



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:29 PM BST

PDB ID : 3JTC  
Title : Importance of Mg<sup>2+</sup> in the Ca<sup>2+</sup>-Dependent Folding of the gamma-Carboxyglutamic Acid Domains of Vitamin K-Dependent clotting and anticlotting Proteins  
Authors : Bajaj, S.P.; Vadivel, K.; Agah, S.; Cascio, D.; Krishnaswamy, S.; Esmon, C.; Padmanabhan, K.  
Deposited on : 2009-09-11  
Resolution : 1.60 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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

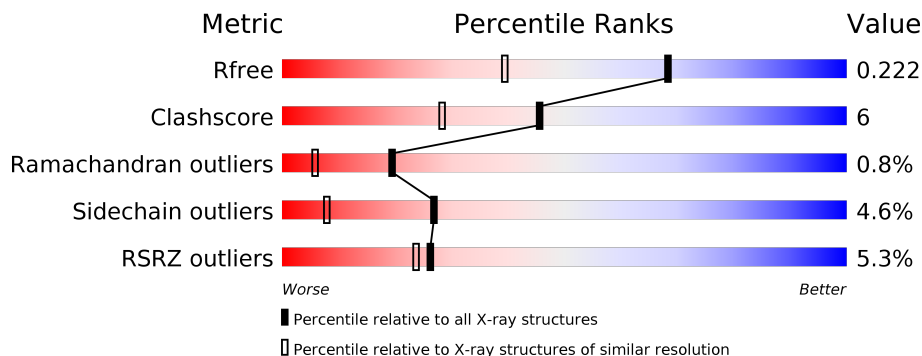
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	193	 3% 73% 15% • 11%
1	B	193	 7% 71% 18% • 10%
2	C	33	 88% 12%
2	D	33	 6% 73% 27%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	603	-	-	X	-
3	NAG	A	605	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4027 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.

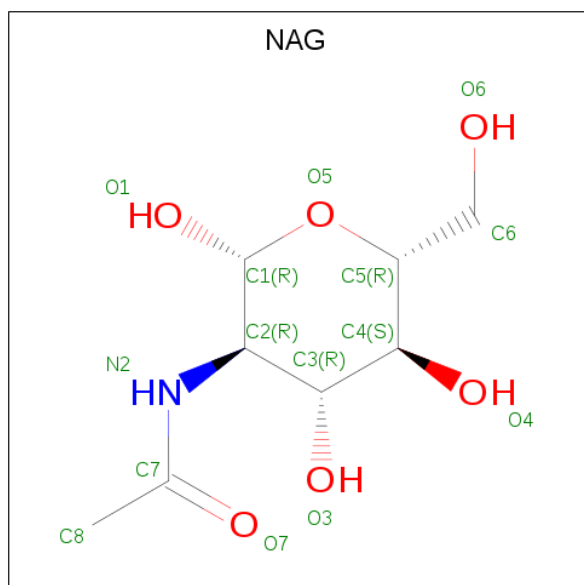
- Molecule 1 is a protein called Endothelial protein C receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	172	Total 1402	C 895	N 249	O 254	S 4	0	0	0
1	B	173	Total 1412	C 901	N 250	O 257	S 4	0	0	0

- Molecule 2 is a protein called Vitamin K-dependent protein C.

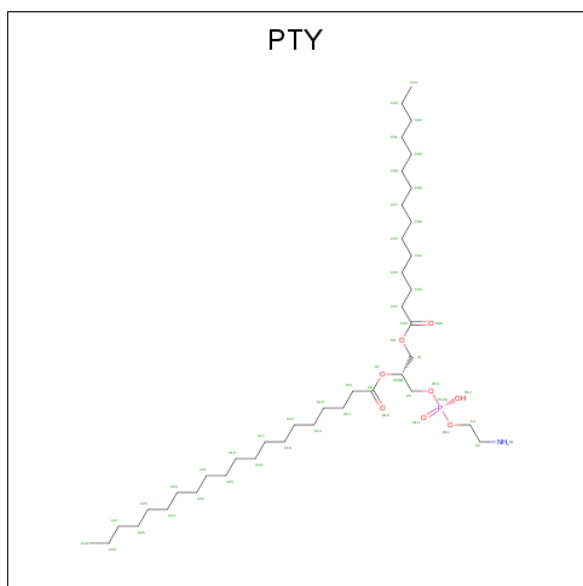
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	33	Total 304	C 179	N 45	O 78	S 2	0	0	0
2	D	33	Total 304	C 179	N 45	O 78	S 2	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
4	B	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Mg	0	0
			2	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	5	Total	Ca	0	0
			5	5		
6	C	5	Total	Ca	0	0
			5	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	179	Total	O	0	0
			179	179		
7	B	115	Total	O	0	0
			115	115		
7	C	66	Total	O	0	0
			66	66		
7	D	47	Total	O	0	0
			47	47		

### 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.

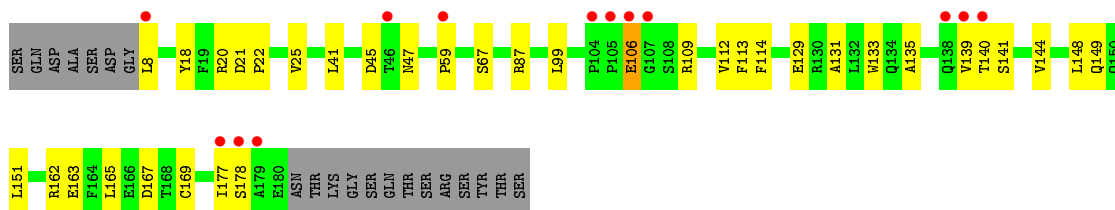
- Molecule 1: Endothelial protein C receptor

Chain A: 




- Molecule 1: Endothelial protein C receptor

Chain B: 



- Molecule 2: Vitamin K-dependent protein C

Chain C: 



- Molecule 2: Vitamin K-dependent protein C

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.22Å 62.36Å 71.03Å 90.00° 101.81° 90.00°	Depositor
Resolution (Å)	23.22 – 1.60 23.22 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.1 (23.22-1.60) 89.1 (23.22-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.191 , 0.226 0.188 , 0.222	Depositor DCC
$R_{free}$ test set	3024 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4027	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.26% 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  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: CGU, MG, CA, NAG, PTY

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	1.23	2/1440 (0.1%)	1.13	3/1960 (0.2%)
1	B	1.24	3/1450 (0.2%)	1.07	2/1974 (0.1%)
2	C	1.33	0/193	1.23	1/246 (0.4%)
2	D	1.24	0/193	1.24	2/246 (0.8%)
All	All	1.24	5/3276 (0.2%)	1.12	8/4426 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	18	TYR	CG-CD1	5.63	1.46	1.39
1	A	172	TYR	CG-CD1	5.56	1.46	1.39
1	A	129	GLU	CD-OE1	5.28	1.31	1.25
1	B	129	GLU	CG-CD	5.16	1.59	1.51
1	B	113	PHE	CE2-CZ	5.09	1.47	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	23	ASP	CB-CG-OD1	5.94	123.65	118.30
1	B	87	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	41	LEU	CB-CG-CD2	-5.78	101.18	111.00
1	A	21	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	123	PHE	CB-CG-CD2	-5.35	117.05	120.80
1	A	87	ARG	NE-CZ-NH1	-5.11	117.75	120.30
2	D	23	ASP	CB-CG-OD2	-5.02	113.78	118.30
2	C	15	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	1402	0	1354	23	0
1	B	1412	0	1362	15	0
2	C	304	0	237	1	0
2	D	304	0	235	4	0
3	A	42	0	39	10	0
3	B	42	0	39	1	0
4	A	50	0	79	2	0
4	B	50	0	79	2	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	1	0
7	A	179	0	0	1	0
7	B	115	0	0	2	0
7	C	66	0	0	0	0
7	D	47	0	0	1	0
All	All	4027	0	3424	45	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 6.

All (45) 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:16:ILE:CG1	3:A:603:NAG:O6	2.02	1.07
1:A:169:CYS:HA	4:A:606:PTY:H291	1.41	1.01
1:A:16:ILE:HG12	3:A:603:NAG:O6	1.63	0.95
1:A:16:ILE:HG13	3:A:603:NAG:O6	1.68	0.92
1:B:169:CYS:HA	4:B:607:PTY:H291	1.56	0.86
1:A:14:LEU:HD23	3:A:603:NAG:H5	1.60	0.82
1:A:20:ARG:HG3	7:A:718:HOH:O	1.83	0.79
2:D:10:HIS:HD2	2:D:11:SER:O	1.67	0.76
1:B:131:ALA:HB2	1:B:162:ARG:HD3	1.70	0.74
1:A:14:LEU:CD2	3:A:603:NAG:H5	2.19	0.73
1:A:169:CYS:CA	4:A:606:PTY:H291	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:SER:OG	1:B:144:VAL:HG23	1.93	0.68
1:B:177:ILE:HD12	1:B:178:SER:N	2.08	0.67
1:A:14:LEU:HD23	3:A:603:NAG:C5	2.27	0.63
6:D:39:CA:CA	7:D:69:HOH:O	1.78	0.61
1:B:149:GLN:NE2	7:B:727:HOH:O	2.34	0.60
2:D:16:CGU:O	2:D:22:CYS:HB3	2.04	0.56
1:A:21:ASP:HB2	1:A:22:PRO:CD	2.37	0.55
1:B:167:ASP:OD1	1:B:167:ASP:C	2.46	0.54
1:A:119:ASN:ND2	3:A:604:NAG:H83	2.24	0.53
1:A:123:PHE:CE1	1:A:144:VAL:HG22	2.45	0.51
1:B:135:ALA:HB2	1:B:148:LEU:HD11	1.91	0.51
1:B:21:ASP:HB2	1:B:22:PRO:CD	2.39	0.51
2:D:17:CYS:SG	2:D:30:ILE:CD1	2.99	0.50
1:A:16:ILE:CD1	1:A:96:ARG:HG3	2.41	0.50
1:A:131:ALA:HB2	1:A:162:ARG:HD3	1.95	0.49
1:A:163:GLU:O	1:A:167:ASP:HB2	2.13	0.48
1:B:25:VAL:CG1	1:B:45:ASP:HB3	2.43	0.48
1:B:169:CYS:CA	4:B:607:PTY:H291	2.38	0.47
1:A:119:ASN:HD22	3:A:604:NAG:H83	1.79	0.46
1:A:25:VAL:HG13	1:A:45:ASP:HB3	1.96	0.46
1:B:165:LEU:O	1:B:169:CYS:HB3	2.15	0.46
1:A:133:TRP:CD1	1:A:151:LEU:HB3	2.51	0.45
1:A:25:VAL:CG1	1:A:45:ASP:HB3	2.47	0.44
2:D:10:HIS:CD2	2:D:11:SER:O	2.58	0.44
1:A:22:PRO:HG3	1:A:91:PHE:CE1	2.53	0.44
1:A:36:HIS:NE2	1:A:54:GLN:OE1	2.38	0.43
3:B:601:NAG:H83	7:B:701:HOH:O	2.18	0.43
2:C:6:CGU:O	2:C:6:CGU:HG	2.18	0.43
1:B:21:ASP:HB2	1:B:22:PRO:HD2	2.01	0.43
1:B:163:GLU:O	1:B:167:ASP:HB3	2.19	0.42
1:A:28:GLN:HG2	3:A:603:NAG:H62	2.01	0.42
1:B:133:TRP:CD1	1:B:151:LEU:HB3	2.56	0.41
1:B:112:VAL:HB	1:B:165:LEU:HB3	2.03	0.41
1:A:16:ILE:CG1	3:A:603:NAG:HO6	2.28	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	170/193 (88%)	160 (94%)	9 (5%)	1 (1%)	25	8
1	B	171/193 (89%)	164 (96%)	5 (3%)	2 (1%)	13	2
2	C	22/33 (67%)	22 (100%)	0	0	100	100
2	D	22/33 (67%)	21 (96%)	1 (4%)	0	100	100
All	All	385/452 (85%)	367 (95%)	15 (4%)	3 (1%)	19	6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	106	GLU
1	B	47	ASN
1	A	88	THR

### 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	153/171 (90%)	148 (97%)	5 (3%)	38	14
1	B	154/171 (90%)	144 (94%)	10 (6%)	17	3
2	C	22/22 (100%)	21 (96%)	1 (4%)	27	8
2	D	22/22 (100%)	22 (100%)	0	100	100
All	All	351/386 (91%)	335 (95%)	16 (5%)	27	8

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	106	GLU
1	A	114	PHE
1	A	161	LEU
1	A	178	SER
1	B	8	LEU
1	B	20	ARG
1	B	59	PRO
1	B	67	SER
1	B	99	LEU
1	B	106	GLU
1	B	109	ARG
1	B	114	PHE
1	B	139	VAL
1	B	140	THR
2	C	33	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	174	GLN
1	B	54	GLN
1	B	149	GLN
1	B	171	GLN
1	B	174	GLN
2	C	33	ASN
2	D	10	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CGU	C	7	2,6	3,11,12	0.97	0	1,14,16	0.11	0
2	CGU	D	20	2,6	3,11,12	0.20	0	1,14,16	3.52	1 (100%)
2	CGU	D	7	2,6	3,11,12	0.62	0	1,14,16	0.37	0
2	CGU	D	16	2,6	3,11,12	0.76	0	1,14,16	1.75	0
2	CGU	C	6	6	3,11,12	1.17	0	1,14,16	0.06	0
2	CGU	C	14	2,5	3,11,12	1.63	1 (33%)	1,14,16	0.90	0
2	CGU	D	19	5	3,11,12	0.60	0	1,14,16	0.89	0
2	CGU	C	19	5	3,11,12	0.86	0	1,14,16	0.53	0
2	CGU	C	25	5	3,11,12	0.69	0	1,14,16	0.39	0
2	CGU	D	26	2,6	3,11,12	1.33	1 (33%)	1,14,16	2.91	1 (100%)
2	CGU	D	29	2,5,6	3,11,12	1.16	0	1,14,16	1.34	0
2	CGU	D	6	6	3,11,12	1.12	0	1,14,16	0.68	0
2	CGU	C	16	2,6	3,11,12	0.61	0	1,14,16	0.47	0
2	CGU	D	25	5	3,11,12	0.68	0	1,14,16	0.43	0
2	CGU	C	26	2,6	3,11,12	0.50	0	1,14,16	1.36	0
2	CGU	C	20	2,6	3,11,12	0.73	0	1,14,16	0.88	0
2	CGU	C	29	2,5,6	3,11,12	1.34	0	1,14,16	0.13	0
2	CGU	D	14	2,5	3,11,12	1.12	0	1,14,16	0.51	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
2	CGU	C	7	2,6	-	0/5/14/16	-
2	CGU	D	20	2,6	-	0/5/14/16	-
2	CGU	D	7	2,6	-	0/5/14/16	-
2	CGU	D	16	2,6	-	0/5/14/16	-
2	CGU	C	6	6	-	3/5/14/16	-
2	CGU	C	14	2,5	-	0/5/14/16	-
2	CGU	D	19	5	-	0/5/14/16	-
2	CGU	C	19	5	-	0/5/14/16	-
2	CGU	C	25	5	-	0/5/14/16	-
2	CGU	D	26	2,6	-	0/5/14/16	-
2	CGU	D	29	2,5,6	-	0/5/14/16	-
2	CGU	D	6	6	-	3/5/14/16	-
2	CGU	C	16	2,6	-	1/5/14/16	-
2	CGU	D	25	5	-	0/5/14/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CGU	C	26	2,6	-	0/5/14/16	-
2	CGU	C	20	2,6	-	0/5/14/16	-
2	CGU	C	29	2,5,6	-	1/5/14/16	-
2	CGU	D	14	2,5	-	0/5/14/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	26	CGU	CB-CG	2.29	1.58	1.53
2	C	14	CGU	CB-CG	-2.03	1.49	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	20	CGU	CB-CA-N	-3.52	102.48	110.32
2	D	26	CGU	CB-CA-N	2.91	116.81	110.32

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6	CGU	O-C-CA-CB
2	C	6	CGU	CA-CB-CG-CD2
2	D	6	CGU	O-C-CA-CB
2	D	6	CGU	CA-CB-CG-CD1
2	D	6	CGU	CA-CB-CG-CD2
2	C	16	CGU	O-C-CA-CB
2	C	29	CGU	O-C-CA-CB
2	C	6	CGU	CA-CB-CG-CD1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	16	CGU	1	0
2	C	6	CGU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry i

Of 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 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	NAG	B	601	1	14,14,15	0.90	1 (7%)	17,19,21	1.49	4 (23%)
3	NAG	A	605	1	14,14,15	0.68	0	17,19,21	0.89	1 (5%)
3	NAG	B	600	1	14,14,15	1.20	1 (7%)	17,19,21	1.53	6 (35%)
4	PTY	A	606	-	49,49,49	1.06	4 (8%)	52,54,54	1.58	11 (21%)
3	NAG	B	602	1	14,14,15	0.51	0	17,19,21	0.71	0
3	NAG	A	604	1	14,14,15	1.10	1 (7%)	17,19,21	1.56	5 (29%)
3	NAG	A	603	1	14,14,15	0.73	0	17,19,21	2.96	8 (47%)
4	PTY	B	607	-	49,49,49	1.09	4 (8%)	52,54,54	1.35	5 (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	NAG	B	601	1	-	2/6/23/26	0/1/1/1
3	NAG	A	605	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	B	600	1	-	0/6/23/26	0/1/1/1
4	PTY	A	606	-	-	19/53/53/53	-
3	NAG	B	602	1	-	2/6/23/26	0/1/1/1
3	NAG	A	604	1	-	2/6/23/26	0/1/1/1
3	NAG	A	603	1	-	2/6/23/26	0/1/1/1
4	PTY	B	607	-	-	16/53/53/53	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	606	PTY	O7-C8	4.64	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	607	PTY	O7-C8	4.48	1.46	1.34
4	B	607	PTY	O4-C30	3.43	1.43	1.33
4	A	606	PTY	O4-C30	3.27	1.42	1.33
4	A	606	PTY	P1-O11	2.68	1.70	1.59
3	A	604	NAG	C1-C2	2.42	1.55	1.52
3	B	601	NAG	O3-C3	-2.37	1.37	1.43
4	A	606	PTY	C2-N1	-2.30	1.27	1.46
3	B	600	NAG	C8-C7	2.30	1.55	1.50
4	B	607	PTY	P1-O11	2.19	1.68	1.59
4	B	607	PTY	C2-N1	-2.13	1.29	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	NAG	C1-O5-C5	6.42	120.89	112.19
4	A	606	PTY	C5-C6-C1	-4.91	100.17	111.79
3	A	603	NAG	O3-C3-C4	-4.90	99.03	110.35
3	A	603	NAG	O5-C1-C2	-4.87	103.60	111.29
4	B	607	PTY	O4-C30-O30	-4.71	111.70	123.59
3	A	603	NAG	C4-C3-C2	-4.31	104.71	111.02
4	A	606	PTY	O7-C8-O10	-4.07	113.86	123.70
4	B	607	PTY	O4-C30-C31	4.02	124.52	111.91
4	A	606	PTY	O4-C30-O30	-3.89	113.76	123.59
3	A	603	NAG	O3-C3-C2	-3.86	101.48	109.47
4	B	607	PTY	C13-C12-C11	-3.25	101.50	113.19
3	B	601	NAG	O6-C6-C5	-3.20	100.31	111.29
3	A	603	NAG	C6-C5-C4	-3.08	105.80	113.00
3	B	601	NAG	C1-O5-C5	-2.91	108.25	112.19
4	A	606	PTY	O4-C30-C31	2.86	120.87	111.91
3	A	604	NAG	O5-C1-C2	-2.85	106.79	111.29
4	B	607	PTY	C5-C6-C1	-2.75	105.29	111.79
3	A	604	NAG	C2-N2-C7	2.59	126.59	122.90
3	A	604	NAG	O6-C6-C5	-2.55	102.56	111.29
4	B	607	PTY	C16-C15-C14	-2.54	101.54	114.42
3	B	600	NAG	O5-C1-C2	-2.52	107.30	111.29
3	B	600	NAG	O7-C7-C8	-2.48	117.44	122.06
3	A	605	NAG	C1-O5-C5	2.40	115.44	112.19
4	A	606	PTY	C26-C25-C24	-2.35	102.50	114.42
4	A	606	PTY	C1-O4-C30	2.33	125.74	117.12
4	A	606	PTY	C24-C23-C22	-2.27	102.92	114.42
3	B	600	NAG	C4-C3-C2	-2.25	107.72	111.02
3	A	603	NAG	C2-N2-C7	2.24	126.09	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	NAG	O4-C4-C3	-2.22	105.22	110.35
3	A	604	NAG	C6-C5-C4	2.21	118.19	113.00
3	A	603	NAG	O5-C5-C6	-2.18	103.79	107.20
3	B	601	NAG	O3-C3-C2	-2.18	104.96	109.47
3	B	600	NAG	O3-C3-C4	2.13	115.28	110.35
3	A	604	NAG	C3-C4-C5	-2.13	106.44	110.24
4	A	606	PTY	C23-C22-C21	-2.08	103.86	114.42
3	B	601	NAG	O5-C5-C4	-2.05	105.83	110.83
4	A	606	PTY	C20-C19-C18	-2.02	104.15	114.42
3	B	600	NAG	C1-O5-C5	2.02	114.93	112.19
4	A	606	PTY	O10-C8-C11	2.02	131.61	123.73
4	A	606	PTY	C41-C40-C39	2.01	124.61	114.42

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	605	NAG	C1

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	605	NAG	O5-C5-C6-O6
3	A	603	NAG	O5-C5-C6-O6
3	A	605	NAG	C4-C5-C6-O6
4	B	607	PTY	C30-C31-C32-C33
3	B	602	NAG	C4-C5-C6-O6
4	A	606	PTY	C30-C31-C32-C33
3	A	604	NAG	C8-C7-N2-C2
3	A	604	NAG	O7-C7-N2-C2
3	B	602	NAG	O5-C5-C6-O6
3	A	603	NAG	C4-C5-C6-O6
4	B	607	PTY	C22-C23-C24-C25
4	B	607	PTY	C23-C24-C25-C26
4	B	607	PTY	C16-C17-C18-C19
4	B	607	PTY	C37-C38-C39-C40
4	A	606	PTY	C23-C24-C25-C26
4	A	606	PTY	C17-C18-C19-C20
4	B	607	PTY	C24-C25-C26-C27
4	B	607	PTY	C34-C35-C36-C37
4	A	606	PTY	C16-C17-C18-C19
4	A	606	PTY	C18-C19-C20-C21
4	B	607	PTY	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
4	A	606	PTY	C22-C23-C24-C25
4	A	606	PTY	C14-C15-C16-C17
4	A	606	PTY	C32-C33-C34-C35
4	A	606	PTY	C35-C36-C37-C38
4	B	607	PTY	C26-C27-C28-C29
4	A	606	PTY	C38-C39-C40-C41
4	A	606	PTY	C25-C26-C27-C28
4	B	607	PTY	C18-C19-C20-C21
4	B	607	PTY	C6-C5-O14-P1
4	A	606	PTY	C6-C5-O14-P1
4	B	607	PTY	C15-C16-C17-C18
4	B	607	PTY	C19-C20-C21-C22
4	A	606	PTY	C34-C35-C36-C37
4	B	607	PTY	C14-C15-C16-C17
4	A	606	PTY	C37-C38-C39-C40
4	A	606	PTY	C19-C20-C21-C22
4	A	606	PTY	C40-C41-C42-C43
4	A	606	PTY	C36-C37-C38-C39
4	A	606	PTY	C21-C22-C23-C24
3	B	601	NAG	O5-C5-C6-O6
4	B	607	PTY	C32-C33-C34-C35
4	A	606	PTY	C26-C27-C28-C29
3	B	601	NAG	C4-C5-C6-O6
4	B	607	PTY	O4-C30-C31-C32

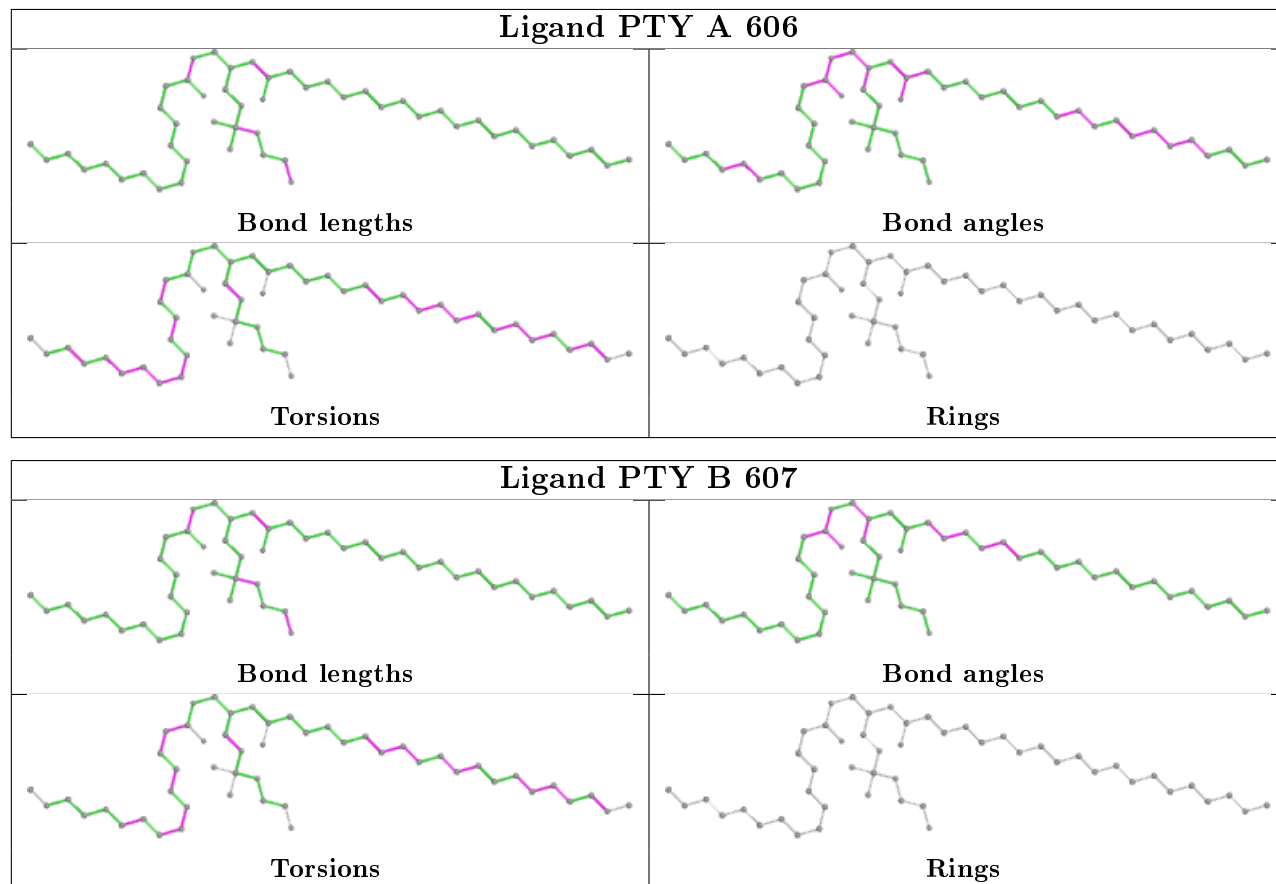
There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	NAG	1	0
4	A	606	PTY	2	0
3	A	604	NAG	2	0
3	A	603	NAG	8	0
4	B	607	PTY	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

### 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<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	172/193 (89%)	0.05	6 (3%) 44 41	13, 21, 39, 58	4 (2%)
1	B	173/193 (89%)	0.26	13 (7%) 14 12	16, 24, 47, 62	7 (4%)
2	C	24/33 (72%)	-0.23	0 100 100	15, 20, 26, 41	0
2	D	24/33 (72%)	0.27	2 (8%) 11 10	20, 23, 30, 46	0
All	All	393/452 (86%)	0.14	21 (5%) 26 24	13, 22, 42, 62	11 (2%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	LEU	9.4
1	B	105	PRO	5.0
1	B	138	GLN	4.9
1	B	178	SER	4.8
1	A	177	ILE	4.8
1	A	178	SER	4.6
1	B	179	ALA	4.6
1	A	105	PRO	4.3
1	B	106	GLU	4.0
1	A	7	GLY	3.9
1	B	107	GLY	3.7
1	B	140	THR	3.5
1	A	20	ARG	3.5
1	B	139	VAL	3.4
1	A	106	GLU	3.4
1	B	177	ILE	3.3
1	B	46	THR	3.2
2	D	33	ASN	3.1
1	B	104	PRO	3.0
2	D	32	GLN	3.0
1	B	59	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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	CGU	D	19	12/13	0.91	0.11	27,31,36,38	0
2	CGU	D	6	12/13	0.91	0.09	20,21,27,27	0
2	CGU	C	19	12/13	0.93	0.13	24,26,29,34	0
2	CGU	C	14	12/13	0.93	0.08	19,23,34,34	0
2	CGU	D	20	12/13	0.94	0.07	19,24,28,29	0
2	CGU	D	14	12/13	0.94	0.07	19,24,28,29	0
2	CGU	D	29	12/13	0.96	0.07	14,20,23,24	0
2	CGU	D	16	12/13	0.96	0.07	18,20,20,21	0
2	CGU	C	20	12/13	0.96	0.06	18,22,25,29	0
2	CGU	D	26	12/13	0.96	0.08	17,18,20,21	0
2	CGU	D	25	12/13	0.97	0.06	19,19,23,23	0
2	CGU	C	25	12/13	0.97	0.06	13,15,18,19	0
2	CGU	C	29	12/13	0.97	0.08	13,15,19,19	0
2	CGU	C	6	12/13	0.97	0.06	14,15,18,20	0
2	CGU	C	26	12/13	0.98	0.08	12,15,17,19	0
2	CGU	C	7	12/13	0.98	0.07	12,13,16,17	0
2	CGU	C	16	12/13	0.98	0.06	14,16,18,18	0
2	CGU	D	7	12/13	0.98	0.05	18,19,21,22	0

## 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
3	NAG	A	605	14/15	0.61	0.24	43,57,61,61	0
3	NAG	B	602	14/15	0.73	0.22	52,55,59,64	0
3	NAG	B	601	14/15	0.79	0.21	34,40,44,45	0
4	PTY	A	606	50/50	0.84	0.17	18,30,38,43	0

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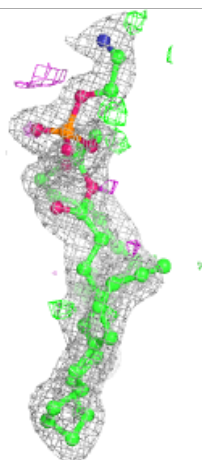
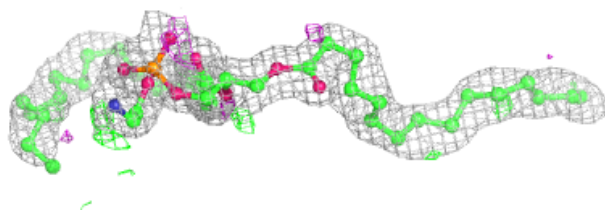
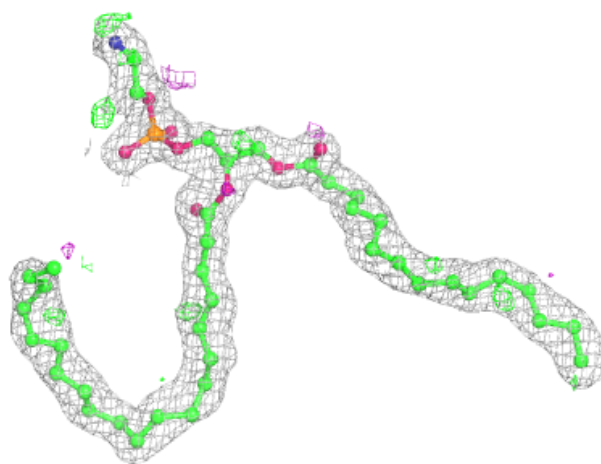
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PTY	B	607	50/50	0.88	0.17	21,31,40,40	0
3	NAG	A	604	14/15	0.88	0.19	30,38,43,44	0
3	NAG	A	603	14/15	0.88	0.17	32,40,53,56	0
5	MG	D	40	1/1	0.93	0.06	33,33,33,33	0
5	MG	C	40	1/1	0.95	0.07	31,31,31,31	0
3	NAG	B	600	14/15	0.96	0.06	15,18,22,24	0
6	CA	D	39	1/1	0.96	0.09	34,34,34,34	0
6	CA	C	39	1/1	0.97	0.07	33,33,33,33	0
5	MG	D	34	1/1	0.98	0.04	21,21,21,21	0
6	CA	D	38	1/1	0.98	0.05	20,20,20,20	0
6	CA	C	38	1/1	0.99	0.05	18,18,18,18	0
5	MG	C	34	1/1	0.99	0.04	15,15,15,15	0
6	CA	D	36	1/1	0.99	0.07	19,19,19,19	0
6	CA	D	35	1/1	0.99	0.05	19,19,19,19	0
6	CA	C	35	1/1	1.00	0.09	14,14,14,14	0
6	CA	C	37	1/1	1.00	0.07	15,15,15,15	0
6	CA	C	36	1/1	1.00	0.09	15,15,15,15	0
6	CA	D	37	1/1	1.00	0.05	18,18,18,18	0

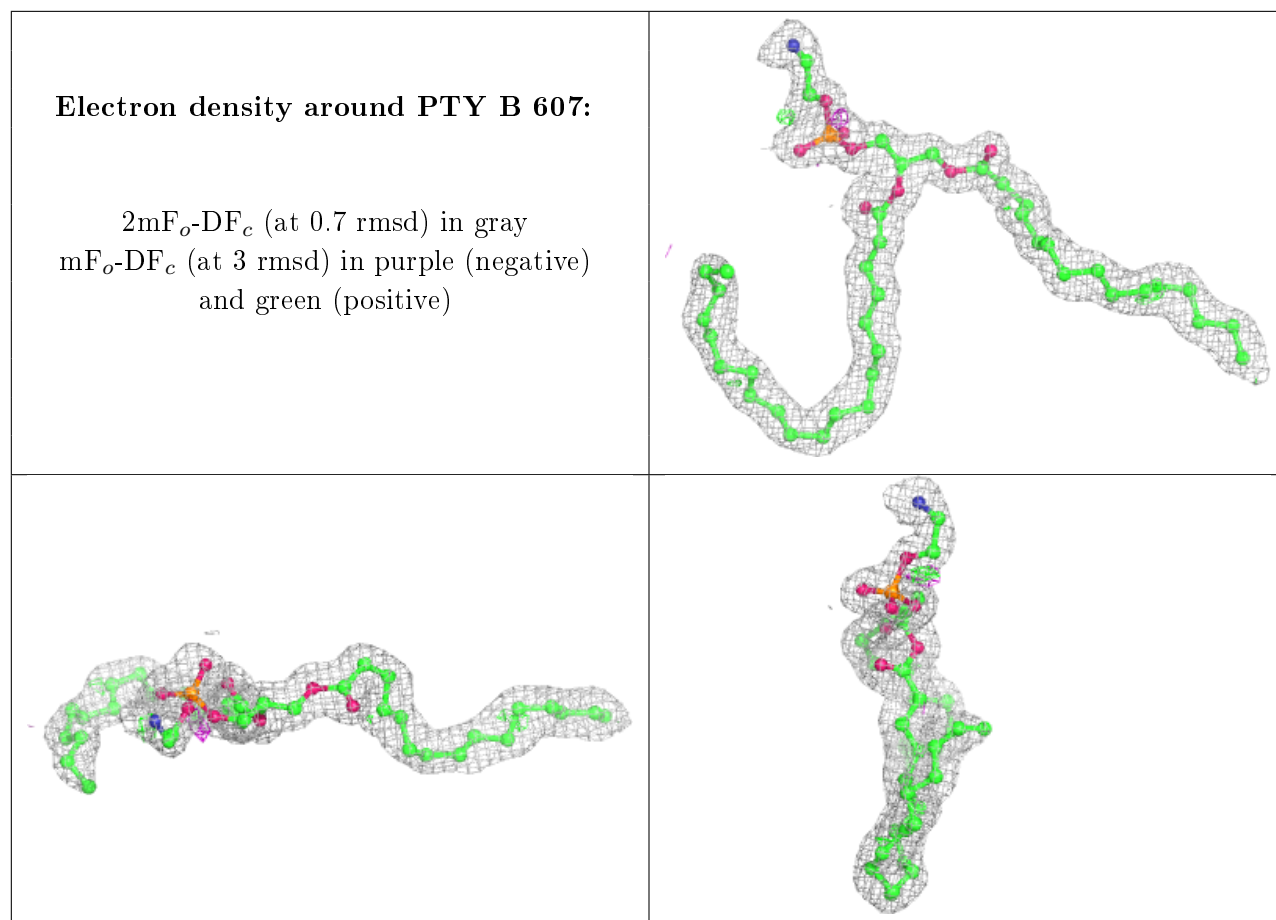
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PTY A 606:**

$2mF_o-DF_c$  (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.