



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:12 PM UTC

PDB ID : 2WIL / pdb_00002wil
Title : AGED FORM OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED BY TABUN ANALOGUE TA5
Authors : Carletti, E.; Aurbek, N.; Gillon, E.; Loiodice, M.; Nicolet, Y.; Fontecilla, J.; Masson, P.; Thiermann, H.; Nachon, F.; Worek, F.
Deposited on : 2009-05-12
Resolution : 3.10 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

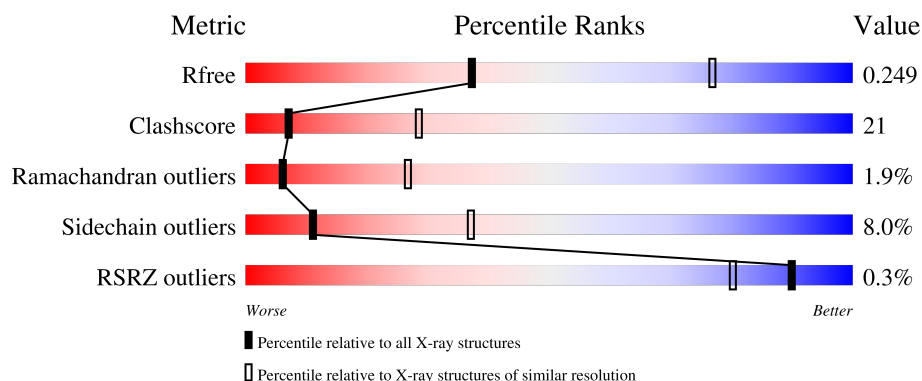
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



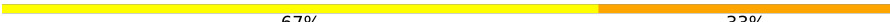
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	529	59% 35% 5%
1	B	529	57% 37% 5%
2	C	3	100%
2	D	3	67% 33%
2	E	3	33% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	3	 67% 33%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8798 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.

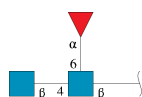
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	526	Total	C	N	O	S	7	2	0
			4205	2714	707	769	15			
1	B	524	Total	C	N	O	S	0	3	0
			4192	2708	705	764	15			

There are 4 discrepancies between the modelled and reference sequences:

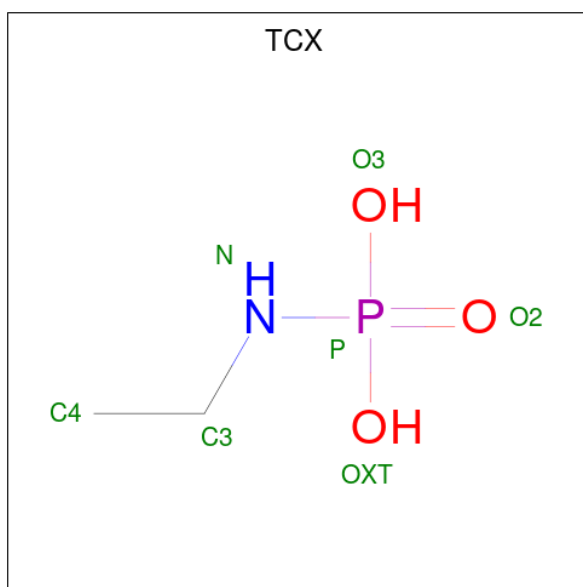
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276
B	17	GLN	ASN	engineered mutation	UNP P06276
B	481	GLN	ASN	engineered mutation	UNP P06276

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	D	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is ethylphosphoramidic acid (CCD ID: TCX) (formula: C₂H₈NO₃P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			6	2	1	2	1		
3	B	1	Total	C	N	O	P	0	0
			6	2	1	2	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



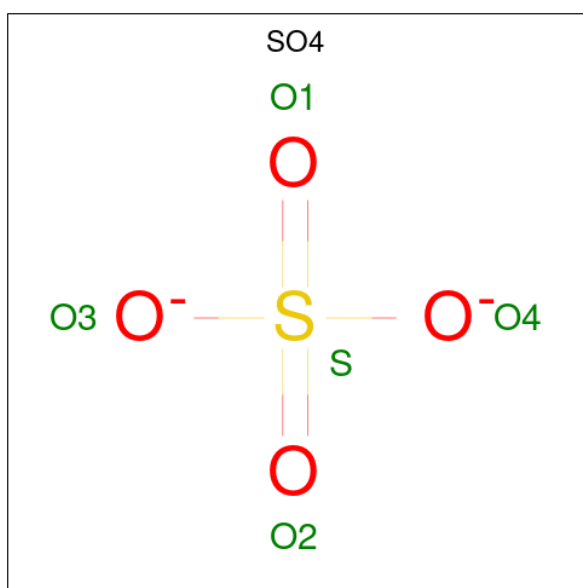
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O S	0	0
			5	4 1		
5	A	1	Total	O S	0	0
			5	4 1		
5	B	1	Total	O S	0	0
			5	4 1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

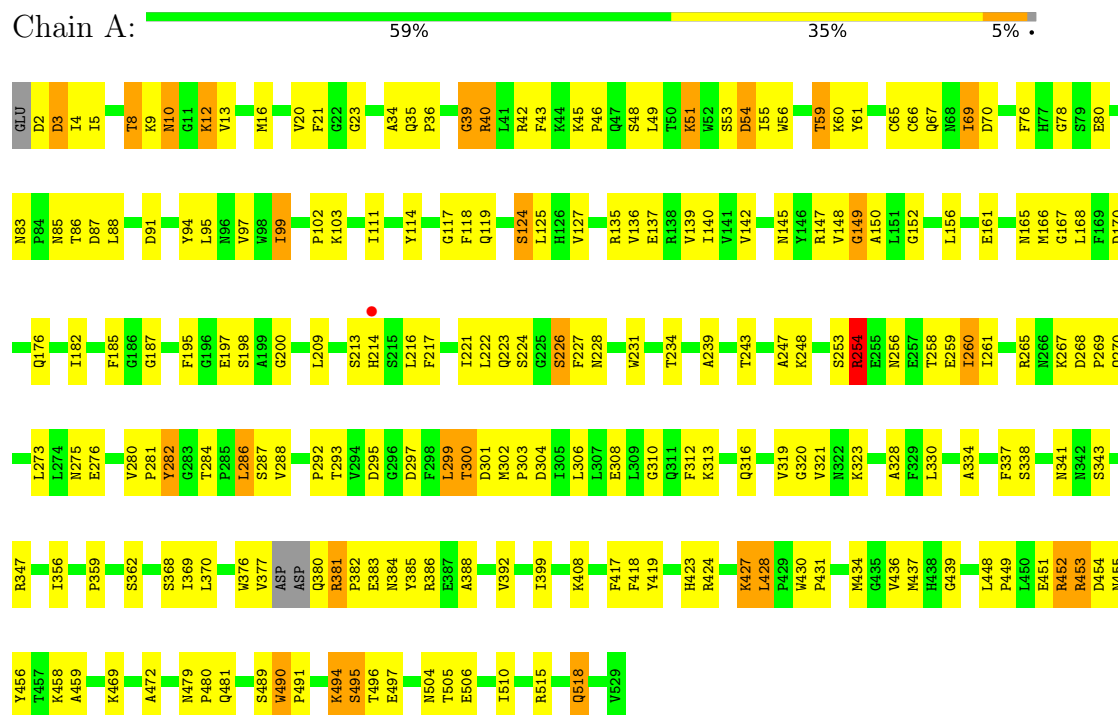
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	65	Total 65	O 65	0	0
7	B	72	Total 72	O 72	0	0

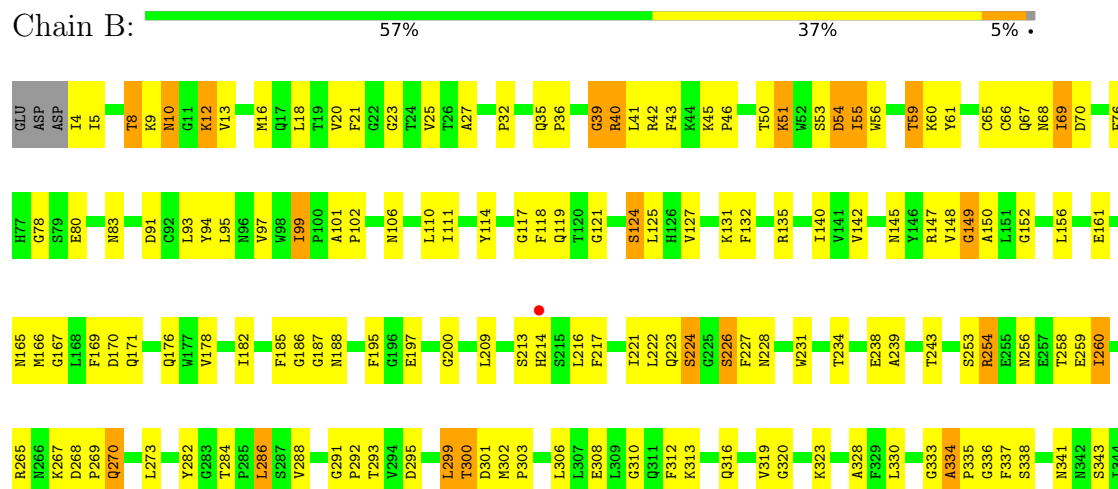
3 Residue-property plots

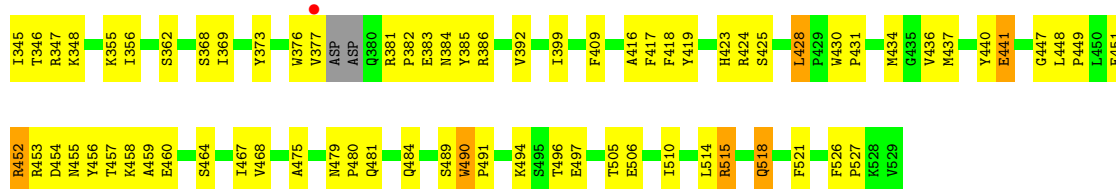
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

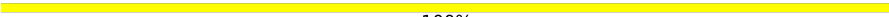


• Molecule 1: CHOLINESTERASE





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  67% 33%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  33% 67%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	150.35Å 150.35Å 139.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 3.10 48.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.39-3.10) 98.2 (48.39-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.220 , 0.253 0.216 , 0.249	Depositor DCC
R_{free} test set	937 reflections (3.22%)	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8798	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: SO4, NAG, CL, FUC, TCX

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	0.78	1/4327 (0.0%)	0.96	12/5874 (0.2%)
1	B	0.71	0/4317	0.98	13/5860 (0.2%)
All	All	0.74	1/8644 (0.0%)	0.97	25/11734 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	TYR	CB-CG	-7.77	1.34	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	437	MET	N-CA-C	6.45	119.26	110.55
1	A	437	MET	N-CA-C	5.99	118.63	110.55
1	B	291	GLY	CA-C-N	5.97	125.91	119.76
1	B	291	GLY	C-N-CA	5.97	125.91	119.76
1	B	490	TRP	CA-C-N	5.97	125.93	119.78
1	B	490	TRP	C-N-CA	5.97	125.93	119.78
1	B	456	TYR	N-CA-C	-5.82	102.69	110.55
1	B	121	GLY	N-CA-C	5.66	117.32	111.95
1	A	334	ALA	CA-C-N	5.57	126.44	119.98
1	A	334	ALA	C-N-CA	5.57	126.44	119.98
1	A	456	TYR	N-CA-C	-5.46	103.18	110.55
1	B	99	ILE	CA-C-N	-5.44	114.64	120.03
1	B	99	ILE	C-N-CA	-5.44	114.64	120.03
1	B	334	ALA	CA-C-N	5.39	126.57	119.84
1	B	334	ALA	C-N-CA	5.39	126.57	119.84
1	A	254	ARG	N-CA-C	5.31	115.55	108.38
1	A	490	TRP	CA-C-N	5.29	125.19	119.85
1	A	490	TRP	C-N-CA	5.29	125.19	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	VAL	N-CA-C	5.23	116.70	111.00
1	A	381	ARG	CA-C-N	5.20	124.82	119.05
1	A	381	ARG	C-N-CA	5.20	124.82	119.05
1	B	399	ILE	N-CA-C	5.18	115.91	110.62
1	B	441	GLU	N-CA-C	-5.15	107.37	113.97
1	A	282	TYR	CB-CG-CD2	5.05	128.37	120.80
1	A	139	VAL	CB-CA-C	-5.00	104.33	111.19

There are no chirality outliers.

There are no planarity outliers.

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	4205	0	4098	176	0
1	B	4192	0	4095	179	0
2	C	38	0	34	0	0
2	D	38	0	34	3	0
2	E	38	0	34	0	0
2	F	38	0	34	1	0
3	A	6	0	7	3	0
3	B	6	0	7	2	0
4	A	42	0	39	0	0
4	B	42	0	39	1	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
6	A	1	0	0	0	0
7	A	65	0	0	16	0
7	B	72	0	0	18	0
All	All	8798	0	8421	356	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 21.

All (356) 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:2:ASP:HA	1:A:3:ASP:O	1.30	1.28
1:A:253:SER:O	1:A:254:ARG:HD3	1.55	1.05
1:B:452:ARG:HE	1:B:452:ARG:HA	1.20	1.04
1:A:494:LYS:HE2	7:A:756:HOH:O	1.58	1.02
1:A:452:ARG:HE	1:A:452:ARG:HA	1.20	1.02
1:A:518:GLN:H	1:A:518:GLN:NE2	1.59	0.99
1:B:518:GLN:H	1:B:518:GLN:NE2	1.61	0.97
1:B:4:ILE:HG12	7:B:752:HOH:O	1.65	0.96
1:B:518:GLN:HE21	1:B:518:GLN:N	1.66	0.93
1:B:53:SER:O	1:B:54:ASP:HB2	1.69	0.91
1:B:253:SER:O	1:B:254:ARG:HD3	1.71	0.90
1:A:2:ASP:HA	1:A:3:ASP:C	1.97	0.90
1:A:518:GLN:HE21	1:A:518:GLN:N	1.70	0.90
1:A:53:SER:O	1:A:54:ASP:HB2	1.72	0.88
1:A:518:GLN:H	1:A:518:GLN:HE21	0.87	0.86
1:B:40:ARG:HD2	7:B:770:HOH:O	1.73	0.86
1:B:156:LEU:HD13	1:B:243:THR:HG21	1.60	0.83
1:B:53:SER:O	1:B:54:ASP:CB	2.27	0.81
1:B:452:ARG:HA	1:B:452:ARG:NE	1.96	0.81
1:A:53:SER:O	1:A:54:ASP:CB	2.25	0.80
1:B:16:MET:HB3	1:B:59:THR:HG22	1.63	0.80
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.63	0.79
1:B:284:THR:HG22	1:B:356:ILE:O	1.82	0.79
1:A:288:VAL:HG12	1:A:288:VAL:O	1.83	0.77
1:A:284:THR:HG22	1:A:356:ILE:O	1.85	0.77
1:B:430:TRP:HB3	1:B:431:PRO:HD2	1.66	0.77
1:A:23:GLY:HA3	1:A:135:ARG:HE	1.50	0.76
1:B:286:LEU:HD23	3:B:601:TCX:H43C	1.67	0.76
1:B:23:GLY:HA3	1:B:135:ARG:HE	1.51	0.75
1:A:452:ARG:HA	1:A:452:ARG:NE	1.99	0.75
1:A:2:ASP:CG	1:A:2:ASP:O	2.31	0.74
1:A:430:TRP:HB3	1:A:431:PRO:HD2	1.69	0.74
1:B:288:VAL:HG12	1:B:288:VAL:O	1.86	0.74
1:B:491:PRO:CD	1:B:510:ILE:HD12	2.19	0.72
1:B:161:GLU:HG3	1:B:258:THR:HG23	1.72	0.72
1:B:213:SER:HA	1:B:216:LEU:HD12	1.71	0.71
1:A:16:MET:HB3	1:A:59:THR:HG22	1.72	0.71
1:A:213:SER:HA	1:A:216:LEU:HD12	1.72	0.70
1:A:217:PHE:O	1:A:313:LYS:NZ	2.24	0.70
1:B:316:GLN:H	1:B:316:GLN:CD	1.98	0.70
1:A:504:ASN:HB2	7:A:739:HOH:O	1.91	0.70
1:B:518:GLN:H	1:B:518:GLN:HE21	0.81	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:PRO:HD3	1:B:147:ARG:NH2	2.08	0.69
1:B:209:LEU:CD2	1:B:312:PHE:HB3	2.23	0.69
1:A:491:PRO:CD	1:A:510:ILE:HD12	2.22	0.69
1:B:221:ILE:C	1:B:222:LEU:HD12	2.18	0.68
1:A:2:ASP:CA	1:A:3:ASP:O	2.26	0.68
1:B:69:ILE:HA	7:B:732:HOH:O	1.94	0.68
1:B:99:ILE:HG22	1:B:140:ILE:HG12	1.74	0.68
1:A:161:GLU:HG3	1:A:258:THR:HG23	1.75	0.67
1:A:39:GLY:O	1:A:265:ARG:HD3	1.94	0.67
1:B:99:ILE:HG21	1:B:185:PHE:HB3	1.77	0.66
1:A:209:LEU:CD2	1:A:312:PHE:HB3	2.26	0.66
1:B:5:ILE:HD11	7:B:734:HOH:O	1.96	0.66
1:B:42:ARG:HH22	1:B:269:PRO:HD3	1.61	0.66
1:B:39:GLY:O	1:B:265:ARG:HD3	1.96	0.65
1:B:69:ILE:HG23	1:B:83:ASN:OD1	1.97	0.65
1:B:491:PRO:HD3	1:B:510:ILE:HD12	1.79	0.65
1:B:209:LEU:HD23	1:B:312:PHE:HB3	1.78	0.64
1:B:452:ARG:HE	1:B:452:ARG:CA	2.05	0.64
1:A:380:GLN:OE1	7:A:701:HOH:O	2.15	0.64
1:B:491:PRO:HD3	1:B:510:ILE:CD1	2.27	0.63
1:B:42:ARG:NH2	1:B:269:PRO:HD3	2.13	0.63
1:A:286:LEU:HD23	3:A:601:TCX:H43C	1.81	0.63
1:A:491:PRO:HD3	1:A:510:ILE:CD1	2.29	0.62
1:B:65:CYS:O	1:B:67:GLN:HG2	1.99	0.62
1:A:209:LEU:HD23	1:A:312:PHE:HB3	1.81	0.62
1:A:3:ASP:OD2	1:A:5:ILE:HD11	2.00	0.62
1:A:65:CYS:O	1:A:67:GLN:HG2	1.99	0.62
1:B:95:LEU:HD12	1:B:95:LEU:C	2.25	0.62
1:A:99:ILE:HG22	1:A:140:ILE:HG12	1.83	0.61
1:A:303:PRO:HA	1:A:306:LEU:HD12	1.81	0.61
1:A:221:ILE:C	1:A:222:LEU:HD12	2.26	0.61
1:A:114:TYR:HE2	1:A:145:ASN:HA	1.65	0.61
1:B:454:ASP:O	1:B:455:ASN:HB2	2.00	0.61
1:A:213:SER:O	1:A:214[A]:HIS:C	2.42	0.60
1:A:453:ARG:HD3	7:A:732:HOH:O	2.02	0.59
1:A:8:THR:C	1:A:10:ASN:H	2.11	0.59
7:A:724:HOH:O	2:D:2:NAG:H5	2.03	0.59
1:A:99:ILE:HG21	1:A:185:PHE:HB3	1.85	0.59
1:A:321:VAL:HG21	1:A:399:ILE:HG12	1.85	0.59
1:B:491:PRO:CD	1:B:510:ILE:CD1	2.80	0.59
1:A:2:ASP:O	1:A:2:ASP:OD2	2.21	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ASP:O	1:A:455:ASN:HB2	2.03	0.58
1:A:491:PRO:HD3	1:A:510:ILE:HD12	1.84	0.58
1:B:8:THR:C	1:B:10:ASN:H	2.11	0.58
1:A:45:LYS:HE3	7:A:737:HOH:O	2.04	0.58
1:A:491:PRO:CD	1:A:510:ILE:CD1	2.82	0.58
1:A:316:GLN:CD	1:A:316:GLN:H	2.11	0.57
1:B:97:VAL:HG22	1:B:142:VAL:HG22	1.86	0.57
1:A:359:PRO:HD2	7:A:714:HOH:O	2.04	0.57
1:A:119:GLN:HE22	1:A:149:GLY:HA2	1.69	0.57
1:B:383:GLU:H	1:B:383:GLU:CD	2.12	0.57
1:A:491:PRO:HG3	1:A:510:ILE:HD12	1.87	0.57
1:A:46:PRO:HD3	1:A:147:ARG:NH2	2.20	0.57
1:B:165:ASN:OD1	1:B:292:PRO:HA	2.05	0.57
1:B:316:GLN:CD	1:B:316:GLN:N	2.63	0.56
1:A:254:ARG:HB2	1:A:260:ILE:HG12	1.85	0.56
1:B:114:TYR:HE2	1:B:145:ASN:HA	1.69	0.56
1:A:99:ILE:HD11	7:A:702:HOH:O	2.06	0.56
1:B:152:GLY:C	1:B:166:MET:HE2	2.30	0.56
1:A:383:GLU:CD	1:A:383:GLU:H	2.13	0.56
1:B:312:PHE:CD1	1:B:409:PHE:CE1	2.94	0.55
1:B:319:VAL:O	1:B:418:PHE:HA	2.06	0.55
1:B:226:SER:HB2	1:B:228:ASN:OD1	2.05	0.55
1:A:268[B]:ASP:OD2	1:A:270:GLN:HB2	2.07	0.55
1:A:308:GLU:OE2	1:A:308:GLU:HA	2.07	0.55
1:B:140:ILE:HG21	1:B:182:ILE:HD11	1.89	0.54
1:B:32:PRO:HB3	1:B:94:TYR:CE2	2.43	0.54
1:B:312:PHE:CE1	1:B:409:PHE:CE1	2.95	0.54
1:B:76:PHE:CE2	1:B:78:GLY:HA3	2.42	0.54
1:B:13:VAL:HG12	1:B:56:TRP:HB3	1.90	0.54
1:B:46:PRO:HD3	1:B:147:ARG:HH22	1.70	0.54
1:B:355:LYS:O	7:B:701:HOH:O	2.18	0.54
1:B:213:SER:O	1:B:214[A]:HIS:C	2.50	0.54
1:B:114:TYR:HB2	7:B:753:HOH:O	2.07	0.54
1:A:95:LEU:C	1:A:95:LEU:HD12	2.33	0.53
1:A:99:ILE:CD1	7:A:702:HOH:O	2.56	0.53
1:B:338:SER:HB3	1:B:341:ASN:OD1	2.08	0.53
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.23	0.53
1:A:491:PRO:CG	1:A:510:ILE:HD12	2.39	0.53
1:B:223:GLN:NE2	1:B:441:GLU:OE2	2.42	0.53
1:A:2:ASP:CA	1:A:3:ASP:C	2.76	0.53
1:B:369:ILE:HD11	1:B:526:PHE:CE1	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:VAL:HG13	1:B:182:ILE:HB	1.90	0.52
1:B:214[A]:HIS:O	1:B:313:LYS:HE3	2.09	0.52
1:A:295:ASP:OD2	1:A:297:ASP:HB3	2.09	0.52
1:B:35:GLN:O	1:B:36:PRO:C	2.52	0.52
1:B:95:LEU:HD12	1:B:95:LEU:O	2.09	0.52
1:B:197:GLU:O	1:B:200:GLY:N	2.43	0.52
1:B:310:GLY:HA2	1:B:312:PHE:CE2	2.44	0.51
1:B:231:TRP:CE2	3:B:601:TCX:H32C	2.44	0.51
1:A:42:ARG:O	1:A:43:PHE:HB2	2.10	0.51
1:A:8:THR:C	1:A:10:ASN:N	2.67	0.51
1:B:254:ARG:HB2	1:B:260:ILE:HG12	1.92	0.51
1:A:423:HIS:ND1	1:A:505:THR:HG23	2.25	0.51
1:B:491:PRO:HG3	1:B:510:ILE:HD12	1.93	0.50
1:B:8:THR:C	1:B:10:ASN:N	2.69	0.50
1:A:12:LYS:HE2	7:A:763:HOH:O	2.11	0.50
1:A:70:ASP:C	1:A:70:ASP:OD2	2.51	0.50
1:B:106:ASN:ND2	4:B:608:NAG:C7	2.75	0.50
1:B:514:LEU:O	1:B:515:ARG:C	2.53	0.50
1:B:10:ASN:HD22	1:B:51:LYS:HA	1.76	0.50
1:A:161:GLU:HA	1:A:161:GLU:OE1	2.12	0.50
1:B:303:PRO:HD2	7:B:722:HOH:O	2.10	0.49
1:A:80:GLU:HG2	7:A:735:HOH:O	2.13	0.49
1:B:491:PRO:CG	1:B:510:ILE:HD12	2.42	0.49
1:A:423:HIS:CE1	1:A:505:THR:CG2	2.95	0.49
1:A:452:ARG:HE	1:A:452:ARG:CA	2.05	0.49
1:B:320:GLY:HA3	1:B:419:TYR:CD1	2.47	0.49
1:A:319:VAL:O	1:A:418:PHE:HA	2.13	0.49
1:B:50:THR:O	1:B:51:LYS:C	2.54	0.49
1:A:337:PHE:HE2	1:A:386:ARG:HG3	1.76	0.49
1:B:42:ARG:O	1:B:43:PHE:HB2	2.13	0.49
1:A:338:SER:HB2	2:D:1:NAG:H62	1.94	0.49
1:B:119:GLN:NE2	1:B:149:GLY:HA2	2.28	0.49
1:B:167:GLY:O	1:B:170:ASP:HB2	2.12	0.49
1:A:69:ILE:HG23	1:A:83:ASN:OD1	2.13	0.49
1:A:119:GLN:NE2	1:A:149:GLY:HA2	2.27	0.49
1:A:152:GLY:C	1:A:166:MET:HE2	2.37	0.49
1:B:301:ASP:OD2	1:B:302:MET:N	2.45	0.49
1:B:320:GLY:HA3	1:B:419:TYR:CE1	2.47	0.49
1:A:388:ALA:O	1:A:392:VAL:HG23	2.12	0.49
1:A:5:ILE:HD12	1:A:5:ILE:N	2.28	0.49
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:TRP:HA	1:A:376:TRP:CE3	2.48	0.48
1:B:140:ILE:HD12	1:B:187:GLY:HA2	1.94	0.48
1:B:214[B]:HIS:O	1:B:313:LYS:HE3	2.13	0.48
1:B:383:GLU:O	1:B:384:ASN:C	2.57	0.48
1:A:167:GLY:O	1:A:170:ASP:HB2	2.13	0.48
1:B:447:GLY:HA2	1:B:464:SER:OG	2.14	0.48
1:B:66:CYS:HB3	1:B:273:LEU:HD11	1.95	0.48
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.49	0.48
1:A:66:CYS:HB3	1:A:273:LEU:HD11	1.96	0.48
1:A:518:GLN:NE2	1:A:518:GLN:N	2.43	0.48
1:A:114:TYR:CE2	1:A:145:ASN:HA	2.48	0.48
1:B:376:TRP:HA	1:B:376:TRP:CE3	2.48	0.48
1:A:95:LEU:HD12	1:A:95:LEU:O	2.14	0.48
1:A:231:TRP:CE2	3:A:601:TCX:H32C	2.49	0.48
1:B:300:THR:O	1:B:301:ASP:HB2	2.13	0.47
1:A:85:ASN:O	1:A:86:THR:HG22	2.13	0.47
1:B:4:ILE:HG22	7:B:762:HOH:O	2.14	0.47
1:B:50:THR:HA	7:B:710:HOH:O	2.15	0.47
1:B:80:GLU:HA	1:B:83:ASN:HD22	1.77	0.47
1:A:140:ILE:HD12	1:A:187:GLY:HA2	1.96	0.47
1:B:209:LEU:HD11	1:B:227:PHE:CE1	2.49	0.47
1:A:140:ILE:HG21	1:A:182:ILE:HD11	1.96	0.47
1:A:227:PHE:C	1:A:227:PHE:CD2	2.93	0.47
1:B:459:ALA:HB1	1:B:505:THR:HB	1.96	0.47
1:A:149:GLY:O	1:A:150:ALA:C	2.57	0.47
1:A:316:GLN:CD	1:A:316:GLN:N	2.72	0.47
1:A:380:GLN:N	7:A:701:HOH:O	2.46	0.47
1:A:491:PRO:HD3	1:A:510:ILE:HD11	1.96	0.47
1:B:119:GLN:HE22	1:B:149:GLY:HA2	1.78	0.47
1:B:303:PRO:HA	1:B:306:LEU:HD12	1.96	0.47
1:A:495:SER:HB3	7:A:746:HOH:O	2.14	0.47
1:A:80:GLU:HA	1:A:83:ASN:HD22	1.79	0.47
1:A:97:VAL:HG22	1:A:142:VAL:HG22	1.95	0.47
1:B:110:LEU:HD11	1:B:475:ALA:CB	2.45	0.47
1:B:312:PHE:CE1	1:B:409:PHE:CD1	3.04	0.46
1:A:80:GLU:HA	1:A:83:ASN:ND2	2.31	0.46
1:A:119:GLN:O	1:A:148:VAL:HG21	2.16	0.46
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.74	0.46
1:A:383:GLU:O	1:A:384:ASN:C	2.59	0.46
1:B:416:ALA:N	7:B:709:HOH:O	2.47	0.46
1:B:417:PHE:HB3	1:B:490:TRP:CE2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:HIS:CE1	1:A:505:THR:HG21	2.50	0.46
1:B:381:ARG:NH2	1:B:383:GLU:OE1	2.49	0.46
1:A:42:ARG:NH2	1:A:269:PRO:HD3	2.31	0.45
1:B:152:GLY:O	1:B:166:MET:HB2	2.16	0.45
1:A:35:GLN:O	1:A:36:PRO:C	2.58	0.45
1:A:197:GLU:O	1:A:200:GLY:N	2.44	0.45
1:B:51:LYS:NZ	7:B:710:HOH:O	2.50	0.45
1:B:268[B]:ASP:OD2	1:B:270:GLN:HB2	2.16	0.45
1:B:328:ALA:HA	1:B:434:MET:CE	2.47	0.45
1:B:13:VAL:HA	1:B:56:TRP:O	2.16	0.45
1:A:137:GLU:OE2	1:A:469:LYS:HE2	2.16	0.45
1:B:91:ASP:OD1	1:B:91:ASP:C	2.59	0.45
1:B:167:GLY:O	1:B:171:GLN:HG3	2.17	0.45
1:B:308:GLU:OE2	1:B:308:GLU:HA	2.16	0.45
1:A:280:VAL:HB	1:A:281:PRO:HD2	1.97	0.45
1:A:424:ARG:HH12	1:A:428:LEU:HD12	1.81	0.45
1:B:334:ALA:HB3	1:B:337:PHE:CD1	2.52	0.45
1:B:518:GLN:NE2	1:B:518:GLN:N	2.43	0.45
1:B:234:THR:O	1:B:293:THR:HG22	2.16	0.45
1:B:479:ASN:OD1	1:B:481:GLN:HG2	2.16	0.45
1:A:247:ALA:O	1:A:248:LYS:C	2.60	0.44
1:B:337:PHE:HE2	1:B:386:ARG:HG3	1.81	0.44
1:B:217:PHE:O	1:B:313:LYS:NZ	2.37	0.44
1:B:341:ASN:ND2	2:F:1:NAG:O7	2.49	0.44
1:A:40:ARG:HG2	7:A:764:HOH:O	2.16	0.44
1:B:68:ASN:OD1	1:B:273:LEU:HB3	2.18	0.44
1:B:381:ARG:HA	1:B:382:PRO:HD3	1.77	0.44
1:A:376:TRP:HA	1:A:376:TRP:HE3	1.83	0.44
1:A:338:SER:HB3	1:A:341:ASN:OD1	2.17	0.44
1:B:61:TYR:CG	1:B:124:SER:HB3	2.53	0.44
1:B:186:GLY:O	7:B:702:HOH:O	2.21	0.44
1:B:424:ARG:NH1	1:B:428:LEU:HD12	2.32	0.44
1:B:491:PRO:HD3	1:B:510:ILE:HD11	2.00	0.44
1:A:165:ASN:OD1	1:A:292:PRO:HA	2.17	0.44
1:A:424:ARG:NH2	1:A:430:TRP:O	2.49	0.44
1:B:101:ALA:HA	1:B:102:PRO:C	2.43	0.44
1:B:282:TYR:HB3	7:B:759:HOH:O	2.17	0.44
1:B:348:LYS:HB2	7:B:760:HOH:O	2.16	0.44
1:B:239:ALA:HB2	1:B:293:THR:HG21	2.00	0.44
1:B:448:LEU:N	1:B:449:PRO:CD	2.81	0.44
1:A:21:PHE:HE2	1:A:451:GLU:HA	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASP:OD1	1:A:91:ASP:C	2.61	0.43
1:A:197:GLU:OE2	1:A:439:GLY:HA2	2.18	0.43
1:B:65:CYS:HB3	7:B:714:HOH:O	2.17	0.43
1:B:70:ASP:OD2	1:B:70:ASP:C	2.61	0.43
1:B:223:GLN:O	1:B:224:SER:C	2.61	0.43
1:B:458:LYS:O	1:B:459:ALA:C	2.62	0.43
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.83	0.43
1:B:111:ILE:HA	1:B:142:VAL:O	2.19	0.43
1:B:213:SER:HA	1:B:216:LEU:CD1	2.43	0.43
1:B:227:PHE:CD2	1:B:227:PHE:C	2.96	0.43
1:B:467:ILE:O	1:B:468:VAL:C	2.61	0.43
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.54	0.43
1:A:34:ALA:C	1:A:49:LEU:HD13	2.44	0.43
1:A:304:ASP:OD1	1:A:304:ASP:N	2.50	0.43
1:A:137:GLU:HG3	1:A:472:ALA:HB2	2.01	0.43
1:B:333:GLY:O	1:B:335:PRO:HD3	2.18	0.43
1:B:440:TYR:HA	7:B:720:HOH:O	2.19	0.43
1:B:515:ARG:NE	7:B:711:HOH:O	2.51	0.43
1:A:4:ILE:HG23	1:A:4:ILE:O	2.19	0.43
1:A:102:PRO:O	1:A:103:LYS:C	2.62	0.43
1:A:341:ASN:ND2	2:D:1:NAG:O7	2.51	0.43
1:B:238:GLU:O	1:B:239:ALA:C	2.59	0.43
1:B:376:TRP:HA	1:B:376:TRP:HE3	1.83	0.43
1:A:119:GLN:O	1:A:148:VAL:CG2	2.67	0.43
1:A:239:ALA:HB2	1:A:293:THR:HG21	2.01	0.43
1:B:12:LYS:HB2	1:B:55:ILE:HG12	2.00	0.43
1:B:21:PHE:HE2	1:B:451:GLU:HA	1.84	0.43
1:A:234:THR:HB	1:A:293:THR:HG22	2.01	0.42
1:A:280:VAL:HG23	1:A:282:TYR:O	2.19	0.42
1:A:328:ALA:HA	1:A:434:MET:CE	2.49	0.42
1:A:341:ASN:C	1:A:343:SER:H	2.27	0.42
1:A:448:LEU:N	1:A:449:PRO:CD	2.82	0.42
1:A:459:ALA:HB1	1:A:505:THR:HB	2.01	0.42
1:A:337:PHE:CE2	1:A:386:ARG:HG3	2.53	0.42
1:B:423:HIS:ND1	1:B:505:THR:HG23	2.34	0.42
1:A:300:THR:O	1:A:301:ASP:HB2	2.19	0.42
1:B:149:GLY:O	1:B:150:ALA:C	2.62	0.42
1:B:457:THR:OG1	1:B:460:GLU:HG3	2.20	0.42
1:B:459:ALA:HA	7:B:743:HOH:O	2.19	0.42
1:A:423:HIS:CE1	1:A:505:THR:HG23	2.54	0.42
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASN:HD22	1:A:51:LYS:HA	1.85	0.42
1:A:118:PHE:O	1:A:148:VAL:HB	2.20	0.42
1:A:275:ASN:O	1:A:276:GLU:C	2.62	0.42
1:A:284:THR:H	1:A:287:SER:HG	1.56	0.42
1:A:427:LYS:HB3	1:A:427:LYS:HE3	1.88	0.42
1:B:188:ASN:OD1	1:B:188:ASN:C	2.61	0.42
1:B:256:ASN:O	1:B:259:GLU:HB2	2.20	0.42
1:B:373:TYR:CD2	1:B:392:VAL:HG22	2.55	0.42
1:A:256:ASN:O	1:A:259:GLU:HB2	2.20	0.42
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.82	0.42
1:B:234:THR:HB	1:B:293:THR:CG2	2.50	0.42
1:B:425:SER:O	1:B:428:LEU:HB2	2.20	0.42
1:B:484:GLN:HE21	1:B:484:GLN:HB2	1.62	0.42
1:A:13:VAL:HA	1:A:56:TRP:O	2.20	0.42
1:A:214[A]:HIS:HE1	7:A:762:HOH:O	2.02	0.42
1:A:376:TRP:HH2	1:A:388:ALA:HB2	1.85	0.42
1:A:408:LYS:HB3	7:A:720:HOH:O	2.20	0.42
1:B:185:PHE:CD1	1:B:185:PHE:N	2.87	0.42
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.75	0.42
1:B:165:ASN:HD22	1:B:295:ASP:CG	2.28	0.42
1:A:76:PHE:CE2	1:A:78:GLY:HA3	2.55	0.41
1:A:85:ASN:C	1:A:86:THR:CG2	2.93	0.41
1:B:45:LYS:HD3	1:B:169:PHE:CE1	2.55	0.41
1:B:284:THR:C	1:B:286:LEU:N	2.78	0.41
1:B:336:GLY:HA3	1:B:345:ILE:HG22	2.02	0.41
1:B:521:PHE:CD2	1:B:521:PHE:C	2.98	0.41
1:B:526:PHE:N	1:B:527:PRO:CD	2.83	0.41
1:A:99:ILE:O	1:A:99:ILE:HG13	2.19	0.41
1:B:347:ARG:HB2	1:B:385:TYR:CZ	2.55	0.41
1:A:198:SER:HA	1:A:224:SER:O	2.21	0.41
1:A:209:LEU:HD11	1:A:227:PHE:CE1	2.55	0.41
1:A:369:ILE:O	1:A:370:LEU:C	2.63	0.41
1:B:18:LEU:HD11	1:B:27:ALA:HB2	2.01	0.41
1:A:111:ILE:HA	1:A:142:VAL:O	2.20	0.41
1:A:347:ARG:HB2	1:A:385:TYR:CZ	2.54	0.41
1:B:337:PHE:HA	1:B:343:SER:OG	2.20	0.41
1:B:480:PRO:HB2	1:B:490:TRP:CE3	2.54	0.41
1:A:234:THR:O	1:A:293:THR:HG22	2.20	0.41
1:A:479:ASN:OD1	1:A:481:GLN:HG2	2.21	0.41
1:A:480:PRO:HB2	1:A:490:TRP:CE3	2.55	0.41
1:B:131:LYS:HE2	1:B:132:PHE:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:THR:O	1:B:347:ARG:C	2.64	0.41
1:A:88:LEU:N	1:A:88:LEU:HD23	2.34	0.41
1:A:156:LEU:HD22	1:A:261:ILE:HD11	2.03	0.41
1:A:227:PHE:CD2	1:A:228:ASN:N	2.89	0.41
1:B:423:HIS:CE1	1:B:505:THR:CG2	3.03	0.41
1:A:226:SER:HB2	1:A:228:ASN:OD1	2.21	0.41
1:A:381:ARG:HA	1:A:382:PRO:HD3	1.78	0.41
1:B:41:LEU:HD23	1:B:41:LEU:HA	1.89	0.41
1:B:93:LEU:HD23	1:B:93:LEU:N	2.34	0.41
1:A:13:VAL:HG12	1:A:56:TRP:HB3	2.02	0.41
1:A:197:GLU:HA	1:A:223:GLN:O	2.21	0.41
1:A:301:ASP:OD2	1:A:302:MET:N	2.54	0.41
1:A:458:LYS:O	1:A:459:ALA:C	2.61	0.41
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.93	0.41
1:A:61:TYR:CG	1:A:124:SER:HB3	2.56	0.40
1:A:268[B]:ASP:OD2	1:A:270:GLN:CB	2.68	0.40
1:B:25:VAL:HG13	1:B:99:ILE:O	2.21	0.40
1:A:417:PHE:HB3	1:A:490:TRP:CE2	2.56	0.40
1:B:5:ILE:N	1:B:5:ILE:HD12	2.35	0.40
1:A:94:TYR:CD1	1:A:94:TYR:N	2.89	0.40
1:B:458:LYS:HD2	1:B:458:LYS:HA	1.76	0.40
1:A:231:TRP:CD2	3:A:601:TCX:H32C	2.56	0.40
1:B:118:PHE:O	1:B:148:VAL:HB	2.22	0.40
1:A:168:LEU:HA	1:A:168:LEU:HD23	1.80	0.40
1:B:76:PHE:O	1:B:80:GLU:HB2	2.21	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	524/529 (99%)	465 (89%)	49 (9%)	10 (2%)	6 27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	523/529 (99%)	466 (89%)	47 (9%)	10 (2%)	6	27
All	All	1047/1058 (99%)	931 (89%)	96 (9%)	20 (2%)	6	27

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	54	ASP
1	B	54	ASP
1	A	39	GLY
1	A	149	GLY
1	A	362	SER
1	A	506	GLU
1	B	39	GLY
1	B	362	SER
1	B	453	ARG
1	B	506	GLU
1	B	224	SER
1	A	9	LYS
1	A	453	ARG
1	B	9	LYS
1	B	436	VAL
1	A	117	GLY
1	A	436	VAL
1	B	117	GLY
1	B	149	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	452/454 (100%)	414 (92%)	38 (8%)	10	35
1	B	451/454 (99%)	417 (92%)	34 (8%)	12	39
All	All	903/908 (99%)	831 (92%)	72 (8%)	11	37

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	10	ASN
1	A	12	LYS
1	A	20	VAL
1	A	40	ARG
1	A	48	SER
1	A	51	LYS
1	A	55	ILE
1	A	59	THR
1	A	60	LYS
1	A	69	ILE
1	A	87	ASP
1	A	99	ILE
1	A	124	SER
1	A	125	LEU
1	A	127	VAL
1	A	176	GLN
1	A	195	PHE
1	A	226	SER
1	A	254	ARG
1	A	260	ILE
1	A	267	LYS
1	A	286	LEU
1	A	299	LEU
1	A	300	THR
1	A	323	LYS
1	A	368	SER
1	A	377	VAL
1	A	427	LYS
1	A	428	LEU
1	A	452	ARG
1	A	489	SER
1	A	494	LYS
1	A	495	SER
1	A	496	THR
1	A	497	GLU
1	A	515	ARG
1	A	518	GLN
1	B	8	THR
1	B	10	ASN
1	B	12	LYS
1	B	20	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	40	ARG
1	B	51	LYS
1	B	55	ILE
1	B	59	THR
1	B	60	LYS
1	B	69	ILE
1	B	124	SER
1	B	125	LEU
1	B	127	VAL
1	B	176	GLN
1	B	195	PHE
1	B	226	SER
1	B	254	ARG
1	B	260	ILE
1	B	267	LYS
1	B	270	GLN
1	B	286	LEU
1	B	299	LEU
1	B	300	THR
1	B	323	LYS
1	B	368	SER
1	B	377	VAL
1	B	428	LEU
1	B	452	ARG
1	B	489	SER
1	B	494	LYS
1	B	496	THR
1	B	497	GLU
1	B	515	ARG
1	B	518	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	17	GLN
1	A	35	GLN
1	A	71	GLN
1	A	119	GLN
1	A	172	GLN
1	A	181	ASN
1	A	223	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	322	ASN
1	A	372	HIS
1	A	484	GLN
1	A	518	GLN
1	B	10	ASN
1	B	17	GLN
1	B	35	GLN
1	B	67	GLN
1	B	71	GLN
1	B	119	GLN
1	B	172	GLN
1	B	181	ASN
1	B	223	GLN
1	B	322	ASN
1	B	372	HIS
1	B	397	ASN
1	B	414	ASN
1	B	484	GLN
1	B	498	GLN
1	B	518	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 ⓘ

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2,1	14,14,15	0.56	0	17,19,21	1.65	2 (11%)
2	NAG	C	2	2	14,14,15	0.44	0	17,19,21	1.51	2 (11%)
2	FUC	C	3	2	10,10,11	0.63	0	14,14,16	0.89	1 (7%)
2	NAG	D	1	2,1	14,14,15	0.67	0	17,19,21	0.68	0
2	NAG	D	2	2	14,14,15	0.43	0	17,19,21	2.26	6 (35%)
2	FUC	D	3	2	10,10,11	0.60	0	14,14,16	1.22	1 (7%)
2	NAG	E	1	2,1	14,14,15	0.64	0	17,19,21	1.89	2 (11%)
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	1.47	1 (5%)
2	FUC	E	3	2	10,10,11	0.72	0	14,14,16	0.92	0
2	NAG	F	1	2,1	14,14,15	0.59	0	17,19,21	0.89	1 (5%)
2	NAG	F	2	2	14,14,15	0.46	0	17,19,21	2.37	6 (35%)
2	FUC	F	3	2	10,10,11	0.65	0	14,14,16	1.30	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	FUC	F	3	2	-	-	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C1-O5-C5	6.54	120.95	112.19
2	D	2	NAG	C1-O5-C5	6.29	120.61	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	5.09	119.00	112.19
2	E	2	NAG	C1-O5-C5	4.97	118.85	112.19
2	E	1	NAG	C1-O5-C5	4.73	118.53	112.19
2	C	1	NAG	C4-C3-C2	4.66	117.84	111.02
2	E	1	NAG	C4-C3-C2	4.55	117.69	111.02
2	F	2	NAG	C6-C5-C4	-3.87	103.51	113.02
2	F	3	FUC	C1-C2-C3	-3.36	104.75	109.64
2	C	1	NAG	C1-O5-C5	3.27	116.57	112.19
2	D	2	NAG	C4-C3-C2	-3.18	106.36	111.02
2	F	2	NAG	C4-C3-C2	-3.11	106.46	111.02
2	D	2	NAG	C6-C5-C4	-2.91	105.86	113.02
2	F	2	NAG	O5-C5-C4	2.83	117.70	110.83
2	D	2	NAG	O5-C5-C4	2.66	117.29	110.83
2	D	3	FUC	C1-C2-C3	-2.58	105.88	109.64
2	F	2	NAG	C1-C2-N2	2.55	114.44	110.43
2	F	1	NAG	O5-C1-C2	-2.51	107.41	111.29
2	F	2	NAG	C3-C4-C5	2.45	114.68	110.23
2	C	3	FUC	C3-C4-C5	2.32	113.34	109.81
2	D	2	NAG	C2-N2-C7	-2.11	120.08	122.90
2	C	2	NAG	C2-N2-C7	-2.03	120.18	122.90
2	D	2	NAG	O5-C1-C2	-2.02	108.16	111.29

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

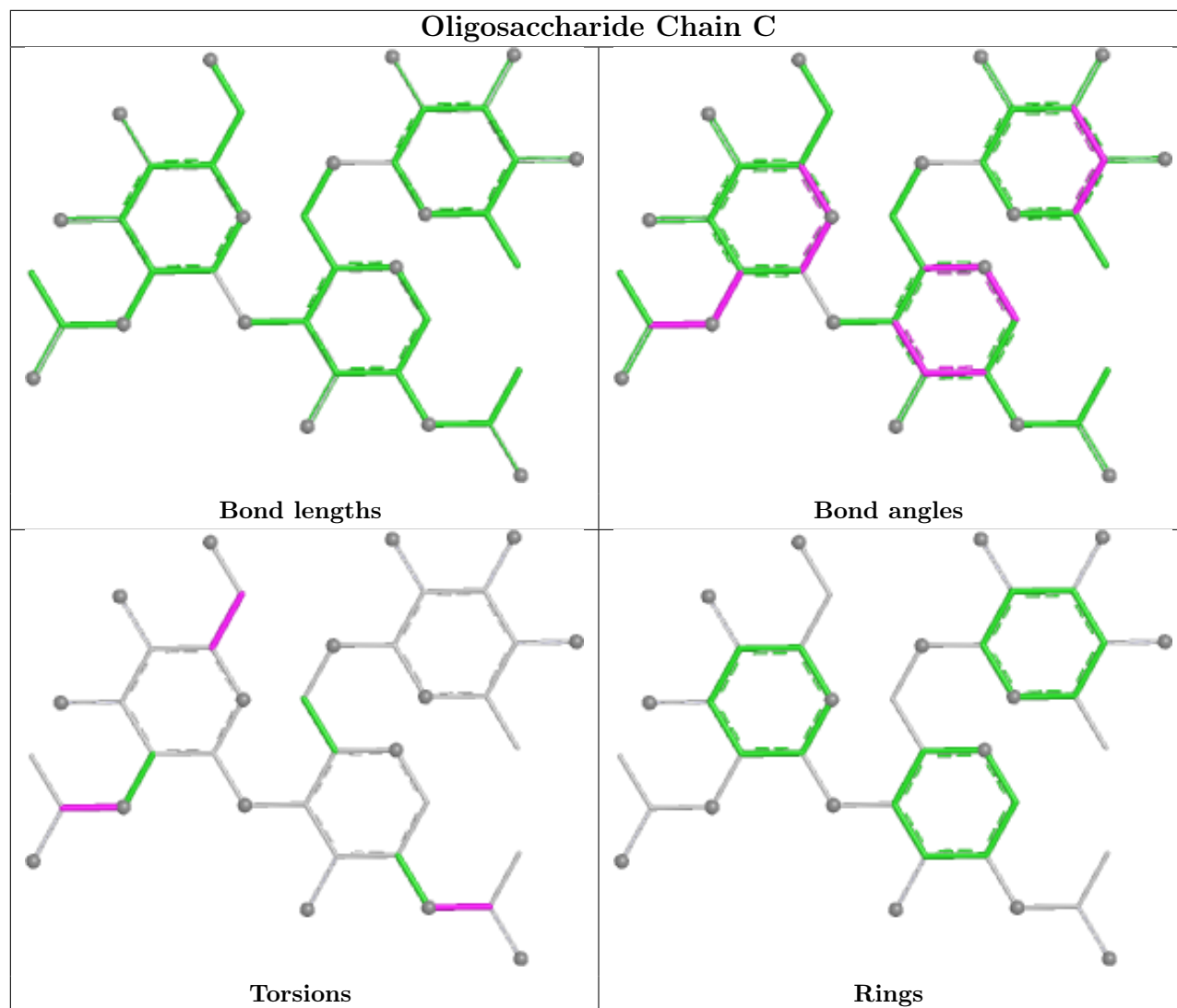
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

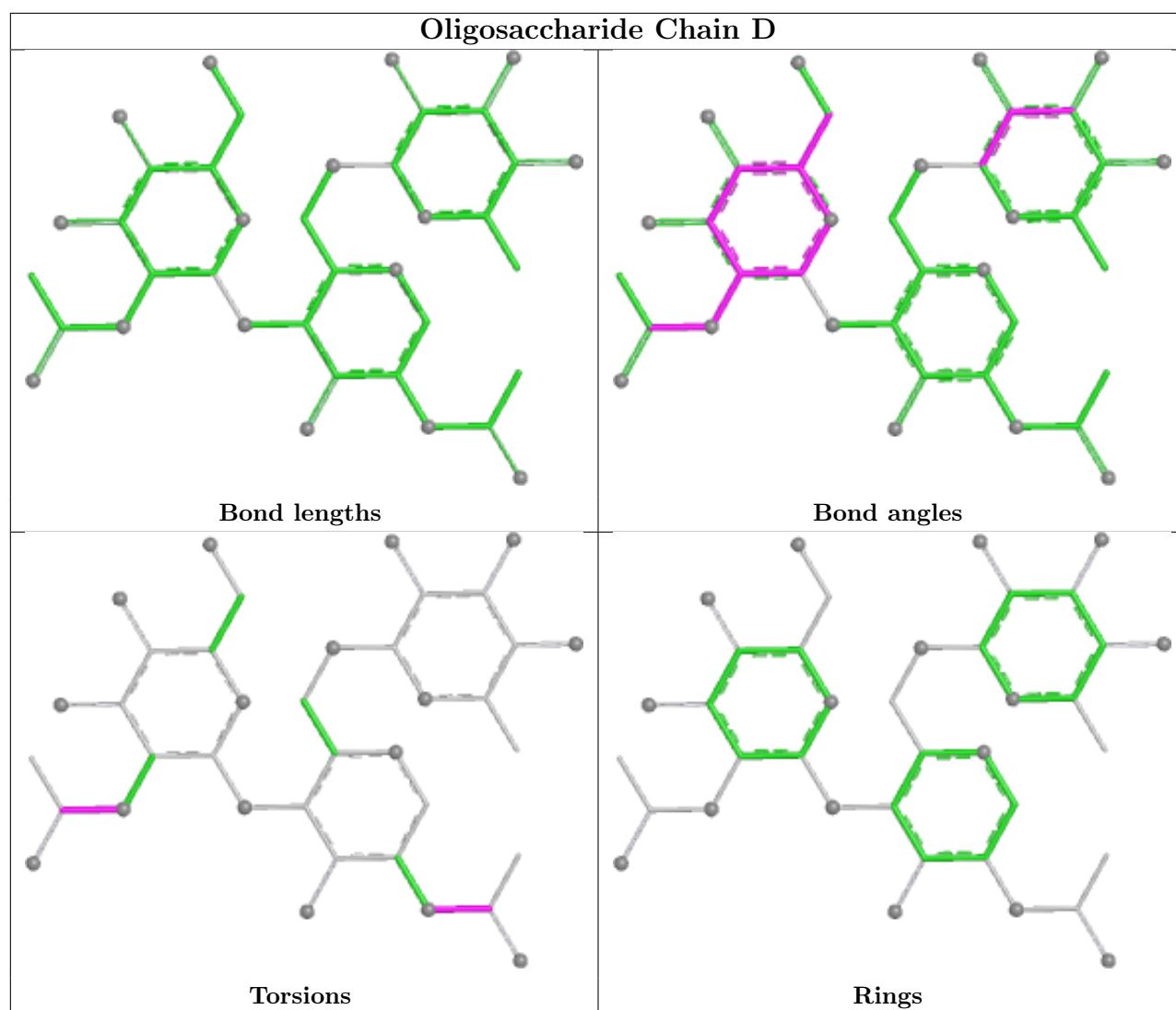
There are no ring outliers.

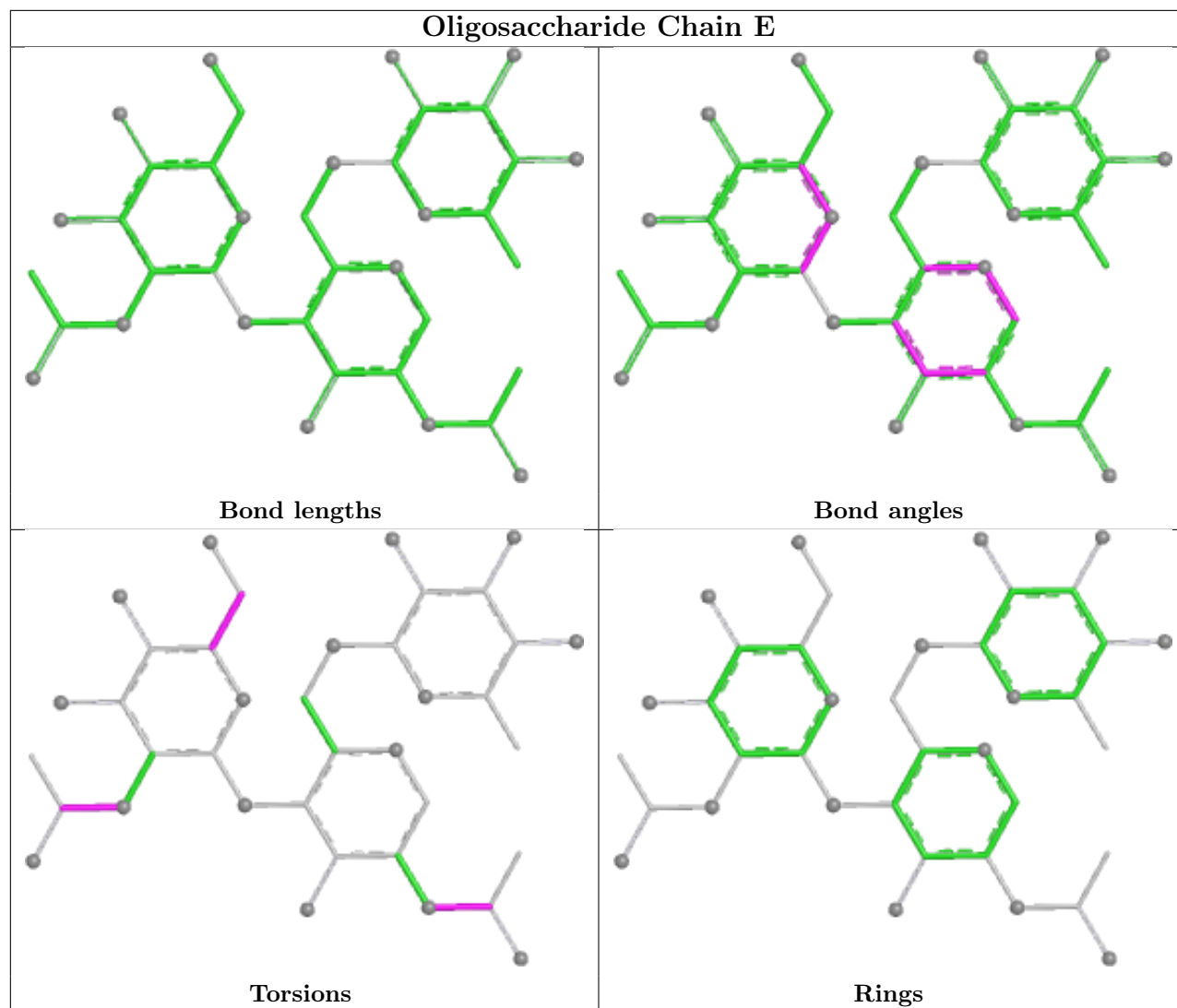
3 monomers are involved in 4 short contacts:

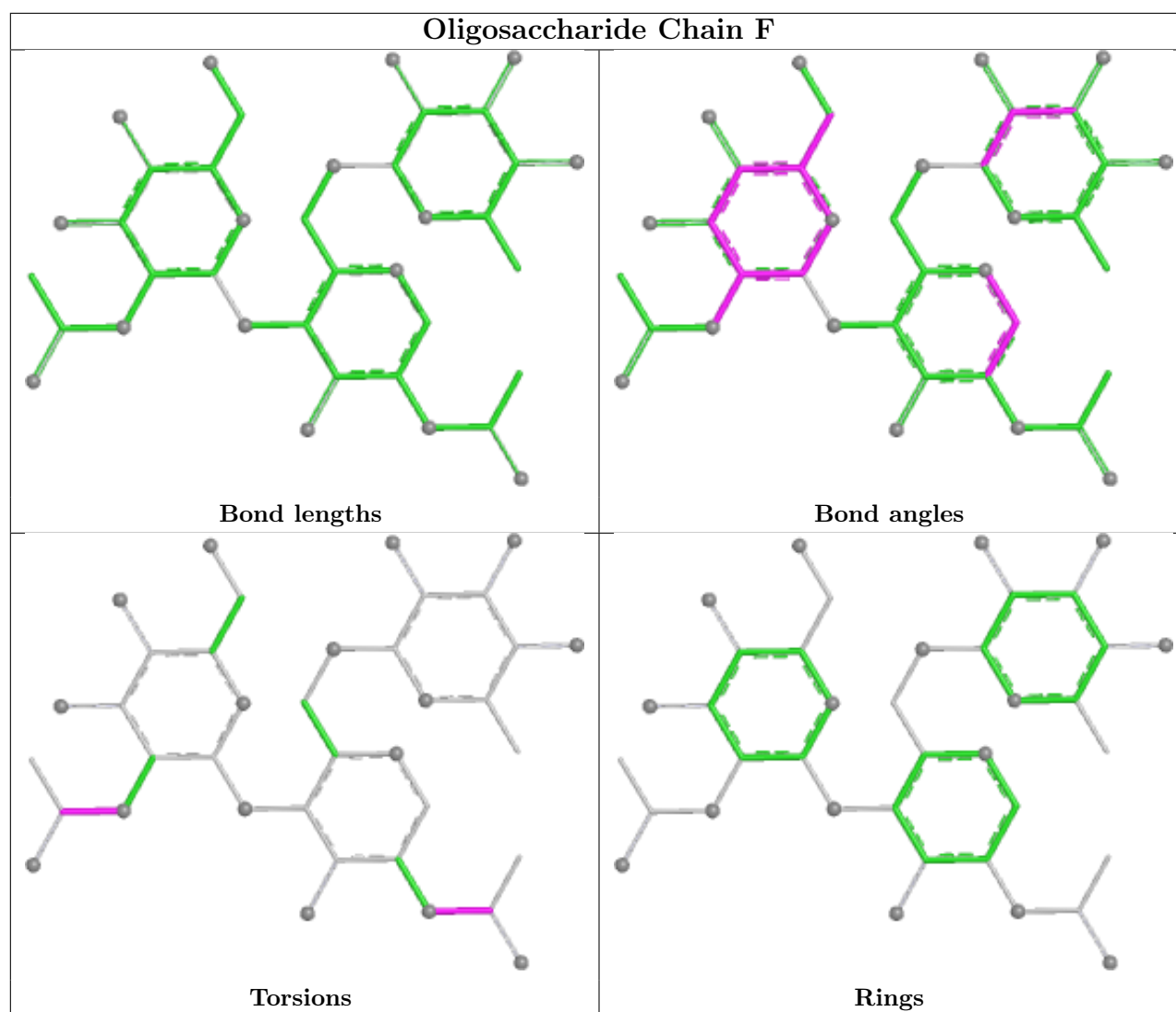
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0
2	D	1	NAG	2	0
2	D	2	NAG	1	0

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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	609	1	14,14,15	0.78	1 (7%)	17,19,21	2.02	5 (29%)
4	NAG	A	608	1	14,14,15	0.61	0	17,19,21	1.87	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	608	1	14,14,15	0.72	0	17,19,21	1.79	4 (23%)
4	NAG	B	609	1	14,14,15	0.50	0	17,19,21	1.86	4 (23%)
5	SO4	A	612	-	4,4,4	0.25	0	6,6,6	0.21	0
5	SO4	A	611	-	4,4,4	0.28	0	6,6,6	0.42	0
4	NAG	A	610	1	14,14,15	0.55	0	17,19,21	1.17	1 (5%)
4	NAG	B	610	1	14,14,15	0.51	0	17,19,21	1.32	2 (11%)
5	SO4	B	611	-	4,4,4	0.26	0	6,6,6	0.27	0
3	TCX	A	601	1	2,5,6	0.62	0	1,5,8	1.59	0
3	TCX	B	601	1	2,5,6	0.57	0	1,5,8	1.13	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
4	NAG	A	609	1	-	3/6/23/26	0/1/1/1
4	NAG	A	608	1	-	4/6/23/26	0/1/1/1
4	NAG	B	608	1	-	4/6/23/26	0/1/1/1
4	NAG	B	609	1	-	3/6/23/26	0/1/1/1
4	NAG	A	610	1	-	0/6/23/26	0/1/1/1
4	NAG	B	610	1	-	1/6/23/26	0/1/1/1
3	TCX	A	601	1	-	0/0/3/4	-
3	TCX	B	601	1	-	0/0/3/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	609	NAG	C1-C2	2.30	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	608	NAG	C1-O5-C5	4.64	118.40	112.19
4	A	609	NAG	C2-N2-C7	-4.54	116.81	122.90
4	A	608	NAG	C2-N2-C7	-4.23	117.23	122.90
4	B	609	NAG	C1-O5-C5	4.14	117.73	112.19
4	B	608	NAG	C4-C3-C2	-4.05	105.08	111.02
4	A	609	NAG	C1-O5-C5	4.04	117.60	112.19
4	B	608	NAG	C2-N2-C7	-3.98	117.56	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	610	NAG	O5-C1-C2	-3.97	105.15	111.29
4	B	609	NAG	C2-N2-C7	-3.90	117.67	122.90
4	B	610	NAG	O5-C1-C2	-3.85	105.34	111.29
4	A	609	NAG	O5-C1-C2	-3.73	105.53	111.29
4	B	609	NAG	O5-C1-C2	-3.41	106.02	111.29
4	A	608	NAG	C4-C3-C2	-3.04	106.56	111.02
4	B	608	NAG	C1-O5-C5	2.79	115.93	112.19
4	A	609	NAG	C3-C4-C5	2.61	114.97	110.23
4	B	609	NAG	C3-C4-C5	2.61	114.96	110.23
4	B	608	NAG	C1-C2-N2	2.58	114.50	110.43
4	B	610	NAG	C2-N2-C7	-2.49	119.56	122.90
4	A	608	NAG	C1-C2-N2	2.30	114.05	110.43
4	A	609	NAG	O5-C5-C4	2.13	116.00	110.83

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	608	NAG	C8-C7-N2-C2
4	A	608	NAG	O7-C7-N2-C2
4	A	609	NAG	C8-C7-N2-C2
4	A	609	NAG	O7-C7-N2-C2
4	B	608	NAG	C8-C7-N2-C2
4	B	608	NAG	O7-C7-N2-C2
4	B	609	NAG	C8-C7-N2-C2
4	B	609	NAG	O7-C7-N2-C2
4	B	608	NAG	C4-C5-C6-O6
4	A	608	NAG	C4-C5-C6-O6
4	A	608	NAG	O5-C5-C6-O6
4	B	608	NAG	O5-C5-C6-O6
4	A	609	NAG	O5-C5-C6-O6
4	B	609	NAG	O5-C5-C6-O6
4	B	610	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	608	NAG	1	0
3	A	601	TCX	3	0
3	B	601	TCX	2	0

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	526/529 (99%)	-0.14	1 (0%) 91 83	32, 70, 95, 107	6 (1%)
1	B	524/529 (99%)	-0.19	2 (0%) 88 76	32, 70, 95, 106	6 (1%)
All	All	1050/1058 (99%)	-0.17	3 (0%) 90 80	32, 70, 95, 107	12 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214[A]	HIS	2.7
1	A	214[A]	HIS	2.5
1	B	377	VAL	2.3

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.

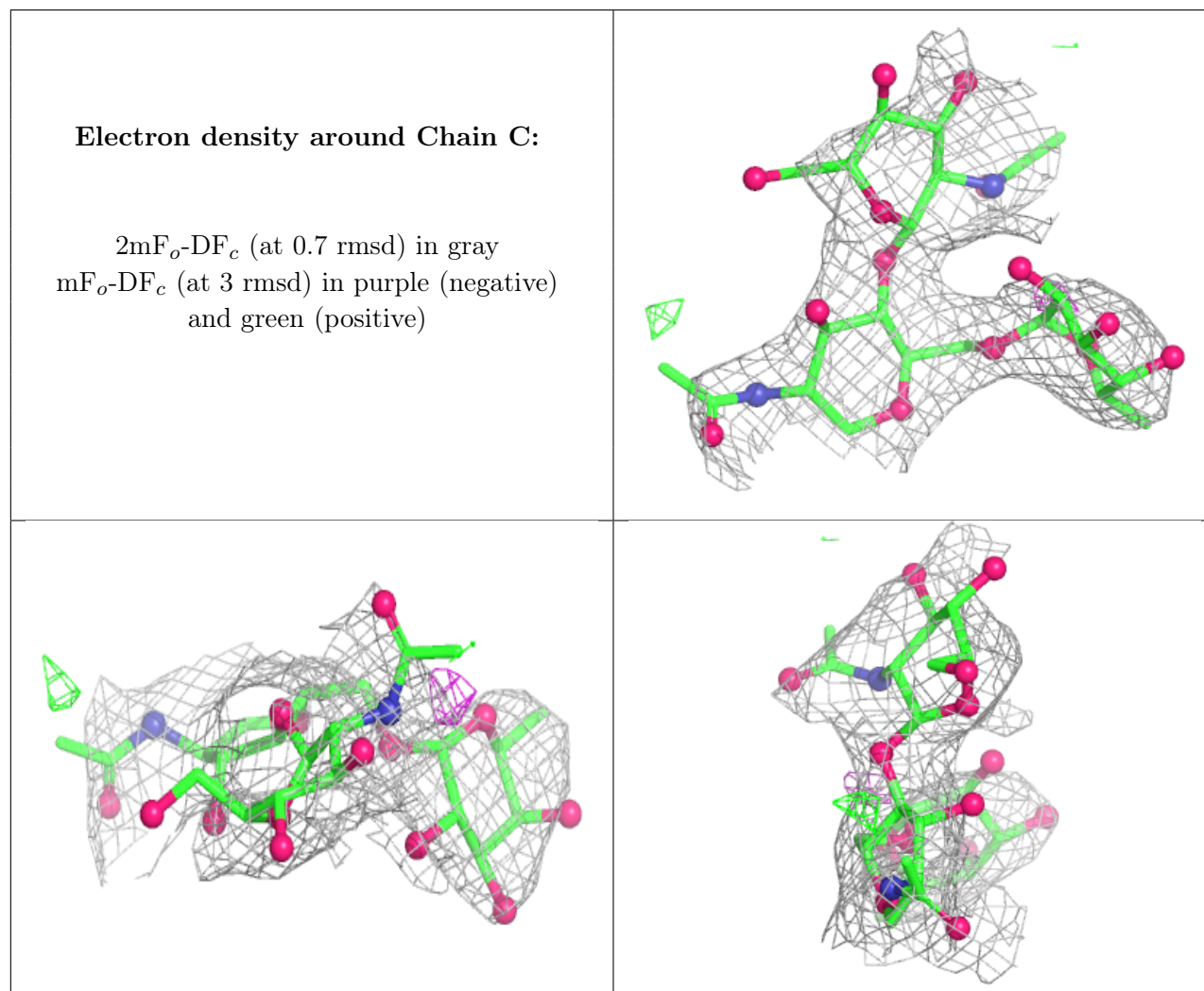
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.53	0.14	124,126,128,128	0
2	NAG	F	2	14/15	0.55	0.15	106,108,110,111	0
2	NAG	E	2	14/15	0.63	0.13	123,125,126,127	0
2	NAG	D	2	14/15	0.68	0.13	106,109,111,112	0
2	NAG	C	1	14/15	0.70	0.12	109,115,117,121	0
2	NAG	E	1	14/15	0.73	0.12	108,114,116,119	0

Continued on next page...

Continued from previous page...

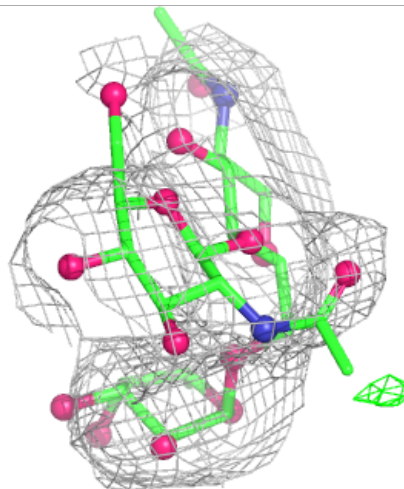
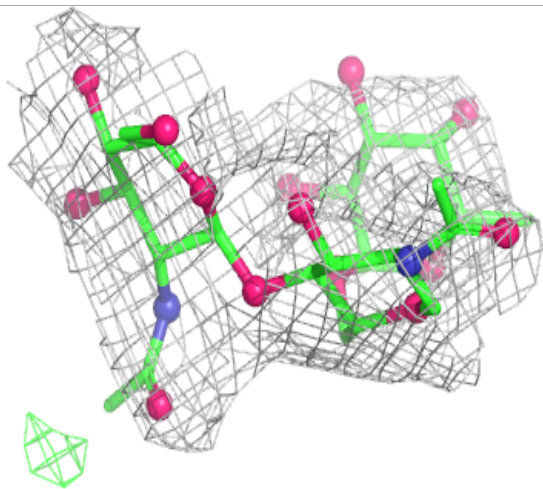
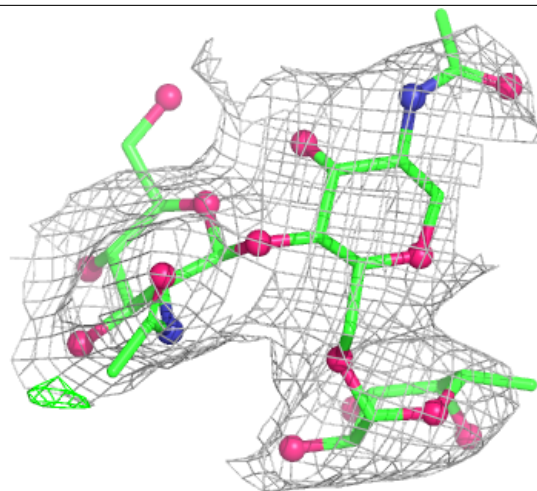
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FUC	C	3	10/11	0.86	0.13	115,116,116,117	0
2	FUC	F	3	10/11	0.89	0.09	105,107,107,108	0
2	FUC	D	3	10/11	0.90	0.11	106,107,108,108	0
2	NAG	F	1	14/15	0.90	0.10	91,96,101,103	0
2	FUC	E	3	10/11	0.91	0.13	114,115,115,116	0
2	NAG	D	1	14/15	0.92	0.10	92,96,102,104	0

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



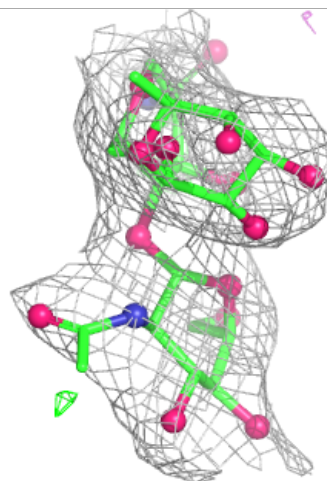
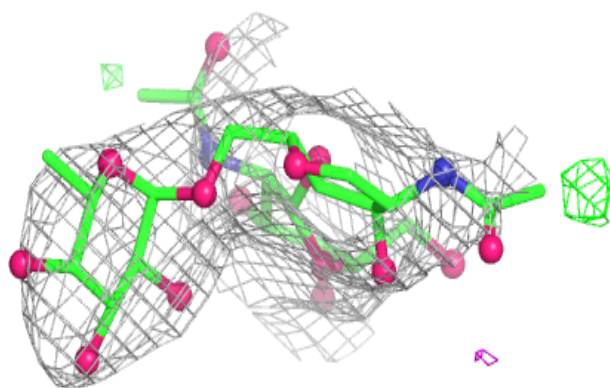
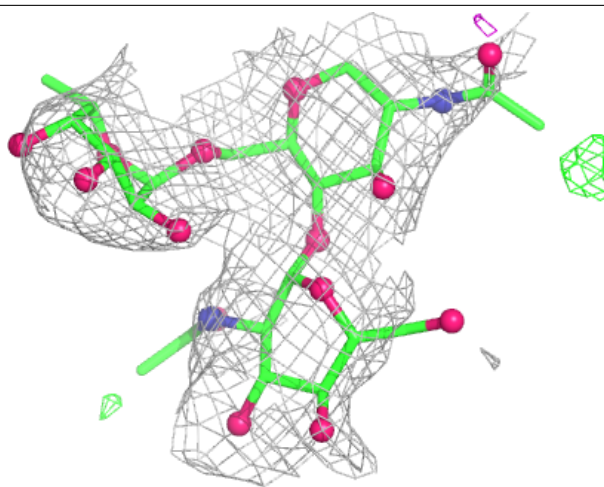
Electron density around Chain D:

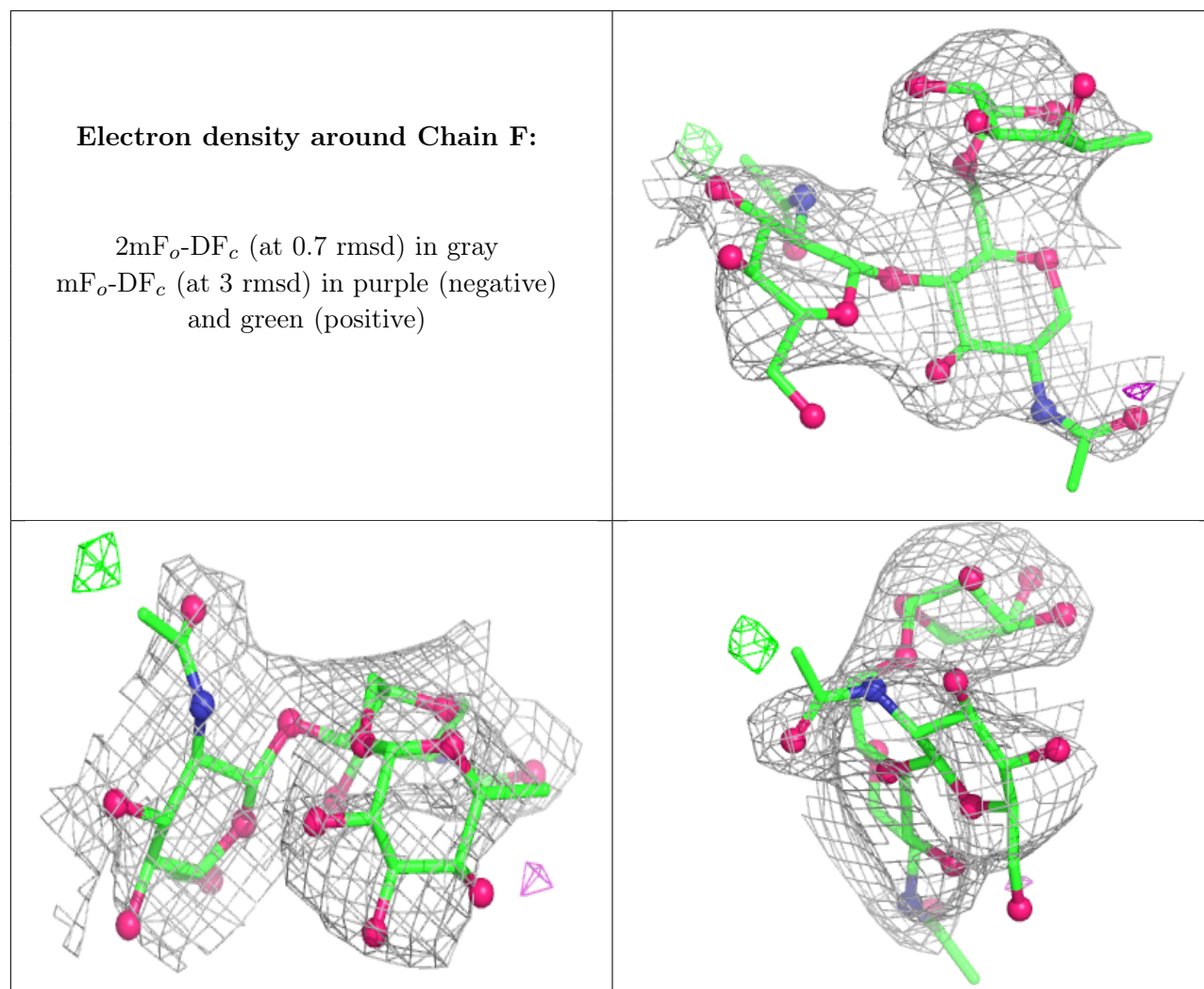
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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(Å ²)	Q<0.9
4	NAG	B	608	14/15	0.64	0.15	91,94,95,96	0
4	NAG	A	609	14/15	0.70	0.15	104,105,106,106	0
4	NAG	B	609	14/15	0.76	0.11	103,105,106,106	0
5	SO4	A	612	5/5	0.80	0.16	137,138,138,138	0
5	SO4	A	611	5/5	0.84	0.13	105,106,106,107	0
4	NAG	A	608	14/15	0.84	0.11	91,94,95,96	0
5	SO4	B	611	5/5	0.85	0.16	112,113,113,113	0
4	NAG	B	610	14/15	0.89	0.10	97,102,104,105	0
4	NAG	A	610	14/15	0.89	0.12	98,102,105,106	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	A	613	1/1	0.96	0.06	70,70,70,70	0
3	TCX	B	601	6/7	0.97	0.09	53,54,54,55	0
3	TCX	A	601	6/7	0.99	0.07	53,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.