



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 25, 2024 – 03:48 PM EST

PDB ID : 1Z7S  
Title : The crystal structure of coxsackievirus A21  
Authors : Xiao, C.; Bator-Kelly, C.M.; Rieder, E.; Chipman, P.R.; Craig, A.; Kuhn, R.J.; Wimmer, E.; Rossmann, M.G.  
Deposited on : 2005-03-28  
Resolution : 3.20 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

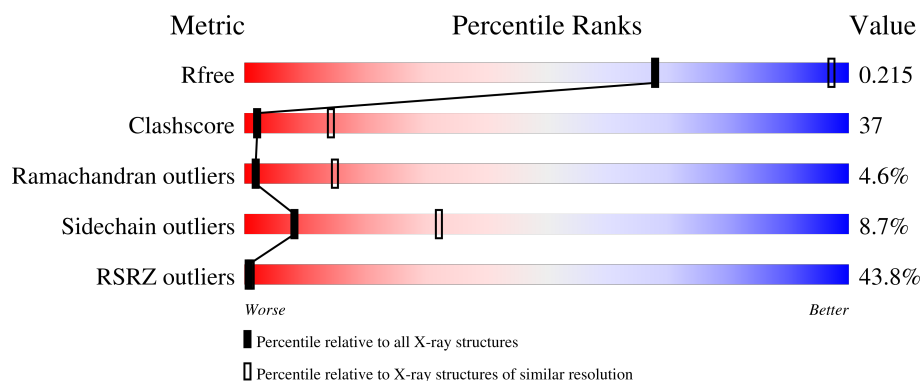
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	1	298	<div> <div>43%</div> <div>38%</div> <div>52%</div> <div>5%</div> <div>5%</div> </div>
2	2	272	<div> <div>44%</div> <div>44%</div> <div>49%</div> <div>5%</div> <div>••</div> </div>
3	3	240	<div> <div>39%</div> <div>42%</div> <div>48%</div> <div>9%</div> </div>
4	4	68	<div> <div>49%</div> <div>49%</div> <div>38%</div> <div>10%</div> <div>•</div> </div>

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
6	MYR	1	300	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6765 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 Human COXSACKIEVIRUS A21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	283	Total	C	N	O	S	0	0	0
			2229	1411	380	428	10			

- Molecule 2 is a protein called Human COXSACKIEVIRUS A21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	267	Total	C	N	O	S	0	0	0
			2069	1314	349	394	12			

- Molecule 3 is a protein called Human coxsackievirus A21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	239	Total	C	N	O	S	0	0	0
			1846	1178	305	343	20			

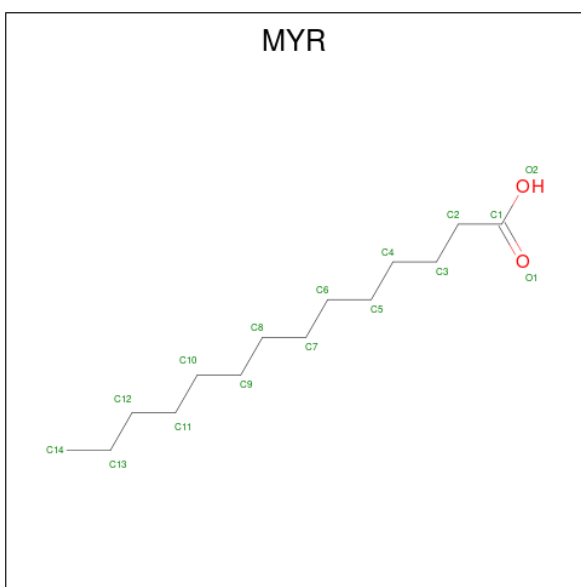
- Molecule 4 is a protein called Human coxsackievirus A21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	68	Total	C	N	O	S	0	0	0
			513	311	90	111	1			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

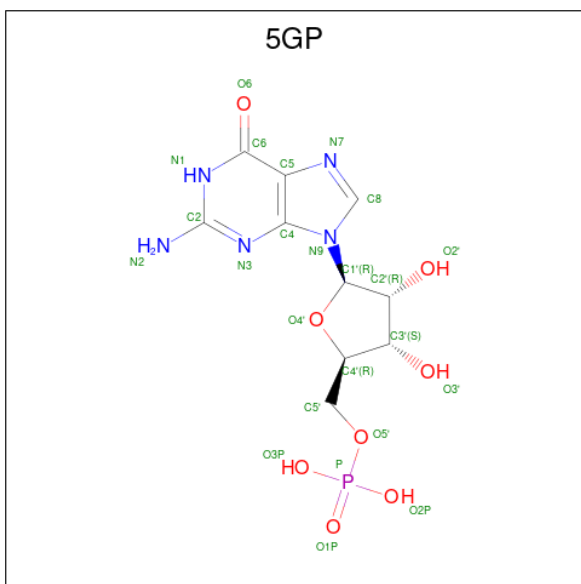
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1	1	Total	Ca	0	0
			1	1		

- Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	1	1	Total	C	O	0	0
			16	14	2		
6	4	1	Total	C	O	0	0
			15	14	1		

- Molecule 7 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula:  $C_{10}H_{14}N_5O_8P$ ).

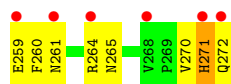


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	2	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

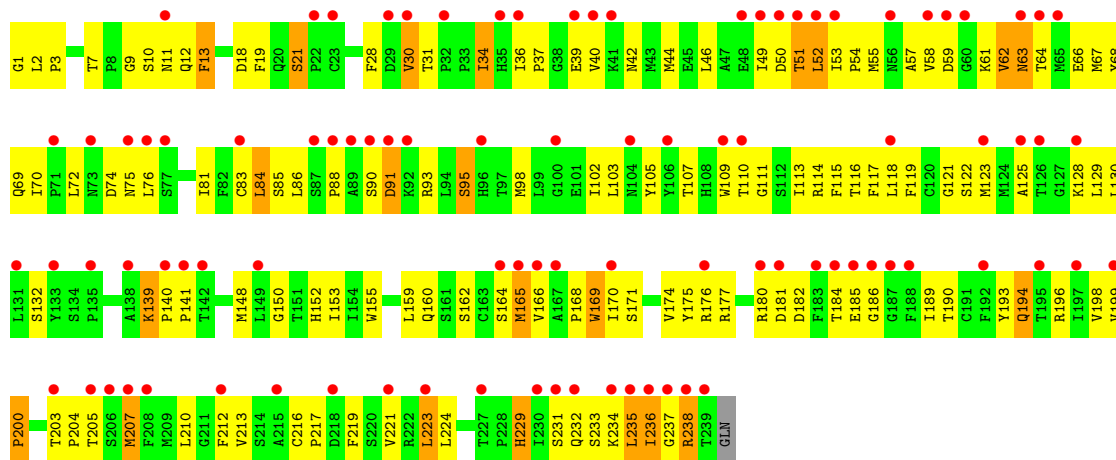
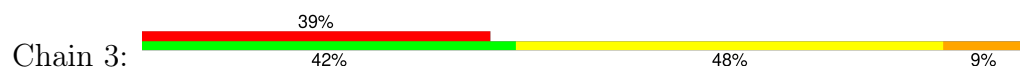
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	1	28	Total 28	O 28	0	0
8	2	9	Total 9	O 9	0	0
8	3	16	Total 16	O 16	0	0

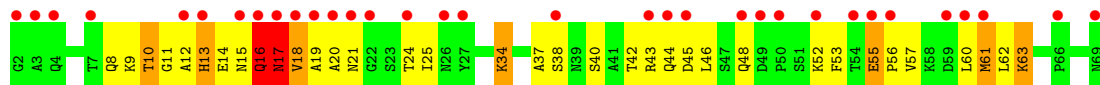




• Molecule 3: Human coxsackievirus A21



• Molecule 4: Human coxsackievirus A21



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	348.01Å 348.01Å 348.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 3.20 49.72 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (49.72-3.20) 94.3 (49.72-3.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.81 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.235 0.203 , 0.215	Depositor DCC
$R_{free}$ test set	8790 reflections (7.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.34	EDS
Total number of atoms	6765	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 5GP, CA, MYR

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	1	0.39	0/2291	0.66	0/3124
2	2	0.41	0/2126	0.68	0/2908
3	3	0.41	0/1895	0.69	0/2579
4	4	0.45	0/520	0.71	1/705 (0.1%)
All	All	0.40	0/6832	0.68	1/9316 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	16	GLN	N-CA-C	-5.39	96.45	111.00

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	1	2229	0	2148	209	0
2	2	2069	0	1988	149	0
3	3	1846	0	1836	166	0
4	4	513	0	493	47	0
5	1	1	0	0	0	0
6	1	16	0	27	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	4	15	0	27	0	0
7	2	23	0	12	0	0
8	1	28	0	0	2	0
8	2	9	0	0	0	0
8	3	16	0	0	1	0
All	All	6765	0	6531	485	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 37.

The worst 5 of 485 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)
1:1:275:ARG:HD3	1:1:282:ILE:HG22	1.28	1.07
4:4:11:GLY:H	4:4:14:GLU:HG3	1.20	1.04
1:1:110:THR:HA	3:3:232:GLN:HE22	1.18	1.04
4:4:34:LYS:H	4:4:34:LYS:HD2	1.14	1.03
3:3:61:LYS:O	3:3:64:THR:HG22	1.60	1.01

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	1	281/298 (94%)	233 (83%)	36 (13%)	12 (4%)	2	16
2	2	265/272 (97%)	226 (85%)	28 (11%)	11 (4%)	2	17
3	3	237/240 (99%)	203 (86%)	24 (10%)	10 (4%)	2	17
4	4	66/68 (97%)	52 (79%)	8 (12%)	6 (9%)	0	3
All	All	849/878 (97%)	714 (84%)	96 (11%)	39 (5%)	2	15

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	168	TYR
1	1	280	ASP
2	2	176	ALA
2	2	241	ALA
3	3	236	ILE

### 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	1	249/261 (95%)	233 (94%)	16 (6%)	14	46
2	2	225/230 (98%)	204 (91%)	21 (9%)	7	29
3	3	212/213 (100%)	192 (91%)	20 (9%)	7	28
4	4	57/57 (100%)	49 (86%)	8 (14%)	3	14
All	All	743/761 (98%)	678 (91%)	65 (9%)	8	32

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	10	THR
4	4	16	GLN
2	2	126	LEU
2	2	100	TYR
4	4	17	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	261	ASN
4	4	48	GLN
3	3	152	HIS
4	4	26	ASN
3	3	108	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z  > 2$
6	MYR	1	300	-	15,15,15	0.68	0	15,15,15	0.71	0
7	5GP	2	273	-	18,25,26	1.09	2 (11%)	17,37,40	0.76	1 (5%)
6	MYR	4	1	4	13,14,15	0.39	0	12,13,15	0.48	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
6	MYR	1	300	-	-	7/13/13/13	-
7	5GP	2	273	-	-	0/3/25/26	0/3/3/3
6	MYR	4	1	4	-	5/12/12/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2	273	5GP	C8-N7	-2.52	1.30	1.34
7	2	273	5GP	C5-C6	-2.37	1.42	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	2	273	5GP	O6-C6-C5	2.21	128.71	124.32

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

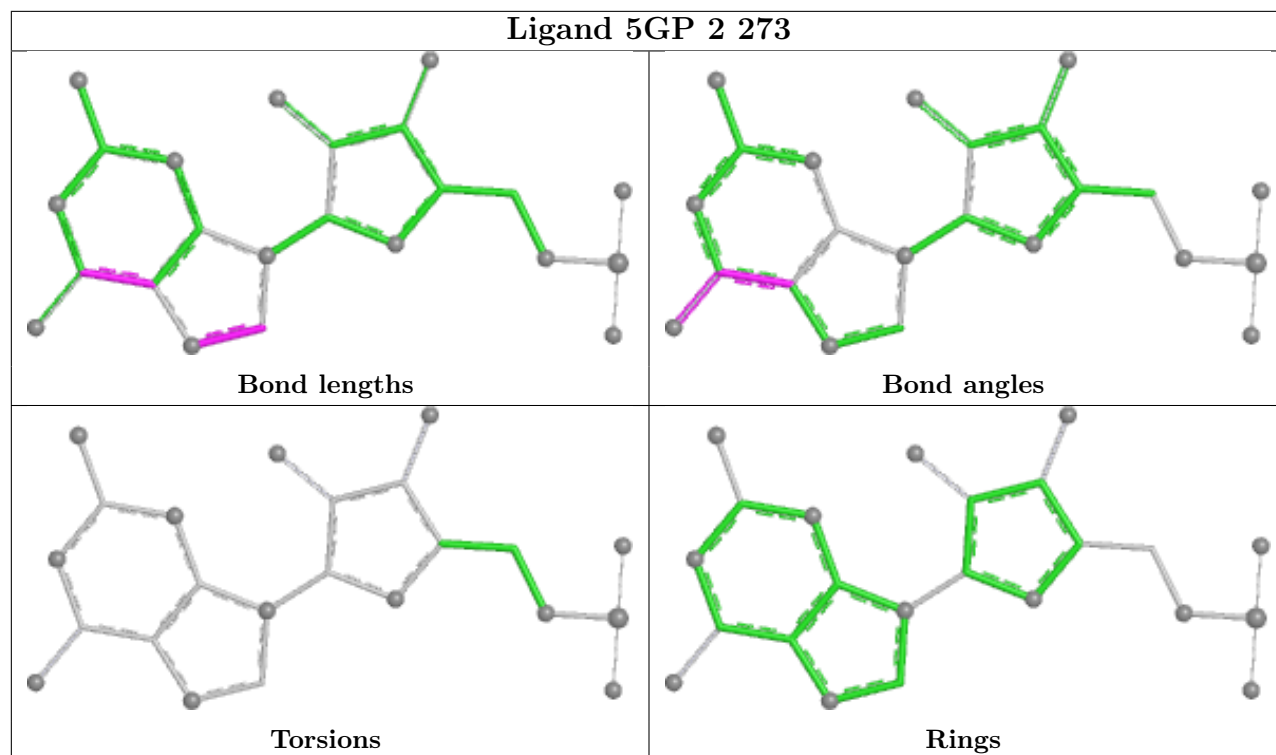
Mol	Chain	Res	Type	Atoms
6	4	1	MYR	O1-C1-C2-C3
6	1	300	MYR	C1-C2-C3-C4
6	1	300	MYR	C4-C5-C6-C7
6	4	1	MYR	C4-C5-C6-C7
6	1	300	MYR	C6-C7-C8-C9

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	300	MYR	12	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 ⓘ

**Warning:** The R factor obtained from EDS is 0.4914, which does not match the depositor's R factor of 0.224. Please interpret the results in this section carefully.

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1	283/298 (94%)	2.19	129 (45%) 1 1	5, 51, 91, 105	4 (1%)
2	2	267/272 (98%)	2.09	120 (44%) 1 1	32, 46, 79, 119	0
3	3	239/240 (99%)	1.80	93 (38%) 1 1	32, 44, 69, 135	0
4	4	68/68 (100%)	2.34	33 (48%) 0 1	32, 50, 93, 108	0
All	All	857/878 (97%)	2.06	375 (43%) 1 1	5, 47, 86, 135	4 (0%)

The worst 5 of 375 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	4	17	ASN	11.8
4	4	2	GLY	9.7
1	1	287	LEU	8.9
1	1	274	TYR	8.0
1	1	277	GLU	7.7

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

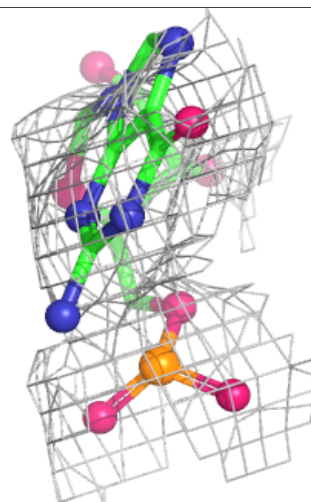
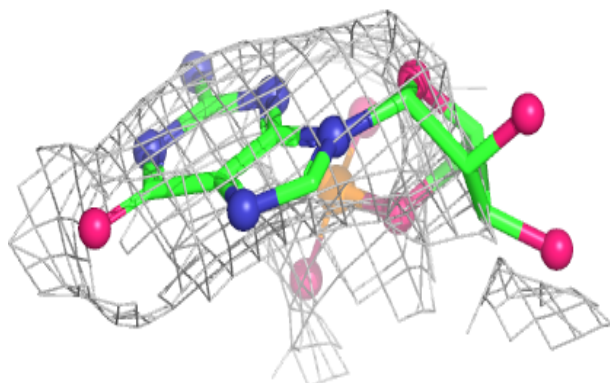
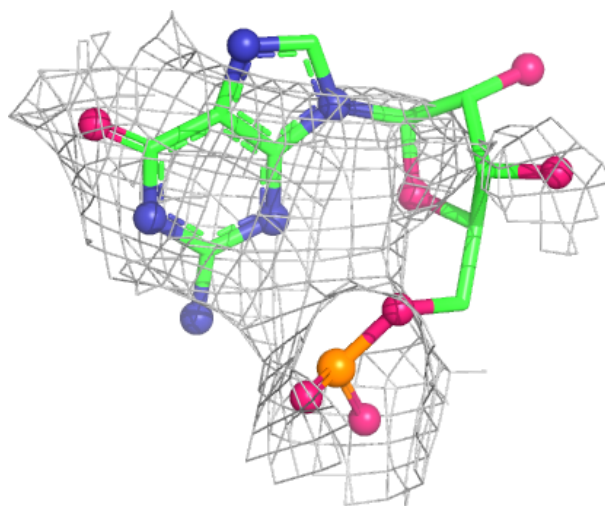
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	5GP	2	273	23/24	0.66	0.45	94,98,113,114	23
6	MYR	4	1	15/16	0.76	0.39	58,70,82,83	0
6	MYR	1	300	16/16	0.84	0.28	36,41,71,72	0
5	CA	1	299	1/1	0.86	0.09	58,58,58,58	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 5GP 2 273:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.