Full wwPDB X-ray Structure Validation Report

May 20, 2024 – 03:06 AM JST

PDB ID	:	8HJH
Title	:	Crystal structure of glycosyltransferase SgUGT94-289-3 in complex with SIA, state 3
Authors	:	Li, M.; Zhang, S.; Cui, S.
Deposited on	:	2022-11-23
Resolution	:	1.76 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:

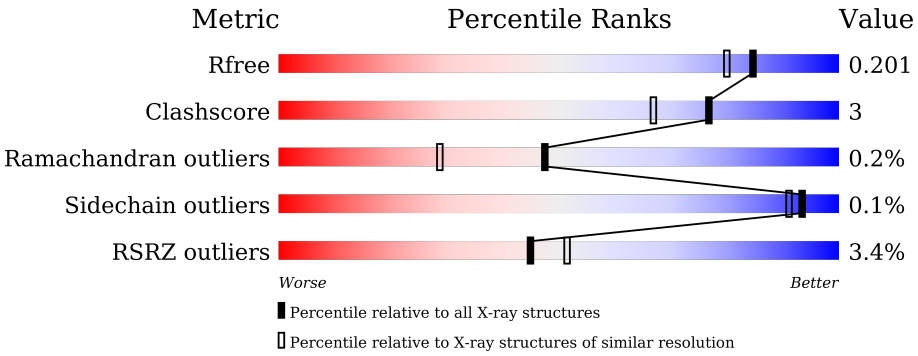
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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	459	2% 89% 6% 5%
1	B	459	4% 88% 7% 5%

2 Entry composition

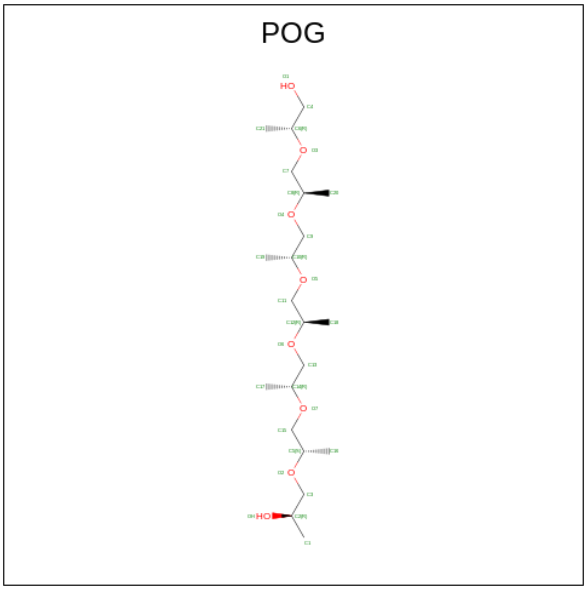
There are 6 unique types of molecules in this entry. The entry contains 7734 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glycosyltransferase.

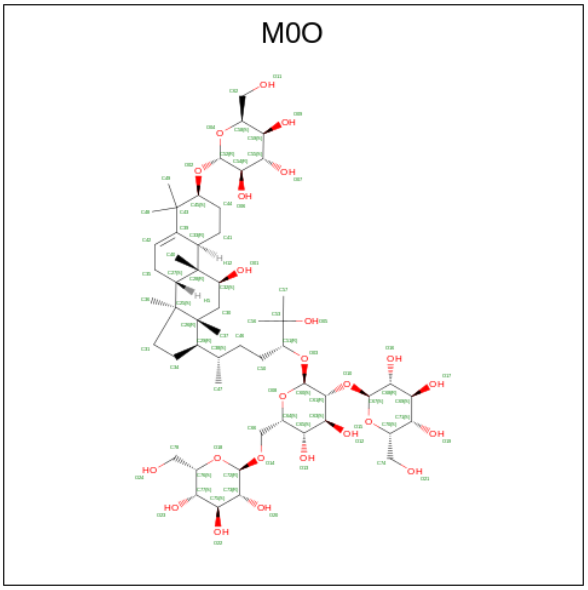
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	1	0
			3435	2222	582	614	17			
1	B	437	Total	C	N	O	S	0	0	0
			3454	2231	582	624	17			

- Molecule 2 is (20S)-2,5,8,11,14,17-HEXAMETHYL-3,6,9,12,15,18-HEXAOXAHENICOSANE-1,20-DIOL (three-letter code: POG) (formula: $C_{21}H_{44}O_8$).



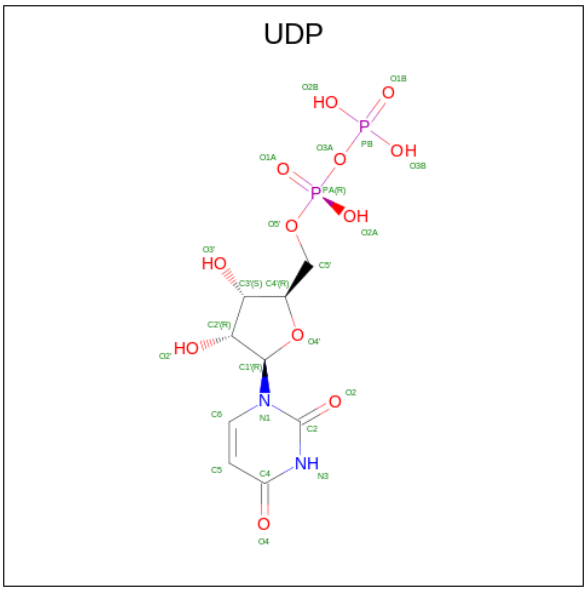
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			13	9	4			
2	A	1	Total	C	O		0	0
			21	15	6			
2	B	1	Total	C	O		0	0
			13	9	4			
2	B	1	Total	C	O		0	0
			21	15	6			

- Molecule 3 is (2S,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[[(2S,3S,4S,5R,6S)-5-[(2S,3R,4S,5S,6S)-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[(3R,6S)-6-[(3S,8S,9R,10R,11S,13R,14S,17R)-3-[(2S,3R,4S,5S,6S)-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,4,9,13,14-pentamethyl-11-oxidanyl-2,3,7,8,10,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-methyl-2-oxidanyl-heptan-3-yl]oxy-3,4-bis(oxidanyl)oxan-2-yl]methoxy]oxane-3,4,5-triol (three-letter code: M0O) (formula: $C_{54}H_{92}O_{24}$) (labeled as "Ligand of Interest" by depositor).



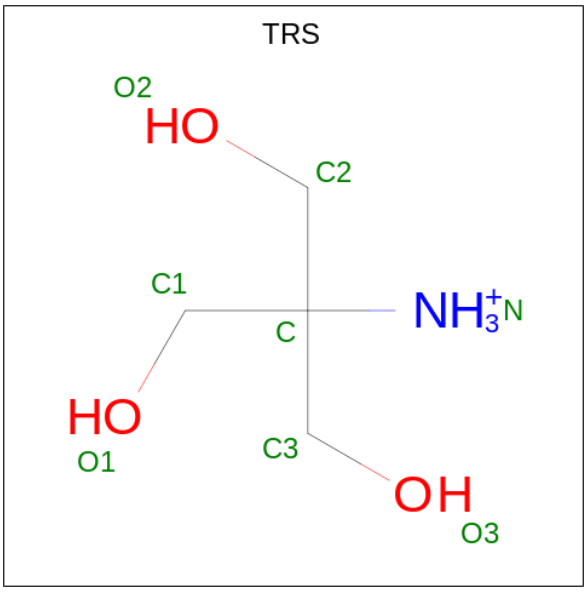
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 78 54 24	0	0
3	B	1	Total C O 78 54 24	0	0

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
4	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is water.

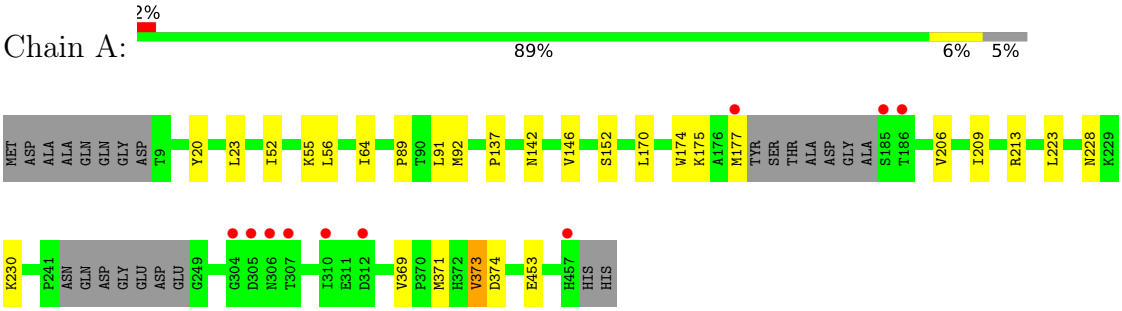
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	292	Total O 292 292	0	0
6	B	271	Total O 271 271	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

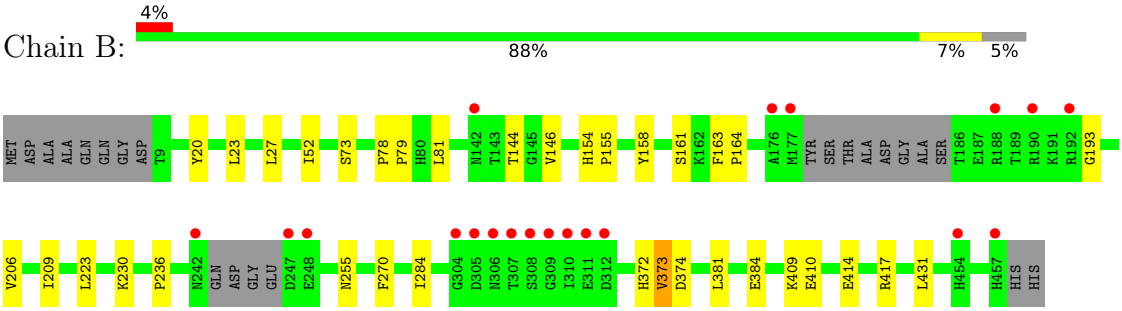
• Molecule 1: glycosyltransferase

Chain A:



• Molecule 1: glycosyltransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.25Å 76.80Å 82.11Å 90.00° 92.63° 90.00°	Depositor
Resolution (Å)	35.93 – 1.76 57.93 – 1.76	Depositor EDS
% Data completeness (in resolution range)	86.5 (35.93-1.76) 84.3 (57.93-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.181 , 0.201 0.181 , 0.201	Depositor DCC
R_{free} test set	4442 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l 0.012 for -k,-h,-l 0.067 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7734	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: UDP, TRS, POG, M0O

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.62	0/3536	0.70	0/4798
1	B	0.62	0/3555	0.70	0/4824
All	All	0.62	0/7091	0.70	0/9622

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

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	3435	0	3362	19	0
1	B	3454	0	3368	20	0
2	A	34	0	50	3	0
2	B	34	0	50	2	0
3	A	78	0	0	0	0
3	B	78	0	0	0	0
4	A	25	0	11	0	0
4	B	25	0	11	0	0
5	B	8	0	12	1	0
6	A	292	0	0	2	0
6	B	271	0	0	1	0
All	All	7734	0	6864	42	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 3.

All (42) 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:142[A]:ASN:HB2	1:A:209:ILE:HD12	1.58	0.84
1:A:142[B]:ASN:HB3	1:A:209:ILE:HD12	1.58	0.83
1:A:146:VAL:HG23	1:A:223:LEU:HD22	1.78	0.65
1:A:137:PRO:HG3	1:A:453:GLU:HG3	1.80	0.64
1:B:144:THR:HG22	5:B:502:TRS:H12	1.81	0.63
1:B:20:TYR:HA	1:B:23:LEU:HD12	1.82	0.60
1:B:27:LEU:HD22	1:B:52:ILE:HG13	1.84	0.60
1:A:52:ILE:HD12	1:A:55:LYS:HD3	1.85	0.57
1:A:170:LEU:HD23	1:A:175:LYS:HG2	1.88	0.54
1:B:236:PRO:HG3	1:B:431:LEU:HD22	1.89	0.54
1:B:146:VAL:HB	1:B:209:ILE:HD13	1.90	0.53
1:A:373:VAL:HG12	1:A:374:ASP:N	2.24	0.52
1:B:78:PRO:HD2	1:B:81:LEU:HD12	1.92	0.52
1:A:89:PRO:O	6:A:601:HOH:O	2.19	0.51
1:B:146:VAL:HG23	1:B:223:LEU:HD22	1.92	0.51
1:B:193:GLY:HA3	2:B:501:POG:H6	1.91	0.51
1:B:409:LYS:HG2	1:B:414:GLU:HG3	1.92	0.50
1:A:174:TRP:HA	1:A:177:MET:HG2	1.94	0.49
1:B:255:ASN:ND2	6:B:604:HOH:O	2.44	0.49
1:B:372:HIS:CD2	1:B:373:VAL:HG23	2.50	0.47
1:B:206:VAL:HG12	1:B:230:LYS:HB3	1.97	0.47
1:A:373:VAL:HG12	1:A:374:ASP:H	1.81	0.45
1:B:381:LEU:HA	1:B:384:GLU:HG2	1.98	0.45
1:A:206:VAL:HG12	1:A:230:LYS:HB3	1.98	0.45
1:B:410:GLU:HB3	1:B:417:ARG:HG2	1.99	0.45
1:B:154:HIS:N	1:B:155:PRO:HD2	2.32	0.45
1:A:152:SER:HB3	2:A:501:POG:H71	1.99	0.45
2:A:503:POG:H31	2:A:503:POG:H151	1.65	0.44
1:A:369:VAL:HG12	1:A:371:MET:HE1	1.98	0.44
1:B:73:SER:OG	1:B:79:PRO:HD3	2.18	0.44
1:B:373:VAL:HG12	1:B:374:ASP:N	2.32	0.44
1:A:56:LEU:HD11	1:A:64:ILE:HD12	1.99	0.43
2:B:504:POG:H111	2:B:504:POG:H131	1.68	0.42
1:A:213:ARG:HD3	6:A:725:HOH:O	2.20	0.42
1:B:270:PHE:CZ	1:B:284:ILE:HD13	2.55	0.41
1:A:20:TYR:HA	1:A:23:LEU:HD12	2.01	0.41
1:B:158:TYR:HB3	1:B:161:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:PHE:HA	1:B:164:PRO:HD3	1.88	0.41
2:A:503:POG:H172	2:A:503:POG:H152	1.90	0.40
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.95	0.40
1:A:92:MET:HE2	1:A:92:MET:HB3	1.94	0.40
1:A:52:ILE:HD12	1:A:52:ILE:HA	1.99	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	430/459 (94%)	424 (99%)	5 (1%)	1 (0%)	47	29
1	B	431/459 (94%)	426 (99%)	4 (1%)	1 (0%)	47	29
All	All	861/918 (94%)	850 (99%)	9 (1%)	2 (0%)	47	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	VAL
1	B	373	VAL

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	371/400 (93%)	370 (100%)	1 (0%)	92 89
1	B	374/400 (94%)	374 (100%)	0	100 100
All	All	745/800 (93%)	744 (100%)	1 (0%)	93 91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	228	ASN
1	A	372	HIS
1	B	255	ASN
1	B	286	HIS
1	B	372	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	POG	A	503	-	15,20,28	1.34	2 (13%)	18,24,34	1.81	4 (22%)
4	UDP	A	504	-	24,26,26	0.58	0	37,40,40	0.92	2 (5%)
2	POG	A	501	-	9,12,28	0.40	0	10,14,34	0.63	0
2	POG	B	501	-	9,12,28	1.11	0	10,14,34	0.94	1 (10%)
3	M0O	A	502	-	85,85,85	1.99	20 (23%)	129,135,135	2.80	45 (34%)
4	UDP	B	505	-	24,26,26	1.15	2 (8%)	37,40,40	1.48	5 (13%)
5	TRS	B	502	-	7,7,7	0.13	0	9,9,9	0.19	0
2	POG	B	504	-	15,20,28	1.10	1 (6%)	18,24,34	1.81	4 (22%)
3	M0O	B	503	-	85,85,85	1.97	17 (20%)	129,135,135	3.03	40 (31%)

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	POG	A	503	-	-	12/22/22/32	-
4	UDP	A	504	-	-	3/16/32/32	0/2/2/2
2	POG	A	501	-	-	0/12/12/32	-
2	POG	B	501	-	-	5/12/12/32	-
3	M0O	A	502	-	-	16/38/194/194	0/8/8/8
4	UDP	B	505	-	-	3/16/32/32	0/2/2/2
5	TRS	B	502	-	-	1/9/9/9	-
2	POG	B	504	-	-	5/22/22/32	-
3	M0O	B	503	-	-	17/38/194/194	0/8/8/8

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	M0O	C42-C39	9.50	1.51	1.33
3	A	502	M0O	C42-C39	9.46	1.51	1.33
3	B	503	M0O	O01-C32	-6.74	1.32	1.43
3	A	502	M0O	O01-C32	-6.72	1.32	1.43
3	B	503	M0O	C38-C29	-4.23	1.47	1.54
3	A	502	M0O	C35-C42	4.18	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	M0O	C35-C42	4.13	1.59	1.50
3	A	502	M0O	C38-C29	-3.96	1.47	1.54
3	A	502	M0O	C33-C39	3.71	1.59	1.52
3	B	503	M0O	C33-C39	3.48	1.59	1.52
3	A	502	M0O	C31-C34	3.15	1.64	1.54
3	B	503	M0O	C31-C34	3.13	1.64	1.54
3	A	502	M0O	C35-C27	3.09	1.58	1.53
3	B	503	M0O	C35-C27	2.87	1.58	1.53
3	A	502	M0O	C30-C32	-2.59	1.49	1.53
3	B	503	M0O	C50-C46	2.55	1.60	1.53
3	A	502	M0O	C44-C41	-2.54	1.46	1.52
3	A	502	M0O	C50-C46	2.54	1.60	1.53
4	B	505	UDP	C4-N3	-2.54	1.34	1.38
2	A	503	POG	O6-C13	-2.45	1.39	1.43
3	B	503	M0O	C44-C41	-2.43	1.46	1.52
3	B	503	M0O	O05-C53	-2.32	1.40	1.44
4	B	505	UDP	C2-N3	-2.32	1.33	1.38
3	A	502	M0O	O04-C52	2.30	1.47	1.41
3	A	502	M0O	O08-C60	2.28	1.47	1.41
3	A	502	M0O	C69-C68	-2.19	1.46	1.52
3	A	502	M0O	C75-C73	-2.17	1.46	1.52
3	B	503	M0O	C30-C32	-2.15	1.50	1.53
3	A	502	M0O	O22-C75	2.14	1.48	1.43
3	A	502	M0O	O05-C53	-2.13	1.40	1.44
3	B	503	M0O	C25-C27	-2.12	1.53	1.56
3	B	503	M0O	C69-C68	-2.11	1.47	1.52
2	B	504	POG	O6-C13	-2.10	1.39	1.43
3	B	503	M0O	O04-C52	2.09	1.47	1.41
3	A	502	M0O	C28-C27	2.08	1.60	1.56
3	A	502	M0O	C71-C69	-2.08	1.47	1.52
3	B	503	M0O	C75-C73	-2.06	1.47	1.52
3	B	503	M0O	C71-C69	-2.06	1.47	1.52
3	A	502	M0O	C55-C54	-2.04	1.47	1.52
3	B	503	M0O	O18-C72	2.03	1.47	1.41
3	A	502	M0O	O18-C72	2.02	1.47	1.41
2	A	503	POG	C9-C10	2.01	1.55	1.51

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	M0O	C37-C26-C30	-13.04	93.09	111.11
3	B	503	M0O	C43-C39-C33	-12.66	104.21	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	M0O	C37-C26-C25	-12.36	91.96	112.39
3	B	503	M0O	C37-C26-C30	-11.42	95.34	111.11
3	A	502	M0O	C37-C26-C25	-11.17	93.92	112.39
3	B	503	M0O	C43-C39-C42	-9.90	116.07	122.08
3	A	502	M0O	C31-C25-C27	7.92	128.05	114.04
3	B	503	M0O	C31-C25-C27	7.32	126.98	114.04
3	B	503	M0O	C36-C25-C26	-6.72	101.28	112.39
3	A	502	M0O	C36-C25-C26	-6.36	101.88	112.39
3	B	503	M0O	C30-C26-C25	5.71	118.26	108.30
3	B	503	M0O	C35-C42-C39	-5.71	114.36	125.07
3	A	502	M0O	C50-C51-C53	-5.57	106.32	115.49
3	A	502	M0O	O03-C51-C53	5.42	113.23	106.42
3	A	502	M0O	C26-C29-C38	5.33	126.20	119.30
3	B	503	M0O	C26-C29-C38	5.33	126.19	119.30
3	B	503	M0O	C37-C26-C29	-5.28	101.56	111.80
3	A	502	M0O	C44-C45-C43	-5.26	109.33	113.28
3	A	502	M0O	C30-C26-C25	5.02	117.06	108.30
2	B	504	POG	C3-O2-C5	4.98	122.45	115.02
3	B	503	M0O	O03-C51-C53	4.93	112.61	106.42
3	B	503	M0O	O18-C76-C77	4.90	118.59	109.69
3	A	502	M0O	C37-C26-C29	-4.88	102.34	111.80
3	A	502	M0O	C35-C42-C39	-4.86	115.95	125.07
3	B	503	M0O	C47-C38-C29	4.74	120.17	112.92
3	A	502	M0O	O15-C70-C71	4.72	118.26	109.69
3	A	502	M0O	C30-C26-C29	4.64	134.28	117.38
3	B	503	M0O	C30-C26-C29	4.60	134.12	117.38
3	A	502	M0O	O18-C76-C77	4.48	117.82	109.69
3	B	503	M0O	O15-C70-C71	4.43	117.74	109.69
4	B	505	UDP	C4-N3-C2	-4.26	120.96	126.58
3	A	502	M0O	C35-C27-C28	4.24	115.56	110.41
2	A	503	POG	O4-C9-C10	4.07	122.59	111.78
3	A	502	M0O	C36-C25-C31	-4.04	97.06	111.86
3	B	503	M0O	O08-C64-C65	4.00	116.95	109.69
3	B	503	M0O	C63-C65-C64	3.97	117.33	110.24
3	A	502	M0O	C47-C38-C29	3.97	118.99	112.92
3	A	502	M0O	C26-C25-C27	3.93	113.89	109.92
4	B	505	UDP	N3-C2-N1	3.91	120.08	114.89
3	B	503	M0O	C35-C27-C25	-3.91	111.00	114.69
3	B	503	M0O	C36-C25-C31	-3.90	97.58	111.86
3	A	502	M0O	C52-O02-C45	3.82	121.18	115.08
3	B	503	M0O	C35-C27-C28	3.75	114.97	110.41
3	B	503	M0O	C26-C25-C27	3.68	113.64	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	M0O	C35-C27-C25	-3.67	111.23	114.69
3	A	502	M0O	C43-C39-C33	-3.64	112.54	115.91
2	A	503	POG	C13-O6-C12	3.59	120.38	115.02
2	A	503	POG	C15-O7-C14	3.53	120.28	115.02
4	B	505	UDP	C5-C4-N3	3.51	120.09	114.84
3	A	502	M0O	O08-C64-C65	3.45	115.96	109.69
3	B	503	M0O	C40-C28-C27	-3.38	104.20	112.73
3	A	502	M0O	C27-C28-C32	3.36	113.89	107.50
3	B	503	M0O	C27-C28-C32	3.31	113.79	107.50
3	A	502	M0O	O06-C54-C55	-3.24	102.87	110.35
2	B	504	POG	C15-O7-C14	3.18	119.76	115.02
3	A	502	M0O	C60-O08-C64	3.15	119.87	113.69
3	B	503	M0O	C50-C51-C53	-3.15	110.31	115.49
3	A	502	M0O	C63-C65-C64	3.15	115.85	110.24
3	A	502	M0O	C40-C28-C27	-3.09	104.94	112.73
3	A	502	M0O	O08-C60-C61	3.04	115.54	109.51
3	A	502	M0O	C75-C77-C76	2.90	115.42	110.24
4	B	505	UDP	O4-C4-C5	-2.87	120.11	125.16
3	A	502	M0O	C69-C71-C70	2.72	115.10	110.24
3	B	503	M0O	O04-C58-C59	2.71	114.61	109.69
3	B	503	M0O	C75-C77-C76	2.68	115.02	110.24
3	A	502	M0O	C43-C39-C42	-2.66	120.47	122.08
3	B	503	M0O	C46-C50-C51	-2.66	106.58	112.71
3	B	503	M0O	C26-C30-C32	2.61	116.94	113.19
3	B	503	M0O	C60-O08-C64	2.57	118.74	113.69
3	A	502	M0O	C36-C25-C27	-2.57	107.87	111.44
3	A	502	M0O	C27-C35-C42	2.57	117.81	113.02
3	B	503	M0O	C28-C33-C39	2.54	117.49	113.47
3	B	503	M0O	C34-C29-C26	-2.51	100.36	103.73
3	A	502	M0O	O02-C52-C54	2.49	114.54	108.10
3	A	502	M0O	C34-C29-C38	-2.46	108.34	112.15
3	A	502	M0O	O12-C63-C65	-2.43	104.74	110.35
3	B	503	M0O	O08-C60-C61	2.41	114.29	109.51
3	B	503	M0O	C46-C38-C29	-2.38	105.37	110.28
3	B	503	M0O	C78-C76-C77	-2.37	107.46	113.00
4	B	505	UDP	O2-C2-N1	-2.31	119.72	122.79
3	A	502	M0O	C67-O15-C70	2.30	118.20	113.69
3	A	502	M0O	O20-C73-C75	-2.29	105.06	110.35
3	B	503	M0O	C52-O02-C45	-2.28	111.44	115.08
3	B	503	M0O	O12-C63-C65	-2.27	105.11	110.35
3	B	503	M0O	C69-C71-C70	2.26	114.28	110.24
3	B	503	M0O	C31-C25-C26	2.24	104.74	101.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	M0O	C59-C55-C54	2.23	114.72	110.82
3	A	502	M0O	C52-C54-C55	2.18	114.53	110.00
2	A	503	POG	C3-O2-C5	2.13	118.20	115.02
3	A	502	M0O	C55-C59-C58	2.13	114.03	110.24
3	A	502	M0O	C78-C76-C77	-2.13	108.02	113.00
3	A	502	M0O	C72-O18-C76	2.10	117.81	113.69
3	B	503	M0O	C67-O10-C61	-2.09	112.79	117.96
4	A	504	UDP	O3A-PB-O1B	-2.07	99.68	111.19
2	B	501	POG	O4-C9-C10	2.07	112.87	108.86
2	B	504	POG	C17-C14-C13	-2.07	106.69	112.63
3	B	503	M0O	C62-C58-C59	-2.05	108.21	113.00
4	A	504	UDP	O4'-C1'-N1	-2.04	103.70	108.36
2	B	504	POG	C19-C10-C9	-2.03	106.81	112.63
3	A	502	M0O	C26-C30-C32	2.01	116.08	113.19
3	A	502	M0O	O04-C52-C54	2.00	114.58	110.35

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	POG	C15-C5-O2-C3
2	A	503	POG	O5-C10-C9-O4
2	A	503	POG	O5-C11-C12-O6
2	A	503	POG	O5-C11-C12-C18
2	A	503	POG	C11-C12-O6-C13
2	A	503	POG	C17-C14-O7-C15
2	B	501	POG	O3-C7-C8-O4
2	B	501	POG	O3-C7-C8-C20
2	B	501	POG	O5-C10-C9-O4
2	B	501	POG	C19-C10-C9-O4
2	B	504	POG	O5-C10-C9-O4
2	B	504	POG	C19-C10-C9-O4
2	B	504	POG	O5-C11-C12-O6
2	B	504	POG	O5-C11-C12-C18
3	A	502	M0O	C26-C29-C38-C46
3	A	502	M0O	C50-C51-C53-O05
3	A	502	M0O	C53-C51-O03-C60
3	A	502	M0O	C54-C52-O02-C45
3	B	503	M0O	C53-C51-O03-C60
3	B	503	M0O	O18-C72-O14-C66
5	B	502	TRS	N-C-C2-O2
3	A	502	M0O	C26-C29-C38-C47

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Mol	Chain	Res	Type	Atoms
3	A	502	M0O	C34-C29-C38-C46
3	A	502	M0O	O08-C64-C66-O14
3	B	503	M0O	O08-C64-C66-O14
3	A	502	M0O	C34-C29-C38-C47
3	B	503	M0O	C47-C38-C46-C50
3	A	502	M0O	O04-C58-C62-O11
3	B	503	M0O	O04-C58-C62-O11
3	B	503	M0O	C26-C29-C38-C47
3	A	502	M0O	O15-C70-C74-O21
3	B	503	M0O	C77-C76-C78-O24
3	B	503	M0O	O15-C70-C74-O21
3	A	502	M0O	C59-C58-C62-O11
3	B	503	M0O	C59-C58-C62-O11
3	A	502	M0O	C65-C64-C66-O14
3	B	503	M0O	C34-C29-C38-C47
3	A	502	M0O	C38-C46-C50-C51
3	B	503	M0O	O18-C76-C78-O24
3	A	502	M0O	O03-C51-C53-C57
3	A	502	M0O	C71-C70-C74-O21
4	B	505	UDP	O4'-C4'-C5'-O5'
4	B	505	UDP	C3'-C4'-C5'-O5'
2	B	501	POG	C8-C7-O3-C6
2	B	504	POG	C12-C11-O5-C10
2	A	503	POG	OH-C2-C3-O2
2	A	503	POG	O7-C15-C5-C16
3	B	503	M0O	C71-C70-C74-O21
2	A	503	POG	O7-C15-C5-O2
4	A	504	UDP	PB-O3A-PA-O5'
4	B	505	UDP	PB-O3A-PA-O5'
3	A	502	M0O	C50-C51-C53-C57
3	B	503	M0O	C29-C38-C46-C50
2	A	503	POG	C19-C10-C9-O4
2	A	503	POG	C18-C12-O6-C13
3	B	503	M0O	O03-C51-C53-C57
4	A	504	UDP	O4'-C4'-C5'-O5'
3	B	503	M0O	C34-C29-C38-C46
3	B	503	M0O	C26-C29-C38-C46
2	A	503	POG	C19-C10-O5-C11
4	A	504	UDP	C3'-C4'-C5'-O5'
3	B	503	M0O	C65-C64-C66-O14

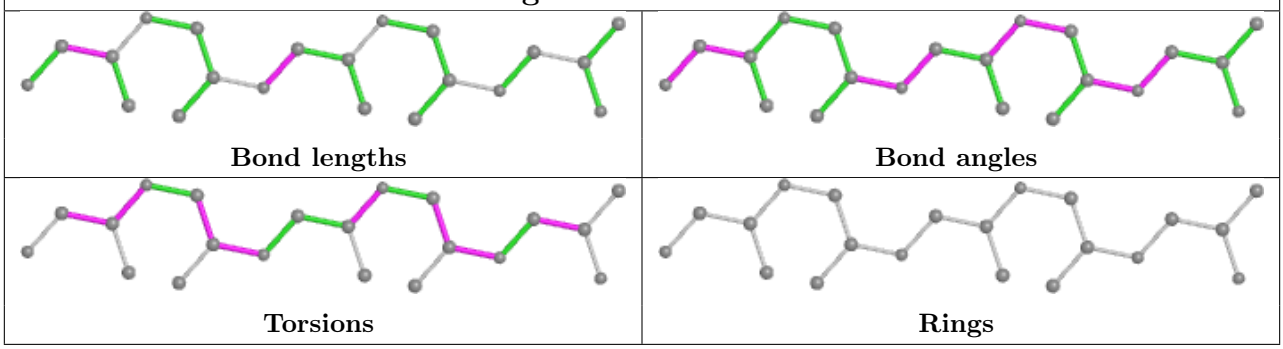
There are no ring outliers.

5 monomers are involved in 6 short contacts:

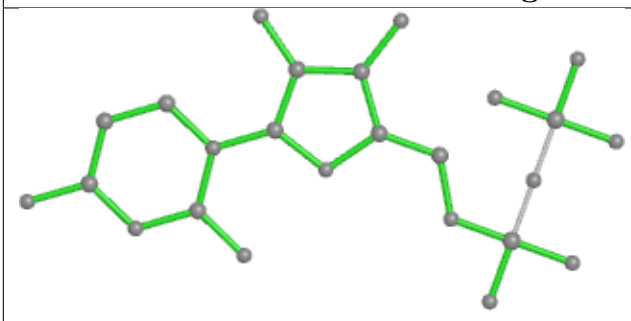
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	POG	2	0
2	A	501	POG	1	0
2	B	501	POG	1	0
5	B	502	TRS	1	0
2	B	504	POG	1	0

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 then 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.

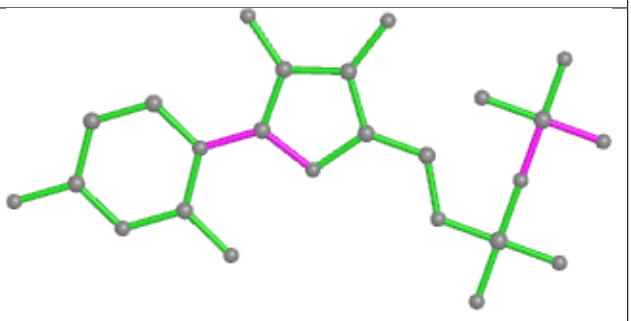
Ligand POG A 503



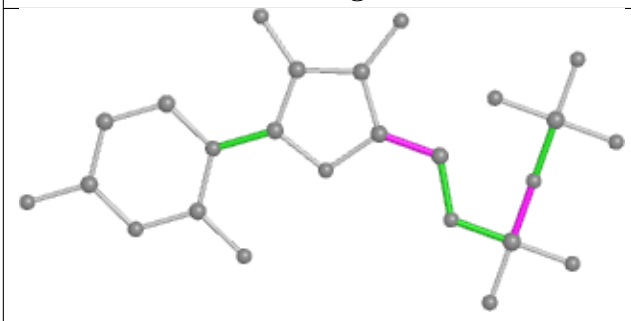
Ligand UDP A 504



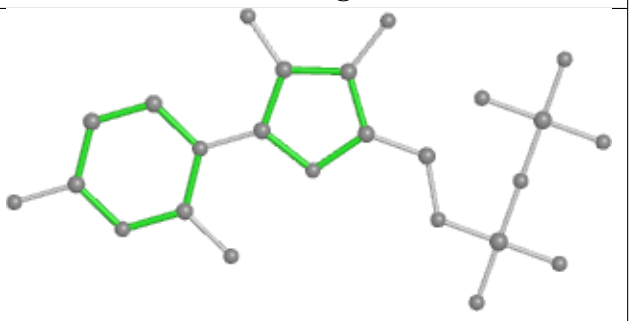
Bond lengths



Bond angles

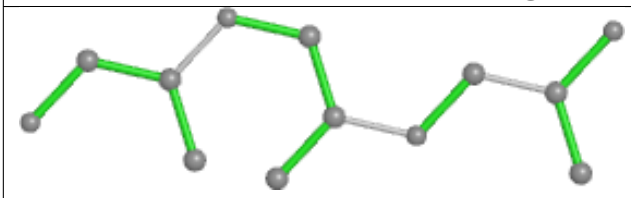


Torsions

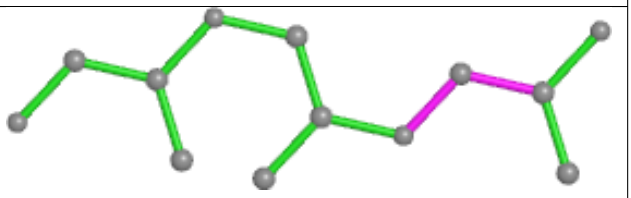


Rings

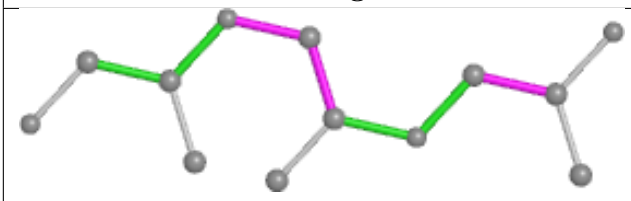
Ligand POG B 501



Bond lengths



Bond angles



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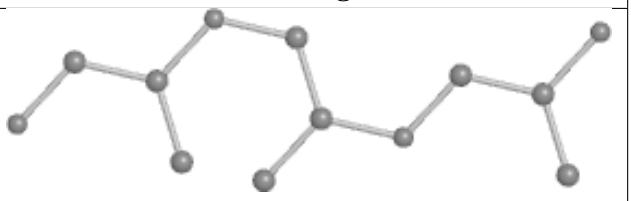
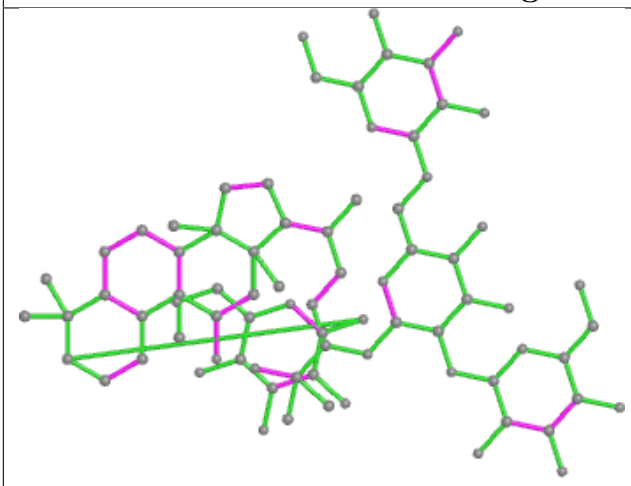
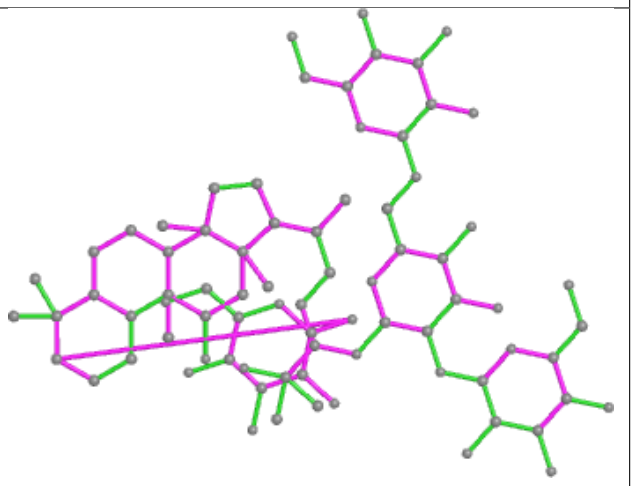


Rings

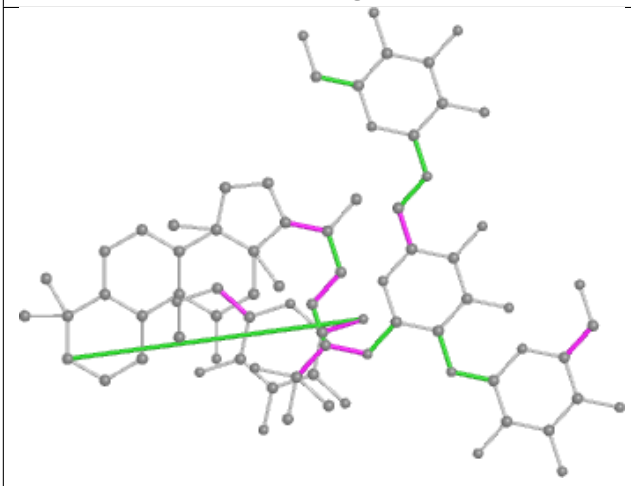
Ligand M0O A 502



Bond lengths



Bond angles



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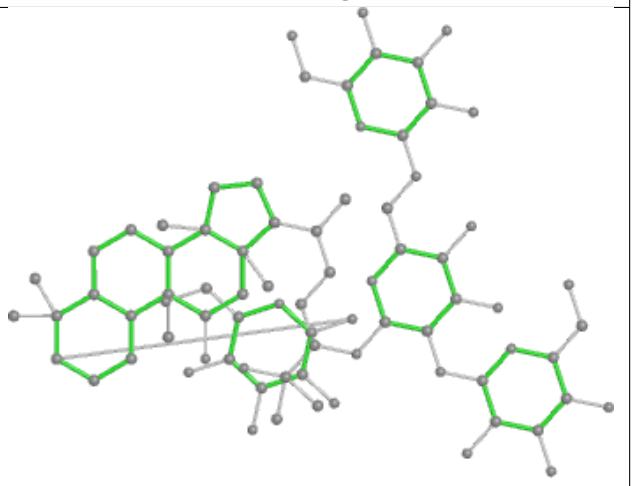
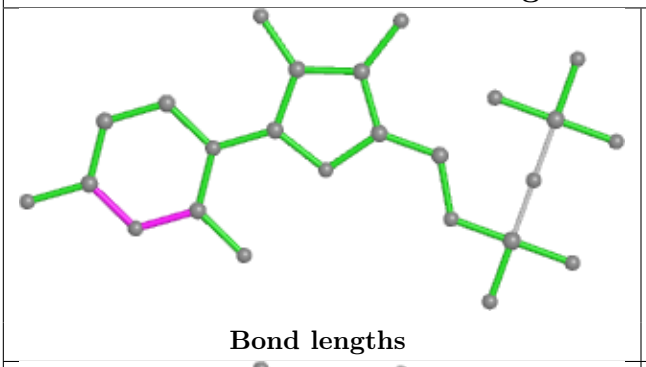


Rings

Ligand UDP B 505



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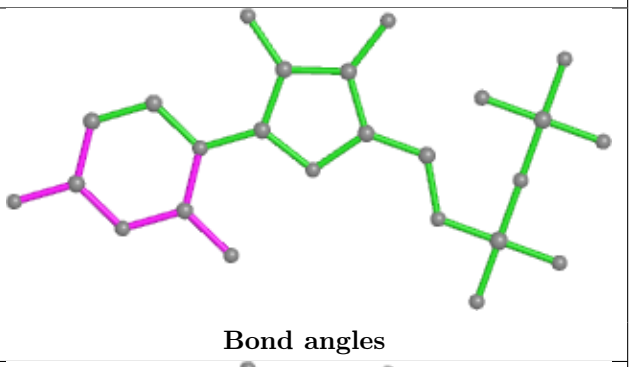
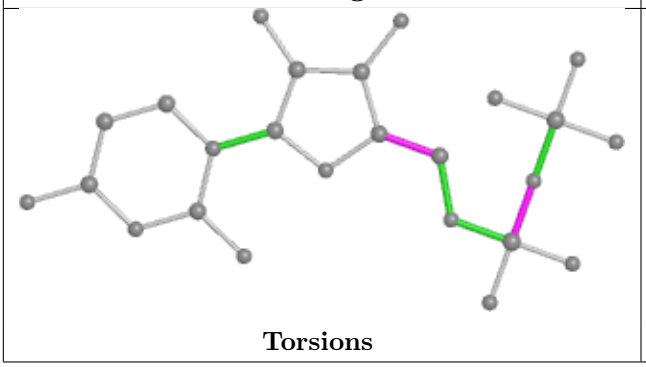
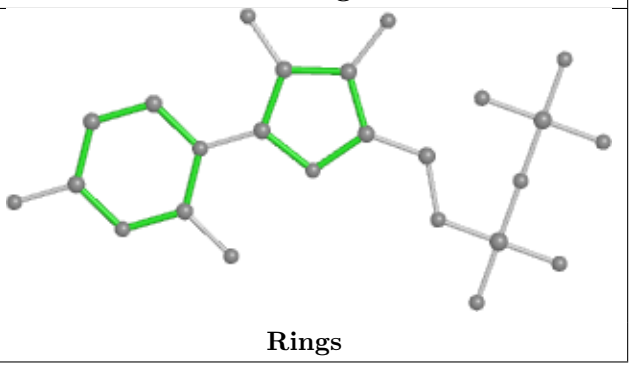


Bond angles

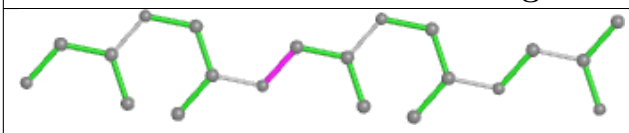


Torsions

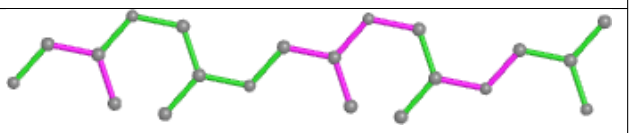


Rings

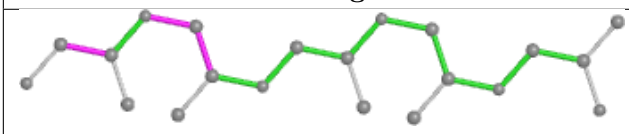
Ligand POG B 504



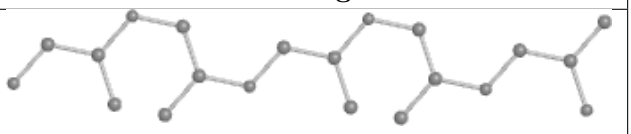
Bond lengths



Bond angles

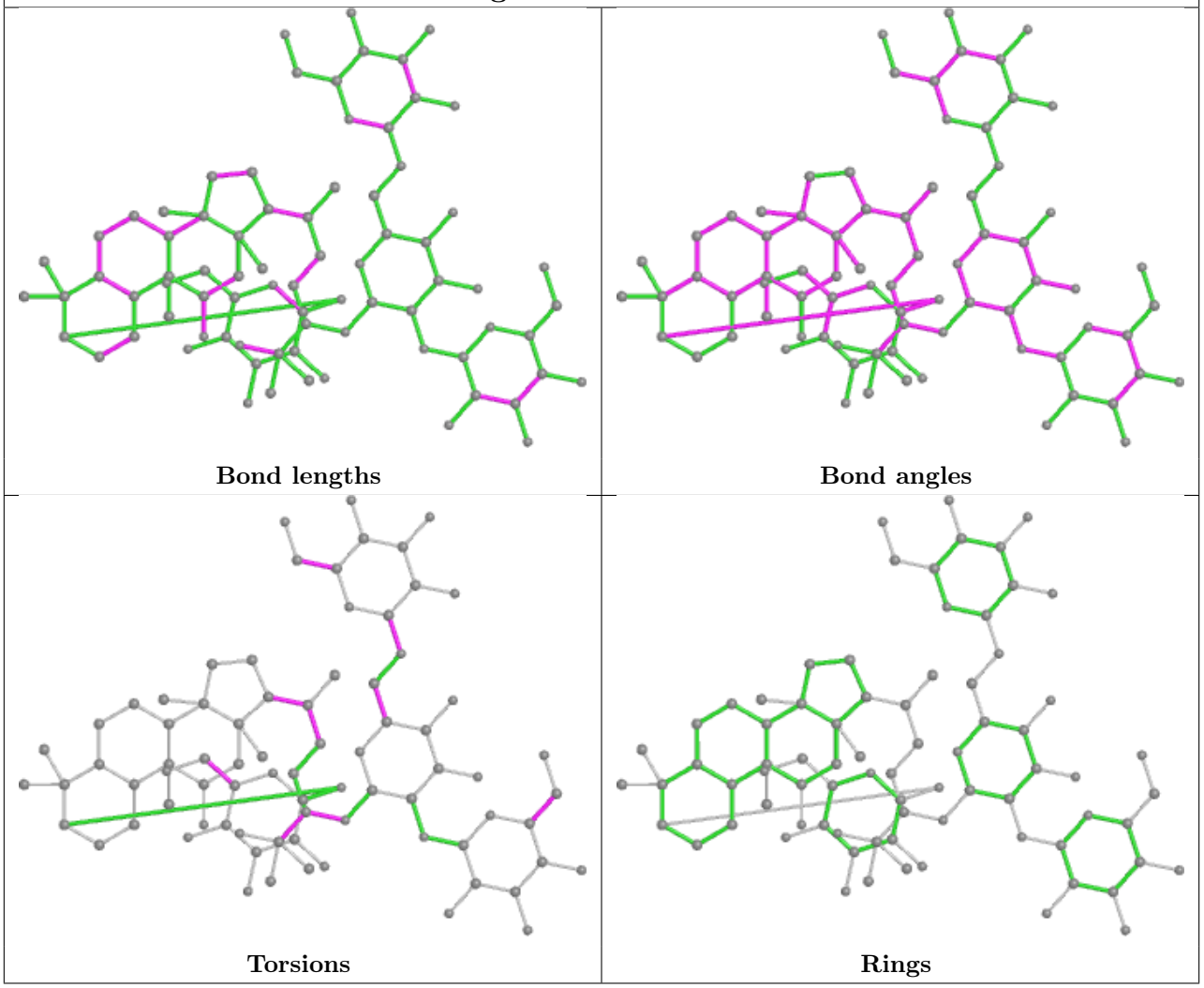


Torsions



Rings

Ligand M0O B 503



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^{th} 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	435/459 (94%)	-0.02	10 (2%)	60	67	16, 26, 50, 84	0
1	B	437/459 (95%)	0.04	20 (4%)	32	38	16, 27, 54, 87	1 (0%)
All	All	872/918 (94%)	0.01	30 (3%)	45	51	16, 27, 52, 87	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	ASN	6.0
1	B	307	THR	4.8
1	A	177	MET	4.7
1	A	312	ASP	4.6
1	A	307	THR	4.2
1	B	312	ASP	4.1
1	B	305	ASP	4.0
1	B	177	MET	3.9
1	B	242	ASN	3.7
1	B	248	GLU	3.7
1	B	309	GLY	3.4
1	B	457	HIS	3.4
1	B	311	GLU	3.2
1	A	305	ASP	3.1
1	A	306	ASN	3.1
1	B	310	ILE	3.0
1	A	457	HIS	3.0
1	A	185	SER	2.9
1	B	176	ALA	2.9
1	B	188	ARG	2.8
1	B	308	SER	2.8
1	A	186	THR	2.8
1	B	192	ARG	2.6
1	A	310	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	142	ASN	2.4
1	B	304	GLY	2.3
1	A	304	GLY	2.3
1	B	247	ASP	2.1
1	B	190	ARG	2.0
1	B	454	HIS	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)

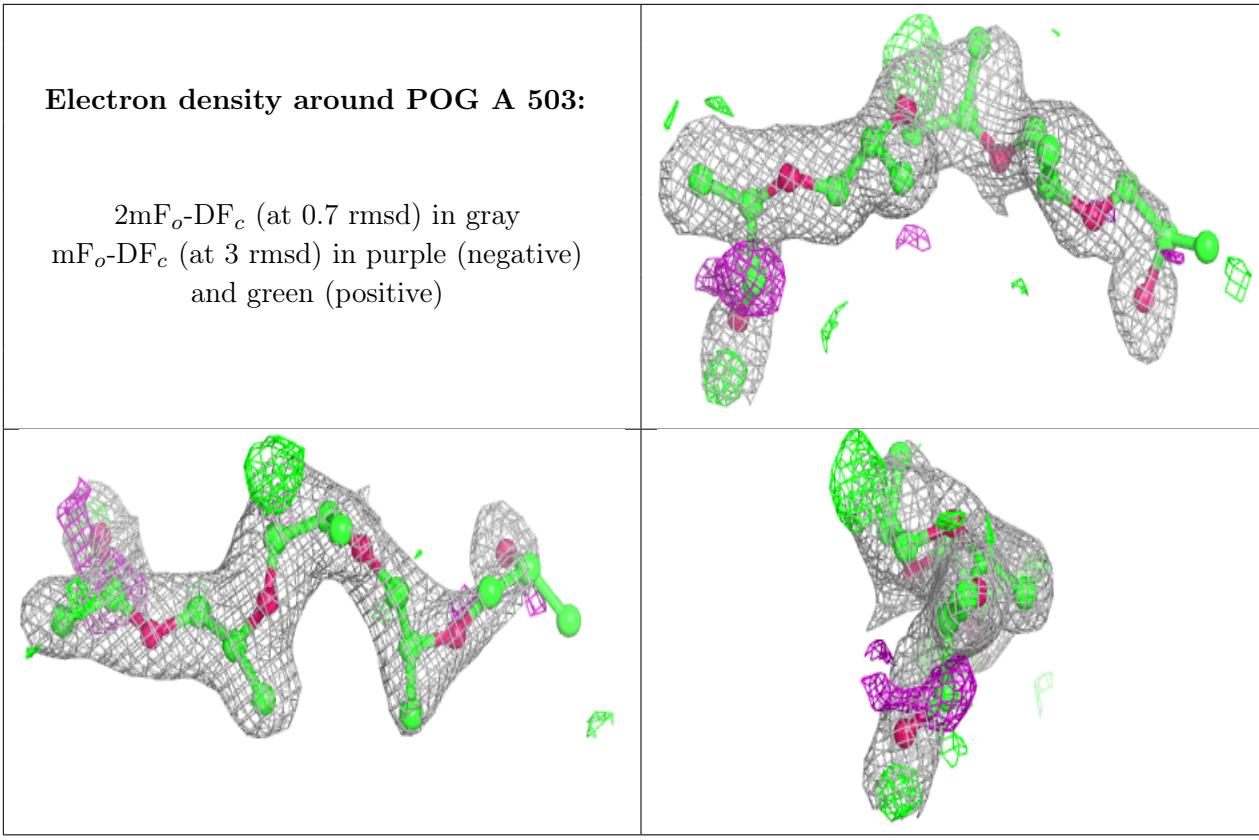
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	POG	A	501	13/29	0.74	0.22	45,49,55,56	0
5	TRS	B	502	8/8	0.74	0.23	25,32,36,36	0
2	POG	A	503	21/29	0.77	0.20	31,42,55,56	0
2	POG	B	504	21/29	0.84	0.15	34,46,54,59	0
3	M0O	A	502	78/78	0.88	0.13	18,29,48,57	0
3	M0O	B	503	78/78	0.89	0.12	19,30,47,51	0
2	POG	B	501	13/29	0.89	0.12	42,47,53,54	0
4	UDP	B	505	25/25	0.96	0.10	19,21,24,25	0
4	UDP	A	504	25/25	0.99	0.07	18,21,23,24	0

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

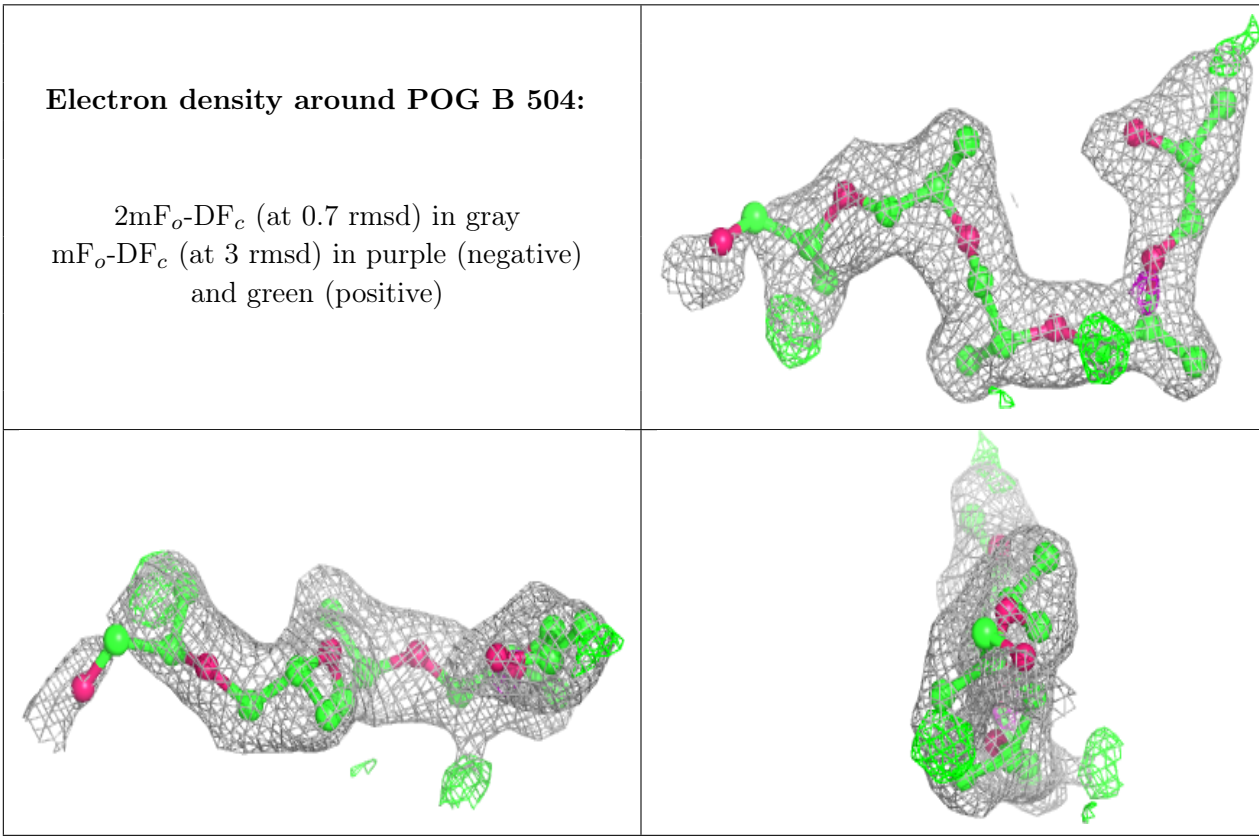
Electron density around POG A 503:

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



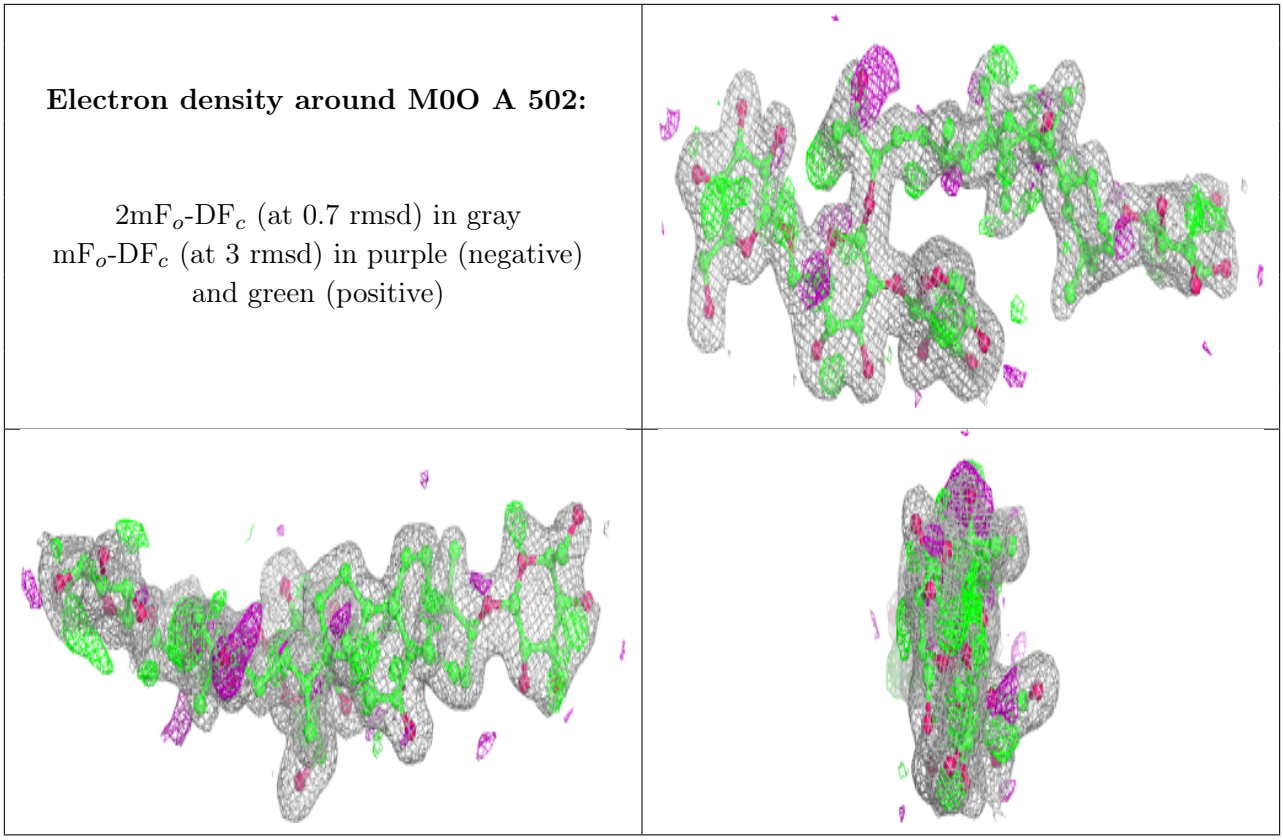
Electron density around POG B 504:

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



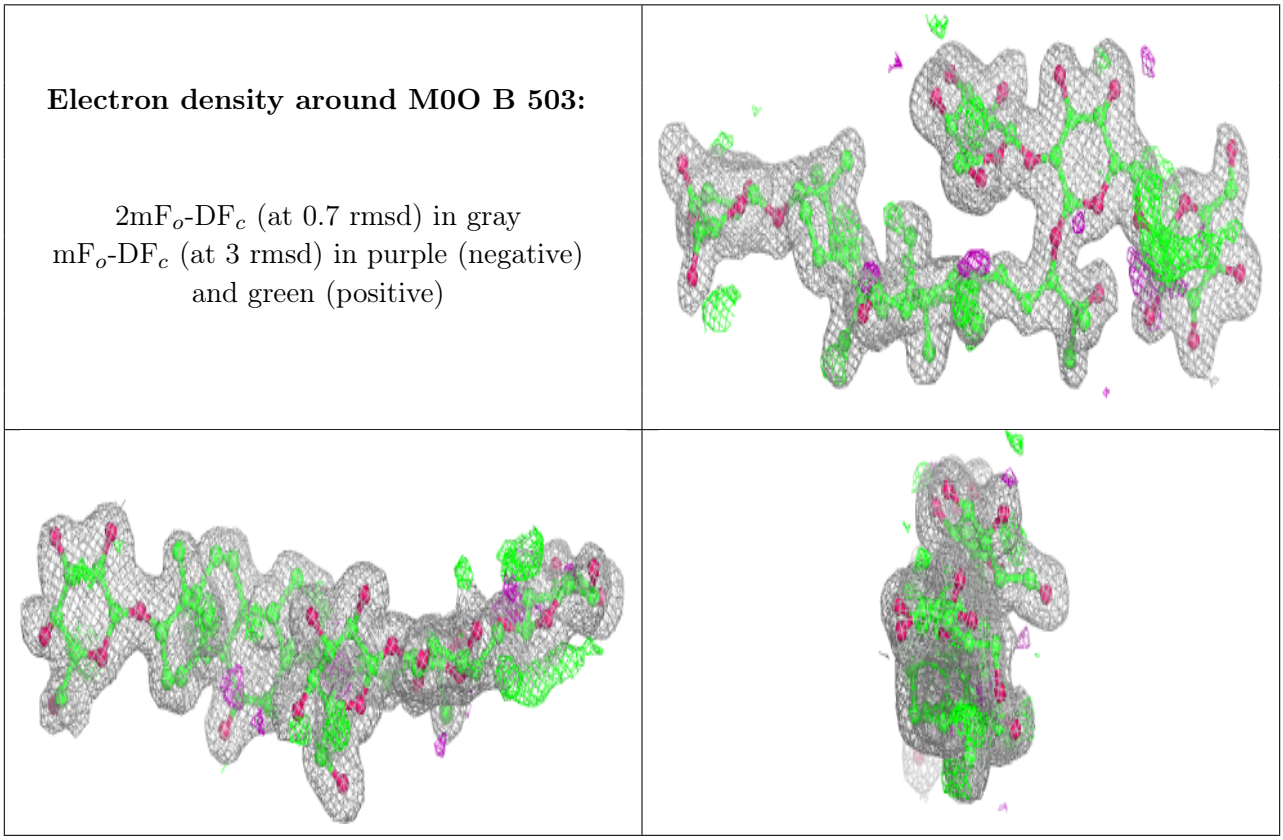
Electron density around M0O A 502:

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



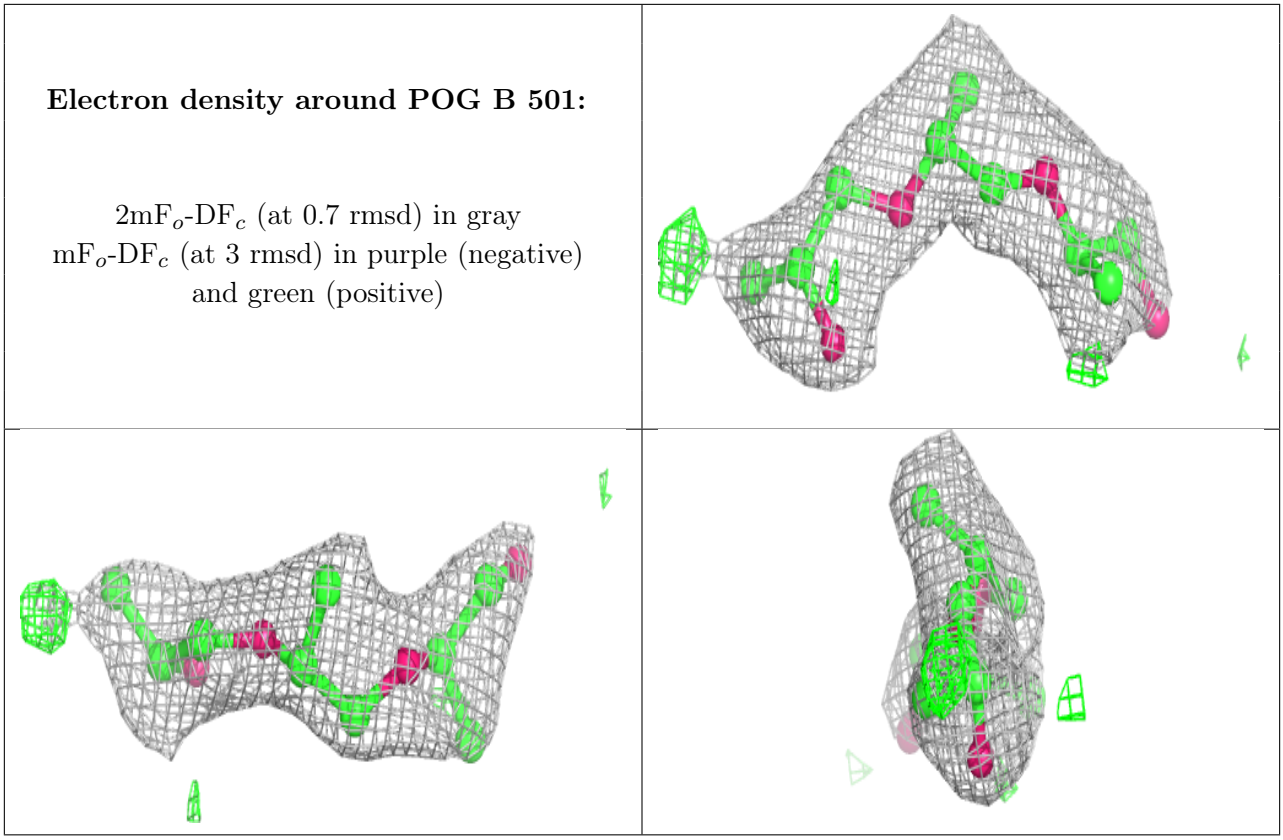
Electron density around M0O B 503:

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



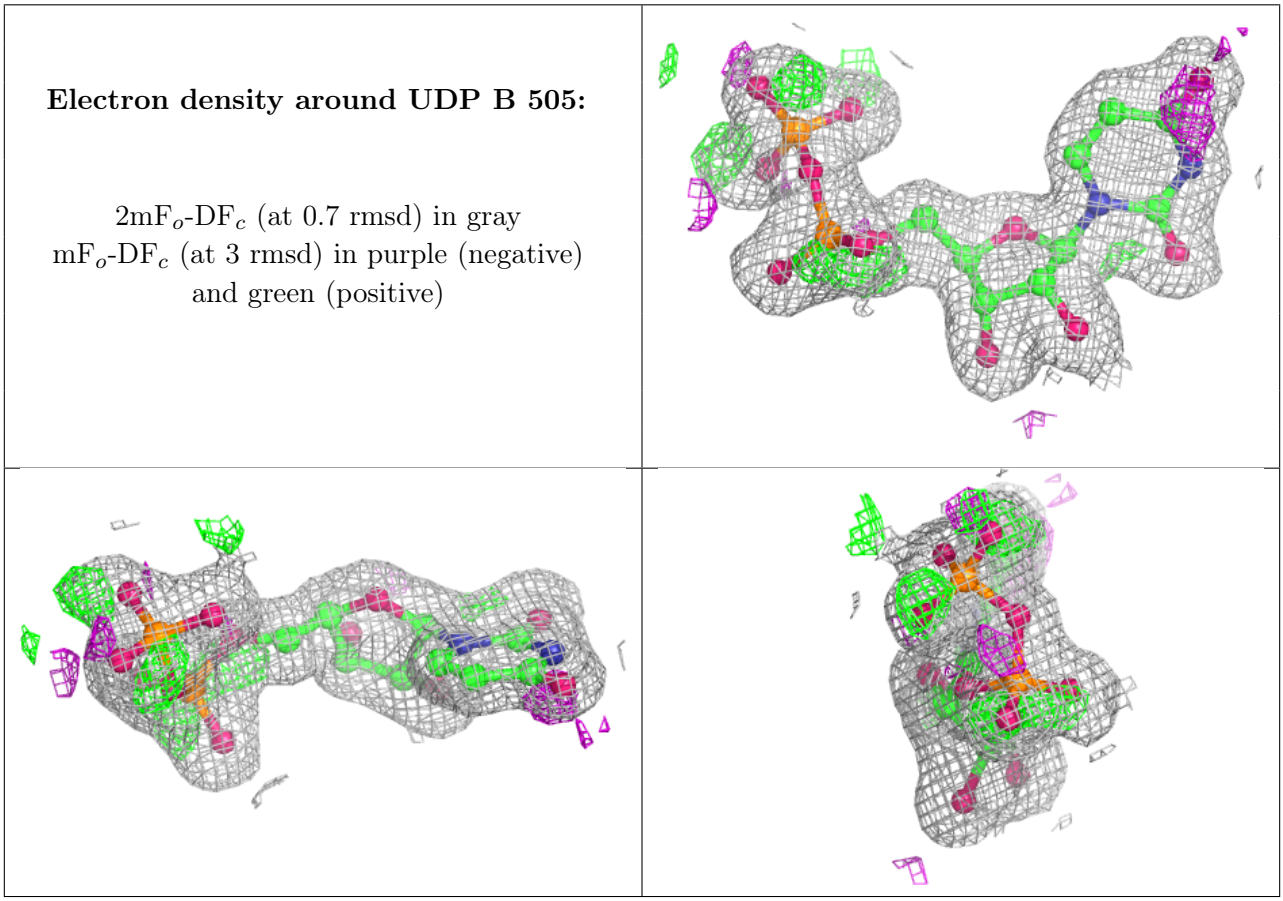
Electron density around POG B 501:

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



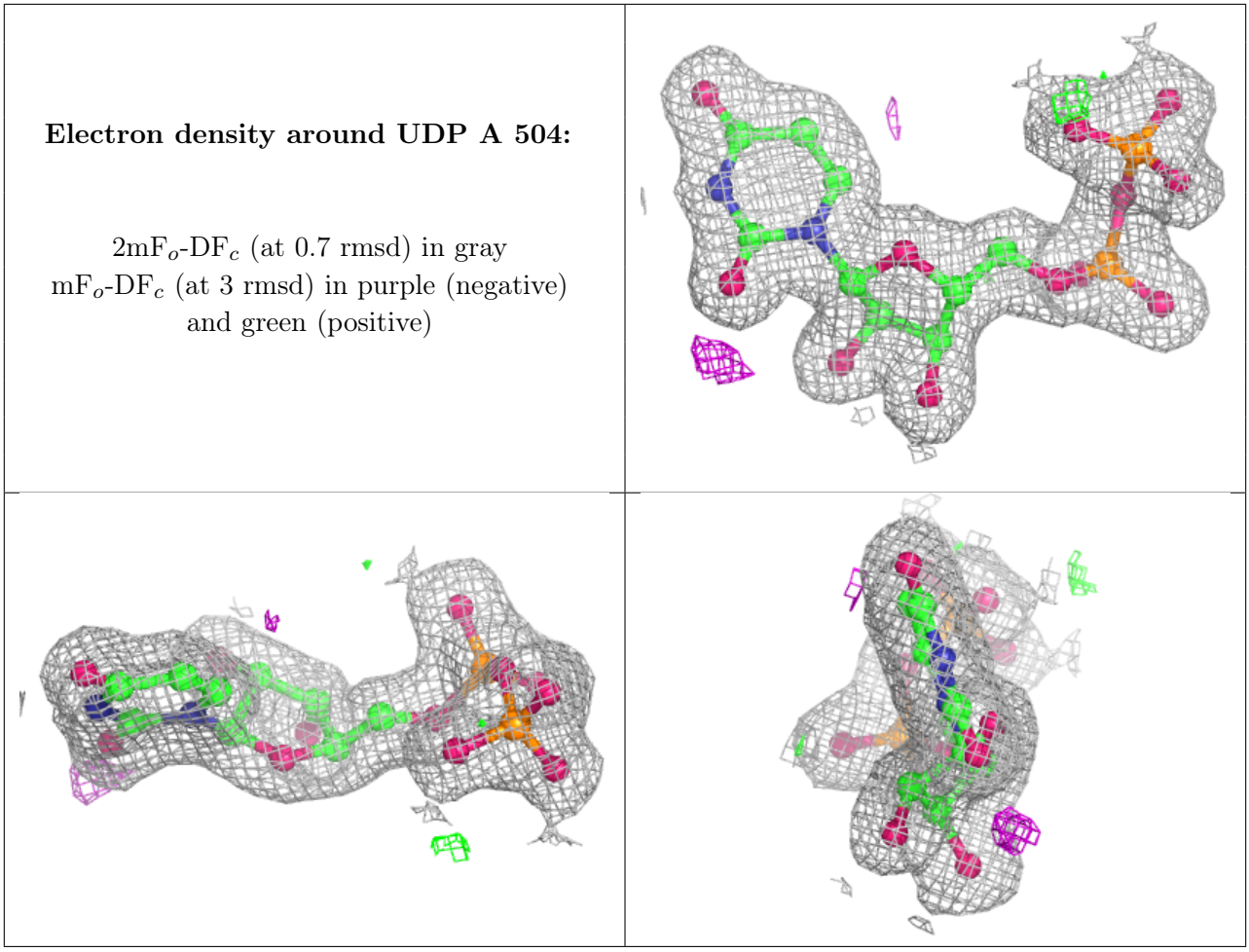
Electron density around UDP B 505:

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



Electron density around UDP A 504:

$2mF_o$-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.