wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2023 – 03:10 PM JST

PDB ID	:	8HCF
Title	:	Crystal structure of mTREX1-UMP complex
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Deposited on	:	2022-11-01
Resolution	:	1.60 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 (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:

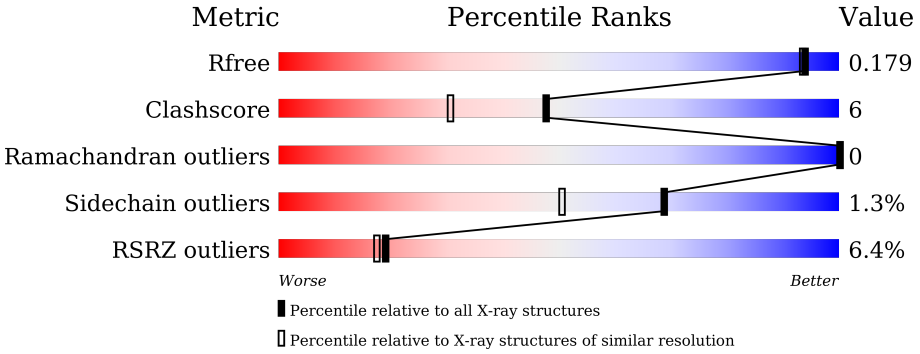
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	250	7% 84% 5% • 10%
1	B	250	4% 82% 8% • 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7636 atoms, of which 3528 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.

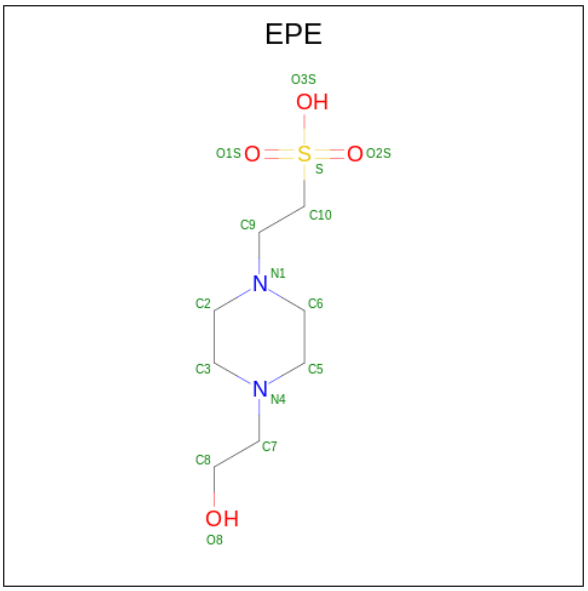
- Molecule 1 is a protein called Three-prime repair exonuclease 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	224	3474	1097	1740	306	322	9	0	0	0
1	B	228	3519	1110	1760	311	329	9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

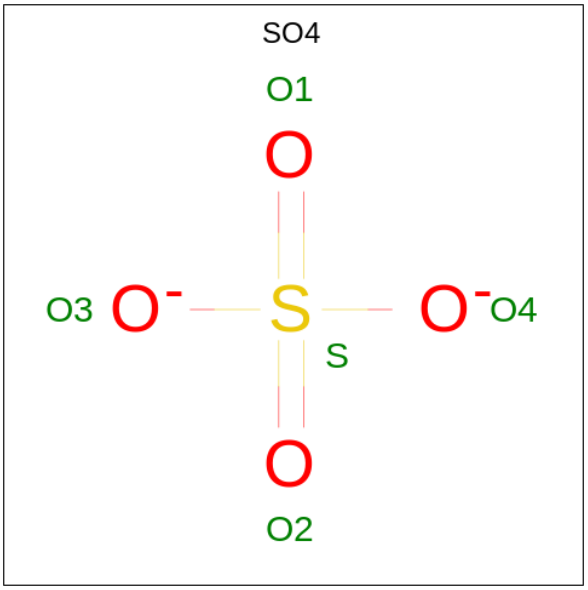
Chain	Residue	Modelled	Actual	Comment	Reference
A	243	LEU	-	expression tag	UNP Q91XB0
A	244	GLU	-	expression tag	UNP Q91XB0
A	245	HIS	-	expression tag	UNP Q91XB0
A	246	HIS	-	expression tag	UNP Q91XB0
A	247	HIS	-	expression tag	UNP Q91XB0
A	248	HIS	-	expression tag	UNP Q91XB0
A	249	HIS	-	expression tag	UNP Q91XB0
A	250	HIS	-	expression tag	UNP Q91XB0
B	243	LEU	-	expression tag	UNP Q91XB0
B	244	GLU	-	expression tag	UNP Q91XB0
B	245	HIS	-	expression tag	UNP Q91XB0
B	246	HIS	-	expression tag	UNP Q91XB0
B	247	HIS	-	expression tag	UNP Q91XB0
B	248	HIS	-	expression tag	UNP Q91XB0
B	249	HIS	-	expression tag	UNP Q91XB0
B	250	HIS	-	expression tag	UNP Q91XB0

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



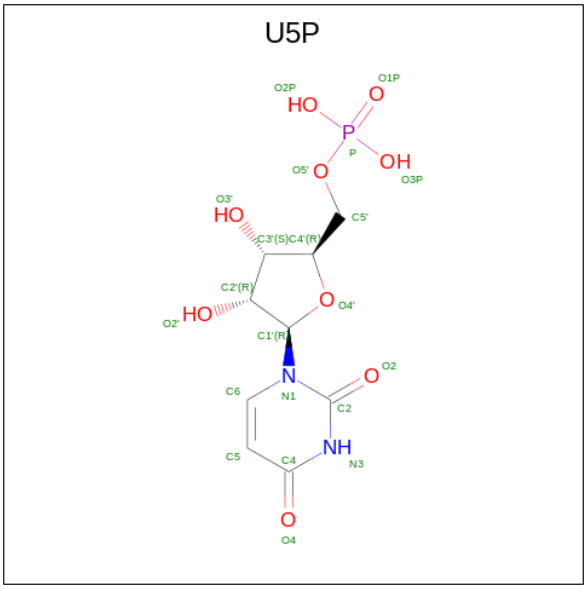
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
2	A	1	32	8	17	2	4	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0

- Molecule 4 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula: $C_9H_{13}N_2O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
4	B	1	32	9	11	2	9	1	0	0

- Molecule 5 is water.

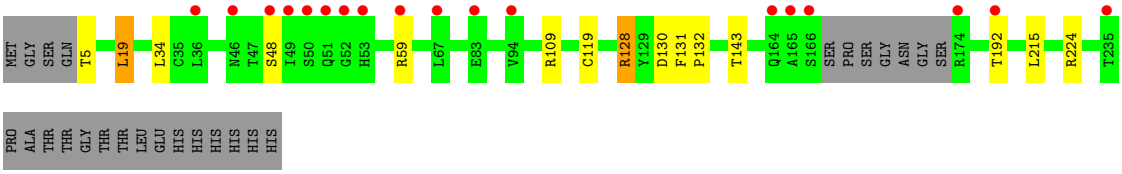
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	282	282	282	0	0
5	B	282	282	282	0	0

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.

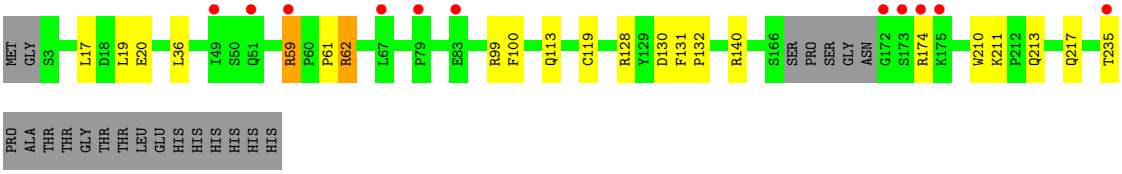
• Molecule 1: Three-prime repair exonuclease 1

Chain A:



• Molecule 1: Three-prime repair exonuclease 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.03Å 85.77Å 100.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.14 – 1.60 29.57 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (23.14-1.60) 99.8 (29.57-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.46 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.152 , 0.179 0.152 , 0.179	Depositor DCC
R_{free} test set	5742 reflections (7.84%)	wwPDB-VP
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 58.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7636	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8871e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: U5P, EPE, SO4

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	0.59	1/1776 (0.1%)	0.77	3/2422 (0.1%)
1	B	0.60	2/1801 (0.1%)	0.81	4/2455 (0.2%)
All	All	0.59	3/3577 (0.1%)	0.79	7/4877 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	119	CYS	CB-SG	-8.85	1.67	1.82
1	B	59	ARG	CZ-NH2	6.29	1.41	1.33
1	A	119	CYS	CB-SG	-5.60	1.72	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	59	ARG	NE-CZ-NH1	-14.92	112.84	120.30
1	B	59	ARG	NH1-CZ-NH2	7.78	127.95	119.40
1	B	59	ARG	CD-NE-CZ	-5.71	115.60	123.60
1	A	224	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	62	ARG	NE-CZ-NH2	-5.23	117.68	120.30

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	1734	1740	1739	14	0
1	B	1759	1760	1760	29	0
2	A	15	17	18	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
4	B	21	11	11	0	0
5	A	282	0	0	7	0
5	B	282	0	0	19	0
All	All	4108	3528	3528	43	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 6.

The worst 5 of 43 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:B:213:GLN:NE2	5:B:402:HOH:O	1.78	0.99
1:A:59:ARG:NH2	5:A:401:HOH:O	2.04	0.90
1:B:20:GLU:OE1	5:B:403:HOH:O	1.88	0.89
1:B:99:ARG:NH2	5:B:405:HOH:O	2.09	0.86
1:B:62:ARG:N	5:B:406:HOH:O	2.09	0.84

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	220/250 (88%)	219 (100%)	1 (0%)	0	100	100
1	B	224/250 (90%)	223 (100%)	1 (0%)	0	100	100
All	All	444/500 (89%)	442 (100%)	2 (0%)	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	193/214 (90%)	190 (98%)	3 (2%)	62	41
1	B	196/214 (92%)	194 (99%)	2 (1%)	76	61
All	All	389/428 (91%)	384 (99%)	5 (1%)	69	50

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	128	ARG
1	A	130	ASP
1	B	130	ASP
1	B	174	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	213	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)

5 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	EPE	A	301	-	15,15,15	0.64	0	18,20,20	1.80	5 (27%)
3	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.16	0
4	U5P	B	301	-	22,22,22	3.37	8 (36%)	33,33,33	1.85	9 (27%)
3	SO4	A	303	-	4,4,4	0.39	0	6,6,6	0.60	0
3	SO4	B	302	-	4,4,4	0.27	0	6,6,6	0.68	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
4	U5P	B	301	-	-	2/10/26/26	0/2/2/2
2	EPE	A	301	-	-	2/9/19/19	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	U5P	C3'-C4'	-7.64	1.33	1.53
4	B	301	U5P	O4'-C4'	7.59	1.62	1.45
4	B	301	U5P	C2-N1	5.72	1.47	1.38
4	B	301	U5P	C2-N3	5.40	1.47	1.38
4	B	301	U5P	C6-C5	5.21	1.47	1.35

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	301	U5P	C4-N3-C2	-5.62	119.17	126.58
2	A	301	EPE	C5-N4-C3	4.02	117.88	108.83
4	B	301	U5P	N3-C2-N1	3.85	120.00	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	301	U5P	C5-C4-N3	3.74	120.43	114.84
2	A	301	EPE	C7-N4-C3	3.59	120.42	111.23

There are no chirality outliers.

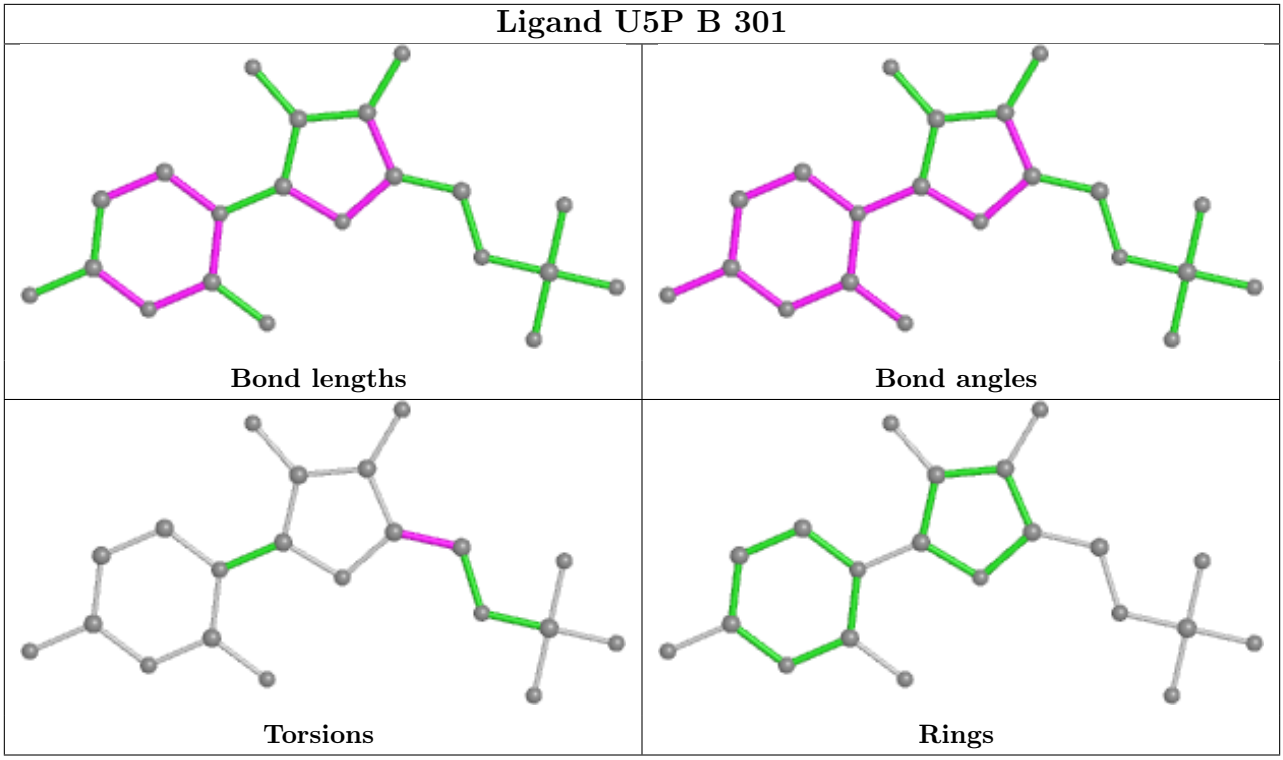
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	EPE	C8-C7-N4-C3
4	B	301	U5P	O4'-C4'-C5'-O5'
2	A	301	EPE	N4-C7-C8-O8
4	B	301	U5P	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.



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	224/250 (89%)	0.05	18 (8%)	12	11	13, 21, 55, 98	0
1	B	228/250 (91%)	0.01	11 (4%)	30	28	14, 23, 49, 103	0
All	All	452/500 (90%)	0.03	29 (6%)	19	17	13, 22, 54, 103	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	SER	9.8
1	B	174	ARG	8.3
1	A	50	SER	7.8
1	A	49	ILE	7.2
1	B	172	GLY	6.7

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)

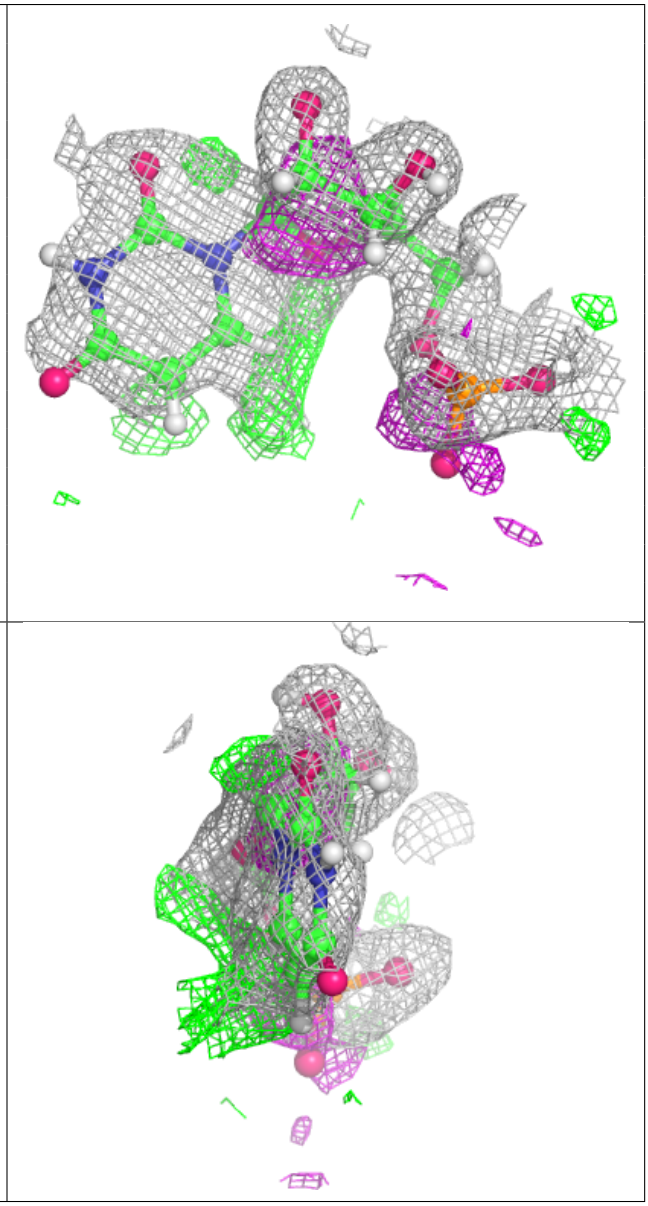
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	303	5/5	0.75	0.28	20,52,67,76	0
4	U5P	B	301	21/21	0.77	0.20	28,50,74,80	0
3	SO4	A	302	5/5	0.82	0.23	61,75,82,84	0
3	SO4	B	302	5/5	0.84	0.21	18,31,40,78	0
2	EPE	A	301	15/15	0.95	0.26	31,55,69,72	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 U5P B 301:

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.