



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 05:02 PM UTC

PDB ID : 5EBE / pdb\_00005ebe  
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)

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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (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

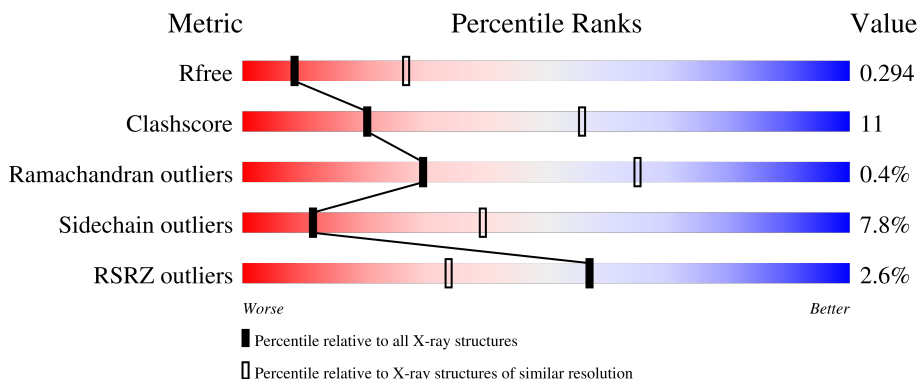
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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  $\geq 3$ , 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	418	 78% 19% ..
2	B	415	 5% 64% 30% 6%
2	C	415	 3% 71% 26% .
3	D	2	 100%

## 2 Entry composition [i](#)

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 (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

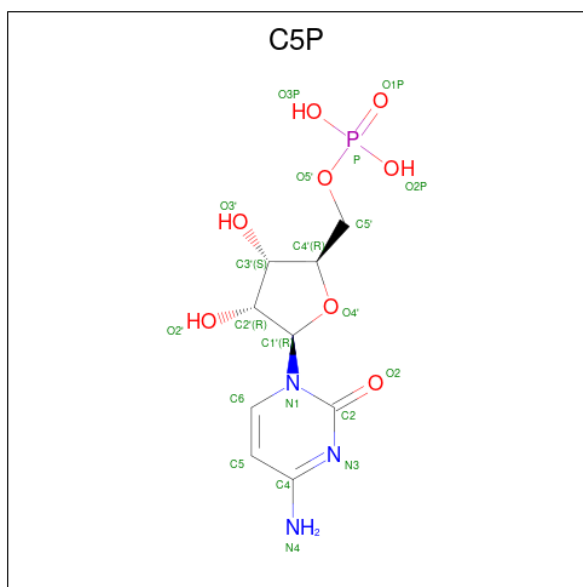
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		

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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 (CCD ID: C5P) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>3</sub>O<sub>8</sub>P).



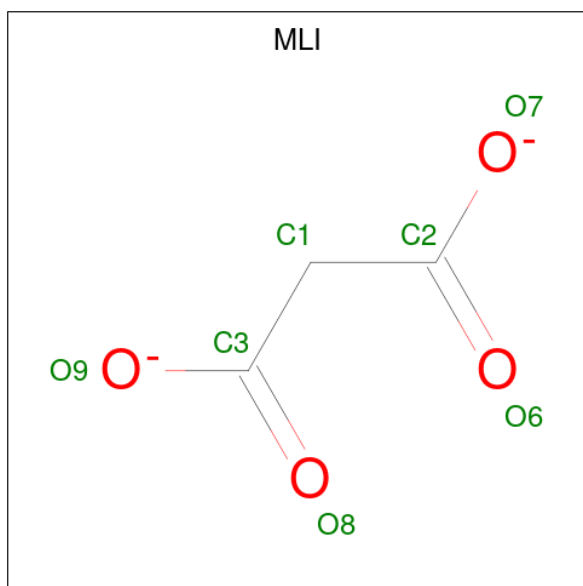
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P 21 9 3 8 1	0	0
6	C	1	Total C N O P 21 9 3 8 1	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



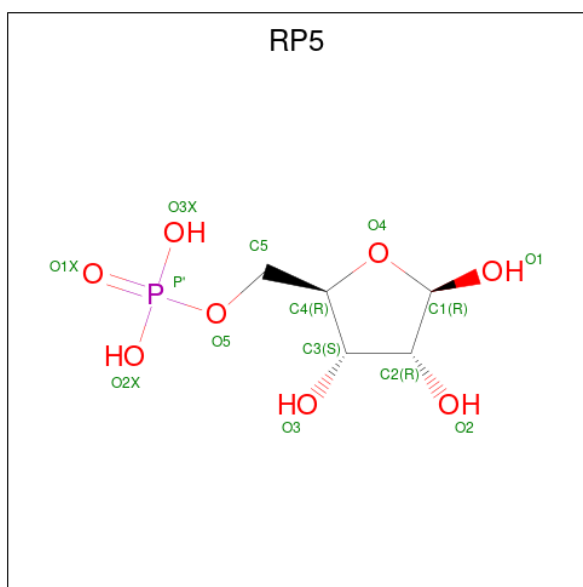
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is MALONATE ION (CCD ID: MLI) (formula:  $C_3H_2O_4$ ).



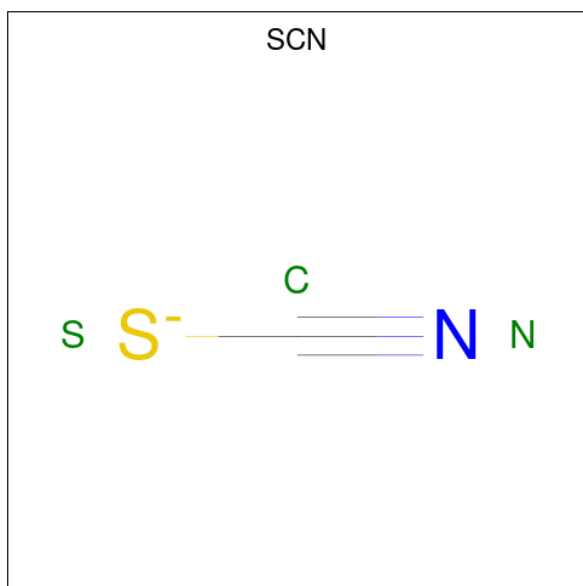
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 9 is 5-O-phosphono-beta-D-ribofuranose (CCD ID: RP5) (formula:  $C_5H_{11}O_8P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
9	B	1	14	5	8	1	0	0

- Molecule 10 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
10	C	1	3	1	1	1	0	0
10	C	1	3	1	1	1	0	0

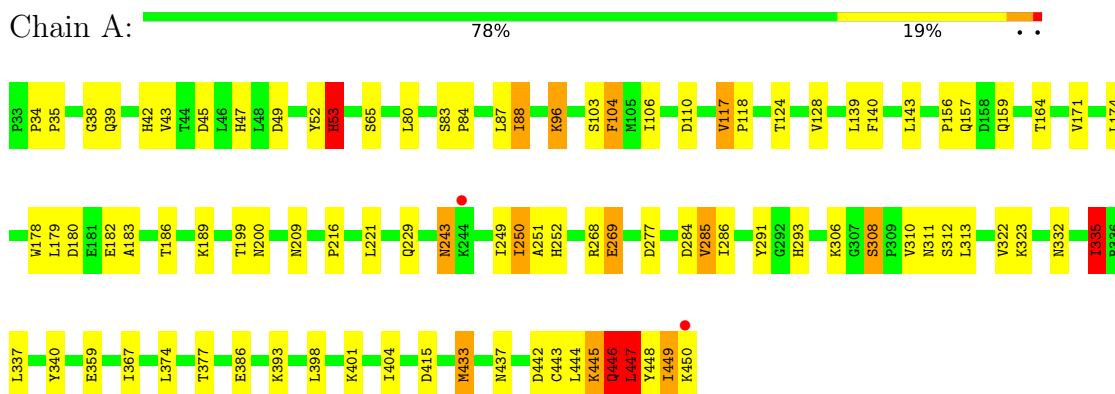
- Molecule 11 is water.

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

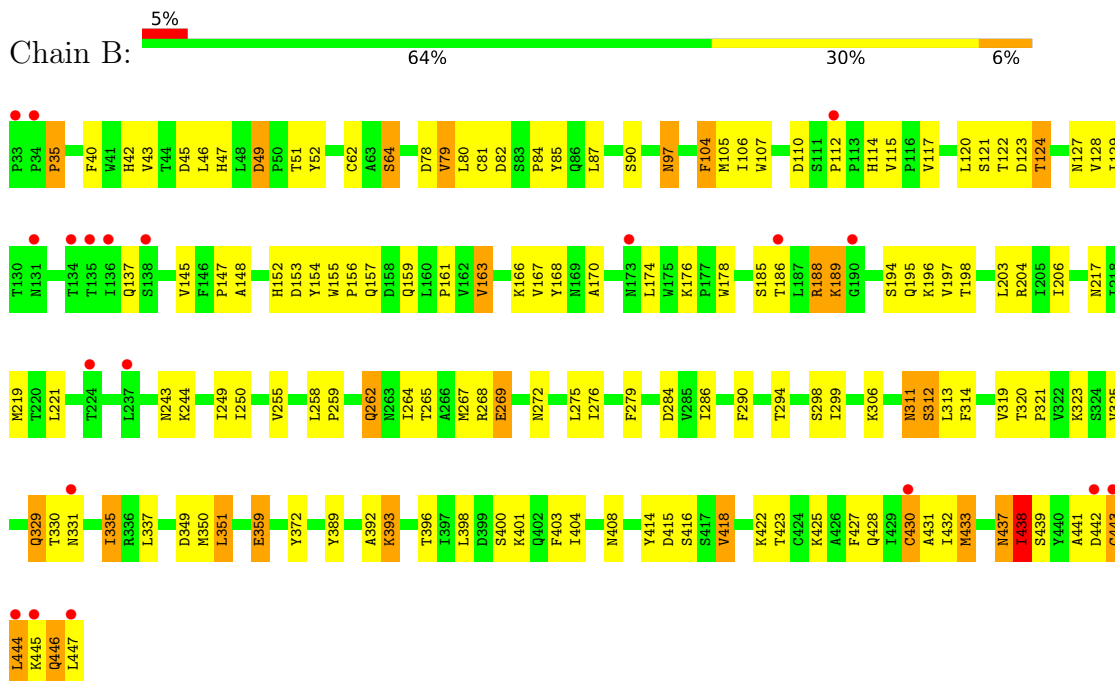
### 3 Residue-property plots

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

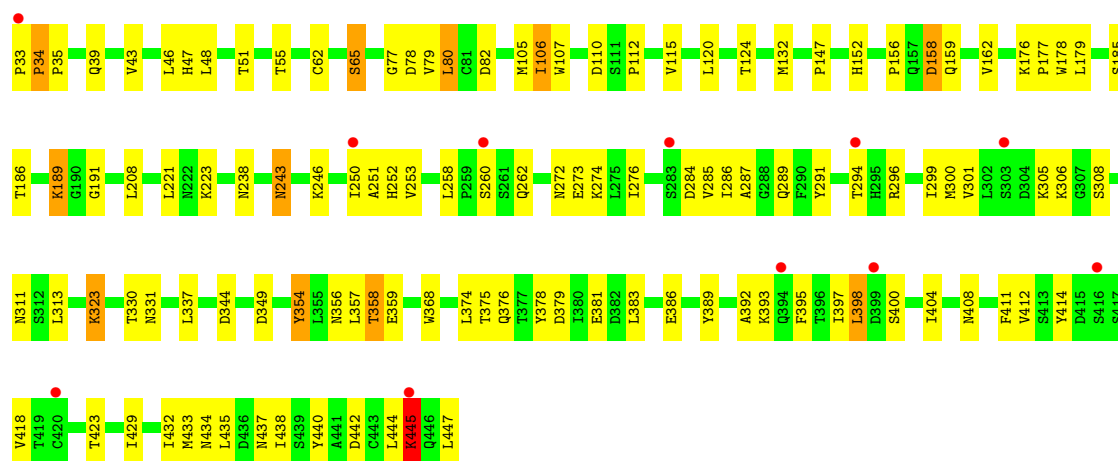


- Molecule 2: Acid sphingomyelinase-like phosphodiesterase 3a



- Molecule 2: Acid sphingomyelinase-like phosphodiesterase 3a





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

100%

MAG1  
MAG2

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.6 (47.56-3.00)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.251 , 0.295 0.251 , 0.294	Depositor DCC
$R_{free}$ test set	1790 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtrriage
Anisotropy	0.364	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage'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.*

<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: MLI, NAG, RP5, SCN, C5P, ZN, GOL

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	0.90	3/3479 (0.1%)	1.09	20/4749 (0.4%)
2	B	0.98	2/3443 (0.1%)	1.20	21/4702 (0.4%)
2	C	0.93	0/3448	1.12	11/4708 (0.2%)
All	All	0.94	5/10370 (0.0%)	1.14	52/14159 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	HIS	C-O	-6.02	1.16	1.24
2	B	431	ALA	CA-C	-5.31	1.45	1.52
1	A	49	ASP	C-O	-5.27	1.19	1.24
1	A	449	ILE	N-CA	5.26	1.52	1.46
2	B	446	GLN	CA-C	5.07	1.57	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	444	LEU	N-CA-C	-13.35	96.35	113.17
2	B	438	ILE	N-CA-C	-10.65	100.49	110.82
2	C	445	LYS	N-CA-C	-9.16	98.20	111.30
1	A	449	ILE	N-CA-C	7.60	119.28	108.42
1	A	117	VAL	CB-CA-C	-7.40	106.67	113.70
2	B	79	VAL	N-CA-C	-7.14	99.37	110.09
1	A	447	LEU	N-CA-CB	-6.92	98.79	110.49
2	C	253	VAL	N-CA-C	-6.79	102.70	109.02
2	B	335	ILE	N-CA-C	-6.61	99.63	108.35
2	B	258	LEU	CA-C-N	-6.43	113.15	119.64
2	B	258	LEU	C-N-CA	-6.43	113.15	119.64
2	B	104	PHE	N-CA-C	6.27	116.35	108.45
2	B	437	ASN	N-CA-C	6.27	120.93	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	GLN	CB-CA-C	6.27	122.89	110.42
2	C	253	VAL	CA-C-N	-6.17	114.19	120.85
2	C	253	VAL	C-N-CA	-6.17	114.19	120.85
1	A	447	LEU	CA-C-N	6.16	132.79	121.70
1	A	447	LEU	C-N-CA	6.16	132.79	121.70
1	A	285	VAL	CB-CA-C	-6.15	104.00	112.24
2	B	443	CYS	N-CA-C	-6.07	104.95	113.20
1	A	53	HIS	CB-CA-C	6.05	122.46	110.42
2	B	359	GLU	N-CA-C	-6.03	104.33	111.03
2	B	51	THR	N-CA-C	5.97	118.75	111.82
1	A	88	ILE	CB-CA-C	-5.95	104.25	112.04
1	A	404	ILE	N-CA-CB	5.92	117.48	110.55
2	C	354	TYR	N-CA-C	5.85	116.81	108.74
1	A	415	ASP	N-CA-C	-5.81	99.93	109.40
1	A	104	PHE	N-CA-C	5.75	115.84	108.24
2	B	117	VAL	CB-CA-C	-5.63	108.35	113.70
1	A	200	ASN	N-CA-C	-5.62	97.38	109.81
1	A	332	ASN	N-CA-C	-5.53	102.95	110.36
1	A	335	ILE	N-CA-C	-5.49	101.10	108.35
2	C	34	PRO	N-CA-C	-5.46	104.04	110.70
2	C	51	THR	CB-CA-C	-5.40	101.50	110.68
2	C	381	GLU	N-CA-C	5.39	117.59	111.02
2	C	77	GLY	N-CA-C	5.38	117.81	111.63
1	A	249	ILE	CB-CA-C	-5.35	104.19	111.15
2	B	128	VAL	N-CA-C	5.34	115.55	110.42
1	A	87	LEU	N-CA-C	-5.29	105.42	111.14
2	B	176	LYS	CA-C-N	-5.26	114.20	119.56
2	B	176	LYS	C-N-CA	-5.26	114.20	119.56
2	B	262	GLN	N-CA-C	5.23	118.14	109.46
1	A	128	VAL	N-CA-C	5.22	115.43	110.42
2	B	51	THR	CB-CA-C	-5.20	100.69	110.67
2	C	33	PRO	CA-C-N	-5.13	115.10	120.38
2	C	33	PRO	C-N-CA	-5.13	115.10	120.38
2	B	329	GLN	N-CA-C	5.12	117.91	109.72
2	B	206	ILE	N-CA-C	5.03	114.42	106.32
2	B	49	ASP	CA-C-N	5.02	125.29	119.47
2	B	49	ASP	C-N-CA	5.02	125.29	119.47
1	A	447	LEU	O-C-N	-5.01	115.92	122.59
1	A	447	LEU	N-CA-C	5.01	121.48	110.80

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	3380	0	3300	54	0
2	B	3344	0	3262	91	0
2	C	3350	0	3263	82	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	229	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 11.

All (229) 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
2:C:408:ASN:HB3	11:C:721:HOH:O	1.68	0.92
2:C:79:VAL:O	2:C:80:LEU:HB2	1.70	0.90
2:C:294[B]:THR:OG1	11:C:702:HOH:O	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:LYS:HD3	11:B:733:HOH:O	1.83	0.78
6:A:607:C5P:H6	6:A:607:C5P:H5'1	1.65	0.77
1:A:293:HIS:O	6:A:607:C5P:H5'2	1.84	0.77
2:B:47:HIS:CD2	11:B:701:HOH:O	2.38	0.76
2:B:428:GLN:O	2:B:432:ILE:HG13	1.84	0.76
3:D:1:NAG:H82	3:D:1:NAG:O3	1.89	0.73
1:A:322:VAL:O	6:A:607:C5P:N4	2.24	0.70
2:C:246:LYS:HE3	2:C:287:ALA:HB2	1.73	0.69
1:A:43:VAL:HG12	1:A:335:ILE:HD12	1.75	0.69
1:A:442:ASP:O	1:A:446:GLN:HB3	1.93	0.69
2:B:47:HIS:CE1	2:B:110:ASP:HB3	2.28	0.69
2:C:191:GLY:O	11:C:703:HOH:O	2.12	0.67
1:A:47:HIS:CE1	1:A:110:ASP:HB3	2.30	0.67
2:C:80:LEU:N	11:C:701:HOH:O	1.78	0.67
2:B:45:ASP:HB3	11:B:701:HOH:O	1.94	0.67
1:A:444:LEU:HG	1:A:449:ILE:HD11	1.78	0.66
2:C:246:LYS:HE2	2:C:344:ASP:O	1.95	0.66
2:C:294[B]:THR:HG22	2:C:296:ARG:HB2	1.77	0.65
2:C:330:THR:O	2:C:411:PHE:HB3	1.97	0.65
2:B:154:TYR:CD1	2:B:167:VAL:HG11	2.32	0.65
1:A:52:TYR:O	1:A:53:HIS:HB3	1.96	0.64
1:A:448:TYR:O	1:A:449:ILE:CD1	2.43	0.63
2:C:110:ASP:OD2	2:C:252:HIS:CE1	2.51	0.63
2:C:392:ALA:O	2:C:395:PHE:HB2	1.98	0.62
2:B:312:SER:HB3	2:B:314:PHE:CE2	2.34	0.62
2:B:442:ASP:C	2:B:444:LEU:H	2.08	0.61
1:A:447:LEU:O	1:A:447:LEU:HD12	2.00	0.60
1:A:286:ILE:HB	1:A:311:ASN:HD21	1.65	0.60
2:B:112[A]:PRO:HB2	11:B:713:HOH:O	2.00	0.60
2:B:286:ILE:HB	2:B:311:ASN:HD21	1.65	0.60
2:B:294:THR:HG21	11:B:727:HOH:O	2.00	0.60
1:A:445:LYS:O	1:A:446:GLN:C	2.43	0.59
2:B:267:MET:HE1	2:B:275:LEU:HD12	1.85	0.59
2:B:350:MET:HE1	2:B:372:TYR:OH	2.03	0.59
2:C:289:GLN:HB2	2:C:313:LEU:HG	1.84	0.58
2:C:112:PRO:HG2	2:C:152:HIS:O	2.05	0.57
2:B:52:TYR:CD1	2:B:84:PRO:HB3	2.40	0.57
2:B:47:HIS:HD2	11:B:701:HOH:O	1.82	0.56
4:C:604:NAG:H3	4:C:604:NAG:H83	1.86	0.56
2:C:185:SER:O	2:C:189:LYS:HD2	2.05	0.56
2:C:374:LEU:O	2:C:374:LEU:HD23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLN:HB3	1:A:337:LEU:HD11	1.88	0.55
1:A:446:GLN:CG	1:A:447:LEU:HD23	2.36	0.55
2:B:49:ASP:OD2	2:B:64:SER:OG	2.15	0.55
2:C:294[A]:THR:HG21	11:C:702:HOH:O	1.84	0.55
2:B:97:ASN:N	2:B:97:ASN:HD22	2.05	0.55
2:B:320:THR:HG22	11:B:701:HOH:O	2.06	0.55
2:C:300:MET:HG2	2:C:435:LEU:HD11	1.90	0.55
1:A:243:ASN:N	1:A:243:ASN:OD1	2.38	0.54
2:C:258:LEU:HD23	11:C:702:HOH:O	2.07	0.54
2:B:137:GLN:HG3	2:B:178:TRP:CZ2	2.42	0.54
2:C:294[B]:THR:CG2	2:C:296:ARG:HB2	2.37	0.54
2:B:35:PRO:CB	2:C:376:GLN:OE1	2.56	0.54
2:C:78:ASP:OD2	2:C:79:VAL:O	2.26	0.54
2:B:313:LEU:HD12	2:B:313:LEU:N	2.24	0.53
2:C:162:VAL:HG21	2:C:223:LYS:NZ	2.23	0.53
2:C:299:ILE:HG13	2:C:432:ILE:HG23	1.91	0.52
2:B:129:ILE:HD11	2:B:153:ASP:HB3	1.91	0.52
2:C:393:LYS:HD3	2:C:433:MET:HE1	1.90	0.52
2:C:392:ALA:HB3	2:C:433:MET:HE3	1.90	0.52
2:B:351:LEU:N	2:B:351:LEU:HD12	2.24	0.52
2:C:43:VAL:HG23	2:C:107:TRP:CD1	2.44	0.52
2:B:85:TYR:CE2	3:D:1:NAG:H4	2.45	0.52
2:B:124:THR:HA	2:B:127:ASN:HD22	1.74	0.52
2:B:329:GLN:HE22	2:B:414:TYR:HD2	1.57	0.52
2:B:185:SER:O	2:B:189:LYS:HD2	2.09	0.52
2:C:79:VAL:O	2:C:80:LEU:CB	2.46	0.52
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.91	0.51
2:C:286:ILE:HB	2:C:311:ASN:HD21	1.75	0.51
2:B:264:ILE:HG22	2:B:265:THR:O	2.10	0.51
2:B:403:PHE:CD2	2:B:425:LYS:HD2	2.45	0.51
2:B:400:SER:O	2:B:404:ILE:HG12	2.10	0.51
2:B:42:HIS:ND1	2:B:106[B]:ILE:HD11	2.24	0.51
2:C:107:TRP:O	2:C:147:PRO:HA	2.11	0.51
2:C:400:SER:O	2:C:404:ILE:HG12	2.11	0.51
2:B:415:ASP:HB3	2:B:418:VAL:HB	1.92	0.51
2:C:357:LEU:O	2:C:358:THR:C	2.54	0.50
2:B:43:VAL:HG12	2:B:335:ILE:HD12	1.91	0.50
2:B:154:TYR:CZ	2:B:161:PRO:HD3	2.47	0.50
2:C:294[B]:THR:HG22	2:C:296:ARG:CB	2.41	0.50
1:A:45:ASP:OD2	1:A:252:HIS:HE1	1.93	0.50
2:B:156:PRO:HG2	2:B:159:GLN:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:CYS:SG	2:B:443:CYS:SG	0.50	0.50
2:B:331:ASN:OD1	2:B:331:ASN:N	2.43	0.49
2:B:441:ALA:C	2:B:443:CYS:N	2.67	0.49
2:B:78:ASP:C	2:B:79:VAL:O	2.47	0.49
2:B:272:ASN:O	2:B:276:ILE:HG12	2.13	0.49
2:C:397:ILE:HG22	2:C:398:LEU:O	2.13	0.49
2:C:445:LYS:O	2:C:445:LYS:HG3	2.12	0.49
1:A:445:LYS:C	1:A:447:LEU:N	2.69	0.48
2:B:35:PRO:HB2	2:C:376:GLN:OE1	2.13	0.48
2:B:115:VAL:HG23	2:B:120:LEU:HG	1.96	0.48
2:C:158:ASP:OD1	2:C:158:ASP:N	2.44	0.48
2:B:40:PHE:O	2:B:337:LEU:HD12	2.13	0.48
2:C:176:LYS:N	2:C:177:PRO:CD	2.76	0.48
2:B:87:LEU:O	2:B:90:SER:OG	2.31	0.48
2:C:48:LEU:HD22	2:C:132:MET:HE3	1.96	0.48
2:C:445:LYS:O	2:C:445:LYS:CG	2.61	0.48
1:A:104:PHE:HA	1:A:143:LEU:HD11	1.96	0.48
1:A:52:TYR:CD1	1:A:84:PRO:HB3	2.49	0.48
11:B:709:HOH:O	3:D:2:NAG:H81	2.14	0.48
2:C:273:GLU:OE2	2:C:437:ASN:N	2.47	0.48
2:C:301:VAL:HG11	2:C:389:TYR:HB2	1.95	0.47
1:A:268:ARG:O	1:A:269:GLU:C	2.57	0.47
2:B:106[A]:ILE:HD12	2:B:250:ILE:HG12	1.95	0.47
1:A:359:GLU:OE1	1:A:367[B]:ILE:HD12	2.14	0.47
2:B:45:ASP:C	11:B:701:HOH:O	2.58	0.47
2:B:194:SER:HB2	2:B:204:ARG:HD3	1.96	0.47
2:B:163:VAL:HG13	11:B:746:HOH:O	2.14	0.47
2:B:78:ASP:HB3	2:B:81:CYS:HB2	1.98	0.46
1:A:171:VAL:HA	1:A:174:LEU:HD12	1.98	0.46
2:B:195:GLN:HG3	2:B:196:LYS:O	2.15	0.46
2:B:393:LYS:O	2:B:396:THR:OG1	2.30	0.46
2:C:272:ASN:O	2:C:276:ILE:HG12	2.16	0.46
2:B:268:ARG:O	2:B:269:GLU:C	2.59	0.46
2:B:80:LEU:HD11	2:B:325:VAL:HA	1.97	0.46
2:C:156:PRO:HG2	2:C:159:GLN:HG3	1.98	0.45
2:C:106[A]:ILE:HG23	2:C:250:ILE:CG1	2.46	0.45
1:A:47:HIS:NE2	1:A:110:ASP:HB3	2.30	0.45
1:A:180:ASP:HB3	1:A:182:GLU:H	1.82	0.45
2:B:47:HIS:HB3	2:B:82:ASP:OD1	2.16	0.45
2:B:107:TRP:O	2:B:147:PRO:HA	2.16	0.45
2:B:299:ILE:O	2:B:432:ILE:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:HIS:HA	1:A:106[B]:ILE:HG13	1.99	0.45
1:A:140:PHE:HB3	1:A:143:LEU:HB3	1.98	0.45
2:B:170:ALA:O	2:B:174:LEU:HG	2.16	0.45
2:B:389:TYR:CE1	2:B:433:MET:HG2	2.52	0.45
2:B:349:ASP:OD1	2:B:350:MET:N	2.49	0.45
2:B:255:VAL:HG11	2:B:279:PHE:HE2	1.81	0.45
2:B:441:ALA:C	2:B:443:CYS:H	2.24	0.45
2:C:208:LEU:HB2	2:C:251:ALA:HB2	1.99	0.45
1:A:157:GLN:O	1:A:159:GLN:HG2	2.17	0.45
2:C:354:TYR:HA	2:C:368:TRP:CZ3	2.51	0.45
2:C:418:VAL:O	2:C:418:VAL:HG13	2.16	0.44
1:A:43:VAL:HG12	1:A:335:ILE:CD1	2.45	0.44
2:C:115:VAL:CG2	2:C:120:LEU:HG	2.47	0.44
1:A:96:LYS:HE2	1:A:139:LEU:HD22	1.99	0.44
2:B:112[B]:PRO:CG	2:B:152:HIS:O	2.66	0.44
2:B:262:GLN:HB3	2:B:427:PHE:CZ	2.52	0.44
11:B:709:HOH:O	3:D:2:NAG:C8	2.65	0.44
1:A:209:ASN:H	1:A:229:GLN:HE22	1.65	0.44
2:B:329:GLN:NE2	2:B:414:TYR:HD2	2.14	0.44
2:C:440:TYR:O	2:C:440:TYR:CD2	2.71	0.44
2:C:349:ASP:OD1	2:C:375:THR:HG23	2.17	0.44
1:A:444:LEU:HG	1:A:449:ILE:CD1	2.45	0.44
2:B:219:MET:HE2	2:B:219:MET:N	2.33	0.44
2:C:323:LYS:N	11:C:701:HOH:O	2.51	0.44
2:C:331:ASN:HA	2:C:411:PHE:O	2.17	0.44
2:B:35:PRO:HB3	2:C:376:GLN:OE1	2.17	0.44
2:B:105:MET:O	2:B:145:VAL:HA	2.18	0.44
1:A:446:GLN:HG2	1:A:447:LEU:HD23	2.00	0.44
2:C:105:MET:O	2:C:106[A]:ILE:HD13	2.18	0.44
2:C:434:ASN:C	2:C:435:LEU:HD12	2.43	0.44
1:A:445:LYS:HB3	1:A:445:LYS:HE3	1.79	0.43
2:C:62:CYS:SG	2:C:65:SER:HB3	2.58	0.43
1:A:323:LYS:HA	6:A:607:C5P:N4	2.33	0.43
2:B:259:PRO:HD2	11:B:728:HOH:O	2.18	0.43
2:B:438:ILE:HA	2:B:438:ILE:HD13	1.73	0.43
2:C:374:LEU:HD23	2:C:374:LEU:C	2.44	0.43
1:A:83:SER:CB	1:A:88:ILE:HD11	2.48	0.43
1:A:393:LYS:HD3	1:A:433:MET:HE1	2.00	0.43
2:B:262:GLN:HB2	2:B:427:PHE:CE1	2.53	0.43
2:C:79:VAL:CA	11:C:701:HOH:O	2.66	0.43
2:C:243:ASN:N	2:C:243:ASN:OD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:TYR:HB3	2:B:188:ARG:HA	2.01	0.43
2:B:40:PHE:CD1	2:B:104:PHE:CZ	3.07	0.43
2:B:154:TYR:CD1	2:B:167:VAL:CG1	3.02	0.42
1:A:443:CYS:O	1:A:447:LEU:HD21	2.19	0.42
2:C:444:LEU:HD22	2:C:447:LEU:HD13	2.02	0.42
2:C:47:HIS:CE1	2:C:110:ASP:HB3	2.55	0.42
2:C:378:TYR:O	2:C:379:ASP:C	2.60	0.42
1:A:38:GLY:C	1:A:340:TYR:CE1	2.97	0.42
1:A:374:LEU:C	1:A:374:LEU:HD23	2.44	0.42
2:B:124:THR:HA	2:B:127:ASN:ND2	2.34	0.42
2:B:442:ASP:C	2:B:444:LEU:N	2.77	0.42
2:C:162:VAL:HG21	2:C:223:LYS:HZ1	1.84	0.42
2:B:62:CYS:O	2:B:62:CYS:SG	2.76	0.42
2:B:79:VAL:O	2:B:80:LEU:HB2	2.18	0.42
1:A:251:ALA:O	1:A:291:TYR:HA	2.19	0.42
1:A:312:SER:C	1:A:313:LEU:HD12	2.45	0.42
2:B:121:SER:HA	2:B:155:TRP:CD1	2.54	0.42
2:B:265:THR:HG21	11:B:715:HOH:O	2.19	0.42
2:C:34:PRO:HA	2:C:35:PRO:HD3	1.90	0.42
2:C:46:LEU:HD12	2:C:107:TRP:CZ2	2.55	0.42
2:C:423:THR:HG23	2:C:447:LEU:HD21	2.02	0.42
2:C:442:ASP:O	2:C:445:LYS:HB3	2.19	0.42
2:C:323:LYS:CG	11:C:701:HOH:O	2.67	0.42
1:A:38:GLY:HA3	1:A:340:TYR:CZ	2.55	0.41
1:A:313:LEU:HD12	1:A:313:LEU:N	2.35	0.41
1:A:443:CYS:O	1:A:447:LEU:CD2	2.68	0.41
2:B:321:PRO:O	2:B:330:THR:HG21	2.20	0.41
1:A:445:LYS:O	1:A:447:LEU:N	2.53	0.41
2:B:249:ILE:O	2:B:290:PHE:N	2.49	0.41
2:C:323:LYS:HG2	11:C:701:HOH:O	2.19	0.41
2:C:412:VAL:HG12	2:C:412:VAL:O	2.20	0.41
2:B:156:PRO:O	2:B:157:GLN:C	2.64	0.41
2:B:122:THR:HG21	2:B:166:LYS:HD3	2.01	0.41
1:A:106[A]:ILE:HD12	1:A:250:ILE:HG12	2.01	0.41
1:A:308:SER:O	1:A:310:VAL:HG13	2.21	0.41
1:A:34:PRO:HA	1:A:35:PRO:HD3	1.92	0.41
1:A:103:SER:HB3	1:A:199:THR:OG1	2.21	0.41
1:A:178:TRP:O	1:A:179:LEU:HD23	2.20	0.41
2:B:46:LEU:HD23	2:B:319:VAL:HG21	2.04	0.41
2:B:217:ASN:O	2:B:268:ARG:NH2	2.52	0.41
2:B:392:ALA:O	2:B:396:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:178:TRP:O	2:C:179:LEU:HD23	2.21	0.40
1:A:110:ASP:CG	1:A:252:HIS:CE1	2.99	0.40
1:A:156:PRO:O	1:A:157:GLN:C	2.64	0.40
2:B:197:VAL:HG21	2:B:203:LEU:HD23	2.02	0.40
2:C:34:PRO:O	2:C:34:PRO:CD	2.69	0.40
2:B:47:HIS:CD2	2:B:114:HIS:HE1	2.39	0.40
2:C:356:ASN:HB3	2:C:359:GLU:HB3	2.04	0.40
2:C:395:PHE:HB3	2:C:429:ILE:HD11	2.01	0.40
2:B:148:ALA:HB2	2:B:250:ILE:HG22	2.03	0.40
2:C:39:GLN:HB3	2:C:337:LEU:HD11	2.04	0.40
2:C:47:HIS:HB3	2:C:82:ASP:OD1	2.22	0.40
2:C:78:ASP:N	11:C:711:HOH:O	2.49	0.40
1:A:180:ASP:HB2	1:A:183:ALA:H	1.87	0.40
2:C:106[A]:ILE:CG2	2:C:250:ILE:HG13	2.52	0.40
2:C:291:TYR:HE2	2:C:313:LEU:HD23	1.87	0.40
2:C:440:TYR:O	2:C:440:TYR:CG	2.74	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	420/418 (100%)	380 (90%)	38 (9%)	2 (0%)	24 60
2	B	416/415 (100%)	367 (88%)	47 (11%)	2 (0%)	24 60
2	C	417/415 (100%)	381 (91%)	35 (8%)	1 (0%)	43 76
All	All	1253/1248 (100%)	1128 (90%)	120 (10%)	5 (0%)	30 65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	35	PRO

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

### 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	384/380 (101%)	357 (93%)	27 (7%)	14	44
2	B	380/377 (101%)	345 (91%)	35 (9%)	8	33
2	C	381/377 (101%)	353 (93%)	28 (7%)	13	42
All	All	1145/1134 (101%)	1055 (92%)	90 (8%)	11	39

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	65	SER
1	A	80	LEU
1	A	96	LYS
1	A	124	THR
1	A	186	THR
1	A	189	LYS
1	A	221	LEU
1	A	243	ASN
1	A	250	ILE
1	A	269	GLU
1	A	277	ASP
1	A	284	ASP
1	A	285	VAL
1	A	306	LYS
1	A	308	SER
1	A	335	ILE
1	A	377	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	386	GLU
1	A	398	LEU
1	A	401	LYS
1	A	433	MET
1	A	437	ASN
1	A	445	LYS
1	A	446	GLN
1	A	447	LEU
1	A	450	LYS
2	B	64	SER
2	B	97	ASN
2	B	123	ASP
2	B	124	THR
2	B	163	VAL
2	B	186	THR
2	B	188	ARG
2	B	189	LYS
2	B	198	THR
2	B	221	LEU
2	B	243	ASN
2	B	244	LYS
2	B	269	GLU
2	B	284	ASP
2	B	298	SER
2	B	306	LYS
2	B	311	ASN
2	B	312	SER
2	B	323	LYS
2	B	351	LEU
2	B	359	GLU
2	B	393	LYS
2	B	398	LEU
2	B	401	LYS
2	B	408	ASN
2	B	416	SER
2	B	418	VAL
2	B	423	THR
2	B	430	CYS
2	B	433	MET
2	B	437	ASN
2	B	438	ILE
2	B	439	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	446	GLN
2	B	447	LEU
2	C	55	THR
2	C	65	SER
2	C	80	LEU
2	C	106[A]	ILE
2	C	106[B]	ILE
2	C	124	THR
2	C	158	ASP
2	C	186	THR
2	C	189	LYS
2	C	221	LEU
2	C	238	ASN
2	C	243	ASN
2	C	260[A]	SER
2	C	260[B]	SER
2	C	262	GLN
2	C	274	LYS
2	C	284	ASP
2	C	285	VAL
2	C	305	LYS
2	C	306	LYS
2	C	308	SER
2	C	323	LYS
2	C	358	THR
2	C	383	LEU
2	C	386	GLU
2	C	398	LEU
2	C	438	ILE
2	C	445	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	39	GLN
1	A	58	HIS
1	A	86	GLN
1	A	169	ASN
1	A	229	GLN
1	A	238	ASN
1	A	262	GLN
1	A	311	ASN

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Mol	Chain	Res	Type
1	A	437	ASN
2	B	47	HIS
2	B	58	HIS
2	B	86	GLN
2	B	97	ASN
2	B	127	ASN
2	B	169	ASN
2	B	173	ASN
2	B	229	GLN
2	B	241	GLN
2	B	295	HIS
2	B	329	GLN
2	B	332	ASN
2	B	434	ASN
2	B	437	ASN
2	C	39	GLN
2	C	58	HIS
2	C	86	GLN
2	C	200	ASN
2	C	211	ASN
2	C	229	GLN
2	C	238	ASN
2	C	280	GLN
2	C	311	ASN
2	C	434	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

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	1.85	3 (21%)	17,19,21	1.92	3 (17%)
3	NAG	D	2	3	14,14,15	1.79	4 (28%)	17,19,21	2.63	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	5.64	1.60	1.52
3	D	2	NAG	O5-C5	4.45	1.52	1.43
3	D	2	NAG	C8-C7	3.09	1.57	1.50
3	D	2	NAG	O5-C1	2.55	1.48	1.43
3	D	2	NAG	C4-C5	2.42	1.58	1.53
3	D	1	NAG	O4-C4	2.40	1.48	1.43
3	D	1	NAG	C2-N2	2.18	1.49	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	6.41	120.78	112.19
3	D	1	NAG	C2-N2-C7	5.05	129.67	122.90
3	D	2	NAG	C4-C3-C2	-4.95	103.77	111.02
3	D	1	NAG	C1-O5-C5	4.34	118.01	112.19
3	D	2	NAG	O5-C1-C2	-3.96	105.17	111.29
3	D	2	NAG	O6-C6-C5	-2.96	101.27	111.33
3	D	2	NAG	O5-C5-C4	2.77	117.56	110.83
3	D	2	NAG	C1-C2-N2	2.68	114.66	110.43
3	D	1	NAG	O7-C7-C8	-2.25	118.06	122.05

There are no chirality outliers.

All (8) torsion outliers are listed below:

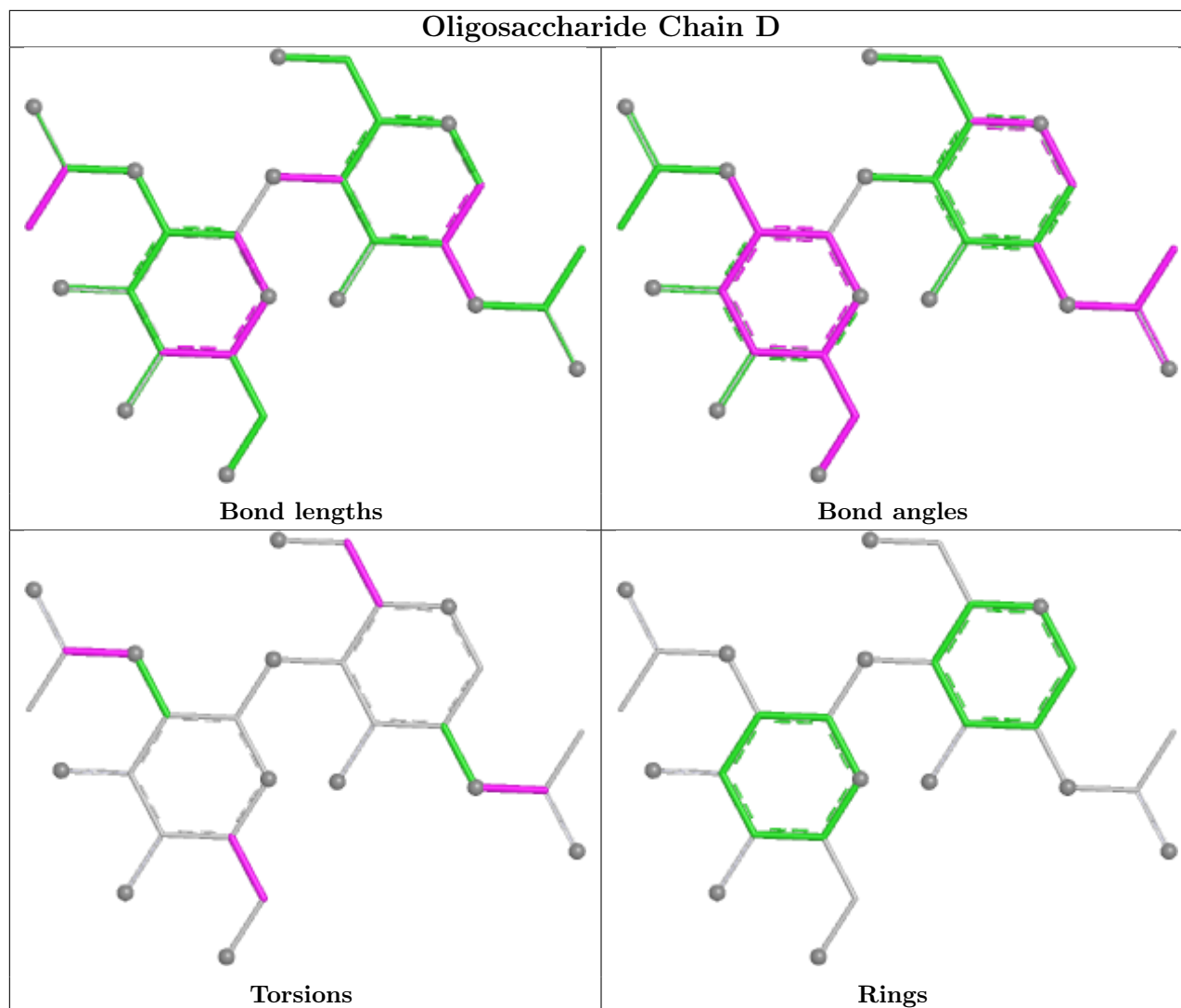
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2

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.



## 5.6 Ligand geometry [i](#)

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$
4	NAG	A	601	1	14,14,15	2.13	4 (28%)	17,19,21	2.11	5 (29%)
7	GOL	B	608	-	5,5,5	0.64	0	5,5,5	0.76	0
4	NAG	C	602	2	14,14,15	1.95	3 (21%)	17,19,21	1.52	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	604	-	13,13,15	3.89	4 (30%)	15,17,21	3.81	8 (53%)
6	C5P	C	607	5	22,22,22	1.23	3 (13%)	32,33,33	1.79	9 (28%)
4	NAG	C	601	2	14,14,15	3.15	5 (35%)	17,19,21	2.41	3 (17%)
4	NAG	A	602	1	14,14,15	2.01	3 (21%)	17,19,21	2.06	2 (11%)
4	NAG	A	603	1	14,14,15	1.23	2 (14%)	17,19,21	2.52	6 (35%)
10	SCN	C	608	-	1,2,2	0.52	0	0,1,1	-	-
4	NAG	B	605	2	14,14,15	3.15	5 (35%)	17,19,21	1.83	6 (35%)
4	NAG	C	603	2	14,14,15	1.95	2 (14%)	17,19,21	2.30	2 (11%)
9	RP5	B	611	5	14,14,14	1.12	1 (7%)	19,21,21	1.63	3 (15%)
10	SCN	C	609	-	1,2,2	0.24	0	0,1,1	-	-
7	GOL	B	609	-	5,5,5	0.85	0	5,5,5	0.56	0
4	NAG	B	604	2	14,14,15	1.40	1 (7%)	17,19,21	1.56	3 (17%)
6	C5P	A	607	5	22,22,22	0.75	0	32,33,33	1.23	4 (12%)
4	NAG	C	604	2	14,14,15	2.09	4 (28%)	17,19,21	1.81	4 (23%)
4	NAG	B	601	2	14,14,15	1.54	2 (14%)	17,19,21	2.35	5 (29%)
8	MLI	B	610	-	6,6,6	3.19	2 (33%)	7,7,7	1.22	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
9	RP5	B	611	5	-	3/6/22/22	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
7	GOL	B	609	-	-	2/4/4/4	-
7	GOL	B	608	-	-	2/4/4/4	-
4	NAG	C	602	2	-	2/6/23/26	0/1/1/1
4	NAG	C	601	2	-	0/6/23/26	0/1/1/1
6	C5P	C	607	5	-	4/10/26/26	0/2/2/2
6	C5P	A	607	5	-	0/10/26/26	0/2/2/2
4	NAG	C	604	2	-	5/6/23/26	0/1/1/1
8	MLI	B	610	-	-	2/4/4/4	-
4	NAG	A	602	1	-	2/6/23/26	0/1/1/1
4	NAG	B	601	2	-	0/6/23/26	0/1/1/1
4	NAG	B	605	2	-	1/6/23/26	0/1/1/1
4	NAG	A	604	-	-	2/6/19/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	604	2	-	2/6/23/26	0/1/1/1
4	NAG	C	603	2	-	2/6/23/26	0/1/1/1
4	NAG	A	603	1	-	2/6/23/26	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	NAG	C1-C2	11.42	1.64	1.51
4	C	601	NAG	C1-C2	7.51	1.62	1.52
4	B	605	NAG	O5-C1	7.38	1.56	1.43
4	C	601	NAG	O5-C1	6.73	1.55	1.43
4	A	604	NAG	O5-C5	5.89	1.54	1.43
4	C	604	NAG	C1-C2	5.79	1.60	1.52
4	B	605	NAG	C1-C2	5.63	1.60	1.52
8	B	610	MLI	C1-C2	5.40	1.59	1.51
4	C	603	NAG	O5-C1	5.25	1.52	1.43
4	A	602	NAG	O5-C1	5.14	1.52	1.43
8	B	610	MLI	C1-C3	5.07	1.58	1.51
4	B	605	NAG	O5-C5	4.70	1.52	1.43
4	B	605	NAG	O4-C4	4.29	1.53	1.43
4	A	604	NAG	O4-C4	4.28	1.52	1.43
4	A	601	NAG	C1-C2	4.19	1.58	1.52
4	A	601	NAG	O5-C1	4.13	1.50	1.43
4	A	601	NAG	O4-C4	4.02	1.52	1.43
4	C	602	NAG	C1-C2	4.02	1.57	1.52
4	C	602	NAG	O5-C1	3.93	1.50	1.43
4	C	601	NAG	O5-C5	3.63	1.50	1.43
4	B	601	NAG	C1-C2	3.40	1.57	1.52
4	B	604	NAG	C1-C2	3.38	1.56	1.52
4	B	601	NAG	O5-C1	3.36	1.49	1.43
4	C	603	NAG	O5-C5	3.30	1.49	1.43
4	C	601	NAG	O4-C4	3.26	1.51	1.43
4	A	602	NAG	O5-C5	3.10	1.49	1.43
4	A	602	NAG	O4-C4	2.71	1.49	1.43
4	A	603	NAG	O5-C1	2.60	1.48	1.43
4	C	604	NAG	O5-C1	2.55	1.48	1.43
4	A	604	NAG	O5-C1	2.40	1.47	1.43
4	C	604	NAG	O4-C4	2.34	1.48	1.43
4	B	605	NAG	C4-C5	2.33	1.58	1.53
6	C	607	C5P	C6-C5	2.31	1.40	1.35
4	C	604	NAG	C8-C7	2.30	1.55	1.50
6	C	607	C5P	C2-N1	2.28	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	C8-C7	2.24	1.55	1.50
4	C	602	NAG	O4-C4	2.15	1.48	1.43
9	B	611	RP5	O4-C1	-2.13	1.40	1.43
4	A	603	NAG	C8-C7	2.11	1.54	1.50
6	C	607	C5P	C5'-C4'	2.10	1.57	1.51
4	C	601	NAG	C4-C5	2.05	1.57	1.53

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	NAG	C3-C2-C1	9.11	117.88	109.50
4	C	601	NAG	C1-O5-C5	8.39	123.42	112.19
4	C	603	NAG	C1-O5-C5	7.79	122.63	112.19
4	B	601	NAG	C1-O5-C5	7.67	122.46	112.19
4	A	603	NAG	C1-O5-C5	7.15	121.76	112.19
4	A	604	NAG	C1-O5-C5	7.01	121.58	112.19
4	A	602	NAG	C1-O5-C5	6.62	121.06	112.19
4	A	601	NAG	C1-O5-C5	6.51	120.91	112.19
4	A	603	NAG	C1-C2-N2	-5.10	102.40	110.43
9	B	611	RP5	O1-C1-O4	-4.84	104.95	111.12
4	A	604	NAG	C6-C5-C4	-4.52	107.35	113.53
4	C	602	NAG	C1-O5-C5	4.43	118.12	112.19
6	C	607	C5P	O2-C2-N3	-4.37	115.44	122.33
4	A	604	NAG	O5-C5-C4	4.36	116.91	109.66
6	C	607	C5P	C1'-N1-C2	4.13	127.55	118.44
4	A	604	NAG	C3-C4-C5	-3.89	105.81	110.76
4	B	605	NAG	C1-O5-C5	3.79	117.26	112.19
4	A	602	NAG	O5-C5-C6	3.67	114.80	107.66
6	C	607	C5P	O5'-C5'-C4'	3.66	121.44	108.99
4	B	604	NAG	C1-O5-C5	3.55	116.94	112.19
4	C	604	NAG	C2-N2-C7	3.53	127.62	122.90
4	A	604	NAG	O6-C6-C5	-3.52	99.36	111.33
4	C	604	NAG	C1-C2-N2	3.43	115.84	110.43
4	C	604	NAG	C8-C7-N2	3.32	121.63	116.12
4	C	604	NAG	O7-C7-C8	-3.07	116.59	122.05
4	B	605	NAG	O5-C5-C6	3.04	113.58	107.66
6	A	607	C5P	C3'-C2'-C1'	2.80	106.75	101.46
6	C	607	C5P	O4'-C1'-N1	2.77	114.63	108.36
4	B	604	NAG	O5-C1-C2	-2.71	107.10	111.29
4	B	601	NAG	C2-N2-C7	-2.67	119.32	122.90
4	B	601	NAG	C1-C2-N2	-2.65	106.26	110.43
6	A	607	C5P	O3P-P-O5'	-2.61	99.87	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	607	C5P	C3'-C2'-C1'	2.58	106.35	101.46
6	C	607	C5P	C6-N1-C2	-2.55	116.15	120.46
6	A	607	C5P	O2P-P-O3P	2.52	117.24	107.80
4	C	603	NAG	O6-C6-C5	-2.48	102.89	111.33
6	C	607	C5P	O2-C2-N1	2.45	123.69	118.90
4	B	605	NAG	O3-C3-C2	-2.39	104.44	109.40
4	A	604	NAG	C3-C2-N2	-2.35	106.76	110.62
4	A	601	NAG	O3-C3-C2	-2.35	104.53	109.40
9	B	611	RP5	O5-C5-C4	-2.33	101.07	108.99
4	B	604	NAG	C3-C4-C5	-2.30	106.05	110.23
4	A	603	NAG	C4-C3-C2	-2.28	107.67	111.02
4	B	605	NAG	C6-C5-C4	-2.27	107.44	113.02
9	B	611	RP5	C1-C2-C3	2.24	105.05	102.29
4	C	601	NAG	O7-C7-N2	2.22	125.90	121.98
4	A	604	NAG	C4-C3-C2	-2.21	109.78	112.50
6	A	607	C5P	O2-C2-N3	-2.21	118.85	122.33
4	B	601	NAG	C3-C4-C5	-2.18	106.28	110.23
4	A	601	NAG	O4-C4-C5	2.17	114.67	109.32
4	C	601	NAG	O5-C5-C6	2.17	111.88	107.66
4	B	601	NAG	O6-C6-C5	-2.13	104.08	111.33
4	B	605	NAG	O6-C6-C5	-2.12	104.10	111.33
4	A	603	NAG	O6-C6-C5	-2.12	104.10	111.33
6	C	607	C5P	O4'-C4'-C5'	2.12	116.13	109.33
6	C	607	C5P	C1'-N1-C6	-2.10	116.30	120.78
4	A	603	NAG	O5-C1-C2	-2.06	108.11	111.29
4	A	601	NAG	C2-N2-C7	-2.06	120.14	122.90
4	A	601	NAG	C3-C4-C5	-2.02	106.57	110.23
4	B	605	NAG	O5-C1-C2	-2.02	108.17	111.29
4	A	603	NAG	C6-C5-C4	-2.01	108.09	113.02

There are no chirality outliers.

All (31) 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
4	C	602	NAG	O5-C5-C6-O6
4	A	604	NAG	O5-C5-C6-O6
4	C	603	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	602	NAG	C4-C5-C6-O6
4	A	602	NAG	C4-C5-C6-O6
4	C	604	NAG	C4-C5-C6-O6
4	A	603	NAG	C4-C5-C6-O6
4	A	604	NAG	C4-C5-C6-O6
4	A	603	NAG	O5-C5-C6-O6
4	C	604	NAG	C8-C7-N2-C2
4	C	604	NAG	O7-C7-N2-C2
6	C	607	C5P	C3'-C4'-C5'-O5'
4	C	603	NAG	C4-C5-C6-O6
4	C	604	NAG	O5-C5-C6-O6
7	B	608	GOL	O1-C1-C2-C3
4	B	605	NAG	O5-C5-C6-O6
7	B	608	GOL	O1-C1-C2-O2
7	B	609	GOL	O1-C1-C2-O2
8	B	610	MLI	C3-C1-C2-O6
9	B	611	RP5	C3-C4-C5-O5
4	C	604	NAG	C3-C2-N2-C7
9	B	611	RP5	C5-O5-P'-O1X
6	C	607	C5P	O4'-C1'-N1-C6
7	B	609	GOL	C1-C2-C3-O3
8	B	610	MLI	C3-C1-C2-O7
6	C	607	C5P	O4'-C1'-N1-C2

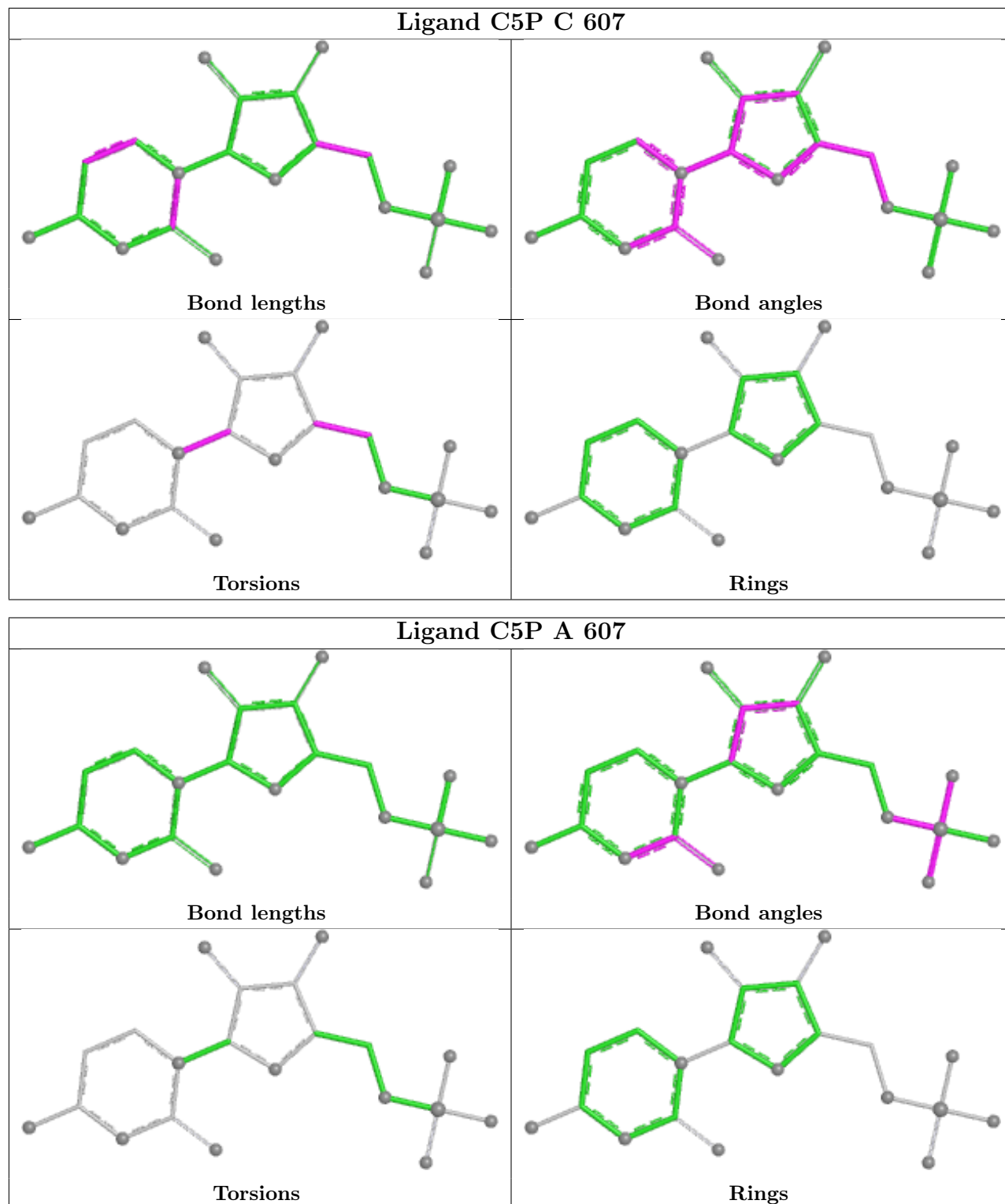
There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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

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	418/418 (100%)	-0.40	2 (0%) 87 72	9, 26, 51, 85	4 (0%)
2	B	415/415 (100%)	0.59	20 (4%) 35 19	13, 44, 72, 119	3 (0%)
2	C	415/415 (100%)	0.44	11 (2%) 56 33	11, 43, 63, 87	4 (0%)
All	All	1248/1248 (100%)	0.21	33 (2%) 57 34	9, 39, 65, 119	11 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	445	LYS	4.0
2	B	430	CYS	3.7
2	B	33	PRO	3.7
2	C	33	PRO	3.4
2	B	447	LEU	3.3
2	B	444	LEU	3.3
2	C	294[A]	THR	3.2
2	C	283	SER	3.2
2	B	224	THR	3.1
1	A	450	LYS	2.9
2	B	445	LYS	2.9
2	C	399	ASP	2.9
2	C	394	GLN	2.8
2	C	420	CYS	2.7
2	B	135	THR	2.7
2	B	331	ASN	2.7
2	C	250	ILE	2.7
2	B	190	GLY	2.7
2	B	134	THR	2.7
2	B	131	ASN	2.7
2	B	34	PRO	2.6
2	B	173	ASN	2.5
2	B	112[A]	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	186	THR	2.5
2	B	138	SER	2.5
2	B	443	CYS	2.4
2	B	237	LEU	2.4
2	C	303	SER	2.4
2	C	260[A]	SER	2.3
2	B	442	ASP	2.3
2	B	136	ILE	2.2
1	A	244	LYS	2.2
2	C	416	SER	2.1

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

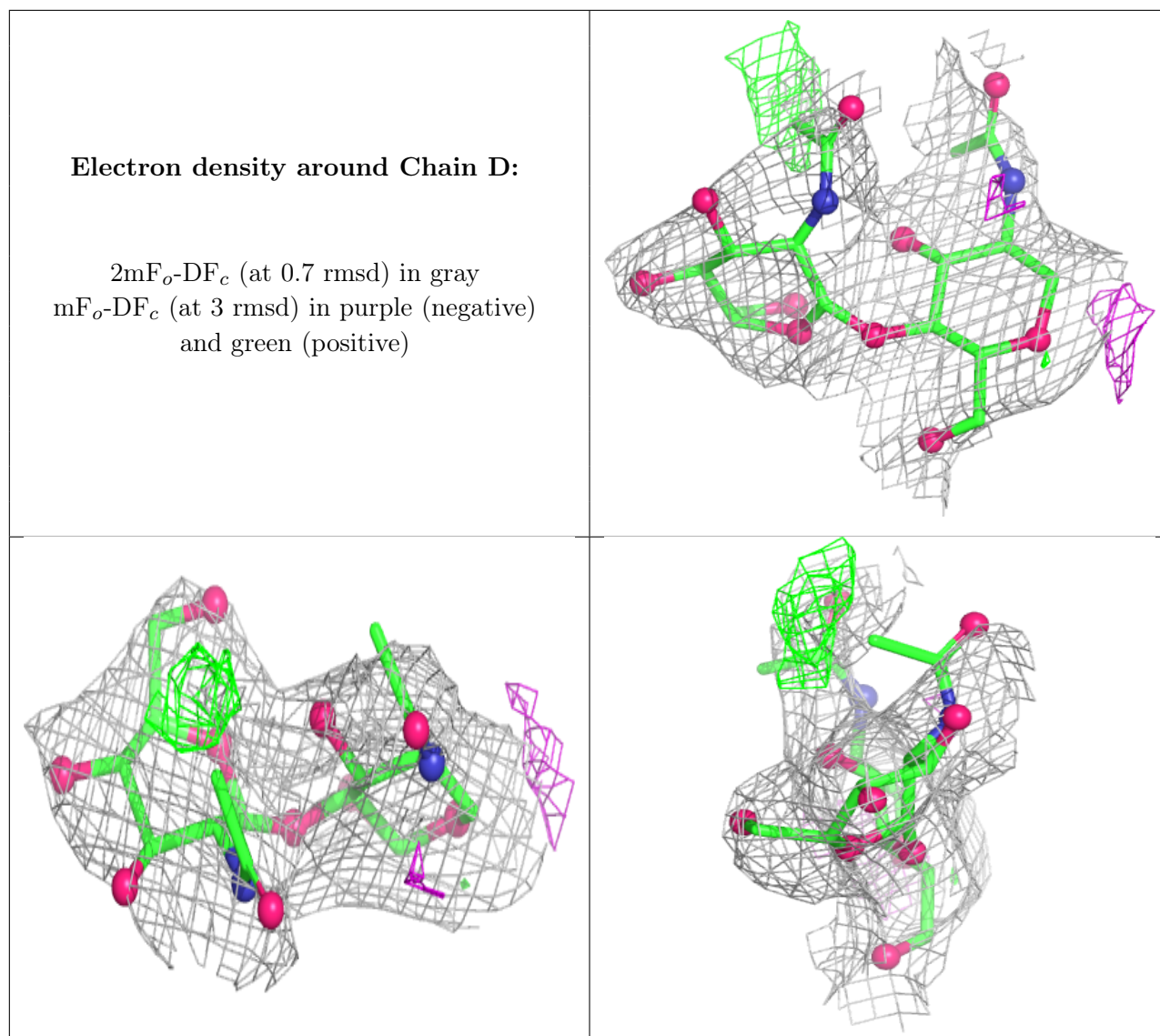
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

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	D	2	14/15	0.73	0.12	62,70,78,78	0
3	NAG	D	1	14/15	0.88	0.14	46,57,70,74	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



## 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
7	GOL	B	609	6/6	0.54	0.20	52,63,67,68	0
10	SCN	C	608	3/3	0.72	0.14	36,36,44,48	0
7	GOL	B	608	6/6	0.73	0.17	41,42,44,44	0
4	NAG	B	604	14/15	0.77	0.12	72,76,79,85	0
8	MLI	B	610	7/7	0.78	0.18	52,63,65,67	0
4	NAG	A	603	14/15	0.79	0.13	45,52,57,61	0
9	RP5	B	611	14/14	0.80	0.15	61,68,78,81	0

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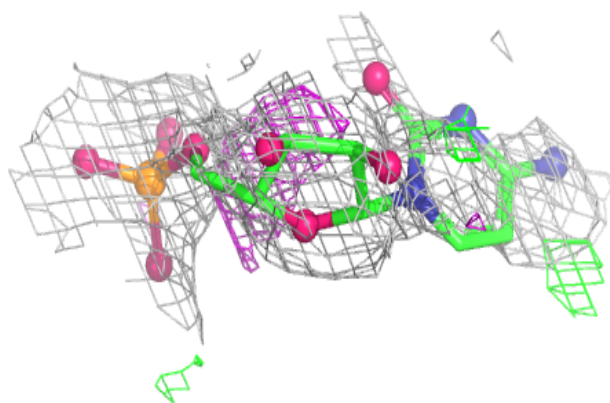
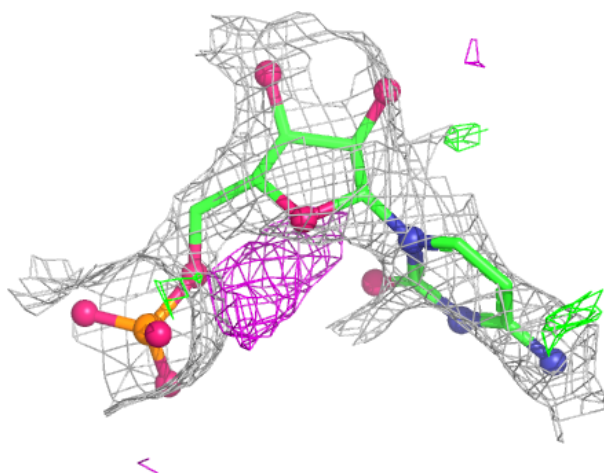
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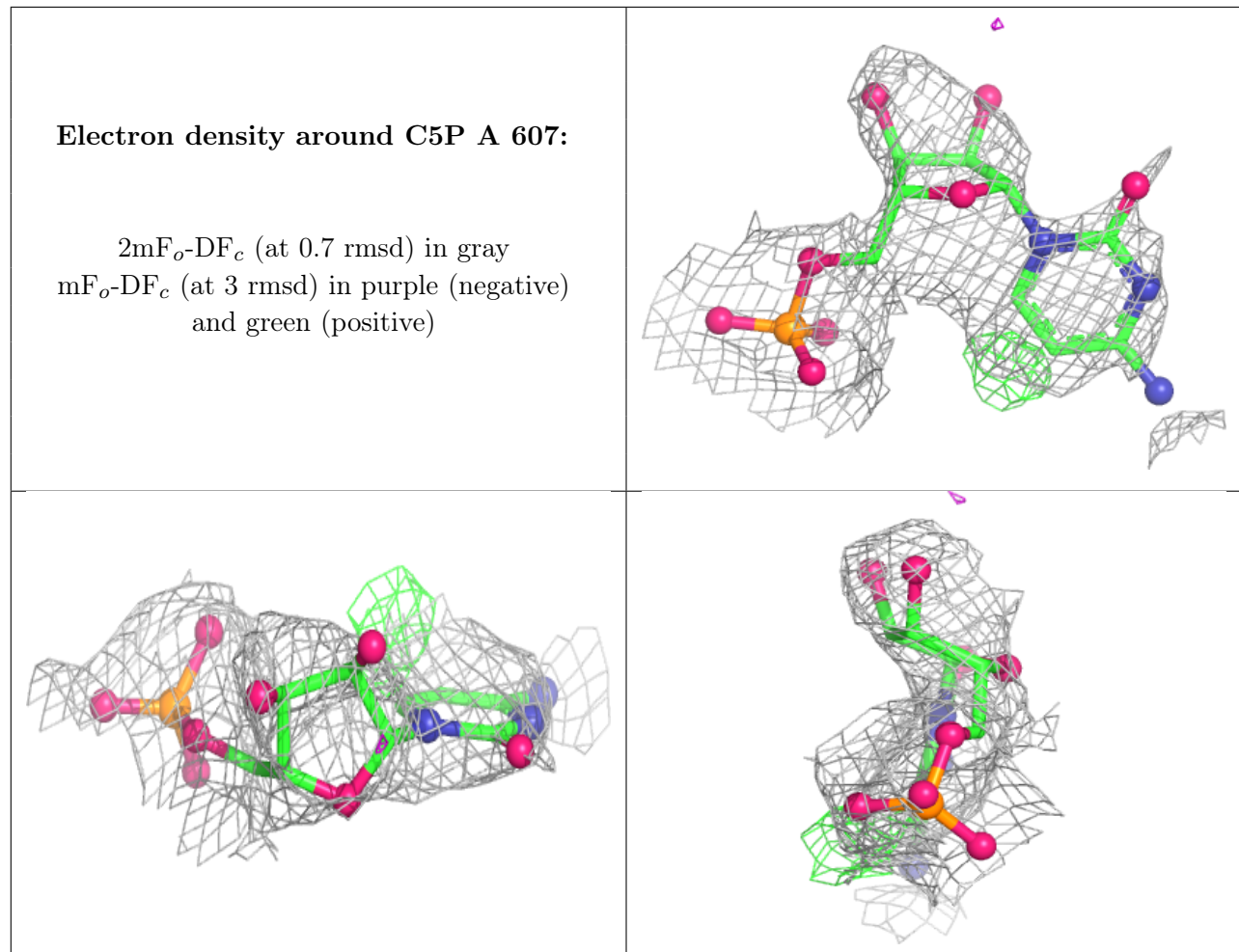
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	C	603	14/15	0.82	0.12	53,63,68,72	0
10	SCN	C	609	3/3	0.82	0.15	40,40,43,52	0
4	NAG	C	604	14/15	0.84	0.12	47,50,54,55	0
4	NAG	A	604	13/15	0.85	0.14	31,34,39,42	0
6	C5P	C	607	21/21	0.86	0.17	53,75,86,90	0
4	NAG	C	602	14/15	0.88	0.10	50,52,54,55	0
4	NAG	B	605	14/15	0.88	0.11	42,47,52,52	0
4	NAG	A	602	14/15	0.89	0.10	35,37,40,40	0
4	NAG	B	601	14/15	0.90	0.10	38,43,46,46	0
4	NAG	C	601	14/15	0.91	0.10	43,47,51,52	0
6	C5P	A	607	21/21	0.94	0.12	48,77,83,84	0
4	NAG	A	601	14/15	0.94	0.08	26,27,29,30	0
5	ZN	C	605	1/1	0.98	0.07	50,50,50,50	0
5	ZN	B	606	1/1	0.99	0.02	35,35,35,35	0
5	ZN	B	607	1/1	0.99	0.05	40,40,40,40	0
5	ZN	A	605	1/1	0.99	0.02	27,27,27,27	0
5	ZN	C	606	1/1	0.99	0.03	32,32,32,32	0
5	ZN	A	606	1/1	1.00	0.02	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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.