



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:30 AM UTC

PDB ID : 5GR8 / pdb_00005gr8
Title : Crystal structure of PEPR1-AtPEP1
Authors : Chai, J.J.; Tang, J.
Deposited on : 2016-08-08
Resolution : 2.59 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

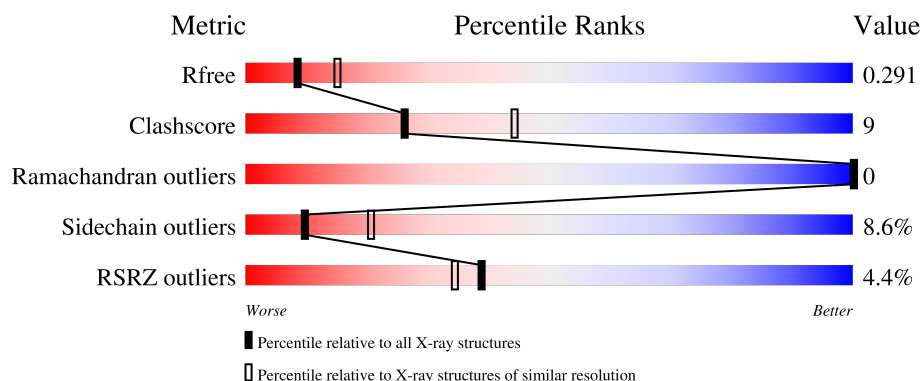
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

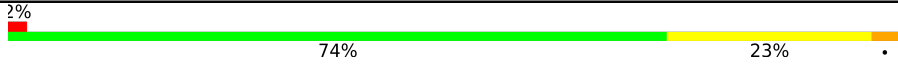
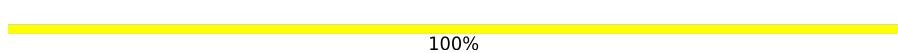
The reported resolution of this entry is 2.59 Å.

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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	710	
1	D	710	
2	J	17	
2	P	17	
3	B	2	

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Mol	Chain	Length	Quality of chain
3	C	2	50% 50%
3	E	2	100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11318 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 Leucine-rich repeat receptor-like protein kinase PEPR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	710	Total	C	N	O	S	0	0	0
			5404	3419	915	1054	16			
1	D	710	Total	C	N	O	S	0	0	0
			5404	3419	915	1054	16			

- Molecule 2 is a protein called Elicitor peptide 1.

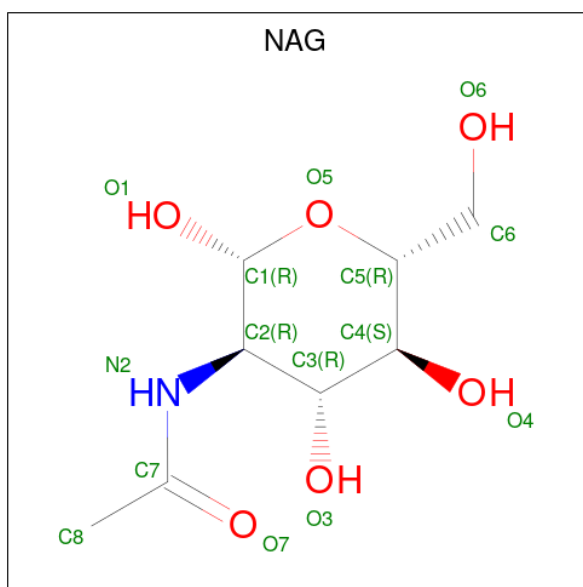
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	17	Total	C	N	O	0	0	0
			133	77	31	25			
2	P	16	Total	C	N	O	0	0	0
			124	71	29	24			

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



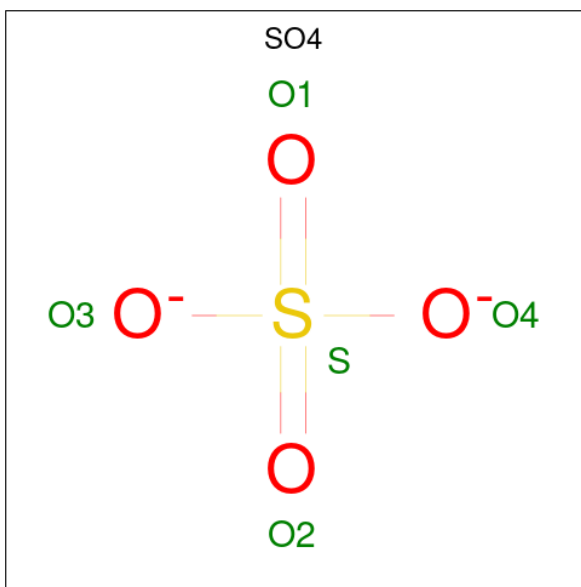
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

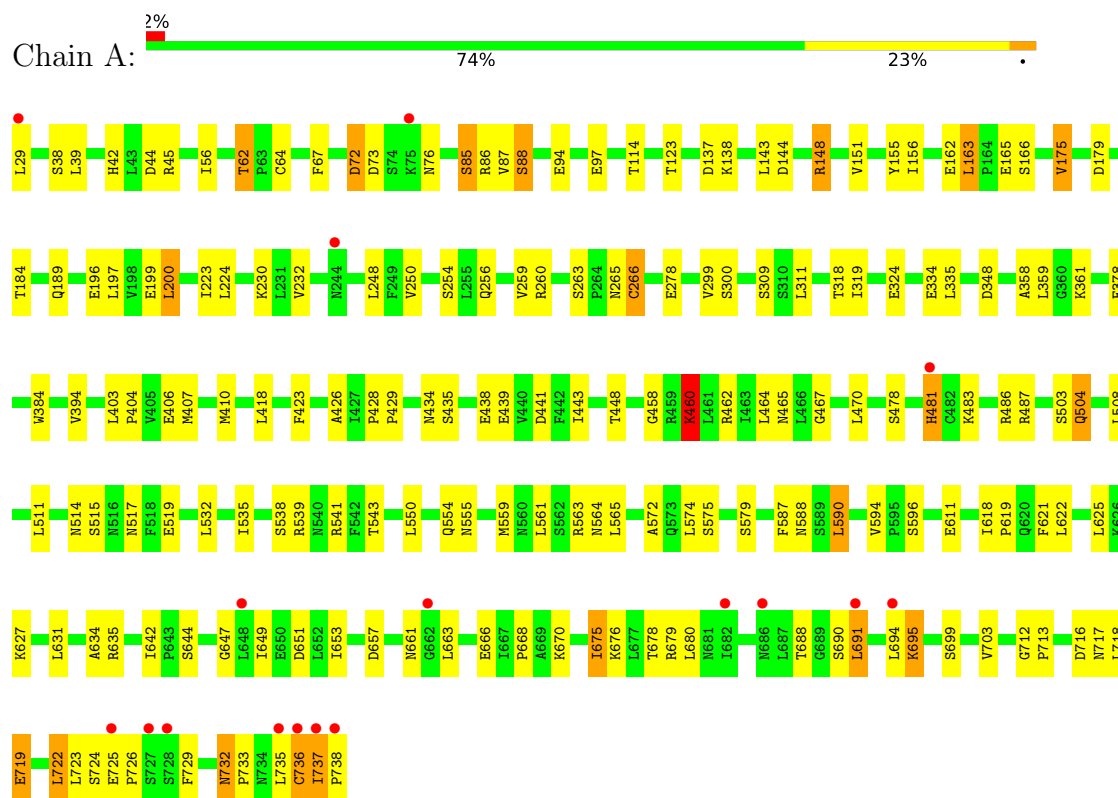
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		
6	D	13	Total	O	0	0
			13	13		
6	J	4	Total	O	0	0
			4	4		
6	P	2	Total	O	0	0
			2	2		

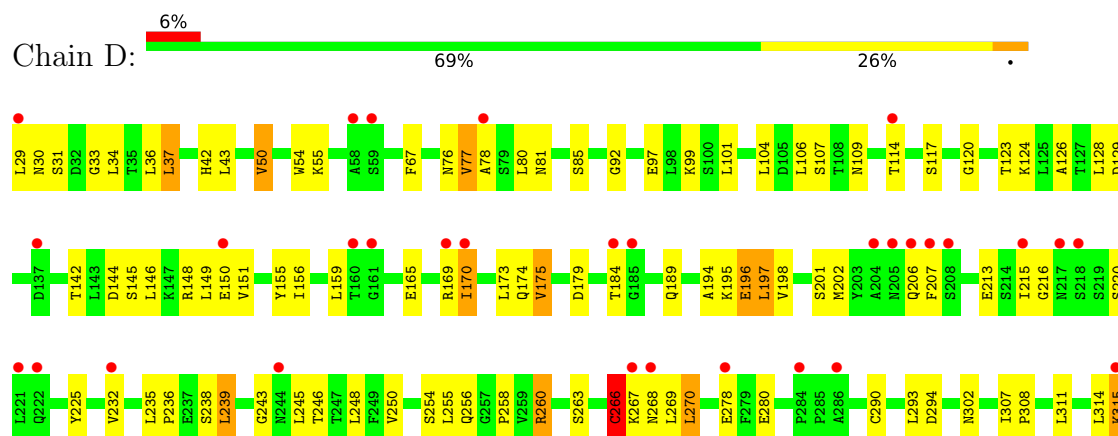
3 Residue-property plots

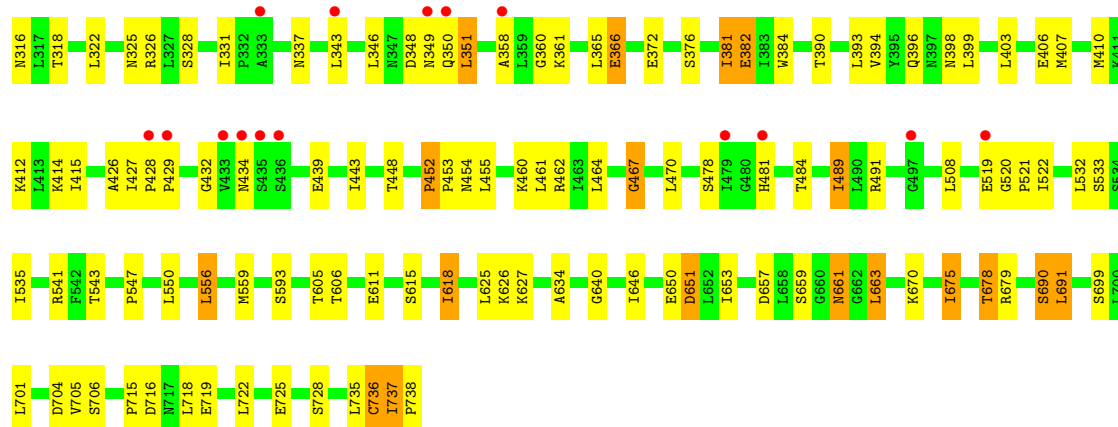
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Leucine-rich repeat receptor-like protein kinase PEPR1



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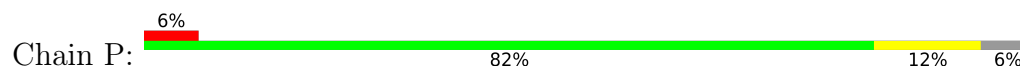




• Molecule 2: Elicitor peptide 1



• Molecule 2: Elicitor peptide 1



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



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• Molecule 3: 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	99.49Å 96.97Å 106.01Å 90.00° 110.79° 90.00°	Depositor
Resolution (Å)	49.55 – 2.59 49.55 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.55-2.59) 99.1 (49.55-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.234 , 0.288 0.241 , 0.291	Depositor DCC
R_{free} test set	2968 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11318	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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: NAG, SO4

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	0.63	0/5500	1.07	24/7470 (0.3%)
1	D	0.57	0/5500	1.06	17/7470 (0.2%)
2	J	0.81	0/134	1.33	2/173 (1.2%)
2	P	0.48	0/125	0.97	0/162
All	All	0.60	0/11259	1.07	43/15275 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	690	SER	N-CA-C	10.65	122.64	111.14
1	A	504	GLN	N-CA-C	-8.66	99.10	110.53
1	D	452	PRO	CA-C-N	8.27	127.91	119.56
1	D	452	PRO	C-N-CA	8.27	127.91	119.56
2	J	9	ARG	N-CA-C	8.08	122.39	109.86
1	A	85	SER	N-CA-C	-7.93	98.53	109.95
1	D	85	SER	N-CA-C	-7.40	98.67	110.14
1	D	266	CYS	N-CA-C	-7.40	95.04	110.80
1	A	67	PHE	N-CA-C	7.26	119.82	111.11
1	D	394	VAL	N-CA-C	6.96	118.78	112.17
2	J	8	GLN	N-CA-C	6.72	125.11	110.80
1	D	328	SER	N-CA-C	6.63	121.08	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	649	ILE	N-CA-C	-6.53	98.04	107.78
1	A	230	LYS	N-CA-C	6.06	119.62	112.72
1	D	640	GLY	N-CA-C	5.97	122.66	111.80
1	D	651	ASP	N-CA-C	5.85	120.12	112.92
1	A	394	VAL	N-CA-C	5.74	117.62	112.17
1	A	73	ASP	N-CA-C	-5.69	105.22	111.82
1	A	661	ASN	N-CA-C	5.62	120.25	113.17
1	A	712	GLY	CA-C-N	5.61	126.86	119.84
1	A	712	GLY	C-N-CA	5.61	126.86	119.84
1	A	62	THR	CA-C-N	5.60	126.34	120.12
1	A	62	THR	C-N-CA	5.60	126.34	120.12
1	A	259	VAL	CA-C-N	-5.59	115.08	122.85
1	A	259	VAL	C-N-CA	-5.59	115.08	122.85
1	D	467	GLY	N-CA-C	5.44	118.32	112.33
1	A	85	SER	CA-C-N	-5.35	115.22	123.14
1	A	85	SER	C-N-CA	-5.35	115.22	123.14
1	D	85	SER	CA-C-N	-5.33	115.44	122.85
1	D	85	SER	C-N-CA	-5.33	115.44	122.85
1	A	732	ASN	CA-C-N	5.33	125.39	119.32
1	A	732	ASN	C-N-CA	5.33	125.39	119.32
1	A	460	LYS	N-CA-C	5.32	120.43	113.30
1	A	517	ASN	N-CA-C	5.29	118.75	112.72
1	A	64	CYS	N-CA-C	5.25	118.78	112.38
1	D	315	LYS	N-CA-C	-5.22	103.15	110.35
1	D	67	PHE	N-CA-C	5.20	117.34	111.11
1	A	690	SER	N-CA-C	5.15	116.71	111.14
1	A	541	ARG	N-CA-C	5.12	119.22	112.92
1	D	706	SER	N-CA-C	5.08	116.85	110.24
1	D	302	ASN	N-CA-C	-5.08	100.80	108.67
1	D	661	ASN	N-CA-C	5.07	120.10	113.30
1	A	299	VAL	N-CA-C	-5.05	101.10	108.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	434	ASN	Peptide

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	5404	0	5464	96	0
1	D	5404	0	5463	116	0
2	J	133	0	134	3	0
2	P	124	0	121	2	0
3	B	28	0	25	0	0
3	C	28	0	25	0	0
3	E	28	0	25	0	0
4	A	56	0	52	0	0
4	D	42	0	39	0	0
5	A	5	0	0	0	0
6	A	47	0	0	5	0
6	D	13	0	0	1	0
6	J	4	0	0	1	0
6	P	2	0	0	0	0
All	All	11318	0	11348	213	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 (213) 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:148:ARG:HG2	1:A:148:ARG:HH11	1.40	0.87
1:D:372:GLU:OE1	1:D:396:GLN:NE2	2.08	0.86
1:A:438:GLU:OE2	1:A:462:ARG:NH1	2.15	0.80
1:D:243:GLY:O	1:D:268:ASN:ND2	2.16	0.79
1:A:45:ARG:HH12	1:A:86:ARG:HH21	1.30	0.78
1:D:194:ALA:HB3	1:D:197:LEU:HD12	1.64	0.78
1:D:81:ASN:ND2	6:D:901:HOH:O	2.16	0.77
1:A:486:ARG:HG3	1:A:487:ARG:HG3	1.65	0.76
1:A:695:LYS:HA	1:A:717:ASN:HD21	1.52	0.74
1:A:736:CYS:SG	1:A:737:ILE:N	2.60	0.73
1:D:550:LEU:HD13	1:D:559:MET:HE1	1.70	0.73
1:A:666:GLU:HG2	1:A:688:THR:O	1.89	0.73
1:D:155:TYR:HD1	1:D:156:ILE:HG13	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:HD21	1:A:200:LEU:HG	1.70	0.72
1:A:588:ASN:HB2	1:A:590:LEU:HD22	1.72	0.71
1:D:184:THR:HG22	1:D:206:GLN:HB2	1.73	0.70
1:A:611:GLU:OE2	1:A:635:ARG:NE	2.22	0.70
1:D:376:SER:HA	1:D:398:ASN:O	1.92	0.69
1:D:151:VAL:HG12	1:D:175:VAL:HG13	1.73	0.69
1:A:378:GLU:OE2	6:A:901:HOH:O	2.11	0.69
1:D:124:LYS:HD2	1:D:148:ARG:HD2	1.75	0.68
1:A:675:ILE:O	1:A:699:SER:OG	2.11	0.68
1:D:448:THR:HG22	1:D:470:LEU:HB2	1.78	0.66
1:D:678:THR:HG22	1:D:679:ARG:HG3	1.76	0.66
1:D:439:GLU:OE1	1:D:462:ARG:NH2	2.27	0.66
1:A:44:ASP:HB3	1:A:88:SER:HB2	1.75	0.66
1:A:726:PRO:O	6:A:902:HOH:O	2.12	0.66
1:D:381:ILE:HA	1:D:384:TRP:HD1	1.63	0.64
1:A:94:GLU:O	1:A:97:GLU:HG2	1.98	0.64
1:D:453:PRO:O	1:D:478:SER:OG	2.12	0.63
1:A:318:THR:HG23	1:A:319:ILE:HG13	1.81	0.63
1:D:165:GLU:OE2	1:D:169:ARG:NH2	2.32	0.62
1:D:704:ASP:HA	1:D:728:SER:HB2	1.83	0.60
1:D:322:LEU:O	1:D:325:ASN:ND2	2.33	0.59
1:A:407:MET:HG3	1:A:410:MET:HE3	1.84	0.59
1:A:441:ASP:HA	1:A:465:ASN:HB2	1.85	0.59
1:A:559:MET:HE2	1:A:561:LEU:HD21	1.84	0.59
1:A:519:GLU:OE2	6:A:903:HOH:O	2.17	0.59
1:A:155:TYR:HD1	1:A:156:ILE:HG13	1.67	0.58
1:D:432:GLY:HA3	1:D:454:ASN:C	2.28	0.58
1:D:216:GLY:HA3	1:D:238:SER:HB2	1.85	0.58
1:D:294:ASP:HA	1:D:316:ASN:O	2.03	0.58
1:A:151:VAL:HG12	1:A:175:VAL:HG13	1.84	0.58
1:A:678:THR:HG22	1:A:679:ARG:HG3	1.86	0.57
1:D:736:CYS:SG	1:D:737:ILE:N	2.77	0.57
2:J:7:LYS:NZ	6:J:101:HOH:O	2.36	0.57
1:A:358:ALA:O	1:A:361:LYS:HB3	2.04	0.57
1:A:622:LEU:HD13	1:A:631:LEU:HD11	1.85	0.57
1:A:435:SER:HB3	1:A:458:GLY:HA3	1.85	0.57
1:D:690:SER:O	1:D:691:LEU:HB2	2.03	0.57
1:D:358:ALA:O	1:D:361:LYS:HB3	2.05	0.56
1:D:366:GLU:OE1	1:D:412:LYS:NZ	2.39	0.56
1:A:561:LEU:O	1:A:564:ASN:ND2	2.35	0.56
1:D:489:ILE:O	1:D:489:ILE:HG13	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:ILE:HG12	1:A:676:LYS:HB3	1.89	0.55
1:D:201:SER:HA	1:D:225:TYR:HB2	1.88	0.55
1:A:137:ASP:CG	1:A:138:LYS:H	2.14	0.55
1:A:539:ARG:HG2	1:A:563:ARG:HD2	1.89	0.55
1:A:266:CYS:HB3	6:A:908:HOH:O	2.05	0.55
1:D:532:LEU:HD13	1:D:535:ILE:HD11	1.89	0.54
1:D:124:LYS:O	1:D:148:ARG:HD3	2.07	0.54
1:A:162:GLU:HG2	1:A:163:LEU:N	2.23	0.54
1:D:30:ASN:O	1:D:34:LEU:HG	2.07	0.54
1:D:149:LEU:HB3	1:D:170:ILE:HD11	1.89	0.53
1:A:72:ASP:OD2	6:A:904:HOH:O	2.19	0.53
1:D:737:ILE:HD12	1:D:738:PRO:HD2	1.91	0.53
1:D:270:LEU:HA	1:D:293:LEU:HA	1.90	0.53
1:A:651:ASP:O	1:A:653:ILE:HG13	2.07	0.53
1:D:266:CYS:HB3	1:D:290:CYS:HA	1.90	0.53
1:D:202:MET:HE2	1:D:207:PHE:CE2	2.44	0.52
1:D:659:SER:O	1:D:661:ASN:ND2	2.42	0.52
1:A:572:ALA:O	1:A:575:SER:OG	2.23	0.52
1:D:432:GLY:HA3	1:D:454:ASN:O	2.10	0.52
1:A:148:ARG:HG2	1:A:148:ARG:NH1	2.14	0.52
1:A:406:GLU:OE2	1:A:406:GLU:N	2.41	0.52
1:D:489:ILE:HD13	1:D:491:ARG:CZ	2.39	0.52
1:D:381:ILE:HD11	1:D:406:GLU:OE1	2.09	0.52
1:D:36:LEU:HD11	1:D:77:VAL:HG11	1.92	0.51
1:D:605:THR:HG23	1:D:606:THR:OG1	2.10	0.51
1:D:678:THR:HG23	1:D:701:LEU:HD12	1.92	0.51
1:D:126:ALA:O	1:D:149:LEU:HD12	2.10	0.51
1:A:45:ARG:NH1	1:A:86:ARG:HH21	2.03	0.51
1:D:246:THR:HA	1:D:269:LEU:HA	1.92	0.51
1:A:691:LEU:HD22	1:A:694:LEU:HD22	1.93	0.51
1:A:713:PRO:HA	1:A:736:CYS:H	1.75	0.51
1:A:29:LEU:HG	1:A:62:THR:HG22	1.93	0.51
1:A:439:GLU:OE1	1:A:462:ARG:NH2	2.44	0.51
1:A:719:GLU:O	1:A:723:LEU:N	2.40	0.51
1:D:427:ILE:HB	1:D:452:PRO:HG3	1.92	0.51
1:D:258:PRO:HA	1:D:280:GLU:O	2.12	0.50
1:D:651:ASP:O	1:D:653:ILE:HG13	2.12	0.50
1:D:360:GLY:HA3	1:D:382:GLU:HB2	1.94	0.50
1:A:72:ASP:HB2	1:A:76:ASN:H	1.77	0.49
1:D:202:MET:HB3	1:D:207:PHE:CE2	2.46	0.49
1:A:334:GLU:OE1	1:A:334:GLU:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:LEU:O	1:D:109:ASN:ND2	2.36	0.48
1:D:315:LYS:CG	1:D:316:ASN:H	2.25	0.48
1:A:403:LEU:HD13	1:A:407:MET:HE1	1.95	0.48
1:A:435:SER:HB3	1:A:458:GLY:CA	2.43	0.48
1:A:543:THR:HG22	1:A:565:LEU:HB2	1.95	0.48
1:D:415:ILE:HG23	1:D:439:GLU:HB2	1.95	0.48
1:D:675:ILE:O	1:D:699:SER:OG	2.21	0.48
1:D:626:LYS:HD2	1:D:650:GLU:OE2	2.14	0.47
1:D:426:ALA:HA	1:D:448:THR:O	2.14	0.47
1:A:515:SER:OG	1:A:539:ARG:NH2	2.47	0.47
1:D:256:GLN:HA	1:D:278:GLU:O	2.13	0.47
1:D:150:GLU:O	1:D:173:LEU:HD12	2.14	0.47
1:D:331:ILE:HG21	1:D:346:LEU:HD13	1.96	0.47
1:A:263:SER:O	1:A:265:ASN:O	2.32	0.47
1:D:170:ILE:HG12	1:D:173:LEU:HB2	1.97	0.47
1:D:196:GLU:O	1:D:198:VAL:HG23	2.15	0.47
1:D:349:ASN:HB3	1:D:351:LEU:HD13	1.97	0.47
1:A:722:LEU:O	1:A:722:LEU:HD22	2.15	0.46
1:A:550:LEU:HD13	1:A:559:MET:HE1	1.98	0.46
1:A:256:GLN:HA	1:A:278:GLU:O	2.15	0.46
1:D:715:PRO:HD2	1:D:718:LEU:HD12	1.95	0.46
1:A:443:ILE:HA	1:A:467:GLY:O	2.16	0.46
1:A:722:LEU:HD23	1:A:729:PHE:CD2	2.50	0.46
1:D:107:SER:HB3	1:D:129:ASP:CG	2.40	0.46
1:D:308:PRO:HG2	1:D:311:LEU:HG	1.96	0.46
1:D:407:MET:HG3	1:D:410:MET:HE3	1.97	0.46
1:A:144:ASP:HB2	1:A:166:SER:HB2	1.98	0.46
1:A:300:SER:HA	1:A:324:GLU:O	2.16	0.46
1:A:737:ILE:HD12	1:A:738:PRO:HD2	1.98	0.46
1:D:519:GLU:CD	1:D:520:GLY:H	2.24	0.46
1:D:170:ILE:HG21	1:D:173:LEU:HD22	1.98	0.46
1:D:653:ILE:O	1:D:678:THR:HB	2.14	0.46
1:A:594:VAL:HB	1:A:619:PRO:HG3	1.98	0.45
1:D:232:VAL:HG12	1:D:254:SER:HB2	1.97	0.45
1:D:315:LYS:HG2	1:D:316:ASN:H	1.80	0.45
1:D:533:SER:HA	1:D:556:LEU:HA	1.98	0.45
1:D:519:GLU:HG2	1:D:541:ARG:HB3	1.97	0.45
1:A:724:SER:C	1:A:726:PRO:HD3	2.40	0.45
1:D:29:LEU:HD21	1:D:31:SER:HB3	1.99	0.45
1:D:461:LEU:O	1:D:484:THR:HG23	2.17	0.45
1:D:236:PRO:HG2	1:D:239:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:LEU:HD21	1:D:248:LEU:HD22	1.99	0.45
1:D:126:ALA:HB2	1:D:148:ARG:HE	1.82	0.45
1:A:428:PRO:HA	1:A:429:PRO:HD3	1.83	0.44
1:A:554:GLN:O	1:A:579:SER:OG	2.26	0.44
1:A:719:GLU:O	1:A:723:LEU:HG	2.17	0.44
1:A:384:TRP:HE3	1:A:410:MET:CE	2.30	0.44
1:D:489:ILE:HD12	1:D:491:ARG:HG2	1.98	0.44
1:D:443:ILE:HD11	1:D:489:ILE:CG1	2.48	0.44
1:D:29:LEU:HB2	1:D:76:ASN:OD1	2.16	0.44
1:D:263:SER:O	1:D:266:CYS:HB2	2.18	0.44
1:D:266:CYS:O	1:D:267:LYS:HB2	2.17	0.44
1:A:508:LEU:HD21	1:A:511:LEU:HD12	1.98	0.44
1:A:587:PHE:CE2	1:A:611:GLU:HG3	2.53	0.44
1:D:55:LYS:HD3	1:D:55:LYS:HA	1.89	0.44
1:A:232:VAL:HA	1:A:254:SER:O	2.17	0.44
1:A:627:LYS:HD3	1:A:627:LYS:HA	1.85	0.44
1:D:142:THR:C	1:D:144:ASP:H	2.24	0.44
1:D:322:LEU:HD23	1:D:322:LEU:HA	1.69	0.44
1:A:532:LEU:HD13	1:A:535:ILE:HD11	1.99	0.44
1:A:642:ILE:O	1:A:668:PRO:HG3	2.18	0.44
1:A:511:LEU:HD23	1:A:511:LEU:C	2.43	0.43
1:D:260:ARG:H	1:D:260:ARG:HG3	1.59	0.43
1:D:294:ASP:O	1:D:318:THR:N	2.47	0.43
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.81	0.43
1:D:202:MET:HB3	1:D:207:PHE:HE2	1.84	0.43
1:A:162:GLU:HG2	1:A:163:LEU:H	1.82	0.43
1:A:634:ALA:HB2	1:A:657:ASP:CG	2.43	0.43
1:D:670:LYS:HD2	1:D:670:LYS:HA	1.83	0.43
1:A:39:LEU:HA	1:A:42:HIS:HD2	1.84	0.43
1:A:719:GLU:HA	1:A:722:LEU:HB3	2.00	0.43
1:A:460:LYS:HE2	1:A:460:LYS:HB3	1.67	0.43
1:D:307:ILE:HD12	1:D:331:ILE:HG22	2.00	0.43
1:D:410:MET:O	1:D:434:ASN:ND2	2.41	0.43
1:A:348:ASP:OD2	2:J:18:ARG:NH2	2.50	0.43
1:D:593:SER:HA	1:D:615:SER:O	2.19	0.43
1:A:448:THR:HG22	1:A:470:LEU:HB2	2.01	0.42
1:D:50:VAL:HA	1:D:54:TRP:CD1	2.55	0.42
1:D:120:GLY:O	1:D:145:SER:HB2	2.19	0.42
1:D:270:LEU:N	1:D:270:LEU:HD23	2.34	0.42
1:A:384:TRP:CD1	1:A:404:PRO:HG2	2.54	0.42
1:A:478:SER:O	1:A:481:HIS:CD2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:THR:C	1:D:144:ASP:N	2.78	0.42
1:D:521:PRO:HA	1:D:543:THR:O	2.20	0.42
1:A:179:ASP:CG	2:J:9:ARG:HH22	2.26	0.42
1:D:174:GLN:O	1:D:198:VAL:N	2.43	0.42
1:D:315:LYS:O	1:D:316:ASN:HB2	2.20	0.42
1:D:443:ILE:HA	1:D:467:GLY:O	2.19	0.42
1:A:426:ALA:HA	1:A:448:THR:O	2.20	0.42
1:A:85:SER:HB2	1:A:87:VAL:HG23	2.01	0.42
1:D:29:LEU:HG	1:D:31:SER:N	2.34	0.42
1:D:522:ILE:O	1:D:547:PRO:HG3	2.20	0.42
1:D:104:LEU:HD23	1:D:128:LEU:HD13	2.02	0.42
1:A:722:LEU:HD23	1:A:729:PHE:CE2	2.55	0.41
1:D:78:ALA:O	1:D:101:LEU:HD12	2.20	0.41
1:A:647:GLY:HA3	1:A:670:LYS:HB3	2.02	0.41
1:A:678:THR:HG22	1:A:679:ARG:CG	2.49	0.41
1:A:732:ASN:HA	1:A:733:PRO:HD2	1.84	0.41
1:D:117:SER:O	1:D:142:THR:OG1	2.37	0.41
1:A:418:LEU:HB3	1:A:423:PHE:CE2	2.56	0.41
1:A:680:LEU:O	1:A:703:VAL:HA	2.20	0.41
1:D:634:ALA:HB2	1:D:657:ASP:CG	2.45	0.41
1:A:199:GLU:CD	1:A:223:ILE:HD12	2.45	0.41
1:A:407:MET:O	1:A:410:MET:HG3	2.19	0.41
1:D:42:HIS:CD2	1:D:92:GLY:HA3	2.55	0.41
1:D:173:LEU:O	1:D:196:GLU:HB3	2.20	0.41
1:D:348:ASP:CG	2:P:18:ARG:HH21	2.28	0.41
1:D:618:ILE:HD11	1:D:663:LEU:HD21	2.02	0.41
1:A:44:ASP:N	1:A:88:SER:O	2.53	0.41
1:A:224:LEU:HD23	1:A:248:LEU:HD13	2.03	0.41
1:A:514:ASN:HA	1:A:538:SER:O	2.21	0.41
1:D:195:LYS:O	1:D:220:SER:OG	2.34	0.41
1:D:390:THR:HA	1:D:412:LYS:O	2.21	0.41
1:D:428:PRO:HA	1:D:429:PRO:HD3	1.85	0.41
1:D:348:ASP:OD2	2:P:18:ARG:NH2	2.54	0.41
1:A:596:SER:HA	1:A:621:PHE:CD2	2.57	0.40
1:D:33:GLY:O	1:D:37:LEU:HD22	2.20	0.40
1:D:455:LEU:HA	1:D:455:LEU:HD23	1.87	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	708/710 (100%)	690 (98%)	18 (2%)	0	100	100
1	D	708/710 (100%)	685 (97%)	23 (3%)	0	100	100
2	J	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
2	P	14/17 (82%)	14 (100%)	0	0	100	100
All	All	1445/1454 (99%)	1403 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	628/628 (100%)	582 (93%)	46 (7%)	13	27
1	D	628/628 (100%)	565 (90%)	63 (10%)	7	15
2	J	14/14 (100%)	14 (100%)	0	100	100
2	P	13/14 (93%)	12 (92%)	1 (8%)	12	25
All	All	1283/1284 (100%)	1173 (91%)	110 (9%)	10	21

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	56	ILE

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Mol	Chain	Res	Type
1	A	72	ASP
1	A	88	SER
1	A	114	THR
1	A	123	THR
1	A	143	LEU
1	A	148	ARG
1	A	163	LEU
1	A	165	GLU
1	A	175	VAL
1	A	184	THR
1	A	189	GLN
1	A	196	GLU
1	A	200	LEU
1	A	250	VAL
1	A	260	ARG
1	A	266	CYS
1	A	309	SER
1	A	311	LEU
1	A	335	LEU
1	A	359	LEU
1	A	460	LYS
1	A	464	LEU
1	A	481	HIS
1	A	483	LYS
1	A	503	SER
1	A	504	GLN
1	A	555	ASN
1	A	574	LEU
1	A	590	LEU
1	A	618	ILE
1	A	625	LEU
1	A	644	SER
1	A	663	LEU
1	A	675	ILE
1	A	691	LEU
1	A	695	LYS
1	A	716	ASP
1	A	718	LEU
1	A	719	GLU
1	A	722	LEU
1	A	725	GLU
1	A	735	LEU

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Mol	Chain	Res	Type
1	A	736	CYS
1	A	737	ILE
1	D	37	LEU
1	D	43	LEU
1	D	50	VAL
1	D	77	VAL
1	D	80	LEU
1	D	97	GLU
1	D	99	LYS
1	D	114	THR
1	D	123	THR
1	D	146	LEU
1	D	159	LEU
1	D	170	ILE
1	D	175	VAL
1	D	179	ASP
1	D	189	GLN
1	D	196	GLU
1	D	197	LEU
1	D	213	GLU
1	D	215	ILE
1	D	235	LEU
1	D	239	LEU
1	D	250	VAL
1	D	255	LEU
1	D	260	ARG
1	D	266	CYS
1	D	270	LEU
1	D	314	LEU
1	D	326	ARG
1	D	337	ASN
1	D	343	LEU
1	D	350	GLN
1	D	351	LEU
1	D	365	LEU
1	D	366	GLU
1	D	381	ILE
1	D	382	GLU
1	D	393	LEU
1	D	399	LEU
1	D	403	LEU
1	D	414	LYS

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Mol	Chain	Res	Type
1	D	460	LYS
1	D	464	LEU
1	D	481	HIS
1	D	489	ILE
1	D	508	LEU
1	D	556	LEU
1	D	611	GLU
1	D	618	ILE
1	D	625	LEU
1	D	627	LYS
1	D	646	ILE
1	D	663	LEU
1	D	675	ILE
1	D	678	THR
1	D	691	LEU
1	D	705	VAL
1	D	716	ASP
1	D	719	GLU
1	D	722	LEU
1	D	725	GLU
1	D	735	LEU
1	D	736	CYS
1	D	737	ILE
2	P	14	VAL

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

Mol	Chain	Res	Type
1	A	434	ASN
1	A	707	ASN
1	A	717	ASN
1	D	189	GLN
1	D	210	ASN
1	D	350	GLN
1	D	396	GLN
1	D	555	ASN
1	D	734	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 ⓘ

6 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	B	1	3,1	14,14,15	0.65	0	17,19,21	1.52	3 (17%)
3	NAG	B	2	3	14,14,15	0.59	0	17,19,21	1.71	4 (23%)
3	NAG	C	1	3,1	14,14,15	1.04	1 (7%)	17,19,21	1.85	2 (11%)
3	NAG	C	2	3	14,14,15	0.54	0	17,19,21	0.85	0
3	NAG	E	1	3,1	14,14,15	0.48	0	17,19,21	1.26	1 (5%)
3	NAG	E	2	3	14,14,15	0.56	0	17,19,21	1.07	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
3	NAG	B	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	O7-C7	-2.16	1.18	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	5.13	119.06	112.19
3	B	1	NAG	C2-N2-C7	-3.82	117.79	122.90
3	B	2	NAG	O5-C1-C2	3.69	116.99	111.29
3	C	1	NAG	O3-C3-C2	-3.57	101.99	109.40
3	E	1	NAG	C1-O5-C5	3.47	116.84	112.19
3	B	2	NAG	C3-C4-C5	-3.31	104.23	110.23
3	B	1	NAG	O5-C1-C2	-2.72	107.08	111.29
3	B	1	NAG	C1-C2-N2	2.65	114.62	110.43
3	B	2	NAG	C1-O5-C5	2.64	115.73	112.19
3	E	2	NAG	C1-O5-C5	2.58	115.65	112.19
3	B	2	NAG	C1-C2-N2	-2.53	106.44	110.43

There are no chirality outliers.

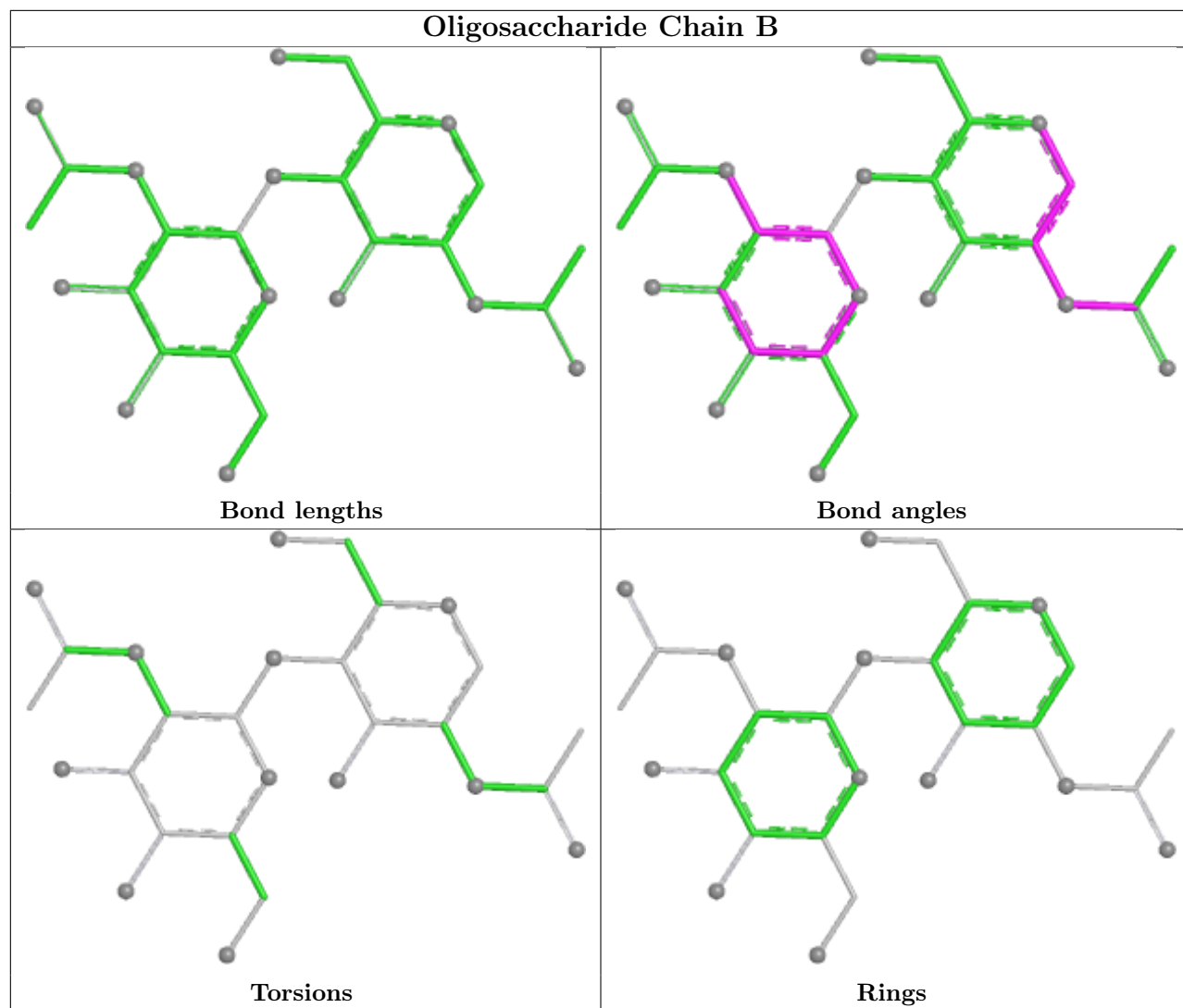
All (9) torsion outliers are listed below:

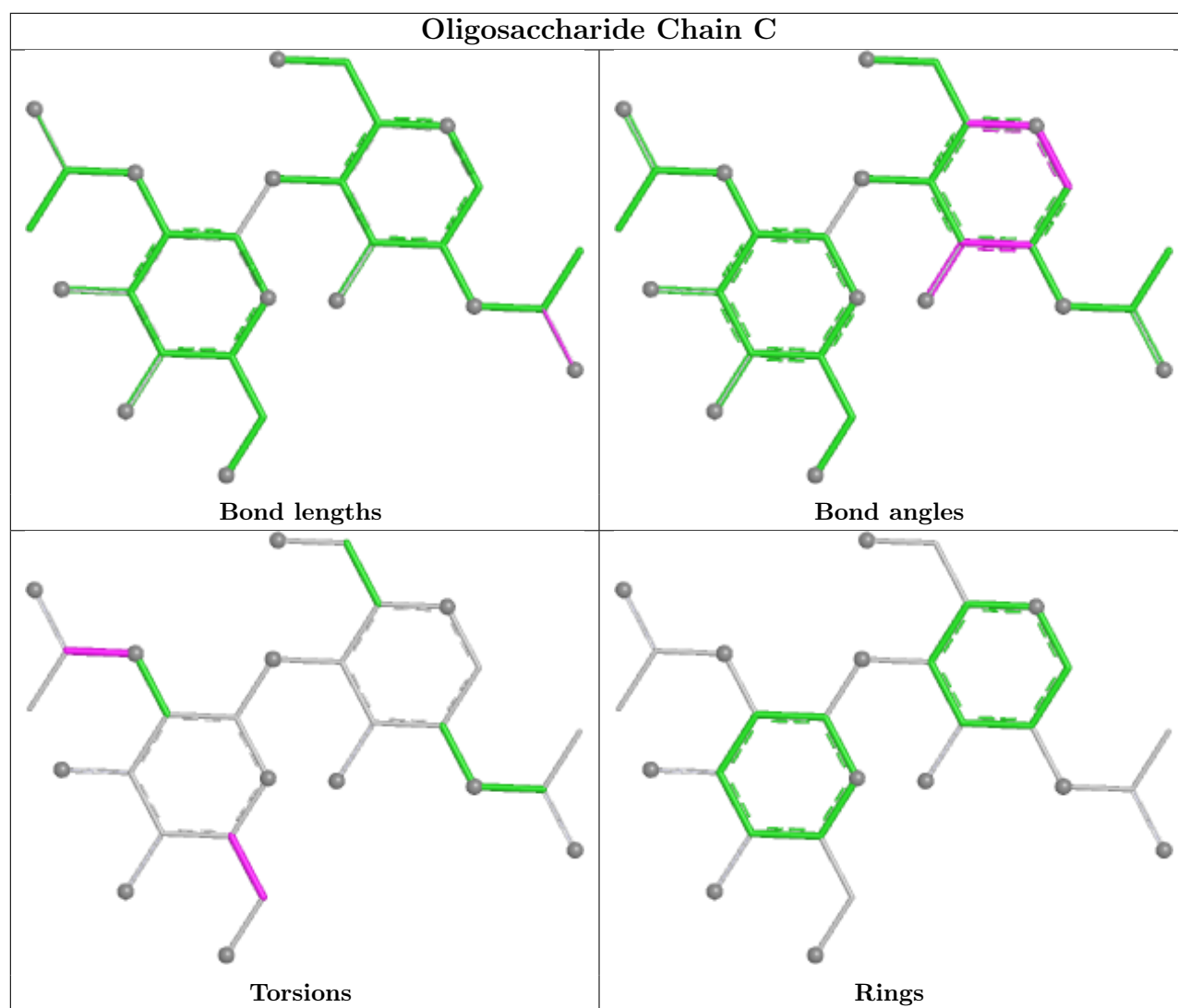
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	E	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O7-C7-N2-C2

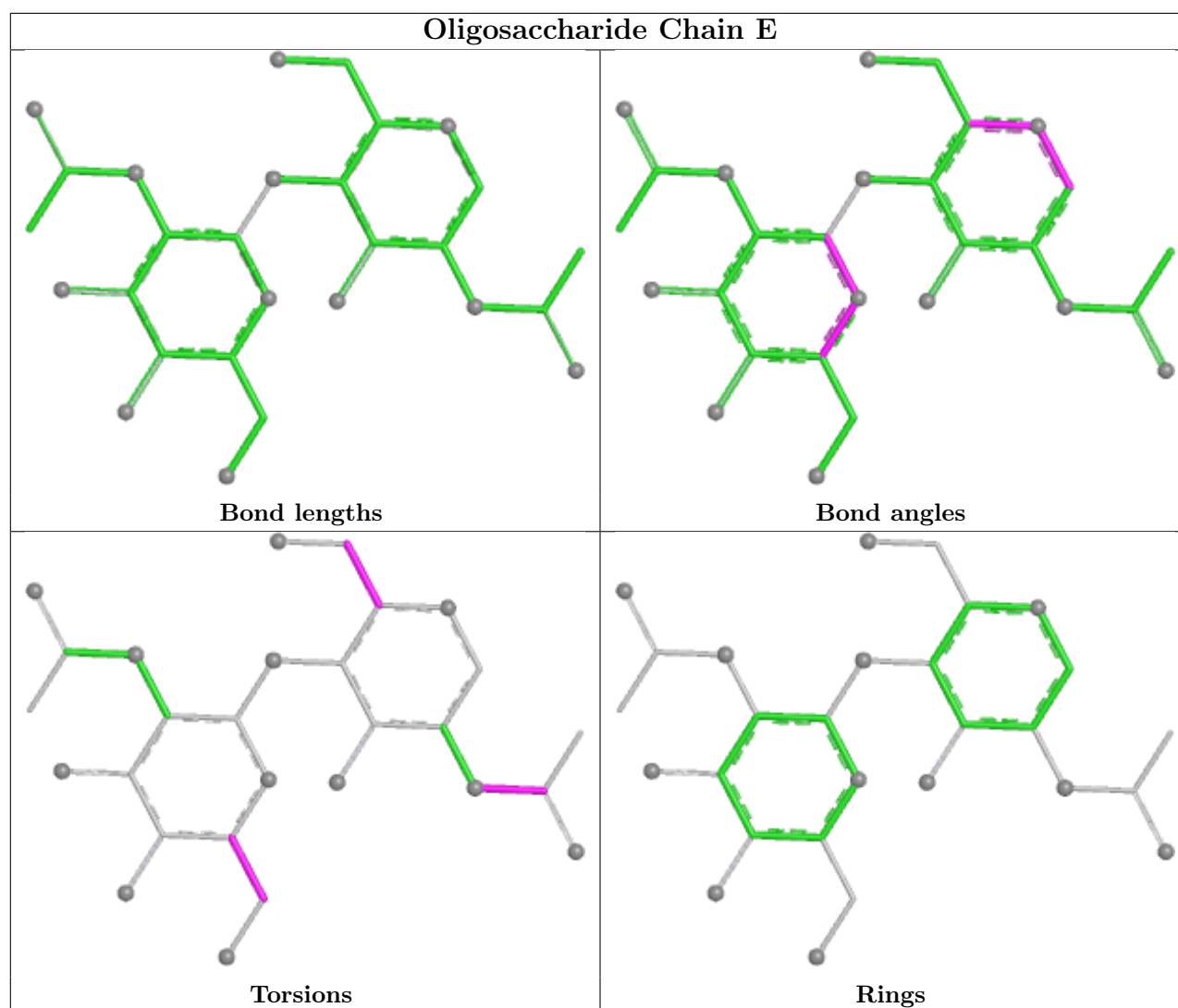
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	D	806	1	14,14,15	0.66	0	17,19,21	1.25	3 (17%)
4	NAG	A	805	1	14,14,15	0.60	0	17,19,21	1.07	0
5	SO4	A	807	-	4,4,4	0.26	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	801	1	14,14,15	0.52	0	17,19,21	1.71	7 (41%)
4	NAG	D	807	1	14,14,15	0.75	0	17,19,21	1.56	2 (11%)
4	NAG	A	802	1	14,14,15	0.52	0	17,19,21	1.51	2 (11%)
4	NAG	D	803	1	14,14,15	0.92	0	17,19,21	1.56	4 (23%)
4	NAG	A	806	1	14,14,15	0.53	0	17,19,21	1.13	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
4	NAG	D	806	1	-	0/6/23/26	0/1/1/1
4	NAG	A	805	1	-	0/6/23/26	0/1/1/1
4	NAG	A	801	1	-	0/6/23/26	0/1/1/1
4	NAG	D	807	1	-	0/6/23/26	0/1/1/1
4	NAG	A	802	1	-	1/6/23/26	0/1/1/1
4	NAG	D	803	1	-	5/6/23/26	0/1/1/1
4	NAG	A	806	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	802	NAG	C1-O5-C5	4.63	118.39	112.19
4	D	807	NAG	C1-O5-C5	3.95	117.49	112.19
4	D	803	NAG	O5-C5-C4	-3.23	102.98	110.83
4	D	803	NAG	C1-O5-C5	3.21	116.49	112.19
4	A	801	NAG	C2-N2-C7	-3.17	118.65	122.90
4	A	801	NAG	O5-C5-C6	2.93	113.37	107.66
4	A	802	NAG	C6-C5-C4	-2.76	106.23	113.02
4	D	806	NAG	O5-C5-C6	2.34	112.22	107.66
4	D	803	NAG	C4-C3-C2	2.33	114.44	111.02
4	A	801	NAG	C3-C4-C5	-2.25	106.14	110.23
4	D	803	NAG	C3-C4-C5	-2.24	106.16	110.23
4	A	801	NAG	O4-C4-C3	2.23	115.64	110.38
4	A	801	NAG	C4-C3-C2	-2.23	107.75	111.02
4	D	806	NAG	C6-C5-C4	-2.23	107.55	113.02
4	A	801	NAG	C1-O5-C5	2.21	115.15	112.19
4	A	801	NAG	C6-C5-C4	-2.09	107.90	113.02
4	D	806	NAG	O7-C7-C8	-2.08	118.35	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	807	NAG	O6-C6-C5	-2.05	104.36	111.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	803	NAG	C8-C7-N2-C2
4	D	803	NAG	O7-C7-N2-C2
4	D	803	NAG	O5-C5-C6-O6
4	D	803	NAG	C4-C5-C6-O6
4	D	803	NAG	C3-C2-N2-C7
4	A	802	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	710/710 (100%)	0.08	17 (2%) 59 55	10, 27, 65, 106	0
1	D	710/710 (100%)	0.56	46 (6%) 25 20	17, 45, 63, 74	0
2	J	17/17 (100%)	0.08	0 100 100	15, 23, 44, 46	0
2	P	16/17 (94%)	0.46	1 (6%) 26 21	28, 38, 63, 80	0
All	All	1453/1454 (99%)	0.32	64 (4%) 39 34	10, 36, 63, 106	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	738	PRO	5.2
1	A	686	ASN	4.7
1	A	29	LEU	4.6
1	D	160	THR	4.6
1	D	217	ASN	4.2
1	D	208	SER	3.9
1	D	481	HIS	3.8
1	D	204	ALA	3.7
1	D	221	LEU	3.7
1	D	435	SER	3.6
1	D	436	SER	3.5
1	A	737	ILE	3.3
1	D	205	ASN	3.2
1	A	735	LEU	3.1
1	A	75	LYS	3.0
1	D	244	ASN	3.0
1	D	185	GLY	2.9
1	D	497	GLY	2.9
1	A	481	HIS	2.9
1	D	218	SER	2.9
1	D	434	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	206	GLN	2.8
1	D	278	GLU	2.7
1	A	694	LEU	2.5
1	D	267	LYS	2.5
1	D	150	GLU	2.5
1	D	343	LEU	2.5
1	A	725	GLU	2.5
1	D	433	VAL	2.5
1	D	286	ALA	2.4
1	A	727	SER	2.4
1	A	648	LEU	2.4
1	D	29	LEU	2.4
1	D	232	VAL	2.4
1	A	728	SER	2.4
1	D	170	ILE	2.4
1	A	736	CYS	2.4
1	D	78	ALA	2.3
1	D	114	THR	2.3
1	D	479	ILE	2.3
1	D	429	PRO	2.3
1	D	161	GLY	2.3
1	A	691	LEU	2.3
1	D	268	ASN	2.2
1	A	682	ILE	2.2
1	D	58	ALA	2.2
1	D	349	ASN	2.2
1	D	428	PRO	2.2
1	D	215	ILE	2.1
1	D	169	ARG	2.1
1	D	137	ASP	2.1
1	D	315	LYS	2.1
1	D	222	GLN	2.1
1	A	662	GLY	2.1
1	D	519	GLU	2.1
1	D	184	THR	2.1
1	D	59	SER	2.1
1	D	284	PRO	2.1
1	D	207	PHE	2.1
1	D	358	ALA	2.1
1	A	244	ASN	2.1
1	D	350	GLN	2.0
1	D	333	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	P	8	GLN	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](#)

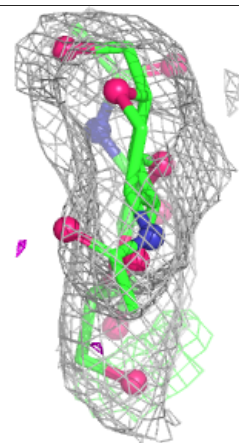
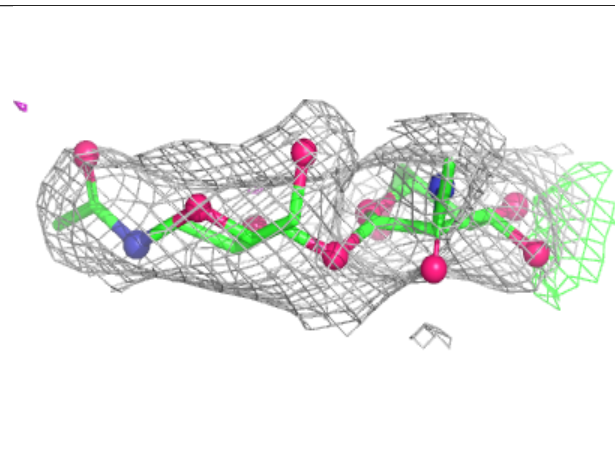
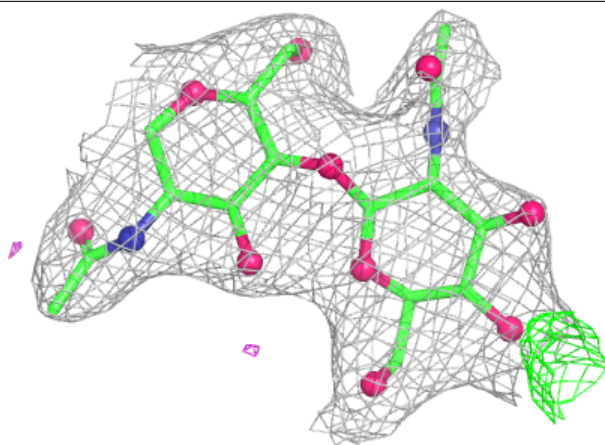
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	NAG	B	1	14/15	-	-	13,19,32,38	0
3	NAG	B	2	14/15	-	-	29,40,53,56	0
3	NAG	C	1	14/15	-	-	33,38,43,54	0
3	NAG	C	2	14/15	-	-	30,45,53,55	0
3	NAG	E	2	14/15	0.71	0.13	36,46,48,51	0
3	NAG	E	1	14/15	0.93	0.07	36,38,49,51	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.

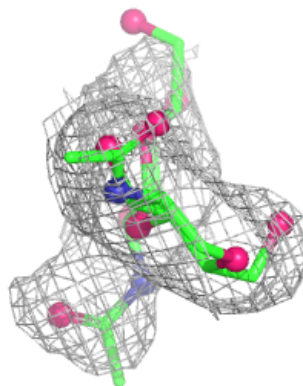
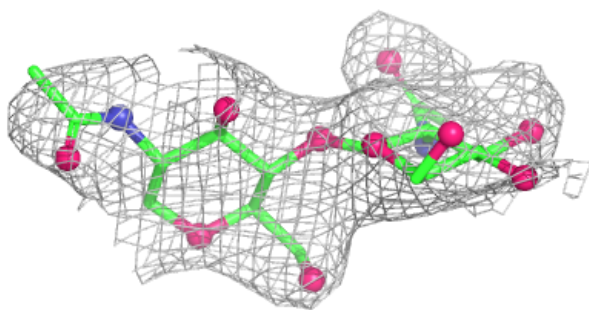
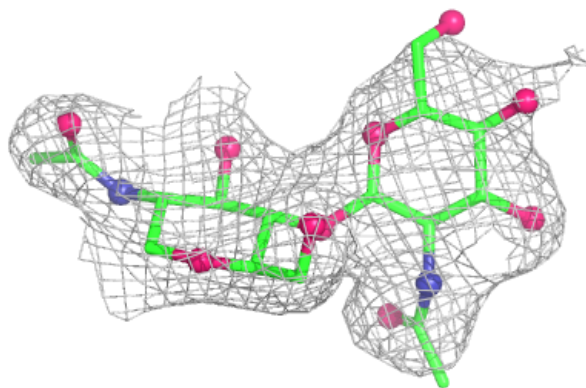
Electron density around Chain B:

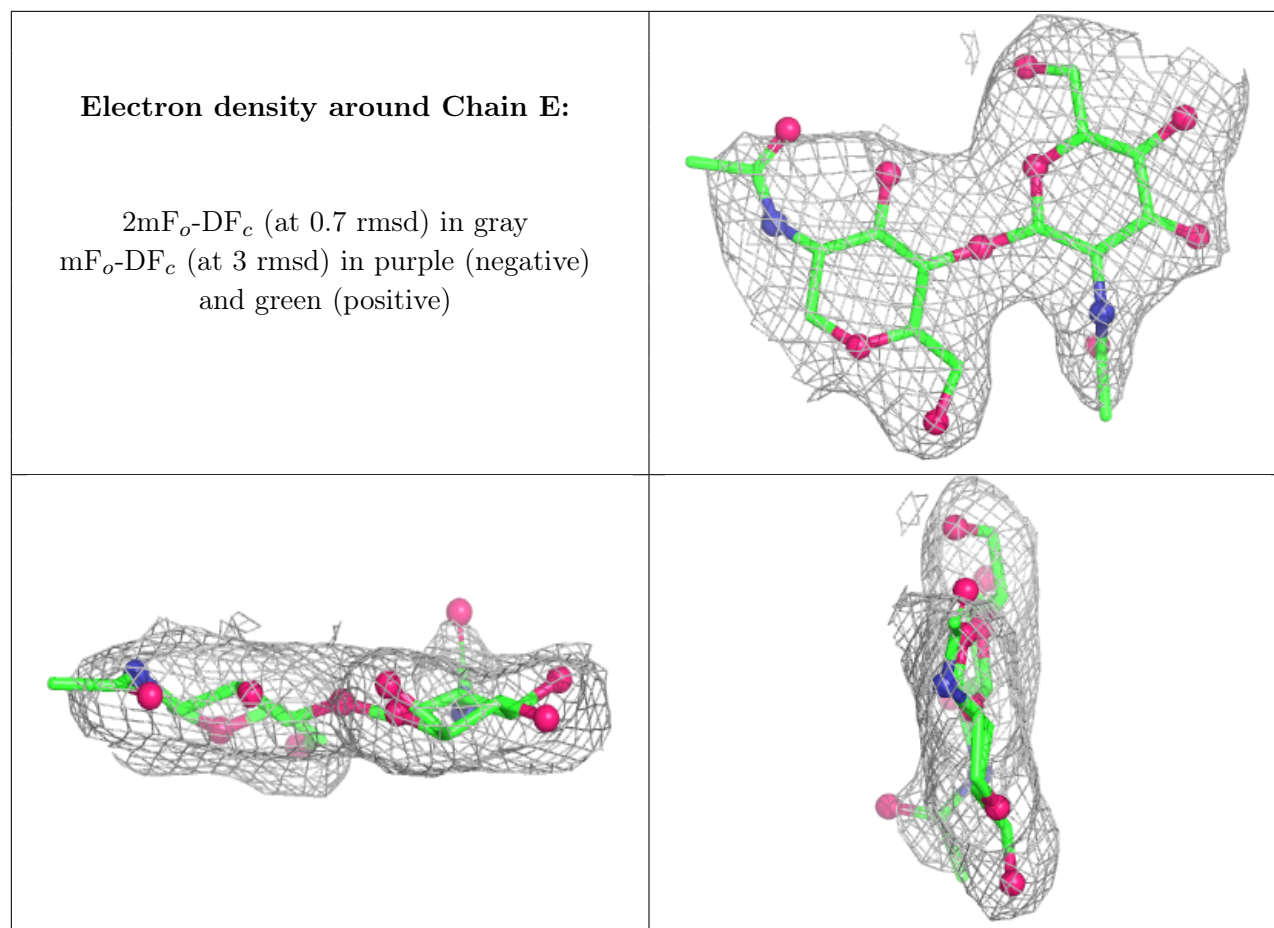
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain C:

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





6.4 Ligands [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
4	NAG	D	807	14/15	0.75	0.12	36,41,50,50	0
4	NAG	D	803	14/15	0.77	0.11	31,40,47,48	0
4	NAG	A	801	14/15	0.83	0.10	28,34,43,46	0
5	SO4	A	807	5/5	0.89	0.10	35,39,45,63	0
4	NAG	D	806	14/15	0.90	0.10	19,25,29,29	0
4	NAG	A	802	14/15	0.92	0.08	20,26,33,33	0
4	NAG	A	806	14/15	0.93	0.07	18,29,34,35	0
4	NAG	A	805	14/15	0.96	0.08	15,19,23,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.