



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:09 AM UTC

PDB ID : 1VFO / pdb_00001vfo
Title : Crystal structure of Thermoactinomyces vulgaris R-47 alpha-amylase 2/beta-cyclodextrin complex
Authors : Ohtaki, A.; Mizuno, M.; Tono-zuka, T.; Sakano, Y.; Kamitori, S.
Deposited on : 2004-04-16
Resolution : 2.81 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

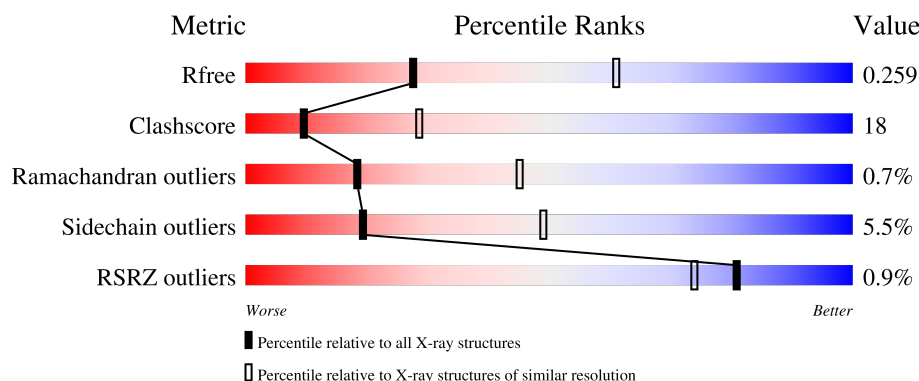
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	585	65% 32% .
1	B	585	2% 62% 33% .
2	C	7	43% 43% 14%
3	D	7	29% 71%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9936 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.

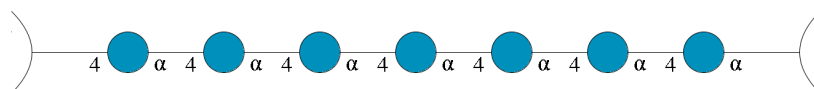
- Molecule 1 is a protein called Neopullulanase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4776	3056	833	872	15			
1	B	585	Total	C	N	O	S	0	0	0
			4776	3056	833	872	15			

There are 4 discrepancies between the modelled and reference sequences:

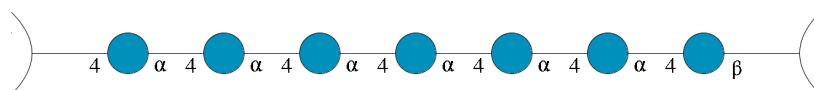
Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ASN	ASP	engineered mutation	UNP Q08751
A	421	ASN	ASP	engineered mutation	UNP Q08751
B	325	ASN	ASP	engineered mutation	UNP Q08751
B	421	ASN	ASP	engineered mutation	UNP Q08751

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	7	Total	C	O	0	0	0
			77	42	35			

- Molecule 3 is an oligosaccharide called Cyclic alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	7	Total	C	O	0	0	0
			77	42	35			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

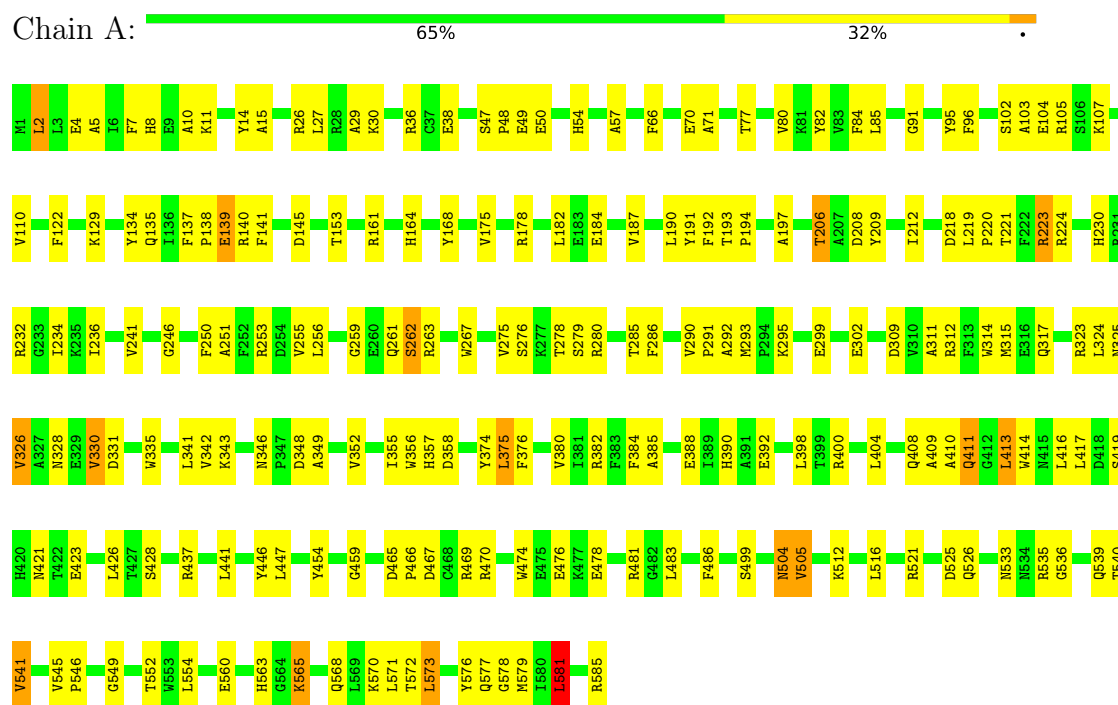
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total	O	0	0
			125	125		
5	B	103	Total	O	0	0
			103	103		

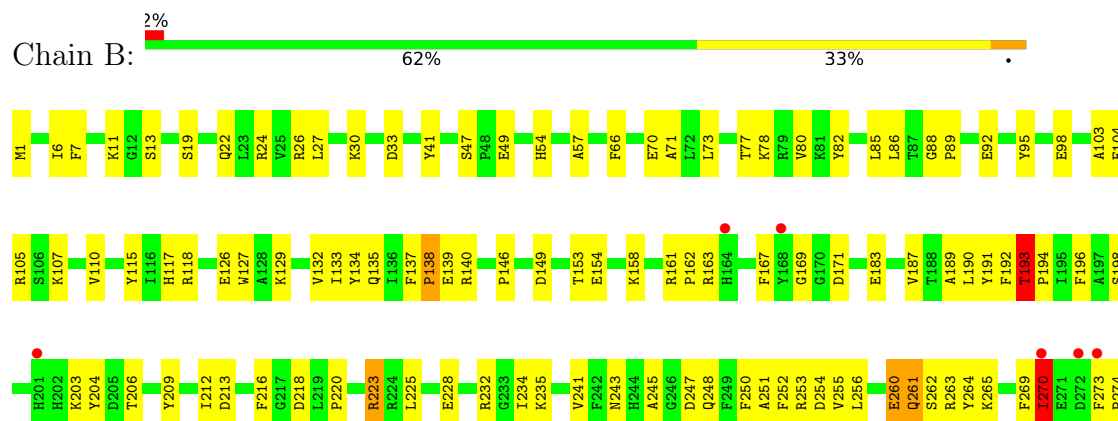
3 Residue-property plots

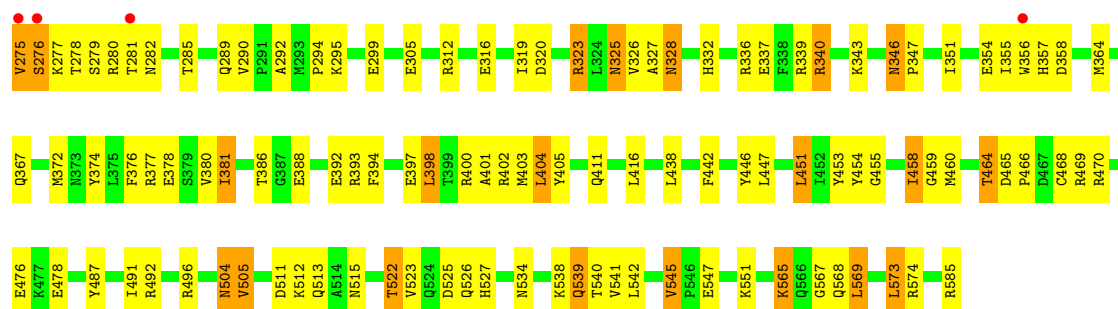
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Neopullulanase 2



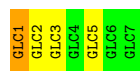
• Molecule 1: Neopullulanase 2





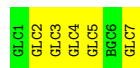
- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain C: 43% 43% 14%



- Molecule 3: Cyclic alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D: 29% 71%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.08Å 118.81Å 114.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.87 – 2.81 38.87 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.87-2.81) 99.3 (38.87-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.256 0.208 , 0.259	Depositor DCC
R_{free} test set	3864 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l 0.023 for -h,-l,-k 0.023 for l,-k,h 0.009 for k,l,h 0.009 for l,h,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9936	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, GLC, CA

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	0.46	0/4906	0.98	24/6641 (0.4%)
1	B	0.44	0/4906	0.96	28/6641 (0.4%)
All	All	0.45	0/9812	0.97	52/13282 (0.4%)

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

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

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	290	VAL	CA-C-N	7.60	129.34	119.84
1	A	290	VAL	C-N-CA	7.60	129.34	119.84
1	A	261	GLN	N-CA-C	-7.50	104.16	113.38
1	A	331	ASP	N-CA-C	6.97	119.31	110.24
1	B	161	ARG	CA-C-N	6.91	128.48	119.84
1	B	161	ARG	C-N-CA	6.91	128.48	119.84
1	A	323	ARG	N-CA-C	-6.79	97.34	108.41
1	A	581	LEU	N-CA-C	6.63	119.09	108.41
1	B	277	LYS	N-CA-C	-6.56	102.62	111.87
1	A	267	TRP	N-CA-C	-6.54	105.30	113.28
1	A	423	GLU	N-CA-C	-6.45	102.02	110.53
1	A	263	ARG	N-CA-C	-6.42	105.31	113.01
1	A	385	ALA	N-CA-C	6.39	118.12	111.03
1	B	193	THR	CA-C-N	-6.37	113.21	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	THR	C-N-CA	-6.37	113.21	119.90
1	A	66	PHE	N-CA-C	6.29	119.39	110.14
1	B	137	PHE	CA-C-N	6.20	127.59	119.84
1	B	137	PHE	C-N-CA	6.20	127.59	119.84
1	B	276	SER	N-CA-C	6.09	119.29	110.28
1	A	137	PHE	CA-C-N	6.04	127.39	119.84
1	A	137	PHE	C-N-CA	6.04	127.39	119.84
1	B	459	GLY	N-CA-C	6.02	123.63	115.32
1	B	346	ASN	CA-C-N	5.98	125.66	119.56
1	B	346	ASN	C-N-CA	5.98	125.66	119.56
1	B	539	GLN	N-CA-C	5.90	118.14	109.24
1	A	459	GLY	N-CA-C	5.88	124.22	115.64
1	B	538	LYS	N-CA-C	-5.87	99.71	109.46
1	A	145	ASP	CA-C-N	5.84	125.70	119.28
1	A	145	ASP	C-N-CA	5.84	125.70	119.28
1	B	323	ARG	N-CA-C	-5.82	99.04	108.52
1	B	522	THR	N-CA-C	5.81	118.23	109.23
1	B	7	PHE	N-CA-C	5.76	118.16	109.23
1	A	161	ARG	CA-C-N	5.72	125.72	119.89
1	A	161	ARG	C-N-CA	5.72	125.72	119.89
1	A	428	SER	N-CA-C	-5.62	105.25	111.71
1	B	80	VAL	N-CA-C	5.42	116.46	108.45
1	A	476	GLU	N-CA-C	5.35	117.80	111.33
1	B	66	PHE	N-CA-C	5.30	117.47	109.41
1	A	417	LEU	N-CA-C	-5.24	107.44	113.88
1	B	270	ILE	N-CA-C	5.24	115.85	108.36
1	B	103	ALA	N-CA-C	-5.21	106.43	112.89
1	B	327	ALA	N-CA-C	5.19	118.39	111.75
1	B	394	PHE	N-CA-C	-5.16	105.57	111.14
1	A	103	ALA	N-CA-C	-5.12	106.99	113.18
1	B	290	VAL	CA-C-N	5.11	125.39	119.47
1	B	290	VAL	C-N-CA	5.11	125.39	119.47
1	B	88	GLY	CA-C-N	5.08	124.69	119.56
1	B	88	GLY	C-N-CA	5.08	124.69	119.56
1	B	254	ASP	N-CA-C	-5.07	106.93	113.01
1	A	206	THR	N-CA-C	5.06	117.80	110.42
1	B	299	GLU	N-CA-C	-5.05	106.63	112.89
1	A	80	VAL	N-CA-C	5.02	114.80	107.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4776	0	4611	137	0
1	B	4776	0	4611	204	0
2	C	77	0	63	3	0
3	D	77	0	63	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	125	0	0	9	0
5	B	103	0	0	10	0
All	All	9936	0	9348	339	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 18.

All (339) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASN:HB3	1:A:355:ILE:HD12	1.37	1.02
1:B:138:PRO:HD2	1:B:193:THR:HG22	1.50	0.91
1:B:512:LYS:HE3	1:B:513:GLN:HE22	1.37	0.90
1:A:278:THR:HG23	1:A:280:ARG:H	1.36	0.89
1:B:476:GLU:HB3	5:B:1052:HOH:O	1.73	0.87
1:B:280:ARG:HE	1:B:280:ARG:HA	1.38	0.86
1:B:276:SER:HB3	1:B:278:THR:HG22	1.59	0.83
1:B:547:GLU:HG2	1:B:551:LYS:HE2	1.64	0.78
1:B:312:ARG:O	1:B:316:GLU:HG3	1.84	0.77
1:A:525:ASP:HB3	1:A:585:ARG:HD2	1.68	0.76
1:B:134:TYR:HB2	1:B:187:VAL:HG11	1.68	0.75
1:A:276:SER:OG	1:A:278:THR:HG22	1.86	0.74
1:B:285:THR:HG22	1:B:294:PRO:HA	1.69	0.74
1:B:196:PHE:HB2	5:B:1013:HOH:O	1.87	0.73
1:A:224:ARG:HE	1:A:224:ARG:HA	1.52	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLU:OE2	1:B:92:GLU:N	2.22	0.72
1:A:572:THR:C	1:A:573:LEU:HD23	2.15	0.71
1:B:54:HIS:HB3	5:B:1055:HOH:O	1.90	0.71
1:B:280:ARG:HA	1:B:280:ARG:NE	2.05	0.71
1:B:253:ARG:NH1	1:B:253:ARG:HB2	2.06	0.70
1:B:263:ARG:HD2	5:B:1069:HOH:O	1.89	0.70
1:A:57:ALA:HA	1:A:71:ALA:HB2	1.73	0.70
1:A:410:ALA:HA	1:A:413:LEU:HD22	1.74	0.69
1:A:346:ASN:ND2	1:A:348:ASP:H	1.91	0.69
1:B:198:SER:HB3	1:B:203:LYS:HG3	1.76	0.68
1:B:328:ASN:HB3	1:B:355:ILE:HG13	1.76	0.68
1:B:241:VAL:HG23	1:B:241:VAL:O	1.95	0.67
1:B:250:PHE:CG	1:B:251:ALA:N	2.63	0.66
1:B:190:LEU:HD13	1:B:234:ILE:HG21	1.77	0.65
1:B:542:LEU:HD21	1:B:568:GLN:NE2	2.11	0.65
1:A:516:LEU:HD13	1:A:541:VAL:CG1	2.26	0.65
1:B:525:ASP:O	1:B:585:ARG:HD2	1.95	0.65
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.32	0.65
1:A:516:LEU:HD13	1:A:541:VAL:HG11	1.77	0.65
1:B:235:LYS:HG3	1:B:320:ASP:CG	2.21	0.65
1:A:328:ASN:CB	1:A:355:ILE:HD12	2.20	0.65
1:B:256:LEU:HA	1:B:275:VAL:HB	1.80	0.64
1:B:565:LYS:HD2	1:B:565:LYS:O	1.97	0.64
1:B:253:ARG:HB2	1:B:253:ARG:HH11	1.63	0.64
1:A:504:ASN:C	1:A:504:ASN:HD22	2.06	0.63
1:B:253:ARG:HH11	1:B:253:ARG:CB	2.12	0.63
1:B:416:LEU:HD23	1:B:416:LEU:H	1.64	0.63
1:A:4:GLU:HG2	1:B:30:LYS:HG3	1.80	0.63
1:B:241:VAL:HG12	1:B:325:ASN:ND2	2.14	0.62
1:A:565:LYS:H	1:A:565:LYS:HD2	1.64	0.62
1:B:337:GLU:HG2	1:B:340:ARG:HH11	1.64	0.62
1:B:57:ALA:HB2	1:B:71:ALA:HB2	1.82	0.62
1:B:223:ARG:HB3	1:B:223:ARG:NH2	2.13	0.62
1:B:146:PRO:HA	1:B:149:ASP:OD2	2.00	0.62
1:B:319:ILE:HD12	1:B:319:ILE:C	2.25	0.61
1:B:270:ILE:HD12	1:B:270:ILE:H	1.65	0.61
1:A:36:ARG:NH2	1:A:38:GLU:OE2	2.34	0.61
1:A:309:ASP:OD2	1:A:312:ARG:NH1	2.34	0.61
1:B:526:GLN:HG3	1:B:585:ARG:OXT	2.00	0.61
1:A:82:TYR:C	1:A:110:VAL:HG23	2.26	0.61
1:B:245:ALA:O	1:B:294:PRO:HD2	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:HG2	1:B:70:GLU:HG3	1.83	0.60
1:A:11:LYS:N	1:A:15:ALA:HB3	2.16	0.60
1:B:212:ILE:HD12	1:B:212:ILE:H	1.65	0.60
1:A:278:THR:HG23	1:A:280:ARG:N	2.14	0.60
1:A:26:ARG:HD3	1:A:70:GLU:OE2	2.02	0.60
1:B:132:VAL:HG11	1:B:491:ILE:HD12	1.84	0.59
1:A:416:LEU:H	1:A:416:LEU:HD23	1.68	0.59
1:A:343:LYS:HE2	1:A:349:ALA:O	2.03	0.59
1:A:447:LEU:HB2	1:A:505:VAL:CG2	2.33	0.59
1:B:163:ARG:HG3	1:B:163:ARG:HH11	1.67	0.58
1:A:138:PRO:HG2	5:A:1018:HOH:O	2.03	0.58
1:A:206:THR:HG21	1:A:209:TYR:CD2	2.38	0.58
1:A:47:SER:HB3	1:A:50:GLU:HG3	1.86	0.58
1:A:212:ILE:HD12	1:A:314:TRP:HH2	1.69	0.58
1:B:243:ASN:HD21	1:B:295:LYS:NZ	2.02	0.57
1:B:328:ASN:N	1:B:328:ASN:HD22	2.02	0.57
1:B:332:HIS:HD2	1:B:367:GLN:OE1	1.86	0.57
1:A:141:PHE:HB3	5:A:1112:HOH:O	2.05	0.57
1:B:542:LEU:HD21	1:B:568:GLN:HE22	1.69	0.57
1:B:253:ARG:HA	1:B:256:LEU:HD12	1.86	0.57
1:B:355:ILE:N	1:B:355:ILE:HD12	2.21	0.56
3:D:2:GLC:H61	3:D:3:GLC:O5	2.05	0.56
1:B:190:LEU:HD13	1:B:234:ILE:CG2	2.36	0.56
1:A:178:ARG:HD2	1:A:474:TRP:CH2	2.41	0.56
1:A:223:ARG:HD2	1:A:317:GLN:OE1	2.05	0.56
1:B:545:VAL:HG21	1:B:569:LEU:HB2	1.87	0.56
1:A:536:GLY:HA2	1:A:576:TYR:CE1	2.41	0.56
1:B:525:ASP:HB3	1:B:585:ARG:HD3	1.87	0.56
1:A:193:THR:HB	1:A:194:PRO:CD	2.36	0.55
1:A:392:GLU:HG3	1:A:512:LYS:HB3	1.89	0.55
1:B:133:ILE:CD1	1:B:189:ALA:HB3	2.36	0.55
1:B:357:HIS:O	1:B:358:ASP:C	2.49	0.55
1:B:104:GLU:OE1	1:B:107:LYS:HE3	2.07	0.55
1:B:465:ASP:OD2	1:B:466:PRO:HA	2.07	0.55
1:B:280:ARG:HE	1:B:280:ARG:CA	2.17	0.55
1:B:400:ARG:O	1:B:404:LEU:HD13	2.06	0.54
1:B:252:PHE:O	1:B:255:VAL:HB	2.07	0.54
1:B:243:ASN:ND2	1:B:295:LYS:NZ	2.55	0.54
1:B:171:ASP:HB2	1:B:216:PHE:O	2.08	0.54
1:B:255:VAL:HG12	1:B:275:VAL:HG21	1.90	0.54
1:B:455:GLY:HA2	1:B:458:ILE:HD11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:SER:OG	1:B:22:GLN:HB2	2.08	0.54
1:A:573:LEU:HD23	1:A:573:LEU:N	2.22	0.54
1:A:579:MET:HE2	1:A:581:LEU:HD11	1.89	0.54
1:B:278:THR:OG1	1:B:279:SER:N	2.41	0.53
1:B:278:THR:C	1:B:280:ARG:H	2.14	0.53
1:B:542:LEU:HD11	1:B:568:GLN:HB3	1.90	0.53
1:A:311:ALA:O	1:A:315:MET:HG3	2.09	0.53
1:A:390:HIS:HD2	1:A:392:GLU:H	1.57	0.53
1:A:330:VAL:HG13	1:A:335:TRP:HE1	1.74	0.53
1:B:204:TYR:HD1	1:B:241:VAL:HG11	1.74	0.52
1:A:26:ARG:HG2	1:A:70:GLU:HG3	1.90	0.52
1:A:82:TYR:O	1:A:110:VAL:HG23	2.09	0.52
1:B:386:THR:OG1	1:B:388:GLU:HG3	2.09	0.52
1:B:138:PRO:CD	1:B:193:THR:HG22	2.32	0.52
1:B:402:ARG:HG2	1:B:403:MET:CE	2.39	0.52
1:A:400:ARG:NH1	1:B:98:GLU:O	2.42	0.52
1:A:437:ARG:HB3	1:A:486:PHE:CE1	2.44	0.52
1:B:193:THR:OG1	1:B:194:PRO:HD3	2.10	0.52
1:A:107:LYS:HD2	5:A:1031:HOH:O	2.10	0.52
1:A:190:LEU:HG	1:A:234:ILE:CG2	2.39	0.52
1:A:299:GLU:OE2	1:B:117:HIS:HB3	2.09	0.52
1:A:376:PHE:O	1:A:380:VAL:HG23	2.10	0.52
1:B:126:GLU:O	1:B:129:LYS:HB2	2.10	0.52
1:B:273:PHE:HB3	1:B:274:PRO:HA	1.91	0.52
1:B:263:ARG:O	1:B:263:ARG:HG3	2.10	0.51
1:A:278:THR:OG1	1:A:279:SER:N	2.43	0.51
1:A:478:GLU:HG3	5:A:1089:HOH:O	2.09	0.51
1:B:250:PHE:CD1	1:B:251:ALA:N	2.78	0.51
1:A:504:ASN:C	1:A:504:ASN:ND2	2.67	0.51
1:A:346:ASN:ND2	1:A:346:ASN:C	2.68	0.51
1:A:552:THR:HG23	1:A:563:HIS:ND1	2.26	0.51
1:B:47:SER:OG	1:B:49:GLU:HG3	2.11	0.51
1:A:95:TYR:CE2	1:A:105:ARG:HB2	2.45	0.51
1:B:192:PHE:CZ	1:B:225:LEU:HD21	2.46	0.51
1:B:354:GLU:C	1:B:355:ILE:HD12	2.36	0.50
1:B:468:CYS:SG	1:B:469:ARG:HG3	2.51	0.50
1:B:504:ASN:C	1:B:504:ASN:HD22	2.18	0.50
1:B:336:ARG:NH1	5:B:1102:HOH:O	2.43	0.50
1:B:512:LYS:HG3	1:B:513:GLN:NE2	2.26	0.50
1:A:224:ARG:HA	1:A:224:ARG:NE	2.25	0.50
1:B:212:ILE:HD12	1:B:212:ILE:N	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ALA:O	1:A:413:LEU:HD13	2.12	0.50
1:B:504:ASN:C	1:B:504:ASN:ND2	2.69	0.50
1:A:2:LEU:HD12	1:A:30:LYS:CD	2.42	0.50
1:A:286:PHE:CZ	2:C:3:GLC:H62	2.47	0.50
1:B:551:LYS:NZ	1:B:567:GLY:H	2.10	0.50
1:A:291:PRO:HG3	5:A:1036:HOH:O	2.11	0.49
1:B:203:LYS:NZ	1:B:213:ASP:OD2	2.40	0.49
1:B:374:TYR:O	1:B:378:GLU:HG3	2.11	0.49
1:A:134:TYR:HB2	1:A:187:VAL:HG11	1.94	0.49
1:B:33:ASP:O	1:B:89:PRO:HD3	2.12	0.49
1:B:41:TYR:HB3	1:B:82:TYR:HB3	1.93	0.49
1:A:2:LEU:HD12	1:A:30:LYS:HD2	1.93	0.49
1:A:38:GLU:OE1	1:A:54:HIS:HB3	2.12	0.49
1:B:515:ASN:HD21	1:B:534:ASN:HD22	1.60	0.49
1:B:260:GLU:HG2	1:B:265:LYS:HD2	1.95	0.48
1:B:295:LYS:HD2	5:B:1007:HOH:O	2.13	0.48
1:B:276:SER:HB2	1:B:282:ASN:OD1	2.13	0.48
1:A:250:PHE:CG	1:A:251:ALA:N	2.81	0.48
1:B:305:GLU:OE2	1:B:305:GLU:HA	2.14	0.48
1:B:416:LEU:H	1:B:416:LEU:CD2	2.25	0.48
1:B:453:TYR:O	1:B:454:TYR:C	2.55	0.48
1:B:573:LEU:N	1:B:573:LEU:HD22	2.29	0.48
1:B:487:TYR:O	1:B:491:ILE:HG12	2.14	0.48
1:A:256:LEU:HD23	1:A:275:VAL:HB	1.95	0.48
1:B:393:ARG:O	1:B:397:GLU:HG3	2.14	0.48
1:A:206:THR:HG21	1:A:209:TYR:CG	2.49	0.48
1:A:504:ASN:O	1:A:521:ARG:HA	2.13	0.48
1:A:565:LYS:HD2	1:A:568:GLN:O	2.14	0.48
1:A:577:GLN:CG	1:A:578:GLY:N	2.77	0.48
1:B:206:THR:HG21	1:B:209:TYR:CD2	2.49	0.48
1:B:351:ILE:N	1:B:351:ILE:HD12	2.29	0.48
1:A:291:PRO:HD2	5:A:1066:HOH:O	2.14	0.48
1:B:206:THR:HG21	1:B:209:TYR:CE2	2.49	0.48
1:B:343:LYS:HE2	1:B:351:ILE:HD13	1.96	0.48
1:A:206:THR:HG21	1:A:209:TYR:CE2	2.49	0.47
1:B:243:ASN:HD21	1:B:295:LYS:HZ3	1.61	0.47
1:B:218:ASP:CG	1:B:220:PRO:HD2	2.38	0.47
1:B:574:ARG:HB2	1:B:574:ARG:HH11	1.79	0.47
1:A:419:SER:C	1:A:421:ASN:H	2.21	0.47
1:B:183:GLU:CD	1:B:232:ARG:HB3	2.39	0.47
1:B:262:SER:C	1:B:264:TYR:H	2.21	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PHE:HB2	1:A:96:PHE:HB3	1.96	0.47
1:B:139:GLU:C	1:B:140:ARG:HG2	2.39	0.47
1:B:377:ARG:HG2	1:B:381:ILE:HD13	1.96	0.47
1:A:255:VAL:HA	1:A:262:SER:OG	2.15	0.47
1:B:492:ARG:HD2	1:B:496:ARG:HH12	1.79	0.47
1:A:140:ARG:HG2	1:A:469:ARG:O	2.14	0.47
1:A:184:GLU:HB2	5:A:1056:HOH:O	2.13	0.47
1:A:218:ASP:OD1	1:A:220:PRO:HD2	2.14	0.47
1:A:392:GLU:CG	1:A:512:LYS:HB3	2.45	0.47
1:A:540:THR:HG21	1:A:570:LYS:HE3	1.96	0.47
1:B:260:GLU:HB2	1:B:273:PHE:CE2	2.50	0.47
1:B:573:LEU:N	1:B:573:LEU:CD2	2.78	0.47
1:A:341:LEU:HD23	1:A:342:VAL:N	2.30	0.47
1:B:247:ASP:OD2	1:B:247:ASP:C	2.58	0.47
1:B:325:ASN:CG	1:B:326:VAL:HG23	2.39	0.47
1:A:554:LEU:HD12	1:A:560:GLU:O	2.15	0.47
1:B:458:ILE:HD13	1:B:458:ILE:N	2.30	0.46
1:A:276:SER:HG	1:A:278:THR:HG22	1.79	0.46
1:A:535:ARG:NH2	1:A:539:GLN:OE1	2.49	0.46
1:B:251:ALA:O	1:B:255:VAL:HG23	2.15	0.46
1:B:447:LEU:HB2	1:B:505:VAL:CG2	2.45	0.46
1:B:133:ILE:HD13	1:B:189:ALA:HB3	1.97	0.46
1:A:26:ARG:CD	1:A:70:GLU:HG3	2.46	0.46
1:A:346:ASN:C	1:A:346:ASN:HD22	2.24	0.46
1:B:256:LEU:HD23	1:B:275:VAL:HG12	1.97	0.46
1:A:129:LYS:HA	1:A:411:GLN:OE1	2.15	0.46
1:B:278:THR:HG23	1:B:280:ARG:H	1.80	0.46
1:B:6:ILE:HD13	1:B:86:LEU:CD1	2.45	0.46
1:B:454:TYR:O	1:B:454:TYR:CG	2.69	0.46
1:B:574:ARG:HB2	1:B:574:ARG:NH1	2.30	0.46
3:D:2:GLC:H61	3:D:3:GLC:C1	2.46	0.46
1:B:339:ARG:HD2	1:B:367:GLN:O	2.16	0.46
1:B:193:THR:OG1	1:B:194:PRO:CD	2.64	0.46
1:B:401:ALA:HA	1:B:404:LEU:HD22	1.96	0.46
1:A:341:LEU:HD23	1:A:341:LEU:C	2.40	0.46
1:A:545:VAL:O	1:A:546:PRO:C	2.59	0.46
1:A:122:PHE:HB3	1:A:408:GLN:NE2	2.31	0.45
1:A:481:ARG:HG2	5:A:1060:HOH:O	2.16	0.45
1:B:158:LYS:HD2	1:B:478:GLU:HB3	1.98	0.45
1:B:243:ASN:ND2	1:B:295:LYS:HZ2	2.13	0.45
1:B:85:LEU:HD13	1:B:95:TYR:CZ	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:THR:OG1	1:B:289:GLN:HG2	2.16	0.45
1:B:402:ARG:HG2	1:B:403:MET:HE3	1.99	0.45
1:A:325:ASN:ND2	1:A:326:VAL:HG23	2.32	0.45
1:B:6:ILE:HG23	1:B:27:LEU:HD21	1.99	0.45
1:A:7:PHE:CG	1:A:8:HIS:N	2.85	0.45
1:A:230:HIS:C	1:A:232:ARG:H	2.25	0.45
1:B:241:VAL:HG12	1:B:325:ASN:CG	2.42	0.45
1:B:376:PHE:O	1:B:380:VAL:HG13	2.17	0.45
1:B:1:MET:HE3	1:B:92:GLU:HG2	1.99	0.45
1:B:118:ARG:NH1	1:B:118:ARG:HG2	2.32	0.45
1:A:253:ARG:NE	5:A:1065:HOH:O	2.49	0.45
1:B:585:ARG:NE	5:B:1075:HOH:O	2.49	0.45
1:A:241:VAL:HG13	1:A:325:ASN:HD22	1.82	0.44
1:A:324:LEU:HD13	1:A:335:TRP:CH2	2.52	0.44
1:A:465:ASP:HA	1:A:466:PRO:HA	1.73	0.44
1:B:447:LEU:HB2	1:B:505:VAL:HG21	1.99	0.44
1:A:286:PHE:CE2	2:C:3:GLC:H62	2.53	0.44
1:A:446:TYR:CG	1:A:447:LEU:N	2.85	0.44
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.81	0.44
1:A:104:GLU:O	1:A:105:ARG:C	2.61	0.44
1:B:223:ARG:HB3	1:B:223:ARG:CZ	2.48	0.44
1:B:269:PHE:CE2	1:B:295:LYS:HG2	2.53	0.44
1:B:328:ASN:HB3	1:B:355:ILE:CG1	2.46	0.44
1:A:8:HIS:HD2	1:A:26:ARG:O	2.00	0.44
1:B:118:ARG:HG2	1:B:118:ARG:HH11	1.82	0.44
1:B:241:VAL:O	1:B:241:VAL:CG2	2.66	0.44
1:B:337:GLU:HG2	1:B:340:ARG:NH1	2.33	0.44
1:B:404:LEU:HB3	1:B:405:TYR:CE2	2.53	0.44
1:A:441:LEU:C	1:A:441:LEU:HD23	2.43	0.43
1:B:525:ASP:HB3	1:B:585:ARG:CD	2.48	0.43
1:A:382:ARG:HG2	1:A:388:GLU:OE1	2.18	0.43
1:B:27:LEU:HD23	1:B:27:LEU:C	2.43	0.43
1:B:77:THR:O	1:B:78:LYS:HB2	2.18	0.43
1:B:504:ASN:HB2	5:B:1096:HOH:O	2.18	0.43
1:B:540:THR:HG22	1:B:541:VAL:N	2.32	0.43
1:A:102:SER:OG	1:A:107:LYS:HB2	2.17	0.43
1:B:241:VAL:HA	1:B:325:ASN:HD22	1.82	0.43
1:A:197:ALA:HB3	1:A:208:ASP:HB3	2.01	0.43
1:B:85:LEU:HD13	1:B:95:TYR:CE2	2.52	0.43
1:B:127:TRP:HD1	5:B:1023:HOH:O	2.00	0.43
1:B:464:THR:O	1:B:465:ASP:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASN:OD1	1:B:326:VAL:HG23	2.19	0.43
1:B:133:ILE:HD12	1:B:189:ALA:HB3	2.01	0.43
1:B:253:ARG:C	1:B:255:VAL:N	2.76	0.43
1:B:270:ILE:H	1:B:270:ILE:CD1	2.27	0.43
1:B:343:LYS:HE2	1:B:351:ILE:CD1	2.49	0.43
1:A:5:ALA:O	1:A:29:ALA:HA	2.19	0.43
1:B:247:ASP:N	1:B:292:ALA:O	2.49	0.43
1:B:261:GLN:NE2	1:B:261:GLN:N	2.66	0.43
1:A:356:TRP:CH2	2:C:1:GLC:H2	2.54	0.43
1:A:374:TYR:CE1	1:A:375:LEU:HD13	2.54	0.43
1:B:346:ASN:HA	1:B:347:PRO:HD2	1.82	0.43
1:B:398:LEU:HD21	1:B:442:PHE:HZ	1.84	0.43
1:A:139:GLU:OE2	1:A:140:ARG:NH1	2.52	0.42
1:B:24:ARG:HD2	1:B:70:GLU:HG2	2.00	0.42
1:B:515:ASN:HD21	1:B:534:ASN:ND2	2.16	0.42
1:A:295:LYS:HE2	1:B:115:TYR:CZ	2.54	0.42
1:B:232:ARG:NH1	5:B:1027:HOH:O	2.52	0.42
1:A:8:HIS:CE1	1:A:82:TYR:OH	2.73	0.42
1:A:467:ASP:O	1:A:470:ARG:HG3	2.19	0.42
1:A:47:SER:OG	1:A:48:PRO:HD2	2.19	0.42
1:A:153:THR:HG23	1:A:168:TYR:HA	2.02	0.42
1:A:285:THR:HB	1:A:293:MET:O	2.19	0.42
1:A:549:GLY:HA2	1:A:585:ARG:HH22	1.84	0.42
1:B:255:VAL:O	1:B:275:VAL:HG21	2.20	0.42
1:B:357:HIS:HA	1:B:374:TYR:OH	2.19	0.42
1:B:460:MET:HE1	1:B:470:ARG:O	2.19	0.42
1:A:499:SER:HB2	1:A:526:GLN:CD	2.45	0.42
1:B:319:ILE:HD12	1:B:320:ASP:N	2.35	0.42
1:B:522:THR:OG1	1:B:527:HIS:HD2	2.02	0.42
1:B:57:ALA:CB	1:B:71:ALA:HB2	2.47	0.42
1:A:390:HIS:HD2	1:A:392:GLU:N	2.18	0.42
1:A:357:HIS:O	1:A:358:ASP:C	2.63	0.42
1:A:374:TYR:CZ	1:A:375:LEU:HD13	2.55	0.42
1:A:380:VAL:HG13	1:A:384:PHE:HD1	1.84	0.42
1:B:135:GLN:HG3	1:B:191:TYR:CD2	2.55	0.41
1:B:392:GLU:OE1	1:B:512:LYS:HG2	2.20	0.41
1:A:441:LEU:HD23	1:A:441:LEU:O	2.20	0.41
1:B:171:ASP:CB	1:B:216:PHE:HA	2.51	0.41
1:B:340:ARG:HE	1:B:340:ARG:HB3	1.61	0.41
1:A:10:ALA:O	1:A:11:LYS:HB3	2.20	0.41
1:A:533:ASN:HB2	1:A:573:LEU:HD12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLU:OE2	1:B:228:GLU:HA	2.19	0.41
1:B:372:MET:HE3	1:B:416:LEU:HD13	2.02	0.41
1:B:446:TYR:CG	1:B:447:LEU:N	2.87	0.41
1:A:565:LYS:O	1:A:565:LYS:HG2	2.20	0.41
1:B:139:GLU:CD	1:B:139:GLU:O	2.64	0.41
1:B:374:TYR:CD1	1:B:374:TYR:C	2.99	0.41
1:B:253:ARG:C	1:B:255:VAL:H	2.27	0.41
1:A:246:GLY:HA2	1:A:292:ALA:O	2.21	0.41
1:B:163:ARG:HG3	1:B:163:ARG:NH1	2.34	0.41
1:A:164:HIS:CE1	1:A:466:PRO:HD3	2.56	0.41
1:A:208:ASP:OD2	1:A:208:ASP:C	2.64	0.41
1:B:398:LEU:HD12	1:B:398:LEU:HA	1.89	0.41
1:B:250:PHE:HA	1:B:253:ARG:NH2	2.36	0.41
1:A:175:VAL:O	1:A:178:ARG:N	2.51	0.41
1:A:192:PHE:HE2	1:A:236:ILE:HD12	1.86	0.41
1:A:218:ASP:CG	1:A:220:PRO:HD2	2.46	0.41
1:A:223:ARG:HB3	1:A:223:ARG:NH1	2.36	0.41
1:B:105:ARG:HG2	1:B:105:ARG:NH1	2.36	0.41
1:A:221:THR:O	1:A:224:ARG:HB3	2.21	0.41
1:B:104:GLU:CD	1:B:107:LYS:HE3	2.46	0.41
1:B:149:ASP:OD1	1:B:169:GLY:HA3	2.21	0.41
1:A:352:VAL:HG21	1:A:414:TRP:CE2	2.56	0.40
1:B:398:LEU:HD21	1:B:442:PHE:CZ	2.56	0.40
1:B:465:ASP:HA	1:B:466:PRO:HA	1.85	0.40
1:B:504:ASN:HD21	1:B:522:THR:HB	1.86	0.40
1:B:511:ASP:OD2	1:B:511:ASP:C	2.62	0.40
1:A:259:GLY:O	1:A:262:SER:HB2	2.21	0.40
1:B:171:ASP:HB2	1:B:216:PHE:HA	2.02	0.40
1:A:135:GLN:HG3	1:A:191:TYR:CD2	2.56	0.40
1:A:454:TYR:O	1:A:454:TYR:CG	2.72	0.40
1:B:1:MET:CE	1:B:92:GLU:HG2	2.52	0.40
1:B:574:ARG:HH11	1:B:574:ARG:CB	2.35	0.40
1:A:27:LEU:HD23	1:A:27:LEU:C	2.46	0.40
1:B:1:MET:HB2	1:B:33:ASP:HB3	2.03	0.40
1:B:135:GLN:HB2	1:B:451:LEU:HD21	2.04	0.40
1:B:153:THR:HG22	1:B:154:GLU:N	2.36	0.40
1:B:523:VAL:O	1:B:523:VAL:HG13	2.20	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	583/585 (100%)	534 (92%)	47 (8%)	2 (0%)	36	64
1	B	583/585 (100%)	522 (90%)	55 (9%)	6 (1%)	12	36
All	All	1166/1170 (100%)	1056 (91%)	102 (9%)	8 (1%)	18	45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	B	11	LYS
1	B	162	PRO
1	B	193	THR
1	B	464	THR
1	A	91	GLY
1	B	138	PRO
1	B	275	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	493/493 (100%)	468 (95%)	25 (5%)	21	52
1	B	493/493 (100%)	464 (94%)	29 (6%)	18	46
All	All	986/986 (100%)	932 (94%)	54 (6%)	19	49

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLU
1	A	77	THR
1	A	85	LEU
1	A	139	GLU
1	A	182	LEU
1	A	219	LEU
1	A	223	ARG
1	A	262	SER
1	A	302	GLU
1	A	326	VAL
1	A	330	VAL
1	A	375	LEU
1	A	398	LEU
1	A	404	LEU
1	A	411	GLN
1	A	413	LEU
1	A	426	LEU
1	A	483	LEU
1	A	504	ASN
1	A	505	VAL
1	A	541	VAL
1	A	565	LYS
1	A	571	LEU
1	A	573	LEU
1	A	581	LEU
1	B	13	SER
1	B	73	LEU
1	B	110	VAL
1	B	167	PHE
1	B	223	ARG
1	B	248	GLN
1	B	260	GLU
1	B	261	GLN
1	B	270	ILE
1	B	323	ARG
1	B	325	ASN
1	B	328	ASN
1	B	340	ARG
1	B	356	TRP
1	B	364	MET
1	B	381	ILE
1	B	398	LEU
1	B	404	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	411	GLN
1	B	438	LEU
1	B	451	LEU
1	B	458	ILE
1	B	504	ASN
1	B	505	VAL
1	B	539	GLN
1	B	545	VAL
1	B	565	LYS
1	B	569	LEU
1	B	573	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	54	HIS
1	A	90	GLN
1	A	135	GLN
1	A	155	GLN
1	A	244	HIS
1	A	261	GLN
1	A	325	ASN
1	A	332	HIS
1	A	346	ASN
1	A	390	HIS
1	A	411	GLN
1	A	443	GLN
1	A	504	ASN
1	A	509	HIS
1	A	526	GLN
1	A	527	HIS
1	A	533	ASN
1	A	544	GLN
1	B	135	GLN
1	B	243	ASN
1	B	244	HIS
1	B	261	GLN
1	B	289	GLN
1	B	325	ASN
1	B	328	ASN
1	B	332	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	357	HIS
1	B	504	ASN
1	B	513	GLN
1	B	527	HIS
1	B	534	ASN
1	B	539	GLN
1	B	544	GLN

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 ⓘ

14 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	C	1	2	11,11,12	0.45	0	15,15,17	0.72	1 (6%)
2	GLC	C	2	2	11,11,12	0.58	0	15,15,17	0.73	1 (6%)
2	GLC	C	3	2	11,11,12	0.76	0	15,15,17	0.65	0
2	GLC	C	4	2	11,11,12	0.59	0	15,15,17	0.61	0
2	GLC	C	5	2	11,11,12	0.57	0	15,15,17	0.63	1 (6%)
2	GLC	C	6	2	11,11,12	0.43	0	15,15,17	0.58	0
2	GLC	C	7	2	11,11,12	0.56	0	15,15,17	0.57	0
3	GLC	D	1	3	11,11,12	0.62	0	15,15,17	0.58	0
3	GLC	D	2	3	11,11,12	0.58	0	15,15,17	0.66	0
3	GLC	D	3	3	11,11,12	0.54	0	15,15,17	0.56	0
3	GLC	D	4	3	11,11,12	0.58	0	15,15,17	0.67	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	D	5	3	11,11,12	0.68	0	15,15,17	1.01	1 (6%)
3	BGC	D	6	3	11,11,12	0.65	0	15,15,17	0.73	0
3	GLC	D	7	3	11,11,12	0.59	0	15,15,17	0.64	1 (6%)

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	C	1	2	-	0/2/19/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	2/2/19/22	0/1/1/1
2	GLC	C	6	2	-	2/2/19/22	0/1/1/1
2	GLC	C	7	2	-	2/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/19/22	0/1/1/1
3	GLC	D	2	3	-	2/2/19/22	0/1/1/1
3	GLC	D	3	3	-	0/2/19/22	0/1/1/1
3	GLC	D	4	3	-	2/2/19/22	0/1/1/1
3	GLC	D	5	3	-	2/2/19/22	0/1/1/1
3	BGC	D	6	3	-	2/2/19/22	0/1/1/1
3	GLC	D	7	3	-	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(°)
3	D	5	GLC	C1-O5-C5	2.68	115.77	112.19
2	C	2	GLC	C1-O5-C5	2.28	115.24	112.19
3	D	4	GLC	C1-O5-C5	2.06	114.95	112.19
2	C	1	GLC	C1-O5-C5	2.03	114.91	112.19
2	C	5	GLC	C1-O5-C5	2.02	114.89	112.19
3	D	7	GLC	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

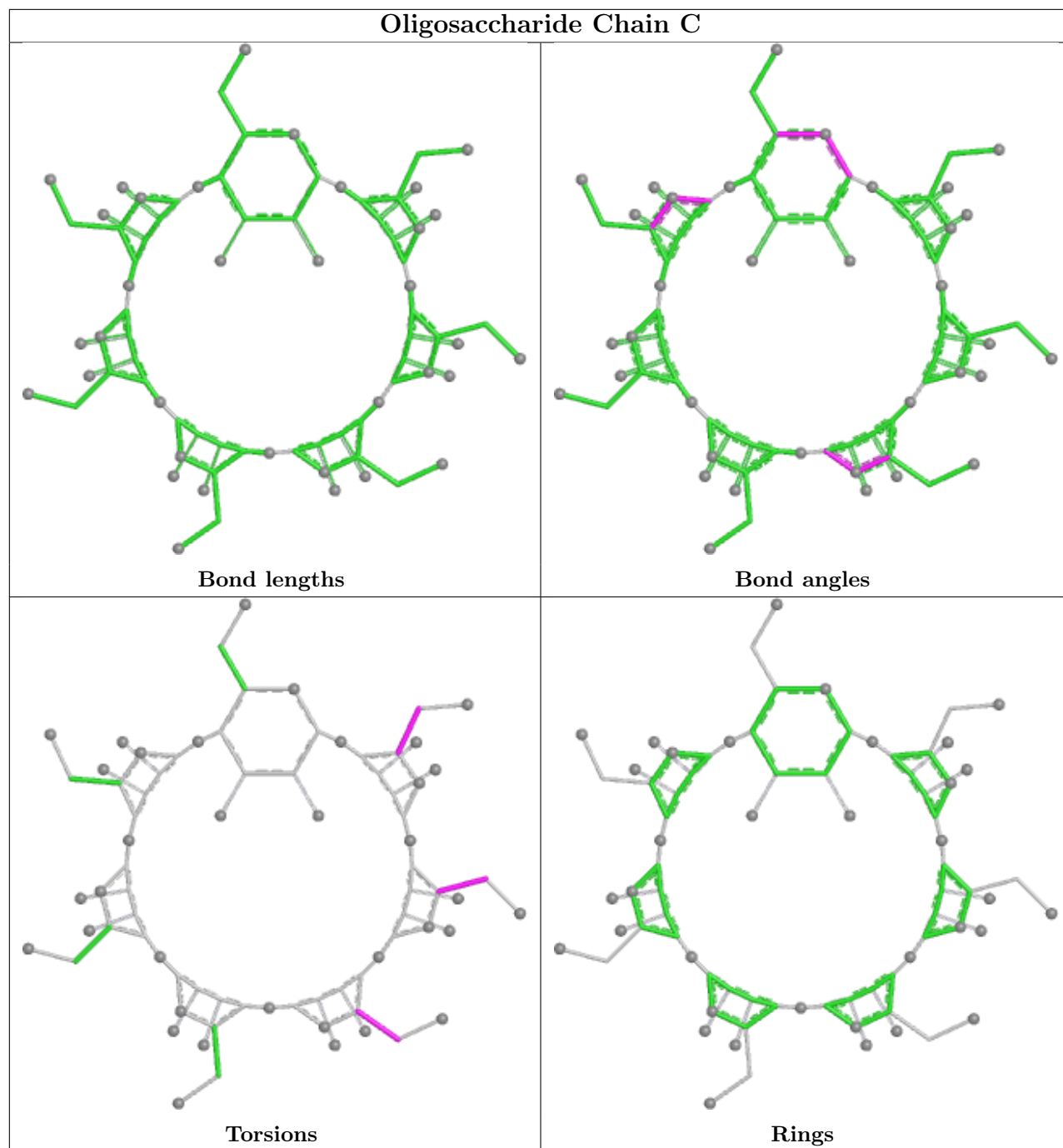
Mol	Chain	Res	Type	Atoms
2	C	6	GLC	O5-C5-C6-O6
2	C	7	GLC	C4-C5-C6-O6
3	D	4	GLC	O5-C5-C6-O6
2	C	6	GLC	C4-C5-C6-O6
3	D	4	GLC	C4-C5-C6-O6
3	D	2	GLC	O5-C5-C6-O6
3	D	2	GLC	C4-C5-C6-O6
3	D	7	GLC	O5-C5-C6-O6
3	D	7	GLC	C4-C5-C6-O6
2	C	7	GLC	O5-C5-C6-O6
3	D	5	GLC	C4-C5-C6-O6
2	C	5	GLC	O5-C5-C6-O6
3	D	6	BGC	C4-C5-C6-O6
3	D	6	BGC	O5-C5-C6-O6
3	D	5	GLC	O5-C5-C6-O6
2	C	5	GLC	C4-C5-C6-O6

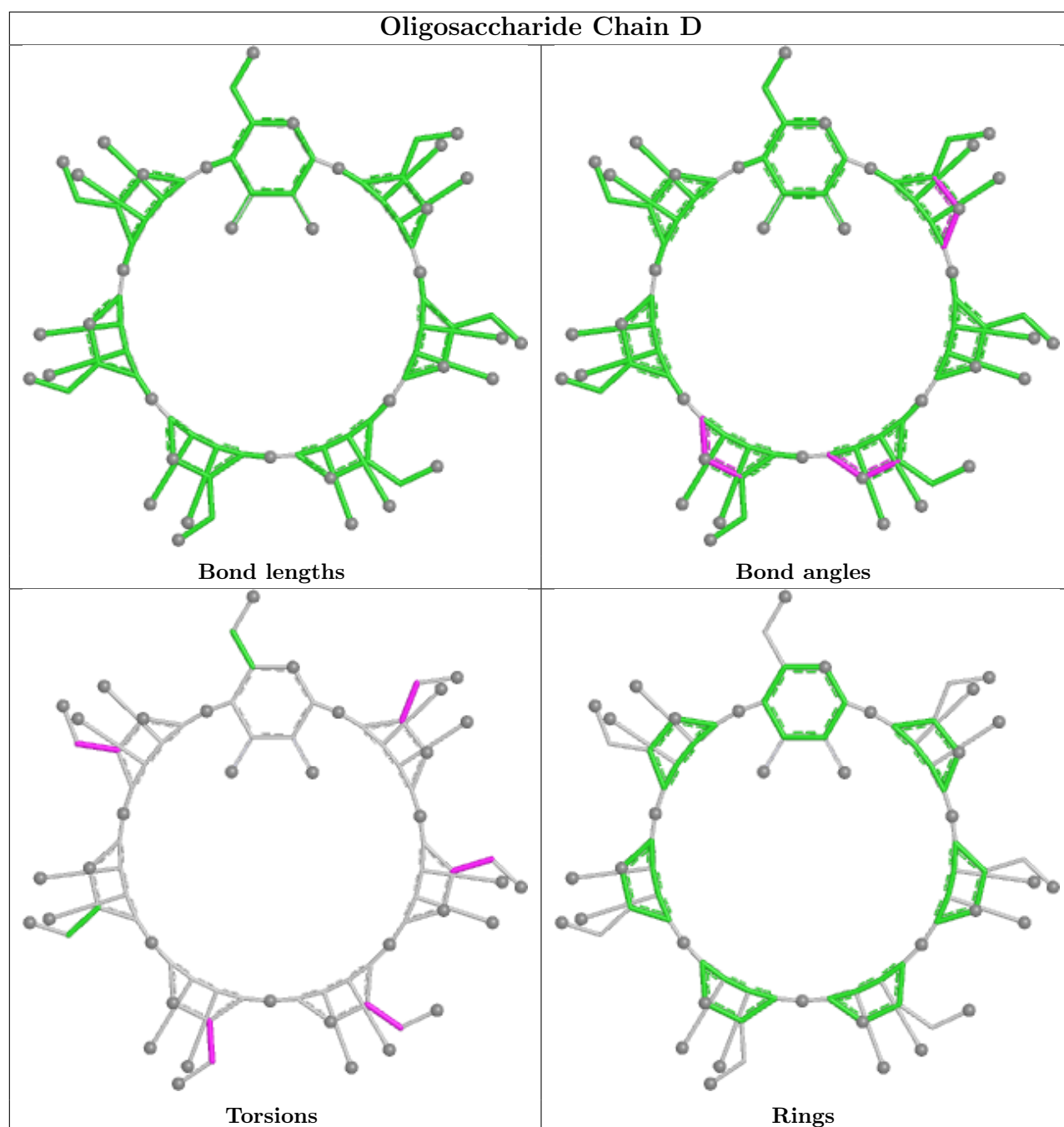
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	GLC	2	0
3	D	2	GLC	2	0
2	C	1	GLC	1	0
3	D	3	GLC	2	0

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





5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	585/585 (100%)	-0.28	0 100 100	14, 38, 69, 85	0
1	B	585/585 (100%)	-0.05	10 (1%) 69 60	18, 45, 83, 100	0
All	All	1170/1170 (100%)	-0.17	10 (0%) 81 74	14, 41, 78, 100	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	TRP	2.7
1	B	275	VAL	2.7
1	B	168	TYR	2.4
1	B	273	PHE	2.4
1	B	276	SER	2.3
1	B	270	ILE	2.3
1	B	281	THR	2.3
1	B	201	HIS	2.2
1	B	272	ASP	2.2
1	B	164	HIS	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](#)

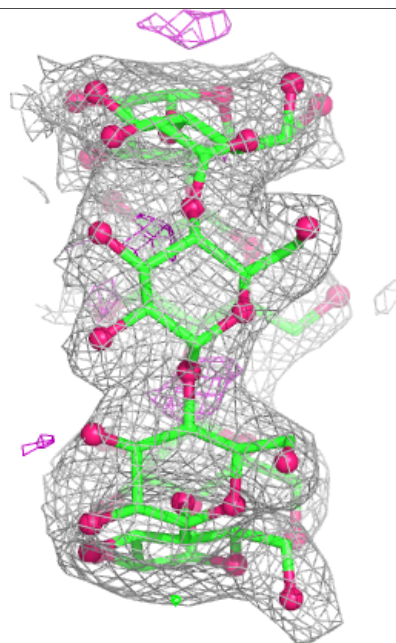
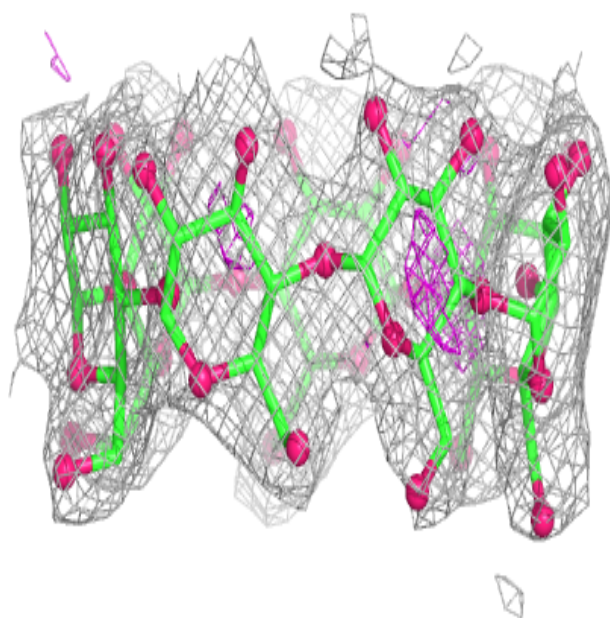
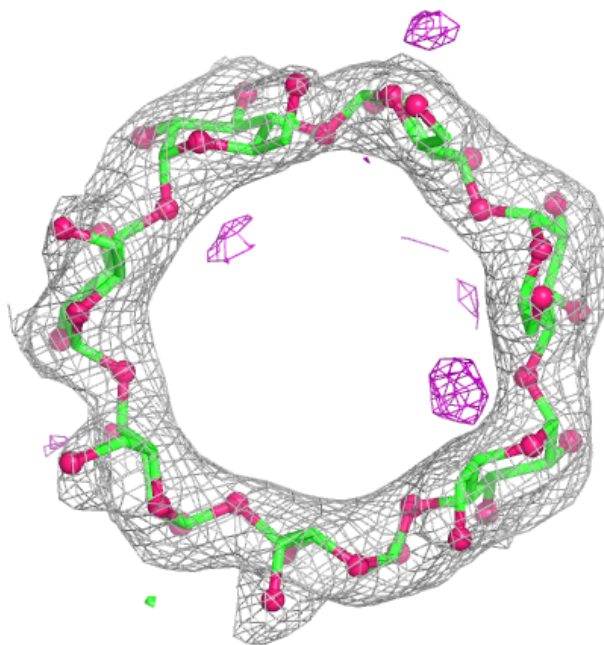
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

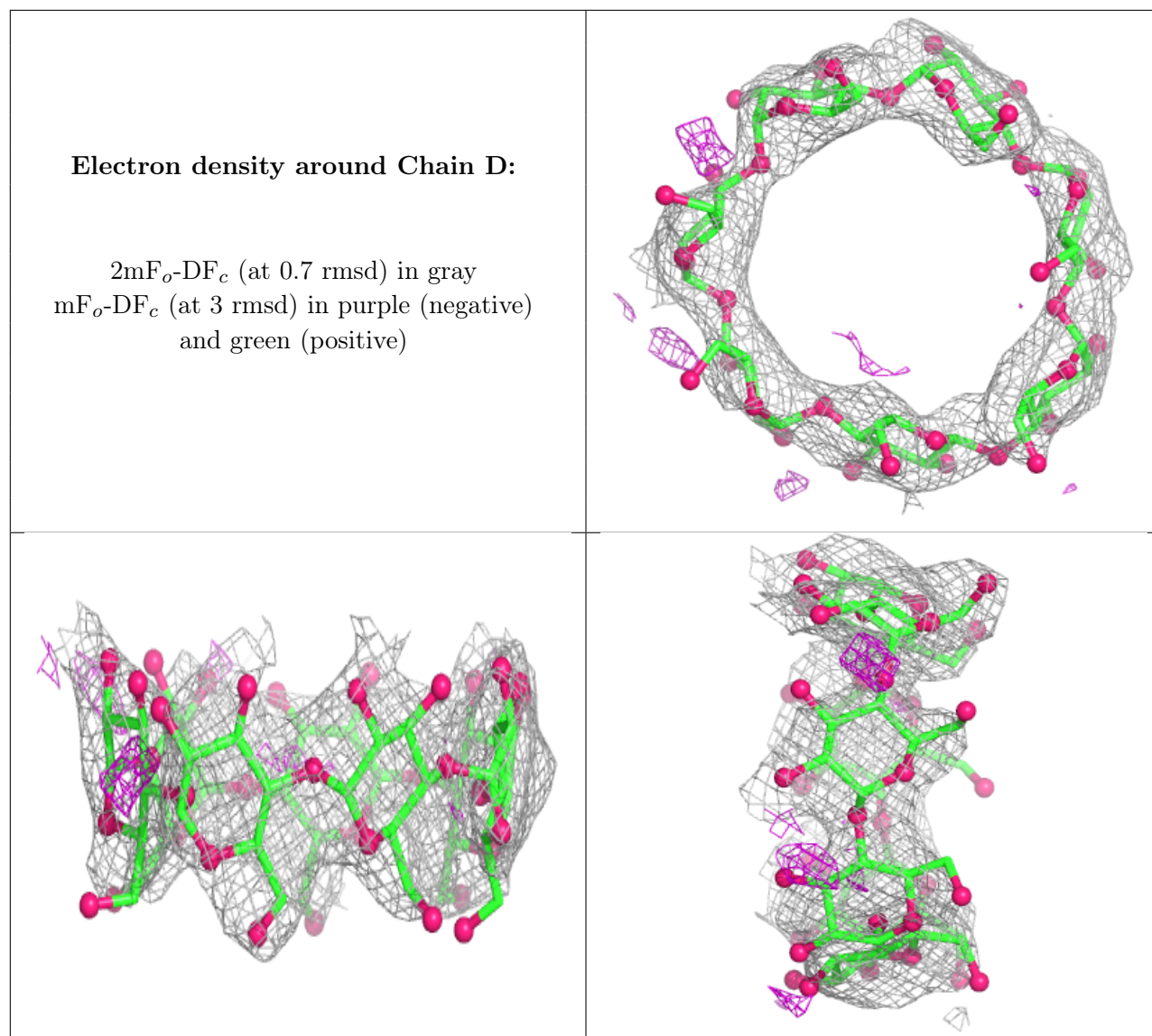
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	D	5	11/12	0.58	0.14	96,97,98,98	0
3	GLC	D	4	11/12	0.69	0.14	97,98,99,99	0
3	GLC	D	1	11/12	0.74	0.15	93,94,94,95	0
3	BGC	D	6	11/12	0.76	0.12	95,97,98,98	0
3	GLC	D	7	11/12	0.77	0.14	92,95,96,96	0
3	GLC	D	3	11/12	0.79	0.14	91,93,94,97	0
3	GLC	D	2	11/12	0.87	0.13	90,92,93,93	0
2	GLC	C	6	11/12	0.91	0.08	49,49,51,51	0
2	GLC	C	7	11/12	0.91	0.08	44,46,48,48	0
2	GLC	C	5	11/12	0.91	0.08	44,47,49,51	0
2	GLC	C	4	11/12	0.92	0.09	37,38,39,40	0
2	GLC	C	3	11/12	0.93	0.09	40,45,47,49	0
2	GLC	C	2	11/12	0.93	0.08	46,47,49,50	0
2	GLC	C	1	11/12	0.95	0.07	45,46,48,50	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)





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(Å ²)	Q<0.9
4	CA	A	1001	1/1	0.98	0.03	35,35,35,35	0
4	CA	B	1002	1/1	0.99	0.04	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.