



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:42 AM UTC

PDB ID : 6YLV / pdb_00006ylv
Title : Translation initiation factor 4E in complex with 4-Cl-Bn7GpppG mRNA 5' cap analog
Authors : Kubacka, D.; Wojcik, R.; Baranowski, M.R.; Kowalska, J.; Jemielity, J.
Deposited on : 2020-04-07
Resolution : 2.66 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

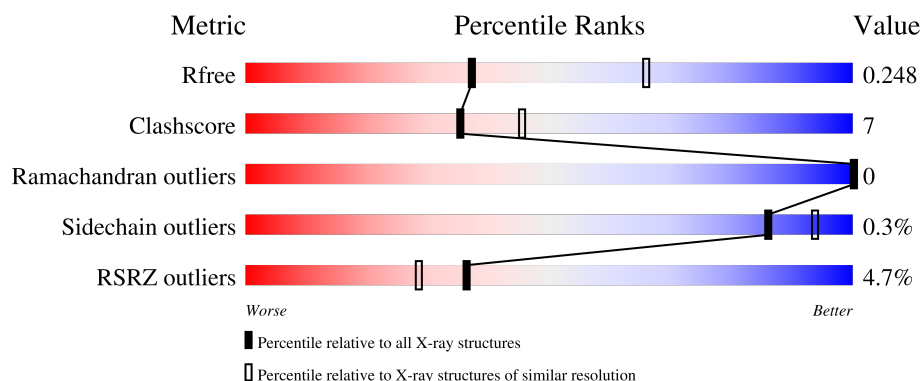
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	191	2% 80% 16% .
1	B	191	4% 84% 13% .
1	C	191	6% 74% 20% 6%
1	D	191	6% 72% 21% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6288 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.

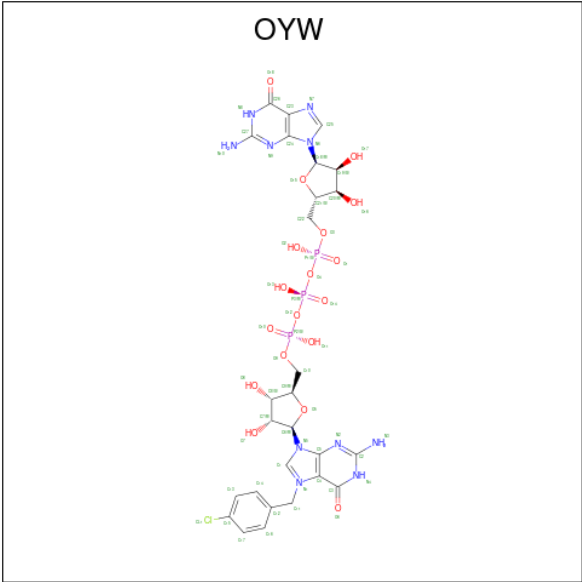
- Molecule 1 is a protein called Eukaryotic translation initiation factor 4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	3	0
			1497	963	262	266	6			
1	B	185	Total	C	N	O	S	0	2	0
			1496	958	261	271	6			
1	C	179	Total	C	N	O	S	0	0	0
			1399	896	244	253	6			
1	D	178	Total	C	N	O	S	0	1	0
			1406	900	244	256	6			

There are 4 discrepancies between the modelled and reference sequences:

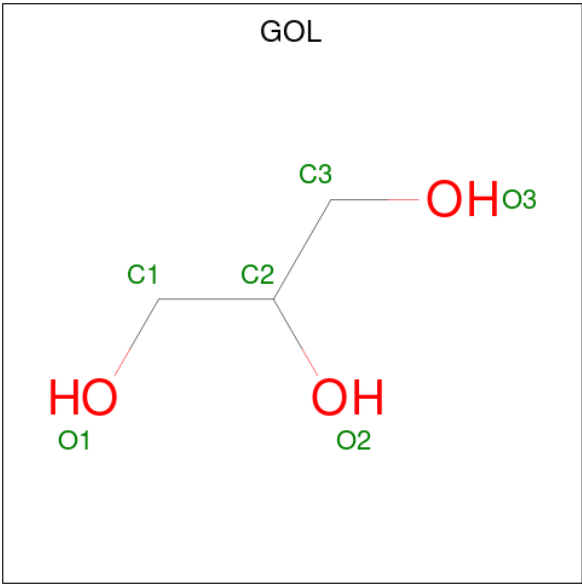
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	initiating methionine	UNP P63073
B	27	MET	-	initiating methionine	UNP P63073
C	27	MET	-	initiating methionine	UNP P63073
D	27	MET	-	initiating methionine	UNP P63073

- Molecule 2 is 4-Cl-Bn7GpppG mRNA 5' cap analog (CCD ID: OYW) (formula: $C_{27}H_{33}ClN_{10}O_{18}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	P		
2	A	1	Total 80	34	2	10	28	6	0	1
2	B	1	Total 80	34	2	10	28	6	0	1
2	C	1	Total 40	17	1	5	14	3	0	0
2	D	1	Total 40	17	1	5	14	3	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

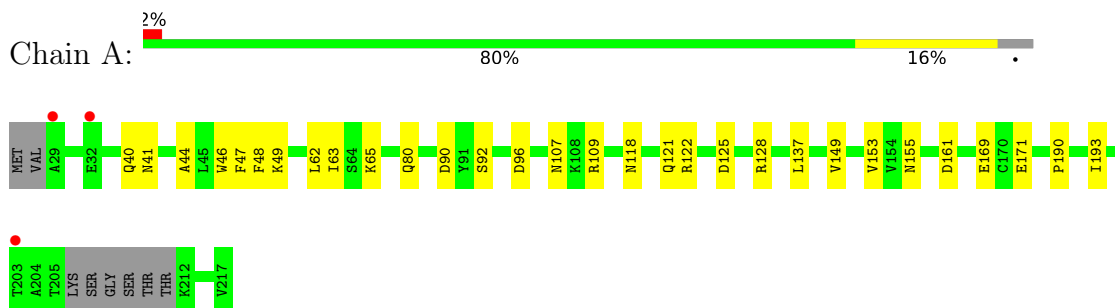
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total	O	0	0
			77	77		
4	B	81	Total	O	0	0
			81	81		
4	C	45	Total	O	0	0
			45	45		
4	D	35	Total	O	0	0
			35	35		

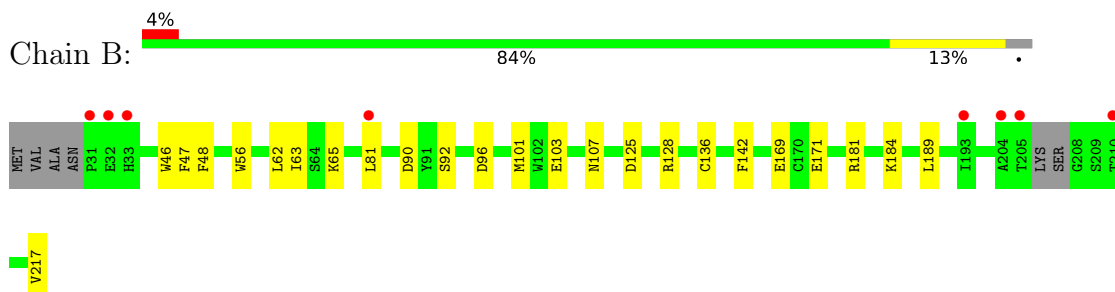
3 Residue-property plots [i](#)

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.

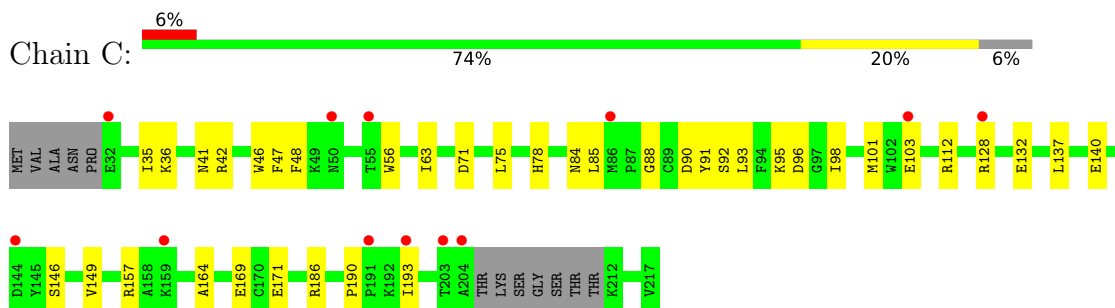
- Molecule 1: Eukaryotic translation initiation factor 4E



- Molecule 1: Eukaryotic translation initiation factor 4E

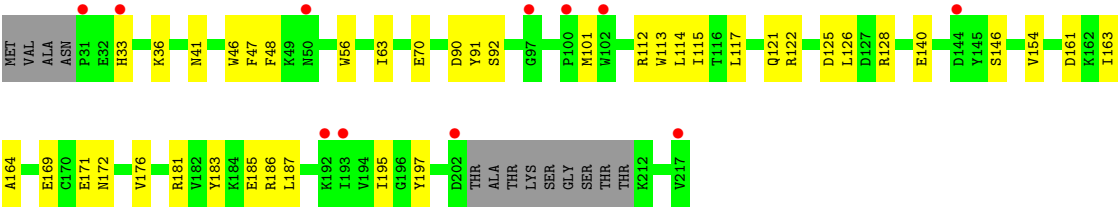


- Molecule 1: Eukaryotic translation initiation factor 4E



- Molecule 1: Eukaryotic translation initiation factor 4E





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.35Å 38.39Å 148.08Å 85.28° 88.42° 77.23°	Depositor
Resolution (Å)	49.19 – 2.66 49.19 – 2.66	Depositor EDS
% Data completeness (in resolution range)	93.6 (49.19-2.66) 93.6 (49.19-2.66)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.201 , 0.255 0.203 , 0.248	Depositor DCC
R_{free} test set	815 reflections (3.69%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6288	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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: GOL, OYW

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	0.12	0/1548	0.34	0/2102
1	B	0.12	0/1543	0.34	0/2096
1	C	0.18	0/1437	0.42	1/1959 (0.1%)
1	D	0.12	0/1449	0.31	0/1976
All	All	0.14	0/5977	0.35	1/8133 (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	128	ARG	CG-CD-NE	8.11	129.84	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1497	0	1426	23	0
1	B	1496	0	1407	14	0
1	C	1399	0	1264	25	0
1	D	1406	0	1262	23	0
2	A	80	0	0	2	0
2	B	80	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	40	0	0	2	0
2	D	40	0	0	1	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
4	A	77	0	0	2	0
4	B	81	0	0	1	0
4	C	45	0	0	0	0
4	D	35	0	0	2	0
All	All	6288	0	5375	84	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 7.

All (84) 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:D:125:ASP:OD2	1:D:128:ARG:NH2	2.16	0.78
1:C:41:ASN:ND2	1:C:140:GLU:OE2	2.20	0.74
1:A:137:LEU:HD22	1:A:149:VAL:HG11	1.71	0.72
1:A:47:PHE:HB2	1:A:63:ILE:HD11	1.72	0.72
1:C:75:LEU:HA	1:C:78:HIS:HD2	1.57	0.67
1:B:48:PHE:HB3	1:B:90:ASP:HB2	1.76	0.67
1:C:132:GLU:OE2	1:C:186:ARG:NH1	2.29	0.66
2:D:300:OYW:CL1	4:D:425:HOH:O	2.50	0.65
1:C:169:GLU:HG3	1:C:171:GLU:H	1.63	0.64
1:D:47:PHE:HB2	1:D:63:ILE:HD11	1.81	0.63
1:B:125:ASP:OD1	1:B:128:ARG:NH2	2.32	0.63
1:A:65:LYS:NZ	1:A:96:ASP:OD1	2.33	0.60
1:B:46:TRP:HB2	1:B:92:SER:HB2	1.83	0.60
1:D:122:ARG:NH1	1:D:161:ASP:OD1	2.35	0.59
1:B:47:PHE:HB2	1:B:63:ILE:HD11	1.85	0.59
1:D:172:ASN:O	1:D:176:VAL:HG23	2.03	0.58
1:C:112:ARG:HB2	1:C:164:ALA:HB1	1.86	0.58
1:C:103:GLU:OE2	1:C:103:GLU:N	2.31	0.58
1:D:126:LEU:HD12	1:D:163:ILE:HD11	1.86	0.58
1:C:48:PHE:HB3	1:C:90:ASP:HB2	1.86	0.57
1:B:184:LYS:HG3	1:B:189:LEU:HB2	1.86	0.57
1:A:122:ARG:NH2	1:A:161:ASP:OD1	2.32	0.56
1:C:46:TRP:HB2	1:C:92:SER:HB2	1.88	0.55
1:A:125:ASP:OD1	1:A:128:ARG:NH1	2.40	0.55
1:C:93:LEU:HD23	1:C:137:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:LYS:NZ	1:B:217:VAL:OXT	2.39	0.55
1:A:92:SER:OG	2:A:300[A]:OYW:CL1	2.59	0.54
1:A:92:SER:OG	2:A:300[B]:OYW:CL1	2.60	0.54
1:B:56:TRP:HZ3	1:B:101:MET:HE3	1.73	0.53
1:D:186:ARG:NH2	4:D:403:HOH:O	2.40	0.53
1:C:137:LEU:HD22	1:C:149:VAL:HG21	1.91	0.53
1:A:80:GLN:HG2	1:D:36:LYS:HG2	1.91	0.53
1:C:190:PRO:HG2	1:C:193:ILE:HG12	1.91	0.53
1:D:46:TRP:HB2	1:D:92:SER:HB2	1.89	0.53
1:C:157:ARG:NH1	2:C:300:OYW:O11	2.40	0.51
1:D:112:ARG:HB2	1:D:164:ALA:HB1	1.93	0.51
1:A:107:ASN:ND2	4:A:403:HOH:O	2.35	0.51
1:A:80:GLN:NE2	1:D:70:GLU:HG2	2.26	0.50
1:A:62:LEU:HD21	1:A:65:LYS:HE2	1.94	0.49
1:A:48:PHE:HB3	1:A:90:ASP:HB2	1.94	0.49
1:B:169:GLU:HG3	1:B:171:GLU:H	1.77	0.49
1:B:107:ASN:ND2	4:B:403:HOH:O	2.35	0.49
1:D:41:ASN:ND2	1:D:140:GLU:OE2	2.44	0.49
1:C:75:LEU:HA	1:C:78:HIS:CD2	2.43	0.49
1:A:190:PRO:HG2	1:A:193:ILE:HG12	1.94	0.48
1:C:103:GLU:OE1	2:C:300:OYW:N3	2.46	0.48
1:D:169:GLU:HG3	1:D:171:GLU:H	1.77	0.48
1:D:91:TYR:HB2	1:D:154:VAL:CG1	2.43	0.48
1:C:36:LYS:NZ	1:C:71:ASP:OD1	2.42	0.48
1:D:181:ARG:O	1:D:185:GLU:HG3	2.14	0.48
1:C:47:PHE:HB2	1:C:63:ILE:HD11	1.96	0.47
1:A:44:ALA:HB1	1:A:62:LEU:HD11	1.95	0.46
1:D:48:PHE:HB3	1:D:90:ASP:HB2	1.98	0.45
1:D:113:TRP:CD2	1:D:197:TYR:HB2	2.51	0.45
1:A:92:SER:OG	1:A:153:VAL:HG22	2.16	0.45
1:A:40:GLN:HG2	1:A:41:ASN:OD1	2.17	0.45
1:A:122:ARG:HH21	1:A:161:ASP:CG	2.23	0.45
1:B:181:ARG:HG2	1:B:217:VAL:HG21	1.99	0.45
1:A:169:GLU:HG3	1:A:171:GLU:H	1.83	0.44
1:A:49:LYS:HD2	1:D:33:HIS:CD2	2.52	0.44
1:A:90:ASP:OD1	1:A:155:ASN:ND2	2.50	0.44
1:D:56:TRP:HZ3	1:D:101:MET:HE3	1.83	0.44
1:C:75:LEU:HD12	1:C:78:HIS:NE2	2.33	0.44
1:C:84:ASN:O	1:C:84:ASN:ND2	2.48	0.44
1:C:95:LYS:HB2	1:C:98:ILE:HD12	1.99	0.43
1:B:65:LYS:NZ	1:B:96:ASP:OD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LEU:HD21	1:B:65:LYS:HE2	2.01	0.43
1:C:42:ARG:HG2	1:C:96:ASP:HB2	2.00	0.43
1:C:88:GLY:HA2	1:C:157:ARG:HH21	1.83	0.43
1:C:85:LEU:HD11	1:C:91:TYR:CE2	2.54	0.42
1:A:46:TRP:HB2	1:A:92:SER:HB2	2.01	0.42
1:C:35:ILE:O	1:C:35:ILE:HG13	2.19	0.42
1:D:183:TYR:CZ	1:D:187:LEU:HD11	2.54	0.42
1:B:136:CYS:HB3	1:B:142:PHE:CE2	2.55	0.42
1:B:101:MET:HE2	1:B:103:GLU:OE1	2.20	0.42
1:D:122:ARG:HH11	1:D:161:ASP:CG	2.28	0.42
1:C:56:TRP:HZ3	1:C:101:MET:HE3	1.86	0.41
1:D:114:LEU:O	1:D:195:ILE:HG23	2.21	0.41
1:D:117:LEU:HG	1:D:121:GLN:HB2	2.02	0.41
1:A:118:ASN:OD1	1:A:121:GLN:HG3	2.20	0.41
1:A:109:ARG:O	1:A:169:GLU:HA	2.22	0.40
1:C:146:SER:O	1:C:149:VAL:HG12	2.20	0.40
1:D:114:LEU:HD12	1:D:115:ILE:N	2.37	0.40
3:A:301:GOL:H32	4:A:401:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	182/191 (95%)	179 (98%)	3 (2%)	0	100	100
1	B	183/191 (96%)	178 (97%)	5 (3%)	0	100	100
1	C	175/191 (92%)	172 (98%)	3 (2%)	0	100	100
1	D	175/191 (92%)	172 (98%)	3 (2%)	0	100	100
All	All	715/764 (94%)	701 (98%)	14 (2%)	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	155/170 (91%)	155 (100%)	0	100	100
1	B	154/170 (91%)	153 (99%)	1 (1%)	78	88
1	C	135/170 (79%)	135 (100%)	0	100	100
1	D	137/170 (81%)	136 (99%)	1 (1%)	76	86
All	All	581/680 (85%)	579 (100%)	2 (0%)	86	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	LEU
1	D	146	SER

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	80	GLN
1	A	178	HIS
1	B	50	ASN
1	B	57	GLN
1	B	121	GLN
1	C	107	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	OYW	B	300[D]	-	42,43,65	2.78	11 (26%)	60,67,101	1.73	13 (21%)
2	OYW	B	300[C]	-	42,43,65	2.13	11 (26%)	60,67,101	1.67	13 (21%)
2	OYW	C	300	-	42,43,65	2.78	12 (28%)	60,67,101	1.70	12 (20%)
2	OYW	A	300[A]	-	42,43,65	2.09	9 (21%)	60,67,101	1.69	13 (21%)
2	OYW	D	300	-	42,43,65	2.99	12 (28%)	60,67,101	1.70	12 (20%)
3	GOL	A	301	-	5,5,5	0.38	0	5,5,5	0.28	0
2	OYW	A	300[B]	-	42,43,65	2.79	11 (26%)	60,67,101	1.75	14 (23%)
3	GOL	B	301	-	5,5,5	0.38	0	5,5,5	0.29	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
2	OYW	B	300[D]	-	-	4/26/42/68	0/4/4/7
2	OYW	B	300[C]	-	-	6/26/42/68	0/4/4/7
2	OYW	C	300	-	-	4/26/42/68	0/4/4/7
2	OYW	A	300[A]	-	-	5/26/42/68	0/4/4/7
2	OYW	D	300	-	-	9/26/42/68	0/4/4/7
3	GOL	A	301	-	-	2/4/4/4	-
2	OYW	A	300[B]	-	-	5/26/42/68	0/4/4/7
3	GOL	B	301	-	-	1/4/4/4	-

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300[D]	OYW	P2-O12	-11.18	1.47	1.59
2	A	300[B]	OYW	P2-O12	-10.52	1.48	1.59
2	C	300	OYW	P2-O12	-9.19	1.49	1.59
2	D	300	OYW	P2-O12	-9.18	1.49	1.59
2	D	300	OYW	P3-O12	8.21	1.68	1.59
2	D	300	OYW	P3-O4	7.90	1.68	1.59
2	A	300[B]	OYW	O6-C3	6.82	1.36	1.23
2	A	300[A]	OYW	O6-C3	6.80	1.36	1.23
2	D	300	OYW	O6-C3	6.78	1.36	1.23
2	B	300[D]	OYW	O6-C3	6.78	1.36	1.23
2	B	300[C]	OYW	O6-C3	6.78	1.36	1.23
2	C	300	OYW	O6-C3	6.77	1.36	1.23
2	C	300	OYW	P3-O12	6.64	1.66	1.59
2	A	300[B]	OYW	C11-C12	-5.95	1.39	1.51
2	C	300	OYW	P3-O4	5.92	1.65	1.59
2	A	300[A]	OYW	C11-C12	-5.80	1.39	1.51
2	B	300[D]	OYW	C11-C12	-5.67	1.39	1.51
2	B	300[C]	OYW	C11-C12	-5.61	1.39	1.51
2	C	300	OYW	C11-C12	-5.51	1.40	1.51
2	D	300	OYW	C11-C12	-5.49	1.40	1.51
2	A	300[B]	OYW	P3-O4	5.25	1.65	1.59
2	A	300[B]	OYW	P3-O12	4.98	1.64	1.59
2	B	300[D]	OYW	P3-O12	4.50	1.64	1.59
2	A	300[A]	OYW	P3-O12	4.44	1.64	1.59
2	B	300[D]	OYW	P3-O4	4.28	1.64	1.59
2	B	300[C]	OYW	P1-O2	-3.99	1.40	1.54
2	B	300[C]	OYW	P3-O4	3.98	1.63	1.59
2	B	300[C]	OYW	P1-O3	-3.88	1.40	1.54
2	C	300	OYW	P1-O1	3.67	1.61	1.50
2	D	300	OYW	P1-O1	3.65	1.61	1.50
2	B	300[D]	OYW	P1-O1	3.61	1.61	1.50
2	A	300[B]	OYW	P1-O1	3.57	1.61	1.50
2	A	300[A]	OYW	P1-O1	3.44	1.61	1.50
2	B	300[D]	OYW	C4-N1	-3.43	1.34	1.39
2	B	300[C]	OYW	C4-N1	-3.43	1.34	1.39
2	A	300[B]	OYW	C4-N1	-3.40	1.34	1.39
2	D	300	OYW	C4-N1	-3.40	1.34	1.39
2	A	300[A]	OYW	C4-N1	-3.39	1.34	1.39
2	C	300	OYW	C4-N1	-3.34	1.34	1.39
2	C	300	OYW	P2-O11	-3.34	1.39	1.55
2	D	300	OYW	P2-O11	-3.29	1.40	1.55
2	A	300[B]	OYW	P2-O11	-3.21	1.40	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300[C]	OYW	C4-C3	-3.20	1.33	1.43
2	B	300[D]	OYW	P2-O11	-3.20	1.40	1.55
2	B	300[D]	OYW	C4-C3	-3.15	1.34	1.43
2	C	300	OYW	C4-C3	-3.15	1.34	1.43
2	A	300[A]	OYW	C4-C3	-3.14	1.34	1.43
2	A	300[A]	OYW	P2-O12	3.08	1.62	1.59
2	A	300[B]	OYW	C4-C3	-3.07	1.34	1.43
2	D	300	OYW	C4-C3	-3.07	1.34	1.43
2	A	300[B]	OYW	P2-O10	-3.05	1.40	1.50
2	B	300[D]	OYW	P2-O10	-3.04	1.40	1.50
2	A	300[A]	OYW	P3-O4	3.03	1.62	1.59
2	D	300	OYW	P2-O10	-3.02	1.40	1.50
2	C	300	OYW	P2-O10	-2.95	1.40	1.50
2	B	300[C]	OYW	P2-O12	2.77	1.62	1.59
2	B	300[C]	OYW	P3-O12	2.57	1.62	1.59
2	B	300[C]	OYW	C3-N4	-2.48	1.34	1.38
2	B	300[D]	OYW	C3-N4	-2.47	1.34	1.38
2	A	300[B]	OYW	C3-N4	-2.40	1.34	1.38
2	A	300[A]	OYW	C3-N4	-2.36	1.34	1.38
2	C	300	OYW	C3-N4	-2.35	1.34	1.38
2	D	300	OYW	C3-N4	-2.35	1.34	1.38
2	B	300[C]	OYW	P1-O1	-2.18	1.43	1.50
2	D	300	OYW	P1-O2	-2.06	1.47	1.54
2	C	300	OYW	P1-O2	-2.04	1.47	1.54

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	300	OYW	C2-N2-C5	4.79	120.55	112.30
2	A	300[B]	OYW	C2-N2-C5	4.75	120.48	112.30
2	D	300	OYW	C4-C3-N4	4.67	121.50	111.84
2	C	300	OYW	O6-C3-C4	-4.67	117.59	128.01
2	A	300[B]	OYW	C4-C3-N4	4.65	121.45	111.84
2	C	300	OYW	C2-N2-C5	4.64	120.30	112.30
2	C	300	OYW	C4-C3-N4	4.64	121.43	111.84
2	B	300[D]	OYW	C2-N2-C5	4.63	120.28	112.30
2	B	300[D]	OYW	C4-C3-N4	4.60	121.35	111.84
2	A	300[A]	OYW	O6-C3-C4	-4.60	117.75	128.01
2	A	300[A]	OYW	C4-C3-N4	4.60	121.34	111.84
2	B	300[C]	OYW	O6-C3-C4	-4.58	117.78	128.01
2	A	300[A]	OYW	C2-N2-C5	4.58	120.19	112.30
2	B	300[D]	OYW	O6-C3-C4	-4.57	117.80	128.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300[B]	OYW	O6-C3-C4	-4.55	117.84	128.01
2	B	300[C]	OYW	C4-C3-N4	4.54	121.23	111.84
2	D	300	OYW	O6-C3-C4	-4.54	117.87	128.01
2	B	300[C]	OYW	C2-N2-C5	4.53	120.10	112.30
2	A	300[B]	OYW	C4-C5-N2	-4.17	120.27	128.15
2	B	300[D]	OYW	C11-N1-C1	-4.08	120.70	124.69
2	D	300	OYW	C4-C5-N2	-4.07	120.45	128.15
2	B	300[D]	OYW	C4-C5-N2	-4.06	120.48	128.15
2	C	300	OYW	C11-N1-C1	-3.99	120.79	124.69
2	B	300[C]	OYW	C11-N1-C1	-3.97	120.81	124.69
2	C	300	OYW	C4-C5-N2	-3.95	120.69	128.15
2	A	300[B]	OYW	C11-N1-C1	-3.93	120.86	124.69
2	B	300[C]	OYW	C4-C5-N2	-3.91	120.76	128.15
2	A	300[A]	OYW	C4-C5-N2	-3.88	120.82	128.15
2	A	300[A]	OYW	C11-N1-C1	-3.71	121.07	124.69
2	A	300[B]	OYW	O5-C9-C8	-3.33	98.55	105.15
2	B	300[D]	OYW	O5-C9-C8	-3.27	98.67	105.15
2	D	300	OYW	C11-N1-C1	-3.21	121.56	124.69
2	A	300[B]	OYW	C2-N4-C3	-3.13	119.44	125.11
2	D	300	OYW	C2-N4-C3	-3.10	119.48	125.11
2	C	300	OYW	C2-N4-C3	-3.05	119.58	125.11
2	A	300[A]	OYW	C2-N4-C3	-3.05	119.58	125.11
2	B	300[D]	OYW	C2-N4-C3	-3.02	119.64	125.11
2	A	300[A]	OYW	O5-C9-C8	-2.93	99.33	105.15
2	B	300[C]	OYW	C2-N4-C3	-2.93	119.79	125.11
2	A	300[B]	OYW	O3-P1-O4	2.92	114.44	104.64
2	D	300	OYW	O5-C9-C8	-2.90	99.39	105.15
2	B	300[D]	OYW	O3-P1-O4	2.87	114.26	104.64
2	A	300[A]	OYW	O3-P1-O4	2.80	114.01	104.64
2	A	300[B]	OYW	N5-C5-N2	2.72	131.40	125.95
2	C	300	OYW	O5-C9-C8	-2.70	99.79	105.15
2	C	300	OYW	O3-P1-O4	2.70	113.68	104.64
2	B	300[D]	OYW	N5-C5-N2	2.69	131.34	125.95
2	B	300[C]	OYW	O5-C9-C8	-2.69	99.81	105.15
2	D	300	OYW	O3-P1-O4	2.67	113.60	104.64
2	C	300	OYW	N5-C5-N2	2.59	131.13	125.95
2	B	300[C]	OYW	N5-C5-N2	2.58	131.11	125.95
2	A	300[B]	OYW	O5-C9-C10	2.54	117.46	109.33
2	D	300	OYW	N5-C5-N2	2.53	131.01	125.95
2	A	300[A]	OYW	C8-C7-C6	-2.50	96.73	101.46
2	A	300[A]	OYW	N5-C5-N2	2.47	130.88	125.95
2	B	300[C]	OYW	O3-P1-O4	2.39	112.64	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300[D]	OYW	O5-C9-C10	2.33	116.79	109.33
2	B	300[C]	OYW	O5-C9-C10	2.30	116.69	109.33
2	A	300[B]	OYW	C12-C11-N1	-2.27	109.24	112.48
2	D	300	OYW	C10-C9-C8	-2.21	107.26	115.21
2	B	300[D]	OYW	C10-C9-C8	-2.20	107.31	115.21
2	C	300	OYW	C10-C9-C8	-2.19	107.32	115.21
2	C	300	OYW	O5-C9-C10	2.18	116.33	109.33
2	D	300	OYW	N4-C2-N2	-2.13	119.42	123.32
2	C	300	OYW	N4-C2-N2	-2.12	119.44	123.32
2	A	300[A]	OYW	C12-C11-N1	-2.12	109.46	112.48
2	B	300[C]	OYW	N4-C2-N2	-2.11	119.46	123.32
2	B	300[D]	OYW	N4-C2-N2	-2.10	119.49	123.32
2	D	300	OYW	O5-C9-C10	2.09	116.03	109.33
2	A	300[A]	OYW	C10-C9-C8	-2.09	107.70	115.21
2	A	300[A]	OYW	N4-C2-N2	-2.08	119.51	123.32
2	A	300[B]	OYW	N4-C2-N2	-2.08	119.52	123.32
2	A	300[B]	OYW	C10-C9-C8	-2.05	107.84	115.21
2	B	300[D]	OYW	O12-P2-O10	2.03	116.82	110.70
2	B	300[C]	OYW	C8-C7-C6	-2.03	97.62	101.46
2	B	300[C]	OYW	C10-C9-C8	-2.03	107.90	115.21
2	A	300[B]	OYW	O12-P2-O10	2.01	116.76	110.70

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	300	OYW	C10-O9-P2-O11
2	D	300	OYW	P3-O4-P1-O2
2	D	300	OYW	P3-O4-P1-O3
2	D	300	OYW	C10-O9-P2-O10
2	D	300	OYW	C10-O9-P2-O11
2	A	300[B]	OYW	P3-O12-P2-O10
2	B	300[C]	OYW	P3-O12-P2-O10
2	D	300	OYW	P2-O12-P3-O14
3	A	301	GOL	O1-C1-C2-O2
2	A	300[B]	OYW	C10-O9-P2-O10
2	B	300[D]	OYW	C10-O9-P2-O10
2	C	300	OYW	C10-O9-P2-O10
2	D	300	OYW	C10-O9-P2-O12
2	B	300[C]	OYW	P1-O4-P3-O14
2	A	300[B]	OYW	C12-C11-N1-C4
2	B	300[D]	OYW	C12-C11-N1-C4

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Mol	Chain	Res	Type	Atoms
3	A	301	GOL	O1-C1-C2-C3
2	A	300[A]	OYW	P1-O4-P3-O14
2	B	300[D]	OYW	P3-O12-P2-O10
2	D	300	OYW	C9-C10-O9-P2
2	A	300[A]	OYW	C12-C11-N1-C4
2	B	300[C]	OYW	C12-C11-N1-C4
2	C	300	OYW	C12-C11-N1-C4
3	B	301	GOL	O1-C1-C2-O2
2	A	300[B]	OYW	C9-C10-O9-P2
2	B	300[C]	OYW	P1-O4-P3-O13
2	B	300[D]	OYW	P3-O12-P2-O11
2	C	300	OYW	C12-C11-N1-C1
2	D	300	OYW	P3-O4-P1-O1
2	A	300[A]	OYW	C12-C11-N1-C1
2	B	300[C]	OYW	C12-C11-N1-C1
2	A	300[A]	OYW	P1-O4-P3-O13
2	A	300[A]	OYW	P3-O12-P2-O11
2	A	300[B]	OYW	P3-O12-P2-O11
2	B	300[C]	OYW	P3-O12-P2-O11
2	D	300	OYW	P1-O4-P3-O13

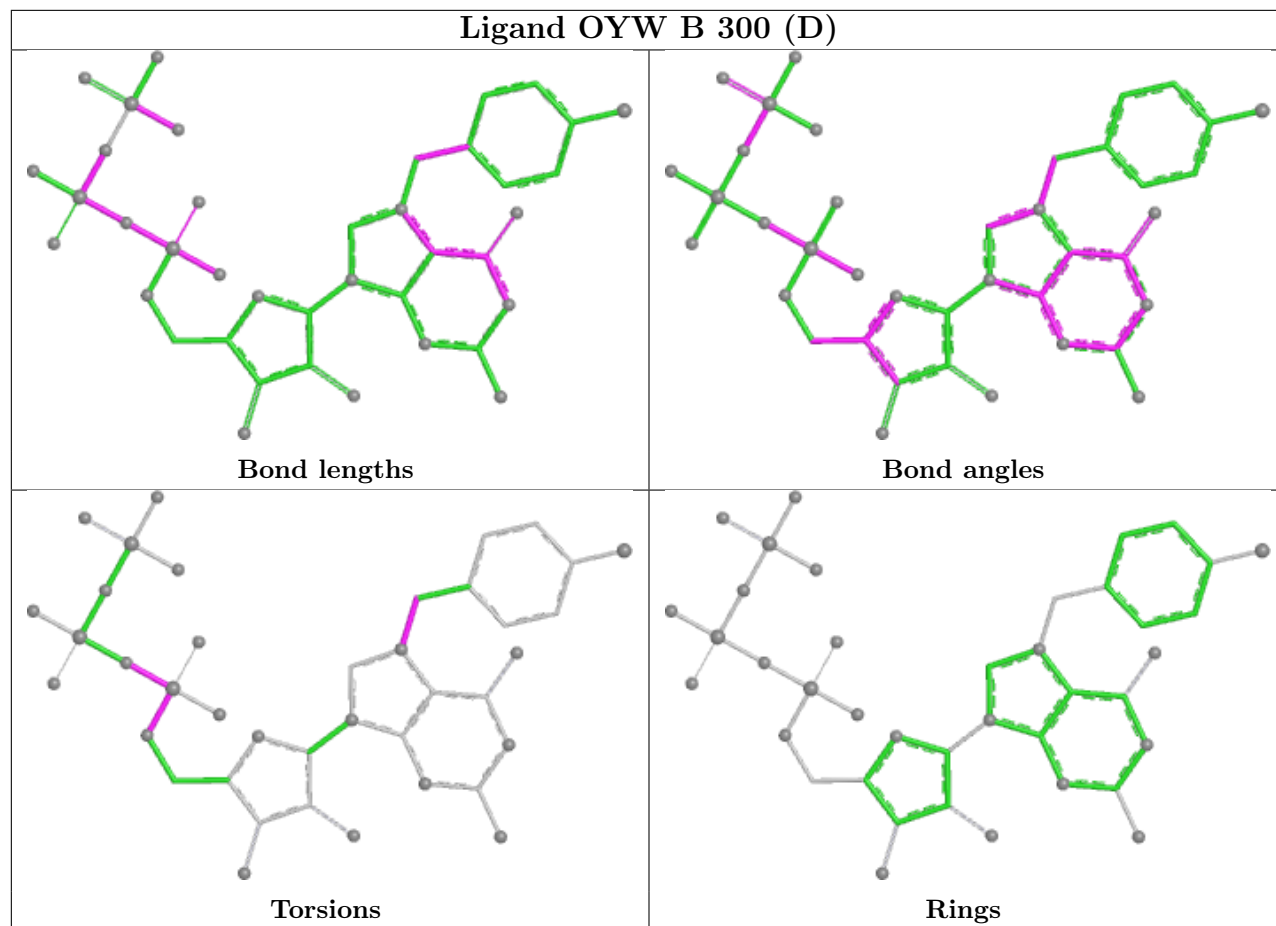
There are no ring outliers.

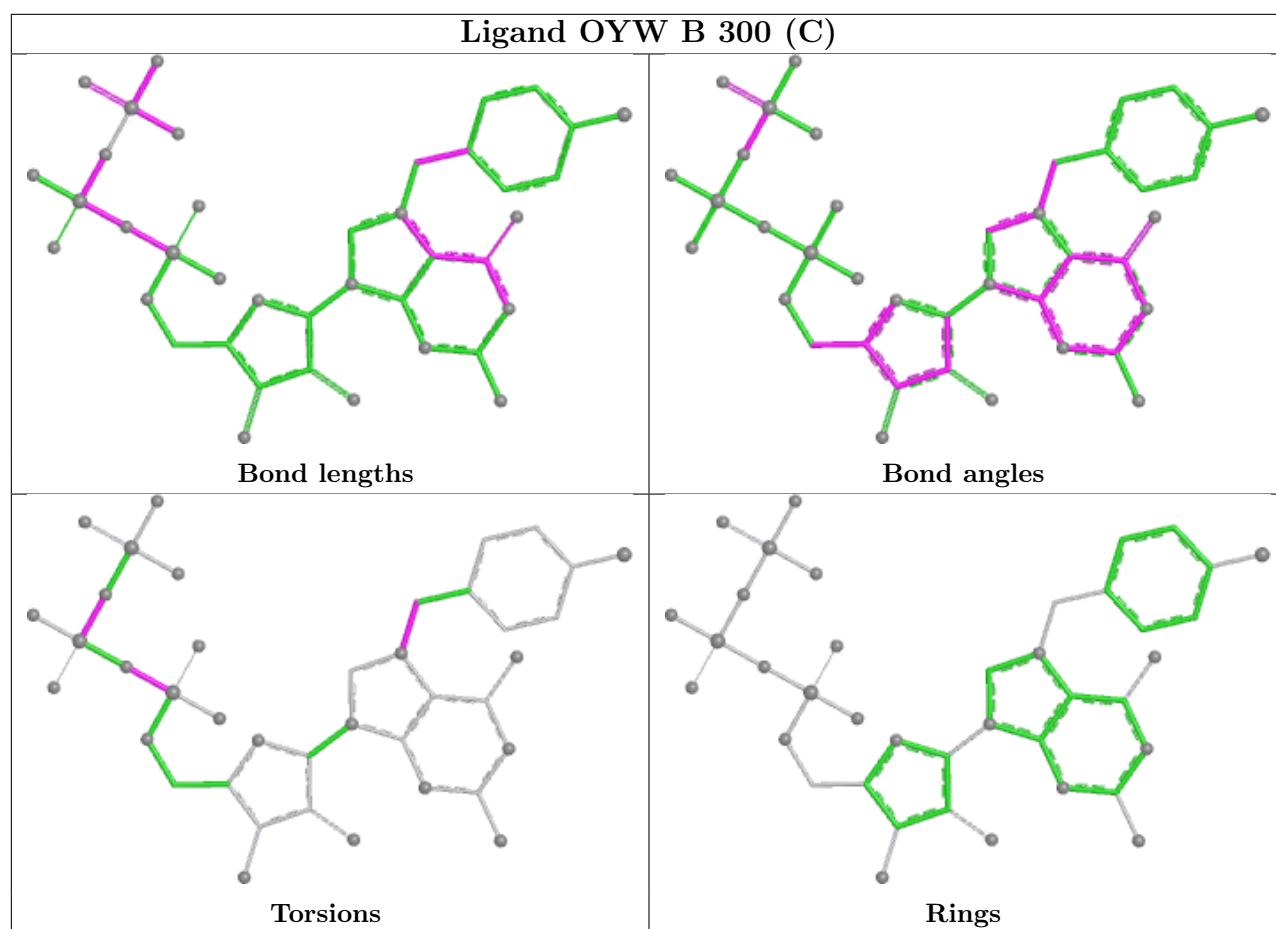
5 monomers are involved in 6 short contacts:

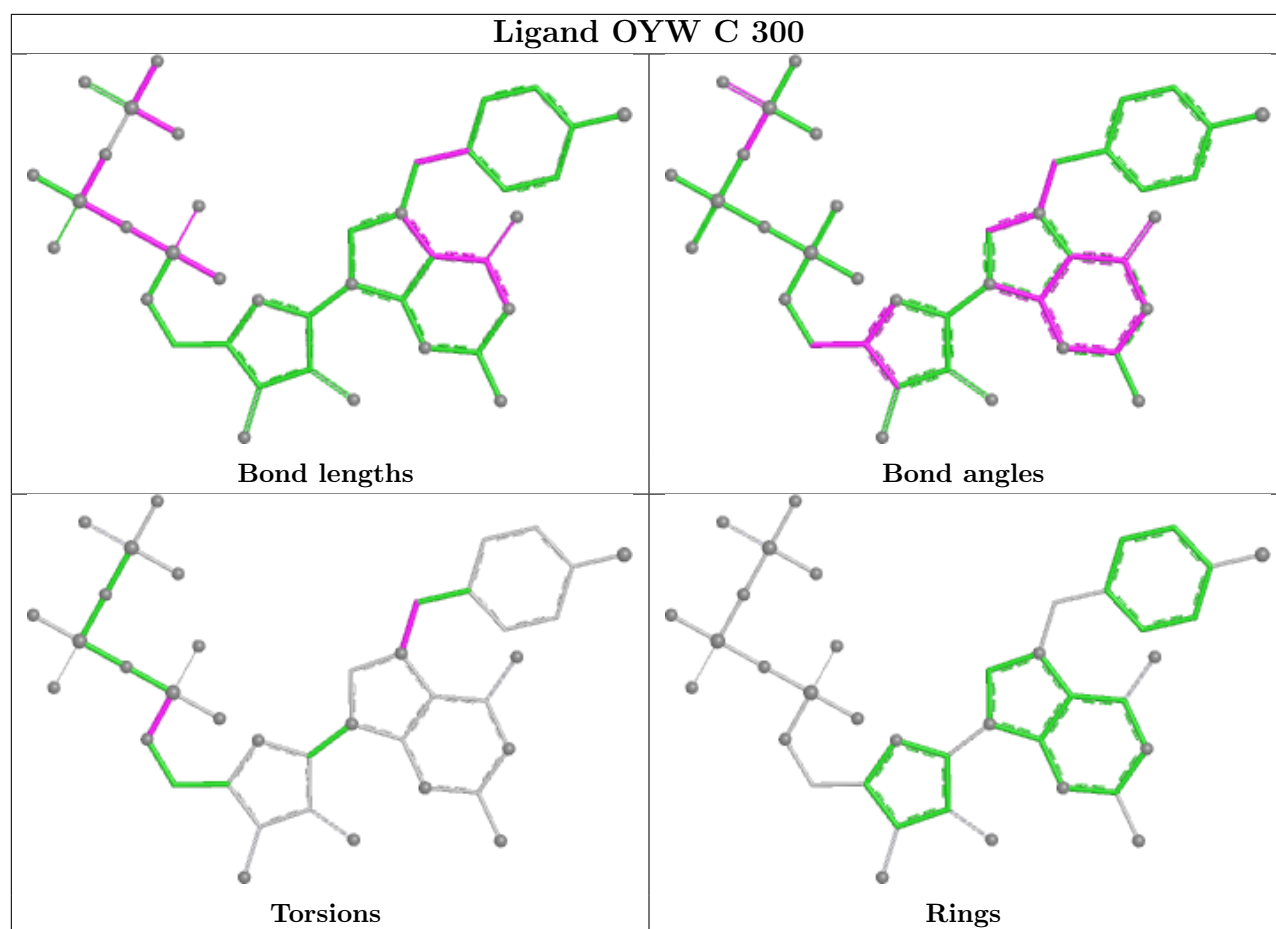
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	300	OYW	2	0
2	A	300[A]	OYW	1	0
2	D	300	OYW	1	0
3	A	301	GOL	1	0
2	A	300[B]	OYW	1	0

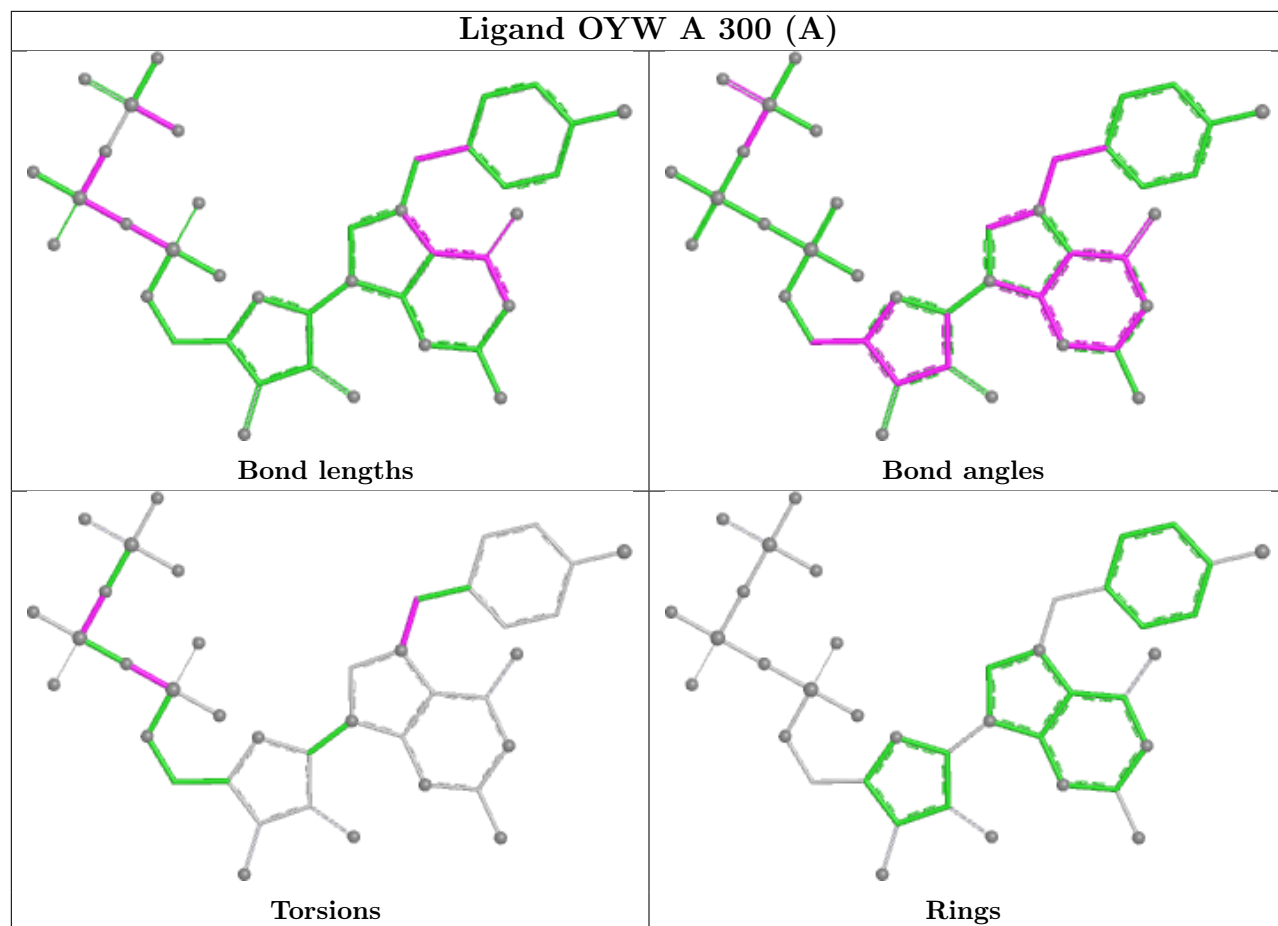
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

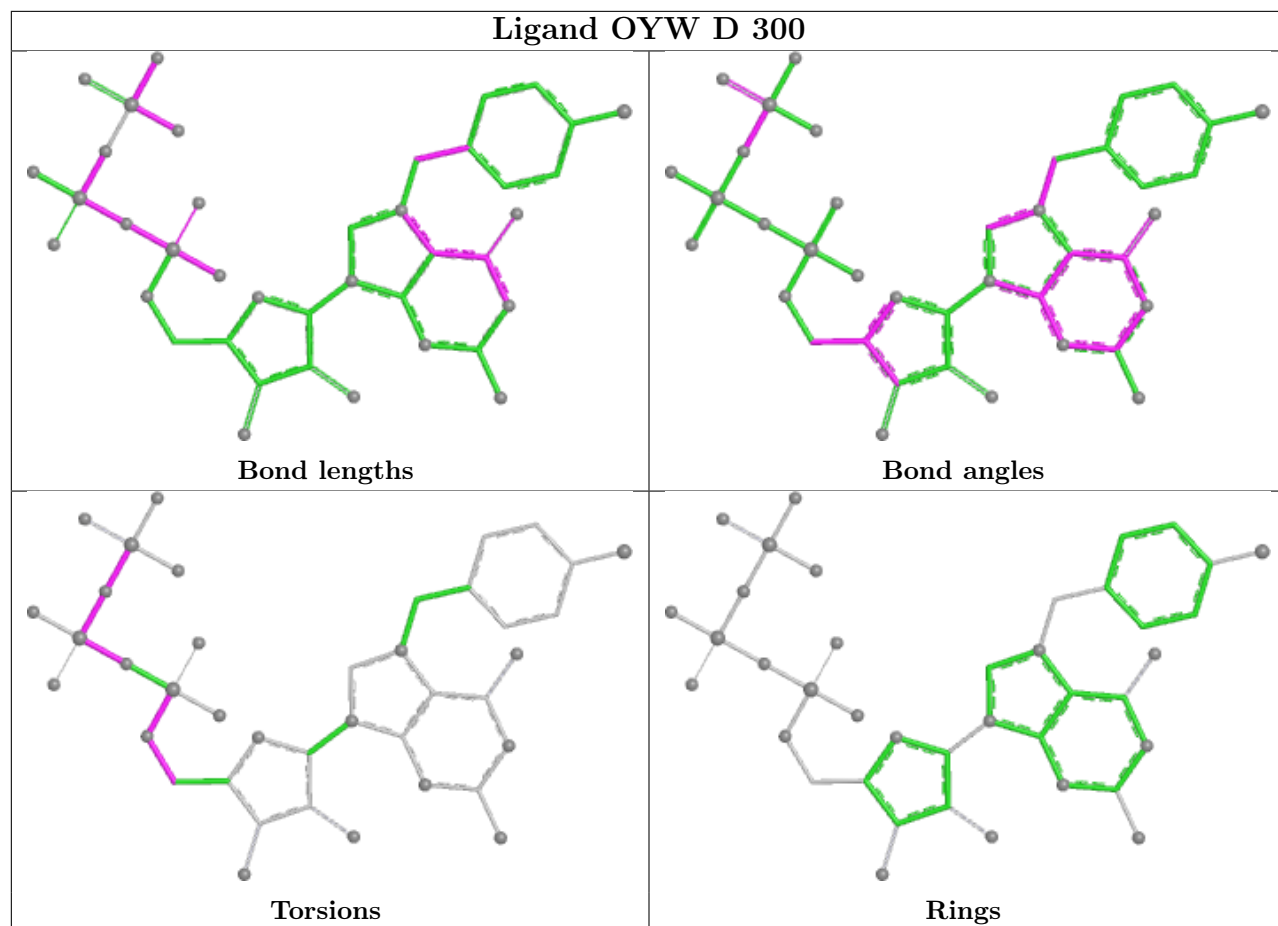
equivalents in the CSD to analyse the geometry.

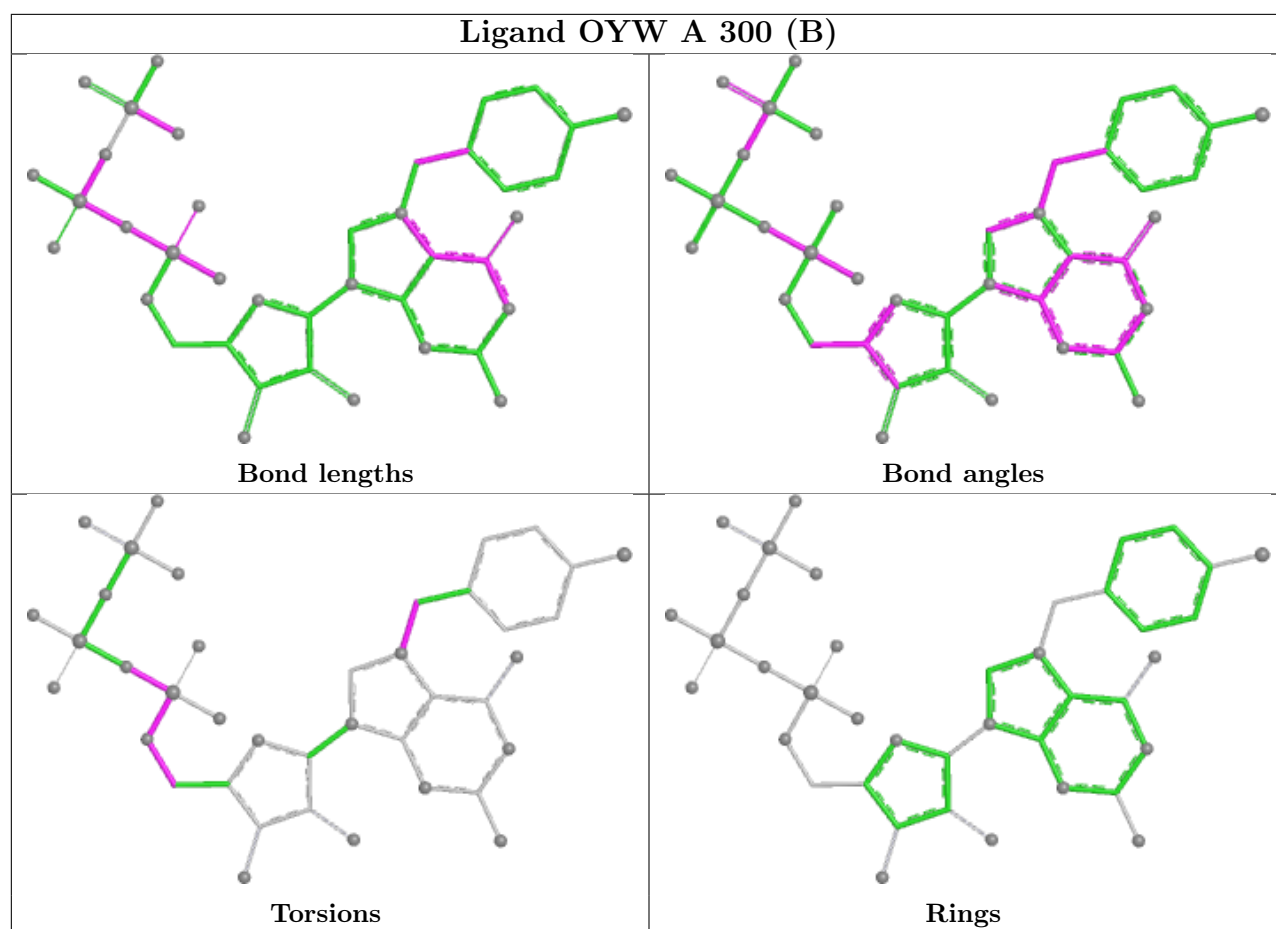












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	183/191 (95%)	0.21	3 (1%) 70 66	19, 35, 59, 83	3 (1%)
1	B	185/191 (96%)	0.22	8 (4%) 40 32	17, 36, 67, 96	2 (1%)
1	C	179/191 (93%)	0.53	12 (6%) 24 18	28, 51, 85, 96	0
1	D	178/191 (93%)	0.51	11 (6%) 26 20	22, 50, 83, 106	1 (0%)
All	All	725/764 (94%)	0.37	34 (4%) 36 28	17, 41, 79, 106	6 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	32	GLU	5.8
1	D	202	ASP	3.9
1	B	32	GLU	3.7
1	D	31	PRO	3.7
1	C	204	ALA	3.3
1	B	205	THR	3.2
1	B	33	HIS	2.9
1	B	31	PRO	2.8
1	A	29	ALA	2.8
1	B	193	ILE	2.8
1	C	193	ILE	2.8
1	D	100	PRO	2.8
1	D	50	ASN	2.7
1	A	32	GLU	2.7
1	D	97	GLY	2.5
1	A	203	THR	2.5
1	B	204	ALA	2.5
1	C	159	LYS	2.4
1	C	103	GLU	2.4
1	C	144	ASP	2.4
1	D	217	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	102	TRP	2.3
1	C	128	ARG	2.3
1	D	192	LYS	2.2
1	B	210	THR	2.2
1	C	50	ASN	2.2
1	D	193	ILE	2.2
1	B	81	LEU	2.2
1	D	33	HIS	2.2
1	D	144	ASP	2.1
1	C	55	THR	2.1
1	C	191	PRO	2.1
1	C	86	MET	2.1
1	C	203	THR	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.

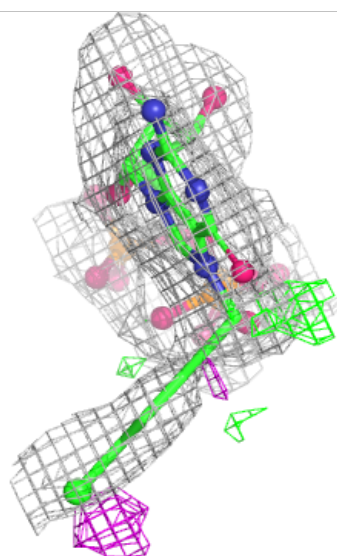
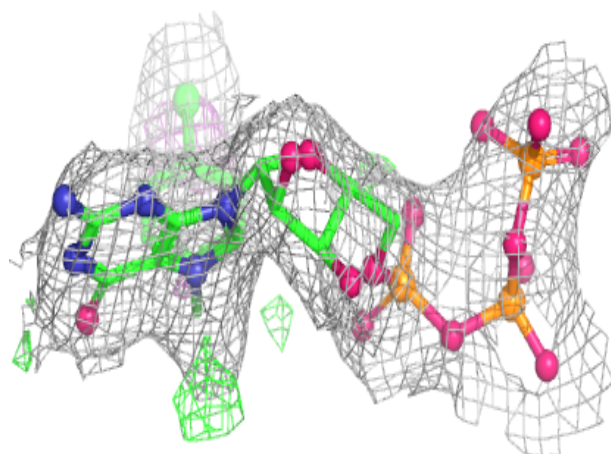
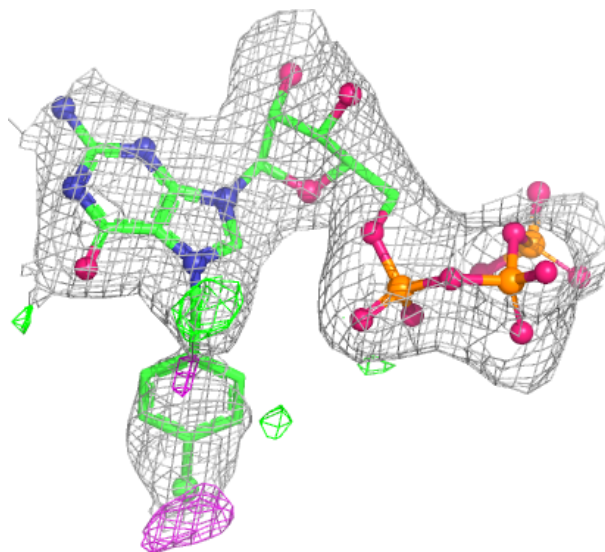
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OYW	A	300[A]	40/59	0.83	0.14	50,56,64,71	40
2	OYW	A	300[B]	40/59	0.83	0.14	50,57,65,71	40
3	GOL	A	301	6/6	0.83	0.13	42,51,53,54	0
2	OYW	D	300	40/59	0.84	0.12	58,68,92,97	0
2	OYW	C	300	40/59	0.84	0.11	55,67,94,97	0
2	OYW	B	300[D]	40/59	0.85	0.13	27,46,58,59	40
2	OYW	B	300[C]	40/59	0.85	0.13	28,45,62,65	40
3	GOL	B	301	6/6	0.86	0.11	42,44,47,49	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.

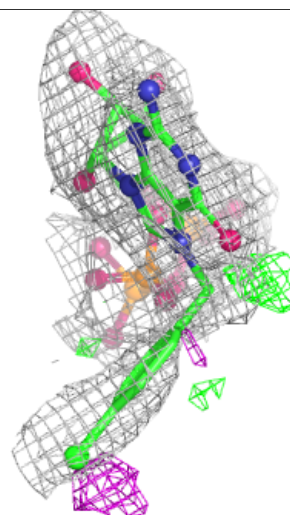
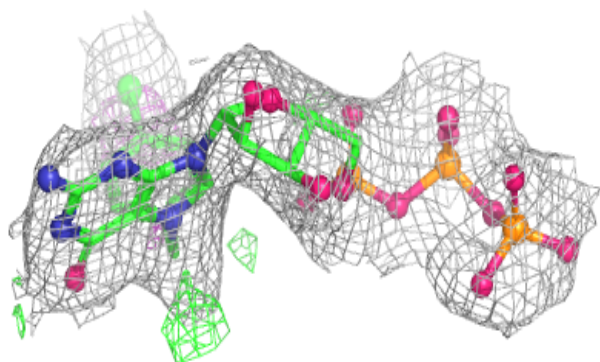
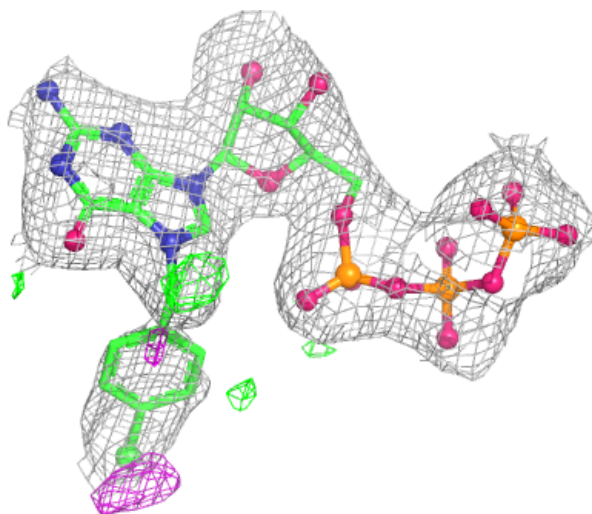
Electron density around OYW A 300 (A):

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



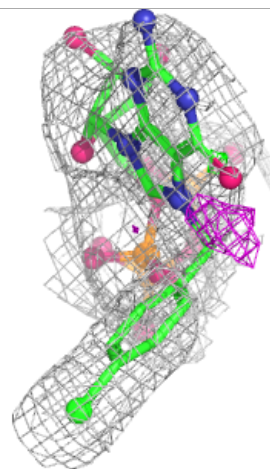
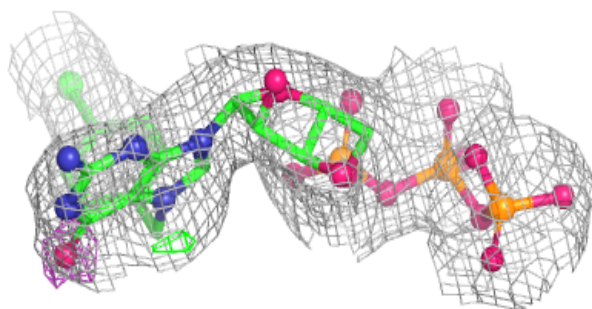
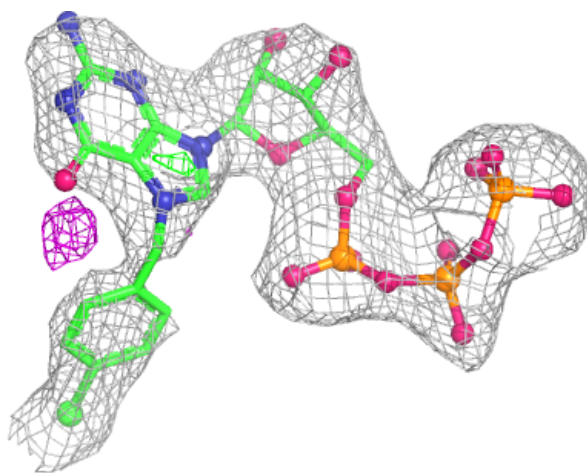
Electron density around OYW A 300 (B):

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



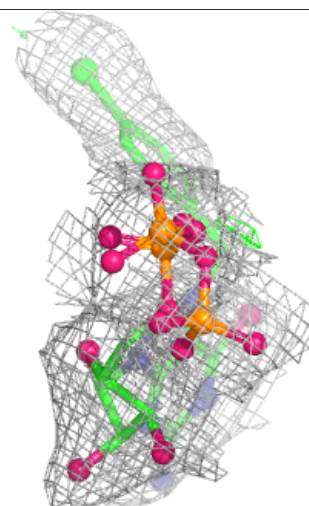
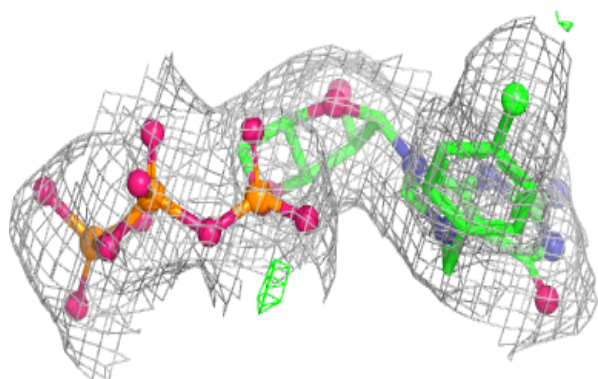
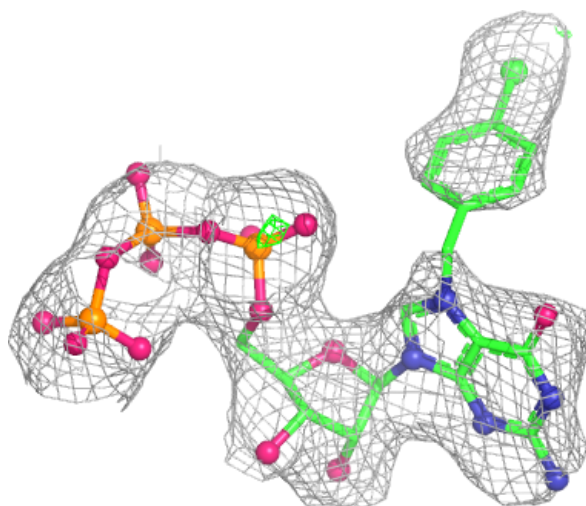
Electron density around OYW D 300:

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



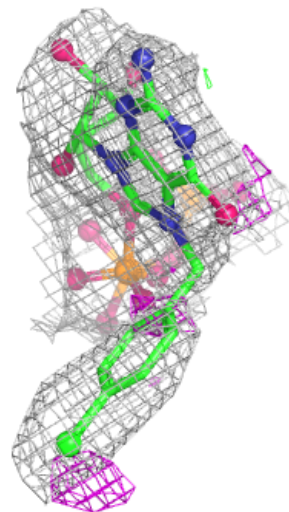
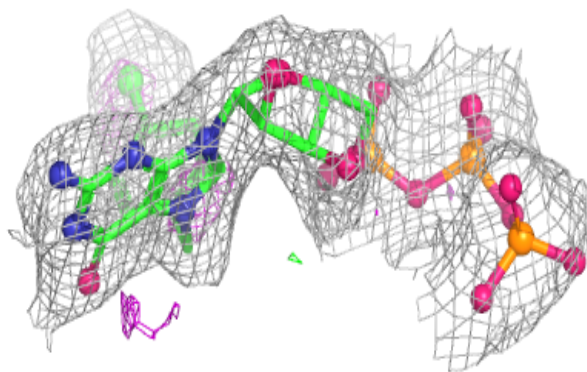
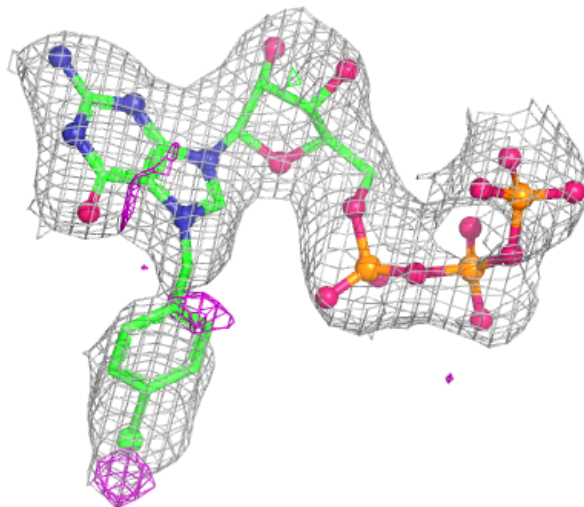
Electron density around OYW C 300:

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



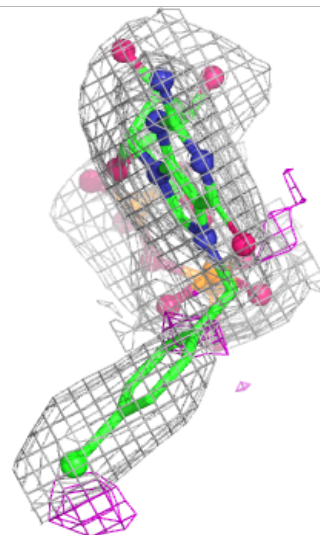
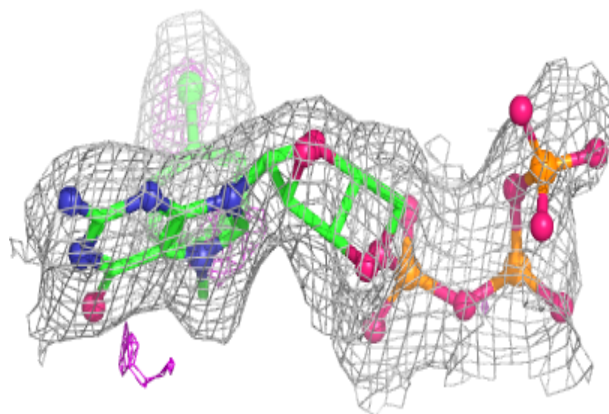
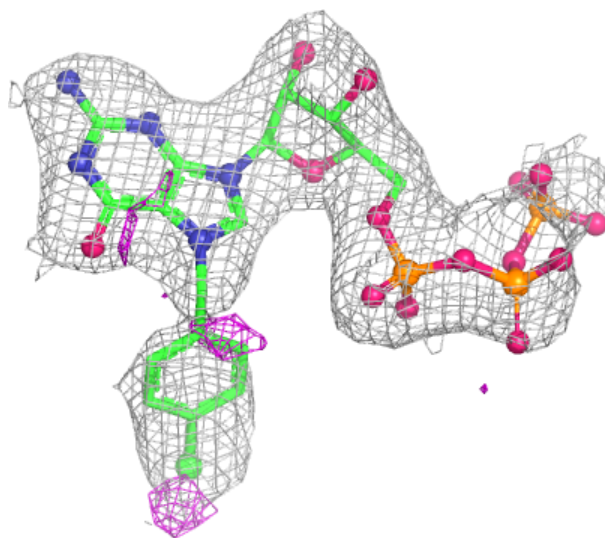
Electron density around OYW B 300 (D):

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



Electron density around OYW B 300 (C):

$2mF_o-DF_c$ (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.