



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:53 PM UTC

PDB ID : 1P5E / pdb_00001p5e
Title : The structure of phospho-CDK2/cyclin A in complex with the inhibitor 4,5,6,7-tetrabromobenzotriazole (TBS)
Authors : De Moliner, E.; Brown, N.R.; Johnson, L.N.
Deposited on : 2003-04-26
Resolution : 2.22 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

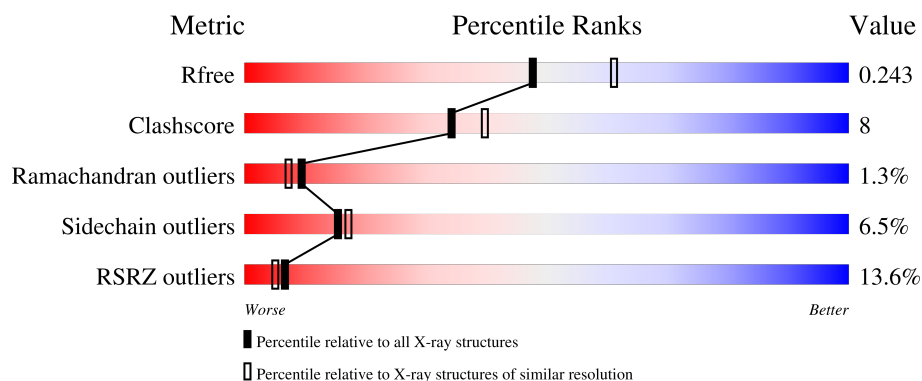
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	299	7% 78% 18% ..
1	C	299	23% 75% 20% ..
2	B	258	4% 83% 15% .
2	D	258	19% 86% 9% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9212 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cell division protein kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			

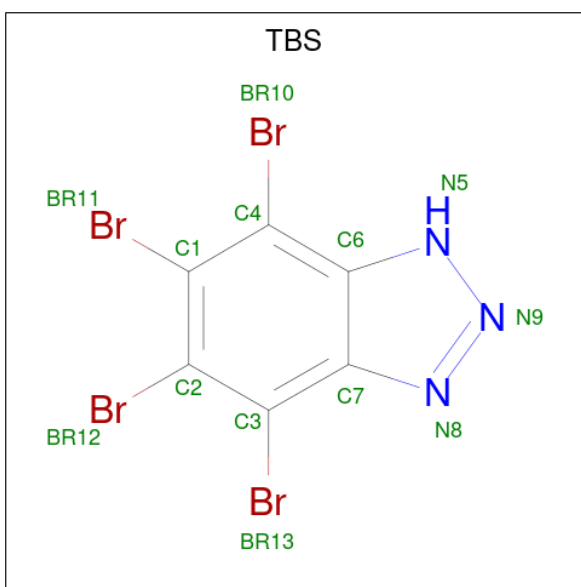
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	cloning artifact	UNP P24941
A	160	TPO	THR	modified residue	UNP P24941
C	0	SER	-	cloning artifact	UNP P24941
C	160	TPO	THR	modified residue	UNP P24941

- Molecule 2 is a protein called Cyclin A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S		0	0	0
			2084	1350	339	384	11				
2	D	258	Total	C	N	O	S		0	0	0
			2084	1350	339	384	11				

- Molecule 3 is 4,5,6,7-TETRABROMOBENZOTRIAZOLE (CCD ID: TBS) (formula: $C_6HBr_4N_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	Br	C	N	0	0
			13	4	6	3		
3	C	1	Total	Br	C	N	0	0
			13	4	6	3		

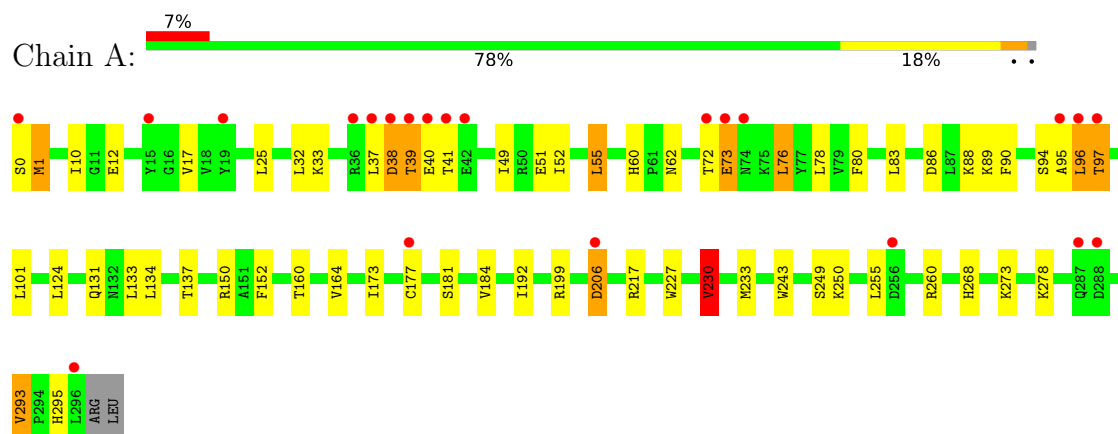
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total	O	0	0
			98	98		
4	B	71	Total	O	0	0
			71	71		
4	C	36	Total	O	0	0
			36	36		
4	D	37	Total	O	0	0
			37	37		

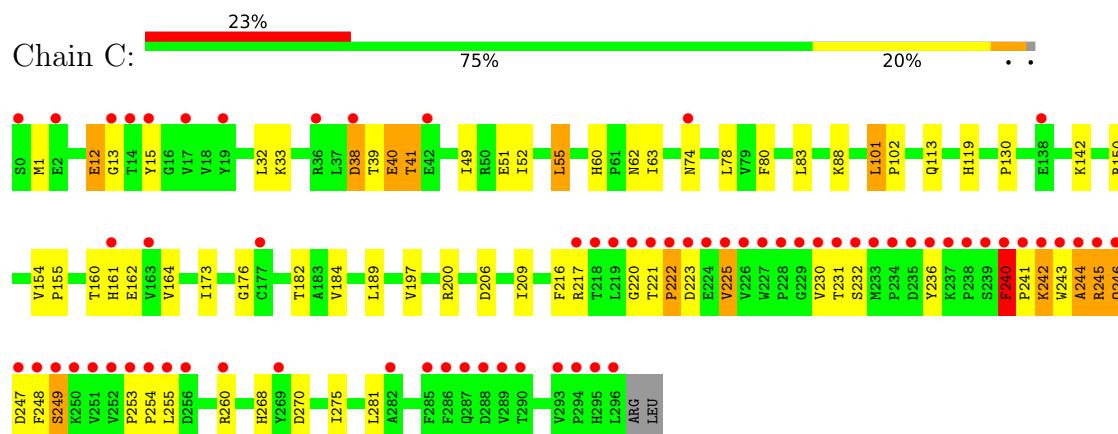
3 Residue-property plots [i](#)

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

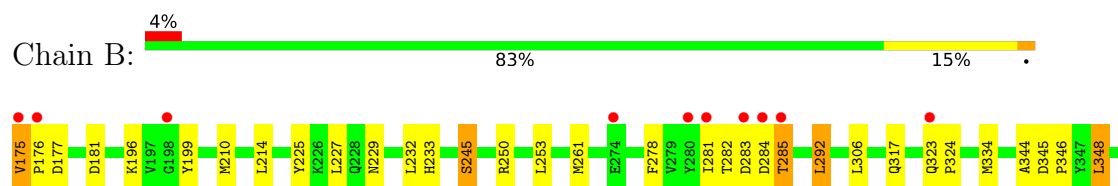
- Molecule 1: Cell division protein kinase 2

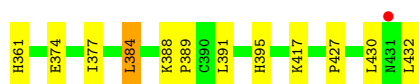


- Molecule 1: Cell division protein kinase 2

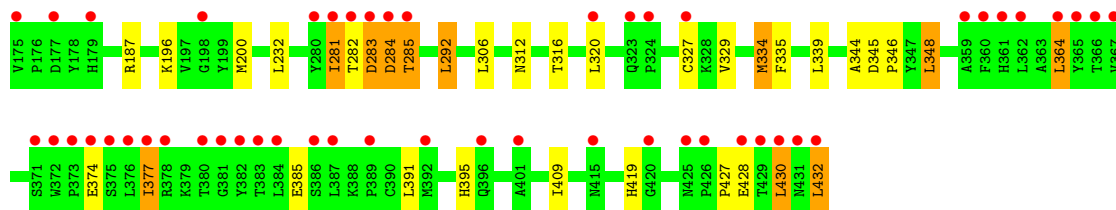
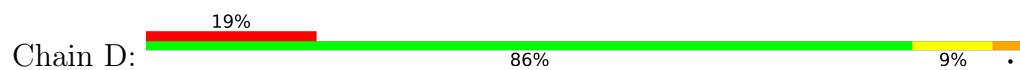


- Molecule 2: Cyclin A2





● Molecule 2: Cyclin A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.54Å 133.95Å 148.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.97 – 2.22 46.97 – 2.22	Depositor EDS
% Data completeness (in resolution range)	92.8 (46.97-2.22) 98.4 (46.97-2.22)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.22Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.257 0.218 , 0.243	Depositor DCC
R_{free} test set	6507 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9212	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TBS, 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	0.54	0/2438	0.87	2/3308 (0.1%)
1	C	0.49	0/2438	0.87	1/3308 (0.0%)
2	B	0.52	0/2134	0.87	0/2897
2	D	0.46	0/2134	0.89	0/2897
All	All	0.50	0/9144	0.87	3/12410 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	VAL	CB-CA-C	-7.39	102.42	111.88
1	C	240	PHE	N-CA-C	5.52	122.01	109.81
1	A	230	VAL	N-CA-CB	5.13	116.20	110.51

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2388	0	2430	42	0
1	C	2388	0	2430	52	0
2	B	2084	0	2107	32	0
2	D	2084	0	2107	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	13	0	1	3	0
3	C	13	0	1	2	0
4	A	98	0	0	4	0
4	B	71	0	0	3	0
4	C	36	0	0	1	0
4	D	37	0	0	2	0
All	All	9212	0	9076	137	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 8.

All (137) 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:B:175:VAL:HB	2:B:176:PRO:CD	1.72	1.18
1:C:216:PHE:CD2	1:C:240:PHE:HE2	1.64	1.12
2:B:175:VAL:HB	2:B:176:PRO:HD2	1.10	1.07
1:C:12:GLU:HG3	1:C:13:GLY:H	1.16	1.04
1:C:216:PHE:HD2	1:C:240:PHE:CE2	1.80	0.99
1:C:216:PHE:HD2	1:C:240:PHE:HE2	0.94	0.91
1:C:216:PHE:CD2	1:C:240:PHE:CE2	2.55	0.90
1:C:220:GLY:HA2	1:C:244:ALA:HB3	1.61	0.83
1:A:206:ASP:HB3	4:A:330:HOH:O	1.78	0.82
1:C:12:GLU:CG	1:C:13:GLY:H	1.96	0.78
2:B:391:LEU:HD23	2:B:432:LEU:HD11	1.65	0.77
1:A:227:TRP:O	1:A:230:VAL:HG22	1.86	0.76
1:A:177:CYS:HB2	1:A:233:MET:CE	2.18	0.74
1:C:161:HIS:HD2	1:C:162:GLU:H	1.37	0.72
1:C:12:GLU:HG3	1:C:13:GLY:N	1.93	0.71
2:B:175:VAL:CB	2:B:176:PRO:HD2	2.05	0.70
1:C:155:PRO:HD2	2:D:316:THR:HG22	1.74	0.69
2:B:175:VAL:CB	2:B:176:PRO:CD	2.61	0.69
1:A:60:HIS:HD2	1:A:62:ASN:H	1.41	0.68
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.76	0.68
1:C:245:ARG:CZ	1:C:246:GLN:HB2	2.24	0.67
1:A:94:SER:O	1:A:97:THR:O	2.12	0.67
1:C:220:GLY:HA2	1:C:244:ALA:CB	2.24	0.66
1:A:137:THR:O	1:A:293:VAL:HG22	1.94	0.66
2:B:395:HIS:HE1	2:B:427:PRO:O	1.79	0.65
1:A:88:LYS:HD3	1:A:131:GLN:HG3	1.78	0.65
1:A:177:CYS:HB3	4:A:312:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:SER:OG	4:B:502:HOH:O	2.14	0.64
2:B:196:LYS:HG3	2:B:199:TYR:HB3	1.78	0.64
1:A:173:ILE:HD11	1:A:184:VAL:HG11	1.80	0.64
1:A:60:HIS:CD2	1:A:62:ASN:H	2.16	0.63
1:C:222:PRO:HB2	1:C:230:VAL:HG11	1.80	0.63
1:C:161:HIS:CD2	1:C:162:GLU:H	2.17	0.63
2:B:210:MET:HE1	2:B:250:ARG:CB	2.29	0.62
1:A:181:SER:HB3	4:A:351:HOH:O	2.00	0.61
2:B:229:ASN:HD22	2:B:334:MET:HE3	1.65	0.61
1:C:1:MET:HE1	1:C:32:LEU:HD13	1.83	0.60
1:C:268:HIS:HD2	1:C:270:ASP:H	1.49	0.60
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.65	0.60
1:C:119:HIS:CD2	1:C:182:THR:HB	2.37	0.60
1:A:95:ALA:HA	1:A:199:ARG:HH11	1.66	0.60
1:C:60:HIS:HD2	1:C:62:ASN:H	1.49	0.59
1:C:216:PHE:CE1	1:C:222:PRO:HD2	2.37	0.59
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.84	0.59
2:D:312:ASN:OD1	2:D:334:MET:HE1	2.03	0.59
1:C:39:THR:O	2:D:292:LEU:HD23	2.04	0.57
1:A:133:LEU:HD11	1:A:192:ILE:HD13	1.88	0.55
2:B:282:THR:O	2:B:285:THR:OG1	2.24	0.55
1:A:268:HIS:CD2	4:A:352:HOH:O	2.59	0.55
1:A:86:ASP:OD2	1:A:89:LYS:HD3	2.06	0.55
1:C:119:HIS:HD2	4:D:438:HOH:O	1.90	0.55
2:B:317:GLN:NE2	4:B:453:HOH:O	2.31	0.54
2:D:282:THR:O	2:D:285:THR:OG1	2.25	0.54
1:C:155:PRO:HD2	2:D:316:THR:CG2	2.39	0.53
1:A:33:LYS:HB3	1:A:78:LEU:HB2	1.91	0.52
1:A:51:GLU:O	1:A:55:LEU:HB2	2.09	0.52
1:A:88:LYS:HD3	1:A:131:GLN:CG	2.40	0.52
1:C:51:GLU:O	1:C:55:LEU:HB2	2.08	0.52
1:C:15:TYR:CZ	1:C:33:LYS:HE3	2.46	0.51
1:C:173:ILE:HD11	1:C:184:VAL:HG11	1.93	0.50
2:B:278:PHE:HA	2:B:281:ILE:HG12	1.93	0.50
1:C:161:HIS:CD2	1:C:162:GLU:N	2.79	0.50
1:A:249:SER:HA	1:A:260:ARG:CD	2.41	0.50
1:C:245:ARG:N	1:C:245:ARG:HD3	2.26	0.50
2:D:374:GLU:HA	2:D:377:ILE:HG22	1.94	0.50
1:A:37:LEU:HD11	1:A:76:LEU:HD13	1.93	0.49
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.46	0.49
1:C:83:LEU:HD11	1:C:142:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.47	0.49
1:A:249:SER:HA	1:A:260:ARG:HD3	1.93	0.49
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.95	0.49
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.95	0.49
2:B:227:LEU:HD12	2:B:261:MET:HE3	1.95	0.48
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.93	0.48
1:C:38:ASP:HB2	1:C:41:THR:OG1	2.13	0.48
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.95	0.48
1:C:41:THR:N	4:C:304:HOH:O	2.46	0.48
2:B:233:HIS:HE1	4:B:491:HOH:O	1.96	0.48
1:C:40:GLU:O	1:C:41:THR:OG1	2.26	0.48
1:C:249:SER:HA	1:C:260:ARG:HD2	1.94	0.48
2:D:430:LEU:HB3	2:D:432:LEU:HG	1.95	0.48
1:C:83:LEU:O	3:C:302:TBS:BR11	2.88	0.47
1:C:60:HIS:HB3	1:C:63:ILE:HD12	1.96	0.47
1:C:243:TRP:HB2	1:C:244:ALA:H	1.53	0.46
1:A:177:CYS:HB2	1:A:233:MET:HE3	1.98	0.46
1:A:217:ARG:HG2	1:A:243:TRP:CD2	2.50	0.46
1:C:80:PHE:CD2	3:C:302:TBS:BR13	3.24	0.46
1:C:221:THR:HG21	1:C:241:PRO:HA	1.97	0.45
1:C:223:ASP:OD1	1:C:225:VAL:HG12	2.15	0.45
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.52	0.45
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.52	0.45
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.97	0.45
1:A:268:HIS:CD2	1:A:273:LYS:HB2	2.52	0.45
1:C:60:HIS:CD2	1:C:62:ASN:H	2.33	0.45
1:C:113:GLN:HG3	1:C:281:LEU:HD21	1.99	0.45
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.78	0.45
2:B:374:GLU:HA	2:B:377:ILE:HD12	1.98	0.45
2:B:345:ASP:HA	2:B:346:PRO:HA	1.70	0.45
2:D:281:ILE:C	2:D:283:ASP:H	2.25	0.45
2:B:229:ASN:ND2	2:B:334:MET:HE3	2.32	0.44
1:A:83:LEU:HD13	1:A:134:LEU:HB2	2.00	0.44
1:A:278:LYS:NZ	2:B:181:ASP:OD2	2.51	0.44
1:A:83:LEU:O	3:A:301:TBS:BR11	2.90	0.44
1:A:295:HIS:H	1:A:295:HIS:CD2	2.36	0.44
1:C:12:GLU:CG	1:C:13:GLY:N	2.67	0.44
1:A:80:PHE:CD2	3:A:301:TBS:BR13	3.26	0.44
1:C:52:ILE:HD11	1:C:78:LEU:HD21	2.00	0.44
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.99	0.44
2:D:345:ASP:HA	2:D:346:PRO:HA	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:327:CYS:HB3	2:D:419:HIS:CE1	2.53	0.43
2:D:187:ARG:HD3	4:D:439:HOH:O	2.19	0.43
1:C:154:VAL:O	2:D:316:THR:HG22	2.18	0.43
1:C:88:LYS:HB2	1:C:130:PRO:HB2	1.99	0.43
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.54	0.43
1:A:1:MET:HE1	1:A:32:LEU:HD13	2.01	0.43
1:C:236:TYR:OH	1:C:241:PRO:HG2	2.18	0.43
1:C:197:VAL:HG21	1:C:255:LEU:HD13	2.00	0.42
2:B:278:PHE:O	2:B:281:ILE:HG13	2.20	0.42
1:C:161:HIS:NE2	1:C:176:GLY:HA2	2.34	0.42
1:A:10:ILE:HD12	3:A:301:TBS:BR11	2.75	0.42
1:A:40:GLU:HB3	1:A:41:THR:H	1.65	0.42
2:D:329:VAL:HG11	2:D:364:LEU:HD13	2.01	0.42
1:A:39:THR:O	2:B:292:LEU:HD23	2.20	0.41
2:D:283:ASP:HB3	2:D:284:ASP:H	1.66	0.41
2:D:395:HIS:HE1	2:D:427:PRO:O	2.03	0.41
1:A:49:ILE:HG23	2:B:306:LEU:HD12	2.02	0.41
2:B:348:LEU:HD12	2:B:348:LEU:HA	1.87	0.41
1:C:101:LEU:N	1:C:102:PRO:CD	2.84	0.41
1:A:95:ALA:HA	1:A:199:ARG:NH1	2.31	0.41
2:B:384:LEU:HD12	2:B:384:LEU:HA	1.96	0.41
1:C:154:VAL:HA	1:C:155:PRO:HA	1.94	0.40
2:D:374:GLU:HA	2:D:377:ILE:CG2	2.51	0.40
2:B:395:HIS:HB2	2:B:430:LEU:HD11	2.03	0.40
1:A:90:PHE:HZ	1:A:295:HIS:CD2	2.40	0.40
1:A:12:GLU:HA	1:A:17:VAL:HA	2.02	0.40
1:A:72:THR:O	1:A:72:THR:HG23	2.22	0.40
2:B:323:GLN:HA	2:B:324:PRO:HA	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/299 (98%)	282 (96%)	8 (3%)	4 (1%)	9	7
1	C	294/299 (98%)	269 (92%)	15 (5%)	10 (3%)	3	1
2	B	256/258 (99%)	255 (100%)	1 (0%)	0	100	100
2	D	256/258 (99%)	253 (99%)	3 (1%)	0	100	100
All	All	1100/1114 (99%)	1059 (96%)	27 (2%)	14 (1%)	9	7

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	96	LEU
1	C	41	THR
1	C	242	LYS
1	C	246	GLN
1	C	12	GLU
1	C	248	PHE
1	A	164	VAL
1	C	164	VAL
1	C	240	PHE
1	C	249	SER
1	C	244	ALA
1	A	73	GLU
1	C	222	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/263 (99%)	244 (94%)	17 (6%)	15	17
1	C	261/263 (99%)	244 (94%)	17 (6%)	15	17
2	B	232/232 (100%)	221 (95%)	11 (5%)	23	29
2	D	232/232 (100%)	213 (92%)	19 (8%)	10	11
All	All	986/990 (100%)	922 (94%)	64 (6%)	15	17

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	1	MET
1	A	25	LEU
1	A	38	ASP
1	A	39	THR
1	A	55	LEU
1	A	73	GLU
1	A	76	LEU
1	A	96	LEU
1	A	97	THR
1	A	101	LEU
1	A	150	ARG
1	A	206	ASP
1	A	230	VAL
1	A	250	LYS
1	A	255	LEU
1	A	293	VAL
2	B	175	VAL
2	B	177	ASP
2	B	232	LEU
2	B	245	SER
2	B	283	ASP
2	B	284	ASP
2	B	285	THR
2	B	292	LEU
2	B	348	LEU
2	B	384	LEU
2	B	417	LYS
1	C	38	ASP
1	C	40	GLU
1	C	55	LEU
1	C	74	ASN
1	C	101	LEU
1	C	150	ARG
1	C	200	ARG
1	C	206	ASP
1	C	209	ILE
1	C	217	ARG
1	C	225	VAL
1	C	231	THR
1	C	232	SER
1	C	242	LYS

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Mol	Chain	Res	Type
1	C	245	ARG
1	C	247	ASP
1	C	275	ILE
2	D	196	LYS
2	D	200	MET
2	D	232	LEU
2	D	281	ILE
2	D	283	ASP
2	D	284	ASP
2	D	285	THR
2	D	292	LEU
2	D	320	LEU
2	D	334	MET
2	D	348	LEU
2	D	364	LEU
2	D	377	ILE
2	D	385	GLU
2	D	391	LEU
2	D	409	ILE
2	D	428	GLU
2	D	430	LEU
2	D	432	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	60	HIS
1	A	62	ASN
1	A	295	HIS
2	B	228	GLN
2	B	233	HIS
2	B	254	GLN
2	B	317	GLN
2	B	395	HIS
2	B	396	GLN
1	C	60	HIS
1	C	119	HIS
1	C	161	HIS
1	C	265	GLN
1	C	268	HIS
2	D	254	GLN

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Mol	Chain	Res	Type
2	D	313	GLN
2	D	395	HIS
2	D	406	GLN
2	D	415	ASN
2	D	419	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	C	160	1	8,10,11	1.30	1 (12%)	10,14,16	0.81	0
1	TPO	A	160	1	8,10,11	1.34	1 (12%)	10,14,16	0.76	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	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-O1P	2.81	1.59	1.50
1	C	160	TPO	P-O1P	2.68	1.58	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	TBS	A	301	-	13,14,14	2.21	5 (38%)	15,21,21	1.63	3 (20%)
3	TBS	C	302	-	13,14,14	2.12	4 (30%)	15,21,21	1.29	1 (6%)

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	TBS	A	301	-	-	-	0/2/2/2
3	TBS	C	302	-	-	-	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	TBS	N8-N9	4.99	1.43	1.31
3	A	301	TBS	N8-N9	4.99	1.43	1.31
3	C	302	TBS	C6-N5	3.46	1.38	1.36
3	C	302	TBS	C6-C7	3.42	1.45	1.40
3	A	301	TBS	C6-N5	3.31	1.38	1.36
3	A	301	TBS	C6-C7	3.11	1.44	1.40
3	A	301	TBS	N5-N9	2.44	1.43	1.34
3	C	302	TBS	N5-N9	2.41	1.43	1.34
3	A	301	TBS	C7-C3	-2.18	1.38	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	TBS	C6-N5-N9	-3.83	103.02	110.01
3	A	301	TBS	C6-N5-N9	-3.82	103.05	110.01
3	A	301	TBS	BR11-C1-C2	-2.99	115.81	120.56
3	A	301	TBS	BR13-C3-C2	-2.32	116.87	120.56

There are no chirality outliers.

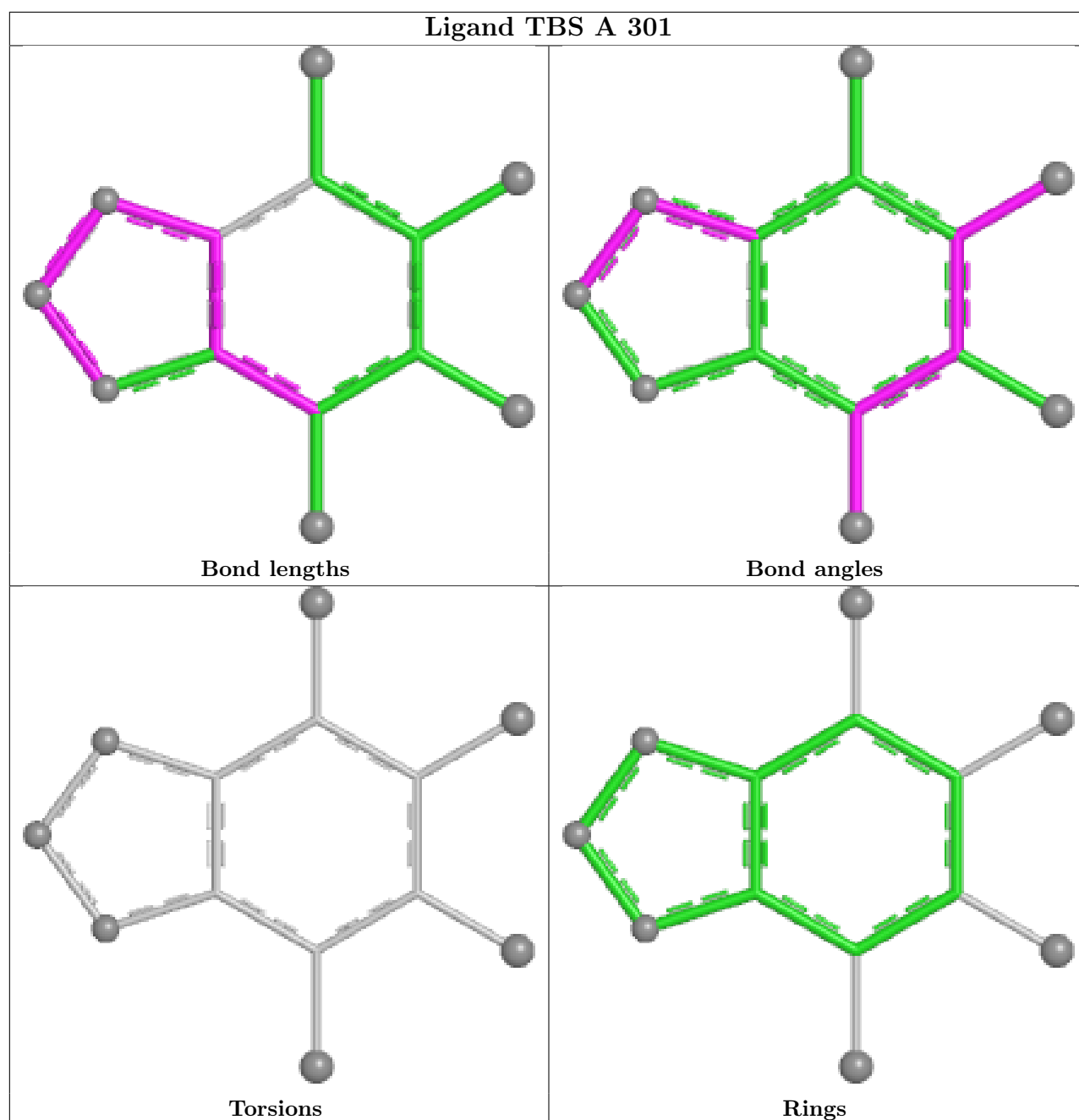
There are no torsion outliers.

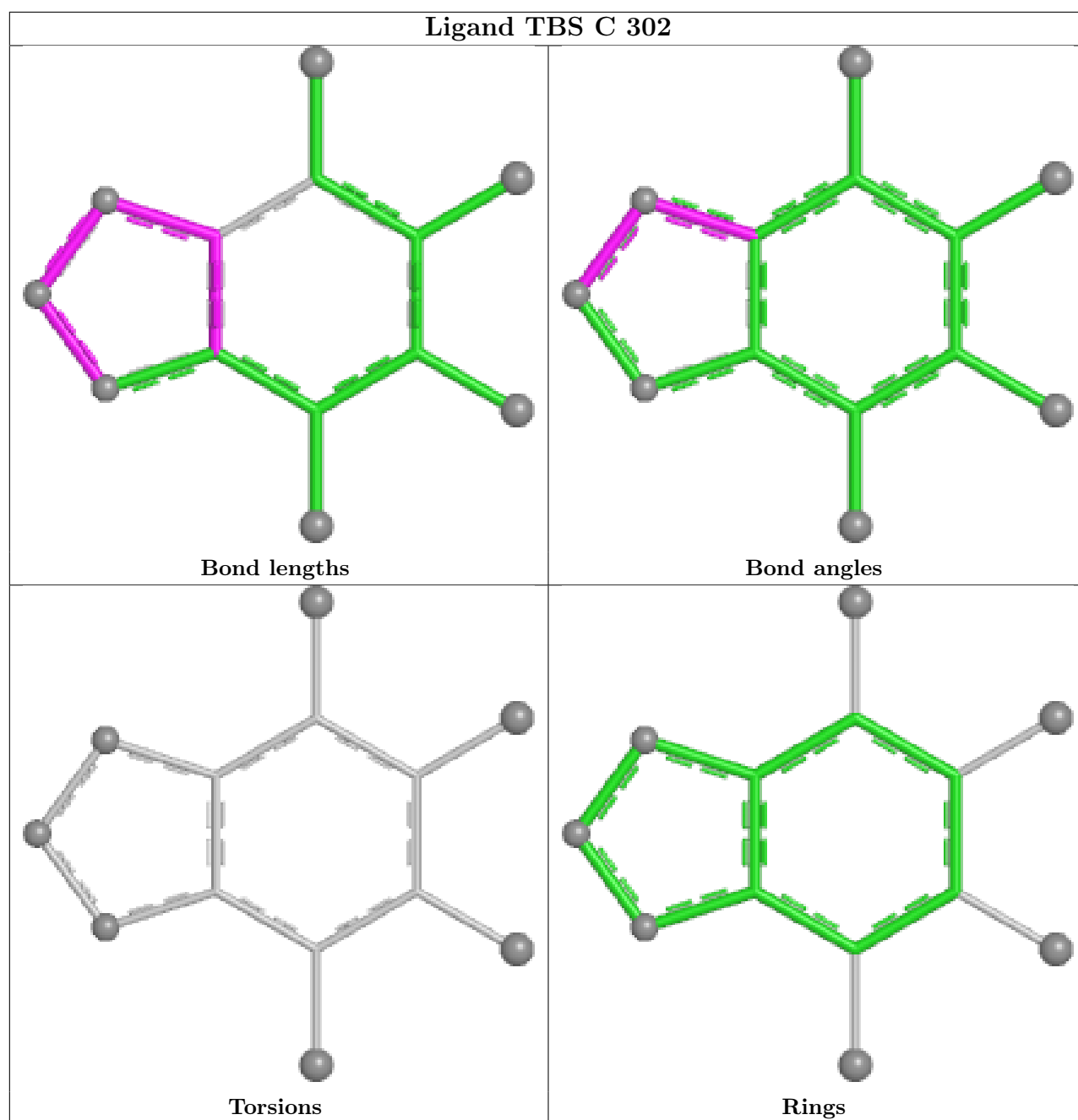
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	TBS	3	0
3	C	302	TBS	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	296/299 (98%)	0.20	22 (7%) 20 18	14, 24, 46, 66	0
1	C	296/299 (98%)	1.43	68 (22%) 2 1	23, 38, 107, 111	0
2	B	258/258 (100%)	0.17	11 (4%) 40 37	17, 26, 41, 55	0
2	D	258/258 (100%)	1.04	50 (19%) 3 2	20, 39, 63, 75	0
All	All	1108/1114 (99%)	0.72	151 (13%) 7 5	14, 32, 63, 111	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	225	VAL	11.4
1	C	244	ALA	10.6
1	C	226	VAL	9.8
1	C	243	TRP	8.8
1	C	240	PHE	8.7
1	C	222	PRO	8.6
1	C	234	PRO	8.0
1	C	241	PRO	7.9
1	C	236	TYR	7.7
1	C	248	PHE	7.4
1	C	14	THR	7.2
1	C	230	VAL	7.1
1	C	238	PRO	6.8
1	C	251	VAL	6.8
1	C	227	TRP	6.6
1	C	13	GLY	6.5
1	C	237	LYS	6.5
1	C	224	GLU	6.3
1	C	239	SER	6.0
1	C	246	GLN	5.9
1	C	15	TYR	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	228	PRO	5.6
1	C	296	LEU	5.4
1	C	221	THR	5.4
1	C	247	ASP	5.3
2	B	284	ASP	5.2
1	A	41	THR	5.2
2	D	175	VAL	5.1
2	D	429	THR	5.0
1	A	96	LEU	5.0
2	D	285	THR	5.0
1	C	229	GLY	4.9
1	C	295	HIS	4.7
2	D	430	LEU	4.6
1	C	245	ARG	4.6
1	A	39	THR	4.4
2	D	365	TYR	4.4
2	D	373	PRO	4.4
1	C	231	THR	4.4
1	A	74	ASN	4.3
1	C	252	VAL	4.2
2	D	383	THR	4.2
1	C	233	MET	4.2
1	A	73	GLU	4.1
2	D	432	LEU	4.1
1	C	0	SER	4.1
1	A	97	THR	4.0
2	D	320	LEU	4.0
1	C	220	GLY	3.9
2	B	285	THR	3.9
1	C	235	ASP	3.9
2	B	175	VAL	3.9
1	C	242	LYS	3.8
1	C	74	ASN	3.7
2	D	420	GLY	3.7
1	C	161	HIS	3.7
1	C	250	LYS	3.6
2	D	428	GLU	3.6
2	D	384	LEU	3.6
2	D	284	ASP	3.6
1	A	40	GLU	3.6
1	C	253	PRO	3.6
1	C	36	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	223	ASP	3.5
2	D	283	ASP	3.5
1	A	38	ASP	3.4
1	C	256	ASP	3.4
2	D	431	ASN	3.4
1	C	287	GLN	3.4
2	D	426	PRO	3.3
2	D	396	GLN	3.3
2	D	362	LEU	3.3
1	A	95	ALA	3.3
2	B	176	PRO	3.3
2	D	372	TRP	3.3
1	C	249	SER	3.2
2	D	386	SER	3.2
1	A	256	ASP	3.1
2	B	283	ASP	3.1
2	D	392	MET	3.1
2	B	198	GLY	3.1
1	A	37	LEU	3.0
1	C	219	LEU	3.0
1	A	287	GLN	3.0
2	D	425	ASN	3.0
1	A	296	LEU	2.9
1	C	232	SER	2.9
2	D	281	ILE	2.9
1	C	217	ARG	2.8
2	D	324	PRO	2.8
1	C	282	ALA	2.8
2	D	374	GLU	2.8
1	C	294	PRO	2.8
2	D	282	THR	2.8
2	D	376	LEU	2.8
2	D	380	THR	2.7
1	C	289	VAL	2.7
1	C	38	ASP	2.7
1	A	177	CYS	2.7
2	D	327	CYS	2.7
1	C	17	VAL	2.7
1	C	255	LEU	2.7
2	B	280	TYR	2.6
2	D	381	GLY	2.6
2	D	378	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	367	VAL	2.6
2	D	179	HIS	2.6
1	C	293	VAL	2.6
2	D	382	TYR	2.6
2	D	323	GLN	2.6
2	B	274	GLU	2.6
2	D	366	THR	2.6
2	D	359	ALA	2.5
2	D	375	SER	2.5
1	A	15	TYR	2.5
1	A	72	THR	2.5
2	D	360	PHE	2.5
1	A	206	ASP	2.5
1	C	163	VAL	2.4
1	C	177	CYS	2.4
2	D	280	TYR	2.4
1	A	36	ARG	2.4
2	D	198	GLY	2.4
2	D	377	ILE	2.4
1	C	269	TYR	2.3
1	C	254	PRO	2.3
1	C	290	THR	2.3
1	A	288	ASP	2.3
2	D	177	ASP	2.3
1	C	19	TYR	2.3
2	D	371	SER	2.2
1	C	42	GLU	2.2
2	D	387	LEU	2.2
1	C	218	THR	2.2
2	D	401	ALA	2.2
2	B	431	ASN	2.2
1	A	42	GLU	2.2
1	C	138	GLU	2.2
2	D	415	ASN	2.1
1	C	286	PHE	2.1
1	A	0	SER	2.1
2	B	281	ILE	2.1
1	C	2	GLU	2.1
2	D	389	PRO	2.1
1	A	19	TYR	2.1
2	B	323	GLN	2.1
2	D	364	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	361	HIS	2.0
1	C	288	ASP	2.0
1	C	285	PHE	2.0
1	C	260	ARG	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	0.10	33,37,40,40	0
1	TPO	A	160	11/12	0.97	0.07	22,23,24,25	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

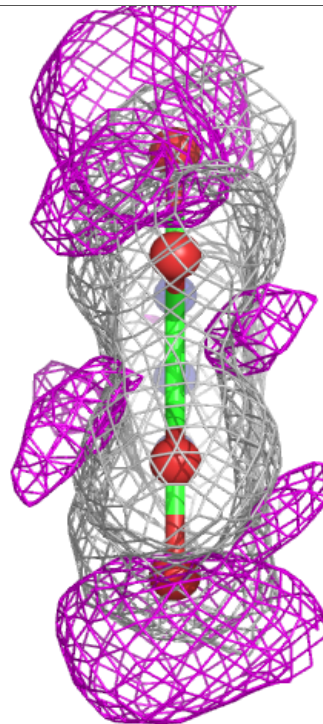
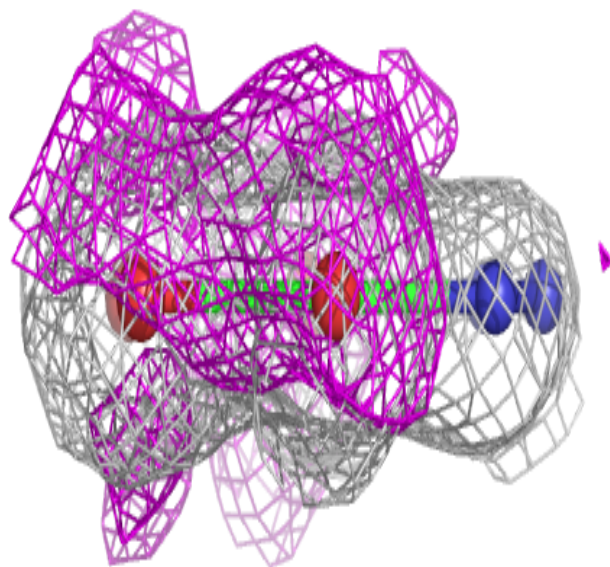
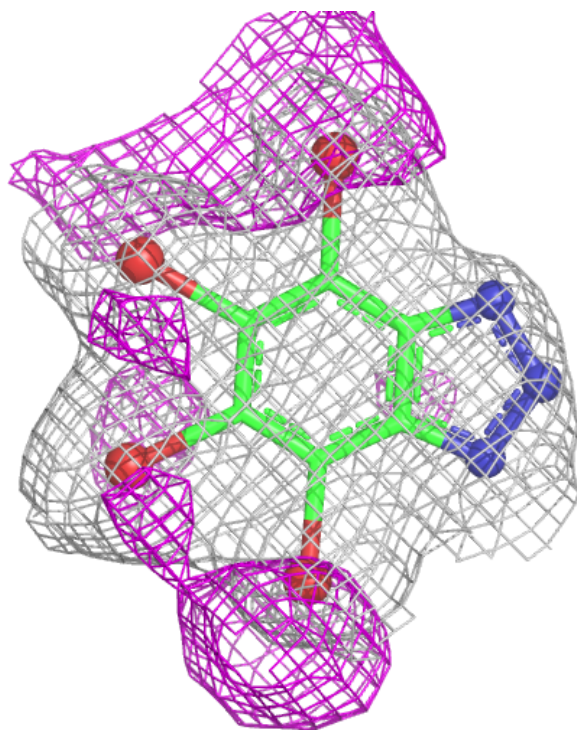
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TBS	A	301	13/13	0.94	0.12	40,58,63,65	0
3	TBS	C	302	13/13	0.94	0.12	53,71,73,78	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.

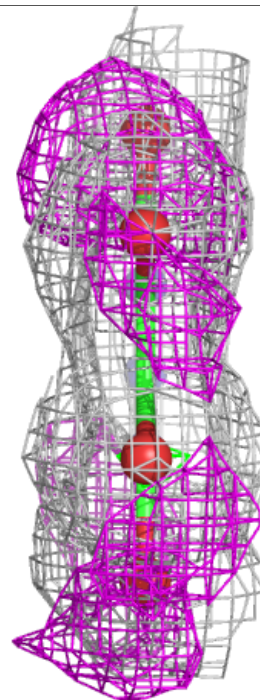
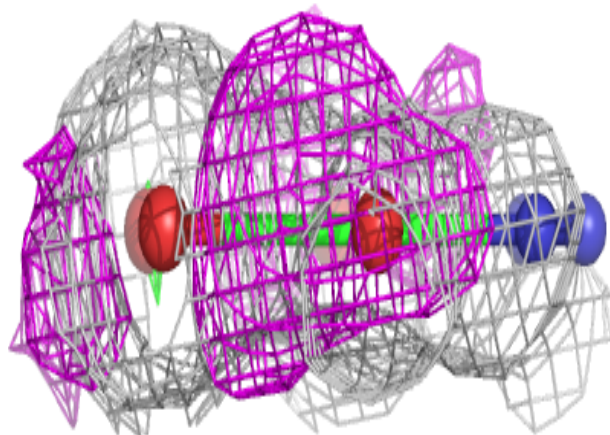
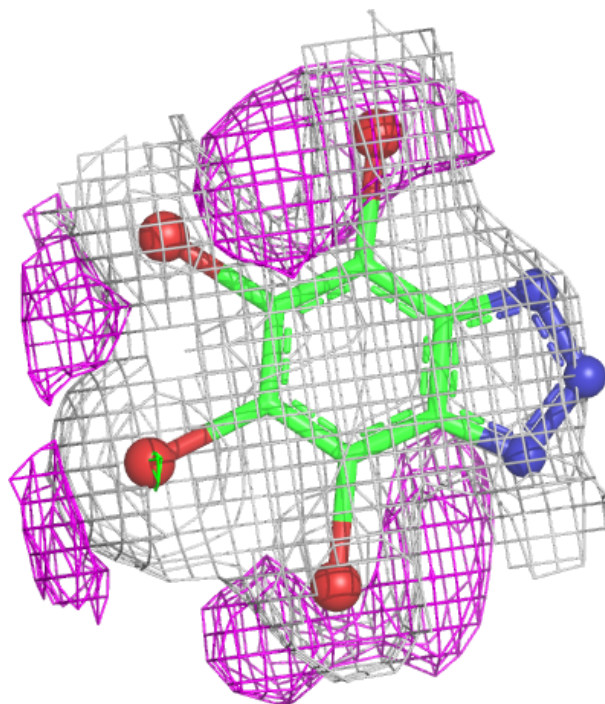
Electron density around TBS A 301:

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



Electron density around TBS C 302:

$2mF_o - DF_c$ (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.