



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:24 AM UTC

PDB ID : 6N95 / pdb_00006n95
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

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:

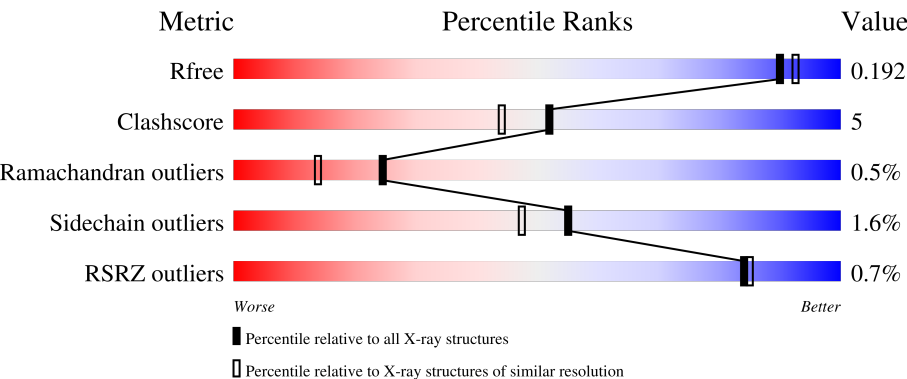
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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	261	90%9%
1	B	261	2% 90%9%
1	C	261	% 90%8%
1	D	261	88%12%
1	E	261	% 92%8%

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Mol	Chain	Length	Quality of chain
1	F	261	 90% 9%

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.

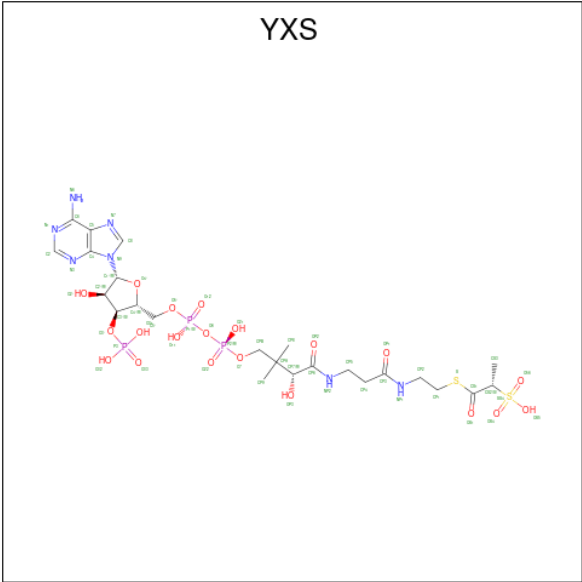
- Molecule 1 is a protein called Methylmalonyl-CoA decarboxylase.

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:

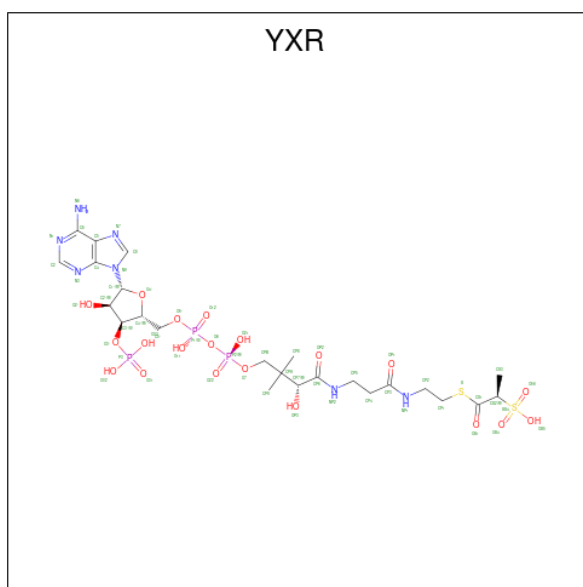
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP P52045
B	2	ALA	SER	engineered mutation	UNP P52045
C	2	ALA	SER	engineered mutation	UNP P52045
D	2	ALA	SER	engineered mutation	UNP P52045
E	2	ALA	SER	engineered mutation	UNP P52045
F	2	ALA	SER	engineered mutation	UNP P52045

- Molecule 2 is (2S)-sulfonatepropionyl-CoA (CCD ID: YXS) (formula: $C_{24}H_{40}N_7O_{20}P_3S_2$).



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 (CCD ID: YXR) (formula: C₂₄H₄₀N₇O₂₀P₃S₂).



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 (CCD ID: 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 (CCD ID: K) (formula: K).

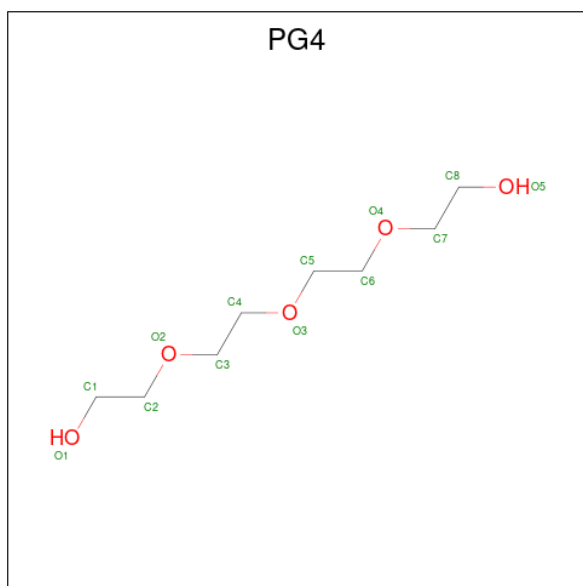
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	K	0	0
			1	1		

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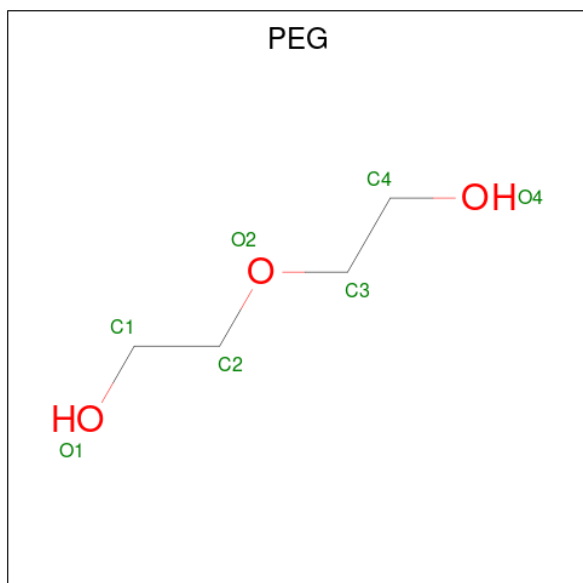
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total K 1 1	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



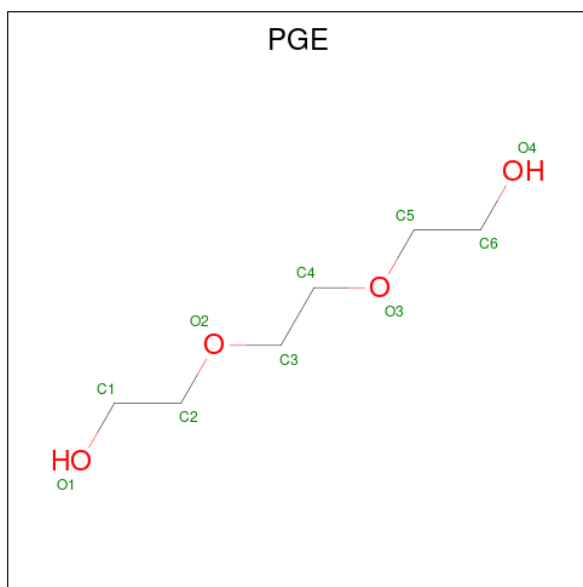
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 13 8 5	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: 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 (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 9 is water.

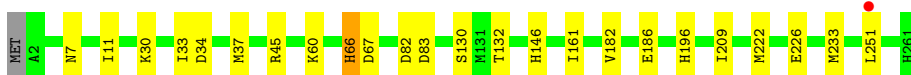
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	305	Total	O	1	19
			322	322		
9	B	265	Total	O	0	9
			274	274		
9	C	283	Total	O	0	19
			301	301		
9	D	282	Total	O	0	14
			295	295		
9	E	271	Total	O	0	14
			285	285		
9	F	288	Total	O	0	13
			301	301		

3 Residue-property plots

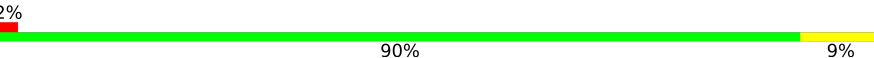
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A: 



- Molecule 1: Methylmalonyl-CoA decarboxylase

Chain B: 



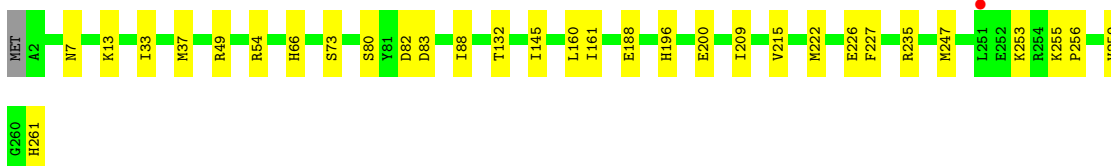
- Molecule 1: Methylmalonyl-CoA decarboxylase

Chain C: 

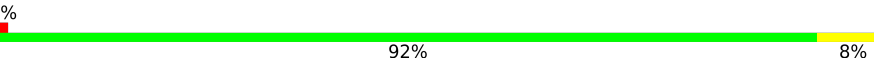


- Molecule 1: Methylmalonyl-CoA decarboxylase

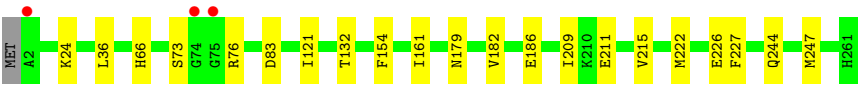
Chain D: 



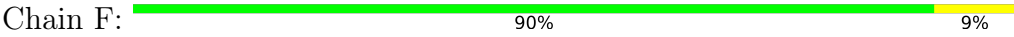
- Molecule 1: Methylmalonyl-CoA decarboxylase

Chain E: 





● 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, α , β , γ	86.93Å 114.42Å 193.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.80) 99.7 (20.00-1.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, K, PGE, NI, YXS, PEG, YXR

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	1.07	0/2253	1.23	0/3045
1	B	1.04	1/2191 (0.0%)	1.24	2/2962 (0.1%)
1	C	1.07	0/2196	1.20	2/2968 (0.1%)
1	D	1.07	1/2186 (0.0%)	1.24	1/2953 (0.0%)
1	E	1.05	0/2206	1.24	0/2985
1	F	1.04	0/2206	1.23	1/2987 (0.0%)
All	All	1.06	2/13238 (0.0%)	1.23	6/17900 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	226	GLU	CD-OE2	-5.04	1.15	1.25
1	D	196	HIS	CG-ND1	5.01	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	82	ASP	CB-CA-C	6.32	121.37	110.94
1	B	83	ASP	CB-CA-C	5.56	118.30	109.52
1	B	238	TYR	CB-CA-C	5.29	120.95	110.17
1	C	82	ASP	CB-CA-C	5.21	119.54	110.94
1	C	83	ASP	CA-CB-CG	5.17	117.77	112.60
1	D	82	ASP	CB-CA-C	5.11	119.19	110.56

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	24	0
1	B	2111	0	2160	26	0
1	C	2114	0	2153	23	0
1	D	2103	0	2139	25	0
1	E	2120	0	2175	21	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	1	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	4	0
9	B	274	0	0	5	0
9	C	301	0	0	3	0
9	D	295	0	0	9	0
9	E	285	0	0	1	0
9	F	301	0	0	1	0
All	All	15205	0	13064	136	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 (136) 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:HE1	1:A:226[B]:GLU:HG2	1.27	1.15
1:A:222[B]:MET:HE2	1:A:226[B]:GLU:CG	1.73	1.11
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:HE2	1:A:226[B]:GLU:HG2	0.90	0.89
1:A:222[B]:MET:HE1	1:A:226[B]:GLU:CG	1.91	0.89
1:B:188:GLU:OE1	9:B:474[B]:HOH:O	1.90	0.88
1:C:222[A]:MET:CE	1:C:226[A]:GLU:CG	2.51	0.84
1:A:222[B]:MET:HE3	1:A:226[B]:GLU:HG2	1.51	0.84
1:D:222[B]:MET:HE3	1:D:227[B]:PHE:CE1	2.15	0.81
1:D:83:ASP:HB2	9:D:471:HOH:O	1.81	0.80
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:243:TYR:CE1	1:C:247:MET:HE3	2.21	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: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
1:F:261:HIS:NE2	7:F:305:PEG:H42	2.10	0.66
1:C:60[B]:LYS:NZ	2:C:301[B]:YXS:O21	2.30	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:82:ASP:O	1:B:87[B]:GLN:NE2	2.32	0.62
1:B:222[A]:MET:SD	1:B:227[A]:PHE:CE1	2.91	0.62
1:E:215[B]:VAL:HG12	1:F:222:MET:HE1	1.81	0.62
1:F:196[B]:HIS:HD2	9:F:563:HOH:O	1.82	0.62
1:A:222[B]:MET:HE2	1:A:226[B]:GLU:CB	2.30	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:E:222[B]:MET:HE2	1:E:227[B]:PHE:CE1	2.37	0.59
1:E:247:MET:HA	1:E:247:MET:HE2	1.83	0.59
1:D:33:ILE:HG22	1:D:37:MET:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:60[A]:LYS:NZ	3:B:302[A]:YXR:O21	2.29	0.58
1:A:33:ILE:HG22	1:A:37:MET:HE2	1.84	0.58
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:F:33:ILE:HG22	1:F:37:MET:HE2	1.86	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:D:73:SER:OG	1:D:247[A]:MET:HE1	2.07	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: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
1:D:54:ARG:HH12	1:D:188[A]:GLU:CD	2.15	0.53
2:E:301[B]:YXS:O11	2:E:301[B]:YXS:C4'	2.56	0.53
1:E:222[B]:MET:HE3	1:E:226:GLU:HB3	1.91	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
1:E:209:ILE:HG21	1:F:161:ILE:HG21	1.92	0.51
1:E:222[B]:MET:HE2	1:E:227[B]:PHE:CD1	2.45	0.50
1:A:233[A]:MET:HE1	1:C:211:GLU:HG2	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: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:OP3	3:B:302[A]:YXR:O12	2.32	0.48
1:D:161:ILE:HG21	1:F:209:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182[B]:VAL:CG1	1:F:186:GLU:HB2	2.44	0.47
1:E:66:HIS:HE1	1:E:83:ASP:OD1	1.98	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:B:247:MET:HA	1:B:247:MET:HE2	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: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
2:A:301[B]:YXS:C2'	2:A:301[B]:YXS:O5'	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:B:250:PHE:CD1	1:B:250:PHE:C	2.95	0.45
1:F:3:TYR:OH	1:F:42:ASP:OD2	2.35	0.44
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: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:E:211:GLU:HG2	1:F:233[B]:MET:HE1	1.99	0.43
1:A:222[B]:MET:HE1	1:A:226[B]:GLU:HG3	1.89	0.43
1:F:146[A]:HIS:CE1	1:F:220:HIS:HD1	2.37	0.43
1:D:259:VAL:HG21	1:D:261[B]:HIS:CE1	2.54	0.43
1:A:222[B]:MET:HE1	1:C:215[B]:VAL:HB	2.01	0.43
1:C:60[A]:LYS:HA	1:C:60[A]:LYS:HD3	1.83	0.43
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:D:222[B]:MET:HE3	1:D:227[B]:PHE:CD1	2.53	0.42
1:D:253:LYS:NZ	2:D:302[B]:YXS:O31	2.35	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215[B]:VAL:CG1	1:F:222:MET:CE	2.99	0.41
1:A:222[B]:MET:CE	1:C:215[B]:VAL:HB	2.50	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:HD23	1:E:36[B]:LEU:HA	1.94	0.40
1:C:227[B]:PHE:CE2	1:C:231[B]:GLN:HG2	2.56	0.40
1:D:37:MET:HG2	1:D:88[A]:ILE:HD13	2.03	0.40
1:D:145:ILE:HD13	1:D:145:ILE:HA	1.94	0.40
1:B:220:HIS:CE1	9:B:543:HOH:O	2.74	0.40
1:D:222[B]:MET:HE3	1:D:227[B]:PHE:CZ	2.56	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

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%)	30	19
1	B	270/261 (103%)	259 (96%)	10 (4%)	1 (0%)	30	19
1	C	271/261 (104%)	264 (97%)	6 (2%)	1 (0%)	30	19
1	D	270/261 (103%)	263 (97%)	6 (2%)	1 (0%)	30	19
1	E	273/261 (105%)	265 (97%)	7 (3%)	1 (0%)	30	19
1	F	273/261 (105%)	263 (96%)	8 (3%)	2 (1%)	18	8
All	All	1635/1566 (104%)	1583 (97%)	45 (3%)	7 (0%)	24	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	74	GLY

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Mol	Chain	Res	Type
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 ⓘ

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%)	236 (97%)	7 (3%)	37	25
1	B	235/224 (105%)	231 (98%)	4 (2%)	53	45
1	C	236/224 (105%)	229 (97%)	7 (3%)	36	24
1	D	236/224 (105%)	232 (98%)	4 (2%)	53	45
1	E	238/224 (106%)	237 (100%)	1 (0%)	84	83
1	F	238/224 (106%)	235 (99%)	3 (1%)	61	54
All	All	1426/1344 (106%)	1400 (98%)	26 (2%)	55	43

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	60	LYS
1	A	66[A]	HIS
1	A	66[B]	HIS
1	A	130[A]	SER
1	A	130[B]	SER
1	A	251	LEU
1	B	66	HIS
1	B	76	ARG
1	B	154	PHE
1	B	247	MET
1	C	23	ARG

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Mol	Chain	Res	Type
1	C	136	LEU
1	C	154	PHE
1	C	204[A]	LEU
1	C	204[B]	LEU
1	C	222[A]	MET
1	C	222[B]	MET
1	D	160	LEU
1	D	215[A]	VAL
1	D	215[B]	VAL
1	D	235	ARG
1	E	154	PHE
1	F	66	HIS
1	F	154	PHE
1	F	185	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
1	B	7	ASN
1	B	26	ASN
1	C	26	ASN
1	C	69	HIS
1	C	244	GLN
1	C	257	ASN
1	C	261	HIS
1	D	7	ASN
1	D	12	ASN
1	D	66	HIS
1	D	87	GLN
1	E	7	ASN
1	E	26	ASN
1	E	66	HIS
1	E	179	ASN
1	E	197	HIS
1	F	26	ASN
1	F	66	HIS
1	F	193	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	C	301[B]	-	54,58,58	1.23	5 (9%)	77,88,88	1.64	13 (16%)
2	YXS	A	301[B]	-	54,58,58	1.33	4 (7%)	77,88,88	1.73	18 (23%)
8	PGE	F	304	5	9,9,9	0.35	0	8,8,8	0.20	0
2	YXS	F	301[B]	-	54,58,58	1.37	8 (14%)	77,88,88	3.11	23 (29%)
2	YXS	B	301[B]	-	54,58,58	1.11	7 (12%)	77,88,88	1.81	21 (27%)
3	YXR	E	302[A]	-	54,58,58	1.42	6 (11%)	77,88,88	3.09	28 (36%)
3	YXR	F	302[A]	-	54,58,58	1.24	6 (11%)	77,88,88	1.87	16 (20%)
3	YXR	A	302[A]	-	54,58,58	1.27	4 (7%)	77,88,88	1.68	15 (19%)
2	YXS	D	302[B]	-	54,58,58	1.15	3 (5%)	77,88,88	3.07	22 (28%)
7	PEG	C	305	-	6,6,6	0.34	0	5,5,5	0.18	0
7	PEG	F	305	-	6,6,6	0.29	0	5,5,5	0.25	0
3	YXR	B	302[A]	-	54,58,58	1.07	5 (9%)	77,88,88	3.35	24 (31%)
3	YXR	D	303[A]	-	54,58,58	1.22	5 (9%)	77,88,88	3.05	22 (28%)
6	PG4	C	304	5	12,12,12	0.26	0	11,11,11	0.25	0
2	YXS	E	301[B]	-	54,58,58	1.24	7 (12%)	77,88,88	1.86	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	YXR	C	302[A]	-	54,58,58	1.22	6 (11%)	77,88,88	1.72	13 (16%)

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	C	301[B]	-	-	5/58/77/77	0/3/3/3
2	YXS	A	301[B]	-	-	3/58/77/77	0/3/3/3
8	PGE	F	304	5	-	0/7/7/7	-
2	YXS	F	301[B]	-	-	13/58/77/77	0/3/3/3
2	YXS	B	301[B]	-	-	7/58/77/77	0/3/3/3
3	YXR	E	302[A]	-	-	15/58/77/77	0/3/3/3
3	YXR	F	302[A]	-	-	7/58/77/77	0/3/3/3
3	YXR	A	302[A]	-	-	1/58/77/77	0/3/3/3
2	YXS	D	302[B]	-	-	7/58/77/77	0/3/3/3
7	PEG	C	305	-	-	0/4/4/4	-
7	PEG	F	305	-	-	1/4/4/4	-
3	YXR	B	302[A]	-	-	10/58/77/77	0/3/3/3
3	YXR	D	303[A]	-	-	6/58/77/77	0/3/3/3
6	PG4	C	304	5	-	2/10/10/10	-
2	YXS	E	301[B]	-	-	8/58/77/77	0/3/3/3
3	YXR	C	302[A]	-	-	3/58/77/77	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	302[A]	YXR	P1-O6	5.47	1.65	1.59
2	A	301[B]	YXS	C5-C4	4.90	1.47	1.39
3	A	302[A]	YXR	C5-C4	4.89	1.47	1.39
2	F	301[B]	YXS	C5-C4	4.83	1.47	1.39
2	C	301[B]	YXS	C5-C4	4.71	1.47	1.39
3	C	302[A]	YXR	C5-C4	4.71	1.47	1.39
3	F	302[A]	YXR	C5-C4	4.66	1.47	1.39
3	E	302[A]	YXR	C5-C4	4.62	1.47	1.39
2	E	301[B]	YXS	C5-C4	4.62	1.47	1.39
3	D	303[A]	YXR	C5-C4	4.37	1.46	1.39
2	A	301[B]	YXS	CS2-CS1	-4.31	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	302[B]	YXS	C5-C4	4.21	1.46	1.39
3	B	302[A]	YXR	C5-C4	3.89	1.46	1.39
2	B	301[B]	YXS	C5-C4	3.83	1.45	1.39
3	E	302[A]	YXR	C4-N9	-3.59	1.30	1.37
2	F	301[B]	YXS	CS2-CS1	-3.52	1.48	1.52
3	A	302[A]	YXR	CS2-CS1	-3.46	1.48	1.52
3	D	303[A]	YXR	OS1-CS1	3.31	1.25	1.20
2	D	302[B]	YXS	OS1-CS1	3.17	1.25	1.20
2	C	301[B]	YXS	CS2-CS1	-2.86	1.49	1.52
3	F	302[A]	YXR	CS2-CS1	-2.83	1.49	1.52
2	F	301[B]	YXS	P1-O6	2.78	1.62	1.59
2	F	301[B]	YXS	C5-C6	2.75	1.48	1.41
3	A	302[A]	YXR	C8-N7	2.68	1.36	1.31
2	A	301[B]	YXS	C8-N7	2.64	1.36	1.31
2	E	301[B]	YXS	P1-O6	2.61	1.62	1.59
3	D	303[A]	YXR	C5-N7	-2.61	1.34	1.39
2	F	301[B]	YXS	C8-N7	2.54	1.36	1.31
2	C	301[B]	YXS	C5-C6	2.53	1.48	1.41
3	C	302[A]	YXR	C5-C6	2.53	1.48	1.41
2	E	301[B]	YXS	CS2-CS1	-2.53	1.49	1.52
2	E	301[B]	YXS	C4-N9	-2.51	1.32	1.37
3	F	302[A]	YXR	C5-C6	2.50	1.47	1.41
2	C	301[B]	YXS	C4-N9	-2.50	1.32	1.37
3	C	302[A]	YXR	C4-N9	-2.50	1.32	1.37
3	B	302[A]	YXR	C5-N7	-2.48	1.34	1.39
2	C	301[B]	YXS	C5-N7	-2.47	1.34	1.39
3	C	302[A]	YXR	C5-N7	-2.47	1.34	1.39
2	E	301[B]	YXS	C5-C6	2.47	1.47	1.41
2	B	301[B]	YXS	C5-N7	-2.46	1.34	1.39
3	F	302[A]	YXR	C4-N9	-2.42	1.32	1.37
3	B	302[A]	YXR	C4-N9	-2.38	1.32	1.37
2	B	301[B]	YXS	CS2-CS1	-2.37	1.49	1.52
3	C	302[A]	YXR	OS1-CS1	2.35	1.24	1.20
2	E	301[B]	YXS	P2-O6	2.35	1.62	1.59
3	E	302[A]	YXR	C5-C6	2.34	1.47	1.41
2	B	301[B]	YXS	C4-N9	-2.33	1.32	1.37
3	C	302[A]	YXR	CS2-CS1	-2.32	1.49	1.52
2	F	301[B]	YXS	C5-N7	-2.31	1.34	1.39
3	D	303[A]	YXR	C4-N9	-2.30	1.32	1.37
2	B	301[B]	YXS	CS1-S	-2.27	1.67	1.75
3	E	302[A]	YXR	CS2-CS1	-2.26	1.49	1.52
3	F	302[A]	YXR	P1-O6	2.26	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301[B]	YXS	OS1-CS1	2.23	1.24	1.20
3	F	302[A]	YXR	C5-N7	-2.23	1.35	1.39
2	A	301[B]	YXS	C4-N9	-2.21	1.33	1.37
2	F	301[B]	YXS	C4-N9	-2.19	1.33	1.37
3	A	302[A]	YXR	C4-N9	-2.17	1.33	1.37
3	D	303[A]	YXR	C8-N7	2.16	1.35	1.31
2	D	302[B]	YXS	C4-N9	-2.13	1.33	1.37
2	B	301[B]	YXS	C8-N7	2.10	1.35	1.31
3	B	302[A]	YXR	C8-N7	2.09	1.35	1.31
3	E	302[A]	YXR	OS1-CS1	2.05	1.23	1.20
3	B	302[A]	YXR	OS1-CS1	2.05	1.23	1.20
2	E	301[B]	YXS	C8-N7	2.00	1.35	1.31
2	F	301[B]	YXS	OS1-CS1	2.00	1.23	1.20

All (238) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302[A]	YXR	CP8-CPA-CPB	-14.48	84.33	108.22
3	E	302[A]	YXR	CP8-CPA-CPB	-13.91	85.25	108.22
2	D	302[B]	YXS	CP8-CPA-CPB	-13.63	85.72	108.22
3	B	302[A]	YXR	CP8-CPA-CP7	-13.59	85.59	108.77
3	D	303[A]	YXR	CP8-CPA-CPB	-13.54	85.87	108.22
2	F	301[B]	YXS	CP8-CPA-CPB	-12.95	86.85	108.22
2	F	301[B]	YXS	CP8-CPA-CP7	-12.65	87.20	108.77
3	E	302[A]	YXR	CP8-CPA-CP7	-11.71	88.81	108.77
3	D	303[A]	YXR	CP8-CPA-CP9	-10.76	87.74	109.20
2	D	302[B]	YXS	CP8-CPA-CP9	-10.65	87.97	109.20
3	B	302[A]	YXR	CP9-CPA-CPB	10.24	125.14	108.22
2	F	301[B]	YXS	CP9-CPA-CP7	10.06	125.92	108.77
3	B	302[A]	YXR	CP8-CPA-CP9	-9.98	89.30	109.20
2	F	301[B]	YXS	CP8-CPA-CP9	-9.84	89.59	109.20
2	D	302[B]	YXS	CP8-CPA-CP7	-9.58	92.44	108.77
3	D	303[A]	YXR	CP8-CPA-CP7	-9.42	92.72	108.77
3	D	303[A]	YXR	CP9-CPA-CPB	8.94	122.99	108.22
2	D	302[B]	YXS	CP9-CPA-CPB	8.48	122.22	108.22
3	E	302[A]	YXR	CP9-CPA-CP7	7.25	121.13	108.77
3	C	302[A]	YXR	OS4-SS4-CS2	-7.16	103.53	109.36
3	E	302[A]	YXR	CP8-CPA-CP9	-7.12	95.01	109.20
2	E	301[B]	YXS	O56-SS4-CS2	-6.35	104.18	109.36
3	F	302[A]	YXR	OS4-SS4-CS2	-6.26	104.26	109.36
2	A	301[B]	YXS	O56-SS4-CS2	-6.25	104.26	109.36
3	A	302[A]	YXR	OS4-SS4-CS2	-6.16	104.34	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301[B]	YXS	O56-SS4-CS2	-5.88	104.57	109.36
3	D	303[A]	YXR	CP9-CPA-CP7	5.62	118.35	108.77
2	D	302[B]	YXS	CP9-CPA-CP7	5.53	118.19	108.77
3	F	302[A]	YXR	C5-C4-N3	-5.45	119.21	126.72
3	E	302[A]	YXR	C4-N9-C8	5.34	111.35	105.74
2	F	301[B]	YXS	C5-C4-N3	-5.29	119.43	126.72
2	D	302[B]	YXS	C4-N9-C8	5.24	111.24	105.74
2	B	301[B]	YXS	C5-C4-N3	-5.23	119.52	126.72
3	B	302[A]	YXR	C5-C4-N3	-5.20	119.55	126.72
3	D	303[A]	YXR	OP3-CP7-CPA	-5.15	98.25	110.18
3	E	302[A]	YXR	C2'-C3'-C4'	-5.11	94.30	103.24
2	D	302[B]	YXS	OP3-CP7-CPA	-5.03	98.54	110.18
3	F	302[A]	YXR	N3-C4-N9	4.96	135.61	127.17
2	C	301[B]	YXS	C5-C4-N3	-4.85	120.03	126.72
3	C	302[A]	YXR	C5-C4-N3	-4.85	120.03	126.72
2	B	301[B]	YXS	N3-C4-N9	4.85	135.41	127.17
3	B	302[A]	YXR	N3-C4-N9	4.82	135.37	127.17
3	E	302[A]	YXR	CP9-CPA-CPB	4.82	116.18	108.22
2	D	302[B]	YXS	N3-C4-N9	4.79	135.31	127.17
3	B	302[A]	YXR	O4'-C1'-N9	4.58	116.88	108.09
2	B	301[B]	YXS	O4'-C1'-N9	4.51	116.75	108.09
2	E	301[B]	YXS	C5-C4-N3	-4.42	120.63	126.72
3	A	302[A]	YXR	C4-N9-C8	4.37	110.33	105.74
3	D	303[A]	YXR	C5-C4-N3	-4.36	120.71	126.72
2	A	301[B]	YXS	C4-N9-C8	4.36	110.32	105.74
2	D	302[B]	YXS	C5-C4-N3	-4.35	120.72	126.72
3	D	303[A]	YXR	N3-C4-N9	4.34	134.55	127.17
3	F	302[A]	YXR	C4-N9-C8	4.26	110.21	105.74
3	E	302[A]	YXR	O6-P1-O12	4.24	123.46	110.70
2	B	301[B]	YXS	O56-SS4-CS2	-4.18	105.95	109.36
2	C	301[B]	YXS	N3-C4-N9	4.16	134.25	127.17
3	C	302[A]	YXR	N3-C4-N9	4.16	134.25	127.17
2	A	301[B]	YXS	OS4-SS4-CS2	-4.11	106.01	109.36
3	B	302[A]	YXR	OS4-SS4-CS2	-4.11	106.01	109.36
3	A	302[A]	YXR	C5-C4-N3	-4.10	121.07	126.72
2	A	301[B]	YXS	C5-C4-N3	-4.05	121.14	126.72
2	B	301[B]	YXS	N1-C2-N3	-4.05	122.45	128.58
2	F	301[B]	YXS	O56-SS4-CS2	-4.05	106.06	109.36
3	B	302[A]	YXR	N1-C2-N3	-4.03	122.48	128.58
2	B	301[B]	YXS	C2-N3-C4	3.98	121.55	111.83
2	D	302[B]	YXS	N1-C2-N3	-3.97	122.58	128.58
3	B	302[A]	YXR	C2-N3-C4	3.96	121.51	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301[B]	YXS	CP5-CP4-CP3	-3.95	105.82	112.39
3	A	302[A]	YXR	N3-C4-N9	3.91	133.82	127.17
2	E	301[B]	YXS	N3-C4-N9	3.89	133.79	127.17
2	A	301[B]	YXS	N3-C4-N9	3.86	133.74	127.17
3	B	302[A]	YXR	C4-N9-C8	3.82	109.75	105.74
2	B	301[B]	YXS	C4-N9-C8	3.78	109.70	105.74
2	F	301[B]	YXS	C4-C5-N7	-3.76	106.28	110.58
2	F	301[B]	YXS	N3-C4-N9	3.74	133.53	127.17
3	F	302[A]	YXR	N1-C2-N3	-3.72	122.95	128.58
2	C	301[B]	YXS	C4-N9-C8	3.71	109.63	105.74
3	C	302[A]	YXR	C4-N9-C8	3.71	109.63	105.74
2	B	301[B]	YXS	CP5-CP4-CP3	-3.70	106.22	112.39
3	F	302[A]	YXR	C2-N3-C4	3.70	120.87	111.83
2	E	301[B]	YXS	C4-N9-C8	3.68	109.60	105.74
2	C	301[B]	YXS	C4-C5-N7	-3.67	106.38	110.58
3	C	302[A]	YXR	C4-C5-N7	-3.67	106.38	110.58
3	F	302[A]	YXR	CP5-CP4-CP3	-3.64	106.33	112.39
3	F	302[A]	YXR	O7-CPB-CPA	-3.61	104.74	110.55
3	E	302[A]	YXR	N1-C2-N3	-3.56	123.19	128.58
3	D	303[A]	YXR	C4-N9-C8	3.55	109.47	105.74
3	E	302[A]	YXR	C4-N9-C1'	-3.49	118.47	126.63
3	D	303[A]	YXR	P3-O3'-C3'	-3.47	114.16	123.43
2	E	301[B]	YXS	O11-P1-O6	3.45	116.61	107.27
3	B	302[A]	YXR	O7-CPB-CPA	-3.44	105.02	110.55
2	E	301[B]	YXS	N1-C2-N3	-3.41	123.42	128.58
2	A	301[B]	YXS	N1-C2-N3	-3.38	123.46	128.58
3	A	302[A]	YXR	N1-C2-N3	-3.35	123.51	128.58
2	F	301[B]	YXS	C2-N3-C4	3.34	119.99	111.83
3	C	302[A]	YXR	N1-C2-N3	-3.33	123.54	128.58
2	C	301[B]	YXS	N1-C2-N3	-3.31	123.57	128.58
3	B	302[A]	YXR	CP5-CP4-CP3	-3.31	106.88	112.39
2	D	302[B]	YXS	N9-C8-N7	-3.30	109.25	113.94
3	E	302[A]	YXR	C4'-O4'-C1'	-3.30	102.18	109.47
3	F	302[A]	YXR	C4-C5-N7	-3.29	106.83	110.58
3	E	302[A]	YXR	C5'-C4'-C3'	-3.27	103.47	114.38
3	E	302[A]	YXR	N3-C4-N9	3.23	132.66	127.17
2	E	301[B]	YXS	P3-O3'-C3'	-3.22	114.84	123.43
2	E	301[B]	YXS	C2-N3-C4	3.20	119.65	111.83
2	D	302[B]	YXS	C2-N3-C4	3.18	119.60	111.83
2	C	301[B]	YXS	C2-N3-C4	3.18	119.60	111.83
3	C	302[A]	YXR	C2-N3-C4	3.18	119.60	111.83
2	F	301[B]	YXS	N1-C2-N3	-3.17	123.78	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301[B]	YXS	C4-C5-N7	-3.13	107.00	110.58
3	D	303[A]	YXR	N6-C6-N1	3.11	125.31	118.38
2	A	301[B]	YXS	CP5-CP4-CP3	-3.03	107.35	112.39
3	A	302[A]	YXR	N9-C8-N7	-3.01	109.67	113.94
3	A	302[A]	YXR	CP5-CP4-CP3	-2.99	107.41	112.39
2	E	301[B]	YXS	O4'-C4'-C5'	2.99	118.93	109.33
2	A	301[B]	YXS	N9-C8-N7	-2.98	109.70	113.94
3	E	302[A]	YXR	CP5-CP4-CP3	-2.96	107.46	112.39
3	B	302[A]	YXR	CP9-CPA-CP7	2.92	113.75	108.77
2	E	301[B]	YXS	O5'-C5'-C4'	2.92	118.93	108.99
3	E	302[A]	YXR	N9-C8-N7	-2.91	109.80	113.94
3	D	303[A]	YXR	N1-C2-N3	-2.88	124.22	128.58
2	F	301[B]	YXS	O4'-C4'-C5'	2.88	118.55	109.33
3	A	302[A]	YXR	C2-N3-C4	2.85	118.79	111.83
3	F	302[A]	YXR	CP1-S-CS1	2.85	109.90	101.73
2	A	301[B]	YXS	C2-N3-C4	2.84	118.77	111.83
2	C	301[B]	YXS	C5-N7-C8	2.81	107.87	103.45
3	C	302[A]	YXR	C5-N7-C8	2.81	107.87	103.45
2	E	301[B]	YXS	CP9-CPA-CP7	2.81	113.56	108.77
3	F	302[A]	YXR	N9-C8-N7	-2.77	110.00	113.94
3	D	303[A]	YXR	O21-P2-O6	-2.77	99.77	107.27
3	E	302[A]	YXR	C2-N1-C6	2.76	123.27	118.73
3	F	302[A]	YXR	C5-N7-C8	2.74	107.76	103.45
2	F	301[B]	YXS	CP9-CPA-CPB	2.72	112.72	108.22
2	A	301[B]	YXS	C4-C5-N7	-2.72	107.47	110.58
3	A	302[A]	YXR	C4-C5-N7	-2.71	107.49	110.58
3	B	302[A]	YXR	C2'-C1'-N9	-2.71	106.58	113.30
3	E	302[A]	YXR	OS4-SS4-CS2	-2.71	107.15	109.36
3	D	303[A]	YXR	CP5-CP4-CP3	-2.70	107.89	112.39
3	E	302[A]	YXR	C5-C4-N3	-2.65	123.06	126.72
2	B	301[B]	YXS	C2'-C1'-N9	-2.65	106.72	113.30
3	C	302[A]	YXR	OP1-CP3-CP4	-2.65	117.22	122.02
3	C	302[A]	YXR	C2-N1-C6	2.64	123.08	118.73
2	B	301[B]	YXS	CP8-CPA-CP9	2.64	114.47	109.20
3	D	303[A]	YXR	O4'-C1'-N9	2.64	113.17	108.09
2	B	301[B]	YXS	C5-C6-N6	-2.63	116.76	123.29
2	D	302[B]	YXS	N6-C6-N1	2.63	124.23	118.38
2	C	301[B]	YXS	C2-N1-C6	2.62	123.04	118.73
3	B	302[A]	YXR	C5-C6-N6	-2.62	116.80	123.29
2	C	301[B]	YXS	OP1-CP3-CP4	-2.62	117.28	122.02
3	E	302[A]	YXR	C6-C5-N7	2.61	137.13	132.09
2	F	301[B]	YXS	C5-N7-C8	2.60	107.54	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302[A]	YXR	C2-N3-C4	2.60	118.17	111.83
2	D	302[B]	YXS	O56-SS4-CS2	-2.59	107.25	109.36
2	D	302[B]	YXS	CP5-CP4-CP3	-2.59	108.08	112.39
2	D	302[B]	YXS	C5-N7-C8	2.58	107.51	103.45
3	B	302[A]	YXR	N9-C8-N7	-2.56	110.30	113.94
2	E	301[B]	YXS	C2-N1-C6	2.54	122.91	118.73
2	B	301[B]	YXS	N9-C8-N7	-2.53	110.34	113.94
3	D	303[A]	YXR	C2-N3-C4	2.53	118.00	111.83
3	A	302[A]	YXR	C5-N7-C8	2.51	107.40	103.45
2	C	301[B]	YXS	N9-C8-N7	-2.51	110.38	113.94
3	C	302[A]	YXR	N9-C8-N7	-2.51	110.38	113.94
2	A	301[B]	YXS	C5-N7-C8	2.50	107.38	103.45
2	F	301[B]	YXS	CP7-CP6-NP2	-2.50	111.74	116.48
2	D	302[B]	YXS	C2-N1-C6	2.50	122.83	118.73
2	F	301[B]	YXS	O5'-C5'-C4'	2.48	117.42	108.99
3	E	302[A]	YXR	CP1-S-CS1	2.45	108.76	101.73
2	E	301[B]	YXS	CS2-CS1-S	2.44	122.34	114.05
2	F	301[B]	YXS	C2-N1-C6	2.40	122.67	118.73
2	E	301[B]	YXS	OS4-SS4-CS2	2.40	111.31	109.36
2	E	301[B]	YXS	C5'-C4'-C3'	-2.39	106.43	114.38
3	B	302[A]	YXR	OS1-CS1-S	-2.38	120.60	123.80
2	E	301[B]	YXS	OP3-CP7-CPA	-2.36	104.72	110.18
2	E	301[B]	YXS	C6-C5-N7	2.35	136.62	132.09
2	A	301[B]	YXS	C2-N1-C6	2.35	122.59	118.73
2	B	301[B]	YXS	OP3-CP7-CPA	-2.33	104.79	110.18
3	D	303[A]	YXR	O32-P3-O33	2.33	116.52	107.80
3	A	302[A]	YXR	C2-N1-C6	2.32	122.54	118.73
3	C	302[A]	YXR	CP1-S-CS1	2.32	108.38	101.73
2	B	301[B]	YXS	O3'-C3'-C2'	-2.31	103.38	111.68
2	A	301[B]	YXS	C4-N9-C1'	-2.30	121.25	126.63
3	A	302[A]	YXR	C4-N9-C1'	-2.28	121.30	126.63
2	F	301[B]	YXS	C6-C5-N7	2.28	136.48	132.09
3	A	302[A]	YXR	O4'-C1'-N9	2.27	112.45	108.09
3	B	302[A]	YXR	CP1-S-CS1	2.27	108.24	101.73
3	D	303[A]	YXR	C5-C6-N6	-2.26	117.70	123.29
3	E	302[A]	YXR	O32-P3-O3'	2.25	114.63	105.85
2	F	301[B]	YXS	C4-N9-C8	2.24	108.09	105.74
2	D	302[B]	YXS	OS1-CS1-S	-2.24	120.79	123.80
2	A	301[B]	YXS	O4'-C1'-N9	2.23	112.38	108.09
2	D	302[B]	YXS	C4-C5-N7	-2.23	108.03	110.58
2	D	302[B]	YXS	CP4-CP3-NP1	2.22	120.40	116.34
3	B	302[A]	YXR	O3'-C3'-C2'	-2.22	103.71	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301[B]	YXS	CP8-CPA-CPB	-2.22	104.57	108.22
3	D	303[A]	YXR	O3'-P3-O31	-2.22	101.44	109.33
3	F	302[A]	YXR	O21-P2-O6	2.21	113.25	107.27
2	F	301[B]	YXS	OP3-CP7-CPA	-2.20	105.08	110.18
2	B	301[B]	YXS	N6-C6-N1	2.20	123.28	118.38
3	E	302[A]	YXR	C4-C5-N7	-2.20	108.07	110.58
2	E	301[B]	YXS	CP9-CPA-CPB	2.18	111.83	108.22
2	E	301[B]	YXS	C5-N7-C8	2.18	106.88	103.45
3	B	302[A]	YXR	N6-C6-N1	2.18	123.23	118.38
3	A	302[A]	YXR	C5'-C4'-C3'	-2.18	107.13	114.38
2	D	302[B]	YXS	OP1-CP3-NP1	-2.17	118.77	123.03
2	C	301[B]	YXS	C6-C5-N7	2.17	136.26	132.09
3	C	302[A]	YXR	C6-C5-N7	2.17	136.26	132.09
2	B	301[B]	YXS	CP1-CP2-NP1	-2.16	107.89	112.41
3	E	302[A]	YXR	O11-P1-O12	-2.16	102.39	112.44
3	F	302[A]	YXR	CP9-CPA-CP7	2.16	112.45	108.77
2	E	301[B]	YXS	C2'-C1'-N9	-2.16	107.94	113.30
3	E	302[A]	YXR	N6-C6-N1	2.16	123.18	118.38
3	B	302[A]	YXR	C4-C5-N7	-2.16	108.12	110.58
3	F	302[A]	YXR	C2-N1-C6	2.15	122.27	118.73
3	B	302[A]	YXR	C6-C5-N7	2.15	136.23	132.09
3	E	302[A]	YXR	CP1-CP2-NP1	-2.15	107.93	112.41
2	F	301[B]	YXS	O2'-C2'-C1'	2.14	117.48	110.10
3	E	302[A]	YXR	P3-O3'-C3'	-2.14	117.72	123.43
3	D	303[A]	YXR	CP4-CP3-NP1	2.13	120.23	116.34
2	B	301[B]	YXS	OS1-CS1-S	-2.12	120.95	123.80
2	E	301[B]	YXS	N9-C8-N7	-2.11	110.94	113.94
3	D	303[A]	YXR	C2-N1-C6	2.10	122.18	118.73
3	B	302[A]	YXR	C5-N7-C8	2.10	106.75	103.45
2	D	302[B]	YXS	C5-C6-N6	-2.10	118.09	123.29
3	D	303[A]	YXR	OP1-CP3-NP1	-2.09	118.93	123.03
3	F	302[A]	YXR	OP3-CP7-CPA	-2.09	105.35	110.18
2	E	301[B]	YXS	CP1-CP2-NP1	-2.08	108.06	112.41
2	B	301[B]	YXS	C4-C5-N7	-2.08	108.20	110.58
2	B	301[B]	YXS	C6-C5-N7	2.08	136.10	132.09
2	A	301[B]	YXS	C5'-C4'-C3'	-2.08	107.46	114.38
3	E	302[A]	YXR	O2'-C2'-C3'	2.08	117.00	111.19
2	A	301[B]	YXS	CP1-CP2-NP1	-2.07	108.09	112.41
2	F	301[B]	YXS	OS4-SS4-CS2	-2.06	107.67	109.36
2	A	301[B]	YXS	N6-C6-N1	2.06	122.97	118.38
2	B	301[B]	YXS	C5-N7-C8	2.05	106.68	103.45
2	F	301[B]	YXS	N9-C8-N7	-2.03	111.06	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302[A]	YXR	N6-C6-N1	2.02	122.89	118.38
2	C	301[B]	YXS	CP1-S-CS1	2.02	107.53	101.73
2	A	301[B]	YXS	C6-C5-N7	2.02	135.98	132.09

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301[B]	YXS	OS1-CS1-CS2-CS3
2	D	302[B]	YXS	CP8-CPA-CPB-O7
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	D	302[B]	YXS	CS3-CS2-SS4-O56
2	E	301[B]	YXS	C4'-C5'-O5'-P1
2	E	301[B]	YXS	C5'-O5'-P1-O12
2	E	301[B]	YXS	C5'-O5'-P1-O6
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
2	F	301[B]	YXS	C5'-O5'-P1-O11
2	F	301[B]	YXS	CP8-CPA-CPB-O7
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	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
3	D	303[A]	YXR	CP8-CPA-CPB-O7
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	C5'-O5'-P1-O6
3	E	302[A]	YXR	P1-O6-P2-O7
3	E	302[A]	YXR	CPB-O7-P2-O6
3	E	302[A]	YXR	CPB-O7-P2-O22
3	E	302[A]	YXR	CP8-CPA-CPB-O7
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

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Mol	Chain	Res	Type	Atoms
3	E	302[A]	YXR	CP6-CP7-CPA-CP9
3	F	302[A]	YXR	CP6-CP7-CPA-CPB
3	E	302[A]	YXR	C3'-C4'-C5'-O5'
7	F	305	PEG	O2-C3-C4-O4
3	E	302[A]	YXR	O4'-C4'-C5'-O5'
2	B	301[B]	YXS	O4'-C4'-C5'-O5'
2	E	301[B]	YXS	C3'-O3'-P3-O33
6	C	304	PG4	O1-C1-C2-O2
2	B	301[B]	YXS	C3'-C4'-C5'-O5'
3	D	303[A]	YXR	CP4-CP5-NP2-CP6
3	F	302[A]	YXR	P1-O6-P2-O7
2	D	302[B]	YXS	CP4-CP5-NP2-CP6
3	F	302[A]	YXR	CP6-CP7-CPA-CP8
2	C	301[B]	YXS	CP9-CPA-CPB-O7
2	F	301[B]	YXS	CP6-CP7-CPA-CPB
3	C	302[A]	YXR	CP9-CPA-CPB-O7
3	F	302[A]	YXR	CP9-CPA-CPB-O7
3	B	302[A]	YXR	C3'-C4'-C5'-O5'
2	F	301[B]	YXS	CP4-CP5-NP2-CP6
3	E	302[A]	YXR	C3'-O3'-P3-O31
2	B	301[B]	YXS	C5'-O5'-P1-O6
2	F	301[B]	YXS	C5'-O5'-P1-O6
2	F	301[B]	YXS	CPB-O7-P2-O22
2	F	301[B]	YXS	OP3-CP7-CPA-CPB
3	B	302[A]	YXR	OP3-CP7-CPA-CPB
3	E	302[A]	YXR	C5'-O5'-P1-O11
3	E	302[A]	YXR	CPB-O7-P2-O21
3	F	302[A]	YXR	CPB-O7-P2-O22
6	C	304	PG4	C3-C4-O3-C5
2	B	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
2	F	301[B]	YXS	OS1-CS1-CS2-CS3
3	A	302[A]	YXR	C3'-C4'-C5'-O5'
3	B	302[A]	YXR	O4'-C4'-C5'-O5'
3	B	302[A]	YXR	C4'-C3'-O3'-P3
2	C	301[B]	YXS	CS3-CS2-SS4-OS5
2	A	301[B]	YXS	OS1-CS1-S-CP1
3	B	302[A]	YXR	C2'-C3'-O3'-P3
3	B	302[A]	YXR	C3'-O3'-P3-O31
2	A	301[B]	YXS	C3'-C4'-C5'-O5'
2	D	302[B]	YXS	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	B	301[B]	YXS	C2'-C3'-O3'-P3
3	F	302[A]	YXR	CP6-CP7-CPA-CP9
2	B	301[B]	YXS	C4'-C3'-O3'-P3
2	F	301[B]	YXS	C3'-O3'-P3-O32
3	D	303[A]	YXR	C3'-O3'-P3-O33
2	B	301[B]	YXS	CP6-CP7-CPA-CPB
2	C	301[B]	YXS	CP8-CPA-CPB-O7
3	B	302[A]	YXR	CP9-CPA-CPB-O7
3	C	302[A]	YXR	CP8-CPA-CPB-O7
3	F	302[A]	YXR	CP8-CPA-CPB-O7
2	C	301[B]	YXS	CP7-CPA-CPB-O7
3	C	302[A]	YXR	CP7-CPA-CPB-O7

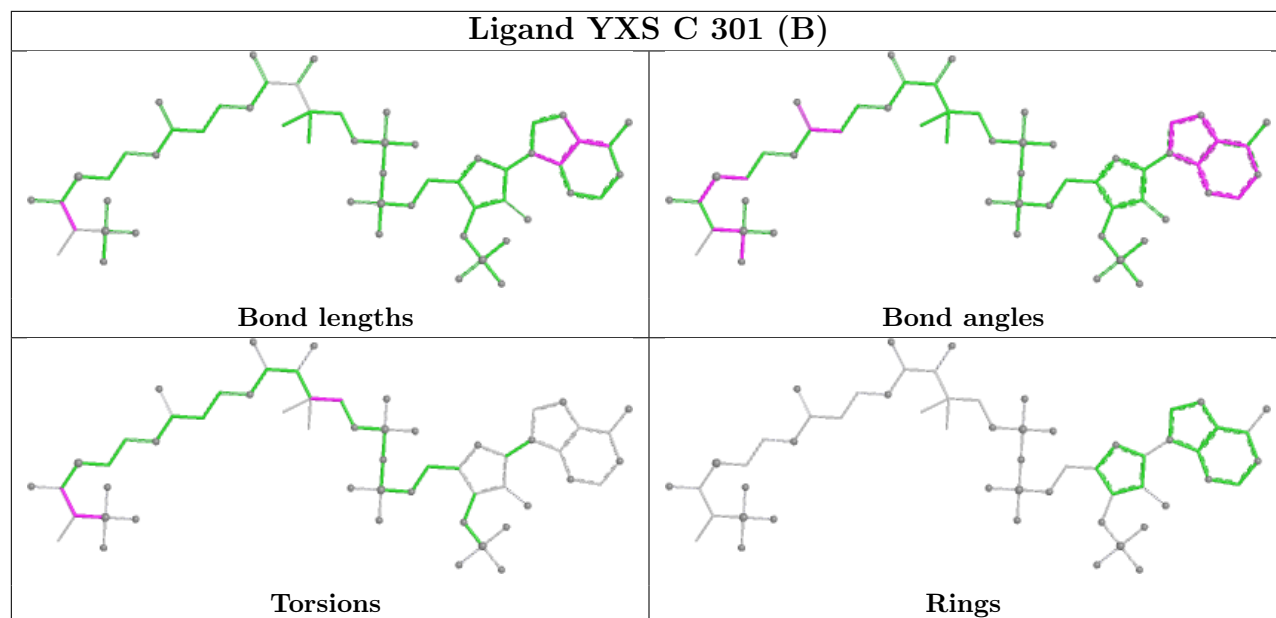
There are no ring outliers.

8 monomers are involved in 13 short contacts:

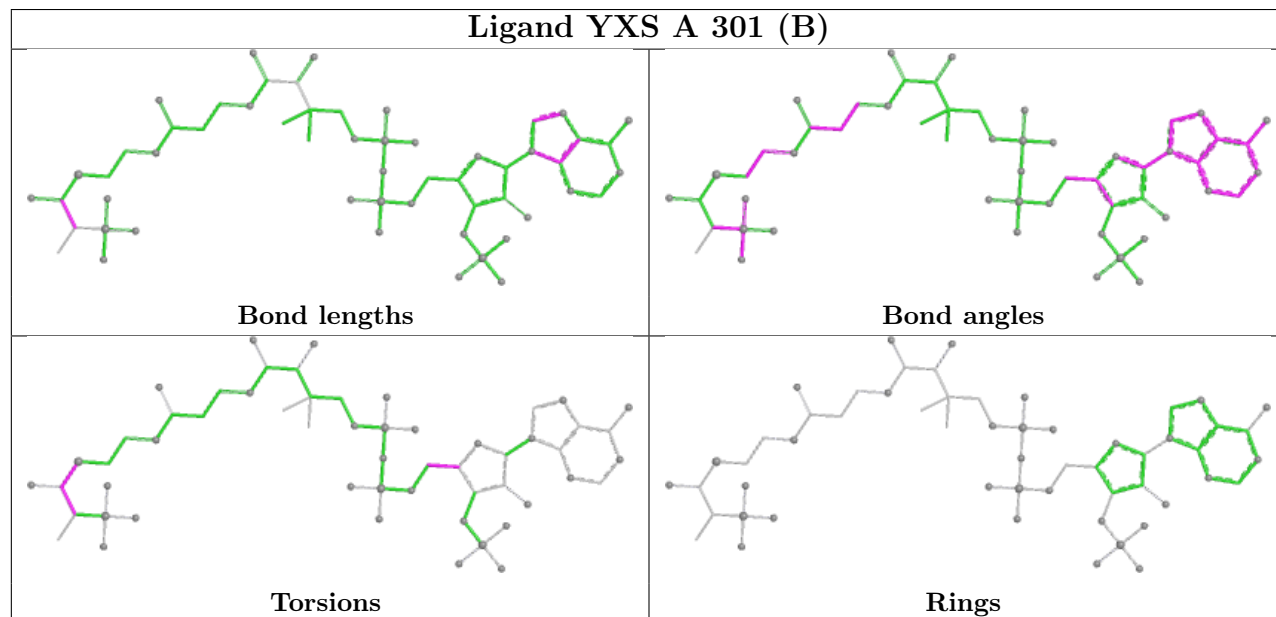
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301[B]	YXS	1	0
2	A	301[B]	YXS	1	0
3	A	302[A]	YXR	1	0
2	D	302[B]	YXS	1	0
7	F	305	PEG	3	0
3	B	302[A]	YXR	2	0
6	C	304	PG4	1	0
2	E	301[B]	YXS	3	0

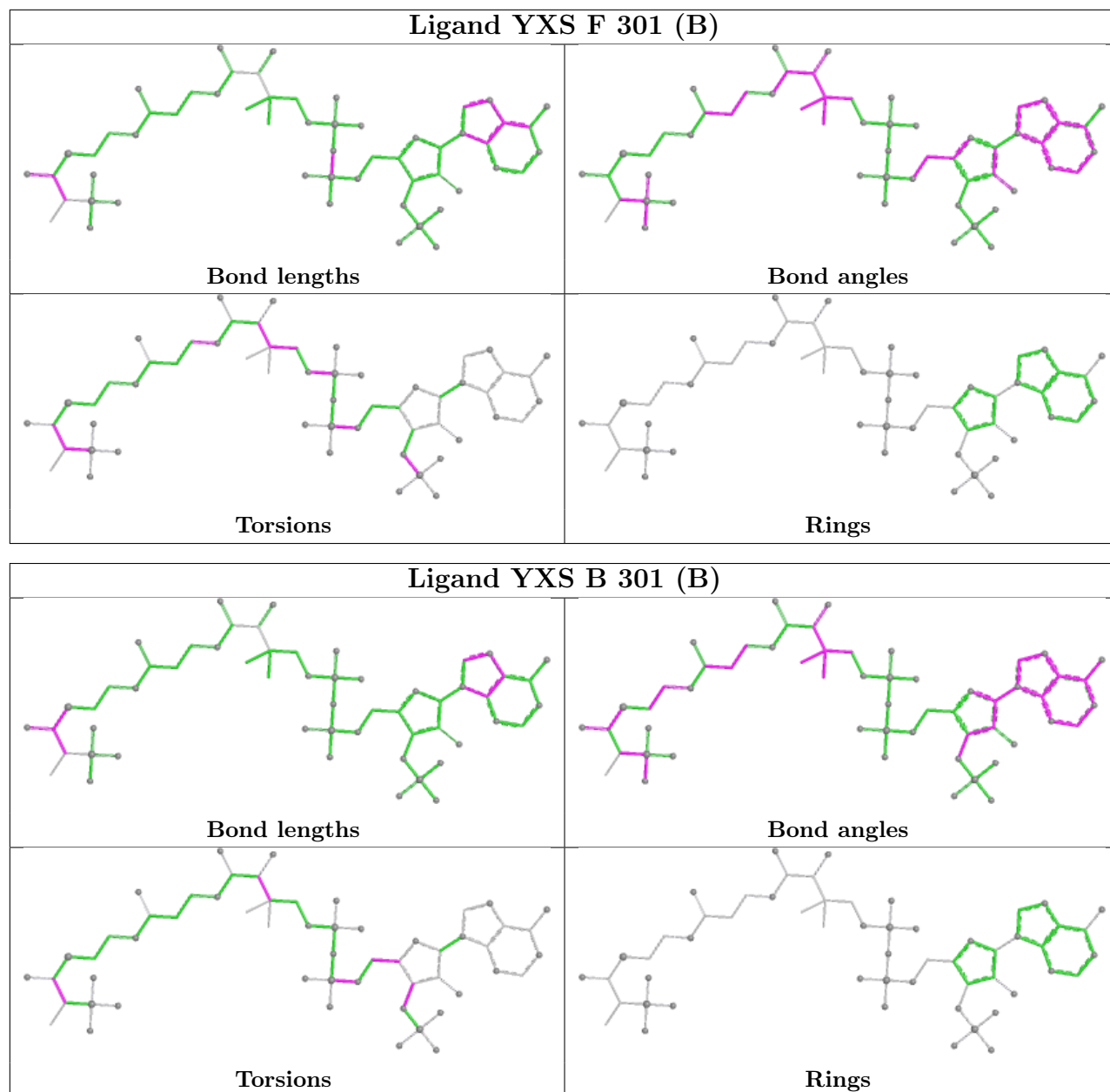
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

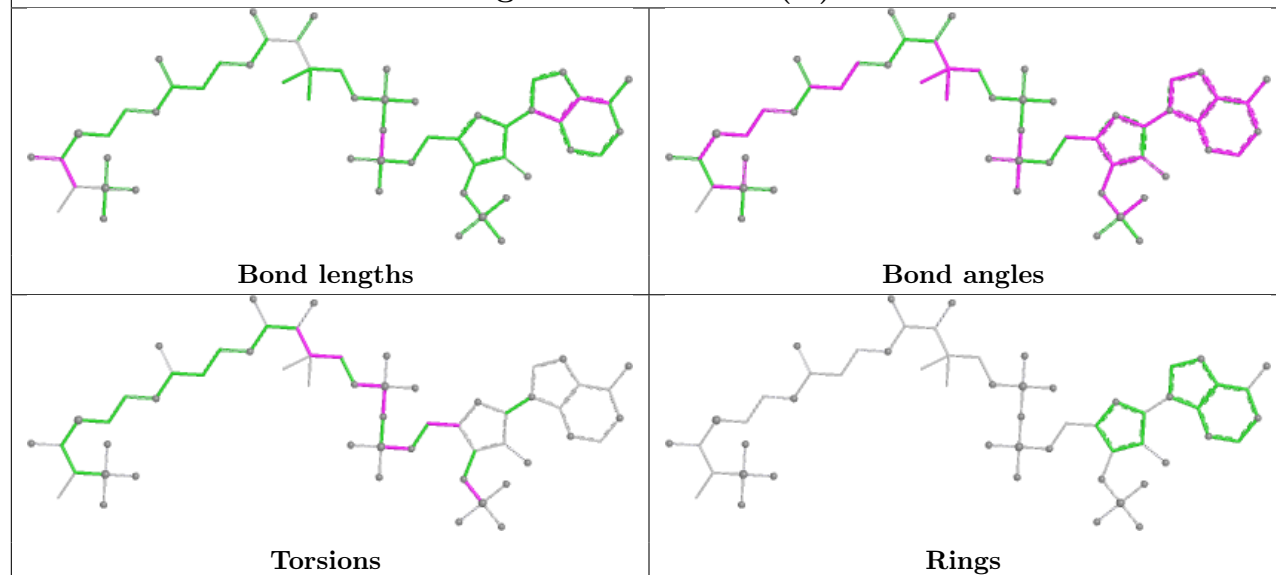
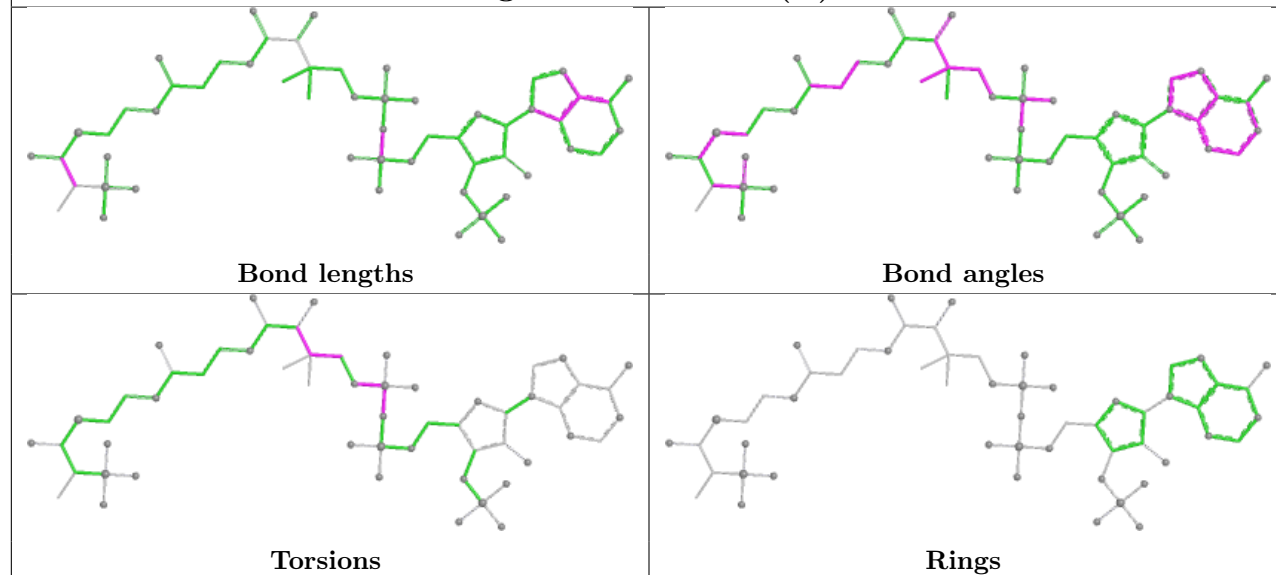
Ligand YXS C 301 (B)

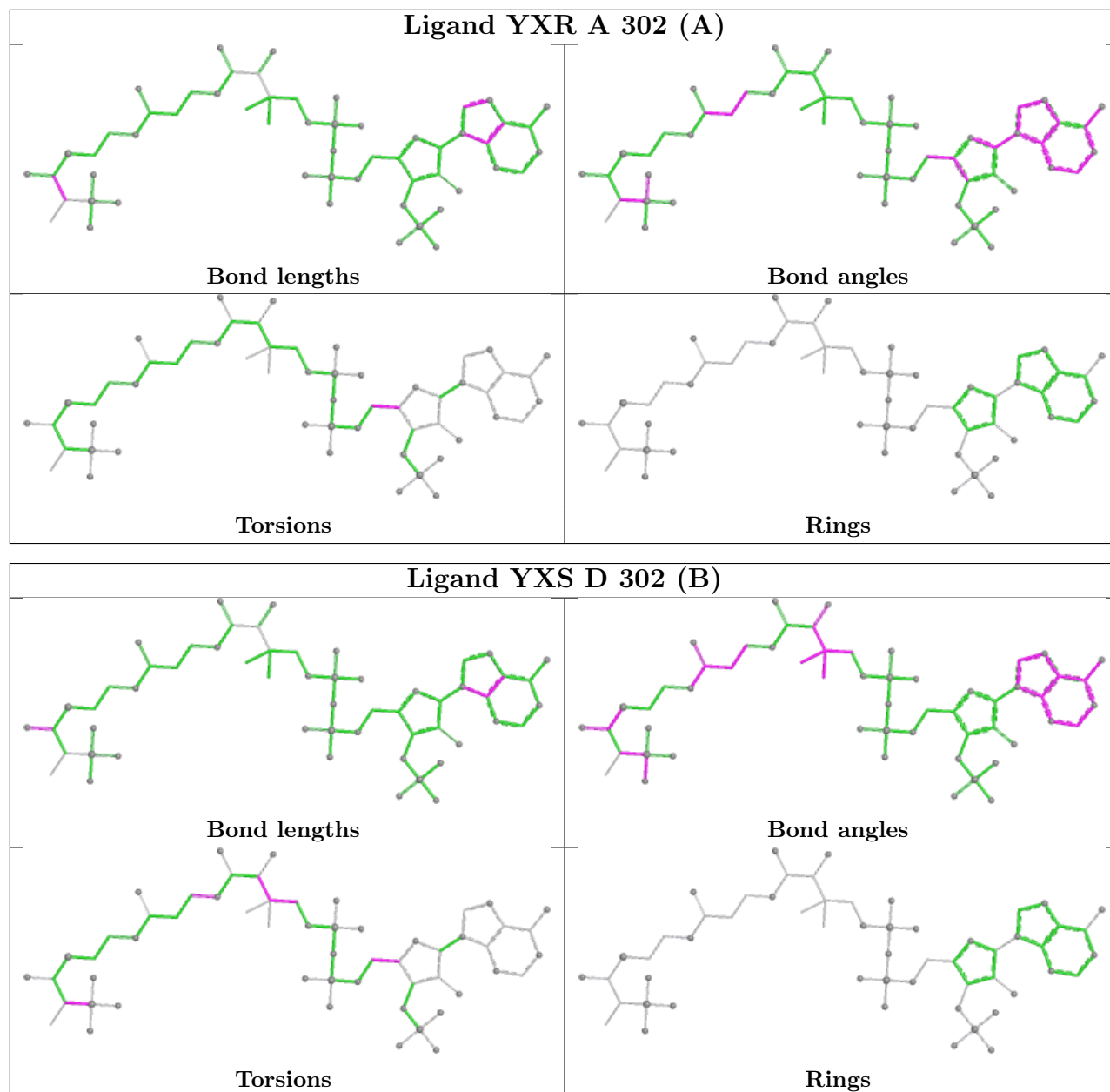


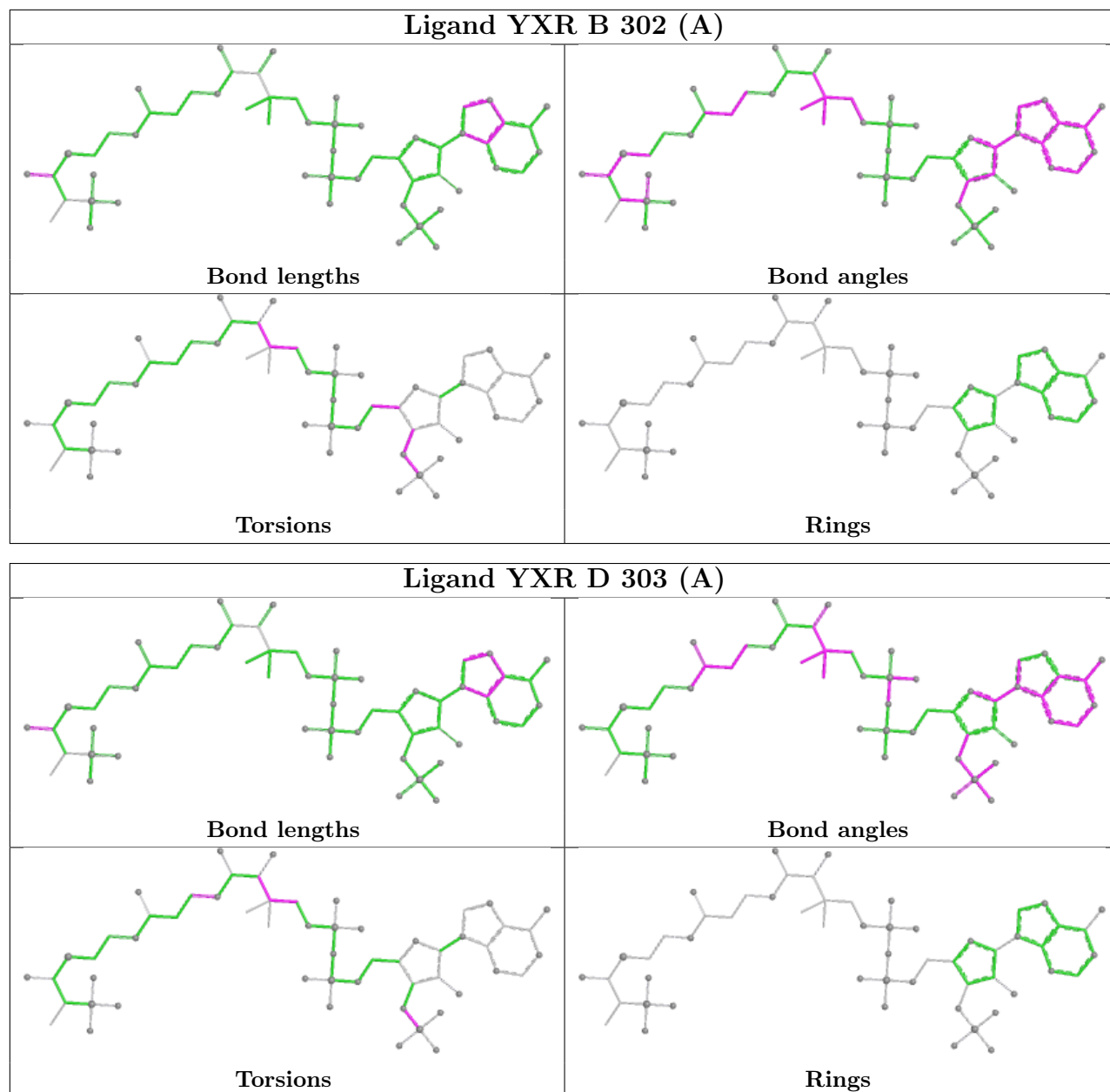
Ligand YXS A 301 (B)

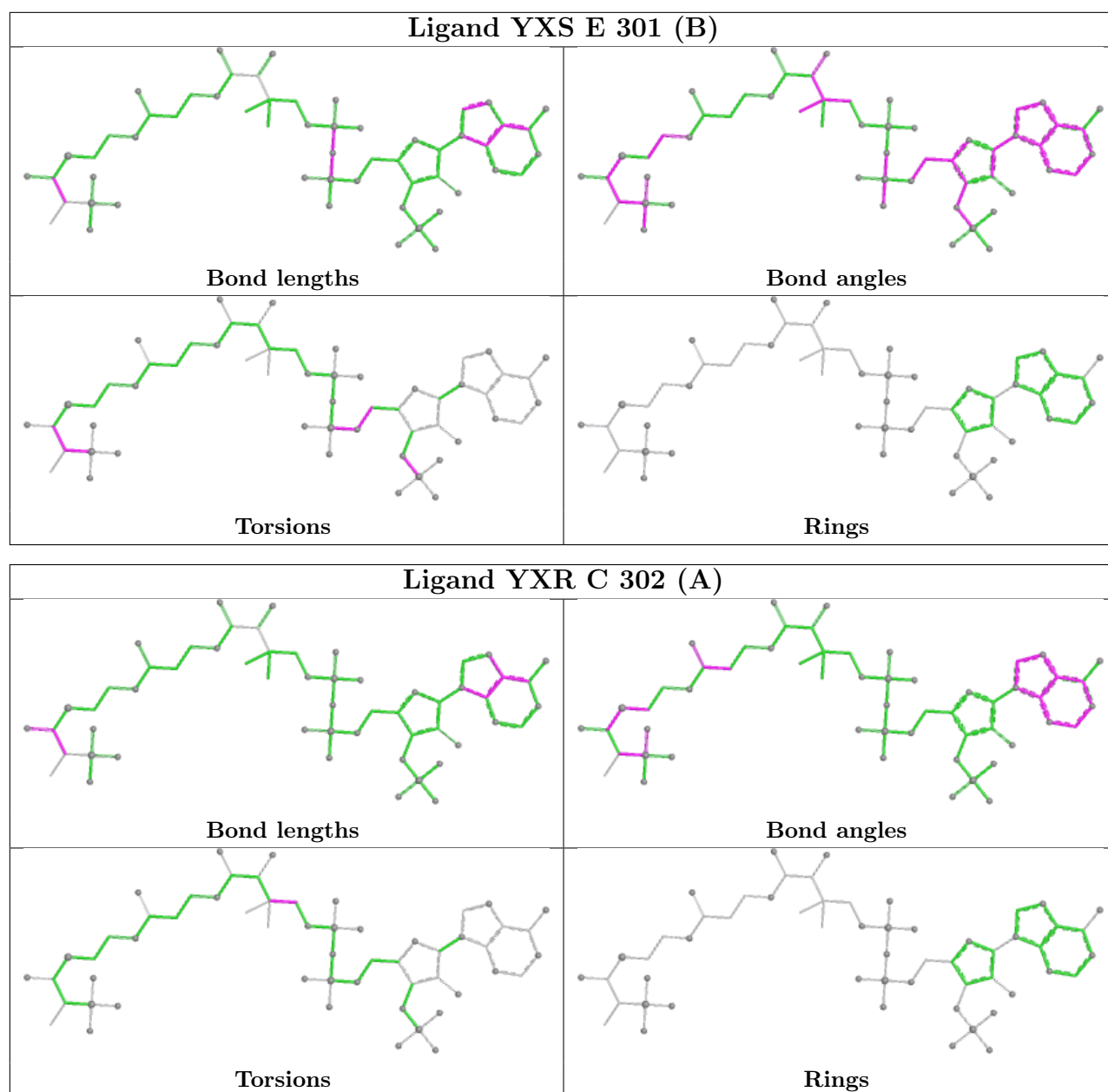




Ligand YXR E 302 (A)**Ligand YXR F 302 (A)**







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	260/261 (99%)	-0.47	1 (0%) 88 89	10, 21, 36, 46	20 (7%)
1	B	260/261 (99%)	-0.30	4 (1%) 72 72	11, 23, 47, 86	11 (4%)
1	C	260/261 (99%)	-0.41	2 (0%) 82 83	10, 21, 42, 90	13 (5%)
1	D	260/261 (99%)	-0.35	1 (0%) 88 89	11, 22, 38, 79	13 (5%)
1	E	260/261 (99%)	-0.32	3 (1%) 76 77	11, 22, 47, 84	15 (5%)
1	F	260/261 (99%)	-0.37	0 100 100	10, 23, 43, 57	15 (5%)
All	All	1560/1566 (99%)	-0.37	11 (0%) 84 85	10, 22, 42, 90	87 (5%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	GLY	3.2
1	E	74	GLY	3.0
1	B	75	GLY	2.9
1	C	23	ARG	2.8
1	B	73	SER	2.8
1	E	2	ALA	2.6
1	A	251	LEU	2.4
1	B	251	LEU	2.3
1	D	251	LEU	2.3
1	E	75	GLY	2.2
1	C	75	GLY	2.1

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

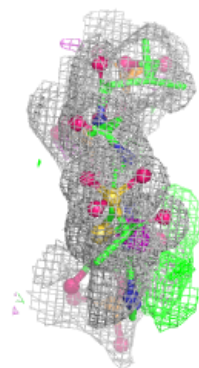
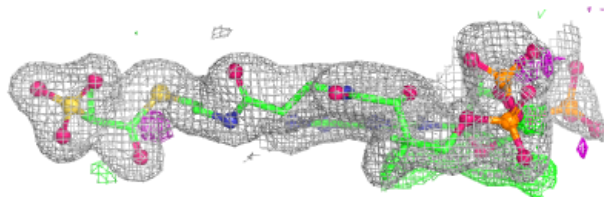
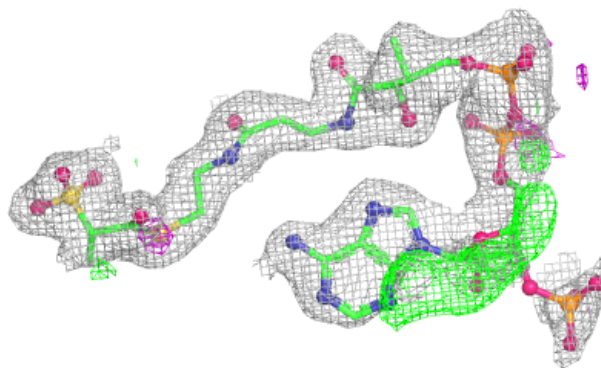
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PEG	C	305	7/7	0.82	0.15	66,69,71,74	0
7	PEG	F	305	7/7	0.85	0.14	56,57,61,62	0
8	PGE	F	304	10/10	0.85	0.12	49,54,61,61	0
2	YXS	F	301[B]	56/56	0.87	0.12	26,50,67,69	56
2	YXS	E	301[B]	56/56	0.90	0.10	26,39,54,57	56
6	PG4	C	304	13/13	0.92	0.09	40,43,49,50	0
3	YXR	B	302[A]	56/56	0.92	0.10	24,46,75,79	56
3	YXR	E	302[A]	56/56	0.92	0.09	23,35,44,46	56
3	YXR	F	302[A]	56/56	0.92	0.09	25,35,49,52	56
2	YXS	D	302[B]	56/56	0.93	0.08	22,34,42,53	56
2	YXS	B	301[B]	56/56	0.93	0.09	25,44,74,79	56
3	YXR	A	302[A]	56/56	0.94	0.08	19,31,54,57	56
2	YXS	A	301[B]	56/56	0.94	0.08	23,31,54,57	56
3	YXR	D	303[A]	56/56	0.94	0.07	22,32,39,51	56
3	YXR	C	302[A]	56/56	0.95	0.07	22,36,49,53	56
2	YXS	C	301[B]	56/56	0.95	0.07	23,36,49,53	56
5	K	F	303	1/1	0.98	0.06	44,44,44,44	0
5	K	C	303	1/1	0.99	0.08	41,41,41,41	0
4	NI	A	303	1/1	0.99	0.02	41,41,41,41	0
4	NI	D	301	1/1	0.99	0.04	39,39,39,39	0

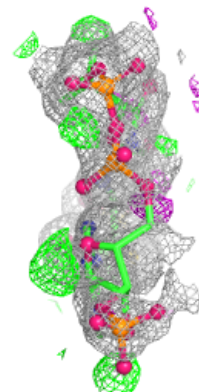
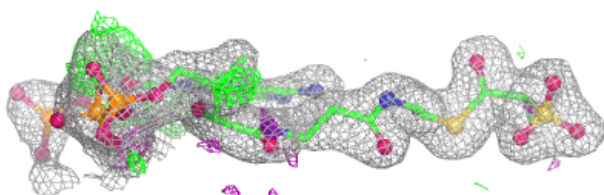
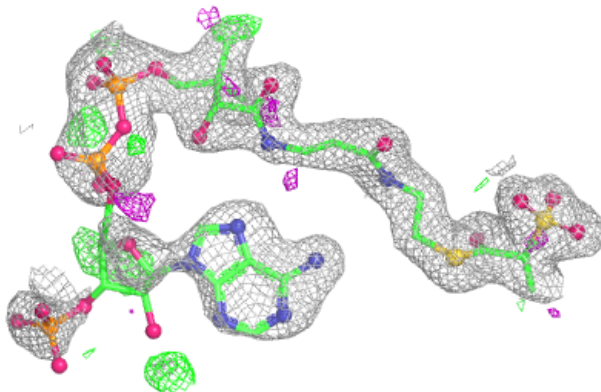
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YXS 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)

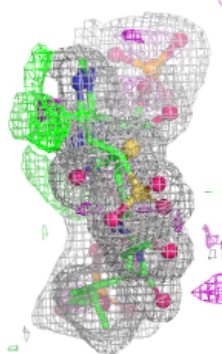
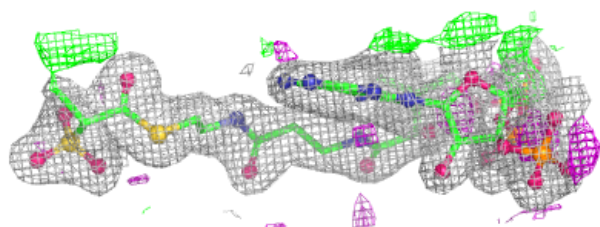
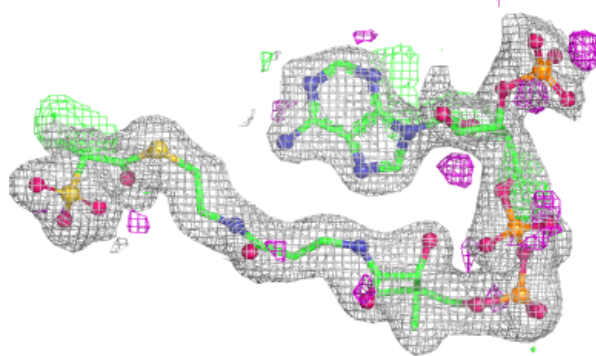
**Electron density around YXS E 301 (B):**

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

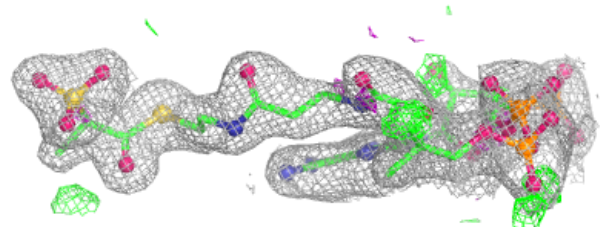
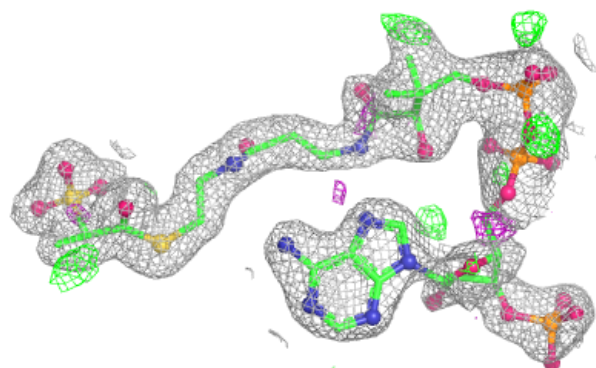


Electron density around YXR B 302 (A):

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

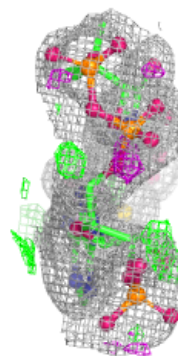
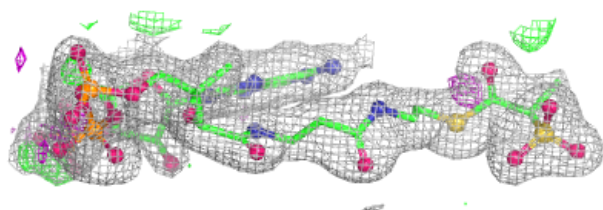
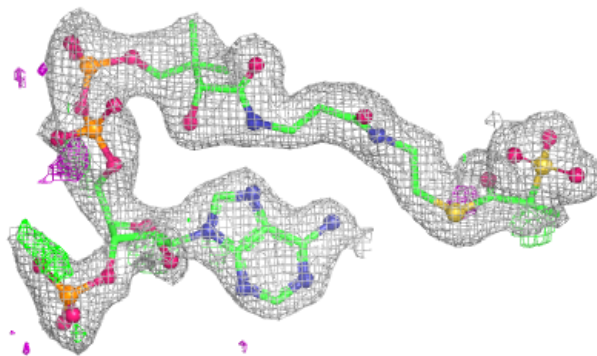
**Electron density around YXR E 302 (A):**

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

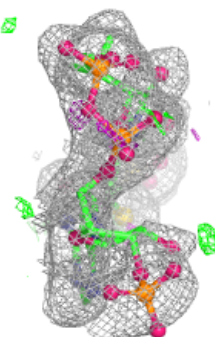
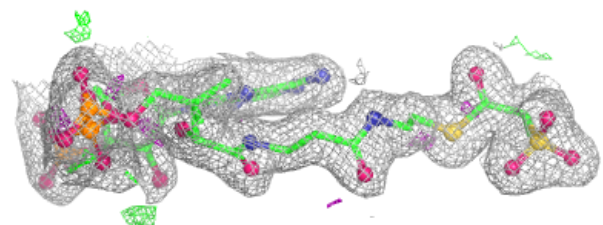
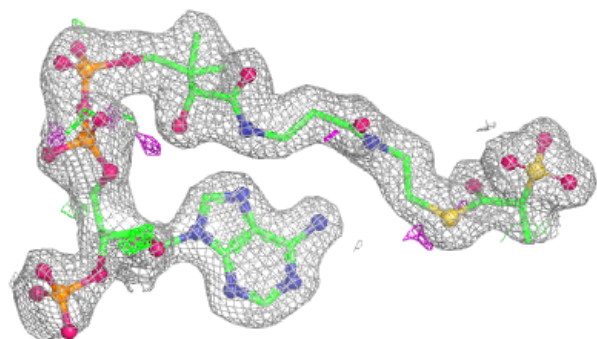


Electron density around YXR F 302 (A):

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and green (positive)

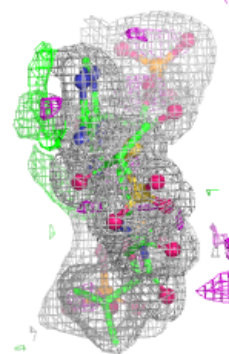
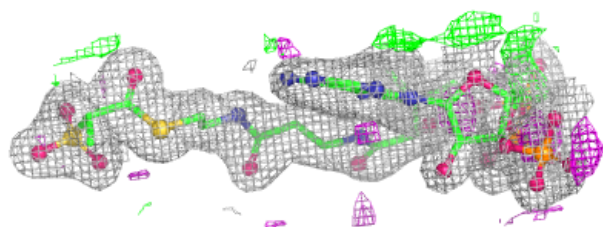
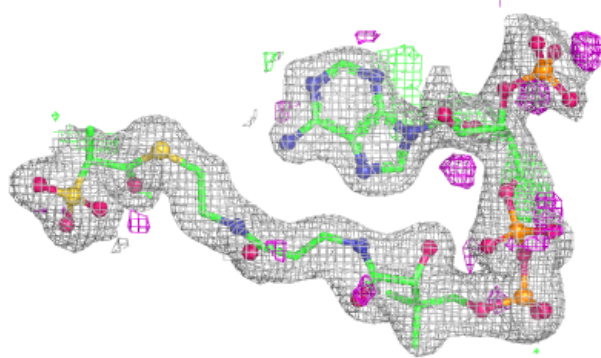
**Electron density around YXS D 302 (B):**

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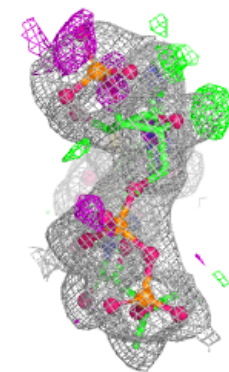
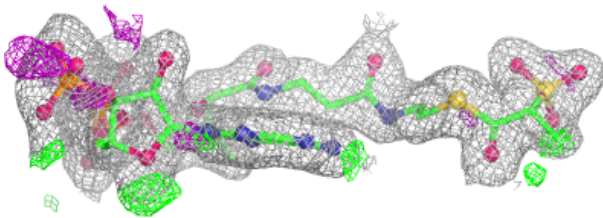
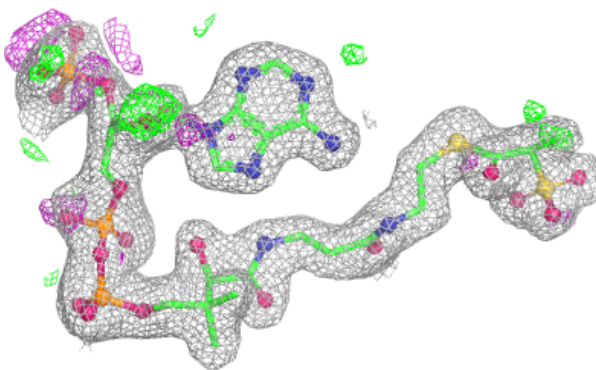


Electron density around YXS B 301 (B):

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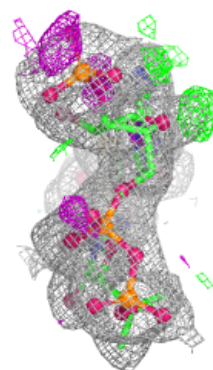
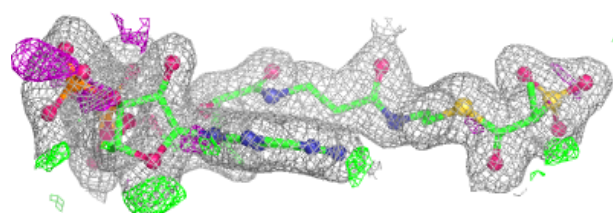
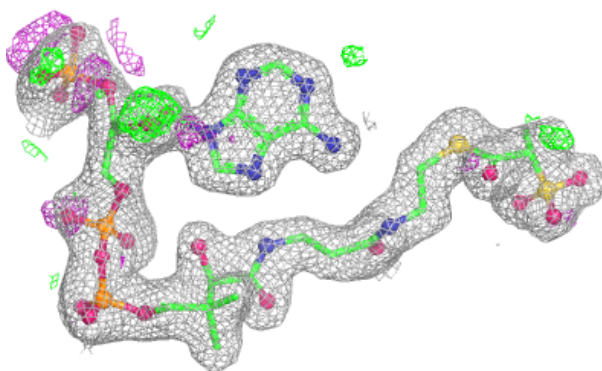
**Electron density around YXR A 302 (A):**

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and green (positive)

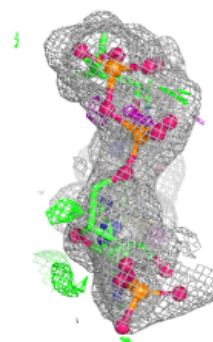
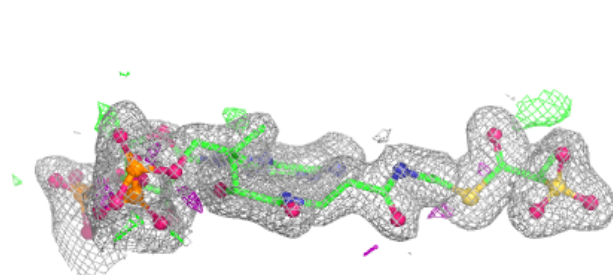
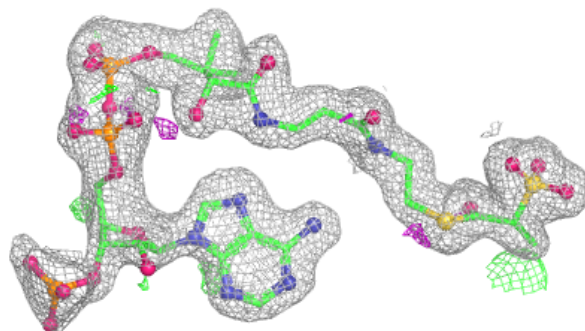


Electron density around YXS A 301 (B):

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

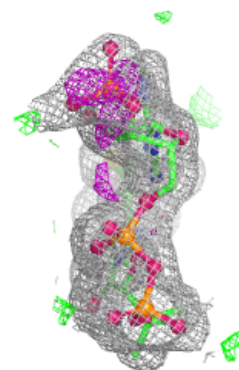
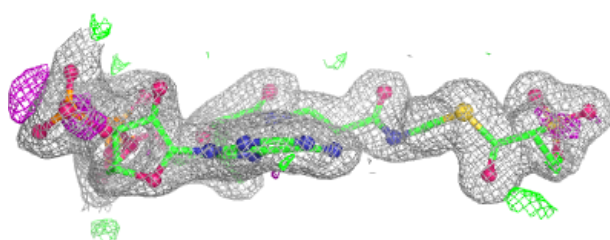
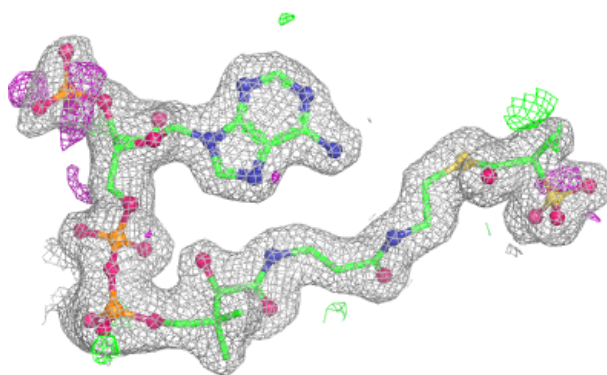
**Electron density around YXR D 303 (A):**

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

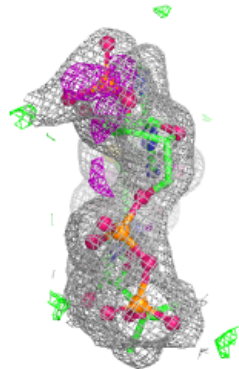
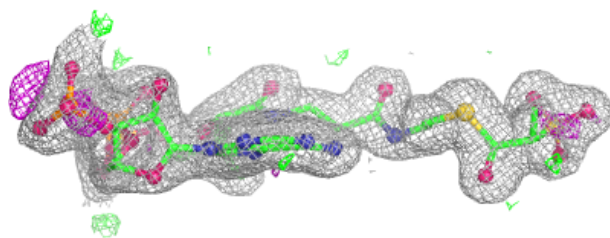
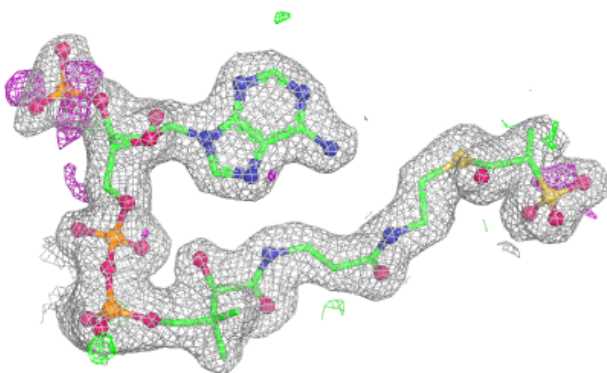


Electron density around YXR C 302 (A):

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.