Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2024 – 12:24 PM JST

PDB ID	:	8Y98
Title	:	Crystal structure of a heterooligomeric aminotransferase from Serratia sp. ATCC 39006, PPE-bound form
Authors	:	Pramono, H.; Yoshida, A.; Nishiyama, M.
Deposited on	:	2024-02-06
Resolution	:	2.31 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:

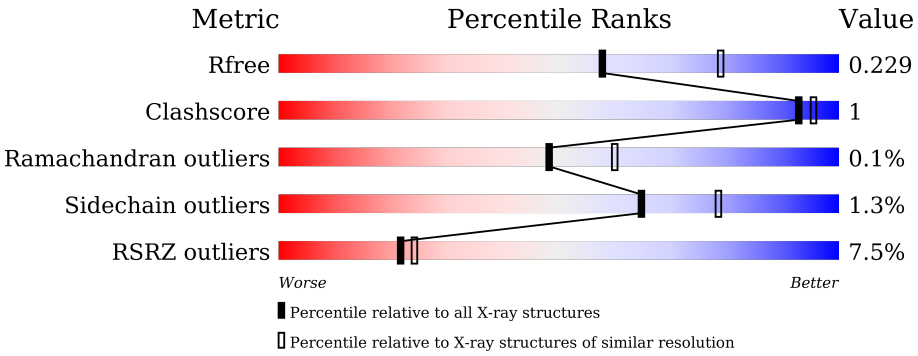
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.31 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}	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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	443	6% 89% 7% ·
1	B	443	5% 91% 5% ·
2	C	218	11% 91% 9%
2	D	218	10% 87% 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10267 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 DegT/DnrJ/EryC1/StrS family aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	3	0
			3383	2175	574	617	17			
1	B	428	Total	C	N	O	S	0	3	0
			3394	2177	580	620	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	HIS	-	expression tag	UNP A0A2I5TIB4
A	439	HIS	-	expression tag	UNP A0A2I5TIB4
A	440	HIS	-	expression tag	UNP A0A2I5TIB4
A	441	HIS	-	expression tag	UNP A0A2I5TIB4
A	442	HIS	-	expression tag	UNP A0A2I5TIB4
A	443	HIS	-	expression tag	UNP A0A2I5TIB4
B	438	HIS	-	expression tag	UNP A0A2I5TIB4
B	439	HIS	-	expression tag	UNP A0A2I5TIB4
B	440	HIS	-	expression tag	UNP A0A2I5TIB4
B	441	HIS	-	expression tag	UNP A0A2I5TIB4
B	442	HIS	-	expression tag	UNP A0A2I5TIB4
B	443	HIS	-	expression tag	UNP A0A2I5TIB4

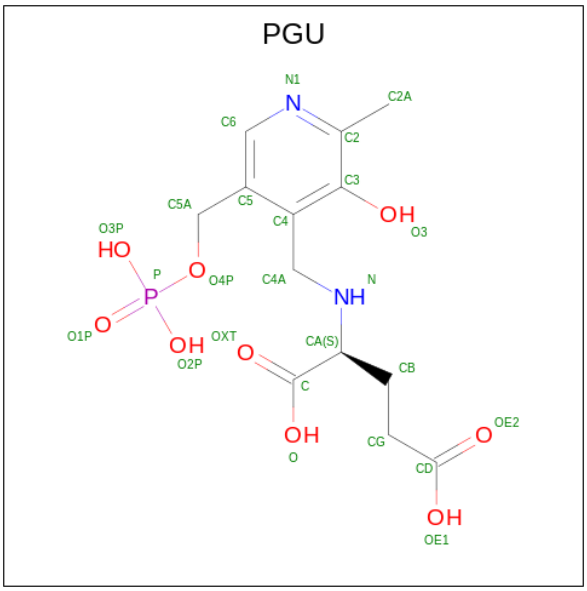
- Molecule 2 is a protein called DegT/DnrJ/EryC1/StrS aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	199	Total	C	N	O	S	0	0	0
			1539	993	255	286	5			
2	D	192	Total	C	N	O	S	0	0	0
			1478	956	246	271	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP A0A2I5T5Y7
C	1	GLY	-	expression tag	UNP A0A2I5T5Y7
C	212	HIS	-	expression tag	UNP A0A2I5T5Y7
C	213	HIS	-	expression tag	UNP A0A2I5T5Y7
C	214	HIS	-	expression tag	UNP A0A2I5T5Y7
C	215	HIS	-	expression tag	UNP A0A2I5T5Y7
C	216	HIS	-	expression tag	UNP A0A2I5T5Y7
C	217	HIS	-	expression tag	UNP A0A2I5T5Y7
D	0	MET	-	initiating methionine	UNP A0A2I5T5Y7
D	1	GLY	-	expression tag	UNP A0A2I5T5Y7
D	212	HIS	-	expression tag	UNP A0A2I5T5Y7
D	213	HIS	-	expression tag	UNP A0A2I5T5Y7
D	214	HIS	-	expression tag	UNP A0A2I5T5Y7
D	215	HIS	-	expression tag	UNP A0A2I5T5Y7
D	216	HIS	-	expression tag	UNP A0A2I5T5Y7
D	217	HIS	-	expression tag	UNP A0A2I5T5Y7

- Molecule 3 is N-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyl)-L-glutamic acid (three-letter code: PGU) (formula: $C_{13}H_{19}N_2O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
3	B	1	Total	C	N	O	P	0	0
			25	13	2	9	1		

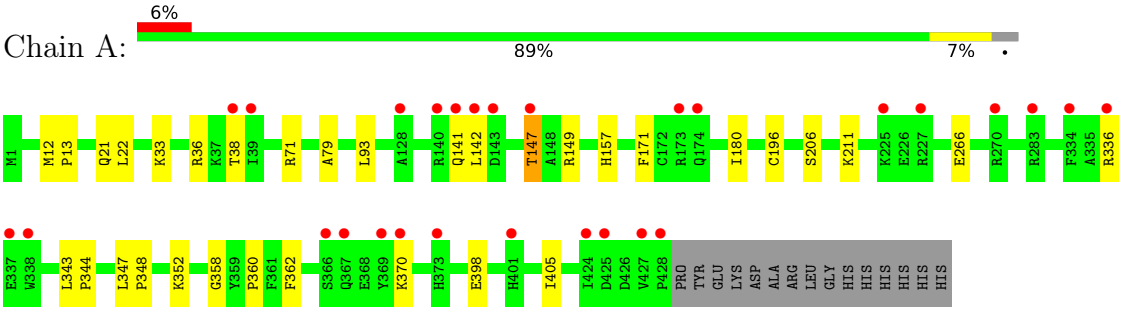
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	144	Total O 144 144	0	0
4	B	170	Total O 170 170	0	0
4	C	62	Total O 62 62	0	0
4	D	47	Total O 47 47	0	0

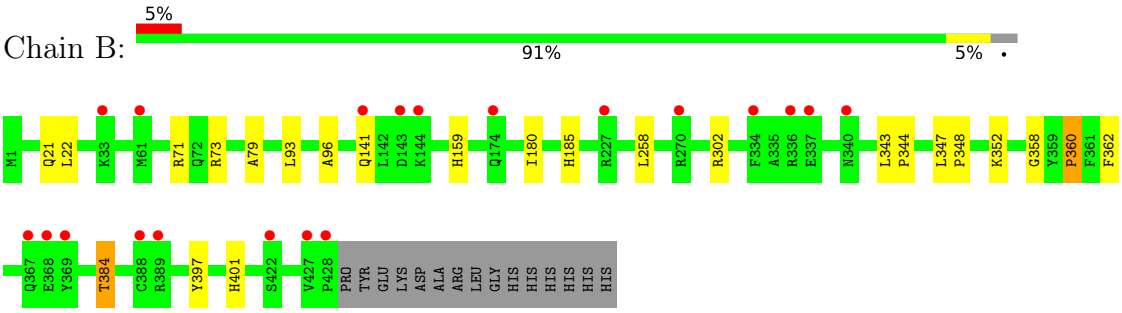
3 Residue-property plots

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.

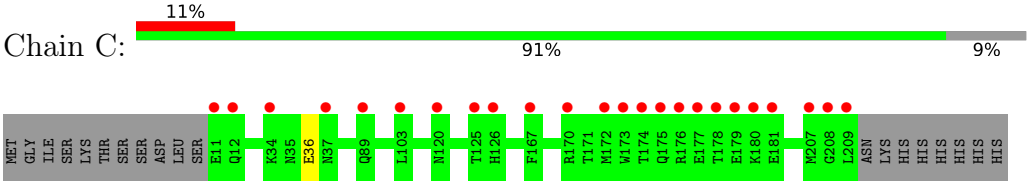
• Molecule 1: DegT/DnrJ/EryC1/StrS family aminotransferase



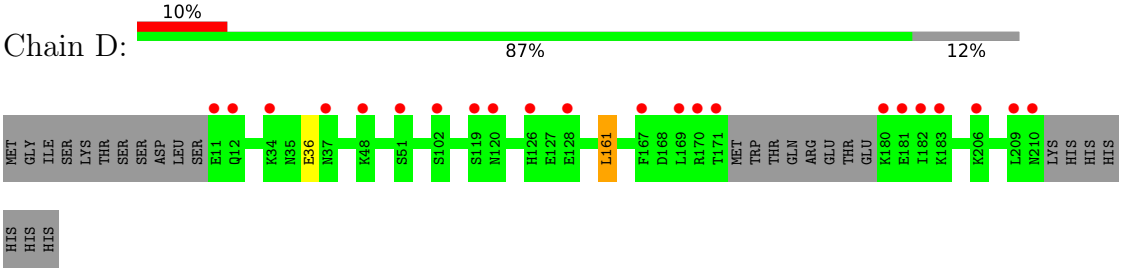
• Molecule 1: DegT/DnrJ/EryC1/StrS family aminotransferase



• Molecule 2: DegT/DnrJ/EryC1/StrS aminotransferase



• Molecule 2: DegT/DnrJ/EryC1/StrS aminotransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.98Å 181.17Å 182.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.86 – 2.31 45.86 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.86-2.31) 99.4 (45.86-2.31)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.193 , 0.223 0.199 , 0.229	Depositor DCC
R_{free} test set	3881 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10267	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.24% 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: PGU

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	0.29	0/3470	0.52	0/4700
1	B	0.29	0/3475	0.52	1/4706 (0.0%)
2	C	0.29	0/1569	0.46	0/2124
2	D	0.29	0/1505	0.48	0/2035
All	All	0.29	0/10019	0.50	1/13565 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	360	PRO	N-CA-CB	-5.52	96.52	102.60

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	3383	0	3360	15	0
1	B	3394	0	3373	12	0
2	C	1539	0	1533	0	0
2	D	1478	0	1486	1	0
3	A	25	0	15	2	0
3	B	25	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	144	0	0	0	0
4	B	170	0	0	0	0
4	C	62	0	0	0	0
4	D	47	0	0	0	0
All	All	10267	0	9782	28	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 (28) 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:206:SER:HB2	3:A:501:PGU:H5A2	1.65	0.78
1:B:21:GLN:HE21	1:B:22:LEU:H	1.47	0.63
1:A:147:THR:HG22	1:A:149:ARG:H	1.65	0.60
2:D:161:LEU:C	2:D:161:LEU:HD23	2.26	0.56
1:A:21:GLN:HE21	1:A:22:LEU:H	1.54	0.56
1:B:302:ARG:HE	1:B:384:THR:HG21	1.73	0.53
1:A:33:LYS:HA	1:A:36:ARG:HD3	1.91	0.52
1:B:93:LEU:HD23	1:B:180:ILE:HG13	1.92	0.52
1:B:159:HIS:H	1:B:185:HIS:HD1	1.60	0.49
1:B:352:LYS:O	1:B:358:GLY:HA2	2.14	0.48
1:A:13:PRO:HG2	1:A:405:ILE:HD12	1.97	0.47
1:B:21:GLN:HE21	1:B:22:LEU:N	2.14	0.46
1:A:211:LYS:HE3	3:A:501:PGU:HB1	1.99	0.45
1:B:343:LEU:N	1:B:344:PRO:CD	2.81	0.44
1:A:352:LYS:O	1:A:358:GLY:HA2	2.17	0.44
1:B:73:ARG:HD2	1:B:258:LEU:HD11	2.00	0.43
1:A:12:MET:HE2	1:A:398:GLU:HG3	2.00	0.43
1:B:397:TYR:CE1	1:B:401[B]:HIS:NE2	2.86	0.43
1:B:96:ALA:CB	1:B:180:ILE:HD11	2.49	0.43
1:A:266[A]:GLU:HA	1:A:266[A]:GLU:OE1	2.18	0.43
1:A:71:ARG:HG3	1:A:79:ALA:HB2	2.01	0.42
1:A:93:LEU:HD23	1:A:180:ILE:HG13	2.02	0.41
1:B:347:LEU:N	1:B:348:PRO:CD	2.84	0.41
1:A:343:LEU:N	1:A:344:PRO:CD	2.84	0.41
1:B:71:ARG:HG3	1:B:79:ALA:HB2	2.03	0.41
1:A:142:LEU:HB3	1:A:171:PHE:CZ	2.56	0.40
1:A:157:HIS:HD1	1:A:196:CYS:HB3	1.86	0.40
1:A:347:LEU:N	1:A:348:PRO:CD	2.84	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	429/443 (97%)	423 (99%)	5 (1%)	1 (0%)	44 54
1	B	429/443 (97%)	425 (99%)	4 (1%)	0	100 100
2	C	197/218 (90%)	191 (97%)	6 (3%)	0	100 100
2	D	188/218 (86%)	181 (96%)	7 (4%)	0	100 100
All	All	1243/1322 (94%)	1220 (98%)	22 (2%)	1 (0%)	48 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	GLN

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	353/369 (96%)	347 (98%)	6 (2%)	56 71
1	B	356/369 (96%)	352 (99%)	4 (1%)	70 83
2	C	164/192 (85%)	163 (99%)	1 (1%)	84 92
2	D	158/192 (82%)	156 (99%)	2 (1%)	65 78
All	All	1031/1122 (92%)	1018 (99%)	13 (1%)	65 78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	147	THR
1	A	336	ARG
1	A	360	PRO
1	A	362	PHE
1	A	370	LYS
1	B	141	GLN
1	B	360	PRO
1	B	362	PHE
1	B	384	THR
2	C	36	GLU
2	D	36	GLU
2	D	161	LEU

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

Mol	Chain	Res	Type
1	A	21	GLN
1	A	42	ASN
1	A	56	GLN
1	A	116	GLN
1	A	269	GLN
1	B	21	GLN
1	B	269	GLN
2	C	72	GLN
2	D	88	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	PGU	B	501	-	25,25,25	0.71	0	31,35,35	1.08	1 (3%)
3	PGU	A	501	-	25,25,25	0.71	0	31,35,35	1.26	3 (9%)

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
3	PGU	B	501	-	-	4/20/20/20	0/1/1/1
3	PGU	A	501	-	-	9/20/20/20	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	PGU	C4A-N-CA	4.09	121.66	113.92
3	B	501	PGU	C4A-N-CA	3.69	120.91	113.92
3	A	501	PGU	O4P-C5A-C5	3.22	115.48	109.35
3	A	501	PGU	C4A-C4-C5	2.29	122.25	119.71

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	PGU	C5-C4-C4A-N
3	A	501	PGU	C5A-O4P-P-O1P
3	A	501	PGU	C5A-O4P-P-O2P
3	A	501	PGU	C5A-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
3	B	501	PGU	C3-C4-C4A-N
3	B	501	PGU	C5-C4-C4A-N
3	A	501	PGU	C3-C4-C4A-N
3	A	501	PGU	C4-C4A-N-CA
3	B	501	PGU	C4-C4A-N-CA
3	B	501	PGU	C-CA-CB-CG
3	A	501	PGU	OE1-CD-CG-CB
3	A	501	PGU	OE2-CD-CG-CB
3	A	501	PGU	CB-CA-N-C4A

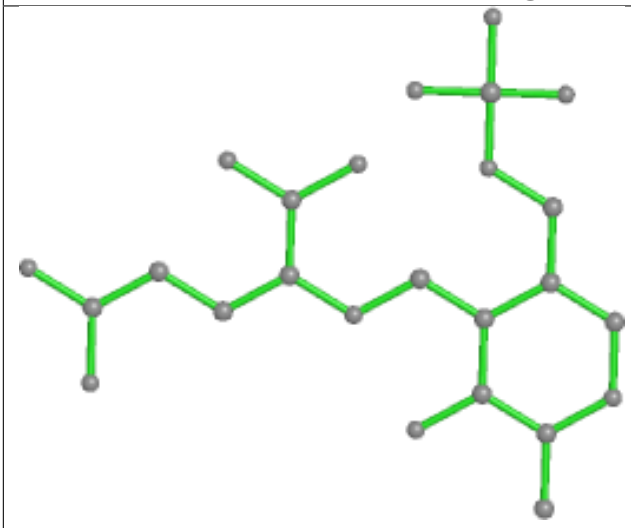
There are no ring outliers.

1 monomer is involved in 2 short contacts:

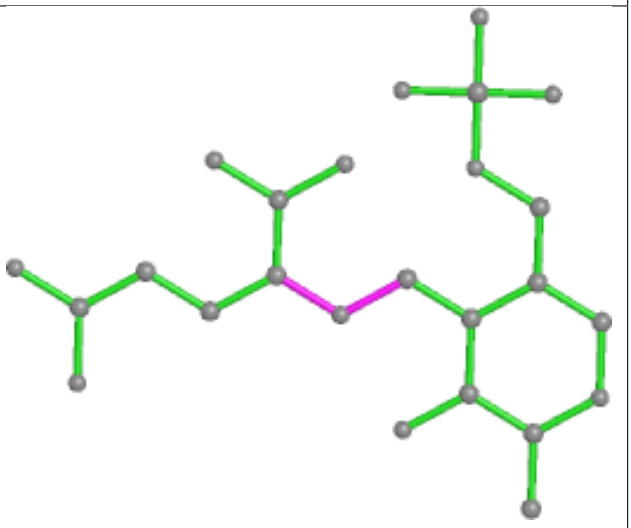
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	PGU	2	0

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 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.

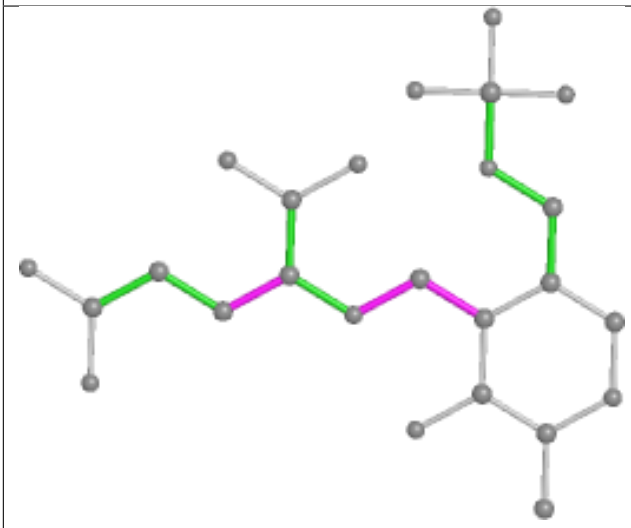
Ligand PGU B 501



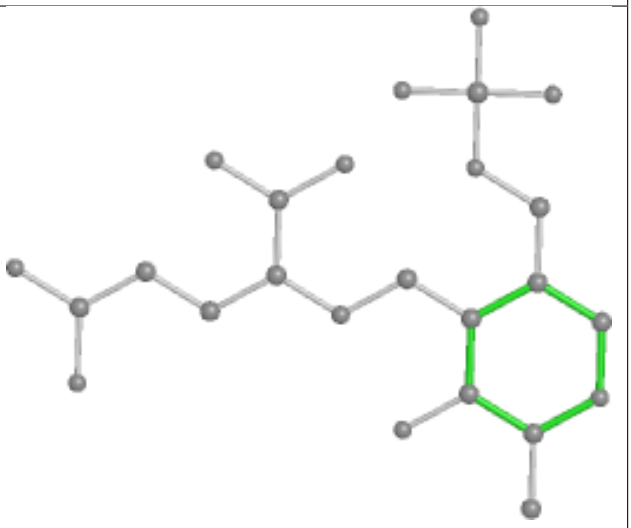
Bond lengths



Bond angles

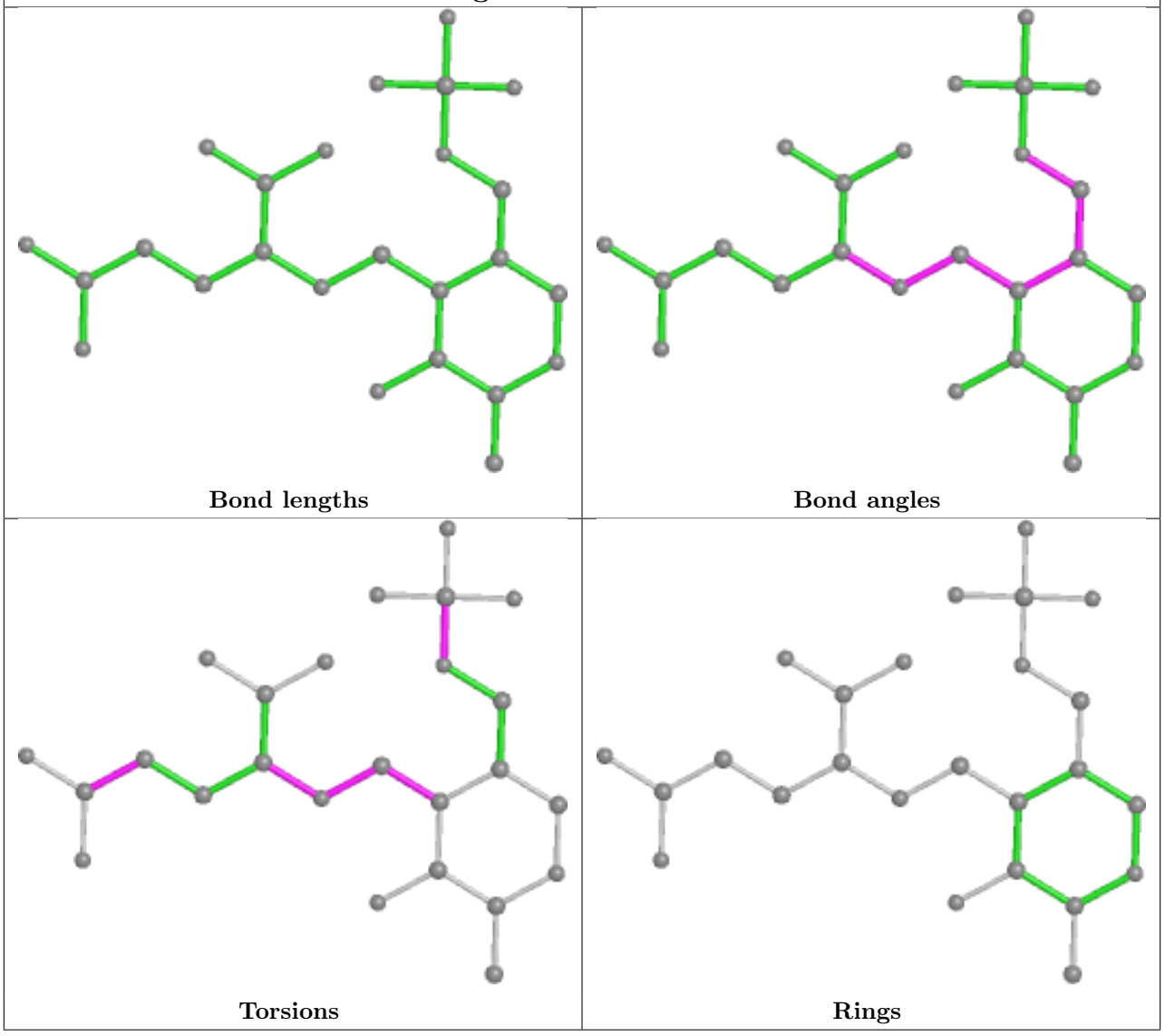


Torsions



Rings

Ligand PGU A 501



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	428/443 (96%)	0.56	28 (6%)	26	29	25, 54, 75, 116	3 (0%)
1	B	428/443 (96%)	0.28	20 (4%)	37	39	24, 51, 69, 107	3 (0%)
2	C	199/218 (91%)	0.70	24 (12%)	10	11	44, 55, 94, 123	0
2	D	192/218 (88%)	0.85	22 (11%)	11	13	45, 58, 85, 96	0
All	All	1247/1322 (94%)	0.53	94 (7%)	22	24	24, 53, 79, 123	6 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	PRO	7.6
1	B	428	PRO	6.3
2	C	176	ARG	5.8
2	C	178	THR	5.7
2	D	171	THR	5.7
2	D	210	ASN	5.6
1	A	427	VAL	5.4
2	C	172	MET	5.2
2	D	170	ARG	5.1
2	D	51	SER	5.1
2	D	180	LYS	5.0
1	B	141	GLN	4.7
1	A	334[A]	PHE	4.6
2	C	174	THR	4.5
1	B	427	VAL	4.4
2	D	181	GLU	4.3
2	D	128	GLU	4.2
2	C	11	GLU	4.2
1	B	334	PHE	4.1
2	C	167	PHE	4.1
1	A	141	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	366	SER	4.0
2	C	125	THR	4.0
1	A	369	TYR	3.8
2	C	179	GLU	3.8
2	C	180	LYS	3.7
2	C	173	TRP	3.7
2	C	175	GLN	3.7
2	D	11	GLU	3.5
2	D	120	ASN	3.5
2	C	209	LEU	3.4
1	A	370	LYS	3.3
1	A	367	GLN	3.2
2	D	209	LEU	3.2
2	D	182	ILE	3.1
2	D	167	PHE	3.0
1	B	389	ARG	3.0
1	B	270	ARG	3.0
2	D	12	GLN	2.9
2	C	120	ASN	2.9
2	C	126	HIS	2.9
1	A	337	GLU	2.9
2	C	177	GLU	2.9
1	A	142	LEU	2.9
1	A	147	THR	2.8
1	A	174	GLN	2.8
2	C	12	GLN	2.8
1	A	39	ILE	2.7
1	A	373	HIS	2.6
2	D	34	LYS	2.6
2	C	181	GLU	2.6
1	A	173	ARG	2.6
2	D	48	LYS	2.5
1	A	336	ARG	2.5
1	B	369	TYR	2.4
1	A	143	ASP	2.4
2	D	206	LYS	2.4
1	A	140	ARG	2.4
1	B	336	ARG	2.4
2	D	126	HIS	2.4
1	A	338	TRP	2.4
2	C	37	ASN	2.4
1	B	33	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	270	ARG	2.4
2	D	102	SER	2.3
1	B	367	GLN	2.3
1	B	61	MET	2.3
1	B	388	CYS	2.3
1	B	143	ASP	2.3
1	A	128	ALA	2.2
1	A	401	HIS	2.2
2	C	89	GLN	2.2
1	A	227[A]	ARG	2.2
1	A	38	THR	2.2
2	C	34	LYS	2.2
1	B	368	GLU	2.2
1	A	425	ASP	2.2
2	C	208	GLY	2.2
1	A	283	ARG	2.2
2	C	170	ARG	2.2
1	A	424	ILE	2.1
1	A	225	LYS	2.1
2	C	207	MET	2.1
1	B	337	GLU	2.1
1	B	422	SER	2.1
2	D	169	LEU	2.1
2	D	119	SER	2.0
1	B	144	LYS	2.0
1	B	340[A]	ASN	2.0
2	C	103	LEU	2.0
2	D	37	ASN	2.0
1	B	227	ARG	2.0
2	D	183	LYS	2.0
1	B	174	GLN	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)

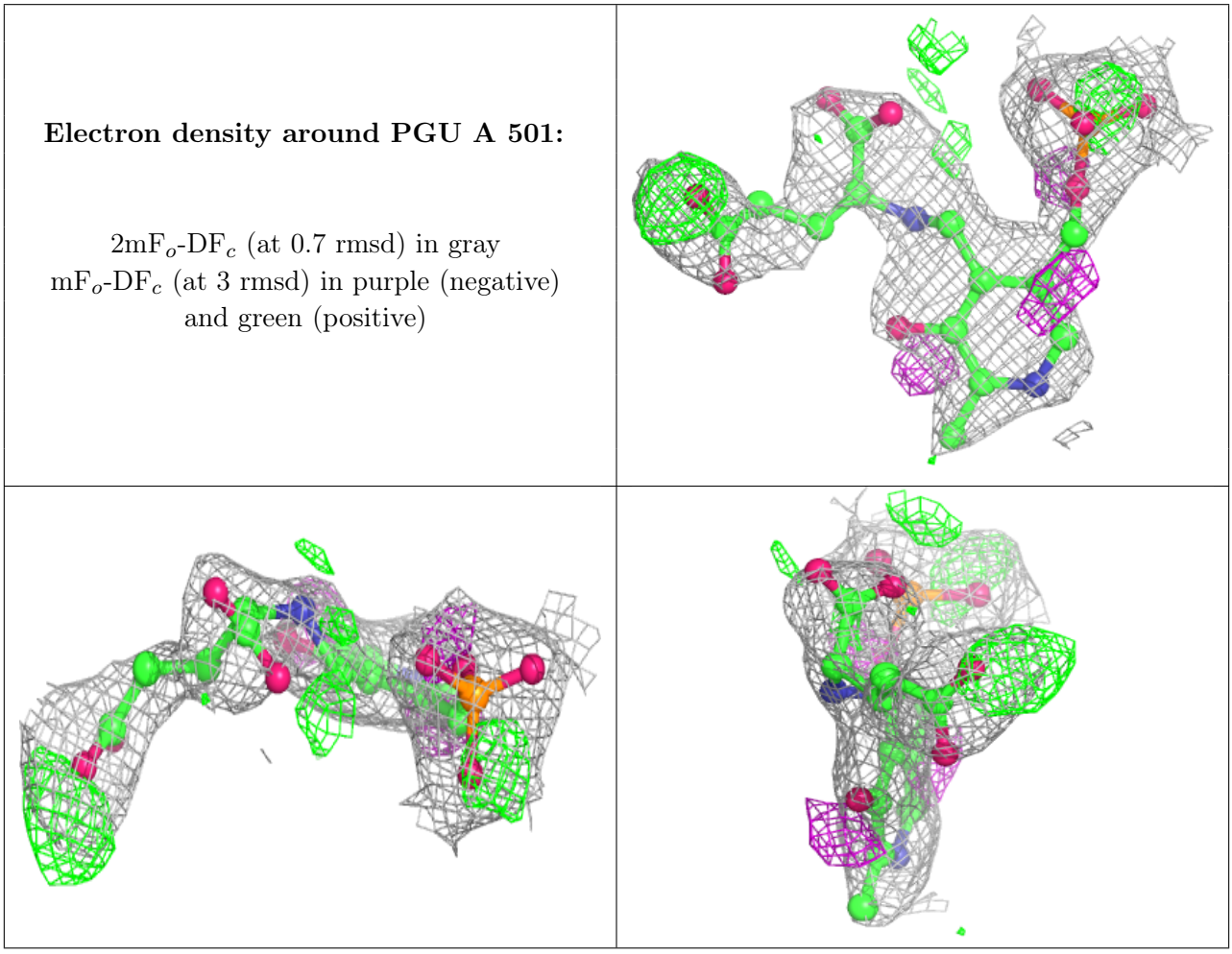
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	PGU	A	501	25/25	0.89	0.19	50,68,86,89	0
3	PGU	B	501	25/25	0.90	0.19	46,67,89,92	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.

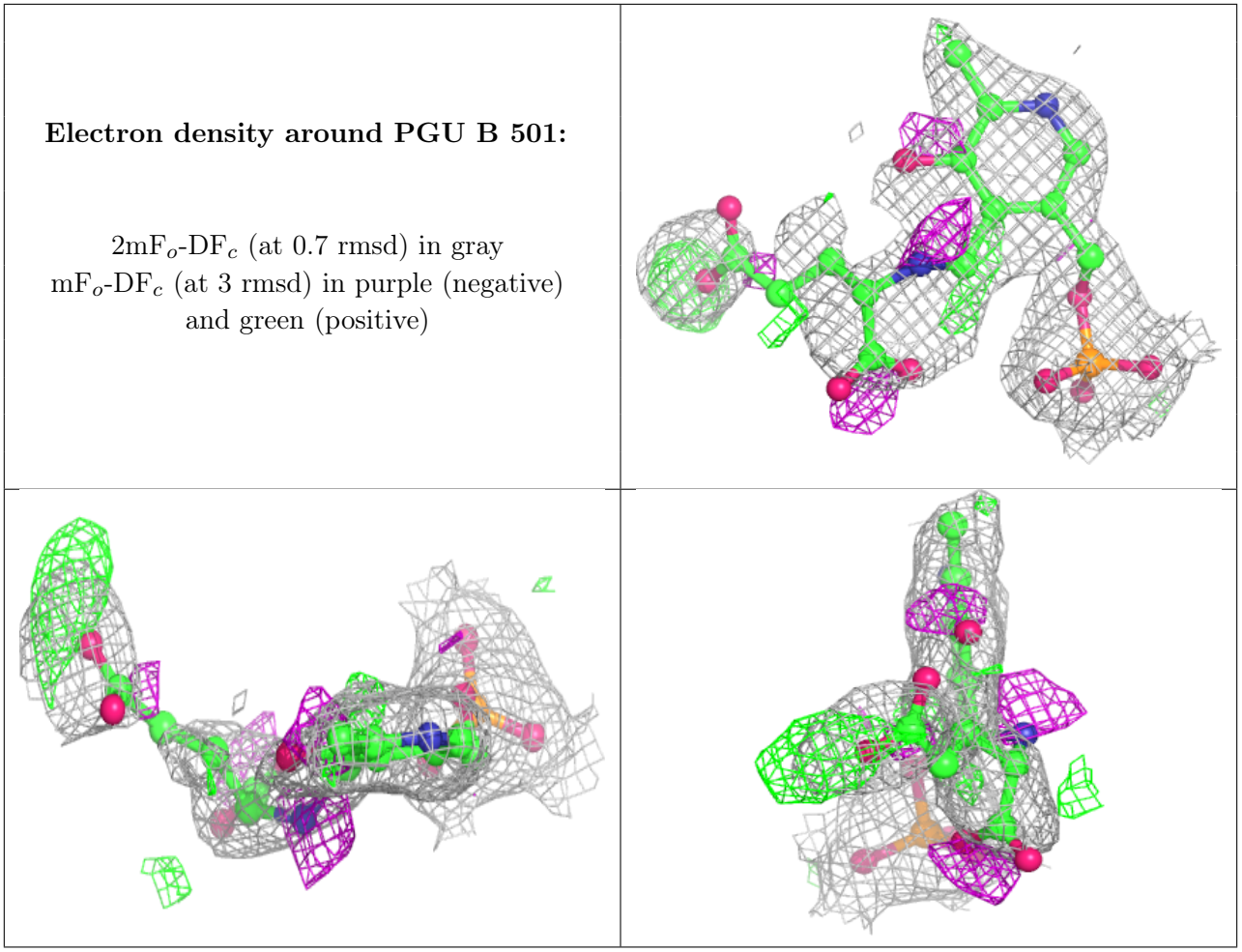
Electron density around PGU A 501:

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



Electron density around PGU 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)



6.5 Other polymers (i)

There are no such residues in this entry.