



# Full wwPDB X-ray Structure Validation Report i

May 20, 2024 – 03:12 AM JST

PDB ID : 8HJG  
Title : Crystal structure of glycosyltransferase SgUGT94-289-3 in complex with M5, state 1  
Authors : Li, M.; Zhang, S.; Cui, S.  
Deposited on : 2022-11-23  
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

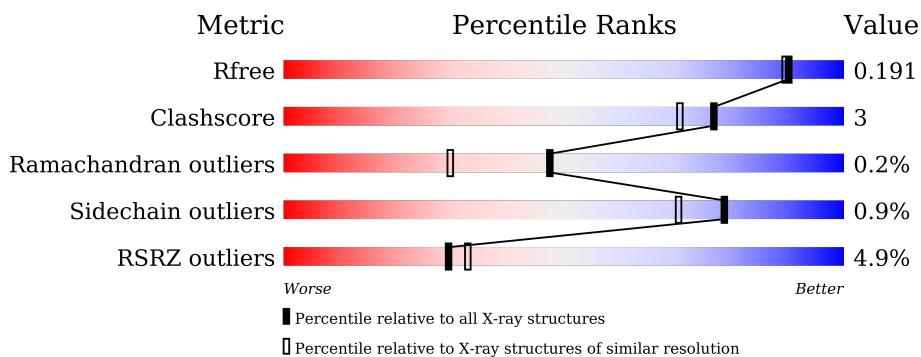
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

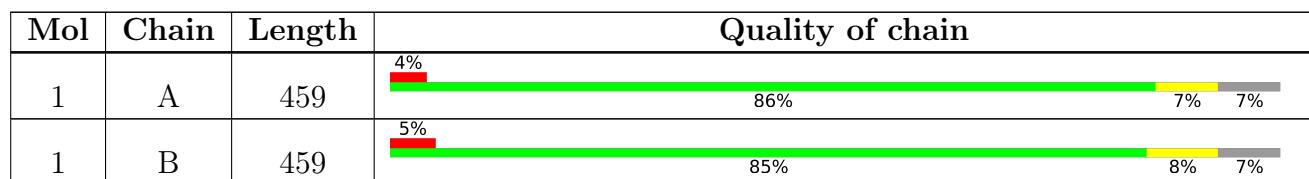
The reported resolution of this entry is 1.70 Å.

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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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.



## 2 Entry composition i

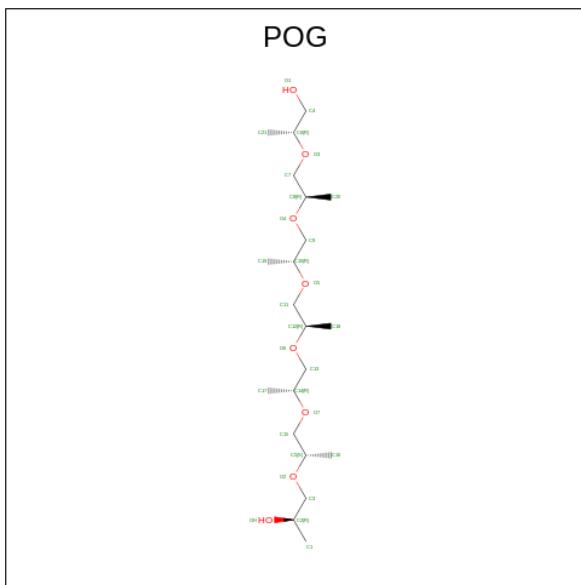
There are 6 unique types of molecules in this entry. The entry contains 7943 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

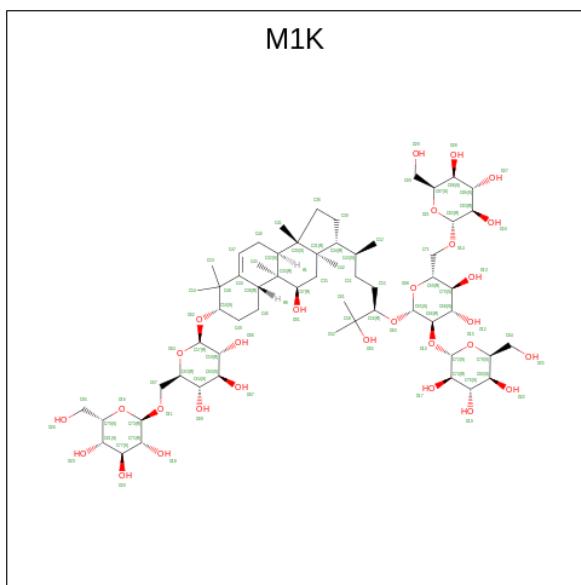
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	15	2	0
			3404	2200	574	614	16			
1	B	426	Total	C	N	O	S	0	1	0
			3372	2185	568	603	16			

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



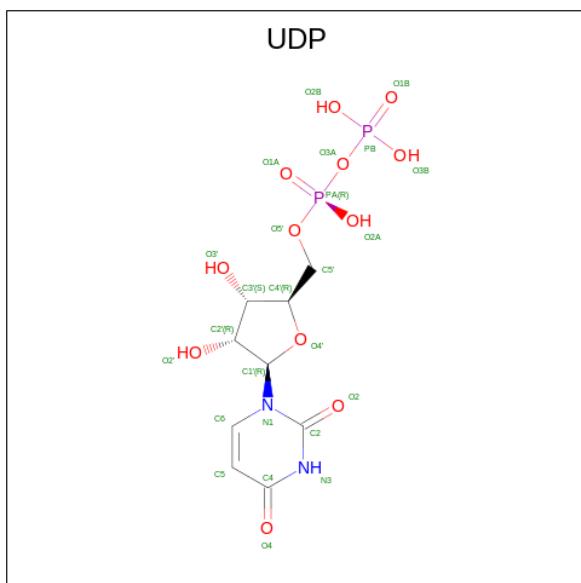
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 29	C 21	O 8	0	0
2	B	1	Total 13	C 9	O 4	0	0

yl)oxan-2-yl]oxymethyl]-4,5-bis(oxidanyl)oxan-2-yl]oxy-6-methyl-6-oxidanyl-heptan-2-yl]-4,4,9,13,14-pentamethyl-11-oxidanyl-2,3,7,8,10,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-3-yl]oxy]-3,4,5-tris(oxidanyl)oxan-2-yl]methoxy]oxane-3,4,5-triol (three-letter code: M1K) (formula: C<sub>60</sub>H<sub>102</sub>O<sub>29</sub>)



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 89 60 29	0	0
3	B	1	Total C O 89 60 29	0	0

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>2</sub>O<sub>12</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

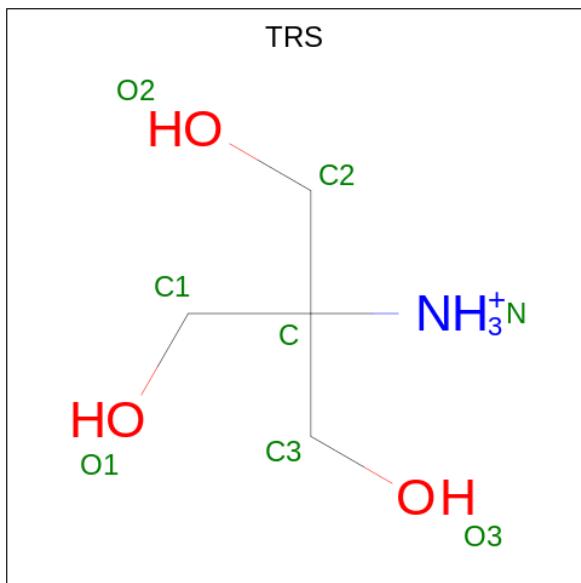


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

Mol	Chain	Residues	Total	C	N	O	P	ZeroOcc	AltConf
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<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



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

Mol	Chain	Residues	Total	C	N	O		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	434	Total	O				0	0
			434	434					

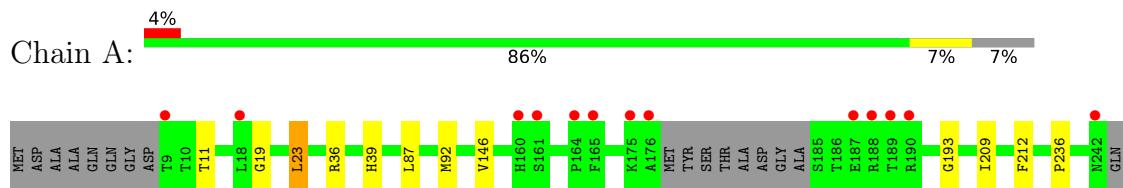
  

Mol	Chain	Residues	Total	O				ZeroOcc	AltConf
6	B	447	Total	O				0	0
			447	447					

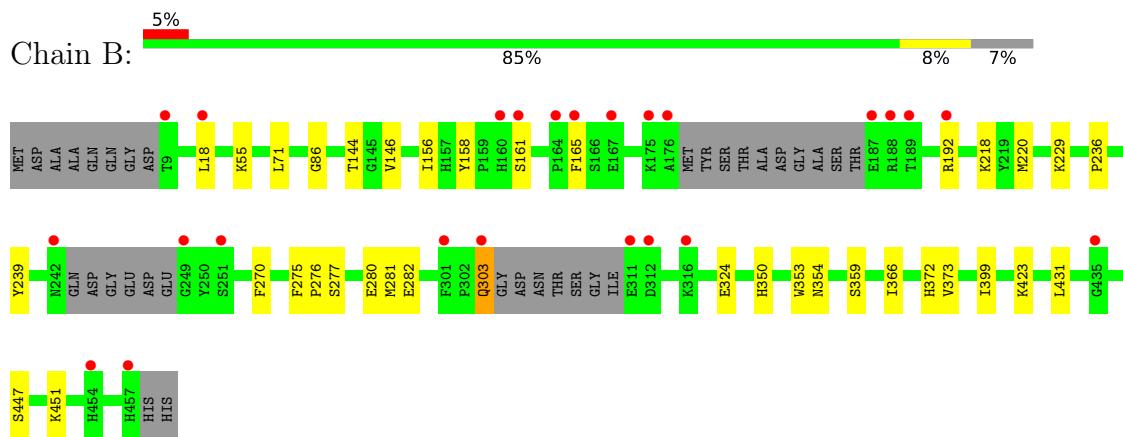
### 3 Residue-property plots

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: glycosyltransferase



- Molecule 1: glycosyltransferase



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.18Å 76.48Å 82.18Å 90.00° 92.64° 90.00°	Depositor
Resolution (Å)	19.65 – 1.70 19.82 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.65-1.70) 95.0 (19.82-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.87 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
$R$ , $R_{free}$	0.180 , 0.191 0.180 , 0.191	Depositor DCC
$R_{free}$ test set	4863 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.4	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50$ , $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l 0.012 for -k,-h,-l 0.060 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, M1K, POG, UDP

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	0.42	0/3504	0.59	0/4749
1	B	0.53	0/3473	0.65	0/4711
All	All	0.48	0/6977	0.62	0/9460

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	3404	0	3355	18	0
1	B	3372	0	3323	22	0
2	A	29	0	44	2	0
2	B	13	0	18	0	0
3	A	89	0	0	0	0
3	B	89	0	0	0	0
4	A	25	0	11	0	0
4	B	25	0	11	1	0
5	A	8	0	12	0	0
5	B	8	0	12	4	0
6	A	434	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	447	0	0	4	0
All	All	7943	0	6786	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:B:236:PRO:HG3	1:B:431:LEU:HD22	1.68	0.75
1:B:447:SER:OG	1:B:451:LYS:HE3	1.94	0.66
1:B:55:LYS:HE3	1:B:239:TYR:CD2	2.34	0.62
1:A:193:GLY:HA3	2:A:501:POG:H72	1.82	0.61
1:B:144:THR:HG22	5:B:504:TRS:H22	1.84	0.59
1:B:366:ILE:HD12	6:B:606:HOH:O	2.03	0.58
1:B:423:LYS:NZ	6:B:605:HOH:O	2.38	0.55
1:A:289:GLU:HG3	6:A:790:HOH:O	2.07	0.54
1:A:278:LYS:HE3	1:A:313:ALA:HA	1.89	0.54
1:A:278:LYS:O	1:A:282:GLU:HG2	2.07	0.54
1:B:277:SER:O	1:B:281:MET:HG2	2.11	0.51
1:A:36[B]:ARG:HH12	1:A:439:PHE:HB2	1.77	0.49
1:B:303:GLN:HG2	6:B:876:HOH:O	2.14	0.48
1:A:87:LEU:HD23	1:A:92:MET:HE2	1.96	0.48
1:B:353:TRP:HB3	5:B:504:TRS:H21	1.97	0.46
1:B:324:GLU:OE2	6:B:601:HOH:O	2.21	0.46
1:A:212:PHE:CE1	1:A:357:MET:HE1	2.51	0.46
1:A:359:SER:HB3	1:A:366:ILE:HD11	1.98	0.46
1:A:410:GLU:HB3	1:A:417:ARG:HG2	1.98	0.46
4:B:503:UDP:O3B	5:B:504:TRS:N	2.38	0.45
1:B:276:PRO:HB2	1:B:281:MET:SD	2.57	0.45
1:A:236:PRO:HG3	1:A:431:LEU:HD22	1.98	0.45
1:B:18:LEU:CD1	1:B:71[B]:LEU:HD11	2.47	0.45
1:A:146:VAL:HG22	1:A:209:ILE:HD13	1.98	0.45
1:B:146:VAL:HG11	1:B:220:MET:HA	1.98	0.45
1:A:19:GLY:O	1:A:23:LEU:HD23	2.17	0.44
1:B:280:GLU:HG2	1:B:399:ILE:HD12	1.99	0.44
2:A:501:POG:H131	2:A:501:POG:H152	1.62	0.44
1:B:158:TYR:HB3	1:B:161:SER:HB2	2.00	0.44
1:B:354:ASN:ND2	5:B:504:TRS:H31	2.34	0.43
1:B:165:PHE:HB3	1:B:218:LYS:HE2	2.00	0.43
1:B:270:PHE:HA	1:B:350:HIS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD21	1:A:328:VAL:HG23	2.00	0.42
1:B:229:LYS:HE2	1:B:229:LYS:HB2	1.83	0.42
1:A:36[B]:ARG:HG2	1:A:443:VAL:HG21	2.02	0.41
1:B:55:LYS:HE3	1:B:239:TYR:CE2	2.55	0.41
1:B:156:ILE:N	1:B:156:ILE:HD13	2.34	0.41
1:A:256:TRP:CD2	1:A:327:MET:HE3	2.55	0.41
1:B:86:GLY:HA2	1:B:275:PHE:HZ	1.86	0.41
1:A:11:THR:HG22	1:A:39:HIS:HB3	2.02	0.41
1:A:319:LEU:HD23	1:A:319:LEU:HA	1.91	0.40
1:A:236:PRO:HD2	1:A:438:LYS:HE2	2.02	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	422/459 (92%)	417 (99%)	4 (1%)	1 (0%)	47 30
1	B	419/459 (91%)	415 (99%)	3 (1%)	1 (0%)	47 30
All	All	841/918 (92%)	832 (99%)	7 (1%)	2 (0%)	47 30

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	373/398 (94%)	371 (100%)	2 (0%)	88   83
1	B	368/398 (92%)	363 (99%)	5 (1%)	67   53
All	All	741/796 (93%)	734 (99%)	7 (1%)	78   70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	372	HIS
1	B	192	ARG
1	B	282	GLU
1	B	303	GLN
1	B	359	SER
1	B	372	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	B	48	ASN
1	B	157	HIS
1	B	303	GLN

### 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)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	UDP	A	503	-	24,26,26	1.29	4 (16%)	37,40,40	1.58	6 (16%)
2	POG	B	502	-	9,12,28	0.46	0	10,14,34	0.79	0
3	M1K	A	502	-	97,97,97	2.69	34 (35%)	147,153,153	1.85	30 (20%)
5	TRS	B	504	-	7,7,7	0.35	0	9,9,9	0.70	0
5	TRS	A	504	-	7,7,7	0.13	0	9,9,9	0.21	0
4	UDP	B	503	-	24,26,26	0.61	0	37,40,40	0.56	0
2	POG	A	501	-	21,28,28	0.50	0	26,34,34	0.68	0
3	M1K	B	501	-	97,97,97	2.68	35 (36%)	147,153,153	1.86	32 (21%)

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
4	UDP	A	503	-	-	4/16/32/32	0/2/2/2
2	POG	B	502	-	-	1/12/12/32	-
3	M1K	A	502	-	-	13/43/219/219	0/9/9/9
5	TRS	B	504	-	-	6/9/9/9	-
5	TRS	A	504	-	-	2/9/9/9	-
4	UDP	B	503	-	-	3/16/32/32	0/2/2/2
2	POG	A	501	-	-	11/32/32/32	-
3	M1K	B	501	-	-	15/43/219/219	0/9/9/9

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	M1K	O02-C50	9.61	1.58	1.45
3	B	501	M1K	O02-C50	9.53	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	M1K	C48-C44	-7.83	1.42	1.54
3	B	501	M1K	C48-C44	-7.63	1.43	1.54
3	A	502	M1K	C48-C50	-7.50	1.41	1.54
3	B	501	M1K	C48-C50	-7.41	1.41	1.54
3	B	501	M1K	C47-C44	6.88	1.46	1.33
3	A	502	M1K	C47-C44	6.83	1.46	1.33
3	A	502	M1K	C60-C59	6.74	1.69	1.52
3	B	501	M1K	C60-C59	6.63	1.69	1.52
3	B	501	M1K	C31-C30	-6.36	1.45	1.56
3	A	502	M1K	C31-C30	-6.25	1.45	1.56
3	B	501	M1K	O16-C79	5.72	1.58	1.44
3	B	501	M1K	O14-C71	5.67	1.54	1.43
3	A	502	M1K	O14-C71	5.62	1.54	1.43
3	A	502	M1K	O16-C79	5.49	1.57	1.44
3	B	501	M1K	C58-C56	5.31	1.63	1.53
3	A	502	M1K	C58-C56	5.31	1.63	1.53
3	B	501	M1K	C81-C79	-4.54	1.43	1.53
3	A	502	M1K	C81-C79	-4.53	1.43	1.53
3	A	502	M1K	O02-C57	4.29	1.53	1.41
3	B	501	M1K	O02-C57	4.27	1.53	1.41
3	B	501	M1K	O11-C67	3.96	1.51	1.43
3	A	502	M1K	O11-C67	3.79	1.50	1.43
3	B	501	M1K	O04-C63	3.50	1.52	1.44
3	A	502	M1K	O04-C63	3.49	1.52	1.44
3	B	501	M1K	C41-C30	3.48	1.61	1.54
3	A	502	M1K	C41-C30	3.29	1.60	1.54
3	A	502	M1K	C54-C48	-3.08	1.47	1.54
3	B	501	M1K	C54-C48	-2.97	1.47	1.54
3	B	501	M1K	C55-C56	2.92	1.59	1.51
3	A	502	M1K	C55-C56	2.90	1.59	1.51
3	A	502	M1K	O06-C59	2.82	1.49	1.43
3	B	501	M1K	C49-C50	-2.79	1.46	1.51
3	A	502	M1K	C49-C50	-2.77	1.46	1.51
3	B	501	M1K	O06-C59	2.75	1.49	1.43
3	B	501	M1K	O25-C84	2.67	1.53	1.42
3	A	502	M1K	O25-C84	2.64	1.53	1.42
3	A	502	M1K	C39-C34	2.64	1.59	1.54
3	A	502	M1K	C33-C38	-2.63	1.51	1.56
3	A	502	M1K	C85-C79	2.62	1.60	1.51
3	A	502	M1K	C40-C47	-2.60	1.44	1.50
3	B	501	M1K	C85-C79	2.58	1.60	1.51
3	B	501	M1K	C40-C47	-2.55	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	UDP	C4-N3	-2.55	1.34	1.38
3	A	502	M1K	O15-C72	2.54	1.48	1.41
3	B	501	M1K	O15-C72	2.53	1.48	1.41
3	B	501	M1K	C33-C38	-2.52	1.51	1.56
3	B	501	M1K	C39-C34	2.50	1.59	1.54
4	A	503	UDP	C2-N3	-2.47	1.33	1.38
3	B	501	M1K	C30-C32	-2.34	1.52	1.56
3	B	501	M1K	C88-C87	-2.32	1.48	1.53
3	A	502	M1K	C30-C32	-2.32	1.52	1.56
3	B	501	M1K	C71-C69	2.28	1.58	1.51
3	A	502	M1K	C71-C69	2.28	1.58	1.51
3	A	502	M1K	O08-C69	-2.28	1.38	1.44
3	A	502	M1K	O14-C82	2.25	1.44	1.40
3	B	501	M1K	O08-C69	-2.25	1.38	1.44
3	A	502	M1K	C88-C87	-2.24	1.48	1.53
3	B	501	M1K	C64-C63	-2.22	1.48	1.53
3	B	501	M1K	O14-C82	2.20	1.44	1.40
3	A	502	M1K	C64-C63	-2.20	1.48	1.53
4	A	503	UDP	PB-O3B	-2.18	1.46	1.54
3	B	501	M1K	C57-C59	-2.12	1.46	1.52
3	A	502	M1K	C57-C59	-2.10	1.46	1.52
3	A	502	M1K	C40-C32	2.08	1.57	1.53
4	A	503	UDP	C5-C4	-2.08	1.39	1.43
3	A	502	M1K	C61-C58	2.06	1.55	1.52
3	B	501	M1K	C73-C75	-2.06	1.46	1.52
3	B	501	M1K	C88-C86	2.05	1.57	1.52
3	B	501	M1K	C61-C58	2.04	1.55	1.52
3	B	501	M1K	C40-C32	2.03	1.57	1.53
3	A	502	M1K	C88-C86	2.02	1.57	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	M1K	C48-C44-C38	5.64	121.12	115.91
3	B	501	M1K	C48-C44-C38	5.58	121.07	115.91
3	B	501	M1K	C33-C38-C44	5.32	121.88	113.47
3	B	501	M1K	C40-C32-C30	-5.31	109.69	114.69
3	A	502	M1K	C48-C44-C47	-5.24	118.90	122.08
3	A	502	M1K	C33-C38-C44	5.10	121.53	113.47
3	A	502	M1K	C40-C32-C30	-5.05	109.93	114.69
3	B	501	M1K	C32-C40-C47	4.74	121.87	113.02
3	A	502	M1K	C32-C40-C47	4.73	121.84	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	M1K	O15-C78-C80	4.69	118.21	109.69
3	A	502	M1K	O03-C56-C58	4.64	112.25	106.42
3	B	501	M1K	O15-C78-C80	4.62	118.09	109.69
3	A	502	M1K	C55-C56-C58	-4.54	108.02	115.49
3	A	502	M1K	C49-C50-C48	-4.44	109.94	113.28
3	B	501	M1K	O03-C56-C58	4.35	111.89	106.42
4	A	503	UDP	C4-N3-C2	-4.19	121.05	126.58
3	B	501	M1K	C49-C50-C48	-4.16	110.15	113.28
3	B	501	M1K	C48-C44-C47	-3.95	119.69	122.08
3	A	502	M1K	C31-C34-C43	3.94	124.40	119.30
3	A	502	M1K	C57-O02-C50	-3.90	108.84	115.08
3	B	501	M1K	C55-C56-C58	-3.89	109.10	115.49
3	B	501	M1K	C57-O02-C50	-3.86	108.91	115.08
4	A	503	UDP	N3-C2-N1	3.69	119.79	114.89
3	B	501	M1K	C31-C34-C43	3.68	124.06	119.30
3	B	501	M1K	O16-C79-C81	3.59	116.22	109.69
3	B	501	M1K	C49-C46-C38	-3.59	102.96	112.03
3	A	502	M1K	C40-C47-C44	-3.57	118.37	125.07
3	B	501	M1K	C40-C47-C44	-3.54	118.42	125.07
3	B	501	M1K	C45-C33-C32	-3.53	103.82	112.73
4	A	503	UDP	C5-C4-N3	3.52	120.11	114.84
3	B	501	M1K	C41-C30-C32	3.50	116.31	111.44
3	A	502	M1K	C45-C33-C32	-3.45	104.02	112.73
3	A	502	M1K	C49-C46-C38	-3.39	103.46	112.03
3	B	501	M1K	C72-O15-C78	3.24	120.04	113.69
3	A	502	M1K	C52-C43-C34	3.22	117.86	112.92
4	A	503	UDP	O3B-PB-O3A	3.21	115.39	104.64
3	A	502	M1K	C72-O15-C78	3.20	119.98	113.69
3	A	502	M1K	C41-C30-C32	3.16	115.84	111.44
4	A	503	UDP	O4-C4-C5	-3.09	119.73	125.16
3	A	502	M1K	C31-C30-C32	3.08	113.03	109.92
3	B	501	M1K	C52-C43-C34	3.07	117.62	112.92
3	B	501	M1K	C41-C30-C31	-3.03	107.39	112.39
3	B	501	M1K	C46-C38-C44	-2.98	102.83	111.28
3	A	502	M1K	C46-C38-C44	-2.92	103.01	111.28
3	A	502	M1K	C67-O11-C73	-2.90	108.07	113.74
3	B	501	M1K	C67-O11-C73	-2.76	108.36	113.74
3	B	501	M1K	C42-C31-C30	-2.73	107.88	112.39
3	B	501	M1K	O02-C50-C49	-2.69	106.83	109.71
3	B	501	M1K	C45-C33-C38	-2.58	104.02	110.13
3	A	502	M1K	C41-C30-C31	-2.58	108.12	112.39
3	B	501	M1K	C31-C30-C32	2.56	112.51	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	M1K	C45-C33-C38	-2.55	104.10	110.13
3	A	502	M1K	C42-C31-C30	-2.49	108.27	112.39
3	A	502	M1K	C46-C49-C50	2.44	115.15	110.81
4	A	503	UDP	O2-C2-N1	-2.42	119.57	122.79
3	A	502	M1K	O16-C79-C81	2.37	113.99	109.69
3	A	502	M1K	C72-O10-C66	-2.29	112.31	117.96
3	B	501	M1K	C72-O10-C66	-2.24	112.42	117.96
3	B	501	M1K	C77-C81-C79	2.23	114.22	110.24
3	B	501	M1K	C55-C51-C43	-2.23	109.51	115.34
3	B	501	M1K	C41-C30-C36	-2.19	103.83	111.86
3	B	501	M1K	C46-C49-C50	2.19	114.71	110.81
3	A	502	M1K	O21-C87-C88	2.18	113.65	109.69
3	A	502	M1K	C41-C30-C36	-2.17	103.90	111.86
3	A	502	M1K	O02-C50-C49	-2.09	107.47	109.71
3	B	501	M1K	O24-C83-C86	-2.09	105.53	110.35
3	A	502	M1K	O24-C83-C86	-2.08	105.54	110.35
3	B	501	M1K	C40-C32-C33	2.04	112.88	110.41

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	POG	C19-C10-O5-C11
2	A	501	POG	O5-C11-C12-O6
2	A	501	POG	O5-C11-C12-C18
2	A	501	POG	O6-C13-C14-C17
2	B	502	POG	C18-C12-O6-C13
3	A	502	M1K	C31-C34-C43-C51
3	A	502	M1K	C39-C34-C43-C51
3	A	502	M1K	C58-C56-O03-C65
3	B	501	M1K	C31-C34-C43-C51
3	B	501	M1K	C39-C34-C43-C51
3	B	501	M1K	C58-C56-O03-C65
3	A	502	M1K	C39-C34-C43-C52
3	B	501	M1K	C39-C34-C43-C52
3	A	502	M1K	C31-C34-C43-C52
3	B	501	M1K	C31-C34-C43-C52
3	A	502	M1K	O16-C79-C85-O26
3	A	502	M1K	O15-C78-C84-O25
3	B	501	M1K	O16-C79-C85-O26
3	B	501	M1K	O15-C78-C84-O25
3	A	502	M1K	C81-C79-C85-O26

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Mol	Chain	Res	Type	Atoms
3	B	501	M1K	C81-C79-C85-O26
3	B	501	M1K	C88-C87-C89-O29
3	A	502	M1K	C80-C78-C84-O25
3	B	501	M1K	O21-C87-C89-O29
3	B	501	M1K	C80-C78-C84-O25
3	A	502	M1K	C88-C87-C89-O29
3	A	502	M1K	C43-C51-C55-C56
3	B	501	M1K	C43-C51-C55-C56
3	A	502	M1K	O21-C87-C89-O29
2	A	501	POG	OH-C2-C3-O2
2	A	501	POG	C1-C2-C3-O2
4	A	503	UDP	PB-O3A-PA-O1A
4	A	503	UDP	C3'-C4'-C5'-O5'
4	A	503	UDP	O4'-C4'-C5'-O5'
2	A	501	POG	O6-C13-C14-O7
4	B	503	UDP	PB-O3A-PA-O5'
4	B	503	UDP	O4'-C4'-C5'-O5'
5	A	504	TRS	N-C-C1-O1
5	B	504	TRS	C2-C-C1-O1
5	B	504	TRS	N-C-C1-O1
5	B	504	TRS	N-C-C2-O2
3	A	502	M1K	O03-C56-C58-C61
3	B	501	M1K	O03-C56-C58-C61
5	A	504	TRS	C2-C-C1-O1
5	B	504	TRS	C3-C-C1-O1
5	B	504	TRS	C3-C-C2-O2
3	B	501	M1K	O04-C63-C67-O11
2	A	501	POG	O5-C10-C9-O4
4	A	503	UDP	PB-O3A-PA-O5'
4	B	503	UDP	C3'-C4'-C5'-O5'
2	A	501	POG	C16-C5-O2-C3
3	B	501	M1K	C64-C63-C67-O11
5	B	504	TRS	C1-C-C2-O2
2	A	501	POG	C4-C6-O3-C7
2	A	501	POG	C13-C14-O7-C15

There are no ring outliers.

3 monomers are involved in 6 short contacts:

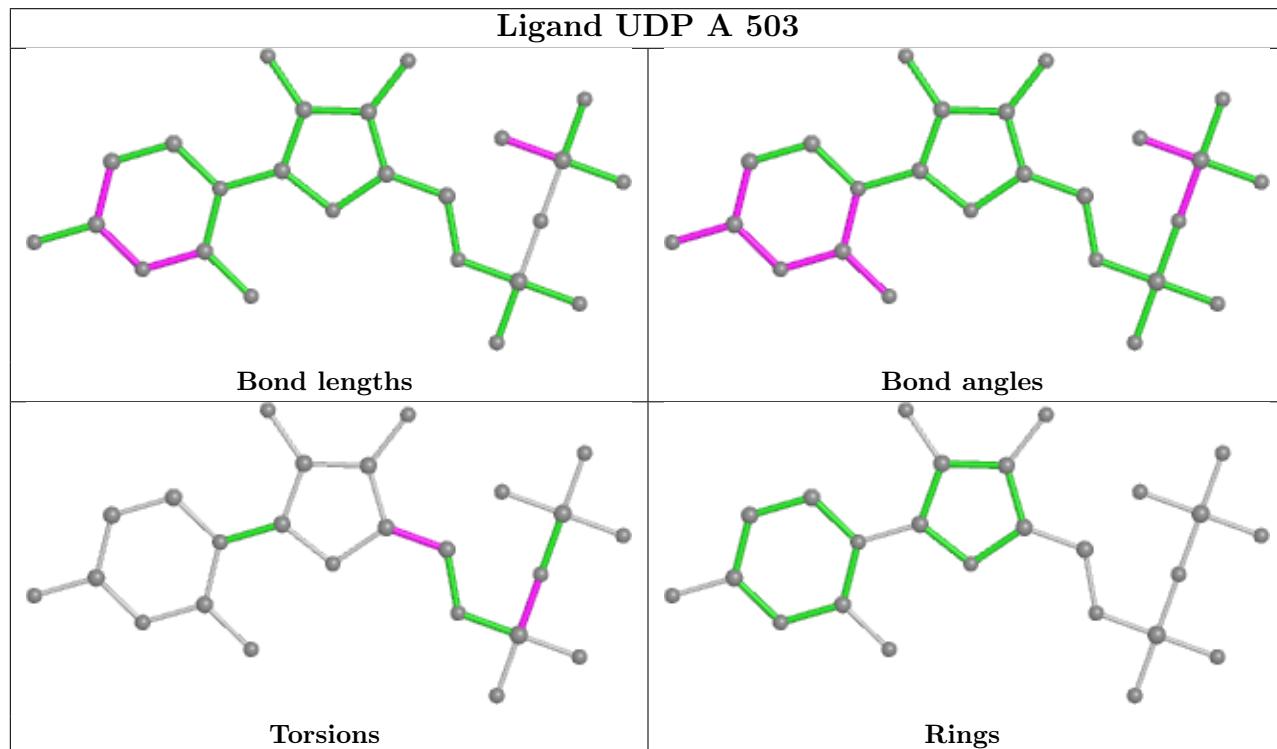
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	TRS	4	0
4	B	503	UDP	1	0

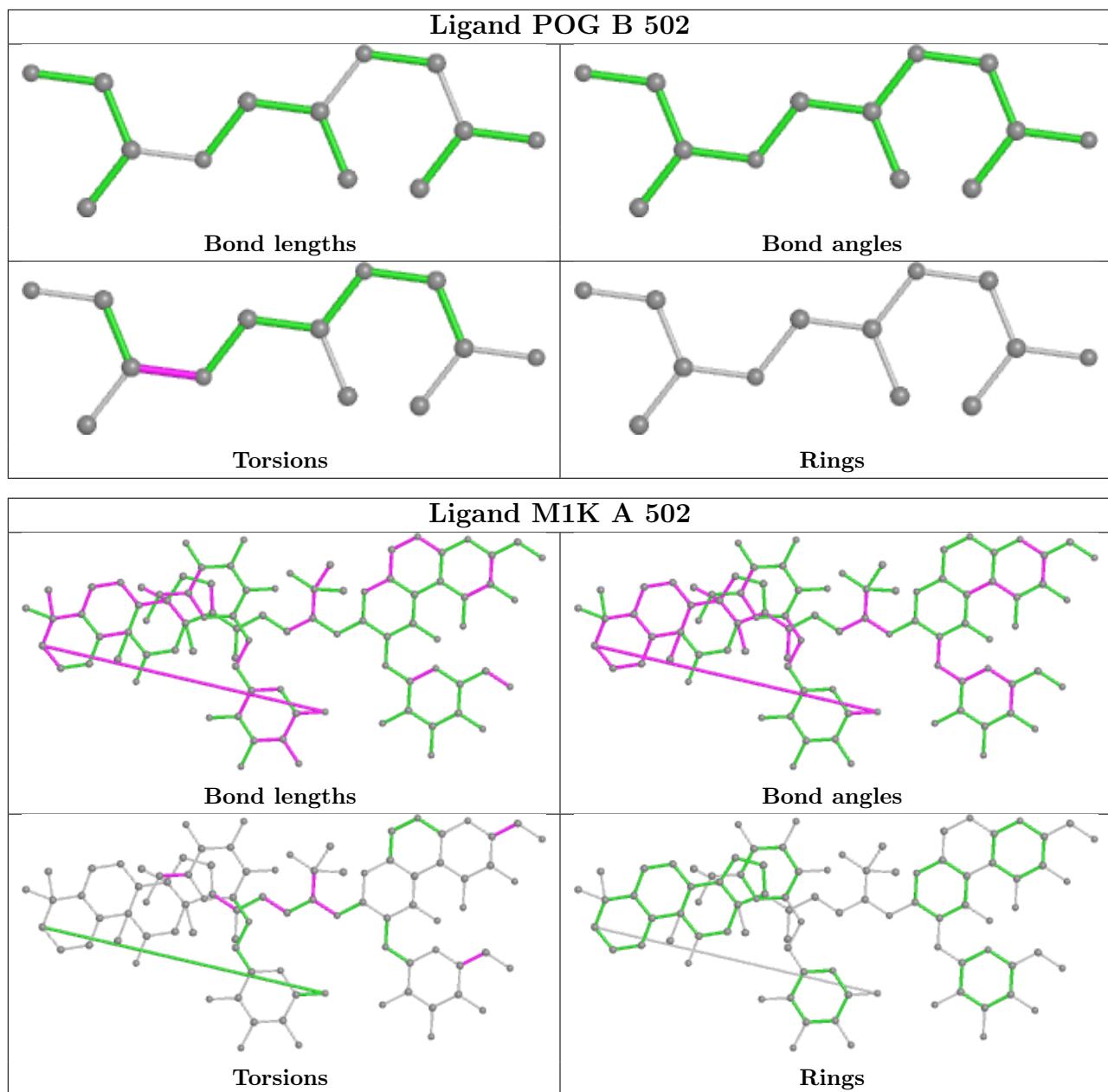
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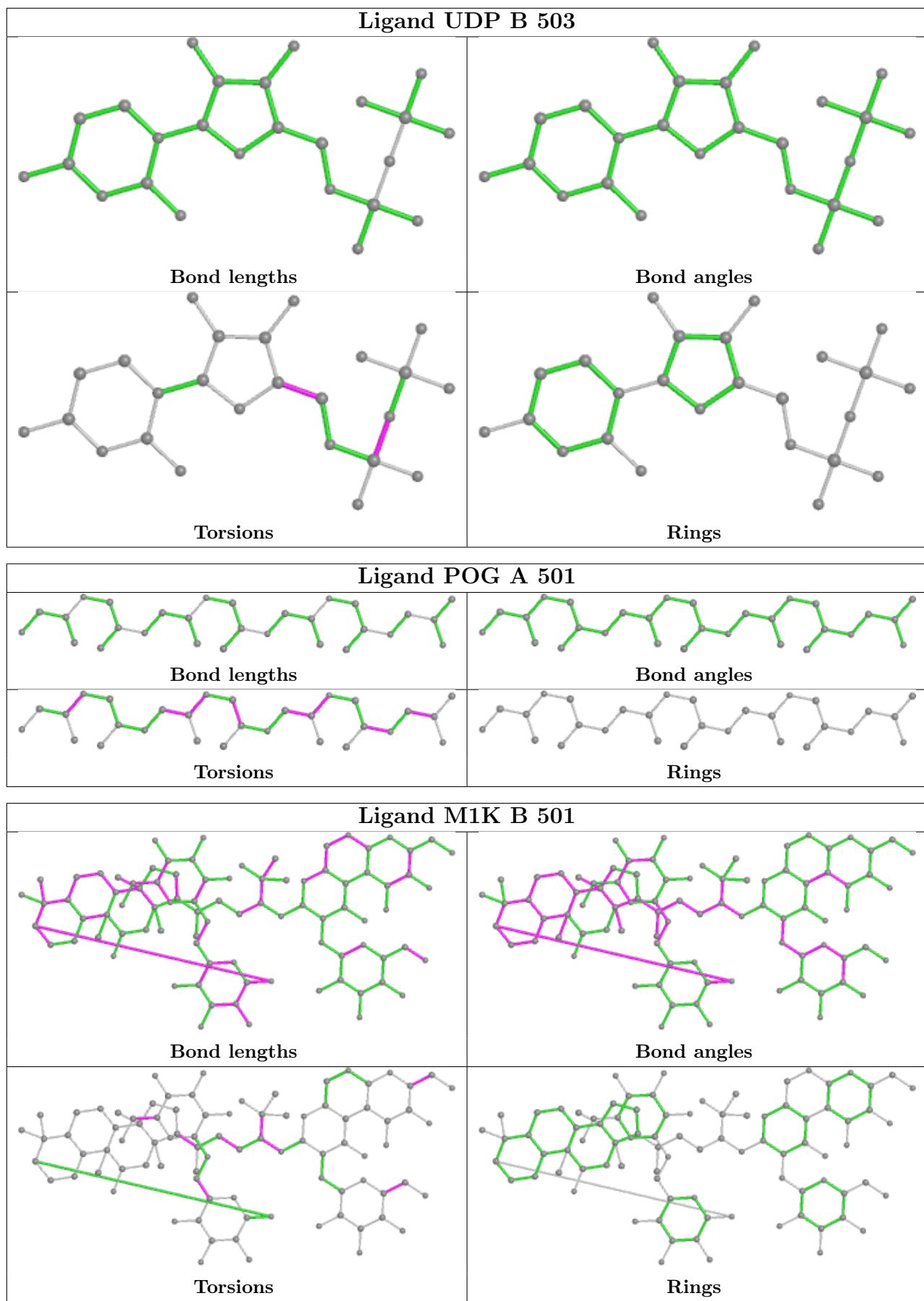
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	POG	2	0

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







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	426/459 (92%)	0.13	18 (4%) 36 40	12, 20, 39, 80	1 (0%)
1	B	426/459 (92%)	0.15	24 (5%) 24 27	12, 20, 38, 58	0
All	All	852/918 (92%)	0.14	42 (4%) 29 33	12, 20, 39, 80	1 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	ARG	5.0
1	A	187	GLU	4.8
1	A	248	GLU	4.8
1	A	160	HIS	4.7
1	A	165	PHE	4.7
1	A	242	ASN	4.7
1	B	165	PHE	4.6
1	B	189	THR	4.5
1	B	187	GLU	4.5
1	A	247	ASP	4.4
1	A	311	GLU	4.2
1	B	312	ASP	4.2
1	A	189	THR	4.1
1	B	457	HIS	4.1
1	B	176	ALA	4.0
1	B	242	ASN	4.0
1	B	160	HIS	4.0
1	B	188	ARG	3.8
1	A	188	ARG	3.8
1	A	176	ALA	3.6
1	A	164	PRO	3.1
1	A	18	LEU	3.0
1	A	175	LYS	2.9
1	B	249	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	164	PRO	2.8
1	B	303	GLN	2.7
1	A	301	PHE	2.7
1	B	9	THR	2.7
1	A	454	HIS	2.7
1	B	301	PHE	2.7
1	B	18	LEU	2.5
1	B	192	ARG	2.5
1	A	9	THR	2.5
1	A	161	SER	2.4
1	B	161	SER	2.3
1	B	251	SER	2.3
1	B	454	HIS	2.3
1	B	435	GLY	2.2
1	B	311	GLU	2.2
1	B	167	GLU	2.1
1	B	316	LYS	2.1
1	B	175	LYS	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 [\(i\)](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

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

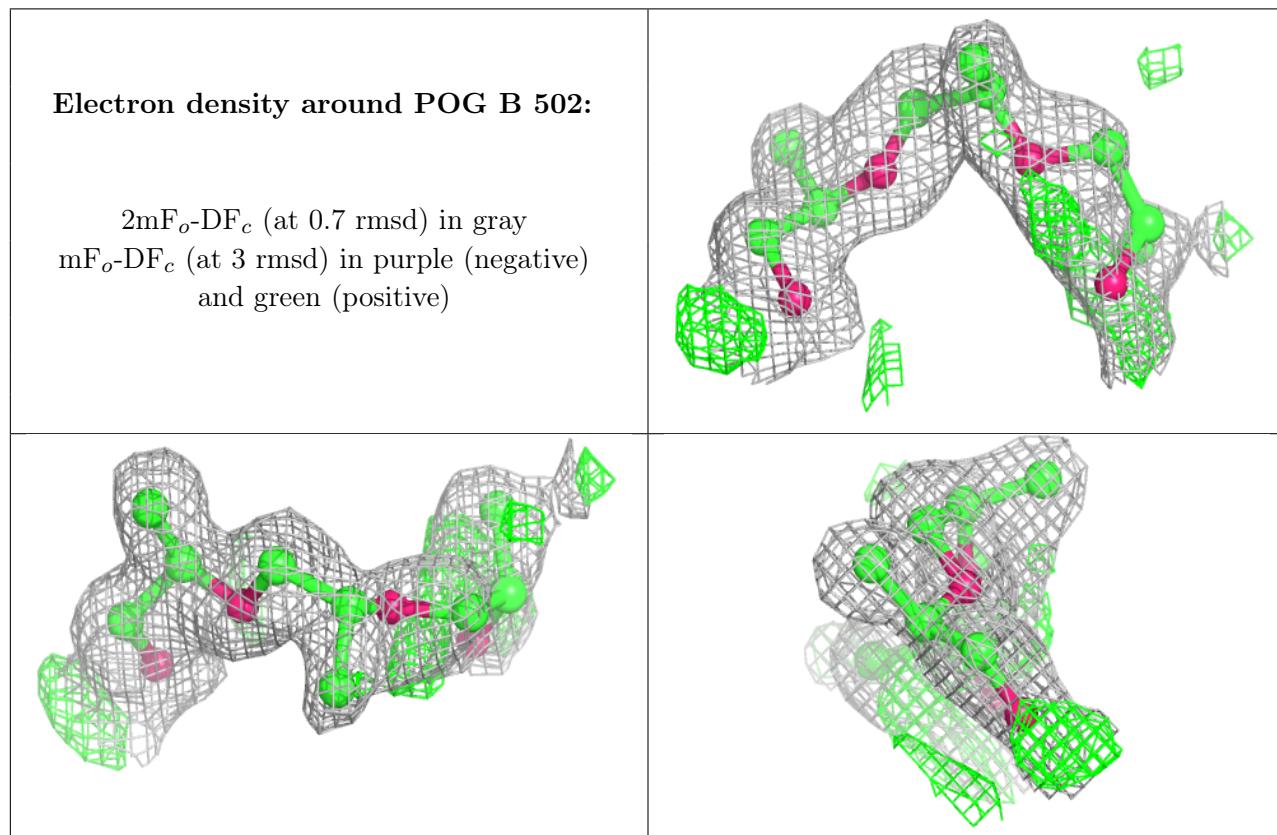
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	POG	B	502	13/29	0.78	0.21	21,30,35,43	10
5	TRS	A	504	8/8	0.78	0.33	21,30,35,36	0
2	POG	A	501	29/29	0.80	0.20	28,37,45,46	19
3	M1K	A	502	89/89	0.89	0.12	14,21,30,36	32
3	M1K	B	501	89/89	0.91	0.11	13,20,33,39	26

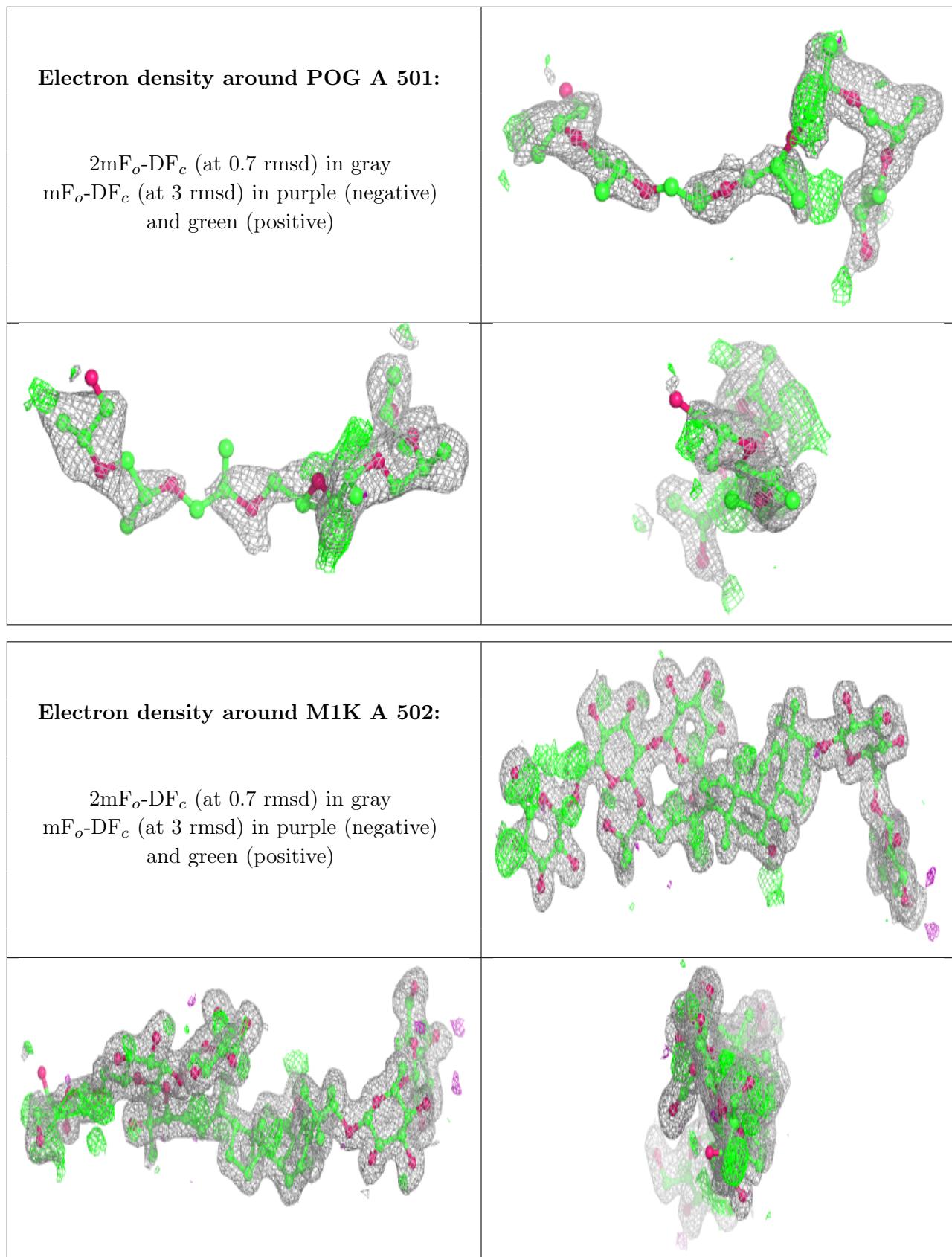
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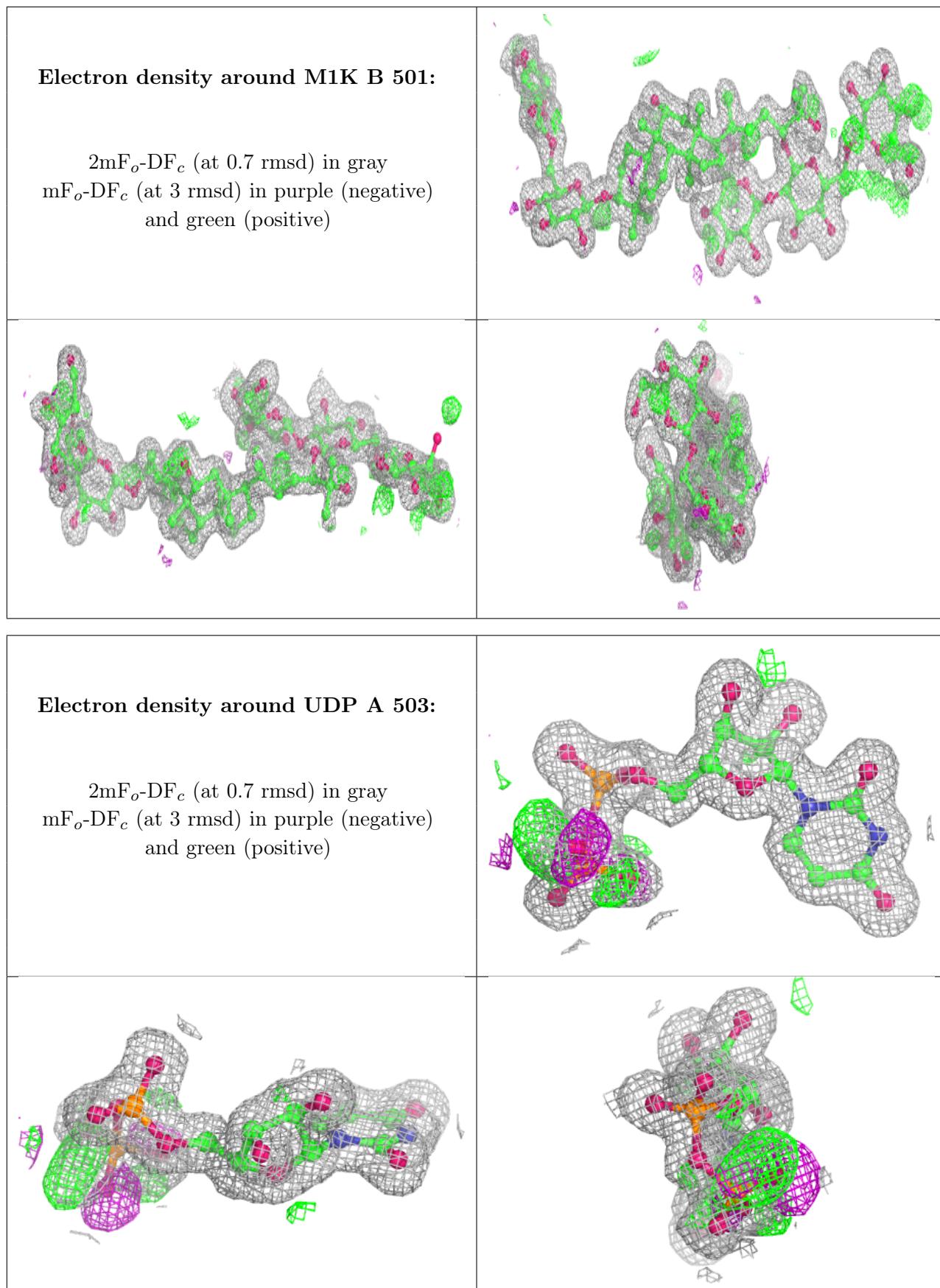
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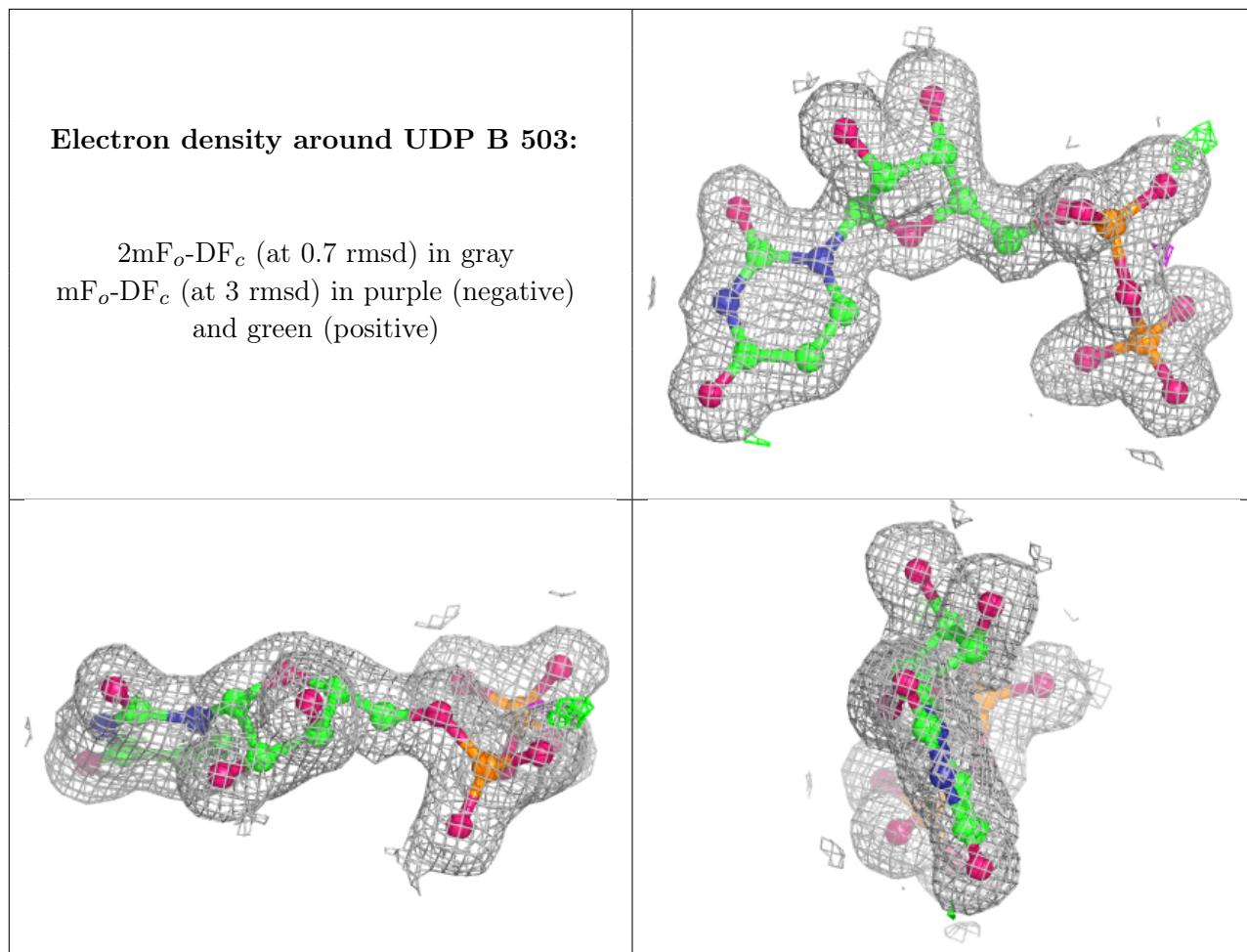
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	TRS	B	504	8/8	0.91	0.21	20,28,36,38	0
4	UDP	A	503	25/25	0.94	0.09	11,14,16,18	1
4	UDP	B	503	25/25	0.98	0.07	13,15,17,19	2

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.









## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.