



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2022 – 04:05 PM EDT

PDB ID : 7UFL
Title : Crystal structure of chimeric omicron RBD (strain BA.2) complexed with chimeric mouse ACE2
Authors : Zhang, W.; Shi, K.; Geng, Q.; Ye, G.; Aihara, H.; Li, F.
Deposited on : 2022-03-22
Resolution : 2.84 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

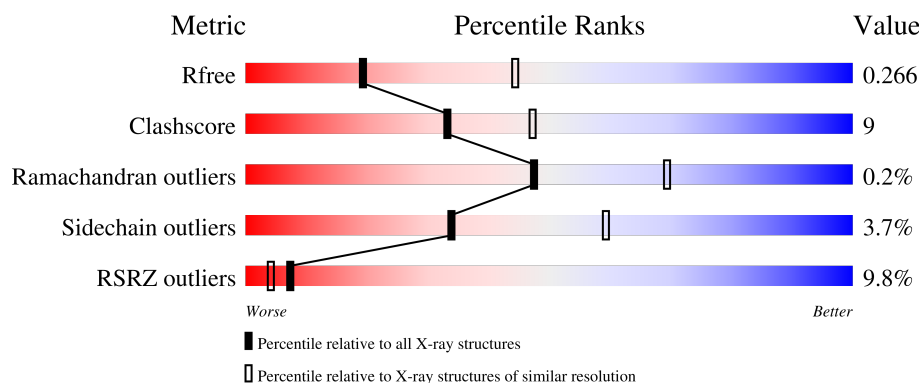
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	<div> <div>9%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>
1	B	597	<div> <div>8%</div> <div>77%</div> <div>21%</div> <div>..</div> </div>
2	E	217	<div> <div>10%</div> <div>73%</div> <div>12%</div> <div>.</div> <div>13%</div> </div>
2	F	217	<div> <div>14%</div> <div>62%</div> <div>24%</div> <div>.</div> <div>12%</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain	
4	D	3		
4	J	3		

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12955 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	595	Total	C	N	O	S	0	1	0
			4860	3103	813	916	28			
1	B	593	Total	C	N	O	S	0	0	0
			4838	3089	809	912	28			

- Molecule 2 is a protein called Spike protein S1.

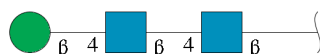
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	188	Total	C	N	O	S	0	1	0
			1504	968	249	277	10			
2	F	190	Total	C	N	O	S	0	0	0
			1517	977	252	279	9			

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

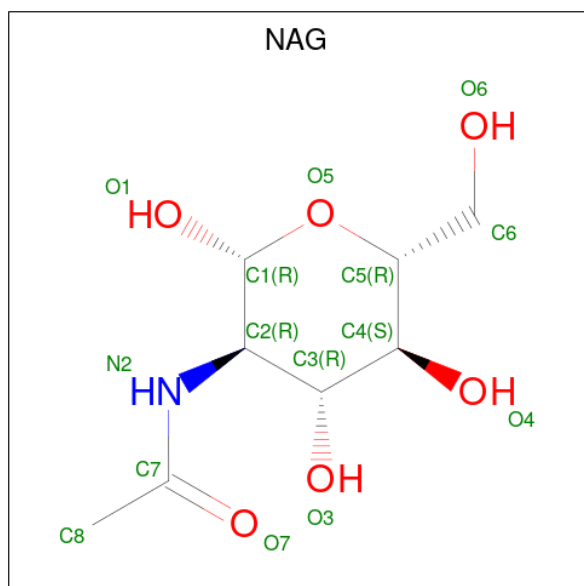
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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 (three-letter code: 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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



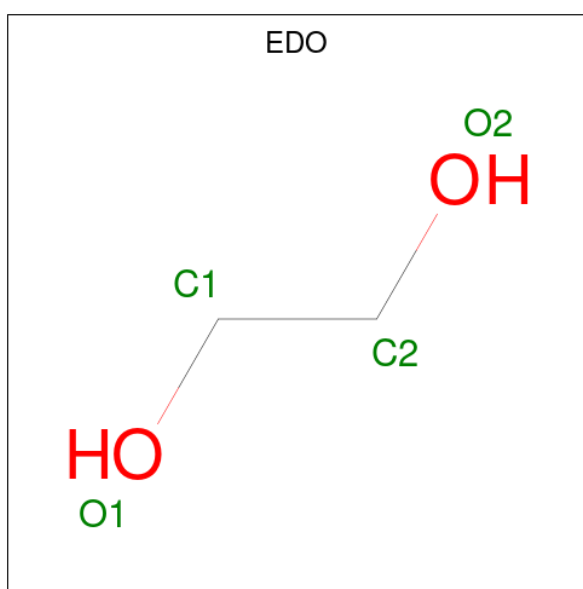
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

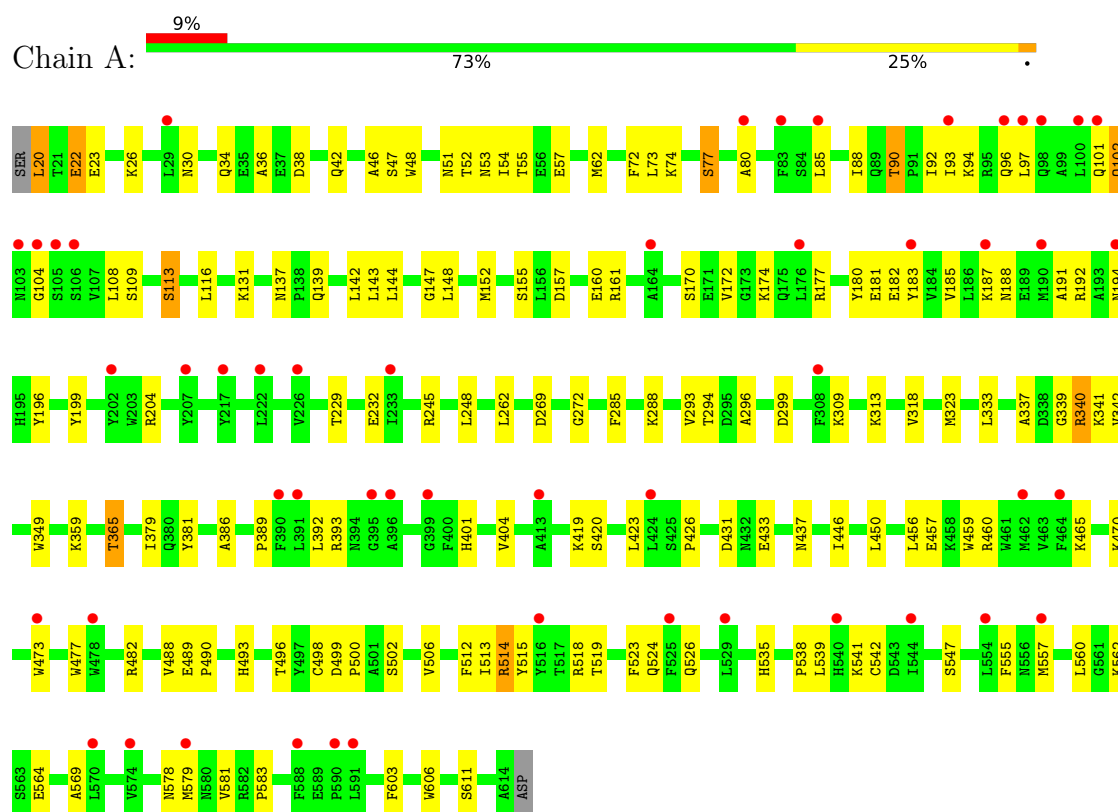
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	9	Total	O	0	0
			9	9		
9	B	9	Total	O	0	0
			9	9		
9	E	1	Total	O	0	0
			1	1		
9	F	1	Total	O	0	0
			1	1		

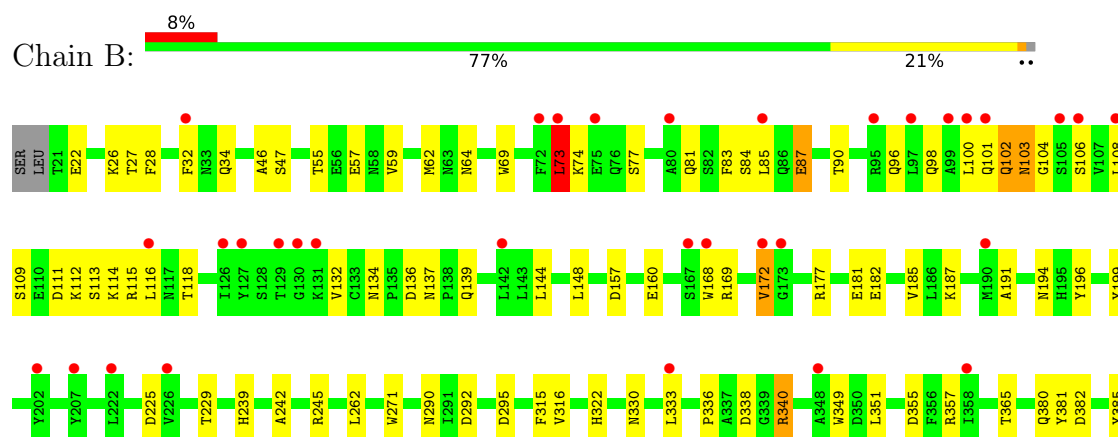
3 Residue-property plots

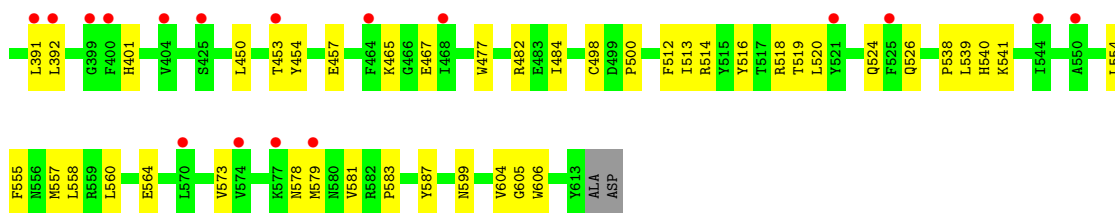
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

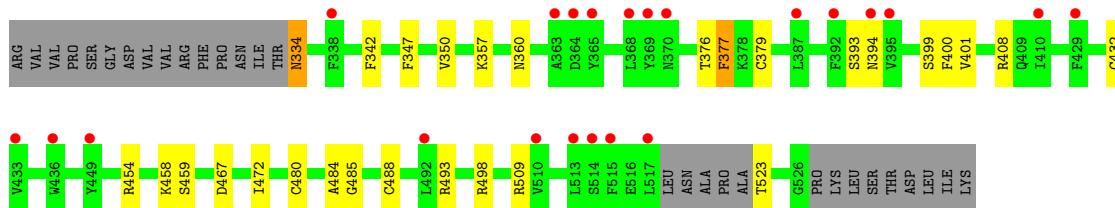
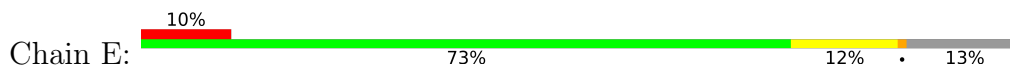


• Molecule 1: Angiotensin-converting enzyme 2

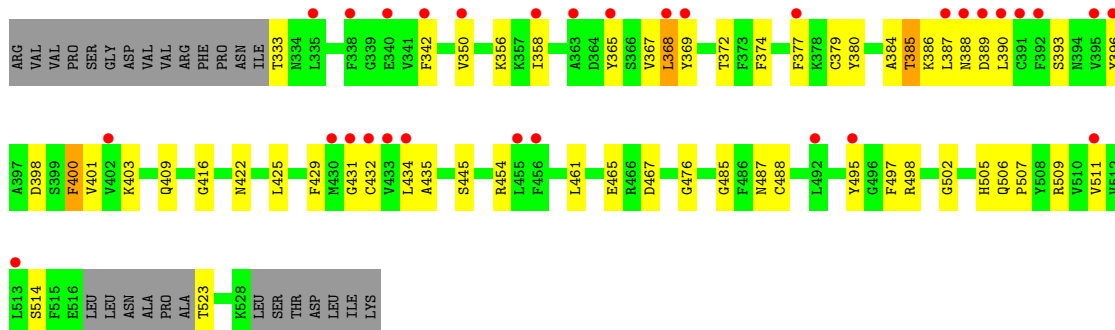




• Molecule 2: Spike protein S1



• Molecule 2: Spike protein S1



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.05Å 118.47Å 110.84Å 90.00° 93.65° 90.00°	Depositor
Resolution (Å)	30.39 – 2.84 80.85 – 2.84	Depositor EDS
% Data completeness (in resolution range)	54.5 (30.39-2.84) 51.0 (80.85-2.84)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.46 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.214 , 0.271 0.219 , 0.266	Depositor DCC
R_{free} test set	1341 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12955	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: BMA, EDO, NAG, CL, 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	0.26	0/4997	0.48	1/6787 (0.0%)
1	B	0.24	0/4975	0.48	1/6757 (0.0%)
2	E	0.26	0/1546	0.53	0/2099
2	F	0.29	0/1560	0.54	1/2117 (0.0%)
All	All	0.26	0/13078	0.49	3/17760 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	LEU	CA-CB-CG	6.24	129.66	115.30
2	F	368	LEU	CB-CG-CD2	-6.18	100.50	111.00
1	A	299	ASP	CB-CG-OD2	-6.05	112.86	118.30

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	4860	0	4630	87	0
1	B	4838	0	4607	73	0
2	E	1504	0	1422	16	0
2	F	1517	0	1447	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	25	1	0
4	D	39	0	34	2	0
4	J	39	0	34	0	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	28	0	26	2	0
7	B	14	0	13	0	0
7	E	14	0	13	1	0
7	F	14	0	13	0	0
8	A	20	0	30	0	0
8	B	16	0	24	1	0
9	A	9	0	0	1	0
9	B	9	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
All	All	12955	0	12318	217	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 9.

All (217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LYS:HE3	1:A:426:PRO:HA	1.48	0.92
1:B:74:LYS:HE3	1:B:106:SER:HB3	1.51	0.88
1:B:340:ARG:HH21	3:C:1:NAG:H81	1.50	0.76
1:A:538:PRO:HD2	1:A:541:LYS:HD3	1.69	0.74
1:B:182:GLU:HA	1:B:185:VAL:HG12	1.70	0.73
1:A:293:VAL:HG21	1:A:423:LEU:HB3	1.73	0.70
2:F:342:PHE:HE2	2:F:368:LEU:HD21	1.56	0.70
2:F:342:PHE:HE2	2:F:368:LEU:CD2	2.04	0.69
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.75	0.69
1:A:26:LYS:O	1:A:30:ASN:ND2	2.26	0.68
1:B:104:GLY:O	1:B:194:ASN:ND2	2.26	0.68
1:B:85:LEU:HD21	1:B:98:GLN:HG2	1.76	0.68
1:A:54:ILE:HB	1:A:341:LYS:HB2	1.76	0.67
1:B:245:ARG:NH2	1:B:605:GLY:O	2.27	0.67
1:B:336:PRO:HB2	1:B:340:ARG:HD3	1.77	0.66
1:B:74:LYS:NZ	1:B:103:ASN:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:LEU:HD22	1:B:579:MET:HE2	1.78	0.65
1:A:46:ALA:HB1	1:A:62:MET:HA	1.78	0.64
2:F:425:LEU:HD22	2:F:429:PHE:CD2	2.32	0.64
1:A:560:LEU:HD21	1:A:564:GLU:HB2	1.81	0.63
1:A:38:ASP:O	1:A:42:GLN:HG2	2.00	0.61
2:F:454:ARG:NH1	2:F:467:ASP:O	2.33	0.61
2:E:334:ASN:OD1	2:E:334:ASN:N	2.33	0.61
1:A:293:VAL:HG22	1:A:296:ALA:HB3	1.84	0.60
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.83	0.60
1:B:69:TRP:O	1:B:73:LEU:HD13	2.01	0.59
1:B:22:GLU:OE2	1:B:90:THR:OG1	2.18	0.59
2:F:485:GLY:N	2:F:488:CYS:O	2.30	0.59
1:A:460:ARG:HD3	1:A:506:VAL:HG13	1.85	0.59
2:F:342:PHE:HE1	2:F:511:VAL:HB	1.67	0.59
1:A:104:GLY:O	1:A:194:ASN:ND2	2.32	0.59
2:F:365:TYR:HB2	2:F:388:ASN:HA	1.85	0.58
1:A:232:GLU:HB2	1:A:581:VAL:HG11	1.85	0.58
2:F:387:LEU:HA	2:F:390:LEU:HD12	1.86	0.58
1:A:323:MET:HE1	1:A:379:ILE:HG21	1.85	0.58
1:A:180:TYR:HA	1:A:183:TYR:HB3	1.86	0.57
1:A:53:ASN:HA	1:A:340:ARG:HG2	1.87	0.56
1:B:187:LYS:HD3	1:B:199:TYR:CE2	2.40	0.56
1:B:46:ALA:HB1	1:B:62:MET:HA	1.87	0.56
1:B:112:LYS:HA	1:B:115:ARG:HB3	1.87	0.56
2:F:425:LEU:HD22	2:F:429:PHE:CE2	2.41	0.56
1:B:229:THR:OG1	1:B:581:VAL:HB	2.06	0.55
2:F:342:PHE:HE1	2:F:511:VAL:CB	2.19	0.55
1:B:116:LEU:HD11	1:B:187:LYS:HG3	1.88	0.55
1:B:482:ARG:O	1:B:606:TRP:NE1	2.40	0.55
1:B:28:PHE:CD2	1:B:83:PHE:HE1	2.24	0.54
2:E:493:ARG:HG3	2:E:493:ARG:HH11	1.71	0.54
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.72	0.54
2:E:472:ILE:HD12	2:E:484:ALA:HB2	1.89	0.54
2:E:454:ARG:NH1	2:E:467:ASP:O	2.37	0.54
2:F:393:SER:O	2:F:523:THR:OG1	2.26	0.54
1:B:144:LEU:HA	1:B:148:LEU:HB2	1.89	0.53
1:A:288:LYS:HE3	1:A:433:GLU:HB2	1.90	0.53
1:B:114:LYS:O	1:B:118:THR:N	2.42	0.53
1:A:420:SER:HB2	4:D:1:NAG:H61	1.90	0.53
2:E:393:SER:O	2:E:523:THR:OG1	2.27	0.53
1:A:52:THR:HA	1:A:342:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:VAL:HG21	1:A:611:SER:HA	1.91	0.52
1:A:182:GLU:HA	1:A:185:VAL:HG12	1.91	0.52
1:A:339:GLY:O	1:A:340:ARG:HB2	2.09	0.52
1:A:562:LYS:NZ	9:A:802:HOH:O	2.37	0.52
1:B:560:LEU:HD13	1:B:564:GLU:HG3	1.90	0.52
2:F:445:SER:O	2:F:498:ARG:NH1	2.43	0.52
2:E:401:VAL:HG22	2:E:509:ARG:HG2	1.92	0.52
2:F:350:VAL:HG23	2:F:400:PHE:HD2	1.75	0.52
1:B:524:GLN:HG2	1:B:583:PRO:HG2	1.92	0.51
1:A:245:ARG:NH2	1:A:603:PHE:O	2.43	0.51
1:B:290:ASN:ND2	1:B:292:ASP:HB3	2.26	0.51
2:F:400:PHE:N	2:F:400:PHE:CD1	2.78	0.51
1:A:97:LEU:O	1:A:101:GLN:HG2	2.10	0.51
1:A:294:THR:HG23	1:A:365:THR:HA	1.92	0.51
1:A:470:LYS:HA	1:A:473:TRP:CD1	2.45	0.51
1:B:229:THR:HG23	1:B:516:TYR:OH	2.12	0.50
2:F:350:VAL:HG23	2:F:400:PHE:CD2	2.47	0.50
1:A:560:LEU:HD22	1:A:569:ALA:HB2	1.92	0.50
2:F:367:VAL:O	2:F:368:LEU:HB2	2.12	0.50
1:B:77:SER:HA	1:B:100:LEU:HD22	1.92	0.50
1:B:538:PRO:HD2	1:B:541:LYS:HD3	1.94	0.50
1:A:177:ARG:NH1	1:A:181:GLU:OE2	2.44	0.50
1:A:157:ASP:HB3	1:A:160:GLU:HB3	1.94	0.49
1:B:134:ASN:HD21	1:B:136:ASP:HB2	1.77	0.49
2:F:342:PHE:CE2	2:F:368:LEU:HD21	2.43	0.49
2:F:350:VAL:HG22	2:F:422:ASN:HB3	1.93	0.49
2:F:384:ALA:C	2:F:386:LYS:H	2.16	0.49
2:F:342:PHE:CE1	2:F:511:VAL:HG21	2.46	0.49
1:A:48:TRP:CZ3	1:A:359:LYS:HB2	2.48	0.49
1:A:204:ARG:HH22	1:A:465:LYS:NZ	2.11	0.49
1:B:578:ASN:OD1	1:B:579:MET:N	2.45	0.49
1:B:454:TYR:HE2	1:B:484:ILE:HD13	1.78	0.49
1:B:28:PHE:CD2	1:B:83:PHE:CE1	3.01	0.48
1:A:47:SER:O	1:A:51:ASN:ND2	2.29	0.48
2:F:401:VAL:HG22	2:F:509:ARG:HG2	1.95	0.48
1:B:177:ARG:NH1	1:B:181:GLU:OE2	2.47	0.48
1:B:290:ASN:HD21	1:B:292:ASP:HB3	1.78	0.48
1:B:32:PHE:HE2	1:B:391:LEU:HD21	1.79	0.48
1:A:482:ARG:O	1:A:606:TRP:NE1	2.44	0.48
2:F:389:ASP:OD1	2:F:389:ASP:N	2.44	0.48
1:A:20:LEU:HD13	1:A:23:GLU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:SER:HB2	1:B:87:GLU:HB2	1.96	0.47
1:B:316:VAL:HG21	1:B:322:HIS:CD2	2.49	0.47
2:F:476:GLY:N	2:F:487:ASN:HB3	2.29	0.47
1:A:386:ALA:HA	1:A:393:ARG:HD3	1.95	0.47
1:A:456:LEU:HD23	1:A:512:PHE:CD2	2.49	0.47
1:B:457:GLU:HG2	1:B:513:ILE:HB	1.96	0.47
2:E:376:THR:OG1	2:E:377:PHE:N	2.48	0.47
1:A:191:ALA:O	1:A:196:TYR:HB2	2.15	0.47
1:B:290:ASN:HD21	8:B:706:EDO:H11	1.80	0.47
1:A:152:MET:O	1:A:161:ARG:NH2	2.48	0.47
2:E:458:LYS:O	2:E:459:SER:OG	2.26	0.47
1:B:351:LEU:HB2	1:B:355:ASP:HB3	1.96	0.46
1:B:477:TRP:CE3	1:B:500:PRO:HG3	2.51	0.46
2:E:342:PHE:HB2	7:E:601:NAG:H82	1.97	0.46
2:E:480[B]:CYS:HB3	2:E:488:CYS:SG	2.55	0.46
2:F:461:LEU:HD22	2:F:465:GLU:HB3	1.98	0.46
1:A:188:ASN:HB3	1:A:192:ARG:HE	1.81	0.46
1:B:239:HIS:CD2	1:B:599:ASN:HD22	2.34	0.46
1:B:239:HIS:HD2	1:B:599:ASN:HD22	1.64	0.46
2:E:357:LYS:HE3	2:E:394:ASN:HD22	1.81	0.46
1:A:318:VAL:HG12	1:A:547:SER:H	1.81	0.45
2:F:369:TYR:CZ	2:F:385:THR:HG22	2.51	0.45
1:B:453:THR:HG23	1:B:512:PHE:CD2	2.51	0.45
1:A:174:LYS:HE3	1:A:496:THR:HB	1.98	0.45
1:A:102:GLN:H	1:A:102:GLN:HG3	1.53	0.45
1:B:177:ARG:HD3	1:B:498:CYS:HB2	1.99	0.45
1:B:526:GLN:HG3	1:B:539:LEU:HD11	1.99	0.45
2:F:400:PHE:N	2:F:400:PHE:HD1	2.13	0.45
1:A:55:THR:HG22	1:A:57:GLU:H	1.81	0.45
1:A:92:ILE:O	1:A:96:GLN:HG3	2.16	0.45
1:A:170:SER:O	1:A:174:LYS:HD3	2.17	0.45
1:A:177:ARG:HD3	1:A:498:CYS:HB2	1.99	0.45
1:A:526:GLN:HG3	1:A:539:LEU:HD11	1.99	0.45
1:B:114:LYS:HD2	1:B:114:LYS:HA	1.82	0.45
1:B:169:ARG:HH22	1:B:271:TRP:HA	1.80	0.45
1:A:309:LYS:O	1:A:313:LYS:HG2	2.16	0.45
1:A:73:LEU:O	1:A:77:SER:HB2	2.16	0.45
1:A:80:ALA:O	1:A:101:GLN:NE2	2.45	0.45
1:A:116:LEU:HD11	1:A:187:LYS:HG3	1.99	0.45
1:A:499:ASP:O	1:A:502:SER:HB3	2.17	0.44
1:A:155:SER:O	1:A:161:ARG:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:O	1:A:94:LYS:HE2	2.17	0.44
1:B:77:SER:OG	1:B:102:GLN:O	2.34	0.44
1:B:144:LEU:HD22	1:B:168:TRP:CZ2	2.52	0.44
2:F:367:VAL:C	2:F:369:TYR:H	2.21	0.44
1:A:144:LEU:HA	1:A:148:LEU:HB2	1.99	0.44
1:B:109:SER:HB3	1:B:112:LYS:HG3	1.99	0.44
1:B:157:ASP:HB3	1:B:160:GLU:HB3	1.99	0.44
1:B:450:LEU:HD21	1:B:519:THR:HG21	1.98	0.44
1:B:134:ASN:ND2	1:B:136:ASP:HB2	2.32	0.44
1:B:242:ALA:HB2	1:B:604:VAL:HA	2.00	0.44
1:B:168:TRP:O	1:B:172:VAL:HG22	2.18	0.43
2:E:379:CYS:HA	2:E:432:CYS:HA	2.00	0.43
2:F:342:PHE:CD1	2:F:511:VAL:HG21	2.53	0.43
1:A:142:LEU:HB3	1:A:147:GLY:HA3	2.01	0.43
1:A:514:ARG:HG2	1:A:515:TYR:N	2.34	0.43
1:B:540:HIS:HA	1:B:587:TYR:CE2	2.53	0.43
2:F:497:PHE:CD2	2:F:507:PRO:HB3	2.53	0.43
1:A:229:THR:OG1	1:A:581:VAL:HB	2.18	0.43
1:A:535:HIS:CD2	1:A:542:CYS:HB2	2.54	0.43
1:A:459:TRP:CG	1:A:477:TRP:HE3	2.37	0.43
1:B:191:ALA:O	1:B:196:TYR:HB2	2.19	0.43
2:F:409:GLN:CD	2:F:416:GLY:HA3	2.39	0.43
1:A:85:LEU:HD13	1:A:101:GLN:HG3	2.01	0.43
1:A:477:TRP:CE3	1:A:500:PRO:HG3	2.54	0.43
2:F:384:ALA:HA	2:F:387:LEU:HD22	2.00	0.43
1:A:340:ARG:CD	7:A:709:NAG:H82	2.49	0.42
1:A:420:SER:HB2	4:D:1:NAG:C6	2.49	0.42
1:A:340:ARG:HD3	7:A:709:NAG:H82	2.00	0.42
1:B:137:ASN:OD1	1:B:139:GLN:HG2	2.19	0.42
1:A:269:ASP:OD1	1:A:272:GLY:N	2.52	0.42
1:B:47:SER:HB3	1:B:349:TRP:HH2	1.84	0.42
1:B:225:ASP:O	1:B:229:THR:HG22	2.19	0.42
2:E:347:PHE:CE2	2:E:399:SER:HB2	2.55	0.42
2:F:396:TYR:HB2	2:F:514:SER:HB2	2.00	0.42
1:A:20:LEU:HD22	1:A:22:GLU:HB2	2.01	0.42
1:A:187:LYS:HD3	1:A:199:TYR:CE2	2.54	0.42
1:A:359:LYS:HB3	1:A:359:LYS:HE3	1.73	0.42
1:B:132:VAL:HG21	1:B:148:LEU:HD21	2.02	0.42
2:F:380:TYR:N	2:F:431:GLY:O	2.49	0.42
1:B:96:GLN:HG2	1:B:392:LEU:HD13	2.01	0.42
1:B:245:ARG:HA	1:B:262:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:OG1	1:A:93:ILE:HD12	2.19	0.42
1:A:108:LEU:HD23	1:A:113:SER:HA	2.02	0.42
1:B:55:THR:O	1:B:59:VAL:HG23	2.20	0.42
2:E:350:VAL:HA	2:E:400:PHE:HB2	2.02	0.42
2:F:379:CYS:HA	2:F:432:CYS:HA	2.00	0.42
1:A:137:ASN:OD1	1:A:139:GLN:HG2	2.19	0.41
2:F:502:GLY:O	2:F:506:GLN:HG3	2.21	0.41
1:A:285:PHE:O	1:A:437:ASN:ND2	2.38	0.41
1:B:336:PRO:C	1:B:338:ASP:H	2.23	0.41
1:B:55:THR:HG22	1:B:57:GLU:H	1.85	0.41
2:F:356:LYS:HE3	2:F:358:ILE:HD11	2.02	0.41
2:F:374:PHE:CD2	2:F:434:LEU:HB3	2.56	0.41
1:A:36:ALA:HB2	1:A:72:PHE:HE2	1.85	0.41
1:A:450:LEU:HD21	1:A:519:THR:HG21	2.03	0.41
1:B:108:LEU:HD23	1:B:113:SER:HA	2.03	0.41
2:F:435:ALA:HA	2:F:509:ARG:O	2.21	0.41
1:A:493:HIS:ND1	1:A:499:ASP:OD2	2.43	0.41
1:B:382:ASP:OD1	1:B:385:TYR:OH	2.25	0.41
1:B:85:LEU:HD13	1:B:101:GLN:HG3	2.03	0.41
2:E:360:ASN:OD1	2:E:360:ASN:N	2.54	0.41
2:F:369:TYR:CE1	2:F:385:THR:HG22	2.56	0.41
1:A:489:GLU:HA	1:A:490:PRO:HD3	1.94	0.41
1:A:578:ASN:OD1	1:A:579:MET:N	2.50	0.41
1:B:330:ASN:HB3	1:B:357:ARG:CZ	2.51	0.41
2:F:403:LYS:HD3	2:F:505:HIS:CD2	2.56	0.41
1:A:20:LEU:HD13	1:A:22:GLU:HB2	2.03	0.41
1:B:81:GLN:HA	1:B:101:GLN:OE1	2.21	0.41
1:A:248:LEU:HD12	1:A:262:LEU:HD22	2.02	0.40
1:A:431:ASP:N	1:A:431:ASP:OD1	2.53	0.40
1:B:315:PHE:CD1	1:B:380:GLN:HG3	2.57	0.40
1:B:465:LYS:HE3	1:B:467:GLU:OE2	2.20	0.40
1:B:554:LEU:O	1:B:558:LEU:HG	2.21	0.40
2:F:398:ASP:O	2:F:511:VAL:HA	2.20	0.40
1:A:389:PRO:HG2	1:A:392:LEU:HD22	2.02	0.40
1:A:465:LYS:HB2	1:A:465:LYS:HE2	1.83	0.40
2:E:485:GLY:N	2:E:488:CYS:O	2.46	0.40
1:A:109:SER:O	1:A:113:SER:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	594/597 (100%)	568 (96%)	24 (4%)	2 (0%)	41	61
1	B	591/597 (99%)	565 (96%)	26 (4%)	0	100	100
2	E	185/217 (85%)	168 (91%)	17 (9%)	0	100	100
2	F	186/217 (86%)	167 (90%)	18 (10%)	1 (0%)	29	51
All	All	1556/1628 (96%)	1468 (94%)	85 (6%)	3 (0%)	47	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	ARG
1	A	337	ALA
2	F	385	THR

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	525/526 (100%)	504 (96%)	21 (4%)	31	57
1	B	523/526 (99%)	502 (96%)	21 (4%)	31	57
2	E	163/189 (86%)	159 (98%)	4 (2%)	47	71
2	F	165/189 (87%)	160 (97%)	5 (3%)	41	65
All	All	1376/1430 (96%)	1325 (96%)	51 (4%)	34	59

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	22	GLU
1	A	34	GLN
1	A	74	LYS
1	A	77	SER
1	A	90	THR
1	A	102	GLN
1	A	113	SER
1	A	131	LYS
1	A	143	LEU
1	A	172	VAL
1	A	333	LEU
1	A	349	TRP
1	A	365	THR
1	A	381	TYR
1	A	401	HIS
1	A	404	VAL
1	A	514	ARG
1	A	518	ARG
1	A	555	PHE
1	A	557	MET
1	B	26	LYS
1	B	27	THR
1	B	34	GLN
1	B	64	ASN
1	B	73	LEU
1	B	87	GLU
1	B	102	GLN
1	B	103	ASN
1	B	111	ASP
1	B	172	VAL
1	B	295	ASP
1	B	333	LEU
1	B	340	ARG
1	B	365	THR
1	B	381	TYR
1	B	401	HIS
1	B	514	ARG
1	B	518	ARG
1	B	555	PHE
1	B	557	MET
1	B	573	VAL
2	E	334	ASN

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Mol	Chain	Res	Type
2	E	377	PHE
2	E	408	ARG
2	E	498	ARG
2	F	333	THR
2	F	372	THR
2	F	377	PHE
2	F	400	PHE
2	F	495	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	117	ASN
1	A	472	GLN
1	B	24	ASN
1	B	34	GLN
1	B	103	ASN
1	B	117	ASN
1	B	121	ASN
1	B	175	GLN
1	B	239	HIS
1	B	290	ASN
1	B	417	HIS
1	B	522	GLN
2	E	334	ASN
2	F	487	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	0.62	0	17,19,21	0.78	0
3	NAG	C	2	3	14,14,15	0.57	0	17,19,21	0.35	0
4	NAG	D	1	4,1	14,14,15	1.03	1 (7%)	17,19,21	0.98	2 (11%)
4	NAG	D	2	4	14,14,15	0.35	0	17,19,21	0.59	0
4	BMA	D	3	4	11,11,12	0.72	0	15,15,17	0.95	0
4	NAG	J	1	4,1	14,14,15	0.56	0	17,19,21	0.55	0
4	NAG	J	2	4	14,14,15	0.29	0	17,19,21	0.48	0
4	BMA	J	3	4	11,11,12	0.59	0	15,15,17	1.12	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	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	O5-C1	-3.55	1.38	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	3	BMA	C1-O5-C5	2.65	115.78	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C3-C4-C5	2.50	114.71	110.24
4	D	1	NAG	O4-C4-C5	-2.26	103.67	109.30

There are no chirality outliers.

All (14) torsion outliers are listed below:

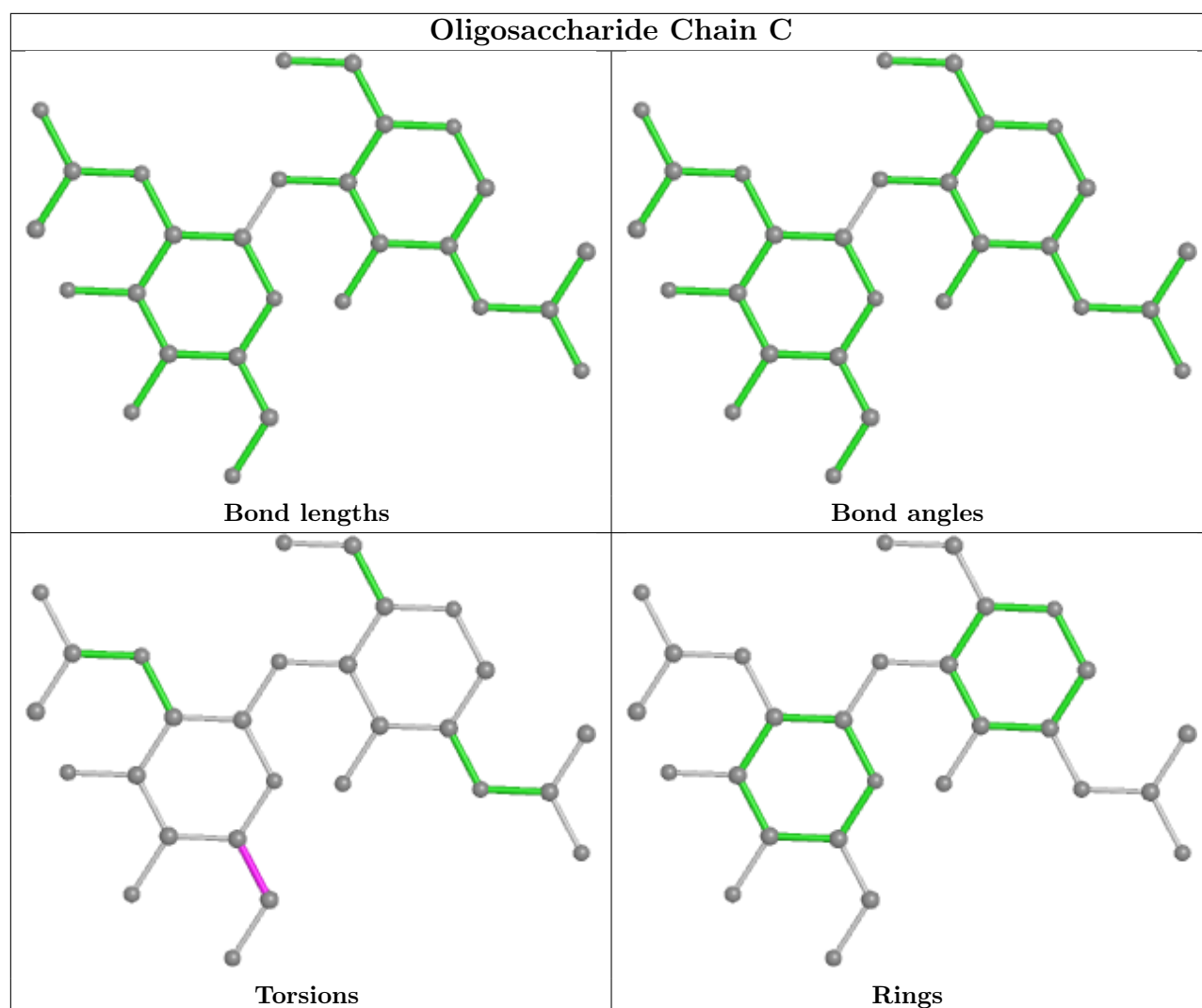
Mol	Chain	Res	Type	Atoms
4	J	3	BMA	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6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

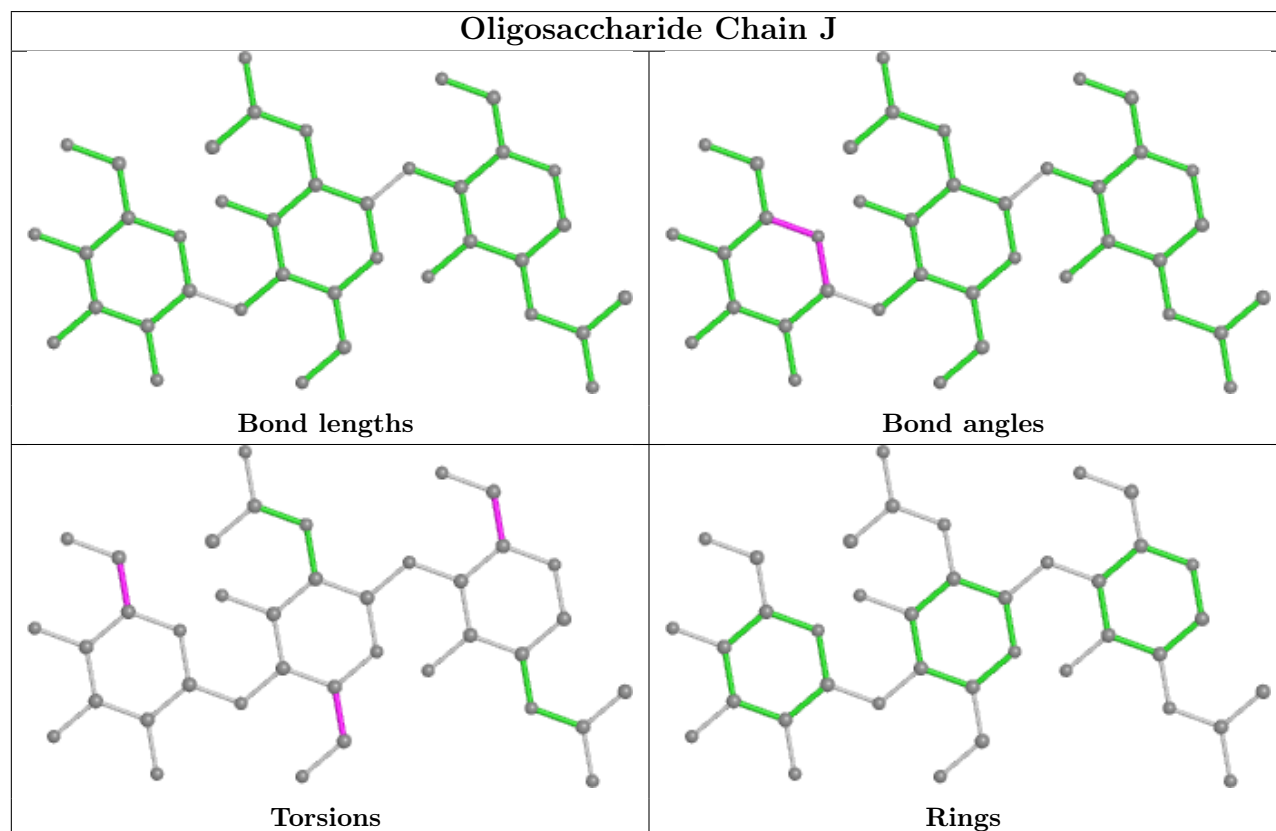
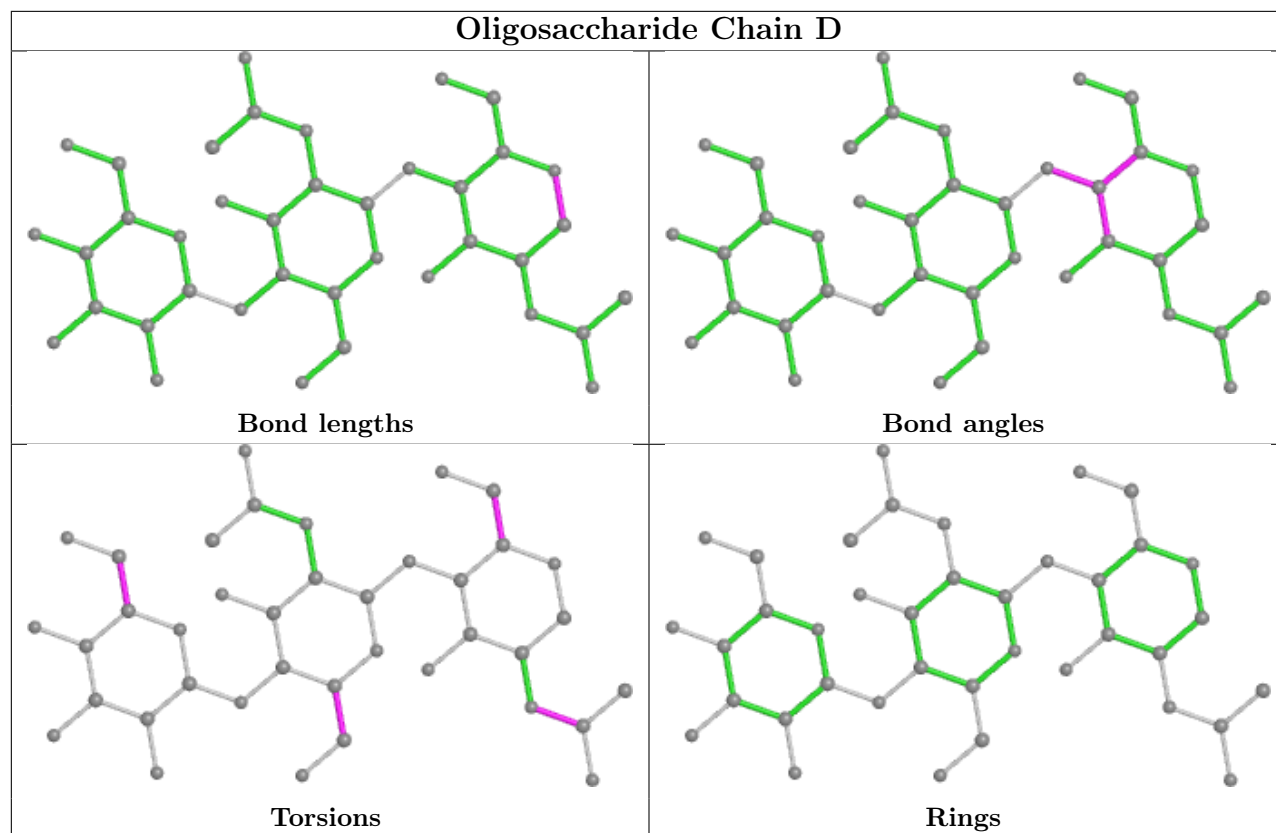
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
4	D	1	NAG	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

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\# Z > 2$
8	EDO	B	703	-	3,3,3	0.46	0	2,2,2	0.34	0
7	NAG	E	601	2	14,14,15	0.30	0	17,19,21	0.42	0
7	NAG	F	601	2	14,14,15	0.42	0	17,19,21	0.49	0
8	EDO	A	706	-	3,3,3	0.46	0	2,2,2	0.32	0
8	EDO	A	704	-	3,3,3	0.46	0	2,2,2	0.26	0
8	EDO	A	708	-	3,3,3	0.46	0	2,2,2	0.31	0
8	EDO	B	706	-	3,3,3	0.47	0	2,2,2	0.33	0
7	NAG	A	709	1	14,14,15	0.29	0	17,19,21	0.45	0
8	EDO	A	707	-	3,3,3	0.45	0	2,2,2	0.35	0
8	EDO	B	704	-	3,3,3	0.47	0	2,2,2	0.27	0
8	EDO	B	707	-	3,3,3	0.47	0	2,2,2	0.29	0
7	NAG	A	703	1	14,14,15	0.49	0	17,19,21	0.56	0
7	NAG	B	705	1	14,14,15	0.43	0	17,19,21	0.57	0
8	EDO	A	705	-	3,3,3	0.47	0	2,2,2	0.27	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
8	EDO	B	703	-	-	1/1/1/1	-
7	NAG	E	601	2	-	1/6/23/26	0/1/1/1
7	NAG	F	601	2	-	1/6/23/26	0/1/1/1
8	EDO	A	706	-	-	0/1/1/1	-
8	EDO	A	704	-	-	0/1/1/1	-
8	EDO	A	708	-	-	0/1/1/1	-
8	EDO	B	706	-	-	1/1/1/1	-
7	NAG	A	709	1	-	2/6/23/26	0/1/1/1
8	EDO	A	707	-	-	0/1/1/1	-
8	EDO	B	704	-	-	0/1/1/1	-

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	703	NAG	O5-C5-C6-O6
7	A	703	NAG	C4-C5-C6-O6
7	A	709	NAG	C4-C5-C6-O6
7	E	601	NAG	O5-C5-C6-O6
7	F	601	NAG	O5-C5-C6-O6
7	A	709	NAG	O5-C5-C6-O6
8	B	703	EDO	O1-C1-C2-O2
8	B	706	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	601	NAG	1	0
8	B	706	EDO	1	0
7	A	709	NAG	2	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	595/597 (99%)	0.59	51 (8%)	10 5	47, 95, 144, 178	0
1	B	593/597 (99%)	0.59	50 (8%)	11 5	47, 83, 154, 195	0
2	E	188/217 (86%)	0.68	22 (11%)	4 2	56, 85, 148, 177	0
2	F	190/217 (87%)	0.82	31 (16%)	1 1	76, 111, 176, 212	0
All	All	1566/1628 (96%)	0.63	154 (9%)	7 4	47, 94, 156, 212	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	GLY	7.9
1	B	129	THR	7.8
1	B	130	GLY	7.5
2	F	363	ALA	6.9
2	E	387	LEU	6.7
2	E	515	PHE	6.6
2	F	434	LEU	6.2
1	B	105	SER	5.4
2	F	368	LEU	5.1
2	F	511	VAL	4.8
2	F	455	LEU	4.8
1	A	399	GLY	4.7
1	A	105	SER	4.5
2	E	395	VAL	4.3
1	B	173	GLY	4.3
1	B	99	ALA	4.2
1	A	85	LEU	4.1
1	A	529	LEU	4.0
1	A	222	LEU	4.0
2	E	392	PHE	3.9
1	B	190	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	570	LEU	3.9
2	F	338	PHE	3.8
2	E	517	LEU	3.7
1	A	413	ALA	3.7
2	E	369	TYR	3.7
1	A	80	ALA	3.6
1	A	187	LYS	3.6
1	B	85	LEU	3.6
2	E	368	LEU	3.6
1	B	80	ALA	3.5
1	B	116	LEU	3.5
1	B	391	LEU	3.5
2	F	369	TYR	3.5
1	A	574	VAL	3.4
2	E	394	ASN	3.4
1	B	127	TYR	3.4
1	A	97	LEU	3.3
2	F	513	LEU	3.3
1	A	101	GLN	3.3
2	E	365	TYR	3.3
2	F	358	ILE	3.3
2	F	342	PHE	3.2
1	B	108	LEU	3.2
2	F	335	LEU	3.2
2	F	432	CYS	3.2
1	A	217	TYR	3.2
1	B	142	LEU	3.2
2	F	388	ASN	3.1
1	B	75	GLU	3.1
2	F	350	VAL	3.1
2	E	513	LEU	3.1
1	A	464	PHE	3.1
1	A	98	GLN	3.0
1	A	396	ALA	3.0
2	E	410	ILE	3.0
1	B	101	GLN	3.0
2	F	433	VAL	3.0
1	A	190	MET	2.9
1	B	202	TYR	2.9
1	B	207	TYR	2.9
2	E	449	TYR	2.9
1	A	194	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	492	LEU	2.9
2	F	387	LEU	2.9
1	A	395	GLY	2.9
1	A	424	LEU	2.9
1	A	183	TYR	2.9
1	B	525	PHE	2.8
2	F	402	VAL	2.8
1	A	462	MET	2.8
1	A	554	LEU	2.8
2	F	390	LEU	2.8
2	F	377	PHE	2.8
1	B	453	THR	2.8
1	A	478	TRP	2.8
2	F	365	TYR	2.7
1	B	126	ILE	2.7
1	A	591	LEU	2.7
1	B	222	LEU	2.7
1	B	73	LEU	2.7
2	E	338	PHE	2.7
1	A	525	PHE	2.6
1	A	106	SER	2.6
1	A	226	VAL	2.6
1	B	72	PHE	2.6
1	A	308	PHE	2.6
1	B	404	VAL	2.6
1	A	233	ILE	2.5
1	B	577	LYS	2.5
1	A	207	TYR	2.5
1	B	425	SER	2.5
2	F	396	TYR	2.5
2	F	456	PHE	2.5
2	F	340	GLU	2.5
1	B	521	TYR	2.5
1	A	588	PHE	2.5
1	B	131	LYS	2.5
2	E	364	ASP	2.5
1	B	167	SER	2.4
1	A	83	PHE	2.4
1	B	226	VAL	2.4
2	F	389	ASP	2.4
1	B	358	ILE	2.4
2	E	510	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	100	LEU	2.4
1	B	168	TRP	2.4
1	B	399	GLY	2.4
2	F	391	CYS	2.4
2	E	433	VAL	2.4
1	A	176	LEU	2.4
1	B	392	LEU	2.4
1	A	516	TYR	2.4
2	F	495	TYR	2.4
1	A	103	ASN	2.4
2	F	392	PHE	2.4
1	A	579	MET	2.4
1	B	97	LEU	2.4
1	B	464	PHE	2.3
1	B	579	MET	2.3
1	B	574	VAL	2.3
1	B	106	SER	2.3
1	B	95	ARG	2.3
1	A	202	TYR	2.3
1	A	391	LEU	2.3
1	A	93	ILE	2.2
1	B	32	PHE	2.2
1	B	550	ALA	2.2
1	A	390	PHE	2.2
2	E	436	TRP	2.2
1	A	29	LEU	2.2
1	A	100	LEU	2.2
2	F	430	MET	2.2
1	A	540	HIS	2.2
1	B	400	PHE	2.1
1	A	557	MET	2.1
1	A	590	PRO	2.1
1	B	570	LEU	2.1
1	B	172	VAL	2.1
1	A	473	TRP	2.1
1	B	348	ALA	2.1
1	A	164	ALA	2.1
1	B	468	ILE	2.1
1	B	333	LEU	2.0
1	B	544	ILE	2.0
2	F	395	VAL	2.0
2	E	514	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	363	ALA	2.0
2	F	431	GLY	2.0
1	A	544	ILE	2.0
1	A	96	GLN	2.0
2	E	370	ASN	2.0
2	E	492	LEU	2.0
2	E	429	PHE	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](#)

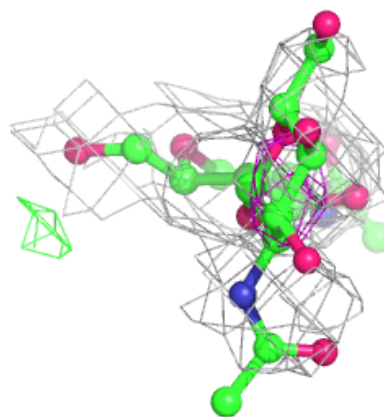
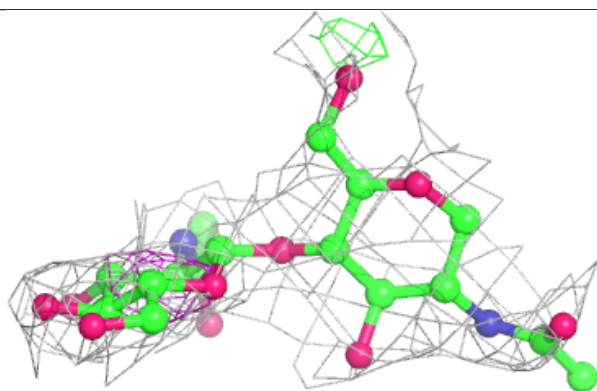
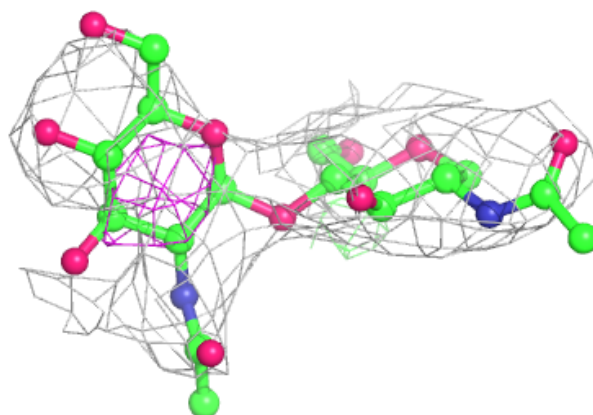
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	2	14/15	0.74	0.30	114,120,123,123	0
4	BMA	D	3	11/12	0.76	0.29	119,126,128,128	0
4	NAG	D	2	14/15	0.81	0.21	108,123,125,126	0
4	NAG	J	2	14/15	0.81	0.18	102,106,113,116	0
4	BMA	J	3	11/12	0.82	0.21	104,114,115,116	0
4	NAG	J	1	14/15	0.84	0.16	79,89,99,103	0
3	NAG	C	1	14/15	0.87	0.24	95,108,113,117	0
4	NAG	D	1	14/15	0.88	0.18	123,126,128,132	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.

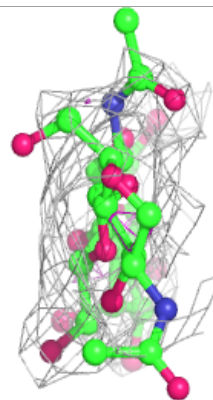
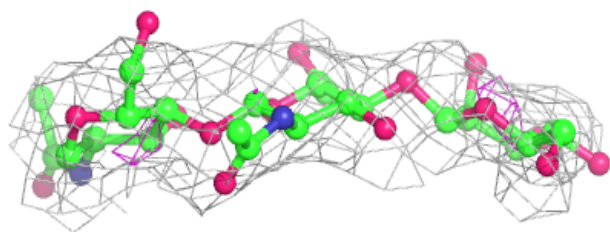
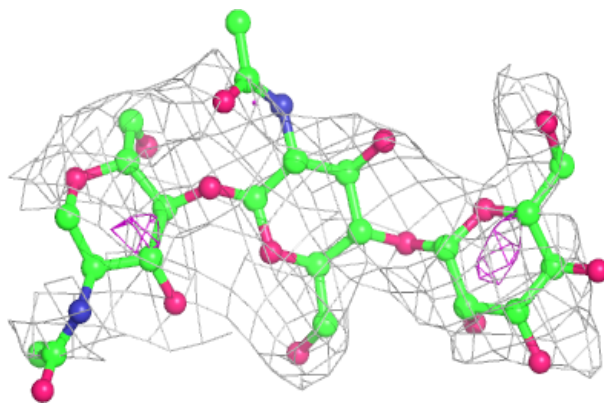
Electron density around Chain C:

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

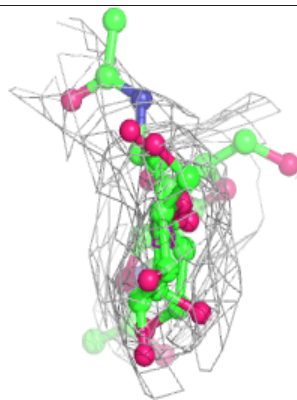
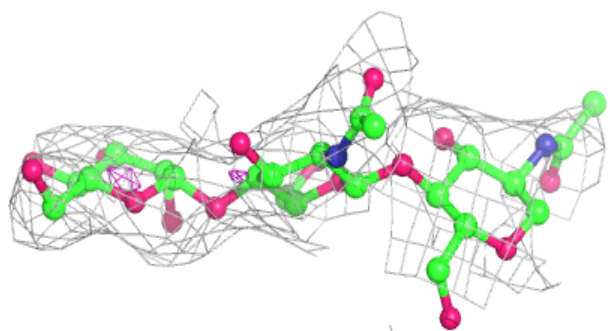
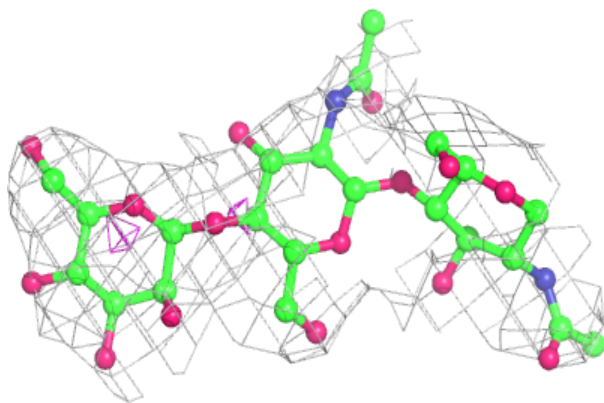


Electron density around Chain D:

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

**Electron density around Chain J:**

$2mF_o-DF_c$ (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	NAG	F	601	14/15	0.67	0.28	122,126,127,127	0
7	NAG	A	703	14/15	0.71	0.20	110,122,124,125	0
7	NAG	E	601	14/15	0.76	0.22	92,98,104,105	0
7	NAG	B	705	14/15	0.76	0.24	80,105,116,116	0
8	EDO	B	703	4/4	0.77	0.25	63,65,68,69	0
8	EDO	B	707	4/4	0.82	0.31	60,63,63,63	0
8	EDO	A	706	4/4	0.83	0.31	65,69,71,73	0
6	CL	B	702	1/1	0.89	0.21	77,77,77,77	0
8	EDO	A	705	4/4	0.91	0.18	56,58,59,61	0
8	EDO	B	704	4/4	0.91	0.18	68,73,74,74	0
8	EDO	B	706	4/4	0.91	0.21	54,55,56,56	0
8	EDO	A	704	4/4	0.91	0.18	54,56,57,57	0
8	EDO	A	707	4/4	0.92	0.23	60,67,70,76	0
7	NAG	A	709	14/15	0.93	0.17	92,93,103,109	0
8	EDO	A	708	4/4	0.93	0.23	42,49,49,50	0
6	CL	A	702	1/1	0.97	0.10	51,51,51,51	0
5	ZN	A	701	1/1	0.97	0.13	89,89,89,89	0
5	ZN	B	701	1/1	0.99	0.21	59,59,59,59	0

6.5 Other polymers

There are no such residues in this entry.