



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:19 AM UTC

PDB ID : 6OH4 / pdb_00006oh4
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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

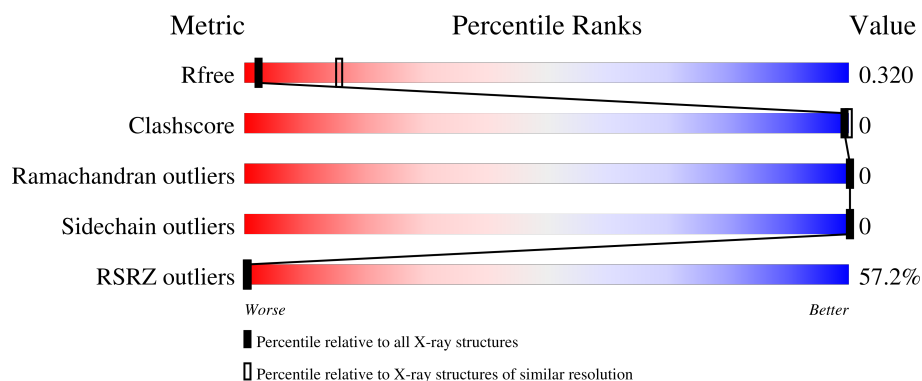
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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}	180053	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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 $\leq 5\%$. 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	345	49% 86% 13%
1	B	345	50% 86% 13%

2 Entry composition

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.

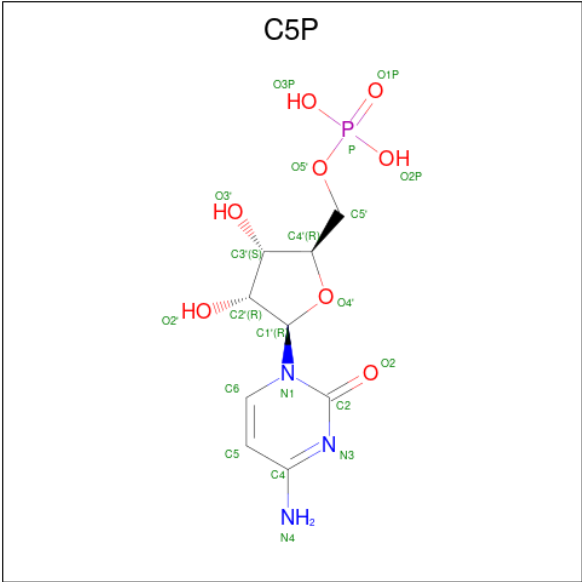
- Molecule 1 is a protein called CMP-sialic acid transporter.

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

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 (CCD ID: C5P) (formula: C₉H₁₄N₃O₈P) (labeled as "Ligand of Interest" by depositor).

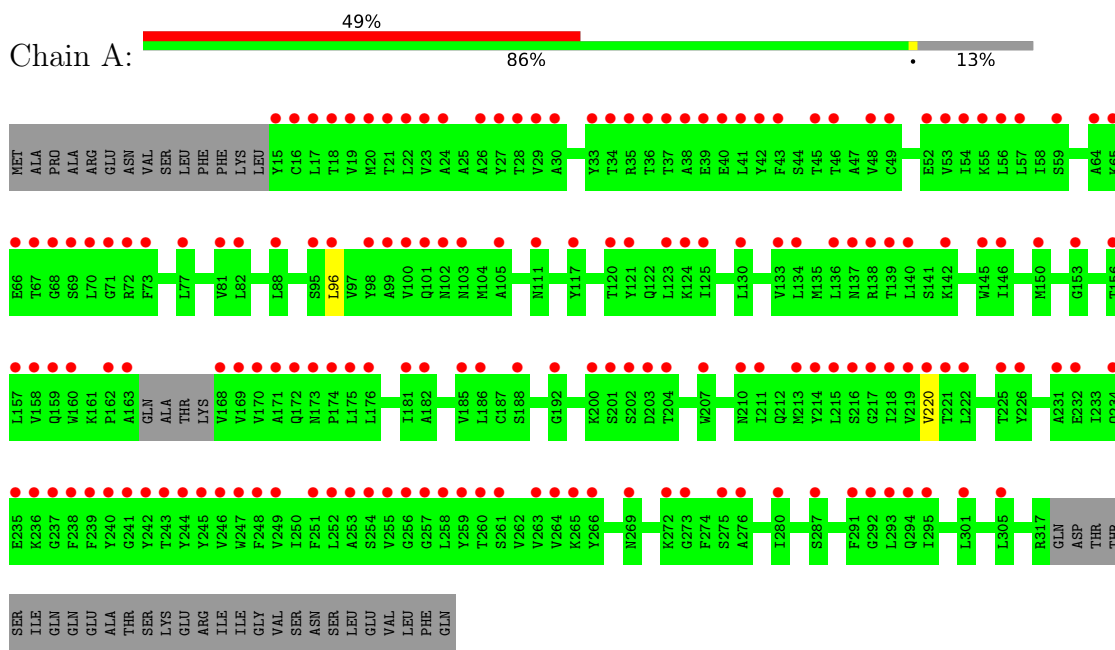


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
2	B	1	Total	C	N	O	P	0	0
			21	9	3	8	1		

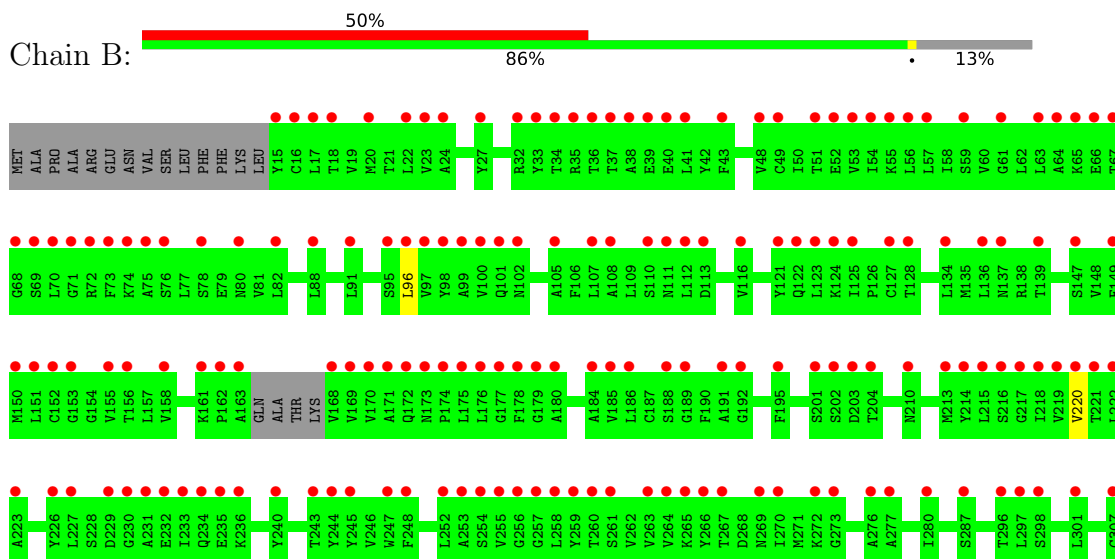
3 Residue-property plots

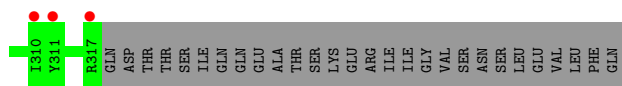
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: CMP-sialic acid transporter





4 Data and refinement statistics

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 49.00 – 3.38	Depositor EDS
% Data completeness (in resolution range)	67.2 (49.00-3.38) 67.2 (49.00-3.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.16 , 11.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	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.*

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

5.1 Standard geometry

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	0.56	0/2275	0.88	0/3105
1	B	0.56	0/2271	0.88	0/3100
All	All	0.56	0/4546	0.88	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

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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	122	GLN
1	A	269	ASN
1	B	111	ASN
1	B	122	GLN
1	B	269	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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(°)	Ideal(°)
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.

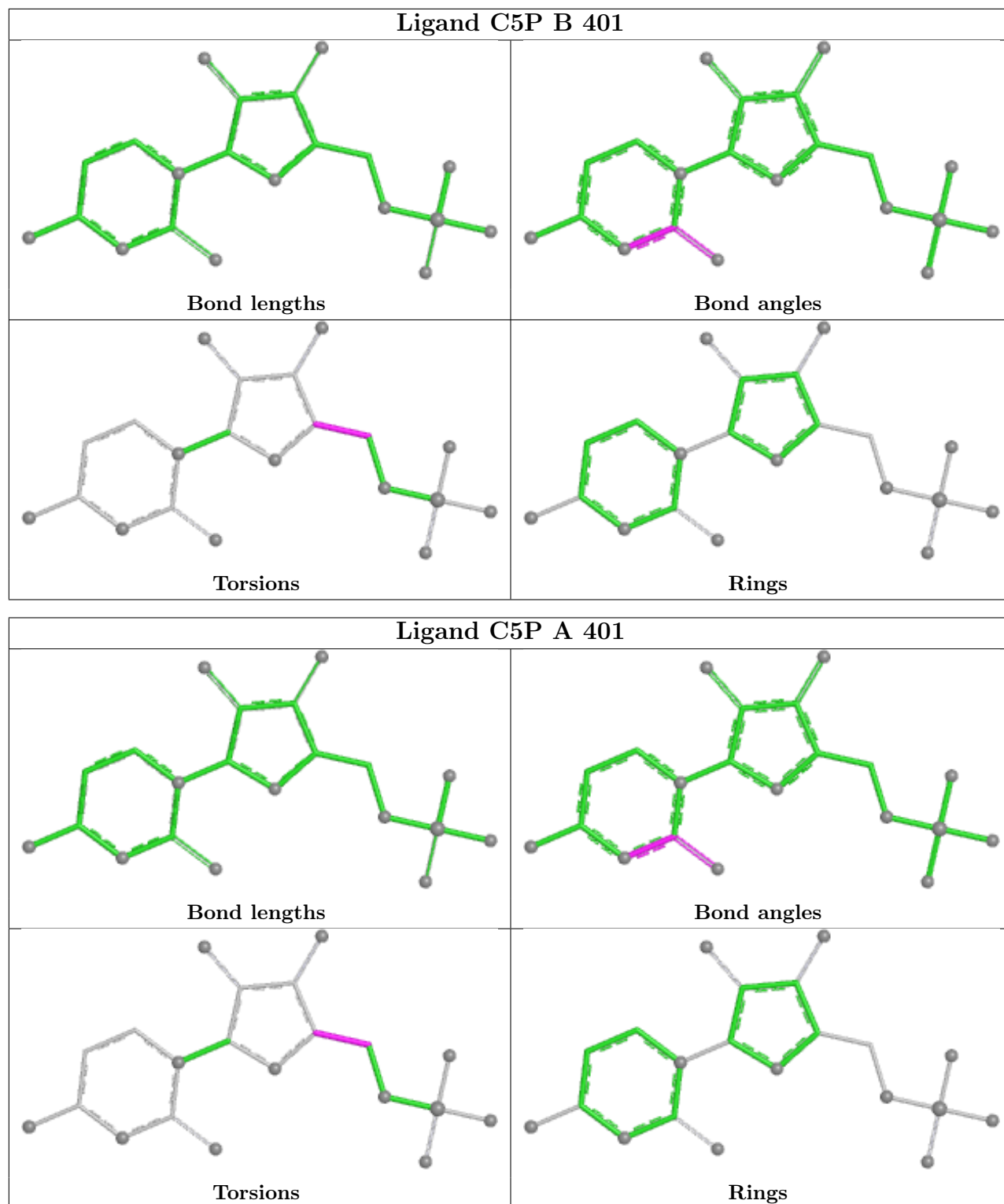
All (4) torsion outliers are listed below:

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 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 ⓘ

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, 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%)	3.49	169 (56%) 0 0	97, 146, 201, 236	0
1	B	299/345 (86%)	4.12	173 (57%) 0 0	105, 145, 199, 232	0
All	All	598/690 (86%)	3.80	342 (57%) 0 0	97, 146, 201, 236	0

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	169	VAL	35.0
1	B	168	VAL	32.8
1	A	245	TYR	28.2
1	B	38	ALA	27.3
1	B	170	VAL	26.1
1	A	171	ALA	21.6
1	A	38	ALA	21.3
1	B	39	GLU	21.3
1	B	70	LEU	20.7
1	A	244	TYR	20.4
1	A	248	PHE	19.9
1	B	175	LEU	19.7
1	A	203	ASP	18.5
1	B	176	LEU	18.2
1	B	171	ALA	17.9
1	A	247	TRP	17.9
1	A	243	THR	17.8
1	B	74	LYS	17.7
1	B	172	GLN	17.4
1	B	174	PRO	16.1
1	B	235	GLU	16.0
1	B	173	ASN	15.4
1	B	71	GLY	15.2
1	B	67	THR	14.9

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Mol	Chain	Res	Type	RSRZ
1	B	245	TYR	14.9
1	B	68	GLY	14.8
1	B	203	ASP	14.6
1	A	170	VAL	13.8
1	A	173	ASN	13.3
1	B	72	ARG	13.0
1	A	69	SER	12.9
1	A	246	VAL	12.8
1	A	169	VAL	12.7
1	A	68	GLY	12.7
1	A	202	SER	12.7
1	B	40	GLU	12.4
1	B	236	LYS	12.4
1	A	172	GLN	12.4
1	B	37	THR	12.3
1	B	111	ASN	12.2
1	B	202	SER	12.0
1	A	70	LEU	11.9
1	A	39	GLU	11.7
1	A	176	LEU	11.5
1	B	65	LYS	11.2
1	B	231	ALA	11.0
1	B	36	THR	10.9
1	A	175	LEU	10.7
1	B	232	GLU	10.6
1	B	69	SER	10.5
1	B	248	PHE	10.2
1	A	235	GLU	10.2
1	A	266	TYR	10.0
1	A	168	VAL	9.8
1	B	178	PHE	9.6
1	B	260	THR	9.5
1	A	34	THR	9.4
1	A	174	PRO	9.4
1	B	110	SER	9.1
1	B	107	LEU	9.0
1	B	311	TYR	8.9
1	B	64	ALA	8.6
1	B	234	GLN	8.6
1	A	33	TYR	8.5
1	A	241	GLY	8.1
1	A	20	MET	8.1

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Mol	Chain	Res	Type	RSRZ
1	B	230	GLY	8.0
1	A	260	THR	7.9
1	A	37	THR	7.9
1	A	72	ARG	7.8
1	B	266	TYR	7.7
1	A	41	LEU	7.7
1	B	272	LYS	7.7
1	B	20	MET	7.6
1	A	236	LYS	7.6
1	A	134	LEU	7.5
1	A	65	LYS	7.5
1	A	272	LYS	7.3
1	A	249	VAL	7.1
1	B	137	ASN	7.1
1	B	52	GLU	7.1
1	A	201	SER	7.0
1	B	125	ILE	7.0
1	A	232	GLU	6.9
1	B	75	ALA	6.9
1	A	231	ALA	6.9
1	B	95	SER	6.8
1	A	242	TYR	6.8
1	B	76	SER	6.8
1	B	41	LEU	6.7
1	A	67	THR	6.7
1	B	16	CYS	6.6
1	B	218	ILE	6.5
1	B	98	TYR	6.4
1	A	40	GLU	6.4
1	B	273	GLY	6.4
1	B	244	TYR	6.4
1	A	137	ASN	6.3
1	B	102	ASN	6.2
1	A	218	ILE	6.2
1	B	112	LEU	6.1
1	B	24	ALA	6.0
1	A	276	ALA	6.0
1	A	102	ASN	5.9
1	B	216	SER	5.9
1	A	36	THR	5.9
1	B	253	ALA	5.9
1	B	188	SER	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	222	LEU	5.8
1	B	257	GLY	5.8
1	B	276	ALA	5.8
1	B	256	GLY	5.8
1	B	33	TYR	5.7
1	B	73	PHE	5.7
1	A	71	GLY	5.6
1	B	80	ASN	5.6
1	A	273	GLY	5.5
1	B	226	TYR	5.4
1	A	256	GLY	5.3
1	A	259	TYR	5.3
1	A	18	THR	5.3
1	B	124	LYS	5.2
1	B	220	VAL	5.2
1	A	17	LEU	5.2
1	A	24	ALA	5.1
1	A	252	LEU	5.1
1	A	257	GLY	5.1
1	B	217	GLY	5.1
1	A	258	LEU	5.1
1	A	216	SER	5.1
1	B	191	ALA	5.1
1	A	52	GLU	5.0
1	A	95	SER	4.9
1	B	27	TYR	4.9
1	A	77	LEU	4.9
1	B	269	ASN	4.9
1	A	22	LEU	4.8
1	B	34	THR	4.8
1	A	42	TYR	4.8
1	A	30	ALA	4.8
1	A	133	VAL	4.8
1	B	227	LEU	4.6
1	B	179	GLY	4.6
1	A	82	LEU	4.6
1	B	240	TYR	4.6
1	A	103	ASN	4.6
1	A	294	GLN	4.6
1	A	188	SER	4.5
1	A	220	VAL	4.5
1	B	63	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	192	GLY	4.5
1	B	213	MET	4.5
1	B	221	THR	4.5
1	A	145	TRP	4.5
1	A	217	GLY	4.4
1	B	113	ASP	4.4
1	A	221	THR	4.4
1	A	57	LEU	4.4
1	B	56	LEU	4.4
1	A	287	SER	4.4
1	B	201	SER	4.4
1	A	219	VAL	4.4
1	A	239	PHE	4.4
1	B	280	ILE	4.4
1	B	53	VAL	4.4
1	B	99	ALA	4.3
1	B	243	THR	4.3
1	B	177	GLY	4.3
1	B	259	TYR	4.3
1	A	96	LEU	4.2
1	A	99	ALA	4.2
1	A	225	THR	4.2
1	B	57	LEU	4.2
1	B	222	LEU	4.2
1	B	258	LEU	4.2
1	B	162	PRO	4.2
1	B	310	ILE	4.2
1	A	27	TYR	4.2
1	B	214	TYR	4.2
1	A	35	ARG	4.2
1	B	161	LYS	4.2
1	B	219	VAL	4.1
1	B	35	ARG	4.1
1	A	253	ALA	4.1
1	B	297	LEU	4.1
1	B	261	SER	4.0
1	B	180	ALA	4.0
1	B	215	LEU	4.0
1	A	139	THR	4.0
1	A	240	TYR	4.0
1	B	66	GLU	4.0
1	A	56	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	280	ILE	3.9
1	B	163	ALA	3.8
1	B	18	THR	3.8
1	A	98	TYR	3.8
1	B	121	TYR	3.8
1	B	82	LEU	3.8
1	A	59	SER	3.8
1	A	160	TRP	3.8
1	B	153	GLY	3.8
1	B	48	VAL	3.7
1	B	15	TYR	3.7
1	B	298	SER	3.7
1	A	66	GLU	3.7
1	A	23	VAL	3.7
1	A	130	LEU	3.6
1	A	293	LEU	3.6
1	B	88	LEU	3.6
1	B	96	LEU	3.6
1	A	124	LYS	3.6
1	B	301	LEU	3.6
1	B	267	THR	3.6
1	A	125	ILE	3.6
1	B	128	THR	3.6
1	A	49	CYS	3.6
1	A	214	TYR	3.6
1	B	247	TRP	3.5
1	A	163	ALA	3.5
1	A	140	LEU	3.5
1	B	185	VAL	3.5
1	B	204	THR	3.5
1	B	101	GLN	3.5
1	A	261	SER	3.5
1	A	146	ILE	3.5
1	A	123	LEU	3.4
1	A	158	VAL	3.4
1	A	234	GLN	3.4
1	B	122	GLN	3.4
1	A	255	VAL	3.4
1	B	55	LYS	3.3
1	A	157	LEU	3.3
1	B	252	LEU	3.3
1	A	153	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	22	LEU	3.3
1	A	48	VAL	3.2
1	B	296	THR	3.2
1	A	29	VAL	3.2
1	B	195	PHE	3.2
1	B	184	ALA	3.2
1	A	263	VAL	3.2
1	A	111	ASN	3.1
1	A	269	ASN	3.0
1	A	215	LEU	3.0
1	B	264	VAL	3.0
1	B	43	PHE	3.0
1	A	186	LEU	3.0
1	B	123	LEU	3.0
1	B	151	LEU	3.0
1	A	251	PHE	3.0
1	A	204	THR	3.0
1	B	139	THR	3.0
1	A	185	VAL	2.9
1	B	317	ARG	2.9
1	A	226	TYR	2.9
1	B	32	ARG	2.9
1	B	229	ASP	2.8
1	B	287	SER	2.8
1	A	21	THR	2.8
1	B	54	ILE	2.8
1	B	210	ASN	2.8
1	B	263	VAL	2.8
1	B	136	LEU	2.7
1	B	155	VAL	2.7
1	A	213	MET	2.7
1	A	28	THR	2.7
1	A	192	GLY	2.7
1	A	64	ALA	2.7
1	A	136	LEU	2.7
1	A	305	LEU	2.7
1	B	189	GLY	2.7
1	A	275	SER	2.7
1	A	55	LYS	2.7
1	B	108	ALA	2.7
1	B	186	LEU	2.7
1	A	210	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	254	SER	2.6
1	A	182	ALA	2.6
1	A	200	LYS	2.6
1	A	121	TYR	2.6
1	B	233	ILE	2.6
1	A	291	PHE	2.6
1	A	142	LYS	2.6
1	A	16	CYS	2.6
1	A	150	MET	2.5
1	A	292	GLY	2.5
1	A	73	PHE	2.5
1	A	105	ALA	2.5
1	A	207	TRP	2.5
1	B	49	CYS	2.5
1	A	45	THR	2.5
1	B	270	ILE	2.5
1	A	265	LYS	2.5
1	A	181	ILE	2.4
1	B	127	CYS	2.4
1	B	265	LYS	2.4
1	B	17	LEU	2.4
1	A	138	ARG	2.4
1	A	254	SER	2.4
1	A	117	TYR	2.4
1	A	19	VAL	2.4
1	B	150	MET	2.4
1	A	264	VAL	2.4
1	A	237	GLY	2.3
1	A	100	VAL	2.3
1	A	211	ILE	2.3
1	B	277	ALA	2.3
1	B	255	VAL	2.3
1	A	295	ILE	2.3
1	B	223	ALA	2.3
1	B	78	SER	2.3
1	B	61	GLY	2.3
1	B	156	THR	2.3
1	A	53	VAL	2.3
1	A	120	THR	2.2
1	A	54	ILE	2.2
1	A	301	LEU	2.2
1	A	15	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	59	SER	2.2
1	B	147	SER	2.2
1	A	46	THR	2.2
1	B	116	VAL	2.2
1	A	159	GLN	2.2
1	A	88	LEU	2.2
1	B	91	LEU	2.2
1	B	134	LEU	2.2
1	A	43	PHE	2.2
1	B	307	CYS	2.1
1	B	23	VAL	2.1
1	A	26	ALA	2.1
1	B	105	ALA	2.1
1	A	101	GLN	2.1
1	B	149	PHE	2.1
1	B	152	CYS	2.1
1	B	100	VAL	2.1
1	A	156	THR	2.1
1	A	162	PRO	2.1
1	B	51	THR	2.0
1	A	238	PHE	2.0
1	A	81	VAL	2.0
1	B	97	VAL	2.0
1	B	158	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

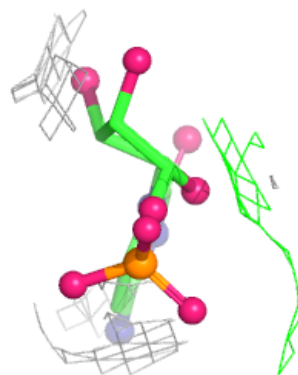
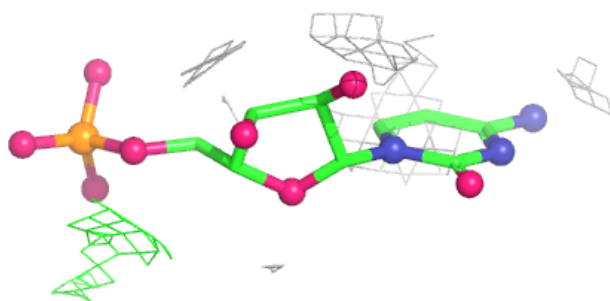
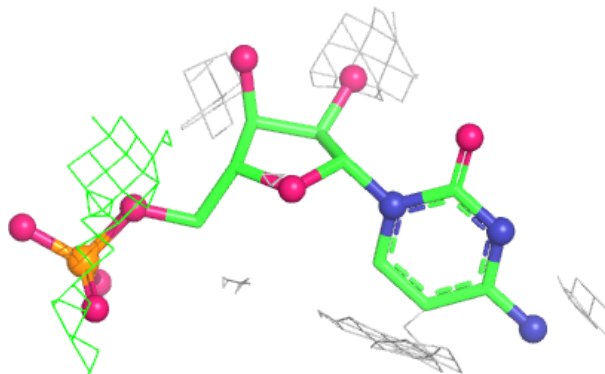
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	C5P	A	401	21/21	0.87	0.10	117,125,133,135	0
2	C5P	B	401	21/21	0.87	0.11	105,115,131,133	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.

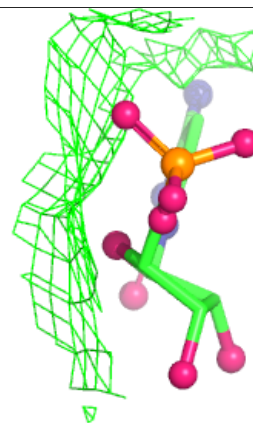
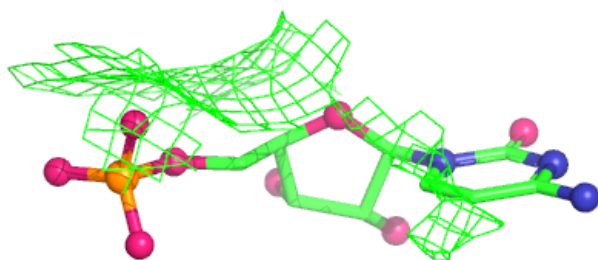
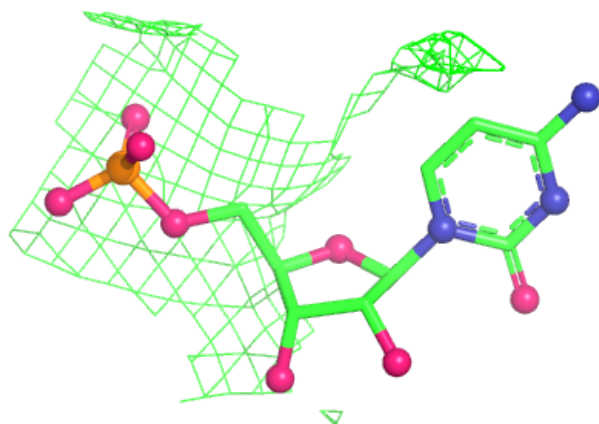
Electron density around C5P A 401:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.