



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 03:20 PM BST

PDB ID : 6N95  
Title : Methylmalonyl-CoA decarboxylase in complex with 2-sulfonate-propionyl-CoA  
Authors : Stunkard, L.M.; Dixon, A.D.; Huth, T.J.; Lohman, J.R.  
Deposited on : 2018-11-30  
Resolution : 1.80 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.13  
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) : 2.13

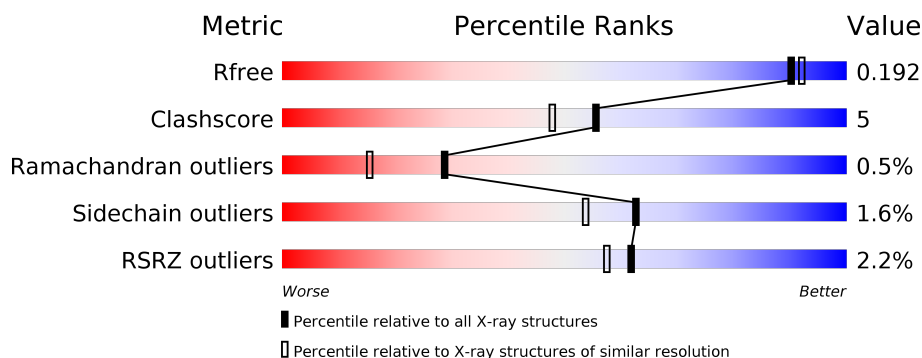
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	261	<div> <div>0%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
1	B	261	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
1	C	261	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	D	261	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
1	E	261	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	F	261	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15205 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.

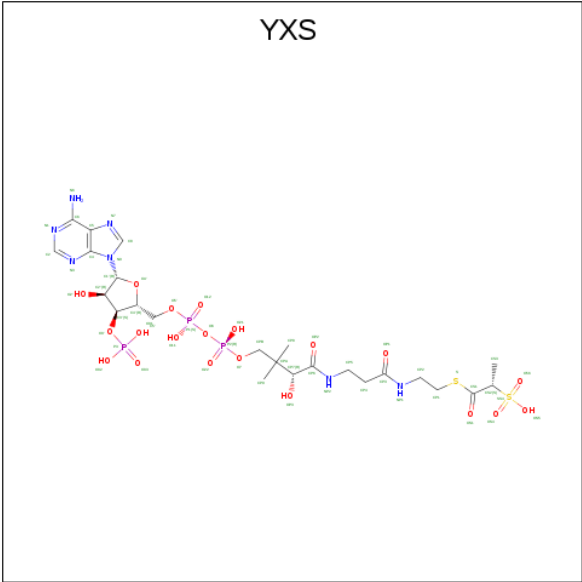
- Molecule 1 is a protein called Methylmalonyl-CoA decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	20	0
			2149	1382	366	388	13			
1	B	260	Total	C	N	O	S	0	11	0
			2111	1357	359	383	12			
1	C	260	Total	C	N	O	S	0	13	0
			2114	1354	359	389	12			
1	D	260	Total	C	N	O	S	0	13	0
			2103	1348	354	388	13			
1	E	260	Total	C	N	O	S	0	15	0
			2120	1363	359	386	12			
1	F	260	Total	C	N	O	S	0	15	0
			2117	1362	356	387	12			

There are 6 discrepancies between the modelled and reference sequences:

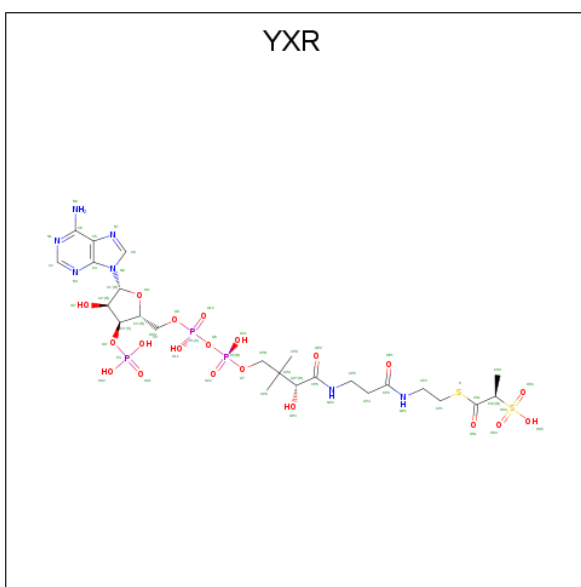
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP P52045
B	2	ALA	SER	engineered mutation	UNP P52045
C	2	ALA	SER	engineered mutation	UNP P52045
D	2	ALA	SER	engineered mutation	UNP P52045
E	2	ALA	SER	engineered mutation	UNP P52045
F	2	ALA	SER	engineered mutation	UNP P52045

- Molecule 2 is (2S)-sulfonatepropionyl-CoA (three-letter code: YXS) (formula: C<sub>24</sub>H<sub>40</sub>N<sub>7</sub>O<sub>20</sub>P<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	1
			56	24	7	20	3	2		
2	B	1	Total	C	N	O	P	S	0	1
			56	24	7	20	3	2		
2	C	1	Total	C	N	O	P	S	0	1
			56	24	7	20	3	2		
2	D	1	Total	C	N	O	P	S	0	1
			56	24	7	20	3	2		
2	E	1	Total	C	N	O	P	S	0	1
			56	24	7	20	3	2		
2	F	1	Total	C	N	O	P	S	0	1
			56	24	7	20	3	2		

- Molecule 3 is (2R)-sulfonatepropionyl-CoA (three-letter code: YXR) (formula: C<sub>24</sub>H<sub>40</sub>N<sub>7</sub>O<sub>20</sub>P<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	1
			56	24	7	20	3	2		
3	B	1	Total	C	N	O	P	S	0	1
			56	24	7	20	3	2		
3	C	1	Total	C	N	O	P	S	0	1
			56	24	7	20	3	2		
3	D	1	Total	C	N	O	P	S	0	1
			56	24	7	20	3	2		
3	E	1	Total	C	N	O	P	S	0	1
			56	24	7	20	3	2		
3	F	1	Total	C	N	O	P	S	0	1
			56	24	7	20	3	2		

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	D	1	Total	Ni	0	0
			1	1		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

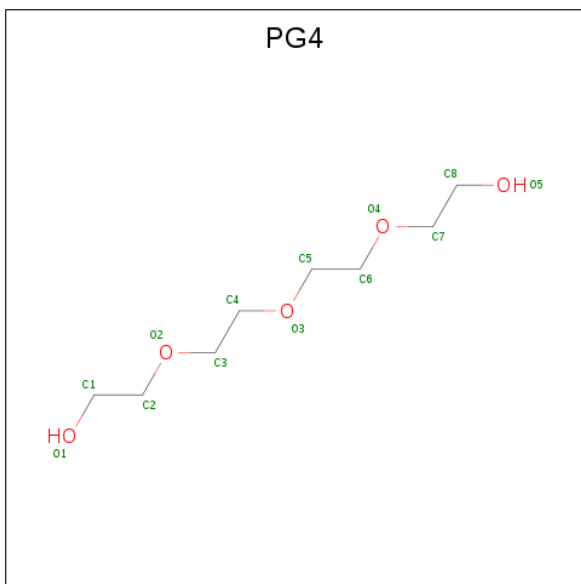
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	K	0	0
			1	1		

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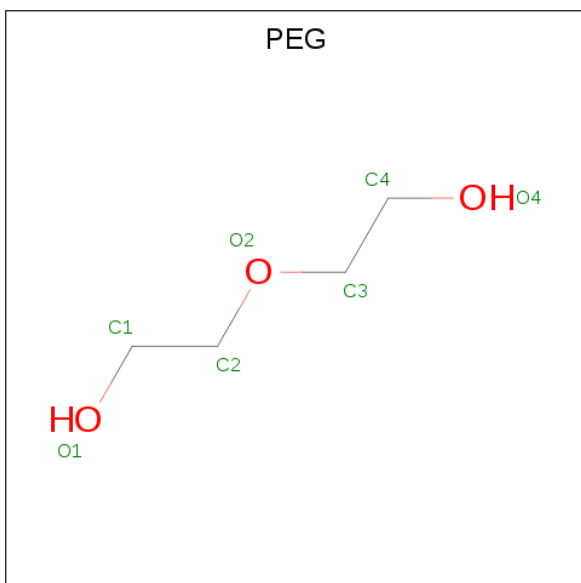
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	K	0	0
			1	1		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



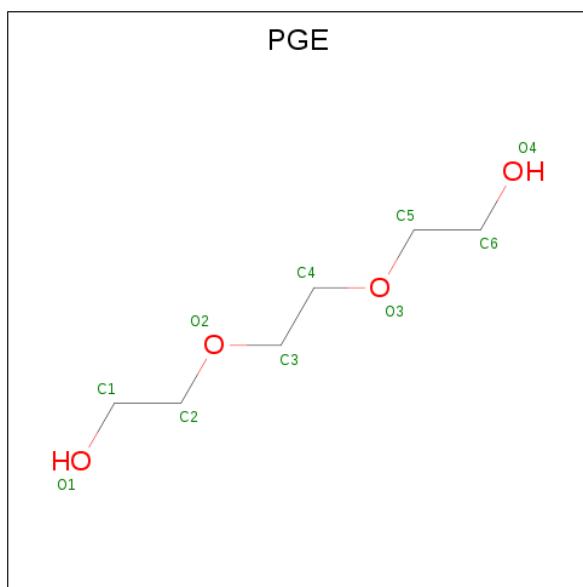
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	4	3		
7	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			10	6	4		

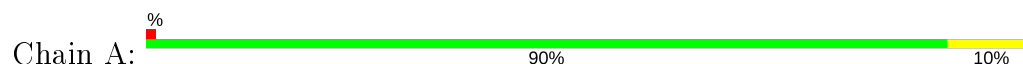
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	305	Total	O	1	19
			322	322		
9	B	265	Total	O	0	9
			274	274		
9	C	283	Total	O	0	19
			301	301		
9	D	282	Total	O	0	14
			295	295		
9	E	271	Total	O	0	14
			285	285		
9	F	288	Total	O	0	13
			301	301		

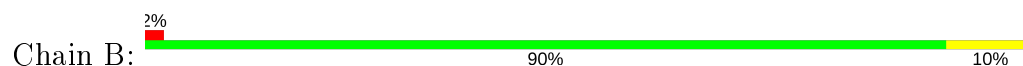
### 3 Residue-property plots

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: Methylmalonyl-CoA decarboxylase



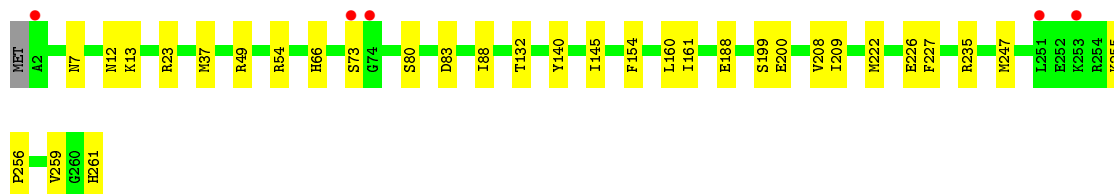
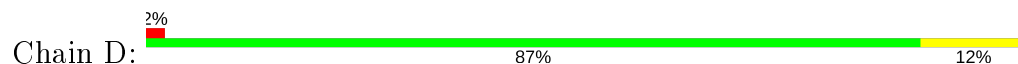
- Molecule 1: Methylmalonyl-CoA decarboxylase



- Molecule 1: Methylmalonyl-CoA decarboxylase



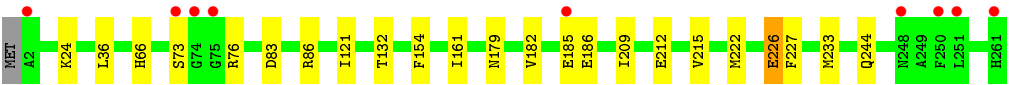
- Molecule 1: Methylmalonyl-CoA decarboxylase



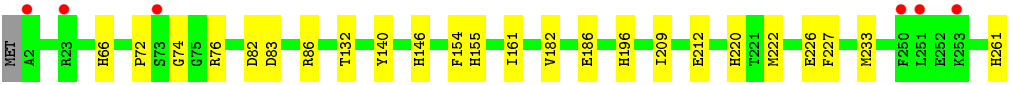
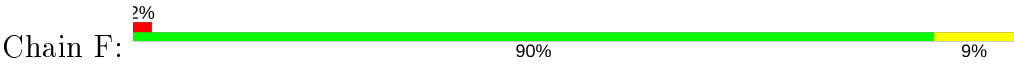
- Molecule 1: Methylmalonyl-CoA decarboxylase







● Molecule 1: Methylmalonyl-CoA decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.93Å 114.42Å 193.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 29.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.80) 99.8 (29.95-1.80)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.159 , 0.192 0.162 , 0.192	Depositor DCC
$R_{free}$ test set	8841 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NI, PGE, YXR, YXS, K, PG4, PEG

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	0.77	0/2253	0.86	2/3045 (0.1%)
1	B	0.77	2/2191 (0.1%)	0.87	2/2962 (0.1%)
1	C	0.77	0/2196	0.83	1/2968 (0.0%)
1	D	0.79	0/2186	0.87	1/2953 (0.0%)
1	E	0.77	3/2206 (0.1%)	0.87	2/2985 (0.1%)
1	F	0.76	2/2206 (0.1%)	0.86	2/2987 (0.1%)
All	All	0.77	7/13238 (0.1%)	0.86	10/17900 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	226	GLU	CD-OE2	-8.97	1.15	1.25
1	F	226	GLU	CD-OE1	-7.83	1.17	1.25
1	E	212	GLU	CD-OE2	-6.29	1.18	1.25
1	F	212	GLU	CD-OE2	-6.26	1.18	1.25
1	B	212	GLU	CD-OE2	-5.69	1.19	1.25
1	E	226	GLU	CD-OE1	-5.53	1.19	1.25
1	E	185	GLU	CD-OE1	5.04	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	E	86	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	86	ARG	NE-CZ-NH1	-6.27	117.16	120.30
1	F	86	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	86	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	D	23	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	F	82	ASP	CB-CA-C	5.49	121.37	110.40
1	E	86	ARG	NE-CZ-NH1	5.34	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	B	238	TYR	CB-CA-C	5.28	120.95	110.40

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	2149	0	2218	23	0
1	B	2111	0	2160	25	0
1	C	2114	0	2153	21	0
1	D	2103	0	2139	25	0
1	E	2120	0	2175	22	0
1	F	2117	0	2167	26	0
2	A	56	0	0	1	0
2	B	56	0	0	0	0
2	C	56	0	0	1	0
2	D	56	0	0	0	0
2	E	56	0	0	3	0
2	F	56	0	0	0	0
3	A	56	0	0	1	0
3	B	56	0	0	2	0
3	C	56	0	0	0	0
3	D	56	0	0	0	0
3	E	56	0	0	0	0
3	F	56	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
6	C	13	0	18	1	0
7	C	7	0	10	0	0
7	F	7	0	10	3	0
8	F	10	0	14	0	0
9	A	322	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	274	0	0	5	0
9	C	301	0	0	4	0
9	D	295	0	0	10	0
9	E	285	0	0	1	0
9	F	301	0	0	2	0
All	All	15205	0	13064	134	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 5.

All (134) 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:222[B]:MET:CE	1:A:226[B]:GLU:HG2	1.14	1.58
1:A:222[B]:MET:CE	1:A:226[B]:GLU:CG	2.09	1.31
1:A:222[B]:MET:HE2	1:A:226[B]:GLU:CG	1.59	1.30
1:A:226[A]:GLU:OE2	9:A:403:HOH:O	1.62	1.16
1:A:222[B]:MET:HE3	1:A:226[B]:GLU:HG2	1.29	1.13
1:C:226[B]:GLU:OE2	9:C:401:HOH:O	1.69	1.09
1:C:222[A]:MET:HE3	1:C:226[A]:GLU:HG2	1.27	1.08
1:C:222[A]:MET:CE	1:C:226[A]:GLU:HG2	1.86	1.04
1:C:222[A]:MET:HE3	1:C:226[A]:GLU:CG	1.89	1.03
1:A:222[B]:MET:HE1	1:A:226[B]:GLU:HG2	1.50	0.93
1:B:188:GLU:OE1	9:B:474[B]:HOH:O	1.90	0.88
1:A:222[B]:MET:HE2	1:A:226[B]:GLU:HG2	0.88	0.87
1:C:222[A]:MET:CE	1:C:226[A]:GLU:CG	2.51	0.84
1:A:222[B]:MET:HE1	1:C:215[B]:VAL:HB	1.62	0.81
1:D:83:ASP:HB2	9:D:471:HOH:O	1.81	0.80
1:D:222[B]:MET:HE3	1:D:227[B]:PHE:CE1	2.17	0.79
1:B:222[A]:MET:CG	1:B:227[A]:PHE:CE2	2.67	0.77
1:D:222[B]:MET:CE	1:D:227[B]:PHE:CE1	2.68	0.76
1:F:222:MET:SD	1:F:227[A]:PHE:CE1	2.79	0.76
1:B:80:SER:HB2	9:E:602[B]:HOH:O	1.86	0.75
1:C:222[A]:MET:HE3	1:C:226[A]:GLU:CB	2.14	0.75
1:F:222:MET:HG2	1:F:227[A]:PHE:CZ	2.22	0.74
1:C:222[A]:MET:HE3	1:C:226[A]:GLU:HB3	1.70	0.72
1:F:83[B]:ASP:OD2	9:F:401:HOH:O	2.07	0.72
1:B:222[A]:MET:HG2	1:B:227[A]:PHE:CE2	2.26	0.71
1:B:222[A]:MET:HG2	1:B:227[A]:PHE:CZ	2.27	0.70
1:D:261[B]:HIS:CD2	9:D:438:HOH:O	2.45	0.69
1:D:200:GLU:OE2	9:D:402:HOH:O	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:HIS:NE2	7:F:305:PEG:H42	2.10	0.66
1:D:199[B]:SER:OG	9:D:402:HOH:O	2.15	0.64
1:C:60[B]:LYS:NZ	2:C:301[B]:YXS:O21	2.30	0.63
1:A:222[B]:MET:HE2	1:A:226[B]:GLU:HG3	1.74	0.63
1:B:222[A]:MET:HG3	1:B:227[A]:PHE:CE2	2.33	0.63
1:F:222:MET:SD	1:F:227[A]:PHE:CD1	2.92	0.63
1:B:222[A]:MET:SD	1:B:227[A]:PHE:CE1	2.91	0.62
1:B:82:ASP:O	1:B:87[B]:GLN:NE2	2.32	0.62
1:F:196[B]:HIS:HD2	9:F:563:HOH:O	1.82	0.62
1:E:24[B]:LYS:HD3	2:E:301[B]:YXS:C2	2.30	0.62
1:F:222:MET:CG	1:F:227[A]:PHE:CE2	2.83	0.61
1:E:179:ASN:HD21	1:F:155:HIS:HB3	1.65	0.61
1:B:60[A]:LYS:NZ	3:B:302[A]:YXR:O21	2.29	0.60
1:E:222[B]:MET:HE3	1:E:226:GLU:HB3	1.84	0.60
1:F:222:MET:CG	1:F:227[A]:PHE:CZ	2.86	0.59
1:F:222:MET:HG2	1:F:227[A]:PHE:CE2	2.38	0.59
1:A:82:ASP:HB3	9:A:614[B]:HOH:O	2.02	0.58
1:B:68:ILE:HD12	1:B:250:PHE:CZ	2.38	0.58
1:B:68:ILE:HD12	1:B:250:PHE:CE1	2.39	0.58
1:C:222[A]:MET:HE1	1:C:226[A]:GLU:CG	2.34	0.57
1:B:222[A]:MET:CG	1:B:227[A]:PHE:CZ	2.88	0.57
1:A:196[B]:HIS:HE1	9:A:608:HOH:O	1.86	0.57
1:D:226:GLU:OE1	9:D:403:HOH:O	2.16	0.57
1:E:222[B]:MET:HE2	1:E:227[B]:PHE:CE1	2.41	0.56
1:D:66:HIS:CE1	9:D:404:HOH:O	2.57	0.56
1:B:182:VAL:HG21	1:B:187:LEU:HA	1.88	0.55
1:E:182[A]:VAL:HG12	1:E:186:GLU:HB2	1.86	0.55
1:F:182[B]:VAL:HG12	1:F:186:GLU:HB2	1.87	0.55
1:A:66[B]:HIS:HD2	1:A:67:ASP:O	1.90	0.55
1:A:261:HIS:ND1	9:A:408:HOH:O	2.33	0.55
1:F:146[B]:HIS:HE2	1:F:220:HIS:HD1	1.52	0.54
1:A:30[B]:LYS:HE3	1:A:34:ASP:OD2	2.07	0.54
1:E:215[B]:VAL:HG12	1:F:222:MET:CE	2.38	0.54
1:B:222[A]:MET:SD	1:B:227[A]:PHE:CD1	3.01	0.54
2:E:301[B]:YXS:O11	2:E:301[B]:YXS:C4'	2.56	0.53
1:B:222[A]:MET:HG3	1:B:227[A]:PHE:CD2	2.44	0.52
1:D:7:ASN:ND2	9:D:405[A]:HOH:O	2.42	0.52
1:C:186:GLU:HG3	9:C:625:HOH:O	2.10	0.52
1:E:121:ILE:H	1:E:179:ASN:HD22	1.56	0.52
1:A:161:ILE:HG21	1:C:209:ILE:HG21	1.93	0.51
1:A:146:HIS:HD2	9:A:652:HOH:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:ILE:HG21	1:F:161:ILE:HG21	1.92	0.51
1:E:215[B]:VAL:HG12	1:F:222:MET:HE2	1.93	0.49
1:F:222:MET:HG3	1:F:227[A]:PHE:CE2	2.48	0.48
1:C:222[A]:MET:CE	1:C:226[A]:GLU:HB3	2.43	0.48
1:D:54:ARG:HH12	1:D:188[A]:GLU:CD	2.15	0.48
1:B:220:HIS:HE1	9:B:543:HOH:O	1.97	0.48
1:D:49:ARG:NH1	9:D:401:HOH:O	1.90	0.48
1:B:76:ARG:HA	1:B:76:ARG:HD2	1.69	0.48
3:B:302[A]:YXR:O12	3:B:302[A]:YXR:OP3	2.32	0.48
1:D:161:ILE:HG21	1:F:209:ILE:HG21	1.96	0.47
1:F:182[B]:VAL:CG1	1:F:186:GLU:HB2	2.44	0.47
1:D:73:SER:OG	1:D:247[A]:MET:HE1	2.15	0.47
1:E:66:HIS:HE1	1:E:83:ASP:OD1	1.98	0.47
1:E:222[B]:MET:HE2	1:E:227[B]:PHE:CD1	2.50	0.47
1:D:83:ASP:OD1	9:D:404:HOH:O	2.20	0.47
1:A:182[B]:VAL:HG12	1:A:186:GLU:HB2	1.97	0.46
1:D:209:ILE:HG21	1:E:161:ILE:HG21	1.97	0.46
1:E:182[A]:VAL:CG1	1:E:186:GLU:HB2	2.46	0.46
3:A:302[A]:YXR:C2'	3:A:302[A]:YXR:O5'	2.64	0.46
6:C:304:PG4:H41	9:C:605:HOH:O	2.16	0.46
1:D:200:GLU:HB2	9:D:513:HOH:O	2.16	0.46
1:A:209:ILE:HG21	1:B:161:ILE:HG21	1.97	0.45
1:B:209:ILE:HG21	1:C:161:ILE:HG21	1.97	0.45
1:D:222[B]:MET:HE3	1:D:227[B]:PHE:CD1	2.51	0.45
1:F:72:PRO:HB2	1:F:76:ARG:HB2	1.97	0.45
1:C:49[B]:ARG:HD2	1:C:203:PRO:HB3	1.99	0.45
1:D:247[A]:MET:HB3	1:D:247[A]:MET:HE3	1.73	0.45
2:A:301[B]:YXS:O5'	2:A:301[B]:YXS:C2'	2.64	0.45
1:D:13:LYS:NZ	1:D:200:GLU:OE2	2.45	0.45
1:A:7:ASN:ND2	9:A:549[B]:HOH:O	2.50	0.45
1:E:215[B]:VAL:CG1	1:F:222:MET:HE2	2.47	0.45
1:E:121:ILE:H	1:E:179:ASN:ND2	2.16	0.44
9:C:613:HOH:O	1:D:80:SER:HB2	2.18	0.44
1:F:261:HIS:CD2	7:F:305:PEG:H22	2.53	0.44
1:A:222[B]:MET:HE1	1:A:226[B]:GLU:CG	2.22	0.44
1:E:73:SER:O	1:E:244:GLN:NE2	2.44	0.44
1:C:72:PRO:HD2	1:C:78:PRO:HA	1.99	0.43
1:F:146[A]:HIS:CE1	1:F:220:HIS:HD1	2.37	0.43
1:D:208:VAL:HG23	1:E:233:MET:HE2	2.00	0.43
1:D:259:VAL:HG21	1:D:261[B]:HIS:CE1	2.54	0.43
1:C:60[A]:LYS:HA	1:C:60[A]:LYS:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36[B]:LEU:HG	1:B:88:ILE:HD11	2.01	0.42
9:B:470:HOH:O	1:E:76:ARG:HD2	2.19	0.42
1:F:222:MET:HG3	1:F:227[A]:PHE:CD2	2.55	0.42
1:F:233[B]:MET:HE2	1:F:233[B]:MET:HB2	1.84	0.42
1:B:182:VAL:CG2	1:B:187:LEU:HA	2.49	0.42
1:D:255:LYS:HG2	1:D:256:PRO:HD2	2.01	0.42
1:A:233[A]:MET:HE2	1:A:233[A]:MET:HB2	1.82	0.41
1:F:261:HIS:NE2	7:F:305:PEG:C4	2.81	0.41
1:E:24[B]:LYS:HD3	2:E:301[B]:YXS:N3	2.35	0.41
1:A:11:ILE:O	1:A:196[A]:HIS:HE1	2.04	0.41
1:C:33:ILE:HD13	1:C:33:ILE:HA	1.93	0.41
1:E:215[B]:VAL:CG1	1:F:222:MET:CE	2.99	0.41
1:E:222[B]:MET:HE3	1:E:226:GLU:CB	2.49	0.41
1:B:83:ASP:HA	1:B:84:PRO:HD3	1.96	0.41
1:B:186:GLU:HB3	9:B:514:HOH:O	2.20	0.40
1:E:36[B]:LEU:HA	1:E:36[B]:LEU:HD23	1.94	0.40
1:C:227[B]:PHE:CE2	1:C:231[B]:GLN:HG2	2.56	0.40
1:D:145:ILE:HD13	1:D:145:ILE:HA	1.94	0.40
1:D:37:MET:HG2	1:D:88[A]:ILE:HD13	2.03	0.40
1:B:220:HIS:CE1	9:B:543:HOH:O	2.74	0.40
1:A:66[B]:HIS:HE1	1:A:83:ASP:OD1	2.04	0.40
1:C:222[A]:MET:CE	1:C:226[A]:GLU:CB	2.92	0.40
1:B:250:PHE:C	1:B:250:PHE:CD1	2.95	0.40

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	278/261 (106%)	269 (97%)	8 (3%)	1 (0%)	34	21
1	B	270/261 (103%)	259 (96%)	10 (4%)	1 (0%)	34	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	271/261 (104%)	264 (97%)	6 (2%)	1 (0%)	34	21
1	D	270/261 (103%)	263 (97%)	6 (2%)	1 (0%)	34	21
1	E	273/261 (105%)	265 (97%)	7 (3%)	1 (0%)	34	21
1	F	273/261 (105%)	263 (96%)	8 (3%)	2 (1%)	22	10
All	All	1635/1566 (104%)	1583 (97%)	45 (3%)	7 (0%)	29	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	74	GLY
1	E	132	THR
1	F	132	THR
1	A	132	THR
1	B	132	THR
1	C	132	THR
1	D	132	THR

### 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	243/224 (108%)	234 (96%)	9 (4%)	34	19
1	B	235/224 (105%)	233 (99%)	2 (1%)	78	75
1	C	236/224 (105%)	231 (98%)	5 (2%)	53	42
1	D	236/224 (105%)	231 (98%)	5 (2%)	53	42
1	E	238/224 (106%)	237 (100%)	1 (0%)	91	89
1	F	238/224 (106%)	235 (99%)	3 (1%)	69	62
All	All	1426/1344 (106%)	1401 (98%)	25 (2%)	62	48

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23[A]	ARG
1	A	23[B]	ARG
1	A	45	ARG
1	A	66[A]	HIS
1	A	66[B]	HIS
1	A	130[A]	SER
1	A	130[B]	SER
1	A	140	TYR
1	A	154	PHE
1	B	76	ARG
1	B	154	PHE
1	C	23	ARG
1	C	136	LEU
1	C	154	PHE
1	C	204[A]	LEU
1	C	204[B]	LEU
1	D	12	ASN
1	D	140	TYR
1	D	154	PHE
1	D	160	LEU
1	D	235	ARG
1	E	154	PHE
1	F	66	HIS
1	F	140	TYR
1	F	154	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
1	B	7	ASN
1	C	244	GLN
1	C	257	ASN
1	D	12	ASN
1	D	66	HIS
1	E	7	ASN
1	E	66	HIS
1	E	179	ASN

### 5.3.3 RNA ⓘ

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 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\# Z  > 2$
2	YXS	B	301[B]	-	48,58,58	0.94	4 (8%)	60,88,88	1.57	13 (21%)
7	PEG	F	305	-	6,6,6	0.29	0	5,5,5	0.26	0
8	PGE	F	304	5	9,9,9	0.35	0	8,8,8	0.20	0
2	YXS	F	301[B]	-	48,58,58	1.12	3 (6%)	60,88,88	3.34	16 (26%)
3	YXR	D	303[A]	-	48,58,58	1.01	2 (4%)	60,88,88	3.26	16 (26%)
3	YXR	E	302[A]	-	48,58,58	0.93	2 (4%)	60,88,88	3.25	18 (30%)
2	YXS	C	301[B]	-	48,58,58	0.96	2 (4%)	60,88,88	1.55	6 (10%)
7	PEG	C	305	-	6,6,6	0.33	0	5,5,5	0.19	0
3	YXR	F	302[A]	-	48,58,58	1.01	3 (6%)	60,88,88	1.75	10 (16%)
3	YXR	C	302[A]	-	48,58,58	0.96	3 (6%)	60,88,88	1.70	8 (13%)
3	YXR	B	302[A]	-	48,58,58	0.87	1 (2%)	60,88,88	3.54	17 (28%)
6	PG4	C	304	5	12,12,12	0.26	0	11,11,11	0.25	0
2	YXS	A	301[B]	-	48,58,58	1.21	3 (6%)	60,88,88	1.72	10 (16%)
2	YXS	D	302[B]	-	48,58,58	1.00	3 (6%)	60,88,88	3.28	17 (28%)
2	YXS	E	301[B]	-	48,58,58	0.91	2 (4%)	60,88,88	1.74	13 (21%)
3	YXR	A	302[A]	-	48,58,58	1.13	3 (6%)	60,88,88	1.62	9 (15%)

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	YXS	B	301[B]	-	-	7/54/77/77	0/3/3/3
7	PEG	F	305	-	-	1/4/4/4	-
8	PGE	F	304	5	-	0/7/7/7	-
2	YXS	F	301[B]	-	-	15/54/77/77	0/3/3/3
3	YXR	D	303[A]	-	-	6/54/77/77	0/3/3/3
3	YXR	E	302[A]	-	-	15/54/77/77	0/3/3/3
2	YXS	C	301[B]	-	-	4/54/77/77	0/3/3/3
7	PEG	C	305	-	-	0/4/4/4	-
3	YXR	F	302[A]	-	-	7/54/77/77	0/3/3/3
3	YXR	C	302[A]	-	-	2/54/77/77	0/3/3/3
3	YXR	B	302[A]	-	-	10/54/77/77	0/3/3/3
6	PG4	C	304	5	-	2/10/10/10	-
2	YXS	A	301[B]	-	-	4/54/77/77	0/3/3/3
2	YXS	D	302[B]	-	-	7/54/77/77	0/3/3/3
2	YXS	E	301[B]	-	-	8/54/77/77	0/3/3/3
3	YXR	A	302[A]	-	-	2/54/77/77	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301[B]	YXS	CS2-CS1	-4.47	1.47	1.52
2	F	301[B]	YXS	CS2-CS1	-3.66	1.48	1.52
3	A	302[A]	YXR	CS2-CS1	-3.60	1.48	1.52
3	D	303[A]	YXR	OS1-CS1	3.21	1.25	1.20
2	A	301[B]	YXS	O4'-C1'	3.19	1.45	1.41
3	A	302[A]	YXR	O4'-C1'	3.13	1.45	1.41
2	D	302[B]	YXS	OS1-CS1	3.07	1.25	1.20
2	C	301[B]	YXS	CS2-CS1	-2.99	1.49	1.52
3	F	302[A]	YXR	CS2-CS1	-2.97	1.49	1.52
2	F	301[B]	YXS	O4'-C1'	2.73	1.44	1.41
2	B	301[B]	YXS	O4'-C1'	2.69	1.44	1.41
2	E	301[B]	YXS	CS2-CS1	-2.66	1.49	1.52
3	B	302[A]	YXR	O4'-C1'	2.64	1.44	1.41
2	A	301[B]	YXS	C5-C4	2.61	1.47	1.40
3	A	302[A]	YXR	C5-C4	2.60	1.47	1.40
2	F	301[B]	YXS	C5-C4	2.56	1.47	1.40
2	B	301[B]	YXS	CS2-CS1	-2.49	1.49	1.52
2	C	301[B]	YXS	C5-C4	2.48	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302[A]	YXR	C5-C4	2.48	1.47	1.40
3	C	302[A]	YXR	CS2-CS1	-2.45	1.49	1.52
3	F	302[A]	YXR	C5-C4	2.45	1.47	1.40
3	E	302[A]	YXR	C5-C4	2.42	1.47	1.40
2	E	301[B]	YXS	C5-C4	2.42	1.47	1.40
3	E	302[A]	YXR	CS2-CS1	-2.39	1.49	1.52
3	C	302[A]	YXR	OS1-CS1	2.27	1.24	1.20
2	B	301[B]	YXS	CS1-S	-2.27	1.67	1.75
3	D	303[A]	YXR	C5-C4	2.25	1.46	1.40
3	F	302[A]	YXR	C2'-C1'	-2.17	1.50	1.53
2	B	301[B]	YXS	OS1-CS1	2.16	1.24	1.20
2	D	302[B]	YXS	C5-C4	2.14	1.46	1.40
2	D	302[B]	YXS	O4'-C1'	2.06	1.44	1.41

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302[A]	YXR	CP8-CPA-CPB	-14.66	84.33	108.23
3	E	302[A]	YXR	CP8-CPA-CPB	-14.09	85.25	108.23
2	D	302[B]	YXS	CP8-CPA-CPB	-13.80	85.72	108.23
3	D	303[A]	YXR	CP8-CPA-CPB	-13.71	85.87	108.23
3	B	302[A]	YXR	CP8-CPA-CP7	-13.40	85.59	108.82
2	F	301[B]	YXS	CP8-CPA-CPB	-13.11	86.85	108.23
2	F	301[B]	YXS	CP8-CPA-CP7	-12.47	87.20	108.82
3	E	302[A]	YXR	CP8-CPA-CP7	-11.54	88.81	108.82
3	D	303[A]	YXR	CP8-CPA-CP9	-10.51	87.74	109.17
2	D	302[B]	YXS	CP8-CPA-CP9	-10.40	87.97	109.17
3	B	302[A]	YXR	CP9-CPA-CPB	10.36	125.14	108.23
2	F	301[B]	YXS	CP9-CPA-CP7	9.86	125.92	108.82
3	B	302[A]	YXR	CP8-CPA-CP9	-9.75	89.30	109.17
2	F	301[B]	YXS	CP8-CPA-CP9	-9.61	89.59	109.17
2	D	302[B]	YXS	CP8-CPA-CP7	-9.45	92.44	108.82
3	D	303[A]	YXR	CP8-CPA-CP7	-9.29	92.72	108.82
3	D	303[A]	YXR	CP9-CPA-CPB	9.05	122.99	108.23
3	C	302[A]	YXR	OS4-SS4-CS2	-8.86	103.53	109.43
2	D	302[B]	YXS	CP9-CPA-CPB	8.57	122.22	108.23
2	E	301[B]	YXS	O56-SS4-CS2	-7.88	104.18	109.43
3	F	302[A]	YXR	OS4-SS4-CS2	-7.76	104.26	109.43
2	A	301[B]	YXS	O56-SS4-CS2	-7.76	104.26	109.43
3	A	302[A]	YXR	OS4-SS4-CS2	-7.65	104.34	109.43
2	C	301[B]	YXS	O56-SS4-CS2	-7.29	104.57	109.43
3	E	302[A]	YXR	CP9-CPA-CP7	7.10	121.13	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302[A]	YXR	CP8-CPA-CP9	-6.95	95.01	109.17
3	D	303[A]	YXR	CP9-CPA-CP7	5.50	118.35	108.82
2	D	302[B]	YXS	CP9-CPA-CP7	5.40	118.19	108.82
2	B	301[B]	YXS	O56-SS4-CS2	-5.22	105.95	109.43
2	A	301[B]	YXS	OS4-SS4-CS2	-5.14	106.01	109.43
3	B	302[A]	YXR	OS4-SS4-CS2	-5.13	106.01	109.43
3	D	303[A]	YXR	OP3-CP7-CPA	-5.10	98.25	110.25
2	F	301[B]	YXS	O56-SS4-CS2	-5.06	106.06	109.43
3	E	302[A]	YXR	C2'-C3'-C4'	-5.04	94.30	103.22
2	D	302[B]	YXS	OP3-CP7-CPA	-4.98	98.54	110.25
3	E	302[A]	YXR	CP9-CPA-CPB	4.87	116.18	108.23
2	D	302[B]	YXS	P2-O6-P1	-4.78	116.42	132.83
3	E	302[A]	YXR	C1'-N9-C4	-4.65	118.47	126.64
3	D	303[A]	YXR	P2-O6-P1	-4.15	118.60	132.83
2	B	301[B]	YXS	N3-C2-N1	-3.99	122.45	128.68
3	B	302[A]	YXR	N3-C2-N1	-3.97	122.48	128.68
2	B	301[B]	YXS	P2-O6-P1	-3.95	119.28	132.83
2	F	301[B]	YXS	CP5-CP4-CP3	-3.92	105.82	112.36
2	D	302[B]	YXS	N3-C2-N1	-3.90	122.58	128.68
3	F	302[A]	YXR	P2-O6-P1	-3.90	119.44	132.83
3	B	302[A]	YXR	P2-O6-P1	-3.75	119.95	132.83
2	B	301[B]	YXS	CP5-CP4-CP3	-3.68	106.22	112.36
3	F	302[A]	YXR	N3-C2-N1	-3.66	122.95	128.68
3	F	302[A]	YXR	CP5-CP4-CP3	-3.62	106.33	112.36
3	F	302[A]	YXR	O7-CPB-CPA	-3.61	104.74	110.55
3	E	302[A]	YXR	N3-C2-N1	-3.51	123.19	128.68
3	B	302[A]	YXR	O7-CPB-CPA	-3.44	105.02	110.55
3	E	302[A]	YXR	OS4-SS4-CS2	-3.42	107.15	109.43
3	E	302[A]	YXR	P2-O6-P1	-3.42	121.10	132.83
2	E	301[B]	YXS	N3-C2-N1	-3.36	123.42	128.68
2	A	301[B]	YXS	N3-C2-N1	-3.34	123.46	128.68
3	A	302[A]	YXR	N3-C2-N1	-3.31	123.51	128.68
3	E	302[A]	YXR	C5'-C4'-C3'	-3.30	103.47	114.40
3	B	302[A]	YXR	CP5-CP4-CP3	-3.29	106.88	112.36
3	C	302[A]	YXR	N3-C2-N1	-3.29	123.54	128.68
2	D	302[B]	YXS	O56-SS4-CS2	-3.28	107.25	109.43
2	C	301[B]	YXS	N3-C2-N1	-3.27	123.57	128.68
3	D	303[A]	YXR	N6-C6-N1	3.24	125.31	118.57
2	F	301[B]	YXS	N3-C2-N1	-3.14	123.78	128.68
3	A	302[A]	YXR	P2-O6-P1	-3.12	122.11	132.83
2	A	301[B]	YXS	C1'-N9-C4	-3.07	121.25	126.64
3	A	302[A]	YXR	C1'-N9-C4	-3.04	121.30	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301[B]	YXS	P2-O6-P1	-3.01	122.50	132.83
2	A	301[B]	YXS	CP5-CP4-CP3	-3.00	107.35	112.36
2	F	301[B]	YXS	C4-C5-N7	-2.99	106.28	109.40
3	A	302[A]	YXR	CP5-CP4-CP3	-2.97	107.41	112.36
3	E	302[A]	YXR	CP5-CP4-CP3	-2.94	107.46	112.36
3	C	302[A]	YXR	P2-O6-P1	-2.92	122.80	132.83
2	C	301[B]	YXS	P2-O6-P1	-2.92	122.82	132.83
2	E	301[B]	YXS	O4'-C4'-C5'	2.90	118.93	109.37
2	C	301[B]	YXS	C4-C5-N7	-2.90	106.38	109.40
3	C	302[A]	YXR	C4-C5-N7	-2.90	106.38	109.40
2	E	301[B]	YXS	O5'-C5'-C4'	2.89	118.93	108.99
3	D	303[A]	YXR	N3-C2-N1	-2.85	124.22	128.68
3	B	302[A]	YXR	CP9-CPA-CP7	2.85	113.75	108.82
2	E	301[B]	YXS	OS4-SS4-CS2	2.82	111.31	109.43
2	F	301[B]	YXS	O4'-C4'-C5'	2.79	118.55	109.37
2	F	301[B]	YXS	CP9-CPA-CPB	2.75	112.72	108.23
2	E	301[B]	YXS	CP9-CPA-CP7	2.73	113.56	108.82
2	D	302[B]	YXS	N6-C6-N1	2.72	124.23	118.57
3	F	302[A]	YXR	CP1-S-CS1	2.71	109.90	101.75
3	D	303[A]	YXR	CP5-CP4-CP3	-2.68	107.89	112.36
3	E	302[A]	YXR	C2-N1-C6	2.64	123.27	118.75
2	F	301[B]	YXS	OS4-SS4-CS2	-2.64	107.67	109.43
2	F	301[B]	YXS	P2-O6-P1	-2.63	123.81	132.83
3	C	302[A]	YXR	OP1-CP3-CP4	-2.62	117.22	122.02
2	B	301[B]	YXS	CP8-CPA-CP9	2.60	114.47	109.17
2	C	301[B]	YXS	OP1-CP3-CP4	-2.59	117.28	122.02
2	D	302[B]	YXS	C1'-N9-C4	-2.59	122.09	126.64
2	D	302[B]	YXS	CP5-CP4-CP3	-2.57	108.08	112.36
3	C	302[A]	YXR	C2-N1-C6	2.53	123.08	118.75
2	C	301[B]	YXS	C2-N1-C6	2.51	123.04	118.75
3	F	302[A]	YXR	C4-C5-N7	-2.47	106.83	109.40
2	F	301[B]	YXS	O5'-C5'-C4'	2.45	117.42	108.99
3	D	303[A]	YXR	O56-SS4-CS2	-2.44	107.80	109.43
2	E	301[B]	YXS	CS2-CS1-S	2.44	122.34	114.05
3	A	302[A]	YXR	O56-SS4-CS2	-2.43	107.81	109.43
2	F	301[B]	YXS	CP7-CP6-NP2	-2.43	111.74	116.58
2	E	301[B]	YXS	C2-N1-C6	2.43	122.91	118.75
2	E	301[B]	YXS	C5'-C4'-C3'	-2.40	106.43	114.40
2	D	302[B]	YXS	C2-N1-C6	2.38	122.83	118.75
3	B	302[A]	YXR	OS1-CS1-S	-2.38	120.60	123.80
2	B	301[B]	YXS	C5-C6-N6	-2.36	116.76	120.35
2	D	302[B]	YXS	CP4-CP3-NP1	2.36	120.40	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301[B]	YXS	OP3-CP7-CPA	-2.35	104.72	110.25
3	B	302[A]	YXR	C5-C6-N6	-2.34	116.80	120.35
3	E	302[A]	YXR	CP1-S-CS1	2.33	108.76	101.75
3	D	303[A]	YXR	O32-P3-O33	2.32	116.52	107.64
2	B	301[B]	YXS	OP3-CP7-CPA	-2.32	104.79	110.25
2	E	301[B]	YXS	C4-C5-N7	-2.30	107.00	109.40
2	B	301[B]	YXS	O3'-C3'-C2'	-2.29	103.38	111.68
2	F	301[B]	YXS	C2-N1-C6	2.29	122.67	118.75
2	B	301[B]	YXS	N6-C6-N1	2.27	123.28	118.57
3	D	303[A]	YXR	CP4-CP3-NP1	2.26	120.23	116.42
2	D	302[B]	YXS	OP1-CP3-NP1	-2.25	118.77	123.01
2	B	301[B]	YXS	CP8-CPA-CPB	-2.25	104.57	108.23
3	B	302[A]	YXR	N6-C6-N1	2.24	123.23	118.57
2	A	301[B]	YXS	C2-N1-C6	2.24	122.59	118.75
2	D	302[B]	YXS	OS1-CS1-S	-2.24	120.79	123.80
3	E	302[A]	YXR	N6-C6-N1	2.22	123.18	118.57
3	A	302[A]	YXR	C2-N1-C6	2.21	122.54	118.75
3	E	302[A]	YXR	O56-SS4-CS2	2.21	110.90	109.43
3	B	302[A]	YXR	O56-SS4-CS2	-2.21	107.96	109.43
3	C	302[A]	YXR	CP1-S-CS1	2.20	108.38	101.75
2	E	301[B]	YXS	CP9-CPA-CPB	2.20	111.83	108.23
3	B	302[A]	YXR	O3'-C3'-C2'	-2.20	103.71	111.68
2	F	301[B]	YXS	OP3-CP7-CPA	-2.20	105.08	110.25
3	A	302[A]	YXR	C5'-C4'-C3'	-2.19	107.13	114.40
3	C	302[A]	YXR	O56-SS4-CS2	-2.17	107.98	109.43
3	D	303[A]	YXR	OP1-CP3-NP1	-2.16	118.93	123.01
3	B	302[A]	YXR	CP1-S-CS1	2.16	108.24	101.75
2	B	301[B]	YXS	CP1-CP2-NP1	-2.15	107.89	112.42
3	E	302[A]	YXR	CP1-CP2-NP1	-2.13	107.93	112.42
2	B	301[B]	YXS	OS1-CS1-S	-2.12	120.95	123.80
2	A	301[B]	YXS	N6-C6-N1	2.12	122.97	118.57
3	B	302[A]	YXR	C1'-N9-C4	-2.10	122.94	126.64
2	A	301[B]	YXS	C5'-C4'-C3'	-2.10	107.46	114.40
3	F	302[A]	YXR	CP9-CPA-CP7	2.09	112.45	108.82
3	F	302[A]	YXR	OP3-CP7-CPA	-2.08	105.35	110.25
3	A	302[A]	YXR	N6-C6-N1	2.08	122.89	118.57
2	E	301[B]	YXS	CP1-CP2-NP1	-2.07	108.06	112.42
2	B	301[B]	YXS	C1'-N9-C4	-2.06	123.01	126.64
2	A	301[B]	YXS	CP1-CP2-NP1	-2.06	108.09	112.42
3	D	303[A]	YXR	O3'-P3-O31	-2.06	101.44	109.39
3	F	302[A]	YXR	C2-N1-C6	2.05	122.27	118.75
3	E	302[A]	YXR	O2'-C2'-C3'	2.05	117.00	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302[B]	YXS	OS4-SS4-CS2	-2.02	108.08	109.43
3	D	303[A]	YXR	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	301[B]	YXS	C5'-O5'-P1-O11
2	F	301[B]	YXS	C5'-O5'-P1-O6
2	F	301[B]	YXS	CP7-CPA-CPB-O7
2	F	301[B]	YXS	OP3-CP7-CPA-CP9
2	F	301[B]	YXS	CP6-CP7-CPA-CP9
2	F	301[B]	YXS	CS3-CS2-SS4-OS5
3	D	303[A]	YXR	CP7-CPA-CPB-O7
3	D	303[A]	YXR	OP3-CP7-CPA-CP9
3	D	303[A]	YXR	CP6-CP7-CPA-CP9
3	E	302[A]	YXR	C3'-O3'-P3-O31
3	E	302[A]	YXR	C3'-C4'-C5'-O5'
3	E	302[A]	YXR	C5'-O5'-P1-O6
3	E	302[A]	YXR	P1-O6-P2-O7
3	E	302[A]	YXR	CPB-O7-P2-O22
3	E	302[A]	YXR	CP7-CPA-CPB-O7
3	E	302[A]	YXR	OP3-CP7-CPA-CPB
3	E	302[A]	YXR	CP6-CP7-CPA-CPB
3	E	302[A]	YXR	OP3-CP7-CPA-CP9
3	E	302[A]	YXR	CP6-CP7-CPA-CP9
2	C	301[B]	YXS	CS3-CS2-SS4-OS5
3	F	302[A]	YXR	CP6-CP7-CPA-CPB
3	B	302[A]	YXR	C3'-O3'-P3-O31
3	B	302[A]	YXR	CP7-CPA-CPB-O7
3	B	302[A]	YXR	OP3-CP7-CPA-CP9
3	B	302[A]	YXR	CP6-CP7-CPA-CP9
2	A	301[B]	YXS	OS1-CS1-CS2-CS3
2	D	302[B]	YXS	CP7-CPA-CPB-O7
2	D	302[B]	YXS	OP3-CP7-CPA-CP9
2	D	302[B]	YXS	CP6-CP7-CPA-CP9
2	E	301[B]	YXS	C3'-O3'-P3-O33
2	E	301[B]	YXS	C4'-C5'-O5'-P1
2	E	301[B]	YXS	C5'-O5'-P1-O12
2	E	301[B]	YXS	CS3-CS2-SS4-O56
2	E	301[B]	YXS	CS3-CS2-SS4-OS5
2	E	301[B]	YXS	CS3-CS2-SS4-OS4

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Mol	Chain	Res	Type	Atoms
7	F	305	PEG	O2-C3-C4-O4
3	E	302[A]	YXR	O4'-C4'-C5'-O5'
2	F	301[B]	YXS	CP8-CPA-CPB-O7
3	E	302[A]	YXR	CP8-CPA-CPB-O7
2	B	301[B]	YXS	O4'-C4'-C5'-O5'
6	C	304	PG4	O1-C1-C2-O2
3	D	303[A]	YXR	CP8-CPA-CPB-O7
2	B	301[B]	YXS	C3'-C4'-C5'-O5'
3	D	303[A]	YXR	CP4-CP5-NP2-CP6
2	D	302[B]	YXS	CP4-CP5-NP2-CP6
3	F	302[A]	YXR	P1-O6-P2-O7
2	D	302[B]	YXS	CP8-CPA-CPB-O7
3	F	302[A]	YXR	CP6-CP7-CPA-CP8
2	B	301[B]	YXS	C5'-O5'-P1-O6
2	F	301[B]	YXS	C3'-O3'-P3-O32
3	D	303[A]	YXR	C3'-O3'-P3-O33
3	E	302[A]	YXR	CPB-O7-P2-O6
2	E	301[B]	YXS	C5'-O5'-P1-O6
2	F	301[B]	YXS	CP4-CP5-NP2-CP6
2	D	302[B]	YXS	CS3-CS2-SS4-O56
2	F	301[B]	YXS	CPB-O7-P2-O22
3	E	302[A]	YXR	C5'-O5'-P1-O11
3	E	302[A]	YXR	CPB-O7-P2-O21
2	A	301[B]	YXS	OS1-CS1-S-CP1
2	F	301[B]	YXS	CP6-CP7-CPA-CPB
3	B	302[A]	YXR	O4'-C4'-C5'-O5'
2	F	301[B]	YXS	OP3-CP7-CPA-CPB
3	B	302[A]	YXR	OP3-CP7-CPA-CPB
3	B	302[A]	YXR	C3'-C4'-C5'-O5'
2	C	301[B]	YXS	CP9-CPA-CPB-O7
3	F	302[A]	YXR	CP9-CPA-CPB-O7
3	C	302[A]	YXR	CP9-CPA-CPB-O7
2	B	301[B]	YXS	OS1-CS1-CS2-CS3
2	F	301[B]	YXS	OS1-CS1-CS2-CS3
2	C	301[B]	YXS	OS1-CS1-CS2-CS3
2	E	301[B]	YXS	OS1-CS1-CS2-CS3
6	C	304	PG4	C3-C4-O3-C5
3	B	302[A]	YXR	C4'-C3'-O3'-P3
3	A	302[A]	YXR	C3'-C4'-C5'-O5'
3	B	302[A]	YXR	CP9-CPA-CPB-O7
3	B	302[A]	YXR	C2'-C3'-O3'-P3
2	C	301[B]	YXS	CP8-CPA-CPB-O7

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Mol	Chain	Res	Type	Atoms
3	F	302[A]	YXR	CP8-CPA-CPB-O7
3	C	302[A]	YXR	CP8-CPA-CPB-O7
2	B	301[B]	YXS	C2'-C3'-O3'-P3
2	A	301[B]	YXS	C3'-C4'-C5'-O5'
2	D	302[B]	YXS	C3'-C4'-C5'-O5'
3	F	302[A]	YXR	CP6-CP7-CPA-CP9
2	B	301[B]	YXS	C4'-C3'-O3'-P3
2	F	301[B]	YXS	CPB-O7-P2-O6
2	A	301[B]	YXS	C3'-O3'-P3-O31
2	F	301[B]	YXS	C5'-O5'-P1-O12
3	F	302[A]	YXR	CPB-O7-P2-O22
2	B	301[B]	YXS	CP6-CP7-CPA-CPB
3	A	302[A]	YXR	O4'-C4'-C5'-O5'

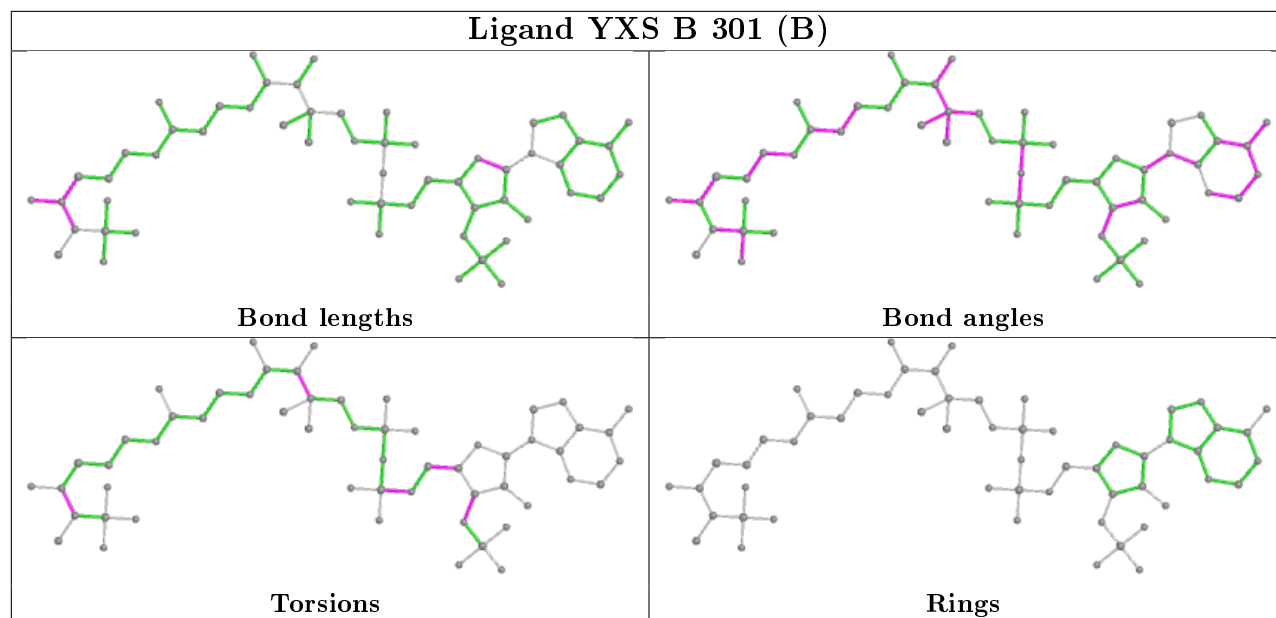
There are no ring outliers.

7 monomers are involved in 12 short contacts:

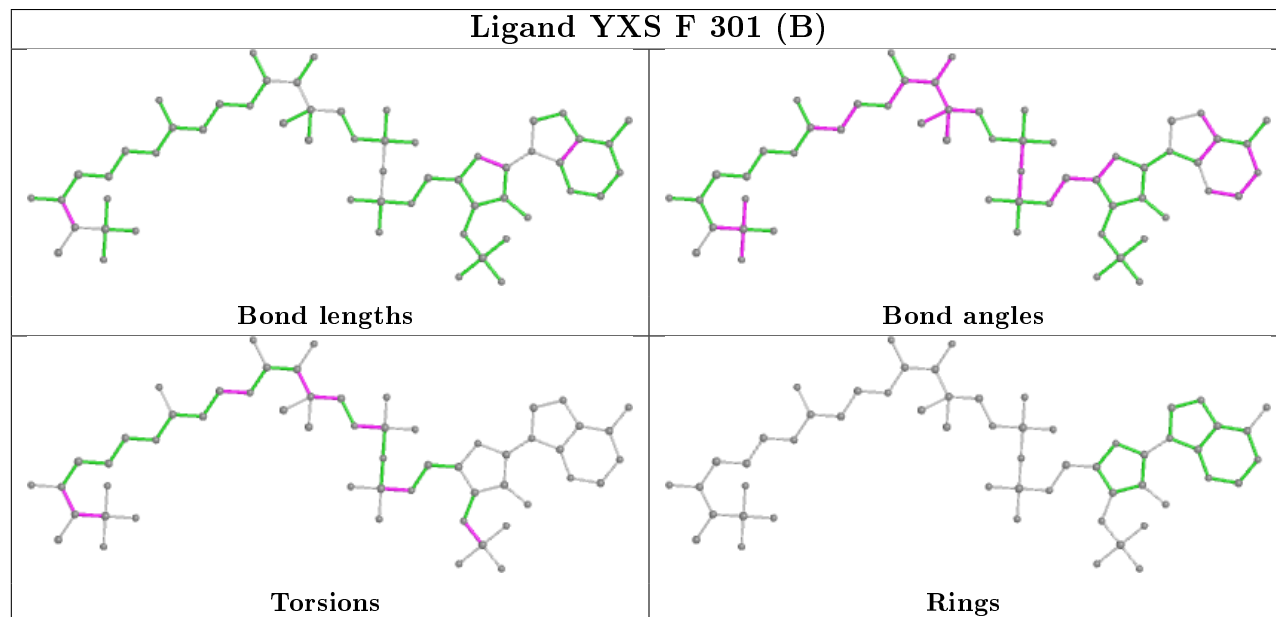
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	305	PEG	3	0
2	C	301[B]	YXS	1	0
3	B	302[A]	YXR	2	0
6	C	304	PG4	1	0
2	A	301[B]	YXS	1	0
2	E	301[B]	YXS	3	0
3	A	302[A]	YXR	1	0

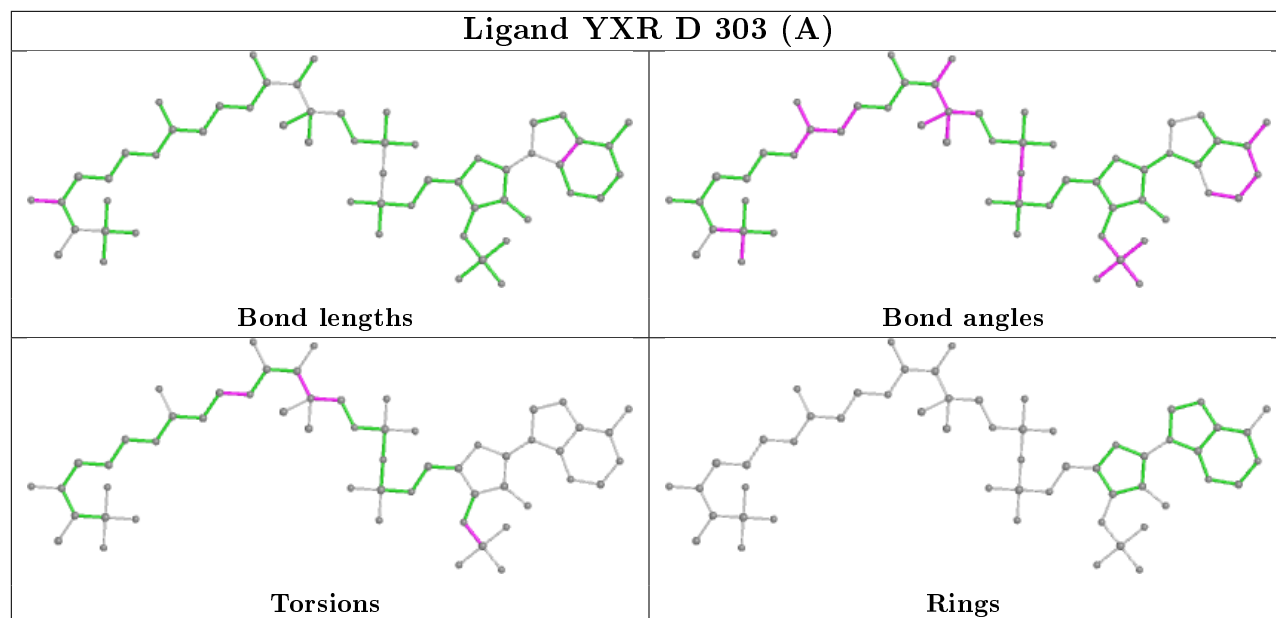
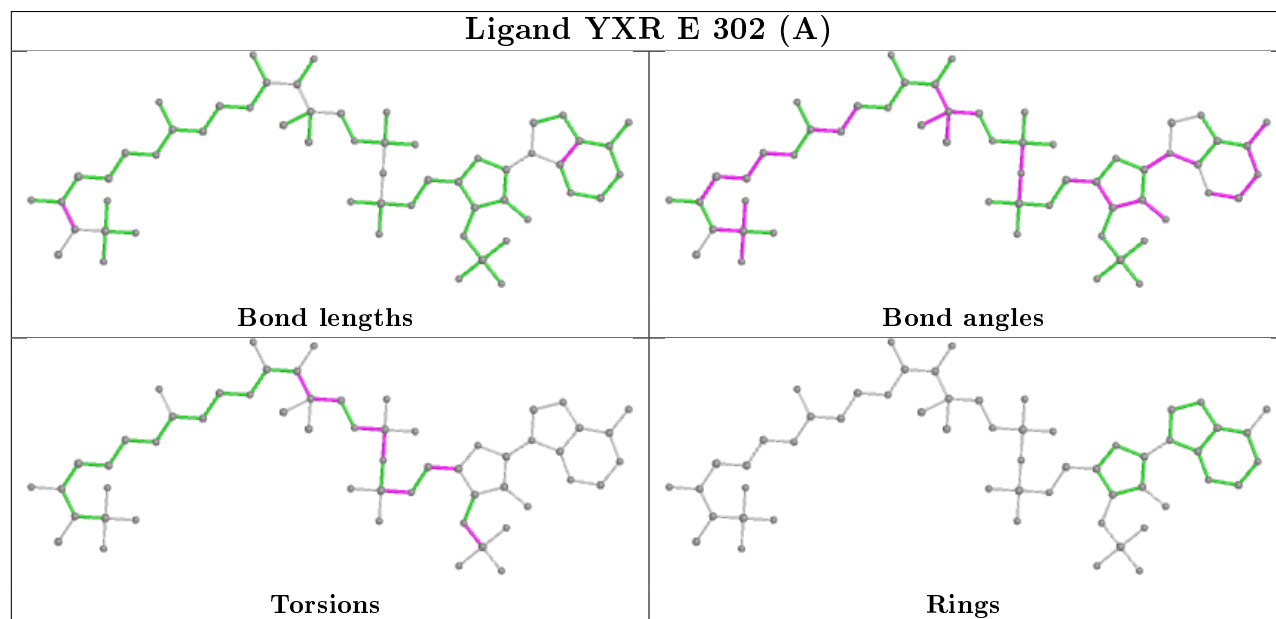
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 YXS B 301 (B)

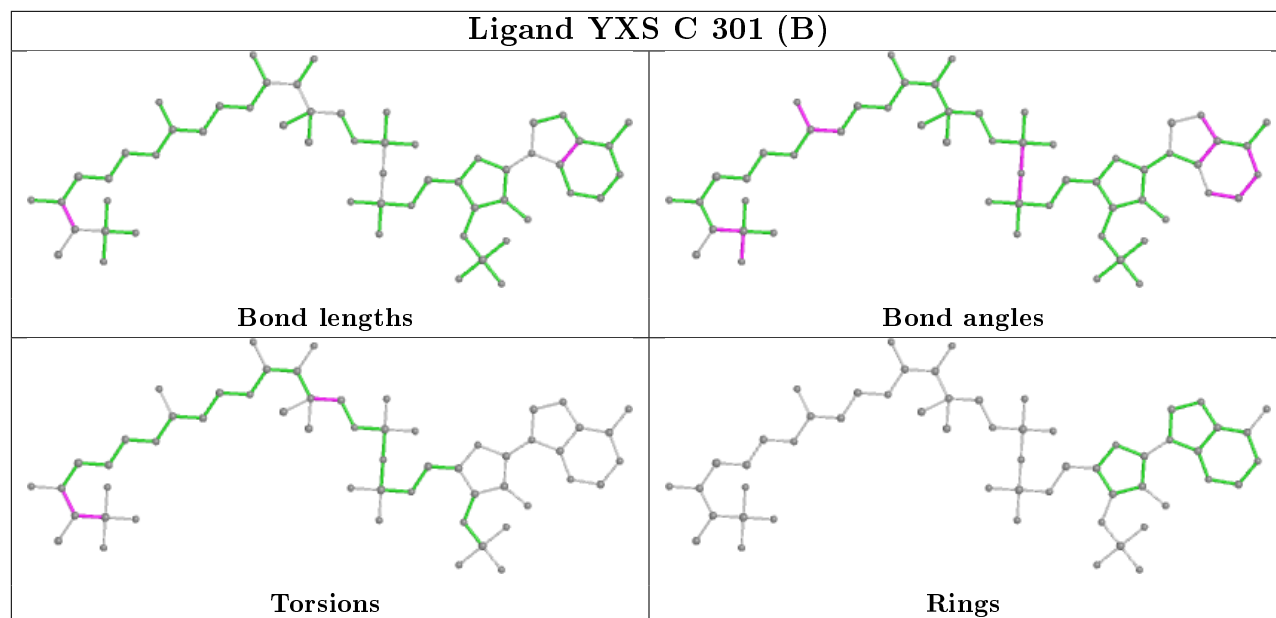


## Ligand YXS F 301 (B)

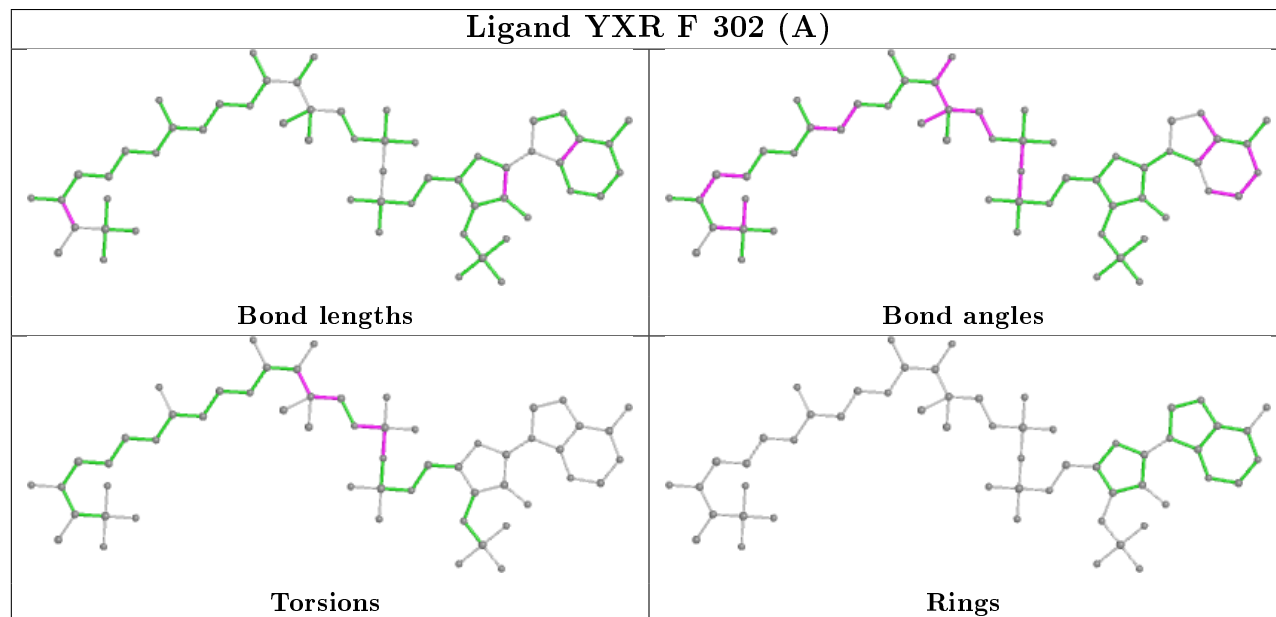


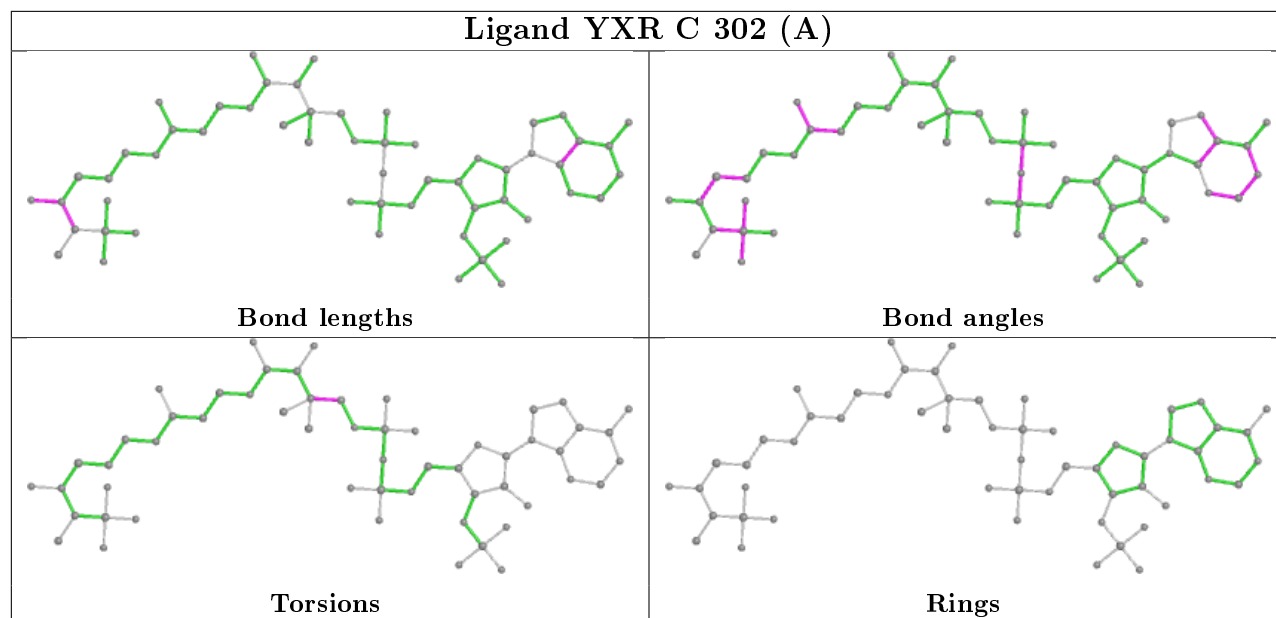
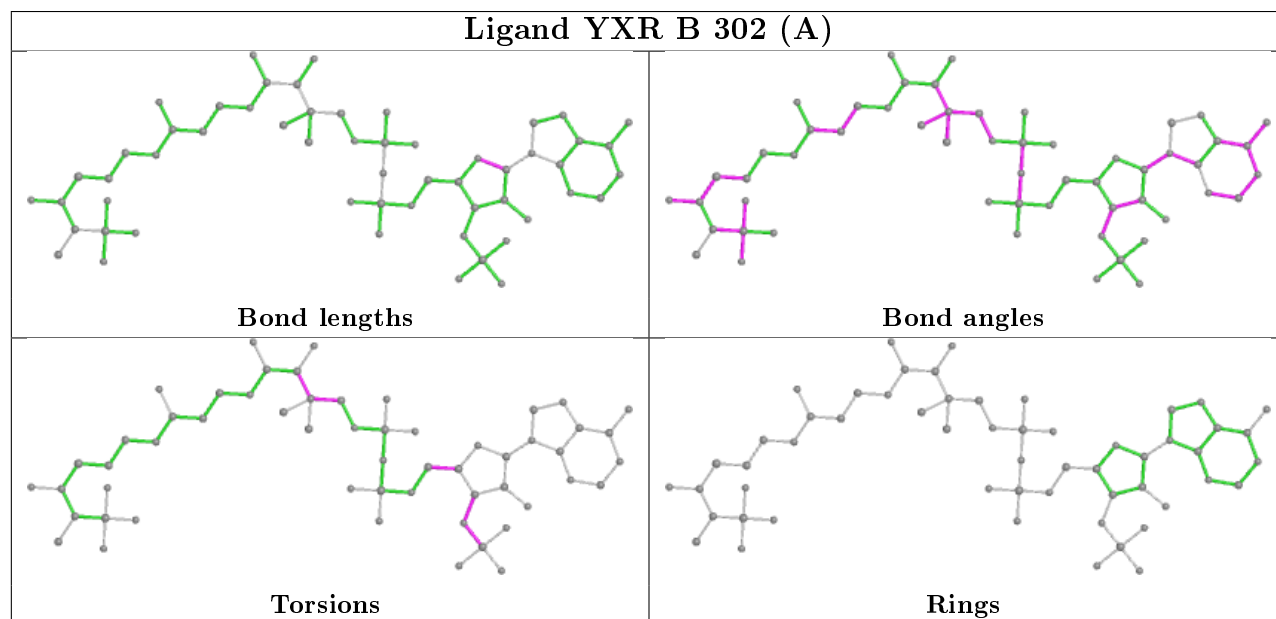
**Ligand YXR D 303 (A)****Ligand YXR E 302 (A)**

## Ligand YXS C 301 (B)

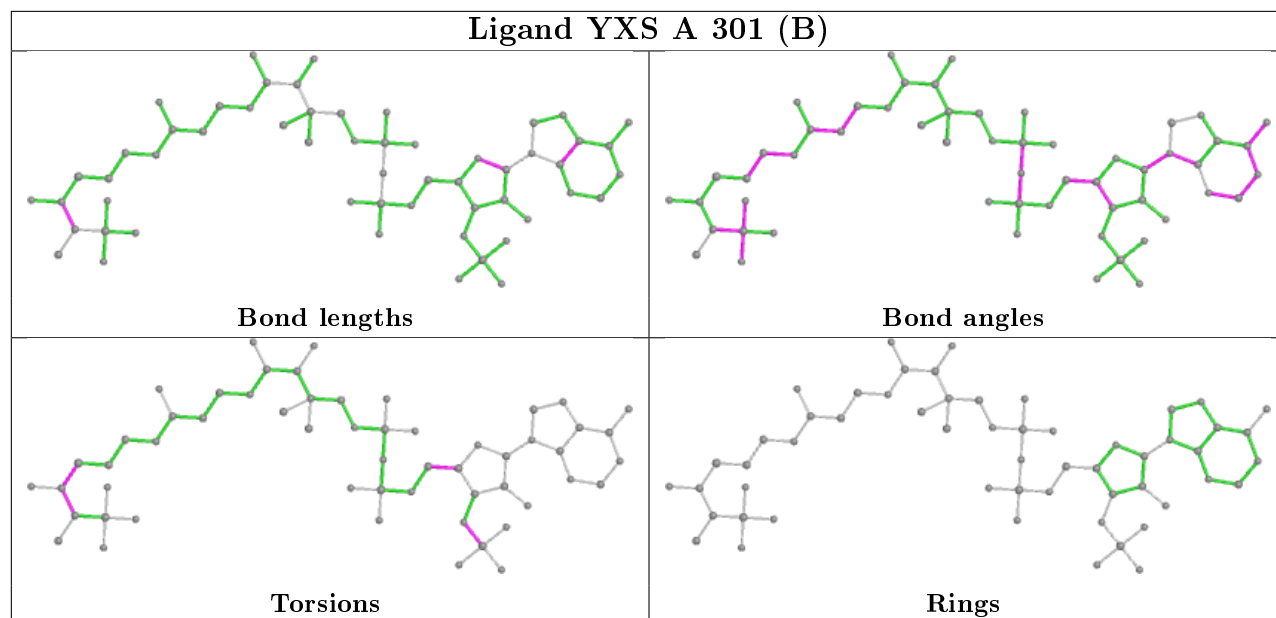


## Ligand YXR F 302 (A)

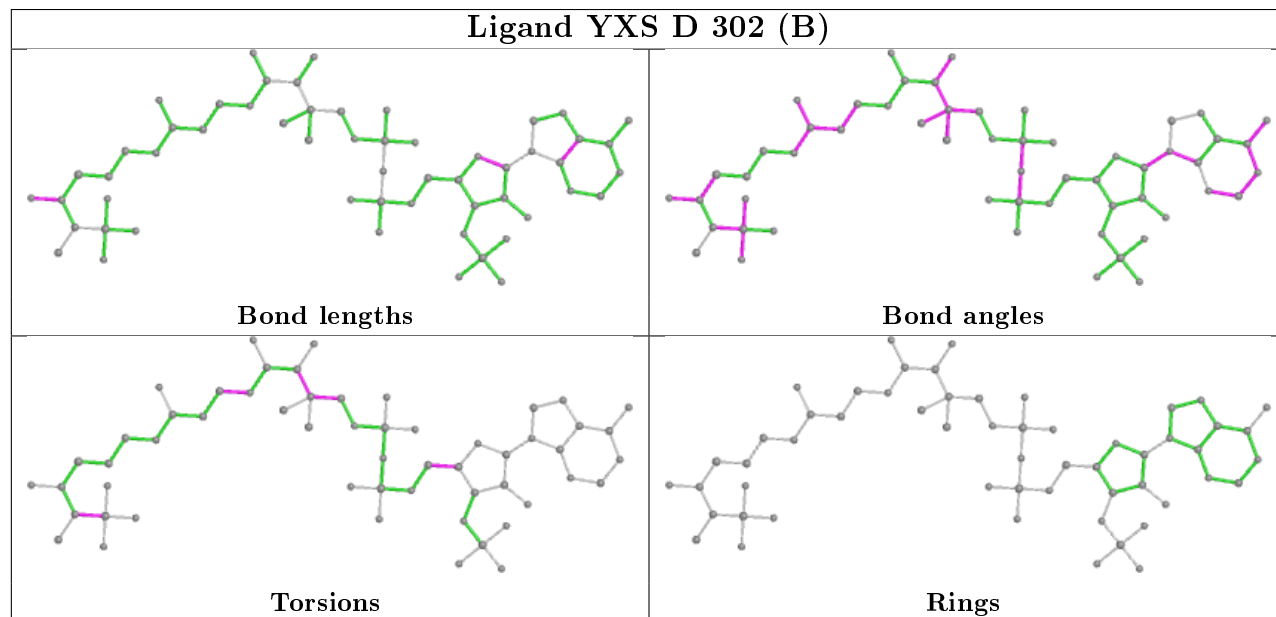


**Ligand YXR C 302 (A)****Ligand YXR B 302 (A)**

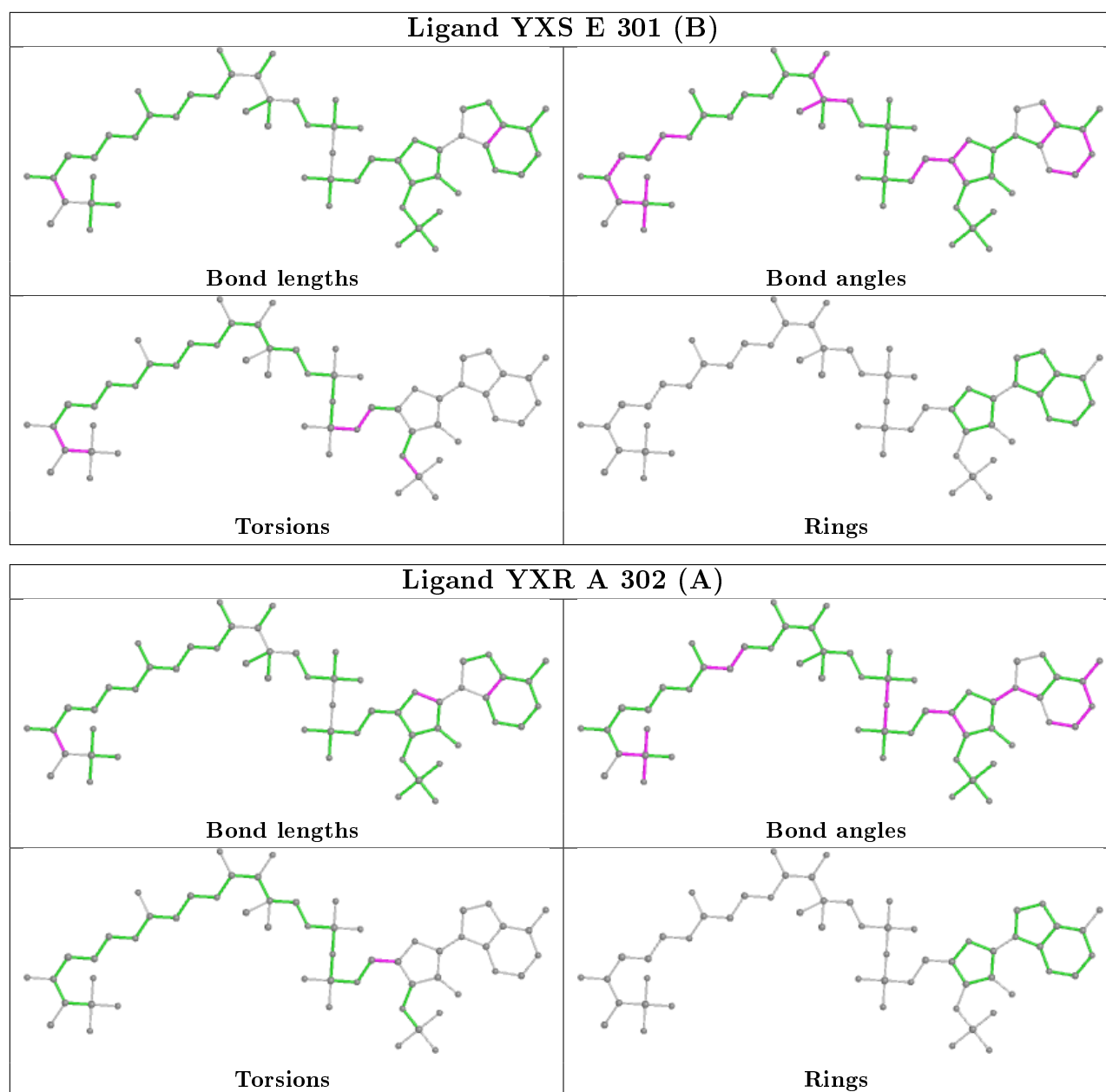
## Ligand YXS A 301 (B)



## Ligand YXS D 302 (B)







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	260/261 (99%)	-0.25	3 (1%) 79 76	17, 21, 37, 46	0
1	B	260/261 (99%)	-0.06	6 (2%) 60 56	17, 23, 47, 86	0
1	C	260/261 (99%)	-0.19	6 (2%) 60 56	16, 22, 42, 90	0
1	D	260/261 (99%)	-0.16	5 (1%) 66 63	17, 22, 38, 79	0
1	E	260/261 (99%)	-0.08	9 (3%) 44 38	17, 23, 47, 84	0
1	F	260/261 (99%)	-0.16	6 (2%) 60 56	17, 23, 43, 57	0
All	All	1560/1566 (99%)	-0.15	35 (2%) 62 57	16, 22, 42, 90	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	74	GLY	9.3
1	B	73	SER	6.6
1	C	74	GLY	5.6
1	D	251	LEU	5.1
1	F	251	LEU	4.8
1	D	2	ALA	4.6
1	E	75	GLY	4.3
1	E	2	ALA	4.3
1	D	74	GLY	4.2
1	A	2	ALA	4.1
1	E	73	SER	3.9
1	E	251	LEU	3.5
1	B	74	GLY	3.4
1	B	251	LEU	3.3
1	B	250	PHE	2.9
1	C	73	SER	2.9
1	F	253	LYS	2.8
1	F	250	PHE	2.6
1	E	261	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	23	ARG	2.6
1	A	23[A]	ARG	2.5
1	F	73	SER	2.5
1	E	248	ASN	2.5
1	B	75	GLY	2.5
1	C	75	GLY	2.4
1	C	261	HIS	2.4
1	E	185	GLU	2.4
1	E	250	PHE	2.2
1	B	2	ALA	2.2
1	D	253	LYS	2.2
1	A	261	HIS	2.2
1	C	23	ARG	2.1
1	F	2	ALA	2.0
1	D	73	SER	2.0
1	C	250	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

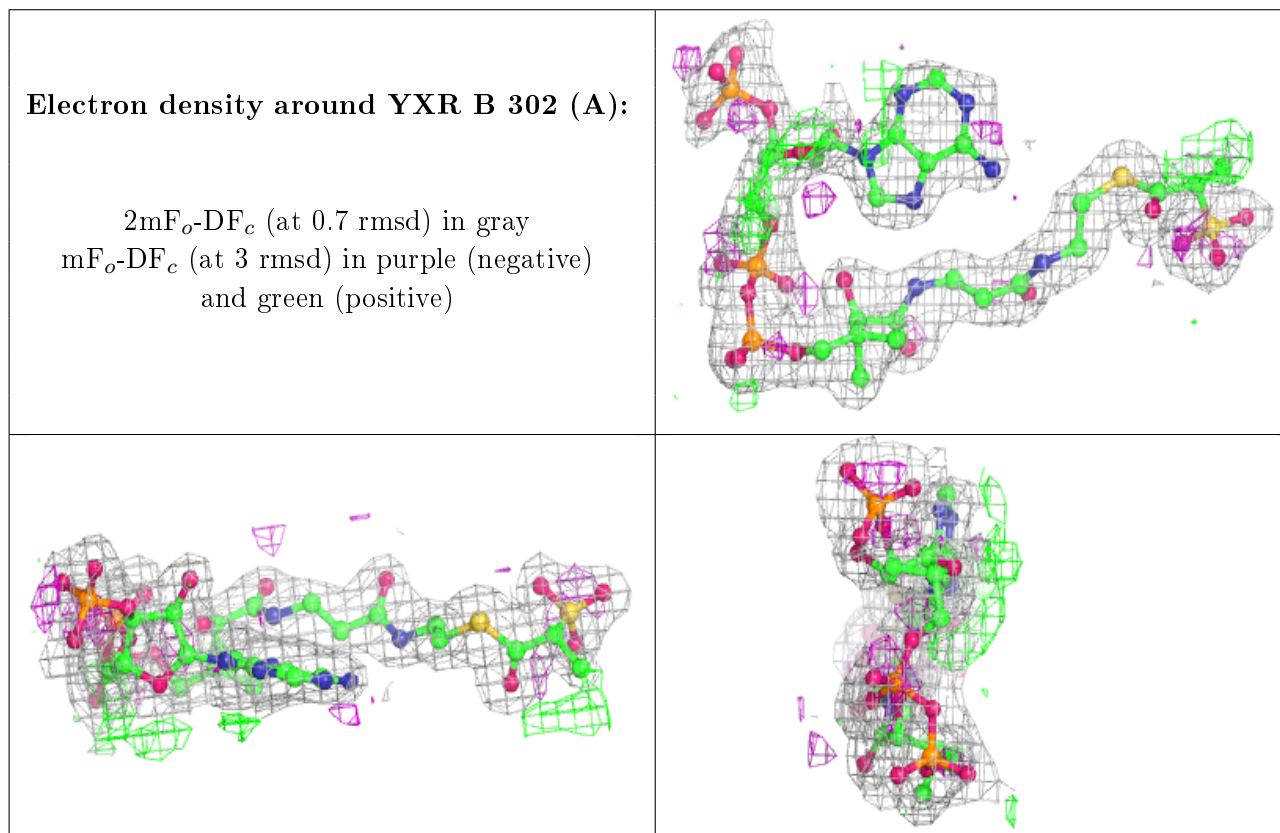
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	PEG	C	305	7/7	0.76	0.17	66,69,71,74	0
7	PEG	F	305	7/7	0.77	0.18	56,57,61,62	0
8	PGE	F	304	10/10	0.80	0.14	49,54,61,61	0
6	PG4	C	304	13/13	0.89	0.12	40,43,49,50	0
3	YXR	B	302[A]	56/56	0.93	0.12	24,46,75,79	56
2	YXS	B	301[B]	56/56	0.93	0.12	25,44,74,79	56
2	YXS	F	301[B]	56/56	0.94	0.13	26,50,67,69	56

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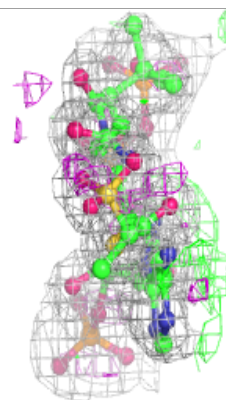
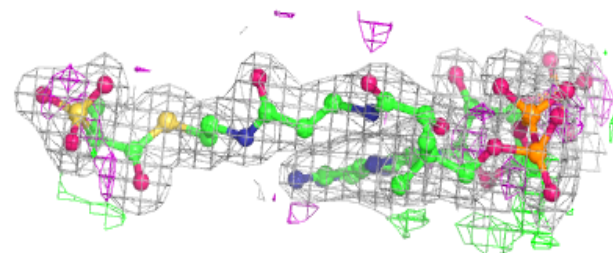
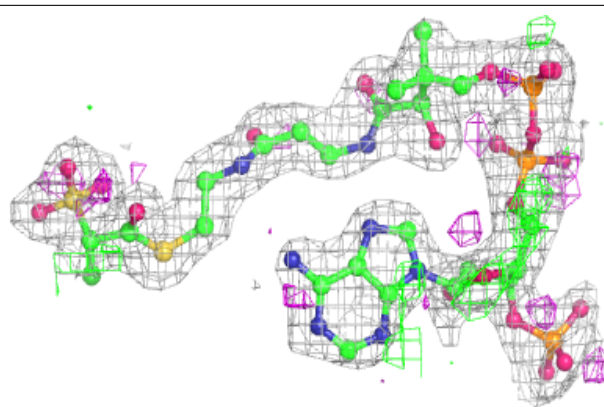
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	YXR	C	302[A]	56/56	0.94	0.10	22,36,49,53	56
2	YXS	C	301[B]	56/56	0.95	0.10	23,36,49,53	56
3	YXR	D	303[A]	56/56	0.95	0.10	22,32,39,51	56
3	YXR	F	302[A]	56/56	0.95	0.11	25,35,49,52	56
3	YXR	A	302[A]	56/56	0.95	0.09	19,31,54,57	56
2	YXS	A	301[B]	56/56	0.96	0.09	23,31,54,57	56
2	YXS	D	302[B]	56/56	0.96	0.10	22,34,42,53	56
2	YXS	E	301[B]	56/56	0.96	0.11	26,39,54,57	56
3	YXR	E	302[A]	56/56	0.96	0.10	23,35,44,46	56
4	NI	D	301	1/1	0.98	0.02	39,39,39,39	0
5	K	F	303	1/1	0.98	0.09	44,44,44,44	0
4	NI	A	303	1/1	0.98	0.03	41,41,41,41	0
5	K	C	303	1/1	0.99	0.11	41,41,41,41	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.

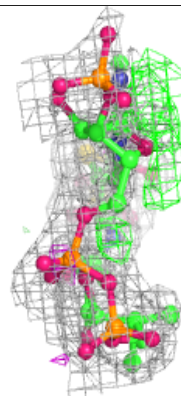
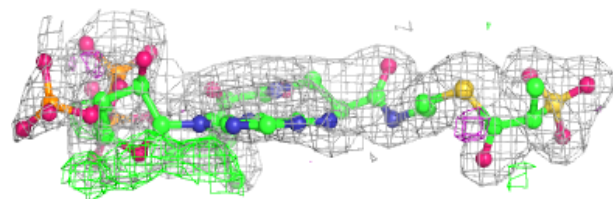
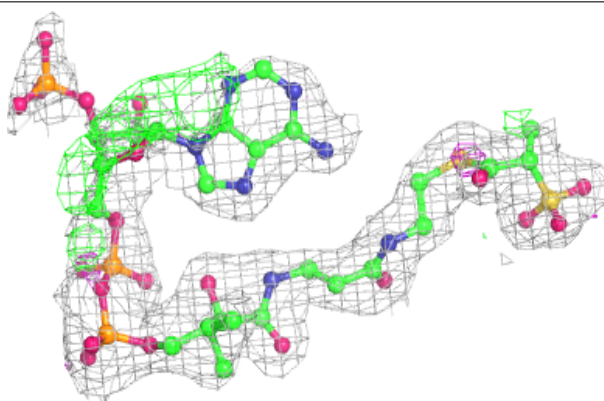


**Electron density around YXS B 301 (B):**

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

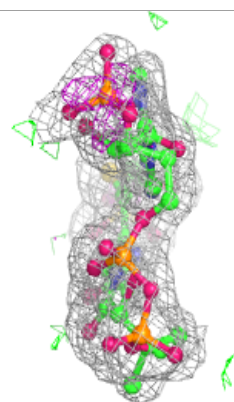
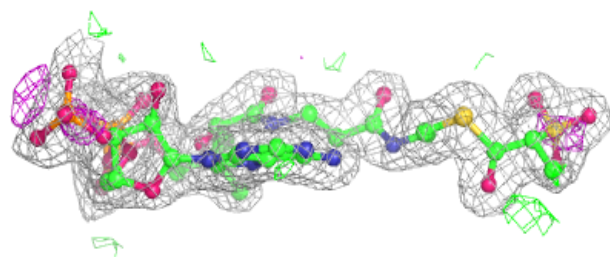
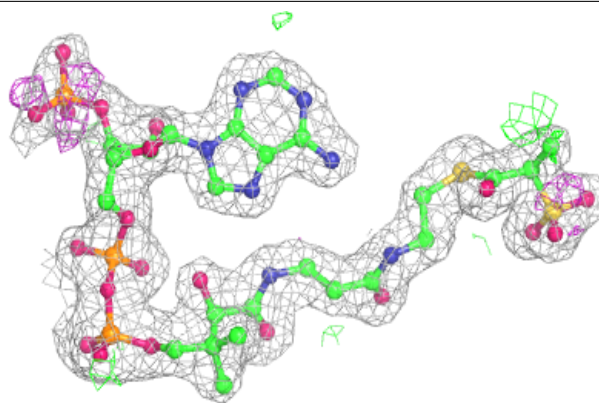
**Electron density around YXS F 301 (B):**

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

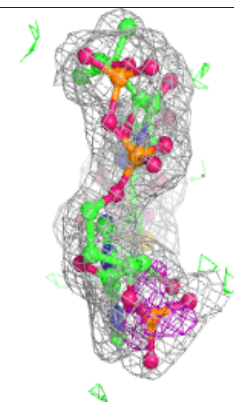
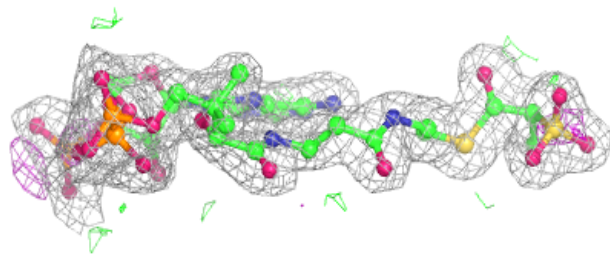
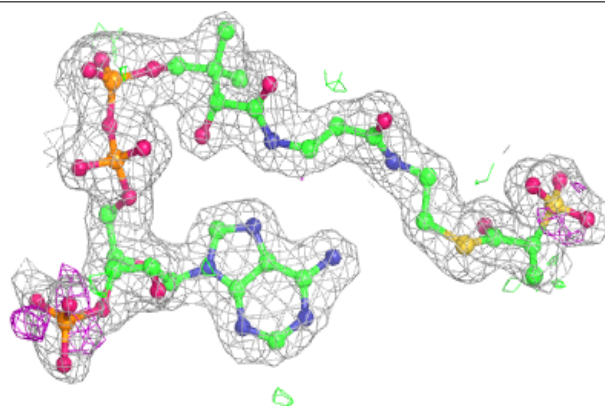


**Electron density around YXR C 302 (A):**

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

**Electron density around YXS C 301 (B):**

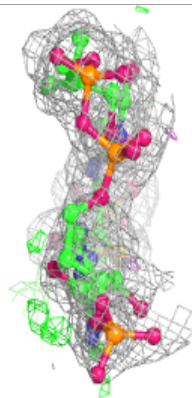
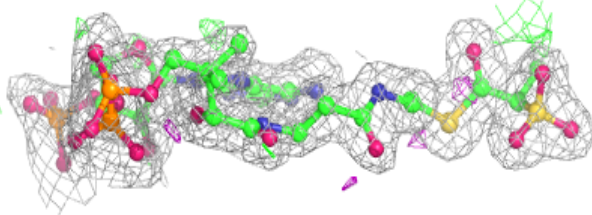
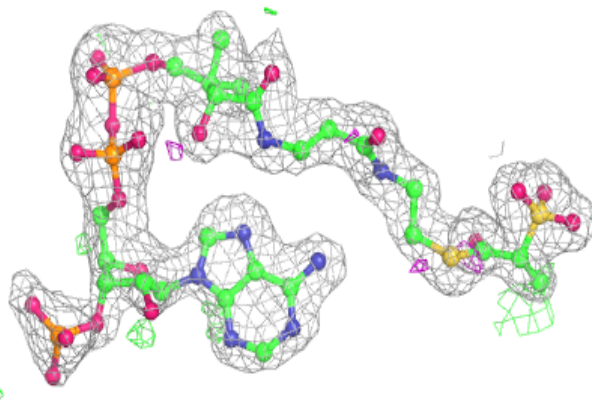
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



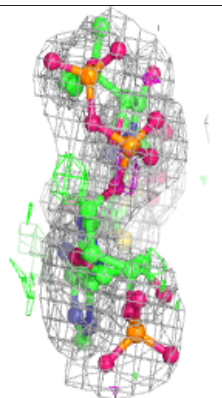
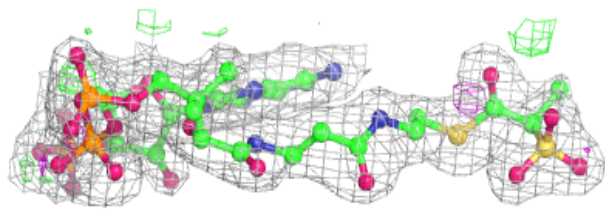
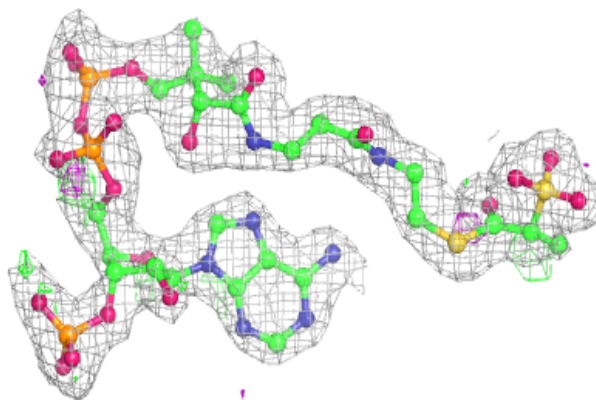


**Electron density around YXR D 303 (A):**

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

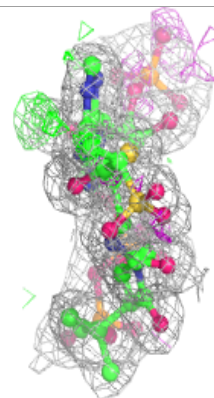
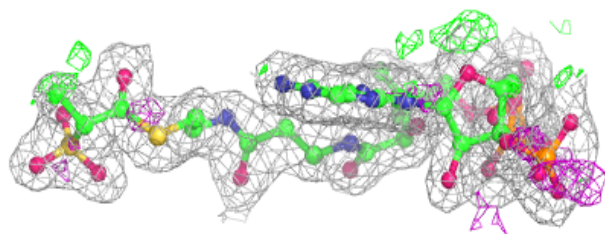
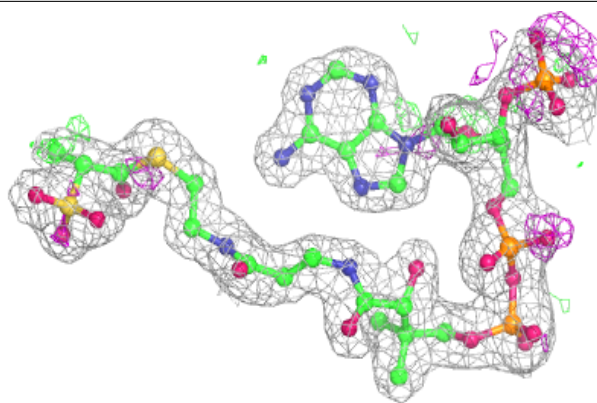
**Electron density around YXR F 302 (A):**

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

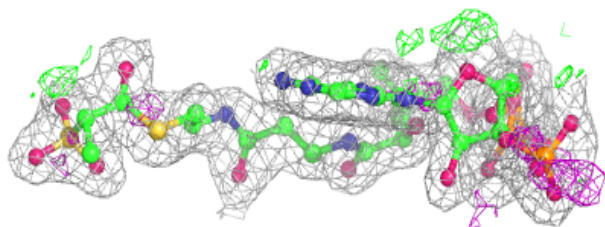
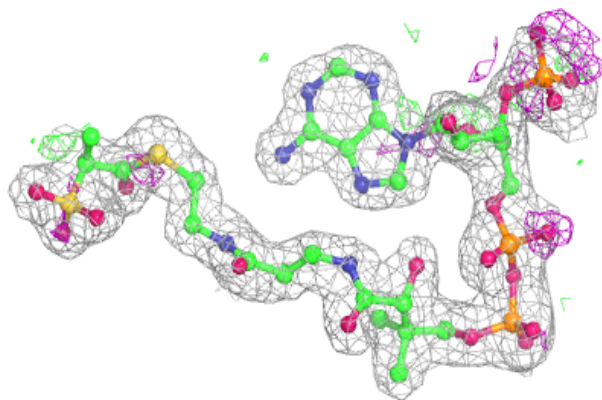


**Electron density around YXR A 302 (A):**

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

**Electron density around YXS A 301 (B):**

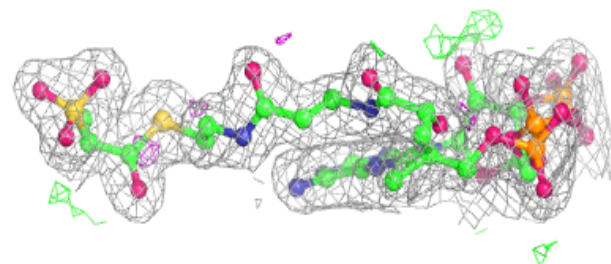
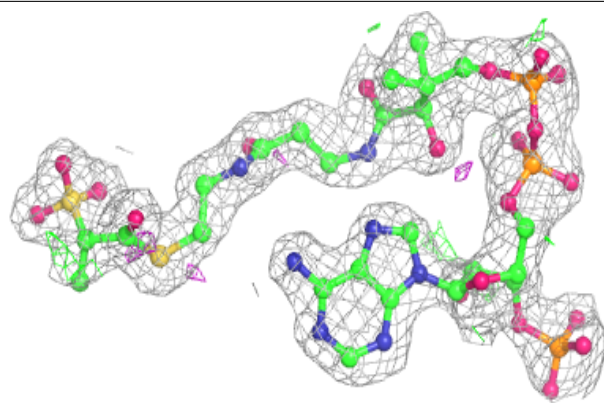
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



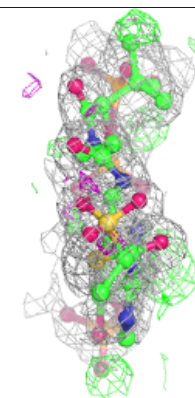
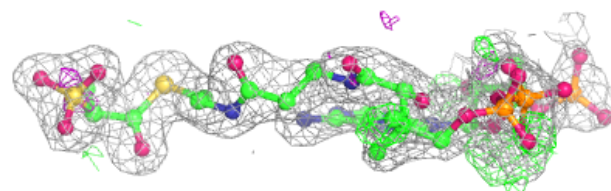
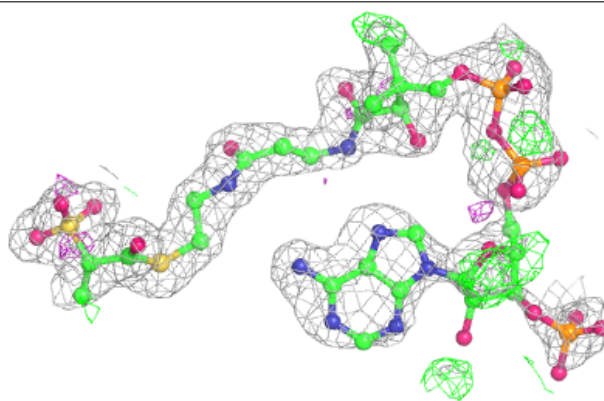


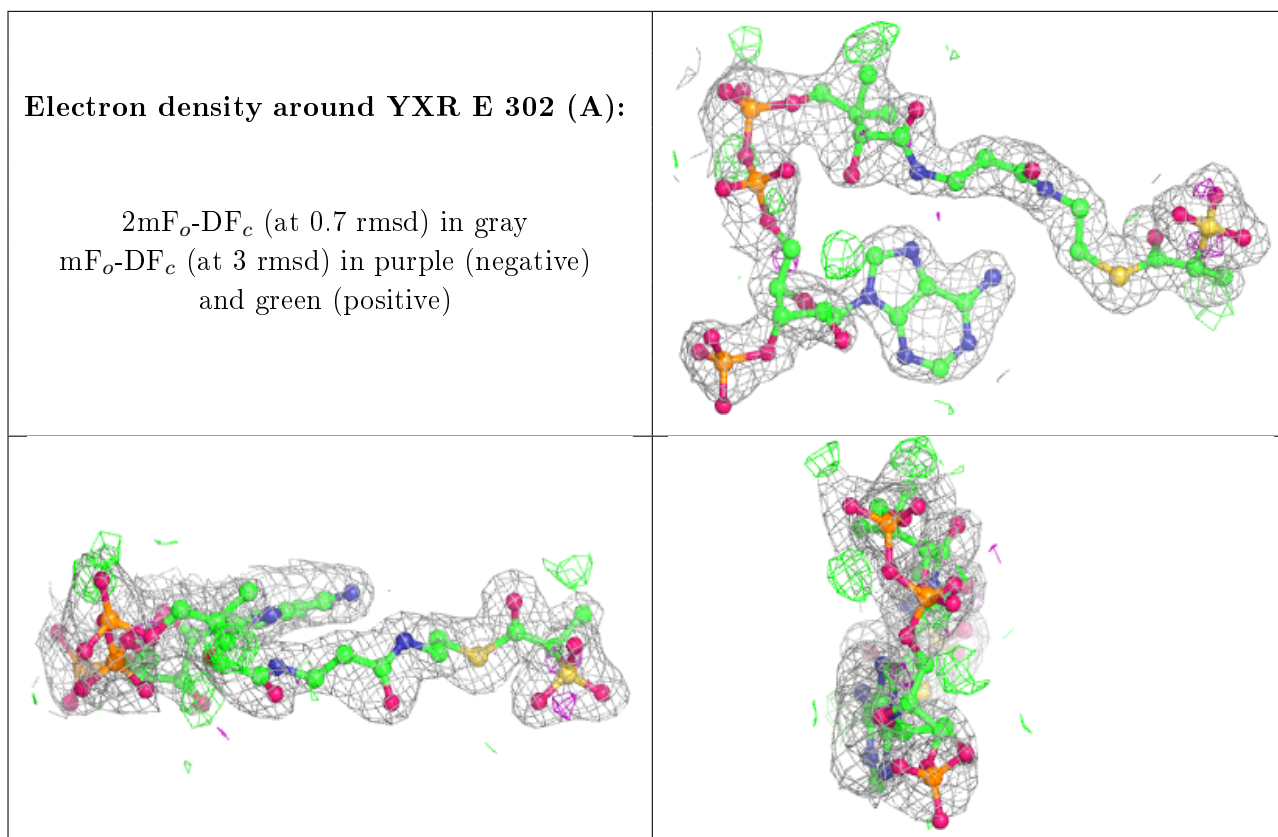
**Electron density around YXS D 302 (B):**

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

**Electron density around YXS E 301 (B):**

$2mF_o-DF_c$  (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.