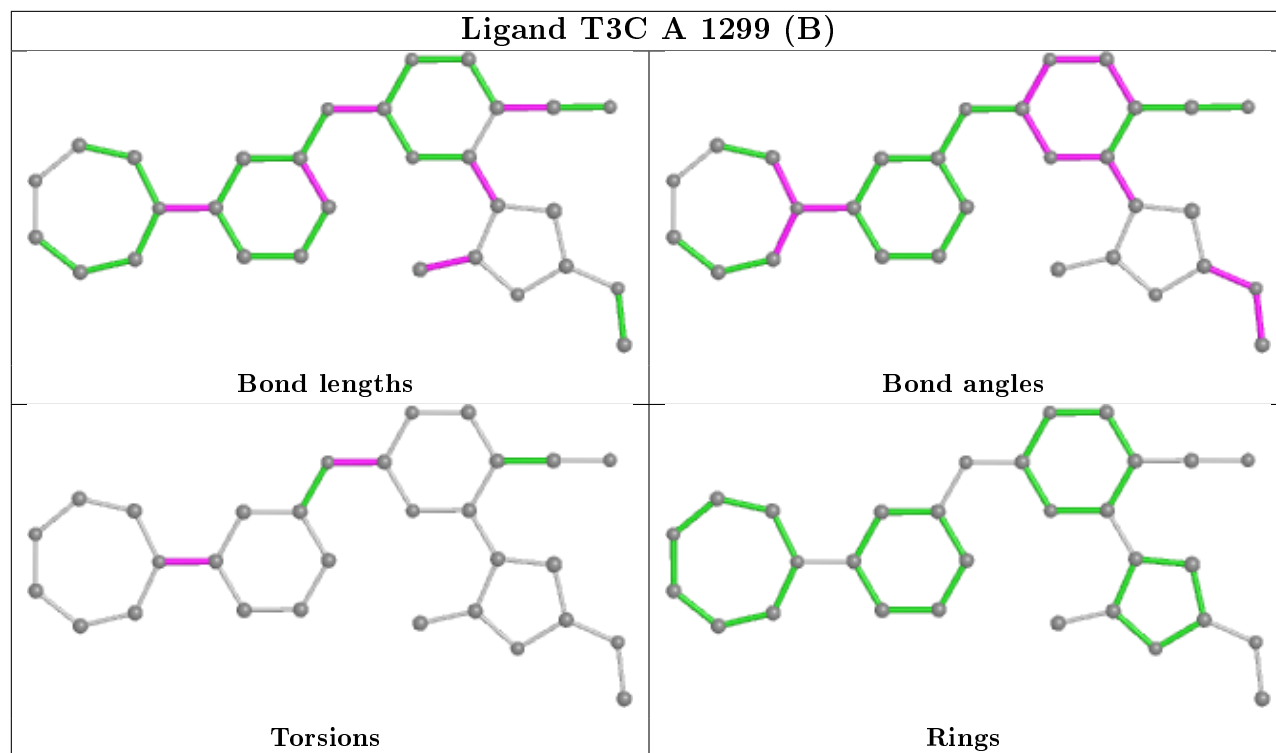
Mol	Chain	Res	Type	Atoms
3	C	1297[B]	T3C	N25-C10-N11-C12
3	A	1299[A]	T3C	N09-C10-N11-C12
3	A	1299[A]	T3C	N25-C10-N11-C12
3	C	1297[A]	T3C	N25-C10-N11-C12
3	C	1297[A]	T3C	N09-C10-N11-C12
5	B	1435	SGM	S1-C1-C2-O2
3	A	1299[B]	T3C	C24-C16-N17-C18
3	C	1297[B]	T3C	C24-C16-N17-C18
5	B	1434	SGM	S1-C1-C2-C3
5	D	1434	SGM	S1-C1-C2-C3
3	C	1297[A]	T3C	C26-C27-C28-N29
5	D	1434	SGM	O2-C2-C3-O3

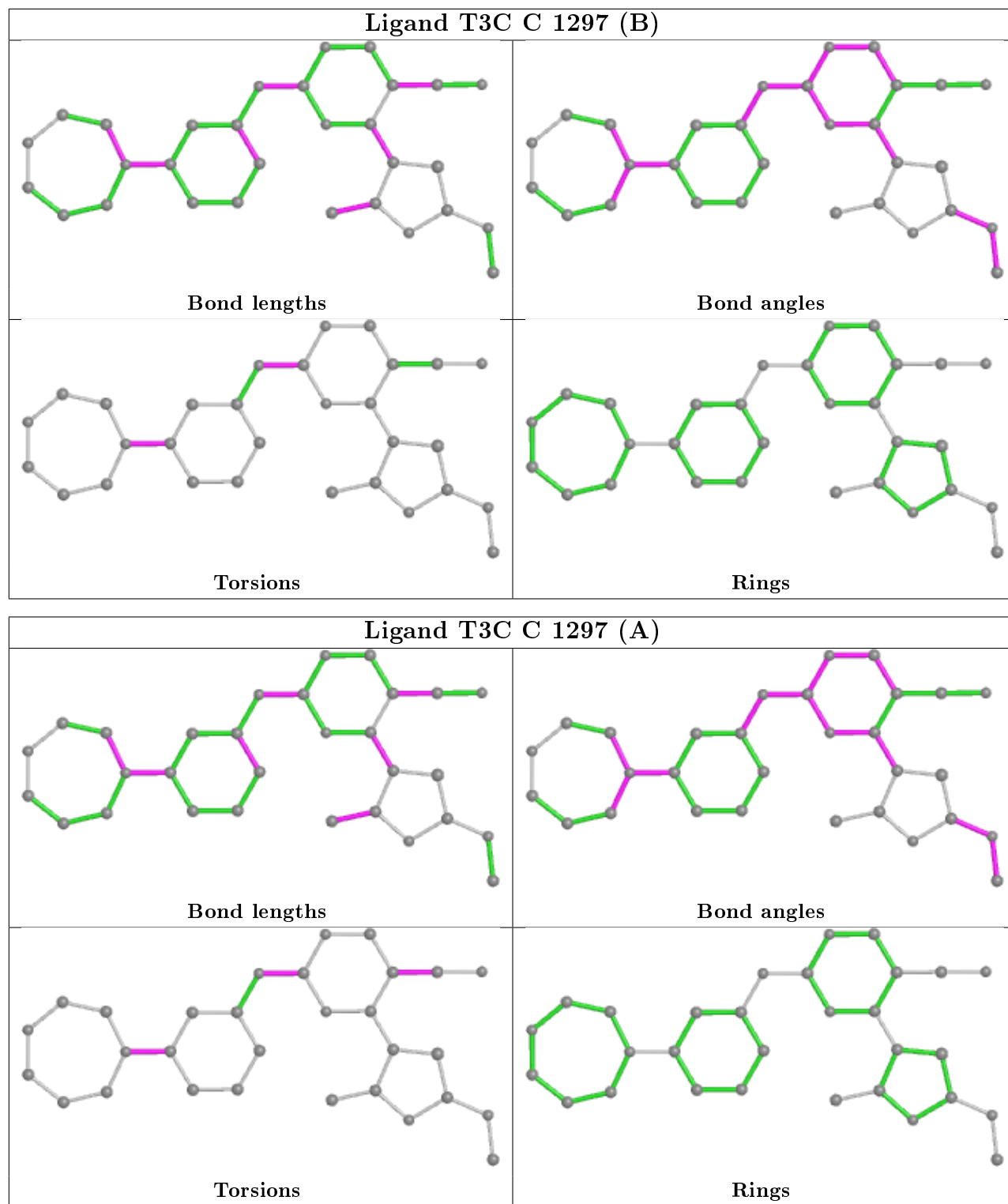
There are no ring outliers.

6 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1299[B]	T3C	5	0
3	A	1299[A]	T3C	13	0
5	B	1434	SGM	2	0
5	D	1434	SGM	2	0
3	C	1297[A]	T3C	5	0
5	B	1435	SGM	3	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	298/300 (99%)	-0.24	9 (3%) 50 53	23, 35, 79, 111	0
1	C	267/300 (89%)	0.26	26 (9%) 7 8	32, 51, 94, 127	0
2	B	257/262 (98%)	-0.12	13 (5%) 28 30	25, 40, 63, 102	0
2	D	257/262 (98%)	0.18	23 (8%) 9 10	31, 51, 87, 125	0
All	All	1079/1124 (95%)	0.01	71 (6%) 18 20	23, 44, 85, 127	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	295	HIS	7.8
2	D	432	LEU	5.4
1	C	221	THR	5.3
1	C	189	LEU	4.9
1	A	38	ASP	4.9
2	D	324	PRO	4.7
1	A	15	TYR	4.4
2	B	323	GLN	4.4
2	D	176	PRO	4.1
1	C	249	SER	4.1
1	A	96	LEU	4.0
1	A	39	THR	3.9
2	B	432	LEU	3.6
1	C	269	TYR	3.6
2	D	323	GLN	3.6
1	C	248	PHE	3.5
1	C	253	PRO	3.4
1	C	73	GLU	3.4
1	C	186	ILE	3.3
1	A	297	ARG	3.2
2	D	311	VAL	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	232	LEU	3.1
2	D	337	GLY	3.1
1	C	287	GLN	3.1
1	C	250	LYS	3.0
1	C	12	GLU	2.9
1	C	128	LEU	2.9
2	B	201	LYS	2.9
2	D	428	GLU	2.9
2	B	431	ASN	2.9
1	A	73	GLU	2.8
1	C	251	VAL	2.8
2	D	423	LEU	2.8
1	A	36	ARG	2.8
2	D	233	HIS	2.8
2	D	336	LEU	2.7
2	B	429	THR	2.7
2	B	177	ASP	2.7
2	B	284	ASP	2.6
2	D	177	ASP	2.6
1	C	111	LEU	2.6
1	C	36	ARG	2.6
2	B	428	GLU	2.6
1	C	191	CYS	2.5
2	D	325	ALA	2.5
1	C	178	LYS	2.5
2	B	176	PRO	2.5
2	B	280	TYR	2.5
1	A	37	LEU	2.5
2	B	311	VAL	2.4
1	C	176	GLY	2.4
1	A	74	ASN	2.4
1	C	192	ILE	2.4
1	C	143	LEU	2.3
2	D	383	THR	2.3
1	C	10	ILE	2.3
2	D	310	THR	2.3
2	D	280	TYR	2.3
2	B	236	VAL	2.2
2	D	388	LYS	2.2
2	D	392	MET	2.2
2	D	420	GLY	2.2
1	C	216	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	283	ASP	2.2
2	D	284	ASP	2.2
1	C	19	TYR	2.1
1	C	270	ASP	2.1
1	C	185	ASP	2.1
2	B	403	GLN	2.0
2	D	327	CYS	2.0
2	D	430	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	TPO	C	160	11/12	0.98	0.06	41,45,47,49	0
1	TPO	A	160	11/12	0.99	0.07	28,34,36,37	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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<sup>th</sup> 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.

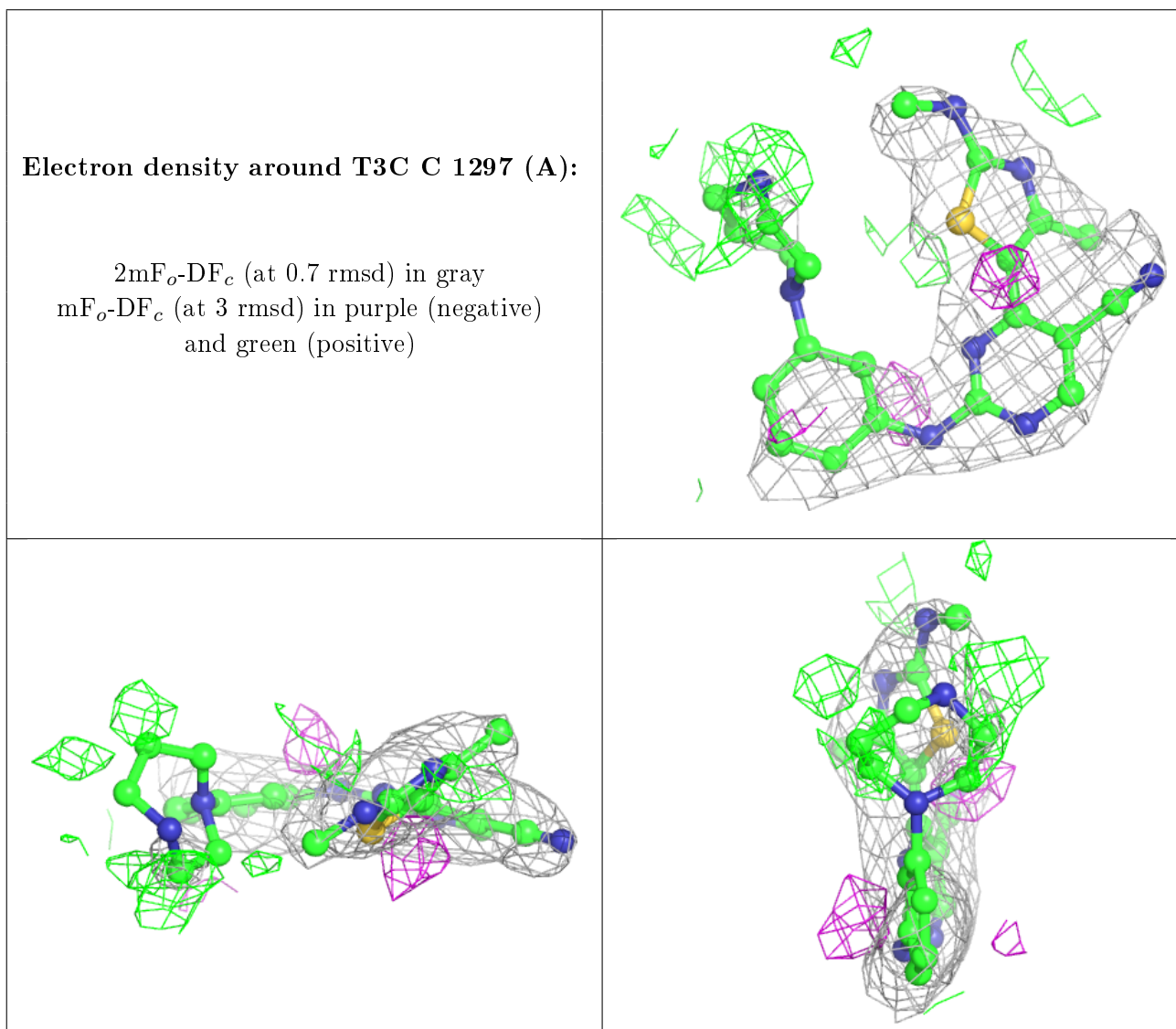
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	SGM	B	1435	6/6	0.70	0.31	86,92,93,161	0
5	SGM	B	1434	6/6	0.81	0.21	42,59,64,81	0
5	SGM	D	1434	6/6	0.82	0.20	65,67,73,132	0
3	T3C	C	1297[A]	30/30	0.88	0.23	54,63,73,125	30
3	T3C	C	1297[B]	30/30	0.88	0.23	53,65,79,125	30
3	T3C	A	1299[A]	30/30	0.91	0.18	51,54,57,57	30
3	T3C	A	1299[B]	30/30	0.91	0.18	52,55,65,67	30
4	SO4	D	1433	5/5	0.93	0.18	103,106,108,114	0

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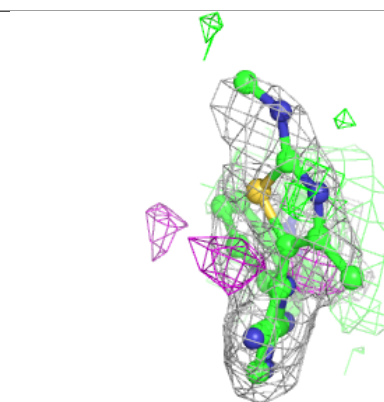
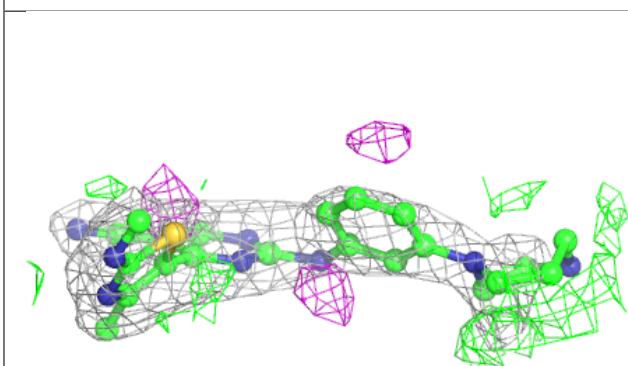
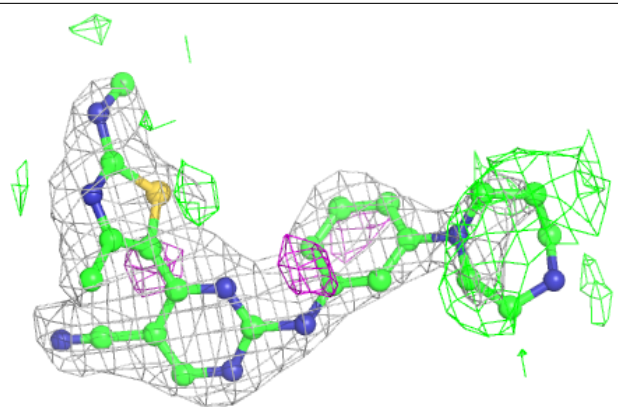
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	1433	5/5	0.96	0.12	102,102,105,116	0

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.



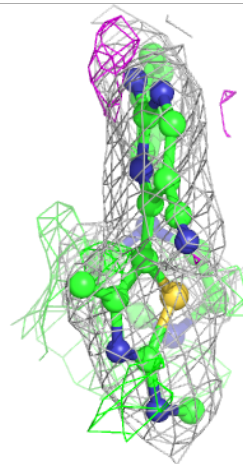
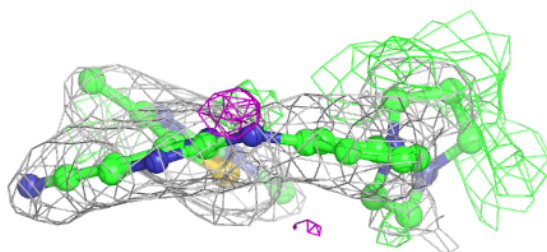
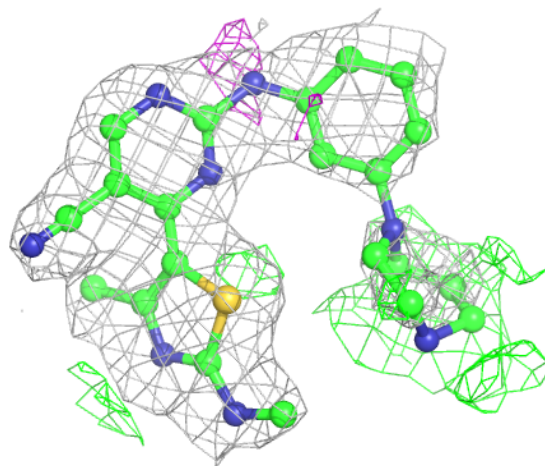
**Electron density around T3C C 1297 (B):**

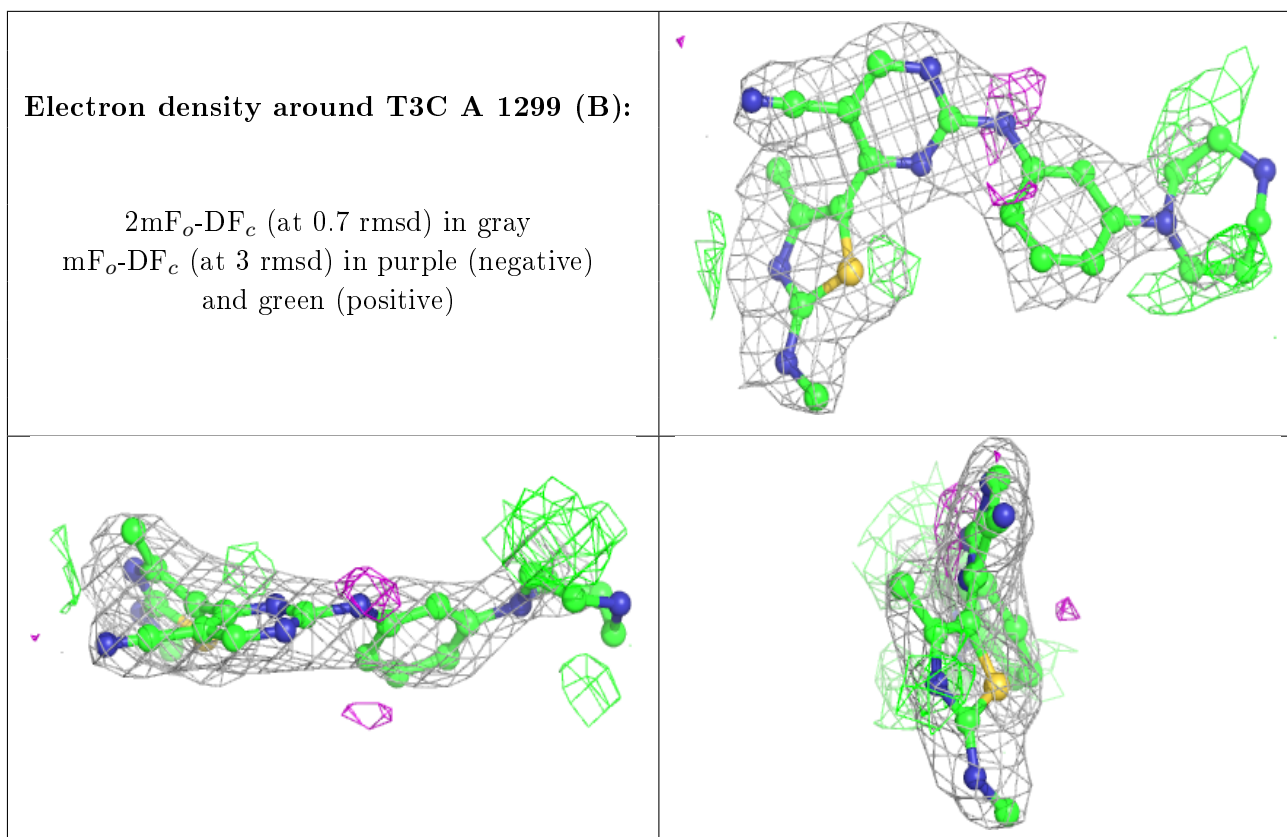
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around T3C A 1299 (A):**

$2mF_o-DF_c$  (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.