



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2020 – 01:46 PM EDT

PDB ID : 6RV8
Title : Crystal Structure of Glucuronoyl Esterase from *Cerrena unicolor* covalent complex with the aldouronic acid UXXR
Authors : Ernst, H.A.; Mosbech, C.; Langkilde, A.; Westh, P.; Meyer, A.; Agger, J.W.; Larsen, S.
Deposited on : 2019-05-31
Resolution : 1.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.8
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
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) : 2.8

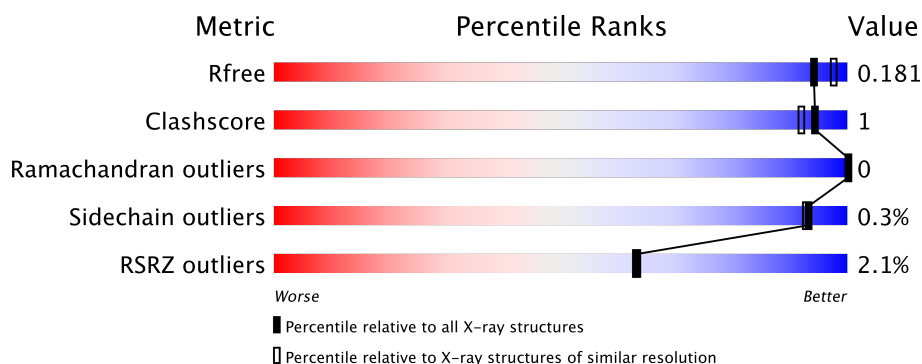
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	111664	2111 (1.86-1.86)
Clashscore	122126	2258 (1.86-1.86)
Ramachandran outliers	120053	2234 (1.86-1.86)
Sidechain outliers	120020	2234 (1.86-1.86)
RSRZ outliers	108989	2075 (1.86-1.86)

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 ≥ 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	481	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -5px; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 3%, orange 3%, yellow 3%, green 76%, grey 21%);"></div> <div style="position: absolute; top: 5px; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 3%, orange 3%, yellow 3%, green 76%, grey 21%);"></div> </div> <div> </div> <div> </div> </div>
1	B	481	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -5px; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 3%, orange 3%, yellow 3%, green 77%, grey 21%);"></div> <div style="position: absolute; top: 5px; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 3%, orange 3%, yellow 3%, green 77%, grey 21%);"></div> </div> <div> </div> <div> </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6590 atoms, of which 105 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 4-O-methyl-glucuronoyl methylesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	4	0
			2891	1826	494	556	15			
1	B	381	Total	C	N	O	S	0	2	0
			2880	1819	493	553	15			

There are 48 discrepancies between the modelled and reference sequences:

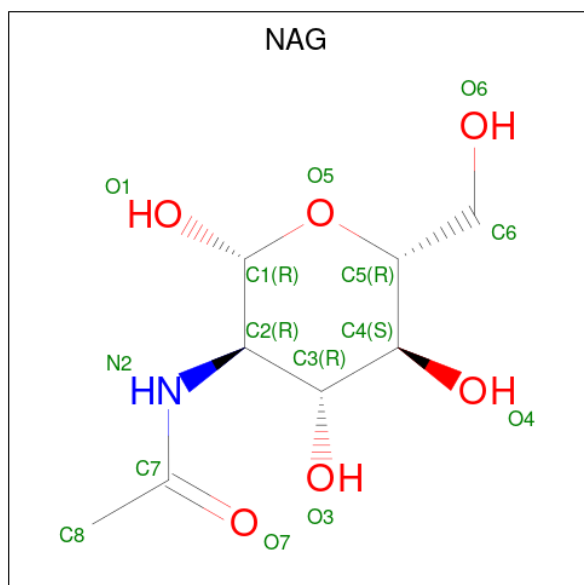
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0A7EQR3
A	459	GLY	-	expression tag	UNP A0A0A7EQR3
A	460	LEU	-	expression tag	UNP A0A0A7EQR3
A	461	GLU	-	expression tag	UNP A0A0A7EQR3
A	462	GLN	-	expression tag	UNP A0A0A7EQR3
A	463	LYS	-	expression tag	UNP A0A0A7EQR3
A	464	LEU	-	expression tag	UNP A0A0A7EQR3
A	465	ILE	-	expression tag	UNP A0A0A7EQR3
A	466	SER	-	expression tag	UNP A0A0A7EQR3
A	467	GLU	-	expression tag	UNP A0A0A7EQR3
A	468	GLU	-	expression tag	UNP A0A0A7EQR3
A	469	ASP	-	expression tag	UNP A0A0A7EQR3
A	470	LEU	-	expression tag	UNP A0A0A7EQR3
A	471	ASN	-	expression tag	UNP A0A0A7EQR3
A	472	SER	-	expression tag	UNP A0A0A7EQR3
A	473	ALA	-	expression tag	UNP A0A0A7EQR3
A	474	VAL	-	expression tag	UNP A0A0A7EQR3
A	475	ASP	-	expression tag	UNP A0A0A7EQR3
A	476	HIS	-	expression tag	UNP A0A0A7EQR3
A	477	HIS	-	expression tag	UNP A0A0A7EQR3
A	478	HIS	-	expression tag	UNP A0A0A7EQR3
A	479	HIS	-	expression tag	UNP A0A0A7EQR3
A	480	HIS	-	expression tag	UNP A0A0A7EQR3
A	481	HIS	-	expression tag	UNP A0A0A7EQR3
B	1	MET	-	initiating methionine	UNP A0A0A7EQR3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	459	GLY	-	expression tag	UNP A0A0A7EQR3
B	460	LEU	-	expression tag	UNP A0A0A7EQR3
B	461	GLU	-	expression tag	UNP A0A0A7EQR3
B	462	GLN	-	expression tag	UNP A0A0A7EQR3
B	463	LYS	-	expression tag	UNP A0A0A7EQR3
B	464	LEU	-	expression tag	UNP A0A0A7EQR3
B	465	ILE	-	expression tag	UNP A0A0A7EQR3
B	466	SER	-	expression tag	UNP A0A0A7EQR3
B	467	GLU	-	expression tag	UNP A0A0A7EQR3
B	468	GLU	-	expression tag	UNP A0A0A7EQR3
B	469	ASP	-	expression tag	UNP A0A0A7EQR3
B	470	LEU	-	expression tag	UNP A0A0A7EQR3
B	471	ASN	-	expression tag	UNP A0A0A7EQR3
B	472	SER	-	expression tag	UNP A0A0A7EQR3
B	473	ALA	-	expression tag	UNP A0A0A7EQR3
B	474	VAL	-	expression tag	UNP A0A0A7EQR3
B	475	ASP	-	expression tag	UNP A0A0A7EQR3
B	476	HIS	-	expression tag	UNP A0A0A7EQR3
B	477	HIS	-	expression tag	UNP A0A0A7EQR3
B	478	HIS	-	expression tag	UNP A0A0A7EQR3
B	479	HIS	-	expression tag	UNP A0A0A7EQR3
B	480	HIS	-	expression tag	UNP A0A0A7EQR3
B	481	HIS	-	expression tag	UNP A0A0A7EQR3

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



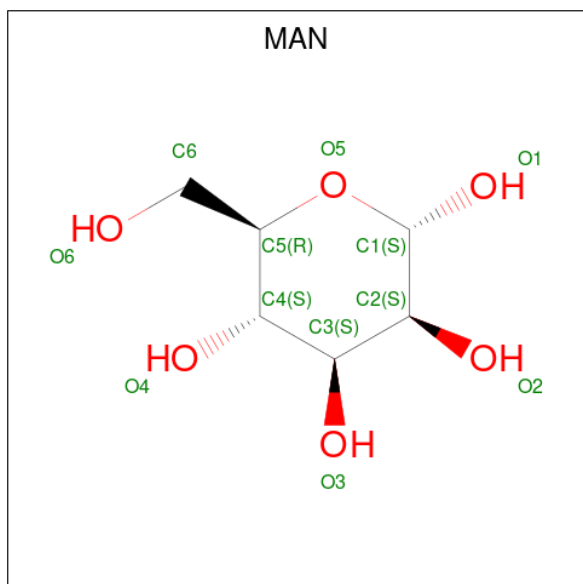
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



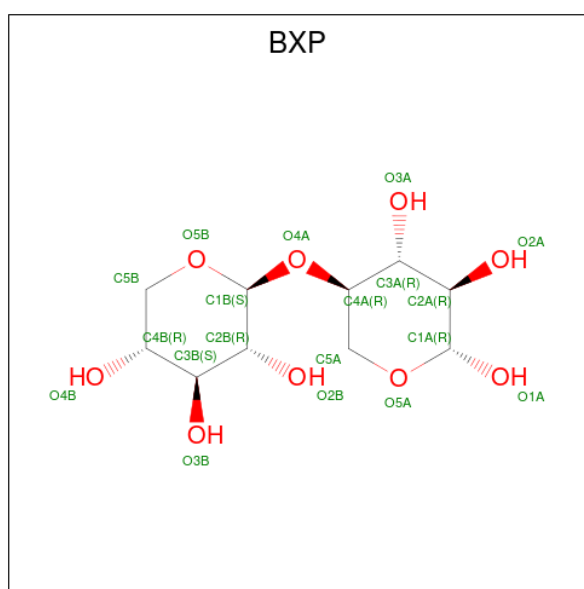
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



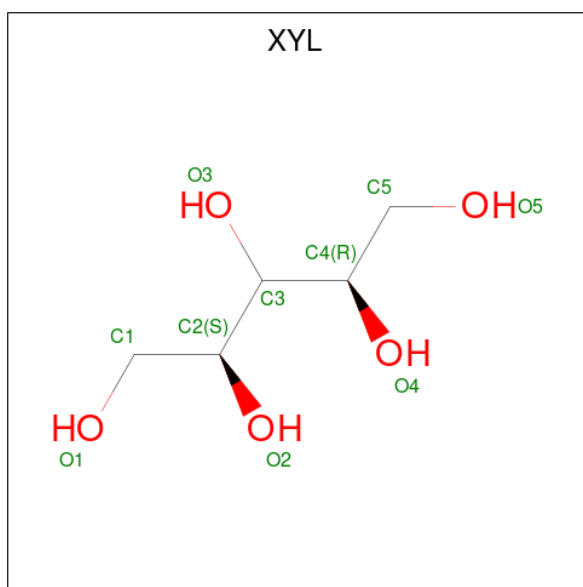
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			22	6	11	5		
4	A	1	Total	C	H	O	0	0
			22	6	11	5		
4	B	1	Total	C	H	O	0	0
			22	6	11	5		
4	B	1	Total	C	H	O	0	0
			22	6	11	5		

- Molecule 5 is 4-O-beta-D-xylopyranosyl-beta-D-xylopyranose (three-letter code: BXP) (formula: C₁₀H₁₈O₉).



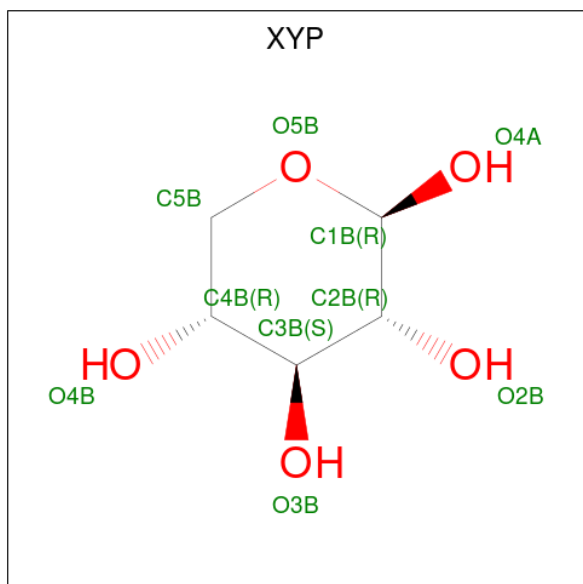
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			37	10	18	9		

- Molecule 6 is D-XYLITOL (three-letter code: XYL) (formula: C₅H₁₂O₅) (labeled as "Ligand of Interest" by author).



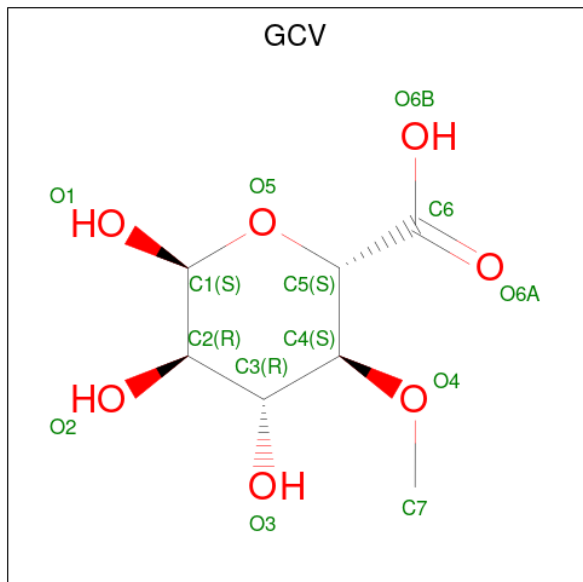
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			21	5	11	5		

- Molecule 7 is BETA-D-XYLOPYRANOSE (three-letter code: XYP) (formula: $C_5H_{10}O_5$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			17	5	8	4		
7	B	1	Total	C	H	O	0	0
			17	5	8	4		

- Molecule 8 is 4-O-METHYL-ALPHA-D-GLUCURONIC ACID (three-letter code: GCV) (formula: $C_7H_{12}O_7$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	H	O	0	0
			22	7	10	5		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	321	Total	O	0	0
			321	321		
9	B	258	Total	O	0	0
			258	258		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.75Å 84.75Å 261.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.45 – 1.85 44.45 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.45-1.85) 95.3 (44.45-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.149 , 0.181 0.149 , 0.181	Depositor DCC
R_{free} test set	4226 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.3	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	6590	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 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XYP, NAG, BXP, EDO, GCV, XYL, MAN

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	0.36	0/2981	0.55	0/4079
1	B	0.34	0/2964	0.54	0/4056
All	All	0.35	0/5945	0.54	0/8135

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2891	0	2779	9	0
1	B	2880	0	2766	8	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	4	6	6	0	0
4	A	22	22	20	0	0
4	B	22	22	20	0	0
5	A	19	18	18	0	0
6	B	10	11	11	0	0
7	B	18	16	14	0	0
8	B	12	10	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	321	0	0	1	0
9	B	258	0	0	2	0
All	All	6485	105	5669	16	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 1.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:PRO:HD2	1:B:159:LEU:HA	1.74	0.68
1:A:255:PRO:HD2	9:A:853:HOH:O	2.05	0.56
1:B:90[B]:ASN:ND2	9:B:601:HOH:O	2.43	0.52
1:B:289:THR:O	1:B:358[B]:MET:HG2	2.10	0.51
1:B:178:PRO:HB3	1:B:183:TRP:NE1	2.27	0.49
1:A:178:PRO:HB3	1:A:183:TRP:NE1	2.28	0.48
1:A:118:ARG:NH2	1:A:284:GLU:HG3	2.31	0.45
1:A:250:ALA:HA	1:A:253:MET:HE2	2.00	0.44
1:A:429:THR:HG21	1:B:338:LYS:NZ	2.33	0.44
1:B:330:THR:HG22	9:B:826:HOH:O	2.18	0.43
1:B:271:ARG:HA	1:B:274:LYS:HE2	2.01	0.43
1:A:178:PRO:HB3	1:A:183:TRP:CE2	2.54	0.42
1:A:159:LEU:HG	1:A:227:LEU:HD11	2.01	0.42
1:B:178:PRO:HB3	1:B:183:TRP:CE2	2.55	0.42
1:A:385:TRP:CD2	1:A:394:HIS:HB2	2.54	0.42
1:A:144:PHE:HB2	1:A:254:THR:HG21	2.01	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/481 (80%)	368 (96%)	15 (4%)	0	100	100
1	B	381/481 (79%)	368 (97%)	13 (3%)	0	100	100
All	All	764/962 (79%)	736 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/378 (82%)	308 (100%)	0	100	100
1	B	306/378 (81%)	304 (99%)	2 (1%)	85	81
All	All	614/756 (81%)	612 (100%)	2 (0%)	93	93

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

Mol	Chain	Res	Type
1	B	162	SER
1	B	433	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	501	1	14,14,15	0.40	0	17,19,21	0.55	0
3	EDO	A	502	-	3,3,3	0.55	0	2,2,2	0.25	0
4	MAN	A	503	1	11,11,12	0.91	0	15,15,17	1.03	1 (6%)
4	MAN	A	504	1	11,11,12	0.80	0	15,15,17	1.11	1 (6%)
5	BXP	A	505	-	20,20,20	2.59	11 (55%)	28,29,29	1.27	3 (10%)
2	NAG	B	501	1	14,14,15	0.36	0	17,19,21	0.45	0
6	XYL	B	502	7	9,9,9	0.77	0	11,11,11	0.96	1 (9%)
7	XYP	B	503	7,6	9,9,10	1.94	3 (33%)	10,12,14	1.35	1 (10%)
7	XYP	B	504	8,7	9,9,10	1.90	3 (33%)	10,12,14	1.27	2 (20%)
8	GCV	B	505	7	10,12,14	1.83	2 (20%)	13,16,20	1.18	1 (7%)
4	MAN	B	506	1	11,11,12	0.87	0	15,15,17	1.10	1 (6%)
4	MAN	B	507	1	11,11,12	0.89	0	15,15,17	1.03	1 (6%)

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	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	EDO	A	502	-	-	0/1/1/1	-
4	MAN	A	503	1	-	0/2/19/22	0/1/1/1
4	MAN	A	504	1	-	2/2/19/22	0/1/1/1
5	BXP	A	505	-	-	0/4/38/38	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
6	XYL	B	502	7	-	4/12/12/12	-
7	XYP	B	503	7,6	-	-	0/1/1/1
7	XYP	B	504	8,7	-	-	0/1/1/1
8	GCV	B	505	7	-	2/3/21/26	0/1/1/1
4	MAN	B	506	1	-	0/2/19/22	0/1/1/1
4	MAN	B	507	1	-	0/2/19/22	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	505	BXP	C4B-C3B	-6.10	1.43	1.52
8	B	505	GCV	O5-C1	4.51	1.51	1.43
5	A	505	BXP	O5B-C1B	4.08	1.50	1.41
5	A	505	BXP	O4A-C1B	-4.02	1.30	1.41
7	B	504	XYP	O5B-C1B	3.91	1.50	1.42
7	B	503	XYP	O5B-C1B	3.83	1.50	1.42
5	A	505	BXP	O3B-C3B	3.02	1.50	1.43
5	A	505	BXP	O5A-C1A	2.95	1.47	1.43
5	A	505	BXP	O5B-C5B	2.86	1.48	1.43
5	A	505	BXP	O4B-C4B	2.74	1.49	1.43
7	B	504	XYP	O5B-C5B	2.73	1.48	1.42
5	A	505	BXP	O5A-C5A	2.63	1.47	1.43
5	A	505	BXP	C3A-C4A	-2.63	1.47	1.53
7	B	503	XYP	C2B-C3B	-2.60	1.48	1.52
7	B	503	XYP	O5B-C5B	2.58	1.47	1.42
7	B	504	XYP	C2B-C3B	-2.45	1.48	1.52
8	B	505	GCV	C4-C5	2.16	1.55	1.52
5	A	505	BXP	C1B-C2B	2.11	1.58	1.52
5	A	505	BXP	O3A-C3A	2.07	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	505	BXP	C1B-O4A-C4A	-3.48	109.95	115.33
7	B	503	XYP	C1B-C2B-C3B	3.19	113.58	109.66
4	A	504	MAN	C1-O5-C5	2.83	116.05	112.20
4	A	503	MAN	C1-O5-C5	2.66	115.81	112.20
4	B	506	MAN	C1-O5-C5	2.65	115.80	112.20
5	A	505	BXP	C5B-C4B-C3B	2.58	112.83	109.66
5	A	505	BXP	O5B-C1B-C2B	-2.57	106.28	110.10
6	B	502	XYL	C5-C4-C3	-2.49	106.98	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	504	XYP	O3B-C3B-C4B	-2.24	105.86	110.02
8	B	505	GCV	O3-C3-C2	-2.14	106.05	110.02
7	B	504	XYP	C5B-C4B-C3B	2.13	112.28	109.66
4	B	507	MAN	C1-O5-C5	2.03	114.96	112.20

There are no chirality outliers.

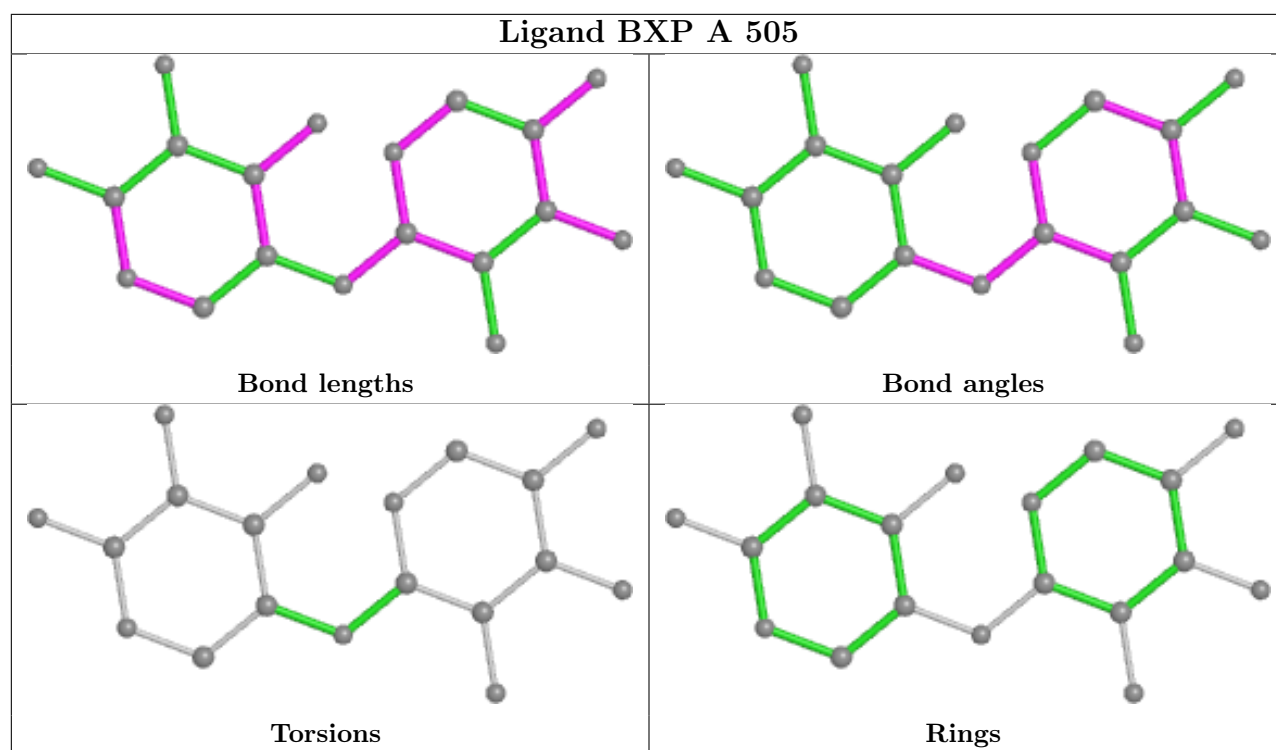
All (8) torsion outliers are listed below:

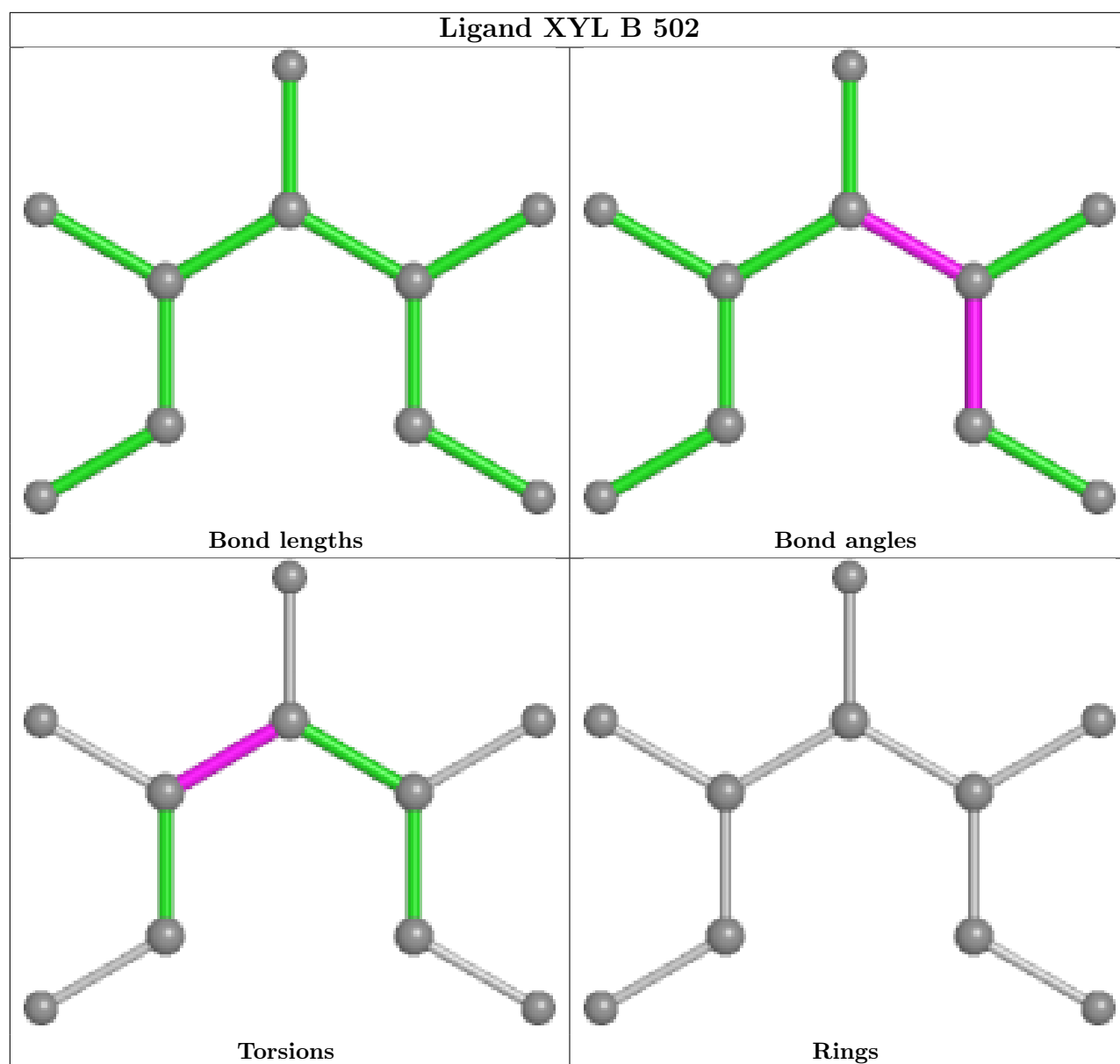
Mol	Chain	Res	Type	Atoms
8	B	505	GCV	C3-C4-O4-C7
4	A	504	MAN	O5-C5-C6-O6
6	B	502	XYL	O2-C2-C3-C4
6	B	502	XYL	C1-C2-C3-O3
6	B	502	XYL	C1-C2-C3-C4
6	B	502	XYL	O2-C2-C3-O3
8	B	505	GCV	C5-C4-O4-C7
4	A	504	MAN	C4-C5-C6-O6

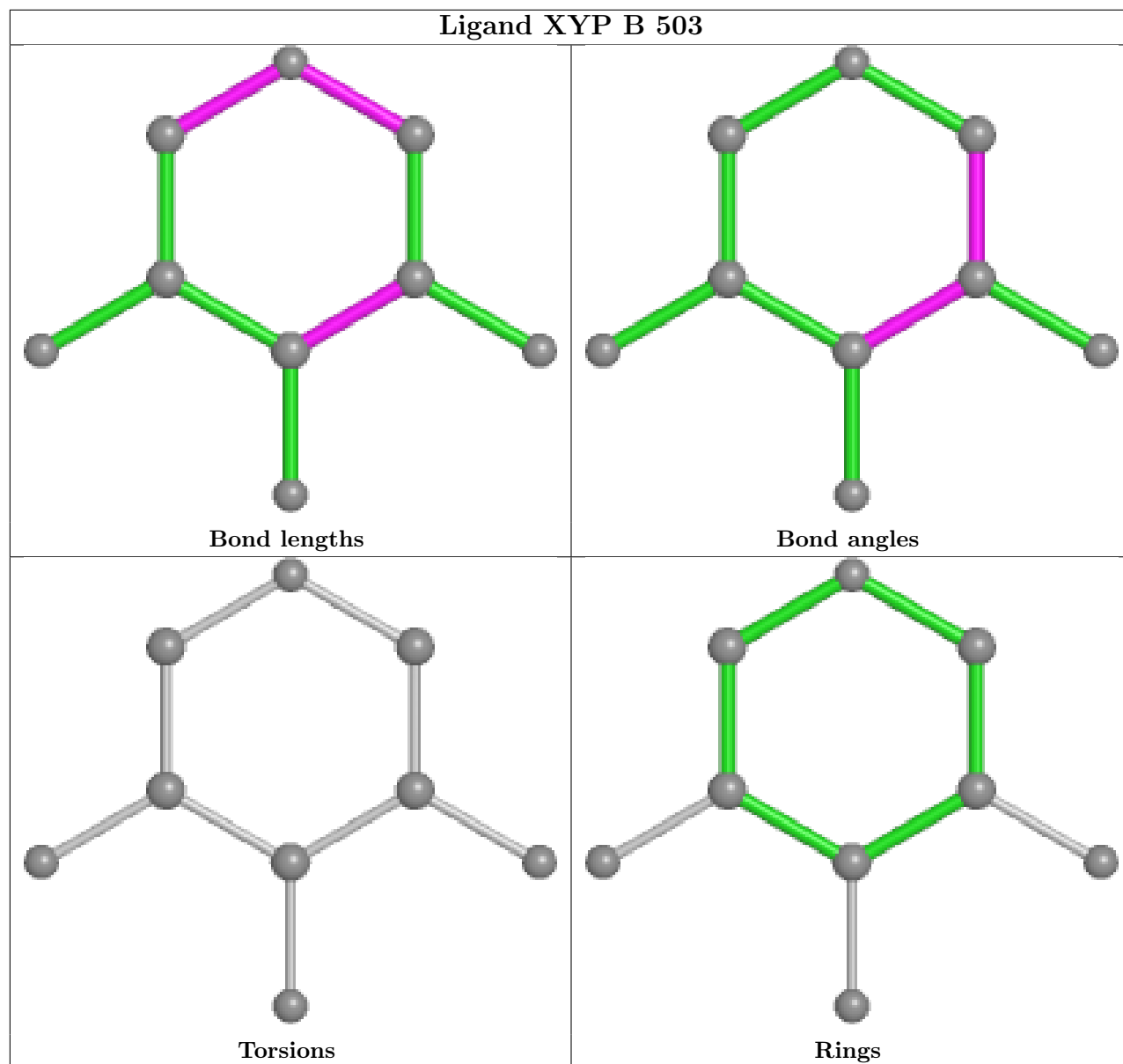
There are no ring outliers.

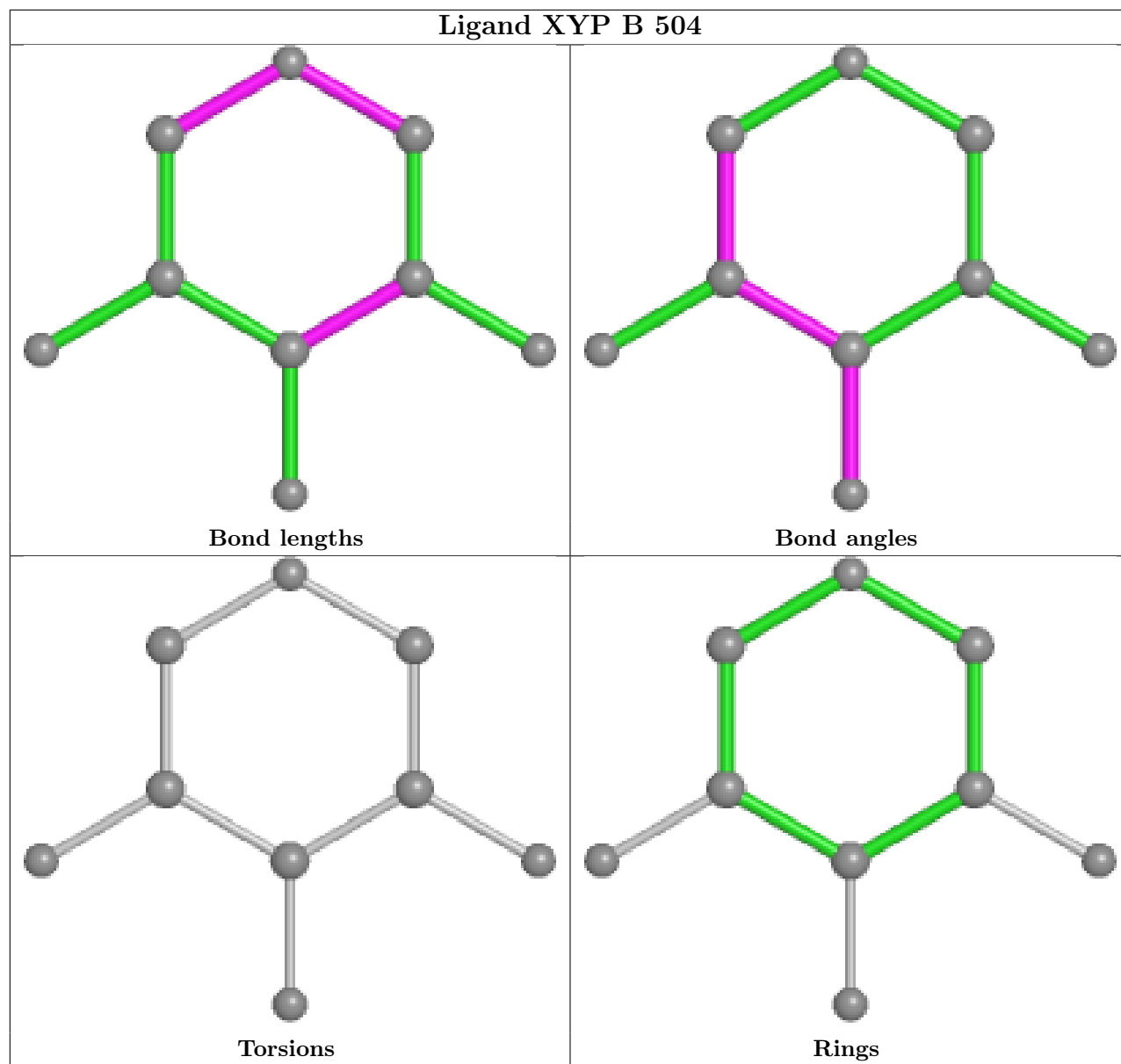
No monomer is involved in short contacts.

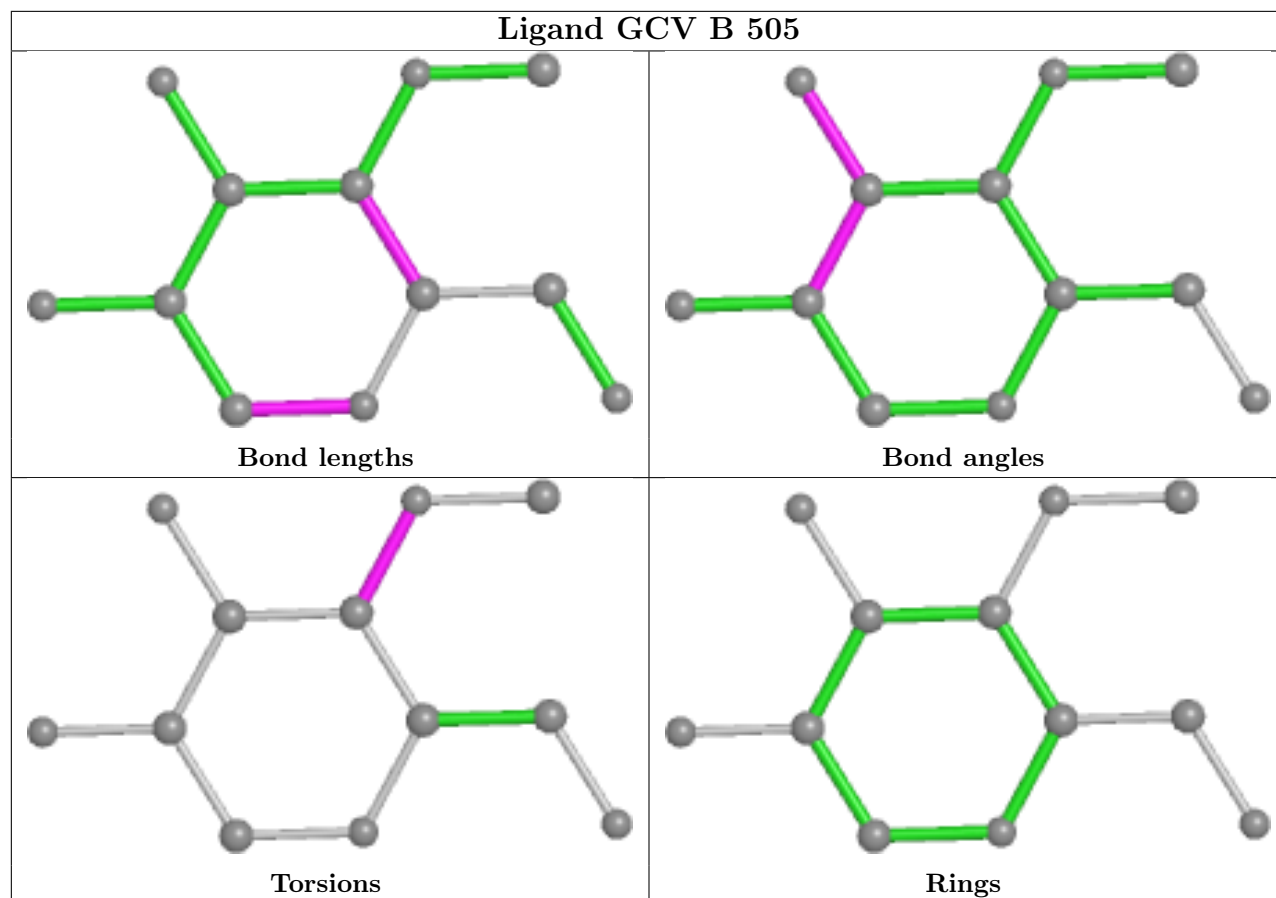
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	381/481 (79%)	-0.60	3 (0%) 86 87	16, 22, 37, 65	0
1	B	381/481 (79%)	-0.39	13 (3%) 45 43	17, 25, 47, 79	0
All	All	762/962 (79%)	-0.50	16 (2%) 63 63	16, 23, 43, 79	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	LEU	4.6
1	B	159	LEU	3.8
1	B	147	SER	3.8
1	B	175	SER	3.7
1	B	176	GLY	3.4
1	A	80	ALA	3.3
1	A	148	GLY	2.6
1	B	82	GLY	2.5
1	A	82	GLY	2.5
1	B	177	THR	2.5
1	B	148	GLY	2.4
1	B	198	ALA	2.4
1	B	80	ALA	2.4
1	B	149	ASN	2.2
1	B	163	GLN	2.1
1	B	459	GLY	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

There are no carbohydrates in this entry.

6.4 Ligands

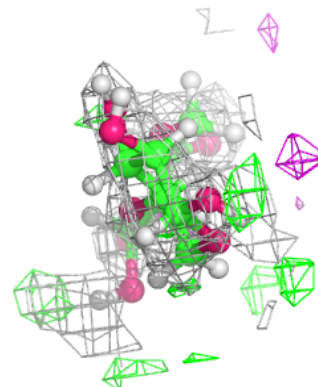
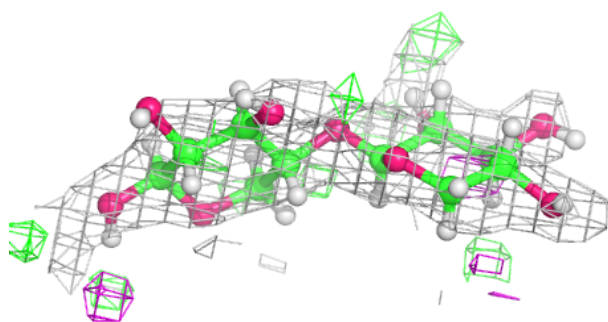
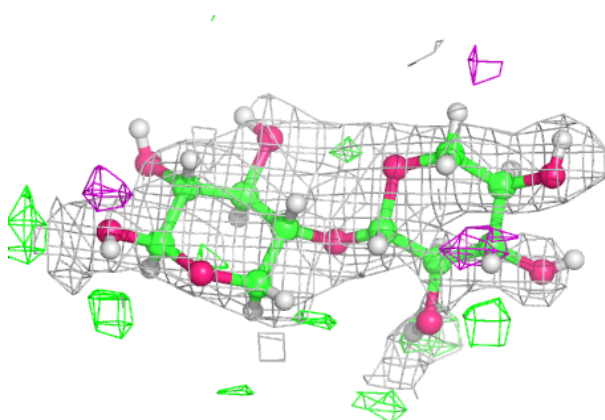
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BXP	A	505	19/19	0.76	0.24	42,59,72,76	37
4	MAN	A	504	11/12	0.77	0.24	56,76,86,91	0
4	MAN	B	507	11/12	0.78	0.15	47,62,74,79	0
4	MAN	A	503	11/12	0.81	0.29	46,72,86,95	0
4	MAN	B	506	11/12	0.85	0.17	49,64,76,79	0
6	XYL	B	502	10/10	0.93	0.25	41,66,84,87	0
7	XYP	B	504	9/10	0.94	0.12	27,37,48,49	0
3	EDO	A	502	4/4	0.96	0.13	22,34,49,49	0
7	XYP	B	503	9/10	0.97	0.14	31,41,53,56	0
2	NAG	A	501	14/15	0.97	0.06	22,27,33,34	0
2	NAG	B	501	14/15	0.97	0.09	20,27,34,34	0
8	GCV	B	505	12/14	0.97	0.06	21,28,35,37	0

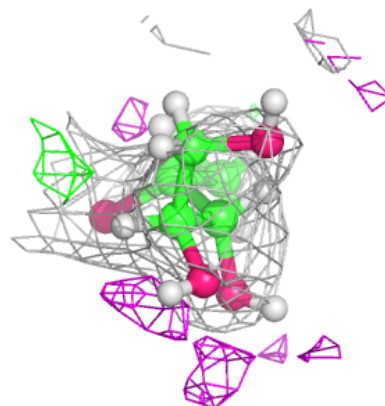
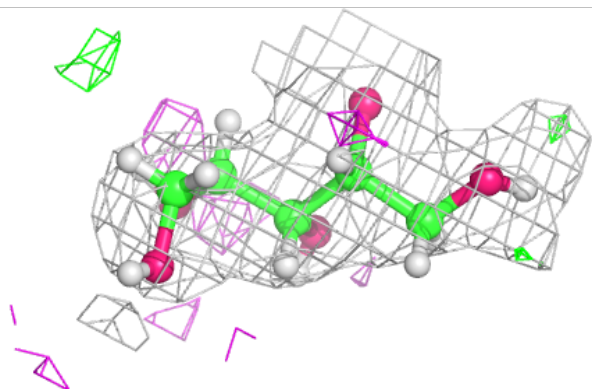
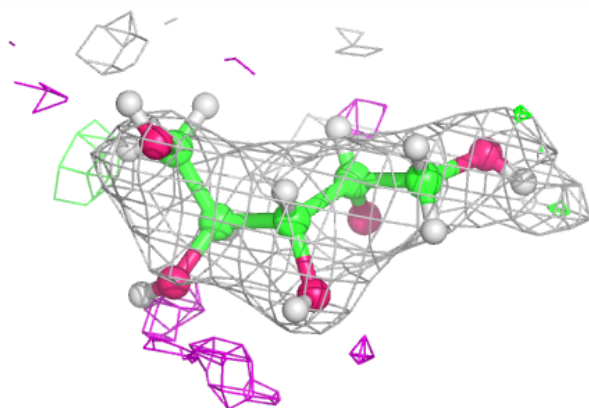
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BXP A 505:

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

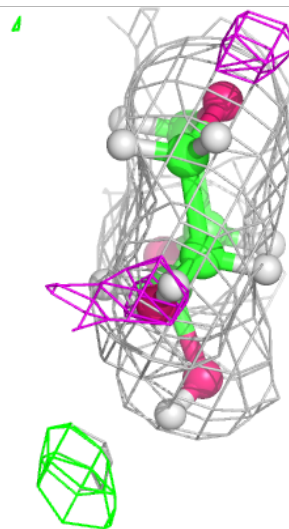
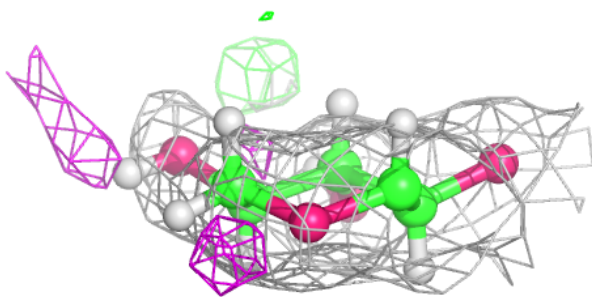
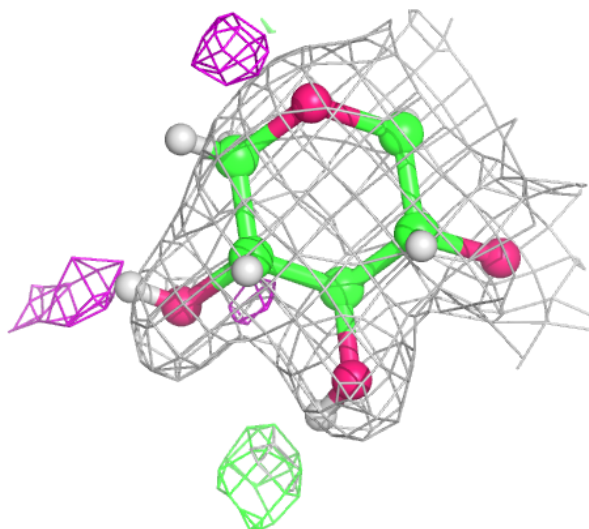
**Electron density around XYL B 502:**

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



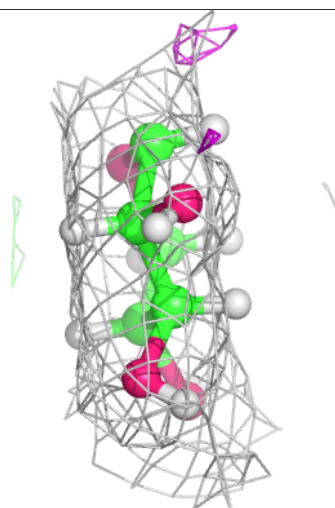
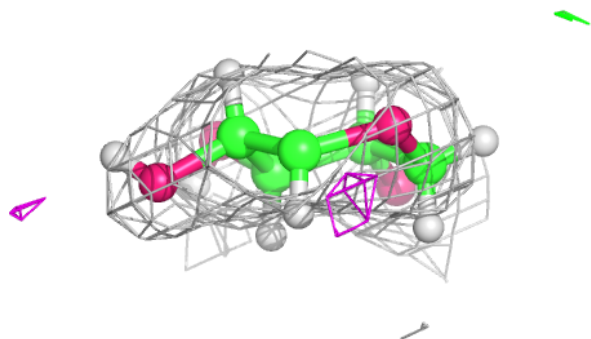
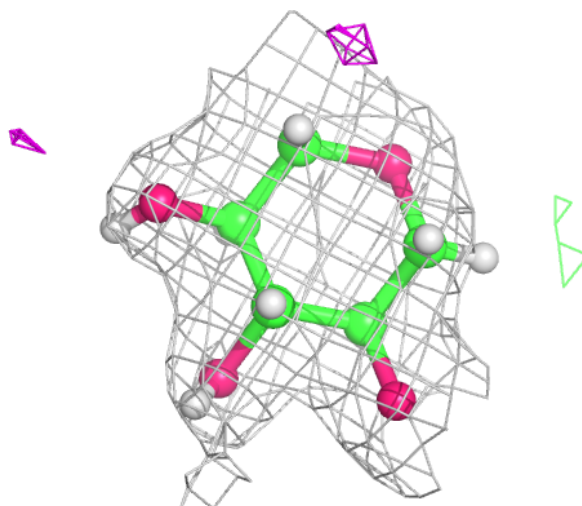
Electron density around XYP B 504:

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



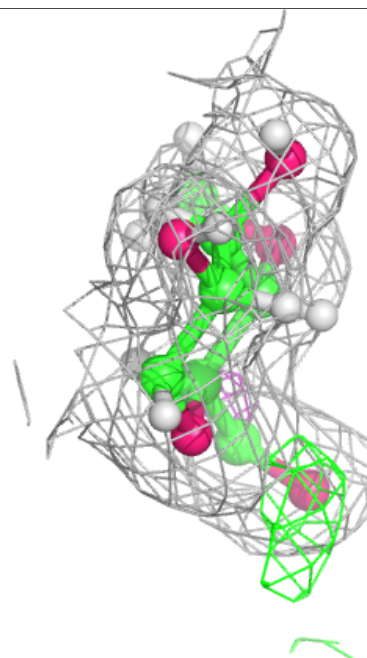
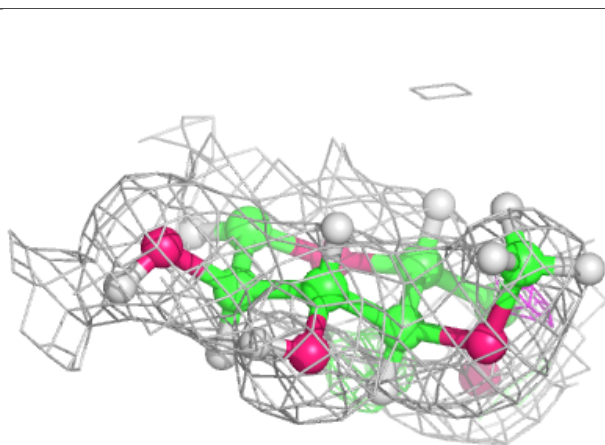
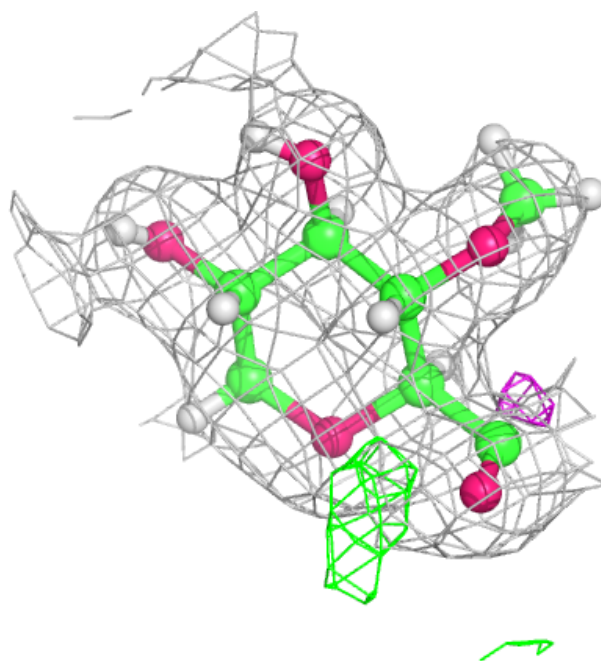
Electron density around XYP B 503:

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



Electron density around GCV B 505:

$2mF_o-DF_c$ (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.