



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:52 AM UTC

PDB ID : 1N5R / pdb_00001n5r
Title : Crystal structure of the mouse acetylcholinesterase-propidium complex
Authors : Bourne, Y.; Taylor, P.; Radic, Z.; Marchot, P.
Deposited on : 2002-11-07
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

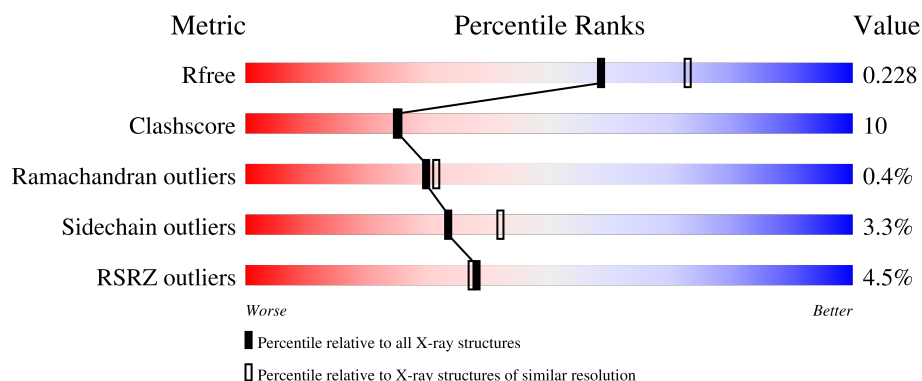
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	543	4% 77% 20% ..
1	B	543	5% 75% 21% ..
2	C	2	50% 50%

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
6	ACY	A	904	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8890 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 acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4184	2684	726	760	14			
1	B	534	Total	C	N	O	S	0	0	0
			4165	2675	719	757	14			

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



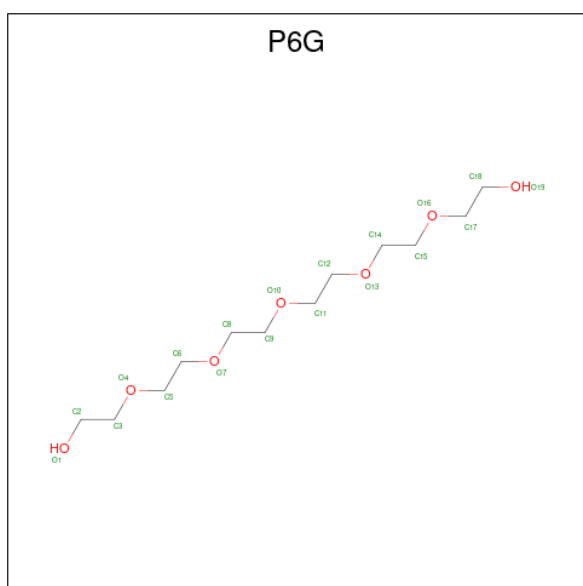
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

- 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	B	1	Total	C	N	O	0	0
			14	8	1	5		

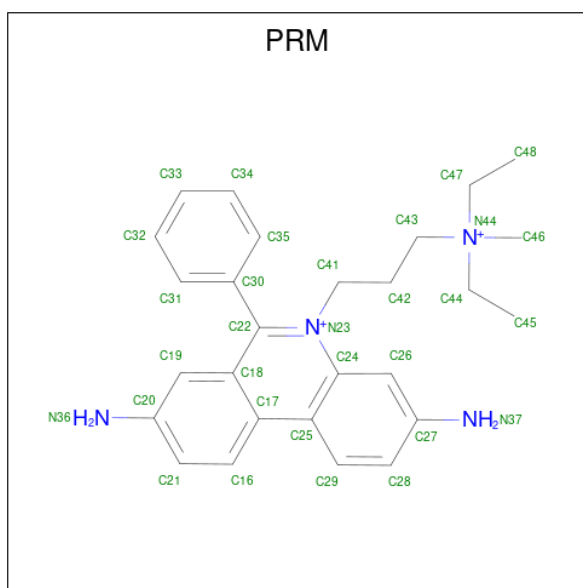
- Molecule 4 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		

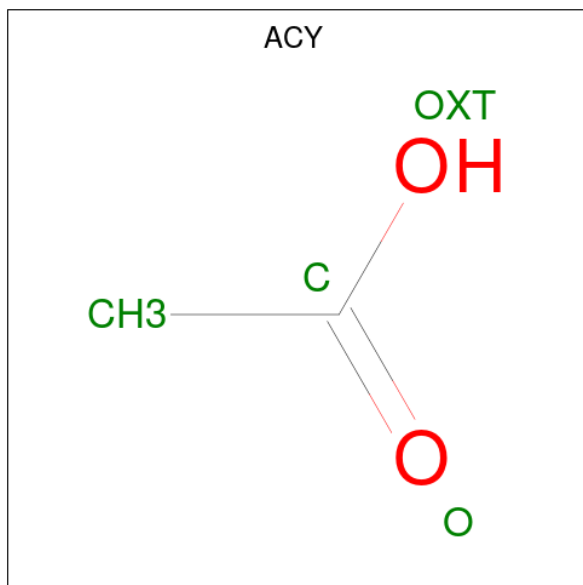
- Molecule 5 is 3,8-DIAMINO-5[3-(DIETHYLMETHYLAMMONIO)PROPYL]-6-PHENYLP

HENANTHRIDINIUM (CCD ID: PRM) (formula: $C_{27}H_{34}N_4$).



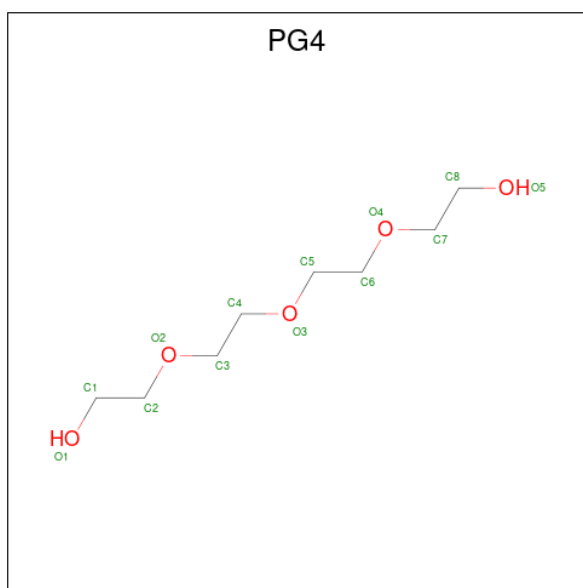
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			31	27	4		

- Molecule 6 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	8	3		

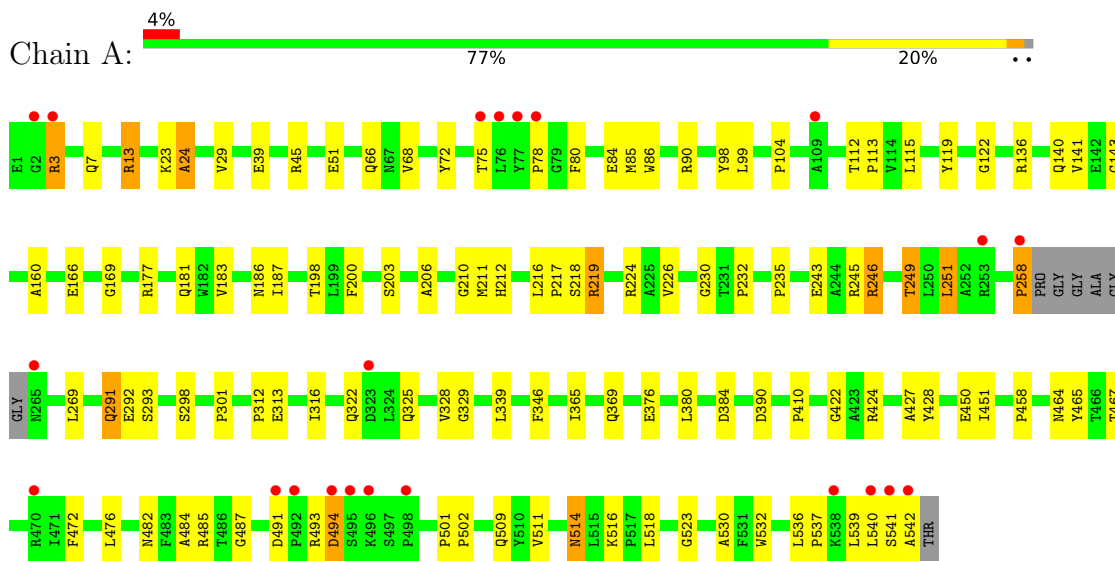
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	243	Total	O	0	0
			243	243		
8	B	177	Total	O	0	0
			177	177		

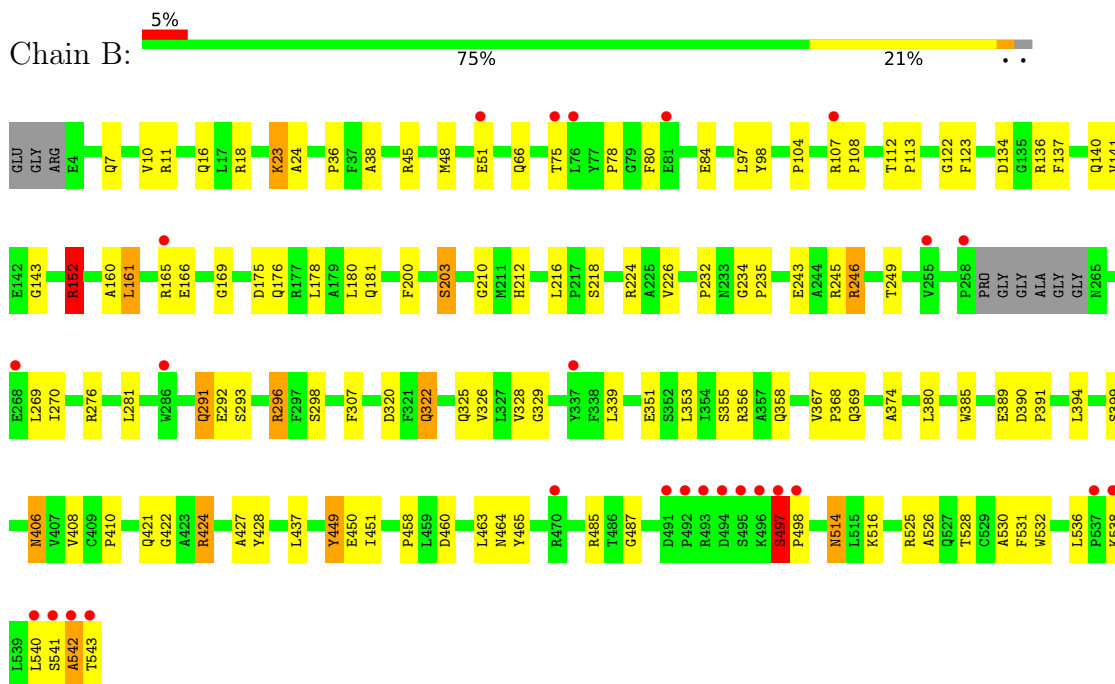
3 Residue-property plots

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: acetylcholinesterase



• Molecule 1: acetylcholinesterase



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.55Å 111.67Å 226.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.79 – 2.25 39.79 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.79-2.25) 99.2 (39.79-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.227 0.206 , 0.228	Depositor DCC
R_{free} test set	1907 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8890	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: NAG, PG4, FUC, ACY, PRM, P6G

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	0.66	0/4308	1.09	21/5887 (0.4%)
1	B	0.64	0/4289	1.09	27/5862 (0.5%)
All	All	0.65	0/8597	1.09	48/11749 (0.4%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	SER	N-CA-C	9.71	121.47	111.07
1	A	298	SER	N-CA-C	7.89	120.65	111.02
1	A	422	GLY	N-CA-C	7.39	123.48	114.69
1	B	450	GLU	N-CA-C	-7.16	104.69	113.50
1	B	235	PRO	N-CA-C	7.05	122.68	113.86
1	B	422	GLY	N-CA-C	6.91	122.92	114.69
1	A	450	GLU	N-CA-C	-6.83	105.09	113.50
1	A	235	PRO	N-CA-C	6.75	122.33	114.03
1	A	322	GLN	N-CA-C	6.75	118.29	111.07
1	B	234	GLY	CA-C-N	6.70	126.33	119.56
1	B	234	GLY	C-N-CA	6.70	126.33	119.56
1	B	292	GLU	N-CA-C	-6.55	100.13	109.96
1	A	539	LEU	N-CA-C	-6.47	104.15	111.14
1	A	451	ILE	N-CA-C	6.26	116.94	110.36
1	A	530	ALA	N-CA-C	-6.21	104.59	111.36
1	A	464	ASN	N-CA-C	6.20	120.14	112.58
1	A	292	GLU	N-CA-C	-5.96	101.02	109.96
1	B	141	VAL	N-CA-C	5.95	116.73	110.72
1	B	464	ASN	N-CA-C	5.91	119.80	112.24
1	B	526	ALA	N-CA-C	5.70	117.95	111.11
1	B	421	GLN	N-CA-C	5.67	119.95	112.25
1	B	322	GLN	N-CA-C	5.63	117.87	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ARG	N-CA-C	5.62	118.18	111.71
1	B	451	ILE	N-CA-C	5.59	115.78	110.42
1	A	24	ALA	N-CA-C	-5.47	102.19	110.50
1	A	482	ASN	N-CA-C	-5.42	105.45	111.36
1	B	390	ASP	CA-C-N	5.40	124.59	118.97
1	B	390	ASP	C-N-CA	5.40	124.59	118.97
1	A	186	ASN	N-CA-C	5.39	120.87	113.97
1	A	390	ASP	CA-C-N	5.39	125.03	119.05
1	A	390	ASP	C-N-CA	5.39	125.03	119.05
1	A	491	ASP	CA-C-N	5.38	125.71	119.47
1	A	491	ASP	C-N-CA	5.38	125.71	119.47
1	A	119	TYR	N-CA-C	5.35	117.59	110.53
1	B	152	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	B	307	PHE	N-CA-C	-5.26	105.44	111.07
1	B	449	TYR	N-CA-C	5.24	118.80	112.93
1	B	367	VAL	CA-C-N	5.22	125.53	119.47
1	B	367	VAL	C-N-CA	5.22	125.53	119.47
1	B	276	ARG	N-CA-C	5.20	116.38	109.93
1	B	530	ALA	N-CA-C	-5.16	105.74	111.36
1	B	406	ASN	N-CA-C	5.15	119.65	112.90
1	B	152	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	166	GLU	N-CA-C	5.13	119.25	112.89
1	B	497	SER	N-CA-C	5.09	121.07	109.81
1	B	161	LEU	N-CA-C	-5.05	98.11	108.21
1	B	385	TRP	N-CA-C	5.03	118.90	112.87
1	A	141	VAL	N-CA-C	5.02	116.47	111.00

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	4184	0	4070	67	0
1	B	4165	0	4050	96	0
2	C	24	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	19	0	26	1	0
5	A	31	0	34	2	0
6	A	4	0	3	2	0
6	B	4	0	3	1	0
7	B	11	0	12	0	0
8	A	243	0	0	4	0
8	B	177	0	0	1	0
All	All	8890	0	8246	162	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.

All (162) 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:B:152:ARG:HH11	1:B:152:ARG:HG3	1.12	1.10
1:B:497:SER:HB2	1:B:498:PRO:C	1.89	0.97
1:B:497:SER:HB2	1:B:498:PRO:O	1.73	0.88
1:B:424:ARG:HH11	1:B:424:ARG:HG3	1.40	0.85
1:B:152:ARG:HH11	1:B:152:ARG:CG	1.90	0.82
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.63	0.80
1:B:152:ARG:HG3	1:B:152:ARG:NH1	1.90	0.79
1:B:245:ARG:O	1:B:249:THR:HG23	1.83	0.78
1:B:424:ARG:HG3	1:B:424:ARG:NH1	2.01	0.74
1:B:11:ARG:NH1	1:B:16:GLN:HG3	2.04	0.72
1:B:351:GLU:OE2	1:B:351:GLU:HA	1.93	0.68
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.74	0.68
1:B:212:HIS:HD2	1:B:218:SER:OG	1.78	0.66
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.31	0.66
1:A:203:SER:OG	6:A:904:ACY:C	2.43	0.66
1:A:80:PHE:O	1:A:84:GLU:HG2	1.95	0.66
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.79	0.65
1:B:514:ASN:C	1:B:514:ASN:HD22	2.04	0.65
1:B:224:ARG:HH11	1:B:325:GLN:HE22	1.45	0.65
1:B:203:SER:OG	6:B:905:ACY:C	2.47	0.62
1:B:45:ARG:HD3	1:B:51:GLU:OE1	1.99	0.62
1:B:134:ASP:OD1	1:B:136:ARG:HD2	1.98	0.62
1:A:245:ARG:O	1:A:249:THR:HG23	2.01	0.60
1:A:13:ARG:NH2	8:A:1031:HOH:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.83	0.60
1:A:3:ARG:HH11	1:A:3:ARG:HG3	1.67	0.59
1:A:7:GLN:O	1:A:7:GLN:HG3	2.03	0.59
1:A:85:MET:HE2	1:A:86:TRP:CZ2	2.38	0.59
1:A:212:HIS:HD2	1:A:218:SER:OG	1.86	0.58
1:B:112:THR:HG21	1:B:143:GLY:O	2.03	0.58
1:A:45:ARG:NH1	1:A:51:GLU:OE1	2.36	0.58
1:B:224:ARG:NH1	1:B:224:ARG:HG3	2.18	0.58
1:B:296:ARG:HH11	1:B:369:GLN:HE22	1.52	0.57
1:B:320:ASP:OD1	1:B:322:GLN:HG3	2.04	0.57
1:A:514:ASN:HD22	1:A:514:ASN:C	2.13	0.57
1:B:11:ARG:HH12	1:B:16:GLN:HG3	1.67	0.57
1:A:537:PRO:O	1:A:540:LEU:HB3	2.05	0.56
1:B:152:ARG:NH1	1:B:175:ASP:OD2	2.39	0.56
1:B:23:LYS:HE3	1:B:23:LYS:HA	1.88	0.56
1:B:224:ARG:HH11	1:B:224:ARG:HG3	1.72	0.55
1:B:161:LEU:HD12	1:B:270:ILE:CG1	2.37	0.55
1:B:296:ARG:HH11	1:B:369:GLN:NE2	2.05	0.54
1:A:514:ASN:HD22	1:A:516:LYS:H	1.55	0.54
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.90	0.54
1:B:224:ARG:HH11	1:B:325:GLN:NE2	2.05	0.54
1:B:497:SER:CB	1:B:498:PRO:C	2.73	0.54
1:A:376:GLU:HG2	1:B:538:LYS:NZ	2.24	0.53
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.43	0.53
1:A:75:THR:O	1:A:78:PRO:HD3	2.09	0.52
1:B:540:LEU:HA	1:B:543:THR:HG23	1.90	0.52
1:B:161:LEU:CD1	1:B:269:LEU:HD22	2.35	0.52
1:A:541:SER:O	1:A:542:ALA:HB2	2.08	0.52
1:B:328:VAL:O	1:B:427:ALA:HA	2.09	0.52
1:A:112:THR:HG21	1:A:143:GLY:O	2.10	0.52
1:B:11:ARG:NH1	1:B:16:GLN:CG	2.72	0.51
1:B:514:ASN:ND2	1:B:516:LYS:H	2.09	0.51
1:B:326:VAL:HG12	1:B:328:VAL:HG13	1.93	0.51
5:A:951:PRM:H34	8:A:1170:HOH:O	2.09	0.51
1:B:355:SER:OG	1:B:358:GLN:HG3	2.11	0.50
1:A:258:PRO:HG2	1:A:269:LEU:HA	1.93	0.50
1:B:80:PHE:O	1:B:84:GLU:HG2	2.12	0.50
1:B:104:PRO:CG	1:B:108:PRO:HG3	2.41	0.50
1:A:291:GLN:HE22	1:A:369:GLN:NE2	2.09	0.49
1:B:75:THR:O	1:B:78:PRO:HD3	2.12	0.49
1:B:104:PRO:HG2	1:B:108:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PRO:HG3	1:B:485:ARG:CG	2.42	0.49
1:A:514:ASN:ND2	1:A:516:LYS:H	2.10	0.49
1:A:376:GLU:O	1:A:380:LEU:HG	2.12	0.48
1:B:528:THR:O	1:B:531:PHE:HB3	2.13	0.48
1:B:152:ARG:HH12	1:B:175:ASP:CG	2.20	0.48
1:B:374:ALA:HB2	1:B:540:LEU:HD21	1.94	0.48
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.95	0.48
1:A:369:GLN:HB2	8:A:974:HOH:O	2.14	0.47
1:A:511:VAL:HB	1:A:518:LEU:HD22	1.95	0.47
1:A:104:PRO:HG3	1:A:143:GLY:HA2	1.97	0.47
1:B:176:GLN:OE1	1:B:212:HIS:HE1	1.96	0.47
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.47	0.47
1:A:206:ALA:HB3	1:A:230:GLY:HA3	1.97	0.47
1:A:339:LEU:HD13	1:A:346:PHE:CE2	2.49	0.47
1:A:99:LEU:C	1:A:99:LEU:HD12	2.40	0.47
1:A:3:ARG:HG3	1:A:3:ARG:NH1	2.29	0.47
1:B:541:SER:O	1:B:542:ALA:HB2	2.15	0.47
1:A:245:ARG:O	1:A:249:THR:CG2	2.63	0.46
1:B:424:ARG:HH11	1:B:424:ARG:CG	2.16	0.46
1:A:29:VAL:HG21	1:A:136:ARG:HB2	1.98	0.46
1:B:243:GLU:OE1	1:B:246:ARG:NH1	2.47	0.46
1:B:532:TRP:CE3	1:B:536:LEU:HD12	2.51	0.46
1:A:72:TYR:CZ	5:A:951:PRM:H16	2.51	0.46
1:B:514:ASN:C	1:B:514:ASN:ND2	2.73	0.46
1:B:514:ASN:HD22	1:B:516:LYS:N	2.14	0.46
1:B:66:GLN:HG3	1:B:98:TYR:CD1	2.51	0.45
1:A:219:ARG:HA	1:A:219:ARG:HD2	1.74	0.45
1:A:211:MET:HG3	1:A:232:PRO:HB3	1.99	0.45
1:B:18:ARG:NH2	8:B:1052:HOH:O	2.49	0.45
1:A:328:VAL:O	1:A:427:ALA:HA	2.15	0.45
1:B:97:LEU:HD11	1:B:152:ARG:NH1	2.32	0.45
1:B:356:ARG:HA	1:B:394:LEU:HD13	1.99	0.45
1:B:428:TYR:C	1:B:428:TYR:CD1	2.95	0.45
1:B:224:ARG:HD3	1:B:487:GLY:HA2	1.98	0.45
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.83	0.44
1:B:134:ASP:CG	1:B:136:ARG:HD2	2.41	0.44
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.52	0.44
1:B:48:MET:HE1	1:B:165:ARG:HH21	1.83	0.44
1:B:224:ARG:HD3	1:B:325:GLN:HE21	1.82	0.44
1:A:183:VAL:HG13	1:A:187:ILE:HB	2.00	0.44
1:B:36:PRO:HB3	1:B:98:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLY:HA3	1:A:232:PRO:HD3	2.00	0.43
1:A:312:PRO:O	1:A:316:ILE:HG23	2.18	0.43
1:B:10:VAL:HG12	1:B:11:ARG:N	2.34	0.43
1:B:291:GLN:HE21	1:B:291:GLN:HB2	1.57	0.43
1:A:122:GLY:H	6:A:904:ACY:C	2.31	0.43
1:B:152:ARG:CG	1:B:152:ARG:NH1	2.63	0.43
1:B:514:ASN:ND2	1:B:516:LYS:N	2.66	0.43
1:B:536:LEU:HD23	1:B:536:LEU:HA	1.67	0.43
1:B:113:PRO:HG3	1:B:485:ARG:HG3	1.99	0.43
1:B:210:GLY:HA3	1:B:232:PRO:HD3	2.01	0.43
1:A:68:VAL:HG23	1:A:90:ARG:HB2	2.01	0.43
1:B:136:ARG:HG2	1:B:137:PHE:N	2.34	0.43
1:B:460:ASP:HB3	1:B:463:LEU:HD12	2.00	0.43
1:B:200:PHE:HB2	1:B:226:VAL:HB	2.01	0.42
1:A:428:TYR:CD1	1:A:428:TYR:C	2.98	0.42
1:B:7:GLN:O	1:B:107:ARG:NH1	2.52	0.42
1:B:122:GLY:O	1:B:123:PHE:HB2	2.19	0.42
1:A:509:GLN:HG3	8:A:1172:HOH:O	2.20	0.42
1:B:166:GLU:HB2	1:B:270:ILE:HD13	2.00	0.42
1:A:115:LEU:HD23	1:A:198:THR:HB	2.00	0.42
1:A:216:LEU:HB3	1:A:217:PRO:HD3	2.02	0.42
1:A:224:ARG:HD3	1:A:325:GLN:NE2	2.35	0.42
1:B:514:ASN:HD21	1:B:516:LYS:HB2	1.84	0.42
1:A:251:LEU:O	1:A:251:LEU:HG	2.20	0.42
1:A:325:GLN:HE21	1:A:487:GLY:HA3	1.84	0.42
1:A:493:ARG:HB2	1:A:494:ASP:H	1.65	0.42
1:A:200:PHE:CB	1:A:226:VAL:HB	2.49	0.42
1:A:224:ARG:HD3	1:A:325:GLN:HE21	1.85	0.42
1:A:115:LEU:HD21	1:A:484:ALA:HB2	2.02	0.41
1:A:243:GLU:OE1	1:A:246:ARG:NH1	2.52	0.41
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.55	0.41
4:A:901:P6G:H81	1:B:380:LEU:HB2	2.02	0.41
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.56	0.41
1:A:291:GLN:HE21	1:A:291:GLN:HB2	1.58	0.41
1:A:160:ALA:HB2	1:A:169:GLY:HA2	2.02	0.41
1:A:384:ASP:OD1	1:A:384:ASP:C	2.63	0.41
1:B:152:ARG:NH1	1:B:175:ASP:CG	2.78	0.41
1:A:291:GLN:NE2	1:A:369:GLN:NE2	2.69	0.41
1:B:224:ARG:HH11	1:B:224:ARG:CG	2.33	0.41
1:A:472:PHE:CZ	1:A:476:LEU:HD11	2.56	0.41
1:A:39:GLU:CB	1:A:45:ARG:NH1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:SER:HA	1:A:365:ILE:HG23	2.03	0.41
1:A:532:TRP:CE3	1:A:536:LEU:HD12	2.55	0.41
1:B:38:ALA:HB2	1:B:178:LEU:HD23	2.03	0.41
1:B:293:SER:HB3	1:B:368:PRO:HB3	2.03	0.41
1:A:177:ARG:O	1:A:181:GLN:HG3	2.21	0.41
1:A:376:GLU:HG2	1:B:538:LYS:HZ3	1.83	0.41
1:B:66:GLN:HG3	1:B:98:TYR:CG	2.56	0.41
1:B:161:LEU:HD11	1:B:269:LEU:CD2	2.42	0.41
1:B:200:PHE:CB	1:B:226:VAL:HB	2.51	0.41
1:A:501:PRO:HA	1:A:502:PRO:HD3	1.94	0.41
1:B:161:LEU:HD12	1:B:270:ILE:HD11	2.03	0.40
1:A:66:GLN:HG3	1:A:98:TYR:CD1	2.56	0.40
1:B:160:ALA:HB2	1:B:169:GLY:CA	2.51	0.40
1:B:339:LEU:HD11	1:B:399:SER:HA	2.04	0.40
1:B:437:LEU:HD11	1:B:449:TYR:CD2	2.56	0.40

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	532/543 (98%)	514 (97%)	16 (3%)	2 (0%)	30	31
1	B	530/543 (98%)	514 (97%)	14 (3%)	2 (0%)	30	31
All	All	1062/1086 (98%)	1028 (97%)	30 (3%)	4 (0%)	30	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	542	ALA
1	A	494	ASP
1	B	497	SER

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Mol	Chain	Res	Type
1	A	523	GLY

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	440/443 (99%)	426 (97%)	14 (3%)	34	43
1	B	438/443 (99%)	423 (97%)	15 (3%)	32	40
All	All	878/886 (99%)	849 (97%)	29 (3%)	33	42

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	13	ARG
1	A	23	LYS
1	A	246	ARG
1	A	249	THR
1	A	251	LEU
1	A	258	PRO
1	A	291	GLN
1	A	301	PRO
1	A	313	GLU
1	A	410	PRO
1	A	424	ARG
1	A	467	THR
1	A	514	ASN
1	B	23	LYS
1	B	152	ARG
1	B	180	LEU
1	B	181	GLN
1	B	203	SER
1	B	216	LEU
1	B	246	ARG
1	B	281	LEU

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Mol	Chain	Res	Type
1	B	291	GLN
1	B	296	ARG
1	B	389	GLU
1	B	410	PRO
1	B	424	ARG
1	B	497	SER
1	B	514	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	184	GLN
1	A	212	HIS
1	A	284	HIS
1	A	291	GLN
1	A	322	GLN
1	A	325	GLN
1	A	474	GLN
1	A	514	ASN
1	B	181	GLN
1	B	212	HIS
1	B	284	HIS
1	B	291	GLN
1	B	325	GLN
1	B	369	GLN
1	B	474	GLN
1	B	514	ASN

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	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.88	1 (7%)	17,19,21	0.86	1 (5%)
2	FUC	C	2	2	10,10,11	0.82	0	14,14,16	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C1-C2	2.26	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	-2.37	119.73	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

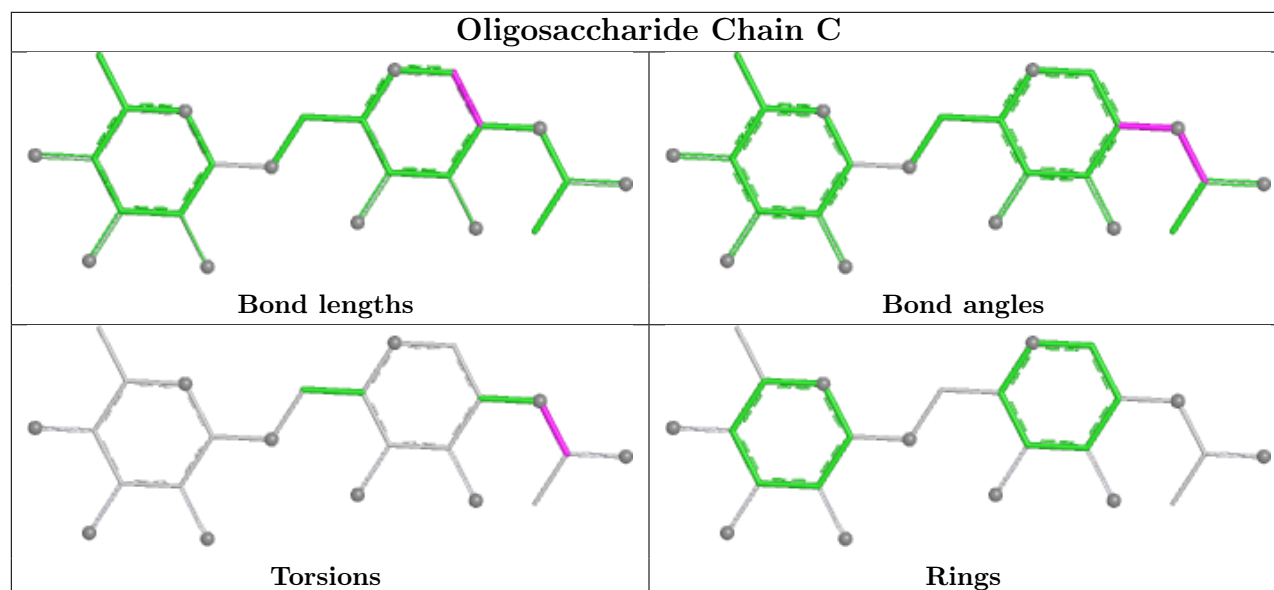
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

7 ligands 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
4	P6G	A	901	-	18,18,18	2.16	6 (33%)	17,17,17	1.19	1 (5%)
5	PRM	A	951	-	32,34,34	1.70	9 (28%)	44,49,49	1.56	4 (9%)
7	PG4	B	902	-	10,10,12	1.86	2 (20%)	9,9,11	0.81	0
6	ACY	A	904	-	3,3,3	1.48	1 (33%)	3,3,3	1.64	1 (33%)
3	NAG	B	601	1	14,14,15	0.80	0	17,19,21	0.86	0
6	ACY	B	905	-	3,3,3	1.26	1 (33%)	3,3,3	1.63	1 (33%)
3	NAG	A	701	1	14,14,15	0.78	0	17,19,21	0.84	1 (5%)

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	P6G	A	901	-	-	7/16/16/16	-
5	PRM	A	951	-	-	1/17/17/17	0/4/4/4
7	PG4	B	902	-	-	1/8/8/10	-
3	NAG	B	601	1	-	4/6/23/26	0/1/1/1
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	902	PG4	O2-C3	4.58	1.61	1.42
4	A	901	P6G	O10-C9	4.37	1.61	1.42
5	A	951	PRM	C25-C24	3.81	1.48	1.41
4	A	901	P6G	O13-C12	3.71	1.58	1.42
4	A	901	P6G	O16-C15	3.58	1.57	1.42
4	A	901	P6G	O4-C3	3.47	1.57	1.42
5	A	951	PRM	C18-C17	3.32	1.47	1.42
4	A	901	P6G	O19-C18	3.27	1.58	1.42
5	A	951	PRM	C29-C28	3.15	1.43	1.36
4	A	901	P6G	O7-C6	2.89	1.54	1.42
5	A	951	PRM	C16-C21	2.87	1.42	1.36
7	B	902	PG4	O3-C5	2.74	1.54	1.42
5	A	951	PRM	C31-C30	2.50	1.44	1.39
5	A	951	PRM	C32-C31	2.48	1.43	1.38
5	A	951	PRM	C19-C20	2.36	1.42	1.39
6	A	904	ACY	O-C	2.30	1.32	1.22
5	A	951	PRM	C34-C35	2.26	1.42	1.38
6	B	905	ACY	O-C	2.09	1.31	1.22
5	A	951	PRM	C34-C33	2.08	1.42	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	951	PRM	C25-C24-N23	6.68	122.77	118.46
5	A	951	PRM	C27-C26-C24	4.04	125.27	119.93
4	A	901	P6G	O1-C2-C3	3.36	131.62	111.82
5	A	951	PRM	C42-C41-N23	3.07	118.70	111.83
5	A	951	PRM	C21-C16-C17	2.46	125.41	121.62
3	A	701	NAG	C2-N2-C7	-2.45	119.62	122.90
6	A	904	ACY	O-C-CH3	-2.25	113.31	122.53
6	B	905	ACY	O-C-CH3	-2.21	113.46	122.53

There are no chirality outliers.

All (15) torsion outliers are listed below:

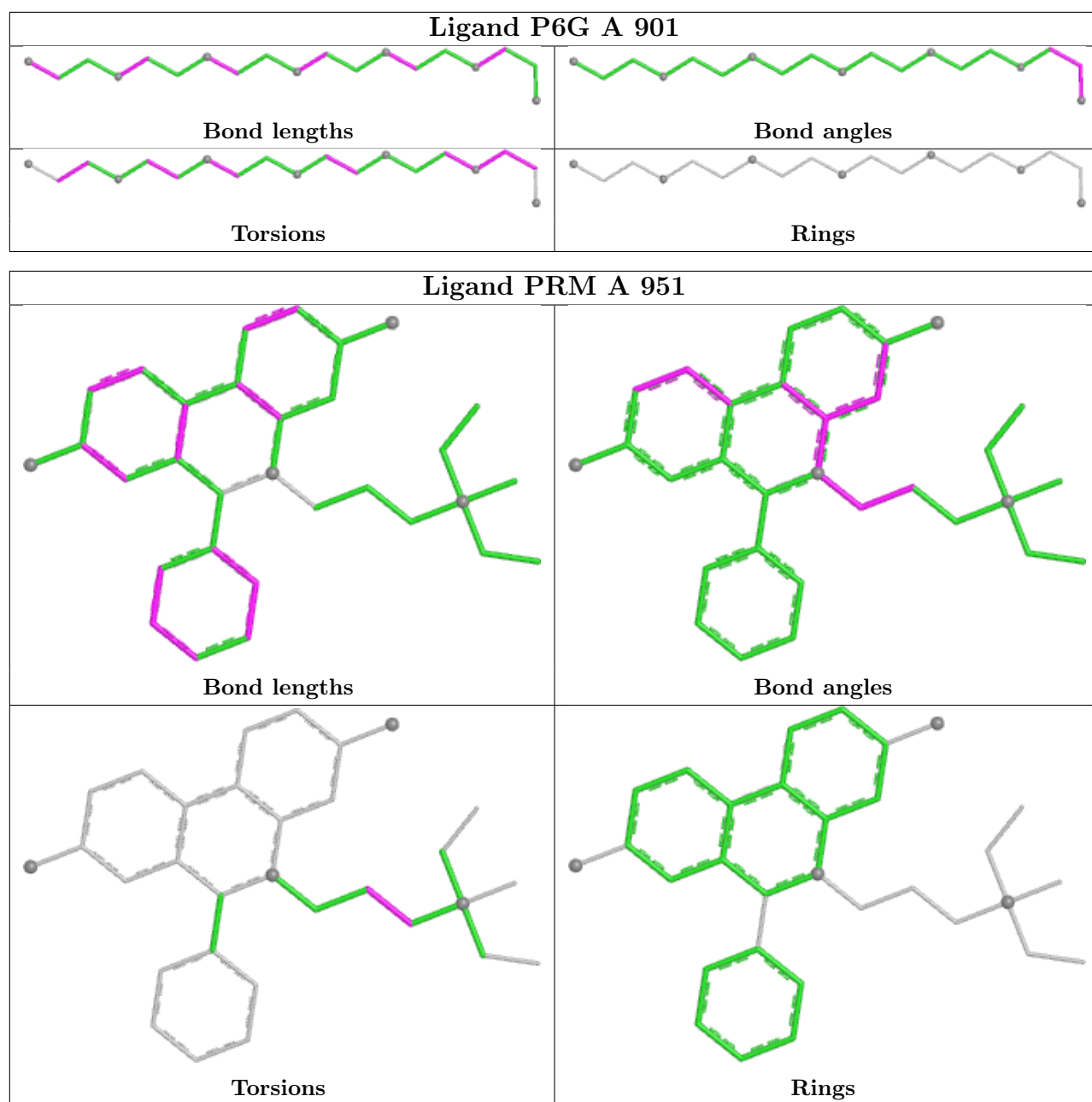
Mol	Chain	Res	Type	Atoms
3	A	701	NAG	O7-C7-N2-C2
3	B	601	NAG	O5-C5-C6-O6
3	A	701	NAG	C8-C7-N2-C2
3	B	601	NAG	C8-C7-N2-C2
3	B	601	NAG	O7-C7-N2-C2
4	A	901	P6G	O1-C2-C3-O4
3	B	601	NAG	C4-C5-C6-O6
4	A	901	P6G	O16-C17-C18-O19
4	A	901	P6G	O13-C14-C15-O16
4	A	901	P6G	C6-C5-O4-C3
4	A	901	P6G	C11-C12-O13-C14
7	B	902	PG4	C5-C6-O4-C7
4	A	901	P6G	O7-C8-C9-O10
4	A	901	P6G	C2-C3-O4-C5
5	A	951	PRM	C41-C42-C43-N44

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	P6G	1	0
5	A	951	PRM	2	0
6	A	904	ACY	2	0
6	B	905	ACY	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	536/543 (98%)	-0.01	22 (4%) 41 41	31, 44, 67, 98	0
1	B	534/543 (98%)	0.21	26 (4%) 35 34	34, 48, 72, 99	0
All	All	1070/1086 (98%)	0.10	48 (4%) 38 37	31, 46, 69, 99	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	542	ALA	5.6
1	B	540	LEU	5.5
1	A	258	PRO	5.4
1	B	542	ALA	5.2
1	B	496	LYS	5.1
1	B	543	THR	4.8
1	B	495	SER	4.5
1	B	541	SER	4.4
1	A	496	LYS	4.3
1	B	258	PRO	4.3
1	B	538	LYS	4.1
1	B	497	SER	4.1
1	A	492	PRO	3.8
1	B	492	PRO	3.6
1	B	493	ARG	3.5
1	A	541	SER	3.5
1	A	498	PRO	3.4
1	A	76	LEU	3.3
1	A	540	LEU	3.2
1	A	470	ARG	3.0
1	B	76	LEU	3.0
1	A	75	THR	2.9
1	A	323	ASP	2.9
1	B	498	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	265	ASN	2.7
1	B	81	GLU	2.7
1	B	491	ASP	2.7
1	B	286	TRP	2.7
1	B	470	ARG	2.6
1	A	495	SER	2.5
1	A	77	TYR	2.5
1	B	165	ARG	2.4
1	A	3	ARG	2.4
1	B	268	GLU	2.3
1	B	337	TYR	2.3
1	A	109	ALA	2.3
1	B	255	VAL	2.3
1	B	537	PRO	2.2
1	A	253	ARG	2.2
1	A	538	LYS	2.2
1	B	75	THR	2.1
1	B	107	ARG	2.1
1	A	494	ASP	2.1
1	B	494	ASP	2.0
1	A	78	PRO	2.0
1	A	2	GLY	2.0
1	B	51	GLU	2.0
1	A	491	ASP	2.0

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

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

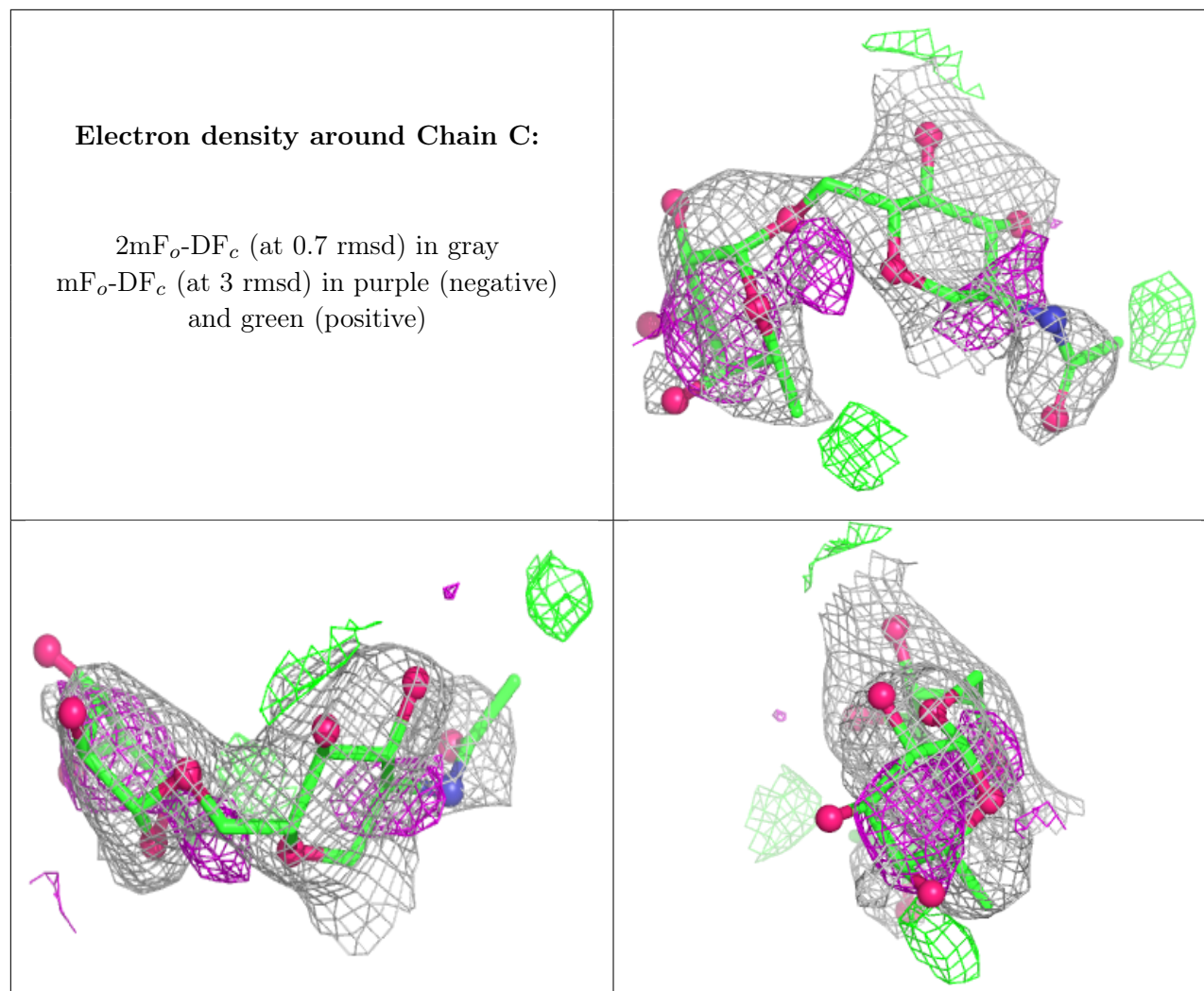
6.3 Carbohydrates [i](#)

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, 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
2	FUC	C	2	10/11	0.56	0.20	96,98,98,98	0
2	NAG	C	1	14/15	0.72	0.19	80,84,89,93	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.



6.4 Ligands [i](#)

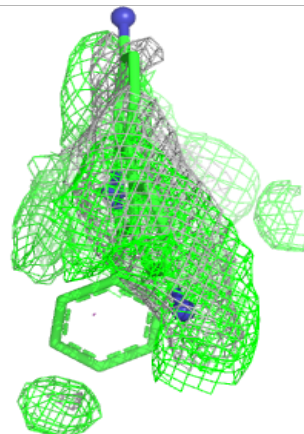
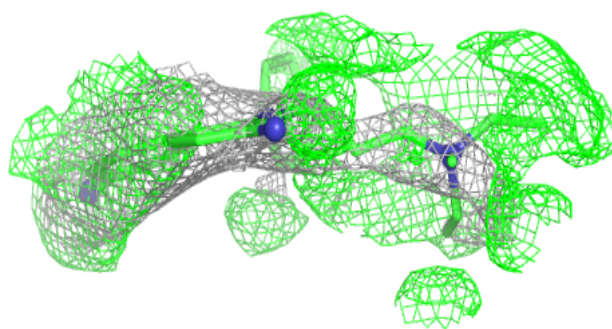
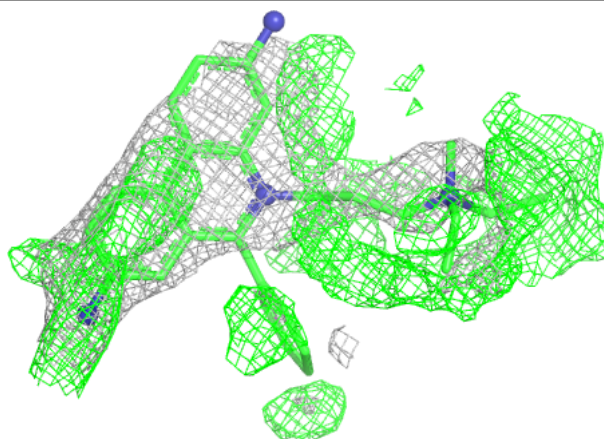
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	B	601	14/15	0.61	0.21	85,89,91,91	0
3	NAG	A	701	14/15	0.69	0.16	85,89,92,93	0
7	PG4	B	902	11/13	0.80	0.35	92,93,94,94	0
5	PRM	A	951	31/31	0.82	0.43	87,90,94,94	31
4	P6G	A	901	19/19	0.90	0.18	63,68,78,79	0
6	ACY	B	905	4/4	0.91	0.19	71,71,72,72	0
6	ACY	A	904	4/4	0.92	0.14	50,50,53,53	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.

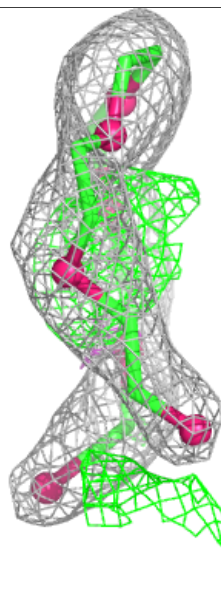
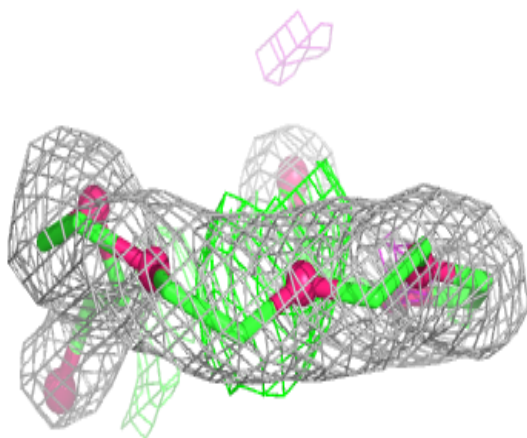
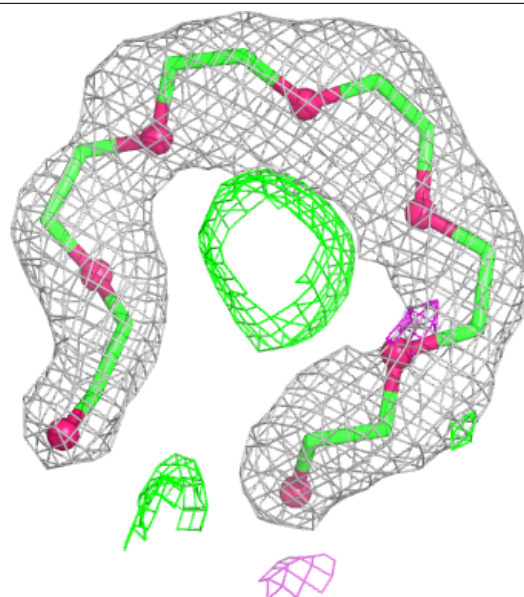
Electron density around PRM A 951:

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



Electron density around P6G A 901:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.