



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:58 AM UTC

PDB ID : 8UZE / pdb_00008uze
Title : Crystal structure of chimeric bat coronavirus BANAL-20-236 RBD complexed with chimeric mouse ACE2
Authors : Zhang, W.; Shi, K.; Aihara, H.; Li, F.
Deposited on : 2023-11-15
Resolution : 3.03 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:

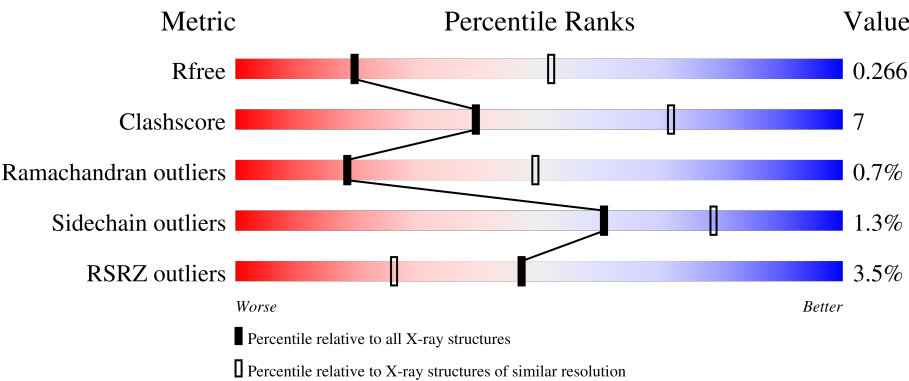
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	597	4% 84% 15% .
1	B	597	3% 77% 21% ..
2	E	217	2% 75% 12% 13%
2	F	217	4% 67% 17% . 13%
3	C	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	G	3	 33% 67%
4	D	2	 50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	NA	A	709	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 12854 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.

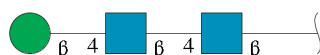
- Molecule 1 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4843	3092	810	913	28			
1	B	593	Total	C	N	O	S	0	0	0
			4838	3089	809	912	28			

- Molecule 2 is a protein called Receptor binding domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	188	Total	C	N	O	S	0	0	0
			1493	962	242	280	9			
2	F	188	Total	C	N	O	S	0	0	0
			1493	962	242	280	9			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

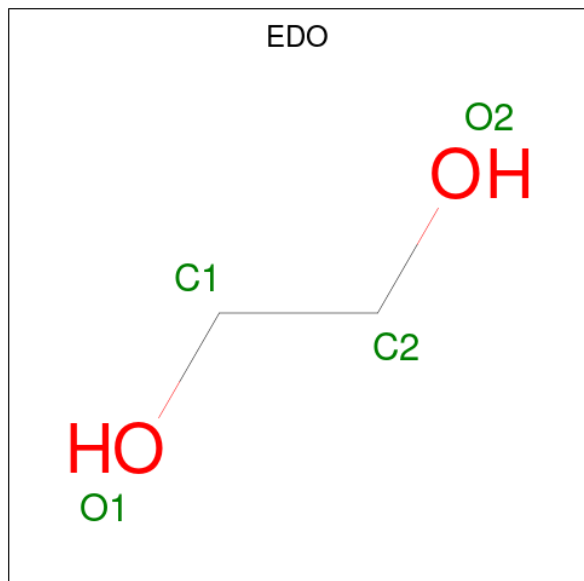
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



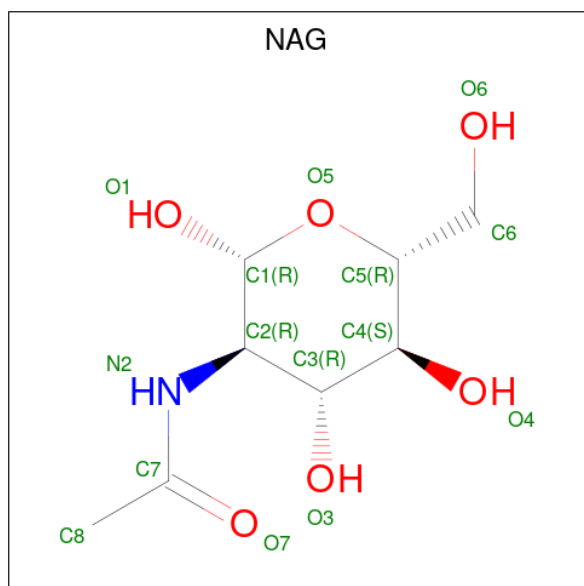
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total 1	Na 1	0	0

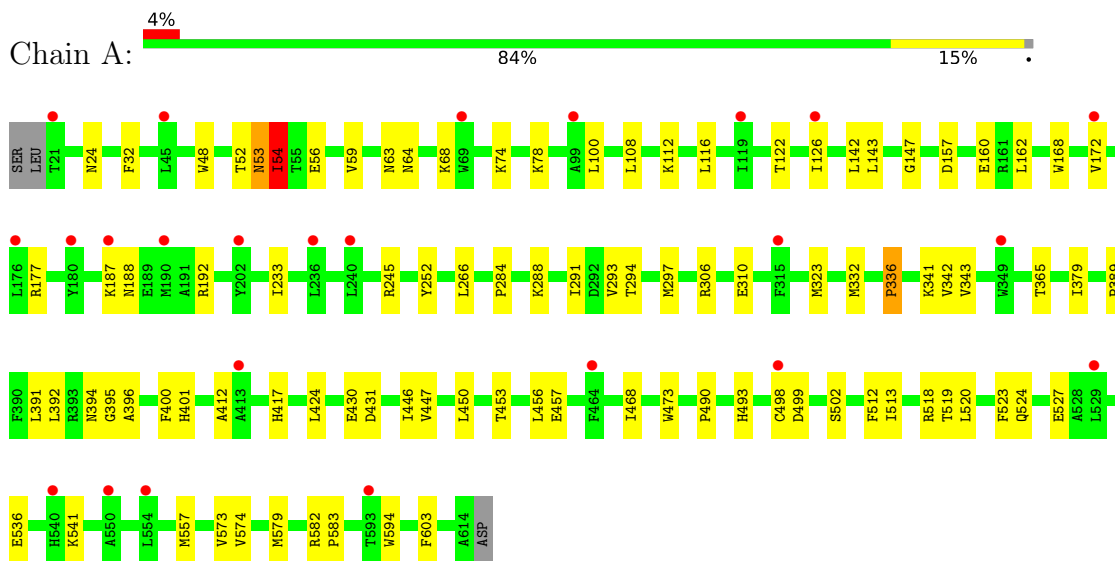
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total 1	O 1	0	0
10	B	1	Total 1	O 1	0	0

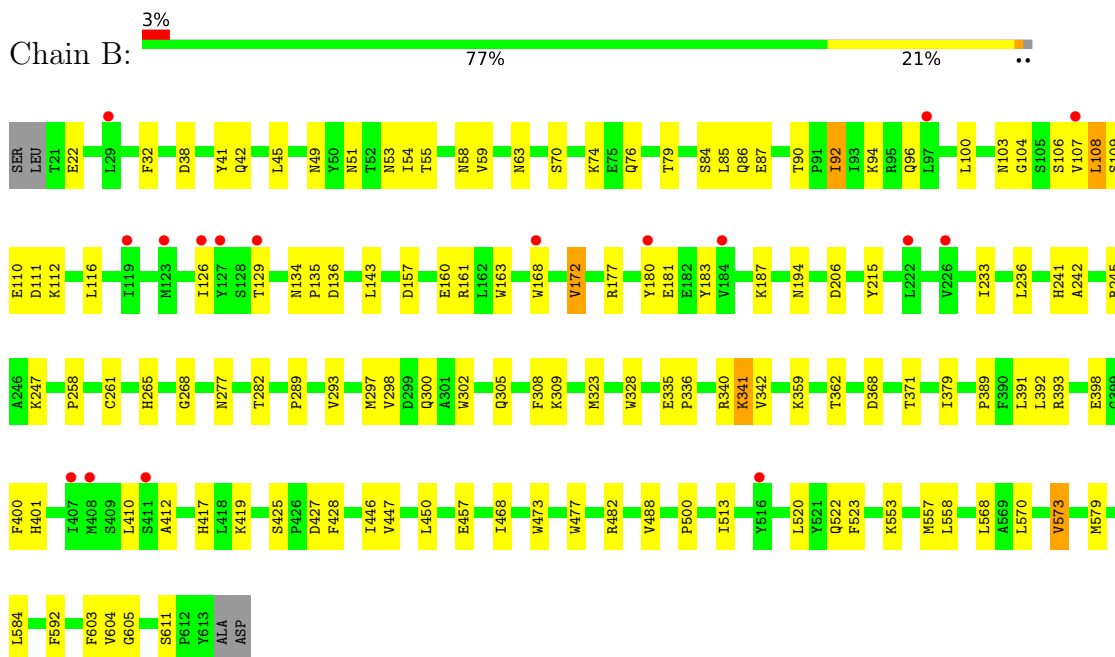
3 Residue-property plots

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: Angiotensin-converting enzyme 2

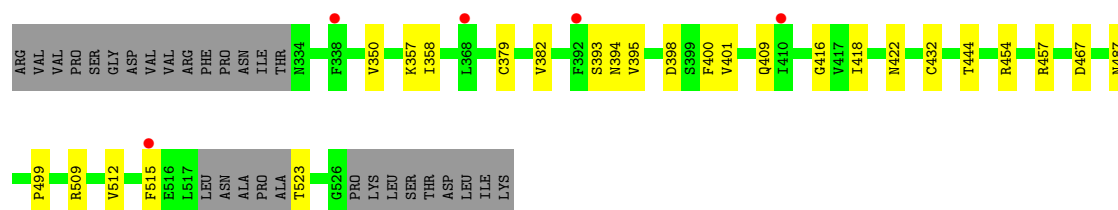


• Molecule 1: Angiotensin-converting enzyme 2



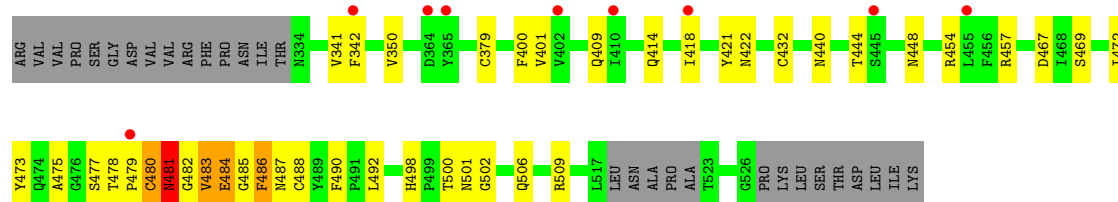
- Molecule 2: Receptor binding domain

Chain E: 



- Molecule 2: Receptor binding domain

Chain F: 



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

Chain C: 



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

Chain G: 



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

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.14Å 118.21Å 107.86Å 90.00° 96.14° 90.00°	Depositor
Resolution (Å)	42.43 – 3.03 42.43 – 3.03	Depositor EDS
% Data completeness (in resolution range)	54.2 (42.43-3.03) 50.8 (42.43-3.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.214 , 0.261 0.246 , 0.266	Depositor DCC
R_{free} test set	993 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å ²)	71.6	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12854	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, EDO, CL, NA, ZN

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	0.09	0/4980	0.27	2/6764 (0.0%)
1	B	0.08	0/4975	0.25	0/6757
2	E	0.08	0/1535	0.23	0/2086
2	F	0.09	0/1535	0.29	0/2086
All	All	0.08	0/13025	0.26	2/17693 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ASN	N-CA-C	-6.41	97.16	110.80
1	A	54	ILE	N-CA-CB	5.54	120.37	111.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4843	0	4613	51	0
1	B	4838	0	4607	74	0
2	E	1493	0	1406	17	0
2	F	1493	0	1407	30	0
3	C	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	39	0	34	0	0
4	D	28	0	25	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	20	0	30	0	0
7	B	12	0	18	0	0
8	A	14	0	13	0	0
8	B	14	0	13	0	0
8	F	14	0	13	0	0
9	A	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
All	All	12854	0	12213	169	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 7.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:478:THR:HG21	2:F:487:ASN:HB2	1.45	0.95
2:F:475:ALA:HB3	2:F:487:ASN:HB3	1.64	0.80
1:A:54:ILE:HD11	1:A:343:VAL:HG23	1.65	0.77
2:F:479:PRO:HG2	2:F:483:VAL:HG21	1.67	0.76
1:A:53:ASN:O	1:A:54:ILE:HG13	1.87	0.75
1:B:336:PRO:HG2	1:B:342:VAL:HG21	1.68	0.73
2:F:409:GLN:HA	2:F:414:GLN:HG3	1.72	0.71
1:B:107:VAL:O	1:B:109:SER:N	2.25	0.69
1:A:59:VAL:O	1:A:63:ASN:ND2	2.27	0.68
1:B:104:GLY:O	1:B:194:ASN:ND2	2.23	0.67
1:A:108:LEU:HD23	1:A:112:LYS:HB3	1.76	0.66
1:B:32:PHE:HD1	1:B:76:GLN:HG3	1.60	0.66
1:A:245:ARG:NH2	1:A:603:PHE:O	2.29	0.65
1:B:59:VAL:O	1:B:63:ASN:ND2	2.29	0.65
1:A:74:LYS:HE3	1:A:78:LYS:HD2	1.79	0.65
1:B:177:ARG:NH1	1:B:181:GLU:OE2	2.30	0.65
1:B:45:LEU:O	1:B:49:ASN:ND2	2.30	0.64
1:B:116:LEU:HD11	1:B:187:LYS:HE2	1.81	0.62
1:B:41:TYR:OH	2:F:500:THR:OG1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:SER:O	1:B:112:LYS:N	2.33	0.61
2:F:480:CYS:O	2:F:482:GLY:N	2.33	0.61
1:B:482:ARG:NH2	1:B:611:SER:OG	2.34	0.61
1:A:54:ILE:HB	1:A:341:LYS:HB3	1.84	0.60
1:B:85:LEU:HG	1:B:86:GLN:H	1.66	0.60
2:F:454:ARG:NH2	2:F:469:SER:O	2.29	0.59
1:A:336:PRO:HG3	1:A:342:VAL:HB	1.84	0.59
1:A:520:LEU:HD22	1:A:579:MET:HE2	1.85	0.59
1:B:85:LEU:HD21	1:B:94:LYS:HE3	1.84	0.59
1:A:323:MET:HE1	1:A:379:ILE:HG21	1.85	0.59
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.85	0.59
1:B:482:ARG:HE	1:B:488:VAL:HG23	1.68	0.58
1:B:241:HIS:CE1	1:B:245:ARG:HH21	2.22	0.58
1:B:520:LEU:HD22	1:B:579:MET:HE2	1.86	0.58
2:F:483:VAL:O	2:F:485:GLY:N	2.34	0.58
1:B:245:ARG:NH2	1:B:605:GLY:O	2.24	0.57
1:A:233:ILE:HD13	1:A:450:LEU:HD13	1.87	0.56
1:B:289:PRO:HB2	1:B:428:PHE:HE1	1.69	0.56
1:A:306:ARG:NH1	1:A:310:GLU:OE1	2.24	0.56
1:A:294:THR:HG23	1:A:365:THR:HA	1.87	0.56
1:B:308:PHE:HE2	1:B:362:THR:HG21	1.71	0.56
1:A:142:LEU:HB3	1:A:147:GLY:HA3	1.89	0.55
1:B:103:ASN:HB3	1:B:106:SER:HB3	1.87	0.55
1:B:54:ILE:HB	1:B:341:LYS:HB3	1.89	0.55
1:B:425:SER:OG	1:B:427:ASP:OD1	2.21	0.55
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.70	0.55
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.89	0.55
1:B:32:PHE:CD1	1:B:76:GLN:HG3	2.42	0.55
2:E:358:ILE:HB	2:E:395:VAL:HB	1.87	0.54
1:A:177:ARG:HD3	1:A:498:CYS:HB2	1.90	0.54
1:B:245:ARG:NH1	1:B:258:PRO:O	2.39	0.54
2:F:341:VAL:HG23	2:F:342:PHE:HD1	1.74	0.53
2:F:473:TYR:O	2:F:488:CYS:HA	2.08	0.53
1:B:446:ILE:HD13	1:B:523:PHE:HZ	1.74	0.53
1:A:430:GLU:OE1	1:A:541:LYS:NZ	2.37	0.53
1:B:305:GLN:O	1:B:309:LYS:HB2	2.09	0.53
1:A:100:LEU:HG	1:A:391:LEU:HD21	1.90	0.53
1:B:233:ILE:HD13	1:B:450:LEU:HD13	1.90	0.52
1:B:55:THR:OG1	1:B:58:ASN:ND2	2.32	0.52
1:A:108:LEU:HB3	1:A:112:LYS:HB2	1.92	0.51
1:B:309:LYS:HD2	1:B:328:TRP:CH2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:PHE:HZ	1:B:570:LEU:HB2	1.76	0.51
1:A:116:LEU:HD11	1:A:187:LYS:HE2	1.92	0.51
1:B:51:ASN:HB3	1:B:359:LYS:HE2	1.93	0.51
2:F:478:THR:HG22	2:F:486:PHE:CE2	2.46	0.51
1:B:410:LEU:HD11	1:B:522:GLN:HE21	1.76	0.51
2:E:379:CYS:HA	2:E:432:CYS:HA	1.92	0.51
1:A:157:ASP:HB3	1:A:160:GLU:HB3	1.93	0.50
1:B:298:VAL:C	1:B:300:GLN:H	2.19	0.50
2:F:401:VAL:HG22	2:F:509:ARG:HG2	1.93	0.50
2:E:357:LYS:HE3	2:E:394:ASN:HD22	1.76	0.50
2:F:484:GLU:H	2:F:484:GLU:CD	2.20	0.50
2:F:421:TYR:HD2	2:F:457:ARG:HB3	1.76	0.50
1:A:291:ILE:HG23	1:A:424:LEU:HD21	1.94	0.49
1:A:64:ASN:O	1:A:68:LYS:HG2	2.12	0.49
2:E:401:VAL:HG22	2:E:509:ARG:HG2	1.93	0.49
1:B:70:SER:O	1:B:74:LYS:HG2	2.12	0.49
1:A:493:HIS:ND1	1:A:499:ASP:OD2	2.46	0.49
1:B:268:GLY:O	1:B:277:ASN:ND2	2.36	0.49
1:A:188:ASN:HB3	1:A:192:ARG:HE	1.78	0.48
1:B:96:GLN:HG2	1:B:392:LEU:HD13	1.95	0.48
1:B:161:ARG:NE	1:B:265:HIS:O	2.44	0.48
2:F:472:ILE:CG2	2:F:488:CYS:HB3	2.43	0.48
1:A:48:TRP:CE2	1:A:52:THR:HG21	2.49	0.48
1:B:323:MET:HE1	1:B:379:ILE:HG21	1.96	0.48
1:A:143:LEU:H	1:A:143:LEU:HD23	1.79	0.48
2:F:457:ARG:NE	2:F:467:ASP:OD2	2.30	0.48
1:B:143:LEU:HD23	1:B:143:LEU:H	1.78	0.47
1:A:288:LYS:NZ	1:A:431:ASP:OD2	2.42	0.47
1:B:523:PHE:CE2	1:B:584:LEU:HD13	2.49	0.47
2:E:444:THR:O	2:E:499:PRO:HD3	2.15	0.47
1:A:284:PRO:HB3	1:A:594:TRP:CH2	2.49	0.46
1:A:168:TRP:NE1	1:A:502:SER:HB2	2.29	0.46
2:F:498:HIS:H	2:F:501:ASN:ND2	2.13	0.46
2:E:393:SER:O	2:E:523:THR:OG1	2.22	0.46
1:B:245:ARG:HH12	1:B:603:PHE:HD2	1.63	0.46
1:B:215:TYR:CZ	1:B:568:LEU:HD23	2.51	0.46
2:E:350:VAL:HG22	2:E:422:ASN:HB3	1.98	0.46
1:A:252:TYR:CZ	1:A:266:LEU:HD22	2.51	0.46
1:B:126:ILE:HA	1:B:129:THR:HG22	1.97	0.46
1:B:157:ASP:HB3	1:B:160:GLU:HB3	1.98	0.46
1:A:389:PRO:HG2	1:A:392:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:482:GLY:O	2:F:483:VAL:C	2.60	0.45
1:A:396:ALA:HB3	1:A:400:PHE:CG	2.52	0.45
1:B:109:SER:O	1:B:111:ASP:N	2.50	0.45
2:F:485:GLY:O	2:F:487:ASN:N	2.50	0.45
1:A:536:GLU:OE1	1:B:419:LYS:NZ	2.37	0.45
1:B:261:CYS:HB2	1:B:488:VAL:HB	1.97	0.45
1:B:206:ASP:OD2	1:B:398:GLU:N	2.46	0.45
1:B:468:ILE:HG22	1:B:473:TRP:HD1	1.81	0.45
1:B:135:PRO:HD3	1:B:163:TRP:HE1	1.82	0.45
1:A:24:ASN:HD21	2:E:487:ASN:CG	2.25	0.44
1:A:412:ALA:HA	1:A:417:HIS:CD2	2.52	0.44
1:B:457:GLU:HG2	1:B:513:ILE:HB	1.98	0.44
2:F:350:VAL:HA	2:F:400:PHE:HB2	1.99	0.44
1:B:557:MET:HE2	1:B:558:LEU:HD23	2.00	0.44
1:A:332:MET:HE1	1:A:342:VAL:HG11	2.00	0.44
2:E:454:ARG:HD3	2:E:457:ARG:HB2	2.00	0.44
1:B:96:GLN:HB3	1:B:391:LEU:HD12	2.00	0.43
1:B:180:TYR:HA	1:B:183:TYR:HB3	2.00	0.43
1:A:168:TRP:CD1	1:A:502:SER:HB2	2.53	0.43
2:F:475:ALA:HB3	2:F:487:ASN:CB	2.42	0.43
1:A:394:ASN:OD1	1:A:395:GLY:N	2.51	0.43
1:B:323:MET:HB2	1:B:328:TRP:NE1	2.33	0.43
2:E:350:VAL:HG21	2:E:418:ILE:HG23	2.00	0.43
1:B:92:ILE:O	1:B:96:GLN:HG3	2.18	0.43
1:A:32:PHE:CE1	1:A:100:LEU:HD21	2.53	0.43
1:B:134:ASN:HD21	1:B:136:ASP:HB2	1.82	0.43
1:A:293:VAL:O	1:A:297:MET:HG2	2.19	0.43
2:F:480:CYS:HA	2:F:488:CYS:SG	2.59	0.43
2:F:502:GLY:O	2:F:506:GLN:HG3	2.19	0.43
2:E:454:ARG:NH1	2:E:467:ASP:O	2.49	0.43
1:A:527:GLU:OE2	1:A:582:ARG:NH2	2.52	0.42
1:B:293:VAL:O	1:B:297:MET:HG3	2.19	0.42
1:B:168:TRP:O	1:B:172:VAL:HG22	2.19	0.42
1:B:389:PRO:O	1:B:393:ARG:HG3	2.20	0.42
2:F:418:ILE:HA	2:F:422:ASN:HD22	1.84	0.42
1:A:122:THR:O	1:A:126:ILE:HG13	2.20	0.42
1:B:368:ASP:HA	1:B:371:THR:OG1	2.20	0.42
2:E:350:VAL:HA	2:E:400:PHE:HB2	2.02	0.42
1:A:456:LEU:HD23	1:A:512:PHE:CD2	2.55	0.42
1:B:340:ARG:HE	4:D:1:NAG:H82	1.85	0.42
2:F:479:PRO:O	2:F:481:ASN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ALA:HB2	1:B:604:VAL:HA	2.00	0.42
1:A:56:GLU:HA	1:A:59:VAL:HG12	2.01	0.42
2:E:409:GLN:CD	2:E:416:GLY:HA3	2.45	0.41
1:A:450:LEU:HD21	1:A:519:THR:HG21	2.02	0.41
2:F:379:CYS:HA	2:F:432:CYS:HA	2.02	0.41
2:F:444:THR:HG22	2:F:448:ASN:HB2	2.02	0.41
1:B:22:GLU:OE2	1:B:90:THR:OG1	2.28	0.41
1:B:32:PHE:CE1	1:B:100:LEU:HD21	2.56	0.41
1:B:412:ALA:HA	1:B:417:HIS:CD2	2.56	0.41
2:E:350:VAL:HG11	2:E:418:ILE:HD12	2.02	0.41
1:B:49:ASN:O	1:B:53:ASN:HB3	2.21	0.41
1:B:85:LEU:C	1:B:87:GLU:H	2.28	0.41
1:B:236:LEU:HD13	1:B:592:PHE:HB2	2.02	0.41
1:B:241:HIS:HE1	1:B:245:ARG:HH21	1.67	0.41
2:E:398:ASP:HB2	2:E:512:VAL:HB	2.02	0.41
2:E:382:VAL:HG11	2:E:515:PHE:HE2	1.86	0.41
1:B:247:LYS:HB2	1:B:282:THR:HG22	2.03	0.40
1:B:477:TRP:CZ3	1:B:500:PRO:HB3	2.55	0.40
1:B:553:LYS:NZ	1:B:573:VAL:HA	2.36	0.40
2:F:440:ASN:OD1	2:F:440:ASN:N	2.50	0.40
2:F:454:ARG:NH1	2:F:467:ASP:O	2.54	0.40
2:F:490:PHE:HE2	2:F:492:LEU:HB2	1.86	0.40
1:A:162:LEU:HD13	1:A:490:PRO:HB2	2.01	0.40
1:A:453:THR:HG23	1:A:512:PHE:CD2	2.56	0.40
2:E:358:ILE:N	2:E:395:VAL:O	2.49	0.40
1:A:468:ILE:HG22	1:A:473:TRP:HD1	1.85	0.40
1:B:38:ASP:O	1:B:42:GLN:HG3	2.21	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	592/597 (99%)	568 (96%)	22 (4%)	2 (0%)	36	67
1	B	591/597 (99%)	560 (95%)	27 (5%)	4 (1%)	18	49
2	E	184/217 (85%)	172 (94%)	12 (6%)	0	100	100
2	F	184/217 (85%)	166 (90%)	13 (7%)	5 (3%)	4	19
All	All	1551/1628 (95%)	1466 (94%)	74 (5%)	11 (1%)	18	49

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ILE
1	B	108	LEU
2	F	480	CYS
2	F	481	ASN
2	F	483	VAL
1	B	84	SER
1	B	110	GLU
1	B	302	TRP
2	F	484	GLU
2	F	486	PHE
1	A	336	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	523/526 (99%)	516 (99%)	7 (1%)	61	79
1	B	523/526 (99%)	514 (98%)	9 (2%)	53	75
2	E	163/190 (86%)	163 (100%)	0	100	100
2	F	163/190 (86%)	161 (99%)	2 (1%)	63	79
All	All	1372/1432 (96%)	1354 (99%)	18 (1%)	61	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	VAL
1	A	401	HIS
1	A	447	VAL
1	A	518	ARG
1	A	557	MET
1	A	573	VAL
1	A	574	VAL
1	B	79	THR
1	B	92	ILE
1	B	108	LEU
1	B	172	VAL
1	B	335	GLU
1	B	341	LYS
1	B	401	HIS
1	B	447	VAL
1	B	573	VAL
2	F	477	SER
2	F	481	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	30	ASN
1	A	58	ASN
1	A	64	ASN
1	A	239	HIS
1	A	330	ASN
1	A	417	HIS
1	A	599	ASN
1	B	49	ASN
1	B	76	GLN
1	B	345	HIS
1	B	417	HIS
1	B	522	GLN
1	B	535	HIS
1	B	552	GLN
2	F	501	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	C	1	3,1	14,14,15	0.43	0	17,19,21	1.58	2 (11%)
3	NAG	C	2	3	14,14,15	0.53	0	17,19,21	0.81	0
3	BMA	C	3	3	11,11,12	0.40	0	15,15,17	0.71	0
4	NAG	D	1	4,1	14,14,15	0.36	0	17,19,21	0.54	0
4	NAG	D	2	4	14,14,15	0.26	0	17,19,21	0.42	0
3	NAG	G	1	3,1	14,14,15	0.25	0	17,19,21	0.64	0
3	NAG	G	2	3	14,14,15	0.50	0	17,19,21	0.94	1 (5%)
3	BMA	G	3	3	11,11,12	0.52	0	15,15,17	0.94	1 (6%)

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
3	NAG	C	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-C2-N2	4.92	118.18	110.43
3	C	1	NAG	C2-N2-C7	3.27	127.28	122.90
3	G	3	BMA	C1-O5-C5	2.89	116.05	112.19
3	G	2	NAG	C2-N2-C7	2.67	126.48	122.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

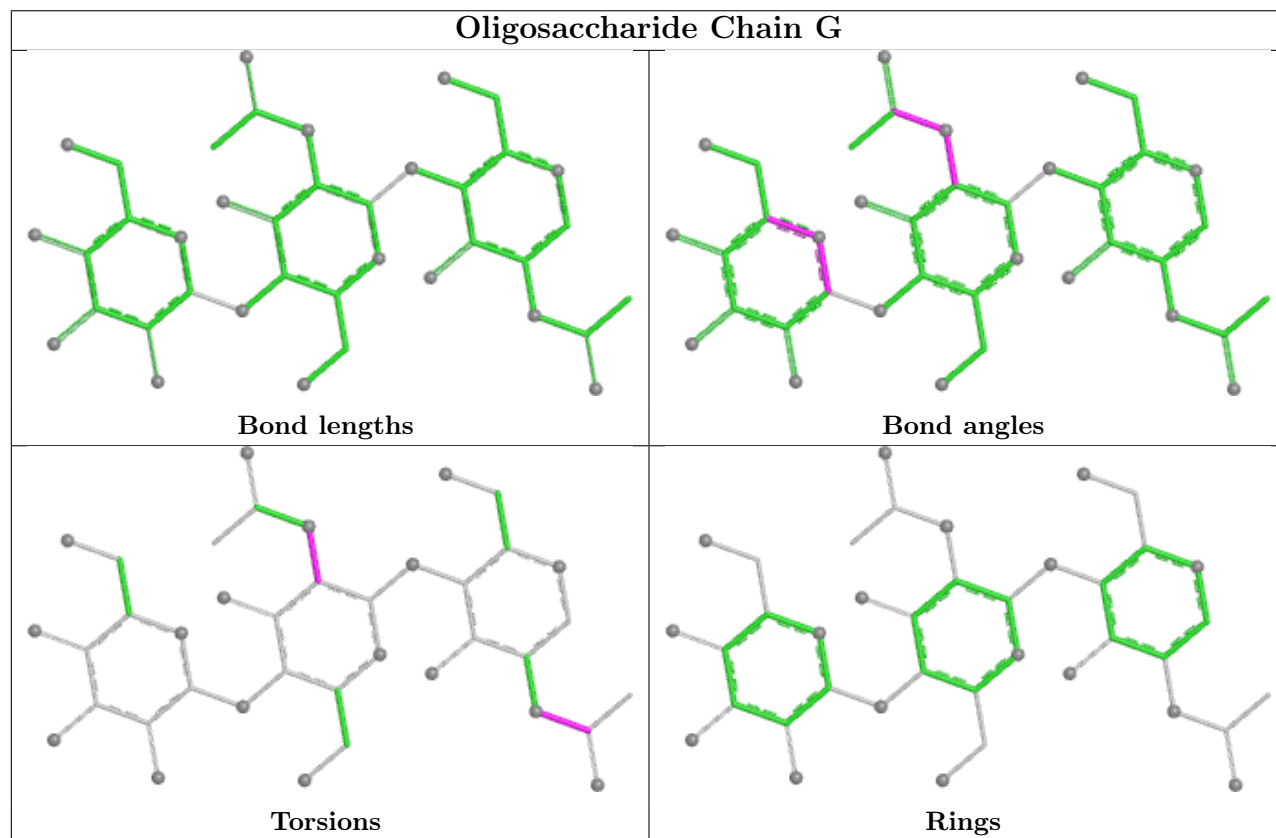
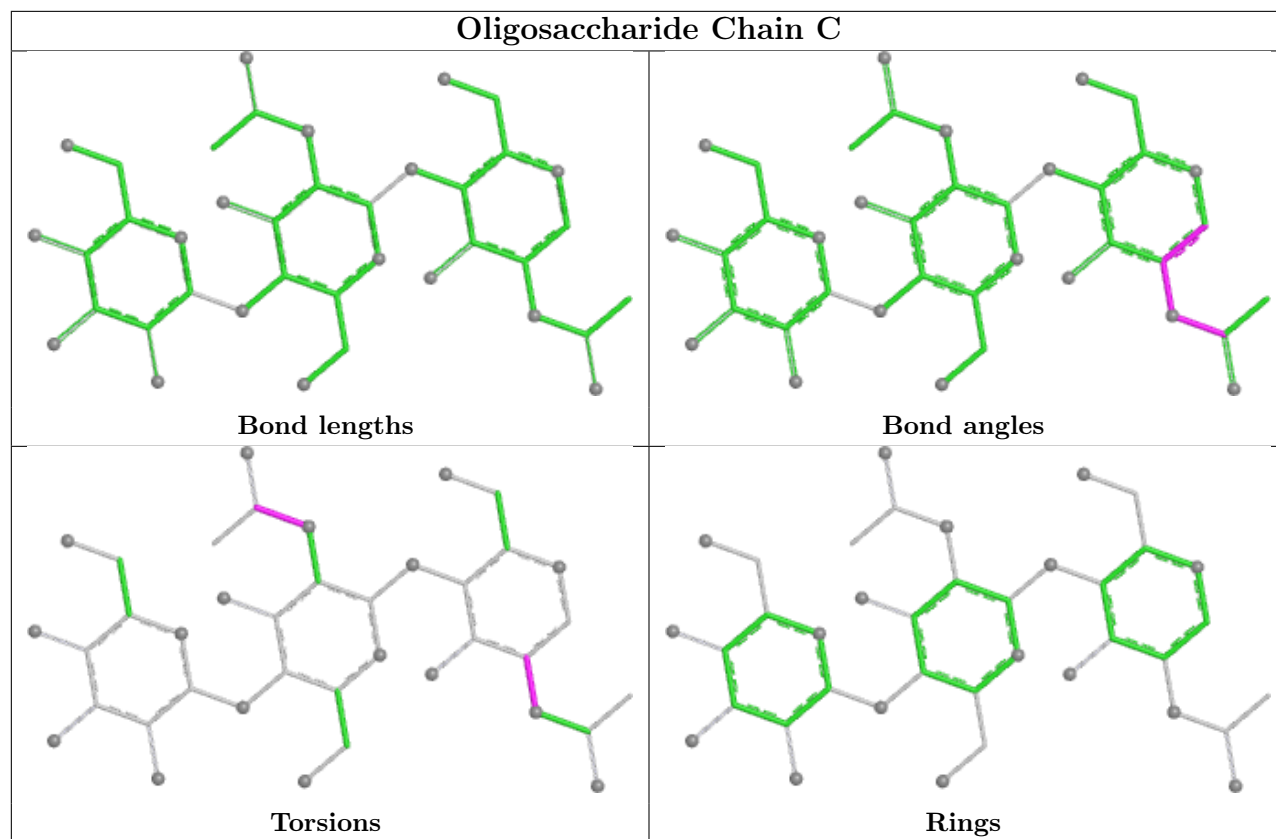
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C3-C2-N2-C7
3	G	2	NAG	C1-C2-N2-C7
4	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6

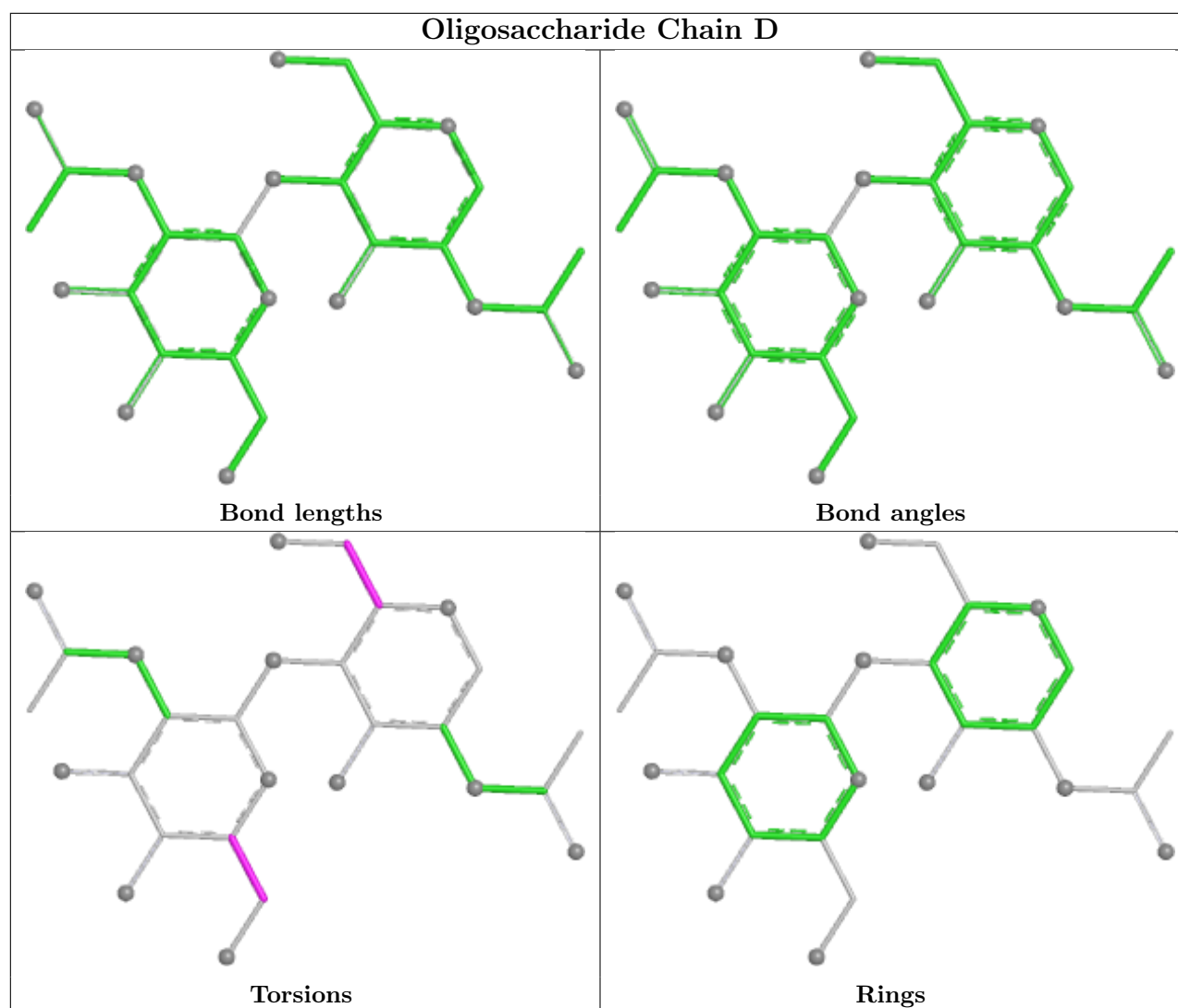
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	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](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	EDO	B	703	-	3,3,3	0.43	0	2,2,2	0.38	0
7	EDO	A	707	-	3,3,3	0.44	0	2,2,2	0.32	0
7	EDO	A	706	-	3,3,3	0.44	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	B	704	-	3,3,3	0.42	0	2,2,2	0.39	0
7	EDO	B	705	-	3,3,3	0.44	0	2,2,2	0.37	0
7	EDO	A	708	-	3,3,3	0.44	0	2,2,2	0.35	0
7	EDO	A	703	-	3,3,3	0.44	0	2,2,2	0.35	0
8	NAG	B	706	1	14,14,15	0.24	0	17,19,21	0.43	0
8	NAG	F	601	2	14,14,15	0.33	0	17,19,21	0.50	0
7	EDO	A	705	-	3,3,3	0.43	0	2,2,2	0.39	0
8	NAG	A	704	1	14,14,15	0.38	0	17,19,21	0.83	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	703	-	-	0/1/1/1	-
7	EDO	A	707	-	-	0/1/1/1	-
7	EDO	A	706	-	-	0/1/1/1	-
7	EDO	B	704	-	-	0/1/1/1	-
7	EDO	B	705	-	-	0/1/1/1	-
7	EDO	A	708	-	-	0/1/1/1	-
7	EDO	A	703	-	-	0/1/1/1	-
8	NAG	B	706	1	-	0/6/23/26	0/1/1/1
8	NAG	F	601	2	-	1/6/23/26	0/1/1/1
7	EDO	A	705	-	-	0/1/1/1	-
8	NAG	A	704	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	704	NAG	C1-O5-C5	2.82	115.96	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	594/597 (99%)	0.38	24 (4%) 42 23	52, 97, 150, 214	0
1	B	593/597 (99%)	0.25	17 (2%) 53 30	38, 83, 148, 222	0
2	E	188/217 (86%)	0.18	5 (2%) 56 32	51, 84, 147, 200	0
2	F	188/217 (86%)	0.35	9 (4%) 35 18	70, 105, 153, 176	0
All	All	1563/1628 (96%)	0.30	55 (3%) 47 26	38, 92, 151, 222	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	455	LEU	4.4
1	A	550	ALA	3.7
2	E	368	LEU	3.7
1	B	127	TYR	3.6
1	A	554	LEU	3.6
1	A	498	CYS	3.5
1	A	176	LEU	3.4
2	E	410	ILE	3.2
1	A	464	PHE	3.1
1	A	180	TYR	2.9
1	A	349	TRP	2.8
1	B	129	THR	2.8
1	A	172	VAL	2.8
2	F	364	ASP	2.7
1	B	123	MET	2.7
2	E	338	PHE	2.7
1	B	226	VAL	2.7
1	A	69	TRP	2.6
1	B	408	MET	2.6
1	B	119	ILE	2.6
2	F	402	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	168	TRP	2.5
1	B	516	TYR	2.5
1	A	529	LEU	2.5
2	F	445	SER	2.5
1	A	240	LEU	2.5
1	B	126	ILE	2.5
1	B	97	LEU	2.5
1	A	593	THR	2.4
2	E	515	PHE	2.4
1	A	45	LEU	2.4
1	A	99	ALA	2.4
1	B	407	ILE	2.4
1	B	29	LEU	2.4
2	F	418	ILE	2.3
1	B	222	LEU	2.3
1	B	411	SER	2.3
1	A	190	MET	2.2
1	B	180	TYR	2.2
2	F	365	TYR	2.2
1	B	107	VAL	2.2
2	F	410	ILE	2.2
1	A	187	LYS	2.2
1	A	315	PHE	2.2
1	B	184	VAL	2.2
1	A	540	HIS	2.1
1	A	236	LEU	2.1
1	A	413	ALA	2.1
2	E	392	PHE	2.1
2	F	342	PHE	2.1
2	F	479	PRO	2.1
1	A	202	TYR	2.0
1	A	119	ILE	2.0
1	A	21	THR	2.0
1	A	126	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

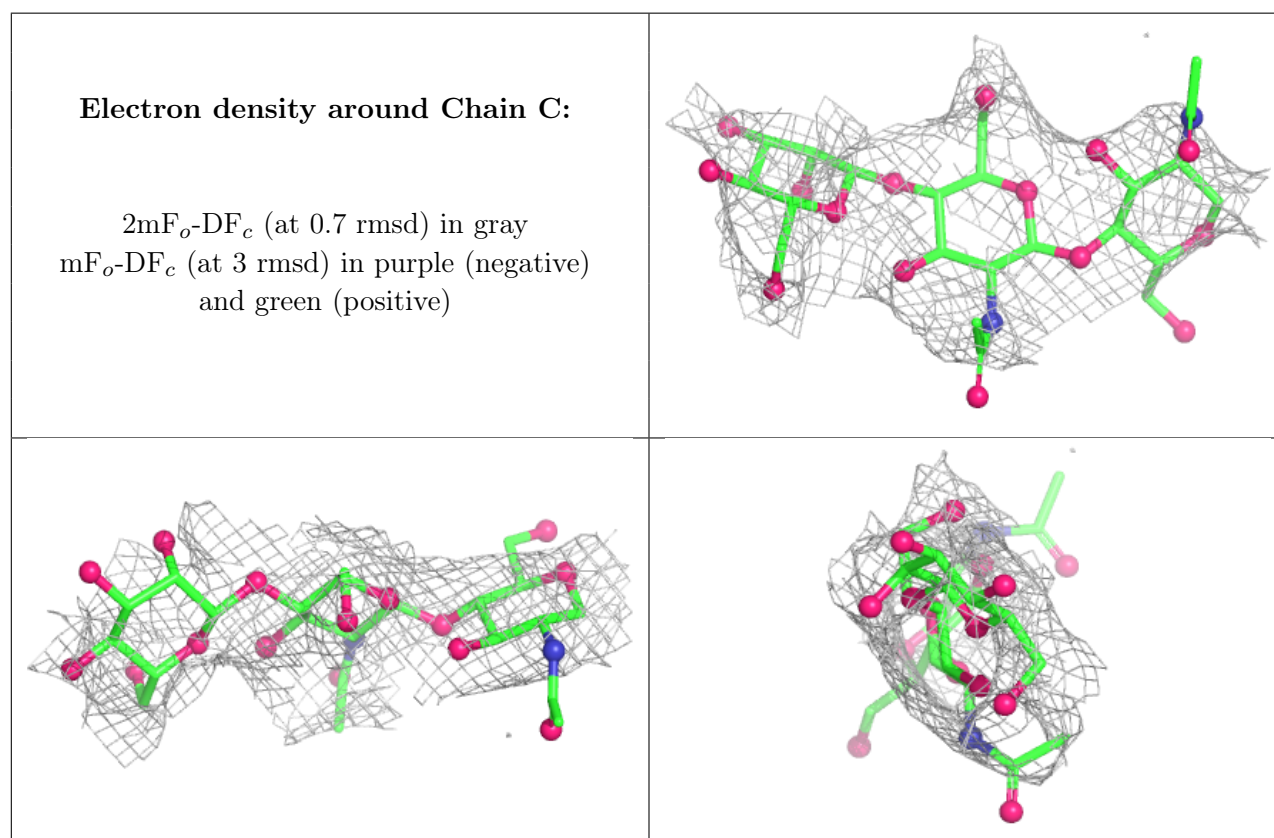
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

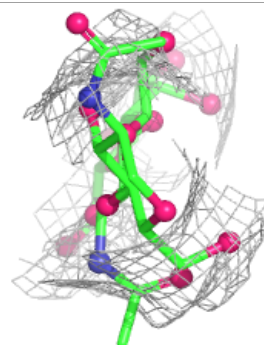
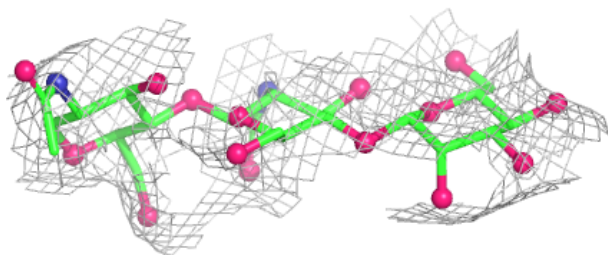
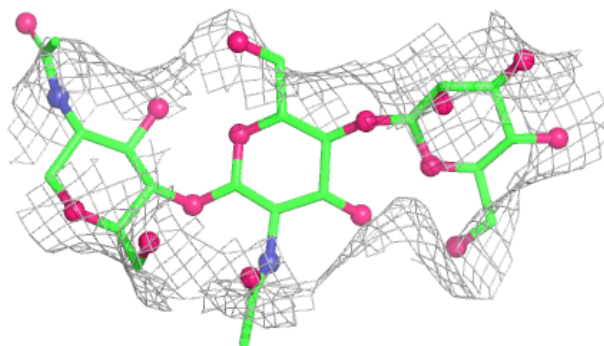
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	129,142,146,149	0
3	NAG	C	2	14/15	-	-	132,149,153,159	0
3	BMA	C	3	11/12	-	-	147,163,169,169	0
3	BMA	G	3	11/12	0.58	0.09	102,114,128,131	0
3	NAG	G	2	14/15	0.78	0.08	97,115,117,121	0
3	NAG	G	1	14/15	0.78	0.10	94,102,109,113	0
4	NAG	D	1	14/15	-	-	108,127,133,134	0
4	NAG	D	2	14/15	-	-	106,143,159,161	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.

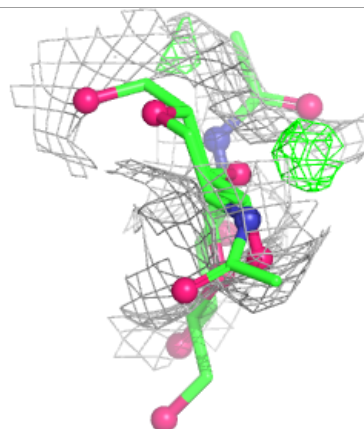
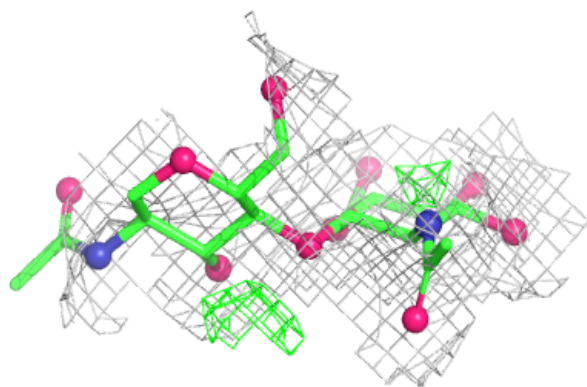
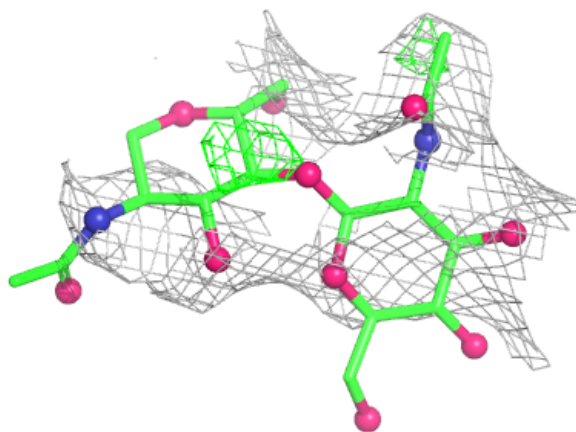


Electron density around Chain G:

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

**Electron density around Chain D:**

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



6.4 Ligands

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
7	EDO	A	706	4/4	0.31	0.18	70,71,72,77	0
9	NA	A	709	1/1	0.62	0.43	66,66,66,66	0
8	NAG	B	706	14/15	0.66	0.11	135,149,158,159	0
7	EDO	B	704	4/4	0.66	0.14	48,56,64,67	0
7	EDO	A	707	4/4	0.68	0.12	47,48,54,63	0
7	EDO	A	705	4/4	0.69	0.15	61,62,63,71	0
7	EDO	A	703	4/4	0.79	0.12	39,40,51,51	0
8	NAG	A	704	14/15	0.79	0.10	94,103,114,118	0
8	NAG	F	601	14/15	0.81	0.09	75,96,110,112	0
7	EDO	B	705	4/4	0.86	0.12	42,52,53,65	0
6	CL	A	702	1/1	0.88	0.08	72,72,72,72	0
6	CL	B	702	1/1	0.89	0.07	63,63,63,63	0
7	EDO	A	708	4/4	0.89	0.10	61,65,65,69	0
7	EDO	B	703	4/4	0.90	0.12	39,50,60,65	0
5	ZN	B	701	1/1	0.94	0.07	61,61,61,61	0
5	ZN	A	701	1/1	0.96	0.10	98,98,98,98	0

6.5 Other polymers

There are no such residues in this entry.