Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 08:21 PM EDT

PDB ID	:	6OH4
Title	:	X-ray crystal structure of the mouse CMP-sialic acid transporter in complex with CMP, by hanging drop vapor diffusion
Authors	:	Ahuja, S.; Whorton, M.R.
Deposited on	:	2019-04-04
Resolution	:	3.38 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 (i) 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 (i)) were used in the production of this report:

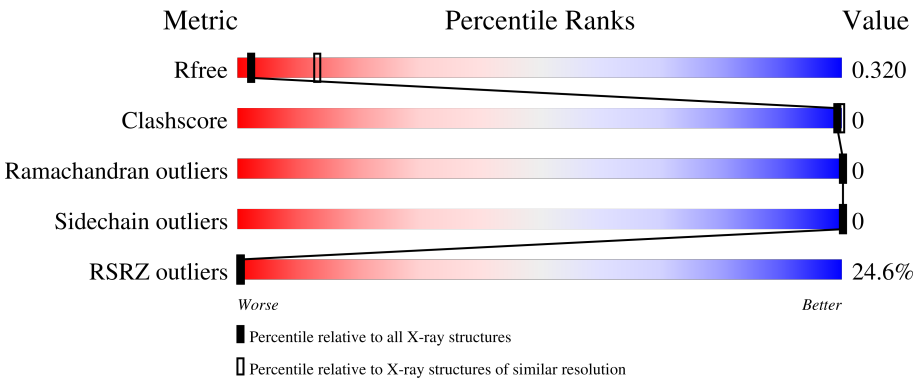
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.38 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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	345	21% 86% • 13%
1	B	345	21% 86% • 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4502 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.

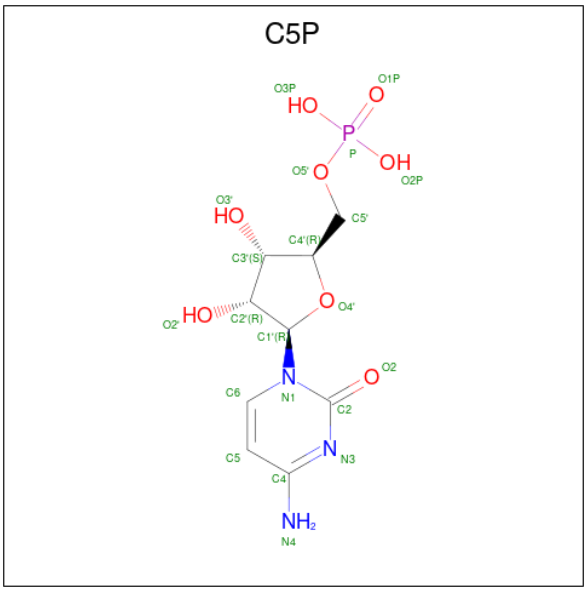
- Molecule 1 is a protein called CMP-sialic acid transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	299	2232	1478	346	395	13	0	0	0
1	B	299	2228	1476	345	394	13	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	SER	-	expression tag	UNP Q61420
A	338	ASN	-	expression tag	UNP Q61420
A	339	SER	-	expression tag	UNP Q61420
A	340	LEU	-	expression tag	UNP Q61420
A	341	GLU	-	expression tag	UNP Q61420
A	342	VAL	-	expression tag	UNP Q61420
A	343	LEU	-	expression tag	UNP Q61420
A	344	PHE	-	expression tag	UNP Q61420
A	345	GLN	-	expression tag	UNP Q61420
B	337	SER	-	expression tag	UNP Q61420
B	338	ASN	-	expression tag	UNP Q61420
B	339	SER	-	expression tag	UNP Q61420
B	340	LEU	-	expression tag	UNP Q61420
B	341	GLU	-	expression tag	UNP Q61420
B	342	VAL	-	expression tag	UNP Q61420
B	343	LEU	-	expression tag	UNP Q61420
B	344	PHE	-	expression tag	UNP Q61420
B	345	GLN	-	expression tag	UNP Q61420

- Molecule 2 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C5P) (formula: $C_9H_{14}N_3O_8P$) (labeled as "Ligand of Interest" by depositor).



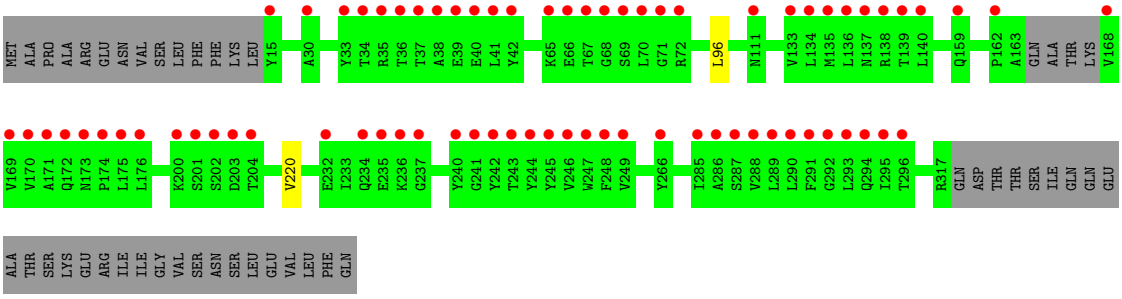
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	21	9	3	8	1	0	0
			Total	C	N	O	P		
2	B	1	21	9	3	8	1	0	0

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.

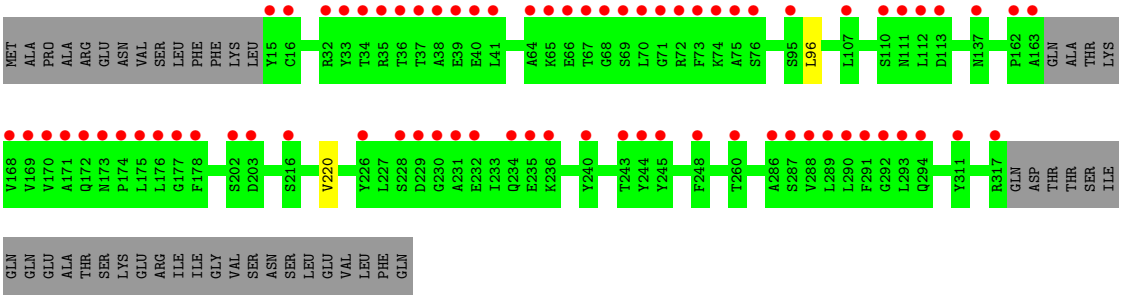
• Molecule 1: CMP-sialic acid transporter

Chain A:



• Molecule 1: CMP-sialic acid transporter

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.82Å 193.96Å 66.44Å 90.00° 101.79° 90.00°	Depositor
Resolution (Å)	49.00 – 3.38 49.08 – 3.38	Depositor EDS
% Data completeness (in resolution range)	67.2 (49.00-3.38) 67.2 (49.08-3.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.289 , 0.321 0.294 , 0.320	Depositor DCC
R_{free} test set	573 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	136.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 96.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	4502	wwPDB-VP
Average B, all atoms (Å^2)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: C5P

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	0.39	0/2275	0.47	0/3105
1	B	0.38	0/2271	0.47	0/3100
All	All	0.39	0/4546	0.47	0/6205

There are no bond length outliers.

There are no bond angle outliers.

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	2232	0	2312	1	0
1	B	2228	0	2306	1	0
2	A	21	0	12	0	0
2	B	21	0	12	0	0
All	All	4502	0	4642	2	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 0.

All (2) 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:96:LEU:HA	1:A:220:VAL:HG11	1.97	0.47
1:B:96:LEU:HA	1:B:220:VAL:HG11	1.97	0.46

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	295/345 (86%)	290 (98%)	5 (2%)	0	100	100
1	B	295/345 (86%)	290 (98%)	5 (2%)	0	100	100
All	All	590/690 (86%)	580 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	236/288 (82%)	236 (100%)	0	100	100
1	B	235/288 (82%)	235 (100%)	0	100	100
All	All	471/576 (82%)	471 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	B	172	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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	$\#\|Z\| > 2$
2	C5P	B	401	-	22,22,22	0.77	0	32,33,33	1.01	1 (3%)
2	C5P	A	401	-	22,22,22	0.78	0	32,33,33	0.96	1 (3%)

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
2	C5P	B	401	-	-	2/10/26/26	0/2/2/2
2	C5P	A	401	-	-	2/10/26/26	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})
2	B	401	C5P	O2-C2-N3	-2.60	118.24	122.33
2	A	401	C5P	O2-C2-N3	-2.54	118.33	122.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

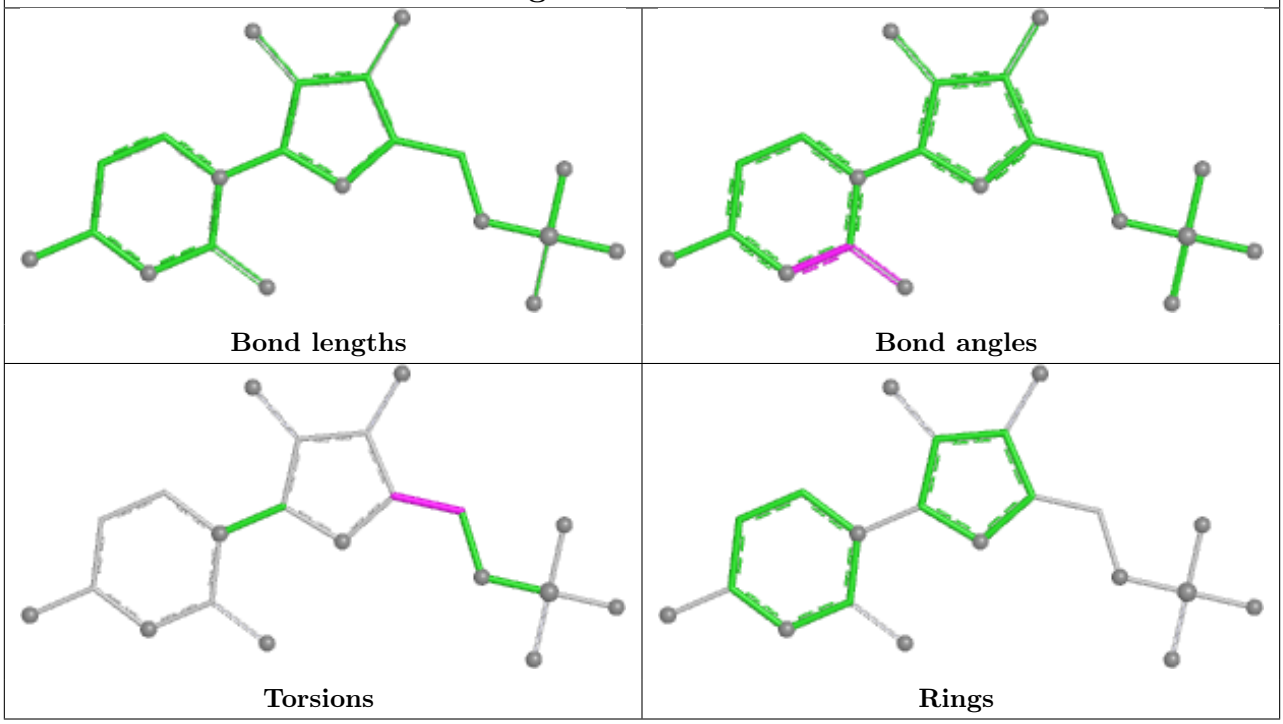
Mol	Chain	Res	Type	Atoms
2	A	401	C5P	O4'-C4'-C5'-O5'
2	A	401	C5P	C3'-C4'-C5'-O5'
2	B	401	C5P	O4'-C4'-C5'-O5'
2	B	401	C5P	C3'-C4'-C5'-O5'

There are no ring outliers.

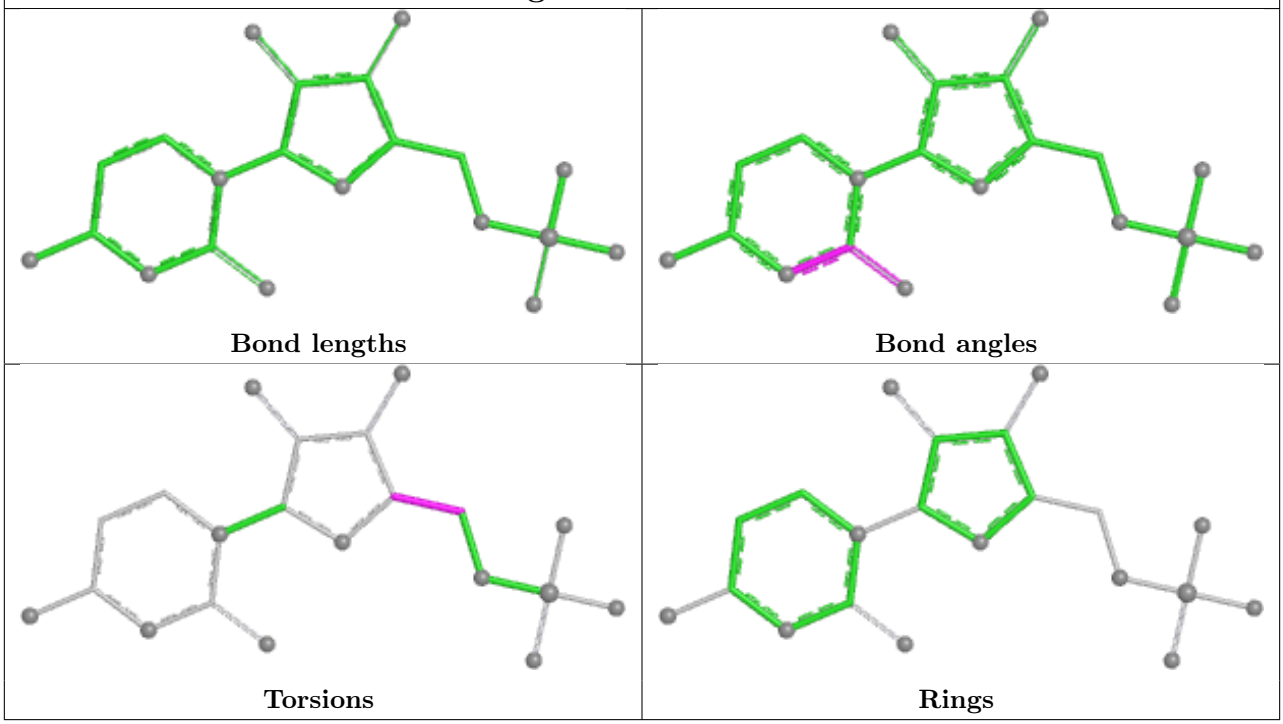
No monomer is involved in short contacts.

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 C5P B 401



Ligand C5P A 401



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	299/345 (86%)	1.28	73 (24%)	0	0	97, 146, 201, 236	0
1	B	299/345 (86%)	1.47	74 (24%)	0	0	105, 145, 199, 232	0
All	All	598/690 (86%)	1.37	147 (24%)	0	0	97, 146, 201, 236	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	VAL	19.6
1	B	38	ALA	15.6
1	B	169	VAL	15.3
1	B	39	GLU	14.9
1	B	68	GLY	13.2
1	A	168	VAL	12.8
1	B	40	GLU	12.5
1	B	170	VAL	12.4
1	B	172	GLN	11.5
1	A	38	ALA	11.4
1	A	172	GLN	11.4
1	B	72	ARG	10.8
1	B	70	LEU	10.8
1	B	69	SER	10.7
1	A	245	TYR	10.3
1	B	236	LYS	10.2
1	A	68	GLY	9.6
1	A	69	SER	9.6
1	A	39	GLU	9.3
1	B	175	LEU	9.2
1	A	243	THR	9.1
1	A	203	ASP	9.0
1	A	171	ALA	8.9
1	B	37	THR	8.9

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Mol	Chain	Res	Type	RSRZ
1	B	36	THR	8.8
1	A	169	VAL	8.6
1	A	170	VAL	8.5
1	B	71	GLY	8.5
1	B	67	THR	8.0
1	B	173	ASN	8.0
1	B	171	ALA	7.9
1	A	248	PHE	7.6
1	B	176	LEU	7.6
1	A	36	THR	7.5
1	A	72	ARG	7.3
1	A	244	TYR	7.3
1	A	37	THR	7.2
1	A	173	ASN	7.2
1	B	111	ASN	7.1
1	A	294	GLN	7.1
1	B	232	GLU	7.0
1	A	70	LEU	6.9
1	A	236	LYS	6.9
1	B	174	PRO	6.9
1	B	230	GLY	6.6
1	A	202	SER	6.6
1	A	247	TRP	6.5
1	B	41	LEU	6.4
1	A	174	PRO	6.4
1	A	201	SER	6.3
1	B	203	ASP	6.1
1	A	67	THR	6.1
1	B	235	GLU	6.1
1	B	245	TYR	6.0
1	A	176	LEU	6.0
1	B	162	PRO	5.8
1	B	15	TYR	5.7
1	A	292	GLY	5.5
1	B	16	CYS	5.5
1	A	65	LYS	5.5
1	A	137	ASN	5.5
1	A	291	PHE	5.4
1	A	241	GLY	5.4
1	A	41	LEU	5.2
1	A	293	LEU	5.2
1	A	295	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	65	LYS	5.1
1	B	74	LYS	5.0
1	A	34	THR	4.9
1	B	113	ASP	4.9
1	A	242	TYR	4.8
1	B	75	ALA	4.8
1	B	163	ALA	4.8
1	A	246	VAL	4.7
1	A	71	GLY	4.7
1	A	40	GLU	4.6
1	B	137	ASN	4.6
1	B	231	ALA	4.6
1	B	112	LEU	4.4
1	B	73	PHE	4.4
1	B	178	PHE	4.4
1	B	110	SER	4.3
1	A	139	THR	4.2
1	B	243	THR	4.2
1	A	266	TYR	4.1
1	B	202	SER	4.0
1	A	287	SER	4.0
1	B	291	PHE	3.9
1	A	175	LEU	3.9
1	B	64	ALA	3.9
1	A	235	GLU	3.8
1	A	237	GLY	3.7
1	A	33	TYR	3.7
1	B	244	TYR	3.6
1	A	35	ARG	3.5
1	B	240	TYR	3.4
1	A	288	VAL	3.4
1	A	138	ARG	3.3
1	A	162	PRO	3.3
1	A	134	LEU	3.3
1	A	240	TYR	3.3
1	B	177	GLY	3.2
1	A	290	LEU	3.2
1	A	232	GLU	3.2
1	B	260	THR	3.2
1	A	111	ASN	3.1
1	A	286	ALA	3.1
1	B	226	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	249	VAL	3.0
1	B	34	THR	3.0
1	A	15	TYR	3.0
1	B	292	GLY	2.9
1	A	42	TYR	2.9
1	B	33	TYR	2.9
1	A	30	ALA	2.9
1	B	66	GLU	2.9
1	A	285	ILE	2.8
1	B	234	GLN	2.8
1	B	289	LEU	2.8
1	B	107	LEU	2.8
1	B	293	LEU	2.8
1	B	35	ARG	2.8
1	A	140	LEU	2.7
1	B	311	TYR	2.7
1	B	290	LEU	2.7
1	B	248	PHE	2.7
1	A	66	GLU	2.5
1	A	133	VAL	2.5
1	B	288	VAL	2.5
1	B	317	ARG	2.4
1	B	287	SER	2.4
1	A	200	LYS	2.4
1	A	135	MET	2.4
1	B	216	SER	2.3
1	A	204	THR	2.3
1	B	228	SER	2.3
1	A	296	THR	2.3
1	A	136	LEU	2.2
1	B	294	GLN	2.2
1	B	95	SER	2.2
1	A	289	LEU	2.2
1	A	159	GLN	2.2
1	B	76	SER	2.1
1	B	286	ALA	2.0
1	B	32	ARG	2.0
1	B	229	ASP	2.0
1	A	234	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

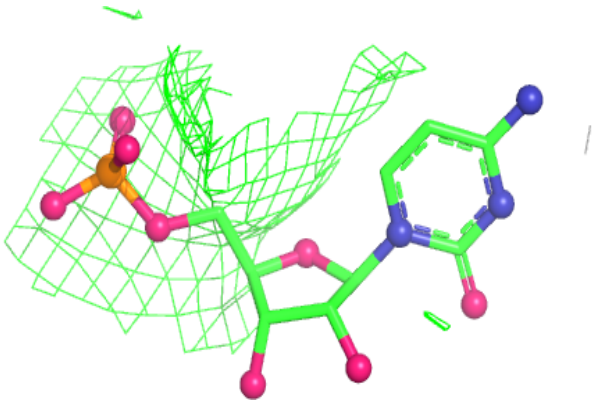
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

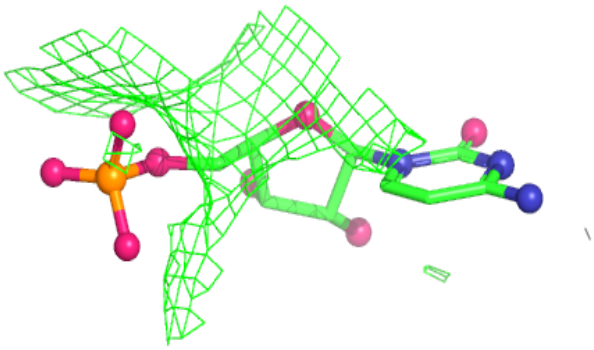
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	C5P	B	401	21/21	0.90	0.44	105,115,131,133	0
2	C5P	A	401	21/21	0.92	0.36	117,125,133,135	0

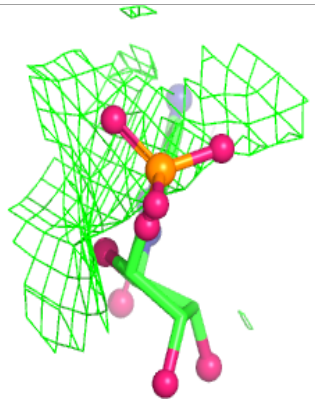
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C5P B 401:

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

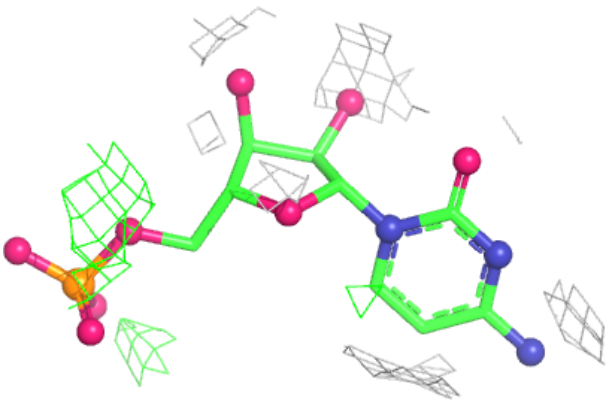


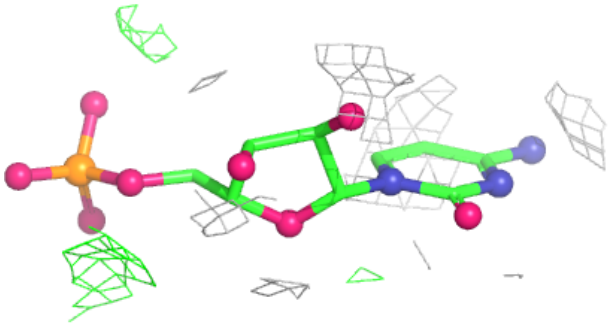


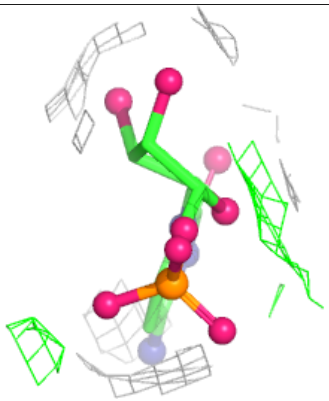


Electron density around C5P A 401:

$2mF_o$-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.