wwPDB X-ray Structure Validation Summary Report (i)

Jan 5, 2024 – 01:05 am GMT

PDB ID	:	5EBE
Title	:	Structure of human sphingomyelinase phosphodiesterase like 3A (SMPDL3A) with 5' CMP
Authors	:	Lim, S.M.; Yeung, K.; Tresaugues, L.; Teo, H.L.; Nordlund, P.
Deposited on	:	2015-10-19
Resolution	:	3.00 Å(reported)

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

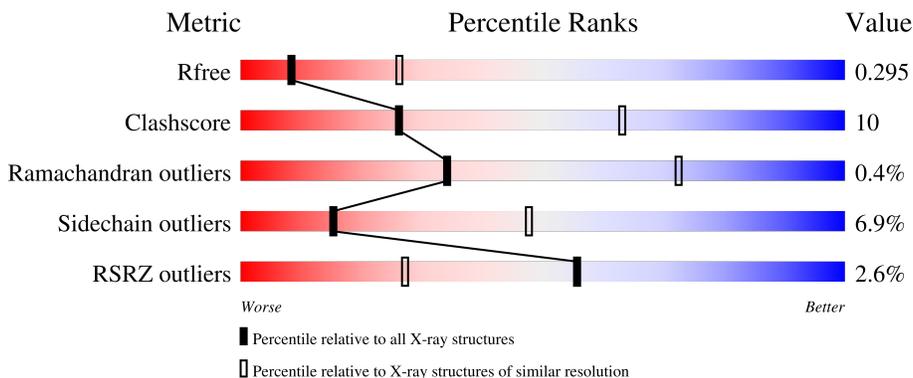|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	Percentile Ranks	Value
Rfree		0.295
Clashscore		10
Ramachandran outliers		0.4%
Sidechain outliers		6.9%
RSRZ outliers		2.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	418	80% 17% ••
2	B	415	4% 68% 29% •
2	C	415	4% 74% 24% •
3	D	2	100%

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
8	MLI	B	610	-	-	-	X

2 Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 10472 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 Acid sphingomyelinase-like phosphodiesterase 3a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	418	3380	2182	541	644	13	0	4	0

- Molecule 2 is a protein called Acid sphingomyelinase-like phosphodiesterase 3a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	415	3344	2157	536	638	13	0	3	0
2	C	415	3350	2159	537	641	13	0	4	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG
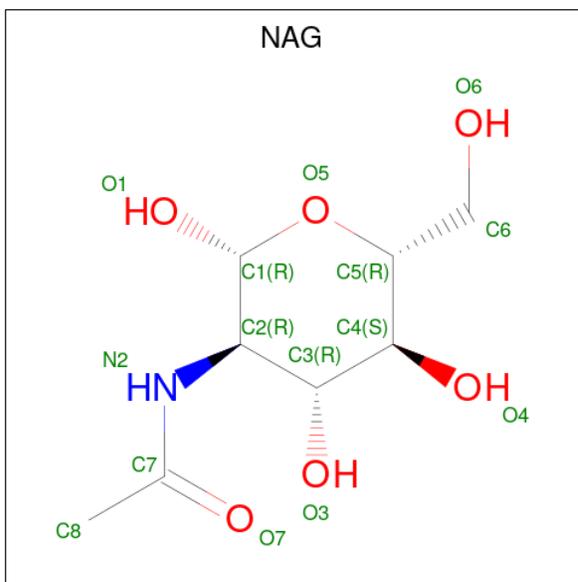
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 13	C 8	N 1	O 4	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	C	1	Total 14	C 8	N 1	O 5	0	0
4	C	1	Total 14	C 8	N 1	O 5	0	0
4	C	1	Total 14	C 8	N 1	O 5	0	0
4	C	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Zn 2	0	0

Continued on next page...

W O R L D W I D E
PDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total Zn 2 2		0	0
5	C	2	Total Zn 2 2		0	0

- Molecule 6 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C5P) (formula: $C_9H_{14}N_3O_8P$).
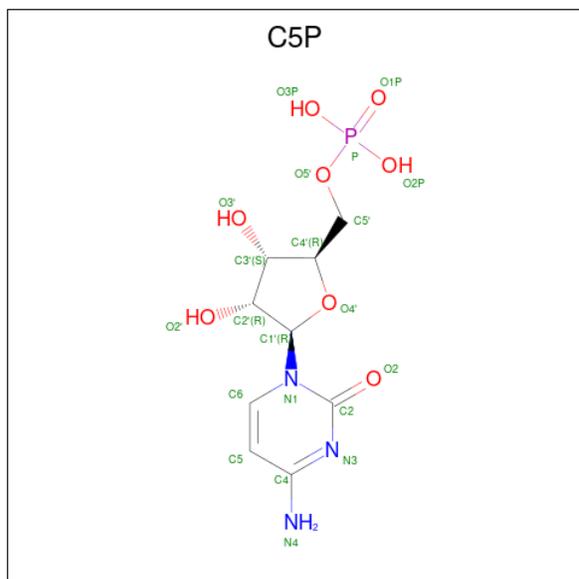
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 21	C 9	N 3	O 8	P 1	0	0
6	C	1	Total 21	C 9	N 3	O 8	P 1	0	0

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

GOL
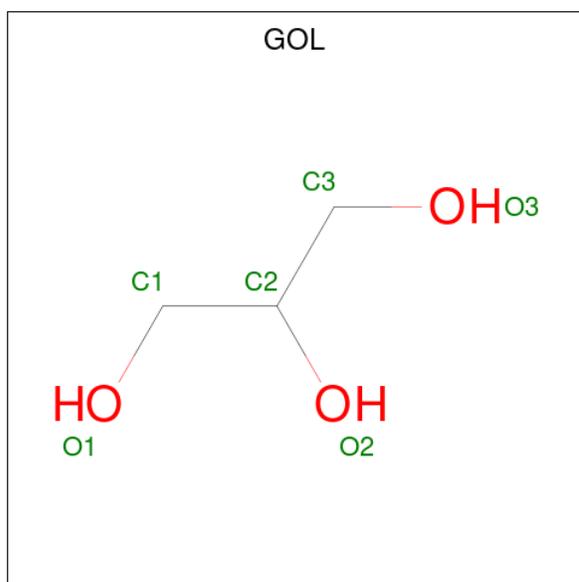
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0

- Molecule 8 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).

MLI
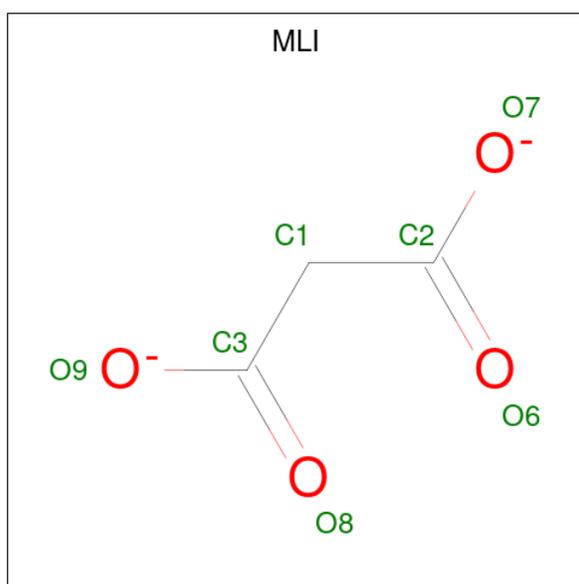
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total 7	C 3	O 4	0	0

- Molecule 9 is 5-O-phosphono-beta-D-ribofuranose (three-letter code: RP5) (formula:

$C_5H_{11}O_8P$).
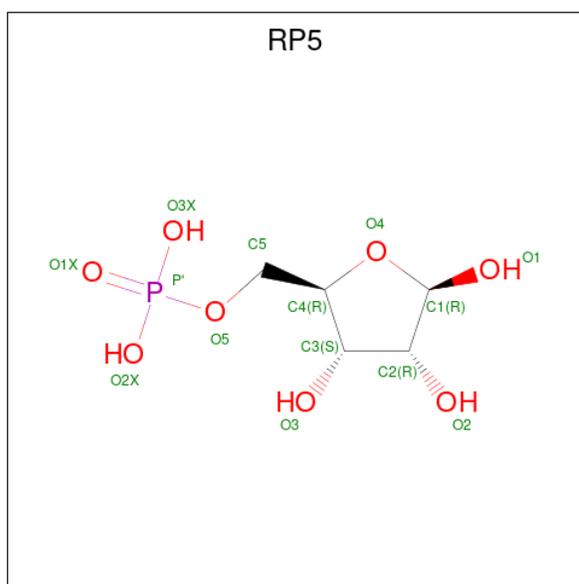
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	O	P	0	0
			14	5	8	1		

- Molecule 10 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).
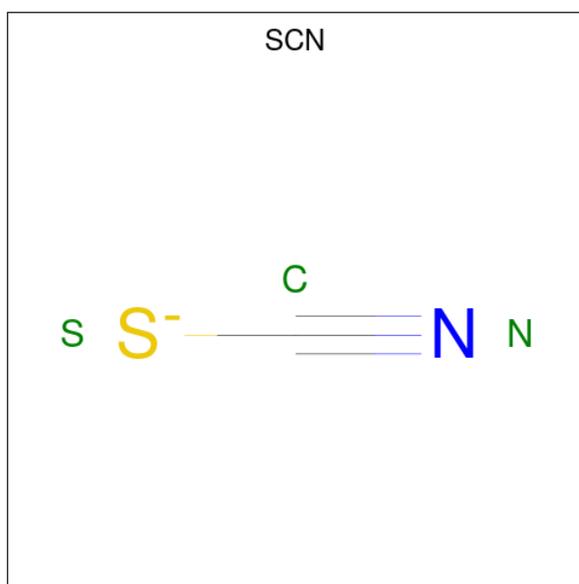
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	N	S	0	0
			3	1	1	1		
10	C	1	Total	C	N	S	0	0
			3	1	1	1		

• Molecule 11 is water.

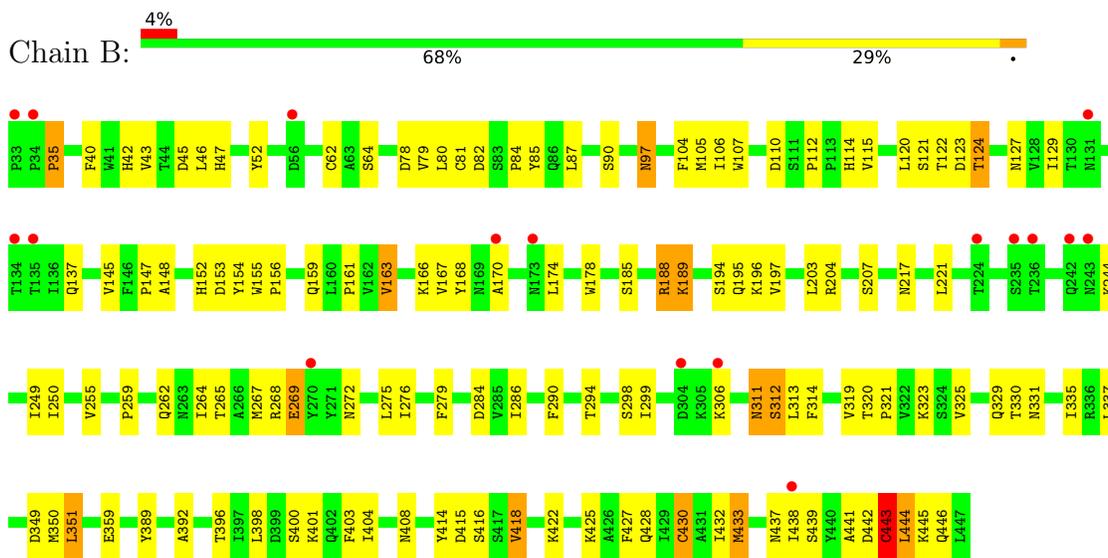| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	19	Total 19	O 19	0	0
11	B	60	Total 60	O 60	0	0
11	C	51	Total 51	O 51	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
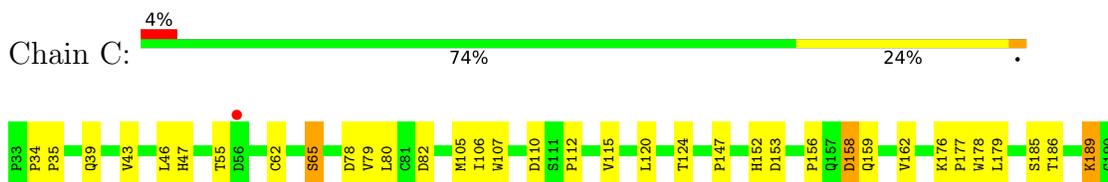
• Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a
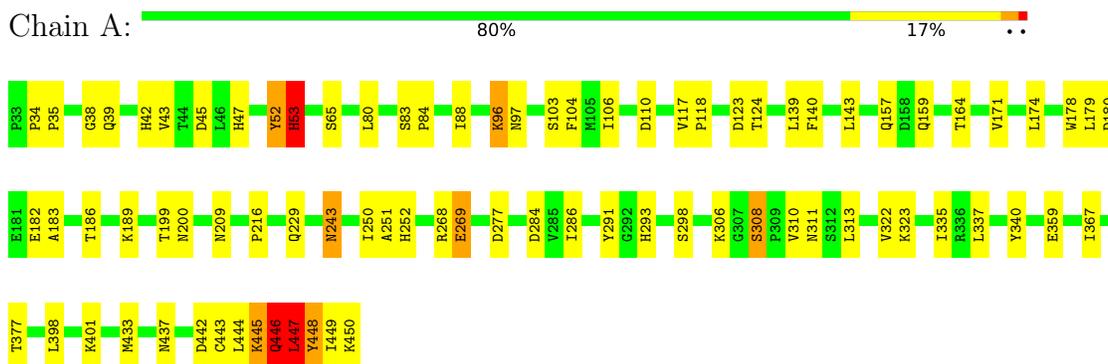
• Molecule 2: Acid sphingomyelinase-like phosphodiesterase 3a

• Molecule 2: Acid sphingomyelinase-like phosphodiesterase 3a

G191 L208 K223 P226 A227 N228 S235 N238 N239 Q242 N243 K244 E245 K246 I250 A251 H252 L258 P259 S260 S261 Q262 N272 E273 K274 L275 I276 D277 Q280 S283 D284 V285 I286 A287 G288 Q289 F290 Y291 T294 H295 R296 I299 M300 V301 L302 S303 D304

K305 K306 G307 S308 N311 S312 L313 K323 T330 N331 L337 D344 D349 Y354 L355 N356 L357 T358 E359 W368 L374 T375 Q376 L383 Y389 A392 F395 T396 I397 L398 D399 S400 I404 N408 F411 V412 S413 Y414 D415 S416 S417 V418 T423

I429 I432 L435 D436 N437 I438 S439 Y440 A441 D442 C443 L444 K445 Q446 L447
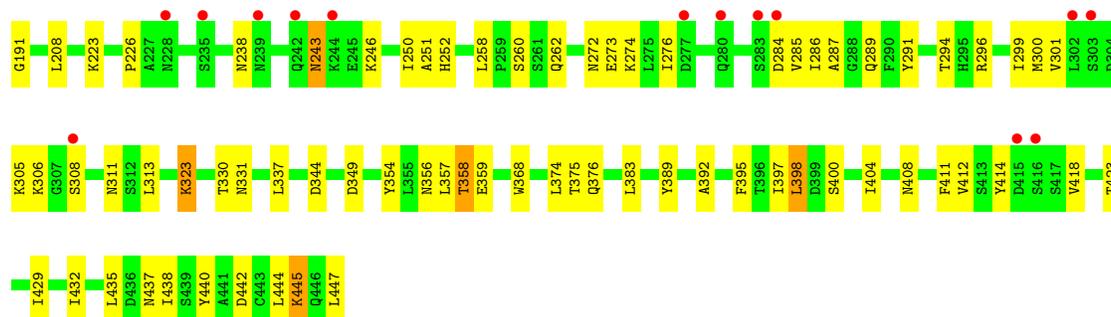
● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

NAG1 NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	147.65Å 147.65Å 142.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.56 – 3.00 47.56 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.56-3.00) 99.7 (47.56-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.251 , 0.295 0.251 , 0.295	Depositor DCC
R_{free} test set	1790 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.3	EDS
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10472	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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 75.71 % 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 1.2003e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: C5P, MLI, ZN, GOL, RP5, NAG, SCN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.68	1/3479 (0.0%)	0.83	5/4749 (0.1%)
2	B	0.70	0/3443	0.84	2/4702 (0.0%)
2	C	0.67	0/3448	0.84	1/4708 (0.0%)
All	All	0.68	1/10370 (0.0%)	0.84	8/14159 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	TYR	CE1-CZ	-5.98	1.30	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	446	GLN	CB-CA-C	6.25	122.89	110.40
1	A	53	HIS	CB-CA-C	6.03	122.46	110.40
1	A	447	LEU	N-CA-CB	-5.81	98.79	110.40
2	B	443	CYS	CA-CB-SG	5.68	124.22	114.00
2	B	444	LEU	N-CA-C	-5.42	96.35	111.00

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	A	3380	0	3300	48	0
2	B	3344	0	3262	86	0
2	C	3350	0	3263	75	0
3	D	28	0	25	4	0
4	A	55	0	50	0	0
4	B	42	0	39	0	0
4	C	56	0	52	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
6	A	21	0	12	4	0
6	C	21	0	12	0	0
7	B	12	0	16	0	0
8	B	7	0	2	0	0
9	B	14	0	0	0	0
10	C	6	0	0	0	0
11	A	19	0	0	0	0
11	B	60	0	0	13	0
11	C	51	0	0	13	0
All	All	10472	0	10033	211	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 10.

The worst 5 of 211 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)
2:B:430:CYS:SG	2:B:443:CYS:CB	2.17	1.31
2:B:430:CYS:CB	2:B:443:CYS:SG	2.29	1.19
2:C:294[A]:THR:CG2	11:C:702:HOH:O	1.97	1.09
1:A:448:TYR:O	1:A:449:ILE:HD13	1.61	0.99
2:C:294[A]:THR:HG22	11:C:702:HOH:O	1.60	0.93

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	420/418 (100%)	380 (90%)	38 (9%)	2 (0%)	29	68
2	B	416/415 (100%)	367 (88%)	47 (11%)	2 (0%)	29	68
2	C	417/415 (100%)	381 (91%)	35 (8%)	1 (0%)	47	82
All	All	1253/1248 (100%)	1128 (90%)	120 (10%)	5 (0%)	34	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	35	PRO
2	B	445	LYS
2	C	414	TYR
1	A	164	THR
1	A	216	PRO

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	384/380 (101%)	359 (94%)	25 (6%)	17	50
2	B	380/377 (101%)	350 (92%)	30 (8%)	12	41
2	C	381/377 (101%)	357 (94%)	24 (6%)	18	51
All	All	1145/1134 (101%)	1066 (93%)	79 (7%)	15	48

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	124	THR
2	C	306	LYS
2	C	186	THR
2	C	260[B]	SER
2	C	383	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	169	ASN
2	C	311	ASN
2	B	295	HIS
2	C	200	ASN
2	B	229	GLN

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 ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	NAG	D	1	3,2	14,14,15	1.75	3 (21%)	17,19,21	1.86	3 (17%)
3	NAG	D	2	3	14,14,15	1.78	4 (28%)	17,19,21	2.60	6 (35%)

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	D	1	3,2	-	5/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	5.15	1.60	1.52
3	D	2	NAG	O5-C5	4.28	1.52	1.43
3	D	2	NAG	C8-C7	3.09	1.57	1.50
3	D	2	NAG	O5-C1	2.67	1.48	1.43
3	D	1	NAG	O4-C4	2.51	1.48	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	6.34	120.78	112.19
3	D	2	NAG	C4-C3-C2	-4.95	103.77	111.02
3	D	1	NAG	C2-N2-C7	4.75	129.67	122.90
3	D	1	NAG	C1-O5-C5	4.29	118.01	112.19
3	D	2	NAG	O5-C1-C2	-3.88	105.17	111.29

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	2	0
3	D	1	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 oligosaccharide.

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings
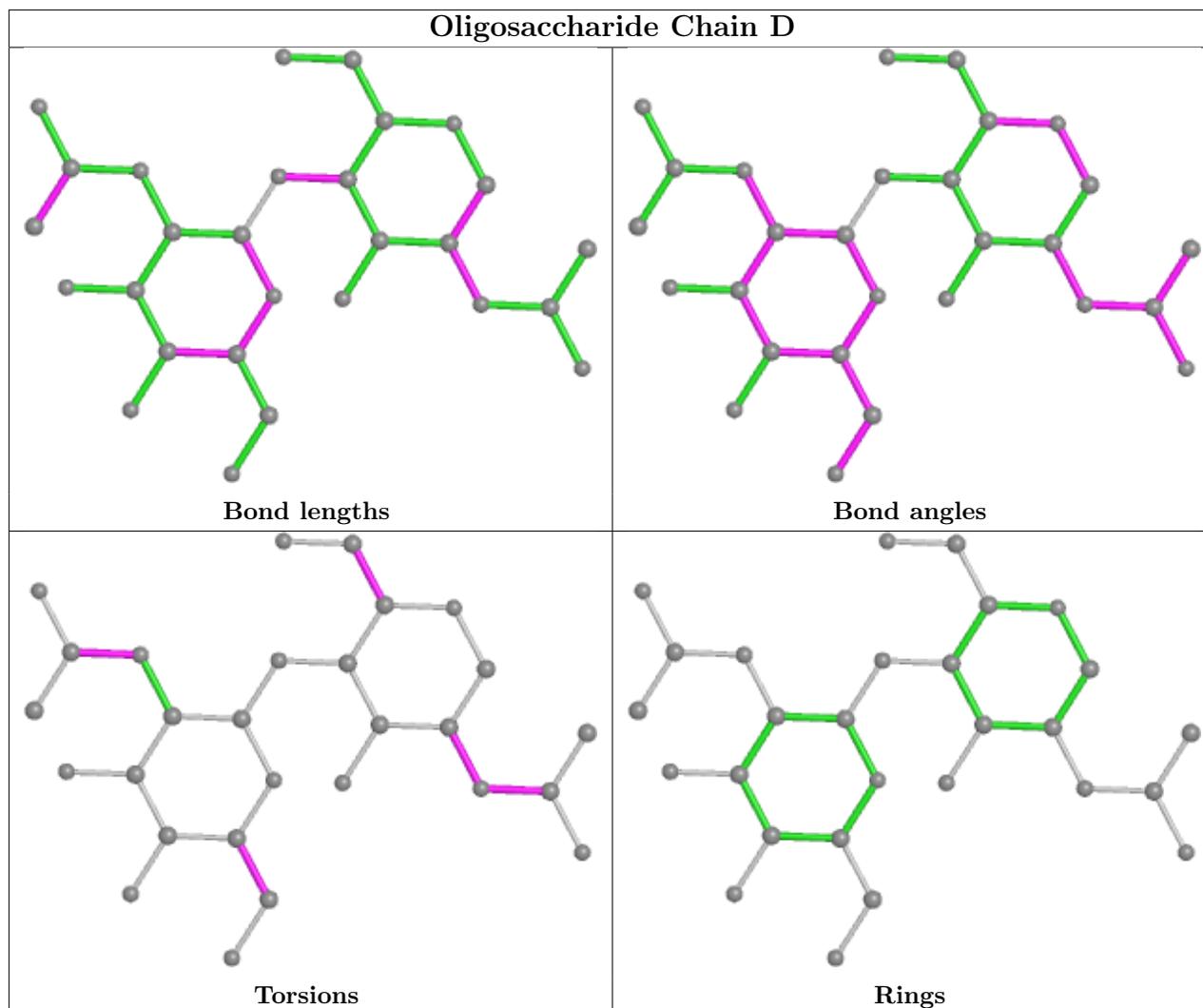
5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 6 are monoatomic - leaving 19 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	$\#|Z| > 2$
8	MLI	B	610	-	6,6,6	3.21	2 (33%)	7,7,7	1.20	0
4	NAG	B	605	2	14,14,15	3.15	5 (35%)	17,19,21	1.94	5 (29%)
4	NAG	A	603	1	14,14,15	1.25	2 (14%)	17,19,21	2.47	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	B	604	2	14,14,15	1.34	1 (7%)	17,19,21	1.56	3 (17%)
10	SCN	C	609	-	1,2,2	0.25	0	0,1,1	-	-
9	RP5	B	611	5	14,14,14	1.13	1 (7%)	20,21,21	1.60	3 (15%)
4	NAG	C	604	2	14,14,15	2.01	4 (28%)	17,19,21	1.74	4 (23%)
4	NAG	C	603	2	14,14,15	1.97	2 (14%)	17,19,21	2.31	3 (17%)
4	NAG	A	604	-	13,13,15	4.06	4 (30%)	16,17,21	3.69	8 (50%)
4	NAG	B	601	2	14,14,15	1.53	3 (21%)	17,19,21	2.31	5 (29%)
6	C5P	C	607	5	22,22,22	1.21	3 (13%)	33,33,33	1.86	10 (30%)
6	C5P	A	607	5	22,22,22	0.75	0	33,33,33	1.21	4 (12%)
4	NAG	C	601	2	14,14,15	3.10	5 (35%)	17,19,21	2.44	3 (17%)
10	SCN	C	608	-	1,2,2	0.53	0	0,1,1	-	-
4	NAG	C	602	2	14,14,15	1.93	4 (28%)	17,19,21	1.57	2 (11%)
7	GOL	B	608	-	5,5,5	0.62	0	5,5,5	0.71	0
4	NAG	A	602	1	14,14,15	2.05	3 (21%)	17,19,21	2.18	2 (11%)
7	GOL	B	609	-	5,5,5	0.81	0	5,5,5	0.54	0
4	NAG	A	601	1	14,14,15	2.13	4 (28%)	17,19,21	2.10	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
4	NAG	A	603	1	-	2/6/23/26	0/1/1/1
4	NAG	B	604	2	-	2/6/23/26	0/1/1/1
8	MLI	B	610	-	-	2/4/4/4	-
4	NAG	A	604	-	-	2/6/19/26	0/1/1/1
9	RP5	B	611	5	-	3/6/22/22	0/1/1/1
4	NAG	B	601	2	-	0/6/23/26	0/1/1/1
4	NAG	C	602	2	-	2/6/23/26	0/1/1/1
4	NAG	C	603	2	-	2/6/23/26	0/1/1/1
6	C5P	C	607	5	-	5/10/26/26	0/2/2/2
7	GOL	B	608	-	-	2/4/4/4	-
4	NAG	C	604	2	-	5/6/23/26	0/1/1/1
4	NAG	A	602	1	-	2/6/23/26	0/1/1/1
6	C5P	A	607	5	-	1/10/26/26	0/2/2/2
7	GOL	B	609	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	605	2	-	1/6/23/26	0/1/1/1
4	NAG	C	601	2	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	NAG	C1-C2	12.26	1.64	1.51
4	B	605	NAG	O5-C1	7.75	1.56	1.43
4	C	601	NAG	O5-C1	7.06	1.55	1.43
4	C	601	NAG	C1-C2	6.85	1.62	1.52
4	A	604	NAG	O5-C5	5.66	1.54	1.43

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	604	NAG	C3-C2-C1	9.11	117.88	109.50
4	C	601	NAG	C1-O5-C5	8.29	123.42	112.19
4	C	603	NAG	C1-O5-C5	7.71	122.63	112.19
4	B	601	NAG	C1-O5-C5	7.58	122.46	112.19
4	A	603	NAG	C1-O5-C5	7.06	121.76	112.19

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	607	C5P	O4'-C4'-C5'-O5'
9	B	611	RP5	C5-O5-P'-O3X
4	B	604	NAG	C4-C5-C6-O6
4	A	602	NAG	O5-C5-C6-O6
4	B	604	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	604	NAG	1	0
6	A	607	C5P	4	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 C5P C 607

Bond lengths

Bond angles

Torsions

Rings

Ligand C5P A 607

Bond lengths

Bond angles

Torsions

Rings
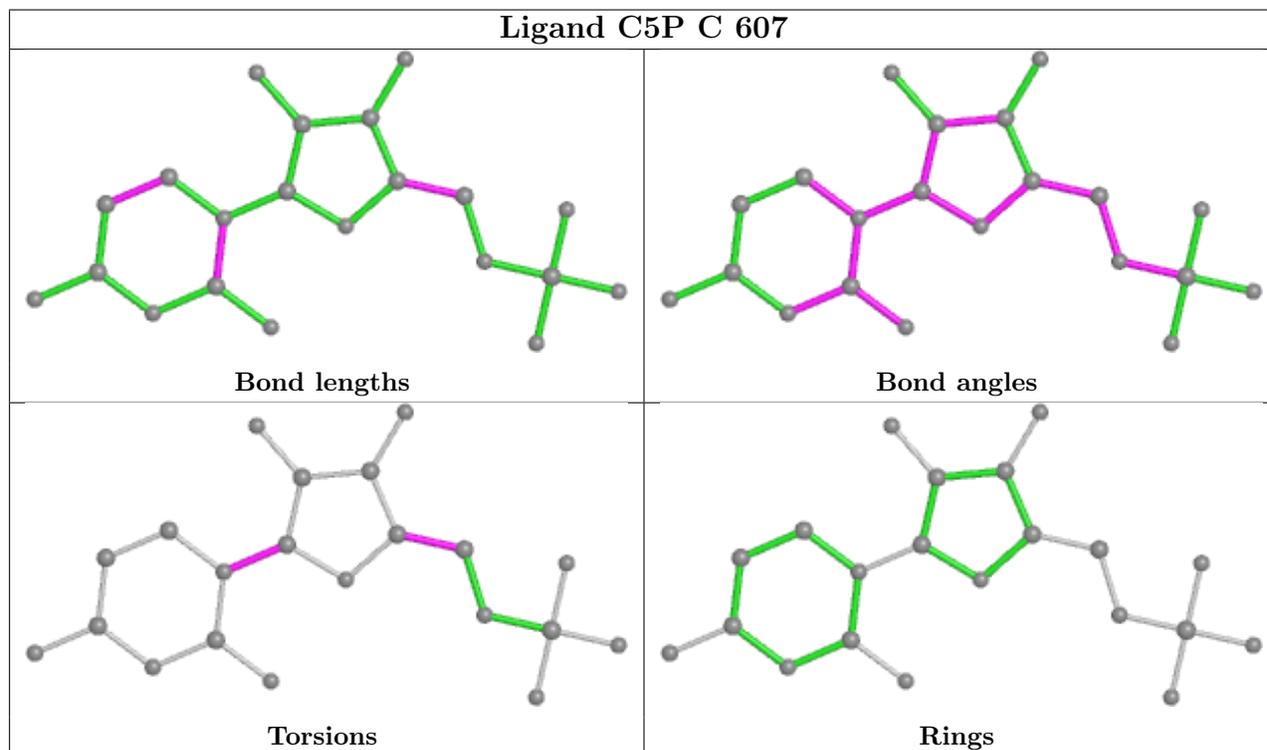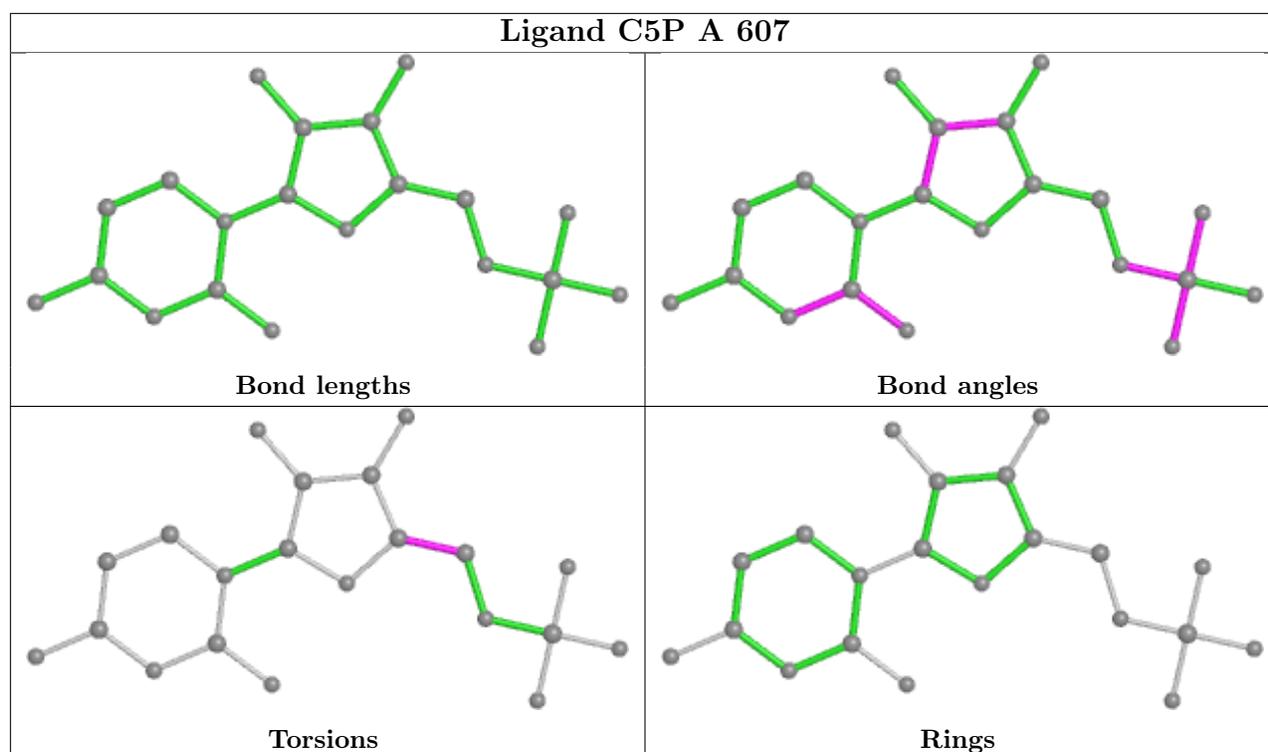
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	418/418 (100%)	-0.56	0	100	100	10, 26, 51, 85	0
2	B	415/415 (100%)	0.03	17 (4%)	37	14	23, 44, 72, 119	0
2	C	415/415 (100%)	-0.06	15 (3%)	42	17	22, 43, 63, 87	0
All	All	1248/1248 (100%)	-0.20	32 (2%)	56	27	10, 39, 65, 119	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	303	SER	4.9
2	C	283	SER	4.0
2	B	235	SER	3.7
2	B	224	THR	3.4
2	B	134	THR	3.2

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

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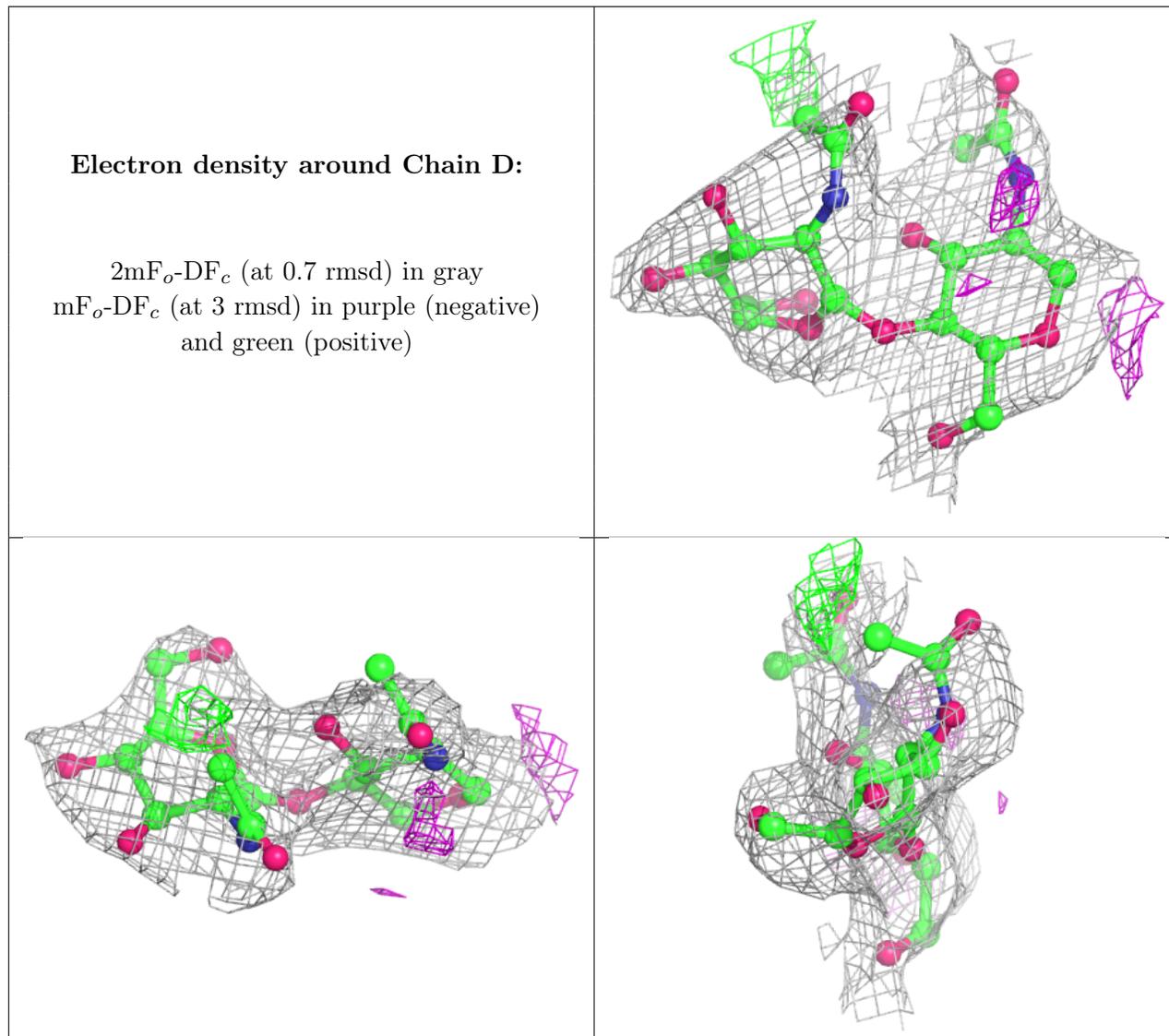
6.3 Carbohydrates ⓘ

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
3	NAG	D	2	14/15	0.87	0.29	62,70,78,78	0
3	NAG	D	1	14/15	0.89	0.27	46,57,70,74	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

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, 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
7	GOL	B	609	6/6	0.49	0.28	52,63,67,68	0
10	SCN	C	608	3/3	0.53	0.30	36,36,44,48	0
7	GOL	B	608	6/6	0.72	0.39	41,42,44,44	0
4	NAG	B	604	14/15	0.78	0.32	72,76,79,85	0
8	MLI	B	610	7/7	0.80	0.45	52,63,65,67	0

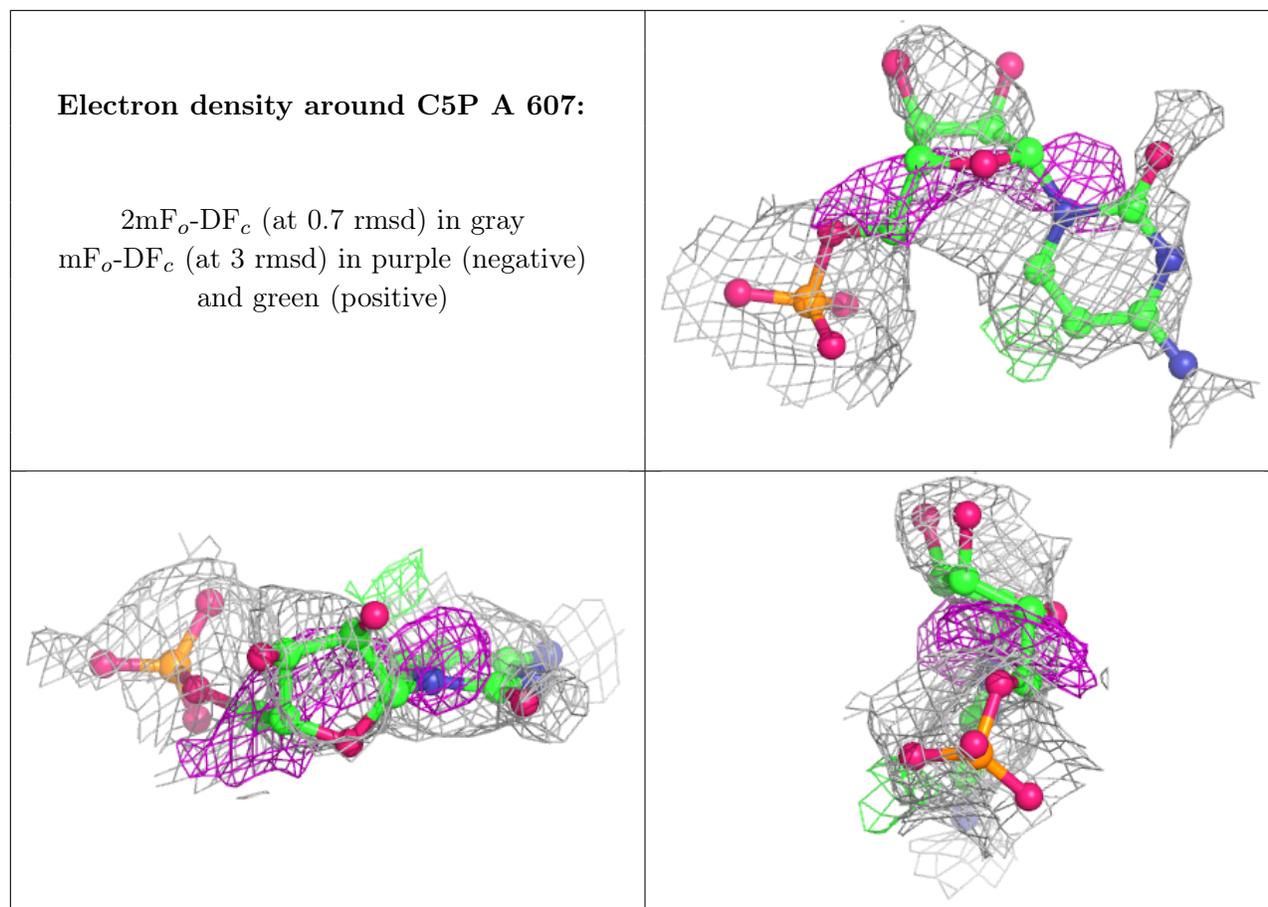*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	C	603	14/15	0.84	0.18	53,63,68,72	0
4	NAG	B	605	14/15	0.85	0.24	42,47,52,52	0
9	RP5	B	611	14/14	0.86	0.25	61,68,78,81	0
4	NAG	C	604	14/15	0.86	0.16	47,50,54,55	0
10	SCN	C	609	3/3	0.86	0.21	40,40,43,52	0
4	NAG	C	601	14/15	0.88	0.28	43,47,51,52	0
4	NAG	A	603	14/15	0.89	0.16	45,52,57,61	0
4	NAG	C	602	14/15	0.90	0.19	50,52,54,55	0
4	NAG	A	604	13/15	0.91	0.16	31,34,39,42	0
4	NAG	B	601	14/15	0.92	0.17	38,43,46,46	0
6	C5P	C	607	21/21	0.92	0.25	53,75,86,90	0
4	NAG	A	601	14/15	0.93	0.20	26,27,29,30	0
4	NAG	A	602	14/15	0.93	0.13	35,37,40,40	0
6	C5P	A	607	21/21	0.94	0.22	48,77,83,84	0
5	ZN	B	607	1/1	0.97	0.05	40,40,40,40	0
5	ZN	C	605	1/1	0.97	0.04	50,50,50,50	0
5	ZN	C	606	1/1	0.99	0.08	32,32,32,32	0
5	ZN	A	605	1/1	0.99	0.10	27,27,27,27	0
5	ZN	B	606	1/1	0.99	0.09	35,35,35,35	0
5	ZN	A	606	1/1	1.00	0.13	14,14,14,14	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 C5P C 607:

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

Electron density around C5P A 607:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.