



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:05 AM UTC

PDB ID : 1J06 / pdb_00001j06
Title : Crystal structure of mouse acetylcholinesterase in the apo form
Authors : Bourne, Y.; Taylor, P.; Radic, Z.; Marchot, P.
Deposited on : 2002-11-07
Resolution : 2.35 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

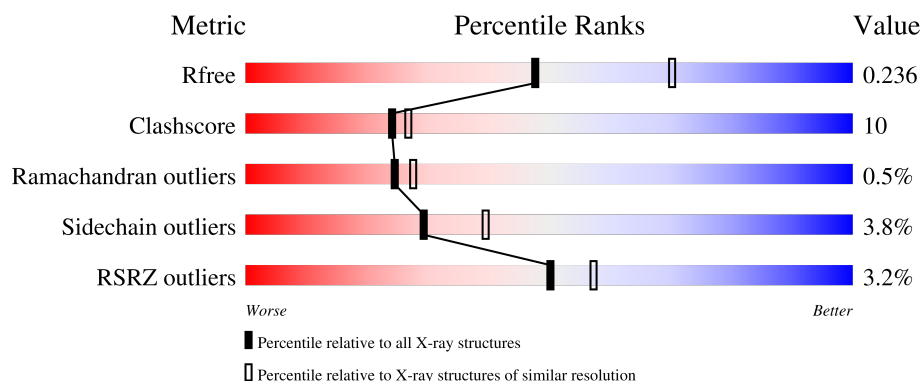
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	3% 74% 22% ..
1	B	543	3% 73% 22% ..
2	C	2	50% 50%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8804 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	535	Total	C	N	O	S	0	0	0
			4177	2679	725	759	14			
1	B	533	Total	C	N	O	S	0	0	0
			4159	2670	718	757	14			

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



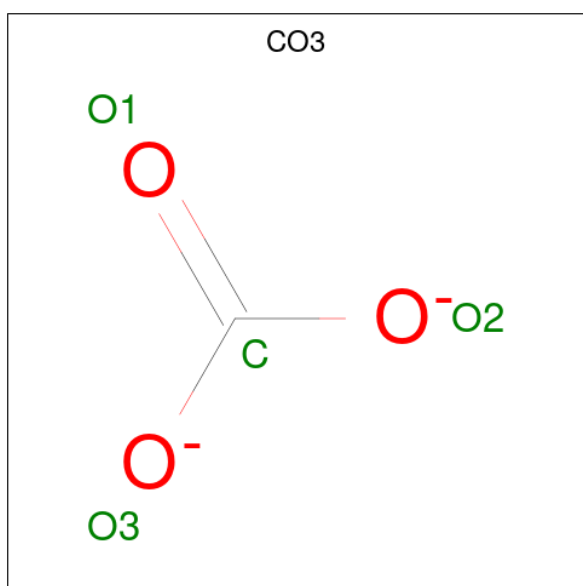
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



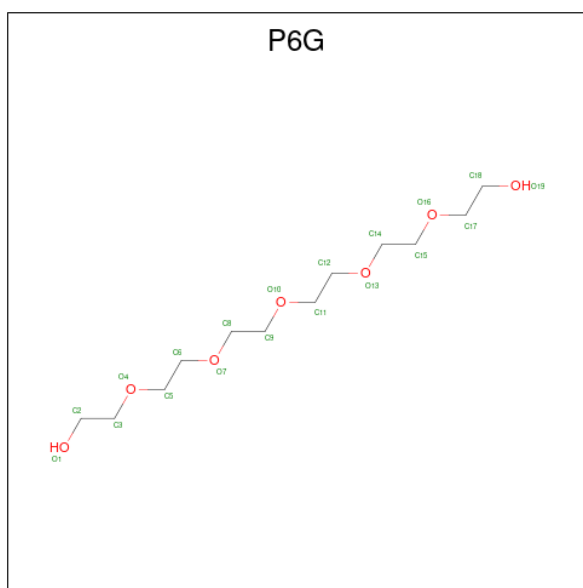
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CARBONATE ION (CCD ID: CO3) (formula: CO_3).



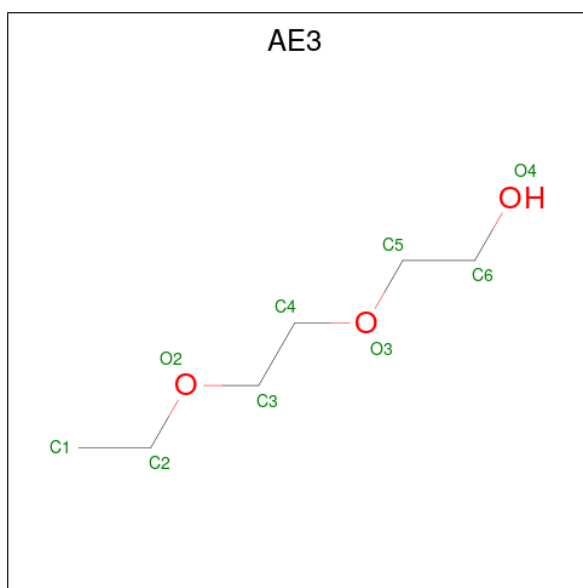
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		
4	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



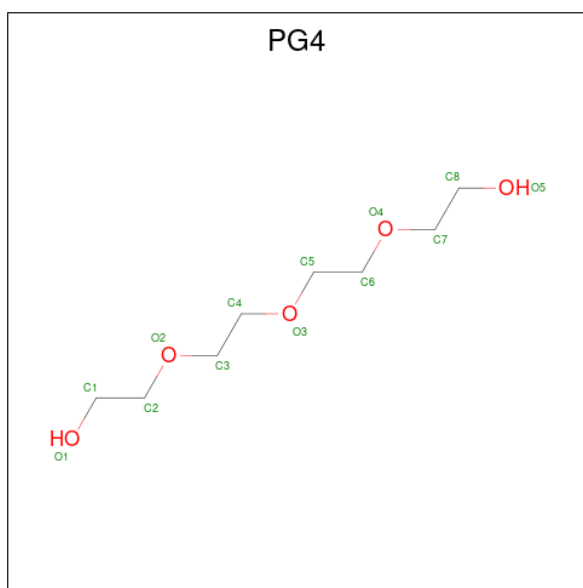
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 6 is 2-(2-ETHOXYETHOXY)ETHANOL (CCD ID: AE3) (formula: $C_6H_{14}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	6	3		
6	B	1	Total	C	O	0	0
			9	6	3		

- 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		

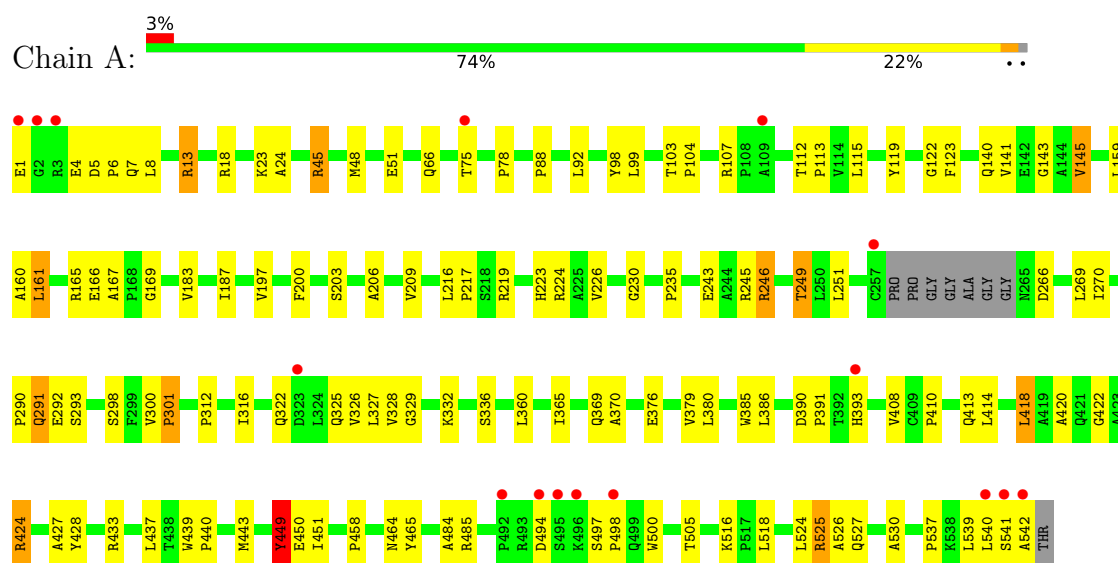
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	210	Total	O	0	0
			210	210		
8	B	150	Total	O	0	0
			150	150		

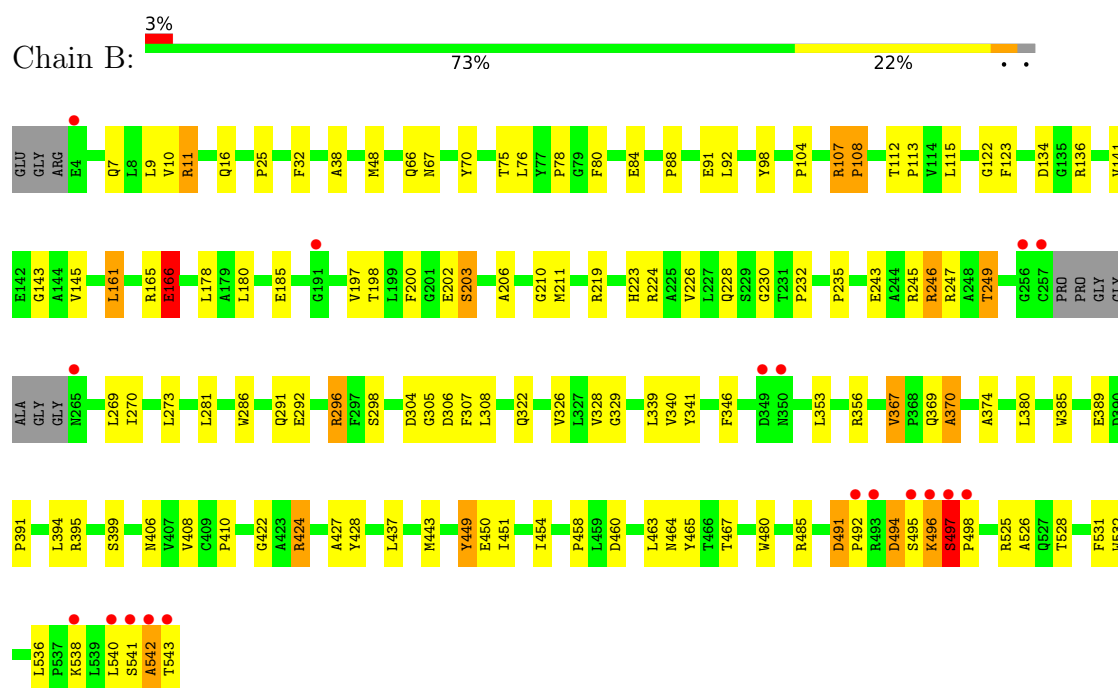
3 Residue-property plots [i](#)

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

• Molecule 1: acetylcholinesterase



• Molecule 1: acetylcholinesterase



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

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.20Å 111.97Å 226.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.35) 98.8 (20.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 2.34Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.232 0.210 , 0.236	Depositor DCC
R_{free} test set	1692 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.847	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.9	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	0.95	EDS
Total number of atoms	8804	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 2.88% 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: P6G, AE3, CO3, FUC, PG4, NAG

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	0.81	0/4300	1.13	27/5875 (0.5%)
1	B	0.71	0/4282	1.12	25/5851 (0.4%)
All	All	0.76	0/8582	1.12	52/11726 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	491	ASP	CA-C-N	9.71	130.73	119.47
1	B	491	ASP	C-N-CA	9.71	130.73	119.47
1	A	298	SER	N-CA-C	8.16	119.80	111.07
1	A	451	ILE	N-CA-C	8.07	118.84	110.36
1	B	298	SER	N-CA-C	7.84	119.46	111.07
1	A	235	PRO	N-CA-C	7.63	123.41	114.03
1	A	450	GLU	N-CA-C	-7.56	103.86	113.23
1	B	450	GLU	N-CA-C	-7.50	104.28	113.50
1	A	422	GLY	N-CA-C	7.25	124.34	114.92
1	B	451	ILE	N-CA-C	7.14	117.86	110.36
1	B	449	TYR	N-CA-C	7.07	120.85	112.93
1	B	235	PRO	N-CA-C	6.71	122.25	113.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	539	LEU	N-CA-C	-6.56	104.05	111.07
1	B	161	LEU	N-CA-C	-6.46	95.28	108.21
1	B	107	ARG	CA-C-N	6.30	127.71	119.84
1	B	107	ARG	C-N-CA	6.30	127.71	119.84
1	A	497	SER	CA-C-N	-6.09	113.51	119.78
1	A	497	SER	C-N-CA	-6.09	113.51	119.78
1	A	449	TYR	N-CA-C	6.08	120.32	113.02
1	B	322	GLN	N-CA-C	6.06	118.42	111.02
1	B	526	ALA	N-CA-C	6.06	118.38	111.11
1	B	219	ARG	N-CA-C	6.00	119.44	111.75
1	B	422	GLY	N-CA-C	5.94	122.94	115.21
1	A	464	ASN	N-CA-C	5.89	119.78	112.24
1	A	141	VAL	N-CA-C	5.86	117.39	111.00
1	A	219	ARG	N-CA-C	5.77	118.34	111.71
1	A	292	GLU	N-CA-C	-5.74	101.78	110.28
1	B	292	GLU	N-CA-C	-5.67	101.46	109.96
1	A	266	ASP	N-CA-C	5.64	117.43	111.28
1	B	367	VAL	CA-C-N	5.59	125.95	119.47
1	B	367	VAL	C-N-CA	5.59	125.95	119.47
1	B	370	ALA	N-CA-C	5.59	118.64	109.76
1	B	185	GLU	N-CA-C	5.58	119.34	112.54
1	B	464	ASN	N-CA-C	5.48	119.14	111.74
1	A	424	ARG	N-CA-C	-5.47	100.27	108.96
1	A	370	ALA	N-CA-C	5.40	118.35	109.76
1	A	167	ALA	CA-C-N	5.37	125.04	119.56
1	A	167	ALA	C-N-CA	5.37	125.04	119.56
1	A	336	SER	N-CA-C	5.34	117.52	111.11
1	B	141	VAL	N-CA-C	5.34	116.11	110.72
1	A	161	LEU	N-CA-C	-5.33	97.54	108.21
1	A	322	GLN	N-CA-C	5.29	117.48	111.02
1	A	145	VAL	N-CA-C	-5.27	100.30	107.99
1	B	305	GLY	N-CA-C	-5.21	108.06	115.30
1	A	119	TYR	N-CA-C	5.18	117.22	110.43
1	B	145	VAL	N-CA-C	-5.16	99.82	107.51
1	B	307	PHE	N-CA-C	-5.14	105.57	111.07
1	A	526	ALA	N-CA-C	5.13	117.27	111.11
1	A	530	ALA	N-CA-C	-5.13	105.77	111.36
1	B	166	GLU	N-CA-C	5.10	119.60	113.17
1	A	209	VAL	N-CA-C	-5.03	105.49	110.62
1	A	408	VAL	N-CA-C	5.02	115.64	110.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	449	TYR	Sidechain
1	B	70	TYR	Sidechain

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	4177	0	4063	81	0
1	B	4159	0	4046	89	0
2	C	24	0	22	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	4	0	0	1	0
4	B	4	0	0	1	0
5	A	19	0	26	1	0
6	A	9	0	14	0	0
6	B	9	0	14	2	0
7	B	11	0	12	0	0
8	A	210	0	0	6	0
8	B	150	0	0	2	0
All	All	8804	0	8223	167	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 (167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:VAL:H	1:A:223:HIS:HD2	1.14	0.94
1:B:197:VAL:H	1:B:223:HIS:HD2	1.03	0.93
1:A:485:ARG:HG3	8:A:1107:HOH:O	1.70	0.92
1:B:497:SER:HB2	1:B:498:PRO:O	1.72	0.90
1:A:4:GLU:OE2	1:A:18:ARG:HD3	1.73	0.88
1:B:497:SER:HB2	1:B:498:PRO:C	2.02	0.84
1:B:245:ARG:O	1:B:249:THR:HG23	1.80	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:VAL:H	1:B:223:HIS:CD2	1.94	0.80
1:A:197:VAL:H	1:A:223:HIS:CD2	1.99	0.78
1:A:245:ARG:O	1:A:249:THR:HG23	1.85	0.77
1:A:48:MET:HE3	1:A:166:GLU:HA	1.68	0.74
1:A:48:MET:CE	1:A:166:GLU:HA	2.18	0.73
1:B:48:MET:CE	1:B:166:GLU:HA	2.18	0.72
1:A:48:MET:HE1	1:A:165:ARG:O	1.89	0.71
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.73	0.70
1:B:424:ARG:HG3	1:B:424:ARG:NH1	2.06	0.70
1:B:424:ARG:HG3	1:B:424:ARG:HH11	1.55	0.70
1:A:203:SER:OG	4:A:951:CO3:C	2.39	0.70
1:B:112:THR:HG21	1:B:143:GLY:O	1.92	0.69
1:B:48:MET:HE3	1:B:166:GLU:HA	1.73	0.69
1:B:203:SER:OG	4:B:952:CO3:C	2.43	0.66
1:B:243:GLU:OE1	1:B:246:ARG:NH1	2.29	0.65
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.79	0.64
1:A:243:GLU:OE1	1:A:246:ARG:NH1	2.31	0.64
1:A:376:GLU:HG2	1:B:538:LYS:NZ	2.15	0.61
1:A:376:GLU:HG2	1:B:538:LYS:CE	2.29	0.61
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.83	0.61
1:A:115:LEU:HD21	1:A:484:ALA:HB2	1.83	0.60
1:A:161:LEU:HD12	1:A:270:ILE:HD11	1.83	0.60
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.37	0.60
1:A:88:PRO:HD3	8:A:1062:HOH:O	2.01	0.59
1:A:433:ARG:HD3	8:A:1080:HOH:O	2.02	0.59
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.84	0.58
1:A:161:LEU:HD12	1:A:270:ILE:CG1	2.32	0.58
1:A:112:THR:HG21	1:A:143:GLY:O	2.03	0.58
1:B:374:ALA:HB2	1:B:540:LEU:HD21	1.86	0.57
1:B:11:ARG:NH1	1:B:16:GLN:HG2	2.19	0.57
1:B:48:MET:HE1	1:B:165:ARG:O	2.04	0.57
1:A:13:ARG:NH2	8:A:1029:HOH:O	2.38	0.57
1:A:537:PRO:O	1:A:540:LEU:HB3	2.04	0.57
1:B:495:SER:O	1:B:496:LYS:O	2.23	0.57
1:A:414:LEU:HG	1:A:418:LEU:HD22	1.86	0.56
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.88	0.56
1:B:48:MET:HE1	1:B:166:GLU:HA	1.89	0.54
1:A:439:TRP:CE3	1:A:443:MET:HE1	2.42	0.54
1:B:11:ARG:HH12	1:B:16:GLN:CG	2.20	0.54
1:B:161:LEU:HD12	1:B:270:ILE:CG1	2.38	0.54
1:A:245:ARG:O	1:A:249:THR:CG2	2.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:LEU:HD11	1:B:449:TYR:CD2	2.43	0.53
1:B:80:PHE:O	1:B:84:GLU:HG2	2.09	0.53
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.90	0.53
1:A:541:SER:O	1:A:542:ALA:CB	2.57	0.53
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.44	0.52
1:B:424:ARG:HH11	1:B:424:ARG:CG	2.20	0.52
1:B:304:ASP:OD2	1:B:306:ASP:HB3	2.09	0.52
1:A:541:SER:O	1:A:542:ALA:HB2	2.10	0.52
1:B:340:VAL:HG11	1:B:443:MET:CE	2.40	0.51
1:A:420:ALA:HB2	1:A:505:THR:HG21	1.92	0.51
1:A:159:LEU:C	1:A:159:LEU:HD23	2.36	0.51
1:B:122:GLY:O	1:B:123:PHE:HB2	2.09	0.51
1:B:210:GLY:HA3	1:B:232:PRO:HD3	1.93	0.51
1:A:75:THR:O	1:A:78:PRO:HD3	2.11	0.51
1:A:224:ARG:HH11	1:A:224:ARG:HG3	1.75	0.51
1:A:326:VAL:HG12	1:A:328:VAL:HG13	1.93	0.51
1:B:497:SER:CB	1:B:498:PRO:C	2.82	0.50
1:A:527:GLN:HE21	5:A:901:P6G:H21	1.77	0.50
1:B:224:ARG:NH1	1:B:224:ARG:HG3	2.26	0.50
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.47	0.50
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.46	0.49
1:B:328:VAL:O	1:B:427:ALA:HA	2.12	0.49
1:B:67:ASN:OD1	1:B:91:GLU:HB2	2.11	0.49
1:B:11:ARG:NH1	1:B:16:GLN:CG	2.74	0.49
1:B:243:GLU:O	1:B:247:ARG:HG3	2.13	0.49
1:A:216:LEU:HB3	1:A:217:PRO:HD3	1.94	0.49
1:B:104:PRO:HG2	1:B:108:PRO:HD3	1.94	0.49
1:A:161:LEU:HD12	1:A:270:ILE:CD1	2.42	0.49
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.95	0.48
1:A:48:MET:HE1	1:A:166:GLU:HA	1.94	0.48
1:A:380:LEU:HD22	1:A:385:TRP:CZ2	2.49	0.48
1:B:369:GLN:HB2	8:B:988:HOH:O	2.12	0.48
1:A:498:PRO:HG2	1:A:518:LEU:HB2	1.96	0.48
1:A:5:ASP:HB3	1:A:8:LEU:HD12	1.96	0.48
1:B:541:SER:O	1:B:542:ALA:HB2	2.13	0.48
1:A:312:PRO:O	1:A:316:ILE:HG23	2.14	0.48
1:B:66:GLN:HG3	1:B:98:TYR:CD1	2.49	0.47
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.49	0.47
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.96	0.47
1:B:7:GLN:OE1	1:B:107:ARG:N	2.43	0.47
1:B:346:PHE:HE2	1:B:395:ARG:HG2	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:HIS:HB2	8:A:1033:HOH:O	2.14	0.47
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.97	0.47
1:A:243:GLU:CD	1:A:246:ARG:NH1	2.73	0.47
1:B:10:VAL:HG23	1:B:32:PHE:CE2	2.50	0.47
1:A:122:GLY:O	1:A:123:PHE:HB2	2.14	0.47
1:A:369:GLN:HB2	8:A:1027:HOH:O	2.14	0.46
1:A:66:GLN:HG3	1:A:98:TYR:CD1	2.51	0.46
1:A:88:PRO:HG2	1:A:92:LEU:HD21	1.97	0.46
1:A:224:ARG:HG3	1:A:224:ARG:NH1	2.29	0.46
1:B:206:ALA:HB3	1:B:230:GLY:HA3	1.97	0.46
1:A:300:VAL:HB	1:A:301:PRO:HD2	1.98	0.46
1:A:380:LEU:HD22	1:A:385:TRP:HZ2	1.81	0.46
1:B:495:SER:C	1:B:496:LYS:O	2.58	0.46
1:A:327:LEU:HD11	1:A:500:TRP:CZ2	2.51	0.45
1:A:166:GLU:HB2	1:A:270:ILE:HD13	1.98	0.45
1:A:524:LEU:O	1:A:525:ARG:C	2.60	0.45
1:B:532:TRP:CE3	1:B:536:LEU:HD12	2.51	0.45
1:B:75:THR:O	1:B:78:PRO:HD3	2.17	0.45
1:A:45:ARG:CZ	1:A:51:GLU:OE1	2.64	0.45
1:A:104:PRO:HG3	1:A:143:GLY:HA2	1.98	0.45
1:B:367:VAL:HG12	1:B:370:ALA:HB2	1.98	0.45
1:B:339:LEU:HD11	1:B:399:SER:HA	1.99	0.45
1:A:433:ARG:NH2	1:A:440:PRO:O	2.50	0.45
1:B:286:TRP:CD2	6:B:903:AE3:H3C1	2.52	0.44
1:B:296:ARG:HG2	8:B:1066:HOH:O	2.16	0.44
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.99	0.44
1:A:293:SER:HA	1:A:365:ILE:HG23	2.00	0.44
1:B:66:GLN:HG3	1:B:98:TYR:CG	2.52	0.44
1:B:161:LEU:HD12	1:B:270:ILE:HD11	2.00	0.44
1:B:496:LYS:HB2	1:B:496:LYS:NZ	2.33	0.44
1:B:528:THR:O	1:B:531:PHE:HB3	2.17	0.44
1:A:7:GLN:O	1:A:107:ARG:NH1	2.52	0.43
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.78	0.43
1:B:536:LEU:HD23	1:B:536:LEU:HA	1.83	0.43
1:B:197:VAL:N	1:B:223:HIS:HD2	1.88	0.43
1:A:428:TYR:CD1	1:A:428:TYR:C	2.97	0.43
1:B:202:GLU:HA	1:B:228:GLN:O	2.18	0.43
1:B:224:ARG:HG3	1:B:224:ARG:HH11	1.84	0.43
1:B:243:GLU:CD	1:B:246:ARG:HH11	2.26	0.43
1:A:99:LEU:C	1:A:99:LEU:HD12	2.43	0.43
1:A:200:PHE:HB2	1:A:226:VAL:HB	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PRO:HG3	1:B:485:ARG:HG2	2.01	0.43
1:B:326:VAL:HG12	1:B:328:VAL:HG13	2.01	0.43
1:B:48:MET:HA	1:B:48:MET:HE2	2.00	0.42
1:A:103:THR:HG22	1:A:145:VAL:HG22	2.00	0.42
1:A:360:LEU:CD2	1:A:379:VAL:HG11	2.49	0.42
1:A:48:MET:HA	1:A:48:MET:HE2	2.00	0.42
1:B:161:LEU:CD1	1:B:269:LEU:HD22	2.48	0.42
1:A:376:GLU:HG2	1:B:538:LYS:HE3	2.00	0.42
1:B:48:MET:HE3	1:B:166:GLU:C	2.44	0.42
1:B:76:LEU:HD22	1:B:341:TYR:CE2	2.54	0.42
1:B:48:MET:HE3	1:B:166:GLU:CA	2.44	0.42
1:B:356:ARG:HA	1:B:394:LEU:HD13	2.02	0.42
1:B:491:ASP:HA	1:B:492:PRO:HD3	1.66	0.42
1:B:107:ARG:HA	1:B:108:PRO:HD3	1.94	0.42
1:A:200:PHE:CB	1:A:226:VAL:HB	2.50	0.41
1:A:328:VAL:O	1:A:427:ALA:HA	2.19	0.41
1:B:491:ASP:HB3	1:B:494:ASP:HB3	2.02	0.41
1:A:48:MET:HE3	1:A:166:GLU:CA	2.45	0.41
1:A:269:LEU:HD23	1:A:269:LEU:C	2.45	0.41
1:A:290:PRO:HG2	1:A:291:GLN:NE2	2.36	0.41
1:B:88:PRO:HG2	1:B:92:LEU:HD21	2.02	0.41
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.88	0.41
1:A:5:ASP:HA	1:A:6:PRO:HD2	1.96	0.41
1:A:160:ALA:HB2	1:A:169:GLY:HA2	2.02	0.41
1:B:38:ALA:HB2	1:B:178:LEU:HD23	2.02	0.41
1:B:104:PRO:CG	1:B:108:PRO:HG3	2.50	0.41
1:B:115:LEU:HD23	1:B:198:THR:HB	2.03	0.41
1:B:286:TRP:CE2	6:B:903:AE3:H3C1	2.55	0.41
1:A:206:ALA:HB3	1:A:230:GLY:HA3	2.03	0.41
1:B:273:LEU:HD23	1:B:273:LEU:HA	1.93	0.40
1:B:454:ILE:HD12	1:B:480:TRP:CE2	2.57	0.40
1:A:494:ASP:OD1	1:A:494:ASP:C	2.65	0.40
1:B:380:LEU:HD22	1:B:385:TRP:CZ2	2.57	0.40
1:A:437:LEU:HD11	1:A:449:TYR:CD2	2.57	0.40
1:A:183:VAL:HG13	1:A:187:ILE:HB	2.04	0.40
1:A:390:ASP:HA	1:A:391:PRO:HD3	1.95	0.40
1:B:134:ASP:OD1	1:B:136:ARG:HD2	2.20	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	531/543 (98%)	506 (95%)	25 (5%)	0	100	100
1	B	529/543 (97%)	507 (96%)	17 (3%)	5 (1%)	14	14
All	All	1060/1086 (98%)	1013 (96%)	42 (4%)	5 (0%)	24	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	542	ALA
1	B	496	LYS
1	B	494	ASP
1	B	497	SER
1	B	108	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	439/443 (99%)	423 (96%)	16 (4%)	31	41
1	B	438/443 (99%)	421 (96%)	17 (4%)	28	39
All	All	877/886 (99%)	844 (96%)	33 (4%)	29	39

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	13	ARG
1	A	23	LYS
1	A	45	ARG
1	A	246	ARG
1	A	249	THR
1	A	251	LEU
1	A	291	GLN
1	A	301	PRO
1	A	332	LYS
1	A	410	PRO
1	A	413	GLN
1	A	418	LEU
1	A	424	ARG
1	A	516	LYS
1	A	525	ARG
1	B	9	LEU
1	B	11	ARG
1	B	25	PRO
1	B	166	GLU
1	B	180	LEU
1	B	203	SER
1	B	246	ARG
1	B	249	THR
1	B	281	LEU
1	B	291	GLN
1	B	296	ARG
1	B	389	GLU
1	B	410	PRO
1	B	424	ARG
1	B	467	THR
1	B	497	SER
1	B	543	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	291	GLN
1	A	421	GLN
1	A	527	GLN
1	B	223	HIS
1	B	291	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	322	GLN
1	B	413	GLN
1	B	499	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	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	1.01	1 (7%)	17,19,21	1.20	3 (17%)
2	FUC	C	2	2	10,10,11	0.78	0	14,14,16	0.79	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	1,2	-	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	2.53	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	-2.46	119.60	122.90
2	C	1	NAG	C4-C3-C2	-2.32	107.62	111.02
2	C	1	NAG	C1-O5-C5	2.25	115.20	112.19

There are no chirality outliers.

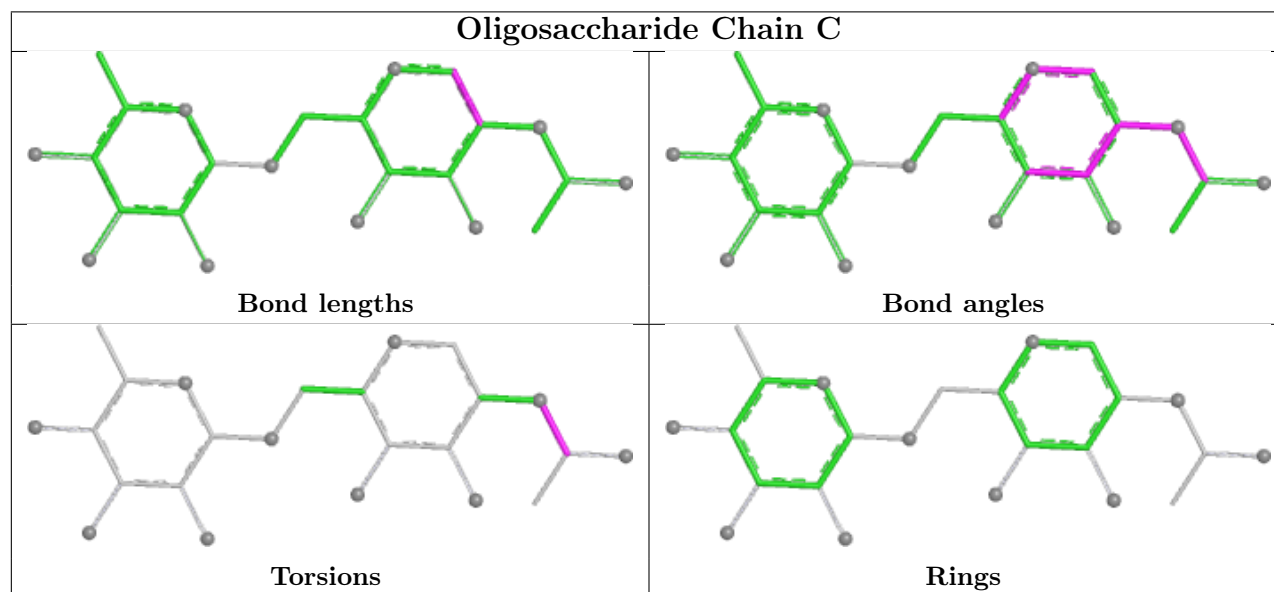
All (2) torsion outliers are listed below:

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](#)

8 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$
7	PG4	B	904	-	10,10,12	1.89	2 (20%)	9,9,11	0.84	0
6	AE3	B	903	-	8,8,8	1.70	2 (25%)	7,7,7	1.49	1 (14%)
3	NAG	A	701	1	14,14,15	0.81	0	17,19,21	0.84	1 (5%)
6	AE3	A	902	-	8,8,8	1.57	2 (25%)	7,7,7	1.36	1 (14%)
4	CO3	A	951	-	3,3,3	0.22	0	2,3,3	0.12	0
4	CO3	B	952	-	3,3,3	0.24	0	2,3,3	0.21	0
5	P6G	A	901	-	18,18,18	2.07	6 (33%)	17,17,17	1.15	1 (5%)
3	NAG	B	601	1	14,14,15	1.05	1 (7%)	17,19,21	0.84	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
7	PG4	B	904	-	-	5/8/8/10	-
6	AE3	B	903	-	-	4/6/6/6	-
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1
6	AE3	A	902	-	-	2/6/6/6	-
5	P6G	A	901	-	-	5/16/16/16	-
3	NAG	B	601	1	-	4/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	904	PG4	O2-C3	4.73	1.62	1.42
5	A	901	P6G	O10-C9	4.00	1.59	1.42
5	A	901	P6G	O13-C12	3.63	1.57	1.42
5	A	901	P6G	O16-C15	3.52	1.57	1.42
6	B	903	AE3	O3-C5	3.50	1.57	1.42
5	A	901	P6G	O4-C3	3.29	1.56	1.42
6	A	902	AE3	O3-C5	3.26	1.56	1.42
5	A	901	P6G	O19-C18	3.26	1.58	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	903	AE3	O2-C3	2.93	1.54	1.42
5	A	901	P6G	O7-C6	2.82	1.54	1.42
7	B	904	PG4	O3-C5	2.76	1.54	1.42
6	A	902	AE3	O2-C3	2.57	1.53	1.42
3	B	601	NAG	C1-C2	2.24	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	P6G	O1-C2-C3	3.34	131.48	111.82
6	B	903	AE3	O4-C6-C5	3.25	130.98	111.82
6	A	902	AE3	O4-C6-C5	3.05	129.76	111.82
3	A	701	NAG	C2-N2-C7	-2.54	119.50	122.90

There are no chirality outliers.

All (22) torsion outliers are listed below:

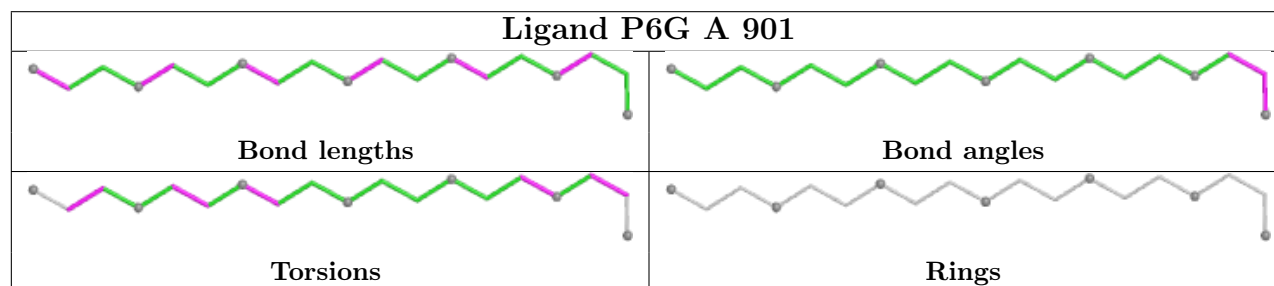
Mol	Chain	Res	Type	Atoms
3	B	601	NAG	O5-C5-C6-O6
3	B	601	NAG	C8-C7-N2-C2
3	B	601	NAG	O7-C7-N2-C2
3	B	601	NAG	C4-C5-C6-O6
7	B	904	PG4	O2-C3-C4-O3
3	A	701	NAG	C8-C7-N2-C2
5	A	901	P6G	O1-C2-C3-O4
7	B	904	PG4	O3-C5-C6-O4
7	B	904	PG4	C4-C3-O2-C2
3	A	701	NAG	O7-C7-N2-C2
5	A	901	P6G	O13-C14-C15-O16
6	B	903	AE3	O2-C3-C4-O3
5	A	901	P6G	O16-C17-C18-O19
6	B	903	AE3	O3-C5-C6-O4
7	B	904	PG4	C8-C7-O4-C6
7	B	904	PG4	C5-C6-O4-C7
5	A	901	P6G	C11-C12-O13-C14
5	A	901	P6G	C6-C5-O4-C3
6	B	903	AE3	C3-C4-O3-C5
6	A	902	AE3	C3-C4-O3-C5
6	A	902	AE3	O2-C3-C4-O3
6	B	903	AE3	C4-C3-O2-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	903	AE3	2	0
4	A	951	CO3	1	0
4	B	952	CO3	1	0
5	A	901	P6G	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	535/543 (98%)	-0.02	16 (2%)	52	59	30, 44, 66, 98	0
1	B	533/543 (98%)	0.18	18 (3%)	48	55	35, 49, 71, 99	0
All	All	1068/1086 (98%)	0.08	34 (3%)	50	57	30, 46, 69, 99	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	497	SER	6.0
1	A	496	LYS	5.3
1	A	542	ALA	4.4
1	B	540	LEU	4.3
1	B	493	ARG	4.3
1	B	542	ALA	4.2
1	B	543	THR	4.0
1	B	257	CYS	3.7
1	B	495	SER	3.7
1	A	492	PRO	3.6
1	A	1	GLU	3.5
1	B	496	LYS	3.5
1	B	492	PRO	3.2
1	A	540	LEU	3.2
1	A	323	ASP	2.8
1	B	498	PRO	2.7
1	A	498	PRO	2.6
1	A	257	CYS	2.6
1	A	109	ALA	2.6
1	A	495	SER	2.5
1	B	538	LYS	2.5
1	B	541	SER	2.3
1	A	75	THR	2.3
1	A	494	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	4	GLU	2.2
1	A	541	SER	2.2
1	A	3	ARG	2.2
1	B	265	ASN	2.2
1	B	350	ASN	2.2
1	B	349	ASP	2.2
1	A	393	HIS	2.1
1	B	191	GLY	2.1
1	A	2	GLY	2.1
1	B	256	GLY	2.1

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

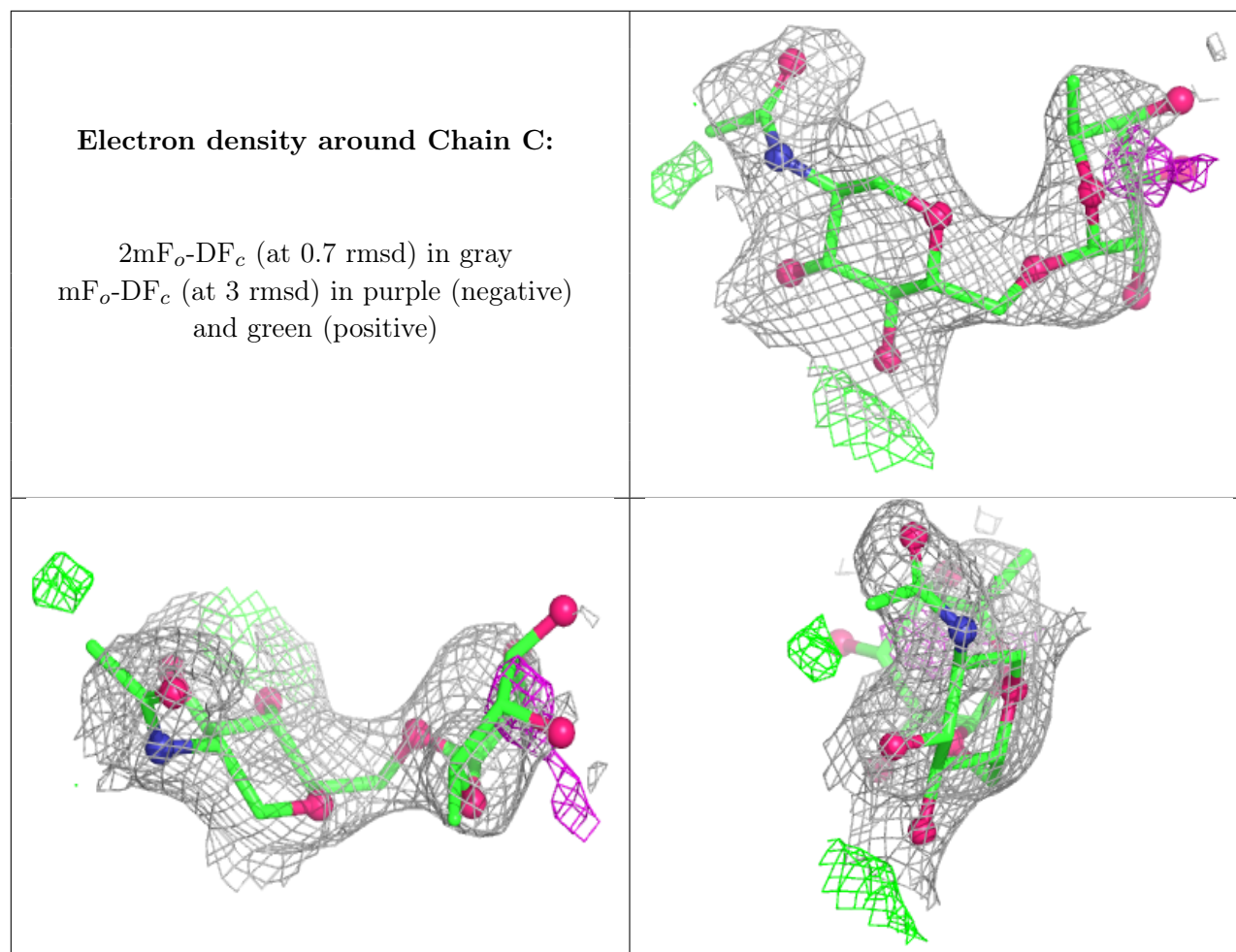
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	1	14/15	0.70	0.14	76,79,85,89	0
2	FUC	C	2	10/11	0.75	0.16	91,93,95,95	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.



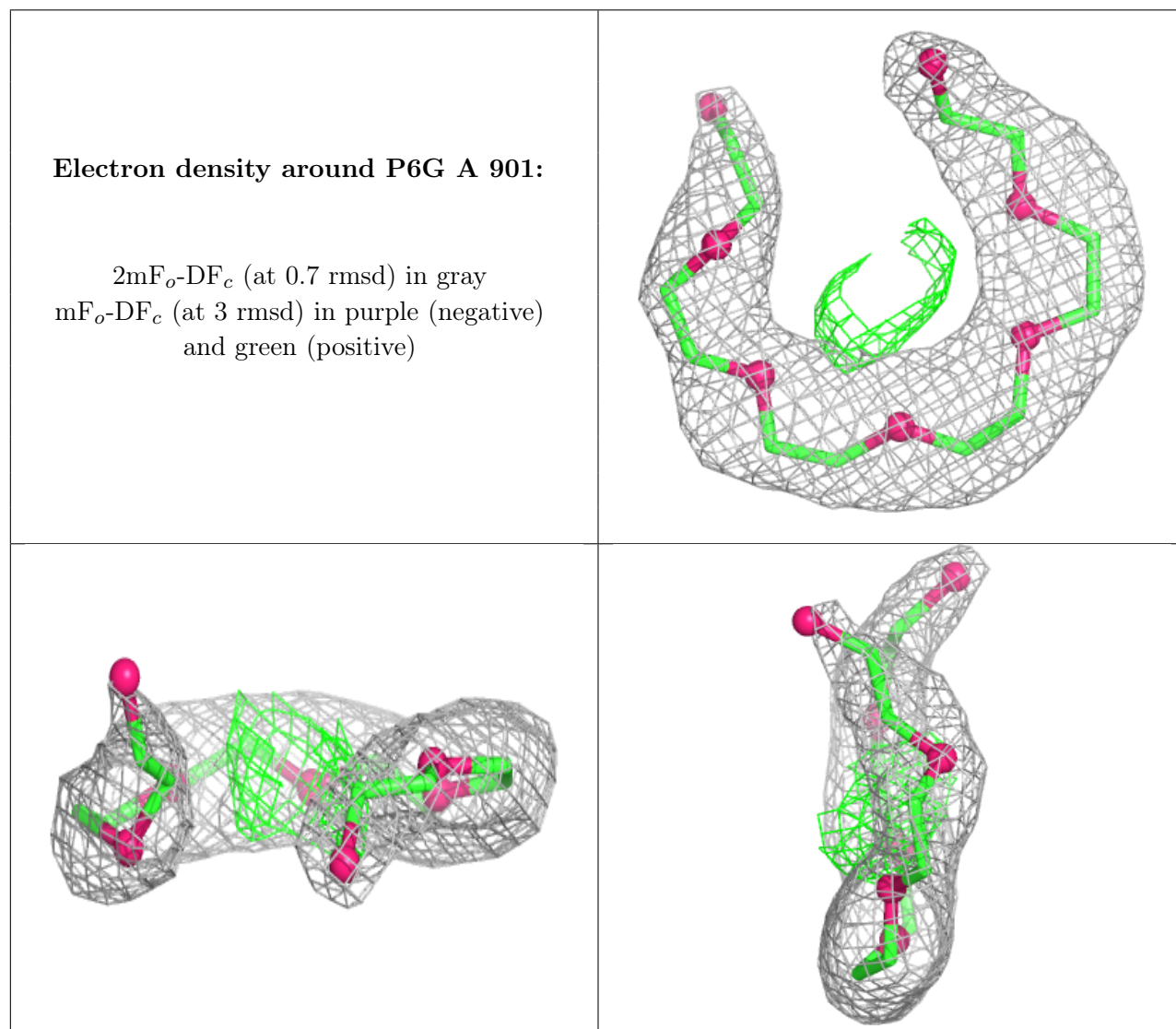
6.4 Ligands [i](#)

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, 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	0.53	0.21	87,89,91,92	0
3	NAG	A	701	14/15	0.69	0.13	81,85,88,89	0
7	PG4	B	904	11/13	0.76	0.23	87,88,90,90	0
6	AE3	A	902	9/9	0.80	0.23	81,82,83,83	0
6	AE3	B	903	9/9	0.87	0.20	83,87,89,89	0
4	CO3	B	952	4/4	0.89	0.15	63,64,64,65	0
4	CO3	A	951	4/4	0.90	0.12	50,50,51,52	0
5	P6G	A	901	19/19	0.93	0.13	61,71,75,76	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.