



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:55 AM UTC

PDB ID : 9ET5 / pdb_00009et5
Title : CDK2-cyclin A in complex with FragLite 8
Authors : Hope, I.; Martin, M.P.; Waring, M.J.; Noble, M.E.M.; Endicott, J.A.; Tatum, N.J.
Deposited on : 2024-03-26
Resolution : 2.53 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

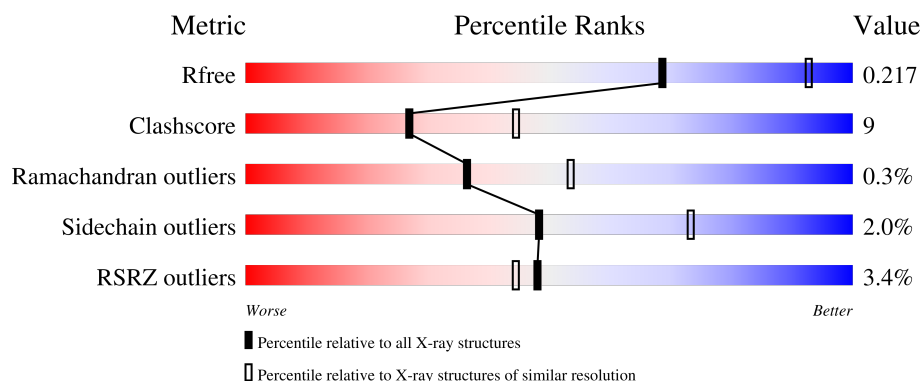
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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 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	B	268	84% 13% .
1	D	268	87% 10% ..
2	A	302	73% 23% ..
2	C	302	77% 20% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	T5G	B	501[A]	-	-	X	X
3	T5G	B	501[B]	-	-	-	X
3	T5G	B	501[C]	-	-	-	X
3	T5G	B	501[D]	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9441 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-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	262	Total	C	N	O	S	0	0	0
			2110	1366	344	390	10			
1	B	262	Total	C	N	O	S	0	2	0
			2124	1373	347	393	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	171	GLY	-	expression tag	UNP P30274
D	433	HIS	-	expression tag	UNP P30274
D	434	HIS	-	expression tag	UNP P30274
D	435	HIS	-	expression tag	UNP P30274
D	436	HIS	-	expression tag	UNP P30274
D	437	HIS	-	expression tag	UNP P30274
D	438	HIS	-	expression tag	UNP P30274
B	171	GLY	-	expression tag	UNP P30274
B	433	HIS	-	expression tag	UNP P30274
B	434	HIS	-	expression tag	UNP P30274
B	435	HIS	-	expression tag	UNP P30274
B	436	HIS	-	expression tag	UNP P30274
B	437	HIS	-	expression tag	UNP P30274
B	438	HIS	-	expression tag	UNP P30274

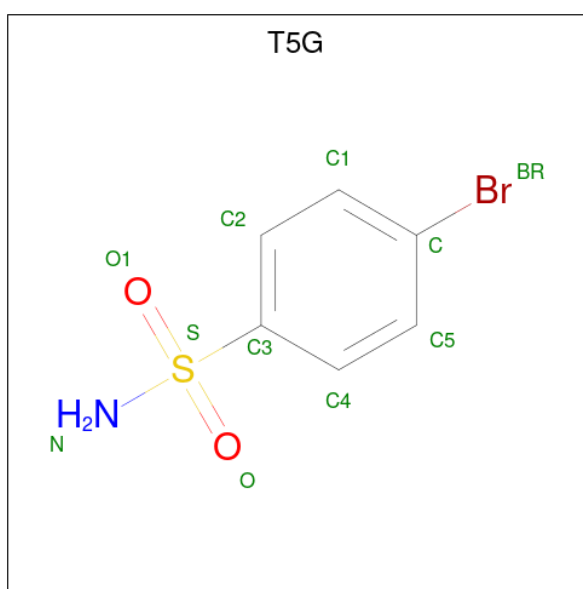
- Molecule 2 is a protein called Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	295	Total	C	N	O	P S	0	3	0
			2394	1551	406	428	1 8			
2	C	297	Total	C	N	O	P S	0	3	0
			2416	1566	409	432	1 8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P24941
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-3	GLY	-	expression tag	UNP P24941
C	-2	PRO	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 3 is 4-bromobenzene-1-sulfonamide (CCD ID: T5G) (formula: $C_6H_5BrNO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	S	0	1
			22	2	12	2	4	2		
3	A	1	Total	Br	C	N	O	S	0	1
			22	2	12	2	4	2		
3	B	1	Total	Br	C	N	O	S	0	1
			44	4	24	4	8	4		
3	B	1	Total	Br	C	N	O	S	0	0
			11	1	6	1	2	1		
3	C	1	Total	Br	C	N	O	S	0	0
			11	1	6	1	2	1		
3	C	1	Total	Br	C	N	O	S	0	0
			11	1	6	1	2	1		

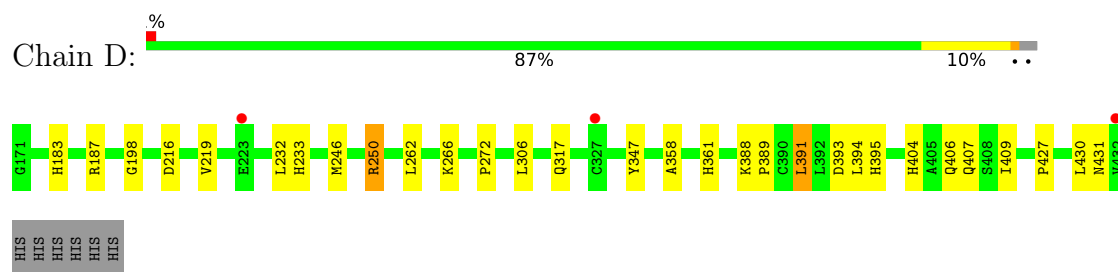
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	48	Total 48	O 48	0	0
4	A	85	Total 85	O 85	0	0
4	B	85	Total 85	O 85	0	0
4	C	58	Total 58	O 58	0	0

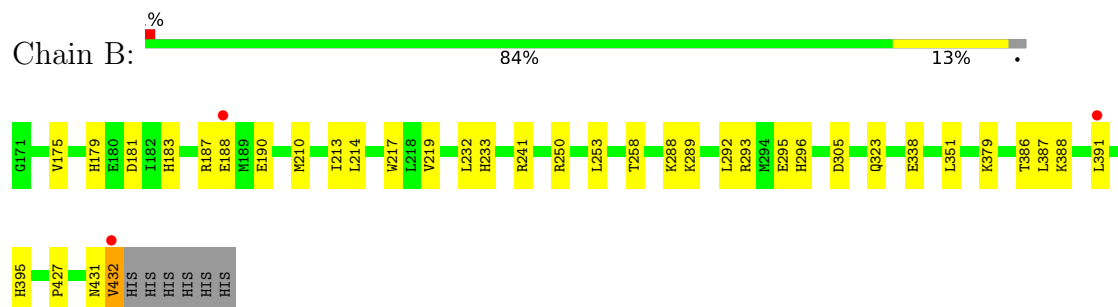
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

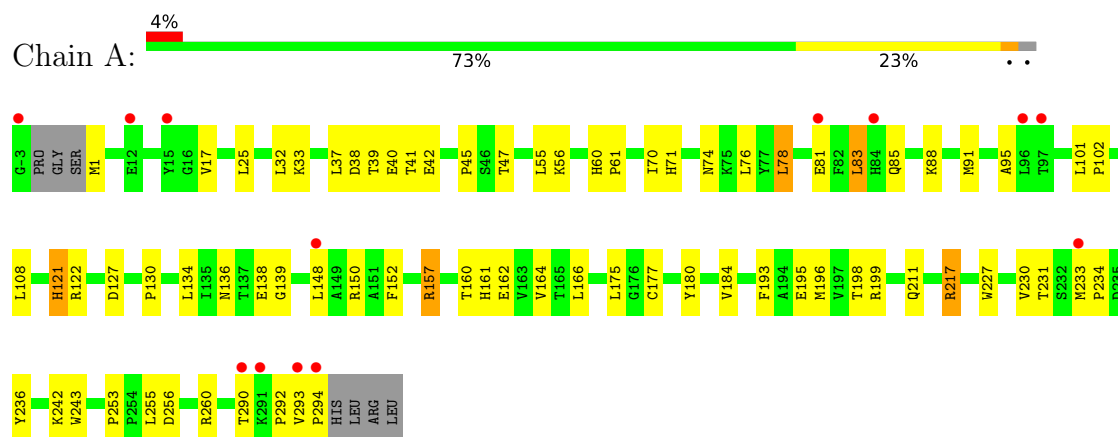
• Molecule 1: Cyclin-A2



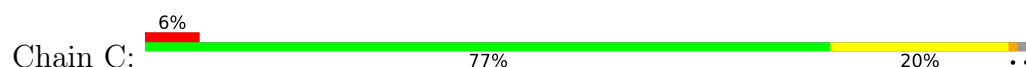
• Molecule 1: Cyclin-A2

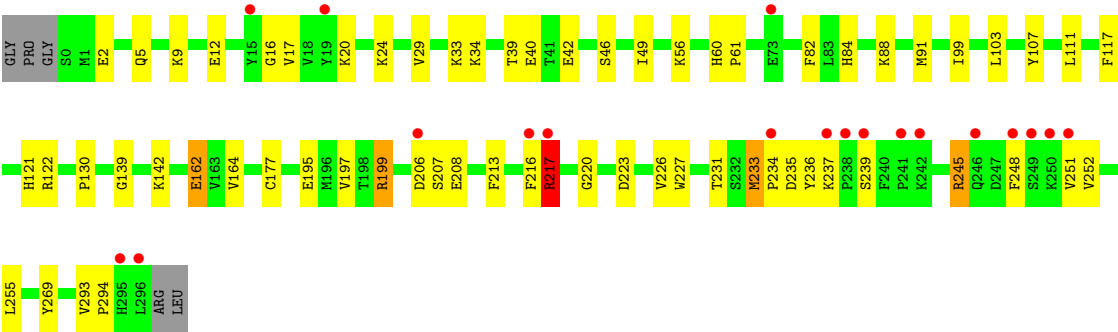


• Molecule 2: Cyclin-dependent kinase 2



• Molecule 2: Cyclin-dependent kinase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.98Å 133.59Å 147.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.13 – 2.53 98.94 – 2.53	Depositor EDS
% Data completeness (in resolution range)	90.4 (99.13-2.53) 90.1 (98.94-2.53)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.200 , 0.221 0.195 , 0.217	Depositor DCC
R_{free} test set	2355 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9441	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: T5G, 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	B	0.61	0/2174	1.16	4/2956 (0.1%)
1	D	0.60	1/2160 (0.0%)	1.18	6/2937 (0.2%)
2	A	0.68	0/2443	1.22	5/3313 (0.2%)
2	C	0.63	0/2467	1.11	2/3347 (0.1%)
All	All	0.63	1/9244 (0.0%)	1.17	17/12553 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	2
2	A	0	4
2	C	0	2
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	198	GLY	C-N	-6.62	1.24	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	152	PHE	CA-CB-CG	7.27	121.07	113.80
2	A	39	THR	N-CA-C	-7.11	104.69	113.15
1	D	250	ARG	CB-CA-C	-6.35	99.89	110.68
1	B	175	VAL	N-CA-CB	6.08	119.73	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	GLN	N-CA-CB	-5.90	102.88	111.20
1	D	272	PRO	N-CA-CB	5.47	106.25	103.19
1	D	393	ASP	CA-CB-CG	5.46	118.06	112.60
2	C	42	GLU	CB-CG-CD	5.46	121.89	112.60
1	B	258	THR	CA-CB-OG1	-5.36	101.56	109.60
2	A	121	HIS	CA-CB-CG	-5.35	108.45	113.80
1	B	181	ASP	CA-CB-CG	5.29	117.89	112.60
1	D	246	MET	CA-C-N	-5.18	114.42	122.09
1	D	246	MET	C-N-CA	-5.18	114.42	122.09
1	D	250	ARG	N-CA-CB	5.10	117.71	110.06
2	A	253	PRO	N-CA-C	5.09	116.92	110.70
2	A	45	PRO	N-CA-CB	5.04	107.74	103.35
2	C	162	GLU	CB-CA-C	5.02	119.87	111.83

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	157	ARG	Sidechain
2	A	217	ARG	Sidechain
2	A	83	LEU	Mainchain
1	B	187	ARG	Sidechain
1	B	241	ARG	Sidechain
2	C	217	ARG	Sidechain
2	C	245	ARG	Sidechain
1	D	187	ARG	Sidechain
1	D	250	ARG	Sidechain

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	B	2124	0	2137	30	0
1	D	2110	0	2128	16	0
2	A	2394	0	2426	66	0
2	C	2416	0	2446	64	0
3	A	44	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	55	0	0	10	0
3	C	22	0	0	3	0
4	A	85	0	0	6	0
4	B	85	0	0	6	0
4	C	58	0	0	3	0
4	D	48	0	0	2	0
All	All	9441	0	9137	168	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 9.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:GLU:CD	2:C:17:VAL:HG22	1.84	1.01
2:A:230:VAL:HA	2:A:233:MET:HE3	1.47	0.94
1:B:217:TRP:CD1	3:B:501[A]:T5G:BR	2.82	0.88
2:A:175:LEU:HD13	2:A:233:MET:SD	2.16	0.86
2:C:12:GLU:CG	2:C:17:VAL:HG22	2.07	0.83
2:C:9:LYS:HE3	2:C:17:VAL:HG13	1.63	0.81
2:C:12:GLU:HG3	2:C:17:VAL:HG22	1.64	0.80
2:C:252:VAL:HG12	2:C:255:LEU:HB2	1.64	0.77
2:C:9:LYS:HE3	2:C:17:VAL:CG1	2.18	0.73
2:A:56:LYS:HD3	1:B:305:ASP:OD1	1.89	0.73
2:A:71:HIS:NE2	1:B:296:HIS:CE1	2.58	0.71
1:B:233:HIS:HD2	4:B:652:HOH:O	1.73	0.71
2:A:175:LEU:CD1	2:A:233:MET:SD	2.79	0.70
2:A:83:LEU:HD22	2:A:136:ASN:HB3	1.73	0.70
2:A:177:CYS:HB2	4:A:629:HOH:O	1.93	0.69
1:B:388:LYS:HA	1:B:391:LEU:HD12	1.75	0.69
2:A:227:TRP:CE2	2:A:233:MET:HE1	2.29	0.68
2:A:71:HIS:CD2	1:B:296:HIS:CE1	2.82	0.68
1:D:233:HIS:HD2	4:D:524:HOH:O	1.77	0.67
2:A:230:VAL:HA	2:A:233:MET:CE	2.23	0.67
2:C:20:LYS:CE	2:C:29:VAL:HG11	2.25	0.66
2:A:148:LEU:HG	4:A:645:HOH:O	1.96	0.65
1:D:183:HIS:HB2	1:D:317:GLN:HE22	1.61	0.65
2:C:197:VAL:HG11	2:C:252:VAL:HG13	1.78	0.65
2:A:37:LEU:HD11	2:A:76:LEU:HB2	1.79	0.65
2:C:252:VAL:HG11	2:C:255:LEU:HD22	1.80	0.64
2:A:38:ASP:C	2:A:40:GLU:H	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:LEU:HD12	2:C:49:ILE:HG23	1.79	0.64
2:A:227:TRP:CZ2	2:A:233:MET:HE1	2.32	0.63
2:A:230:VAL:CA	2:A:233:MET:HE3	2.27	0.63
2:C:197:VAL:HG11	2:C:252:VAL:CG1	2.29	0.63
2:A:127:ASP:OD2	2:A:148:LEU:HD12	1.99	0.62
2:C:12:GLU:OE1	2:C:17:VAL:HG22	1.98	0.62
1:B:217:TRP:CG	3:B:501[A]:T5G:BR	3.08	0.62
2:C:12:GLU:OE1	2:C:17:VAL:CG2	2.48	0.61
2:A:91:MET:HE3	2:A:196:MET:HA	1.82	0.61
1:B:431:ASN:O	1:B:432:VAL:HB	2.00	0.60
2:C:20:LYS:HE2	2:C:29:VAL:HG11	1.82	0.60
2:A:139:GLY:HA2	2:A:294:PRO:HD3	1.83	0.60
2:C:177:CYS:HB2	4:C:624:HOH:O	2.01	0.60
2:C:208[B]:GLU:CD	2:C:208[B]:GLU:H	2.10	0.60
2:A:41:THR:HB	1:B:288:LYS:HZ1	1.66	0.59
1:B:190:GLU:HG3	1:B:351:LEU:HD22	1.85	0.59
2:A:41:THR:HB	1:B:288:LYS:NZ	2.18	0.59
2:A:95:ALA:O	2:A:199:ARG:HD3	2.02	0.59
1:D:219:VAL:HG22	1:D:232:LEU:HD21	1.85	0.57
2:C:234:PRO:C	2:C:236:TYR:H	2.13	0.57
2:C:88:LYS:HB2	2:C:130:PRO:HB2	1.87	0.56
2:C:234:PRO:O	2:C:236:TYR:N	2.39	0.56
2:C:16:GLY:HA3	2:C:34:LYS:O	2.06	0.55
2:C:99:ILE:HG13	2:C:199:ARG:HD3	1.87	0.55
2:A:78:LEU:N	2:A:78:LEU:HD23	2.21	0.54
2:A:127:ASP:CG	2:A:148:LEU:HD12	2.32	0.54
2:A:83:LEU:HD12	2:A:134:LEU:HB2	1.89	0.54
1:D:404:HIS:O	1:D:407:GLN:NE2	2.39	0.54
2:C:227:TRP:CE3	2:C:269:TYR:HB3	2.42	0.54
2:A:81:GLU:O	3:A:501[B]:T5G:BR	2.81	0.53
2:C:20:LYS:HE3	2:C:29:VAL:HG11	1.90	0.53
2:C:248:PHE:HA	2:C:251:VAL:HB	1.90	0.53
2:A:231:THR:HA	2:A:236:TYR:CD2	2.44	0.53
1:D:395:HIS:HE1	1:D:427:PRO:O	1.91	0.52
2:C:33:LYS:CE	3:C:501:T5G:N	2.72	0.52
2:C:121:HIS:C	2:C:122:ARG:HG3	2.34	0.52
2:A:95:ALA:O	2:A:199:ARG:CD	2.58	0.52
1:D:361:HIS:CD2	1:D:361:HIS:C	2.89	0.51
2:A:38:ASP:C	2:A:40:GLU:N	2.68	0.51
1:B:293:ARG:NH2	4:B:602:HOH:O	2.40	0.50
1:D:216:ASP:HB2	1:D:406:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:MET:HE2	2:C:130:PRO:HB3	1.92	0.50
2:A:71:HIS:CD2	1:B:296:HIS:HE1	2.30	0.50
2:C:33:LYS:HE2	3:C:501:T5G:N	2.26	0.50
1:B:387:LEU:O	1:B:391:LEU:HG	2.12	0.50
2:A:177:CYS:HB3	4:A:659:HOH:O	2.12	0.49
1:B:395:HIS:HE1	1:B:427:PRO:O	1.95	0.49
2:A:138:GLU:O	2:A:293:VAL:HG12	2.12	0.49
2:C:5:GLN:HB2	2:C:24:LYS:HE3	1.93	0.49
2:C:91:MET:CE	2:C:130:PRO:HB3	2.43	0.49
2:C:216:PHE:O	2:C:220:GLY:N	2.45	0.49
2:A:101:LEU:HB3	2:A:102:PRO:HD3	1.94	0.49
2:C:142:LYS:NZ	4:C:601:HOH:O	2.31	0.49
1:B:179:HIS:HD2	1:B:379:LYS:NZ	2.11	0.48
2:C:12:GLU:HG3	2:C:17:VAL:CG2	2.39	0.48
1:D:347:TYR:OH	1:D:394:LEU:HA	2.12	0.48
2:A:1:MET:HE1	2:A:32:LEU:HD13	1.95	0.48
2:A:56:LYS:HE3	3:B:502:T5G:C5	2.43	0.48
1:B:183:HIS:HE1	4:B:621:HOH:O	1.97	0.48
2:A:91:MET:HE1	2:A:195:GLU:HG2	1.95	0.48
1:B:183:HIS:CE1	4:B:621:HOH:O	2.66	0.48
2:A:121:HIS:C	2:A:122:ARG:HG3	2.38	0.47
2:A:83:LEU:CD2	2:A:136:ASN:HB3	2.42	0.47
2:C:213:PHE:O	2:C:217:ARG:HG2	2.15	0.47
1:B:210:MET:HE2	3:B:501[D]:T5G:N	2.30	0.47
2:C:12:GLU:CD	2:C:17:VAL:CG2	2.70	0.47
2:C:237:LYS:C	2:C:239:SER:H	2.23	0.47
2:C:20:LYS:HE2	2:C:29:VAL:CG1	2.45	0.47
2:C:20:LYS:HD2	2:C:82:PHE:CE1	2.49	0.47
2:C:177:CYS:SG	2:C:233:MET:HG2	2.54	0.47
2:C:60:HIS:CG	2:C:61:PRO:HD2	2.50	0.47
2:C:91:MET:HE1	2:C:130:PRO:CG	2.45	0.47
1:B:289:LYS:O	1:B:293:ARG:HG3	2.15	0.46
2:C:231:THR:HA	2:C:236:TYR:CD1	2.50	0.46
2:A:91:MET:CE	2:A:196:MET:HA	2.44	0.46
2:A:166:LEU:HD11	2:A:211:GLN:HB2	1.96	0.46
1:B:214:LEU:HB2	3:B:501[A]:T5G:N	2.31	0.46
2:C:139:GLY:HA2	2:C:294:PRO:HD3	1.98	0.46
2:C:197:VAL:CG1	2:C:252:VAL:HG13	2.46	0.46
2:A:227:TRP:CE2	2:A:233:MET:CE	2.98	0.45
1:B:210:MET:HG2	3:B:501[D]:T5G:C3	2.46	0.45
2:C:20:LYS:CE	2:C:29:VAL:CG1	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:180:TYR:HB2	2:A:184:VAL:HG11	1.97	0.45
2:C:234:PRO:C	2:C:236:TYR:N	2.75	0.45
2:C:121:HIS:O	2:C:122:ARG:HG3	2.16	0.45
2:A:33:LYS:CE	3:A:501[A]:T5G:O	2.65	0.45
2:A:37:LEU:HA	2:A:40:GLU:HG3	1.98	0.45
2:A:55:LEU:HA	2:A:55:LEU:HD23	1.79	0.45
2:A:148:LEU:CG	4:A:645:HOH:O	2.61	0.45
1:D:409:ILE:HB	4:D:508:HOH:O	2.16	0.45
1:B:250:ARG:HG3	3:B:501[B]:T5G:N	2.32	0.45
2:C:103:LEU:HD21	2:C:294:PRO:HB3	1.99	0.44
2:A:198:THR:O	2:A:199:ARG:HB2	2.16	0.44
1:B:338:GLU:HG3	4:B:667:HOH:O	2.17	0.44
1:D:266:LYS:HB3	2:C:46:SER:HB3	1.99	0.44
2:C:84:HIS:HB2	4:C:654:HOH:O	2.18	0.44
1:B:253:LEU:HG	3:B:501[A]:T5G:O	2.18	0.44
2:A:227:TRP:CD2	2:A:233:MET:HE1	2.52	0.43
2:C:252:VAL:CG1	2:C:255:LEU:HB2	2.41	0.43
2:C:117:PHE:O	2:C:121:HIS:ND1	2.48	0.43
2:A:88:LYS:HB2	2:A:130:PRO:HB2	2.00	0.43
2:A:227:TRP:CH2	2:A:233:MET:HE1	2.52	0.43
2:A:242:LYS:NZ	4:A:603:HOH:O	2.39	0.43
2:A:139:GLY:HA3	2:A:293:VAL:HA	2.00	0.43
2:A:290:THR:OG1	2:A:292:PRO:HD3	2.19	0.42
1:B:214:LEU:HD13	3:B:501[A]:T5G:O	2.18	0.42
2:C:216:PHE:O	2:C:217:ARG:C	2.62	0.42
1:D:262:LEU:HD11	1:D:266:LYS:HE3	2.02	0.42
1:B:213:ILE:HD12	3:B:501[D]:T5G:C4	2.50	0.42
2:C:56:LYS:HD2	3:C:502:T5G:C5	2.49	0.42
2:C:9:LYS:HE3	2:C:17:VAL:HG11	1.99	0.42
2:C:12:GLU:HG3	2:C:17:VAL:HA	2.02	0.42
2:C:195:GLU:O	2:C:199:ARG:N	2.50	0.42
2:A:108:LEU:HD22	2:A:193:PHE:CG	2.55	0.41
2:A:230:VAL:HA	2:A:233:MET:SD	2.60	0.41
2:C:107:TYR:O	2:C:111:LEU:HG	2.20	0.41
1:D:358:ALA:CB	1:D:391:LEU:HD22	2.49	0.41
2:A:217:ARG:HG2	2:A:243:TRP:CD2	2.56	0.41
2:A:71:HIS:CD2	2:A:76:LEU:HD13	2.55	0.41
2:A:60:HIS:CG	2:A:61:PRO:HD2	2.55	0.41
1:B:219:VAL:HG22	1:B:232:LEU:HD21	2.02	0.41
1:B:386:THR:HB	4:B:630:HOH:O	2.20	0.41
2:C:20:LYS:HE3	2:C:82:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:HIS:HB2	1:D:430:LEU:HD11	2.03	0.41
2:A:256[A]:ASP:O	2:A:260:ARG:HG3	2.20	0.41
2:A:33:LYS:HE3	3:A:501[A]:T5G:O	2.21	0.41
2:A:139:GLY:CA	2:A:293:VAL:HA	2.51	0.41
2:A:227:TRP:CZ2	2:A:233:MET:CE	3.02	0.41
2:A:233:MET:HA	2:A:234:PRO:HD3	1.94	0.41
2:A:255:LEU:HD12	2:A:255:LEU:HA	1.92	0.41
2:C:227:TRP:NE1	2:C:233:MET:HE1	2.37	0.40
1:D:388:LYS:HB3	1:D:389:PRO:HD3	2.03	0.40
2:A:161:HIS:HD2	4:A:681:HOH:O	2.05	0.40
2:C:20:LYS:HE3	2:C:29:VAL:CG1	2.51	0.40
2:C:39:THR:OG1	2:C:40:GLU:OE1	2.37	0.40
2:A:25:LEU:HD23	2:A:25:LEU:HA	1.94	0.40
1:B:292:LEU:O	1:B:295:GLU:HB3	2.21	0.40
2:C:206:ASP:O	2:C:207:SER:HB3	2.22	0.40
2:C:223:ASP:H	2:C:226:VAL:HG12	1.86	0.40
1:D:430:LEU:O	1:D:431:ASN:C	2.65	0.40
2:A:37:LEU:O	2:A:40:GLU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	B	262/268 (98%)	260 (99%)	2 (1%)	0	100	100
1	D	260/268 (97%)	258 (99%)	2 (1%)	0	100	100
2	A	294/302 (97%)	285 (97%)	8 (3%)	1 (0%)	36	53
2	C	297/302 (98%)	284 (96%)	11 (4%)	2 (1%)	18	32
All	All	1113/1140 (98%)	1087 (98%)	23 (2%)	3 (0%)	36	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	164	VAL
2	A	164	VAL
2	C	235	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	236/240 (98%)	234 (99%)	2 (1%)	73	88
1	D	234/240 (98%)	233 (100%)	1 (0%)	84	92
2	A	261/264 (99%)	251 (96%)	10 (4%)	29	53
2	C	264/264 (100%)	257 (97%)	7 (3%)	39	65
All	All	995/1008 (99%)	975 (98%)	20 (2%)	48	73

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	391	LEU
2	A	17	VAL
2	A	42	GLU
2	A	47	THR
2	A	70	ILE
2	A	74	ASN
2	A	78	LEU
2	A	85	GLN
2	A	150	ARG
2	A	157	ARG
2	A	162	GLU
1	B	188	GLU
1	B	432	VAL
2	C	2	GLU
2	C	162	GLU
2	C	199	ARG
2	C	217	ARG
2	C	233	MET
2	C	245	ARG

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Mol	Chain	Res	Type
2	C	293	VAL

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

Mol	Chain	Res	Type
1	D	233	HIS
1	D	254	GLN
1	D	317	GLN
1	D	395	HIS
1	D	425	ASN
2	A	85	GLN
2	A	265	GLN
1	B	179	HIS
1	B	183	HIS
1	B	254	GLN
1	B	296	HIS
1	B	317	GLN
1	B	378	GLN
1	B	395	HIS
1	B	396	GLN
1	B	425	ASN
1	B	431	ASN
2	C	59	ASN

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
2	TPO	A	160	2	8,10,11	0.75	0	10,14,16	1.04	1 (10%)
2	TPO	C	160	2	8,10,11	0.78	0	10,14,16	1.03	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
2	TPO	A	160	2	-	1/9/11/13	-
2	TPO	C	160	2	-	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(°)	Ideal(°)
2	A	160	TPO	O-C-CA	-2.69	117.84	124.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	T5G	A	501[B]	-	11,11,11	0.31	0	16,16,16	0.42	0
3	T5G	B	501[A]	-	11,11,11	0.22	0	16,16,16	0.14	0
3	T5G	B	501[B]	-	11,11,11	0.21	0	16,16,16	0.21	0
3	T5G	B	502	-	11,11,11	0.34	0	16,16,16	0.78	0
3	T5G	A	503[A]	-	11,11,11	0.34	0	16,16,16	0.76	0
3	T5G	A	503[B]	-	11,11,11	0.31	0	16,16,16	0.50	0
3	T5G	C	501	-	11,11,11	0.37	0	16,16,16	1.09	2 (12%)
3	T5G	C	502	-	11,11,11	0.38	0	16,16,16	0.90	0
3	T5G	B	501[C]	-	11,11,11	0.26	0	16,16,16	0.33	0
3	T5G	B	501[D]	-	11,11,11	0.29	0	16,16,16	0.72	0
3	T5G	A	501[A]	-	11,11,11	0.30	0	16,16,16	0.46	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	T5G	A	501[B]	-	-	0/6/6/6	0/1/1/1
3	T5G	B	501[A]	-	-	0/6/6/6	0/1/1/1
3	T5G	B	501[B]	-	-	0/6/6/6	0/1/1/1
3	T5G	B	502	-	-	4/6/6/6	0/1/1/1
3	T5G	A	503[A]	-	-	4/6/6/6	0/1/1/1
3	T5G	A	503[B]	-	-	4/6/6/6	0/1/1/1
3	T5G	C	501	-	-	0/6/6/6	0/1/1/1
3	T5G	C	502	-	-	0/6/6/6	0/1/1/1
3	T5G	B	501[C]	-	-	0/6/6/6	0/1/1/1
3	T5G	B	501[D]	-	-	4/6/6/6	0/1/1/1
3	T5G	A	501[A]	-	-	4/6/6/6	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	T5G	O1-S-N	2.57	111.06	107.35
3	C	501	T5G	O-S-N	-2.27	104.08	107.35

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501[A]	T5G	C4-C3-S-N
3	A	501[A]	T5G	C2-C3-S-O
3	A	503[A]	T5G	C2-C3-S-O
3	A	503[A]	T5G	C2-C3-S-N
3	B	501[D]	T5G	C2-C3-S-N
3	A	503[A]	T5G	C4-C3-S-O
3	A	501[A]	T5G	C4-C3-S-O
3	A	503[A]	T5G	C4-C3-S-N
3	B	501[D]	T5G	C4-C3-S-N
3	B	502	T5G	C2-C3-S-O1
3	A	503[B]	T5G	C4-C3-S-O1
3	A	501[A]	T5G	C2-C3-S-N
3	B	501[D]	T5G	C4-C3-S-O
3	B	502	T5G	C2-C3-S-N
3	A	503[B]	T5G	C4-C3-S-N
3	A	503[B]	T5G	C2-C3-S-O1
3	B	502	T5G	C4-C3-S-O1
3	B	501[D]	T5G	C2-C3-S-O
3	A	503[B]	T5G	C2-C3-S-N
3	B	502	T5G	C4-C3-S-N

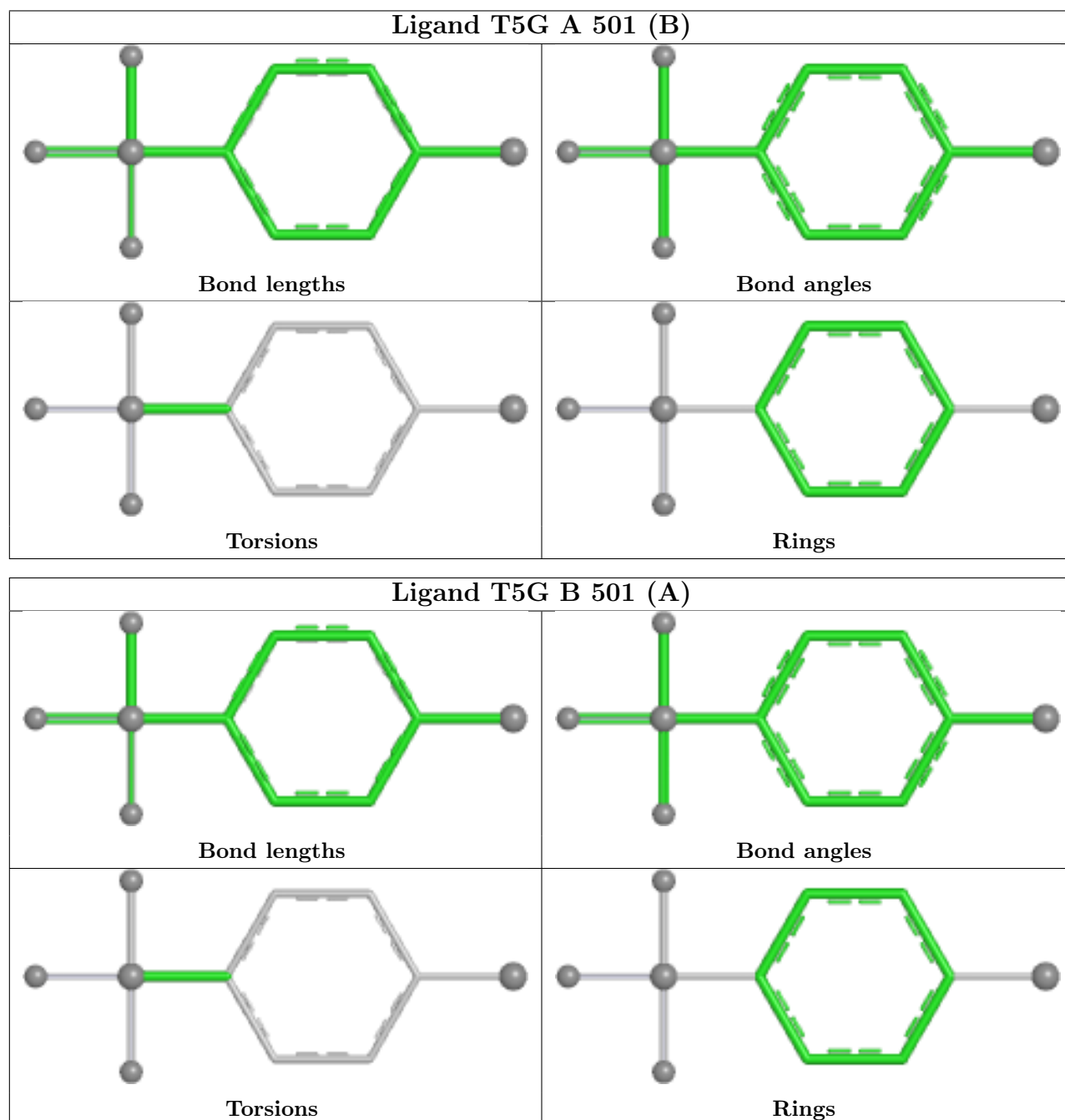
There are no ring outliers.

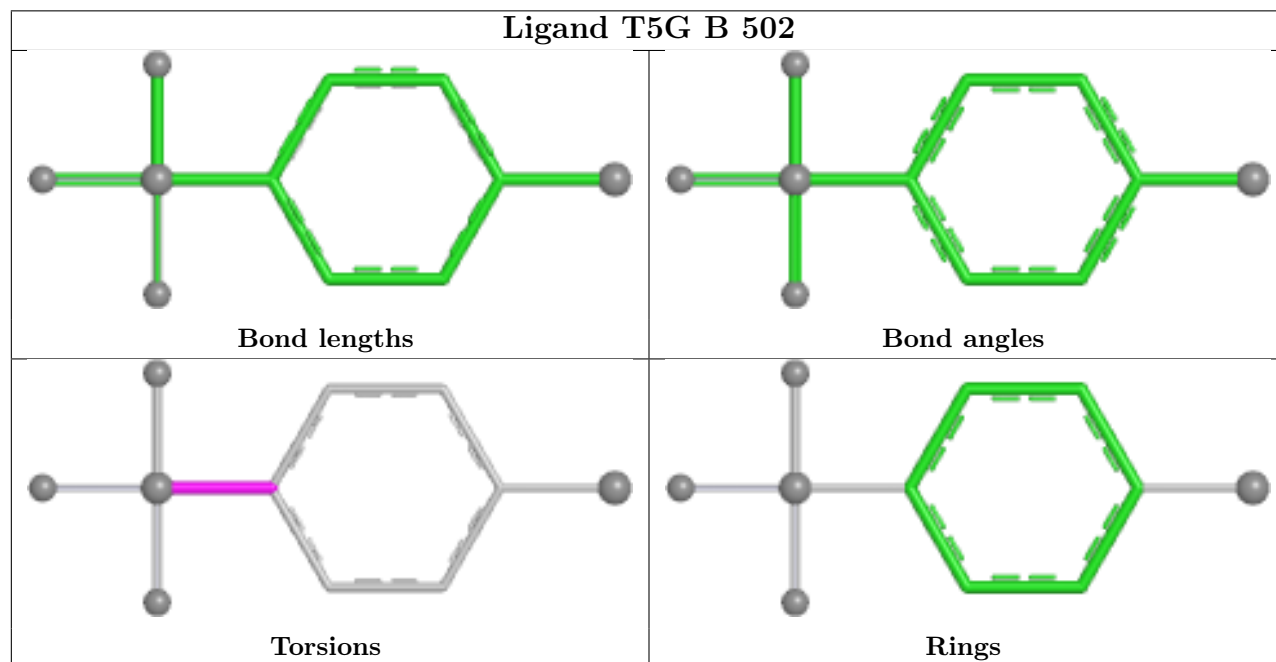
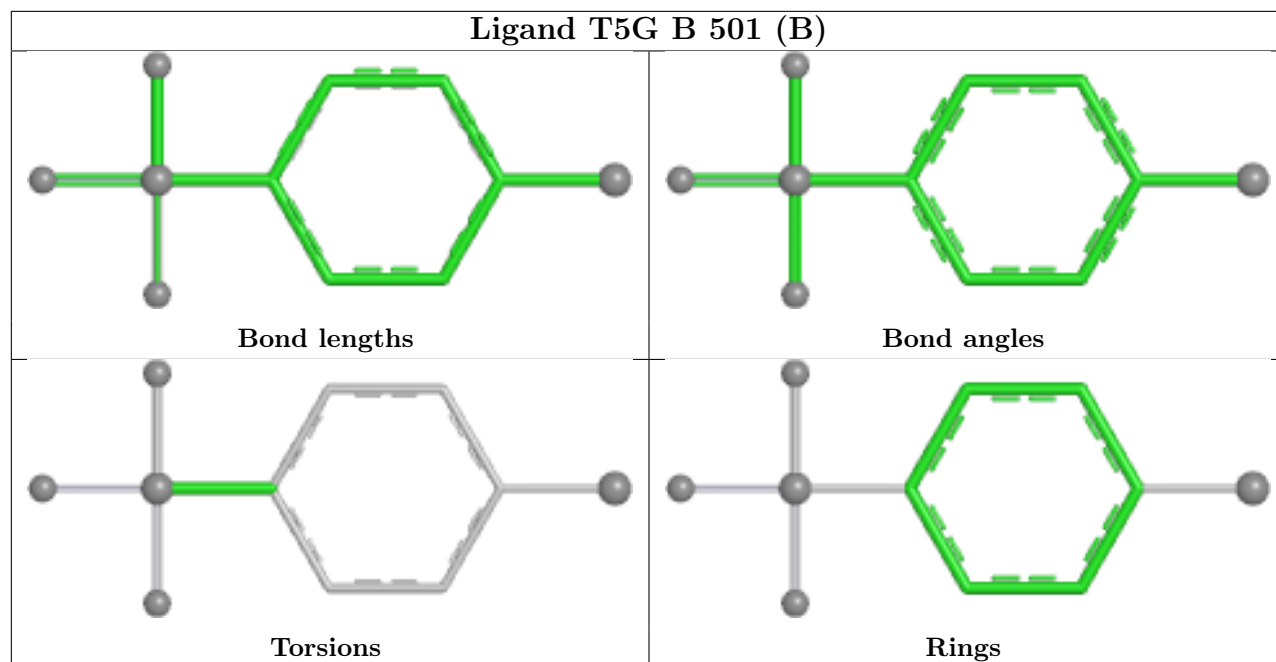
8 monomers are involved in 16 short contacts:

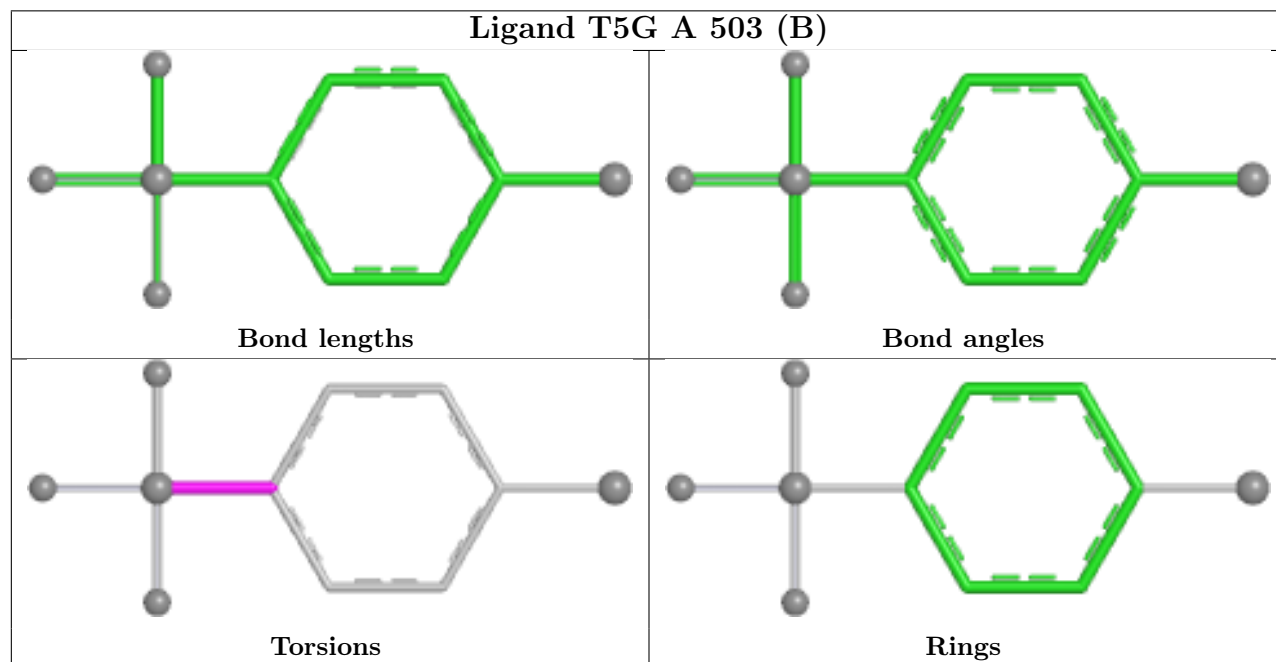
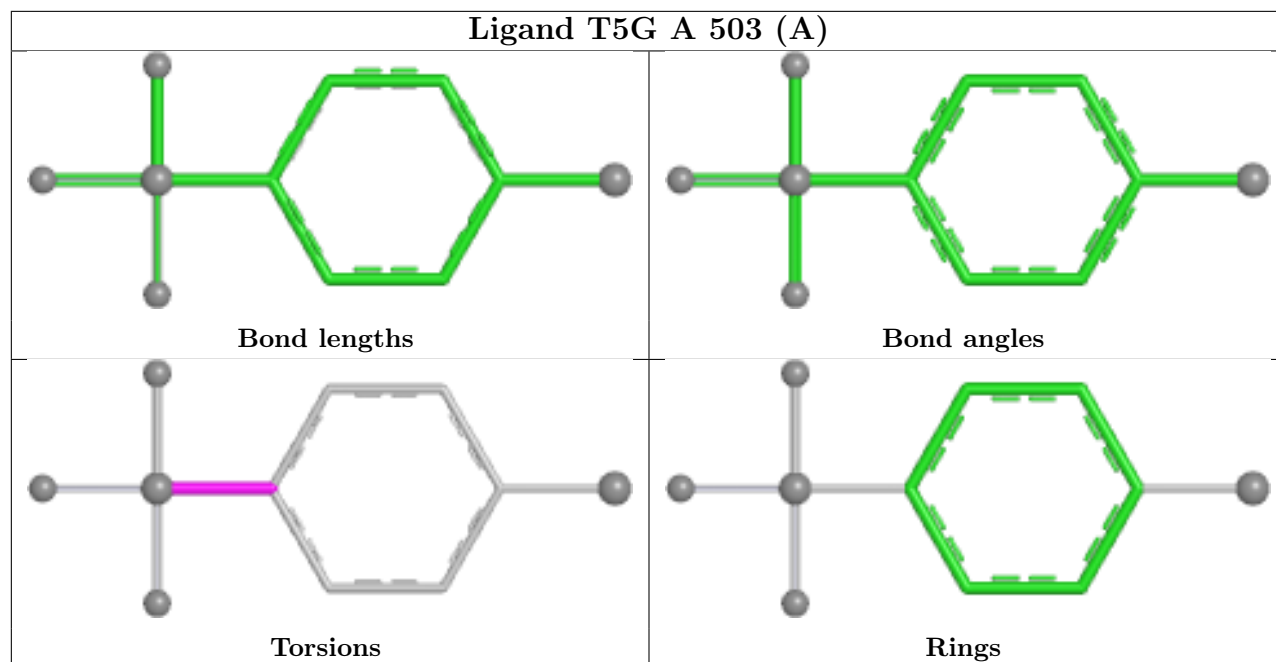
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501[B]	T5G	1	0
3	B	501[A]	T5G	5	0
3	B	501[B]	T5G	1	0
3	B	502	T5G	1	0
3	C	501	T5G	2	0
3	C	502	T5G	1	0
3	B	501[D]	T5G	3	0
3	A	501[A]	T5G	2	0

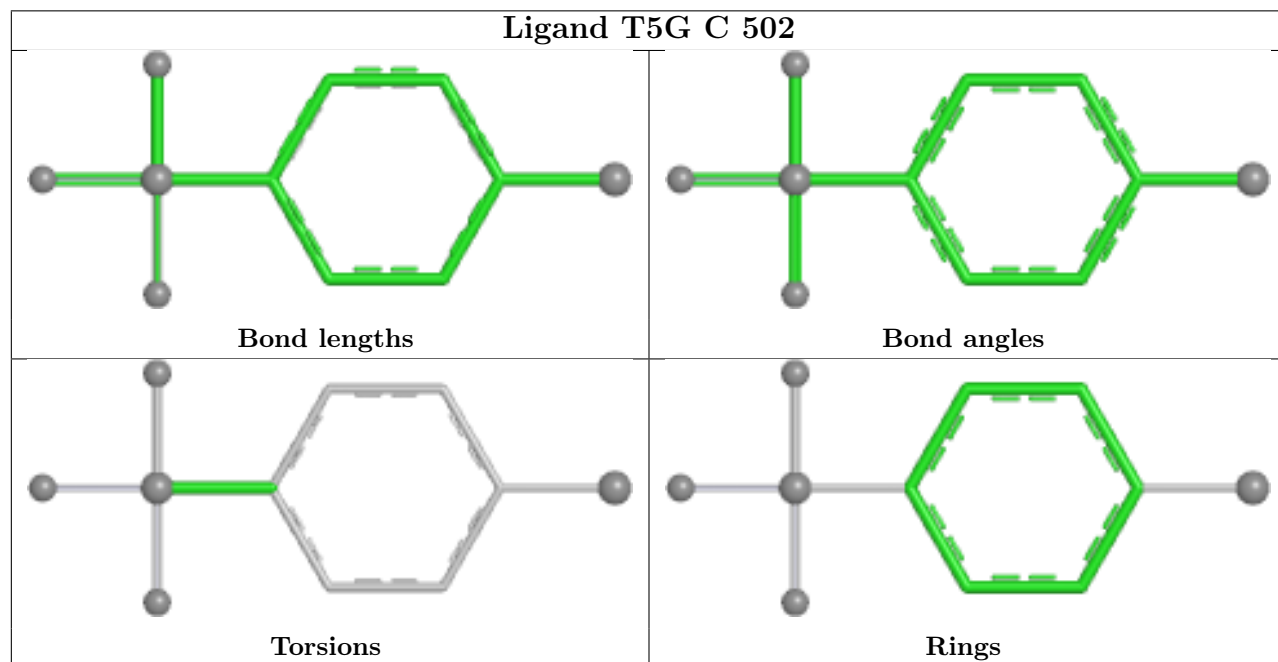
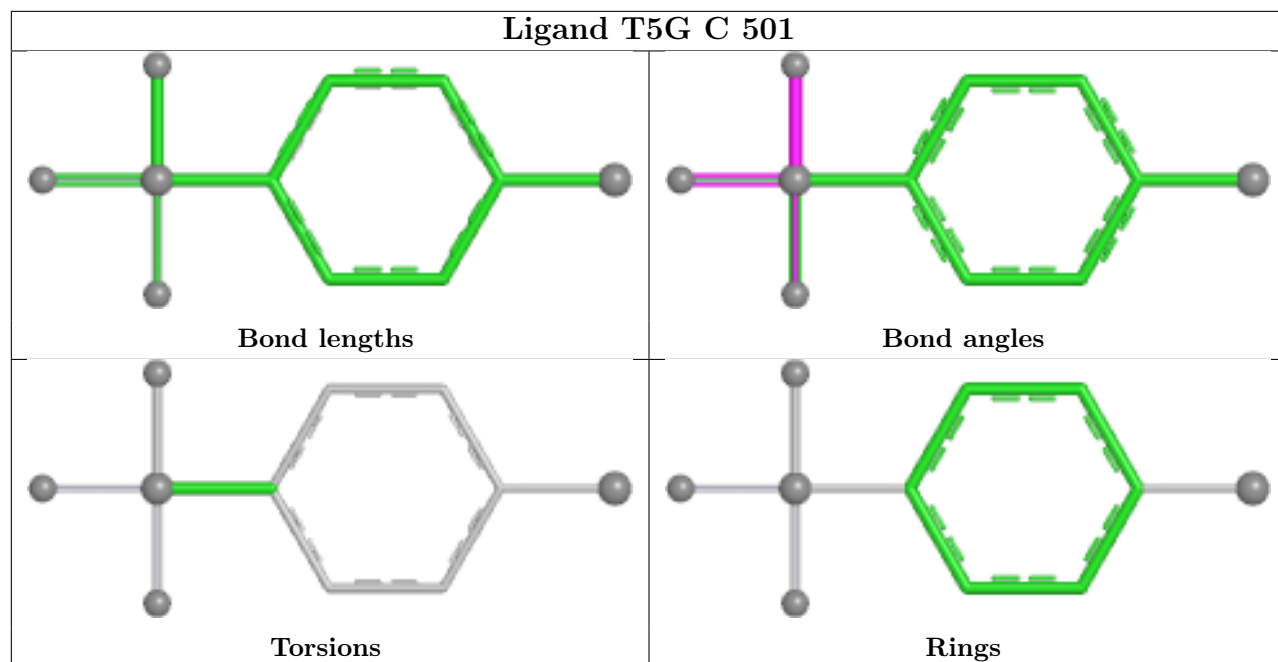
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

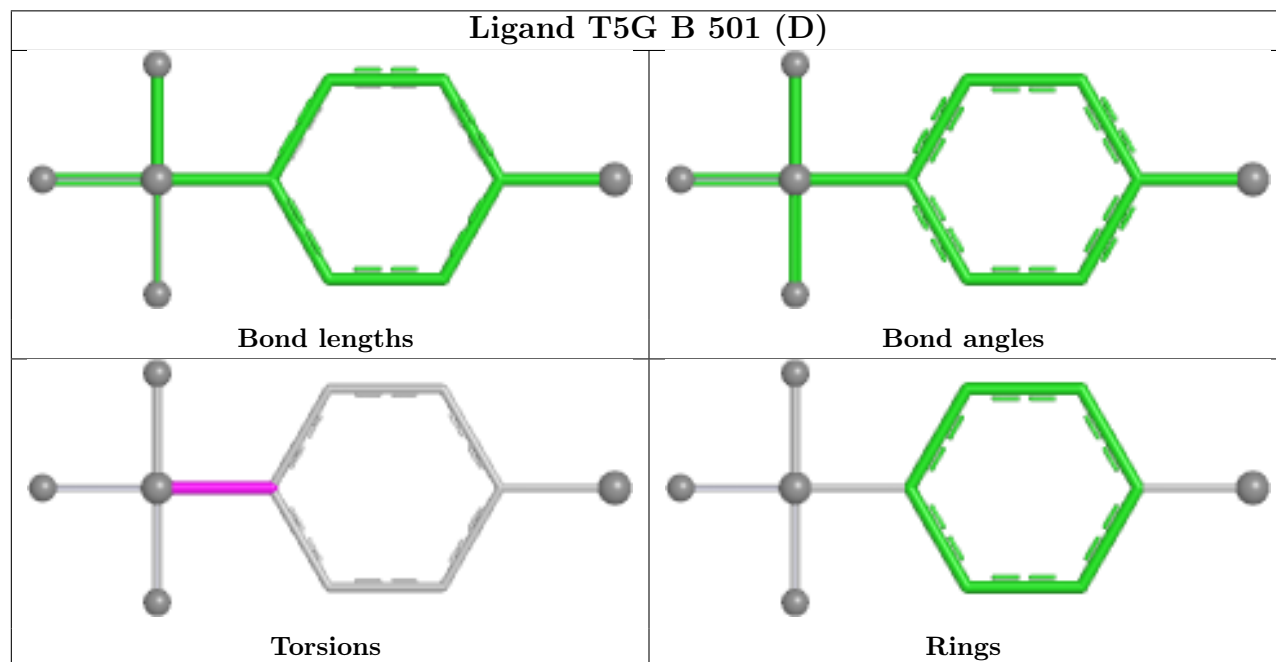
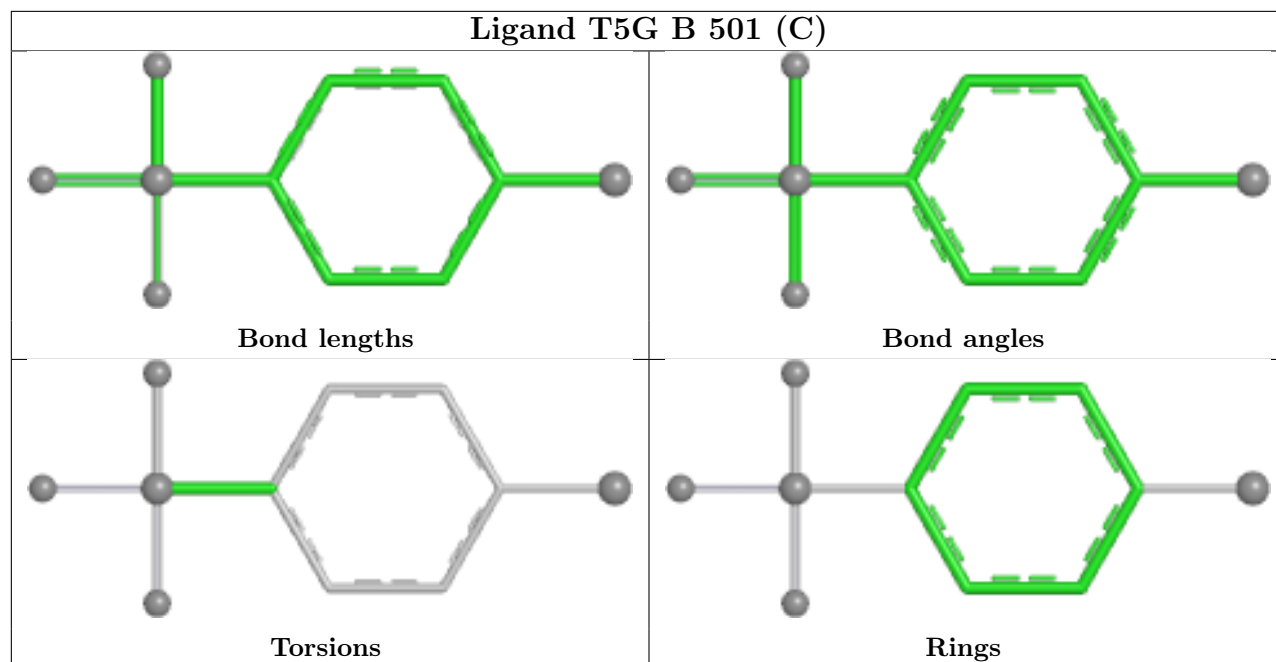
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

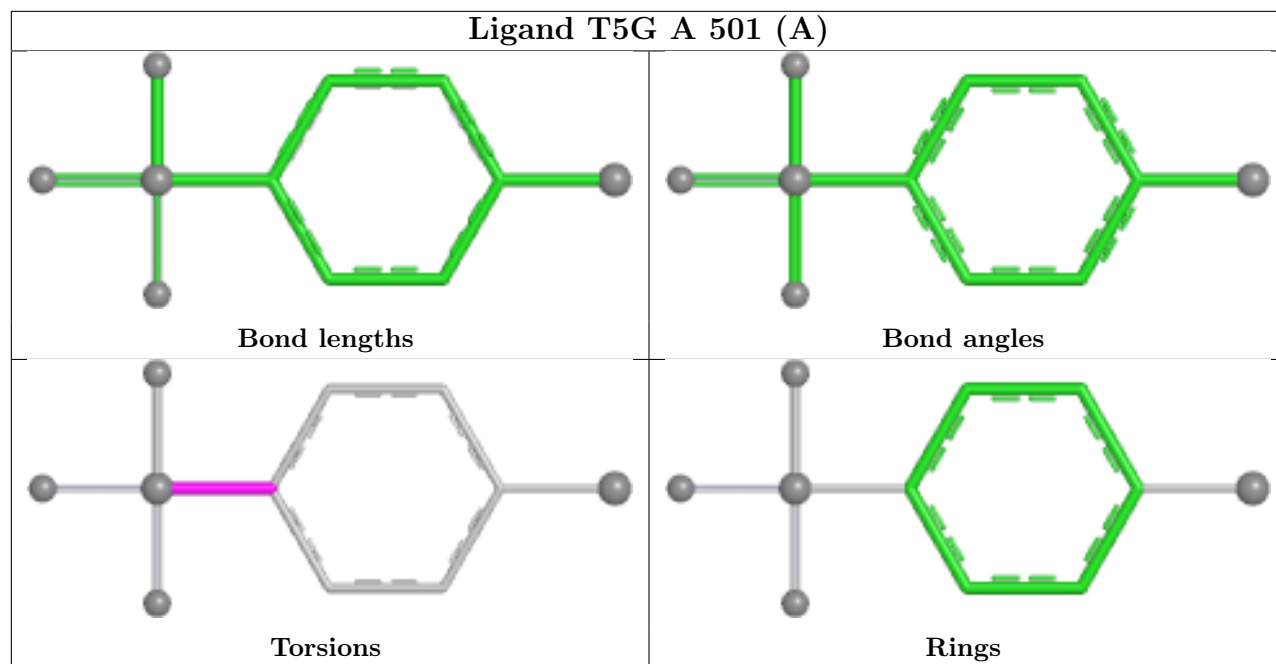












5.7 Other polymers [i](#)

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	B	262/268 (97%)	-0.21	3 (1%) 78 76	19, 44, 68, 104	2 (0%)
1	D	262/268 (97%)	0.14	3 (1%) 78 76	34, 54, 85, 134	0
2	A	294/302 (97%)	0.02	13 (4%) 39 35	20, 41, 92, 134	3 (1%)
2	C	296/302 (98%)	0.27	19 (6%) 25 22	27, 52, 100, 130	3 (1%)
All	All	1114/1140 (97%)	0.06	38 (3%) 48 44	19, 48, 92, 134	8 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	432	VAL	6.6
2	C	295[A]	HIS	5.7
2	C	15	TYR	5.7
2	A	-3	GLY	5.2
2	A	233	MET	5.0
1	B	432	VAL	4.5
2	C	234	PRO	4.1
2	C	249	SER	4.0
2	C	217	ARG	3.6
2	C	19	TYR	3.5
2	A	293	VAL	3.4
2	A	96	LEU	3.3
2	C	73[A]	GLU	3.0
2	C	248	PHE	2.9
2	A	81	GLU	2.9
1	B	188	GLU	2.9
2	C	241	PRO	2.8
2	A	84[A]	HIS	2.8
2	A	291	LYS	2.8
2	C	206	ASP	2.7
2	A	15	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	97	THR	2.6
1	B	391	LEU	2.6
2	C	216	PHE	2.6
2	C	238	PRO	2.6
2	C	242	LYS	2.5
2	C	237	LYS	2.3
2	C	251	VAL	2.3
1	D	327	CYS	2.3
2	A	290	THR	2.3
2	C	239	SER	2.3
2	A	148	LEU	2.2
1	D	223	GLU	2.2
2	C	296	LEU	2.2
2	A	294	PRO	2.1
2	C	250	LYS	2.1
2	C	246	GLN	2.1
2	A	12	GLU	2.1

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
2	TPO	A	160	11/12	0.97	0.07	36,38,42,45	0
2	TPO	C	160	11/12	0.98	0.05	38,47,52,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

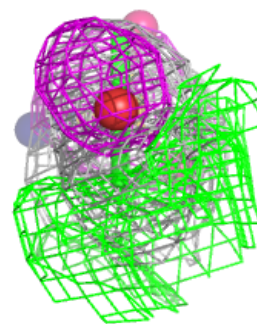
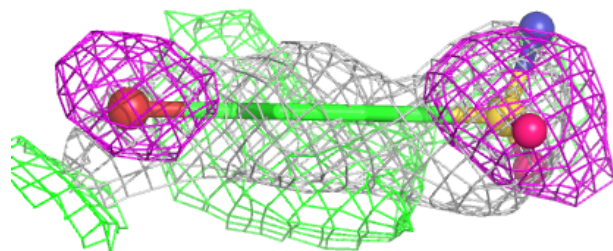
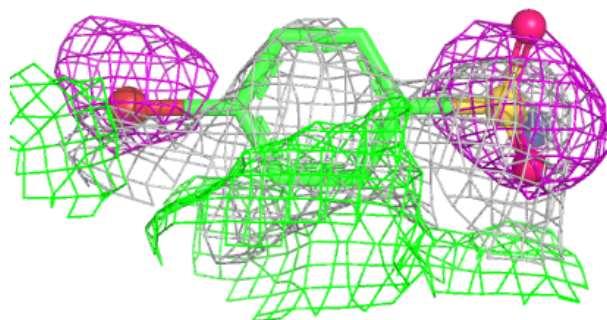
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	T5G	B	501[A]	11/11	0.63	0.53	30,30,30,30	11
3	T5G	B	501[B]	11/11	0.63	0.53	42,43,45,45	11
3	T5G	B	501[C]	11/11	0.63	0.53	49,51,59,60	11
3	T5G	B	501[D]	11/11	0.63	0.53	71,76,97,101	11
3	T5G	A	503[A]	11/11	0.77	0.31	96,100,108,109	11
3	T5G	A	503[B]	11/11	0.77	0.31	86,95,108,125	11
3	T5G	C	502	11/11	0.87	0.14	89,95,117,120	0
3	T5G	A	501[B]	11/11	0.88	0.17	51,59,63,64	11
3	T5G	B	502	11/11	0.88	0.14	101,111,122,131	0
3	T5G	A	501[A]	11/11	0.88	0.17	35,46,56,57	11
3	T5G	C	501	11/11	0.95	0.10	57,64,69,76	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.

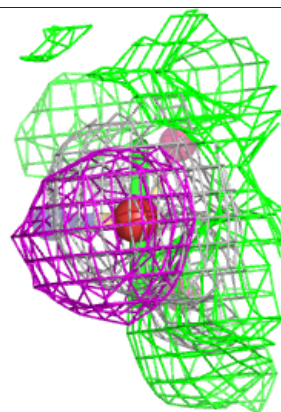
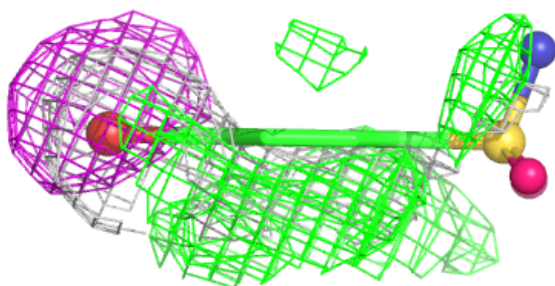
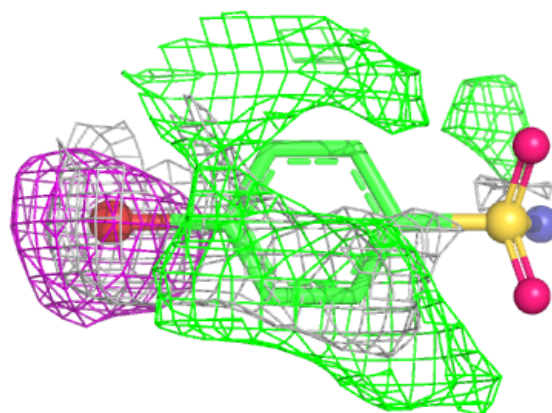
Electron density around T5G B 501 (A):

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



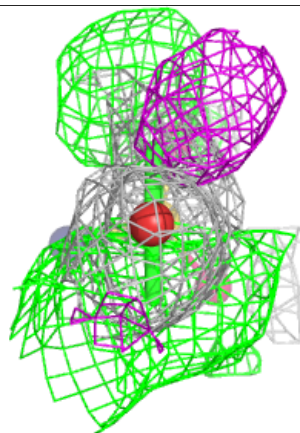
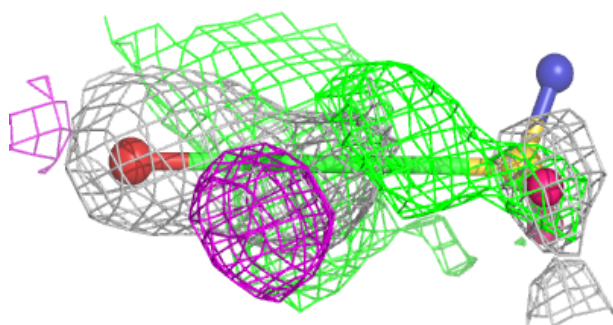
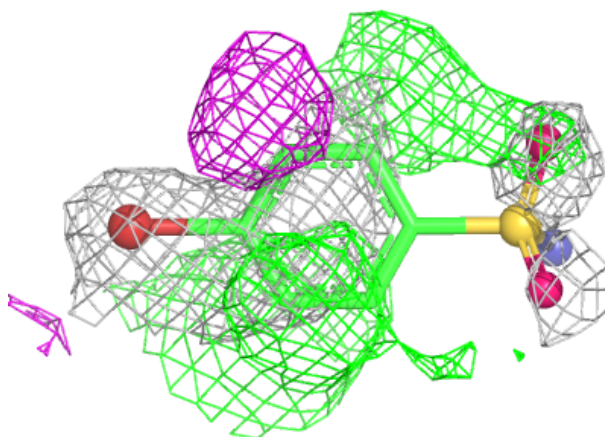
Electron density around T5G B 501 (B):

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and green (positive)

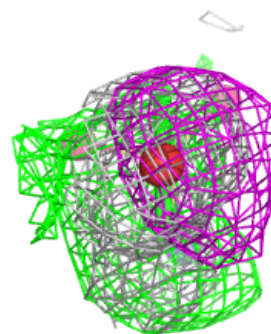
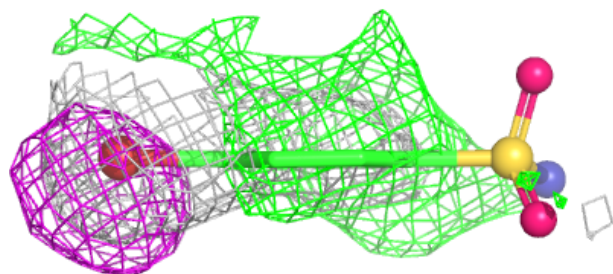
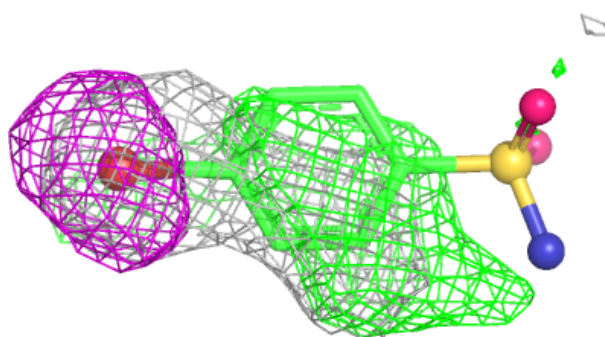


Electron density around T5G B 501 (C):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

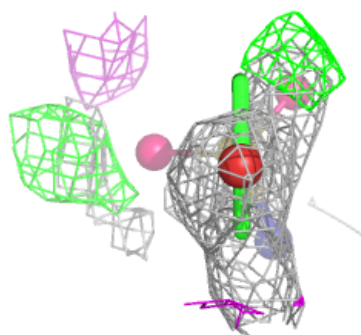
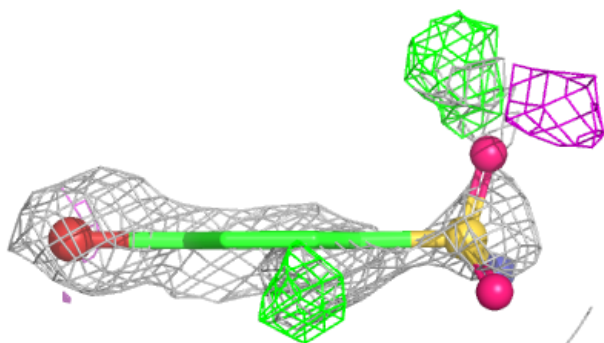
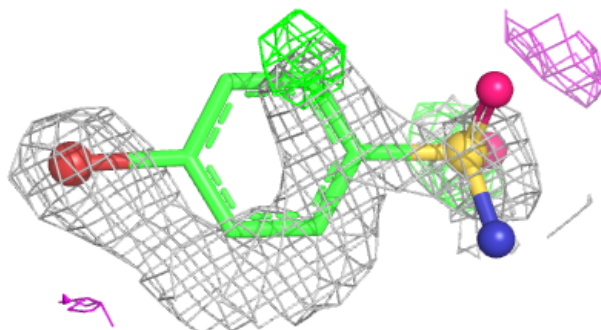
**Electron density around T5G B 501 (D):**

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and green (positive)

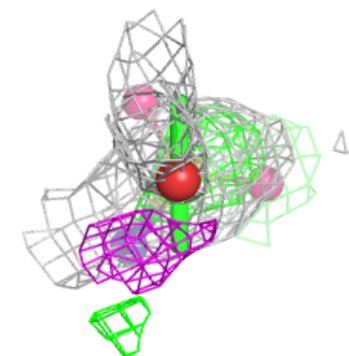
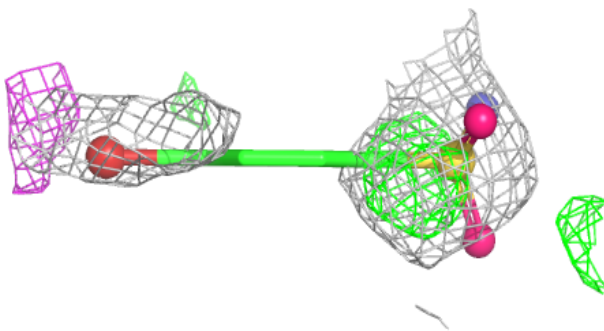
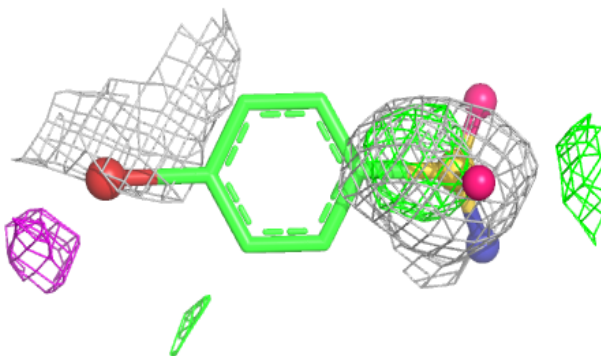


Electron density around T5G A 503 (A):

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

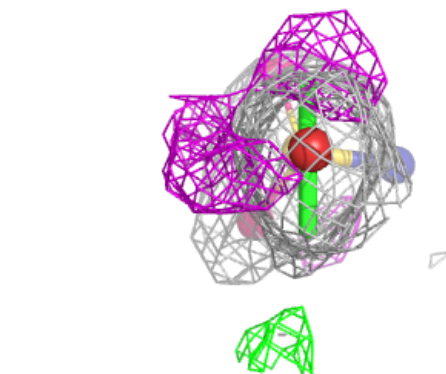
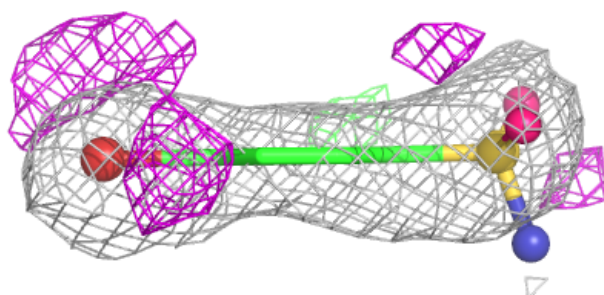
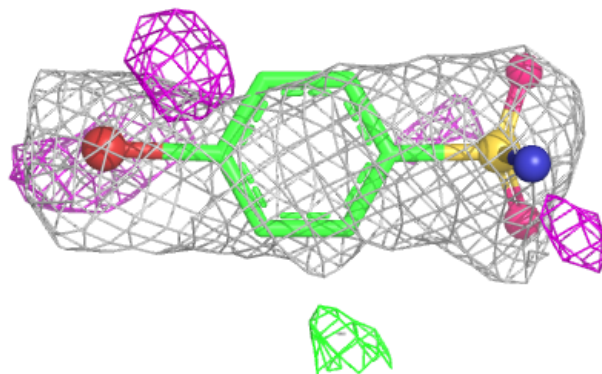
**Electron density around T5G A 503 (B):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

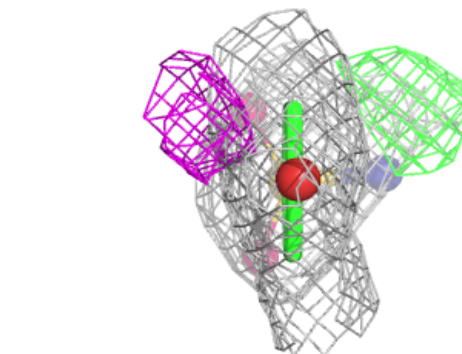
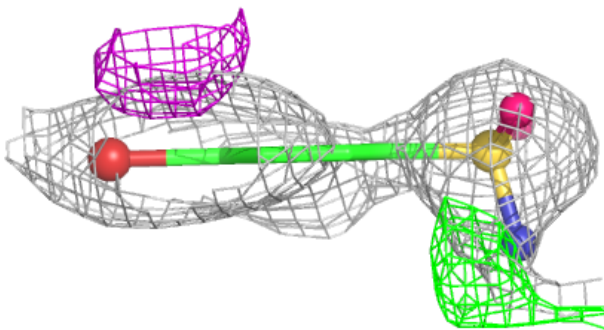
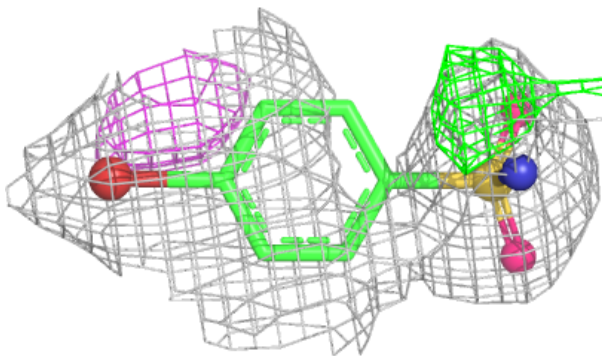


Electron density around T5G C 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

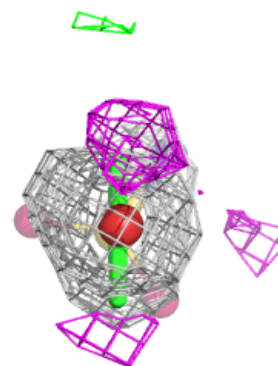
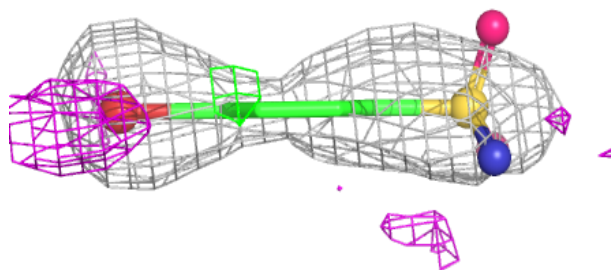
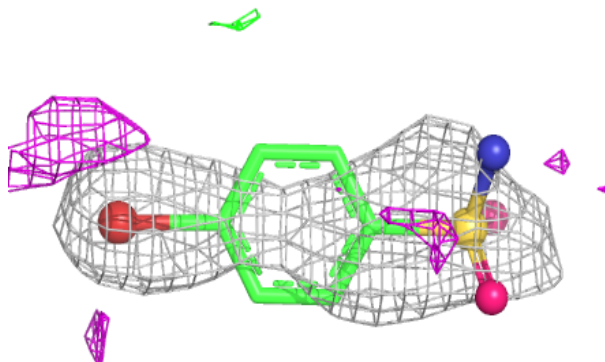
**Electron density around T5G A 501 (B):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

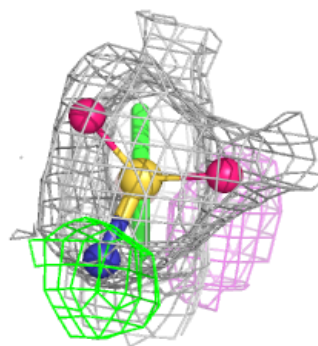
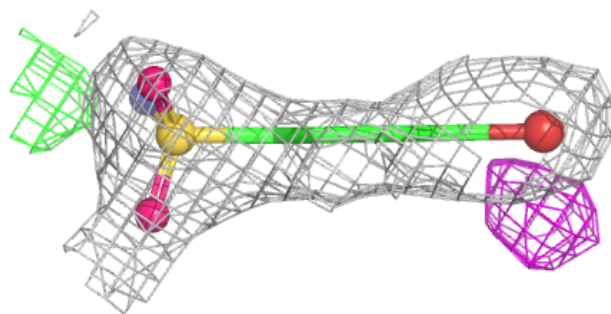
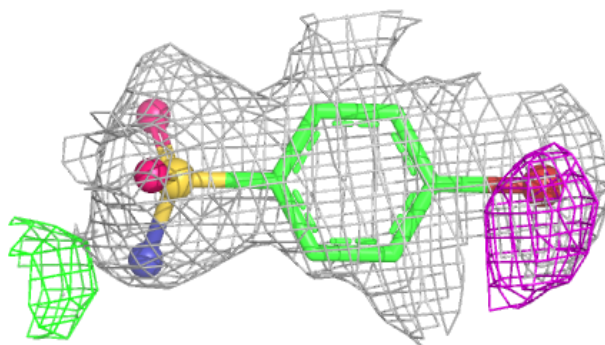


Electron density around T5G B 502:

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

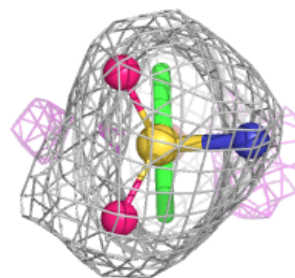
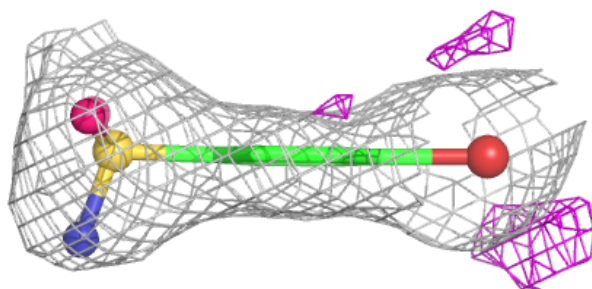
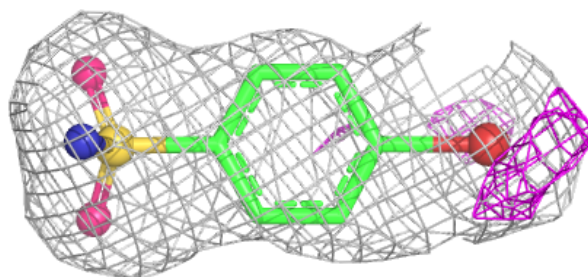
**Electron density around T5G A 501 (A):**

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



Electron density around T5G C 501:

$2mF_o-DF_c$ (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.