wwPDB X-ray Structure Validation Summary Report (i)

Jun 26, 2024 – 12:38 AM EDT

PDB ID	:	6TAH
Title	:	Crystal structure of a Nu-class Glutathione-S-Transferase from Pseudomonas aeruginosa PACS2 bound to glutathione
Authors	:	Feiler, C.G.; Blankenfeldt, W.
Deposited on	:	2019-10-29
Resolution	:	1.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

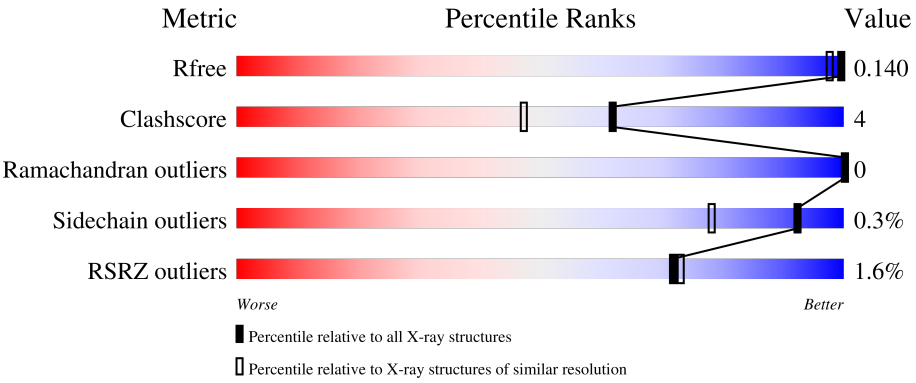
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

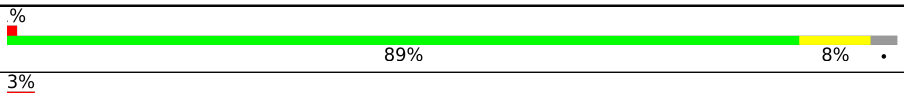
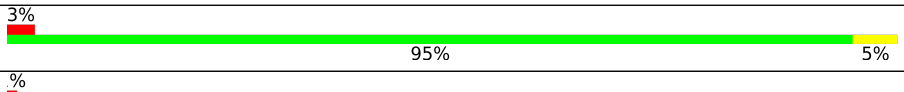
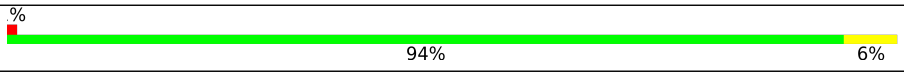
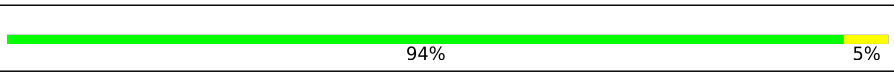
The reported resolution of this entry is 1.30 Å.

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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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	AAA	214	
2	B	213	
3	CAA	204	
4	DAA	203	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15077 atoms, of which 6942 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 Glutathione S-transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	Se			
1	AAA	208	3481	1111	1754	303	306	7	0	13	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	GLY	-	expression tag	UNP A0A485ICL5
AAA	0	PRO	-	expression tag	UNP A0A485ICL5
AAA	1	MSE	-	expression tag	UNP A0A485ICL5
AAA	35	LYS	ARG	conflict	UNP A0A485ICL5

- Molecule 2 is a protein called Glutathione S-transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	Se			
2	B	213	3457	1108	1726	301	315	7	0	8	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP A0A485ICL5
B	0	PRO	-	expression tag	UNP A0A485ICL5
B	1	MSE	-	expression tag	UNP A0A485ICL5
B	35	LYS	ARG	conflict	UNP A0A485ICL5

- Molecule 3 is a protein called Glutathione S-transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	Se			
3	CAA	204	3342	1072	1670	294	300	6	0	9	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CAA	-1	GLY	-	expression tag	UNP A0A485ICL5
CAA	0	PRO	-	expression tag	UNP A0A485ICL5
CAA	1	MSE	-	expression tag	UNP A0A485ICL5
CAA	35	LYS	ARG	conflict	UNP A0A485ICL5

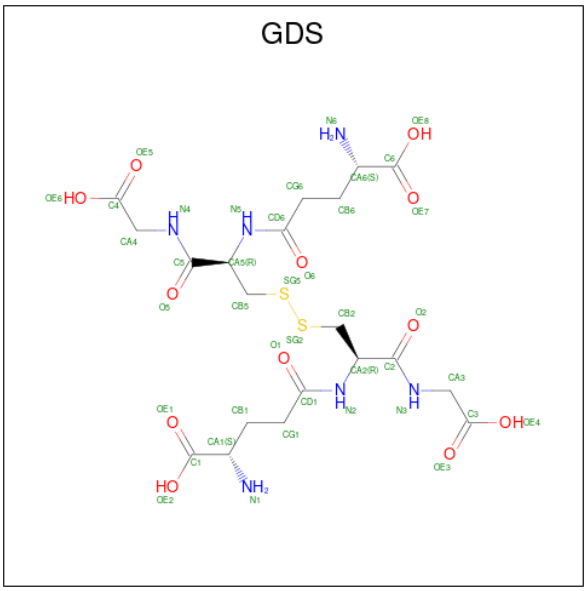
- Molecule 4 is a protein called Glutathione S-transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	Se			
4	DAA	203	3275	1054	1634	284	296	7	0	6	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DAA	0	PRO	-	expression tag	UNP A0A485ICL5
DAA	1	MSE	-	expression tag	UNP A0A485ICL5
DAA	35	LYS	ARG	conflict	UNP A0A485ICL5

- Molecule 5 is OXIDIZED GLUTATHIONE DISULFIDE (three-letter code: GDS) (formula: $C_{20}H_{32}N_6O_{12}S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
5	AAA	1	68	20	28	6	12	2	0	0
5	B	1	Total	C	H	N	O	S	0	0
			68	20	28	6	12	2		

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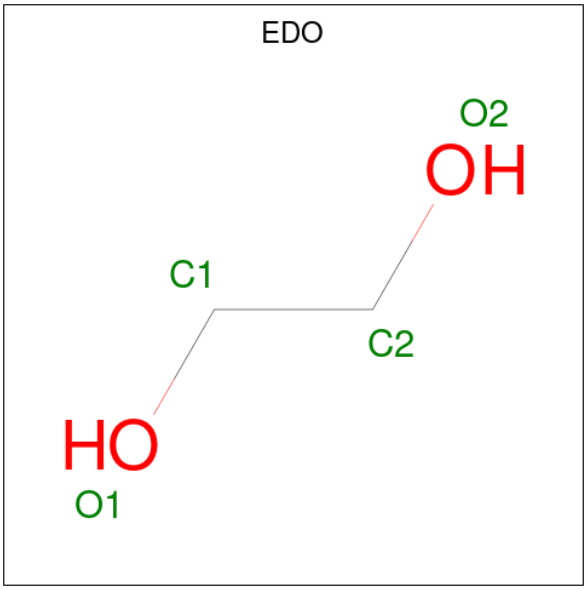
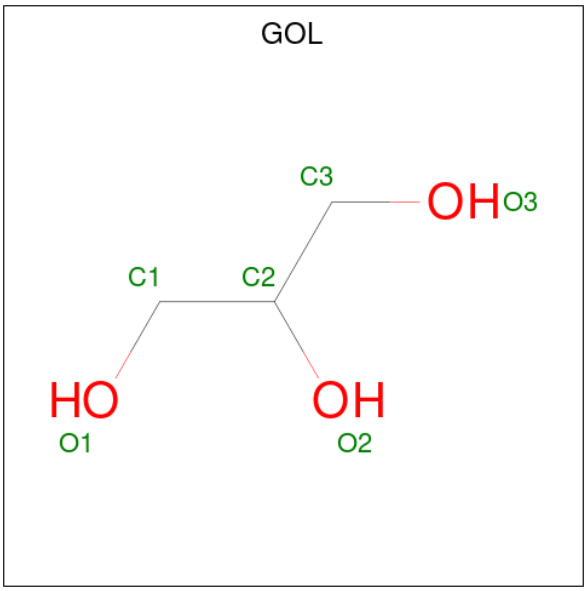
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	CAA	1	Total	C	H	N	O	S	0	0
			68	20	28	6	12	2		
5	DAA	1	Total	C	H	N	O	S	0	0
			68	20	28	6	12	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	CAA	1	Total	C	H	O	0	0
			10	2	6	2		
6	CAA	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total C H O 28 6 16 6	0	1

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	270	Total O 271 271	0	1
8	B	273	Total O 273 273	0	0
8	CAA	324	Total O 324 324	0	0
8	DAA	304	Total O 304 304	0	0

3 Residue-property plots (i)

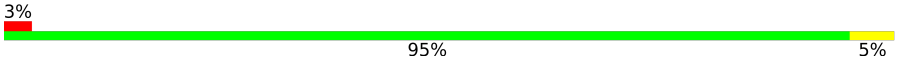
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain AAA:

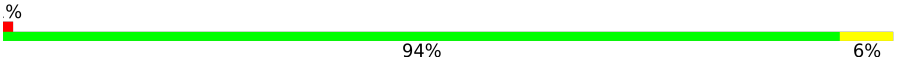
• Molecule 2: Glutathione S-transferase

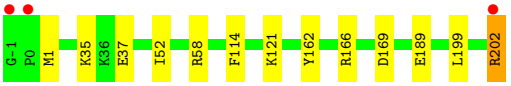
Chain B:



• Molecule 3: Glutathione S-transferase

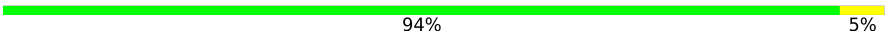
Chain CAA:

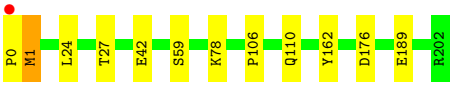




• Molecule 4: Glutathione S-transferase

Chain DAA:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.50Å 96.61Å 100.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.75 – 1.30 19.75 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.75-1.30) 99.9 (19.75-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 1.30Å)	Xtriage
Refinement program	PHENIX 1.17_3644, PHENIX 1.17_3644	Depositor
R, R_{free}	0.120 , 0.140 0.120 , 0.140	Depositor DCC
R_{free} test set	10019 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	8.7	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	15077	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8153e-05.*

[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: GOL, GDS, EDO

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	AAA	0.44	0/1801	0.69	2/2426 (0.1%)
2	B	0.38	0/1790	0.60	0/2415
3	CAA	0.50	2/1735 (0.1%)	0.69	1/2342 (0.0%)
4	DAA	0.39	0/1694	0.63	0/2288
All	All	0.43	2/7020 (0.0%)	0.65	3/9471 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CAA	202	ARG	CZ-NH2	8.50	1.44	1.33
3	CAA	202	ARG	CZ-NH1	7.41	1.42	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CAA	202	ARG	NE-CZ-NH2	-11.99	114.31	120.30
1	AAA	116[A]	ARG	CB-CA-C	-7.64	95.11	110.40
1	AAA	116[B]	ARG	CB-CA-C	-7.64	95.11	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	-1	GLY	Peptide

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	AAA	1727	1754	1757	28	0
2	B	1731	1726	1728	9	1
3	CAA	1672	1670	1676	10	0
4	DAA	1641	1634	1637	14	0
5	AAA	40	28	28	3	0
5	B	40	28	28	0	0
5	CAA	40	28	28	0	0
5	DAA	40	28	28	0	0
6	AAA	4	6	6	1	0
6	B	8	12	12	0	0
6	CAA	8	12	12	0	0
7	AAA	12	16	16	0	0
8	AAA	271	0	0	15	1
8	B	273	0	0	3	3
8	CAA	324	0	0	4	5
8	DAA	304	0	0	3	1
All	All	8135	6942	6956	61	6

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 4.

The worst 5 of 61 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)
4:DAA:42:GLU:O	8:DAA:401:HOH:O	1.61	1.19
3:CAA:169[B]:ASP:OD2	8:CAA:401:HOH:O	1.79	1.00
3:CAA:114:PHE:O	8:CAA:402:HOH:O	1.89	0.90
4:DAA:0:PRO:HG3	4:DAA:78:LYS:HE2	1.53	0.89
2:B:62:ASP:OD2	8:B:401:HOH:O	1.91	0.88

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes

the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:401:HOH:O	8:CAA:695:HOH:O[3_555]	1.82	0.38
8:CAA:582:HOH:O	8:DAA:630:HOH:O[2_465]	1.98	0.22
8:AAA:588:HOH:O	8:CAA:696:HOH:O[4_555]	2.03	0.17
8:B:640:HOH:O	8:CAA:721:HOH:O[3_555]	2.08	0.12
2:B:59:SER:OG	8:CAA:602:HOH:O[3_555]	2.14	0.06

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	AAA	217/214 (101%)	206 (95%)	11 (5%)	0	100	100
2	B	219/213 (103%)	214 (98%)	5 (2%)	0	100	100
3	CAA	211/204 (103%)	206 (98%)	5 (2%)	0	100	100
4	DAA	207/203 (102%)	203 (98%)	4 (2%)	0	100	100
All	All	854/834 (102%)	829 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	182/168 (108%)	180 (99%)	2 (1%)	73	45
2	B	180/167 (108%)	180 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	CAA	175/160 (109%)	175 (100%)	0	100 100
4	DAA	171/160 (107%)	169 (99%)	2 (1%)	71 40
All	All	708/655 (108%)	704 (99%)	4 (1%)	92 65

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	9[A]	THR
1	AAA	9[B]	THR
4	DAA	1[A]	MSE
4	DAA	1[B]	MSE

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

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)

11 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	$\#\|Z\|>2$
5	GDS	B	301	-	37,39,39	1.51	6 (16%)	48,50,50	0.97	1 (2%)
5	GDS	DAA	301	-	37,39,39	1.54	7 (18%)	48,50,50	1.07	1 (2%)
6	EDO	CAA	302	-	3,3,3	0.48	0	2,2,2	0.14	0
7	GOL	AAA	303[A]	-	5,5,5	0.62	0	5,5,5	1.06	0
6	EDO	CAA	303	-	3,3,3	0.44	0	2,2,2	0.35	0
7	GOL	AAA	303[B]	-	5,5,5	0.51	0	5,5,5	1.12	0
5	GDS	AAA	301	-	37,39,39	1.46	6 (16%)	48,50,50	0.97	1 (2%)
6	EDO	B	303	-	3,3,3	0.47	0	2,2,2	0.20	0
6	EDO	AAA	302	-	3,3,3	0.42	0	2,2,2	0.29	0
5	GDS	CAA	301	-	37,39,39	1.45	5 (13%)	48,50,50	1.05	2 (4%)
6	EDO	B	302	-	3,3,3	0.52	0	2,2,2	0.05	0

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
5	GDS	B	301	-	-	2/51/51/51	-
5	GDS	DAA	301	-	-	2/51/51/51	-
6	EDO	CAA	302	-	-	1/1/1/1	-
7	GOL	AAA	303[A]	-	-	0/4/4/4	-
6	EDO	CAA	303	-	-	1/1/1/1	-
7	GOL	AAA	303[B]	-	-	1/4/4/4	-
5	GDS	AAA	301	-	-	0/51/51/51	-
6	EDO	B	303	-	-	1/1/1/1	-
6	EDO	AAA	302	-	-	1/1/1/1	-
5	GDS	CAA	301	-	-	1/51/51/51	-
6	EDO	B	302	-	-	1/1/1/1	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301	GDS	CD6-N5	4.31	1.43	1.34
5	AAA	301	GDS	CD6-N5	4.21	1.43	1.34
5	DAA	301	GDS	C2-N3	3.72	1.41	1.33
5	B	301	GDS	C2-N3	3.69	1.41	1.33
5	DAA	301	GDS	CD6-N5	3.66	1.41	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	CAA	301	GDS	OE4-C3-CA3	2.54	121.55	112.74
5	AAA	301	GDS	CB2-CA2-C2	-2.13	105.12	109.73
5	CAA	301	GDS	CB5-CA5-C5	-2.10	105.17	109.73
5	DAA	301	GDS	OE8-C6-CA6	2.04	120.33	113.38
5	B	301	GDS	CB2-CA2-C2	-2.03	105.33	109.73

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	AAA	303[B]	GOL	C1-C2-C3-O3
6	CAA	303	EDO	O1-C1-C2-O2
6	AAA	302	EDO	O1-C1-C2-O2
6	CAA	302	EDO	O1-C1-C2-O2
5	B	301	GDS	C3-CA3-N3-C2

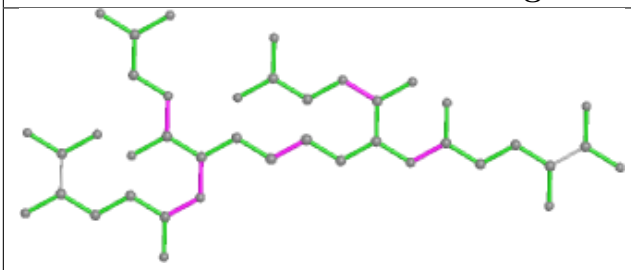
There are no ring outliers.

2 monomers are involved in 4 short contacts:

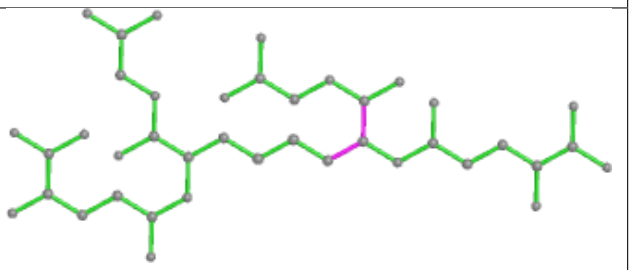
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	301	GDS	3	0
6	AAA	302	EDO	1	0

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.

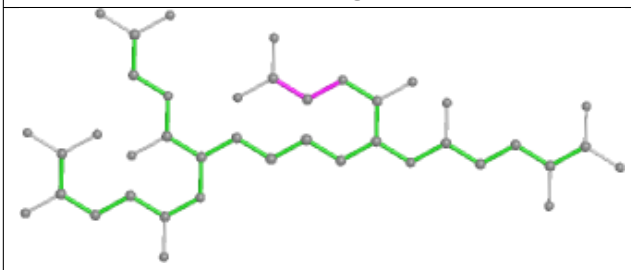
Ligand GDS B 301



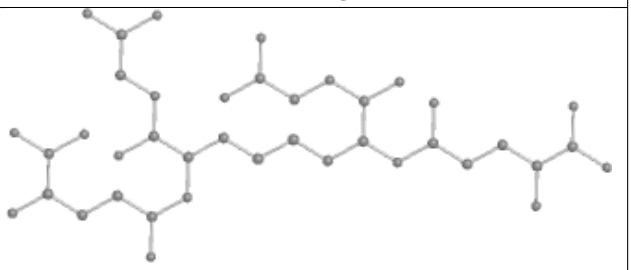
Bond lengths



Bond angles

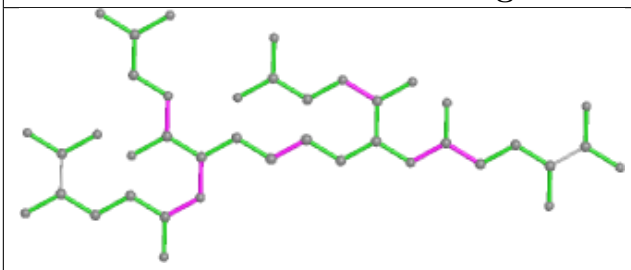


Torsions

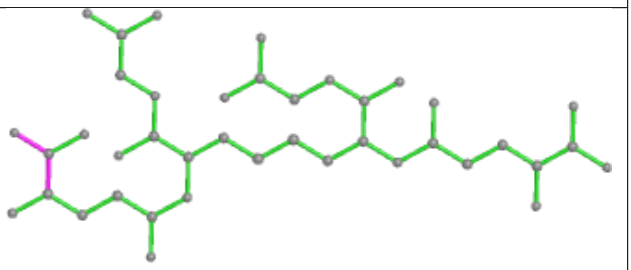


Rings

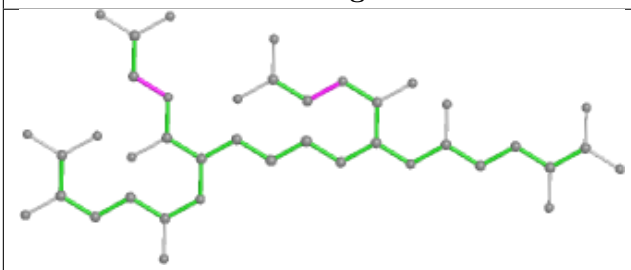
Ligand GDS DAA 301



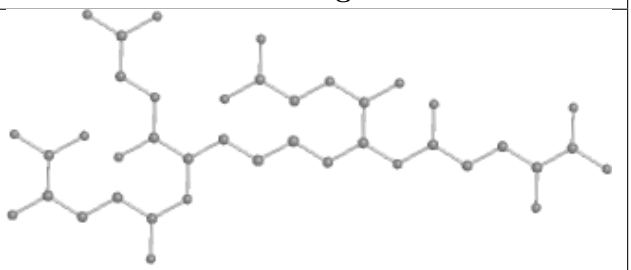
Bond lengths



Bond angles

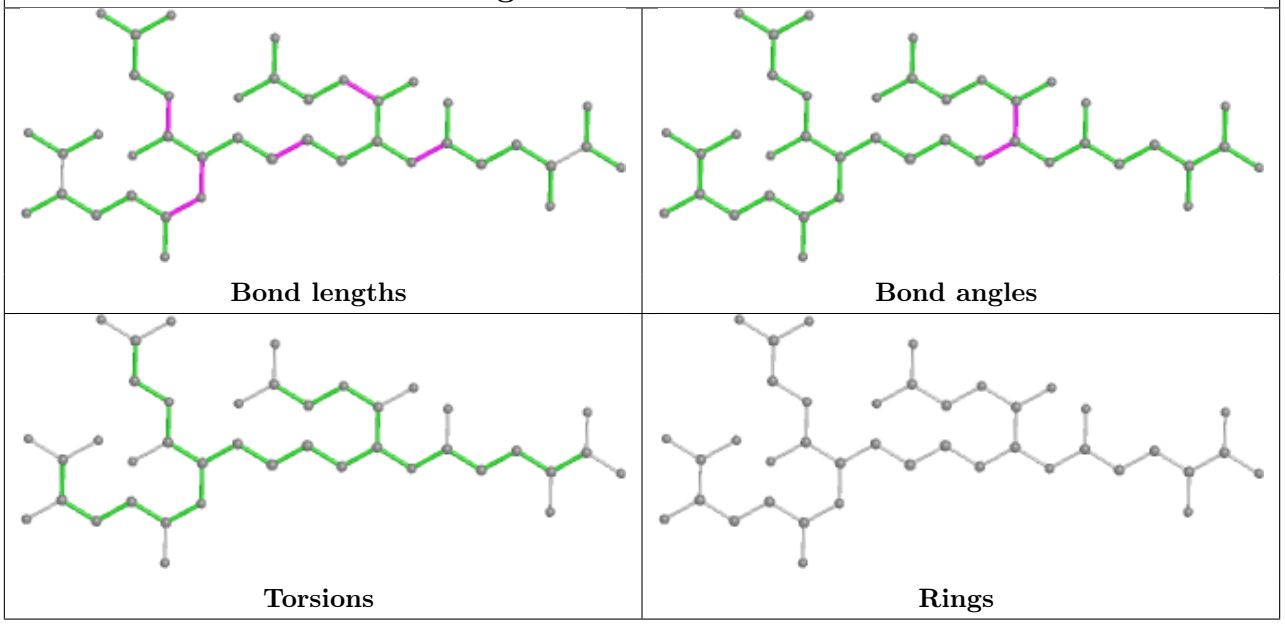


Torsions

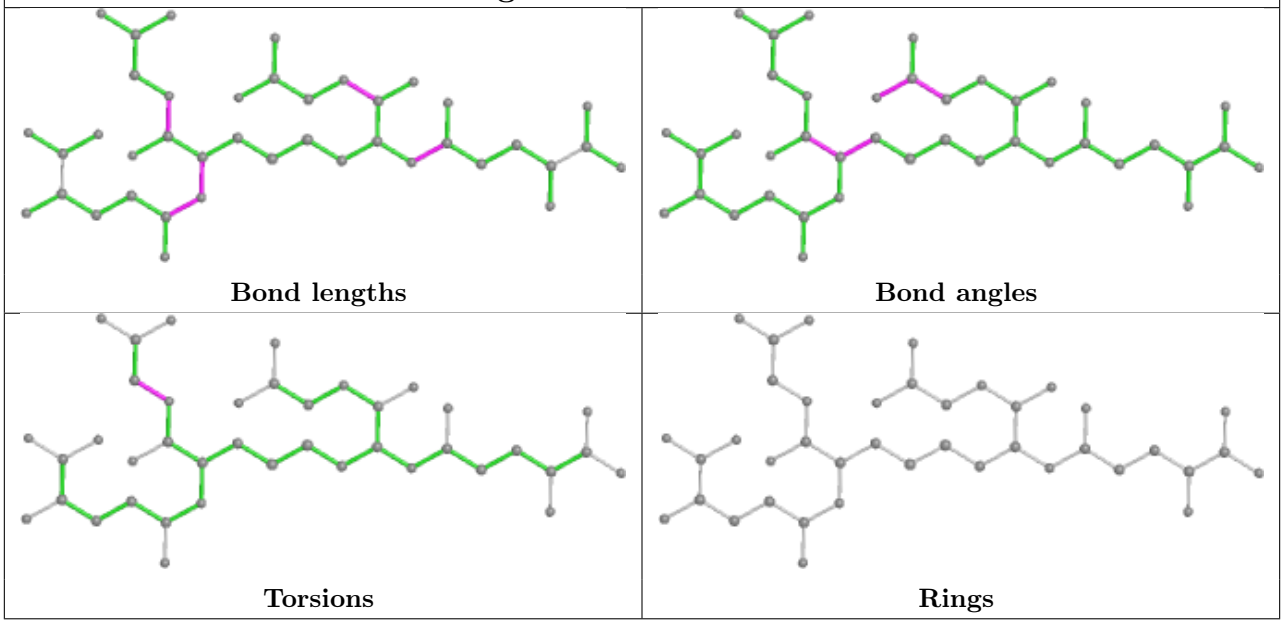


Rings

Ligand GDS AAA 301



Ligand GDS CAA 301



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	AAA	202/214 (94%)	-0.71	3 (1%)	73	75	5, 9, 23, 33	4 (1%)
2	B	207/213 (97%)	-0.57	6 (2%)	51	49	5, 11, 29, 43	11 (5%)
3	CAA	198/204 (97%)	-0.71	3 (1%)	73	75	5, 9, 21, 47	0
4	DAA	197/203 (97%)	-0.65	1 (0%)	91	91	5, 10, 22, 48	0
All	All	804/834 (96%)	-0.66	13 (1%)	72	73	5, 10, 24, 48	15 (1%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	DAA	0	PRO	7.4
2	B	-1	GLY	5.2
3	CAA	-1	GLY	3.8
2	B	206	GLU	3.6
3	CAA	202	ARG	3.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

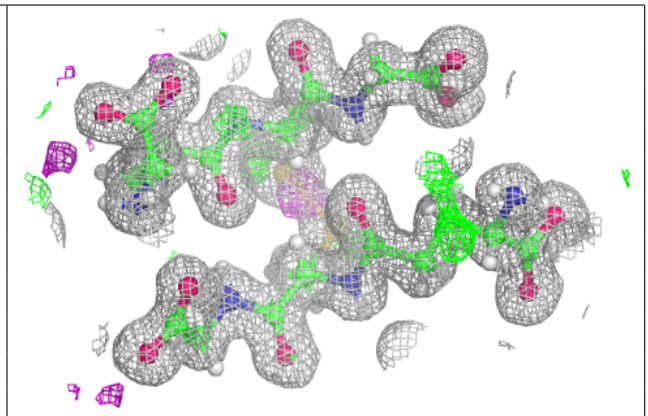
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

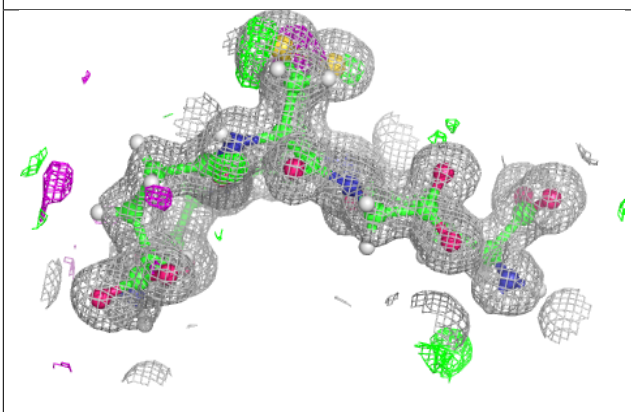
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	B	302	4/4	0.67	0.25	42,50,50,50	0
6	EDO	AAA	302	4/4	0.68	0.28	31,38,38,38	10
6	EDO	B	303	4/4	0.69	0.25	44,53,54,54	0
6	EDO	CAA	303	4/4	0.76	0.23	42,51,51,51	0
6	EDO	CAA	302	4/4	0.82	0.14	32,38,39,39	0
7	GOL	AAA	303[A]	6/6	0.92	0.11	16,19,21,22	14
7	GOL	AAA	303[B]	6/6	0.92	0.11	19,23,24,24	14
5	GDS	DAA	301	40/40	0.98	0.04	5,10,17,17	0
5	GDS	CAA	301	40/40	0.99	0.04	6,9,16,17	0
5	GDS	AAA	301	40/40	0.99	0.04	4,8,13,14	0
5	GDS	B	301	40/40	0.99	0.04	5,9,13,15	0

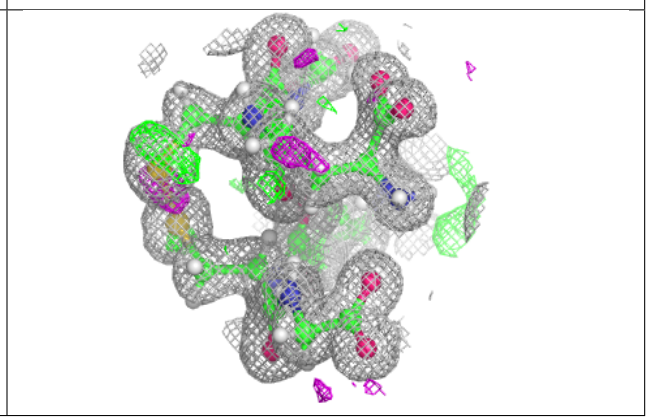
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDS DAA 301:

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

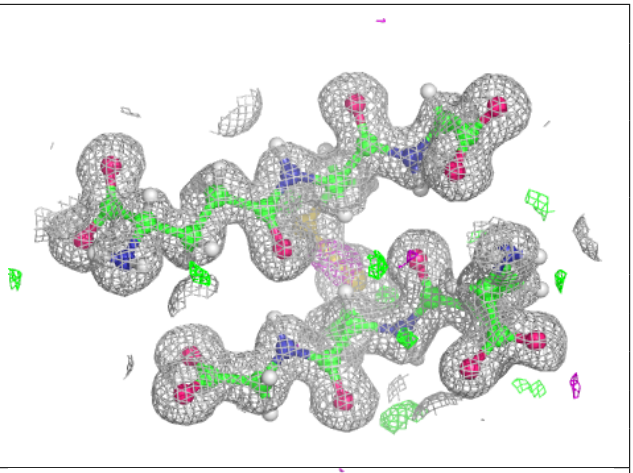


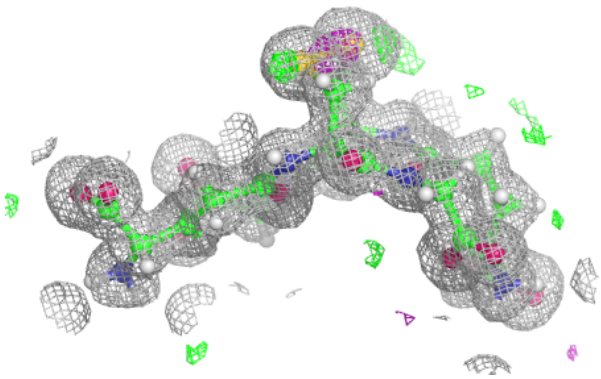


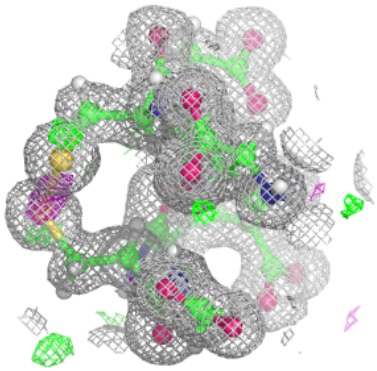


Electron density around GDS CAA 301:

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

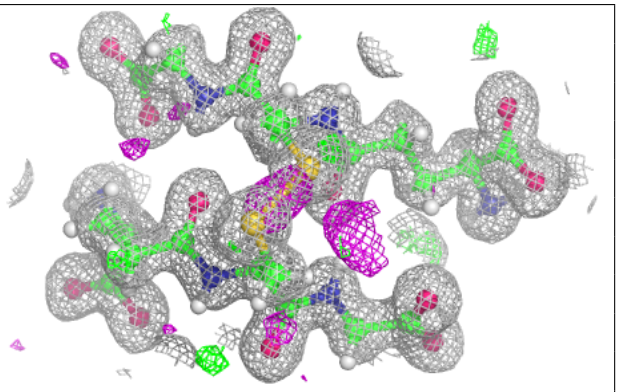


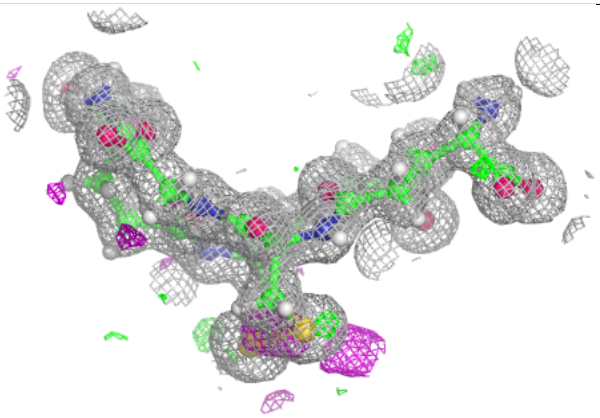


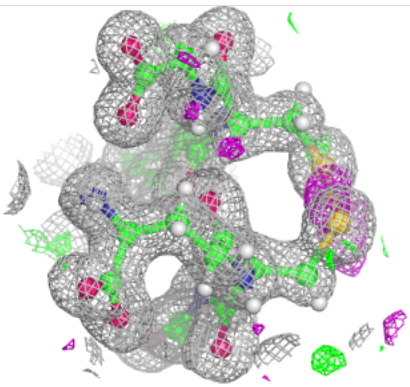


Electron density around GDS AAA 301:

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

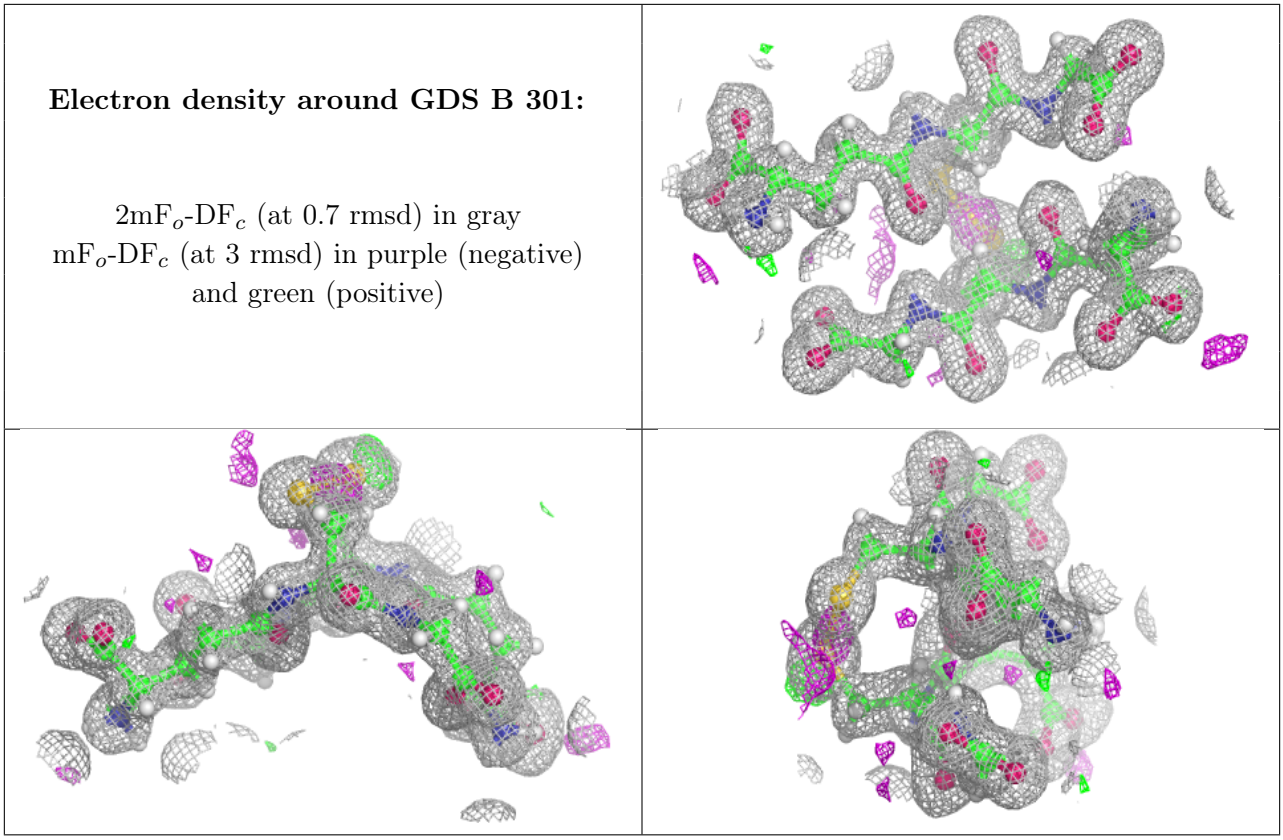






Electron density around GDS B 301:

$2mF_o$-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.