



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 29, 2022 – 12:34 AM EST

PDB ID : 7TUX
Title : Crystal Structure of Plasmodium falciparum Hypoxanthine-Guanine-Xanthine Phosphoribosyltransferase in complex with [(3S)-4-Hydroxy-3-[(2-amino-4-hydroxy-5H-pyrrolo[3,2-d]pyrimidin-7-yl)methyl]amino]butyl]phosphonic acid
Authors : Harijan, R.K.; Minnow, Y.V.T.; Bonanno, J.B.; Almo, S.C.; Schramm, V.L.
Deposited on : 2022-02-03
Resolution : 1.62 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](#) ①) 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	:	2.31.2
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)	:	2.31.2

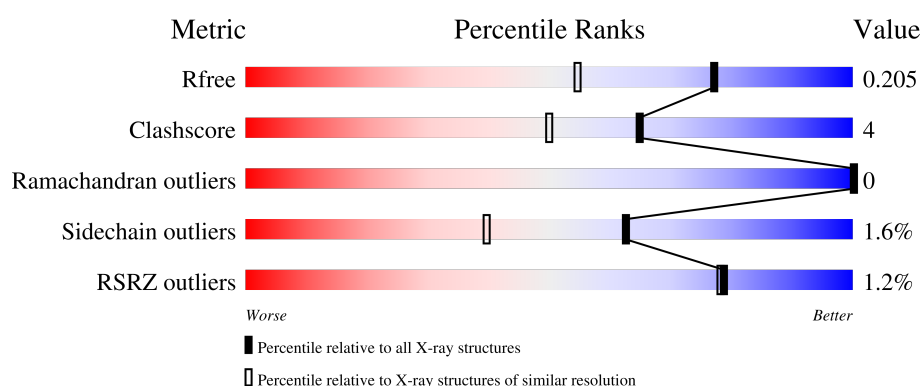
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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 $\leq 5\%$. 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	250	<div> <div>85%</div> <div>8%</div> <div>8%</div> </div>
1	B	250	<div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
1	C	250	<div> <div>83%</div> <div>8%</div> <div>8%</div> </div>
1	D	250	<div> <div>84%</div> <div>9%</div> <div>7%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8671 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 Hypoxanthine-guanine-xanthine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	7	0
			1909	1239	311	351	8			
1	B	230	Total	C	N	O	S	0	9	0
			1919	1246	312	351	10			
1	C	229	Total	C	N	O	S	0	3	0
			1859	1208	305	337	9			
1	D	232	Total	C	N	O	S	0	8	0
			1917	1240	315	352	10			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P20035
A	-17	GLY	-	expression tag	UNP P20035
A	-16	GLY	-	expression tag	UNP P20035
A	-15	SER	-	expression tag	UNP P20035
A	-14	HIS	-	expression tag	UNP P20035
A	-13	HIS	-	expression tag	UNP P20035
A	-12	HIS	-	expression tag	UNP P20035
A	-11	HIS	-	expression tag	UNP P20035
A	-10	HIS	-	expression tag	UNP P20035
A	-9	HIS	-	expression tag	UNP P20035
A	-8	GLY	-	expression tag	UNP P20035
A	-7	GLY	-	expression tag	UNP P20035
A	-6	LEU	-	expression tag	UNP P20035
A	-5	VAL	-	expression tag	UNP P20035
A	-4	PRO	-	expression tag	UNP P20035
A	-3	ARG	-	expression tag	UNP P20035
A	-2	GLY	-	expression tag	UNP P20035
A	-1	SER	-	expression tag	UNP P20035
A	0	HIS	-	expression tag	UNP P20035
B	-18	MET	-	initiating methionine	UNP P20035
B	-17	GLY	-	expression tag	UNP P20035

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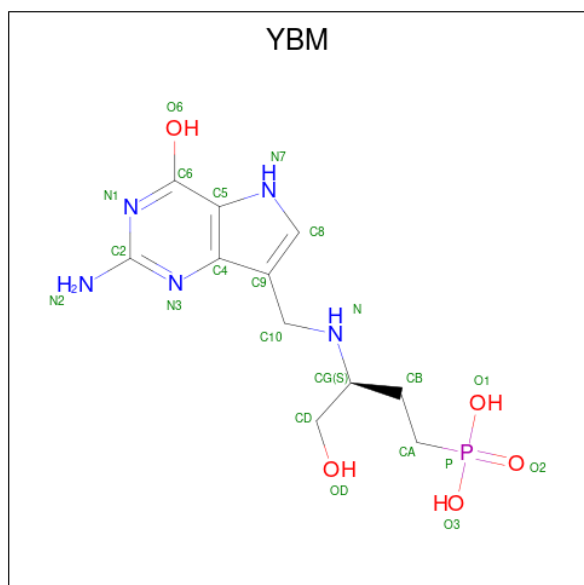
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	GLY	-	expression tag	UNP P20035
B	-15	SER	-	expression tag	UNP P20035
B	-14	HIS	-	expression tag	UNP P20035
B	-13	HIS	-	expression tag	UNP P20035
B	-12	HIS	-	expression tag	UNP P20035
B	-11	HIS	-	expression tag	UNP P20035
B	-10	HIS	-	expression tag	UNP P20035
B	-9	HIS	-	expression tag	UNP P20035
B	-8	GLY	-	expression tag	UNP P20035
B	-7	GLY	-	expression tag	UNP P20035
B	-6	LEU	-	expression tag	UNP P20035
B	-5	VAL	-	expression tag	UNP P20035
B	-4	PRO	-	expression tag	UNP P20035
B	-3	ARG	-	expression tag	UNP P20035
B	-2	GLY	-	expression tag	UNP P20035
B	-1	SER	-	expression tag	UNP P20035
B	0	HIS	-	expression tag	UNP P20035
C	-18	MET	-	initiating methionine	UNP P20035
C	-17	GLY	-	expression tag	UNP P20035
C	-16	GLY	-	expression tag	UNP P20035
C	-15	SER	-	expression tag	UNP P20035
C	-14	HIS	-	expression tag	UNP P20035
C	-13	HIS	-	expression tag	UNP P20035
C	-12	HIS	-	expression tag	UNP P20035
C	-11	HIS	-	expression tag	UNP P20035
C	-10	HIS	-	expression tag	UNP P20035
C	-9	HIS	-	expression tag	UNP P20035
C	-8	GLY	-	expression tag	UNP P20035
C	-7	GLY	-	expression tag	UNP P20035
C	-6	LEU	-	expression tag	UNP P20035
C	-5	VAL	-	expression tag	UNP P20035
C	-4	PRO	-	expression tag	UNP P20035
C	-3	ARG	-	expression tag	UNP P20035
C	-2	GLY	-	expression tag	UNP P20035
C	-1	SER	-	expression tag	UNP P20035
C	0	HIS	-	expression tag	UNP P20035
D	-18	MET	-	initiating methionine	UNP P20035
D	-17	GLY	-	expression tag	UNP P20035
D	-16	GLY	-	expression tag	UNP P20035
D	-15	SER	-	expression tag	UNP P20035
D	-14	HIS	-	expression tag	UNP P20035
D	-13	HIS	-	expression tag	UNP P20035

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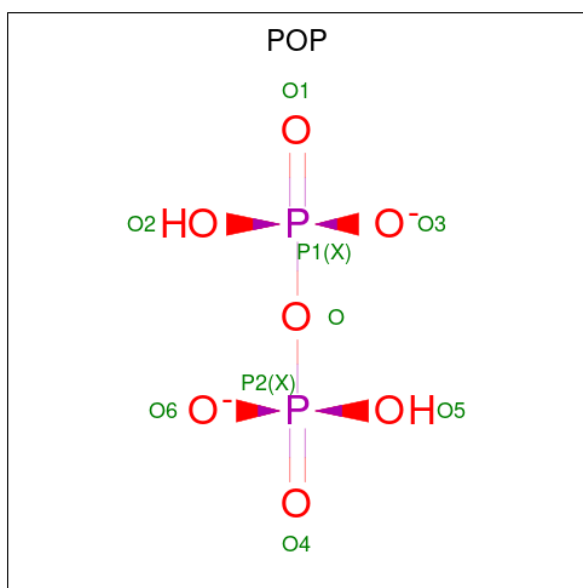
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP P20035
D	-11	HIS	-	expression tag	UNP P20035
D	-10	HIS	-	expression tag	UNP P20035
D	-9	HIS	-	expression tag	UNP P20035
D	-8	GLY	-	expression tag	UNP P20035
D	-7	GLY	-	expression tag	UNP P20035
D	-6	LEU	-	expression tag	UNP P20035
D	-5	VAL	-	expression tag	UNP P20035
D	-4	PRO	-	expression tag	UNP P20035
D	-3	ARG	-	expression tag	UNP P20035
D	-2	GLY	-	expression tag	UNP P20035
D	-1	SER	-	expression tag	UNP P20035
D	0	HIS	-	expression tag	UNP P20035

- Molecule 2 is [(3S)-3-{[(2-amino-4-hydroxy-5H-pyrrolo[3,2-d]pyrimidin-7-yl)methyl]amino}-4-hydroxybutyl]phosphonic acid (three-letter code: YBM) (formula: C₁₁H₁₈N₅O₅P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 22	C 11	N 5	O 5	P 1	0	0
2	B	1	Total 22	C 11	N 5	O 5	P 1	0	0
2	C	1	Total 22	C 11	N 5	O 5	P 1	0	0
2	D	1	Total 22	C 11	N 5	O 5	P 1	0	0

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			9	7	2		
3	B	1	Total	O	P	0	0
			9	7	2		
3	C	1	Total	O	P	0	0
			9	7	2		
3	D	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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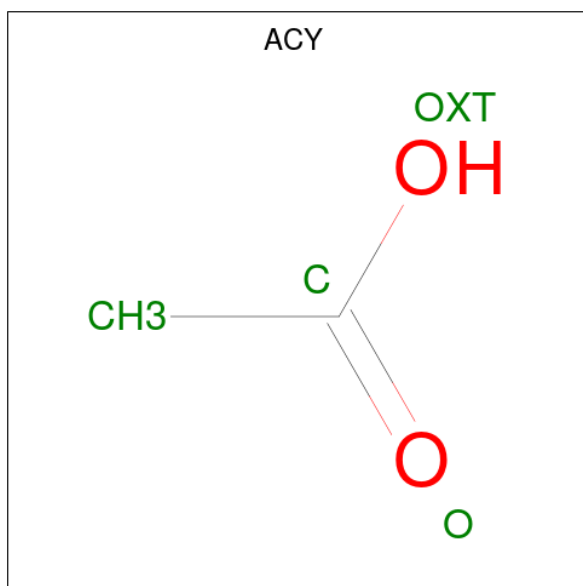
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	198	Total	O	0	0
			198	198		
7	B	199	Total	O	0	0
			199	199		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	196	Total 196	O 196	0	0
7	D	178	Total 178	O 178	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	105.44Å 111.20Å 173.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.47 – 1.62 57.40 – 1.62	Depositor EDS
% Data completeness (in resolution range)	99.9 (57.47-1.62) 99.9 (57.40-1.62)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.170 , 0.195 0.184 , 0.205	Depositor DCC
R_{free} test set	6509 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8671	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: MG, POP, EDO, ACY, YBM

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	0.62	0/1954	0.71	0/2640
1	B	0.62	0/1964	0.71	0/2655
1	C	0.62	0/1904	0.74	1/2573 (0.0%)
1	D	0.62	0/1963	0.72	0/2652
All	All	0.62	0/7785	0.72	1/10520 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	ARG	NE-CZ-NH1	-8.09	116.25	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	1909	0	1908	10	0
1	B	1919	0	1917	18	0
1	C	1859	0	1859	15	0
1	D	1917	0	1903	17	0
2	A	22	0	0	1	0
2	B	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	22	0	0	0	0
2	D	22	0	0	0	0
3	A	9	0	0	1	0
3	B	9	0	0	1	0
3	C	9	0	0	2	0
3	D	9	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	36	0	54	0	0
5	B	48	0	72	2	0
5	C	40	0	60	0	0
5	D	20	0	30	1	0
6	A	4	0	3	0	0
6	B	4	0	3	1	0
6	C	8	0	6	0	0
6	D	8	0	6	0	0
7	A	198	0	0	4	1
7	B	199	0	0	9	0
7	C	196	0	0	4	0
7	D	178	0	0	3	1
All	All	8671	0	7821	65	2

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 4.

All (65) 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:113[A]:VAL:HG13	1:B:125:LEU:HD11	1.40	1.02
1:B:185:LYS:NZ	7:B:401:HOH:O	1.97	0.97
1:D:113:VAL:HG13	1:D:125:LEU:HD11	1.50	0.90
1:B:113[A]:VAL:CG1	1:B:125:LEU:HD11	2.08	0.82
1:D:42:LYS:NZ	7:D:402:HOH:O	2.11	0.82
1:D:113:VAL:CG1	1:D:125:LEU:HD11	2.11	0.80
1:C:112:ARG:NH1	3:C:302:POP:O5	2.15	0.79
1:D:130:GLU:OE2	7:D:401:HOH:O	2.04	0.75
5:B:314:EDO:H12	7:B:405:HOH:O	1.87	0.73
1:A:100[B]:GLU:OE1	7:A:401:HOH:O	2.07	0.72
1:C:113:VAL:CG1	1:C:125:LEU:HD11	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:SER:OG	7:C:401:HOH:O	2.03	0.68
3:B:302:POP:O6	7:B:402:HOH:O	2.13	0.66
1:C:113:VAL:HG13	1:C:125:LEU:HD11	1.79	0.65
1:B:113[A]:VAL:HG13	1:B:125:LEU:CD1	2.23	0.63
1:D:5:ASN:OD1	5:D:308:EDO:O1	2.03	0.62
1:A:73[B]:LEU:HD11	1:A:111:VAL:HG23	1.81	0.62
1:C:42:LYS:NZ	7:C:404:HOH:O	2.33	0.60
1:C:73:LEU:HD11	1:C:111:VAL:HG23	1.83	0.60
1:B:75[B]:LEU:HD23	1:B:111[B]:VAL:CG2	2.31	0.60
3:A:302:POP:O2	7:A:402:HOH:O	2.16	0.60
2:A:301:YBM:OD	7:A:402:HOH:O	2.16	0.58
1:B:128:VAL:HB	7:B:403:HOH:O	2.04	0.58
1:A:142:ILE:HD12	1:A:170[A]:ILE:CD1	2.34	0.58
3:C:302:POP:O4	7:C:402:HOH:O	2.17	0.56
1:B:42:LYS:NZ	7:B:407:HOH:O	2.38	0.56
6:B:316:ACY:H1	7:B:481:HOH:O	2.05	0.55
1:C:142:ILE:HD12	1:C:170[A]:ILE:CD1	2.38	0.54
1:D:113:VAL:HG13	1:D:125:LEU:CD1	2.30	0.52
1:D:150:GLY:O	1:D:154[B]:VAL:HG22	2.09	0.52
1:A:123:GLY:O	1:A:155:LYS:NZ	2.43	0.52
2:B:301:YBM:OD	7:B:402:HOH:O	2.19	0.52
1:A:196:HIS:HE1	7:A:460:HOH:O	1.93	0.51
1:C:62:LYS:NZ	1:C:94:HIS:HD2	2.10	0.50
1:B:73[B]:LEU:HD11	1:B:111[B]:VAL:HG13	1.95	0.49
1:D:62:LYS:NZ	1:D:94:HIS:HD2	2.10	0.49
1:D:70:PHE:O	1:D:106:PHE:HA	2.13	0.49
1:A:70:PHE:O	1:A:106:PHE:HA	2.13	0.48
1:B:70:PHE:O	1:B:106:PHE:HA	2.14	0.47
1:C:35:HIS:H	1:C:35:HIS:CD2	2.32	0.47
1:B:74:CYS:HG	1:B:79[B]:SER:HG	1.64	0.45
1:C:74:CYS:HG	1:C:79[B]:SER:HG	1.65	0.45
1:A:35:HIS:H	1:A:35:HIS:CD2	2.34	0.45
1:B:75[B]:LEU:CD2	1:B:111[B]:VAL:CG2	2.95	0.44
1:C:196:HIS:HE1	7:C:458:HOH:O	2.00	0.44
1:C:70:PHE:O	1:C:106:PHE:HA	2.17	0.44
1:A:124:THR:HG21	1:C:163:PHE:CE1	2.54	0.43
1:A:179:PRO:HB3	1:B:162:LYS:HB3	2.02	0.42
1:B:128:VAL:O	7:B:403:HOH:O	2.21	0.42
1:D:186:ALA:HB3	1:D:189:VAL:HG22	2.01	0.42
1:A:186:ALA:HB3	1:A:189:VAL:HG22	2.01	0.41
1:D:35:HIS:CD2	1:D:35:HIS:H	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:GLU:O	1:D:172[B]:CYS:HA	2.19	0.41
1:C:111:VAL:HG13	1:C:129:SER:HB3	2.02	0.41
1:D:196:HIS:HE1	7:D:425:HOH:O	2.03	0.41
1:B:75[B]:LEU:HD23	1:B:111[B]:VAL:HG23	2.01	0.41
1:B:113[B]:VAL:HA	1:B:126[B]:GLU:O	2.20	0.41
1:B:120:GLN:NE2	7:B:411:HOH:O	2.53	0.41
1:D:113:VAL:HG11	1:D:152:THR:HG23	2.02	0.41
1:C:186:ALA:HB3	1:C:189:VAL:HG22	2.03	0.41
1:D:123:GLY:O	1:D:155:LYS:NZ	2.54	0.41
1:D:172[B]:CYS:SG	1:D:175:ILE:HG23	2.61	0.41
1:D:62:LYS:HZ2	1:D:94:HIS:HD2	1.69	0.40
1:B:26:ASP:OD2	5:B:313:EDO:C2	2.69	0.40
1:B:186:ALA:HB3	1:B:189:VAL:HG22	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:584:HOH:O	7:A:584:HOH:O[3_554]	1.41	0.79
7:D:567:HOH:O	7:D:567:HOH:O[3_454]	1.70	0.50

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	236/250 (94%)	229 (97%)	7 (3%)	0	100	100
1	B	237/250 (95%)	230 (97%)	7 (3%)	0	100	100
1	C	230/250 (92%)	223 (97%)	7 (3%)	0	100	100
1	D	238/250 (95%)	232 (98%)	6 (2%)	0	100	100
All	All	941/1000 (94%)	914 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	213/221 (96%)	209 (98%)	4 (2%)	57	32
1	B	214/221 (97%)	211 (99%)	3 (1%)	67	46
1	C	206/221 (93%)	203 (98%)	3 (2%)	65	43
1	D	214/221 (97%)	210 (98%)	4 (2%)	57	32
All	All	847/884 (96%)	833 (98%)	14 (2%)	62	36

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	63	LYS
1	A	112	ARG
1	A	162	LYS
1	B	11	GLU
1	B	112	ARG
1	B	165	ILE
1	C	11	GLU
1	C	63	LYS
1	C	112	ARG
1	D	112	ARG
1	D	154[A]	VAL
1	D	154[B]	VAL
1	D	162	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	47	ASN
1	A	52	ASN

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Mol	Chain	Res	Type
1	A	196	HIS
1	B	52	ASN
1	C	35	HIS
1	C	47	ASN
1	C	52	ASN
1	C	94	HIS
1	C	196	HIS
1	D	35	HIS
1	D	52	ASN
1	D	89	HIS
1	D	94	HIS
1	D	196	HIS

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](#)

Of 54 ligands modelled in this entry, 4 are monoatomic - leaving 50 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	$\# Z > 2$
5	EDO	A	308	-	3,3,3	0.08	0	2,2,2	0.10	0
2	YBM	A	301	-	21,23,23	1.22	1 (4%)	19,33,33	1.64	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	308	-	3,3,3	0.17	0	2,2,2	0.65	0
2	YBM	D	301	-	21,23,23	1.13	1 (4%)	19,33,33	1.56	4 (21%)
5	EDO	B	310	-	3,3,3	0.34	0	2,2,2	0.37	0
5	EDO	C	306	-	3,3,3	0.28	0	2,2,2	0.46	0
5	EDO	A	305	-	3,3,3	0.12	0	2,2,2	0.19	0
5	EDO	C	308	-	3,3,3	0.08	0	2,2,2	0.40	0
5	EDO	C	309	-	3,3,3	0.08	0	2,2,2	0.31	0
5	EDO	B	314	-	3,3,3	0.30	0	2,2,2	0.44	0
3	POP	D	302	4	6,8,8	0.77	0	13,13,13	1.21	2 (15%)
5	EDO	C	311	-	3,3,3	0.08	0	2,2,2	0.16	0
5	EDO	B	312	-	3,3,3	0.24	0	2,2,2	0.44	0
5	EDO	A	312	-	3,3,3	0.04	0	2,2,2	0.13	0
5	EDO	B	309	-	3,3,3	0.19	0	2,2,2	0.24	0
5	EDO	B	306	-	3,3,3	0.22	0	2,2,2	0.41	0
2	YBM	B	301	-	21,23,23	0.96	2 (9%)	19,33,33	1.47	4 (21%)
5	EDO	C	312	-	3,3,3	0.14	0	2,2,2	0.36	0
5	EDO	C	307	-	3,3,3	0.08	0	2,2,2	0.22	0
5	EDO	B	305	-	3,3,3	0.12	0	2,2,2	0.30	0
6	ACY	A	313	-	3,3,3	0.99	0	3,3,3	0.76	0
6	ACY	B	316	-	3,3,3	0.89	0	3,3,3	0.94	0
6	ACY	C	314	-	3,3,3	1.08	0	3,3,3	0.68	0
5	EDO	A	304	-	3,3,3	0.03	0	2,2,2	0.11	0
2	YBM	C	301	-	21,23,23	1.08	2 (9%)	19,33,33	1.54	5 (26%)
6	ACY	C	315	-	3,3,3	0.96	0	3,3,3	0.77	0
5	EDO	B	307	-	3,3,3	0.11	0	2,2,2	0.43	0
5	EDO	D	307	-	3,3,3	0.15	0	2,2,2	0.49	0
5	EDO	C	304	-	3,3,3	0.08	0	2,2,2	0.13	0
5	EDO	B	313	-	3,3,3	0.21	0	2,2,2	0.55	0
3	POP	C	302	4	6,8,8	0.63	0	13,13,13	1.06	1 (7%)
3	POP	B	302	4	6,8,8	0.95	0	13,13,13	1.23	1 (7%)
5	EDO	B	304	-	3,3,3	0.16	0	2,2,2	0.11	0
6	ACY	D	309	-	3,3,3	0.86	0	3,3,3	0.96	0
5	EDO	A	310	-	3,3,3	0.11	0	2,2,2	0.14	0
5	EDO	D	308	-	3,3,3	0.19	0	2,2,2	0.25	0
6	ACY	D	310	-	3,3,3	0.99	0	3,3,3	0.84	0
5	EDO	C	313	-	3,3,3	0.07	0	2,2,2	0.40	0
5	EDO	C	305	-	3,3,3	0.13	0	2,2,2	0.20	0
5	EDO	A	309	-	3,3,3	0.03	0	2,2,2	0.09	0
5	EDO	A	306	-	3,3,3	0.11	0	2,2,2	0.14	0
5	EDO	D	306	-	3,3,3	0.14	0	2,2,2	0.27	0
5	EDO	A	311	-	3,3,3	0.05	0	2,2,2	0.21	0
5	EDO	A	307	-	3,3,3	0.22	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	315	-	3,3,3	0.06	0	2,2,2	0.25	0
5	EDO	D	304	-	3,3,3	0.15	0	2,2,2	0.24	0
5	EDO	D	305	-	3,3,3	0.10	0	2,2,2	0.32	0
3	POP	A	302	4	6,8,8	0.64	0	13,13,13	1.16	1 (7%)
5	EDO	C	310	-	3,3,3	0.09	0	2,2,2	0.17	0
5	EDO	B	311	-	3,3,3	0.06	0	2,2,2	0.22	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
5	EDO	A	308	-	-	1/1/1/1	-
2	YBM	A	301	-	-	2/11/13/13	0/2/2/2
5	EDO	B	308	-	-	1/1/1/1	-
2	YBM	D	301	-	-	1/11/13/13	0/2/2/2
5	EDO	B	310	-	-	0/1/1/1	-
5	EDO	C	306	-	-	1/1/1/1	-
5	EDO	A	305	-	-	1/1/1/1	-
5	EDO	C	308	-	-	1/1/1/1	-
5	EDO	C	309	-	-	0/1/1/1	-
5	EDO	B	314	-	-	0/1/1/1	-
3	POP	D	302	4	-	0/6/6/6	-
5	EDO	C	311	-	-	0/1/1/1	-
5	EDO	B	312	-	-	0/1/1/1	-
5	EDO	A	312	-	-	0/1/1/1	-
5	EDO	B	309	-	-	0/1/1/1	-
5	EDO	B	306	-	-	1/1/1/1	-
2	YBM	B	301	-	-	2/11/13/13	0/2/2/2
5	EDO	C	312	-	-	0/1/1/1	-
5	EDO	C	307	-	-	1/1/1/1	-
5	EDO	B	305	-	-	0/1/1/1	-
5	EDO	A	304	-	-	0/1/1/1	-
2	YBM	C	301	-	-	3/11/13/13	0/2/2/2
5	EDO	B	307	-	-	1/1/1/1	-
5	EDO	D	307	-	-	1/1/1/1	-
5	EDO	C	304	-	-	0/1/1/1	-
5	EDO	B	313	-	-	1/1/1/1	-
3	POP	C	302	4	-	0/6/6/6	-
3	POP	B	302	4	-	0/6/6/6	-
5	EDO	B	304	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	310	-	-	1/1/1/1	-
5	EDO	D	308	-	-	1/1/1/1	-
5	EDO	C	313	-	-	0/1/1/1	-
5	EDO	C	305	-	-	1/1/1/1	-
5	EDO	A	309	-	-	0/1/1/1	-
5	EDO	A	306	-	-	0/1/1/1	-
5	EDO	D	306	-	-	1/1/1/1	-
5	EDO	A	311	-	-	1/1/1/1	-
5	EDO	A	307	-	-	1/1/1/1	-
5	EDO	B	315	-	-	1/1/1/1	-
5	EDO	D	304	-	-	0/1/1/1	-
5	EDO	D	305	-	-	1/1/1/1	-
3	POP	A	302	4	-	0/6/6/6	-
5	EDO	C	310	-	-	1/1/1/1	-
5	EDO	B	311	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	YBM	P-CA	4.31	1.83	1.78
2	D	301	YBM	P-CA	3.88	1.82	1.78
2	C	301	YBM	P-CA	3.45	1.82	1.78
2	B	301	YBM	P-O3	-2.33	1.49	1.54
2	B	301	YBM	P-CA	2.26	1.81	1.78
2	C	301	YBM	P-O1	-2.06	1.50	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	YBM	N3-C2-N1	-4.21	121.61	127.22
2	C	301	YBM	N3-C2-N1	-3.73	122.25	127.22
2	B	301	YBM	N3-C2-N1	-3.73	122.25	127.22
2	A	301	YBM	N3-C2-N1	-3.51	122.54	127.22
2	A	301	YBM	CB-CG-CD	-2.89	107.44	111.78
2	C	301	YBM	C9-C10-N	2.49	119.99	112.75
2	A	301	YBM	C9-C10-N	2.39	119.69	112.75
3	B	302	POP	P2-O-P1	-2.30	124.93	132.83
3	D	302	POP	O6-P2-O5	2.28	116.33	107.64
2	D	301	YBM	C9-C10-N	2.20	119.14	112.75
2	C	301	YBM	CB-CG-CD	-2.13	108.58	111.78
2	B	301	YBM	C9-C10-N	2.09	118.81	112.75
2	C	301	YBM	C10-C9-C8	2.06	130.57	127.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	YBM	C2-N1-C6	2.06	121.63	116.43
2	D	301	YBM	CB-CG-CD	-2.06	108.69	111.78
3	D	302	POP	P2-O-P1	-2.05	125.81	132.83
3	A	302	POP	O3-P1-O2	2.04	115.43	107.64
2	B	301	YBM	C2-N1-C6	2.04	121.56	116.43
2	A	301	YBM	O2-P-CA	-2.03	107.64	111.40
2	B	301	YBM	CB-CG-CD	-2.02	108.74	111.78
2	C	301	YBM	C2-N1-C6	2.02	121.52	116.43
3	C	302	POP	O3-P1-O2	2.01	115.30	107.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

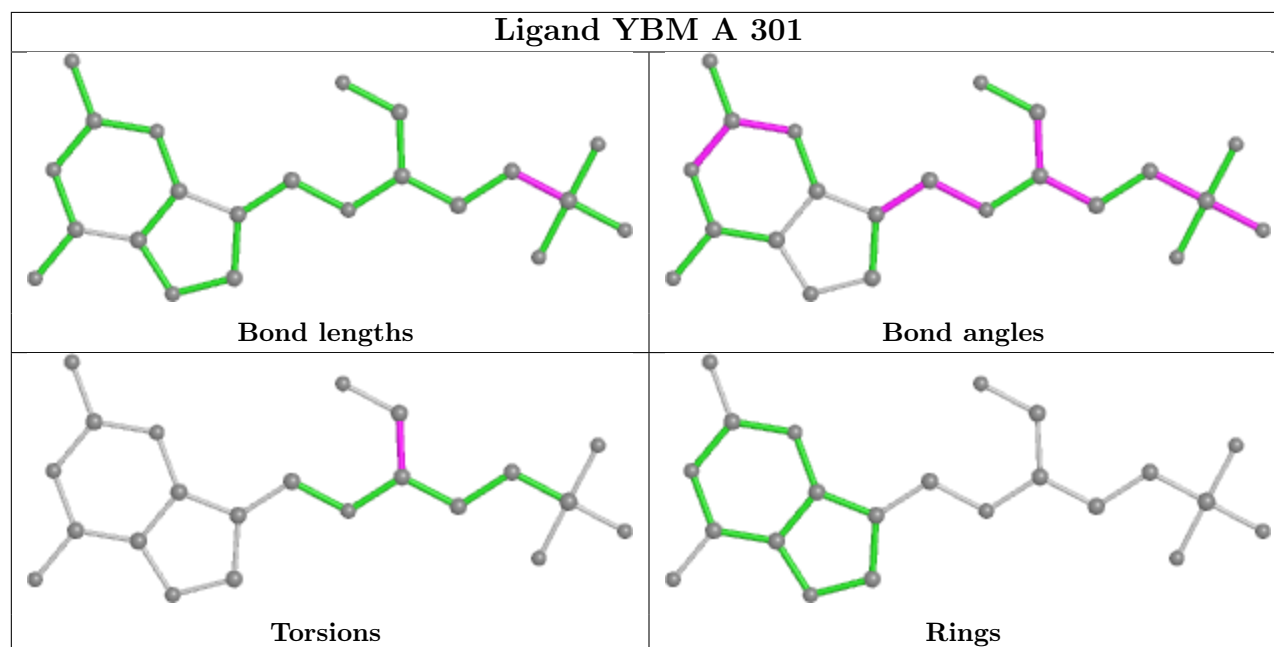
Mol	Chain	Res	Type	Atoms
2	A	301	YBM	OD-CD-CG-N
2	B	301	YBM	OD-CD-CG-N
2	C	301	YBM	OD-CD-CG-N
2	A	301	YBM	OD-CD-CG-CB
2	C	301	YBM	OD-CD-CG-CB
5	B	306	EDO	O1-C1-C2-O2
5	B	307	EDO	O1-C1-C2-O2
5	C	306	EDO	O1-C1-C2-O2
5	C	307	EDO	O1-C1-C2-O2
5	C	308	EDO	O1-C1-C2-O2
5	D	305	EDO	O1-C1-C2-O2
5	D	306	EDO	O1-C1-C2-O2
5	D	307	EDO	O1-C1-C2-O2
5	A	305	EDO	O1-C1-C2-O2
5	B	313	EDO	O1-C1-C2-O2
5	A	310	EDO	O1-C1-C2-O2
5	A	311	EDO	O1-C1-C2-O2
5	C	310	EDO	O1-C1-C2-O2
5	B	308	EDO	O1-C1-C2-O2
5	A	308	EDO	O1-C1-C2-O2
5	C	305	EDO	O1-C1-C2-O2
2	C	301	YBM	C9-C10-N-CG
5	A	307	EDO	O1-C1-C2-O2
5	B	315	EDO	O1-C1-C2-O2
5	D	308	EDO	O1-C1-C2-O2
2	D	301	YBM	OD-CD-CG-N
2	B	301	YBM	OD-CD-CG-CB

There are no ring outliers.

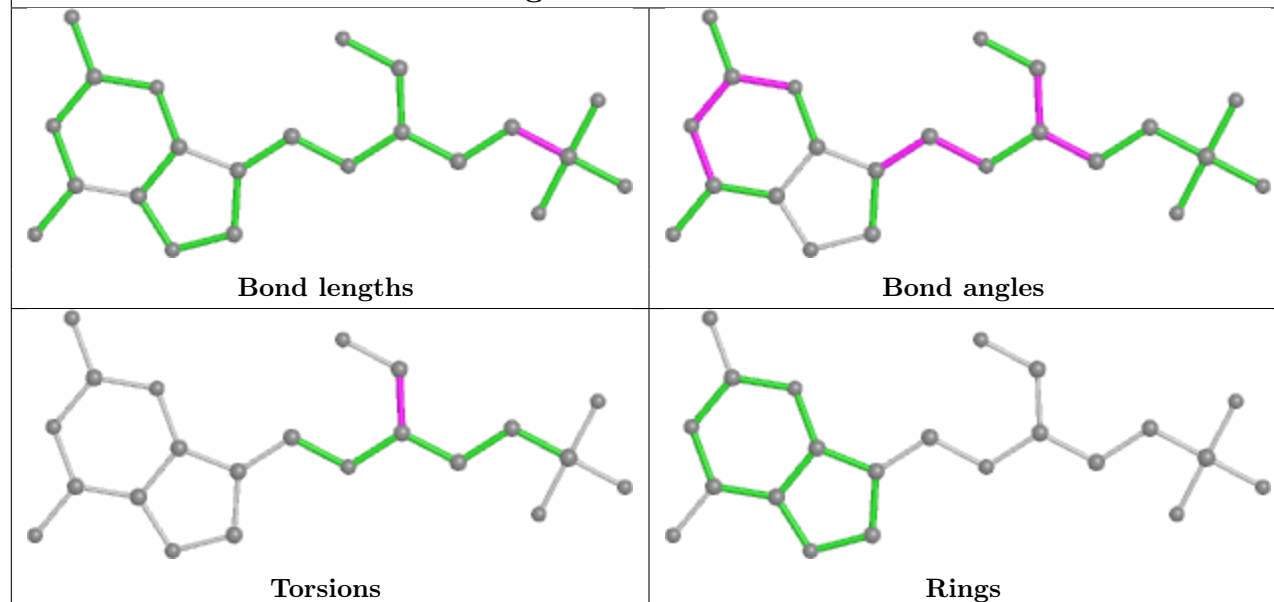
9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	YBM	1	0
5	B	314	EDO	1	0
2	B	301	YBM	1	0
6	B	316	ACY	1	0
5	B	313	EDO	1	0
3	C	302	POP	2	0
3	B	302	POP	1	0
5	D	308	EDO	1	0
3	A	302	POP	1	0

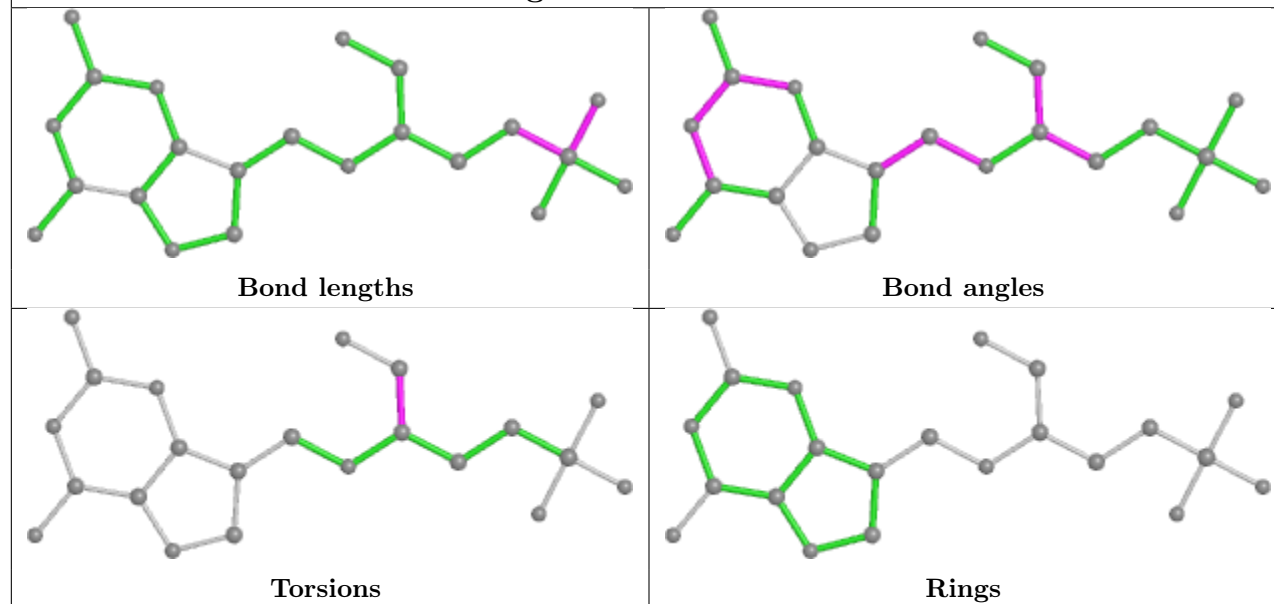
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

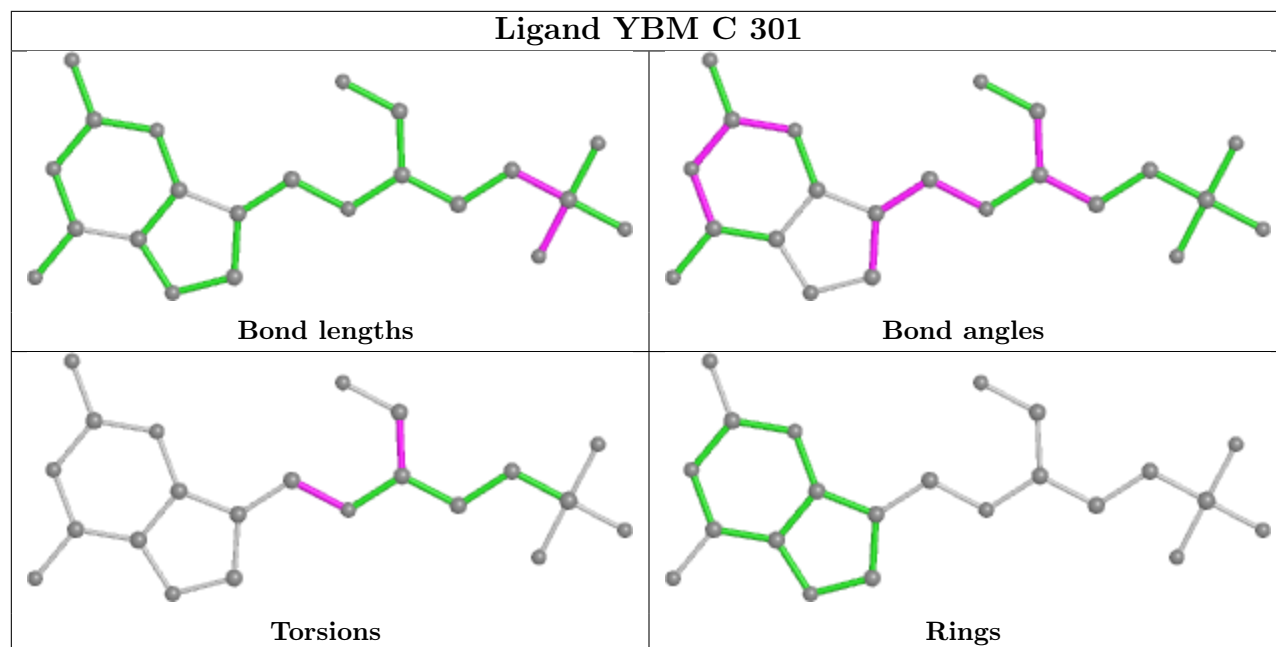


Ligand YBM D 301



Ligand YBM B 301





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	231/250 (92%)	-0.39	2 (0%) 84 84	18, 25, 40, 66	0
1	B	230/250 (92%)	-0.33	3 (1%) 77 76	15, 22, 37, 60	0
1	C	229/250 (91%)	-0.44	1 (0%) 92 92	17, 24, 38, 61	0
1	D	232/250 (92%)	-0.24	5 (2%) 62 60	17, 26, 50, 62	0
All	All	922/1000 (92%)	-0.35	11 (1%) 79 78	15, 24, 43, 66	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	124	THR	4.1
1	B	229	THR	4.0
1	D	229	THR	3.0
1	A	231	LEU	3.0
1	A	129	SER	2.8
1	B	0	HIS	2.7
1	B	129	SER	2.5
1	C	1	MET	2.4
1	D	115	SER	2.4
1	D	96	TYR	2.3
1	D	117	CYS	2.3

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

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
5	EDO	D	307	4/4	0.43	0.20	53,53,54,55	0
6	ACY	B	316	4/4	0.53	0.24	45,48,52,61	0
5	EDO	B	313	4/4	0.54	0.27	52,58,59,61	0
5	EDO	B	312	4/4	0.64	0.26	47,50,51,53	0
5	EDO	C	308	4/4	0.69	0.19	51,53,55,57	0
6	ACY	A	313	4/4	0.70	0.19	61,64,67,67	0
6	ACY	C	314	4/4	0.72	0.17	53,54,55,56	0
5	EDO	C	312	4/4	0.80	0.19	40,44,46,50	0
5	EDO	D	306	4/4	0.80	0.12	36,37,37,40	0
5	EDO	C	305	4/4	0.81	0.15	39,41,41,42	0
5	EDO	B	314	4/4	0.81	0.16	31,31,35,35	0
6	ACY	C	315	4/4	0.83	0.14	46,48,49,55	0
6	ACY	D	310	4/4	0.83	0.15	57,60,61,62	0
5	EDO	B	311	4/4	0.84	0.12	51,51,51,51	0
5	EDO	C	309	4/4	0.84	0.12	49,49,50,51	0
5	EDO	D	308	4/4	0.84	0.20	33,37,39,42	0
5	EDO	C	306	4/4	0.84	0.12	33,38,38,38	0
5	EDO	B	308	4/4	0.85	0.11	38,42,42,42	0
5	EDO	A	312	4/4	0.85	0.10	52,52,53,53	0
5	EDO	C	310	4/4	0.88	0.13	40,41,44,44	0
6	ACY	D	309	4/4	0.89	0.13	47,49,50,52	0
5	EDO	A	305	4/4	0.89	0.10	37,38,40,40	0
5	EDO	C	307	4/4	0.90	0.14	35,39,41,41	0
5	EDO	B	306	4/4	0.91	0.09	32,33,35,35	0
5	EDO	C	311	4/4	0.91	0.12	60,61,61,62	0
5	EDO	A	309	4/4	0.92	0.15	42,42,43,43	0
5	EDO	B	307	4/4	0.92	0.11	28,32,34,35	0
5	EDO	A	310	4/4	0.92	0.16	46,47,47,49	0
5	EDO	B	309	4/4	0.92	0.11	24,24,25,26	0
5	EDO	A	307	4/4	0.92	0.12	38,40,41,42	0
5	EDO	B	310	4/4	0.93	0.12	25,29,30,30	0
5	EDO	B	315	4/4	0.93	0.13	52,53,54,56	0
5	EDO	C	304	4/4	0.93	0.10	23,28,28,29	0
5	EDO	A	311	4/4	0.93	0.07	51,51,52,55	0
5	EDO	A	304	4/4	0.94	0.10	27,28,29,30	0
5	EDO	D	304	4/4	0.94	0.11	24,27,28,28	0
5	EDO	D	305	4/4	0.94	0.12	30,32,33,34	0

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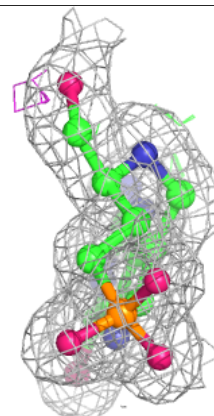
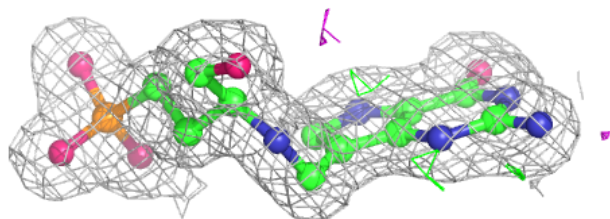
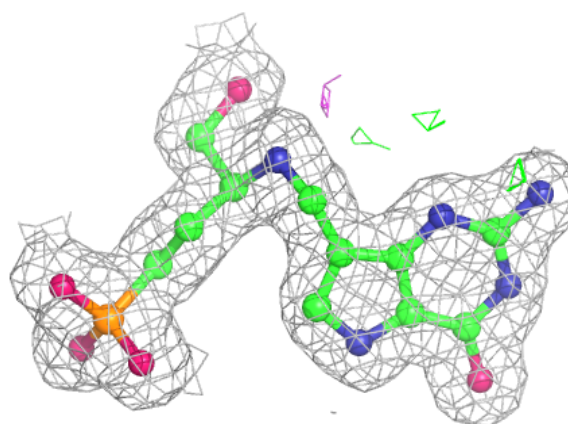
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	A	306	4/4	0.95	0.10	34,35,36,37	0
5	EDO	B	304	4/4	0.95	0.10	20,24,25,27	0
5	EDO	C	313	4/4	0.96	0.12	36,40,41,45	0
5	EDO	A	308	4/4	0.96	0.11	32,33,34,34	0
5	EDO	B	305	4/4	0.97	0.08	27,27,28,28	0
2	YBM	A	301	22/22	0.98	0.06	18,20,21,25	0
2	YBM	B	301	22/22	0.98	0.07	17,19,20,22	0
2	YBM	C	301	22/22	0.98	0.06	19,21,23,26	0
2	YBM	D	301	22/22	0.98	0.06	18,21,24,28	0
3	POP	C	302	9/9	0.98	0.05	23,23,25,25	0
3	POP	D	302	9/9	0.98	0.09	30,31,33,34	0
4	MG	A	303	1/1	0.98	0.04	20,20,20,20	0
4	MG	B	303	1/1	0.99	0.03	20,20,20,20	0
4	MG	C	303	1/1	0.99	0.08	22,22,22,22	0
4	MG	D	303	1/1	0.99	0.11	29,29,29,29	0
3	POP	B	302	9/9	0.99	0.05	20,22,22,23	0
3	POP	A	302	9/9	0.99	0.05	19,21,22,24	0

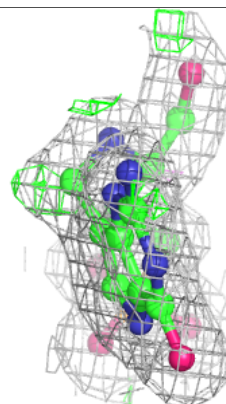
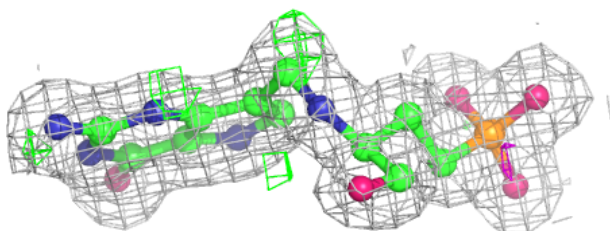
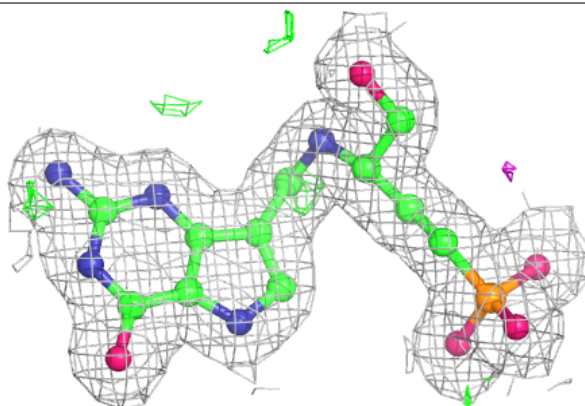
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YBM A 301:

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

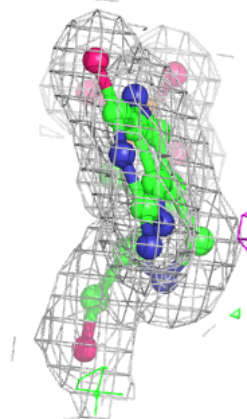
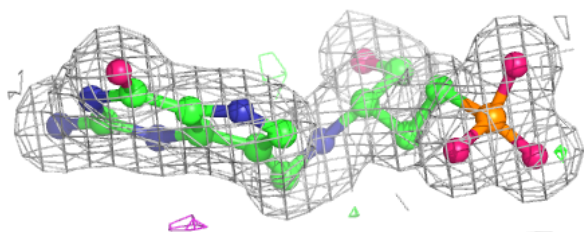
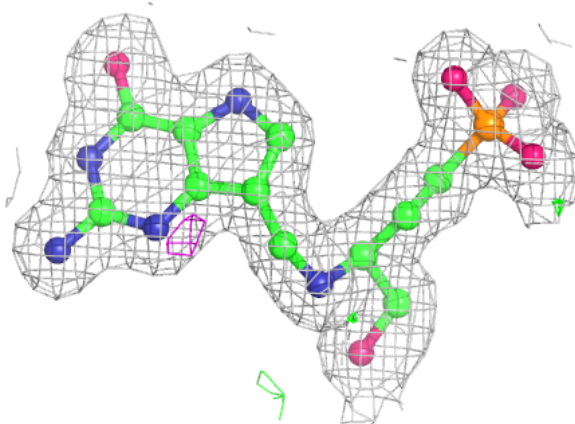
**Electron density around YBM B 301:**

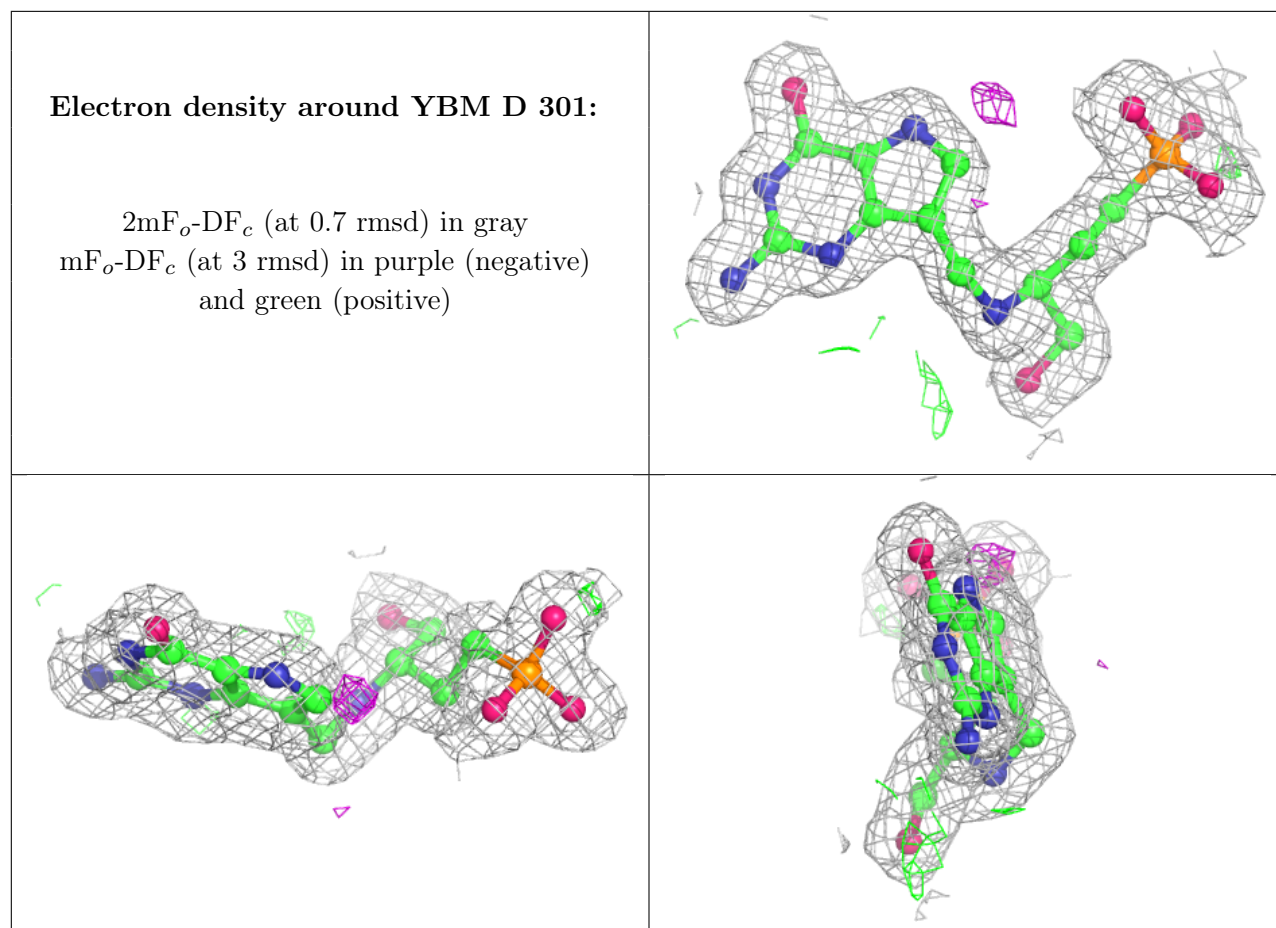
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around YBM C 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 ⓘ

There are no such residues in this entry.