



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:05 PM UTC

PDB ID : 3JTC / pdb_00003jtc
Title : Importance of Mg²⁺ in the Ca²⁺-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 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 ⓘ 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](#) ①) 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

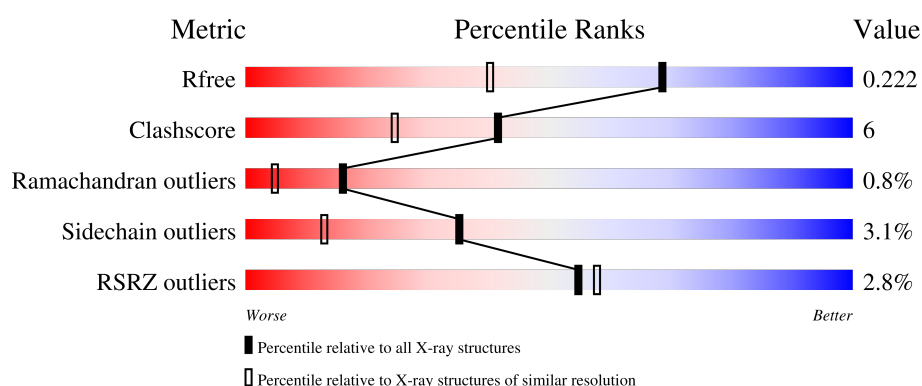
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 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	A	193	2% 73% 16% • 11%
1	B	193	4% 73% 16% • 10%
2	C	33	70% 27% •
2	D	33	52% 42% 6%

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 criteria:

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.

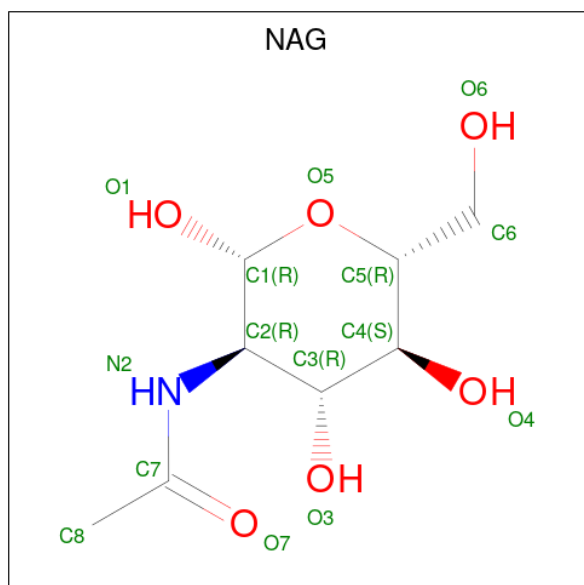
- Molecule 1 is a protein called Endothelial protein C receptor.

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

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

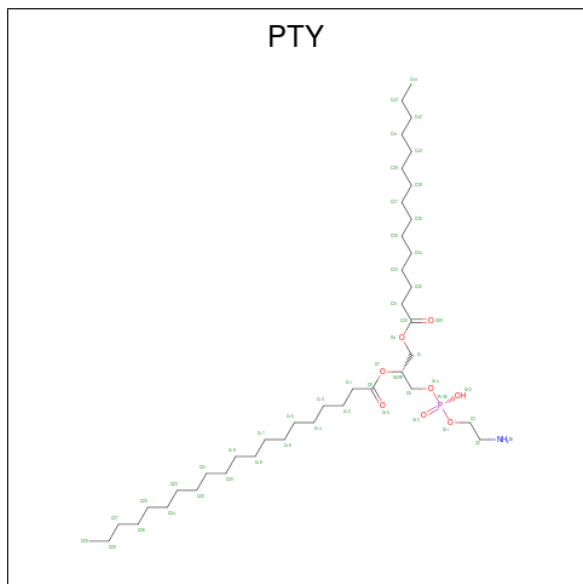
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	33	Total	C	N	O	S	0	0	0
			304	179	45	78	2			
2	D	33	Total	C	N	O	S	0	0	0
			304	179	45	78	2			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 7 is water.

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.60Å)	Xtriage
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 ²)	21.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4027	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage'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.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PTY, CA, CGU, NAG, MG

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	1.43	3/1440 (0.2%)	1.33	4/1960 (0.2%)
1	B	1.45	3/1450 (0.2%)	1.22	3/1974 (0.2%)
2	C	1.42	1/193 (0.5%)	1.20	0/246
2	D	1.42	2/193 (1.0%)	1.20	0/246
All	All	1.43	9/3276 (0.3%)	1.27	7/4426 (0.2%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	11	SER	N-CA	5.95	1.53	1.46
1	B	63	ALA	CA-CB	5.91	1.62	1.53
1	A	15	GLN	N-CA	5.88	1.53	1.46
1	A	12	HIS	CA-C	-5.61	1.45	1.52
1	A	87	ARG	C-O	5.46	1.30	1.24

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	ILE	CB-CA-C	-6.13	102.65	112.16
1	A	174	GLN	CA-CB-CG	-5.75	102.59	114.10
1	B	46	THR	N-CA-C	5.56	119.16	112.38
1	A	104	PRO	O-C-N	5.54	123.75	121.15
1	B	161	LEU	N-CA-C	-5.20	105.51	111.07

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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	21	7
1	B	171/193 (89%)	164 (96%)	5 (3%)	2 (1%)	10	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%)	16	5

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

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%)	150 (98%)	3 (2%)	48	24
1	B	154/171 (90%)	147 (96%)	7 (4%)	24	7
2	C	22/22 (100%)	22 (100%)	0	100	100
2	D	22/22 (100%)	21 (96%)	1 (4%)	24	7
All	All	351/386 (91%)	340 (97%)	11 (3%)	35	13

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	106	GLU
1	B	139	VAL
2	D	32	GLN
1	B	140	THR
1	B	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	171	GLN
2	C	33	ASN
2	D	10	HIS
1	A	57	GLN
1	A	9	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	D	19	5	9,11,12	1.51	2 (22%)	10,14,16	1.35	2 (20%)
2	CGU	D	29	6,2,5	9,11,12	1.72	2 (22%)	10,14,16	1.68	2 (20%)
2	CGU	D	26	6,2	9,11,12	2.31	2 (22%)	10,14,16	1.47	3 (30%)
2	CGU	C	26	6,2	9,11,12	1.43	3 (33%)	10,14,16	2.46	5 (50%)
2	CGU	C	7	6,2	9,11,12	1.58	2 (22%)	10,14,16	1.56	2 (20%)
2	CGU	C	14	2,5	9,11,12	2.09	3 (33%)	10,14,16	1.12	1 (10%)
2	CGU	D	7	6,2	9,11,12	1.47	2 (22%)	10,14,16	2.01	4 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CGU	D	14	2,5	9,11,12	1.71	2 (22%)	10,14,16	0.86	0
2	CGU	D	16	6,2	9,11,12	0.97	0	10,14,16	1.63	2 (20%)
2	CGU	D	20	6,2	9,11,12	1.51	2 (22%)	10,14,16	2.29	6 (60%)
2	CGU	C	25	5	9,11,12	1.74	3 (33%)	10,14,16	1.42	1 (10%)
2	CGU	C	6	6	9,11,12	1.55	2 (22%)	10,14,16	2.66	3 (30%)
2	CGU	C	16	6,2	9,11,12	1.55	1 (11%)	10,14,16	2.81	6 (60%)
2	CGU	C	20	6,2	9,11,12	1.10	1 (11%)	10,14,16	2.17	4 (40%)
2	CGU	D	6	6	9,11,12	1.97	2 (22%)	10,14,16	1.96	4 (40%)
2	CGU	C	19	5	9,11,12	1.53	3 (33%)	10,14,16	0.70	0
2	CGU	D	25	5	9,11,12	0.94	0	10,14,16	1.19	1 (10%)
2	CGU	C	29	6,2,5	9,11,12	1.02	0	10,14,16	1.22	1 (10%)

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	D	19	5	-	2/13/14/16	-
2	CGU	D	29	6,2,5	-	1/13/14/16	-
2	CGU	D	26	6,2	-	4/13/14/16	-
2	CGU	C	26	6,2	-	4/13/14/16	-
2	CGU	C	7	6,2	-	2/13/14/16	-
2	CGU	C	14	2,5	-	0/13/14/16	-
2	CGU	D	7	6,2	-	2/13/14/16	-
2	CGU	D	14	2,5	-	2/13/14/16	-
2	CGU	D	16	6,2	-	5/13/14/16	-
2	CGU	D	20	6,2	-	1/13/14/16	-
2	CGU	C	25	5	-	1/13/14/16	-
2	CGU	C	6	6	-	4/13/14/16	-
2	CGU	C	16	6,2	-	5/13/14/16	-
2	CGU	C	20	6,2	-	2/13/14/16	-
2	CGU	D	6	6	-	3/13/14/16	-
2	CGU	C	19	5	-	3/13/14/16	-
2	CGU	D	25	5	-	3/13/14/16	-
2	CGU	C	29	6,2,5	-	4/13/14/16	-

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	26	CGU	CG-CD1	5.99	1.59	1.52
2	C	14	CGU	CG-CD1	3.90	1.57	1.52
2	D	6	CGU	CG-CD1	3.89	1.57	1.52
2	C	16	CGU	CG-CD1	-3.77	1.47	1.52
2	C	7	CGU	CG-CD1	3.71	1.56	1.52

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	CGU	CB-CG-CD1	4.99	123.24	113.11
2	C	6	CGU	CB-CG-CD2	-4.97	103.02	113.11
2	C	20	CGU	CB-CA-C	-4.86	103.51	110.99
2	C	26	CGU	OE22-CD2-OE21	-4.57	113.72	124.08
2	C	16	CGU	OE22-CD2-OE21	-4.40	114.10	124.08

There are no chirality outliers.

5 of 48 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-CD1
2	C	6	CGU	CA-CB-CG-CD2
2	C	16	CGU	O-C-CA-CB
2	C	16	CGU	OE12-CD1-CG-CB

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 oligosaccharides 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	602	1	14,14,15	0.52	0	17,19,21	0.74	0
4	PTY	A	606	-	49,49,49	1.08	4 (8%)	52,54,54	1.60	11 (21%)
3	NAG	B	601	1	14,14,15	0.88	1 (7%)	17,19,21	1.46	4 (23%)
3	NAG	A	603	1	14,14,15	0.72	0	17,19,21	2.96	7 (41%)
3	NAG	A	605	1	14,14,15	0.69	0	17,19,21	0.89	1 (5%)
4	PTY	B	607	-	49,49,49	1.10	4 (8%)	52,54,54	1.36	5 (9%)
3	NAG	B	600	1	14,14,15	1.20	1 (7%)	17,19,21	1.55	7 (41%)
3	NAG	A	604	1	14,14,15	1.14	1 (7%)	17,19,21	1.55	5 (29%)

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	602	1	-	2/6/23/26	0/1/1/1
4	PTY	A	606	-	-	19/53/53/53	-
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	A	603	1	-	2/6/23/26	0/1/1/1
4	PTY	B	607	-	-	15/53/53/53	-
3	NAG	B	600	1	-	0/6/23/26	0/1/1/1
3	NAG	A	604	1	-	2/6/23/26	0/1/1/1

The worst 5 of 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
4	B	607	PTY	O7-C8	4.48	1.46	1.34
4	B	607	PTY	O4-C30	3.44	1.43	1.33
4	A	606	PTY	O4-C30	3.27	1.42	1.33
4	A	606	PTY	P1-O11	2.75	1.70	1.59

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	NAG	C1-O5-C5	6.49	120.89	112.19
4	A	606	PTY	C5-C6-C1	-4.98	100.17	111.78
3	A	603	NAG	O5-C1-C2	-4.97	103.60	111.29
3	A	603	NAG	O3-C3-C4	-4.81	99.03	110.38
4	B	607	PTY	O4-C30-O30	-4.77	111.70	123.63

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	605	NAG	C1

5 of 44 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
4	B	607	PTY	C30-C31-C32-C33
3	A	605	NAG	C4-C5-C6-O6
3	B	602	NAG	C4-C5-C6-O6

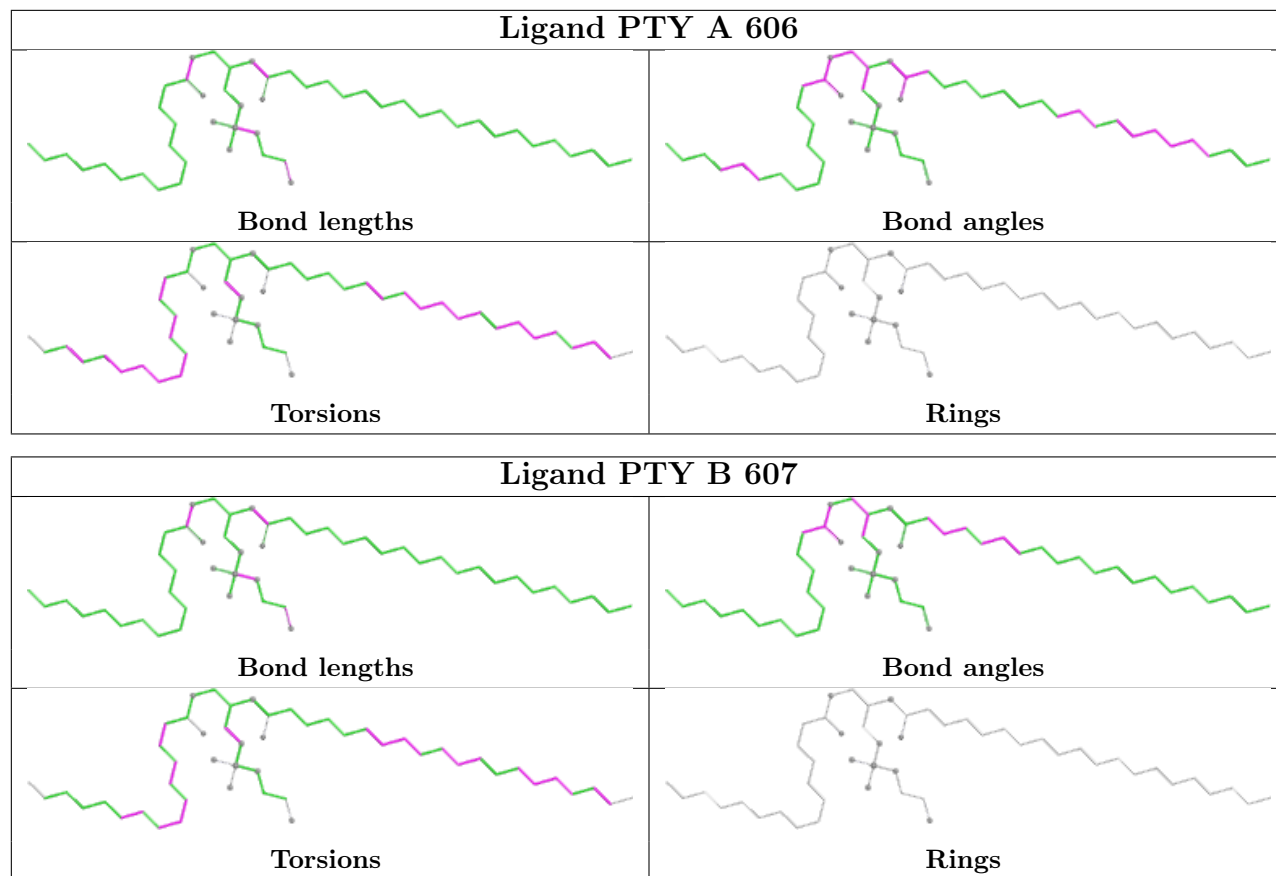
There are no ring outliers.

5 monomers are involved in 15 short contacts:

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

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

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	172/193 (89%)	-0.11	3 (1%) 69 72	13, 21, 39, 58	4 (2%)
1	B	173/193 (89%)	0.08	8 (4%) 37 39	16, 23, 47, 62	7 (4%)
2	C	24/33 (72%)	-0.30	0 100 100	15, 20, 26, 41	0
2	D	24/33 (72%)	0.22	0 100 100	20, 23, 30, 46	0
All	All	393/452 (86%)	-0.02	11 (2%) 55 58	13, 22, 42, 62	11 (2%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	LEU	5.3
1	A	177	ILE	4.5
1	B	139	VAL	3.5
1	A	178	SER	3.4
1	B	26	TRP	3.3

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, 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
2	CGU	C	19	12/13	0.93	0.09	24,26,29,34	0
2	CGU	D	6	12/13	0.93	0.08	20,21,27,27	0
2	CGU	D	19	12/13	0.93	0.08	27,31,36,38	0
2	CGU	C	14	12/13	0.94	0.07	19,23,34,34	0
2	CGU	D	14	12/13	0.95	0.07	19,24,28,29	0
2	CGU	D	26	12/13	0.95	0.07	17,18,20,21	0
2	CGU	D	20	12/13	0.96	0.06	19,24,28,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CGU	C	20	12/13	0.96	0.06	18,22,25,29	0
2	CGU	C	25	12/13	0.97	0.05	13,15,18,19	0
2	CGU	D	16	12/13	0.97	0.05	18,20,20,21	0
2	CGU	C	29	12/13	0.97	0.05	13,15,19,19	0
2	CGU	C	6	12/13	0.97	0.06	14,15,18,20	0
2	CGU	D	25	12/13	0.97	0.05	19,19,23,23	0
2	CGU	D	7	12/13	0.97	0.05	18,19,21,22	0
2	CGU	D	29	12/13	0.97	0.06	14,20,23,24	0
2	CGU	C	7	12/13	0.98	0.04	12,13,16,17	0
2	CGU	C	26	12/13	0.98	0.05	12,15,17,19	0
2	CGU	C	16	12/13	0.98	0.05	14,16,18,18	0

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.

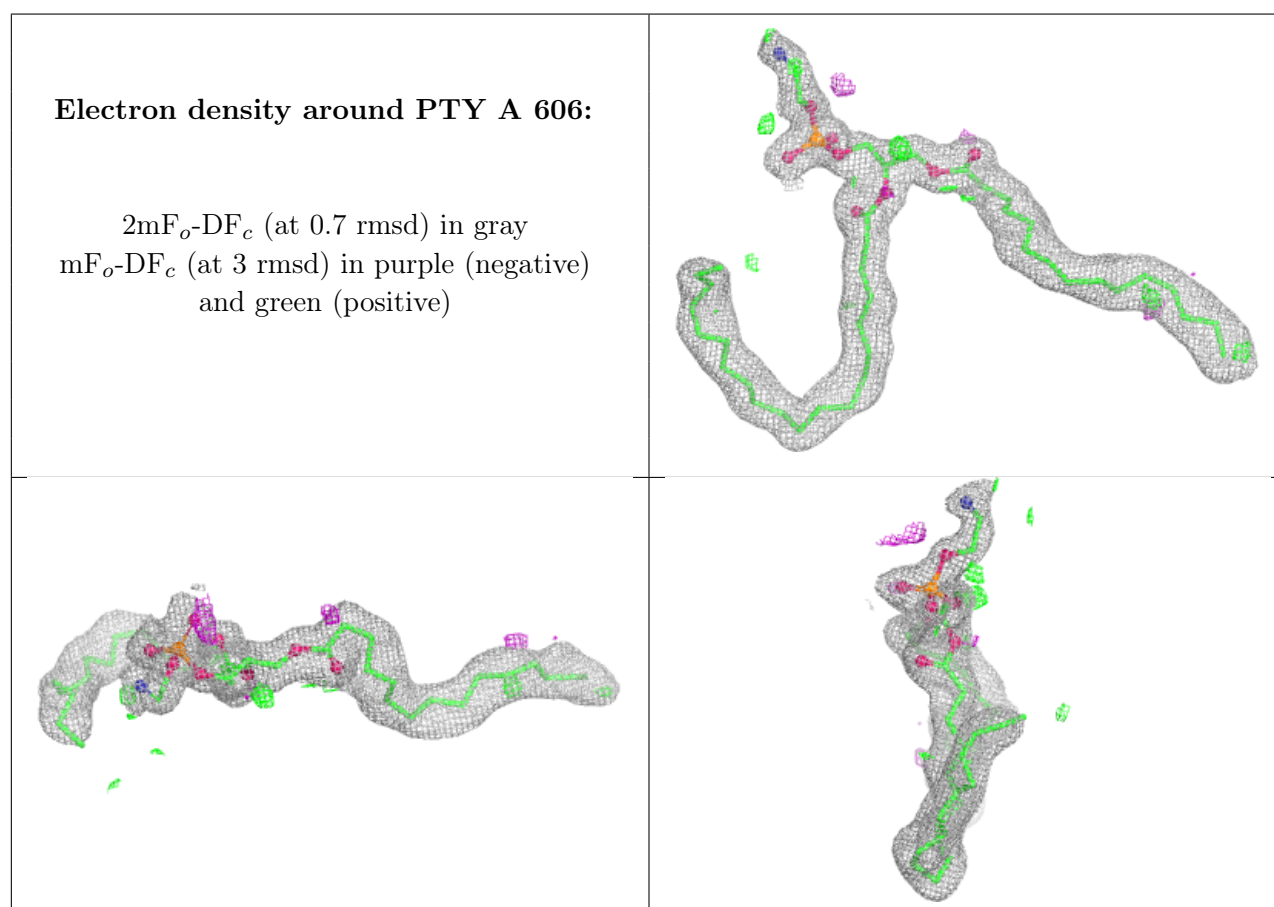
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	605	14/15	0.67	0.15	43,57,61,61	0
3	NAG	B	602	14/15	0.72	0.15	52,55,59,64	0
3	NAG	A	603	14/15	0.78	0.14	32,40,53,56	0
3	NAG	B	601	14/15	0.82	0.11	34,40,44,45	0
3	NAG	A	604	14/15	0.86	0.09	30,38,43,44	0
4	PTY	A	606	50/50	0.91	0.10	18,30,38,43	0
4	PTY	B	607	50/50	0.91	0.09	21,31,40,40	0
5	MG	D	40	1/1	0.93	0.07	33,33,33,33	0
5	MG	C	40	1/1	0.95	0.05	31,31,31,31	0
6	CA	D	39	1/1	0.96	0.08	34,34,34,34	0
6	CA	C	39	1/1	0.97	0.05	33,33,33,33	0
3	NAG	B	600	14/15	0.97	0.05	15,18,22,24	0
6	CA	C	37	1/1	0.99	0.02	15,15,15,15	0
6	CA	C	38	1/1	0.99	0.03	18,18,18,18	0
5	MG	D	34	1/1	0.99	0.04	21,21,21,21	0
6	CA	D	35	1/1	0.99	0.03	19,19,19,19	0
6	CA	D	36	1/1	0.99	0.03	19,19,19,19	0

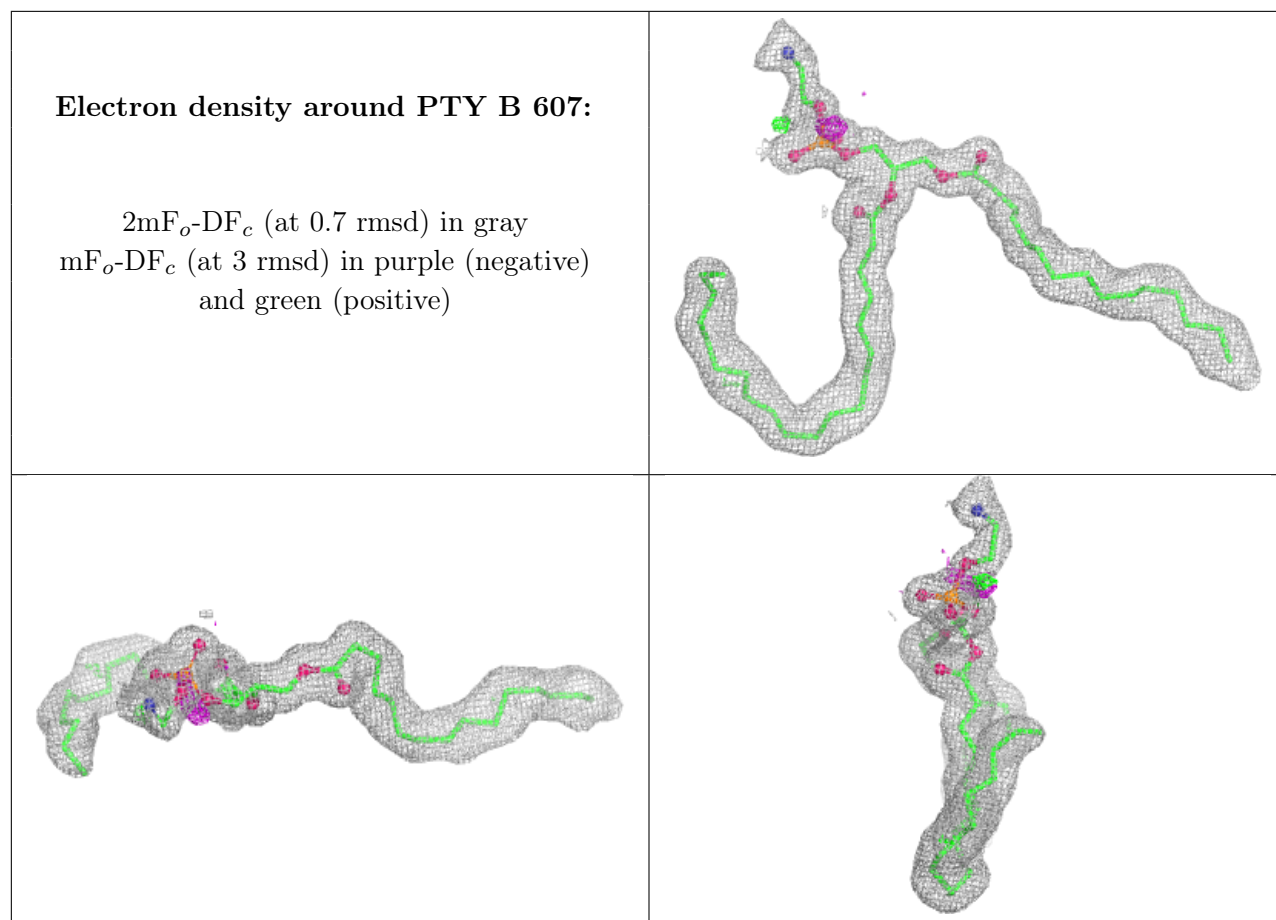
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	D	37	1/1	0.99	0.02	18,18,18,18	0
6	CA	D	38	1/1	0.99	0.03	20,20,20,20	0
5	MG	C	34	1/1	0.99	0.02	15,15,15,15	0
6	CA	C	35	1/1	1.00	0.03	14,14,14,14	0
6	CA	C	36	1/1	1.00	0.02	15,15,15,15	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.