



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:13 AM UTC

PDB ID : 3V8C / pdb_00003v8c
Title : Crystal structure of monoclonal human anti-rhesus D Fc IgG1 t125(yb2/0) double mutant (H310 and H435 in K)
Authors : Menez, R.; Stura, E.A.; Bourel, D.; Siberil, S.; Jorieux, S.; De Romeuf, C.; Ducancel, F.; Fridman, W.H.; Teillaud, J.L.
Deposited on : 2011-12-22
Resolution : 2.77 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

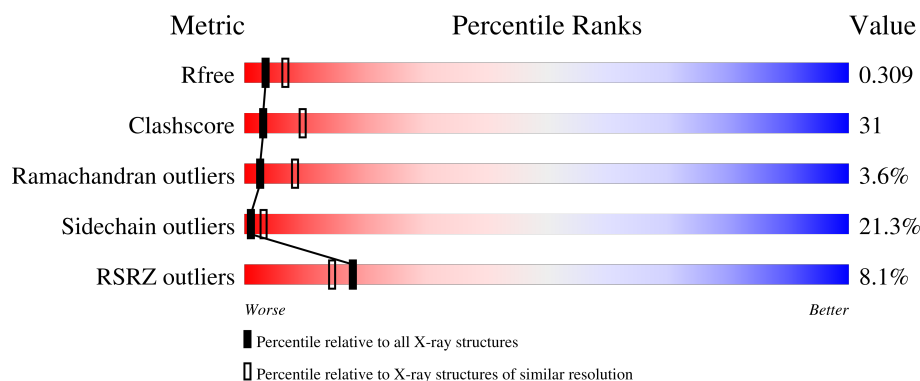
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	212	2% 48% 39% 13%
1	B	212	14% 39% 44% 15%
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
3	NAG	A	502	-	-	X	-
3	NAG	A	505	-	-	X	-
5	MAN	A	503	-	-	X	-
5	MAN	A	507	-	-	X	-
6	GAL	A	506	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3668 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1687	1074	283	324	6			
1	B	209	Total	C	N	O	S	0	0	0
			1665	1062	278	319	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	LYS	HIS	engineered mutation	UNP P01857
A	435	LYS	HIS	engineered mutation	UNP P01857
B	310	LYS	HIS	engineered mutation	UNP P01857
B	435	LYS	HIS	engineered mutation	UNP P01857

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			25	14	1	10			

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



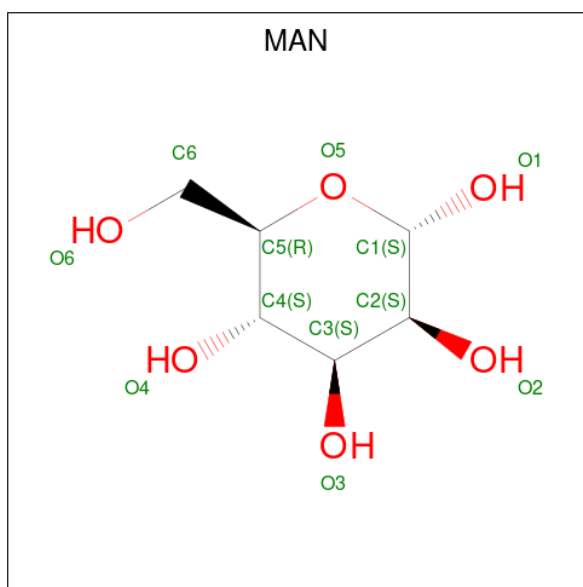
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



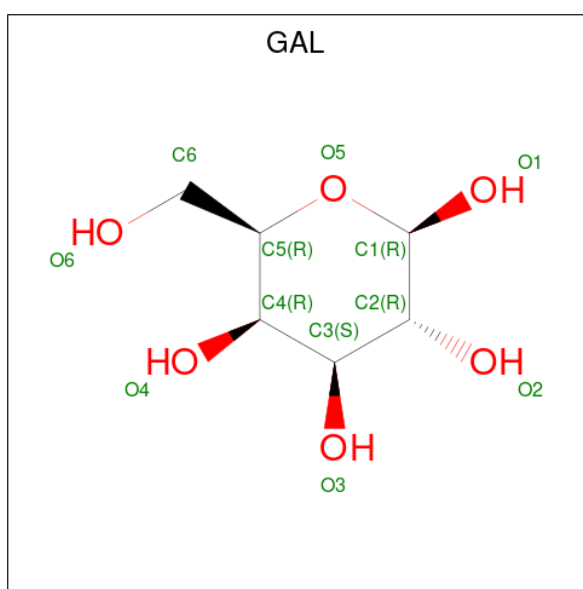
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		

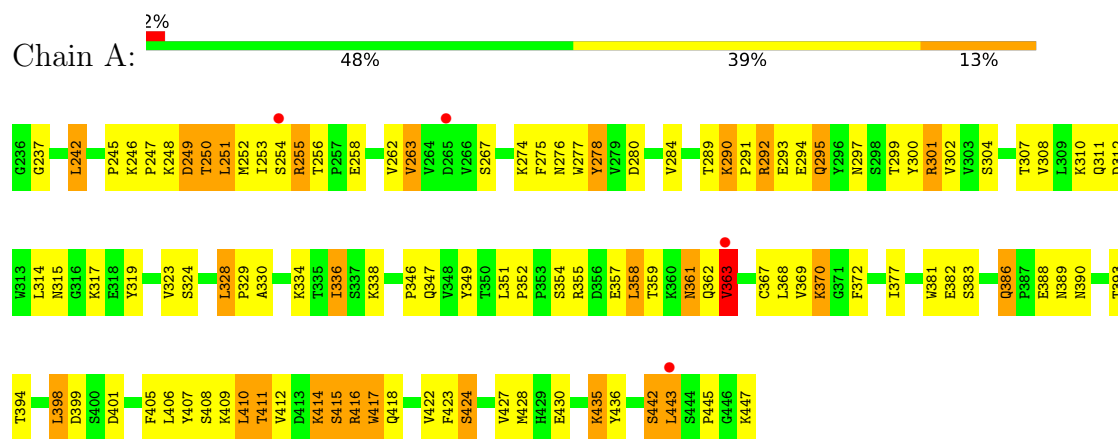
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	50	Total	O	0	0
			50	50		
7	B	48	Total	O	0	0
			48	48		

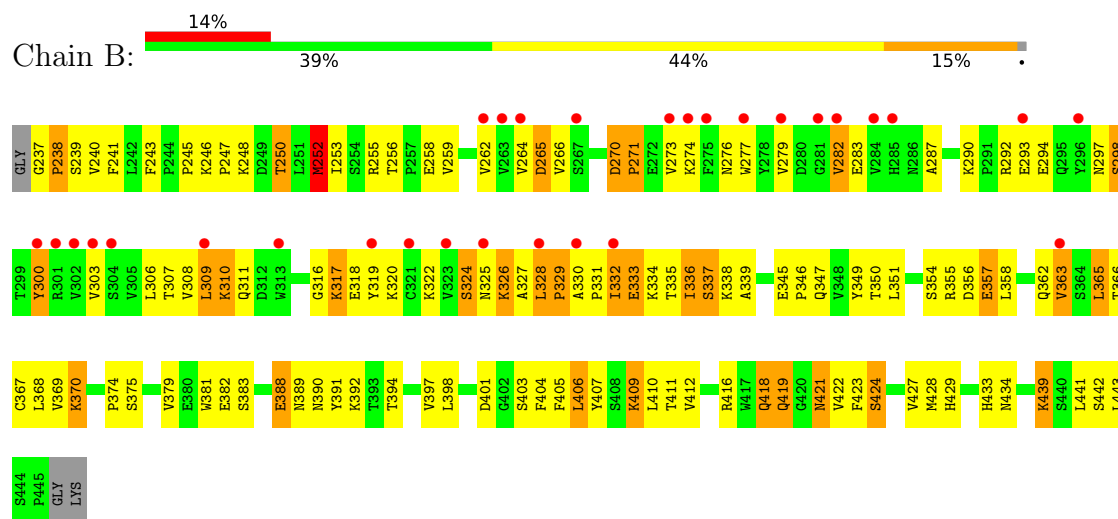
3 Residue-property plots [i](#)

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: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.54Å 79.40Å 139.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.03 – 2.77 42.03 – 2.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.03-2.77) 99.2 (42.03-2.77)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.254 , 0.316 0.251 , 0.309	Depositor DCC
R_{free} test set	723 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3668	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.49% 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: GAL, NAG, GOL, MAN

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	0.88	0/1732	1.23	14/2355 (0.6%)
1	B	0.85	0/1710	1.04	3/2329 (0.1%)
All	All	0.87	0/3442	1.14	17/4684 (0.4%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	GLU	CA-C-N	8.50	130.47	119.84
1	B	345	GLU	C-N-CA	8.50	130.47	119.84
1	A	442	SER	N-CA-C	-8.02	97.02	108.96
1	A	256	THR	CA-C-N	7.90	128.36	119.83
1	A	256	THR	C-N-CA	7.90	128.36	119.83
1	A	237	GLY	CA-C-N	6.09	126.05	119.78
1	A	237	GLY	C-N-CA	6.09	126.05	119.78
1	A	351	LEU	CA-C-N	5.75	123.80	119.66
1	A	351	LEU	C-N-CA	5.75	123.80	119.66
1	B	252	MET	N-CA-C	5.72	118.28	109.07
1	A	389	ASN	N-CA-C	5.48	118.97	112.72
1	A	424	SER	N-CA-C	5.48	118.38	109.06
1	A	352	PRO	O-C-N	5.38	123.68	121.15
1	A	249	ASP	CB-CA-C	-5.38	102.21	110.81
1	A	442	SER	CA-C-N	-5.34	115.53	123.11
1	A	442	SER	C-N-CA	-5.34	115.53	123.11
1	A	363	VAL	N-CA-C	5.09	117.35	108.95

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	1687	0	1669	84	0
1	B	1665	0	1644	111	0
2	C	25	0	22	2	0
3	A	56	0	51	26	0
3	B	42	0	39	6	0
4	A	12	0	16	0	0
4	B	6	0	8	1	0
5	A	33	0	30	20	0
5	B	22	0	20	4	0
6	A	11	0	9	8	0
6	B	11	0	10	5	0
7	A	50	0	0	1	0
7	B	48	0	0	2	0
All	All	3668	0	3518	223	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 31.

All (223) 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)
3:A:505:NAG:O4	6:A:506:GAL:C2	1.64	1.43
3:A:502:NAG:O4	5:A:503:MAN:C1	1.72	1.36
1:B:328:LEU:CB	1:B:329:PRO:HD3	1.86	1.05
1:A:247:PRO:O	1:A:251:LEU:HD12	1.54	1.03
3:A:505:NAG:O4	6:A:506:GAL:C1	2.07	1.02
1:B:328:LEU:HB2	1:B:329:PRO:HD3	1.02	1.01
1:A:242:LEU:HD13	1:A:336:ILE:HB	1.42	1.01
1:B:328:LEU:HB2	1:B:329:PRO:CD	1.91	0.99
1:B:347:GLN:NE2	1:B:349:TYR:OH	1.98	0.97
1:B:266:VAL:HG13	1:B:300:TYR:HB3	1.49	0.95
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.30	0.95
1:A:361:ASN:HD22	1:A:361:ASN:H	1.11	0.95
3:A:502:NAG:O4	5:A:503:MAN:C2	2.17	0.92
1:B:418:GLN:HE21	1:B:418:GLN:HA	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:507:MAN:O2	3:A:508:NAG:H2	1.71	0.89
1:B:282:VAL:HG12	1:B:283:GLU:H	1.42	0.84
1:B:330:ALA:HB1	1:B:331:PRO:HD2	1.58	0.83
1:A:297:ASN:HD21	3:A:501:NAG:C1	1.92	0.83
1:B:391:TYR:HB3	1:B:410:LEU:HD12	1.60	0.83
1:A:361:ASN:H	1:A:361:ASN:ND2	1.77	0.80
1:A:255:ARG:HH11	1:A:255:ARG:CG	1.94	0.79
1:A:357:GLU:HG3	1:B:349:TYR:CZ	2.19	0.77
1:B:406:LEU:O	1:B:406:LEU:HD12	1.84	0.76
1:A:398:LEU:HD13	1:A:399:ASP:O	1.86	0.76
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.01	0.76
1:B:418:GLN:HE21	1:B:418:GLN:CA	1.98	0.76
3:A:502:NAG:C4	5:A:503:MAN:C1	2.65	0.75
1:B:406:LEU:HD12	1:B:406:LEU:C	2.11	0.75
1:A:263:VAL:HG11	1:A:323:VAL:HG11	1.69	0.75
5:A:504:MAN:O2	3:A:505:NAG:C1	2.35	0.75
1:B:248:LYS:HE2	1:B:255:ARG:NH1	2.02	0.75
1:B:306:LEU:HD23	1:B:308:VAL:HG22	1.70	0.73
3:A:502:NAG:O4	5:A:503:MAN:H2	1.88	0.72
1:B:336:ILE:HD12	1:B:337:SER:H	1.53	0.72
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.69	0.72
1:A:361:ASN:HD22	1:A:361:ASN:N	1.83	0.72
1:B:297:ASN:O	1:B:298:SER:HB3	1.87	0.72
1:A:393:THR:OG1	1:A:408:SER:HB2	1.90	0.71
5:A:507:MAN:O2	3:A:508:NAG:C2	2.38	0.71
1:A:338:LYS:NZ	1:A:430:GLU:OE2	2.25	0.70
1:A:255:ARG:O	1:A:310:LYS:NZ	2.25	0.69
5:B:503:MAN:O3	2:C:1:MAN:H3	1.91	0.69
1:B:347:GLN:CD	1:B:349:TYR:OH	2.35	0.69
1:A:311:GLN:O	1:A:315:ASN:HB2	1.93	0.68
1:A:415:SER:O	1:A:418:GLN:N	2.27	0.67
1:B:332:ILE:CG2	1:B:333:GLU:N	2.58	0.67
1:A:247:PRO:O	1:A:251:LEU:CD1	2.38	0.66
3:A:502:NAG:HO4	5:A:503:MAN:C1	2.08	0.66
5:A:503:MAN:O3	5:A:507:MAN:H2	1.95	0.66
1:A:328:LEU:HD11	1:A:330:ALA:O	1.96	0.66
1:B:347:GLN:CD	1:B:349:TYR:HH	2.03	0.66
1:A:246:LYS:NZ	3:A:505:NAG:O3	2.24	0.65
1:B:293:GLU:HG2	1:B:294:GLU:HG3	1.77	0.65
1:B:317:LYS:HB2	1:B:319:TYR:HE1	1.61	0.65
1:A:297:ASN:ND2	3:A:501:NAG:C1	2.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:LEU:HG	1:B:411:THR:N	2.12	0.64
1:A:346:PRO:HG3	1:A:372:PHE:HB3	1.79	0.64
1:B:287:ALA:HB2	1:B:306:LEU:HD12	1.80	0.64
1:A:293:GLU:HG2	1:A:301:ARG:HG3	1.80	0.64
1:A:293:GLU:HG3	1:A:295:GLN:HE22	1.62	0.63
1:B:332:ILE:HG23	1:B:333:GLU:H	1.64	0.63
1:A:377:ILE:HD11	1:A:427:VAL:CG1	2.29	0.62
5:B:504:MAN:O2	3:B:505:NAG:C1	2.48	0.62
5:B:503:MAN:H4	2:C:1:MAN:C1	2.30	0.62
3:A:505:NAG:C4	6:A:506:GAL:C2	2.76	0.62
3:A:502:NAG:C3	5:A:503:MAN:C1	2.77	0.62
1:B:350:THR:HB	1:B:441:LEU:HD22	1.82	0.62
5:A:507:MAN:HO2	3:A:508:NAG:H2	1.65	0.61
1:B:365:LEU:CD1	1:B:410:LEU:HD23	2.29	0.61
1:B:433:HIS:O	1:B:434:ASN:HB2	2.00	0.61
1:B:318:GLU:C	1:B:319:TYR:HD1	2.08	0.61
1:A:275:PHE:CE2	1:A:304:SER:HB2	2.36	0.60
5:A:503:MAN:O6	5:A:504:MAN:H3	2.02	0.60
1:A:280:ASP:OD1	1:A:317:LYS:HG3	2.02	0.59
1:B:246:LYS:HG2	6:B:506:GAL:O4	2.01	0.59
1:B:351:LEU:HB2	1:B:366:THR:HB	1.83	0.59
1:A:394:THR:HG23	1:A:407:TYR:O	2.02	0.59
1:B:406:LEU:C	1:B:406:LEU:CD1	2.74	0.59
1:B:243:PHE:HE2	1:B:262:VAL:HG22	1.67	0.58
1:B:397:VAL:HB	1:B:405:PHE:CE2	2.38	0.58
1:B:336:ILE:HD12	1:B:337:SER:N	2.18	0.58
1:B:357:GLU:O	1:B:357:GLU:HG2	2.02	0.58
1:B:394:THR:HG23	1:B:407:TYR:O	2.02	0.58
1:A:312:ASP:HB3	1:A:319:TYR:OH	2.04	0.58
1:A:328:LEU:CD1	1:A:330:ALA:O	2.51	0.58
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.38	0.58
1:A:361:ASN:ND2	1:A:361:ASN:N	2.47	0.57
1:B:241:PHE:CE2	3:B:502:NAG:H62	2.39	0.57
1:B:246:LYS:HE3	6:B:506:GAL:H61	1.86	0.57
3:B:505:NAG:O4	6:B:506:GAL:C1	2.53	0.57
1:A:245:PRO:HA	6:A:506:GAL:H4	1.86	0.57
1:B:397:VAL:O	1:B:404:PHE:HA	2.04	0.57
1:B:318:GLU:C	1:B:319:TYR:CD1	2.83	0.56
1:B:308:VAL:HG11	1:B:319:TYR:CE2	2.40	0.56
1:B:332:ILE:CG2	1:B:333:GLU:H	2.15	0.56
1:B:388:GLU:OE2	1:B:416:ARG:NH1	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:TRP:HA	1:B:424:SER:O	2.05	0.56
1:A:347:GLN:NE2	1:A:349:TYR:OH	2.36	0.56
1:B:252:MET:HG3	1:B:428:MET:HE3	1.87	0.56
1:A:297:ASN:OD1	3:A:501:NAG:C1	2.53	0.56
1:B:274:LYS:HB3	1:B:324:SER:HB3	1.88	0.56
5:A:503:MAN:O3	5:A:507:MAN:C2	2.54	0.56
1:B:245:PRO:HA	6:B:506:GAL:O3	2.06	0.56
1:A:443:LEU:O	1:A:445:PRO:HD3	2.06	0.55
5:A:503:MAN:O3	5:A:507:MAN:C1	2.55	0.55
1:A:383:SER:HB2	1:A:423:PHE:CD2	2.41	0.55
5:B:504:MAN:O2	3:B:505:NAG:O5	2.24	0.55
1:B:309:LEU:HD23	1:B:311:GLN:H	1.71	0.54
1:B:308:VAL:HG11	1:B:319:TYR:HE2	1.71	0.54
1:B:401:ASP:OD1	1:B:403:SER:OG	2.25	0.54
3:A:501:NAG:O4	3:A:502:NAG:C1	2.56	0.54
4:B:509:GOL:H12	7:B:629:HOH:O	2.07	0.54
1:B:270:ASP:N	1:B:271:PRO:HD3	2.22	0.53
1:B:356:ASP:C	1:B:358:LEU:H	2.16	0.53
1:B:332:ILE:HG22	1:B:333:GLU:N	2.23	0.53
1:A:393:THR:HA	1:A:408:SER:HA	1.90	0.53
1:A:407:TYR:OH	1:B:409:LYS:HG3	2.08	0.53
1:B:306:LEU:CD2	1:B:308:VAL:HG22	2.38	0.53
1:B:347:GLN:NE2	1:B:349:TYR:HH	2.05	0.52
1:A:294:GLU:C	1:A:295:GLN:HE21	2.18	0.52
1:B:388:GLU:OE2	1:B:423:PHE:HE2	1.93	0.52
1:B:418:GLN:CA	1:B:418:GLN:NE2	2.71	0.52
1:A:377:ILE:HD11	1:A:427:VAL:HG13	1.90	0.52
1:A:414:LYS:O	1:A:415:SER:C	2.53	0.52
1:A:246:LYS:HZ1	3:A:505:NAG:C3	2.22	0.51
1:B:421:ASN:OD1	1:B:421:ASN:N	2.43	0.51
1:B:237:GLY:HA2	1:B:329:PRO:HD2	1.92	0.51
1:B:308:VAL:CG1	1:B:319:TYR:HE2	2.24	0.51
1:A:289:THR:HG22	1:A:290:LYS:N	2.24	0.51
1:B:243:PHE:O	1:B:259:VAL:HG23	2.11	0.51
1:B:390:ASN:OD1	1:B:411:THR:HG23	2.11	0.51
1:A:390:ASN:ND2	1:A:411:THR:O	2.37	0.50
1:B:317:LYS:HB2	1:B:319:TYR:CE1	2.43	0.50
1:A:278:TYR:N	1:A:278:TYR:CD2	2.80	0.50
1:A:358:LEU:O	1:A:414:LYS:HE3	2.12	0.49
1:A:382:GLU:HB2	1:A:386:GLN:O	2.11	0.49
1:A:290:LYS:HB3	1:A:291:PRO:CD	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:LEU:HD12	1:B:410:LEU:CD2	2.41	0.49
1:A:292:ARG:HD3	1:A:300:TYR:CD1	2.47	0.48
1:B:350:THR:HG23	1:B:439:LYS:HB3	1.96	0.48
1:B:282:VAL:HG12	1:B:283:GLU:N	2.20	0.48
1:A:377:ILE:HD11	1:A:427:VAL:HG11	1.95	0.48
1:B:356:ASP:O	1:B:358:LEU:N	2.47	0.48
1:A:354:SER:HB2	1:B:349:TYR:HB3	1.96	0.48
1:B:368:LEU:HD13	1:B:407:TYR:CZ	2.49	0.48
1:A:245:PRO:HA	6:A:506:GAL:C4	2.44	0.47
1:A:249:ASP:OD2	6:A:506:GAL:H62	2.14	0.47
1:B:379:VAL:HG22	1:B:427:VAL:HG22	1.97	0.47
1:A:436:TYR:C	1:A:436:TYR:CD2	2.91	0.47
1:B:316:GLY:O	1:B:317:LYS:C	2.57	0.47
1:B:390:ASN:O	1:B:411:THR:HG22	2.13	0.47
3:A:502:NAG:O3	5:A:503:MAN:C1	2.63	0.47
1:B:346:PRO:HD3	1:B:429:HIS:CD2	2.50	0.47
1:A:368:LEU:HD12	1:A:369:VAL:N	2.31	0.47
1:A:398:LEU:HD13	1:A:398:LEU:C	2.40	0.46
1:B:388:GLU:OE1	1:B:388:GLU:HA	2.15	0.46
1:B:418:GLN:HA	1:B:418:GLN:NE2	2.17	0.46
1:B:243:PHE:HE2	1:B:262:VAL:CG2	2.28	0.46
1:A:263:VAL:CG1	1:A:323:VAL:HG11	2.43	0.46
1:B:401:ASP:CG	1:B:403:SER:HG	2.22	0.46
1:B:258:GLU:O	6:B:506:GAL:O3	2.25	0.46
1:B:241:PHE:CE2	3:B:502:NAG:C6	3.00	0.45
1:B:255:ARG:H	1:B:310:LYS:NZ	2.15	0.45
1:B:266:VAL:O	1:B:300:TYR:HB2	2.17	0.45
1:A:295:GLN:HE21	1:A:295:GLN:N	2.15	0.44
1:A:289:THR:CG2	1:A:290:LYS:N	2.79	0.44
1:A:388:GLU:OE1	1:A:416:ARG:NH2	2.50	0.44
1:B:247:PRO:O	1:B:250:THR:HG22	2.16	0.44
1:B:264:VAL:O	1:B:265:ASP:HB2	2.17	0.44
1:B:356:ASP:C	1:B:358:LEU:N	2.75	0.44
1:B:290:LYS:HZ1	1:B:293:GLU:HG3	1.82	0.44
1:B:273:VAL:HG13	1:B:325:ASN:HB2	1.99	0.44
1:B:252:MET:HG3	1:B:428:MET:CE	2.47	0.44
1:A:401:ASP:C	1:A:401:ASP:OD2	2.59	0.44
1:A:246:LYS:O	1:A:249:ASP:HB2	2.16	0.44
1:B:241:PHE:HE2	3:B:502:NAG:C6	2.31	0.44
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.53	0.44
1:B:290:LYS:HD2	1:B:303:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:MET:HB2	1:A:435:LYS:O	2.18	0.43
1:A:293:GLU:CD	1:A:301:ARG:HD2	2.43	0.43
1:A:295:GLN:OE1	1:A:301:ARG:HG2	2.17	0.43
1:B:328:LEU:CB	1:B:329:PRO:CD	2.68	0.43
1:A:422:VAL:HG22	1:A:442:SER:HB3	2.01	0.43
1:B:347:GLN:HB2	1:B:370:LYS:O	2.18	0.43
1:B:363:VAL:HG23	1:B:412:VAL:CG2	2.49	0.43
1:A:295:GLN:HE21	1:A:295:GLN:CA	2.32	0.43
1:A:297:ASN:CG	3:A:501:NAG:C1	2.92	0.42
1:A:388:GLU:HB3	1:A:410:LEU:CD1	2.49	0.42
1:A:247:PRO:O	1:A:250:THR:HB	2.19	0.42
5:A:507:MAN:O2	3:A:508:NAG:N2	2.52	0.42
1:B:238:PRO:HB2	1:B:239:SER:H	1.69	0.42
1:B:336:ILE:CD1	1:B:337:SER:H	2.29	0.42
1:B:241:PHE:HB2	1:B:262:VAL:CG2	2.49	0.42
1:B:354:SER:O	1:B:355:ARG:C	2.62	0.42
1:A:276:ASN:HB3	1:A:278:TYR:HE2	1.85	0.42
1:B:256:THR:HG23	1:B:307:THR:HG23	2.01	0.42
1:A:258:GLU:O	6:A:506:GAL:H4	2.19	0.42
1:B:240:VAL:HG12	1:B:334:LYS:HG3	2.02	0.41
1:B:410:LEU:HG	1:B:411:THR:H	1.83	0.41
1:A:370:LYS:HB2	1:A:370:LYS:HE2	1.46	0.41
1:A:363:VAL:HG23	1:A:412:VAL:HG23	2.02	0.41
1:A:415:SER:O	1:A:417:TRP:N	2.53	0.41
5:A:503:MAN:C3	5:A:507:MAN:C1	2.98	0.41
5:A:504:MAN:C2	3:A:505:NAG:C1	2.99	0.41
1:B:241:PHE:HB2	1:B:262:VAL:HG22	2.02	0.41
1:A:369:VAL:O	1:A:405:PHE:HA	2.20	0.41
1:A:277:TRP:C	1:A:278:TYR:CD2	2.99	0.41
3:A:502:NAG:HO4	5:A:503:MAN:C2	2.31	0.41
1:B:419:GLN:HB2	1:B:421:ASN:OD1	2.21	0.41
1:A:246:LYS:NZ	3:A:505:NAG:C3	2.84	0.41
1:A:249:ASP:OD2	6:A:506:GAL:C6	2.69	0.40
1:A:275:PHE:CD2	1:A:304:SER:HB2	2.55	0.40
1:A:284:VAL:HG12	7:A:601:HOH:O	2.20	0.40
1:B:369:VAL:O	1:B:405:PHE:HA	2.21	0.40
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.93	0.40
1:B:339:ALA:HB3	1:B:374:PRO:HB3	2.04	0.40
1:B:422:VAL:HG12	1:B:442:SER:HB3	2.02	0.40
1:A:394:THR:HG23	1:A:394:THR:H	1.65	0.40
3:A:501:NAG:C4	3:A:502:NAG:C1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:503:MAN:O6	5:A:504:MAN:C3	2.69	0.40
1:B:319:TYR:CD1	1:B:319:TYR:N	2.90	0.40
1:B:246:LYS:O	1:B:247:PRO:C	2.65	0.40
1:B:382:GLU:CB	7:B:626:HOH:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	210/212 (99%)	183 (87%)	23 (11%)	4 (2%)	6	19
1	B	207/212 (98%)	173 (84%)	23 (11%)	11 (5%)	1	4
All	All	417/424 (98%)	356 (85%)	46 (11%)	15 (4%)	2	8

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ARG
1	B	271	PRO
1	B	328	LEU
1	B	329	PRO
1	B	238	PRO
1	B	326	LYS
1	B	327	ALA
1	B	298	SER
1	B	357	GLU
1	B	265	ASP
1	A	267	SER
1	B	270	ASP
1	B	282	VAL
1	A	253	ILE

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Mol	Chain	Res	Type
1	A	329	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	196/196 (100%)	152 (78%)	44 (22%)	1	2
1	B	194/196 (99%)	155 (80%)	39 (20%)	1	4
All	All	390/392 (100%)	307 (79%)	83 (21%)	1	3

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	LEU
1	A	248	LYS
1	A	250	THR
1	A	251	LEU
1	A	252	MET
1	A	254	SER
1	A	255	ARG
1	A	262	VAL
1	A	263	VAL
1	A	274	LYS
1	A	278	TYR
1	A	290	LYS
1	A	295	GLN
1	A	299	THR
1	A	301	ARG
1	A	302	VAL
1	A	307	THR
1	A	308	VAL
1	A	314	LEU
1	A	324	SER
1	A	328	LEU
1	A	334	LYS

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Mol	Chain	Res	Type
1	A	336	ILE
1	A	355	ARG
1	A	358	LEU
1	A	359	THR
1	A	361	ASN
1	A	362	GLN
1	A	363	VAL
1	A	370	LYS
1	A	386	GLN
1	A	398	LEU
1	A	406	LEU
1	A	409	LYS
1	A	410	LEU
1	A	411	THR
1	A	414	LYS
1	A	415	SER
1	A	416	ARG
1	A	417	TRP
1	A	424	SER
1	A	435	LYS
1	A	443	LEU
1	A	447	LYS
1	B	250	THR
1	B	252	MET
1	B	253	ILE
1	B	276	ASN
1	B	277	TRP
1	B	279	VAL
1	B	292	ARG
1	B	300	TYR
1	B	309	LEU
1	B	310	LYS
1	B	317	LYS
1	B	320	LYS
1	B	322	LYS
1	B	324	SER
1	B	326	LYS
1	B	332	ILE
1	B	333	GLU
1	B	335	THR
1	B	336	ILE
1	B	337	SER

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Mol	Chain	Res	Type
1	B	338	LYS
1	B	362	GLN
1	B	363	VAL
1	B	365	LEU
1	B	370	LYS
1	B	375	SER
1	B	383	SER
1	B	388	GLU
1	B	389	ASN
1	B	392	LYS
1	B	398	LEU
1	B	406	LEU
1	B	409	LYS
1	B	418	GLN
1	B	419	GLN
1	B	421	ASN
1	B	424	SER
1	B	439	LYS
1	B	443	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	295	GLN
1	A	325	ASN
1	A	347	GLN
1	A	361	ASN
1	A	390	ASN
1	A	433	HIS
1	B	315	ASN
1	B	347	GLN
1	B	362	GLN
1	B	384	ASN
1	B	418	GLN
1	B	438	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	MAN	C	1	2	11,11,12	0.68	0	15,15,17	0.87	0
2	NAG	C	2	2	14,14,15	0.66	0	17,19,21	1.40	2 (11%)

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	MAN	C	1	2	-	2/2/19/22	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C3-C4-C5	4.01	117.50	110.23
2	C	2	NAG	C4-C3-C2	2.82	115.16	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

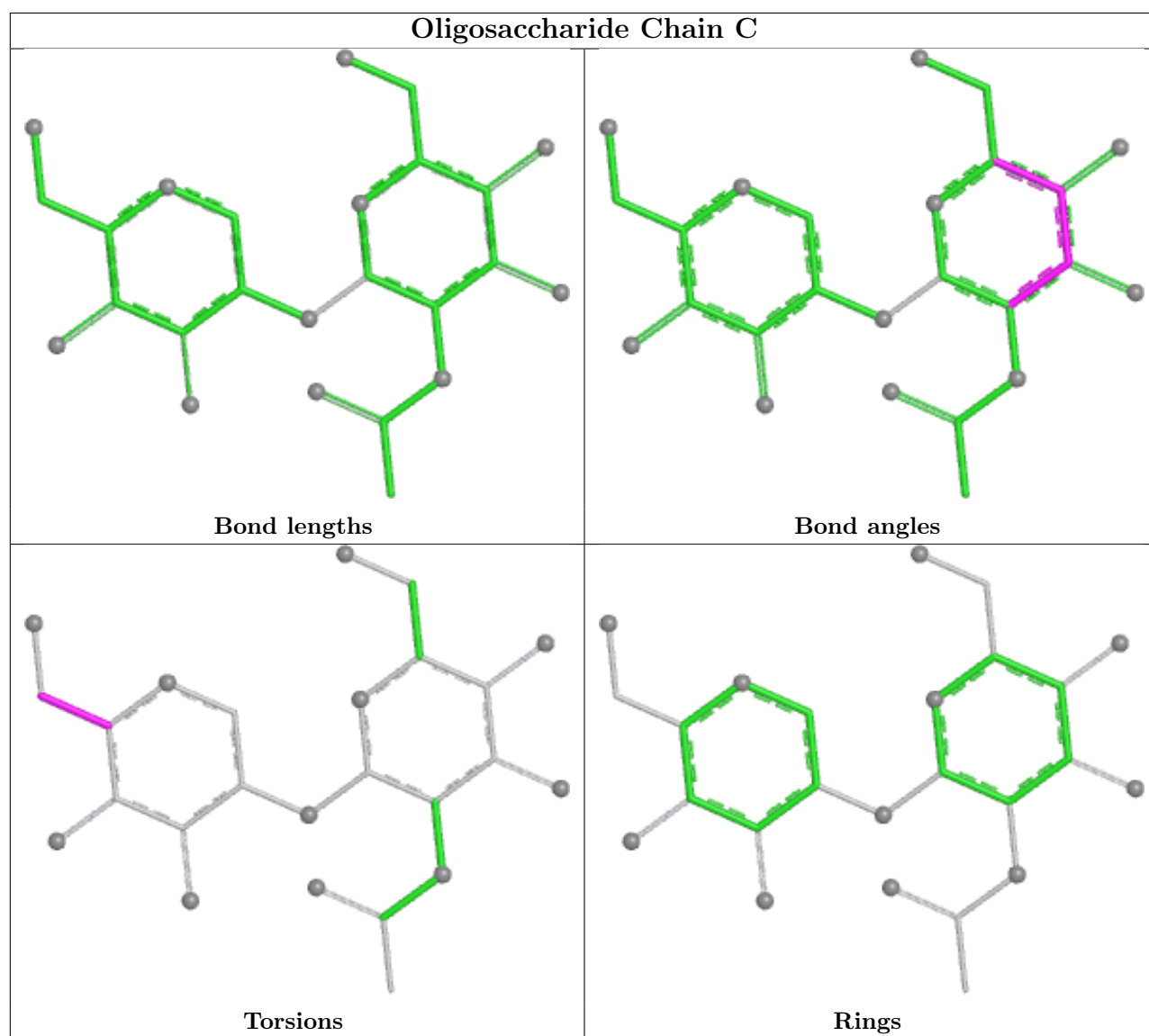
Mol	Chain	Res	Type	Atoms
2	C	1	MAN	O5-C5-C6-O6
2	C	1	MAN	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	MAN	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

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	MAN	A	507	-	11,11,12	0.96	1 (9%)	15,15,17	1.54	3 (20%)
6	GAL	B	506	-	11,11,12	0.76	0	15,15,17	0.98	1 (6%)
3	NAG	B	501	-	14,14,15	0.51	0	17,19,21	0.99	0
5	MAN	B	503	-	11,11,12	0.73	0	15,15,17	1.36	3 (20%)
3	NAG	A	505	-	14,14,15	0.82	0	17,19,21	1.51	3 (17%)
3	NAG	A	502	-	14,14,15	0.89	1 (7%)	17,19,21	1.86	4 (23%)
3	NAG	A	508	-	14,14,15	0.70	0	17,19,21	3.17	8 (47%)
5	MAN	B	504	-	11,11,12	0.54	0	15,15,17	2.00	5 (33%)
6	GAL	A	506	-	11,11,12	0.70	0	15,15,17	2.19	5 (33%)
3	NAG	B	502	-	14,14,15	0.74	1 (7%)	17,19,21	1.14	2 (11%)
3	NAG	A	501	-	14,14,15	0.63	0	17,19,21	1.56	2 (11%)
4	GOL	B	509	-	5,5,5	0.38	0	5,5,5	0.49	0
3	NAG	B	505	-	14,14,15	0.49	0	17,19,21	2.62	7 (41%)
4	GOL	A	510	-	5,5,5	0.39	0	5,5,5	0.37	0
5	MAN	A	503	-	11,11,12	0.65	0	15,15,17	1.37	2 (13%)
5	MAN	A	504	-	11,11,12	0.83	0	15,15,17	1.59	3 (20%)
4	GOL	A	509	-	5,5,5	0.32	0	5,5,5	0.52	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	MAN	A	507	-	-	2/2/19/22	0/1/1/1
6	GAL	B	506	-	-	0/2/19/22	0/1/1/1
3	NAG	B	501	-	-	0/6/23/26	0/1/1/1
5	MAN	B	503	-	-	2/2/19/22	0/1/1/1
3	NAG	A	505	-	-	1/6/23/26	0/1/1/1
3	NAG	A	502	-	-	0/6/23/26	0/1/1/1
3	NAG	A	508	-	-	5/6/23/26	0/1/1/1
5	MAN	B	504	-	-	2/2/19/22	0/1/1/1
6	GAL	A	506	-	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	502	-	-	2/6/23/26	0/1/1/1
3	NAG	A	501	-	-	2/6/23/26	0/1/1/1
4	GOL	B	509	-	-	2/4/4/4	-
3	NAG	B	505	-	-	3/6/23/26	0/1/1/1
4	GOL	A	510	-	-	4/4/4/4	-
5	MAN	A	503	-	-	2/2/19/22	1/1/1/1
5	MAN	A	504	-	-	0/2/19/22	0/1/1/1
4	GOL	A	509	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAG	O5-C1	-2.42	1.39	1.43
3	B	502	NAG	C1-C2	2.16	1.55	1.52
5	A	507	MAN	C2-C3	2.00	1.55	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	NAG	C2-N2-C7	8.42	134.19	122.90
3	A	508	NAG	C1-C2-N2	6.26	120.29	110.43
3	B	505	NAG	C1-O5-C5	5.77	119.92	112.19
6	A	506	GAL	C1-C2-C3	5.34	117.42	109.64
3	B	505	NAG	C1-C2-N2	4.85	118.08	110.43
5	A	504	MAN	C1-C2-C3	4.24	115.82	109.64
3	A	502	NAG	O5-C1-C2	-4.24	104.73	111.29
3	A	508	NAG	C4-C3-C2	-4.09	105.02	111.02
3	A	501	NAG	C3-C4-C5	3.93	117.36	110.23
5	B	504	MAN	C3-C4-C5	3.87	117.24	110.23
5	A	503	MAN	C1-O5-C5	3.77	117.24	112.19
5	A	507	MAN	C1-C2-C3	3.74	115.10	109.64
3	B	505	NAG	C4-C3-C2	-3.69	105.61	111.02
3	A	502	NAG	C1-O5-C5	-3.58	107.38	112.19
3	B	505	NAG	C2-N2-C7	3.54	127.65	122.90
3	A	508	NAG	C8-C7-N2	3.52	121.96	116.12
3	A	505	NAG	C3-C4-C5	3.34	116.30	110.23
6	A	506	GAL	C1-O5-C5	3.34	116.67	112.19
5	B	504	MAN	C2-C3-C4	3.33	116.72	110.86
6	A	506	GAL	O5-C5-C6	3.32	114.13	107.66
3	A	502	NAG	C2-N2-C7	-3.31	118.46	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	505	NAG	O5-C1-C2	-3.25	106.26	111.29
5	B	503	MAN	C2-C3-C4	3.19	116.48	110.86
3	A	505	NAG	O4-C4-C3	-3.01	103.28	110.38
3	B	505	NAG	O5-C5-C4	2.98	118.09	110.83
6	A	506	GAL	C3-C4-C5	-2.88	105.01	110.23
3	A	508	NAG	C1-O5-C5	2.88	116.05	112.19
3	B	502	NAG	C2-N2-C7	2.78	126.62	122.90
5	B	504	MAN	C1-C2-C3	2.72	113.61	109.64
5	B	504	MAN	O2-C2-C3	-2.67	104.62	110.15
5	B	504	MAN	O3-C3-C2	-2.59	104.77	110.05
3	A	502	NAG	C1-C2-N2	-2.59	106.35	110.43
3	B	502	NAG	C4-C3-C2	2.57	114.78	111.02
3	A	508	NAG	O5-C1-C2	-2.51	107.40	111.29
3	A	505	NAG	O5-C1-C2	-2.46	107.49	111.29
5	B	503	MAN	C1-C2-C3	2.45	113.21	109.64
5	A	507	MAN	C2-C3-C4	2.43	115.13	110.86
5	A	504	MAN	C2-C3-C4	2.39	115.06	110.86
5	A	503	MAN	O5-C5-C6	2.37	112.28	107.66
3	A	508	NAG	C3-C4-C5	2.37	114.53	110.23
3	A	501	NAG	C2-N2-C7	2.25	125.92	122.90
5	B	503	MAN	C3-C4-C5	2.24	114.29	110.23
3	A	508	NAG	O7-C7-C8	-2.18	118.17	122.05
5	A	507	MAN	O2-C2-C3	2.15	114.61	110.15
6	B	506	GAL	O5-C1-C2	-2.09	105.81	110.79
3	B	505	NAG	O3-C3-C2	2.05	113.67	109.40
6	A	506	GAL	C6-C5-C4	-2.04	108.00	113.02
5	A	504	MAN	O2-C2-C1	-2.04	104.54	109.22

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	508	NAG	C1-C2-N2-C7
3	B	505	NAG	C1-C2-N2-C7
4	A	509	GOL	O1-C1-C2-C3
4	B	509	GOL	O1-C1-C2-C3
5	B	504	MAN	O5-C5-C6-O6
6	A	506	GAL	C4-C5-C6-O6
5	A	503	MAN	O5-C5-C6-O6
3	A	501	NAG	C4-C5-C6-O6
3	B	505	NAG	O5-C5-C6-O6
5	B	503	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	504	MAN	C4-C5-C6-O6
3	A	508	NAG	O5-C5-C6-O6
6	A	506	GAL	O5-C5-C6-O6
5	A	503	MAN	C4-C5-C6-O6
5	B	503	MAN	C4-C5-C6-O6
3	A	508	NAG	C4-C5-C6-O6
3	A	501	NAG	O5-C5-C6-O6
3	A	508	NAG	C8-C7-N2-C2
3	A	508	NAG	O7-C7-N2-C2
4	A	509	GOL	C1-C2-C3-O3
4	A	510	GOL	O1-C1-C2-C3
4	A	510	GOL	C1-C2-C3-O3
4	A	509	GOL	O1-C1-C2-O2
4	A	510	GOL	O2-C2-C3-O3
4	B	509	GOL	O1-C1-C2-O2
3	B	502	NAG	C4-C5-C6-O6
3	A	505	NAG	O5-C5-C6-O6
4	A	509	GOL	O2-C2-C3-O3
3	B	502	NAG	O5-C5-C6-O6
5	A	507	MAN	C4-C5-C6-O6
4	A	510	GOL	O1-C1-C2-O2
3	B	505	NAG	C4-C5-C6-O6
5	A	507	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	503	MAN	C1-C2-C3-C4-C5-O5

14 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	507	MAN	8	0
6	B	506	GAL	5	0
5	B	503	MAN	2	0
3	A	505	NAG	8	0
3	A	502	NAG	10	0
3	A	508	NAG	4	0
5	B	504	MAN	2	0
6	A	506	GAL	8	0
3	B	502	NAG	3	0
3	A	501	NAG	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	509	GOL	1	0
3	B	505	NAG	3	0
5	A	503	MAN	14	0
5	A	504	MAN	4	0

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	212/212 (100%)	0.28	4 (1%) 66 59	19, 49, 74, 89	1 (0%)
1	B	209/212 (98%)	0.80	30 (14%) 6 5	22, 60, 102, 105	1 (0%)
All	All	421/424 (99%)	0.54	34 (8%) 18 14	19, 54, 99, 105	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	VAL	5.1
1	B	302	VAL	4.7
1	B	275	PHE	4.0
1	B	263	VAL	3.9
1	B	284	VAL	3.5
1	B	273	VAL	3.5
1	B	264	VAL	3.4
1	B	323	VAL	3.3
1	B	325	ASN	3.2
1	B	330	ALA	3.1
1	B	332	ILE	3.1
1	B	363	VAL	3.1
1	B	274	LYS	3.1
1	B	279	VAL	2.9
1	B	300	TYR	2.8
1	B	313	TRP	2.7
1	A	363	VAL	2.6
1	B	285	HIS	2.6
1	B	301	ARG	2.6
1	B	277	TRP	2.5
1	B	328	LEU	2.5
1	B	262	VAL	2.5
1	B	281	GLY	2.4
1	A	254	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	319	TYR	2.3
1	B	304	SER	2.3
1	B	296	TYR	2.2
1	B	267	SER	2.2
1	B	293	GLU	2.2
1	B	282	VAL	2.1
1	B	321	CYS	2.1
1	A	265	ASP	2.0
1	A	443	LEU	2.0
1	B	309	LEU	2.0

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

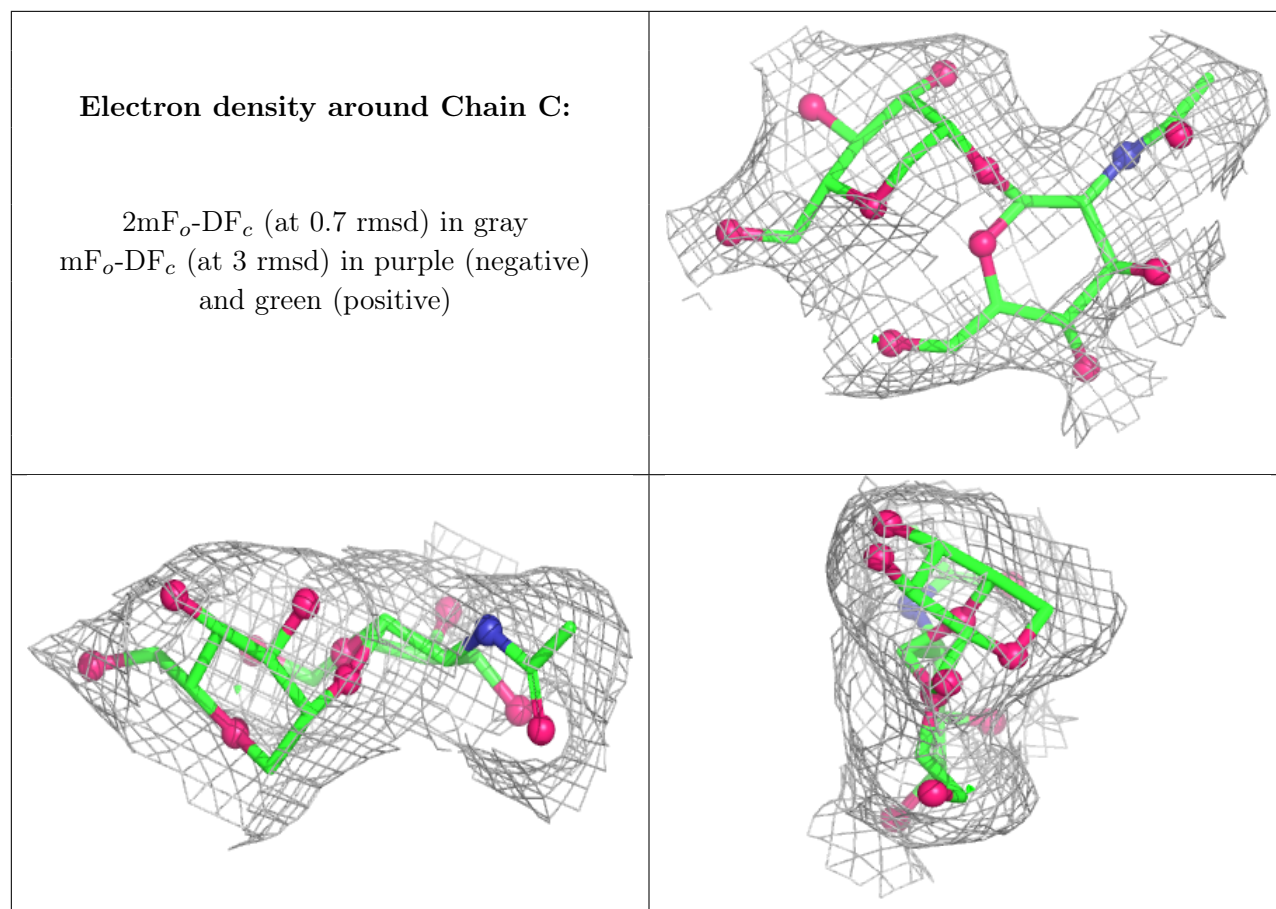
There are no non-standard protein/DNA/RNA residues in this entry.

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	NAG	C	2	14/15	0.77	0.12	78,83,84,85	0
2	MAN	C	1	11/12	0.84	0.11	79,79,79,80	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	B	502	14/15	0.39	0.21	147,149,149,150	0
3	NAG	B	501	14/15	0.51	0.19	144,146,147,147	0
3	NAG	A	508	14/15	0.71	0.12	84,86,87,88	0
5	MAN	B	503	11/12	0.71	0.20	128,129,129,129	0
4	GOL	A	510	6/6	0.73	0.10	79,80,80,80	0
4	GOL	A	509	6/6	0.74	0.11	59,62,63,64	0
6	GAL	A	506	11/12	0.74	0.19	48,51,53,53	11
6	GAL	B	506	11/12	0.74	0.20	54,56,57,57	11
4	GOL	B	509	6/6	0.75	0.10	66,67,68,69	0
5	MAN	B	504	11/12	0.76	0.11	68,70,72,73	0
5	MAN	A	503	11/12	0.79	0.14	59,60,62,63	0
3	NAG	B	505	14/15	0.81	0.12	60,64,66,66	0
5	MAN	A	507	11/12	0.83	0.12	73,74,75,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MAN	A	504	11/12	0.86	0.10	67,68,70,71	0
3	NAG	A	502	14/15	0.87	0.11	59,62,68,68	0
3	NAG	A	501	14/15	0.88	0.10	59,60,62,62	0
3	NAG	A	505	14/15	0.91	0.10	59,62,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.