



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:39 PM UTC

PDB ID : 2PM8 / pdb_00002pm8
Title : Crystal structure of recombinant full length human butyrylcholinesterase
Authors : Ngamelue, M.N.; Homma, K.; Lockridge, O.; Asojo, O.A.
Deposited on : 2007-04-20
Resolution : 2.80 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
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

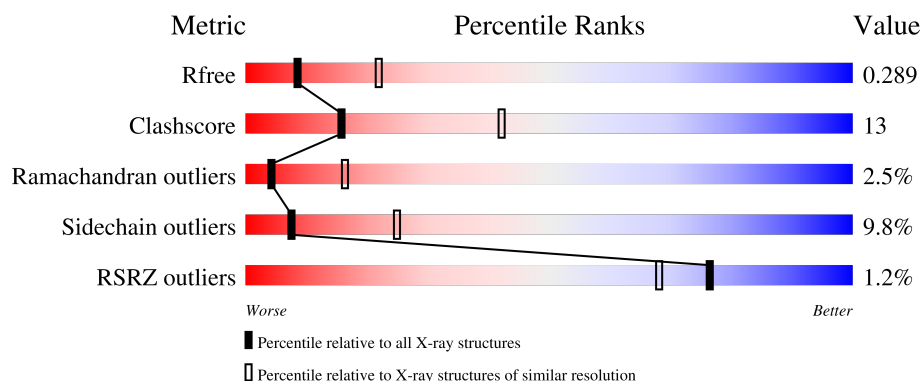
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	574	% 63% 24% 5% 8%
1	B	574	2% 60% 28% . . 8%
2	C	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	606	-	-	X	-
4	SO4	A	608	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8699 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 Cholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4221	2725	708	772	16			
1	B	530	Total	C	N	O	S	0	0	0
			4221	2725	708	772	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	conflict	UNP P06276
A	455	GLN	ASN	conflict	UNP P06276
A	481	GLN	ASN	conflict	UNP P06276
A	486	GLN	ASN	conflict	UNP P06276
B	17	GLN	ASN	conflict	UNP P06276
B	455	GLN	ASN	conflict	UNP P06276
B	481	GLN	ASN	conflict	UNP P06276
B	486	GLN	ASN	conflict	UNP P06276

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



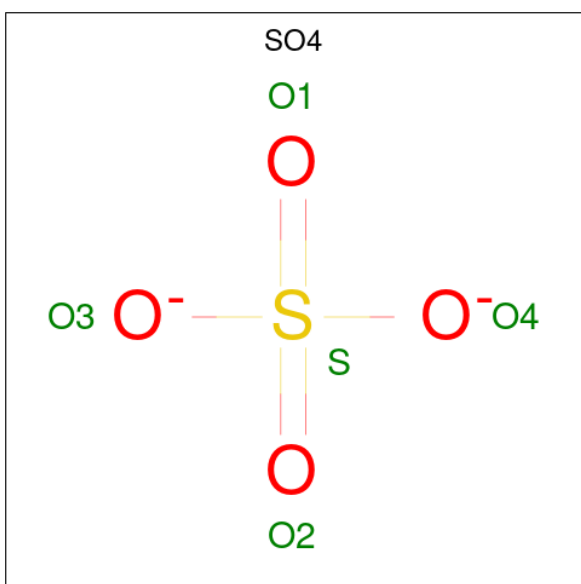
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



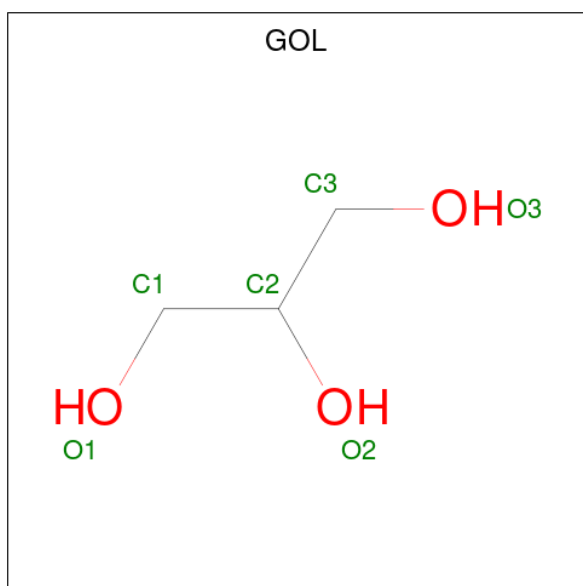
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

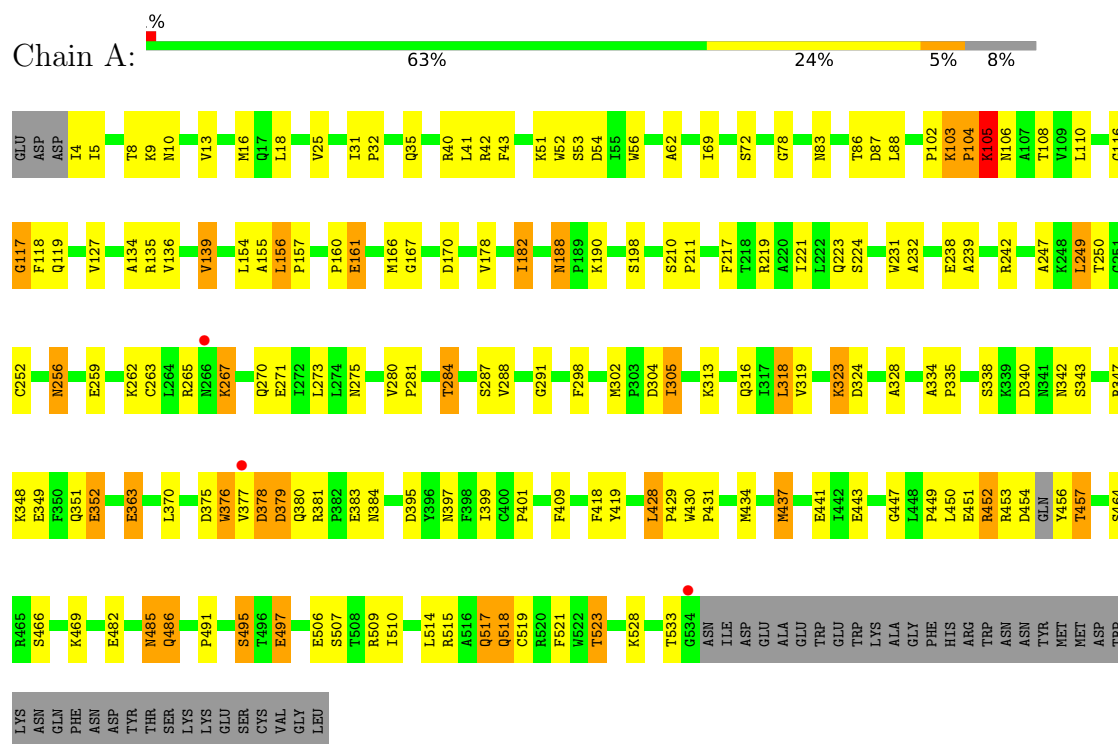
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	52	Total 52	O 52	0	0
6	B	42	Total 42	O 42	0	0

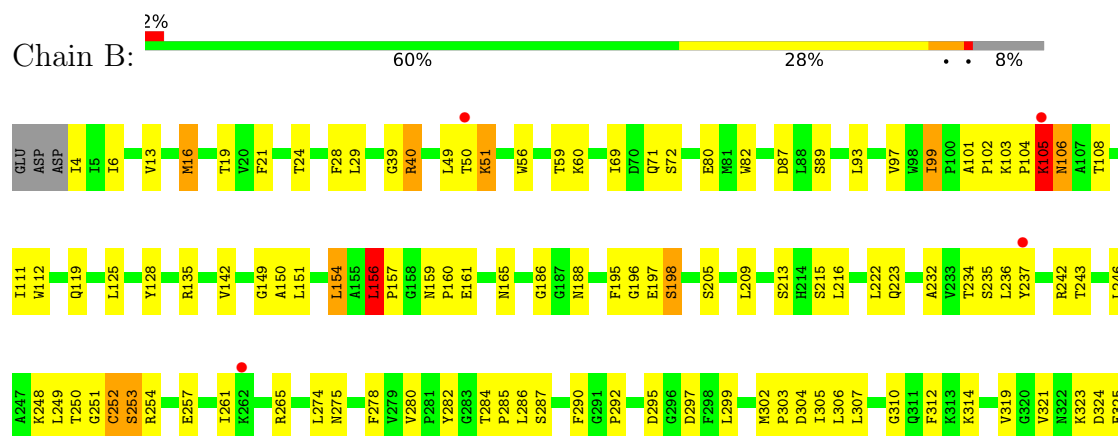
3 Residue-property plots

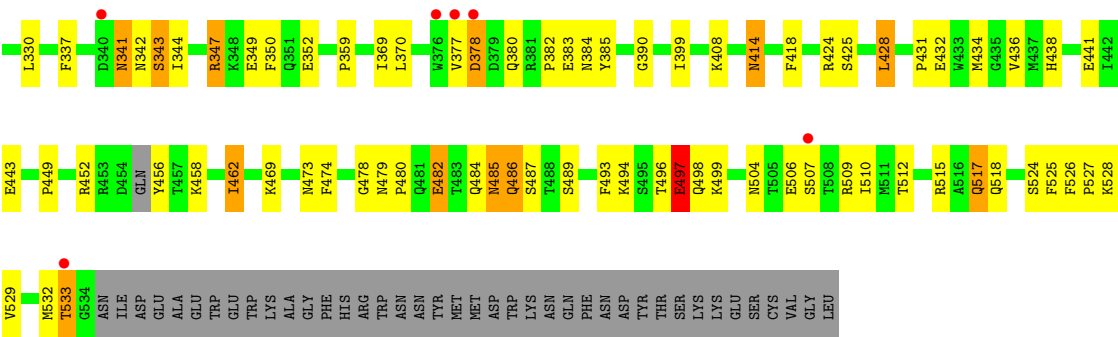
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cholinesterase



• Molecule 1: Cholinesterase





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

Chain C: 100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	150.80Å 150.80Å 142.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.80) 98.8 (50.00-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.292 0.220 , 0.289	Depositor DCC
R_{free} test set	2026 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8699	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: SO4, NAG, 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	0.72	1/4339 (0.0%)	1.02	13/5889 (0.2%)
1	B	0.69	0/4339	0.98	5/5889 (0.1%)
All	All	0.71	1/8678 (0.0%)	1.00	18/11778 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	ASP	CB-CG	6.37	1.68	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	PRO	CA-C-N	7.59	135.36	121.70
1	A	104	PRO	C-N-CA	7.59	135.36	121.70
1	A	104	PRO	N-CA-C	-6.99	101.43	111.22
1	A	305	ILE	CB-CA-C	-6.96	103.59	111.80
1	A	352	GLU	N-CA-C	-5.96	103.96	111.11
1	B	232	ALA	N-CA-C	5.94	119.00	111.69
1	A	232	ALA	N-CA-C	5.85	117.74	111.36
1	A	291	GLY	CA-C-N	5.67	125.61	119.78
1	A	291	GLY	C-N-CA	5.67	125.61	119.78
1	A	156	LEU	CA-C-N	5.48	126.69	119.84
1	A	156	LEU	C-N-CA	5.48	126.69	119.84
1	B	341	ASN	N-CA-C	5.41	116.20	108.74
1	A	273	LEU	N-CA-C	5.27	116.70	111.07
1	B	156	LEU	CA-C-N	5.20	126.34	119.84
1	B	156	LEU	C-N-CA	5.20	126.34	119.84
1	A	238	GLU	N-CA-C	-5.19	105.63	111.28
1	A	284	THR	N-CA-C	-5.15	102.27	108.25
1	B	497	GLU	N-CA-C	5.02	117.40	111.33

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	4221	0	4126	114	0
1	B	4221	0	4129	114	1
2	C	28	0	25	2	0
3	A	42	0	39	0	0
3	B	28	0	26	3	0
4	A	25	0	0	6	1
4	B	10	0	0	0	0
5	A	18	0	24	1	0
5	B	12	0	16	1	0
6	A	52	0	0	3	0
6	B	42	0	0	8	0
All	All	8699	0	8385	226	1

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 13.

All (226) 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:341:ASN:HD21	3:B:601:NAG:C1	1.57	1.16
1:B:517:GLN:H	1:B:517:GLN:HE21	1.05	0.95
1:B:341:ASN:ND2	3:B:601:NAG:C1	2.30	0.95
1:B:425:SER:HB3	1:B:428:LEU:HD23	1.54	0.88
1:A:105:LYS:HG3	1:A:106:ASN:H	1.37	0.88
1:A:509:ARG:NH2	6:A:701:HOH:O	2.09	0.83
1:B:103:LYS:NZ	6:B:701:HOH:O	1.70	0.83
1:A:105:LYS:CG	1:A:106:ASN:H	1.91	0.82
1:B:517:GLN:HE21	1:B:517:GLN:N	1.79	0.81
1:A:449:PRO:HG2	1:A:464:SER:HB2	1.61	0.81
1:A:518:GLN:H	1:A:518:GLN:HE21	1.28	0.80
1:B:104:PRO:CA	1:B:105:LYS:HB3	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:NAG:H61	2:C:2:NAG:HN2	1.45	0.79
1:B:157:PRO:HB3	1:B:236:LEU:HD22	1.66	0.77
1:B:103:LYS:CE	6:B:701:HOH:O	2.24	0.77
1:A:231:TRP:HD1	1:A:397:ASN:HD22	1.33	0.75
1:B:104:PRO:CB	1:B:105:LYS:HB3	2.18	0.74
1:B:246:LEU:O	1:B:250:THR:HG22	1.87	0.74
1:B:156:LEU:HD23	1:B:261:ILE:HD11	1.72	0.72
1:B:314:LYS:HB3	1:B:414:ASN:HD21	1.55	0.72
1:B:104:PRO:O	1:B:186:GLY:HA3	1.89	0.71
1:A:518:GLN:H	1:A:518:GLN:NE2	1.88	0.71
1:A:376:TRP:HD1	1:A:379:ASP:HB3	1.55	0.70
1:A:319:VAL:O	1:A:418:PHE:HA	1.92	0.70
1:A:104:PRO:HA	1:A:105:LYS:HB3	1.75	0.68
1:A:249:LEU:HD22	1:A:275:ASN:HD22	1.59	0.68
1:A:69:ILE:HG23	1:A:83:ASN:ND2	2.09	0.67
1:B:378:ASP:HB3	1:B:380:GLN:HG2	1.77	0.67
1:A:401:PRO:HA	4:A:607:SO4:O1	1.94	0.67
1:A:105:LYS:HG3	1:A:106:ASN:N	2.10	0.66
1:B:504:ASN:HB2	6:B:711:HOH:O	1.94	0.66
1:A:519:CYS:O	1:A:523:THR:HB	1.96	0.65
1:A:434:MET:HE2	1:A:437:MET:SD	2.37	0.65
1:B:104:PRO:HA	1:B:105:LYS:HB3	1.79	0.64
1:A:376:TRP:CD1	1:A:379:ASP:HB3	2.32	0.64
1:B:105:LYS:O	1:B:106:ASN:HB2	1.98	0.64
1:A:42:ARG:O	1:A:43:PHE:HB2	1.97	0.63
1:B:165:ASN:OD1	1:B:292:PRO:HA	1.99	0.63
1:A:198:SER:HA	1:A:224:SER:O	1.97	0.63
1:B:21:PHE:O	1:B:135:ARG:NH1	2.18	0.63
1:A:188:ASN:C	1:A:188:ASN:HD22	2.07	0.61
1:A:252:CYS:SG	1:A:267:LYS:NZ	2.73	0.61
1:A:528:LYS:HE3	4:A:606:SO4:O3	2.01	0.61
1:B:205:SER:HB3	1:B:222:LEU:HD21	1.83	0.61
1:A:381:ARG:NH2	1:A:384:ASN:OD1	2.33	0.61
1:B:104:PRO:HA	1:B:105:LYS:CB	2.31	0.61
1:B:443:GLU:OE1	6:B:702:HOH:O	2.16	0.60
1:A:370:LEU:HD12	4:A:608:SO4:O1	2.02	0.60
1:B:319:VAL:O	1:B:418:PHE:HA	2.02	0.60
1:A:69:ILE:HD11	1:A:88:LEU:HD11	1.82	0.60
1:B:494:LYS:HB2	1:B:497:GLU:OE1	2.02	0.59
1:A:347:ARG:O	1:A:351:GLN:HG3	2.03	0.59
1:B:13:VAL:HG12	1:B:56:TRP:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASP:O	1:A:380:GLN:N	2.34	0.59
1:B:16:MET:HG2	1:B:59:THR:HG22	1.84	0.58
1:A:399:ILE:HG21	1:A:515:ARG:HG3	1.83	0.58
1:A:62:ALA:O	1:A:86:THR:HG21	2.02	0.58
1:B:51:LYS:H	1:B:51:LYS:HD3	1.69	0.58
1:B:249:LEU:HB3	1:B:275:ASN:HD22	1.69	0.58
1:A:381:ARG:HB3	1:A:383:GLU:CD	2.30	0.57
1:B:213:SER:HA	1:B:216:LEU:HD12	1.87	0.57
1:A:454:ASP:O	1:A:456:TYR:N	2.37	0.57
1:A:515:ARG:H	1:B:509:ARG:HH22	1.53	0.56
1:B:104:PRO:CA	1:B:105:LYS:CB	2.83	0.56
1:A:363:GLU:H	1:A:363:GLU:CD	2.14	0.56
1:B:370:LEU:HD12	6:B:741:HOH:O	2.04	0.56
1:A:370:LEU:HD12	4:A:608:SO4:O2	2.06	0.56
1:B:302:MET:HB2	1:B:305:ILE:HD12	1.87	0.56
1:B:103:LYS:HE2	6:B:701:HOH:O	1.96	0.56
1:A:514:LEU:HG	1:A:515:ARG:HG2	1.87	0.55
1:B:458:LYS:O	1:B:462:ILE:HD12	2.07	0.55
1:B:40:ARG:HA	1:B:265:ARG:HD2	1.87	0.55
1:B:324:ASP:O	1:B:325:GLU:C	2.49	0.55
1:B:209:LEU:HD23	1:B:312:PHE:HB3	1.89	0.55
1:B:159:ASN:HD21	1:B:161:GLU:HG2	1.72	0.55
1:B:342:ASN:HB2	1:B:344:ILE:HG12	1.88	0.55
1:A:449:PRO:HA	1:A:456:TYR:CD1	2.41	0.55
1:B:474:PHE:HB2	1:B:480:PRO:HB3	1.89	0.55
1:B:369:ILE:HD11	1:B:526:PHE:CE1	2.42	0.54
1:A:250:THR:O	1:A:267:LYS:NZ	2.39	0.54
1:A:370:LEU:HD12	4:A:608:SO4:S	2.48	0.54
1:A:104:PRO:CA	1:A:105:LYS:HB3	2.37	0.53
1:B:515:ARG:HD2	1:B:518:GLN:HE21	1.73	0.53
1:A:217:PHE:O	1:A:313:LYS:HE2	2.08	0.53
1:A:102:PRO:O	1:A:103:LYS:C	2.51	0.53
1:A:302:MET:HB2	1:A:305:ILE:HD12	1.90	0.53
1:A:338:SER:C	1:A:340:ASP:H	2.17	0.53
1:A:105:LYS:CD	1:A:106:ASN:H	2.21	0.53
1:A:323:LYS:HD2	1:A:324:ASP:OD2	2.08	0.53
1:B:242:ARG:HH12	5:B:605:GOL:H2	1.74	0.53
1:A:249:LEU:HD22	1:A:275:ASN:ND2	2.24	0.52
1:B:151:LEU:HB2	6:B:712:HOH:O	2.08	0.52
1:A:349:GLU:HA	1:A:352:GLU:HB2	1.91	0.52
1:B:349:GLU:HA	1:B:352:GLU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ASN:OD1	1:B:188:ASN:HB2	2.09	0.52
1:A:134:ALA:HA	1:A:139:VAL:O	2.09	0.52
1:B:449:PRO:HA	1:B:456:TYR:CD1	2.45	0.52
1:B:347:ARG:HD2	1:B:385:TYR:OH	2.09	0.51
1:A:395:ASP:OD2	1:A:399:ILE:HD12	2.10	0.51
1:A:188:ASN:C	1:A:188:ASN:ND2	2.68	0.51
1:A:469:LYS:HG2	1:A:482:GLU:HG2	1.91	0.51
1:B:197:GLU:HA	1:B:223:GLN:O	2.10	0.51
1:A:105:LYS:CG	1:A:106:ASN:N	2.64	0.50
1:B:125:LEU:HD12	1:B:128:TYR:CE2	2.46	0.50
1:B:97:VAL:HG22	1:B:142:VAL:HG22	1.92	0.50
1:B:484:GLN:O	1:B:486:GLN:N	2.45	0.50
1:A:517:GLN:HB2	6:A:726:HOH:O	2.12	0.50
1:B:303:PRO:HA	1:B:306:LEU:HD12	1.93	0.50
1:A:188:ASN:ND2	1:A:190:LYS:H	2.10	0.50
1:A:221:ILE:HG23	1:A:318:LEU:HB3	1.92	0.50
1:A:223:GLN:NE2	1:A:441:GLU:OE2	2.45	0.49
1:A:25:VAL:CG2	1:A:135:ARG:HB2	2.42	0.49
1:B:197:GLU:O	1:B:198:SER:C	2.56	0.49
1:B:215:SER:O	1:B:216:LEU:HD23	2.13	0.49
1:B:284:THR:HB	1:B:285:PRO:HD2	1.94	0.49
1:B:493:PHE:CZ	1:B:498:GLN:HG2	2.48	0.49
1:A:119:GLN:HE21	1:A:288:VAL:HG13	1.77	0.48
1:B:341:ASN:ND2	3:B:601:NAG:O7	2.47	0.48
1:B:525:PHE:O	1:B:529:VAL:HG23	2.13	0.48
1:A:155:ALA:HB3	1:A:239:ALA:HB1	1.95	0.48
1:A:160:PRO:HG2	1:A:161:GLU:OE1	2.14	0.48
1:A:219:ARG:HD3	1:A:316:GLN:OE1	2.13	0.48
1:B:524:SER:C	1:B:527:PRO:HD2	2.38	0.48
1:A:491:PRO:HG2	1:A:510:ILE:CG2	2.44	0.48
1:A:78:GLY:HA2	1:A:429:PRO:HG2	1.96	0.47
1:A:347:ARG:HG2	1:A:351:GLN:HE21	1.79	0.47
1:A:41:LEU:O	1:A:42:ARG:C	2.58	0.47
1:A:31:ILE:HG22	1:A:32:PRO:O	2.15	0.47
1:B:344:ILE:HG23	1:B:382:PRO:O	2.13	0.47
1:A:69:ILE:HD12	1:A:69:ILE:N	2.29	0.47
1:A:328:ALA:HB2	1:A:437:MET:HE3	1.97	0.47
1:B:198:SER:HB2	1:B:438:HIS:CE1	2.49	0.47
1:A:116:GLY:O	1:A:118:PHE:N	2.47	0.47
1:A:430:TRP:HB3	1:A:431:PRO:HD2	1.96	0.47
1:B:284:THR:HB	1:B:285:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:SER:HB2	1:B:438:HIS:NE2	2.29	0.47
1:A:40:ARG:HA	1:A:265:ARG:HD2	1.96	0.46
1:B:150:ALA:O	1:B:154:LEU:HB2	2.15	0.46
1:A:428:LEU:HD13	1:A:430:TRP:H	1.80	0.46
1:B:105:LYS:HD3	1:B:106:ASN:C	2.41	0.46
1:A:495:SER:HB2	6:A:725:HOH:O	2.15	0.46
1:B:323:LYS:HB3	1:B:436:VAL:HB	1.98	0.46
1:B:251:GLY:O	1:B:253:SER:N	2.49	0.45
1:A:231:TRP:CD1	1:A:231:TRP:H	2.33	0.45
1:A:521:PHE:HA	4:A:605:SO4:O1	2.16	0.45
1:B:99:ILE:HD12	1:B:104:PRO:HD2	1.98	0.45
1:B:40:ARG:H	1:B:40:ARG:HG2	1.47	0.45
1:B:489:SER:O	1:B:510:ILE:HD11	2.16	0.45
1:A:447:GLY:HA2	1:A:464:SER:OG	2.16	0.45
1:B:112:TRP:CZ3	1:B:196:GLY:HA2	2.52	0.45
1:B:330:LEU:HD11	1:B:390:GLY:HA2	1.99	0.45
1:A:491:PRO:HD3	1:A:510:ILE:HD12	1.99	0.44
1:B:321:VAL:HG11	1:B:399:ILE:HA	1.98	0.44
1:B:359:PRO:HD2	6:B:721:HOH:O	2.17	0.44
1:A:231:TRP:CD1	1:A:397:ASN:HD22	2.23	0.44
1:A:256:ASN:O	1:A:259:GLU:HB2	2.18	0.44
1:B:159:ASN:ND2	1:B:161:GLU:HG2	2.31	0.44
1:A:167:GLY:O	1:A:170:ASP:HB2	2.18	0.44
1:B:80:GLU:C	1:B:82:TRP:H	2.24	0.44
1:B:252:CYS:HA	1:B:254:ARG:NH2	2.33	0.44
1:A:104:PRO:HB2	1:A:105:LYS:CG	2.47	0.44
1:A:136:VAL:HG21	1:A:450:LEU:HD13	2.00	0.44
1:B:119:GLN:HE22	1:B:290:PHE:H	1.66	0.43
1:A:395:ASP:HA	1:A:399:ILE:HB	2.00	0.43
1:B:149:GLY:O	1:B:150:ALA:C	2.60	0.43
1:B:111:ILE:HG12	1:B:142:VAL:HB	2.00	0.43
1:A:104:PRO:HB2	1:A:105:LYS:HG3	2.00	0.43
1:A:334:ALA:HA	1:A:335:PRO:HD2	1.80	0.43
1:A:428:LEU:HA	1:A:429:PRO:HD3	1.80	0.43
1:B:104:PRO:HB2	1:B:105:LYS:HB3	1.98	0.43
1:A:250:THR:HB	1:A:267:LYS:HD3	2.00	0.43
1:A:338:SER:HB2	2:C:1:NAG:H62	2.00	0.43
1:A:485:ASN:O	1:A:486:GLN:C	2.61	0.43
1:B:24:THR:HB	1:B:101:ALA:HB3	2.00	0.43
1:B:474:PHE:O	1:B:478:GLY:N	2.51	0.43
1:B:280:VAL:HG12	1:B:282:TYR:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:GLN:H	1:A:517:GLN:HG3	1.42	0.43
1:B:482:GLU:CD	1:B:482:GLU:C	2.86	0.43
1:B:310:GLY:O	1:B:314:LYS:NZ	2.49	0.43
1:A:452:ARG:HG3	1:A:453:ARG:N	2.34	0.43
1:A:457:THR:HB	1:B:378:ASP:OD2	2.19	0.43
1:A:223:GLN:HG2	1:A:419:TYR:OH	2.19	0.42
1:A:491:PRO:HG2	1:A:510:ILE:HG23	2.01	0.42
1:B:223:GLN:NE2	1:B:441:GLU:OE2	2.52	0.42
1:B:248:LYS:HA	1:B:253:SER:OG	2.19	0.42
1:A:210:SER:HA	1:A:211:PRO:HD2	1.87	0.42
1:B:431:PRO:HG2	1:B:434:MET:HG3	2.02	0.42
1:A:13:VAL:HG12	1:A:56:TRP:HB3	2.02	0.42
1:A:116:GLY:O	1:A:117:GLY:C	2.63	0.42
1:B:469:LYS:HG3	1:B:473:ASN:ND2	2.35	0.42
1:A:178:VAL:O	1:A:182:ILE:HB	2.19	0.41
1:B:424:ARG:NH2	1:B:432:GLU:HA	2.35	0.41
1:A:156:LEU:HA	1:A:157:PRO:HD2	1.85	0.41
1:A:247:ALA:HA	1:A:252:CYS:HB2	2.02	0.41
1:A:284:THR:H	1:A:287:SER:HB2	1.85	0.41
1:B:479:ASN:HA	1:B:480:PRO:HD3	1.92	0.41
1:B:80:GLU:C	1:B:82:TRP:N	2.76	0.41
1:B:275:ASN:HA	1:B:278:PHE:HD1	1.85	0.41
1:B:493:PHE:HD2	1:B:499:LYS:O	2.02	0.41
1:A:154:LEU:N	1:A:166:MET:HE1	2.36	0.41
1:B:28:PHE:N	1:B:28:PHE:CD1	2.89	0.41
1:B:102:PRO:O	1:B:103:LYS:C	2.63	0.41
1:B:261:ILE:O	1:B:265:ARG:HB2	2.20	0.41
1:A:182:ILE:HD12	1:A:182:ILE:HA	1.74	0.41
1:A:259:GLU:O	1:A:263:CYS:N	2.44	0.41
1:B:156:LEU:HD22	1:B:243:THR:HG21	2.03	0.41
1:B:249:LEU:HB3	1:B:275:ASN:ND2	2.33	0.41
1:B:532:MET:O	1:B:533:THR:C	2.63	0.41
1:A:409:PHE:CD2	1:A:409:PHE:C	2.99	0.41
1:B:337:PHE:HA	1:B:343:SER:OG	2.21	0.41
1:B:485:ASN:O	1:B:487:SER:N	2.54	0.41
1:A:497:GLU:H	1:A:497:GLU:HG3	1.67	0.41
1:B:159:ASN:HA	1:B:160:PRO:HD2	1.88	0.41
1:B:497:GLU:H	1:B:497:GLU:HG3	1.60	0.41
1:A:242:ARG:HH12	5:A:610:GOL:H2	1.86	0.40
1:B:295:ASP:OD2	1:B:297:ASP:HB3	2.21	0.40
1:B:307:LEU:HD12	1:B:312:PHE:CE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:GLN:O	1:B:485:ASN:C	2.64	0.40
1:A:86:THR:HG22	1:A:87:ASP:N	2.36	0.40
1:A:449:PRO:HG2	1:A:464:SER:CB	2.42	0.40
1:A:514:LEU:HA	1:B:509:ARG:HH12	1.87	0.40
1:B:347:ARG:O	1:B:350:PHE:HB3	2.22	0.40
1:A:10:ASN:HB3	1:A:52:TRP:CZ3	2.56	0.40
1:A:348:LYS:H	1:A:348:LYS:HG3	1.73	0.40
1:A:380:GLN:O	1:A:381:ARG:C	2.64	0.40
1:A:259:GLU:HG2	1:A:262:LYS:HD2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:LYS:NZ	4:A:606:SO4:O2[4_545]	2.18	0.02

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	526/574 (92%)	463 (88%)	50 (10%)	13 (2%)	4	16
1	B	526/574 (92%)	454 (86%)	59 (11%)	13 (2%)	4	16
All	All	1052/1148 (92%)	917 (87%)	109 (10%)	26 (2%)	4	16

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	LYS
1	A	379	ASP
1	B	105	LYS
1	B	106	ASN

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Mol	Chain	Res	Type
1	B	252	CYS
1	B	486	GLN
1	A	117	GLY
1	A	485	ASN
1	A	507	SER
1	B	39	GLY
1	B	198	SER
1	B	485	ASN
1	A	256	ASN
1	A	486	GLN
1	B	93	LEU
1	B	533	THR
1	A	9	LYS
1	A	54	ASP
1	A	298	PHE
1	A	451	GLU
1	B	89	SER
1	B	347	ARG
1	B	384	ASN
1	A	342	ASN
1	B	507	SER
1	A	281	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	454/494 (92%)	410 (90%)	44 (10%)	8	25
1	B	454/494 (92%)	409 (90%)	45 (10%)	7	24
All	All	908/988 (92%)	819 (90%)	89 (10%)	7	25

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE

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Mol	Chain	Res	Type
1	A	5	ILE
1	A	8	THR
1	A	16	MET
1	A	18	LEU
1	A	35	GLN
1	A	51	LYS
1	A	53	SER
1	A	72	SER
1	A	103	LYS
1	A	105	LYS
1	A	108	THR
1	A	110	LEU
1	A	127	VAL
1	A	139	VAL
1	A	161	GLU
1	A	182	ILE
1	A	188	ASN
1	A	249	LEU
1	A	267	LYS
1	A	270	GLN
1	A	271	GLU
1	A	280	VAL
1	A	318	LEU
1	A	323	LYS
1	A	343	SER
1	A	363	GLU
1	A	375	ASP
1	A	376	TRP
1	A	377	VAL
1	A	378	ASP
1	A	428	LEU
1	A	437	MET
1	A	443	GLU
1	A	452	ARG
1	A	457	THR
1	A	466	SER
1	A	495	SER
1	A	497	GLU
1	A	506	GLU
1	A	517	GLN
1	A	518	GLN
1	A	523	THR

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Mol	Chain	Res	Type
1	A	533	THR
1	B	4	ILE
1	B	6	ILE
1	B	16	MET
1	B	19	THR
1	B	29	LEU
1	B	40	ARG
1	B	49	LEU
1	B	50	THR
1	B	51	LYS
1	B	60	LYS
1	B	69	ILE
1	B	71	GLN
1	B	72	SER
1	B	87	ASP
1	B	99	ILE
1	B	105	LYS
1	B	108	THR
1	B	154	LEU
1	B	156	LEU
1	B	195	PHE
1	B	234	THR
1	B	235	SER
1	B	237	TYR
1	B	253	SER
1	B	257	GLU
1	B	274	LEU
1	B	286	LEU
1	B	287	SER
1	B	299	LEU
1	B	304	ASP
1	B	343	SER
1	B	377	VAL
1	B	378	ASP
1	B	383	GLU
1	B	408	LYS
1	B	414	ASN
1	B	428	LEU
1	B	452	ARG
1	B	462	ILE
1	B	482	GLU
1	B	496	THR

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Mol	Chain	Res	Type
1	B	497	GLU
1	B	506	GLU
1	B	512	THR
1	B	517	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	126	HIS
1	A	176	GLN
1	A	188	ASN
1	A	270	GLN
1	A	275	ASN
1	A	311	GLN
1	A	351	GLN
1	A	372	HIS
1	A	397	ASN
1	A	518	GLN
1	B	83	ASN
1	B	159	ASN
1	B	172	GLN
1	B	176	GLN
1	B	223	GLN
1	B	241	ASN
1	B	256	ASN
1	B	275	ASN
1	B	311	GLN
1	B	341	ASN
1	B	397	ASN
1	B	414	ASN
1	B	473	ASN
1	B	517	GLN
1	B	518	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	0.80	0	17,19,21	1.92	3 (17%)
2	NAG	C	2	2	14,14,15	0.81	0	17,19,21	2.02	4 (23%)

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	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	5.89	130.79	122.90
2	C	2	NAG	O5-C1-C2	-4.39	104.50	111.29
2	C	2	NAG	C1-C2-N2	4.01	116.75	110.43
2	C	2	NAG	C3-C4-C5	3.84	117.20	110.23
2	C	2	NAG	O5-C5-C4	2.95	117.99	110.83
2	C	1	NAG	C4-C3-C2	2.79	115.11	111.02
2	C	1	NAG	O7-C7-C8	-2.04	118.43	122.05

There are no chirality outliers.

All (8) torsion outliers are listed below:

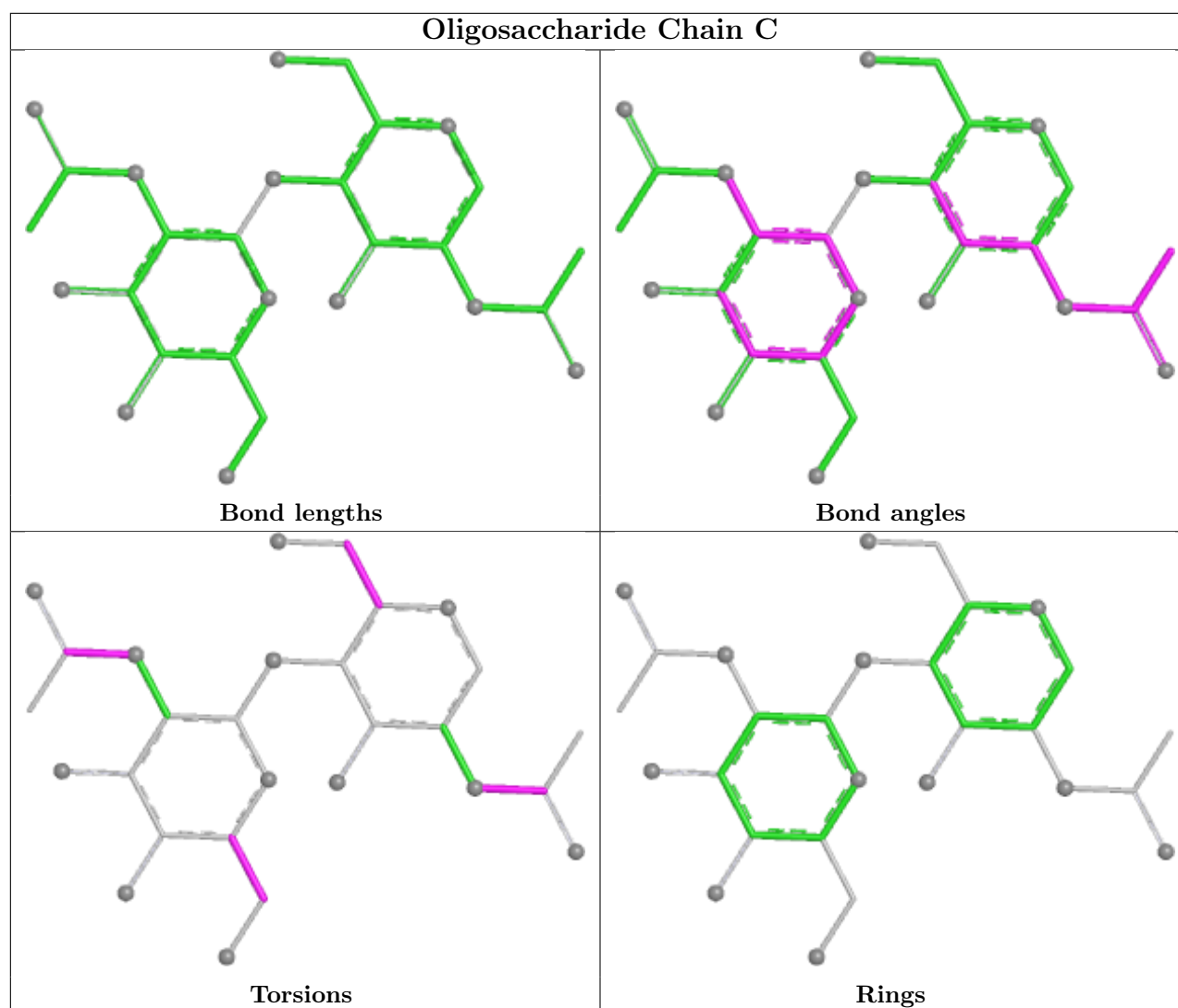
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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



5.6 Ligand geometry [i](#)

17 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	$\# Z > 2$
5	GOL	B	605	-	5,5,5	0.43	0	5,5,5	0.40	0
4	SO4	A	605	-	4,4,4	0.19	0	6,6,6	1.13	0
3	NAG	B	601	-	14,14,15	0.55	0	17,19,21	1.53	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	602	1	14,14,15	0.86	1 (7%)	17,19,21	2.08	2 (11%)
4	SO4	A	604	-	4,4,4	0.30	0	6,6,6	0.43	0
4	SO4	A	608	-	4,4,4	0.16	0	6,6,6	0.75	0
3	NAG	A	601	1	14,14,15	0.69	0	17,19,21	1.41	3 (17%)
4	SO4	A	607	-	4,4,4	0.24	0	6,6,6	0.74	0
4	SO4	B	603	-	4,4,4	0.29	0	6,6,6	0.23	0
4	SO4	B	604	-	4,4,4	0.23	0	6,6,6	0.65	0
3	NAG	B	602	1	14,14,15	0.58	0	17,19,21	0.89	0
5	GOL	A	610	-	5,5,5	0.41	0	5,5,5	0.23	0
5	GOL	B	606	-	5,5,5	0.42	0	5,5,5	0.20	0
5	GOL	A	611	-	5,5,5	0.46	0	5,5,5	1.09	0
4	SO4	A	606	-	4,4,4	0.42	0	6,6,6	1.28	1 (16%)
3	NAG	A	603	1	14,14,15	0.55	0	17,19,21	1.89	3 (17%)
5	GOL	A	609	-	5,5,5	0.34	0	5,5,5	0.60	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
5	GOL	B	605	-	-	2/4/4/4	-
3	NAG	B	601	-	-	4/6/23/26	0/1/1/1
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
5	GOL	B	606	-	-	2/4/4/4	-
3	NAG	B	602	1	-	3/6/23/26	0/1/1/1
5	GOL	A	611	-	-	4/4/4/4	-
5	GOL	A	610	-	-	2/4/4/4	-
3	NAG	A	603	1	-	4/6/23/26	0/1/1/1
5	GOL	A	609	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NAG	C1-C2	2.54	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NAG	C1-O5-C5	7.19	121.82	112.19
3	A	603	NAG	C4-C3-C2	5.31	118.80	111.02
3	A	603	NAG	C3-C4-C5	3.55	116.67	110.23
3	A	601	NAG	C1-O5-C5	3.08	116.32	112.19
3	A	601	NAG	O4-C4-C5	2.94	116.57	109.32
3	A	603	NAG	O5-C5-C6	2.84	113.19	107.66
3	B	601	NAG	C3-C4-C5	-2.72	105.30	110.23
3	B	601	NAG	C2-N2-C7	2.69	126.51	122.90
3	B	601	NAG	O7-C7-C8	-2.49	117.62	122.05
4	A	606	SO4	O3-S-O1	-2.43	96.88	109.56
3	B	601	NAG	O5-C1-C2	2.17	114.64	111.29
3	A	601	NAG	O7-C7-C8	-2.16	118.21	122.05
3	A	602	NAG	O5-C5-C6	2.01	111.57	107.66

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	NAG	O7-C7-N2-C2
3	B	602	NAG	C8-C7-N2-C2
3	B	602	NAG	O7-C7-N2-C2
5	A	611	GOL	C1-C2-C3-O3
5	A	611	GOL	O2-C2-C3-O3
5	B	605	GOL	C1-C2-C3-O3
5	B	605	GOL	O2-C2-C3-O3
3	B	601	NAG	C8-C7-N2-C2
3	A	603	NAG	O5-C5-C6-O6
3	A	603	NAG	C8-C7-N2-C2
3	A	603	NAG	O7-C7-N2-C2
3	A	603	NAG	C4-C5-C6-O6
5	A	609	GOL	C1-C2-C3-O3
5	A	611	GOL	O1-C1-C2-C3
5	B	606	GOL	O1-C1-C2-C3
5	A	611	GOL	O1-C1-C2-O2
3	B	601	NAG	C3-C2-N2-C7
5	A	609	GOL	O2-C2-C3-O3
5	A	610	GOL	C1-C2-C3-O3
3	B	601	NAG	C1-C2-N2-C7
5	A	610	GOL	O2-C2-C3-O3
5	B	606	GOL	O1-C1-C2-O2
3	B	602	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	605	GOL	1	0
4	A	605	SO4	1	0
3	B	601	NAG	3	0
4	A	608	SO4	3	0
4	A	607	SO4	1	0
5	A	610	GOL	1	0
4	A	606	SO4	1	1

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	530/574 (92%)	-0.15	3 (0%) 85 80	31, 50, 74, 86	0
1	B	530/574 (92%)	0.05	10 (1%) 66 57	39, 59, 82, 95	0
All	All	1060/1148 (92%)	-0.05	13 (1%) 76 68	31, 56, 79, 95	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	VAL	5.2
1	B	237	TYR	4.2
1	B	507	SER	3.4
1	B	377	VAL	2.5
1	B	340	ASP	2.5
1	B	533	THR	2.5
1	A	534	GLY	2.4
1	B	262	LYS	2.4
1	A	266	ASN	2.2
1	B	378	ASP	2.2
1	B	376	TRP	2.1
1	B	50	THR	2.0
1	B	105	LYS	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.

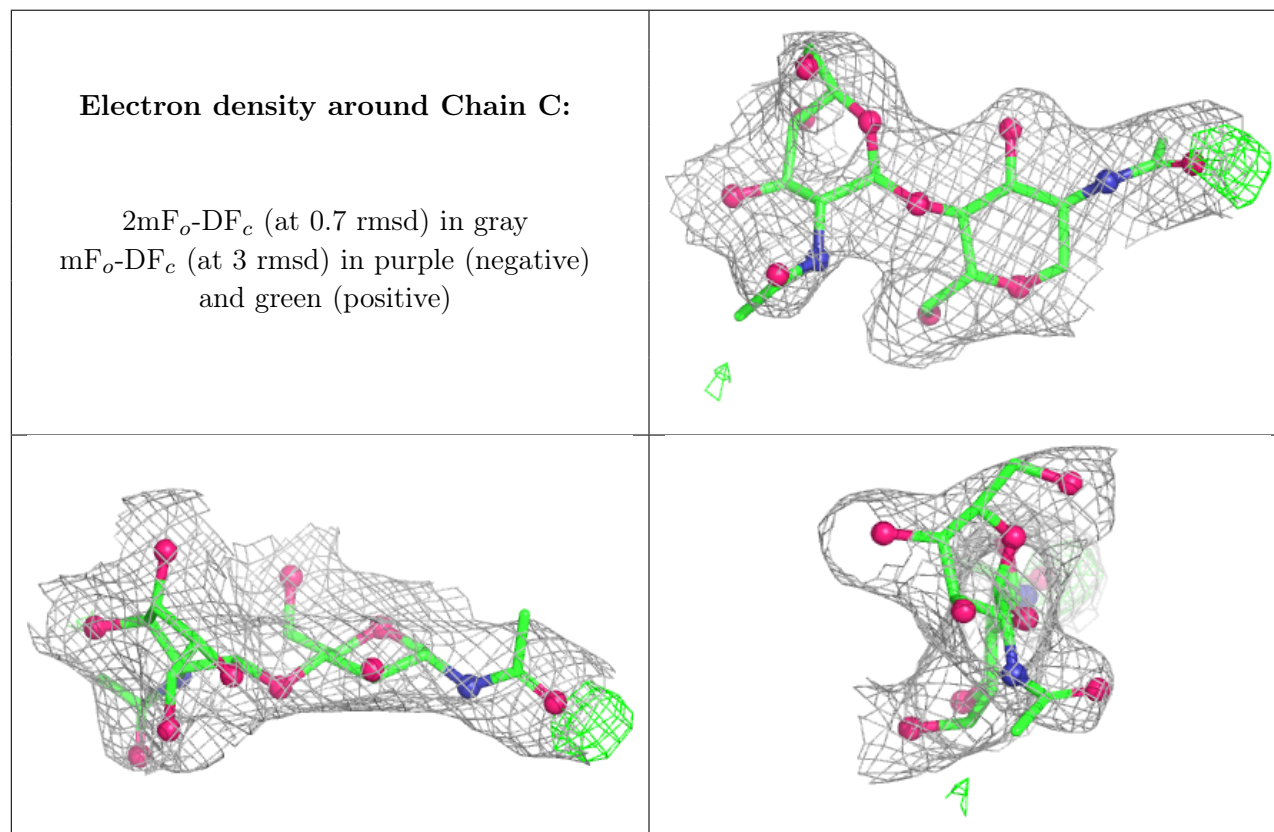
6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.84	0.12	66,68,70,70	0
2	NAG	C	1	14/15	0.88	0.10	54,56,57,61	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(Å ²)	Q<0.9
3	NAG	A	603	14/15	0.57	0.17	71,74,76,77	0
3	NAG	B	602	14/15	0.78	0.14	62,64,67,68	0
5	GOL	B	606	6/6	0.79	0.17	84,86,87,87	0
5	GOL	B	605	6/6	0.81	0.14	58,60,61,61	0
3	NAG	A	601	14/15	0.81	0.11	54,55,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	611	6/6	0.86	0.17	45,48,53,54	0
3	NAG	B	601	14/15	0.86	0.13	69,71,74,76	0
3	NAG	A	602	14/15	0.86	0.11	64,71,72,72	0
5	GOL	A	610	6/6	0.88	0.13	54,62,62,62	0
5	GOL	A	609	6/6	0.88	0.13	61,62,62,63	0
4	SO4	A	608	5/5	0.97	0.08	33,33,34,37	0
4	SO4	A	604	5/5	0.98	0.12	50,50,51,51	0
4	SO4	A	605	5/5	0.98	0.08	34,34,37,39	0
4	SO4	A	606	5/5	0.99	0.04	19,21,24,27	0
4	SO4	B	603	5/5	0.99	0.07	44,44,45,45	0
4	SO4	B	604	5/5	0.99	0.04	41,42,43,45	0
4	SO4	A	607	5/5	0.99	0.04	33,34,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.