



wwPDB X-ray Structure Validation Summary Report

Feb 14, 2017 – 04:55 pm GMT

PDB ID : 2IW9
Title : STRUCTURE OF HUMAN THR160-PHOSPHO CDK2-CYCLIN A COM-
PLEXED WITH A BISANILINOPYRIMIDINE INHIBITOR
Authors : Pratt, D.J.; Bentley, J.; Jewsbury, P.; Boyle, F.T.; Endicott, J.A.; Noble,
M.E.M.
Deposited on : 2006-06-27
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

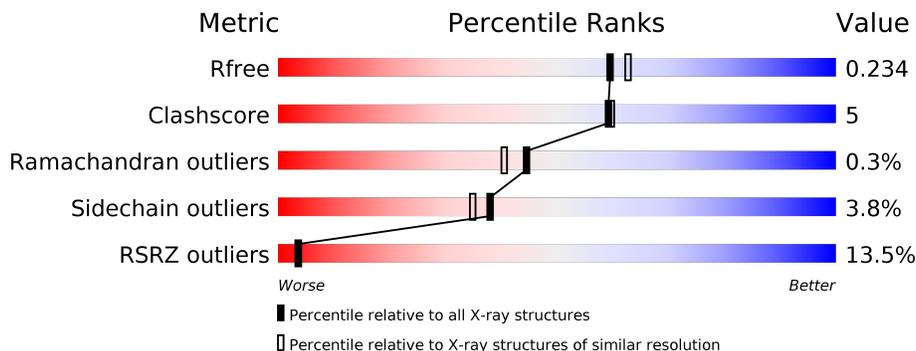
1 Overall quality at a glance

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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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. 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	302	
1	C	302	
2	B	260	
2	D	260	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9155 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	294	Total	C	N	O	P	S	0	5	0
			2391	1552	409	421	1	8			
1	C	269	Total	C	N	O	P	S	0	3	0
			2166	1405	368	385	1	7			

There are 10 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
A	89	THR	LYS	ENGINEERED MUTATION	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
C	89	THR	LYS	ENGINEERED MUTATION	UNP P24941

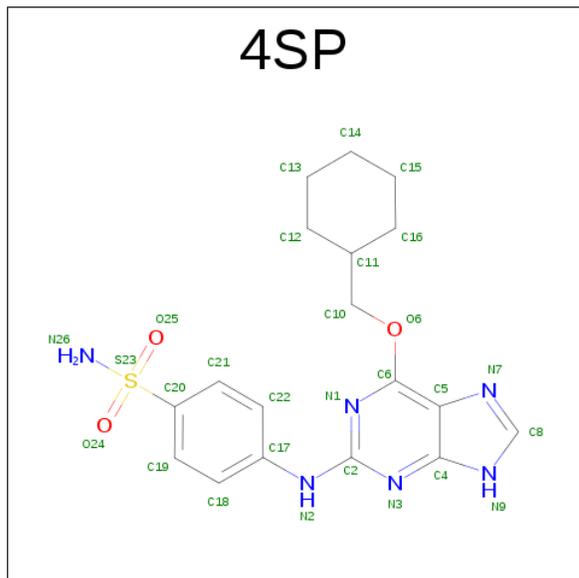
- Molecule 2 is a protein called CYCLIN-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	255	Total	C	N	O	S	0	4	0
			2076	1347	336	381	12			
2	D	255	Total	C	N	O	S	0	1	0
			2068	1340	339	378	11			

There are 2 discrepancies between the modelled and reference sequences:

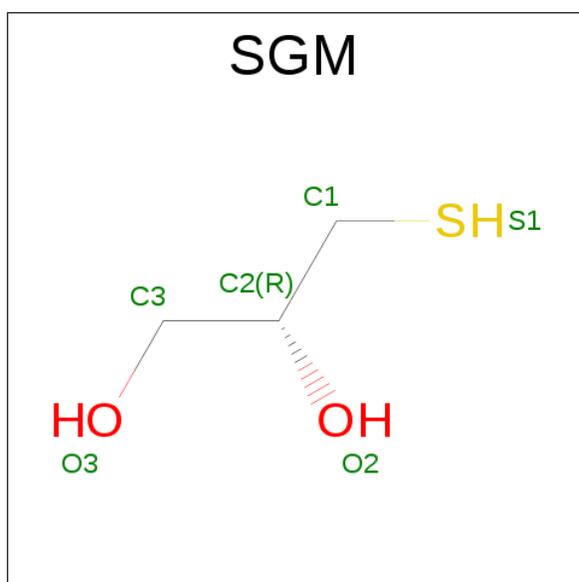
Chain	Residue	Modelled	Actual	Comment	Reference
B	173	MET	-	EXPRESSION TAG	UNP P20248
D	173	MET	-	EXPRESSION TAG	UNP P20248

- Molecule 3 is O6-CYCLOHEXYLMETHOXY-2-(4'-SULPHAMOYLANILINO) PURINE (three-letter code: 4SP) (formula: $C_{18}H_{22}N_6O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
3	A	1	Total	28	18	6	3	1	0	0
3	C	1	Total	28	18	6	3	1	0	0

- Molecule 4 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: $C_3H_8O_2S$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

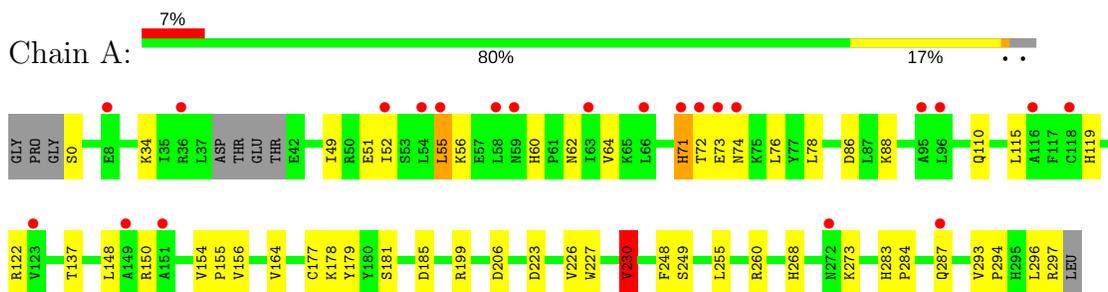
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	171	Total	O	0	0
			171	171		
6	B	122	Total	O	0	0
			122	122		
6	C	49	Total	O	0	0
			49	49		
6	D	42	Total	O	0	0
			42	42		

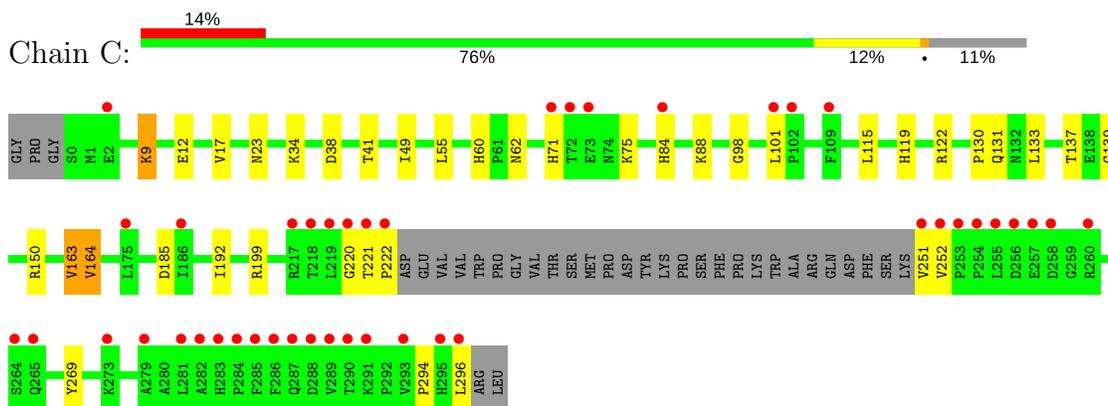
3 Residue-property plots [i](#)

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.

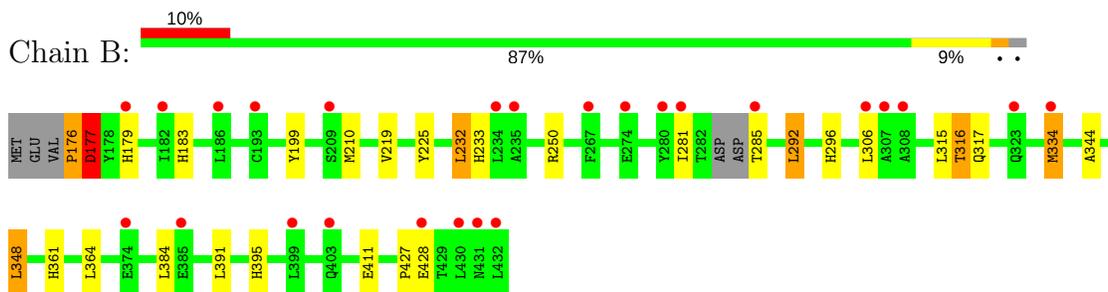
- Molecule 1: CELL DIVISION PROTEIN KINASE 2



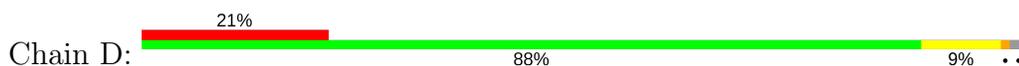
- Molecule 1: CELL DIVISION PROTEIN KINASE 2

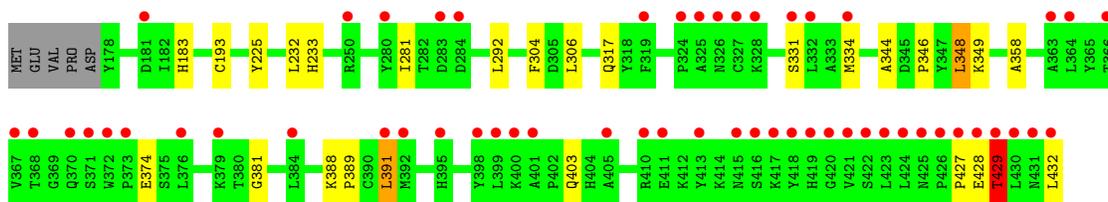


- Molecule 2: CYCLIN-A2



- 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	73.76Å 134.10Å 148.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.00 47.04 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (100.00-2.00) 97.6 (47.04-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.240 0.206 , 0.234	Depositor DCC
R_{free} test set	4861 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	32.0	Xtrriage
Anisotropy	0.332	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.7	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	9155	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 4SP

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	0.60	0/2462	0.70	2/3339 (0.1%)
1	C	0.44	0/2217	0.58	0/3006
2	B	0.54	0/2141	0.60	1/2903 (0.0%)
2	D	0.86	7/2121 (0.3%)	0.61	1/2878 (0.0%)
All	All	0.62	7/8941 (0.1%)	0.63	4/12126 (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
2	B	0	2
2	D	0	1
All	All	0	3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	374	GLU	CD-OE1	18.38	1.45	1.25
2	D	374	GLU	CD-OE2	18.13	1.45	1.25
2	D	429	THR	C-O	13.29	1.48	1.23
2	D	429	THR	C-N	8.42	1.53	1.34
2	D	403	GLN	CD-OE1	6.74	1.38	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	374	GLU	OE1-CD-OE2	9.90	135.18	123.30
1	A	230	VAL	CB-CA-C	-6.00	100.01	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ARG	NE-CZ-NH2	-5.27	117.67	120.30
2	B	364	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	176	PRO	Peptide
2	B	177	ASP	Peptide
2	D	429	THR	Mainchain

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	2391	0	2424	38	0
1	C	2166	0	2217	25	0
2	B	2076	0	2099	27	0
2	D	2068	0	2096	12	0
3	A	28	0	22	2	0
3	C	28	0	22	1	0
4	B	6	0	7	0	0
4	D	6	0	8	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	171	0	0	3	0
6	B	122	0	0	4	0
6	C	49	0	0	1	0
6	D	42	0	0	2	0
All	All	9155	0	8895	95	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 5.

The worst 5 of 95 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:D:193:CYS:SG	4:D:1433:SGM:S1	2.54	0.91
1:A:154:VAL:O	2:B:316:THR:HG22	1.75	0.86
1:A:137:THR:O	1:A:293:VAL:HG13	1.80	0.82
1:A:227:TRP:O	1:A:230:VAL:HG22	1.85	0.77
1:A:268[B]:HIS:CD2	1:A:273:LYS:HB2	2.21	0.76

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	294/302 (97%)	289 (98%)	4 (1%)	1 (0%)	44	40
1	C	267/302 (88%)	259 (97%)	7 (3%)	1 (0%)	38	33
2	B	255/260 (98%)	251 (98%)	3 (1%)	1 (0%)	38	33
2	D	254/260 (98%)	252 (99%)	2 (1%)	0	100	100
All	All	1070/1124 (95%)	1051 (98%)	16 (2%)	3 (0%)	44	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	A	164	VAL
2	B	177	ASP

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	263/264 (100%)	249 (95%)	14 (5%)	26	21
1	C	238/264 (90%)	231 (97%)	7 (3%)	48	47
2	B	233/234 (100%)	220 (94%)	13 (6%)	25	19
2	D	230/234 (98%)	225 (98%)	5 (2%)	57	60
All	All	964/996 (97%)	925 (96%)	39 (4%)	38	32

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	285	THR
2	B	334[B]	MET
2	D	348	LEU
2	B	292	LEU
2	B	316	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	425	ASN
1	C	84	HIS
2	D	395	HIS
1	C	60	HIS
1	C	62	ASN

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	9,10,11	0.77	0	10,14,16	1.03	1 (10%)
1	TPO	C	160	1	9,10,11	0.89	0	10,14,16	1.09	1 (10%)

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	-	0/8/11/13	0/0/0/0
1	TPO	C	160	1	-	0/8/11/13	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	160	TPO	O-C-CA	-2.26	119.88	125.15
1	C	160	TPO	O-C-CA	-2.10	120.24	125.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	4SP	A	1298	-	28,31,31	2.03	5 (17%)	35,44,44	1.78	6 (17%)
4	SGM	B	1433	-	5,5,5	0.63	0	5,5,5	0.84	0
3	4SP	C	1297	-	28,31,31	1.97	5 (17%)	35,44,44	2.28	13 (37%)
4	SGM	D	1433	-	5,5,5	0.40	0	5,5,5	0.42	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	4SP	A	1298	-	-	0/15/23/23	0/4/4/4
4	SGM	B	1433	-	-	0/4/4/4	0/0/0/0
3	4SP	C	1297	-	-	0/15/23/23	0/4/4/4
4	SGM	D	1433	-	-	0/4/4/4	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1298	4SP	C20-S23	-8.41	1.62	1.77
3	C	1297	4SP	C20-S23	-7.82	1.63	1.77
3	A	1298	4SP	S23-N26	-3.74	1.52	1.60
3	C	1297	4SP	S23-N26	-3.51	1.53	1.60
3	A	1298	4SP	O24-S23	2.04	1.48	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1297	4SP	O25-S23-O24	-6.39	106.98	118.70
3	A	1298	4SP	O25-S23-O24	-4.48	110.47	118.70
3	C	1297	4SP	N3-C2-N1	-4.12	119.99	126.23
3	A	1298	4SP	N3-C2-N1	-3.41	121.07	126.23
3	A	1298	4SP	C15-C16-C11	-3.25	106.24	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1298	4SP	2	0
3	C	1297	4SP	1	0
4	D	1433	SGM	1	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	293/302 (97%)	0.76	22 (7%) 15 15	29, 35, 45, 51	5 (1%)
1	C	268/302 (88%)	1.02	43 (16%) 2 2	27, 35, 43, 47	3 (1%)
2	B	255/260 (98%)	0.79	25 (9%) 8 8	30, 35, 43, 51	4 (1%)
2	D	255/260 (98%)	1.21	55 (21%) 1 1	30, 36, 43, 50	1 (0%)
All	All	1071/1124 (95%)	0.94	145 (13%) 3 3	27, 35, 44, 51	13 (1%)

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	432	LEU	14.4
2	D	367	VAL	10.8
2	D	423	LEU	8.4
1	C	287	GLN	7.9
2	D	324	PRO	6.9

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	TPO	A	160	11/12	0.98	0.13	-	29,33,35,36	0
1	TPO	C	160	11/12	0.94	0.12	-	28,32,35,35	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	SGM	D	1433	6/6	0.77	0.19	1.63	66,67,68,69	0
5	MG	B	1434	1/1	0.92	0.19	1.10	43,43,43,43	0
5	MG	D	1434	1/1	0.92	0.15	0.25	38,38,38,38	0
3	4SP	C	1297	28/28	0.92	0.14	-0.13	33,35,39,40	0
3	4SP	A	1298	28/28	0.96	0.14	-0.36	35,38,45,45	0
4	SGM	B	1433	6/6	0.94	0.14	-3.51	45,52,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.