



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:21 AM UTC

PDB ID : 4ZEL / pdb_00004zel
Title : Human dopamine beta-hydroxylase
Authors : Vendelboe, T.V.; Harris, P.; Christensen, H.E.M.; Harlos, K.; Walter, T.;
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Deposited on : 2015-04-20
Resolution : 2.90 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

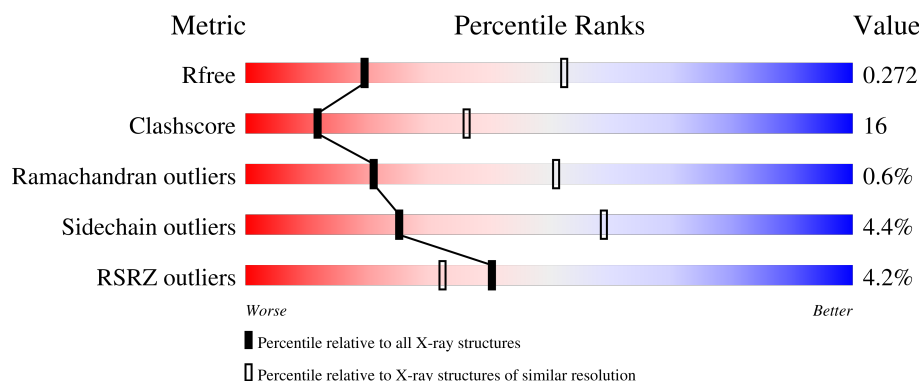
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	578	 4% 61% 30% 5%
1	B	578	 4% 63% 26% 6%
2	C	2	 50% 50%
3	D	3	 33% 33% 33%
3	F	3	 100%

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Mol	Chain	Length	Quality of chain
4	E	4	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8939 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 Dopamine beta-hydroxylase.

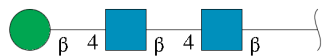
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	1	0
			4396	2813	747	810	26			
1	B	544	Total	C	N	O	S	0	2	0
			4346	2784	742	795	25			

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



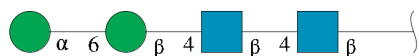
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 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	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

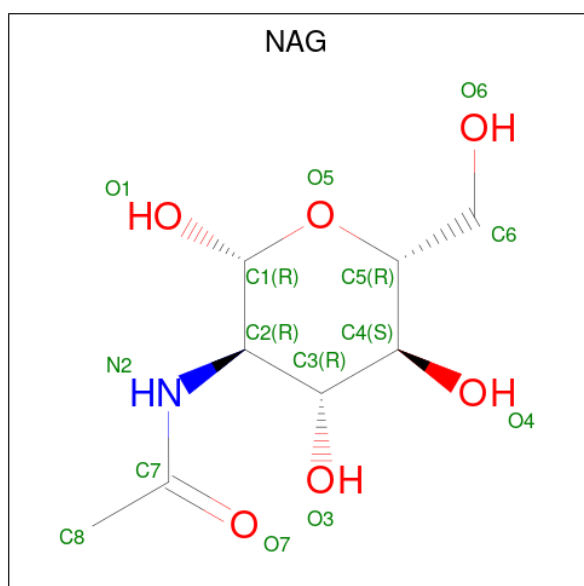


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

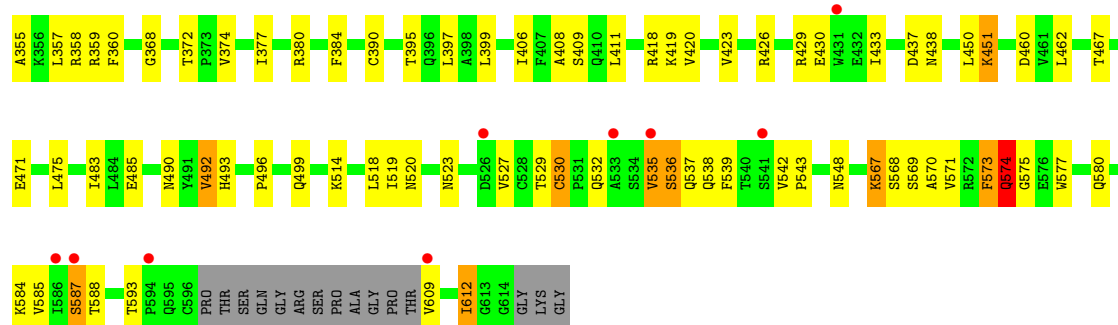
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	4	Total	O	0	0
			4	4		



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

Chain C: 50% 50%



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

Chain D: 33% 33% 33%



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

Chain F: 100%



- Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.81Å 119.06Å 224.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.53 – 2.90 59.53 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (59.53-2.90) 99.8 (59.53-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.230 , 0.270 0.232 , 0.272	Depositor DCC
R_{free} test set	1560 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8939	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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, MAN, NAG, CU

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	0.49	0/4516	1.13	27/6144 (0.4%)
1	B	0.45	0/4466	1.04	24/6073 (0.4%)
All	All	0.47	0/8982	1.09	51/12217 (0.4%)

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	7
1	B	0	5
All	All	0	12

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	ARG	N-CA-C	15.10	130.35	108.00
1	A	311	TYR	CA-C-N	14.04	133.58	119.82
1	A	311	TYR	C-N-CA	14.04	133.58	119.82
1	A	285	SER	N-CA-C	-9.84	92.43	108.07
1	A	270	ALA	CA-C-N	9.34	129.96	119.32
1	A	270	ALA	C-N-CA	9.34	129.96	119.32
1	B	276	VAL	CA-C-N	-9.10	111.02	120.03
1	B	276	VAL	C-N-CA	-9.10	111.02	120.03
1	B	575	GLY	N-CA-C	8.51	122.47	110.38
1	A	326	ARG	CB-CA-C	-8.39	104.59	116.34
1	A	368	GLY	N-CA-C	8.19	120.86	110.38
1	A	357	LEU	N-CA-C	8.18	121.77	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	LYS	N-CA-C	7.95	122.14	110.14
1	A	325	SER	N-CA-C	7.84	121.88	109.65
1	B	542	VAL	CA-C-N	7.79	129.58	119.84
1	B	542	VAL	C-N-CA	7.79	129.58	119.84
1	B	530	CYS	N-CA-C	7.76	122.21	109.79
1	B	536	SER	N-CA-C	7.11	120.36	108.20
1	B	298	VAL	N-CA-C	7.02	118.44	107.28
1	A	587	SER	N-CA-C	7.02	120.08	109.41
1	B	529	THR	CA-C-N	-6.98	115.08	122.89
1	B	529	THR	C-N-CA	-6.98	115.08	122.89
1	B	285	SER	N-CA-C	6.96	120.87	112.38
1	A	399	LEU	CA-C-N	6.92	124.64	119.66
1	A	399	LEU	C-N-CA	6.92	124.64	119.66
1	A	258	GLU	CA-C-N	6.90	130.09	120.29
1	A	258	GLU	C-N-CA	6.90	130.09	120.29
1	B	236	GLU	N-CA-C	6.85	119.84	109.23
1	A	575	GLY	N-CA-C	-6.64	101.53	110.56
1	A	279	PHE	N-CA-C	6.58	120.25	109.06
1	B	537	GLN	N-CA-C	6.41	121.17	113.23
1	B	368	GLY	N-CA-C	6.18	118.29	110.38
1	A	289	PRO	CA-C-O	-6.13	114.38	121.86
1	B	293	ASN	CA-C-N	-6.06	114.25	122.86
1	B	293	ASN	C-N-CA	-6.06	114.25	122.86
1	B	535	VAL	N-CA-C	6.04	121.90	109.34
1	A	290	ASP	CA-C-N	5.85	130.98	121.74
1	A	290	ASP	C-N-CA	5.85	130.98	121.74
1	B	567	LYS	N-CA-C	-5.84	100.63	109.85
1	A	257	ASN	N-CA-C	5.77	120.44	113.17
1	B	295	CYS	N-CA-C	-5.51	106.14	112.92
1	A	275	SER	N-CA-C	5.50	118.89	110.36
1	A	288	LYS	CB-CG-CD	-5.39	98.90	111.30
1	A	207	LEU	N-CA-C	5.38	116.85	110.07
1	B	539	PHE	N-CA-C	5.36	117.13	111.28
1	B	574	GLN	CA-C-N	-5.34	114.89	121.83
1	B	574	GLN	C-N-CA	-5.34	114.89	121.83
1	B	210	ASP	N-CA-C	-5.22	105.66	112.23
1	B	538	GLN	N-CA-C	5.19	118.18	110.14
1	A	258	GLU	O-C-N	5.02	127.44	122.12
1	A	267	PHE	N-CA-C	5.01	117.77	109.85

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	ARG	Peptide
1	A	189	GLN	Peptide
1	A	206	GLU	Peptide
1	A	288	LYS	Peptide
1	A	289	PRO	Peptide
1	A	291	ARG	Peptide
1	A	324	SER	Peptide
1	B	293	ASN	Peptide
1	B	296	ARG	Peptide
1	B	530	CYS	Peptide
1	B	573	PHE	Peptide
1	B	587	SER	Peptide

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	4396	0	4284	172	0
1	B	4346	0	4245	111	1
2	C	28	0	25	0	0
3	D	39	0	34	2	0
3	F	39	0	34	0	0
4	E	50	0	43	0	0
5	A	1	0	0	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
7	A	8	0	0	1	1
7	B	4	0	0	1	1
All	All	8939	0	8691	278	2

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 16.

All (278) 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:288:LYS:HE2	1:A:289:PRO:HD3	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:C	1:A:294:TYR:H	1.85	0.85
1:B:243:ARG:HA	1:B:320:GLY:HA3	1.60	0.84
1:A:235:LYS:HD2	1:A:236:GLU:H	1.43	0.83
1:A:429:ARG:NH1	1:A:587:SER:OG	2.12	0.83
1:A:248:LYS:HB3	1:A:352:TYR:HB2	1.61	0.83
1:B:408:ALA:HB3	1:B:493:HIS:HB2	1.62	0.82
1:A:408:ALA:HB3	1:A:493:HIS:HB2	1.60	0.81
1:B:573:PHE:O	1:B:577:TRP:NE1	2.15	0.80
1:A:313:GLU:HA	1:A:358:ARG:HH11	1.45	0.80
1:B:296:ARG:O	1:B:297:HIS:ND1	2.16	0.79
1:A:279:PHE:CE1	1:A:288:LYS:HD2	2.18	0.78
1:B:67:TYR:OH	1:B:199:LYS:O	2.02	0.77
1:B:243:ARG:NH1	1:B:324:SER:OG	2.19	0.76
1:A:235:LYS:HD2	1:A:236:GLU:N	2.00	0.76
1:B:248:LYS:HB3	1:B:352:TYR:HB2	1.66	0.75
1:A:253:VAL:HG11	1:A:258:GLU:HA	1.68	0.74
1:B:103:LEU:HD12	1:B:145:LEU:HD21	1.70	0.73
1:A:292:LEU:O	1:A:294:TYR:N	2.22	0.72
1:A:326:ARG:NH1	1:A:327:TYR:O	2.23	0.72
1:A:184:ASN:HD21	3:D:1:NAG:C7	1.99	0.72
1:A:221:ILE:HG21	1:A:280:SER:OG	1.89	0.72
1:A:534:SER:HB3	1:A:537:GLN:HB3	1.72	0.72
1:B:236:GLU:OE1	1:B:327:TYR:HA	1.91	0.71
1:A:149:ARG:HH22	1:A:158:ASP:HB3	1.56	0.70
1:B:243:ARG:HD3	1:B:318:ALA:HB1	1.73	0.70
1:A:252:ILE:HD11	1:A:350:ARG:HB2	1.74	0.70
1:A:269:CYS:N	1:A:326:ARG:HD3	2.07	0.70
1:A:426:ARG:NH2	1:A:458:PRO:O	2.24	0.70
1:A:355:ALA:C	1:A:356:LYS:HD2	2.16	0.70
1:A:83:ALA:O	1:A:105:THR:OG1	2.07	0.70
1:A:126:ASP:OD1	1:A:157:LYS:NZ	2.26	0.69
1:A:289:PRO:HB2	1:A:290:ASP:OD1	1.93	0.69
1:A:518:LEU:HG	1:B:518:LEU:HD22	1.74	0.69
1:B:475:LEU:O	7:B:801:HOH:O	2.11	0.69
1:B:215:GLU:O	1:B:235:LYS:NZ	2.17	0.68
1:B:252:ILE:HD11	1:B:350:ARG:HB2	1.75	0.67
1:A:130:ASP:OD2	1:A:149:ARG:NH1	2.28	0.66
1:B:429:ARG:HH12	1:B:588:THR:C	2.04	0.66
1:B:84:GLY:HA3	1:B:173:LEU:HD12	1.77	0.66
1:A:247:ILE:HG12	1:A:354:THR:HG23	1.78	0.65
1:A:259:ALA:O	1:A:262:HIS:NE2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ARG:HH22	1:B:532:GLN:NE2	1.95	0.64
1:A:590:GLU:N	1:A:590:GLU:OE1	2.29	0.63
1:A:290:ASP:CG	1:A:291:ARG:H	2.06	0.63
1:B:269:CYS:HA	1:B:295:CYS:HA	1.81	0.62
1:A:426:ARG:NE	1:A:460:ASP:OD1	2.31	0.62
1:A:139:THR:HG23	1:A:141:GLU:H	1.65	0.62
1:B:307:LYS:HG3	1:B:308:ALA:N	2.15	0.61
1:A:269:CYS:H	1:A:326:ARG:HD3	1.62	0.61
1:B:335:HIS:ND1	1:B:337:PRO:HD3	2.15	0.61
1:A:529:THR:HG22	1:A:531:PRO:HD3	1.82	0.61
1:B:419:LYS:HB2	1:B:467:THR:HB	1.83	0.61
1:A:326:ARG:HG3	1:A:327:TYR:N	2.15	0.61
1:A:325:SER:OG	1:A:326:ARG:N	2.33	0.61
1:A:524:ASN:OD1	1:A:525:GLU:N	2.33	0.61
1:A:104:TRP:HE3	1:A:111:TYR:HB2	1.65	0.61
1:B:128:GLN:H	1:B:128:GLN:CD	2.09	0.61
1:A:524:ASN:HB2	1:B:514:LYS:HE2	1.82	0.60
1:A:104:TRP:CE3	1:A:111:TYR:HB2	2.36	0.60
1:A:290:ASP:OD1	1:A:291:ARG:N	2.34	0.60
1:B:294:TYR:HB2	1:B:296:ARG:HG3	1.82	0.60
1:A:357:LEU:HG	1:A:358:ARG:O	2.01	0.60
1:A:219:PRO:HD3	1:A:233:TYR:CD1	2.37	0.59
1:A:295:CYS:O	1:A:329:ARG:NH1	2.35	0.59
1:A:236:GLU:HG2	1:A:327:TYR:CD2	2.37	0.59
1:A:243:ARG:HB2	1:A:321:GLY:HA3	1.84	0.59
1:A:67:TYR:OH	1:A:199:LYS:O	2.12	0.59
1:A:231:TRP:CH2	1:A:281:GLY:HA2	2.38	0.59
1:B:184:ASN:OD1	1:B:185:GLY:N	2.35	0.58
1:A:275:SER:OG	1:A:276:VAL:N	2.35	0.58
1:A:279:PHE:CZ	1:A:288:LYS:HD2	2.38	0.58
1:A:219:PRO:HD3	1:A:233:TYR:CE1	2.39	0.58
1:B:568:SER:C	1:B:570:ALA:H	2.12	0.58
1:B:426:ARG:NH1	1:B:460:ASP:OD1	2.32	0.58
1:A:233:TYR:CE2	1:A:235:LYS:HB2	2.39	0.57
1:A:440:TYR:OH	1:A:445:GLN:NE2	2.35	0.57
1:B:397:LEU:HD21	1:B:574:GLN:HB2	1.84	0.57
1:B:227:GLU:O	1:B:336:ASN:N	2.27	0.57
1:A:200:PRO:HA	1:A:451:LYS:HG2	1.86	0.57
1:A:210:ASP:OD2	1:A:355:ALA:N	2.21	0.57
1:A:269:CYS:HB2	1:A:326:ARG:NE	2.19	0.57
1:B:66:SER:OG	1:B:69:GLN:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LYS:C	1:A:288:LYS:N	2.61	0.57
1:B:149:ARG:NH1	1:B:150:PRO:O	2.37	0.57
1:A:286:LYS:C	1:A:288:LYS:H	2.13	0.56
1:A:585:VAL:C	1:A:587:SER:H	2.11	0.56
1:B:208:PRO:HD2	1:B:211:ALA:HB2	1.87	0.56
1:A:356:LYS:HD2	1:A:356:LYS:N	2.20	0.56
1:B:247:ILE:HB	1:B:358:ARG:HH21	1.71	0.56
1:B:208:PRO:C	1:B:210:ASP:H	2.14	0.56
1:A:104:TRP:HZ3	1:A:609:VAL:HG11	1.71	0.56
1:B:217:GLN:HB3	1:B:346:SER:O	2.05	0.56
1:A:113:ALA:HB2	1:A:609:VAL:HG13	1.88	0.56
1:B:322:PRO:HA	1:B:324:SER:N	2.21	0.55
1:A:326:ARG:CG	1:A:327:TYR:H	2.17	0.55
1:A:414:HIS:ND1	1:A:485:GLU:O	2.30	0.55
1:A:527:VAL:HG12	1:A:527:VAL:O	2.08	0.54
1:B:236:GLU:CD	1:B:237:LEU:H	2.16	0.54
1:B:235:LYS:HG3	1:B:236:GLU:N	2.22	0.54
1:A:243:ARG:O	1:A:356:LYS:HE3	2.07	0.54
1:A:573:PHE:O	1:A:577:TRP:NE1	2.20	0.54
1:A:269:CYS:H	1:A:326:ARG:NH1	2.05	0.54
1:A:196:GLN:NE2	7:A:802:HOH:O	2.30	0.54
1:A:181:GLU:OE1	1:A:181:GLU:N	2.38	0.54
1:A:83:ALA:HB3	1:A:173:LEU:O	2.08	0.53
1:B:263[B]:HIS:CE1	1:B:333:HIS:HD1	2.27	0.53
1:B:188:LEU:HG	1:B:190:MET:HG2	1.91	0.53
1:A:271:PRO:HA	1:A:325:SER:HB3	1.91	0.53
1:A:429:ARG:HH22	1:A:589:LEU:HD12	1.73	0.53
1:A:429:ARG:HH11	1:A:430:GLU:H	1.54	0.53
1:A:576:GLU:O	1:A:580:GLN:NE2	2.41	0.53
1:B:181:GLU:OE2	1:B:181:GLU:N	2.42	0.52
1:A:235:LYS:CD	1:A:236:GLU:H	2.18	0.52
1:A:177:PHE:CE1	3:D:1:NAG:H62	2.43	0.52
1:A:299:LEU:HA	1:A:317:LEU:HD21	1.92	0.52
1:B:372:THR:HB	1:B:374:VAL:HG22	1.90	0.52
1:B:139:THR:HG23	1:B:141:GLU:H	1.74	0.52
1:A:221:ILE:HD13	1:A:231:TRP:CZ2	2.45	0.52
1:A:313:GLU:HA	1:A:358:ARG:NH1	2.22	0.52
1:A:409:SER:OG	1:A:490:ASN:OD1	2.27	0.52
1:B:125:LEU:HD11	1:B:609:VAL:HG22	1.91	0.52
1:B:216:VAL:HG12	1:B:330:LEU:HD22	1.91	0.51
1:A:295:CYS:C	1:A:296:ARG:HD3	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:VAL:HG22	1:A:334:TYR:CE1	2.46	0.51
1:A:326:ARG:CG	1:A:327:TYR:N	2.71	0.51
1:B:171:GLY:HA2	1:B:189:GLN:O	2.10	0.51
1:A:236:GLU:OE1	1:A:237:LEU:N	2.36	0.51
1:A:288:LYS:HB3	1:A:289:PRO:HD3	1.92	0.51
1:A:587:SER:OG	1:A:588:THR:N	2.43	0.51
1:B:165:THR:H	1:B:437:ASP:CG	2.19	0.51
1:A:104:TRP:HB3	1:A:106:ASP:CG	2.36	0.51
1:A:336:ASN:OD1	1:A:338:LEU:HB3	2.10	0.51
1:A:390:CYS:HA	1:A:563:MET:HE1	1.92	0.51
1:B:242:SER:HA	1:B:321:GLY:H	1.76	0.51
1:A:64:ASN:OD1	1:A:73:HIS:HB2	2.11	0.50
1:B:88:GLY:HA3	1:B:100:LEU:HD23	1.92	0.50
1:A:585:VAL:HG12	1:A:587:SER:HB3	1.94	0.50
1:B:251:PRO:HG3	1:B:302:TRP:NE1	2.27	0.50
1:B:170:TYR:CZ	1:B:191:GLY:HA3	2.46	0.50
1:A:326:ARG:HG3	1:A:327:TYR:H	1.76	0.49
1:A:276:VAL:HG21	1:A:289:PRO:HG2	1.94	0.49
1:A:48:PRO:HD2	1:A:64:ASN:HB3	1.94	0.49
1:B:411:LEU:HD13	1:B:420:VAL:HB	1.95	0.49
1:A:379:PRO:O	1:A:549:ARG:NH1	2.31	0.49
1:A:395:THR:O	1:A:399:LEU:HB2	2.13	0.49
1:A:222:GLN:HG3	1:A:342:GLY:HA3	1.94	0.49
1:A:521:ARG:NH2	1:B:532:GLN:NE2	2.61	0.49
1:A:104:TRP:CZ3	1:A:609:VAL:HG11	2.48	0.49
1:A:406:ILE:HG23	1:A:492:VAL:HG13	1.94	0.49
1:A:231:TRP:O	1:A:331:GLU:HA	2.13	0.48
1:B:69:GLN:HE21	1:B:148:LYS:HD3	1.77	0.48
1:A:263:HIS:HB3	1:A:333:HIS:HB3	1.94	0.48
1:B:177:PHE:CE2	1:B:183:ILE:HA	2.48	0.48
1:A:92:ARG:NH2	1:A:439:HIS:O	2.45	0.48
1:A:326:ARG:NH2	1:A:327:TYR:HB2	2.29	0.48
1:A:521:ARG:HH12	1:B:532:GLN:HE21	1.62	0.48
1:B:72:ILE:HD11	1:B:198:LEU:HD23	1.94	0.48
1:B:543:PRO:O	1:B:548:ASN:ND2	2.47	0.48
1:B:225:SER:O	1:B:226:GLN:HG3	2.14	0.48
1:A:270:ALA:HB1	1:A:272:GLU:OE1	2.14	0.48
1:B:257:ASN:HA	1:B:260:LEU:HD23	1.96	0.48
1:A:380:ARG:NH2	1:A:474:GLU:HG2	2.29	0.48
1:A:214:MET:HE1	1:A:237:LEU:HD23	1.94	0.47
1:A:231:TRP:CZ2	1:A:281:GLY:HA2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:HIS:CD2	1:B:357:LEU:HD22	2.49	0.47
1:A:139:THR:HG23	1:A:141:GLU:N	2.27	0.47
1:A:268:GLN:O	1:A:297:HIS:HB3	2.15	0.47
1:A:269:CYS:HA	1:A:295:CYS:HA	1.96	0.47
1:A:534:SER:O	1:A:538:GLN:N	2.48	0.47
1:A:139:THR:OG1	1:A:140:PRO:HD2	2.14	0.47
1:A:419:LYS:HB2	1:A:467:THR:HB	1.95	0.47
1:B:395:THR:O	1:B:399:LEU:HB2	2.14	0.47
1:A:149:ARG:NH2	1:A:159:TYR:O	2.48	0.47
1:A:266:VAL:HG23	1:A:349:ILE:HD12	1.97	0.47
1:A:288:LYS:HE2	1:A:288:LYS:HB3	1.57	0.47
1:A:289:PRO:HB2	1:A:290:ASP:CG	2.39	0.47
1:A:167:HIS:HE1	1:A:439:HIS:O	1.97	0.47
1:A:265:GLU:HB3	1:A:267:PHE:CE1	2.50	0.47
1:A:292:LEU:O	1:A:294:TYR:HD2	1.98	0.47
1:A:326:ARG:HG3	1:A:327:TYR:O	2.14	0.47
1:A:446:GLU:OE2	1:A:448:ARG:NH1	2.48	0.46
1:B:337:PRO:C	1:B:339:VAL:H	2.23	0.46
1:A:243:ARG:NH2	1:A:361:ASN:HD21	2.14	0.46
1:A:286:LYS:NZ	1:A:288:LYS:O	2.42	0.46
1:A:88:GLY:HA3	1:A:100:LEU:HD23	1.98	0.46
1:A:295:CYS:O	1:A:296:ARG:HD3	2.16	0.46
1:B:49:TYR:CE1	1:B:199:LYS:HD2	2.52	0.45
1:A:242:SER:O	1:A:244:HIS:ND1	2.48	0.45
1:B:390:CYS:HB3	1:B:462:LEU:HB2	1.97	0.45
1:B:429:ARG:NH1	1:B:587:SER:HB3	2.32	0.45
1:B:535:VAL:HG23	1:B:536:SER:H	1.81	0.45
1:B:406:ILE:HG23	1:B:492:VAL:HG13	1.98	0.45
1:A:221:ILE:HD13	1:A:231:TRP:CE2	2.52	0.45
1:A:279:PHE:CZ	1:A:288:LYS:CD	2.99	0.45
1:A:289:PRO:O	1:A:291:ARG:O	2.34	0.45
1:B:430:GLU:OE1	1:B:588:THR:OG1	2.35	0.45
1:A:165:THR:H	1:A:437:ASP:CG	2.25	0.45
1:A:225:SER:O	1:A:339:VAL:HG23	2.17	0.45
1:A:610:VAL:HG12	1:A:611:SER:H	1.82	0.45
1:B:269:CYS:HA	1:B:295:CYS:CB	2.47	0.45
1:B:139:THR:HG23	1:B:141:GLU:N	2.32	0.45
1:B:267:PHE:CE1	1:B:298:VAL:HG22	2.52	0.45
1:A:315:ALA:HB1	1:A:362:ALA:HB2	1.99	0.45
1:B:226:GLN:O	1:B:336:ASN:HB3	2.17	0.45
1:B:177:PHE:HD2	1:B:183:ILE:HG12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:GLN:O	1:B:567:LYS:HB3	2.16	0.44
1:A:297:HIS:HA	1:A:501:GLU:OE1	2.18	0.44
1:A:390:CYS:HB3	1:A:462:LEU:HB2	2.00	0.44
1:A:525:GLU:HG3	1:A:527:VAL:HG23	2.00	0.44
1:A:522:PHE:C	1:A:524:ASN:H	2.26	0.44
1:B:200:PRO:HB3	1:B:451:LYS:HA	1.99	0.44
1:B:577:TRP:HA	1:B:580:GLN:HE21	1.82	0.44
1:B:360:PHE:CD1	1:B:496:PRO:HB3	2.52	0.44
1:A:262:HIS:N	1:A:262:HIS:CD2	2.84	0.44
1:B:236:GLU:CD	1:B:237:LEU:N	2.75	0.44
1:B:568:SER:OG	1:B:571:VAL:HG22	2.18	0.44
1:A:429:ARG:HD2	1:A:587:SER:CB	2.48	0.44
1:B:573:PHE:HB3	1:B:574:GLN:HG2	1.99	0.44
1:A:419:LYS:HG2	1:A:438:ASN:O	2.18	0.43
1:B:419:LYS:HG2	1:B:438:ASN:O	2.17	0.43
1:A:396:GLN:HA	1:A:458:PRO:HB3	1.99	0.43
1:B:269:CYS:HA	1:B:295:CYS:CA	2.47	0.43
1:A:414:HIS:HB2	1:A:486:GLU:CD	2.44	0.43
1:B:110:ALA:HB3	1:B:612:ILE:O	2.19	0.43
1:B:302:TRP:CD1	1:B:306:ALA:HB3	2.54	0.43
1:B:423:VAL:HG12	1:B:433:ILE:HD13	1.99	0.43
1:A:233:TYR:HE2	1:A:235:LYS:HB2	1.80	0.43
1:A:128:GLN:HE22	1:A:157:LYS:NZ	2.16	0.43
1:A:437:ASP:HB3	1:A:440:TYR:HB2	2.01	0.43
1:A:429:ARG:HD2	1:A:429:ARG:HA	1.73	0.43
1:A:149:ARG:HG2	1:A:150:PRO:O	2.18	0.43
1:A:235:LYS:CD	1:A:236:GLU:N	2.77	0.43
1:A:538:GLN:O	1:A:542:VAL:HG23	2.19	0.43
1:B:243:ARG:NH1	1:B:319:PHE:HA	2.34	0.43
1:B:244:HIS:CD2	1:B:355:ALA:HA	2.54	0.43
1:A:134:LEU:HD11	1:A:148:LYS:HB2	2.01	0.42
1:B:130:ASP:OD1	1:B:130:ASP:N	2.42	0.42
1:B:139:THR:OG1	1:B:140:PRO:HD2	2.18	0.42
1:A:104:TRP:O	1:A:110:ALA:HA	2.20	0.42
1:B:202:ILE:H	1:B:202:ILE:HG13	1.73	0.42
1:B:206:GLU:HG2	1:B:207:LEU:N	2.34	0.42
1:B:519:ILE:HG13	1:B:520:ASN:N	2.34	0.42
1:A:233:TYR:CD1	1:A:279:PHE:O	2.73	0.42
1:A:272:GLU:H	1:A:272:GLU:CD	2.26	0.42
1:B:612:ILE:HD13	1:B:612:ILE:HA	1.89	0.42
1:A:312:PRO:HG2	1:A:407:PHE:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:PHE:CD2	1:B:183:ILE:HG12	2.55	0.42
1:A:297:HIS:HA	1:A:501:GLU:CD	2.44	0.42
1:B:95:LEU:HB2	1:B:190:MET:HE2	2.01	0.42
1:B:247:ILE:HG21	1:B:358:ARG:HE	1.84	0.42
1:B:377:ILE:HG23	1:B:384:PHE:CD2	2.54	0.42
1:B:409:SER:OG	1:B:490:ASN:OD1	2.36	0.42
1:A:311:TYR:HA	1:A:312:PRO:HD3	1.63	0.42
1:A:355:ALA:HB1	1:A:356:LYS:HD2	2.03	0.41
1:A:269:CYS:H	1:A:326:ARG:CD	2.31	0.41
1:B:585:VAL:C	1:B:587:SER:H	2.27	0.41
1:B:92:ARG:CZ	1:B:418[B]:ARG:HG2	2.51	0.41
1:B:568:SER:OG	1:B:571:VAL:N	2.53	0.41
1:A:417:GLY:O	1:A:418:ARG:NH1	2.51	0.41
1:A:238:PRO:O	1:A:241:PHE:HB2	2.21	0.41
1:A:232:CYS:N	1:A:283:CYS:SG	2.94	0.41
1:A:279:PHE:CZ	1:A:281:GLY:N	2.88	0.41
1:B:408:ALA:HA	1:B:450:LEU:HD13	2.01	0.41
1:A:559:ALA:HA	1:A:560:PRO:HD3	1.91	0.41
1:B:286:LYS:HD2	1:B:286:LYS:HA	1.91	0.41
1:A:577:TRP:HA	1:A:580:GLN:HE21	1.86	0.41
1:B:202:ILE:O	1:B:202:ILE:HD12	2.21	0.41
1:B:380:ARG:HA	1:B:471:GLU:HA	2.03	0.41
1:B:223:ILE:HA	1:B:224:PRO:HD3	1.83	0.41
1:B:243:ARG:CA	1:B:320:GLY:HA3	2.41	0.41
1:A:177:PHE:CD2	1:A:183:ILE:HA	2.57	0.40
1:A:423:VAL:HG12	1:A:433:ILE:HD13	2.03	0.40
1:A:286:LYS:HD2	1:A:286:LYS:HA	1.52	0.40
1:B:210:ASP:OD2	1:B:355:ALA:N	2.55	0.40
1:B:227:GLU:HA	1:B:336:ASN:O	2.20	0.40
1:A:297:HIS:HA	1:A:501:GLU:OE2	2.22	0.40
1:B:69:GLN:NE2	1:B:148:LYS:HD3	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:807:HOH:O	7:B:804:HOH:O[5_555]	2.08	0.12
1:B:359:ARG:NH1	1:B:593:THR:OG1[4_555]	2.17	0.03

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	545/578 (94%)	513 (94%)	27 (5%)	5 (1%)	14	41
1	B	536/578 (93%)	507 (95%)	27 (5%)	2 (0%)	30	59
All	All	1081/1156 (94%)	1020 (94%)	54 (5%)	7 (1%)	21	51

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	A	190[A]	MET
1	A	190[B]	MET
1	B	569	SER
1	A	527	VAL
1	A	339	VAL
1	B	339	VAL

5.3.2 Protein sidechains [i](#)

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	485/504 (96%)	465 (96%)	20 (4%)	27	61
1	B	479/504 (95%)	455 (95%)	24 (5%)	22	53
All	All	964/1008 (96%)	920 (95%)	44 (5%)	25	57

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	VAL
1	A	119	GLN
1	A	148	LYS
1	A	190[A]	MET
1	A	190[B]	MET
1	A	202	ILE
1	A	227	GLU
1	A	276	VAL
1	A	286	LYS
1	A	288	LYS
1	A	339	VAL
1	A	340	ILE
1	A	346	SER
1	A	356	LYS
1	A	357	LEU
1	A	377	ILE
1	A	492	VAL
1	A	588	THR
1	A	589	LEU
1	A	591	GLU
1	B	64	ASN
1	B	103	LEU
1	B	128	GLN
1	B	129	GLN
1	B	202	ILE
1	B	204	GLU
1	B	225	SER
1	B	227	GLU
1	B	263[A]	HIS
1	B	263[B]	HIS
1	B	268	GLN
1	B	272	GLU
1	B	276	VAL
1	B	286	LYS
1	B	294	TYR
1	B	451	LYS
1	B	483	ILE
1	B	485	GLU
1	B	492	VAL
1	B	523	ASN
1	B	527	VAL
1	B	574	GLN
1	B	584	LYS

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Mol	Chain	Res	Type
1	B	612	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	257	ASN
1	A	333	HIS
1	A	335	HIS
1	A	410	GLN
1	A	457	HIS
1	A	513	GLN
1	B	226	GLN
1	B	396	GLN
1	B	532	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.72	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	C	2	2	14,14,15	0.26	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	1	1,3	14,14,15	0.91	1 (7%)	17,19,21	0.88	1 (5%)
3	NAG	D	2	3	14,14,15	0.53	0	17,19,21	0.45	0
3	BMA	D	3	3	11,11,12	0.54	0	15,15,17	0.92	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.35	0	17,19,21	0.66	0
4	NAG	E	2	4	14,14,15	0.45	0	17,19,21	0.77	0
4	BMA	E	3	4	11,11,12	0.82	0	15,15,17	1.36	2 (13%)
4	MAN	E	4	4	11,11,12	0.76	0	15,15,17	1.52	2 (13%)
3	NAG	F	1	1,3	14,14,15	0.49	0	17,19,21	0.43	0
3	NAG	F	2	3	14,14,15	0.26	0	17,19,21	0.46	0
3	BMA	F	3	3	11,11,12	0.69	0	15,15,17	0.71	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
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	1/1/1/1
4	MAN	E	4	4	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	2.52	1.47	1.43
3	D	1	NAG	O5-C1	-2.48	1.39	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	MAN	C1-O5-C5	4.54	118.27	112.19
2	C	1	NAG	C1-O5-C5	4.31	117.97	112.19
4	E	3	BMA	C1-O5-C5	4.07	117.64	112.19
4	E	3	BMA	O2-C2-C3	-2.27	105.44	110.15
3	D	3	BMA	O2-C2-C3	-2.26	105.46	110.15
3	D	1	NAG	C3-C4-C5	2.10	114.03	110.23
4	E	4	MAN	O2-C2-C3	-2.03	105.95	110.15

There are no chirality outliers.

All (26) torsion outliers are listed below:

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

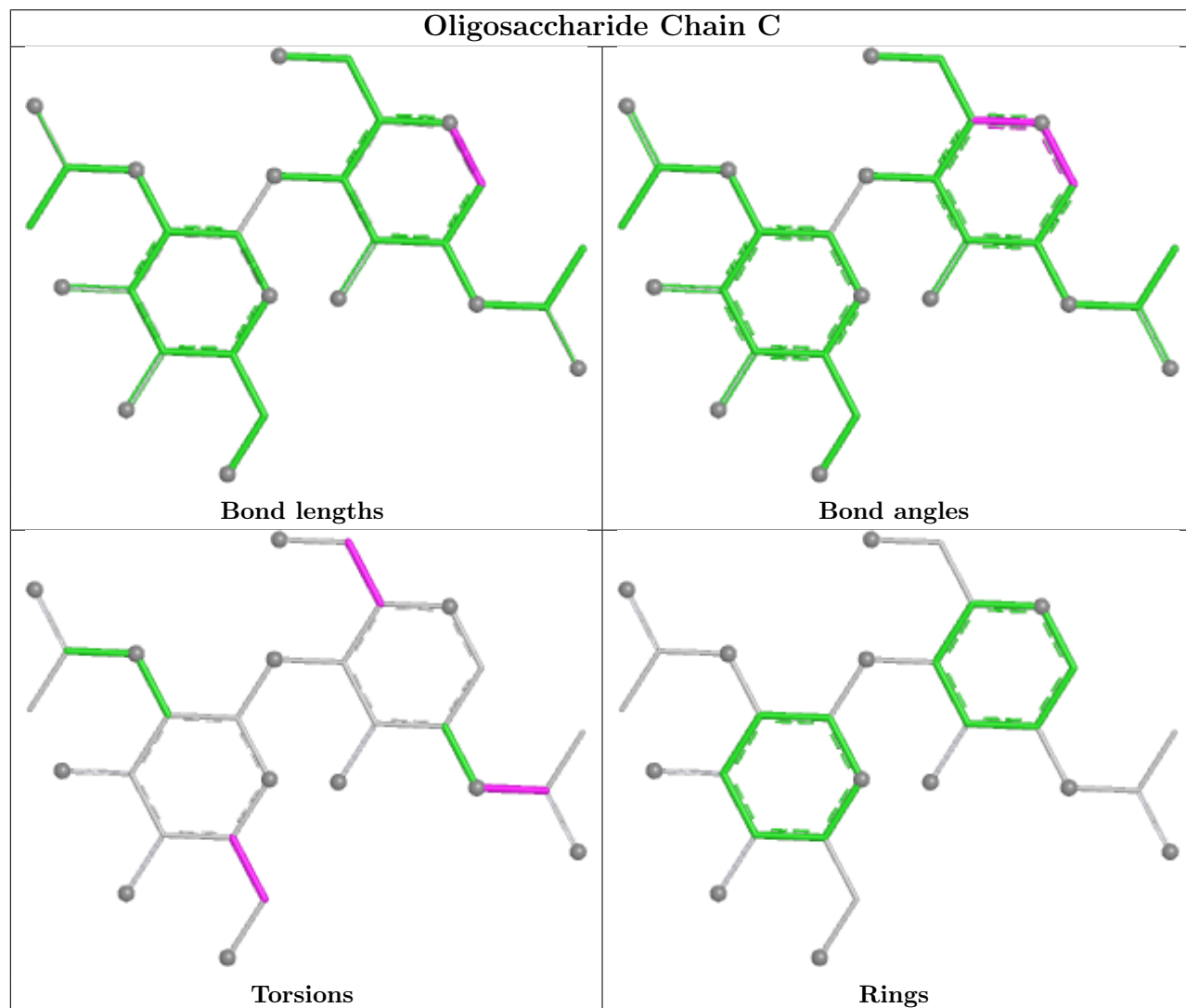
All (1) ring outliers are listed below:

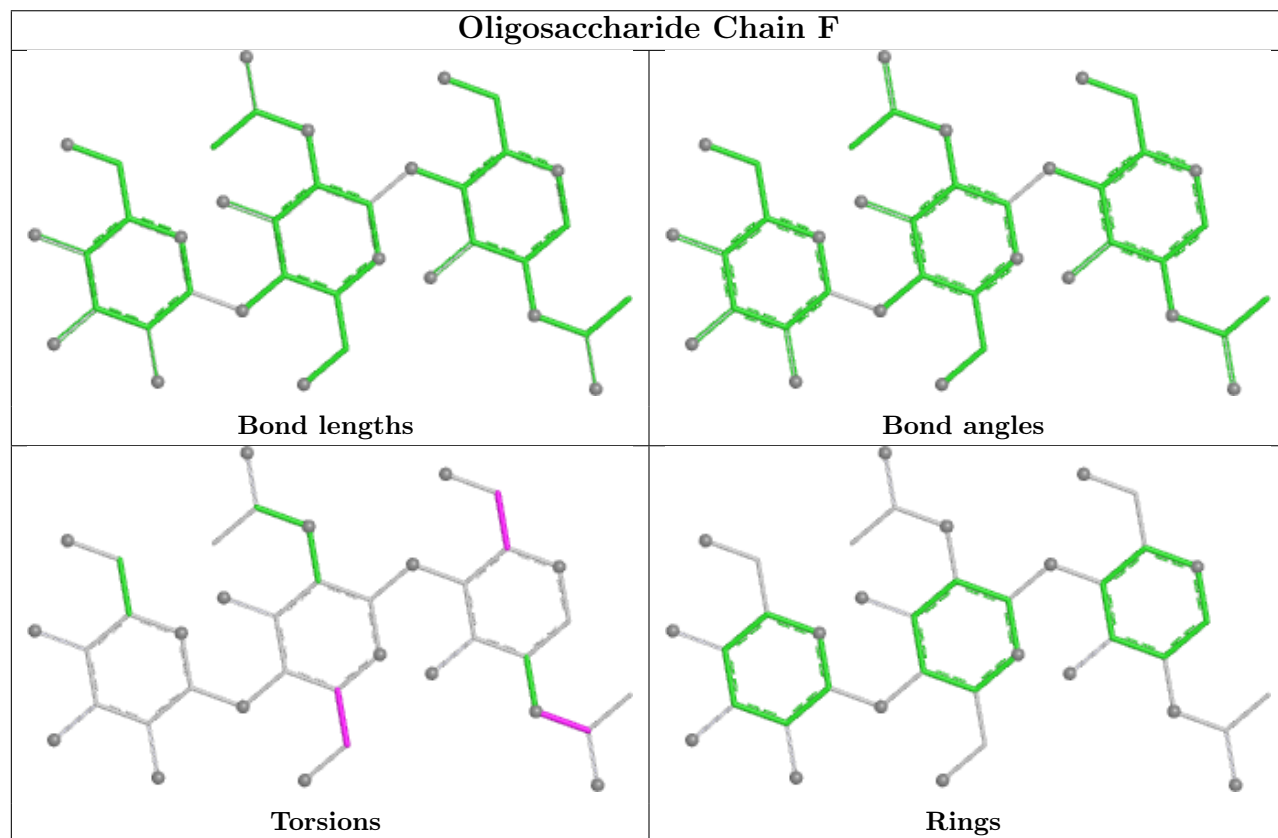
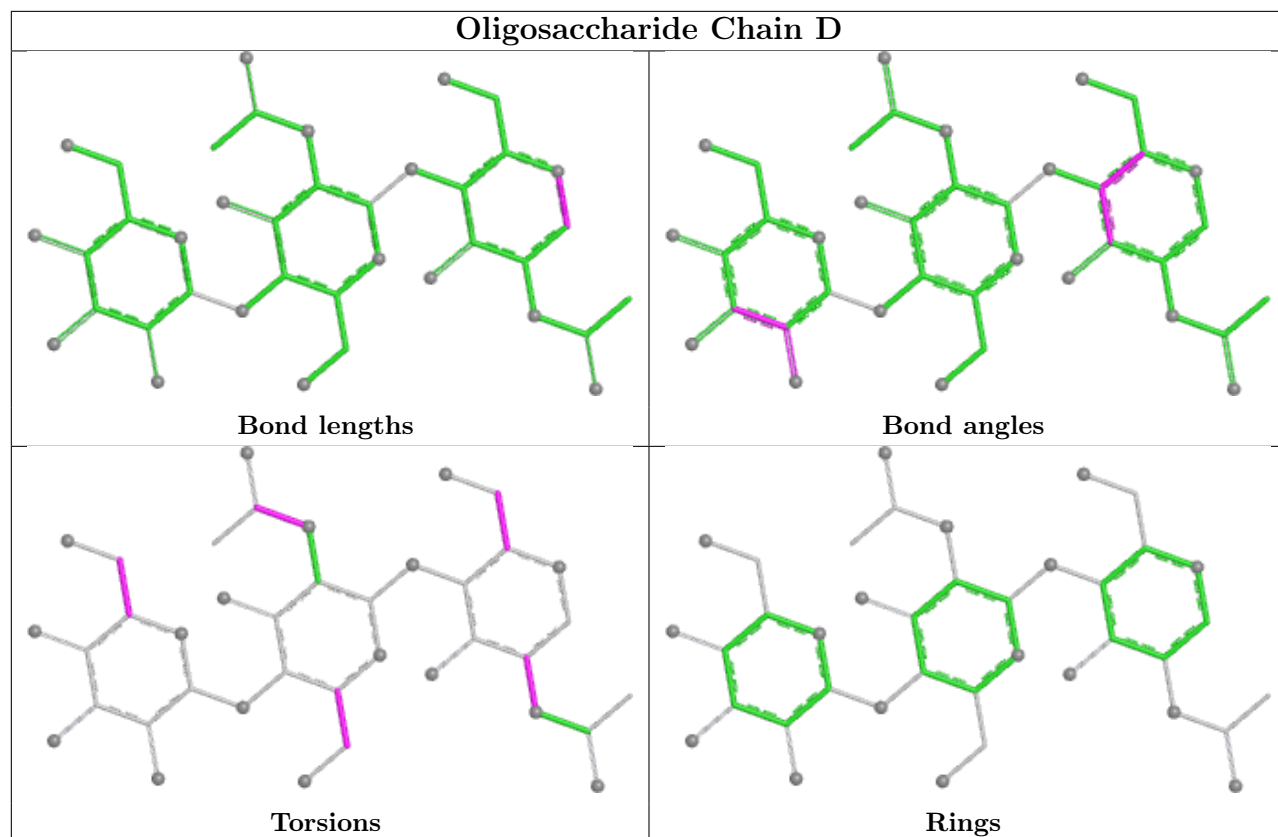
Mol	Chain	Res	Type	Atoms
4	E	3	BMA	C1-C2-C3-C4-C5-O5

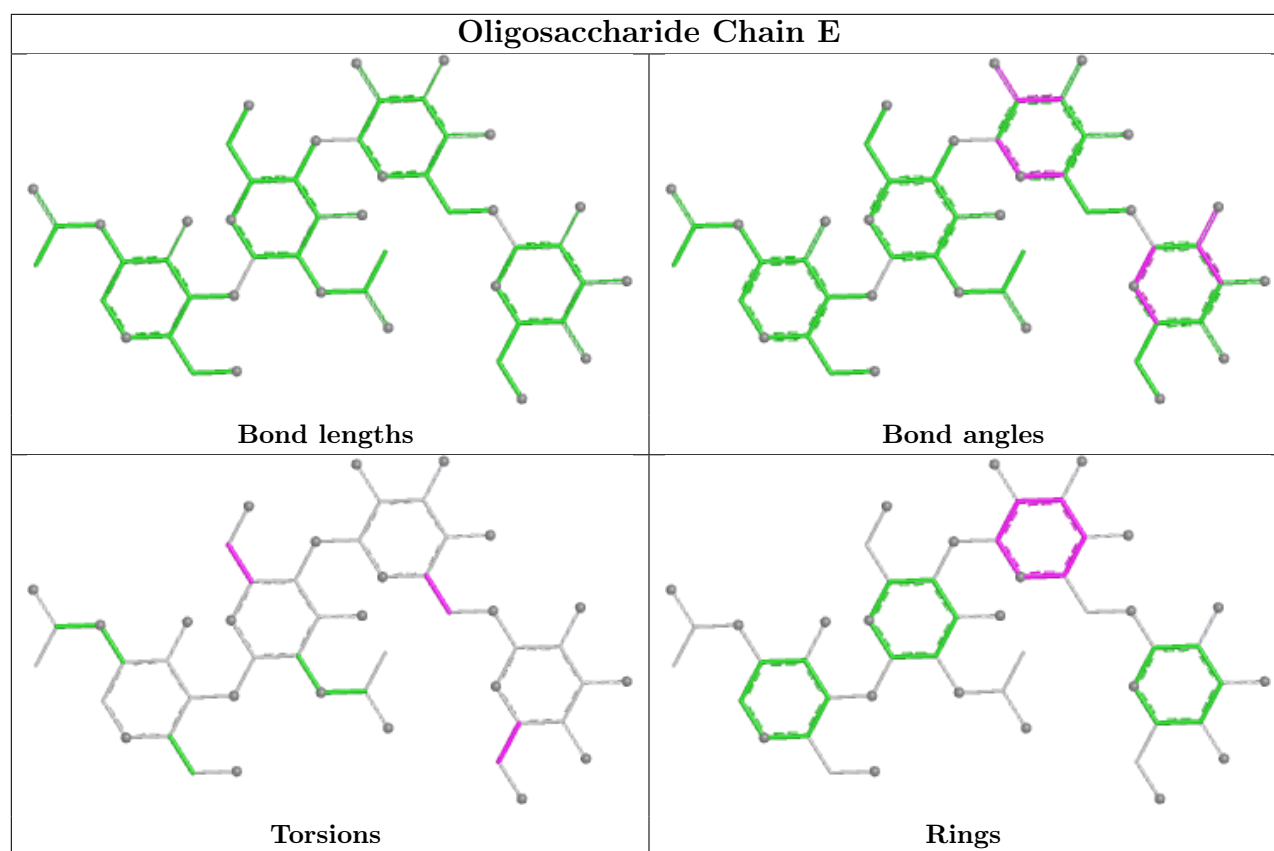
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	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 [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
6	NAG	A	702	1	14,14,15	0.32	0	17,19,21	0.49	0
6	NAG	B	705	1	14,14,15	1.46	2 (14%)	17,19,21	1.82	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	702	1	-	4/6/23/26	0/1/1/1
6	NAG	B	705	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	705	NAG	O5-C1	4.22	1.50	1.43
6	B	705	NAG	C1-C2	2.47	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	705	NAG	C1-O5-C5	5.73	119.86	112.19
6	B	705	NAG	O5-C1-C2	-4.05	105.03	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	NAG	O5-C5-C6-O6
6	A	702	NAG	C4-C5-C6-O6
6	B	705	NAG	O5-C5-C6-O6
6	A	702	NAG	C8-C7-N2-C2
6	A	702	NAG	O7-C7-N2-C2
6	B	705	NAG	C4-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	550/578 (95%)	0.41	25 (4%)	38 30	28, 69, 137, 197	1 (0%)
1	B	544/578 (94%)	0.29	21 (3%)	43 35	24, 64, 116, 170	2 (0%)
All	All	1094/1156 (94%)	0.35	46 (4%)	40 32	24, 67, 131, 197	3 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	587	SER	5.1
1	A	190[A]	MET	4.9
1	A	592	PRO	4.6
1	B	67	TYR	3.9
1	A	260	LEU	3.7
1	A	338	LEU	3.6
1	A	357	LEU	3.6
1	A	340	ILE	3.4
1	B	594	PRO	3.4
1	A	280	SER	3.3
1	A	569	SER	3.2
1	A	355	ALA	3.2
1	B	535	VAL	3.0
1	B	287	MET	2.9
1	A	282	PRO	2.9
1	A	277	PRO	2.8
1	A	180	LEU	2.8
1	B	292	LEU	2.8
1	B	263[A]	HIS	2.7
1	A	110	ALA	2.7
1	B	111	TYR	2.7
1	B	526	ASP	2.7
1	A	356	LYS	2.5
1	B	431	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	290	ASP	2.5
1	A	230	TYR	2.5
1	B	236	GLU	2.5
1	A	269	CYS	2.5
1	A	587	SER	2.5
1	B	103	LEU	2.4
1	A	483	ILE	2.4
1	B	586	ILE	2.3
1	A	104	TRP	2.3
1	A	105	THR	2.3
1	B	533	ALA	2.2
1	B	297	HIS	2.2
1	A	328	LEU	2.2
1	A	106	ASP	2.1
1	B	294	TYR	2.1
1	B	541	SER	2.1
1	B	276	VAL	2.0
1	B	46	PRO	2.0
1	A	262	HIS	2.0
1	A	332	VAL	2.0
1	B	313	GLU	2.0
1	B	609	VAL	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.

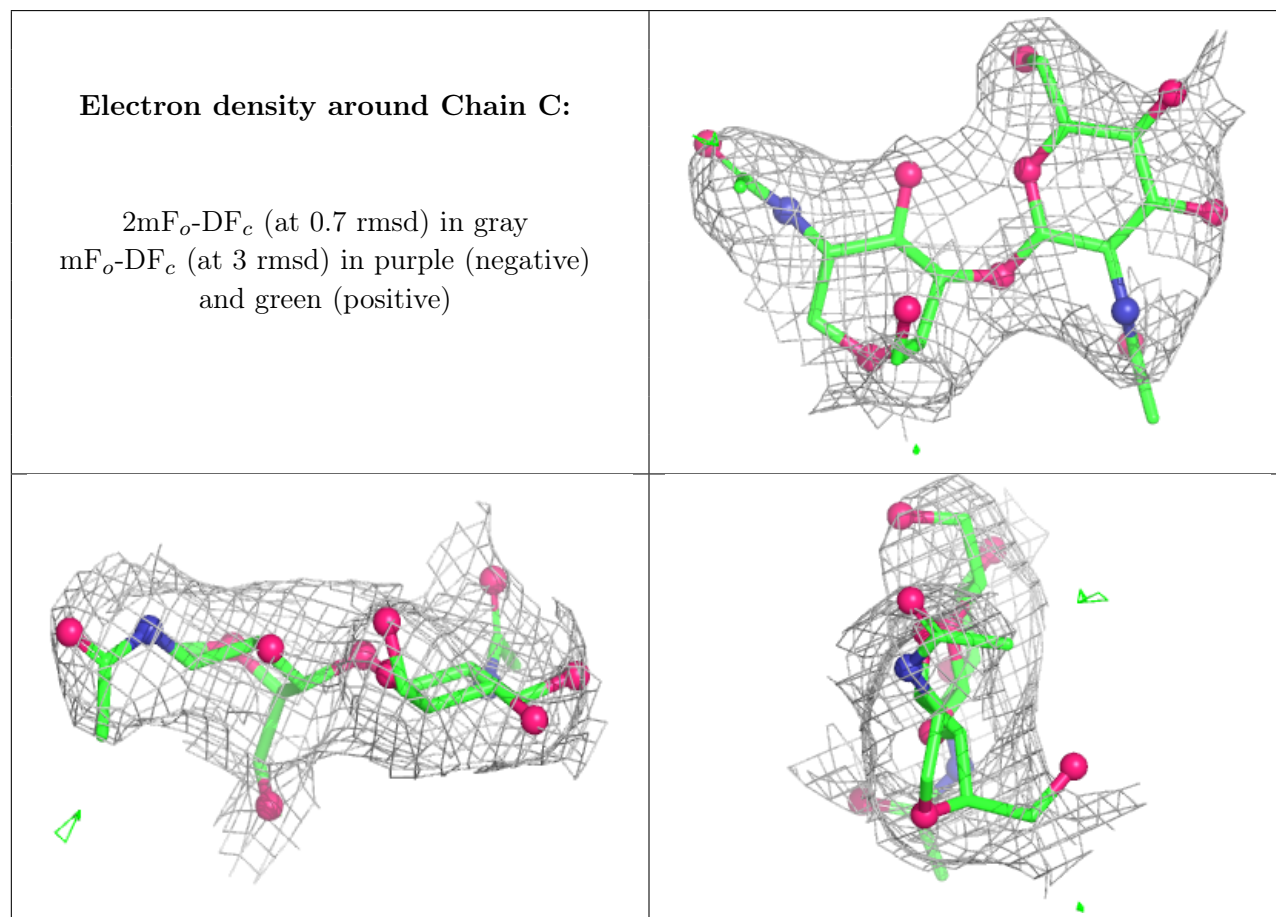
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	D	3	11/12	0.36	0.12	155,156,159,160	0
3	BMA	F	3	11/12	0.51	0.13	121,129,147,152	0
3	NAG	F	2	14/15	0.58	0.14	105,113,121,125	0
4	BMA	E	3	11/12	0.61	0.14	105,107,115,117	0
3	NAG	D	2	14/15	0.67	0.12	153,155,166,169	0
4	MAN	E	4	11/12	0.71	0.20	100,110,119,127	0

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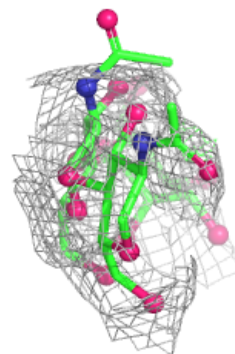
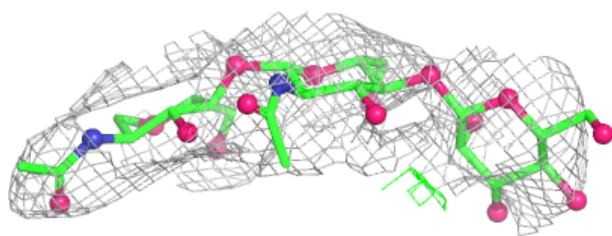
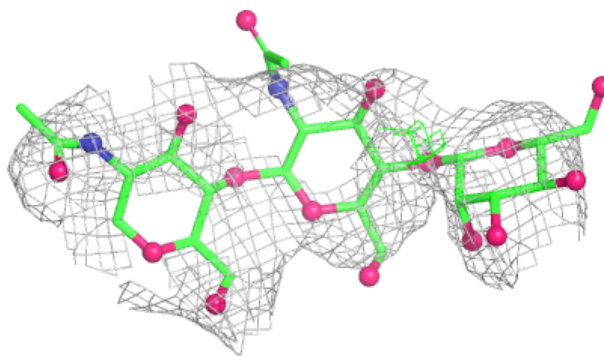
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	2	14/15	0.77	0.10	89,97,101,102	0
4	NAG	E	2	14/15	0.82	0.13	71,94,103,105	0
2	NAG	C	1	14/15	0.84	0.10	64,77,94,99	0
3	NAG	D	1	14/15	0.85	0.11	70,99,122,134	0
3	NAG	F	1	14/15	0.86	0.13	61,74,94,98	0
4	NAG	E	1	14/15	0.92	0.09	43,48,57,63	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.

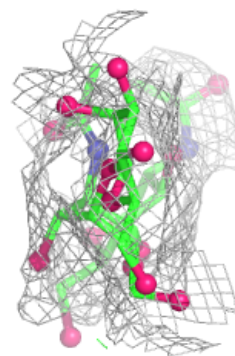
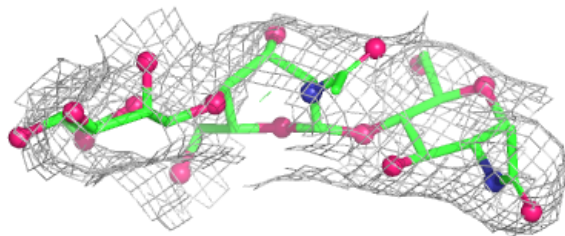
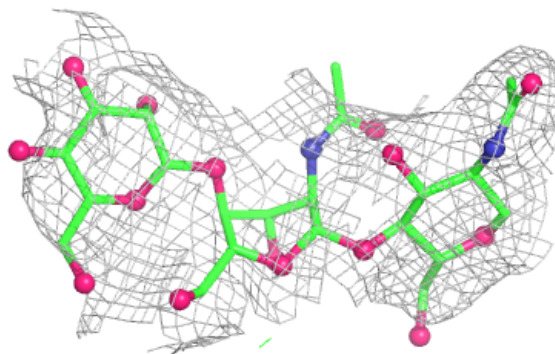


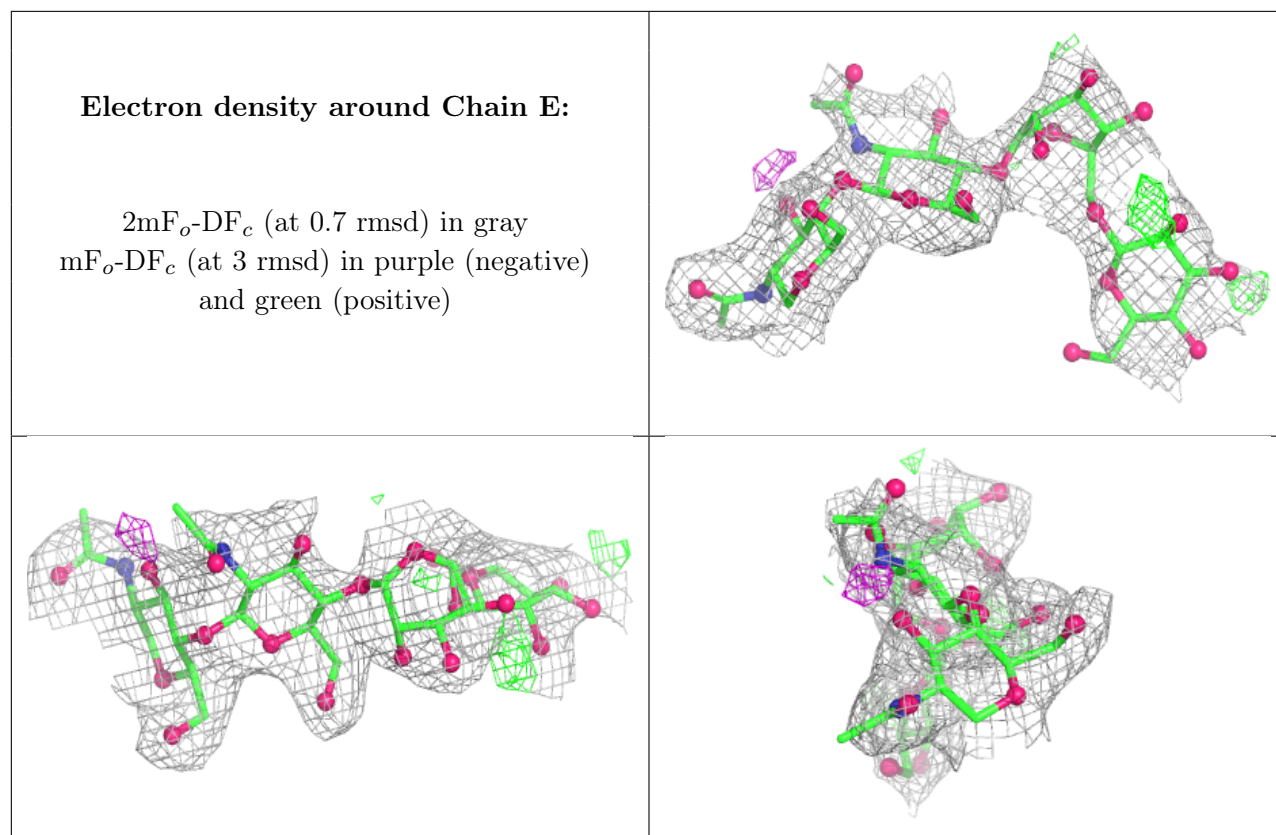
Electron density around Chain D:

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

**Electron density around Chain F:**

$2mF_o-DF_c$ (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
6	NAG	B	705	14/15	0.72	0.14	79,91,103,104	0
6	NAG	A	702	14/15	0.73	0.13	69,78,83,90	0
5	CU	A	701	1/1	0.91	0.09	151,151,151,151	0

6.5 Other polymers [i](#)

There are no such residues in this entry.