



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2024 – 12:51 AM EST

PDB ID : 3V8X
Title : The crystal structure of transferrin binding protein A (TbpA) from *Neisseria meningitidis* serogroup B in complex with full length human transferrin
Authors : Noinaj, N.; Easley, N.; Buchanan, S.K.
Deposited on : 2011-12-23
Resolution : 2.60 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

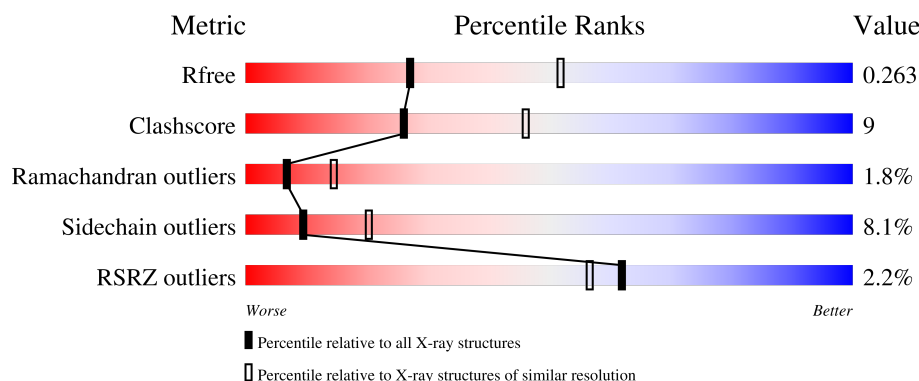
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	904	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• 6%</div> </div> </div>
2	B	698	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• • •</div> </div> </div>
3	C	10	<div> <div>10%</div> <div>50%</div> <div>40%</div> </div>
4	D	9	<div> <div>11%</div> <div>67%</div> <div>22%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12233 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 Transferrin-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	853	Total	C	N	O	S	0	2	0
			6686	4176	1218	1282	10			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	expression tag	UNP Q9K0U9
A	13	ASP	-	expression tag	UNP Q9K0U9
A	14	ILE	-	expression tag	UNP Q9K0U9
A	15	HIS	-	expression tag	UNP Q9K0U9
A	16	HIS	-	expression tag	UNP Q9K0U9
A	17	HIS	-	expression tag	UNP Q9K0U9
A	18	HIS	-	expression tag	UNP Q9K0U9
A	19	HIS	-	expression tag	UNP Q9K0U9
A	20	HIS	-	expression tag	UNP Q9K0U9
A	21	HIS	-	expression tag	UNP Q9K0U9
A	22	HIS	-	expression tag	UNP Q9K0U9
A	23	HIS	-	expression tag	UNP Q9K0U9
A	24	HIS	-	expression tag	UNP Q9K0U9
A	435	VAL	ILE	variant	UNP Q9K0U9
A	913	TYR	MET	engineered mutation	UNP Q9K0U9

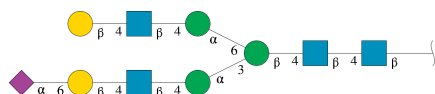
- Molecule 2 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	676	Total	C	N	O	S	0	0	0
			5050	3160	868	977	45			

There is a discrepancy between the modelled and reference sequences:

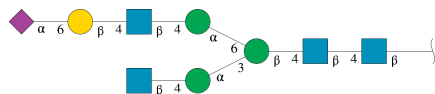
Chain	Residue	Modelled	Actual	Comment	Reference
B	429	VAL	ILE	variant	UNP P02787

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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.



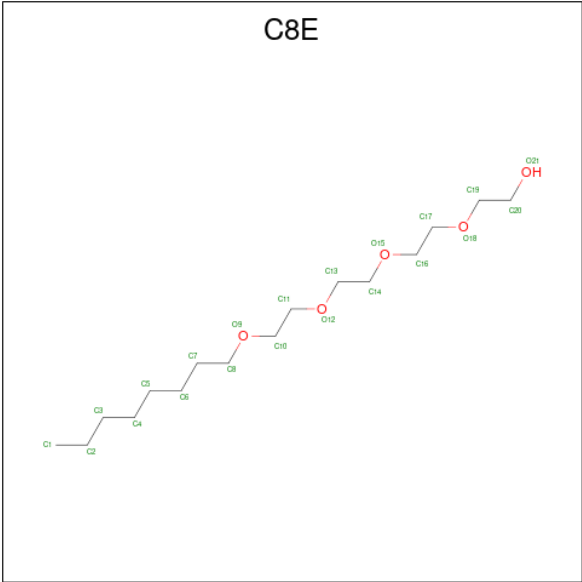
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			131	73	5	53			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-3)]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	9	Total	C	N	O	0	0	0
			120	67	5	48			

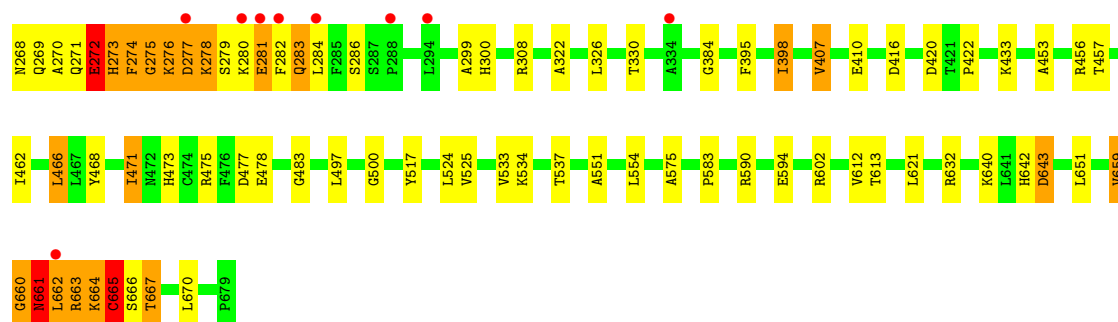
- Molecule 5 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			21	16	5		
5	A	1	Total	C	O	0	0
			21	16	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	142	Total	O	0	0
			142	142		
6	B	62	Total	O	0	0
			62	62		



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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 C: 10% 50% 40%



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 11% 67% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.01Å 129.36Å 198.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.60 29.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.92-2.60) 98.1 (29.92-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.208 , 0.267 0.208 , 0.263	Depositor DCC
R_{free} test set	3602 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12233	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, SIA, GAL, BMA, C8E

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	0.29	0/6834	0.47	1/9244 (0.0%)
2	B	0.29	0/5166	0.44	1/7025 (0.0%)
All	All	0.29	0/12000	0.45	2/16269 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	275	GLY	N-CA-C	-5.57	99.18	113.10
1	A	448	ALA	N-CA-C	-5.07	97.30	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6686	0	6396	91	0
2	B	5050	0	4646	120	0
3	C	131	0	110	7	0
4	D	120	0	101	2	0
5	A	42	0	68	6	0
6	A	142	0	0	2	0
6	B	62	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12233	0	11321	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)
2:B:282:PHE:O	2:B:283:GLN:HG2	1.46	1.15
2:B:275:GLY:HA2	2:B:281:GLU:O	1.48	1.12
2:B:659:VAL:HG23	2:B:660:GLY:H	0.91	1.05
2:B:269:GLN:HA	2:B:272:GLU:HG3	1.39	1.02
2:B:659:VAL:CG2	2:B:660:GLY:H	1.69	1.00
2:B:659:VAL:HG23	2:B:660:GLY:N	1.54	1.00
2:B:274:PHE:HB2	2:B:279:SER:HB3	1.40	0.98
2:B:661:ASN:H	2:B:661:ASN:ND2	1.65	0.94
2:B:274:PHE:CB	2:B:279:SER:HB3	2.01	0.89
2:B:277:ASP:CB	2:B:283:GLN:HA	2.02	0.89
2:B:283:GLN:HE21	2:B:286:SER:HB3	1.38	0.87
2:B:661:ASN:N	2:B:661:ASN:HD22	1.77	0.82
2:B:277:ASP:HA	2:B:283:GLN:HA	1.62	0.81
1:A:229:GLU:HG2	1:A:305:LEU:H	1.45	0.81
2:B:660:GLY:O	2:B:663:ARG:CB	2.30	0.80
2:B:270:ALA:O	2:B:276:LYS:CB	2.30	0.79
2:B:275:GLY:CA	2:B:281:GLU:O	2.30	0.79
2:B:274:PHE:C	2:B:276:LYS:N	2.29	0.78
2:B:277:ASP:CA	2:B:283:GLN:HA	2.13	0.78
2:B:282:PHE:O	2:B:283:GLN:CG	2.30	0.77
2:B:269:GLN:CA	2:B:272:GLU:HG3	2.15	0.77
1:A:510:LEU:HB3	1:A:575:ARG:HG3	1.67	0.76
2:B:52:ILE:HD11	2:B:60:VAL:HG23	1.67	0.76
2:B:659:VAL:CG2	2:B:660:GLY:N	2.30	0.75
2:B:10:ALA:HB1	2:B:15:GLU:HG3	1.66	0.75
2:B:277:ASP:CB	2:B:284:LEU:H	2.00	0.74
2:B:661:ASN:H	2:B:661:ASN:HD22	1.31	0.73
2:B:274:PHE:HB2	2:B:279:SER:CB	2.18	0.72
2:B:661:ASN:ND2	2:B:661:ASN:N	2.30	0.72
2:B:271:GLN:O	2:B:272:GLU:C	2.30	0.70
1:A:631:VAL:HG12	1:A:641:THR:HG22	1.74	0.70
2:B:48:CYS:HB3	2:B:60:VAL:HG21	1.73	0.69
1:A:256:ALA:HB1	1:A:279:ASP:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:HD13	1:A:643:ARG:HD2	1.76	0.68
2:B:663:ARG:O	2:B:664:LYS:C	2.29	0.68
2:B:273:HIS:C	2:B:275:GLY:H	1.98	0.68
1:A:779:GLN:NE2	1:A:835:THR:OG1	2.26	0.67
2:B:660:GLY:O	2:B:661:ASN:C	2.33	0.67
2:B:283:GLN:HG2	2:B:283:GLN:O	1.93	0.67
2:B:274:PHE:C	2:B:276:LYS:H	1.99	0.66
2:B:273:HIS:C	2:B:275:GLY:N	2.47	0.66
2:B:273:HIS:O	2:B:275:GLY:N	2.29	0.66
2:B:276:LYS:O	2:B:284:LEU:N	2.29	0.65
2:B:661:ASN:O	2:B:663:ARG:N	2.29	0.65
2:B:268:ASN:O	2:B:272:GLU:HG2	1.96	0.65
2:B:61:THR:HG1	2:B:249:HIS:HD1	1.43	0.65
2:B:272:GLU:O	2:B:274:PHE:N	2.30	0.65
2:B:660:GLY:O	2:B:663:ARG:N	2.31	0.64
1:A:760:ALA:HB3	1:A:792:VAL:HG13	1.81	0.62
1:A:755:TRP:HB3	1:A:797:TYR:HD2	1.65	0.62
2:B:272:GLU:O	2:B:274:PHE:HD2	1.82	0.61
1:A:358:LYS:NZ	6:A:1195:HOH:O	2.32	0.61
2:B:433:LYS:NZ	2:B:524:LEU:O	2.34	0.60
2:B:272:GLU:O	2:B:274:PHE:CD2	2.54	0.60
2:B:269:GLN:HA	2:B:272:GLU:CG	2.22	0.60
2:B:277:ASP:CB	2:B:284:LEU:N	2.64	0.60
1:A:755:TRP:HE3	1:A:797:TYR:HB2	1.67	0.59
2:B:659:VAL:O	2:B:661:ASN:N	2.35	0.59
1:A:911:LEU:HD22	1:A:913:TYR:HE2	1.68	0.59
2:B:663:ARG:O	2:B:665:CYS:HB3	2.03	0.59
2:B:277:ASP:CB	2:B:283:GLN:CA	2.79	0.58
2:B:274:PHE:CB	2:B:279:SER:CB	2.79	0.58
2:B:271:GLN:O	2:B:276:LYS:CB	2.52	0.58
1:A:73:VAL:HG23	1:A:78:ASP:HB2	1.85	0.58
1:A:524:TYR:H	3:C:4:MAN:H61	1.67	0.58
2:B:61:THR:HA	2:B:251:VAL:HA	1.86	0.57
2:B:273:HIS:O	2:B:276:LYS:N	2.29	0.57
1:A:662:GLY:O	2:B:602:ARG:NH2	2.34	0.57
2:B:662:LEU:C	2:B:663:ARG:O	2.40	0.57
1:A:313:LEU:HD11	1:A:330:ILE:HD11	1.86	0.57
1:A:674:LYS:HD2	1:A:701:ARG:HH12	1.70	0.57
1:A:197:SER:HA	1:A:908:THR:HG22	1.88	0.56
2:B:274:PHE:HD1	2:B:278:LYS:C	2.08	0.56
2:B:517:TYR:CZ	2:B:534:LYS:HD3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:661:ASN:C	2:B:663:ARG:N	2.57	0.56
1:A:861:THR:HG23	1:A:912:GLU:HB2	1.87	0.55
1:A:221:ILE:HD12	1:A:313:LEU:HD23	1.89	0.55
1:A:732:ARG:HG3	1:A:767:ARG:HB2	1.89	0.55
1:A:453:LYS:O	1:A:456:ARG:NH2	2.41	0.54
2:B:283:GLN:CG	2:B:283:GLN:O	2.55	0.54
1:A:449:ASP:CG	1:A:451:SER:OG	2.46	0.54
2:B:664:LYS:O	2:B:665:CYS:CB	2.55	0.54
2:B:8:TRP:HD1	2:B:9:CYS:O	1.91	0.54
2:B:279:SER:OG	2:B:280:LYS:N	2.40	0.53
1:A:842:THR:HG21	1:A:877:TRP:HB2	1.90	0.53
1:A:55:VAL:HG13	1:A:631:VAL:HG22	1.91	0.53
3:C:4:MAN:H3	3:C:5:NAG:C7	2.39	0.52
2:B:158:CYS:HB2	2:B:173:LEU:HB2	1.91	0.52
1:A:482:ALA:HB3	1:A:501:LEU:HB2	1.91	0.52
1:A:869:LEU:O	1:A:905:ARG:NH1	2.41	0.52
2:B:283:GLN:HE21	2:B:286:SER:CB	2.18	0.51
1:A:484:PHE:HB2	1:A:499:VAL:HG22	1.93	0.51
2:B:8:TRP:HD1	2:B:9:CYS:H	1.58	0.51
1:A:816:LYS:HB2	1:A:842:THR:HG22	1.93	0.51
1:A:449:ASP:OD1	1:A:451:SER:OG	2.29	0.50
2:B:662:LEU:O	2:B:663:ARG:O	2.29	0.50
2:B:282:PHE:O	2:B:283:GLN:O	2.30	0.50
1:A:870:LEU:O	1:A:872:TYR:N	2.42	0.50
1:A:103:GLY:HA2	1:A:786:ILE:HG12	1.93	0.50
2:B:666:SER:OG	2:B:667:THR:N	2.44	0.50
2:B:661:ASN:O	2:B:662:LEU:C	2.50	0.49
1:A:729:GLN:NE2	1:A:780:SER:O	2.37	0.49
2:B:271:GLN:O	2:B:272:GLU:O	2.30	0.49
2:B:433:LYS:HE3	2:B:525:VAL:HA	1.93	0.49
2:B:661:ASN:O	2:B:663:ARG:O	2.30	0.49
1:A:257:TYR:CZ	1:A:278:LYS:HE2	2.48	0.49
2:B:660:GLY:O	2:B:661:ASN:O	2.30	0.49
1:A:640:LEU:HD12	1:A:682:ILE:HD13	1.94	0.49
1:A:473:TYR:HH	1:A:508:SER:HG	1.58	0.49
1:A:502:GLY:HA3	1:A:583:TYR:CE2	2.47	0.49
1:A:843:ARG:HE	5:A:1002:C8E:H172	1.77	0.49
2:B:280:LYS:O	2:B:281:GLU:O	2.30	0.49
1:A:332:GLU:HB3	1:A:407:ARG:HB3	1.96	0.48
1:A:398:PHE:CG	1:A:453:LYS:HG3	2.49	0.48
1:A:449:ASP:OD2	1:A:451:SER:OG	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:PHE:CD1	2:B:278:LYS:CB	2.97	0.48
1:A:108:ARG:HG2	1:A:167:LEU:HD12	1.95	0.47
2:B:272:GLU:O	2:B:273:HIS:C	2.50	0.47
1:A:744:TRP:NE1	1:A:757:SER:HB2	2.30	0.47
1:A:101:ILE:HG22	1:A:102:ARG:HG2	1.97	0.47
1:A:479:LEU:HD13	1:A:504:ASP:HB2	1.97	0.47
1:A:892:LYS:HA	1:A:893:ASN:HA	1.68	0.47
2:B:471:ILE:HB	2:B:473:HIS:NE2	2.30	0.47
1:A:782:LEU:HG	1:A:837:ALA:HB2	1.97	0.47
1:A:450:GLY:HA3	1:A:451:SER:HA	1.57	0.47
2:B:178:GLY:HA3	2:B:183:ASN:HB2	1.97	0.47
1:A:876:THR:O	1:A:880:VAL:HG23	2.15	0.47
1:A:91:GLN:HG3	1:A:139:ALA:HB2	1.96	0.46
2:B:422:PRO:HG3	2:B:640:LYS:O	2.15	0.46
2:B:643:ASP:OD1	2:B:643:ASP:N	2.48	0.46
1:A:56:THR:HA	1:A:57:GLY:HA2	1.48	0.46
2:B:9:CYS:HB3	2:B:60:VAL:HG22	1.98	0.46
2:B:8:TRP:CD1	2:B:9:CYS:N	2.83	0.46
5:A:1002:C8E:H171	5:A:1002:C8E:H142	1.51	0.46
2:B:134:LEU:HD13	2:B:322:ALA:HB2	1.97	0.46
1:A:524:TYR:H	3:C:4:MAN:C6	2.28	0.45
2:B:130:ILE:HD11	2:B:246:VAL:HG21	1.97	0.45
1:A:555:ASN:OD1	3:C:7:SIA:O4	2.28	0.45
1:A:639:ASP:HB2	1:A:683:VAL:HG13	1.98	0.45
1:A:759:PHE:CD1	1:A:793:VAL:HG12	2.51	0.45
2:B:398:ILE:HD11	2:B:670:LEU:HG	1.99	0.45
1:A:755:TRP:HB3	1:A:797:TYR:CD2	2.47	0.45
2:B:283:GLN:NE2	2:B:286:SER:HB3	2.19	0.45
1:A:190:ILE:HG23	1:A:915:PHE:HB2	1.99	0.45
5:A:1002:C8E:H192	5:A:1002:C8E:H162	1.59	0.45
2:B:281:GLU:HA	2:B:282:PHE:HA	1.55	0.45
2:B:395:PHE:HA	2:B:398:ILE:HG23	1.98	0.45
1:A:649:ARG:HD3	1:A:673:GLU:OE1	2.17	0.44
1:A:149:LYS:HD3	1:A:180:ASP:OD1	2.17	0.44
1:A:607[B]:ARG:O	1:A:607[B]:ARG:NH1	2.50	0.44
1:A:759:PHE:HD1	1:A:793:VAL:HG12	1.82	0.44
2:B:214:LEU:HG	2:B:219:ASP:HB3	2.00	0.44
2:B:407:VAL:HG13	2:B:594:GLU:HG3	1.99	0.44
1:A:341:ARG:CZ	1:A:451:SER:HB2	2.48	0.44
2:B:151:ALA:HB1	2:B:169:GLN:HB2	1.99	0.44
2:B:274:PHE:HB3	2:B:279:SER:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:LYS:O	2:B:277:ASP:CB	2.64	0.44
2:B:583:PRO:HG3	2:B:651:LEU:HD23	1.99	0.44
1:A:894:VAL:HA	1:A:895:GLY:HA3	1.61	0.44
2:B:410:GLU:OE1	2:B:632:ARG:HG2	2.17	0.44
1:A:575:ARG:H	1:A:575:ARG:HG2	1.58	0.44
1:A:836:LYS:HD3	5:A:1002:C8E:H31	1.98	0.44
2:B:136:TYR:HA	2:B:139:LEU:HD22	2.00	0.44
1:A:366:GLY:HA2	1:A:524:TYR:CZ	2.53	0.43
2:B:121:GLY:HA2	2:B:160:PRO:HG2	2.00	0.43
1:A:132:ARG:O	1:A:467:LYS:NZ	2.52	0.43
1:A:74:LEU:O	1:A:225:ARG:NH2	2.51	0.43
2:B:468:TYR:CD2	2:B:661:ASN:HB3	2.54	0.43
2:B:575:ALA:HB1	3:C:3:BMA:O6	2.19	0.43
1:A:683:VAL:HB	1:A:692:GLU:HG3	2.01	0.43
2:B:533:VAL:HG21	2:B:537:THR:HG21	2.00	0.43
2:B:31:PRO:HB2	2:B:32:SER:H	1.56	0.42
1:A:635:THR:C	1:A:637:TRP:H	2.22	0.42
2:B:255:SER:OG	2:B:256:MET:N	2.51	0.42
2:B:274:PHE:HB3	2:B:279:SER:HB3	1.94	0.42
2:B:85:TYR:CD2	2:B:299:ALA:HA	2.55	0.42
2:B:384:GLY:HA2	2:B:590:ARG:NH1	2.34	0.42
2:B:134:LEU:HD12	2:B:134:LEU:HA	1.86	0.42
3:C:7:SIA:H8	3:C:7:SIA:N5	2.34	0.42
1:A:479:LEU:HG	1:A:481:GLN:HG3	2.02	0.42
1:A:700:TYR:N	1:A:731:ALA:O	2.51	0.42
4:D:3:BMA:H61	4:D:4:MAN:H2	1.22	0.42
1:A:815:ALA:HB2	1:A:844:PRO:HD3	2.01	0.42
1:A:229:GLU:H	1:A:229:GLU:HG3	1.42	0.41
1:A:840:ARG:HH21	5:A:1002:C8E:H141	1.85	0.41
2:B:59:ALA:HB2	2:B:263:ILE:HD13	2.02	0.41
1:A:167:LEU:HD13	1:A:700:TYR:HD1	1.85	0.41
1:A:260:VAL:HA	1:A:549:VAL:O	2.20	0.41
1:A:524:TYR:O	3:C:4:MAN:H62	2.20	0.41
1:A:879:ASN:HB3	1:A:900:TYR:HB3	2.02	0.41
2:B:233:LYS:HD2	2:B:241:CYS:HB2	2.03	0.41
2:B:274:PHE:HD1	2:B:278:LYS:CB	2.32	0.41
2:B:326:LEU:HD12	2:B:326:LEU:HA	1.90	0.41
2:B:462:ILE:O	2:B:466:LEU:HD22	2.20	0.41
2:B:151:ALA:HB2	2:B:170:LEU:HD13	2.03	0.41
1:A:633:LYS:HG2	1:A:639:ASP:OD1	2.19	0.41
1:A:369:LYS:HD3	1:A:549:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:4:MAN:H3	4:D:5:NAG:C7	2.50	0.41
1:A:186:ARG:NH1	1:A:188:TRP:O	2.53	0.41
1:A:421:THR:HG22	1:A:422:TRP:H	1.85	0.41
2:B:96:TYR:HB2	2:B:207:HIS:HB3	2.03	0.41
5:A:1001:C8E:H51	5:A:1001:C8E:H82	1.91	0.41
2:B:453:ALA:HB3	2:B:456:ARG:HD3	2.03	0.41
1:A:164:SER:HB2	1:A:650:LEU:HD22	2.02	0.41
1:A:245:ARG:HG2	1:A:348:PHE:HB3	2.02	0.41
1:A:485:LYS:HE3	1:A:485:LYS:HB2	1.91	0.41
1:A:818:ILE:HG12	1:A:822:LEU:HD22	2.03	0.41
1:A:858:LYS:O	1:A:914:LYS:HB2	2.21	0.41
2:B:475:ARG:O	2:B:478:GLU:HG2	2.21	0.41
2:B:269:GLN:C	2:B:272:GLU:HG3	2.42	0.40
1:A:698:ASN:HB2	6:A:1158:HOH:O	2.21	0.40
2:B:551:ALA:HA	2:B:554:LEU:HG	2.03	0.40
2:B:483:GLY:HA2	2:B:497:LEU:HD11	2.04	0.40
1:A:517:TYR:CZ	1:A:559:GLY:HA3	2.57	0.40
2:B:660:GLY:O	2:B:663:ARG:CA	2.69	0.40
1:A:649:ARG:HH22	1:A:655:GLU:CD	2.25	0.40
1:A:892:LYS:HB2	1:A:893:ASN:OD1	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	849/904 (94%)	807 (95%)	39 (5%)	3 (0%)	30	52
2	B	674/698 (97%)	593 (88%)	57 (8%)	24 (4%)	3	4
All	All	1523/1602 (95%)	1400 (92%)	96 (6%)	27 (2%)	7	14

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	780	SER
2	B	31	PRO
2	B	272	GLU
2	B	281	GLU
2	B	283	GLN
2	B	659	VAL
2	B	663	ARG
2	B	665	CYS
1	A	871	ASN
2	B	273	HIS
2	B	274	PHE
2	B	276	LYS
2	B	277	ASP
2	B	660	GLY
2	B	661	ASN
2	B	24	ASP
2	B	9	CYS
2	B	278	LYS
2	B	457	THR
2	B	500	GLY
2	B	662	LEU
2	B	664	LYS
1	A	158	ASN
2	B	55	ASN
2	B	248	SER
2	B	54	ALA
2	B	612	VAL

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	685/741 (92%)	616 (90%)	69 (10%)	6	12
2	B	520/585 (89%)	490 (94%)	30 (6%)	17	36
All	All	1205/1326 (91%)	1106 (92%)	99 (8%)	9	20

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	58	LEU
1	A	73	VAL
1	A	76	ILE
1	A	86	ILE
1	A	89	VAL
1	A	109	VAL
1	A	111	LEU
1	A	119	ILE
1	A	160	VAL
1	A	167	LEU
1	A	188	TRP
1	A	190	ILE
1	A	194	THR
1	A	204	THR
1	A	219	LEU
1	A	220	LEU
1	A	229	GLU
1	A	240	VAL
1	A	245	ARG
1	A	260	VAL
1	A	279	ASP
1	A	280	VAL
1	A	286	ARG
1	A	299	ARG
1	A	301	LEU
1	A	321	GLU
1	A	334	THR
1	A	353	VAL
1	A	364	LEU
1	A	376	TYR
1	A	395	THR
1	A	421	THR
1	A	451	SER
1	A	511	ARG
1	A	515	TYR
1	A	533	ASN
1	A	550	THR
1	A	556	VAL
1	A	575	ARG
1	A	592	LEU
1	A	607[A]	ARG
1	A	607[B]	ARG

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Mol	Chain	Res	Type
1	A	618	THR
1	A	622	ARG
1	A	631	VAL
1	A	650	LEU
1	A	678	LYS
1	A	683	VAL
1	A	687	ASP
1	A	691	LEU
1	A	698	ASN
1	A	729	GLN
1	A	747	VAL
1	A	755	TRP
1	A	757	SER
1	A	776	THR
1	A	782	LEU
1	A	822	LEU
1	A	828	LEU
1	A	855	THR
1	A	858	LYS
1	A	861	THR
1	A	862	LEU
1	A	873	ARG
1	A	888	VAL
1	A	892	LYS
1	A	894	VAL
1	A	899	ARG
2	B	9	CYS
2	B	11	VAL
2	B	49	ILE
2	B	55	ASN
2	B	56	GLU
2	B	92	GLN
2	B	134	LEU
2	B	139	LEU
2	B	170	LEU
2	B	228	LEU
2	B	249	HIS
2	B	251	VAL
2	B	272	GLU
2	B	300	HIS
2	B	308	ARG
2	B	330	THR

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Mol	Chain	Res	Type
2	B	398	ILE
2	B	407	VAL
2	B	416	ASP
2	B	420	ASP
2	B	466	LEU
2	B	471	ILE
2	B	477	ASP
2	B	613	THR
2	B	621	LEU
2	B	642	HIS
2	B	643	ASP
2	B	661	ASN
2	B	665	CYS
2	B	667	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	779	GLN
2	B	283	GLN
2	B	469	ASN
2	B	661	ASN

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](#)

19 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	3,2	14,14,15	0.68	0	17,19,21	1.02	2 (11%)
3	GAL	C	10	3	11,11,12	0.67	0	15,15,17	1.48	1 (6%)
3	NAG	C	2	3	14,14,15	0.51	0	17,19,21	1.02	2 (11%)
3	BMA	C	3	3	11,11,12	1.07	1 (9%)	15,15,17	1.61	4 (26%)
3	MAN	C	4	3	11,11,12	0.82	0	15,15,17	1.73	3 (20%)
3	NAG	C	5	3	14,14,15	0.58	0	17,19,21	1.52	2 (11%)
3	GAL	C	6	3	11,11,12	0.65	0	15,15,17	0.53	0
3	SIA	C	7	3	20,20,21	0.73	0	21,28,31	1.87	5 (23%)
3	MAN	C	8	3	11,11,12	0.64	0	15,15,17	1.34	1 (6%)
3	NAG	C	9	3	14,14,15	0.61	0	17,19,21	0.97	1 (5%)
4	NAG	D	1	4,2	14,14,15	0.70	0	17,19,21	1.25	1 (5%)
4	NAG	D	2	4	14,14,15	0.51	0	17,19,21	1.71	3 (17%)
4	BMA	D	3	4	11,11,12	1.94	3 (27%)	15,15,17	1.95	6 (40%)
4	MAN	D	4	4	11,11,12	0.57	0	15,15,17	0.66	0
4	NAG	D	5	4	14,14,15	0.50	0	17,19,21	0.97	1 (5%)
4	GAL	D	6	4	11,11,12	0.56	0	15,15,17	2.06	4 (26%)
4	SIA	D	7	4	20,20,21	0.68	0	21,28,31	1.04	3 (14%)
4	MAN	D	8	4	11,11,12	0.65	0	15,15,17	1.29	1 (6%)
4	NAG	D	9	4	14,14,15	0.53	0	17,19,21	0.58	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
3	NAG	C	1	3,2	-	0/6/23/26	0/1/1/1
3	GAL	C	10	3	-	1/2/19/22	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	0/6/23/26	0/1/1/1
3	GAL	C	6	3	-	2/2/19/22	0/1/1/1
3	SIA	C	7	3	-	5/18/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	C	8	3	-	2/2/19/22	1/1/1/1
3	NAG	C	9	3	-	3/6/23/26	0/1/1/1
4	NAG	D	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	NAG	D	5	4	-	0/6/23/26	0/1/1/1
4	GAL	D	6	4	-	1/2/19/22	0/1/1/1
4	SIA	D	7	4	-	3/18/34/38	0/1/1/1
4	MAN	D	8	4	-	1/2/19/22	0/1/1/1
4	NAG	D	9	4	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	BMA	C1-C2	4.85	1.63	1.52
4	D	3	BMA	C2-C3	2.26	1.56	1.52
3	C	3	BMA	C2-C3	2.07	1.55	1.52
4	D	3	BMA	O5-C1	2.07	1.47	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	7	SIA	O6-C2-C3	5.11	117.43	110.56
4	D	6	GAL	O2-C2-C3	4.93	120.37	110.15
4	D	2	NAG	C1-O5-C5	4.78	118.59	112.19
3	C	7	SIA	C6-C5-N5	4.54	118.14	110.91
4	D	6	GAL	O2-C2-C1	4.44	119.39	109.22
3	C	5	NAG	C1-O5-C5	4.34	118.00	112.19
3	C	10	GAL	C1-C2-C3	4.30	115.91	109.64
3	C	4	MAN	O4-C4-C3	4.26	120.43	110.38
4	D	1	NAG	C4-C3-C2	3.94	116.79	111.02
4	D	8	MAN	C3-C4-C5	3.36	116.33	110.23
3	C	4	MAN	C6-C5-C4	-3.21	105.14	113.02
4	D	3	BMA	C3-C4-C5	-3.16	104.50	110.23
3	C	5	NAG	O5-C1-C2	3.12	116.12	111.29
4	D	3	BMA	C1-O5-C5	3.09	116.33	112.19
4	D	2	NAG	O5-C1-C2	2.98	115.90	111.29
4	D	6	GAL	O6-C6-C5	-2.84	101.66	111.33
4	D	2	NAG	O4-C4-C3	2.74	116.83	110.38
3	C	3	BMA	C2-C3-C4	-2.58	106.33	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C4-C3-C2	2.56	114.77	111.02
4	D	5	NAG	C1-O5-C5	2.56	115.61	112.19
4	D	7	SIA	O6-C2-C1	2.52	112.47	107.72
3	C	2	NAG	C2-N2-C7	-2.46	119.60	122.90
4	D	3	BMA	C1-C2-C3	2.46	113.22	109.64
4	D	3	BMA	O2-C2-C3	-2.42	105.14	110.15
3	C	3	BMA	C1-C2-C3	-2.41	106.14	109.64
3	C	4	MAN	C2-C3-C4	2.35	114.99	110.86
3	C	3	BMA	C3-C4-C5	-2.33	106.01	110.23
3	C	7	SIA	O1B-C1-C2	2.27	118.61	112.71
4	D	6	GAL	O5-C5-C6	2.25	112.05	107.66
3	C	8	MAN	O4-C4-C5	2.25	114.87	109.32
3	C	7	SIA	C8-C7-C6	2.23	117.24	113.05
4	D	7	SIA	O6-C2-C3	2.18	113.49	110.56
3	C	3	BMA	C6-C5-C4	-2.16	107.71	113.02
4	D	3	BMA	O3-C3-C4	-2.15	105.31	110.38
3	C	7	SIA	C5-N5-C10	2.14	128.11	123.11
3	C	2	NAG	C1-O5-C5	2.13	115.04	112.19
4	D	3	BMA	O5-C1-C2	2.11	115.83	110.79
4	D	7	SIA	O1B-C1-C2	2.06	118.06	112.71
3	C	9	NAG	C2-N2-C7	2.02	125.61	122.90
3	C	1	NAG	C3-C4-C5	2.01	113.89	110.23

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	9	NAG	C3-C2-N2-C7
3	C	9	NAG	C8-C7-N2-C2
3	C	9	NAG	O7-C7-N2-C2
3	C	3	BMA	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	8	MAN	O5-C5-C6-O6
4	D	7	SIA	C11-C10-N5-C5
4	D	7	SIA	O10-C10-N5-C5
4	D	9	NAG	C8-C7-N2-C2
4	D	9	NAG	O7-C7-N2-C2
3	C	8	MAN	C4-C5-C6-O6
3	C	7	SIA	C4-C5-N5-C10
3	C	6	GAL	C4-C5-C6-O6
4	D	6	GAL	O5-C5-C6-O6
4	D	8	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	6	GAL	O5-C5-C6-O6
3	C	7	SIA	O1A-C1-C2-O6
3	C	7	SIA	C6-C5-N5-C10
4	D	7	SIA	O8-C8-C9-O9
3	C	7	SIA	O1A-C1-C2-C3
3	C	7	SIA	O1B-C1-C2-C3
3	C	10	GAL	C4-C5-C6-O6

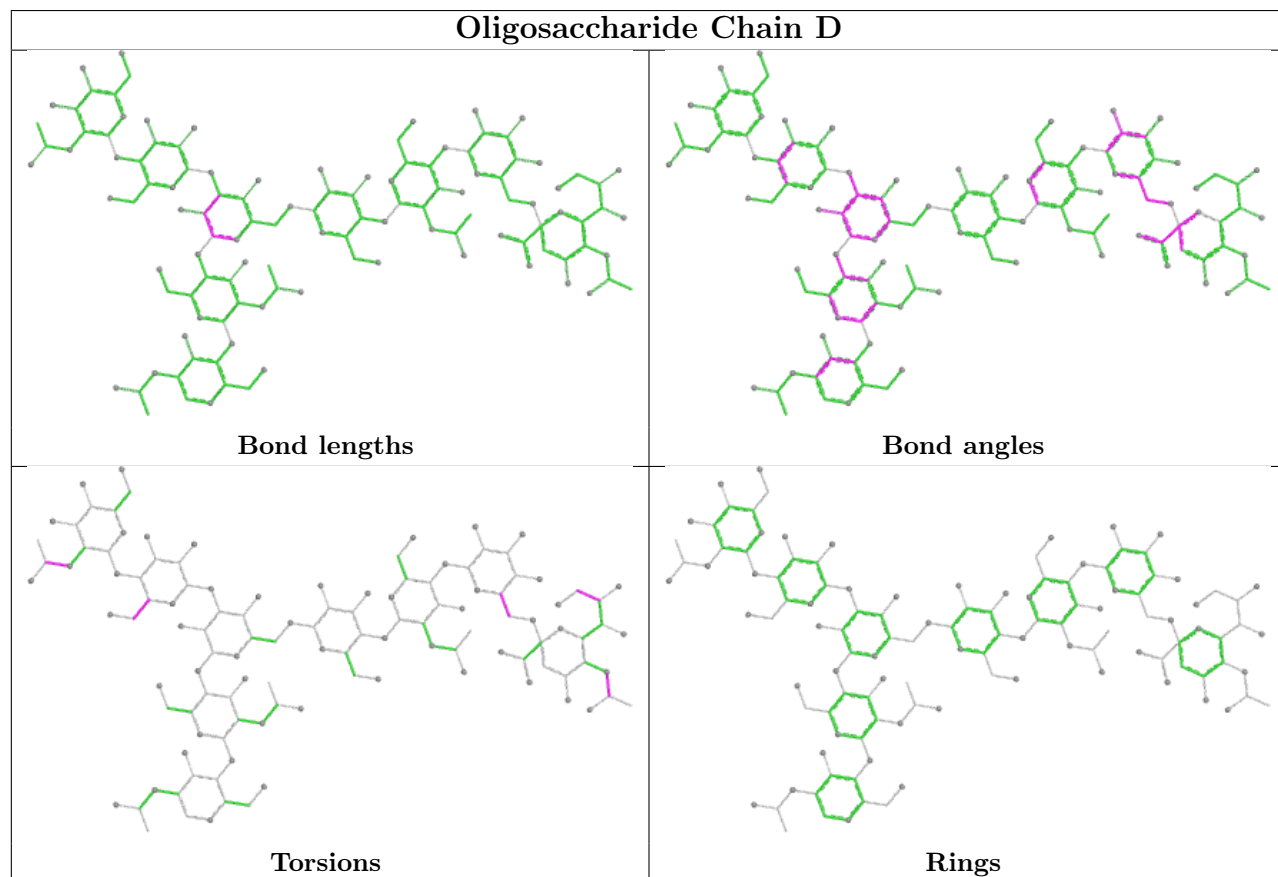
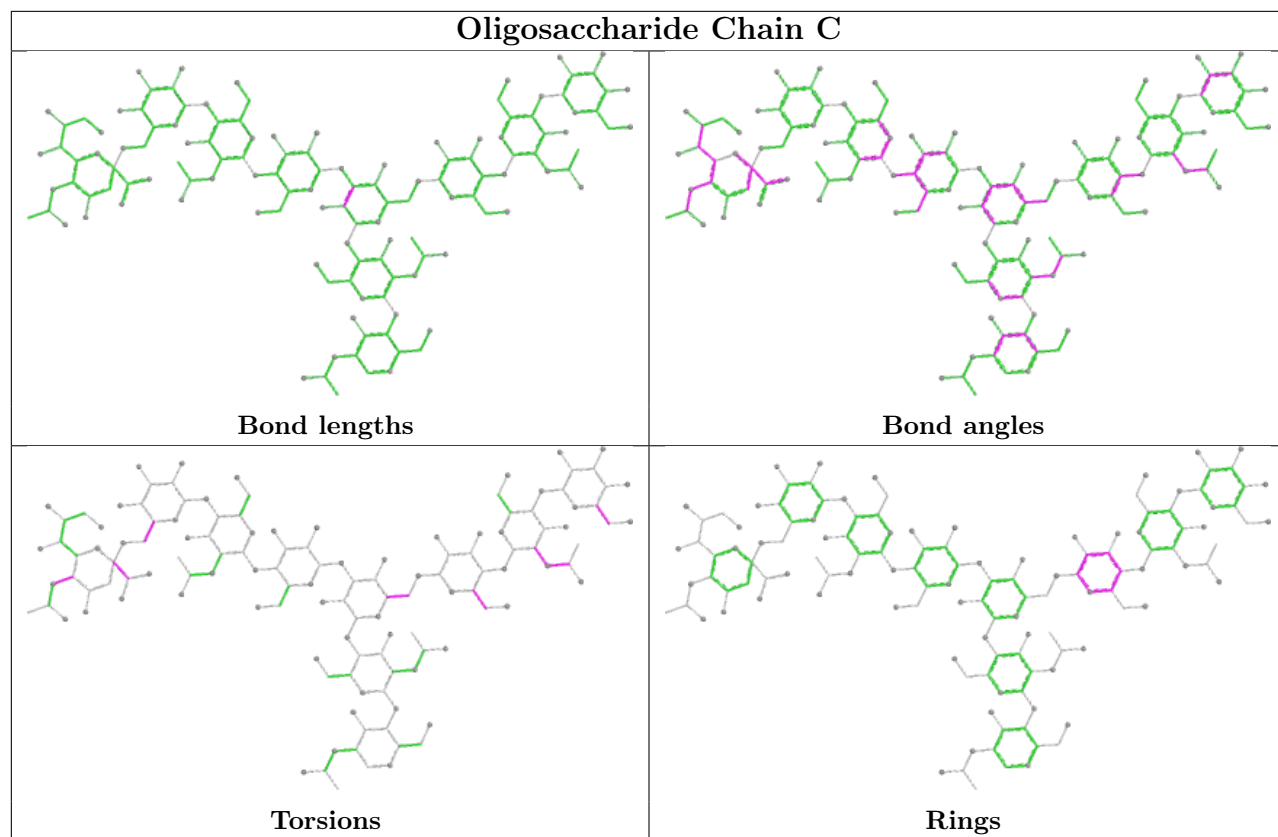
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	8	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	7	SIA	2	0
4	D	5	NAG	1	0
4	D	4	MAN	2	0
3	C	3	BMA	1	0
3	C	5	NAG	1	0
3	C	4	MAN	4	0
4	D	3	BMA	1	0

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



5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	C8E	A	1002	-	20,20,20	0.43	0	19,19,19	0.65	0
5	C8E	A	1001	-	20,20,20	0.39	0	19,19,19	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	C8E	A	1002	-	-	12/18/18/18	-
5	C8E	A	1001	-	-	9/18/18/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1002	C8E	C17-C16-O15-C14
5	A	1001	C8E	O12-C13-C14-O15
5	A	1002	C8E	O15-C16-C17-O18
5	A	1002	C8E	C16-C17-O18-C19
5	A	1001	C8E	O18-C19-C20-O21
5	A	1002	C8E	O18-C19-C20-O21
5	A	1001	C8E	C2-C3-C4-C5
5	A	1002	C8E	C2-C3-C4-C5
5	A	1001	C8E	C6-C7-C8-O9
5	A	1002	C8E	O9-C10-C11-O12
5	A	1001	C8E	C3-C4-C5-C6

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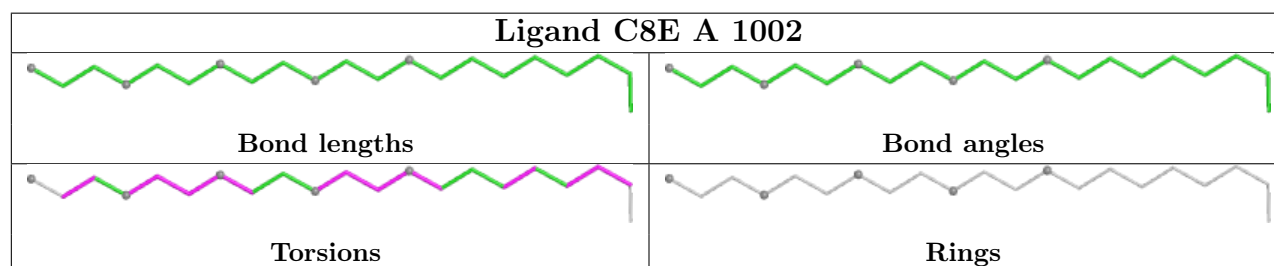
Mol	Chain	Res	Type	Atoms
5	A	1001	C8E	C10-C11-O12-C13
5	A	1002	C8E	C11-C10-O9-C8
5	A	1002	C8E	C10-C11-O12-C13
5	A	1002	C8E	C13-C14-O15-C16
5	A	1001	C8E	C20-C19-O18-C17
5	A	1002	C8E	C1-C2-C3-C4
5	A	1001	C8E	C13-C14-O15-C16
5	A	1001	C8E	C5-C6-C7-C8
5	A	1002	C8E	C4-C5-C6-C7
5	A	1002	C8E	C7-C8-O9-C10

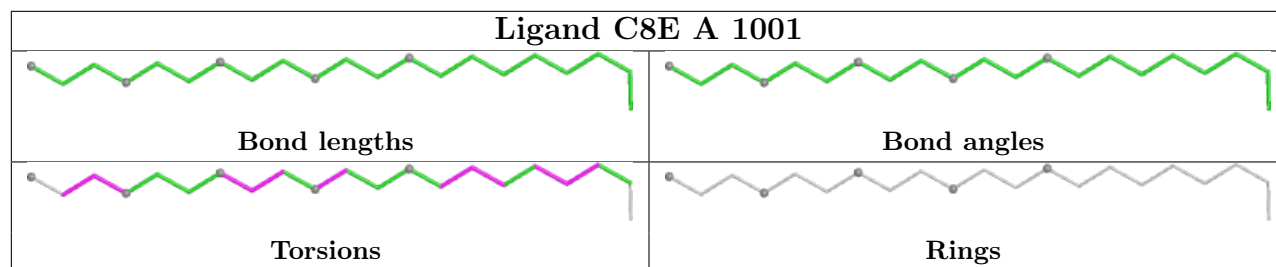
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1002	C8E	5	0
5	A	1001	C8E	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	853/904 (94%)	-0.38	7 (0%) 82 79	27, 69, 111, 155	2 (0%)
2	B	676/698 (96%)	-0.05	26 (3%) 44 38	43, 82, 152, 212	0
All	All	1529/1602 (95%)	-0.23	33 (2%) 62 57	27, 74, 136, 212	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	281	GLU	4.2
2	B	282	PHE	3.6
2	B	24	ASP	3.3
2	B	33	ASP	3.2
2	B	4	LYS	3.1
1	A	747	VAL	3.1
2	B	30	ILE	2.9
1	A	714	ASP	2.8
2	B	32	SER	2.8
1	A	755	TRP	2.8
2	B	22	PHE	2.7
2	B	662	LEU	2.7
2	B	31	PRO	2.7
2	B	284	LEU	2.7
2	B	334	ALA	2.7
2	B	238	TYR	2.6
1	A	492	LYS	2.5
2	B	280	LYS	2.5
2	B	253	ALA	2.5
2	B	35	PRO	2.5
2	B	277	ASP	2.5
1	A	637	TRP	2.4
2	B	37	VAL	2.4
2	B	294	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	8	TRP	2.3
2	B	288	PRO	2.3
1	A	237	GLY	2.2
2	B	254	ARG	2.2
2	B	25	HIS	2.1
1	A	301	LEU	2.1
2	B	23	ARG	2.1
2	B	68	TYR	2.1
2	B	262	LEU	2.1

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

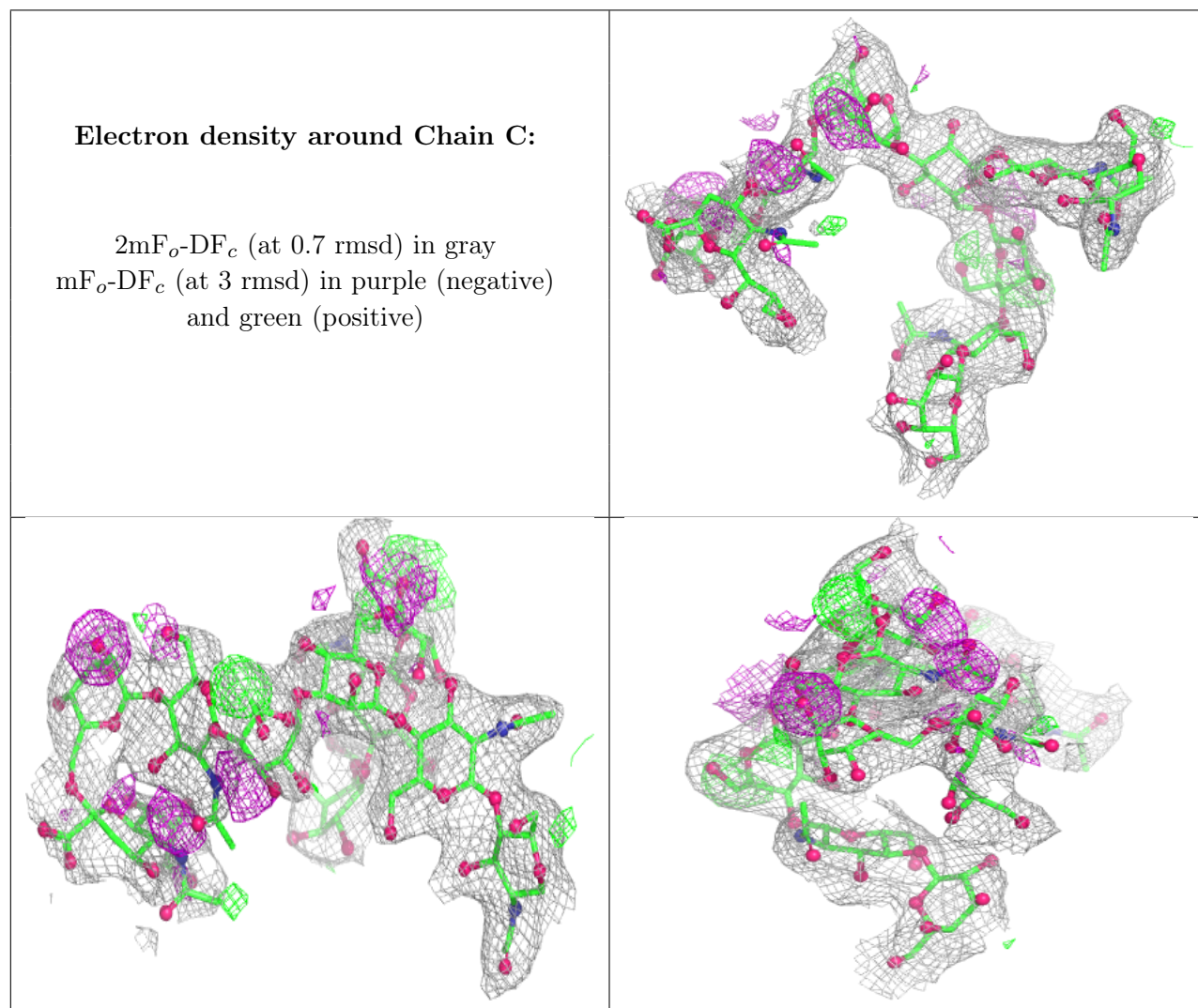
There are no non-standard protein/DNA/RNA residues in this entry.

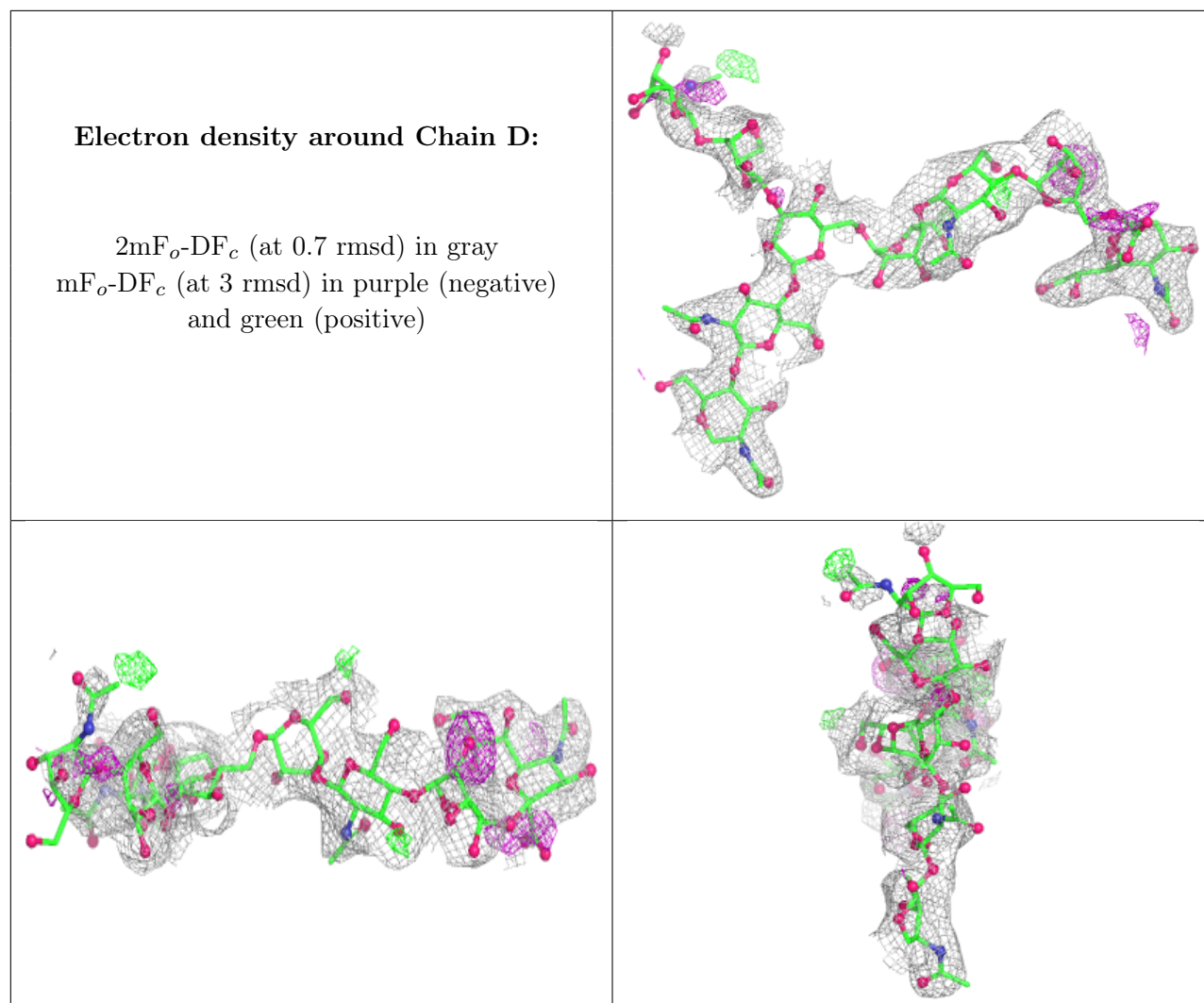
6.3 Carbohydrates [i](#)

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
4	NAG	D	9	14/15	0.07	0.18	157,178,187,187	0
3	GAL	C	10	11/12	0.34	0.15	139,154,157,160	0
4	MAN	D	8	11/12	0.37	0.12	167,175,185,187	0
4	MAN	D	4	11/12	0.42	0.13	137,153,155,157	0
3	GAL	C	6	11/12	0.48	0.14	30,142,156,165	0
4	GAL	D	6	11/12	0.55	0.17	30,133,150,153	0
4	BMA	D	3	11/12	0.56	0.11	150,169,201,202	0
3	SIA	C	7	20/21	0.60	0.14	149,166,174,174	0
4	NAG	D	2	14/15	0.64	0.14	111,144,158,162	0
4	NAG	D	5	14/15	0.72	0.13	113,135,143,144	0
3	MAN	C	8	11/12	0.73	0.18	85,118,141,153	0
3	NAG	C	9	14/15	0.79	0.12	118,125,145,150	0
3	MAN	C	4	11/12	0.81	0.18	79,95,116,128	0
3	NAG	C	5	14/15	0.84	0.15	81,103,113,123	0
4	NAG	D	1	14/15	0.87	0.13	67,113,122,131	0
4	SIA	D	7	20/21	0.89	0.15	73,91,144,146	0
3	BMA	C	3	11/12	0.90	0.11	54,64,85,108	0
3	NAG	C	1	14/15	0.92	0.09	54,67,82,86	0
3	NAG	C	2	14/15	0.93	0.08	55,66,71,80	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands ⓘ

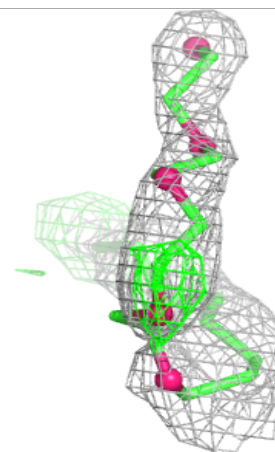
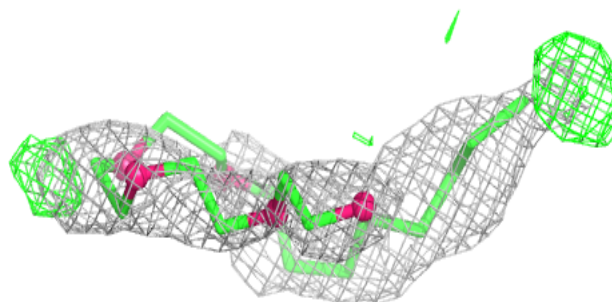
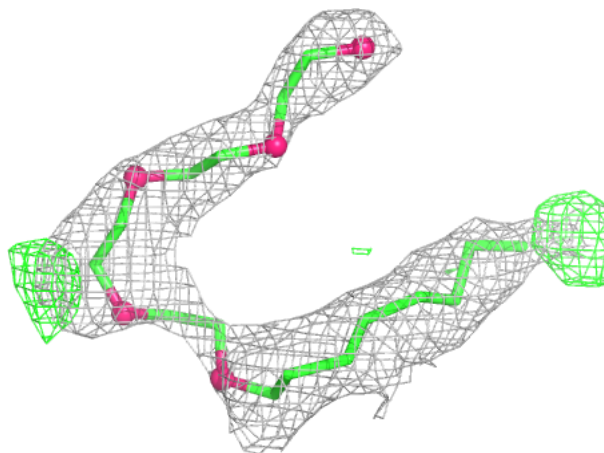
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

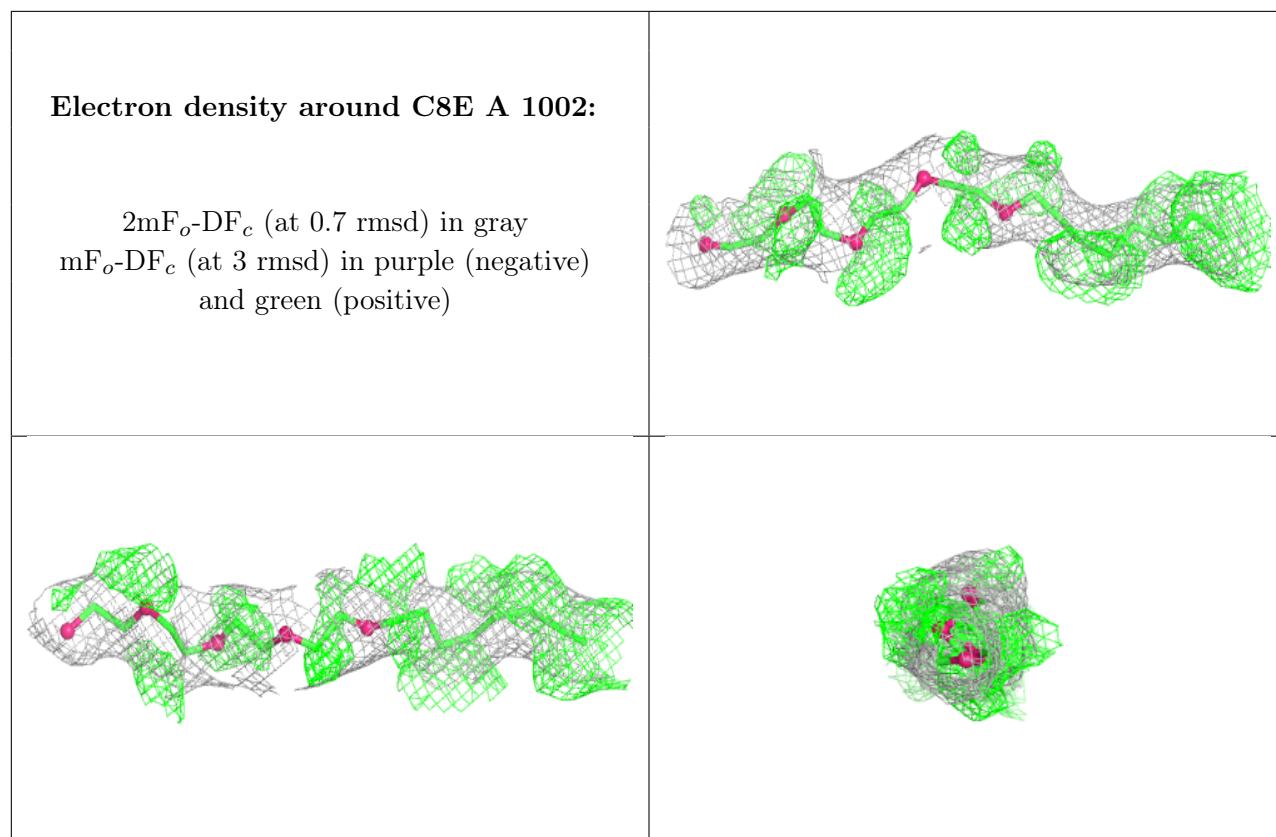
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	C8E	A	1001	21/21	0.78	0.24	70,101,117,118	0
5	C8E	A	1002	21/21	0.88	0.13	48,77,98,106	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around C8E A 1001:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.