Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:28 PM EDT

PDB ID	:	1P5E
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:

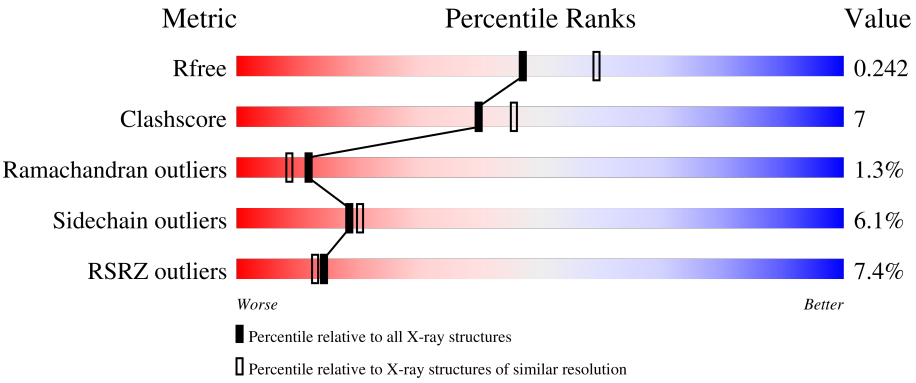
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.22 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}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (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 <=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	3% 77% 19%
1	C	299	16% 74% 20% 5%
2	B	258	2% 83% 14%
2	D	258	8% 86% 11%

2 Entry composition (i)

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			

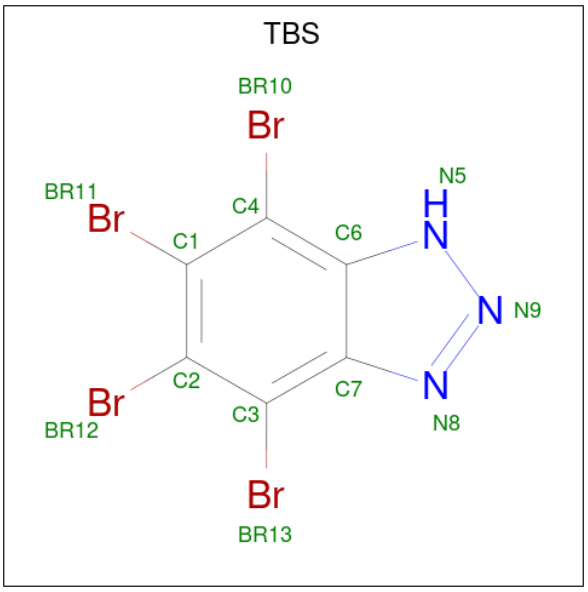
There are 4 discrepancies between the modelled and reference sequences:

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 (three-letter code: TBS) (formula: $C_6HBr_4N_3$).



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

- Molecule 4 is water.

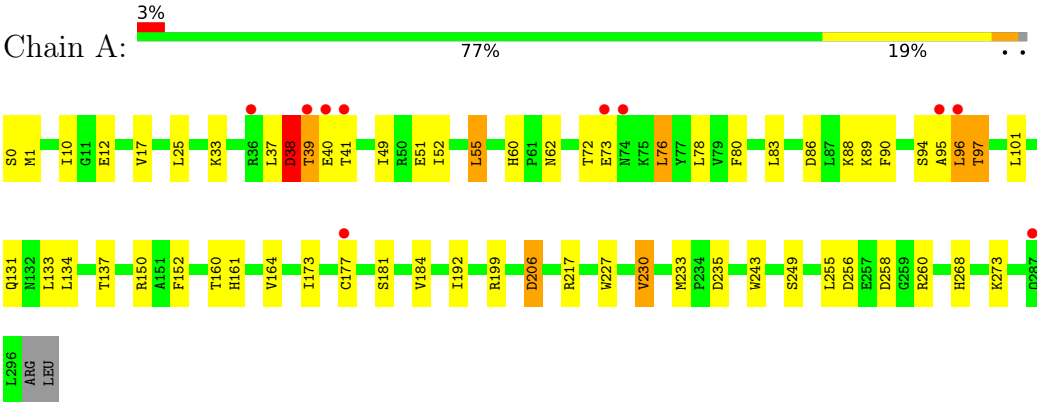
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	98	Total O 98 98	0	0
4	B	71	Total O 71 71	0	0
4	C	36	Total O 36 36	0	0
4	D	37	Total O 37 37	0	0

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.

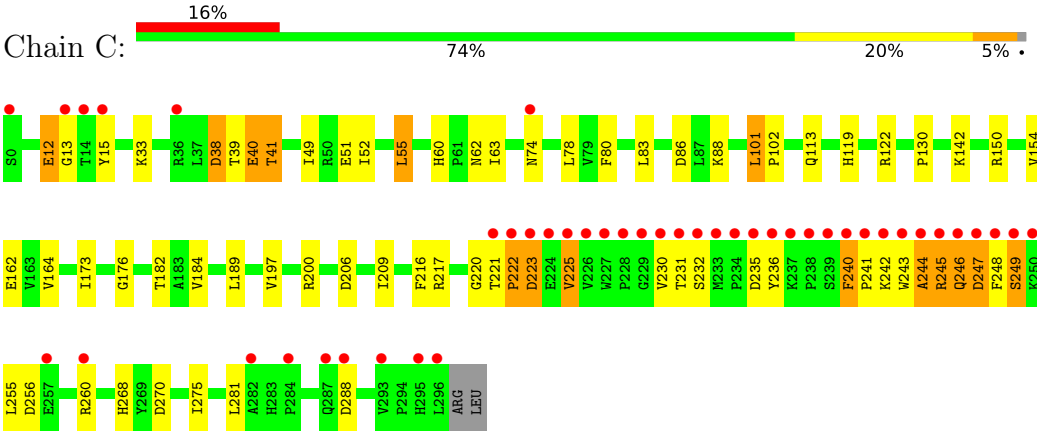
• Molecule 1: Cell division protein kinase 2

Chain A:



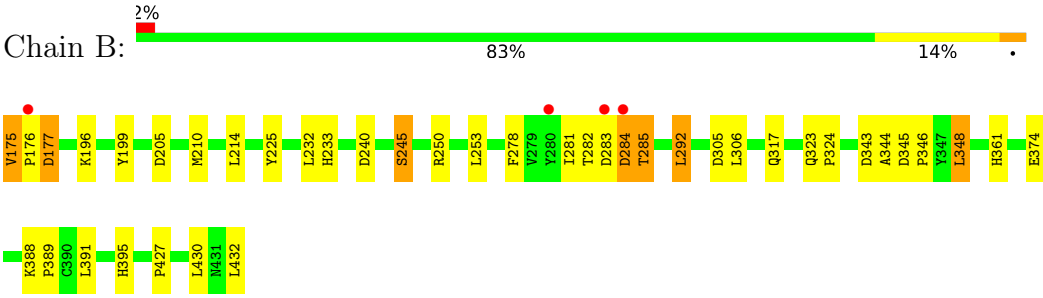
• Molecule 1: Cell division protein kinase 2

Chain C:



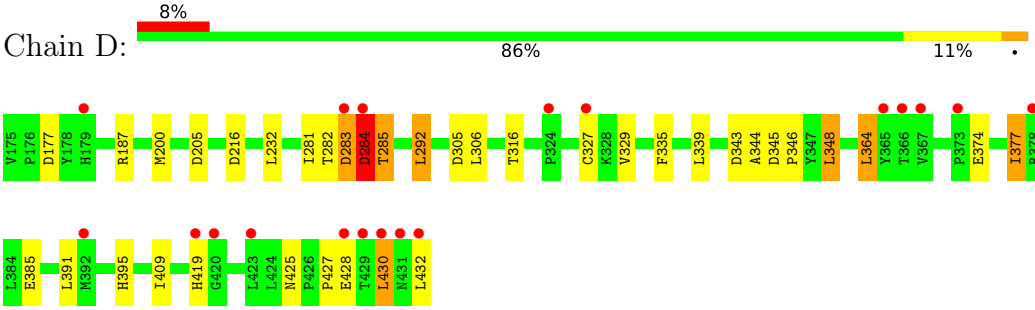
• Molecule 2: Cyclin A2

Chain B:



• Molecule 2: Cyclin A2

Chain D:



4 Data and refinement statistics (i)

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 52.24 – 2.22	Depositor EDS
% Data completeness (in resolution range)	92.8 (46.97-2.22) 98.4 (52.24-2.22)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.22Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.257 0.218 , 0.242	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)	0.38 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TPO, TBS

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	0.45	0/2438	0.71	4/3308 (0.1%)
1	C	0.38	0/2438	0.70	6/3308 (0.2%)
2	B	0.41	0/2134	0.67	6/2897 (0.2%)
2	D	0.36	0/2134	0.67	6/2897 (0.2%)
All	All	0.40	0/9144	0.69	22/12410 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	235	ASP	CB-CG-OD2	5.91	123.62	118.30
2	B	305	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	256	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	38	ASP	CB-CG-OD2	5.38	123.14	118.30
2	B	343	ASP	CB-CG-OD2	5.37	123.13	118.30
2	D	216	ASP	CB-CG-OD2	5.36	123.12	118.30
2	D	177	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	258	ASP	CB-CG-OD2	5.28	123.06	118.30
2	B	177	ASP	CB-CG-OD2	5.25	123.03	118.30
2	B	205	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	223	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	288	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	86	ASP	CB-CG-OD2	5.18	122.96	118.30
2	B	284	ASP	CB-CG-OD2	5.17	122.95	118.30
2	D	305	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	256	ASP	CB-CG-OD2	5.16	122.94	118.30
2	D	205	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	235	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	247	ASP	CB-CG-OD2	5.14	122.92	118.30
2	D	343	ASP	CB-CG-OD2	5.12	122.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	240	ASP	CB-CG-OD2	5.11	122.90	118.30
2	D	284	ASP	CB-CG-OD2	5.03	122.83	118.30

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	2388	0	2430	40	0
1	C	2388	0	2430	51	0
2	B	2084	0	2107	30	0
2	D	2084	0	2107	17	0
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	131	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 (131) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:GLU:HG3	1:C:13:GLY:N	1.93	0.82
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
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
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
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
1:A:181:SER:HB3	4:A:351:HOH:O	2.00	0.61
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:MET:HB3	2:B:210:MET:HE2	1.86	0.45
2:B:345:ASP:HA	2:B:346:PRO:HA	1.70	0.45
1:A:83:LEU:HD13	1:A:134:LEU:HB2	2.00	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
2:B:210:MET:HE1	2:B:250:ARG:CB	2.48	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:B:210:MET:HE1	2:B:250:ARG:HB2	2.00	0.43
2:D:345:ASP:HA	2:D:346:PRO:HA	1.76	0.43
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:177:CYS:HB2	1:A:233:MET:HE2	1.95	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:210:MET:CE	2:B:250:ARG:HB2	2.50	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%)	11 8
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%)	12 9

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 (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	261/263 (99%)	244 (94%)	17 (6%)	17	18
1	C	261/263 (99%)	244 (94%)	17 (6%)	17	18
2	B	232/232 (100%)	222 (96%)	10 (4%)	29	35
2	D	232/232 (100%)	216 (93%)	16 (7%)	15	15
All	All	986/990 (100%)	926 (94%)	60 (6%)	18	20

All (60) 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	76	LEU
1	A	96	LEU
1	A	97	THR
1	A	101	LEU
1	A	122	ARG
1	A	150	ARG
1	A	161	HIS
1	A	206	ASP
1	A	230	VAL
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
1	C	38	ASP

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Mol	Chain	Res	Type
1	C	40	GLU
1	C	55	LEU
1	C	74	ASN
1	C	101	LEU
1	C	122	ARG
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	245	ARG
1	C	247	ASP
1	C	275	ILE
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	348	LEU
2	D	364	LEU
2	D	377	ILE
2	D	385	GLU
2	D	391	LEU
2	D	409	ILE
2	D	425	ASN
2	D	428	GLU
2	D	430	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	60	HIS
1	A	161	HIS
1	A	295	HIS
2	B	179	HIS
2	B	233	HIS

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Mol	Chain	Res	Type
2	B	254	GLN
2	B	370	GLN
2	B	395	HIS
2	B	396	GLN
1	C	60	HIS
1	C	119	HIS
1	C	161	HIS
1	C	268	HIS
2	D	254	GLN
2	D	395	HIS
2	D	406	GLN
2	D	415	ASN
2	D	419	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPO	C	160	1	8,10,11	1.25	1 (12%)	10,14,16	0.76	0
1	TPO	A	160	1	8,10,11	1.29	1 (12%)	10,14,16	0.70	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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	2.69	1.59	1.50
1	C	160	TPO	P-O1P	2.57	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TBS	A	301	-	10,14,14	1.00	0	11,21,21	1.75	2 (18%)
3	TBS	C	302	-	10,14,14	0.57	0	11,21,21	1.10	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	TBS	A	301	-	-	-	0/2/2/2
3	TBS	C	302	-	-	-	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	TBS	BR13-C3-C2	-3.20	116.87	120.97
3	A	301	TBS	BR11-C1-C2	-3.19	115.81	120.60

There are no chirality outliers.

There are no torsion outliers.

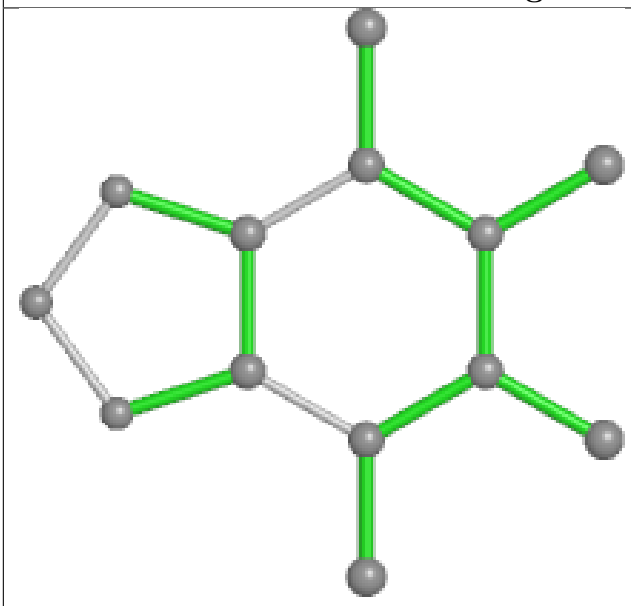
There are no ring outliers.

2 monomers are involved in 5 short contacts:

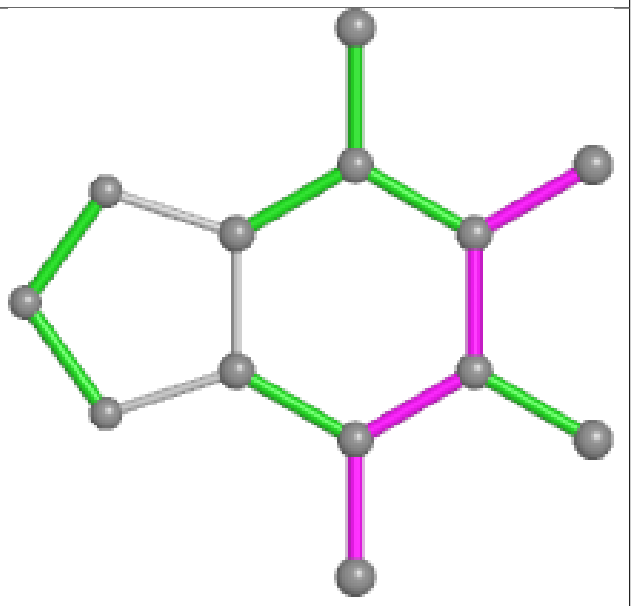
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	TBS	3	0
3	C	302	TBS	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

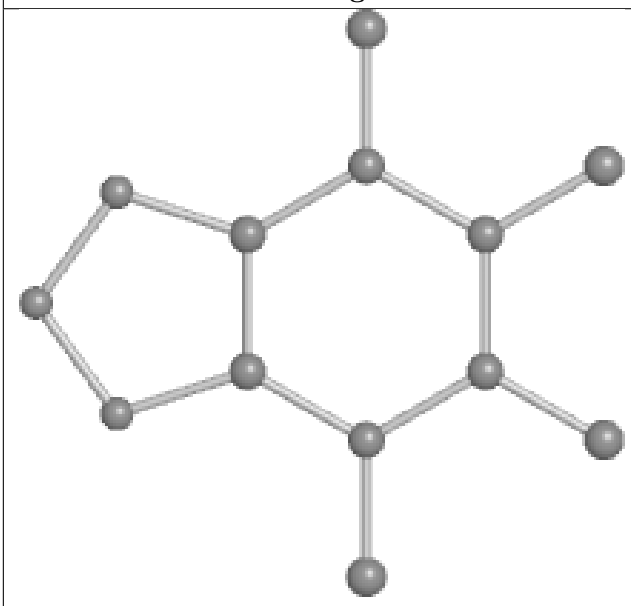
Ligand TBS A 301



Bond lengths



Bond angles



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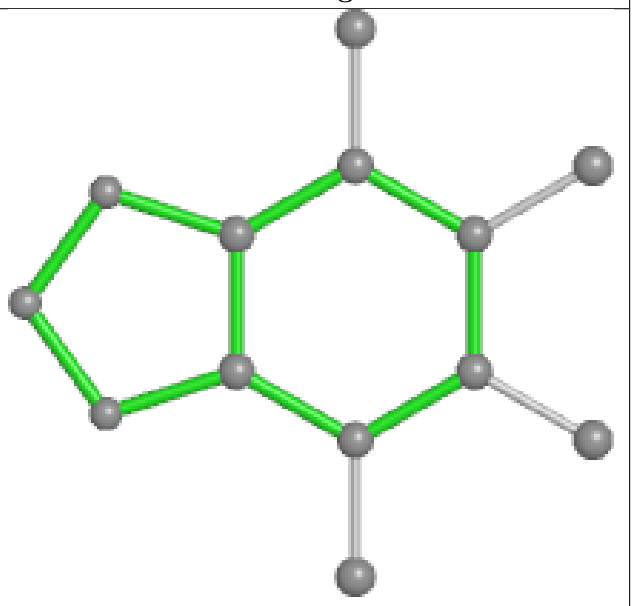

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.19	10 (3%) 45 43	14, 24, 46, 66	0
1	C	296/299 (98%)	1.20	47 (15%) 1 1	23, 38, 107, 111	0
2	B	258/258 (100%)	0.02	4 (1%) 72 70	17, 26, 41, 55	0
2	D	258/258 (100%)	0.57	21 (8%) 12 10	20, 39, 63, 75	0
All	All	1108/1114 (99%)	0.51	82 (7%) 14 13	14, 32, 63, 111	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	225	VAL	15.8
1	C	243	TRP	14.1
1	C	13	GLY	14.0
1	C	244	ALA	13.2
1	C	226	VAL	13.1
1	C	246	GLN	11.9
1	C	240	PHE	11.5
1	C	236	TYR	10.7
1	C	238	PRO	10.4
1	C	233	MET	10.1
1	C	232	SER	9.9
1	C	224	GLU	9.7
1	C	231	THR	9.6
1	C	221	THR	9.3
1	C	234	PRO	9.3
1	C	222	PRO	8.1
1	C	229	GLY	7.4
1	C	247	ASP	6.9
1	C	245	ARG	6.5
1	C	235	ASP	6.4
1	C	227	TRP	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	251	VAL	6.1
1	C	239	SER	6.0
1	C	223	ASP	5.9
1	C	228	PRO	5.8
1	A	96	LEU	5.8
1	C	248	PHE	5.6
1	A	40	GLU	5.6
1	C	15	TYR	5.5
1	C	230	VAL	4.7
1	C	241	PRO	4.5
1	A	41	THR	4.2
1	A	39	THR	4.1
2	D	283	ASP	4.0
1	A	73	GLU	4.0
1	C	237	LYS	4.0
2	D	430	LEU	3.9
1	C	14	THR	3.8
2	B	284	ASP	3.6
2	D	423	LEU	3.6
1	C	287	GLN	3.5
2	B	283	ASP	3.5
2	D	324	PRO	3.4
1	C	282	ALA	3.4
1	C	242	LYS	3.4
2	D	432	LEU	3.3
2	D	381	GLY	3.3
2	D	284	ASP	3.3
2	D	327	CYS	3.2
1	C	36	ARG	3.2
2	D	420	GLY	3.2
1	C	295	HIS	3.1
1	C	250	LYS	3.1
1	C	296	LEU	3.0
1	C	293	VAL	2.9
2	D	373	PRO	2.8
1	C	161	HIS	2.8
1	C	249	SER	2.8
2	D	419	HIS	2.7
2	B	176	PRO	2.7
1	C	0	SER	2.6
2	D	383	THR	2.5
1	A	74	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	365	TYR	2.5
2	D	367	VAL	2.4
1	A	95	ALA	2.4
2	D	428	GLU	2.3
1	C	288	ASP	2.3
1	A	177	CYS	2.3
1	A	36	ARG	2.2
2	B	280	TYR	2.1
1	C	257	GLU	2.1
2	D	431	ASN	2.1
2	D	429	THR	2.1
1	C	284	PRO	2.1
2	D	179	HIS	2.1
1	A	287	GLN	2.1
2	D	378	ARG	2.1
2	D	392	MET	2.0
1	C	74	ASN	2.0
1	C	260	ARG	2.0
2	D	366	THR	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^{th} 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	0.14	33,37,40,40	0
1	TPO	A	160	11/12	0.97	0.13	22,23,24,25	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

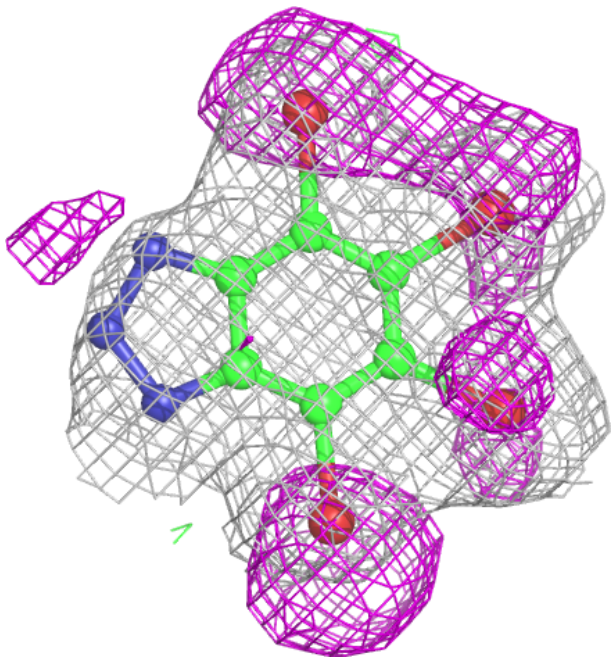
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

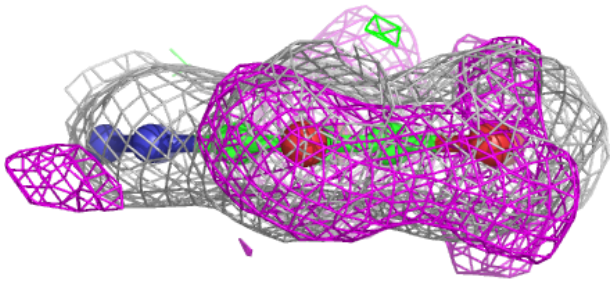
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TBS	C	302	13/13	0.91	0.17	53,71,73,78	0
3	TBS	A	301	13/13	0.93	0.14	40,58,63,65	0

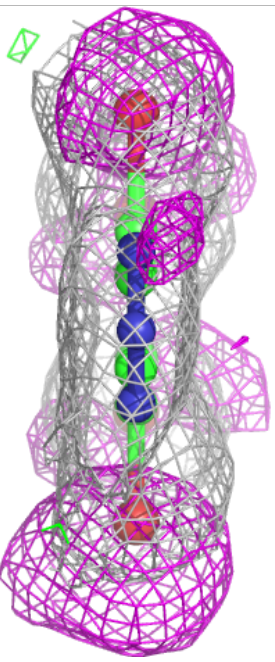
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)







6.5 Other polymers (i)

There are no such residues in this entry.