



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:37 PM UTC

PDB ID : 7K7M / pdb_00007k7m
Title : Crystal Structure of a membrane protein
Authors : Su, C.-C.
Deposited on : 2020-09-23
Resolution : 3.33 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

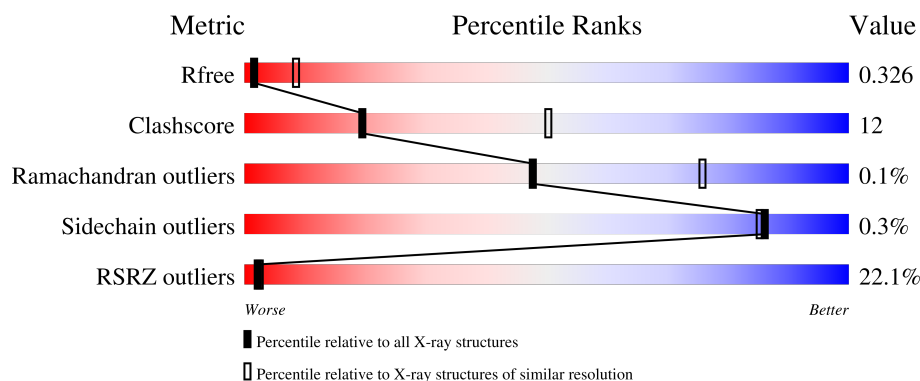
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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	786	17% 69% 26% .
1	B	786	25% 73% 23% .
2	C	2	50% 50%
2	D	2	100%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11641 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 Drug exporters of the RND superfamily-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	756	Total	C	N	O	S	0	0	0
			5751	3721	956	1046	28			
1	B	757	Total	C	N	O	S	0	0	0
			5754	3724	956	1046	28			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	781	HIS	-	expression tag	UNP I7G2R2
A	782	HIS	-	expression tag	UNP I7G2R2
A	783	HIS	-	expression tag	UNP I7G2R2
A	784	HIS	-	expression tag	UNP I7G2R2
A	785	HIS	-	expression tag	UNP I7G2R2
A	786	HIS	-	expression tag	UNP I7G2R2
B	781	HIS	-	expression tag	UNP I7G2R2
B	782	HIS	-	expression tag	UNP I7G2R2
B	783	HIS	-	expression tag	UNP I7G2R2
B	784	HIS	-	expression tag	UNP I7G2R2
B	785	HIS	-	expression tag	UNP I7G2R2
B	786	HIS	-	expression tag	UNP I7G2R2

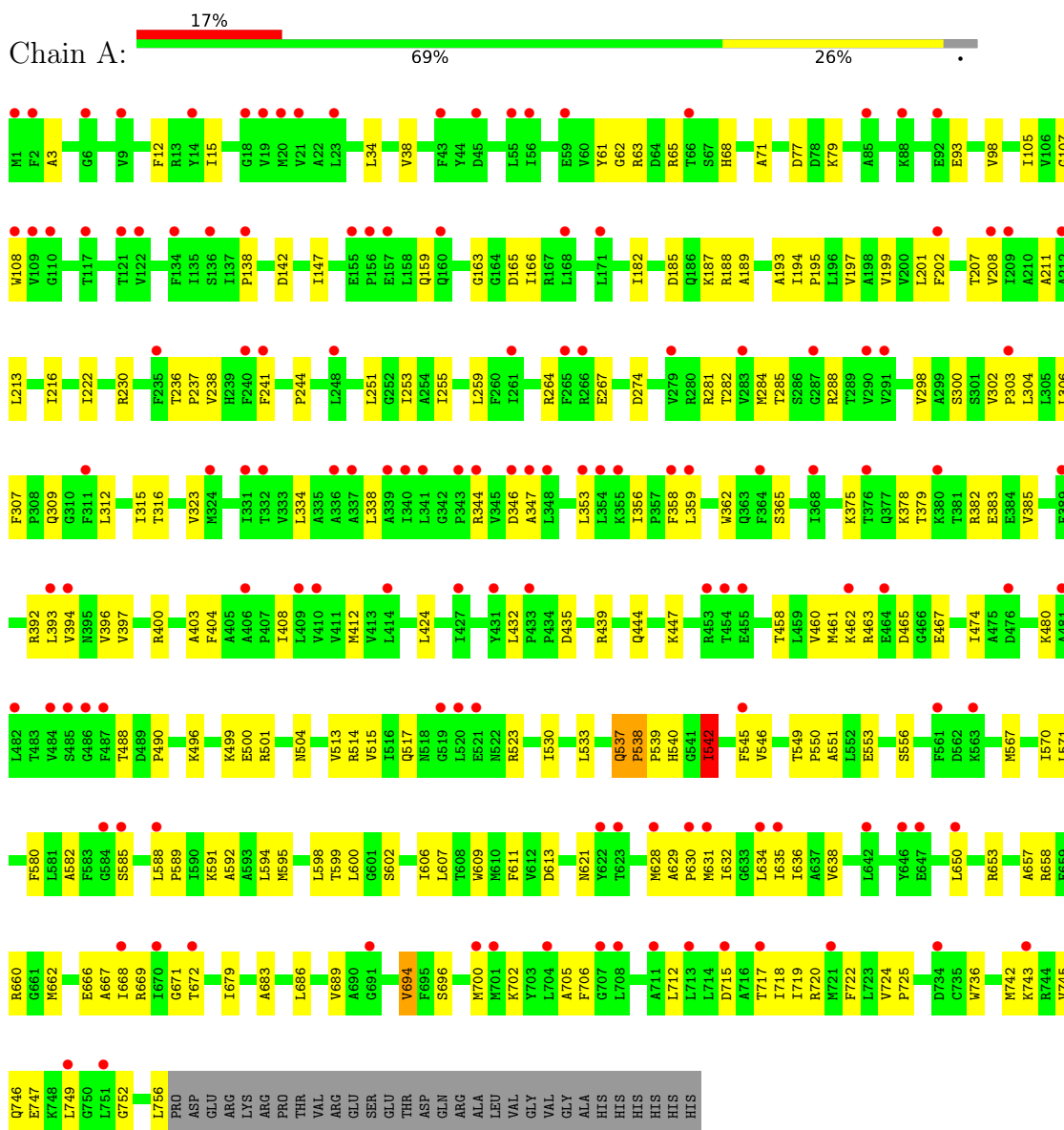
- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-1)-6-O-decanoyl-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			34	22	12			
2	D	2	Total	C	O	0	0	0
			34	22	12			
2	E	2	Total	C	O	0	0	0
			34	22	12			
2	F	2	Total	C	O	0	0	0
			34	22	12			

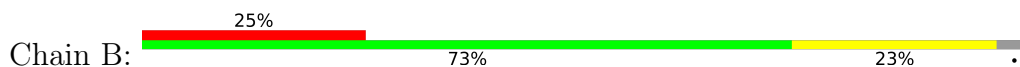
3 Residue-property plots [i](#)

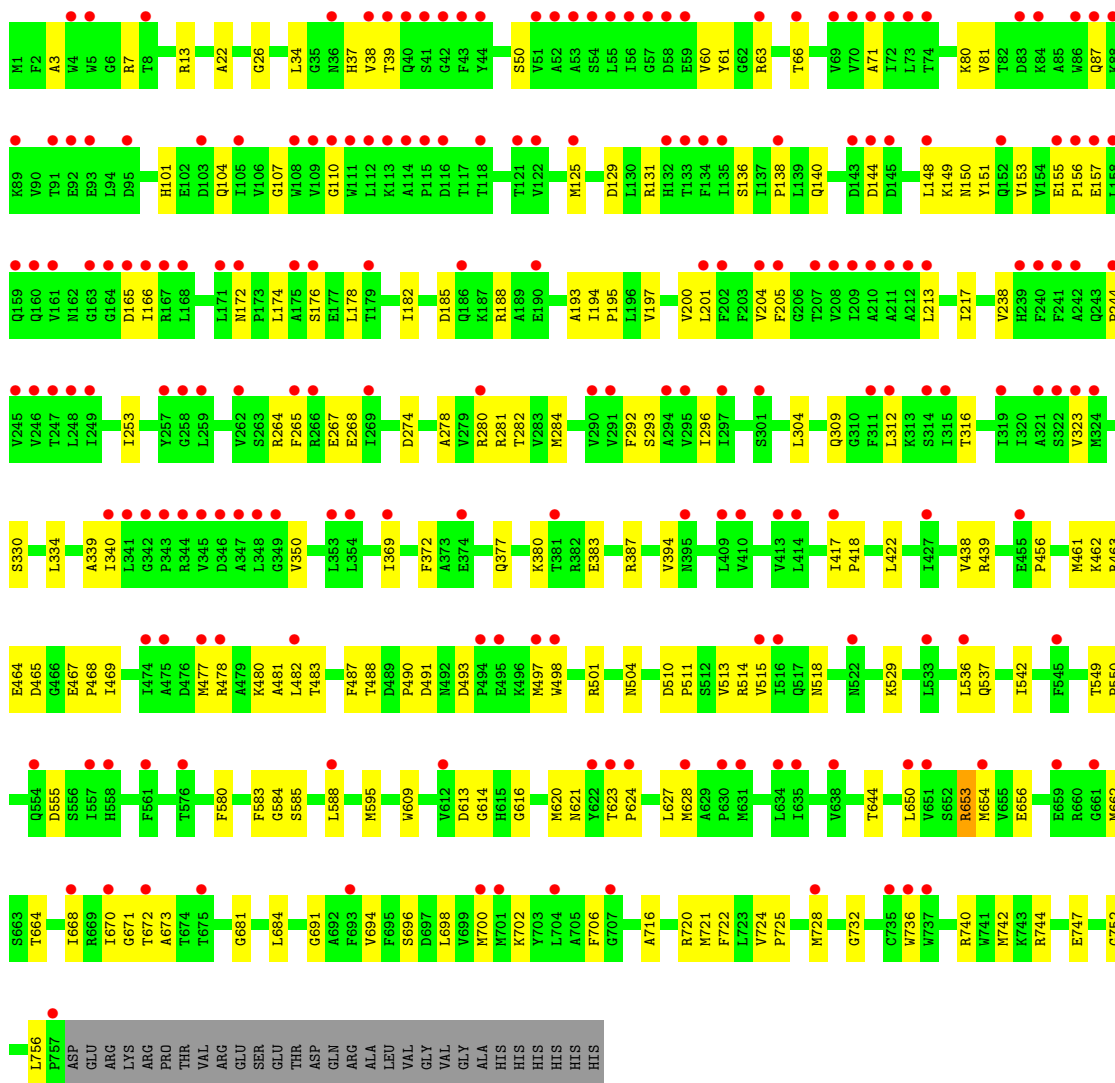
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Drug exporters of the RND superfamily-like protein





- Molecule 2: α -D-glucopyranose-(1-1)-6-O-decanoyl- α -D-glucopyranose

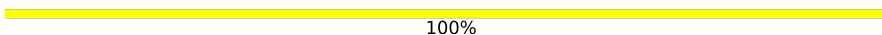
Chain C:



U2D1	GLC2
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- Molecule 2: alpha-D-glucopyranose-(1-1)-6-O-decanoyl-alpha-D-glucopyranose

Chain D:



U2D1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-1)-6-O-decanoyl-alpha-D-glucopyranose

Chain E:





- Molecule 2: alpha-D-glucopyranose-(1-1)-6-O-decanoyl-alpha-D-glucopyranose

Chain F:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.38Å 147.71Å 138.19Å 90.00° 120.89° 90.00°	Depositor
Resolution (Å)	98.66 – 3.33 98.66 – 3.33	Depositor EDS
% Data completeness (in resolution range)	97.6 (98.66-3.33) 98.5 (98.66-3.33)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.8	Depositor
R, R_{free}	0.267 , 0.321 0.274 , 0.326	Depositor DCC
R_{free} test set	2139 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	125.9	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 115.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	11641	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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, U2D

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	0.13	0/5867	0.40	6/7987 (0.1%)
1	B	0.16	0/5871	0.40	6/7993 (0.1%)
All	All	0.14	0/11738	0.40	12/15980 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	538	PRO	CA-C-N	11.65	131.56	120.03
1	A	538	PRO	C-N-CA	11.65	131.56	120.03
1	A	542	ILE	N-CA-C	8.14	119.41	110.21
1	B	621	ASN	N-CA-C	7.36	121.82	111.52
1	B	165	ASP	N-CA-C	6.64	119.74	107.99
1	B	583	PHE	N-CA-C	6.20	120.92	112.68
1	B	464	GLU	CA-C-N	6.09	128.76	120.54
1	B	464	GLU	C-N-CA	6.09	128.76	120.54
1	B	584	GLY	N-CA-C	-5.86	106.93	113.79
1	A	537	GLN	N-CA-C	5.28	116.47	109.93
1	A	537	GLN	CA-C-N	5.05	125.58	120.38
1	A	537	GLN	C-N-CA	5.05	125.58	120.38

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	5751	0	5886	146	0
1	B	5754	0	5890	131	0
2	C	34	0	11	1	0
2	D	34	0	11	0	0
2	E	34	0	11	1	0
2	F	34	0	11	0	0
All	All	11641	0	11820	273	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 12.

All (273) 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:B:620:MET:HE2	1:B:706:PHE:CE1	1.98	0.98
1:A:462:LYS:C	1:A:542:ILE:HG22	1.93	0.93
1:B:620:MET:HE2	1:B:706:PHE:CZ	2.04	0.91
1:A:394:VAL:HG21	1:A:672:THR:HG21	1.58	0.84
1:B:71:ALA:HB1	1:B:166:ILE:HD11	1.61	0.82
1:B:477:MET:HA	1:B:480:LYS:HB2	1.60	0.81
1:A:463:ARG:N	1:A:542:ILE:HG22	1.96	0.80
1:A:747:GLU:HA	1:A:752:GLY:HA3	1.66	0.76
1:B:264:ARG:NH1	1:B:268:GLU:OE2	2.22	0.73
1:B:380:LYS:HA	1:B:383:GLU:HG2	1.71	0.73
1:A:523:ARG:NH2	1:A:553:GLU:OE1	2.22	0.72
1:B:664:THR:HG21	1:B:732:GLY:HA2	1.72	0.70
1:B:80:LYS:NZ	1:B:129:ASP:O	2.25	0.70
1:A:34:LEU:HB2	1:A:230:ARG:HB2	1.74	0.70
1:A:460:VAL:HB	1:A:545:PHE:HB2	1.74	0.69
1:A:62:GLY:HA3	1:A:504:ASN:HB2	1.73	0.69
1:A:264:ARG:HG3	1:A:282:THR:HG22	1.73	0.68
1:A:432:LEU:O	1:A:439:ARG:NH2	2.28	0.67
1:B:185:ASP:OD1	1:B:188:ARG:NH2	2.28	0.67
1:A:264:ARG:NH1	1:A:267:GLU:OE1	2.29	0.66
1:A:264:ARG:HH21	1:A:285:THR:HG21	1.61	0.66
1:B:585:SER:HB2	1:B:736:TRP:HD1	1.60	0.66
1:B:194:ILE:HA	1:B:197:VAL:HG22	1.79	0.64
1:B:60:VAL:HG21	1:B:513:VAL:HG21	1.80	0.64
1:A:208:VAL:HG11	1:A:353:LEU:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:VAL:HA	1:A:515:VAL:HG12	1.80	0.63
1:B:264:ARG:NH2	1:B:656:GLU:OE2	2.31	0.63
1:B:204:VAL:HG11	1:B:681:GLY:HA3	1.79	0.63
1:B:387:ARG:HG3	1:B:673:ALA:HB1	1.80	0.63
1:B:620:MET:CE	1:B:706:PHE:CE1	2.80	0.62
1:B:620:MET:HE2	1:B:706:PHE:HE1	1.56	0.62
1:A:344:ARG:HG2	1:A:347:ALA:HB2	1.80	0.62
1:A:666:GLU:OE1	1:A:669:ARG:NH2	2.33	0.62
1:B:481:ALA:HB1	1:B:498:TRP:CE2	2.34	0.62
1:A:628:MET:HE2	1:A:700:MET:HG3	1.82	0.61
1:B:595:MET:HE1	1:B:724:VAL:HG22	1.81	0.61
1:B:101:HIS:NE2	1:B:157:GLU:OE1	2.34	0.61
1:A:288:ARG:NH2	1:A:582:ALA:O	2.33	0.60
1:A:302:VAL:HG23	1:A:303:PRO:HD3	1.84	0.60
1:A:480:LYS:NZ	1:A:537:GLN:O	2.34	0.59
1:B:477:MET:O	1:B:481:ALA:N	2.32	0.59
1:A:163:GLY:O	1:B:744:ARG:NH1	2.35	0.59
1:A:696:SER:O	1:A:702:LYS:NZ	2.30	0.59
1:A:93:GLU:OE2	1:B:740:ARG:NH1	2.35	0.59
1:A:12:PHE:HD2	1:A:15:ILE:HD11	1.67	0.58
1:B:580:PHE:CZ	1:B:742:MET:HB3	2.38	0.58
1:B:480:LYS:HZ1	1:B:537:GLN:HB2	1.68	0.58
1:A:274:ASP:OD1	1:A:274:ASP:N	2.36	0.58
1:B:265:PHE:HA	1:B:282:THR:HG21	1.86	0.58
1:A:653:ARG:HB3	1:A:671:GLY:HA2	1.86	0.58
1:A:253:ILE:HD11	1:A:323:VAL:HG12	1.86	0.58
1:A:306:LEU:HD11	1:A:570:ILE:HD12	1.84	0.58
1:A:694:VAL:HG13	1:A:706:PHE:CE1	2.39	0.58
1:A:694:VAL:HG23	1:A:705:ALA:HB1	1.85	0.58
1:B:620:MET:CE	1:B:706:PHE:HE1	2.15	0.57
1:A:63:ARG:NH2	1:A:142:ASP:O	2.38	0.57
1:A:444:GLN:HA	1:A:447:LYS:HG2	1.87	0.57
1:A:359:LEU:HA	1:A:365:SER:HB2	1.87	0.56
1:B:267:GLU:OE1	1:B:653:ARG:NH2	2.37	0.56
1:A:660:ARG:HD3	1:A:662:MET:HE1	1.88	0.56
1:B:110:GLY:HA2	1:B:125:MET:HE1	1.88	0.56
1:B:66:THR:O	1:B:136:SER:OG	2.22	0.56
1:B:140:GLN:O	1:B:150:ASN:ND2	2.39	0.56
1:A:393:LEU:HD11	1:A:722:PHE:HE1	1.70	0.56
1:A:304:LEU:HB2	1:A:316:THR:HG21	1.87	0.55
1:A:185:ASP:HA	1:A:188:ARG:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:LYS:HA	1:B:513:VAL:HG12	1.89	0.54
1:B:628:MET:HE2	1:B:700:MET:HG3	1.88	0.54
1:B:696:SER:O	1:B:702:LYS:NZ	2.26	0.54
1:A:68:HIS:CE1	1:A:147:ILE:HG21	2.42	0.54
1:A:668:ILE:O	1:A:672:THR:HG22	2.08	0.54
1:B:50:SER:OG	1:B:555:ASP:OD2	2.24	0.54
1:B:620:MET:HE2	1:B:706:PHE:HZ	1.70	0.54
1:B:668:ILE:O	1:B:672:THR:HG22	2.08	0.53
1:A:463:ARG:HD3	1:A:465:ASP:HB2	1.90	0.53
1:A:98:VAL:HG22	1:A:105:ILE:HG21	1.91	0.53
1:A:580:PHE:CZ	1:A:742:MET:HB3	2.43	0.53
1:B:280:ARG:HG2	1:B:284:MET:HE2	1.90	0.53
1:A:501:ARG:HB3	1:A:515:VAL:HG23	1.90	0.53
1:A:34:LEU:HA	1:A:230:ARG:HD3	1.91	0.53
1:B:463:ARG:HD3	1:B:467:GLU:O	2.09	0.53
1:A:213:LEU:HD23	1:A:216:ILE:HD12	1.90	0.52
1:A:694:VAL:HG13	1:A:706:PHE:HE1	1.72	0.52
1:B:197:VAL:O	1:B:201:LEU:HB2	2.09	0.52
1:B:721:MET:HE3	1:B:722:PHE:HE1	1.73	0.52
1:B:588:LEU:HD11	1:B:736:TRP:HE1	1.74	0.52
1:B:60:VAL:HG11	1:B:513:VAL:HG23	1.91	0.52
1:B:744:ARG:HA	1:B:747:GLU:HB2	1.91	0.52
1:A:71:ALA:HB1	1:A:166:ILE:HD11	1.92	0.51
1:B:63:ARG:O	1:B:504:ASN:ND2	2.43	0.51
1:A:657:ALA:HB3	1:A:667:ALA:HA	1.92	0.51
1:A:300:SER:HA	1:A:571:LEU:HD12	1.92	0.51
1:A:194:ILE:HA	1:A:197:VAL:HG22	1.93	0.51
1:A:93:GLU:HG2	1:B:740:ARG:HH12	1.76	0.51
1:A:694:VAL:O	1:A:702:LYS:HG2	2.11	0.51
1:B:200:VAL:HG11	1:B:684:LEU:HB2	1.93	0.51
1:A:65:ARG:HB3	1:A:138:PRO:HB3	1.93	0.50
1:B:309:GLN:OE1	1:B:309:GLN:N	2.44	0.50
1:B:439:ARG:HH12	1:B:623:THR:HG21	1.77	0.50
1:B:491:ASP:OD2	1:B:493:ASP:HB3	2.11	0.50
1:A:530:ILE:HD13	1:A:551:ALA:HA	1.94	0.50
1:B:487:PHE:HB3	1:B:518:ASN:ND2	2.27	0.50
1:A:382:ARG:HA	1:A:385:VAL:HG22	1.93	0.50
1:A:199:VAL:HA	1:A:202:PHE:CE2	2.47	0.50
1:A:201:LEU:HB3	1:A:211:ALA:HB1	1.93	0.49
1:A:588:LEU:HA	1:A:591:LYS:HE3	1.94	0.49
1:A:496:LYS:O	1:A:499:LYS:NZ	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ILE:HD12	1:A:244:PRO:HG2	1.94	0.49
1:B:61:TYR:CE1	1:B:515:VAL:HG12	2.48	0.49
1:B:480:LYS:O	1:B:483:THR:OG1	2.22	0.49
1:B:81:VAL:O	1:B:87:GLN:NE2	2.43	0.49
1:A:98:VAL:HG21	1:A:108:TRP:HD1	1.76	0.48
1:A:207:THR:HG21	1:A:346:ASP:HA	1.95	0.48
1:B:151:TYR:CD2	1:B:172:ASN:HB3	2.49	0.48
1:B:204:VAL:HG23	1:B:205:PHE:CD1	2.48	0.48
1:B:107:GLY:O	1:B:138:PRO:HD2	2.13	0.48
1:A:222:ILE:HG21	1:A:251:LEU:HB2	1.95	0.48
1:A:356:ILE:O	1:A:358:PHE:N	2.45	0.48
1:A:255:ILE:O	1:A:259:LEU:N	2.46	0.48
1:A:679:ILE:HB	1:A:720:ARG:HH21	1.80	0.47
1:B:3:ALA:O	1:B:7:ARG:HG3	2.14	0.47
1:B:480:LYS:HD2	1:B:536:LEU:HD22	1.96	0.47
1:A:334:LEU:O	1:A:338:LEU:HG	2.14	0.47
1:A:397:VAL:HA	1:A:404:PHE:CD2	2.49	0.47
1:A:686:LEU:HA	1:A:689:VAL:HG22	1.97	0.47
1:B:588:LEU:HD21	1:B:728:MET:HE3	1.95	0.47
1:B:744:ARG:HD2	1:B:747:GLU:HB2	1.95	0.47
1:B:101:HIS:HB3	1:B:104:GLN:HB2	1.97	0.47
1:B:478:ARG:HG3	1:B:498:TRP:HB2	1.97	0.47
1:B:478:ARG:O	1:B:482:LEU:HG	2.14	0.47
1:B:653:ARG:HA	1:B:653:ARG:HD2	1.63	0.47
1:A:662:MET:HB3	1:A:666:GLU:HB2	1.97	0.47
1:A:461:MET:HE1	1:A:474:ILE:HA	1.97	0.47
1:A:600:LEU:HD11	1:A:636:ILE:HG23	1.97	0.46
1:B:461:MET:HG3	1:B:514:ARG:O	2.15	0.46
1:B:650:LEU:HG	1:B:654:MET:HE3	1.96	0.46
1:B:38:VAL:HG13	1:B:238:VAL:HG23	1.97	0.46
1:A:461:MET:HB3	1:A:542:ILE:HD12	1.98	0.46
1:B:580:PHE:HZ	1:B:742:MET:HB3	1.80	0.46
1:A:412:MET:HE1	1:A:719:ILE:HD11	1.97	0.46
1:A:435:ASP:OD2	1:A:621:ASN:ND2	2.38	0.46
1:A:165:ASP:OD2	1:B:744:ARG:NH2	2.48	0.46
1:A:189:ALA:O	1:A:193:ALA:HB3	2.16	0.46
1:B:350:VAL:HG22	1:B:372:PHE:CZ	2.51	0.46
1:B:654:MET:HG2	1:B:671:GLY:HA3	1.98	0.46
1:B:480:LYS:NZ	1:B:537:GLN:HB2	2.31	0.46
1:A:743:LYS:O	1:A:747:GLU:HG3	2.16	0.46
1:A:400:ARG:HG2	1:A:403:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:GLN:HG3	1:A:447:LYS:HZ3	1.81	0.45
1:A:717:THR:OG1	1:A:718:ILE:N	2.50	0.45
1:B:61:TYR:CZ	1:B:515:VAL:HG12	2.52	0.45
1:B:296:ILE:HG21	1:B:644:THR:HG21	1.98	0.45
1:A:463:ARG:HB3	1:A:542:ILE:HG23	1.98	0.45
1:A:159:GLN:NE2	1:A:166:ILE:O	2.43	0.45
1:A:538:PRO:HA	1:A:539:PRO:HD3	1.60	0.45
1:A:658:ARG:HG2	1:A:736:TRP:CG	2.51	0.45
1:B:281:ARG:NH2	1:B:756:LEU:HB3	2.32	0.45
1:B:491:ASP:OD1	1:B:491:ASP:N	2.49	0.45
1:A:588:LEU:HB2	1:A:589:PRO:HD3	1.99	0.45
1:A:629:ALA:HB3	1:A:630:PRO:HD3	1.98	0.45
1:A:105:ILE:HG22	1:A:107:GLY:H	1.80	0.45
1:A:298:VAL:O	1:A:302:VAL:HG22	2.17	0.45
1:A:362:TRP:CD1	1:A:362:TRP:C	2.95	0.45
1:A:683:ALA:O	1:A:712:LEU:HD21	2.17	0.45
1:B:144:ASP:OD2	2:E:1:U2D:O11	2.36	0.44
1:A:462:LYS:HB2	1:A:513:VAL:HG22	1.99	0.44
1:A:530:ILE:HG23	1:A:546:VAL:HG11	1.98	0.44
1:B:609:TRP:O	1:B:613:ASP:HB2	2.17	0.44
1:A:3:ALA:HB2	1:A:284:MET:SD	2.57	0.44
1:A:61:TYR:OH	1:A:514:ARG:NH1	2.50	0.44
1:A:312:LEU:O	1:A:316:THR:HG23	2.17	0.44
1:A:424:LEU:H	2:C:2:GLC:H62	1.82	0.44
1:A:634:LEU:O	1:A:638:VAL:HG23	2.17	0.44
1:A:756:LEU:HD12	1:A:756:LEU:H	1.82	0.44
1:A:38:VAL:HG22	1:A:238:VAL:HG23	1.98	0.44
1:A:77:ASP:HB2	1:A:79:LYS:HE2	1.98	0.44
1:A:408:ILE:HD11	1:A:722:PHE:HD2	1.83	0.44
1:B:292:PHE:O	1:B:296:ILE:HG13	2.17	0.44
1:B:501:ARG:HB3	1:B:515:VAL:HG13	2.00	0.44
1:A:195:PRO:O	1:A:199:VAL:HG13	2.17	0.44
1:A:632:ILE:HA	1:A:635:ILE:HG22	2.00	0.44
1:B:394:VAL:HG13	1:B:725:PRO:HB3	1.99	0.44
1:B:510:ASP:HB3	1:B:513:VAL:HG22	1.99	0.44
1:A:12:PHE:CD2	1:A:15:ILE:HD11	2.49	0.44
1:A:592:ALA:HA	1:A:595:MET:HE2	1.99	0.44
1:A:609:TRP:O	1:A:613:ASP:HB2	2.18	0.44
1:A:650:LEU:HD22	1:A:720:ARG:HA	1.99	0.44
1:A:724:VAL:HB	1:A:725:PRO:HD3	2.00	0.43
1:B:13:ARG:HD2	1:B:340:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:THR:HG22	1:B:490:PRO:HD3	1.99	0.43
1:B:194:ILE:HG13	1:B:195:PRO:HD3	2.00	0.43
1:B:274:ASP:OD1	1:B:274:ASP:N	2.42	0.43
1:A:488:THR:HG22	1:A:490:PRO:HD3	2.00	0.43
1:B:691:GLY:O	1:B:694:VAL:HG22	2.18	0.43
1:B:744:ARG:HA	1:B:744:ARG:HD2	1.72	0.43
1:A:303:PRO:HB2	1:A:567:MET:HG3	2.00	0.43
1:B:662:MET:HE1	1:B:670:ILE:HB	2.00	0.43
1:A:444:GLN:HE21	1:A:447:LYS:NZ	2.17	0.43
1:B:178:LEU:HD22	1:B:698:LEU:HD13	2.00	0.43
1:B:372:PHE:HA	1:B:377:GLN:CB	2.49	0.43
1:A:236:THR:OG1	1:A:237:PRO:HD2	2.19	0.43
1:A:379:THR:O	1:A:383:GLU:HG3	2.18	0.43
1:A:463:ARG:HD2	1:A:467:GLU:N	2.33	0.43
1:B:22:ALA:O	1:B:26:GLY:N	2.48	0.43
1:A:599:THR:HG21	1:A:715:ASP:OD1	2.19	0.43
1:A:658:ARG:HG2	1:A:736:TRP:CD2	2.53	0.43
1:A:194:ILE:N	1:A:195:PRO:HD2	2.34	0.43
1:B:155:GLU:N	1:B:156:PRO:HD2	2.33	0.43
1:A:304:LEU:HA	1:A:307:PHE:HD2	1.83	0.43
1:A:585:SER:HB2	1:A:736:TRP:HA	1.99	0.43
1:B:213:LEU:HB3	1:B:334:LEU:HD11	2.01	0.42
1:B:34:LEU:O	1:B:37:HIS:N	2.48	0.42
1:B:182:ILE:HG23	1:B:244:PRO:HG3	2.00	0.42
1:A:694:VAL:CG1	1:A:706:PHE:CE1	3.02	0.42
1:B:148:LEU:HD11	1:B:176:SER:HB2	2.02	0.42
1:B:468:PRO:HA	1:B:511:PRO:HB2	2.01	0.42
1:B:487:PHE:HB2	1:B:497:MET:HE3	2.01	0.42
1:B:716:ALA:O	1:B:720:ARG:NH1	2.47	0.42
1:A:542:ILE:H	1:A:542:ILE:HG12	1.57	0.42
1:A:746:GLN:HE21	1:A:752:GLY:HA2	1.84	0.42
1:B:13:ARG:HD3	1:B:339:ALA:HB1	2.00	0.42
1:B:461:MET:HB2	1:B:469:ILE:HD13	2.00	0.42
1:A:105:ILE:HG22	1:A:107:GLY:N	2.34	0.42
1:B:417:ILE:N	1:B:418:PRO:HD2	2.35	0.42
1:A:194:ILE:HG23	1:A:195:PRO:HD3	2.02	0.42
1:B:278:ALA:O	1:B:282:THR:HG23	2.19	0.42
1:B:616:GLY:O	1:B:620:MET:HB2	2.20	0.42
1:A:253:ILE:HG22	1:A:686:LEU:HD21	2.02	0.42
1:A:458:THR:HG22	1:A:517:GLN:HB3	2.00	0.42
1:A:500:GLU:OE2	1:A:514:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD23	1:B:438:VAL:HG12	2.02	0.42
1:B:463:ARG:HG3	1:B:469:ILE:HG12	2.02	0.42
1:A:375:LYS:HA	1:A:379:THR:HG22	2.02	0.42
1:A:378:LYS:O	1:A:382:ARG:HD3	2.20	0.42
1:B:131:ARG:HD2	1:B:131:ARG:HA	1.70	0.42
1:B:304:LEU:HB2	1:B:316:THR:HG21	2.02	0.42
1:B:330:SER:O	1:B:334:LEU:HB3	2.19	0.42
1:B:461:MET:HE3	1:B:477:MET:SD	2.60	0.42
1:B:461:MET:HE2	1:B:542:ILE:CD1	2.50	0.42
1:B:149:LYS:O	1:B:153:VAL:HG23	2.20	0.42
1:A:61:TYR:HH	1:A:514:ARG:HH11	1.67	0.41
1:A:549:THR:OG1	1:A:550:PRO:HD3	2.20	0.41
1:B:312:LEU:O	1:B:316:THR:HG23	2.20	0.41
1:A:241:PHE:HD2	1:A:315:ILE:HD11	1.85	0.41
1:A:392:ARG:O	1:A:396:VAL:HG23	2.20	0.41
1:A:594:LEU:O	1:A:598:LEU:N	2.51	0.41
1:B:422:LEU:HD11	1:B:627:LEU:HD12	2.01	0.41
1:A:281:ARG:HE	1:A:281:ARG:HB3	1.68	0.41
1:B:194:ILE:HG13	1:B:195:PRO:CD	2.50	0.41
1:B:293:SER:HA	1:B:296:ILE:HD12	2.02	0.41
1:B:549:THR:OG1	1:B:550:PRO:HD3	2.21	0.41
1:A:304:LEU:HD12	1:A:316:THR:HG22	2.02	0.41
1:B:253:ILE:HD11	1:B:323:VAL:HG12	2.02	0.41
1:A:628:MET:HB3	1:A:631:MET:HB2	2.02	0.41
1:B:194:ILE:N	1:B:195:PRO:HD2	2.35	0.41
1:B:217:ILE:HD13	1:B:217:ILE:HA	1.91	0.41
1:B:747:GLU:HA	1:B:752:GLY:HA3	2.03	0.41
1:A:309:GLN:NE2	1:A:556:SER:OG	2.49	0.41
1:B:369:ILE:HG12	1:B:372:PHE:HE2	1.86	0.41
1:A:539:PRO:O	1:A:540:HIS:C	2.64	0.41
1:A:607:LEU:O	1:A:611:PHE:HB2	2.21	0.41
1:A:745:VAL:O	1:A:749:LEU:HB2	2.20	0.41
1:B:529:LYS:HD3	1:B:529:LYS:HA	1.75	0.41
1:B:193:ALA:O	1:B:197:VAL:HG13	2.21	0.41
1:B:724:VAL:HB	1:B:725:PRO:HD3	2.02	0.41
1:B:614:GLY:HA2	1:B:624:PRO:HB3	2.02	0.40
1:B:480:LYS:NZ	1:B:537:GLN:O	2.50	0.40
1:A:187:LYS:HB3	1:A:187:LYS:HE3	1.89	0.40
1:A:533:LEU:HD23	1:A:533:LEU:HA	1.90	0.40
1:B:39:THR:HG22	1:B:238:VAL:O	2.22	0.40
1:A:474:ILE:HD11	1:A:514:ARG:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:SER:O	1:A:606:ILE:HG13	2.21	0.40
1:B:304:LEU:HD12	1:B:316:THR:HG22	2.03	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	754/786 (96%)	719 (95%)	35 (5%)	0	100	100
1	B	755/786 (96%)	720 (95%)	34 (4%)	1 (0%)	48	76
All	All	1509/1572 (96%)	1439 (95%)	69 (5%)	1 (0%)	48	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	456	PRO

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	608/646 (94%)	606 (100%)	2 (0%)	86	85
1	B	608/646 (94%)	606 (100%)	2 (0%)	86	85
All	All	1216/1292 (94%)	1212 (100%)	4 (0%)	86	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	542	ILE
1	A	694	VAL
1	B	465	ASP
1	B	653	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	440	GLN
1	A	444	GLN
1	A	518	ASN
1	A	625	GLN
1	B	492	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	U2D	C	1	2	22,22,23	1.79	2 (9%)	27,27,29	1.53	2 (7%)
2	GLC	C	2	2	12,12,12	1.04	0	17,17,17	1.66	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	U2D	D	1	2	22,22,23	1.89	2 (9%)	27,27,29	1.51	3 (11%)
2	GLC	D	2	2	12,12,12	1.28	2 (16%)	17,17,17	1.51	3 (17%)
2	U2D	E	1	2	22,22,23	1.79	2 (9%)	27,27,29	1.54	2 (7%)
2	GLC	E	2	2	12,12,12	0.75	0	17,17,17	0.74	0
2	U2D	F	1	2	22,22,23	1.76	2 (9%)	27,27,29	1.61	3 (11%)
2	GLC	F	2	2	12,12,12	0.71	0	17,17,17	0.78	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	U2D	C	1	2	-	2/14/31/34	0/1/1/1
2	GLC	C	2	2	-	2/2/22/22	0/1/1/1
2	U2D	D	1	2	-	8/14/31/34	0/1/1/1
2	GLC	D	2	2	-	0/2/22/22	0/1/1/1
2	U2D	E	1	2	-	7/14/31/34	0/1/1/1
2	GLC	E	2	2	-	2/2/22/22	0/1/1/1
2	U2D	F	1	2	-	3/14/31/34	0/1/1/1
2	GLC	F	2	2	-	0/2/22/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	U2D	O11-CAX	7.24	1.44	1.22
2	C	1	U2D	O11-CAX	7.05	1.43	1.22
2	F	1	U2D	O11-CAX	7.04	1.43	1.22
2	E	1	U2D	O11-CAX	7.02	1.43	1.22
2	D	1	U2D	O6-CAX	4.14	1.45	1.33
2	C	1	U2D	O6-CAX	3.62	1.43	1.33
2	E	1	U2D	O6-CAX	3.59	1.43	1.33
2	F	1	U2D	O6-CAX	3.58	1.43	1.33
2	D	2	GLC	C1-C2	2.78	1.58	1.52
2	D	2	GLC	O1-C1	2.61	1.47	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	U2D	O6-CAX-O11	-5.94	108.76	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	U2D	O6-CAX-O11	-5.73	109.28	123.63
2	C	1	U2D	O6-CAX-O11	-5.72	109.33	123.63
2	C	2	GLC	O5-C5-C6	5.60	120.31	106.44
2	D	1	U2D	O6-CAX-O11	-5.27	110.45	123.63
2	E	1	U2D	O11-CAX-CAY	-3.73	109.19	123.78
2	D	1	U2D	O11-CAX-CAY	-3.65	109.51	123.78
2	C	1	U2D	O11-CAX-CAY	-3.61	109.67	123.78
2	F	1	U2D	O11-CAX-CAY	-3.57	109.83	123.78
2	D	2	GLC	O5-C5-C6	2.98	113.82	106.44
2	D	2	GLC	O2-C2-C1	2.96	116.08	109.25
2	F	1	U2D	C6-O6-CAX	-2.65	107.44	117.12
2	C	2	GLC	C1-O5-C5	2.46	118.40	113.65
2	D	1	U2D	O6-C6-C5	2.16	112.97	108.41
2	D	2	GLC	C6-C5-C4	-2.04	108.00	113.02

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	U2D	CAY-CAX-O6-C6
2	D	1	U2D	O11-CAX-O6-C6
2	E	1	U2D	O11-CAX-O6-C6
2	E	1	U2D	CAY-CAX-O6-C6
2	C	1	U2D	O11-CAX-O6-C6
2	F	1	U2D	CAY-CAX-O6-C6
2	E	2	GLC	O5-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	F	1	U2D	O11-CAX-O6-C6
2	C	1	U2D	CAY-CAX-O6-C6
2	C	2	GLC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	E	1	U2D	CAX-CAY-CAZ-CBA
2	E	1	U2D	CBA-CBB-CBC-CBD
2	D	1	U2D	CAY-CAZ-CBA-CBB
2	D	1	U2D	CAZ-CBA-CBB-CBC
2	E	1	U2D	CBC-CBD-CBE-CBF
2	E	1	U2D	CAY-CAZ-CBA-CBB
2	E	1	U2D	CBB-CBC-CBD-CBE
2	D	1	U2D	C4-C5-C6-O6
2	D	1	U2D	CBA-CBB-CBC-CBD
2	D	1	U2D	CBB-CBC-CBD-CBE
2	D	1	U2D	O6-CAX-CAY-CAZ

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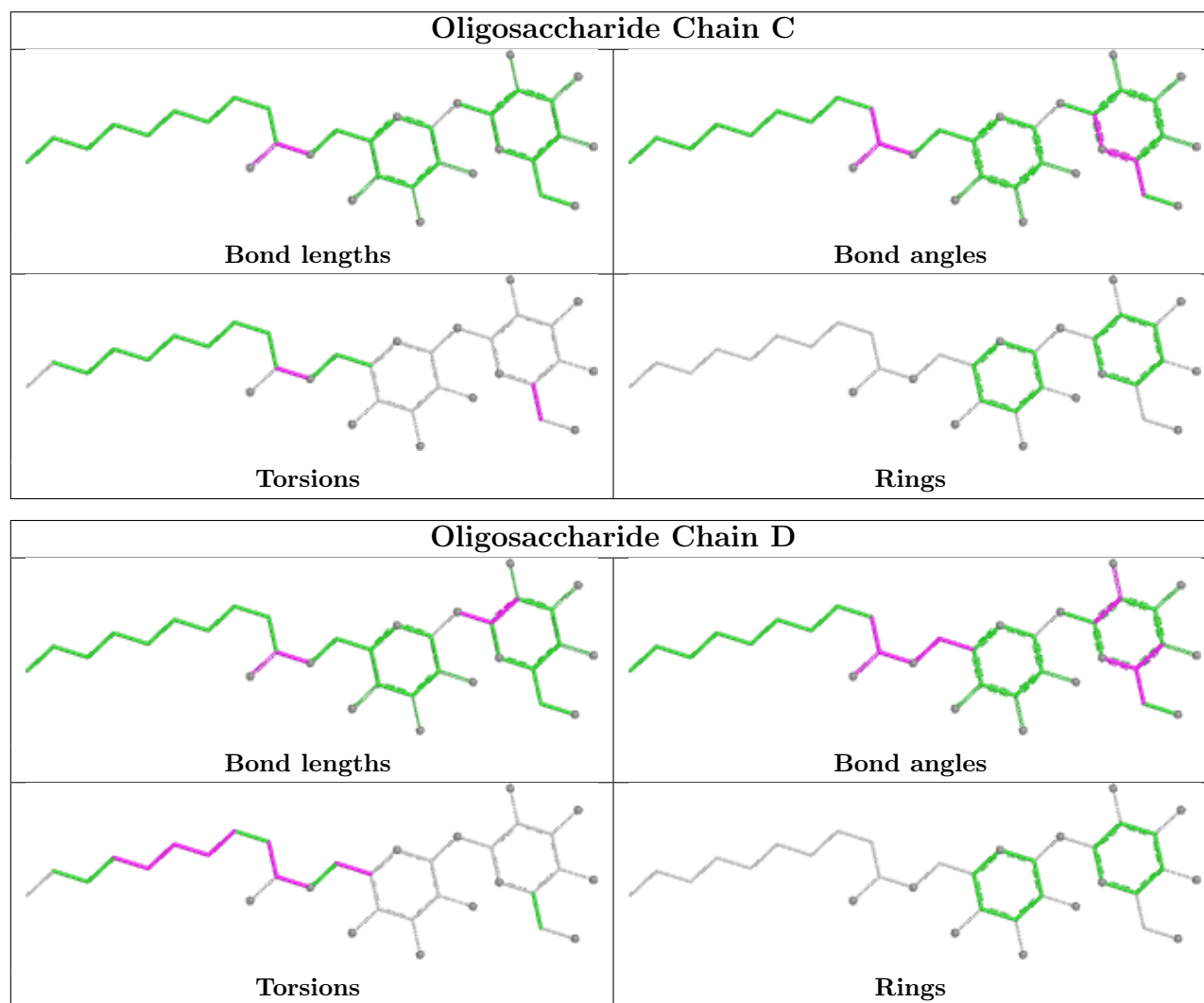
Mol	Chain	Res	Type	Atoms
2	F	1	U2D	O5-C5-C6-O6

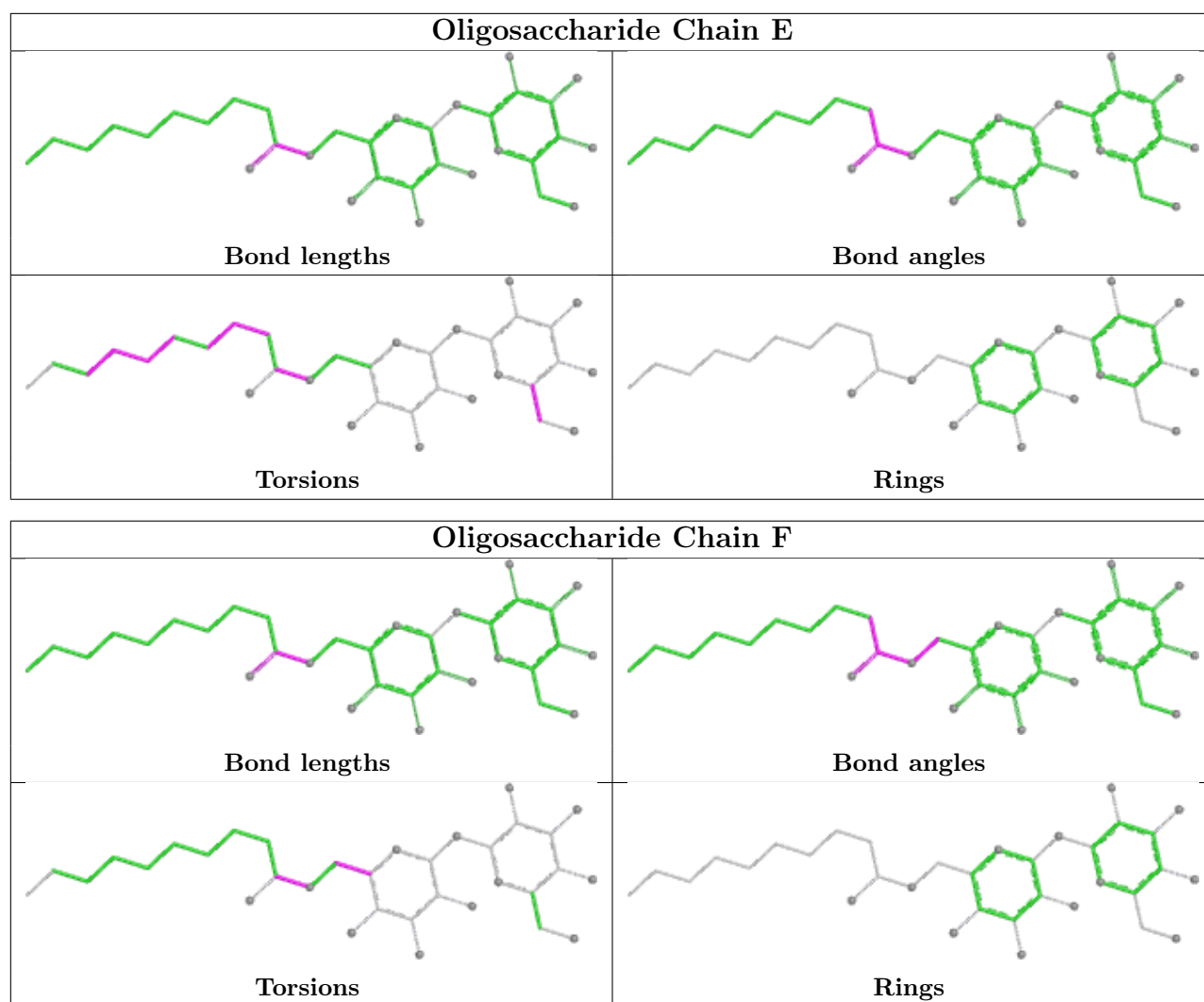
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	U2D	1	0
2	C	2	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](#)

There are no ligands in this entry.

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	756/786 (96%)	1.05	134 (17%)  	91, 137, 194, 213	0
1	B	757/786 (96%)	1.65	200 (26%)  	92, 130, 188, 215	0
All	All	1513/1572 (96%)	1.35	334 (22%)  	91, 134, 192, 215	0

All (334) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	347	ALA	26.7
1	B	346	ASP	23.3
1	B	113	LYS	19.8
1	B	348	LEU	19.2
1	B	343	PRO	19.0
1	B	41	SER	14.1
1	B	55	LEU	13.8
1	B	110	GLY	13.3
1	B	40	GLN	13.0
1	B	344	ARG	12.8
1	B	345	VAL	12.0
1	B	114	ALA	11.9
1	B	209	ILE	11.8
1	B	84	LYS	11.6
1	B	266	ARG	11.5
1	B	210	ALA	11.3
1	B	43	PHE	10.2
1	B	240	PHE	10.1
1	B	208	VAL	10.0
1	B	56	ILE	10.0
1	B	341	LEU	9.9
1	A	341	LEU	9.6
1	B	239	HIS	9.4
1	B	88	LYS	9.0

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Mol	Chain	Res	Type	RSRZ
1	B	58	ASP	8.8
1	B	241	PHE	8.7
1	A	156	PRO	8.5
1	A	348	LEU	8.4
1	B	311	PHE	8.4
1	B	156	PRO	8.4
1	B	342	GLY	8.1
1	A	241	PHE	8.1
1	A	455	GLU	8.1
1	A	208	VAL	7.9
1	A	209	ILE	7.8
1	B	108	TRP	7.7
1	B	87	GLN	7.5
1	A	353	LEU	7.4
1	B	52	ALA	7.4
1	B	205	PHE	7.3
1	B	262	VAL	7.3
1	B	71	ALA	7.3
1	B	168	LEU	7.3
1	B	324	MET	7.1
1	B	160	GLN	7.0
1	A	704	LEU	7.0
1	B	39	THR	6.9
1	B	349	GLY	6.8
1	B	427	ILE	6.6
1	A	485	SER	6.6
1	B	115	PRO	6.6
1	A	340	ILE	6.6
1	B	109	VAL	6.5
1	B	144	ASP	6.5
1	B	661	GLY	6.4
1	B	73	LEU	6.4
1	B	340	ILE	6.4
1	B	704	LEU	6.3
1	B	207	THR	6.3
1	A	364	PHE	6.3
1	B	161	VAL	6.0
1	A	486	GLY	5.9
1	A	202	PHE	5.9
1	A	631	MET	5.9
1	B	112	LEU	5.9
1	B	143	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	159	GLN	5.9
1	A	355	LYS	5.9
1	B	54	SER	5.8
1	A	14	TYR	5.8
1	B	164	GLY	5.8
1	B	125	MET	5.7
1	B	145	ASP	5.6
1	A	337	ALA	5.6
1	B	353	LEU	5.6
1	B	59	GLU	5.5
1	A	2	PHE	5.4
1	B	413	VAL	5.3
1	A	454	THR	5.2
1	B	72	ILE	5.1
1	A	212	ALA	5.1
1	B	631	MET	5.0
1	A	92	GLU	4.8
1	B	133	THR	4.8
1	A	291	VAL	4.8
1	B	455	GLU	4.8
1	B	322	SER	4.7
1	B	257	TYR	4.7
1	A	346	ASP	4.7
1	B	111	TRP	4.7
1	B	248	LEU	4.7
1	A	427	ILE	4.6
1	B	116	ASP	4.6
1	B	522	ASN	4.6
1	B	57	GLY	4.6
1	A	19	VAL	4.6
1	A	157	GLU	4.6
1	B	628	MET	4.6
1	B	152	GLN	4.4
1	B	179	THR	4.4
1	A	711	ALA	4.4
1	A	708	LEU	4.4
1	A	628	MET	4.3
1	B	171	LEU	4.3
1	A	121	THR	4.3
1	A	109	VAL	4.3
1	B	167	ARG	4.2
1	A	464	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	42	GLY	4.2
1	A	462	LYS	4.1
1	A	59	GLU	4.1
1	A	700	MET	4.1
1	A	160	GLN	4.1
1	B	91	THR	4.1
1	B	158	LEU	4.0
1	A	344	ARG	4.0
1	A	406	ALA	4.0
1	A	43	PHE	4.0
1	A	487	PHE	3.9
1	B	245	VAL	3.9
1	A	343	PRO	3.9
1	B	122	VAL	3.9
1	B	175	ALA	3.9
1	A	324	MET	3.9
1	B	494	PRO	3.9
1	B	135	ILE	3.9
1	B	638	VAL	3.8
1	A	88	LYS	3.8
1	A	18	GLY	3.8
1	A	110	GLY	3.8
1	B	258	GLY	3.8
1	B	93	GLU	3.8
1	B	558	HIS	3.7
1	B	634	LEU	3.7
1	A	519	GLY	3.7
1	B	672	THR	3.6
1	A	393	LEU	3.6
1	B	312	LEU	3.6
1	A	481	ALA	3.6
1	B	247	THR	3.6
1	A	9	VAL	3.5
1	B	630	PRO	3.5
1	A	707	GLY	3.5
1	B	475	ALA	3.5
1	A	623	THR	3.5
1	A	23	LEU	3.5
1	A	290	VAL	3.4
1	A	749	LEU	3.4
1	B	132	HIS	3.4
1	B	213	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	521	GLU	3.4
1	A	311	PHE	3.3
1	B	323	VAL	3.3
1	A	635	ILE	3.3
1	A	520	LEU	3.3
1	A	55	LEU	3.3
1	A	20	MET	3.3
1	B	417	ILE	3.3
1	B	477	MET	3.3
1	B	212	ALA	3.3
1	A	354	LEU	3.2
1	B	265	PHE	3.2
1	B	249	ILE	3.2
1	B	201	LEU	3.2
1	B	735	CYS	3.2
1	A	484	VAL	3.2
1	B	92	GLU	3.1
1	A	117	THR	3.1
1	B	516	ILE	3.1
1	B	410	VAL	3.1
1	B	315	ILE	3.1
1	A	171	LEU	3.0
1	A	545	PHE	3.0
1	B	314	SER	3.0
1	B	557	ILE	3.0
1	B	5	TRP	3.0
1	B	157	GLU	3.0
1	B	369	ILE	3.0
1	B	700	MET	3.0
1	B	728	MET	3.0
1	A	279	VAL	3.0
1	A	168	LEU	3.0
1	B	259	LEU	3.0
1	B	414	LEU	3.0
1	B	176	SER	3.0
1	A	266	ARG	2.9
1	B	172	ASN	2.9
1	B	165	ASP	2.9
1	A	717	THR	2.9
1	B	44	TYR	2.9
1	B	63	ARG	2.9
1	B	670	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	108	TRP	2.9
1	B	736	TRP	2.9
1	A	134	PHE	2.9
1	B	83	ASP	2.9
1	B	533	LEU	2.9
1	B	354	LEU	2.8
1	B	409	LEU	2.8
1	B	561	PHE	2.8
1	A	721	MET	2.8
1	A	6	GLY	2.8
1	B	693	PHE	2.8
1	B	301	SER	2.8
1	A	482	LEU	2.8
1	A	672	THR	2.8
1	A	283	VAL	2.8
1	B	38	VAL	2.8
1	A	642	LEU	2.8
1	B	166	ILE	2.8
1	B	319	ILE	2.8
1	B	211	ALA	2.7
1	A	585	SER	2.7
1	A	261	ILE	2.7
1	B	134	PHE	2.7
1	A	136	SER	2.7
1	B	74	THR	2.7
1	A	21	VAL	2.7
1	A	347	ALA	2.7
1	B	515	VAL	2.7
1	B	668	ILE	2.7
1	B	155	GLU	2.7
1	B	659	GLU	2.7
1	B	242	ALA	2.7
1	A	155	GLU	2.6
1	B	498	TRP	2.6
1	A	339	ALA	2.6
1	A	331	ILE	2.6
1	A	453	ARG	2.6
1	A	691	GLY	2.6
1	B	4	TRP	2.6
1	B	651	VAL	2.6
1	B	202	PHE	2.6
1	B	163	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	670	ILE	2.6
1	B	269	ILE	2.6
1	B	69	VAL	2.6
1	A	376	THR	2.6
1	B	95	ASP	2.5
1	B	291	VAL	2.5
1	A	56	ILE	2.5
1	A	701	MET	2.5
1	A	235	PHE	2.5
1	B	70	VAL	2.5
1	B	707	GLY	2.5
1	A	668	ILE	2.5
1	B	474	ILE	2.5
1	A	1	MET	2.5
1	A	66	THR	2.5
1	A	240	PHE	2.5
1	A	414	LEU	2.5
1	A	410	VAL	2.5
1	B	246	VAL	2.5
1	A	45	ASP	2.5
1	B	103	ASP	2.5
1	B	478	ARG	2.5
1	B	321	ALA	2.4
1	B	381	THR	2.4
1	B	737	TRP	2.4
1	A	138	PRO	2.4
1	B	295	VAL	2.4
1	B	701	MET	2.4
1	B	36	ASN	2.4
1	B	66	THR	2.4
1	B	53	ALA	2.4
1	B	8	THR	2.4
1	B	89	LYS	2.4
1	A	409	LEU	2.4
1	B	290	VAL	2.4
1	A	584	GLY	2.4
1	A	715	ASP	2.4
1	A	368	ILE	2.4
1	A	561	PHE	2.4
1	A	713	LEU	2.4
1	A	647	GLU	2.3
1	B	757	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	634	LEU	2.3
1	B	545	PHE	2.3
1	B	554	GLN	2.3
1	A	433	PRO	2.3
1	A	630	PRO	2.3
1	A	85	ALA	2.3
1	B	204	VAL	2.3
1	B	624	PRO	2.3
1	A	431	TYR	2.3
1	A	588	LEU	2.3
1	B	482	LEU	2.3
1	B	186	GLN	2.3
1	B	495	GLU	2.2
1	A	287	GLY	2.2
1	B	536	LEU	2.2
1	B	588	LEU	2.2
1	B	650	LEU	2.2
1	B	623	THR	2.2
1	A	751	LEU	2.2
1	B	497	MET	2.2
1	B	622	TYR	2.2
1	B	244	PRO	2.2
1	A	622	TYR	2.2
1	A	650	LEU	2.2
1	A	743	LYS	2.2
1	A	646	TYR	2.1
1	A	359	LEU	2.1
1	B	148	LEU	2.1
1	A	380	LYS	2.1
1	B	374	GLU	2.1
1	A	476	ASP	2.1
1	A	394	VAL	2.1
1	B	51	VAL	2.1
1	B	294	ALA	2.1
1	B	612	VAL	2.1
1	A	332	THR	2.1
1	A	303	PRO	2.1
1	B	190	GLU	2.1
1	A	563	LYS	2.1
1	A	248	LEU	2.1
1	B	118	THR	2.1
1	A	336	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	122	VAL	2.1
1	A	734	ASP	2.1
1	B	121	THR	2.1
1	B	675	THR	2.1
1	A	358	PHE	2.1
1	B	138	PRO	2.1
1	B	576	THR	2.0
1	A	265	PHE	2.0
1	A	389	PHE	2.0
1	B	280	ARG	2.0
1	B	105	ILE	2.0
1	B	297	ILE	2.0
1	B	635	ILE	2.0
1	B	395	ASN	2.0
1	B	86	TRP	2.0
1	B	654	MET	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](#)

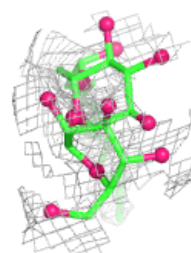
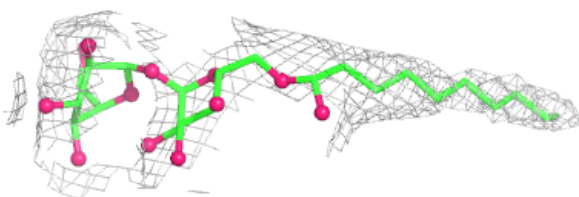
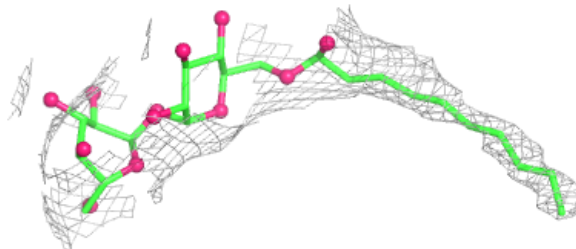
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	F	2	12/12	0.64	0.15	138,161,167,169	0
2	U2D	D	1	22/23	0.70	0.27	121,140,151,154	0
2	U2D	E	1	22/23	0.72	0.19	168,186,194,197	0
2	GLC	C	2	12/12	0.75	0.10	142,150,161,162	0
2	U2D	C	1	22/23	0.78	0.16	82,146,158,160	0
2	U2D	F	1	22/23	0.85	0.15	89,158,167,174	0
2	GLC	D	2	12/12	0.88	0.18	112,135,141,143	0
2	GLC	E	2	12/12	0.91	0.20	166,177,187,188	0

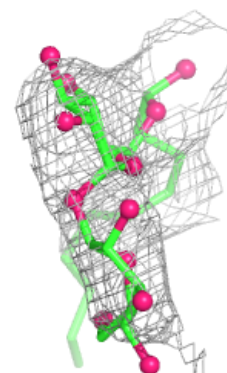
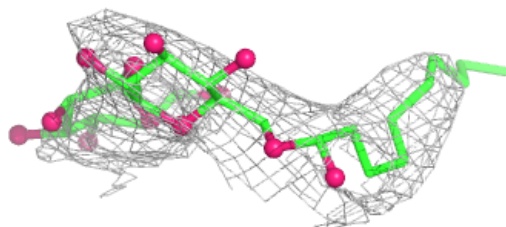
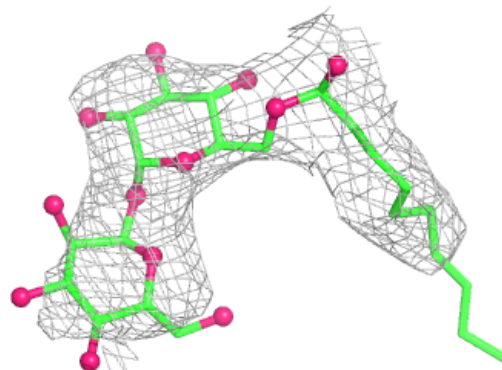
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

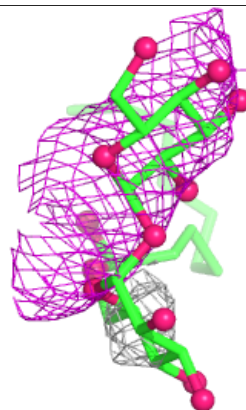
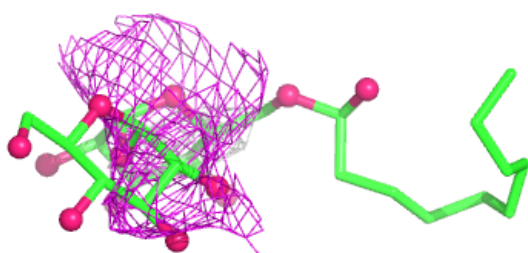
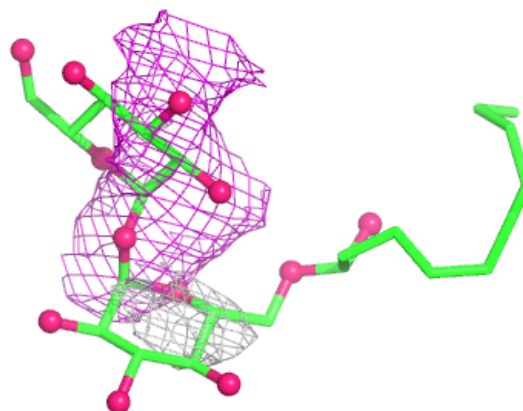
**Electron density around Chain D:**

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

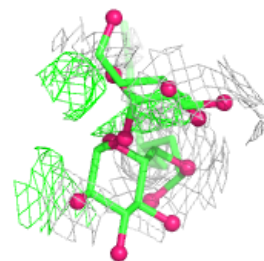
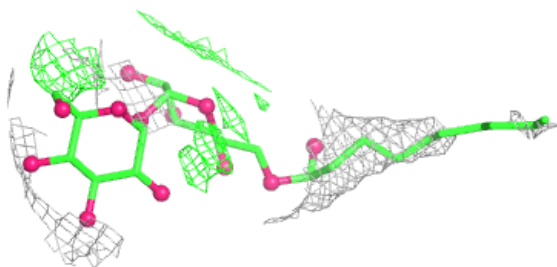
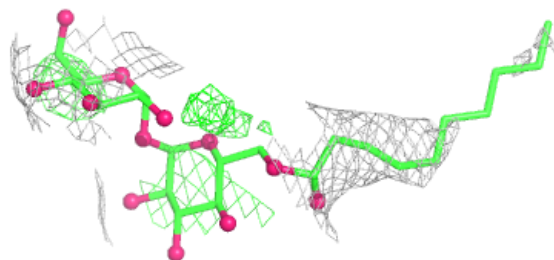


Electron density around Chain E:

$2mF_o-DF_c$ (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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.