



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:41 AM UTC

PDB ID : 7OZA / pdb_00007oza
Title : Sulfated host glycan recognition by carbohydrate sulfatases of the human gut microbiota (BT3796_S1_16)
Authors : Cartmell, A.
Deposited on : 2021-06-27
Resolution : 1.50 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

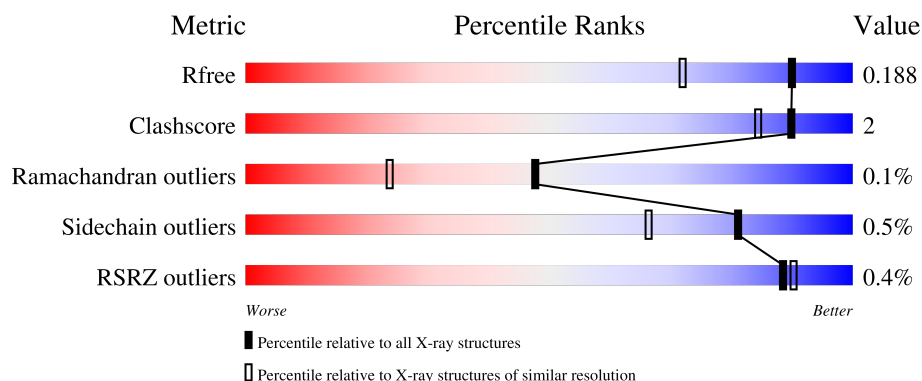
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	522	 92% 7%
1	CCC	522	 89% 5% 7%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8630 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 Putative secreted sulfatase ydeN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	487	Total	C	N	O	S	0	6	0
			3853	2451	646	735	21			
1	CCC	488	Total	C	N	O	S	0	12	0
			3923	2492	662	747	22			

There are 46 discrepancies between the modelled and reference sequences:

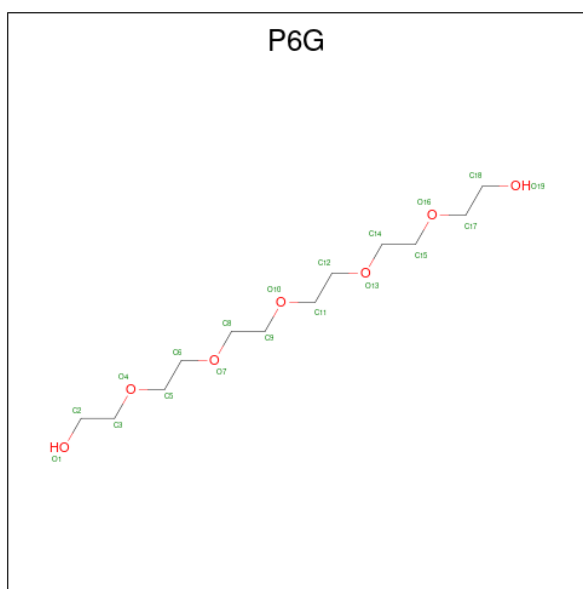
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-3	MET	-	initiating methionine	UNP Q8A171
AAA	-2	GLY	-	expression tag	UNP Q8A171
AAA	-1	SER	-	expression tag	UNP Q8A171
AAA	0	SER	-	expression tag	UNP Q8A171
AAA	1	HIS	-	expression tag	UNP Q8A171
AAA	2	HIS	-	expression tag	UNP Q8A171
AAA	3	HIS	-	expression tag	UNP Q8A171
AAA	4	HIS	-	expression tag	UNP Q8A171
AAA	5	HIS	-	expression tag	UNP Q8A171
AAA	6	HIS	-	expression tag	UNP Q8A171
AAA	7	SER	-	expression tag	UNP Q8A171
AAA	8	SER	-	expression tag	UNP Q8A171
AAA	9	GLY	-	expression tag	UNP Q8A171
AAA	10	LEU	-	expression tag	UNP Q8A171
AAA	11	VAL	-	expression tag	UNP Q8A171
AAA	12	PRO	-	expression tag	UNP Q8A171
AAA	13	ARG	-	expression tag	UNP Q8A171
AAA	14	GLY	-	expression tag	UNP Q8A171
AAA	15	SER	-	expression tag	UNP Q8A171
AAA	16	HIS	-	expression tag	UNP Q8A171
AAA	17	MET	-	expression tag	UNP Q8A171
AAA	18	ALA	-	expression tag	UNP Q8A171
AAA	19	SER	-	expression tag	UNP Q8A171
CCC	-3	MET	-	initiating methionine	UNP Q8A171
CCC	-2	GLY	-	expression tag	UNP Q8A171

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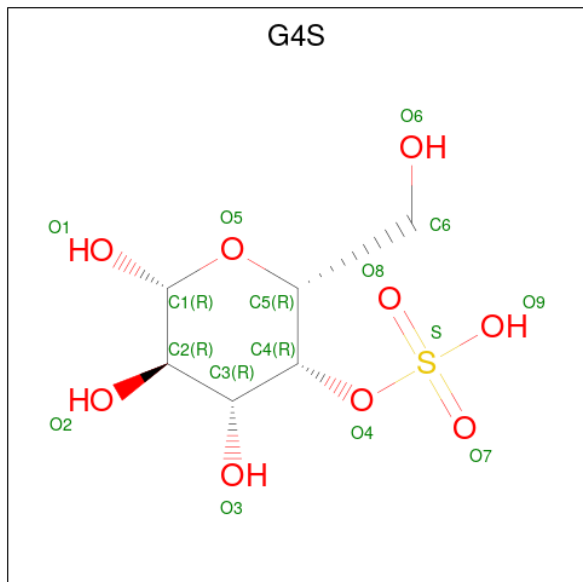
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-1	SER	-	expression tag	UNP Q8A171
CCC	0	SER	-	expression tag	UNP Q8A171
CCC	1	HIS	-	expression tag	UNP Q8A171
CCC	2	HIS	-	expression tag	UNP Q8A171
CCC	3	HIS	-	expression tag	UNP Q8A171
CCC	4	HIS	-	expression tag	UNP Q8A171
CCC	5	HIS	-	expression tag	UNP Q8A171
CCC	6	HIS	-	expression tag	UNP Q8A171
CCC	7	SER	-	expression tag	UNP Q8A171
CCC	8	SER	-	expression tag	UNP Q8A171
CCC	9	GLY	-	expression tag	UNP Q8A171
CCC	10	LEU	-	expression tag	UNP Q8A171
CCC	11	VAL	-	expression tag	UNP Q8A171
CCC	12	PRO	-	expression tag	UNP Q8A171
CCC	13	ARG	-	expression tag	UNP Q8A171
CCC	14	GLY	-	expression tag	UNP Q8A171
CCC	15	SER	-	expression tag	UNP Q8A171
CCC	16	HIS	-	expression tag	UNP Q8A171
CCC	17	MET	-	expression tag	UNP Q8A171
CCC	18	ALA	-	expression tag	UNP Q8A171
CCC	19	SER	-	expression tag	UNP Q8A171

- Molecule 2 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is 4-O-sulfo-beta-D-galactopyranose (CCD ID: G4S) (formula: $C_6H_{12}O_9S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	O	S	0	1
			32	12	18	2		
3	CCC	1	Total	C	O	S	0	0
			16	6	9	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

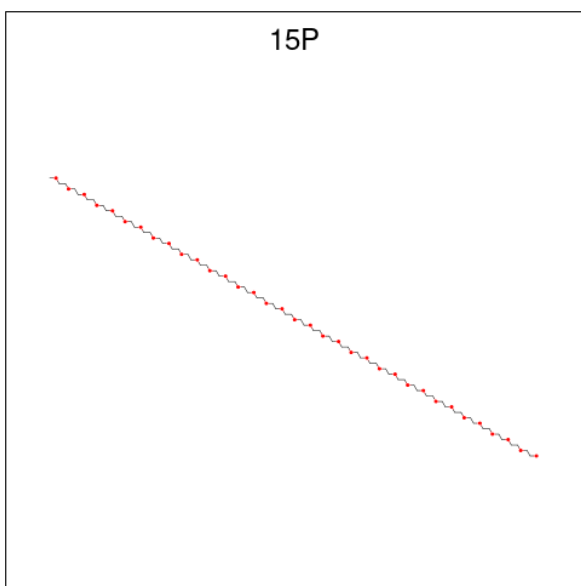
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Ca	0	0
			1	1		
4	CCC	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	CCC	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	CCC	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is POLYETHYLENE GLYCOL (N=34) (CCD ID: 15P) (formula: $C_{69}H_{140}O_{35}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	CCC	1	Total	C	O	0	0
			11	7	4		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	CCC	1	Total 1	Cl 1	0	0

- Molecule 8 is water.

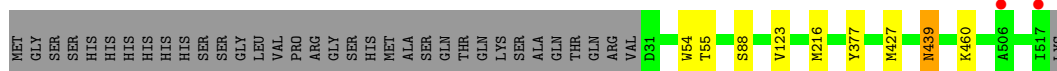
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	355	Total 355	O 355	0	0
8	CCC	400	Total 400	O 400	0	0

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.

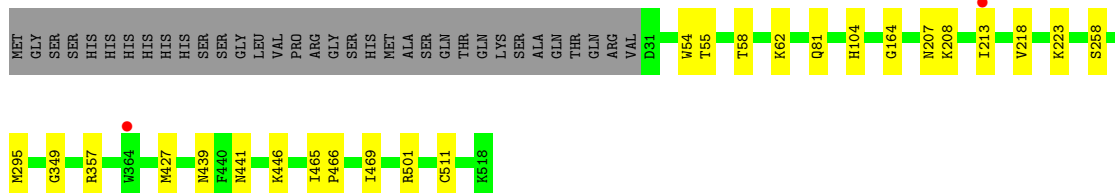
- Molecule 1: Putative secreted sulfatase ydeN

Chain AAA:  92% 7%



- Molecule 1: Putative secreted sulfatase ydeN

Chain CCC:  89% 5% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.18Å 88.95Å 87.91Å 90.00° 112.05° 90.00°	Depositor
Resolution (Å)	81.61 – 1.50 81.48 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (81.61-1.50) 99.5 (81.48-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.141 , 0.176 (Not available) , 0.188	Depositor DCC
R_{free} test set	9115 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8630	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P6G, 15P, G4S, CA, CL, MES

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	0.94	1/3959 (0.0%)	1.11	0/5383
1	CCC	1.00	2/4029 (0.0%)	1.12	1/5474 (0.0%)
All	All	0.97	3/7988 (0.0%)	1.12	1/10857 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	104	HIS	CE1-NE2	7.13	1.39	1.32
1	AAA	123	VAL	C-O	5.70	1.29	1.23
1	CCC	218	VAL	N-CA	5.45	1.50	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	295	MET	N-CA-C	-5.06	105.77	111.28

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	AAA	3853	0	3655	6	0
1	CCC	3923	0	3732	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AAA	13	0	16	2	0
3	AAA	32	0	22	1	0
3	CCC	16	0	11	0	0
4	AAA	1	0	0	0	0
4	CCC	1	0	0	0	0
5	CCC	24	0	26	0	0
6	CCC	11	0	13	9	0
7	CCC	1	0	0	0	0
8	AAA	355	0	0	2	0
8	CCC	400	0	0	1	1
All	All	8630	0	7475	28	1

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 2.

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:AAA:427[A]:MET:HE2	8:AAA:945:HOH:O	1.98	0.63
1:CCC:427[A]:MET:HE3	1:CCC:439:ASN:H	1.62	0.63
1:CCC:81:GLN:HE22	6:CCC:602:15P:H16	1.68	0.59
1:CCC:357:ARG:HH22	6:CCC:602:15P:C2	2.16	0.58
1:CCC:427[A]:MET:O	1:CCC:427[A]:MET:HG2	2.05	0.57
1:AAA:88[B]:SER:OG	3:AAA:802[B]:G4S:O9	2.24	0.55
2:AAA:801:P6G:C6	8:AAA:910:HOH:O	2.55	0.53
1:CCC:427[A]:MET:CE	1:CCC:439:ASN:H	2.21	0.53
1:AAA:427[A]:MET:HE1	1:AAA:439:ASN:H	1.74	0.51
1:CCC:427[A]:MET:O	1:CCC:427[A]:MET:CG	2.60	0.50
1:CCC:357:ARG:HH22	6:CCC:602:15P:H12	1.76	0.50
1:AAA:54:TRP:CG	1:AAA:55:THR:H	2.31	0.48
1:CCC:357:ARG:HH12	6:CCC:602:15P:H12	1.79	0.48
1:CCC:466:PRO:HG3	6:CCC:602:15P:C5	2.43	0.48
1:CCC:466:PRO:HG3	6:CCC:602:15P:H15	1.96	0.48
1:CCC:427[A]:MET:HE3	1:CCC:439:ASN:N	2.30	0.47
1:CCC:58:THR:O	1:CCC:62[A]:LYS:HE3	2.17	0.44
1:CCC:446:LYS:HE3	8:CCC:798:HOH:O	2.16	0.44
1:AAA:460:LYS:HD2	2:AAA:801:P6G:H112	2.00	0.44
1:CCC:207:ASN:HB3	1:CCC:213[B]:ILE:HD11	2.01	0.43
1:CCC:469:ILE:HG13	6:CCC:602:15P:H21	1.99	0.43
1:CCC:357:ARG:NH2	6:CCC:602:15P:H12	2.35	0.42
1:CCC:54:TRP:CG	1:CCC:55:THR:H	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:465:ILE:O	6:CCC:602:15P:C1	2.68	0.42
1:CCC:501:ARG:HD2	1:CCC:511:CYS:O	2.21	0.41
1:CCC:349:GLY:O	1:CCC:427[A]:MET:HE1	2.20	0.41
1:AAA:216:MET:HE2	1:AAA:216:MET:N	2.36	0.40
1:CCC:164:GLY:HA3	1:CCC:258:SER:O	2.21	0.40

All (1) 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:CCC:983:HOH:O	8:CCC:1044:HOH:O[2_655]	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	491/522 (94%)	479 (98%)	11 (2%)	1 (0%)	43	22
1	CCC	499/522 (96%)	487 (98%)	12 (2%)	0	100	100
All	All	990/1044 (95%)	966 (98%)	23 (2%)	1 (0%)	48	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	439	ASN

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	404/444 (91%)	403 (100%)	1 (0%)	87	77
1	CCC	412/444 (93%)	409 (99%)	3 (1%)	76	57
All	All	816/888 (92%)	812 (100%)	4 (0%)	81	66

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

Mol	Chain	Res	Type
1	AAA	377	TYR
1	CCC	208	LYS
1	CCC	223	LYS
1	CCC	441	ASN

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

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	G4S	AAA	802[B]	4	16,16,16	0.43	0	21,24,24	0.58	0
5	MES	CCC	601	-	12,12,12	0.73	0	15,16,16	0.44	0
2	P6G	AAA	801	-	12,12,18	0.35	0	11,11,17	0.32	0
6	15P	CCC	602	-	10,10,103	0.34	0	9,9,102	0.21	0
3	G4S	AAA	802[A]	4	16,16,16	0.44	0	21,24,24	0.63	0
5	MES	CCC	603	-	12,12,12	0.71	0	15,16,16	0.43	0
3	G4S	CCC	604	4	16,16,16	0.61	0	21,24,24	0.74	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
3	G4S	AAA	802[B]	4	-	2/7/27/27	0/1/1/1
5	MES	CCC	601	-	-	0/6/14/14	0/1/1/1
2	P6G	AAA	801	-	-	6/10/10/16	-
6	15P	CCC	602	-	-	7/8/8/101	-
3	G4S	AAA	802[A]	4	-	1/7/27/27	0/1/1/1
5	MES	CCC	603	-	-	1/6/14/14	0/1/1/1
3	G4S	CCC	604	4	-	1/7/27/27	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	CCC	603	MES	N4-C7-C8-S
6	CCC	602	15P	C3-C4-O2-C5
6	CCC	602	15P	O1-C3-C4-O2
3	AAA	802[B]	G4S	O5-C5-C6-O6
6	CCC	602	15P	C5-C6-O3-C7
3	AAA	802[B]	G4S	C4-C5-C6-O6
6	CCC	602	15P	C1-C2-O1-C3
2	AAA	801	P6G	O10-C11-C12-O13
2	AAA	801	P6G	O13-C14-C15-O16
6	CCC	602	15P	OXT-C1-C2-O1
6	CCC	602	15P	O2-C5-C6-O3
2	AAA	801	P6G	O4-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
3	CCC	604	G4S	O5-C5-C6-O6
3	AAA	802[A]	G4S	O5-C5-C6-O6
2	AAA	801	P6G	O7-C8-C9-O10
2	AAA	801	P6G	C8-C9-O10-C11
6	CCC	602	15P	C6-C5-O2-C4
2	AAA	801	P6G	C12-C11-O10-C9

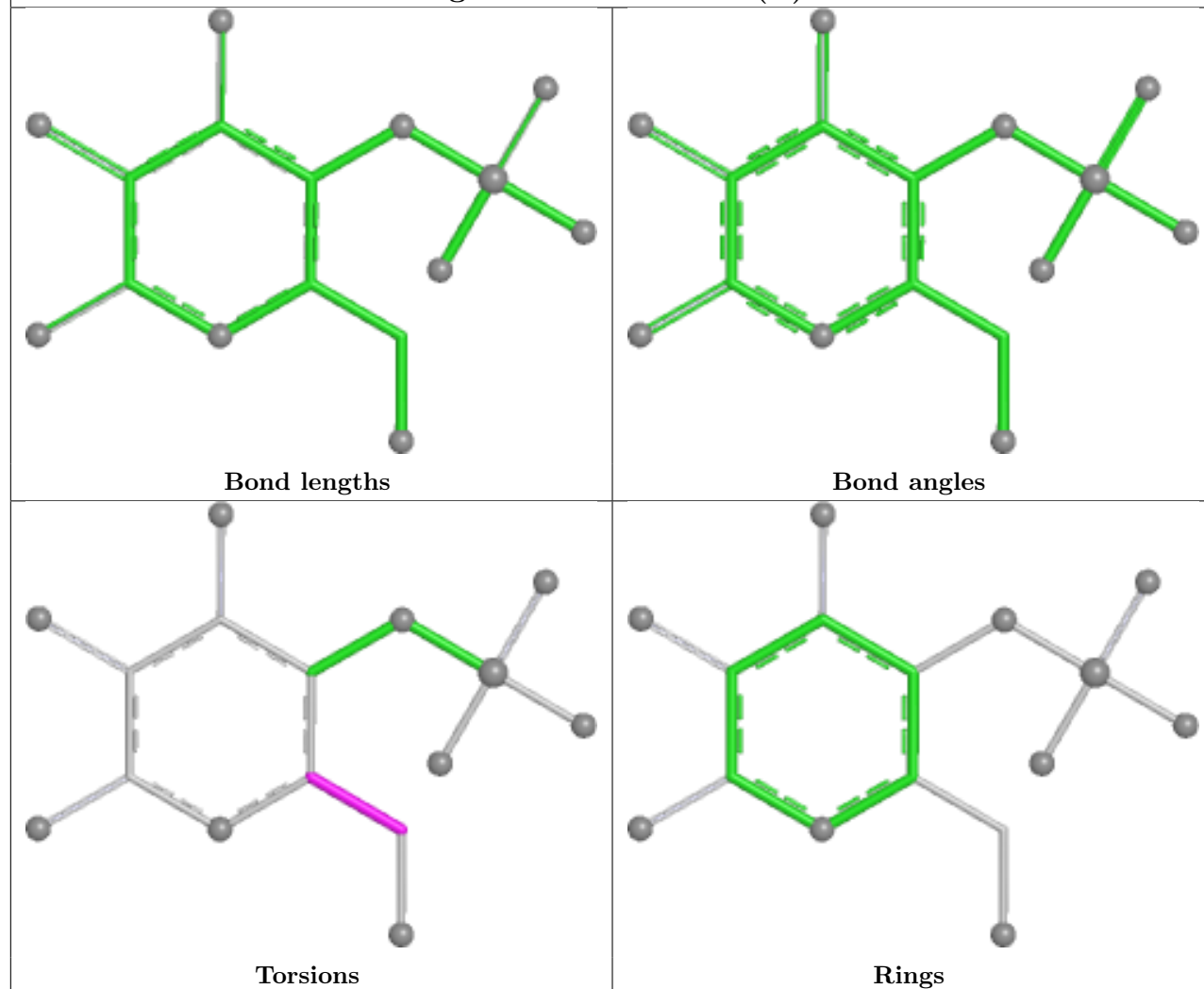
There are no ring outliers.

3 monomers are involved in 12 short contacts:

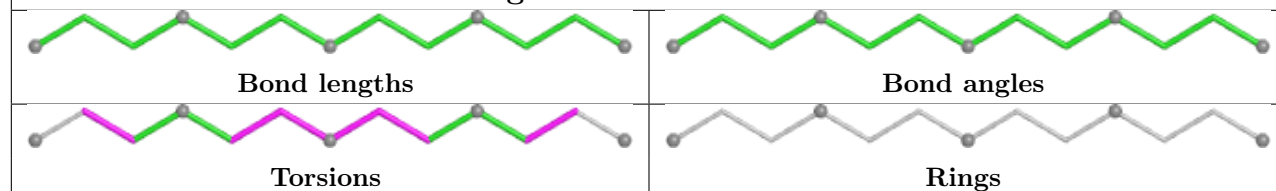
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	802[B]	G4S	1	0
2	AAA	801	P6G	2	0
6	CCC	602	15P	9	0

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.

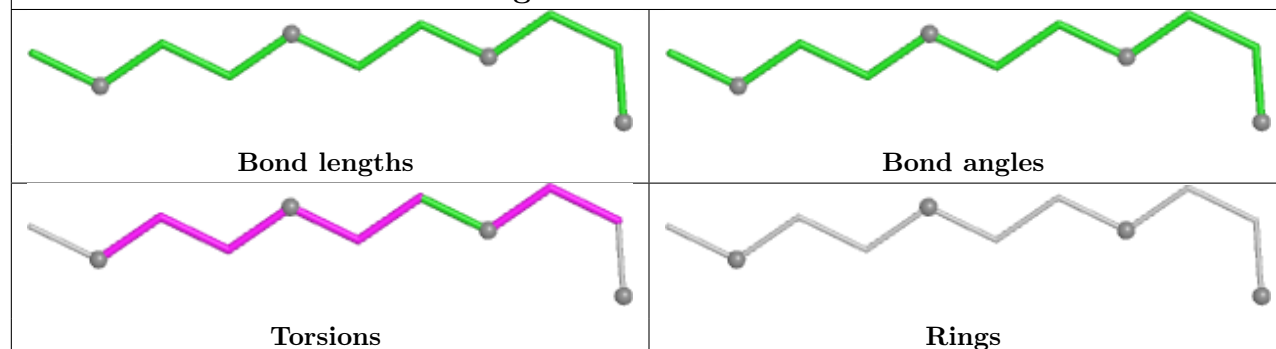
Ligand G4S AAA 802 (B)



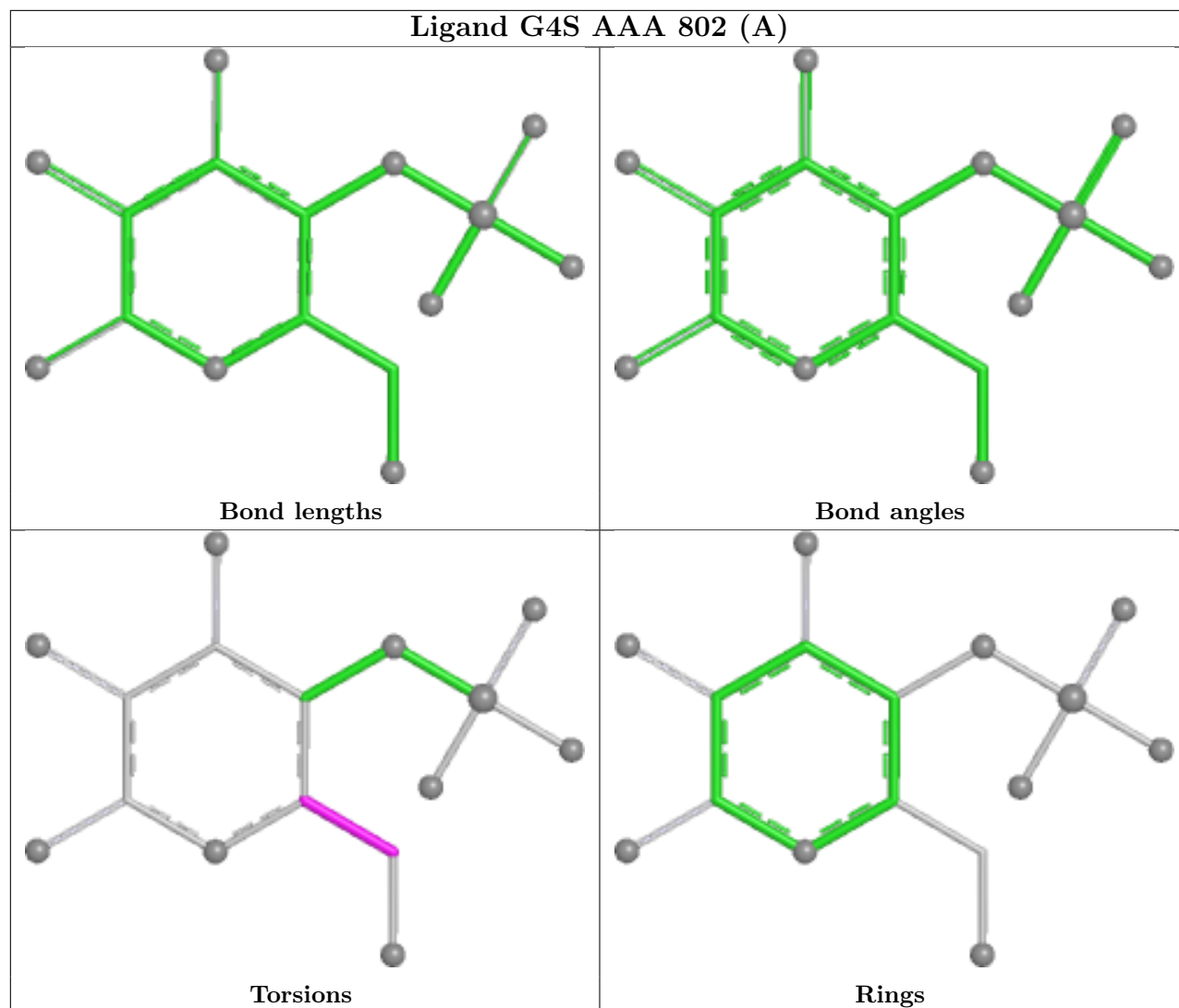
Ligand P6G AAA 801

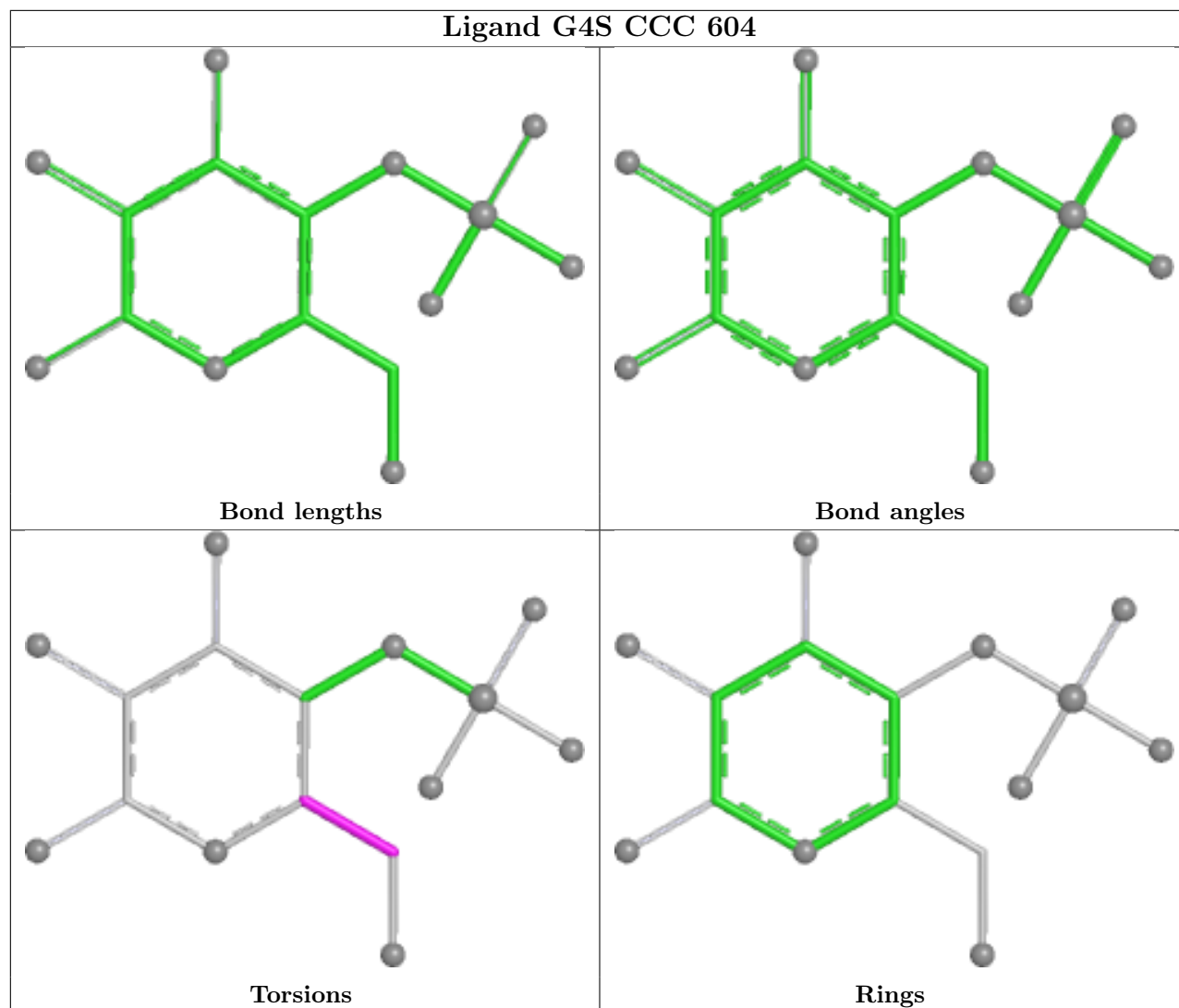


Ligand 15P CCC 602



Ligand G4S AAA 802 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	487/522 (93%)	-0.41	2 (0%) 88 90	7, 17, 32, 52	6 (1%)
1	CCC	488/522 (93%)	-0.53	2 (0%) 88 90	6, 15, 25, 52	12 (2%)
All	All	975/1044 (93%)	-0.47	4 (0%) 88 90	6, 16, 30, 52	18 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	364	TRP	3.4
1	AAA	517	ILE	3.1
1	AAA	506	ALA	3.0
1	CCC	213[A]	ILE	2.9

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MES	CCC	603	12/12	0.74	0.19	50,64,81,90	0

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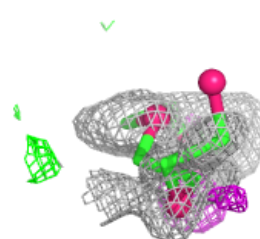
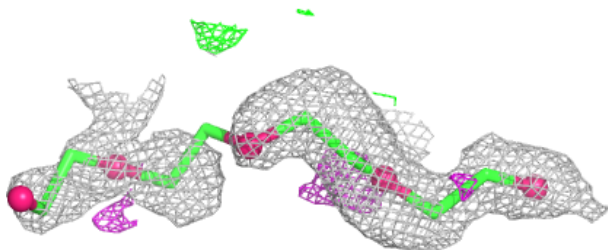
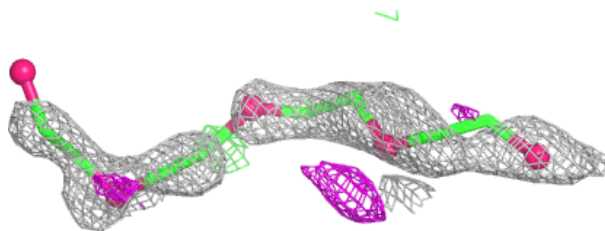
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	P6G	AAA	801	13/19	0.81	0.18	47,57,62,66	0
6	15P	CCC	602	11/104	0.84	0.15	17,22,28,31	11
5	MES	CCC	601	12/12	0.95	0.10	28,33,37,39	0
3	G4S	AAA	802[B]	16/16	0.97	0.07	21,26,32,36	16
3	G4S	AAA	802[A]	16/16	0.97	0.07	16,21,23,28	16
3	G4S	CCC	604	16/16	0.99	0.03	12,13,16,16	0
4	CA	AAA	803	1/1	0.99	0.03	15,15,15,15	1
4	CA	CCC	605	1/1	0.99	0.05	14,14,14,14	1
7	CL	CCC	606	1/1	0.99	0.07	27,27,27,27	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.

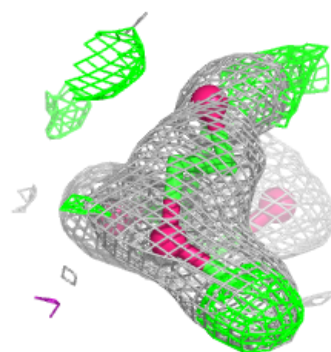
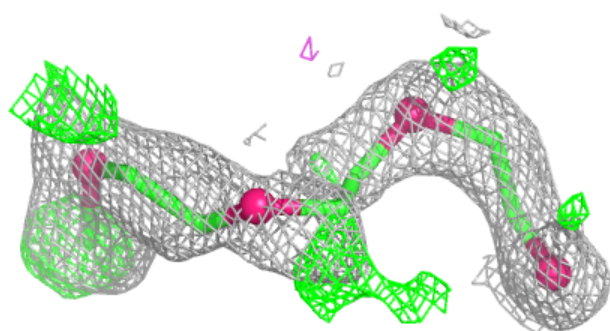
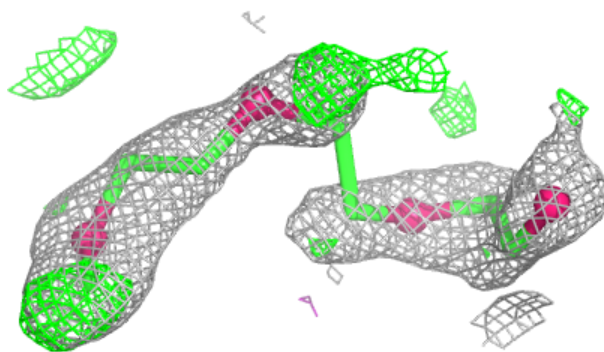
Electron density around P6G AAA 801:

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



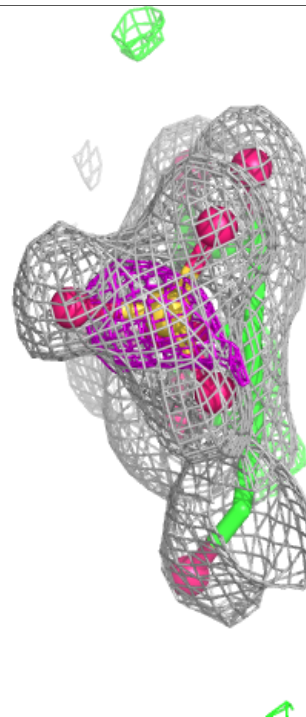
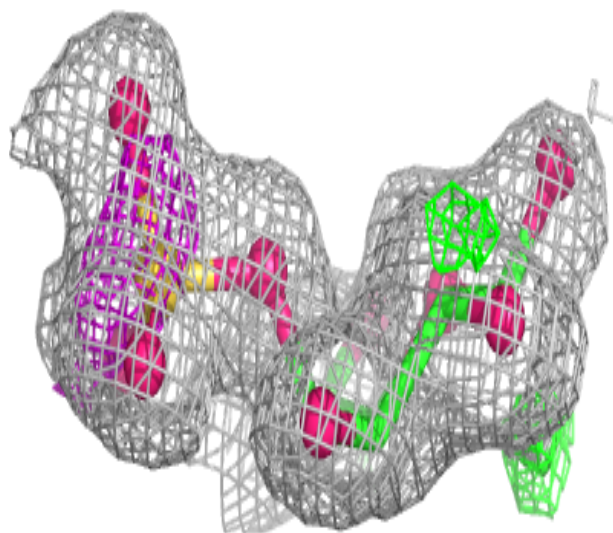
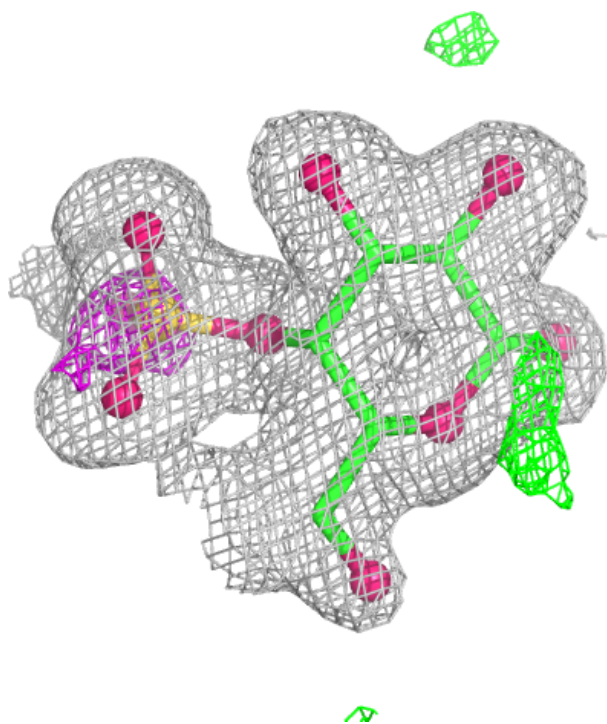
Electron density around 15P CCC 602:

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



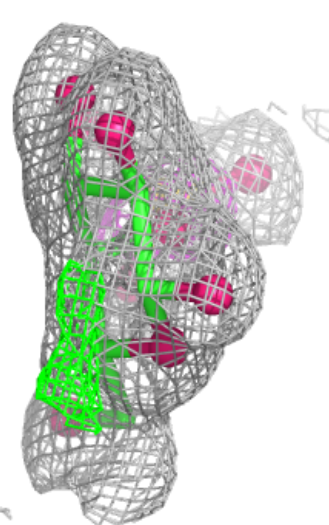
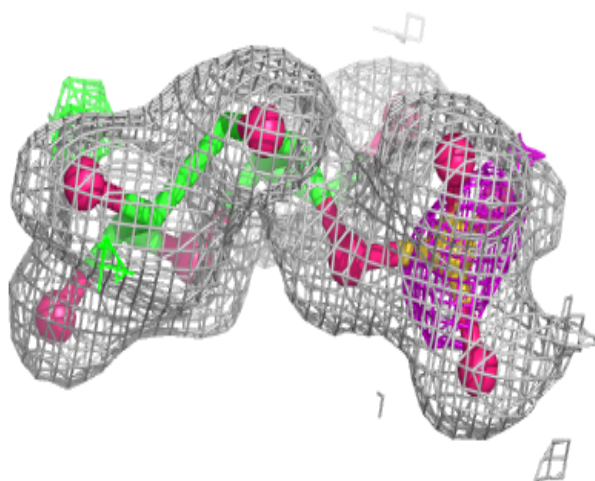
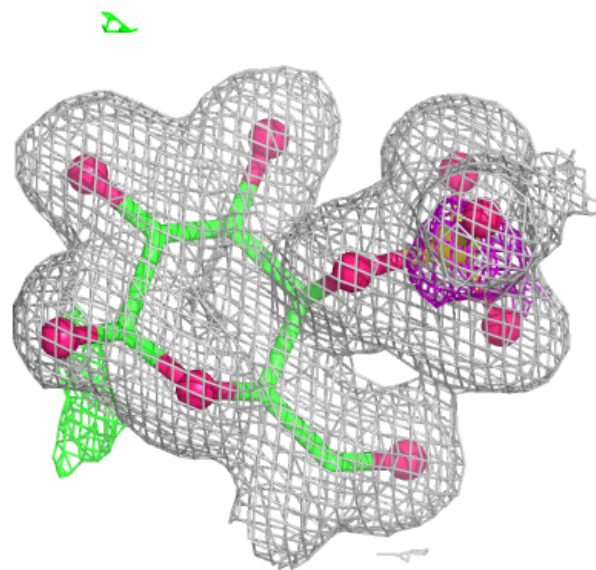
Electron density around G4S AAA 802 (B):

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



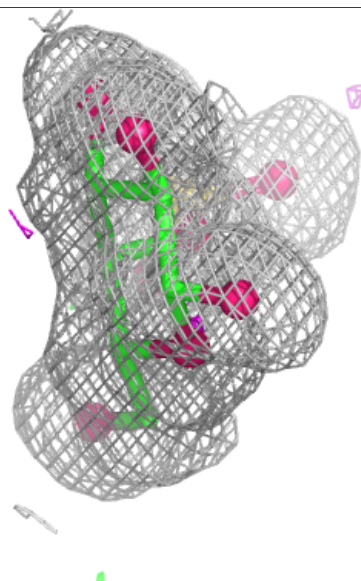
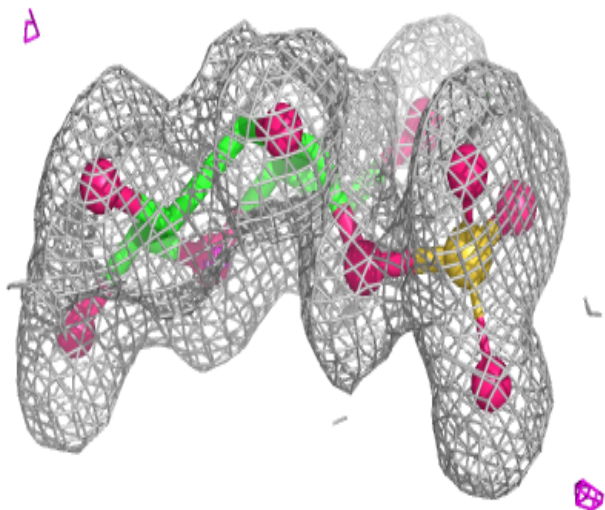
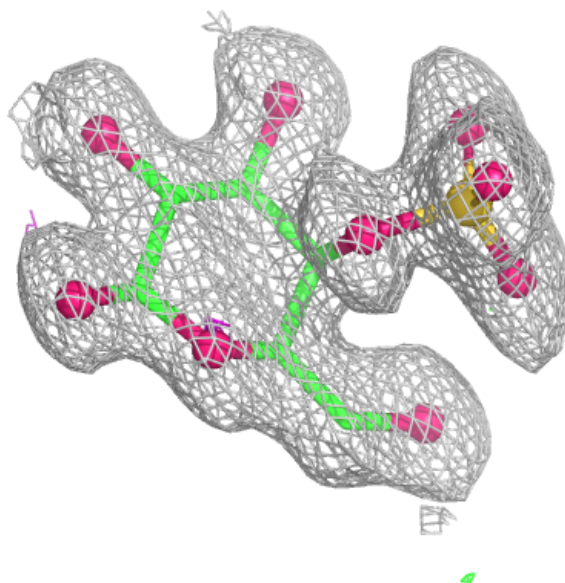
Electron density around G4S AAA 802 (A):

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



Electron density around G4S CCC 604:

$2mF_o-DF_c$ (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.