



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:47 PM UTC

PDB ID : 6RUX / pdb_00006rux
Title : P46, an immunodominant surface protein from Mycoplasma hyopneumoniae
Authors : Guasch, A.; Gonzalez-Gonzalez, L.; Fita, I.
Deposited on : 2019-05-29
Resolution : 2.50 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

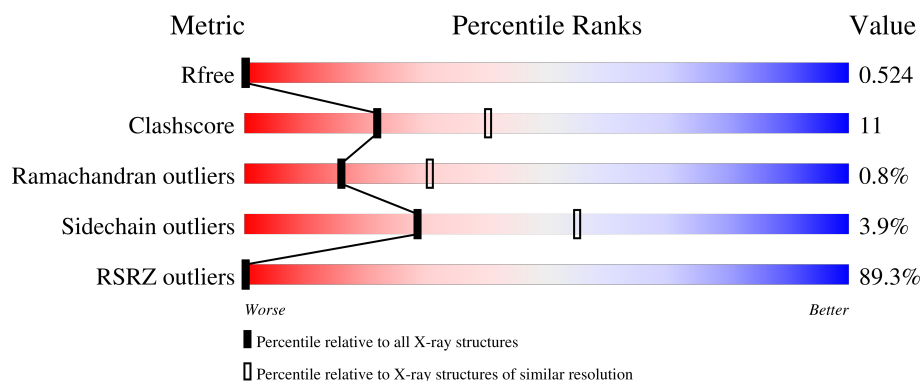
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	387	86% 75% 19% . .
1	B	387	83% 70% 24% . .
1	C	387	87% 68% 25% . 6%
2	D	2	100%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	F	2	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8771 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 46 kDa surface antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2886	1821	485	574	6			
1	B	373	Total	C	N	O	S	0	0	0
			2886	1821	485	574	6			
1	C	365	Total	C	N	O	S	0	0	0
			2832	1789	474	563	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	initiating methionine	UNP P0C0J8
A	417	LEU	-	expression tag	UNP P0C0J8
A	418	GLU	-	expression tag	UNP P0C0J8
B	32	MET	-	initiating methionine	UNP P0C0J8
B	417	LEU	-	expression tag	UNP P0C0J8
B	418	GLU	-	expression tag	UNP P0C0J8
C	32	MET	-	initiating methionine	UNP P0C0J8
C	417	LEU	-	expression tag	UNP P0C0J8
C	418	GLU	-	expression tag	UNP P0C0J8

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	2	Total	C	O	0	0	0
			23	12	11			
2	E	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

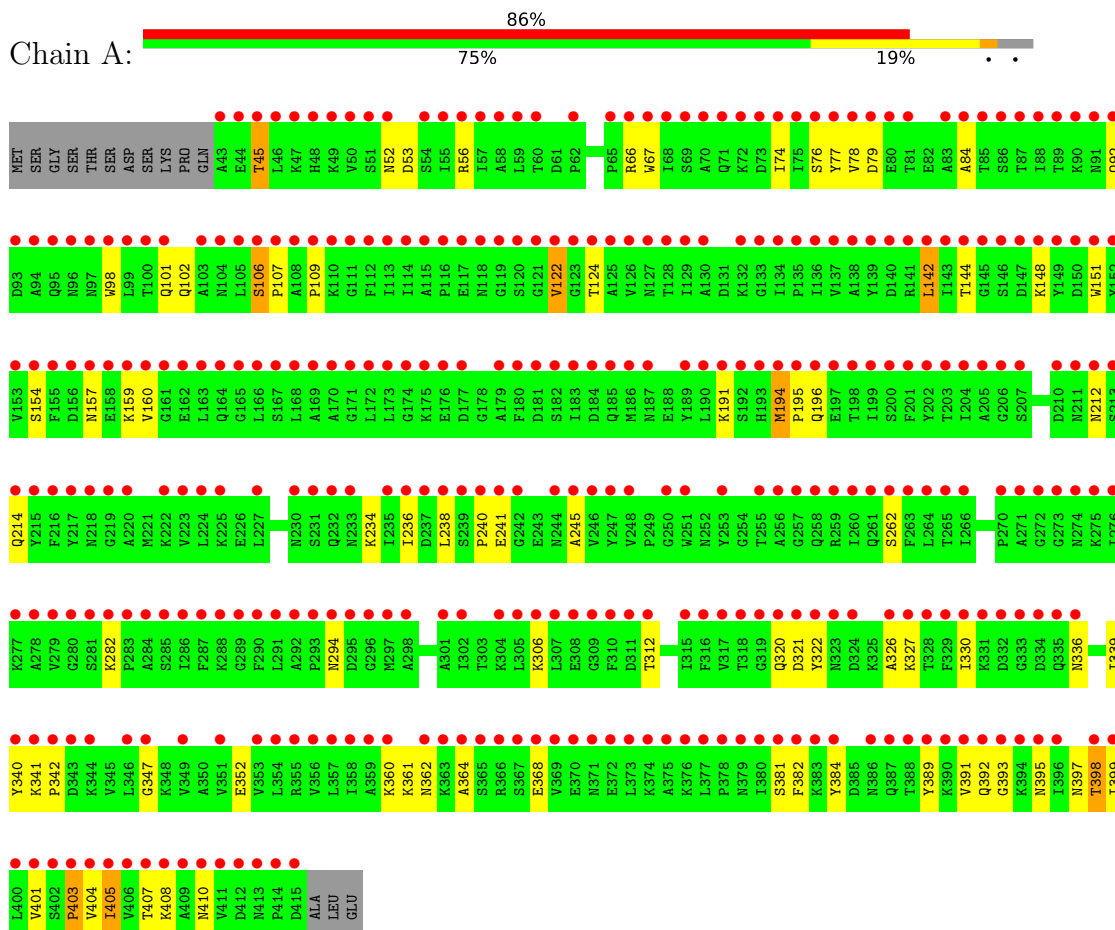
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	44	Total	O	0	0
			44	44		
4	C	13	Total	O	0	0
			13	13		

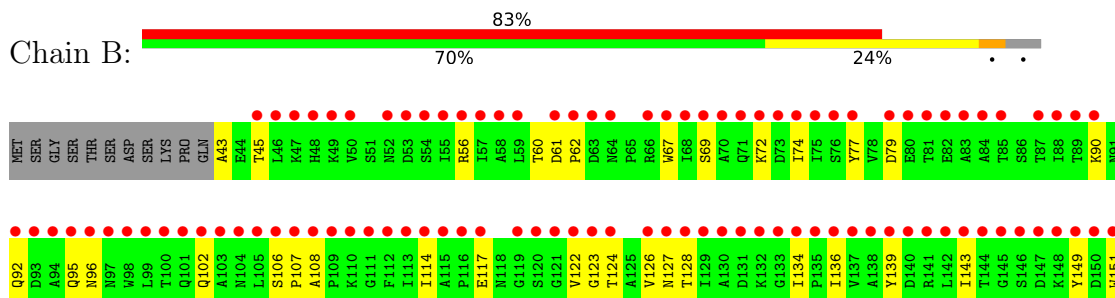
3 Residue-property plots

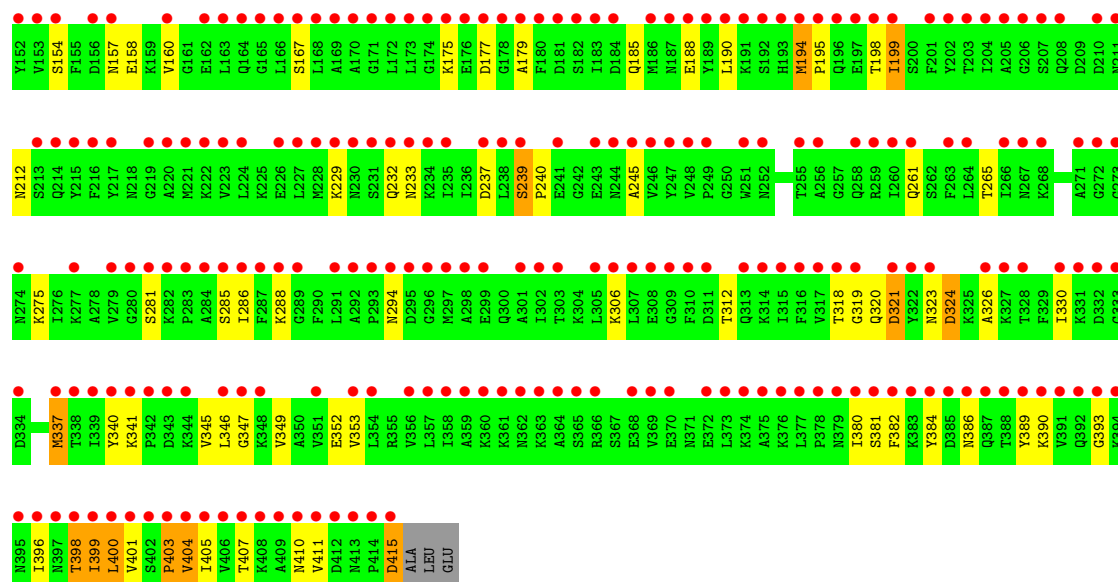
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 46 kDa surface antigen

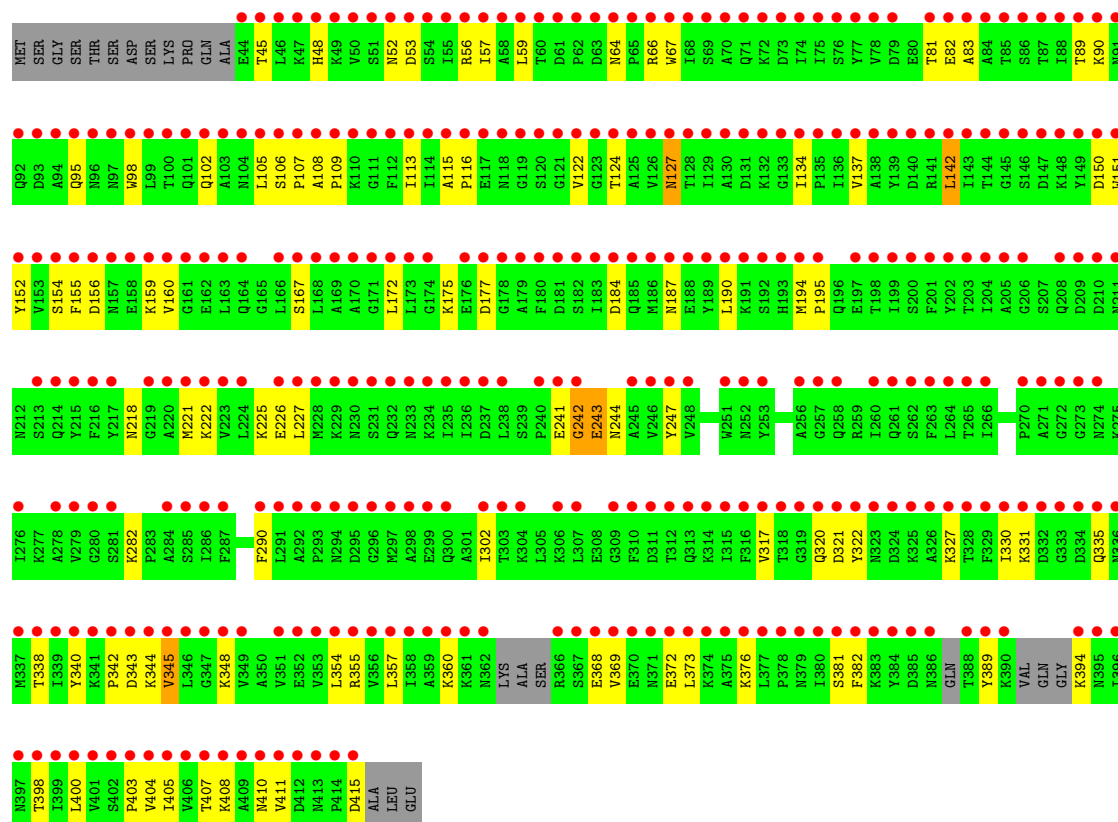
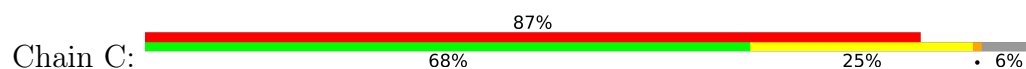


- Molecule 1: 46 kDa surface antigen





• Molecule 1: 46 kDa surface antigen



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:  50% 50%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:  50% 50%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.18Å 136.18Å 139.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.00 – 2.50 60.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (60.00-2.50) 99.9 (60.00-2.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.209 , 0.268 0.539 , 0.524	Depositor DCC
R_{free} test set	2650 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.60	EDS
Total number of atoms	8771	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 9.89% 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: GLC, NA

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	0.42	0/2937	0.61	0/3976
1	B	0.46	0/2937	0.66	0/3976
1	C	0.29	0/2880	0.50	0/3895
All	All	0.40	0/8754	0.60	0/11847

There are no bond length outliers.

There are no bond angle outliers.

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	2886	0	2875	48	0
1	B	2886	0	2875	72	0
1	C	2832	0	2816	65	0
2	D	23	0	21	1	0
2	E	23	0	21	1	0
2	F	23	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	38	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	44	0	0	3	0
4	C	13	0	0	0	0
All	All	8771	0	8629	185	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 11.

All (185) 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:C:56:ARG:NH1	1:C:102:GLN:OE1	2.14	0.81
1:B:72:LYS:NZ	4:B:622:HOH:O	2.12	0.80
1:A:151:TRP:HE1	1:A:364:ALA:HB1	1.45	0.79
1:A:340:TYR:HB3	1:A:405:ILE:HG23	1.66	0.77
1:B:381:SER:O	1:B:403:PRO:HD2	1.86	0.75
1:A:381:SER:O	1:A:403:PRO:HD2	1.88	0.74
1:B:194:MET:HG3	1:B:195:PRO:HD2	1.68	0.73
1:B:323:ASN:O	1:B:324:ASP:HB2	1.86	0.72
1:B:340:TYR:HB3	1:B:405:ILE:HG23	1.71	0.72
1:A:151:TRP:HE1	1:A:364:ALA:CB	2.03	0.71
1:B:399:ILE:HG12	1:B:400:LEU:N	2.05	0.69
1:B:390:LYS:HG2	1:B:396:ILE:HG23	1.74	0.69
1:C:81:THR:OG1	1:C:355:ARG:NH2	2.24	0.69
1:B:318:THR:HB	1:B:337:MET:HE2	1.75	0.67
1:B:382:PHE:HA	1:B:403:PRO:HD2	1.77	0.66
1:A:194:MET:HG3	1:A:195:PRO:HD2	1.78	0.66
1:C:82:GLU:HG2	1:C:83:ALA:H	1.61	0.66
1:A:160:VAL:HG22	1:A:404:VAL:HG21	1.78	0.65
1:C:372:GLU:HG3	1:C:376:LYS:HD3	1.77	0.65
1:B:326:ALA:O	1:B:330:ILE:HG13	1.96	0.64
1:A:294:ASN:HD22	2:D:1:GLC:H61	1.63	0.64
1:B:319:GLY:H	1:B:337:MET:CE	2.11	0.64
1:C:241:GLU:OE1	1:C:282:LYS:NZ	2.31	0.64
1:A:159:LYS:HD2	1:A:403:PRO:HG3	1.78	0.63
1:B:175:LYS:NZ	1:B:177:ASP:O	2.31	0.63
1:B:345:VAL:HG13	1:B:380:ILE:HD13	1.80	0.63
1:A:382:PHE:HA	1:A:403:PRO:HD2	1.81	0.63
1:B:403:PRO:HD3	4:B:601:HOH:O	2.00	0.62
1:C:137:VAL:HG23	1:C:354:LEU:HD13	1.83	0.61
1:C:317:VAL:CG2	1:C:335:GLN:HA	2.30	0.61
1:B:319:GLY:H	1:B:337:MET:HE2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLU:OE1	1:A:282:LYS:NZ	2.35	0.60
1:A:384:TYR:HE1	1:A:398:THR:HG22	1.65	0.60
1:B:340:TYR:HB3	1:B:405:ILE:CG2	2.32	0.60
1:C:302:ILE:HD11	1:C:317:VAL:HG21	1.82	0.59
1:B:160:VAL:HG22	1:B:404:VAL:HG21	1.83	0.59
1:B:275:LYS:HG2	1:B:286:ILE:HD13	1.84	0.59
1:C:290:PHE:HB3	1:C:317:VAL:HG12	1.85	0.59
1:C:360:LYS:HE2	1:C:368:GLU:HG3	1.84	0.59
1:C:369:VAL:HG12	1:C:373:LEU:HD11	1.84	0.58
1:B:92:GLN:O	1:B:96:ASN:ND2	2.34	0.58
1:B:341:LYS:HG2	1:B:404:VAL:HG11	1.85	0.57
1:A:157:ASN:ND2	1:A:212:ASN:OD1	2.37	0.57
1:A:361:LYS:HG2	1:A:362:ASN:H	1.69	0.57
1:C:64:ASN:HD22	1:C:67:TRP:CD1	2.23	0.57
1:A:106:SER:HB3	1:A:107:PRO:HD3	1.86	0.57
1:B:167:SER:HB3	1:B:179:ALA:HB2	1.87	0.57
1:C:48:HIS:HB3	1:C:83:ALA:HB2	1.87	0.56
1:B:410:ASN:O	1:B:410:ASN:ND2	2.38	0.56
1:C:160:VAL:HG22	1:C:404:VAL:HG21	1.88	0.55
1:C:242:GLY:O	1:C:244:ASN:N	2.39	0.55
1:B:74:ILE:HG12	1:B:347:GLY:HA3	1.88	0.55
1:B:237:ASP:OD1	1:B:239:SER:OG	2.20	0.55
1:B:62:PRO:HG2	1:B:90:LYS:HG3	1.89	0.55
1:C:124:THR:O	1:C:127:ASN:ND2	2.39	0.55
1:B:60:THR:HG21	1:B:117:GLU:HB2	1.90	0.54
1:B:154:SER:O	1:B:401:VAL:HA	2.07	0.54
1:A:56:ARG:NH1	1:A:102:GLN:OE1	2.40	0.53
1:A:74:ILE:HG12	1:A:347:GLY:HA3	1.90	0.53
1:C:330:ILE:HA	1:C:335:GLN:O	2.09	0.53
1:A:391:VAL:HG12	1:A:392:GLN:HG2	1.89	0.53
1:B:43:ALA:N	4:B:622:HOH:O	2.40	0.53
1:C:340:TYR:HB3	1:C:405:ILE:HG23	1.91	0.53
1:B:194:MET:SD	1:B:232:GLN:NE2	2.69	0.53
1:C:151:TRP:CZ2	1:C:369:VAL:HG21	2.43	0.53
1:B:139:TYR:CZ	1:B:346:LEU:HD23	2.44	0.52
1:A:322:TYR:OH	1:A:327:LYS:HE3	2.10	0.52
1:A:240:PRO:HB2	1:A:245:ALA:HB1	1.91	0.51
1:B:114:ILE:HD12	1:B:136:ILE:HG23	1.91	0.51
1:B:415:ASP:OD1	1:B:415:ASP:N	2.35	0.51
1:B:341:LYS:HA	1:B:404:VAL:HG12	1.92	0.51
1:C:321:ASP:O	1:C:338:THR:OG1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:NZ	1:A:234:LYS:HB3	2.26	0.50
1:B:384:TYR:HE1	1:B:398:THR:HG22	1.76	0.50
1:A:326:ALA:O	1:A:330:ILE:HG13	2.11	0.50
1:A:98:TRP:O	1:A:102:GLN:HG2	2.12	0.50
1:C:331:LYS:HG2	1:C:411:VAL:HG21	1.92	0.50
1:C:142:LEU:HD13	1:C:389:TYR:HB3	1.92	0.50
1:A:236:ILE:HD12	1:A:238:LEU:HD21	1.94	0.50
1:A:336:ASN:O	1:A:408:LYS:HD3	2.12	0.50
1:B:386:ASN:O	1:B:396:ILE:HG21	2.12	0.50
1:C:243:GLU:HG3	1:C:244:ASN:OD1	2.11	0.50
1:B:143:ILE:HB	1:B:149:TYR:CZ	2.47	0.49
1:B:108:ALA:HB1	1:B:134:ILE:HD11	1.94	0.49
1:B:390:LYS:HB3	1:B:393:GLY:O	2.12	0.49
1:C:66:ARG:NH1	1:C:343:ASP:OD2	2.45	0.49
1:B:157:ASN:ND2	1:B:212:ASN:OD1	2.45	0.49
1:A:403:PRO:HD3	4:A:611:HOH:O	2.12	0.49
1:B:190:LEU:HG	1:B:194:MET:HE2	1.95	0.49
1:B:294:ASN:HA	1:B:320:GLN:HB3	1.93	0.49
1:C:381:SER:O	1:C:403:PRO:HD2	2.12	0.49
1:B:126:VAL:HG13	1:B:136:ILE:HD13	1.96	0.48
1:C:175:LYS:C	1:C:177:ASP:H	2.21	0.48
1:A:306:LYS:NZ	1:A:312:THR:OG1	2.46	0.48
1:C:45:THR:HG21	1:C:83:ALA:HA	1.94	0.48
1:B:106:SER:HB2	1:B:107:PRO:HD3	1.96	0.48
1:B:321:ASP:OD1	2:E:2:GLC:O3	2.29	0.48
1:B:306:LYS:HZ2	1:B:312:THR:HG22	1.78	0.48
1:C:89:THR:HG21	1:C:95:GLN:HA	1.95	0.48
1:A:341:LYS:HG2	1:A:404:VAL:HG11	1.96	0.47
1:A:320:GLN:HA	1:A:339:ILE:H	1.79	0.47
1:C:342:PRO:HB2	1:C:345:VAL:HG12	1.95	0.47
1:B:92:GLN:HG3	1:B:96:ASN:HD21	1.79	0.47
1:C:382:PHE:CD2	1:C:400:LEU:HD11	2.50	0.47
1:C:354:LEU:HA	1:C:357:LEU:HB2	1.97	0.46
1:C:57:ILE:HG23	1:C:113:ILE:HB	1.97	0.46
1:C:53:ASP:HB3	1:C:107:PRO:HB2	1.97	0.46
1:B:124:THR:O	1:B:128:THR:HG23	2.16	0.46
1:B:349:VAL:O	1:B:353:VAL:HG23	2.16	0.46
1:B:261:GLN:O	1:B:265:THR:HG23	2.16	0.46
1:C:317:VAL:HG23	1:C:335:GLN:HA	1.97	0.46
1:C:190:LEU:HD22	1:C:227:LEU:HD12	1.98	0.45
1:C:408:LYS:HB2	1:C:408:LYS:HE2	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLN:NE2	1:A:122:VAL:HG13	2.31	0.45
1:A:66:ARG:NH1	1:A:67:TRP:CZ2	2.85	0.45
1:B:384:TYR:OH	1:B:398:THR:HG23	2.16	0.45
1:C:221:MET:O	1:C:225:LYS:HB2	2.16	0.45
1:B:61:ASP:HB3	1:B:67:TRP:CD1	2.52	0.45
1:B:45:THR:HB	1:B:79:ASP:OD1	2.16	0.45
1:B:77:TYR:OH	1:B:352:GLU:OE2	2.33	0.45
1:C:116:PRO:HB3	1:C:122:VAL:HG11	1.98	0.45
1:A:148:LYS:HD2	1:A:148:LYS:N	2.32	0.45
1:B:318:THR:CB	1:B:337:MET:HE2	2.43	0.44
1:C:320:GLN:HG2	1:C:321:ASP:N	2.31	0.44
1:B:123:GLY:O	1:B:127:ASN:ND2	2.50	0.44
1:A:194:MET:HG3	1:A:195:PRO:CD	2.46	0.44
1:B:229:LYS:N	1:B:229:LYS:HD3	2.32	0.44
1:C:53:ASP:HA	1:C:109:PRO:HA	1.99	0.44
1:C:218:ASN:O	1:C:222:LYS:HG2	2.17	0.44
1:C:108:ALA:HB1	1:C:134:ILE:HD11	2.00	0.44
1:C:410:ASN:O	1:C:410:ASN:ND2	2.51	0.44
1:A:52:ASN:ND2	4:A:605:HOH:O	2.35	0.44
1:A:391:VAL:O	1:A:395:ASN:HB3	2.18	0.44
1:B:390:LYS:HG2	1:B:396:ILE:HA	2.00	0.43
1:C:184:ASP:HA	1:C:187:ASN:HB2	1.99	0.43
1:B:151:TRP:HA	1:B:398:THR:O	2.17	0.43
1:A:234:LYS:HB3	1:A:234:LYS:HZ3	1.81	0.43
1:A:389:TYR:HD2	1:A:399:ILE:HD13	1.82	0.43
1:B:199:ILE:HD12	1:B:288:LYS:HD2	1.99	0.43
1:B:381:SER:C	1:B:403:PRO:HD2	2.42	0.43
1:A:194:MET:O	1:A:196:GLN:NE2	2.50	0.43
1:A:154:SER:O	1:A:401:VAL:HA	2.18	0.43
1:C:52:ASN:HB2	1:C:107:PRO:HD2	2.00	0.43
1:C:382:PHE:HB2	1:C:400:LEU:HD11	2.01	0.43
1:C:344:LYS:O	1:C:348:LYS:HD3	2.19	0.43
1:A:77:TYR:OH	1:A:352:GLU:OE2	2.33	0.42
1:A:294:ASN:HA	1:A:320:GLN:HB3	1.99	0.42
1:B:240:PRO:HB2	1:B:245:ALA:HB1	2.00	0.42
1:A:45:THR:HG22	1:A:79:ASP:HB2	2.01	0.42
1:B:185:GLN:O	1:B:188:GLU:HG3	2.19	0.42
1:B:61:ASP:HB3	1:B:67:TRP:HD1	1.84	0.42
1:C:175:LYS:NZ	1:C:177:ASP:HB3	2.34	0.42
1:C:408:LYS:C	1:C:410:ASN:H	2.27	0.42
1:A:53:ASP:HA	1:A:109:PRO:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ARG:NE	1:B:102:GLN:OE1	2.52	0.42
1:C:415:ASP:OD2	1:C:415:ASP:N	2.52	0.42
1:A:360:LYS:HE2	1:A:368:GLU:CD	2.45	0.42
1:A:340:TYR:CZ	1:A:342:PRO:HB3	2.54	0.42
1:B:389:TYR:CE1	1:B:399:ILE:HD12	2.54	0.42
1:C:244:ASN:HB3	1:C:247:TYR:CD2	2.54	0.42
1:B:404:VAL:H	1:B:404:VAL:HG22	1.52	0.41
1:A:389:TYR:HB2	1:A:399:ILE:HD11	2.01	0.41
1:C:52:ASN:HB3	1:C:105:LEU:HB3	2.02	0.41
1:C:150:ASP:O	1:C:398:THR:OG1	2.37	0.41
1:A:78:VAL:HG11	1:A:84:ALA:HB2	2.01	0.41
1:B:92:GLN:NE2	1:B:122:VAL:HG13	2.36	0.41
1:C:154:SER:OG	1:C:155:PHE:N	2.53	0.41
1:C:322:TYR:CZ	1:C:327:LYS:HD3	2.55	0.41
1:B:198:THR:HG22	1:B:285:SER:HB3	2.02	0.41
1:C:152:TYR:CZ	1:C:154:SER:HB2	2.55	0.41
1:C:156:ASP:OD2	1:C:159:LYS:HB2	2.20	0.41
1:C:98:TRP:O	1:C:102:GLN:HG2	2.20	0.41
1:C:408:LYS:O	1:C:411:VAL:HG13	2.21	0.41
1:B:160:VAL:HG11	1:B:320:GLN:OE1	2.20	0.41
1:B:382:PHE:HA	1:B:403:PRO:CD	2.47	0.41
1:C:372:GLU:O	1:C:376:LYS:HG2	2.20	0.41
1:C:394:LYS:HB3	1:C:394:LYS:HE2	1.89	0.41
1:C:194:MET:HG3	1:C:195:PRO:HD2	2.02	0.41
1:C:52:ASN:HA	1:C:56:ARG:NH2	2.36	0.40
1:C:59:LEU:HA	1:C:115:ALA:HB3	2.02	0.40
1:A:142:LEU:HD12	1:A:144:THR:HG22	2.03	0.40
1:A:191:LYS:HB2	1:A:191:LYS:HE3	1.66	0.40
1:B:60:THR:HG23	1:B:95:GLN:NE2	2.36	0.40
1:B:306:LYS:HZ2	1:B:312:THR:CG2	2.35	0.40
1:C:172:LEU:HD23	1:C:172:LEU:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/387 (96%)	351 (95%)	17 (5%)	3 (1%)	16	31
1	B	371/387 (96%)	346 (93%)	23 (6%)	2 (0%)	24	43
1	C	357/387 (92%)	326 (91%)	27 (8%)	4 (1%)	11	22
All	All	1099/1161 (95%)	1023 (93%)	67 (6%)	9 (1%)	16	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	324	ASP
1	A	321	ASP
1	A	393	GLY
1	B	321	ASP
1	C	90	LYS
1	C	243	GLU
1	A	410	ASN
1	C	106	SER
1	C	242	GLY

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	315/327 (96%)	300 (95%)	15 (5%)	23	46
1	B	315/327 (96%)	299 (95%)	16 (5%)	21	43
1	C	310/327 (95%)	304 (98%)	6 (2%)	50	76
All	All	940/981 (96%)	903 (96%)	37 (4%)	28	55

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR

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Mol	Chain	Res	Type
1	A	76	SER
1	A	101	GLN
1	A	106	SER
1	A	122	VAL
1	A	124	THR
1	A	142	LEU
1	A	194	MET
1	A	214	GLN
1	A	262	SER
1	A	397	ASN
1	A	398	THR
1	A	403	PRO
1	A	405	ILE
1	A	407	THR
1	B	69	SER
1	B	158	GLU
1	B	194	MET
1	B	199	ILE
1	B	233	ASN
1	B	239	SER
1	B	281	SER
1	B	337	MET
1	B	398	THR
1	B	399	ILE
1	B	400	LEU
1	B	403	PRO
1	B	404	VAL
1	B	407	THR
1	B	411	VAL
1	B	415	ASP
1	C	127	ASN
1	C	142	LEU
1	C	167	SER
1	C	226	GLU
1	C	345	VAL
1	C	407	THR

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

Mol	Chain	Res	Type
1	A	52	ASN
1	A	193	HIS

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Mol	Chain	Res	Type
1	A	313	GLN
1	A	387	GLN
1	A	397	ASN
1	A	413	ASN
1	B	71	GLN
1	B	214	GLN
1	B	230	ASN
1	B	300	GLN
1	B	313	GLN
1	C	157	ASN
1	C	261	GLN
1	C	267	ASN
1	C	313	GLN
1	C	410	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	$\# Z > 2$
2	GLC	D	1	2	12,12,12	0.61	0	17,17,17	0.61	0
2	GLC	D	2	2	11,11,12	0.72	0	15,15,17	1.18	2 (13%)
2	GLC	E	1	2	12,12,12	0.46	0	17,17,17	0.53	0
2	GLC	E	2	2	11,11,12	0.78	0	15,15,17	1.16	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	F	1	2	12,12,12	0.56	0	17,17,17	0.57	0
2	GLC	F	2	2	11,11,12	0.70	0	15,15,17	1.41	2 (13%)

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	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	GLC	C1-C2-C3	3.36	114.54	109.64
2	D	2	GLC	C1-C2-C3	3.18	114.28	109.64
2	F	2	GLC	C1-O5-C5	2.67	115.77	112.19
2	E	2	GLC	C1-C2-C3	2.54	113.34	109.64
2	D	2	GLC	C2-C3-C4	2.18	114.70	110.86
2	E	2	GLC	C1-O5-C5	2.09	114.99	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

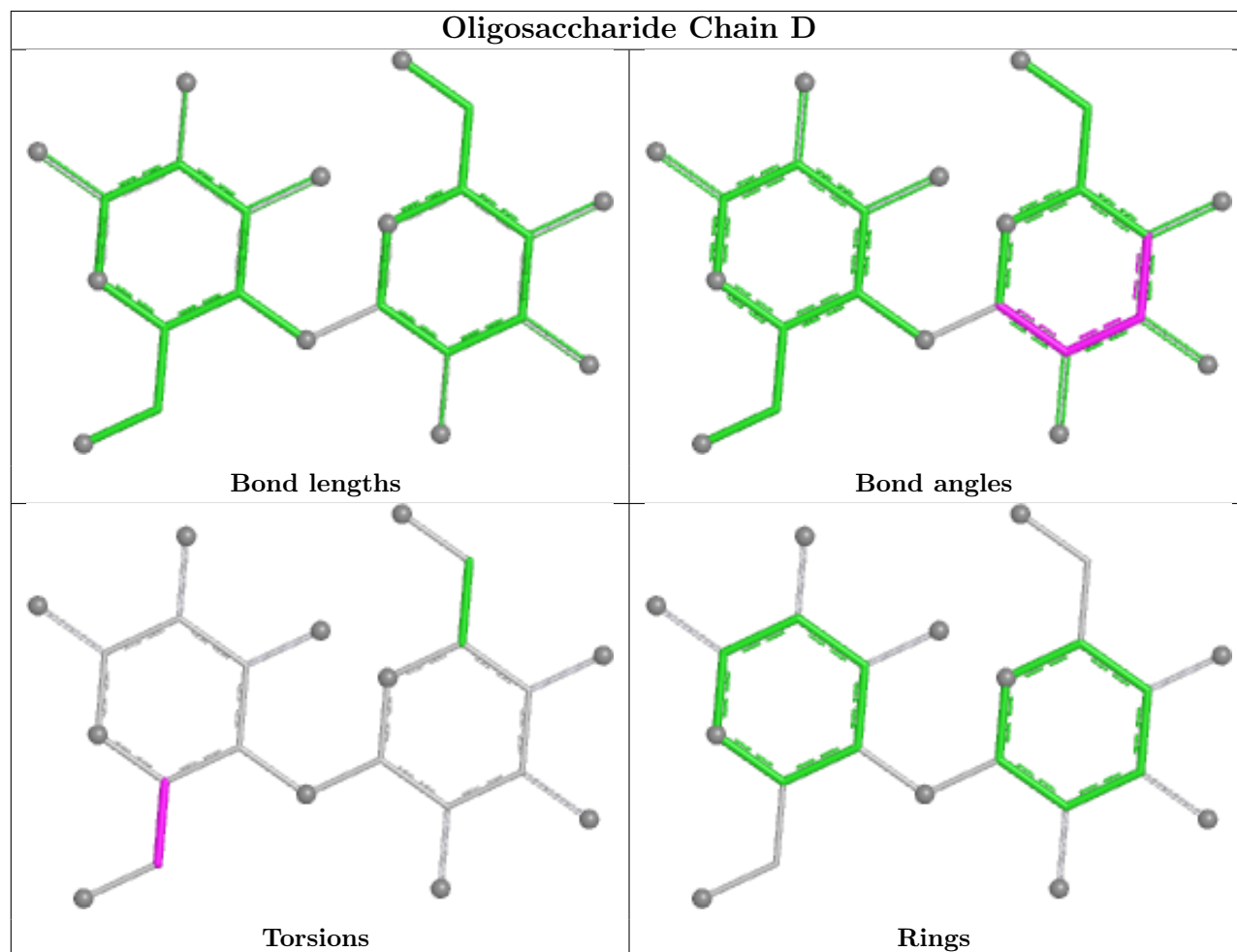
Mol	Chain	Res	Type	Atoms
2	F	2	GLC	O5-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6

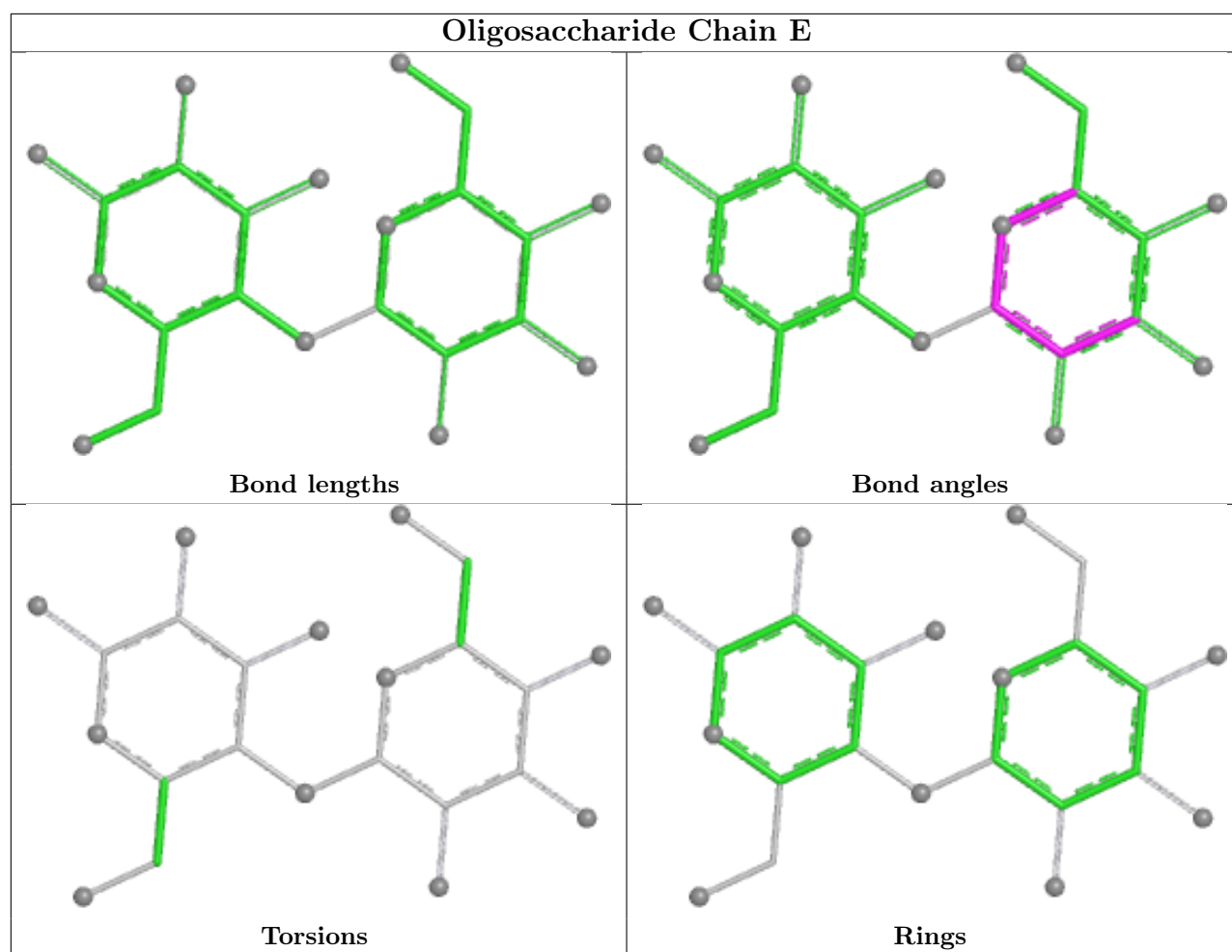
There are no ring outliers.

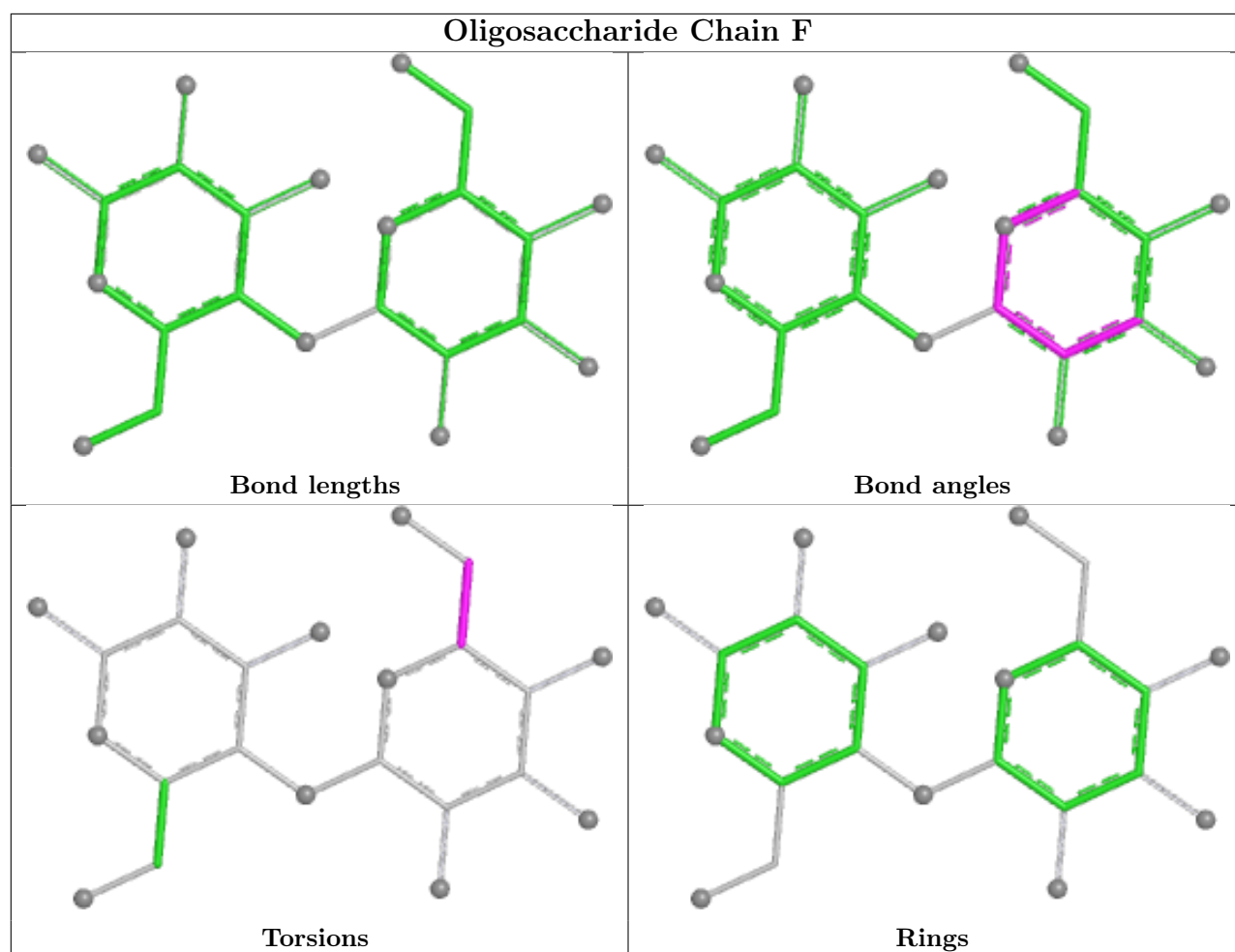
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	GLC	1	0
2	D	1	GLC	1	0

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







5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

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	373/387 (96%)	3.83	334 (89%) 0 0	39, 60, 94, 115	0
1	B	373/387 (96%)	3.82	322 (86%) 0 0	37, 57, 97, 114	0
1	C	365/387 (94%)	4.35	336 (92%) 0 0	42, 103, 149, 163	0
All	All	1111/1161 (95%)	4.00	992 (89%) 0 0	37, 66, 136, 163	0

All (992) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	187	ASN	15.6
1	C	401	VAL	15.5
1	C	192	SER	14.1
1	C	161	GLY	13.9
1	B	307	LEU	12.9
1	B	375	ALA	12.7
1	B	283	PRO	12.5
1	A	135	PRO	12.3
1	C	399	ILE	12.2
1	B	169	ALA	12.0
1	B	393	GLY	11.9
1	A	277	LYS	11.8
1	B	284	ALA	11.6
1	A	272	GLY	11.5
1	A	44	GLU	11.5
1	C	397	ASN	11.1
1	B	108	ALA	11.1
1	B	298	ALA	10.9
1	A	242	GLY	10.8
1	A	239	SER	10.5
1	B	199	ILE	10.5
1	C	371	ASN	10.5
1	A	282	LYS	10.5

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Mol	Chain	Res	Type	RSRZ
1	A	318	THR	10.4
1	A	70	ALA	10.4
1	A	108	ALA	10.3
1	B	170	ALA	10.3
1	C	354	LEU	10.3
1	C	395	ASN	10.2
1	A	317	VAL	10.2
1	C	160	VAL	10.0
1	A	211	ASN	9.9
1	C	357	LEU	9.7
1	C	368	GLU	9.7
1	C	396	ILE	9.6
1	C	235	ILE	9.6
1	C	193	HIS	9.5
1	A	205	ALA	9.4
1	C	54	SER	9.3
1	B	116	PRO	9.0
1	C	295	ASP	8.8
1	B	220	ALA	8.7
1	C	233	ASN	8.7
1	C	88	ILE	8.7
1	B	165	GLY	8.6
1	C	232	GLN	8.6
1	B	58	ALA	8.6
1	B	403	PRO	8.6
1	B	184	ASP	8.6
1	C	265	THR	8.5
1	C	389	TYR	8.5
1	B	406	VAL	8.4
1	A	288	LYS	8.3
1	A	276	ILE	8.2
1	C	59	LEU	8.2
1	B	277	LYS	8.2
1	B	343	ASP	8.1
1	C	414	PRO	8.1
1	A	170	ALA	8.0
1	A	45	THR	8.0
1	C	67	TRP	8.0
1	C	197	GLU	7.7
1	A	362	ASN	7.7
1	B	174	GLY	7.6
1	A	400	LEU	7.6

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Mol	Chain	Res	Type	RSRZ
1	C	366	ARG	7.6
1	C	312	THR	7.6
1	B	340	TYR	7.5
1	C	52	ASN	7.4
1	B	129	ILE	7.4
1	A	375	ALA	7.4
1	A	122	VAL	7.4
1	A	238	LEU	7.3
1	C	262	SER	7.3
1	C	378	PRO	7.3
1	C	77	TYR	7.2
1	A	319	GLY	7.2
1	B	187	ASN	7.2
1	A	298	ALA	7.2
1	C	199	ILE	7.2
1	A	289	GLY	7.2
1	B	407	THR	7.1
1	C	258	GLN	7.0
1	C	398	THR	7.0
1	B	404	VAL	7.0
1	A	51	SER	7.0
1	B	145	GLY	7.0
1	C	296	GLY	7.0
1	C	413	ASN	7.0
1	A	367	SER	6.9
1	B	330	ILE	6.9
1	B	317	VAL	6.9
1	A	198	THR	6.8
1	A	146	SER	6.8
1	C	208	GLN	6.8
1	C	242	GLY	6.7
1	B	63	ASP	6.7
1	B	322	TYR	6.7
1	B	171	GLY	6.7
1	C	109	PRO	6.7
1	B	70	ALA	6.7
1	B	131	ASP	6.7
1	B	213	SER	6.7
1	B	173	LEU	6.6
1	A	372	GLU	6.6
1	B	206	GLY	6.6
1	C	400	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	339	ILE	6.6
1	C	57	ILE	6.6
1	A	284	ALA	6.6
1	B	273	GLY	6.5
1	C	202	TYR	6.5
1	A	406	VAL	6.5
1	A	111	GLY	6.5
1	A	43	ALA	6.5
1	A	271	ALA	6.5
1	C	369	VAL	6.5
1	C	328	THR	6.5
1	C	345	VAL	6.4
1	C	89	THR	6.4
1	C	411	VAL	6.4
1	A	321	ASP	6.4
1	B	288	LYS	6.4
1	C	361	LYS	6.4
1	C	313	GLN	6.3
1	B	293	PRO	6.3
1	C	339	ILE	6.3
1	B	52	ASN	6.3
1	C	173	LEU	6.3
1	B	235	ILE	6.3
1	A	86	SER	6.3
1	A	214	GLN	6.2
1	B	266	ILE	6.2
1	A	46	LEU	6.2
1	B	106	SER	6.2
1	A	240	PRO	6.2
1	A	251	TRP	6.2
1	C	151	TRP	6.2
1	C	70	ALA	6.2
1	C	58	ALA	6.1
1	C	260	ILE	6.1
1	C	108	ALA	6.1
1	A	125	ALA	6.1
1	C	140	ASP	6.1
1	C	118	ASN	6.1
1	B	237	ASP	6.0
1	C	64	ASN	6.0
1	C	66	ARG	6.0
1	B	248	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	286	ILE	6.0
1	A	150	ASP	6.0
1	C	362	ASN	6.0
1	A	396	ILE	6.0
1	B	109	PRO	6.0
1	A	290	PHE	6.0
1	A	157	ASN	5.9
1	A	307	LEU	5.9
1	C	412	ASP	5.9
1	A	152	TYR	5.9
1	B	195	PRO	5.9
1	C	136	ILE	5.9
1	A	283	PRO	5.8
1	C	318	THR	5.8
1	A	52	ASN	5.8
1	A	395	ASN	5.8
1	B	179	ALA	5.8
1	B	198	THR	5.8
1	B	126	VAL	5.8
1	B	153	VAL	5.8
1	B	397	ASN	5.8
1	A	173	LEU	5.7
1	C	377	LEU	5.7
1	A	376	LYS	5.7
1	A	139	TYR	5.7
1	B	319	GLY	5.7
1	A	405	ILE	5.7
1	B	66	ARG	5.7
1	B	204	ILE	5.7
1	C	107	PRO	5.7
1	C	91	ASN	5.7
1	B	251	TRP	5.7
1	C	189	TYR	5.7
1	B	196	GLN	5.7
1	C	227	LEU	5.7
1	A	197	GLU	5.7
1	A	124	THR	5.7
1	C	404	VAL	5.7
1	A	109	PRO	5.7
1	A	87	THR	5.6
1	B	347	GLY	5.6
1	A	183	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	322	TYR	5.6
1	C	142	LEU	5.6
1	C	158	GLU	5.6
1	C	46	LEU	5.6
1	B	292	ALA	5.6
1	C	279	VAL	5.6
1	A	365	SER	5.5
1	B	314	LYS	5.5
1	C	230	ASN	5.5
1	B	376	LYS	5.5
1	C	385	ASP	5.5
1	B	372	GLU	5.5
1	C	204	ILE	5.5
1	A	341	LYS	5.4
1	B	362	ASN	5.4
1	C	317	VAL	5.4
1	A	199	ILE	5.4
1	A	49	LYS	5.4
1	A	202	TYR	5.4
1	C	388	THR	5.4
1	C	211	ASN	5.4
1	B	272	GLY	5.4
1	C	174	GLY	5.4
1	C	143	ILE	5.4
1	C	390	LYS	5.3
1	C	133	GLY	5.3
1	C	172	LEU	5.3
1	C	246	VAL	5.3
1	B	205	ALA	5.3
1	C	298	ALA	5.3
1	C	65	PRO	5.3
1	A	136	ILE	5.3
1	B	96	ASN	5.3
1	A	155	PHE	5.3
1	C	105	LEU	5.3
1	B	389	TYR	5.2
1	C	114	ILE	5.2
1	B	122	VAL	5.2
1	C	384	TYR	5.2
1	B	62	PRO	5.2
1	C	90	LYS	5.2
1	C	93	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	245	ALA	5.2
1	A	358	ILE	5.2
1	B	172	LEU	5.2
1	C	266	ILE	5.2
1	C	74	ILE	5.2
1	A	309	GLY	5.1
1	B	178	GLY	5.1
1	B	364	ALA	5.1
1	A	293	PRO	5.1
1	B	414	PRO	5.1
1	C	119	GLY	5.1
1	A	291	LEU	5.1
1	B	274	ASN	5.1
1	A	354	LEU	5.1
1	B	285	SER	5.1
1	C	113	ILE	5.1
1	C	222	LYS	5.0
1	A	116	PRO	5.0
1	A	163	LEU	5.0
1	B	399	ILE	5.0
1	C	55	ILE	5.0
1	C	128	THR	5.0
1	A	119	GLY	5.0
1	A	71	GLN	5.0
1	B	409	ALA	5.0
1	B	167	SER	5.0
1	C	359	ALA	4.9
1	C	247	TYR	4.9
1	C	314	LYS	4.9
1	C	101	GLN	4.9
1	C	171	GLY	4.9
1	B	183	ILE	4.9
1	C	147	ASP	4.9
1	A	222	LYS	4.9
1	B	197	GLU	4.9
1	B	202	TYR	4.9
1	A	112	PHE	4.9
1	B	258	GLN	4.9
1	C	333	GLY	4.9
1	A	286	ILE	4.9
1	B	49	LYS	4.8
1	C	278	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	104	ASN	4.8
1	B	394	LYS	4.8
1	C	87	THR	4.8
1	C	104	ASN	4.8
1	B	302	ILE	4.8
1	A	92	GLN	4.8
1	B	229	LYS	4.8
1	B	381	SER	4.8
1	A	233	ASN	4.8
1	C	115	ALA	4.8
1	C	99	LEU	4.8
1	C	156	ASP	4.7
1	A	133	GLY	4.7
1	C	75	ILE	4.7
1	A	106	SER	4.7
1	C	139	TYR	4.7
1	C	374	LYS	4.7
1	B	214	GLN	4.7
1	B	59	LEU	4.7
1	B	142	LEU	4.7
1	C	86	SER	4.7
1	B	415	ASP	4.7
1	C	201	PHE	4.7
1	A	308	GLU	4.6
1	C	144	THR	4.6
1	B	309	GLY	4.6
1	C	261	GLN	4.6
1	C	63	ASP	4.6
1	B	390	LYS	4.6
1	B	386	ASN	4.6
1	B	193	HIS	4.6
1	B	128	THR	4.6
1	B	296	GLY	4.6
1	C	126	VAL	4.6
1	C	380	ILE	4.6
1	A	215	TYR	4.6
1	A	148	LYS	4.6
1	C	370	GLU	4.5
1	B	207	SER	4.5
1	C	76	SER	4.5
1	B	387	GLN	4.5
1	A	246	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	50	VAL	4.5
1	C	116	PRO	4.5
1	C	186	MET	4.5
1	A	190	LEU	4.5
1	B	99	LEU	4.5
1	C	415	ASP	4.5
1	A	219	GLY	4.5
1	C	122	VAL	4.5
1	C	183	ILE	4.5
1	A	371	ASN	4.5
1	A	381	SER	4.5
1	C	320	GLN	4.5
1	C	79	ASP	4.5
1	C	340	TYR	4.4
1	A	401	VAL	4.4
1	B	227	LEU	4.4
1	A	295	ASP	4.4
1	A	57	ILE	4.4
1	B	256	ALA	4.4
1	A	118	ASN	4.4
1	A	364	ALA	4.4
1	B	74	ILE	4.3
1	B	190	LEU	4.3
1	C	125	ALA	4.3
1	B	280	GLY	4.3
1	C	124	THR	4.3
1	C	309	GLY	4.3
1	B	405	ILE	4.3
1	A	105	LEU	4.3
1	C	213	SER	4.3
1	A	270	PRO	4.3
1	A	126	VAL	4.3
1	C	78	VAL	4.3
1	C	97	ASN	4.3
1	B	295	ASP	4.3
1	C	53	ASP	4.3
1	A	62	PRO	4.3
1	C	98	TRP	4.3
1	A	85	THR	4.3
1	B	315	ILE	4.3
1	A	349	VAL	4.3
1	C	166	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	123	GLY	4.2
1	A	74	ILE	4.2
1	C	349	VAL	4.2
1	C	106	SER	4.2
1	A	47	LYS	4.2
1	B	222	LYS	4.2
1	A	312	THR	4.2
1	A	137	VAL	4.2
1	C	135	PRO	4.2
1	A	181	ASP	4.2
1	C	117	GLU	4.2
1	B	67	TRP	4.2
1	A	326	ALA	4.2
1	C	245	ALA	4.2
1	A	394	LYS	4.2
1	B	217	TYR	4.2
1	B	281	SER	4.2
1	C	343	ASP	4.2
1	A	204	ILE	4.2
1	C	129	ILE	4.2
1	C	176	GLU	4.2
1	C	356	VAL	4.2
1	B	263	PHE	4.1
1	C	360	LYS	4.1
1	C	188	GLU	4.1
1	C	291	LEU	4.1
1	C	180	PHE	4.1
1	C	216	PHE	4.1
1	C	221	MET	4.1
1	B	378	PRO	4.1
1	C	127	ASN	4.1
1	C	336	ASN	4.1
1	B	71	GLN	4.1
1	A	210	ASP	4.1
1	C	44	GLU	4.1
1	C	257	GLY	4.1
1	C	273	GLY	4.1
1	C	141	ARG	4.1
1	A	331	LYS	4.1
1	C	348	LYS	4.1
1	A	96	ASN	4.1
1	A	257	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	121	GLY	4.1
1	A	363	LYS	4.1
1	B	175	LYS	4.1
1	C	45	THR	4.1
1	A	281	SER	4.0
1	C	182	SER	4.0
1	A	134	ILE	4.0
1	B	338	THR	4.0
1	A	273	GLY	4.0
1	A	334	ASP	4.0
1	C	72	LYS	4.0
1	B	365	SER	4.0
1	C	149	TYR	4.0
1	C	190	LEU	4.0
1	A	329	PHE	4.0
1	A	408	LYS	4.0
1	C	321	ASP	4.0
1	C	146	SER	4.0
1	C	281	SER	4.0
1	A	389	TYR	4.0
1	C	226	GLU	4.0
1	A	103	ALA	4.0
1	A	220	ALA	4.0
1	A	278	ALA	4.0
1	A	347	GLY	4.0
1	A	143	ILE	4.0
1	B	396	ILE	4.0
1	C	394	LYS	3.9
1	B	410	ASN	3.9
1	C	123	GLY	3.9
1	A	55	ILE	3.9
1	A	330	ILE	3.9
1	A	83	ALA	3.9
1	A	415	ASP	3.9
1	C	68	ILE	3.9
1	A	166	LEU	3.9
1	C	402	SER	3.9
1	B	107	PRO	3.9
1	B	342	PRO	3.9
1	B	411	VAL	3.9
1	C	293	PRO	3.9
1	B	186	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	386	ASN	3.9
1	B	163	LEU	3.9
1	C	69	SER	3.9
1	C	256	ALA	3.9
1	A	192	SER	3.9
1	C	82	GLU	3.9
1	C	381	SER	3.9
1	C	215	TYR	3.8
1	A	212	ASN	3.8
1	B	48	HIS	3.8
1	B	244	ASN	3.8
1	C	224	LEU	3.8
1	C	346	LEU	3.8
1	B	368	GLU	3.8
1	C	81	THR	3.8
1	C	351	VAL	3.8
1	A	384	TYR	3.8
1	A	132	LYS	3.8
1	B	140	ASP	3.8
1	C	71	GLN	3.8
1	A	351	VAL	3.8
1	C	304	LYS	3.8
1	C	410	ASN	3.8
1	B	88	ILE	3.8
1	C	236	ILE	3.8
1	B	124	THR	3.8
1	C	405	ILE	3.8
1	C	150	ASP	3.8
1	C	209	ASP	3.8
1	A	76	SER	3.7
1	B	341	LYS	3.7
1	C	284	ALA	3.7
1	C	403	PRO	3.7
1	B	297	MET	3.7
1	B	363	LYS	3.7
1	A	120	SER	3.7
1	B	231	SER	3.7
1	B	351	VAL	3.7
1	C	353	VAL	3.7
1	A	413	ASN	3.7
1	B	157	ASN	3.7
1	A	237	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	340	TYR	3.7
1	C	60	THR	3.7
1	A	130	ALA	3.7
1	C	94	ALA	3.7
1	B	260	ILE	3.7
1	B	332	ASP	3.7
1	A	72	LYS	3.7
1	A	344	LYS	3.7
1	B	189	TYR	3.7
1	B	408	LYS	3.7
1	B	144	THR	3.7
1	C	179	ALA	3.7
1	C	409	ALA	3.7
1	C	214	GLN	3.7
1	C	330	ILE	3.7
1	A	294	ASN	3.7
1	C	376	LYS	3.7
1	A	217	TYR	3.7
1	B	401	VAL	3.6
1	C	103	ALA	3.6
1	B	92	GLN	3.6
1	B	148	LYS	3.6
1	A	378	PRO	3.6
1	C	379	ASN	3.6
1	B	181	ASP	3.6
1	C	100	THR	3.6
1	B	54	SER	3.6
1	B	47	LYS	3.6
1	A	171	GLY	3.6
1	B	216	PHE	3.6
1	A	260	ILE	3.6
1	B	230	ASN	3.6
1	C	157	ASN	3.6
1	B	306	LYS	3.6
1	C	159	LYS	3.6
1	C	130	ALA	3.6
1	C	169	ALA	3.6
1	C	326	ALA	3.6
1	A	59	LEU	3.6
1	B	400	LEU	3.6
1	C	316	PHE	3.6
1	A	311	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	386	ASN	3.6
1	B	384	TYR	3.6
1	B	305	LEU	3.6
1	B	357	LEU	3.6
1	C	280	GLY	3.6
1	A	75	ILE	3.6
1	B	55	ILE	3.6
1	A	336	ASN	3.6
1	A	60	THR	3.5
1	C	85	THR	3.5
1	C	153	VAL	3.5
1	C	253	TYR	3.5
1	A	54	SER	3.5
1	C	56	ARG	3.5
1	A	335	GLN	3.5
1	C	92	GLN	3.5
1	B	238	LEU	3.5
1	B	377	LEU	3.5
1	A	274	ASN	3.5
1	A	56	ARG	3.5
1	B	328	THR	3.5
1	C	152	TYR	3.5
1	A	67	TRP	3.5
1	A	161	GLY	3.5
1	B	245	ALA	3.5
1	C	292	ALA	3.5
1	A	88	ILE	3.5
1	C	48	HIS	3.5
1	B	282	LYS	3.5
1	C	132	LYS	3.5
1	A	141	ARG	3.5
1	B	402	SER	3.5
1	C	251	TRP	3.5
1	A	187	ASN	3.5
1	A	323	ASN	3.5
1	B	252	ASN	3.5
1	B	395	ASN	3.5
1	A	297	MET	3.5
1	B	105	LEU	3.5
1	A	322	TYR	3.5
1	A	94	ALA	3.5
1	B	359	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	100	THR	3.4
1	C	375	ALA	3.4
1	B	112	PHE	3.4
1	C	382	PHE	3.4
1	C	237	ASP	3.4
1	B	264	LEU	3.4
1	C	264	LEU	3.4
1	C	240	PRO	3.4
1	C	138	ALA	3.4
1	A	285	SER	3.4
1	C	315	ILE	3.4
1	B	287	PHE	3.4
1	B	412	ASP	3.4
1	A	89	THR	3.4
1	A	383	LYS	3.4
1	C	110	LYS	3.4
1	A	368	GLU	3.4
1	A	191	LYS	3.4
1	A	142	LEU	3.4
1	A	195	PRO	3.4
1	C	195	PRO	3.4
1	A	393	GLY	3.4
1	B	119	GLY	3.4
1	B	138	ALA	3.4
1	B	326	ALA	3.4
1	A	140	ASP	3.3
1	B	385	ASP	3.3
1	B	294	ASN	3.3
1	A	196	GLN	3.3
1	C	344	LYS	3.3
1	A	153	VAL	3.3
1	A	414	PRO	3.3
1	B	373	LEU	3.3
1	A	193	HIS	3.3
1	C	162	GLU	3.3
1	B	192	SER	3.3
1	C	120	SER	3.3
1	A	201	PHE	3.3
1	C	155	PHE	3.3
1	C	290	PHE	3.3
1	B	152	TYR	3.3
1	B	331	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	334	ASP	3.3
1	A	101	GLN	3.3
1	B	392	GLN	3.3
1	B	82	GLU	3.3
1	A	179	ALA	3.3
1	C	51	SER	3.3
1	B	180	PHE	3.3
1	A	189	TYR	3.3
1	C	217	TYR	3.3
1	A	227	LEU	3.3
1	A	369	VAL	3.3
1	B	223	VAL	3.3
1	C	145	GLY	3.3
1	C	206	GLY	3.3
1	A	129	ILE	3.3
1	A	399	ILE	3.3
1	B	115	ALA	3.3
1	C	194	MET	3.3
1	A	182	SER	3.3
1	A	382	PHE	3.3
1	A	324	ASP	3.3
1	C	252	ASN	3.3
1	B	391	VAL	3.3
1	B	146	SER	3.2
1	A	232	GLN	3.2
1	B	413	ASN	3.2
1	A	117	GLU	3.2
1	A	162	GLU	3.2
1	B	84	ALA	3.2
1	C	84	ALA	3.2
1	B	69	SER	3.2
1	B	164	GLN	3.2
1	C	167	SER	3.2
1	C	287	PHE	3.2
1	A	73	ASP	3.2
1	A	99	LEU	3.2
1	A	224	LEU	3.2
1	B	46	LEU	3.2
1	B	308	GLU	3.2
1	B	132	LYS	3.2
1	B	114	ILE	3.2
1	C	164	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	287	PHE	3.2
1	A	355	ARG	3.2
1	B	316	PHE	3.2
1	B	79	ASP	3.2
1	C	131	ASP	3.2
1	A	77	TYR	3.2
1	B	77	TYR	3.2
1	B	279	VAL	3.2
1	A	81	THR	3.2
1	B	289	GLY	3.2
1	A	113	ILE	3.2
1	B	68	ILE	3.2
1	B	313	GLN	3.2
1	C	154	SER	3.2
1	B	147	ASP	3.2
1	A	48	HIS	3.2
1	A	327	LYS	3.2
1	B	72	LYS	3.2
1	B	374	LYS	3.2
1	C	307	LEU	3.2
1	C	358	ILE	3.2
1	A	180	PHE	3.1
1	A	262	SER	3.1
1	C	112	PHE	3.1
1	B	150	ASP	3.1
1	C	184	ASP	3.1
1	A	342	PRO	3.1
1	A	357	LEU	3.1
1	A	296	GLY	3.1
1	B	353	VAL	3.1
1	A	275	LYS	3.1
1	B	76	SER	3.1
1	C	263	PHE	3.1
1	A	244	ASN	3.1
1	B	398	THR	3.1
1	A	320	GLN	3.1
1	A	304	LYS	3.1
1	B	168	LEU	3.1
1	A	127	ASN	3.1
1	B	64	ASN	3.1
1	C	50	VAL	3.1
1	B	85	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	134	ILE	3.1
1	B	101	GLN	3.1
1	C	327	LYS	3.1
1	A	310	PHE	3.1
1	B	166	LEU	3.1
1	A	69	SER	3.1
1	A	174	GLY	3.1
1	B	221	MET	3.0
1	B	226	GLU	3.0
1	C	297	MET	3.0
1	C	329	PHE	3.0
1	B	56	ARG	3.0
1	B	267	ASN	3.0
1	C	148	LYS	3.0
1	A	380	ILE	3.0
1	B	113	ILE	3.0
1	B	130	ALA	3.0
1	B	346	LEU	3.0
1	B	61	ASP	3.0
1	C	73	ASP	3.0
1	C	334	ASP	3.0
1	B	361	LYS	3.0
1	B	57	ILE	3.0
1	B	98	TRP	3.0
1	A	100	THR	3.0
1	A	169	ALA	3.0
1	B	103	ALA	3.0
1	B	117	GLU	3.0
1	A	305	LEU	3.0
1	B	360	LYS	3.0
1	C	274	ASN	3.0
1	A	123	GLY	3.0
1	A	78	VAL	3.0
1	B	176	GLU	3.0
1	B	299	GLU	3.0
1	C	62	PRO	3.0
1	B	224	LEU	3.0
1	C	355	ARG	3.0
1	A	159	LYS	3.0
1	C	229	LYS	3.0
1	A	95	GLN	3.0
1	C	352	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	115	ALA	2.9
1	B	154	SER	2.9
1	A	186	MET	2.9
1	A	302	ILE	2.9
1	B	87	THR	2.9
1	C	338	THR	2.9
1	C	306	LYS	2.9
1	A	149	TYR	2.9
1	A	250	GLY	2.9
1	A	370	GLU	2.9
1	A	68	ILE	2.9
1	A	266	ILE	2.9
1	A	409	ALA	2.9
1	A	151	TRP	2.9
1	A	412	ASP	2.9
1	B	201	PHE	2.9
1	C	185	GLN	2.9
1	B	188	GLU	2.9
1	C	49	LYS	2.9
1	B	301	ALA	2.9
1	C	205	ALA	2.9
1	A	184	ASP	2.9
1	A	261	GLN	2.9
1	A	165	GLY	2.9
1	C	219	GLY	2.9
1	A	97	ASN	2.8
1	B	97	ASN	2.8
1	B	233	ASN	2.8
1	A	110	LYS	2.8
1	B	191	LYS	2.8
1	B	94	ALA	2.8
1	B	232	GLN	2.8
1	A	176	GLU	2.8
1	C	299	GLU	2.8
1	A	66	ARG	2.8
1	B	344	LYS	2.8
1	C	331	LYS	2.8
1	A	114	ILE	2.8
1	A	160	VAL	2.8
1	B	135	PRO	2.8
1	C	198	THR	2.8
1	C	168	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	156	ASP	2.8
1	B	73	ASP	2.8
1	C	181	ASP	2.8
1	A	98	TRP	2.8
1	C	234	LYS	2.8
1	A	206	GLY	2.8
1	A	247	TYR	2.8
1	B	111	GLY	2.8
1	A	379	ASN	2.8
1	C	276	ILE	2.8
1	C	220	ALA	2.8
1	C	337	MET	2.8
1	A	241	GLU	2.8
1	B	259	ARG	2.8
1	C	383	LYS	2.8
1	B	121	GLY	2.8
1	A	356	VAL	2.8
1	C	228	MET	2.8
1	C	341	LYS	2.8
1	A	258	GLN	2.8
1	B	95	GLN	2.8
1	C	300	GLN	2.8
1	C	372	GLU	2.8
1	C	61	ASP	2.8
1	C	332	ASP	2.8
1	A	316	PHE	2.8
1	C	96	ASN	2.7
1	A	411	VAL	2.7
1	B	303	THR	2.7
1	A	194	MET	2.7
1	B	90	LYS	2.7
1	C	325	LYS	2.7
1	A	333	GLY	2.7
1	B	127	ASN	2.7
1	B	379	ASN	2.7
1	A	200	SER	2.7
1	A	402	SER	2.7
1	B	246	VAL	2.7
1	A	346	LEU	2.7
1	B	110	LYS	2.7
1	A	259	ARG	2.7
1	A	80	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	158	GLU	2.7
1	C	95	GLN	2.7
1	A	147	ASP	2.7
1	B	136	ILE	2.7
1	B	143	ILE	2.7
1	A	223	VAL	2.7
1	B	160	VAL	2.7
1	C	137	VAL	2.7
1	A	264	LEU	2.7
1	A	128	THR	2.7
1	B	318	THR	2.7
1	C	102	GLN	2.7
1	C	178	GLY	2.7
1	C	270	PRO	2.7
1	B	211	ASN	2.7
1	C	408	LYS	2.7
1	A	404	VAL	2.7
1	A	253	TYR	2.7
1	C	83	ALA	2.7
1	A	332	ASP	2.6
1	B	210	ASP	2.6
1	C	294	ASN	2.6
1	A	50	VAL	2.6
1	C	367	SER	2.6
1	A	265	THR	2.6
1	A	145	GLY	2.6
1	A	107	PRO	2.6
1	B	137	VAL	2.6
1	A	144	THR	2.6
1	A	359	ALA	2.6
1	B	327	LYS	2.6
1	B	133	GLY	2.6
1	C	238	LEU	2.6
1	A	410	ASN	2.6
1	A	387	GLN	2.6
1	A	255	THR	2.6
1	A	388	THR	2.6
1	B	89	THR	2.6
1	C	210	ASP	2.6
1	C	310	PHE	2.6
1	A	377	LEU	2.6
1	C	373	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	353	VAL	2.6
1	A	301	ALA	2.6
1	B	255	THR	2.6
1	B	53	ASP	2.5
1	B	194	MET	2.5
1	C	177	ASP	2.5
1	A	235	ILE	2.5
1	B	358	ILE	2.5
1	C	163	LEU	2.5
1	C	323	ASN	2.5
1	B	348	LYS	2.5
1	B	228	MET	2.5
1	A	164	GLN	2.5
1	A	175	LYS	2.5
1	C	223	VAL	2.5
1	A	292	ALA	2.5
1	C	347	GLY	2.5
1	B	234	LYS	2.5
1	C	47	LYS	2.5
1	B	83	ALA	2.5
1	C	170	ALA	2.5
1	B	203	THR	2.5
1	A	315	ILE	2.5
1	C	286	ILE	2.5
1	A	172	LEU	2.5
1	A	263	PHE	2.5
1	B	333	GLY	2.4
1	C	319	GLY	2.4
1	B	247	TYR	2.4
1	B	354	LEU	2.4
1	A	218	ASN	2.4
1	B	81	THR	2.4
1	A	65	PRO	2.4
1	B	177	ASP	2.4
1	B	208	GLN	2.4
1	B	261	GLN	2.4
1	A	167	SER	2.4
1	B	182	SER	2.4
1	B	243	GLU	2.4
1	C	285	SER	2.4
1	C	335	GLN	2.4
1	A	366	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	215	TYR	2.4
1	A	306	LYS	2.4
1	B	45	THR	2.4
1	C	200	SER	2.4
1	A	79	ASP	2.4
1	A	343	ASP	2.4
1	B	139	TYR	2.4
1	A	391	VAL	2.4
1	B	162	GLU	2.4
1	C	303	THR	2.3
1	C	342	PRO	2.3
1	A	213	SER	2.3
1	B	310	PHE	2.3
1	A	91	ASN	2.3
1	C	271	ALA	2.3
1	B	388	THR	2.3
1	C	111	GLY	2.3
1	B	102	GLN	2.3
1	B	268	LYS	2.3
1	B	382	PHE	2.3
1	C	406	VAL	2.3
1	B	323	ASN	2.3
1	A	58	ALA	2.3
1	A	407	THR	2.3
1	A	231	SER	2.3
1	A	373	LEU	2.3
1	B	75	ILE	2.3
1	B	149	TYR	2.3
1	A	84	ALA	2.3
1	A	138	ALA	2.3
1	B	271	ALA	2.3
1	A	121	GLY	2.3
1	A	280	GLY	2.3
1	B	321	ASP	2.3
1	B	370	GLU	2.3
1	C	241	GLU	2.3
1	A	360	LYS	2.2
1	A	177	ASP	2.2
1	C	311	ASP	2.2
1	A	403	PRO	2.2
1	B	104	ASN	2.2
1	A	203	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	328	THR	2.2
1	B	291	LEU	2.2
1	A	154	SER	2.2
1	C	302	ILE	2.2
1	B	156	ASP	2.2
1	B	80	GLU	2.2
1	B	249	PRO	2.2
1	B	356	VAL	2.2
1	C	248	VAL	2.2
1	A	230	ASN	2.2
1	A	374	LYS	2.2
1	A	398	THR	2.2
1	A	168	LEU	2.2
1	B	134	ILE	2.2
1	B	380	ILE	2.2
1	A	390	LYS	2.2
1	B	383	LYS	2.2
1	C	191	LYS	2.2
1	A	256	ALA	2.1
1	C	272	GLY	2.1
1	C	324	ASP	2.1
1	C	203	THR	2.1
1	C	407	THR	2.1
1	A	236	ILE	2.1
1	B	241	GLU	2.1
1	B	366	ARG	2.1
1	A	185	GLN	2.1
1	A	392	GLN	2.1
1	A	279	VAL	2.1
1	B	151	TRP	2.1
1	B	141	ARG	2.1
1	A	225	LYS	2.1
1	B	93	ASP	2.1
1	A	216	PHE	2.0
1	A	248	VAL	2.0
1	B	219	GLY	2.0
1	B	120	SER	2.0
1	B	239	SER	2.0
1	B	369	VAL	2.0
1	A	90	LYS	2.0
1	A	93	ASP	2.0
1	B	311	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	337	MET	2.0
1	A	207	SER	2.0
1	C	231	SER	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](#)

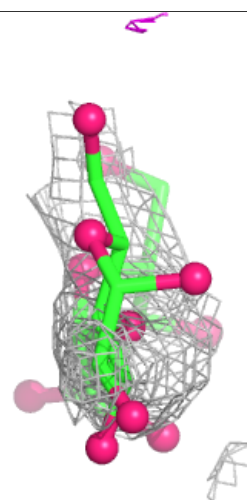
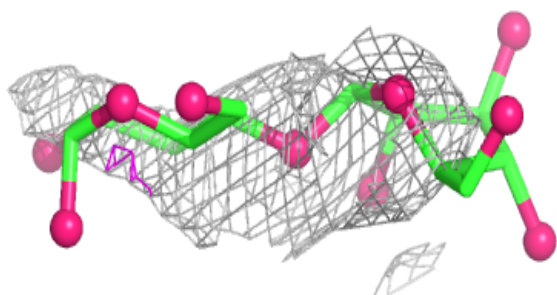
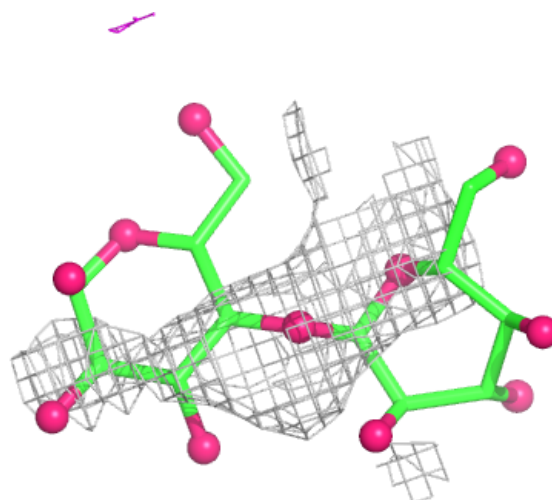
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	E	1	12/12	0.15	0.23	103,113,122,130	12
2	GLC	F	1	12/12	0.32	0.34	152,153,154,156	12
2	GLC	F	2	11/12	0.34	0.41	155,156,160,162	11
2	GLC	D	2	11/12	0.36	0.31	155,156,161,162	11
2	GLC	E	2	11/12	0.55	0.37	90,92,95,98	11
2	GLC	D	1	12/12	0.69	0.32	148,151,153,154	12

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.

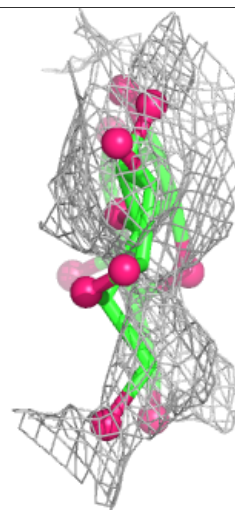
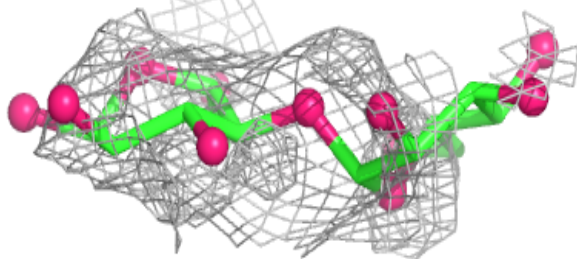
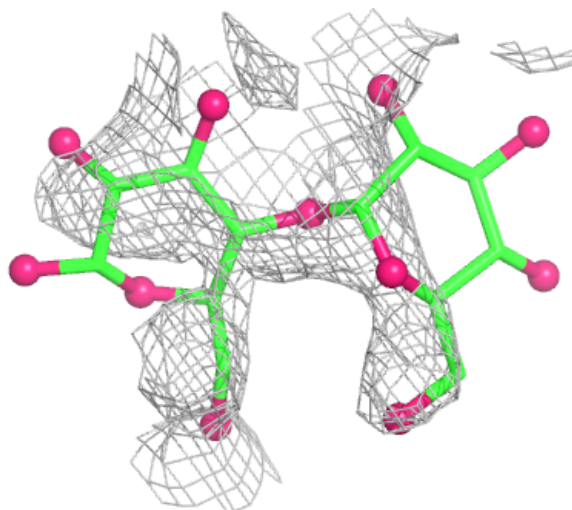
Electron density around Chain D:

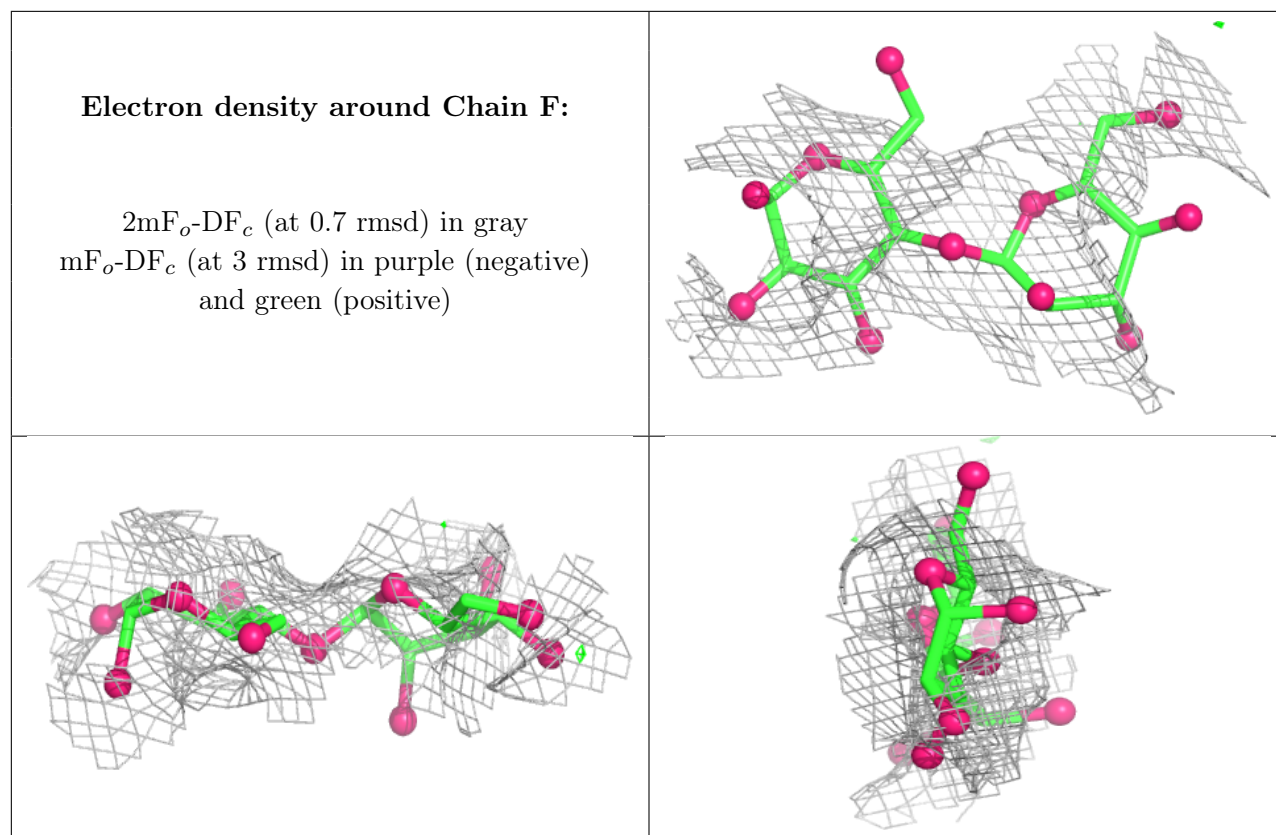
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

$2mF_o-DF_c$ (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
3	NA	C	502	1/1	0.36	0.34	71,71,71,71	0
3	NA	A	502	1/1	0.70	0.26	72,72,72,72	0
3	NA	B	502	1/1	0.80	0.12	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.