



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 07:26 pm BST

PDB ID : 3BHT
Title : Structure of phosphorylated Thr160 CDK2/cyclin A in complex with the inhibitor meriolin 3
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Deposited on : 2007-11-29
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

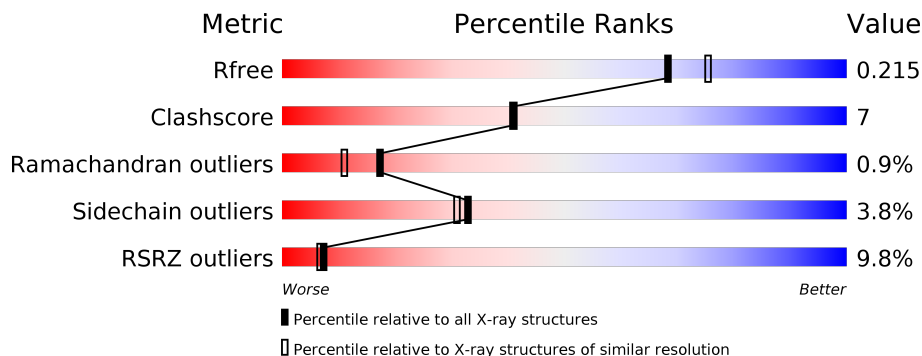
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	300	
1	C	300	
2	B	262	
2	D	262	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SGM	B	5	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9983 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	
			Total	C	N	O	P				S
1	A	298	Total	C	N	O	P	S	0	4	0
			2416	1568	412	426	1	9			
1	C	271	Total	C	N	O	P	S	0	2	0
			2185	1417	373	387	1	7			

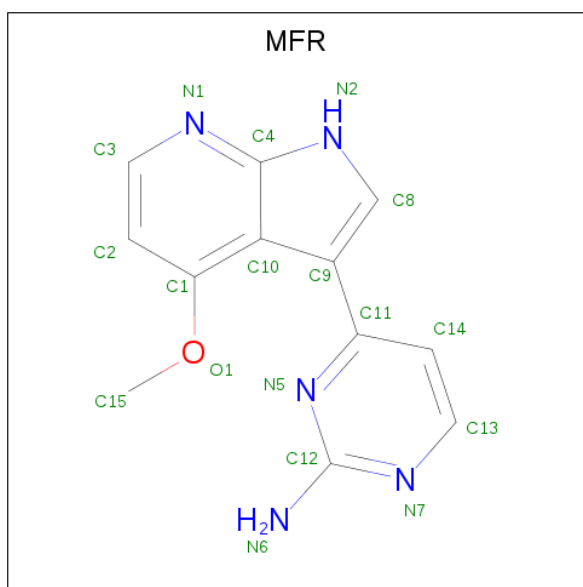
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P24941
A	0	SER	-	EXPRESSION TAG	UNP P24941
C	-1	GLY	-	EXPRESSION TAG	UNP P24941
C	0	SER	-	EXPRESSION TAG	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	262	Total	C	N	O	S	0	3	0
			2130	1379	346	395	10			
2	D	262	Total	C	N	O	S	0	1	0
			2118	1371	344	393	10			

- Molecule 3 is 4-(4-methoxy-1H-pyrrolo[2,3-b]pyridin-3-yl)pyrimidin-2-amine (three-letter code: MFR) (formula: C₁₂H₁₁N₅O).

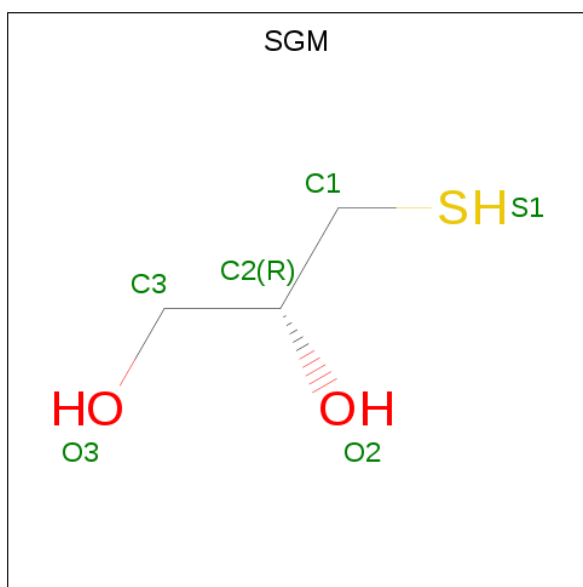


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	18	12	5	1	0	0
3	C	1	18	12	5	1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	B	1	1	1	0	0
4	D	1	1	1	0	0

- Molecule 5 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: C₃H₈O₂S).



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

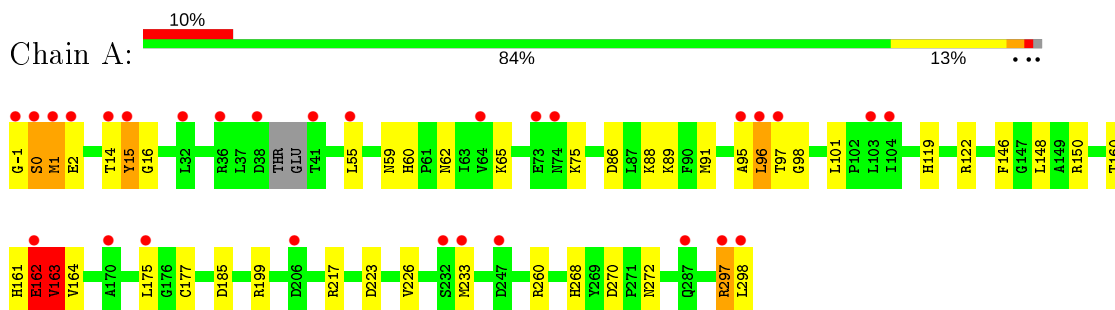
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	345	Total	O	0	0
			345	345		
6	B	292	Total	O	0	0
			292	292		
6	C	227	Total	O	0	0
			227	227		
6	D	214	Total	O	0	0
			214	214		

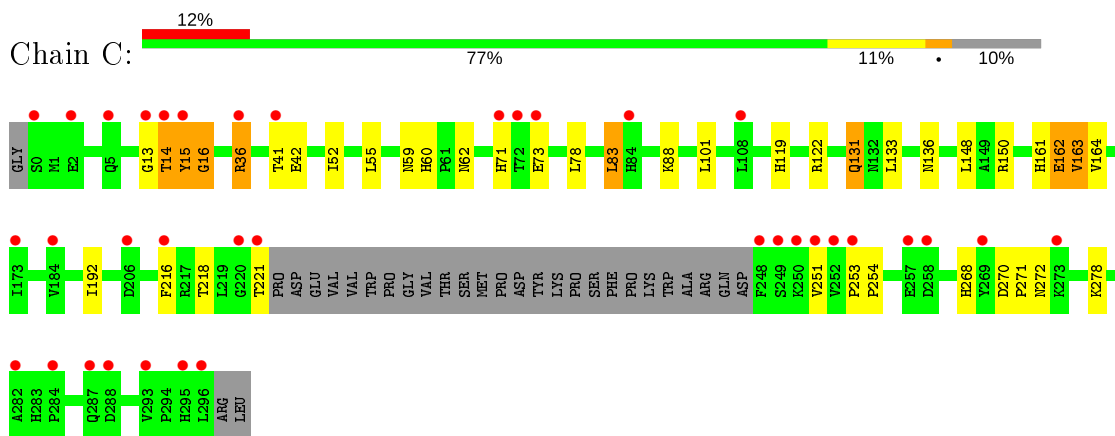
3 Residue-property plots [i](#)

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

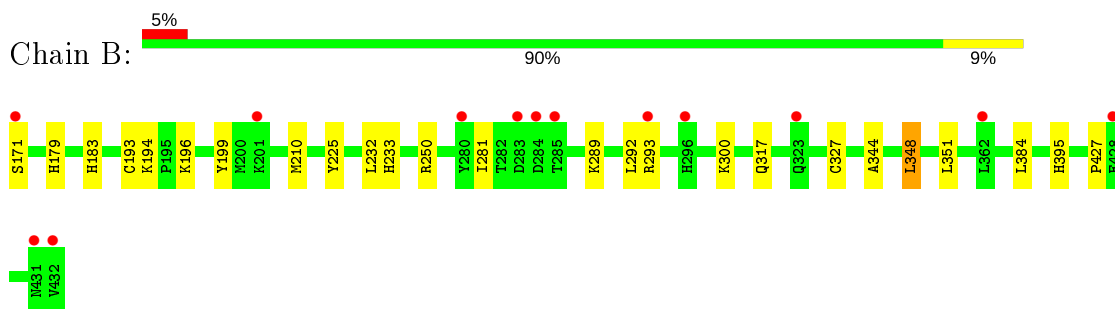
- Molecule 1: Cell division protein kinase 2



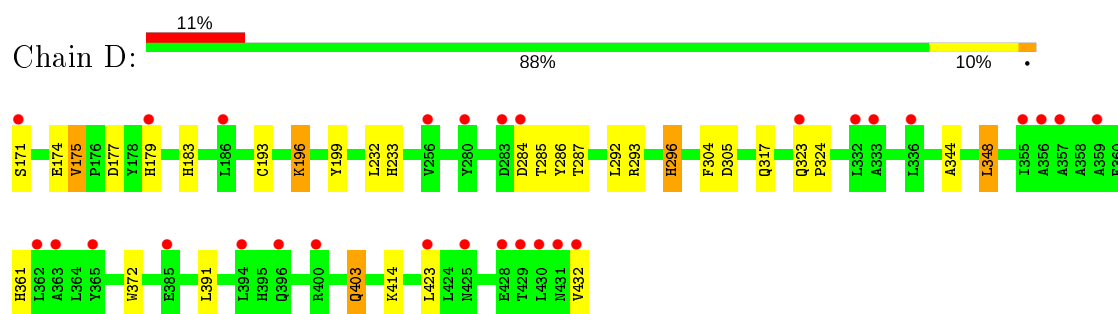
- Molecule 1: Cell division protein kinase 2



- 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	74.13Å 133.77Å 147.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.5 (20.00-2.00) 95.5 (19.87-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.01Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.220 0.181 , 0.215	Depositor DCC
R_{free} test set	4777 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9983	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: TPO, MG, SGM, MFR

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	0.71	0/2477	0.74	2/3357 (0.1%)
1	C	0.54	0/2229	0.62	0/3016
2	B	0.55	0/2190	0.58	0/2978
2	D	0.51	0/2171	0.67	2/2952 (0.1%)
All	All	0.59	0/9067	0.66	4/12303 (0.0%)

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	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	174	GLU	N-CA-C	10.17	138.45	111.00
1	A	217	ARG	NE-CZ-NH2	-8.40	116.10	120.30
2	D	175	VAL	N-CA-C	-6.80	92.63	111.00
1	A	163	VAL	N-CA-C	-6.39	93.75	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	THR	Peptide

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	2416	0	2471	52	1
1	C	2185	0	2250	41	1
2	B	2130	0	2146	19	0
2	D	2118	0	2136	34	0
3	A	18	0	11	0	0
3	C	18	0	11	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	12	0	15	3	0
5	D	6	0	8	3	0
6	A	345	0	0	9	0
6	B	292	0	0	6	0
6	C	227	0	0	5	0
6	D	214	0	0	8	0
All	All	9983	0	9048	128	1

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.

The worst 5 of 128 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177[A]:CYS:SG	1:A:233:MET:HE3	1.45	1.54
2:B:193:CYS:SG	5:B:4:SGM:S1	2.31	1.27
2:D:193:CYS:SG	5:D:3:SGM:S1	2.38	1.22
2:B:171:SER:OG	6:B:595:HOH:O	1.68	1.12
1:C:272:ASN:OD1	2:D:171:SER:HB3	1.47	1.11

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:NH2	1:C:251:VAL:CG2[3_454]	2.18	0.02

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	297/300 (99%)	283 (95%)	9 (3%)	5 (2%)	9	4
1	C	267/300 (89%)	254 (95%)	8 (3%)	5 (2%)	8	3
2	B	263/262 (100%)	261 (99%)	2 (1%)	0	100	100
2	D	261/262 (100%)	256 (98%)	5 (2%)	0	100	100
All	All	1088/1124 (97%)	1054 (97%)	24 (2%)	10 (1%)	17	11

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	15	TYR
1	A	162	GLU
1	C	162	GLU
1	C	163	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/263 (101%)	254 (96%)	11 (4%)	30	27
1	C	239/263 (91%)	228 (95%)	11 (5%)	27	23
2	B	238/235 (101%)	232 (98%)	6 (2%)	47	49
2	D	236/235 (100%)	227 (96%)	9 (4%)	33	31
All	All	978/996 (98%)	941 (96%)	37 (4%)	33	31

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	384	LEU
1	C	55	LEU
2	D	348	LEU
1	C	14	THR
1	C	15	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	84	HIS
1	C	119	HIS
2	D	296	HIS
1	C	85	GLN
1	C	161	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	A	160	1	8,10,11	2.18	3 (37%)	10,14,16	1.41	2 (20%)
1	TPO	C	160	1	8,10,11	2.25	3 (37%)	10,14,16	0.92	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	A	160	1	-	0/9/11/13	-
1	TPO	C	160	1	-	1/9/11/13	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-O3P	-4.11	1.39	1.54
1	C	160	TPO	P-O3P	-3.92	1.39	1.54
1	C	160	TPO	P-O2P	-3.51	1.41	1.54
1	A	160	TPO	P-O2P	-3.46	1.41	1.54
1	C	160	TPO	P-O1P	-2.94	1.41	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	OG1-P-O1P	-2.76	98.73	109.39
1	A	160	TPO	O3P-P-O2P	2.33	116.53	107.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	160	TPO	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	MFR	C	299	-	19,20,20	1.28	2 (10%)	20,28,28	3.44	12 (60%)
5	SGM	B	4	-	5,5,5	0.44	0	5,5,5	0.49	0
5	SGM	D	3	-	5,5,5	0.39	0	5,5,5	0.45	0
3	MFR	A	299	-	19,20,20	1.22	2 (10%)	20,28,28	3.43	10 (50%)
5	SGM	B	5	-	5,5,5	0.43	0	5,5,5	0.27	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	MFR	C	299	-	-	0/2/6/6	0/3/3/3
5	SGM	B	4	-	-	2/4/4/4	-
5	SGM	D	3	-	-	0/4/4/4	-
3	MFR	A	299	-	-	0/2/6/6	0/3/3/3
5	SGM	B	5	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	299	MFR	C1-C10	3.08	1.49	1.42
3	A	299	MFR	C1-C10	2.98	1.49	1.42
3	C	299	MFR	C9-C10	2.26	1.45	1.41
3	A	299	MFR	C9-C10	2.09	1.45	1.41

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	299	MFR	C11-N5-C12	10.14	122.12	116.34
3	C	299	MFR	C11-N5-C12	8.94	121.44	116.34
3	A	299	MFR	N7-C12-N5	-4.75	119.92	125.70
3	C	299	MFR	O1-C1-C10	4.65	122.73	115.89
3	C	299	MFR	C13-N7-C12	4.49	120.84	116.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	4	SGM	S1-C1-C2-O2
5	B	5	SGM	C1-C2-C3-O3
5	B	5	SGM	O2-C2-C3-O3
5	B	4	SGM	S1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	4	SGM	1	0
5	D	3	SGM	3	0
5	B	5	SGM	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/300 (99%)	0.69	29 (9%) 7 7	2, 5, 22, 43	0
1	C	270/300 (90%)	0.93	36 (13%) 3 2	2, 6, 33, 59	0
2	B	262/262 (100%)	0.44	13 (4%) 28 28	2, 5, 16, 27	0
2	D	262/262 (100%)	0.76	29 (11%) 5 4	2, 6, 21, 43	0
All	All	1091/1124 (97%)	0.71	107 (9%) 7 7	2, 6, 24, 59	0

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	SER	10.9
1	C	221	THR	8.8
1	A	96	LEU	8.6
1	A	14	THR	7.3
2	D	171	SER	6.8

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	A	160	11/12	0.98	0.11	2,4,6,7	0
1	TPO	C	160	11/12	0.98	0.10	2,4,7,7	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	SGM	B	5	6/6	0.42	0.41	61,63,63,64	0
5	SGM	D	3	6/6	0.76	0.28	41,43,43,44	0
5	SGM	B	4	6/6	0.88	0.27	30,31,33,34	0
4	MG	B	1	1/1	0.95	0.15	15,15,15,15	0
3	MFR	C	299	18/18	0.95	0.10	2,2,4,5	0
3	MFR	A	299	18/18	0.96	0.10	2,2,2,2	0
4	MG	D	2	1/1	0.98	0.23	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.