



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2024 – 11:42 am BST

PDB ID : 5MU1
Title : UDP-Glucose Glycoprotein Glucosyltransferase from *Chaetomium thermophilum* soaked with K2PtI6
Authors : Roversi, P.; Caputo, A.T.; Hill, J.; Alonzi, D.S.; Zitzmann, N.
Deposited on : 2017-01-11
Resolution : 3.48 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

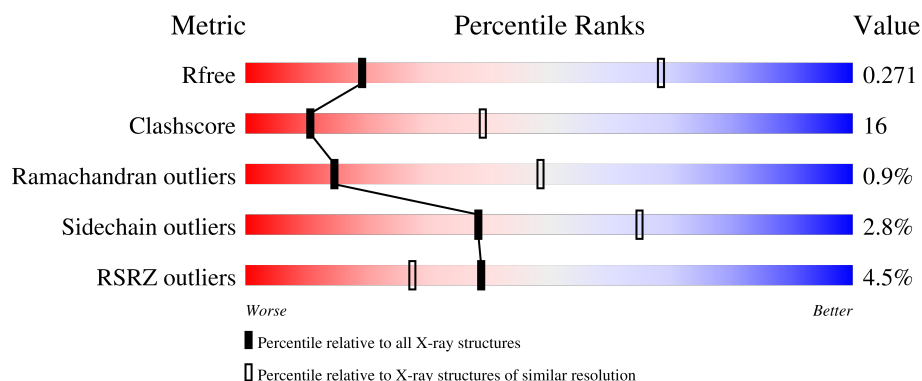
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1099 (3.54-3.42)
Clashscore	180529	1048 (3.52-3.44)
Ramachandran outliers	177936	1033 (3.52-3.44)
Sidechain outliers	177891	1034 (3.52-3.44)
RSRZ outliers	164620	1098 (3.54-3.42)

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	1494	<div> <div>4%</div> <div>66%</div> <div>25%</div> <div>8%</div> </div>
2	B	7	<div> <div>29%</div> <div>43%</div> <div>29%</div> </div>
3	C	5	<div> <div>40%</div> <div>60%</div> </div>
4	D	5	<div> <div>20%</div> <div>60%</div> <div>20%</div> </div>
5	E	7	<div> <div>71%</div> <div>29%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	IOD	A	1606	-	-	X	-
6	IOD	A	1607	-	-	X	-
6	IOD	A	1614	-	-	X	-
6	IOD	A	1618	-	-	X	-
6	IOD	A	1619	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11720 atoms, of which 345 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.

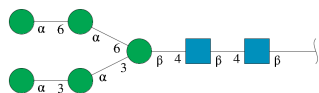
- Molecule 1 is a protein called UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1377	Total	C	H	N	O	S	0	0	0
			11411	7080	345	1884	2070	32			

There are 12 discrepancies between the modelled and reference sequences:

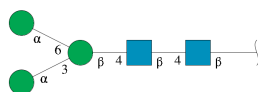
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	UNP G0SB58
A	1510	HIS	-	expression tag	UNP G0SB58
A	1511	HIS	-	expression tag	UNP G0SB58
A	1512	HIS	-	expression tag	UNP G0SB58
A	1513	HIS	-	expression tag	UNP G0SB58
A	1514	HIS	-	expression tag	UNP G0SB58

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



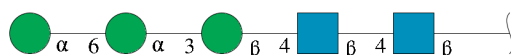
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



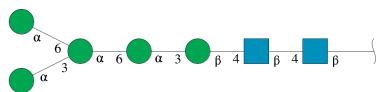
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	I	0	0
			14	14		

- Molecule 7 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total 6	Pt 6	0	0

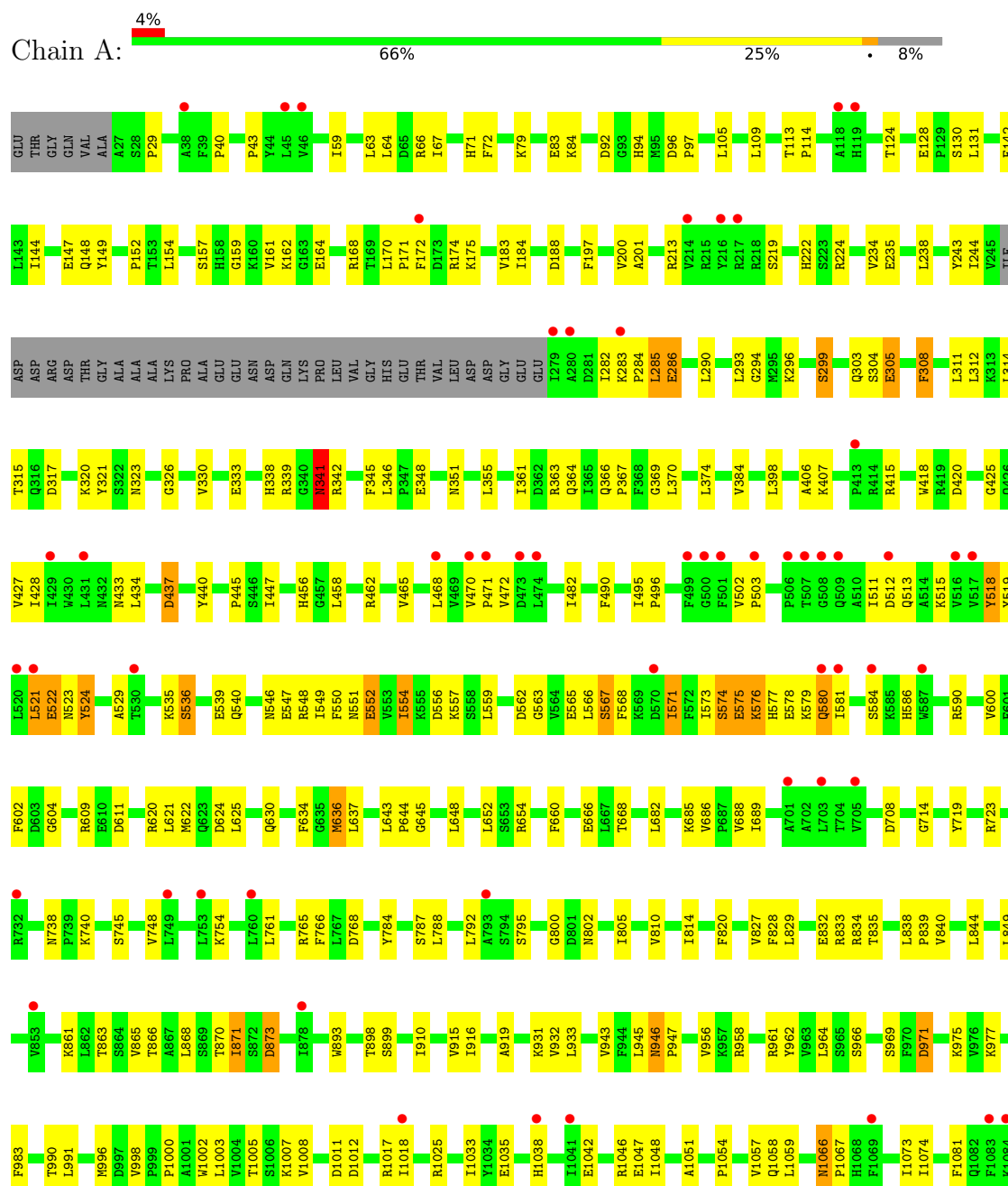
- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

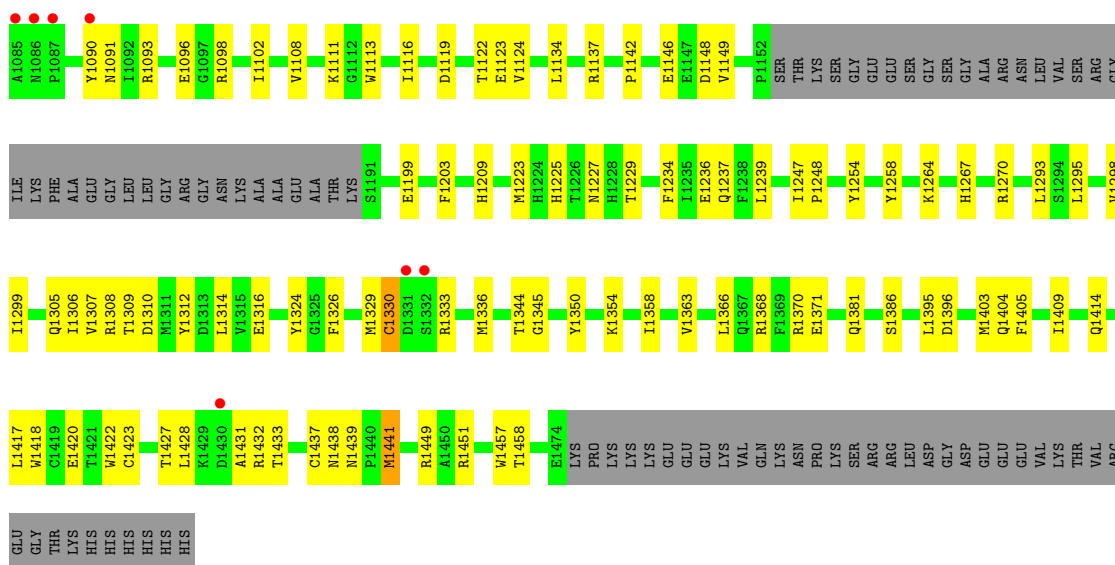
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	Ca 1	0	0

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.

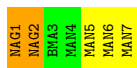
- Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein





- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 29% 43% 29%



- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 40% 60%



- Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 20% 60% 20%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 71% 29%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	116.95Å 116.95Å 301.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	101.28 – 3.48 101.28 – 3.48	Depositor EDS
% Data completeness (in resolution range)	86.8 (101.28-3.48) 86.8 (101.28-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.49Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.237 , 0.252 0.254 , 0.271	Depositor DCC
R_{free} test set	1455 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	123.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 140.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.074 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11720	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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: CA, MAN, BMA, PT, IOD, NAG

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	0.47	0/11331	0.77	7/15369 (0.0%)

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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	GLU	C-N-CA	9.11	144.49	121.70
1	A	523	ASN	N-CA-CB	6.74	122.72	110.60
1	A	341	ASN	CB-CA-C	5.90	122.20	110.40
1	A	523	ASN	C-N-CA	5.87	136.38	121.70
1	A	243	TYR	C-N-CA	5.48	135.40	121.70
1	A	285	LEU	N-CA-C	5.21	125.07	111.00
1	A	1441	MET	CB-CG-SD	-5.09	97.14	112.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	518	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	11066	345	10936	365	0
2	B	83	0	70	4	0
3	C	61	0	52	0	0
4	D	61	0	52	1	0
5	E	83	0	70	2	0
6	A	14	0	0	12	0
7	A	6	0	0	1	0
8	A	1	0	0	0	0
All	All	11375	345	11180	372	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 16.

All (372) 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:1329:MET:SD	1:A:1358:ILE:HD11	1.68	1.33
1:A:244:ILE:CA	1:A:285:LEU:HD21	1.73	1.17
1:A:149:TYR:CE1	1:A:157:SER:HB3	1.83	1.13
1:A:1225:HIS:ND1	1:A:1308:ARG:HA	1.62	1.12
1:A:1295:LEU:HD21	1:A:1298:VAL:CG2	1.79	1.12
1:A:244:ILE:HA	1:A:285:LEU:CD2	1.83	1.07
1:A:67:ILE:HG22	1:A:72:PHE:CD2	1.91	1.05
1:A:67:ILE:HG22	1:A:72:PHE:HD2	1.15	1.04
1:A:1149:VAL:HG13	1:A:1371:GLU:O	1.57	1.02
1:A:72:PHE:CE1	1:A:84:LYS:HG3	1.99	0.97
1:A:1225:HIS:CE1	1:A:1308:ARG:HA	1.98	0.97
1:A:1329:MET:SD	1:A:1358:ILE:CD1	2.53	0.95
1:A:149:TYR:HE1	1:A:157:SER:HB3	1.21	0.93
1:A:458:LEU:HD23	1:A:496:PRO:HG2	1.51	0.92
1:A:1324:TYR:CD1	1:A:1326:PHE:HE1	1.86	0.92
1:A:546:ASN:HB3	1:A:549:ILE:HG22	1.50	0.91
1:A:1048:ILE:HD11	1:A:1137:ARG:HD2	1.53	0.89
1:A:1058:GLN:HG2	1:A:1073:ILE:HG22	1.54	0.89
1:A:338:HIS:HD2	1:A:898:THR:HG23	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PHE:HE1	1:A:84:LYS:HG3	1.35	0.88
1:A:1438:ASN:HA	1:A:1449:ARG:HH22	1.39	0.87
1:A:1441:MET:SD	6:A:1618:IOD:I	3.04	0.86
1:A:1441:MET:SD	6:A:1619:IOD:I	3.04	0.85
1:A:244:ILE:HA	1:A:285:LEU:HD21	0.89	0.85
1:A:67:ILE:CG2	1:A:72:PHE:HD2	1.89	0.84
1:A:456:HIS:HB2	6:A:1614:IOD:I	2.46	0.84
1:A:482:ILE:HD12	1:A:609:ARG:HH22	1.43	0.84
1:A:1441:MET:SD	7:A:1620:PT:PT	1.58	0.84
1:A:1422:TRP:CZ3	1:A:1437:CYS:SG	2.71	0.83
1:A:445:PRO:HG3	1:A:462:ARG:NH2	1.95	0.82
1:A:551:ASN:HA	1:A:554:ILE:HD12	1.60	0.81
1:A:686:VAL:O	1:A:754:LYS:HE2	1.79	0.81
2:B:1:NAG:H3	2:B:2:NAG:HN2	1.45	0.81
1:A:1007:LYS:HG3	1:A:1035:GLU:HB2	1.60	0.81
1:A:1324:TYR:CD1	1:A:1326:PHE:CE1	2.70	0.80
5:E:3:BMA:H3	5:E:4:MAN:H5	1.63	0.79
1:A:1059:LEU:HD11	1:A:1074:ILE:HD11	1.62	0.79
1:A:433:ASN:O	1:A:437:ASP:HB2	1.85	0.77
1:A:1350:TYR:CE1	1:A:1405:PHE:HE2	2.02	0.77
1:A:1314:LEU:HG	1:A:1363:VAL:CG2	2.15	0.76
1:A:384:VAL:HG23	1:A:865:VAL:HG11	1.67	0.76
1:A:1225:HIS:ND1	1:A:1308:ARG:CA	2.48	0.75
1:A:285:LEU:O	1:A:286:GLU:HB2	1.87	0.74
1:A:546:ASN:HB3	1:A:549:ILE:CG2	2.17	0.73
1:A:342:ARG:HD2	1:A:348:GLU:HG3	1.68	0.73
1:A:142:PHE:HE1	1:A:197:PHE:HD2	1.35	0.73
1:A:1295:LEU:HD21	1:A:1298:VAL:HG23	1.68	0.73
1:A:67:ILE:CG2	1:A:72:PHE:CD2	2.67	0.73
1:A:519:TYR:CG	1:A:576:LYS:HG2	2.24	0.72
1:A:1267:HIS:CD2	6:A:1606:IOD:I	3.13	0.72
1:A:338:HIS:CD2	1:A:898:THR:HG23	2.23	0.71
1:A:66:ARG:O	1:A:71:HIS:HB3	1.91	0.70
1:A:130:SER:O	1:A:161:VAL:HG13	1.92	0.70
1:A:1295:LEU:HD21	1:A:1298:VAL:HG22	1.73	0.70
1:A:1422:TRP:HZ3	1:A:1437:CYS:SG	2.13	0.69
1:A:420:ASP:HB3	1:A:425:GLY:HA2	1.74	0.69
1:A:1428:LEU:HD12	1:A:1431:ALA:HB3	1.74	0.69
1:A:515:LYS:CG	1:A:581:ILE:HD11	2.21	0.69
1:A:1048:ILE:HD11	1:A:1137:ARG:HB3	1.73	0.69
1:A:282:ILE:HG13	1:A:990:THR:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PRO:HG3	1:A:462:ARG:HH21	1.55	0.69
1:A:1354:LYS:NZ	1:A:1405:PHE:CE1	2.57	0.69
1:A:188:ASP:OD1	1:A:219:SER:HB3	1.93	0.69
1:A:550:PHE:CD2	1:A:568:PHE:CZ	2.81	0.69
1:A:1324:TYR:CE1	1:A:1326:PHE:HE1	2.12	0.68
1:A:29:PRO:HB2	1:A:1018:ILE:HD13	1.74	0.68
1:A:1307:VAL:HG13	1:A:1433:THR:HG22	1.76	0.68
1:A:834:ARG:O	1:A:839:PRO:HD3	1.95	0.67
1:A:346:LEU:HD12	1:A:893:TRP:HH2	1.58	0.67
1:A:311:LEU:O	1:A:315:THR:HG22	1.93	0.67
1:A:326:GLY:HA2	1:A:330:VAL:HG11	1.75	0.67
1:A:142:PHE:CE1	1:A:197:PHE:HD2	2.12	0.67
1:A:296:LYS:HE2	1:A:330:VAL:HG13	1.77	0.67
1:A:152:PRO:HB3	1:A:200:VAL:HG21	1.76	0.66
1:A:304:SER:O	1:A:305:GLU:HB3	1.94	0.66
1:A:1098:ARG:HH21	1:A:1102:ILE:HD11	1.59	0.66
1:A:1042:GLU:CD	6:A:1606:IOD:I	3.04	0.66
1:A:1418:TRP:HE1	1:A:1427:THR:HB	1.61	0.65
1:A:341:ASN:HB2	1:A:893:TRP:CD1	2.31	0.65
1:A:550:PHE:HD2	1:A:568:PHE:CZ	2.14	0.65
1:A:346:LEU:HD12	1:A:893:TRP:CH2	2.32	0.65
1:A:546:ASN:CB	1:A:549:ILE:HG22	2.23	0.65
1:A:170:LEU:HD11	1:A:172:PHE:CE1	2.32	0.65
1:A:519:TYR:OH	1:A:577:HIS:HA	1.96	0.65
1:A:1366:LEU:O	1:A:1370:ARG:HG3	1.97	0.65
1:A:384:VAL:CG2	1:A:865:VAL:HG11	2.27	0.64
1:A:1324:TYR:CE1	1:A:1326:PHE:CE1	2.86	0.64
1:A:482:ILE:HD12	1:A:609:ARG:NH2	2.10	0.64
1:A:515:LYS:HG2	1:A:581:ILE:HD11	1.80	0.64
1:A:518:TYR:CD1	1:A:580:GLN:HG2	2.33	0.64
1:A:1048:ILE:CD1	1:A:1137:ARG:HB3	2.28	0.64
5:E:3:BMA:H3	5:E:4:MAN:C5	2.27	0.64
1:A:600:VAL:CG2	1:A:609:ARG:HG2	2.29	0.63
1:A:1108:VAL:HG12	1:A:1134:LEU:HD22	1.79	0.63
1:A:96:ASP:HB2	1:A:97:PRO:HD2	1.79	0.63
1:A:1350:TYR:CE1	1:A:1405:PHE:CE2	2.86	0.62
1:A:1042:GLU:OE2	6:A:1606:IOD:I	2.87	0.62
2:B:1:NAG:H3	2:B:2:NAG:N2	2.13	0.62
1:A:124:THR:HA	1:A:128:GLU:OE1	2.00	0.62
1:A:829:LEU:O	1:A:833:ARG:HB2	2.00	0.62
1:A:458:LEU:HD12	1:A:625:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:MET:CG	1:A:1358:ILE:HD11	2.29	0.62
1:A:304:SER:O	1:A:305:GLU:CB	2.46	0.62
1:A:346:LEU:CD1	1:A:893:TRP:HH2	2.13	0.61
1:A:40:PRO:HB3	1:A:224:ARG:HD2	1.83	0.61
1:A:1058:GLN:HG2	1:A:1073:ILE:CG2	2.30	0.61
1:A:1354:LYS:NZ	1:A:1405:PHE:CZ	2.63	0.61
1:A:398:LEU:HD23	1:A:866:THR:HG22	1.82	0.61
1:A:418:TRP:HE1	1:A:648:LEU:HD11	1.66	0.61
1:A:1058:GLN:CG	1:A:1073:ILE:HG22	2.30	0.60
1:A:1247:ILE:HG13	1:A:1248:PRO:HD3	1.82	0.60
1:A:600:VAL:HG23	1:A:609:ARG:CG	2.31	0.60
1:A:420:ASP:OD1	1:A:427:VAL:CG1	2.49	0.60
1:A:470:VAL:HG23	1:A:600:VAL:HG22	1.82	0.60
1:A:345:PHE:HB3	1:A:893:TRP:CZ2	2.37	0.59
1:A:1199:GLU:HB2	1:A:1229:THR:O	2.01	0.59
1:A:634:PHE:CG	6:A:1607:IOD:I	3.26	0.59
1:A:1054:PRO:HB2	1:A:1057:VAL:HG21	1.84	0.59
1:A:1333:ARG:HG2	1:A:1423:CYS:C	2.22	0.59
1:A:515:LYS:HG3	1:A:581:ILE:HD11	1.84	0.59
1:A:482:ILE:CD1	1:A:609:ARG:NH2	2.66	0.59
1:A:899:SER:HA	1:A:943:VAL:O	2.03	0.58
1:A:458:LEU:CD2	1:A:496:PRO:HG2	2.31	0.58
1:A:1422:TRP:CE3	1:A:1437:CYS:SG	2.96	0.58
1:A:519:TYR:CD1	1:A:576:LYS:HG2	2.39	0.57
2:B:2:NAG:O7	2:B:2:NAG:H3	2.04	0.57
1:A:932:VAL:HG11	1:A:964:LEU:HG	1.86	0.57
1:A:630:GLN:O	1:A:634:PHE:HD1	1.87	0.57
1:A:805:ILE:HG12	1:A:810:VAL:HG22	1.85	0.57
1:A:1438:ASN:HA	1:A:1449:ARG:NH2	2.15	0.57
1:A:144:ILE:HG12	1:A:183:VAL:HG12	1.86	0.57
1:A:420:ASP:OD1	1:A:427:VAL:HG12	2.04	0.56
1:A:600:VAL:HG23	1:A:609:ARG:HG2	1.86	0.56
1:A:174:ARG:O	1:A:213:ARG:HB3	2.04	0.56
1:A:142:PHE:HE1	1:A:197:PHE:CD2	2.21	0.56
1:A:142:PHE:HE2	1:A:201:ALA:HB2	1.71	0.56
1:A:458:LEU:HD22	1:A:621:LEU:HD21	1.88	0.56
1:A:1324:TYR:HD1	1:A:1326:PHE:CE1	2.22	0.56
1:A:602:PHE:HZ	1:A:621:LEU:HD13	1.70	0.56
1:A:1354:LYS:HD2	1:A:1404:GLN:HG3	1.87	0.56
1:A:1199:GLU:HG3	1:A:1229:THR:OG1	2.06	0.55
1:A:998:VAL:HG22	1:A:1002:TRP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ARG:HB3	1:A:827:VAL:HG21	1.88	0.55
1:A:535:LYS:C	1:A:549:ILE:HD11	2.26	0.55
1:A:294:GLY:HA3	1:A:947:PRO:HB3	1.89	0.55
1:A:551:ASN:HA	1:A:554:ILE:CD1	2.35	0.55
1:A:296:LYS:HG2	1:A:330:VAL:HG22	1.89	0.55
1:A:519:TYR:HA	1:A:576:LYS:NZ	2.21	0.55
1:A:840:VAL:HG21	1:A:863:THR:HA	1.89	0.55
1:A:915:VAL:HG12	1:A:946:ASN:ND2	2.22	0.55
1:A:1295:LEU:HD21	1:A:1298:VAL:HG21	1.78	0.55
1:A:1091:ASN:OD1	1:A:1122:THR:HG23	2.07	0.54
1:A:547:GLU:HA	1:A:550:PHE:HB3	1.90	0.54
1:A:1059:LEU:CD1	1:A:1074:ILE:HD11	2.35	0.54
1:A:370:LEU:HD13	1:A:933:LEU:HD11	1.89	0.54
1:A:374:LEU:HD22	1:A:910:ILE:HG13	1.90	0.54
1:A:465:VAL:HG22	1:A:643:LEU:CD1	2.37	0.54
1:A:682:LEU:HD13	1:A:788:LEU:HG	1.90	0.54
1:A:234:VAL:HG22	1:A:996:MET:CE	2.38	0.54
1:A:536:SER:HA	1:A:549:ILE:HD13	1.89	0.54
1:A:600:VAL:CG2	1:A:609:ARG:CG	2.86	0.53
1:A:835:THR:O	1:A:839:PRO:HD2	2.07	0.53
1:A:546:ASN:O	1:A:549:ILE:HG22	2.08	0.53
1:A:518:TYR:CE1	1:A:580:GLN:HG2	2.43	0.53
1:A:636:MET:CE	6:A:1607:IOD:I	3.27	0.53
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.44	0.53
1:A:284:PRO:O	1:A:323:ASN:HB2	2.09	0.53
1:A:622:MET:CE	6:A:1614:IOD:I	3.27	0.53
1:A:447:ILE:HD11	1:A:637:LEU:HB3	1.91	0.53
1:A:468:LEU:HD11	1:A:600:VAL:CG1	2.38	0.53
1:A:1306:ILE:HD11	1:A:1457:TRP:HD1	1.74	0.53
1:A:355:LEU:HD11	1:A:910:ILE:HG23	1.90	0.53
1:A:1003:LEU:HD21	1:A:1264:LYS:HB2	1.90	0.52
1:A:1354:LYS:NZ	1:A:1354:LYS:HB2	2.24	0.52
1:A:458:LEU:HD23	1:A:496:PRO:CG	2.32	0.52
1:A:406:ALA:HB2	1:A:839:PRO:HG2	1.91	0.52
1:A:1247:ILE:HD12	1:A:1258:TYR:CD2	2.44	0.52
1:A:652:LEU:CD1	1:A:660:PHE:CZ	2.93	0.52
1:A:745:SER:O	1:A:748:VAL:HG22	2.08	0.52
1:A:689:ILE:HD13	1:A:761:LEU:HD23	1.90	0.52
1:A:147:GLU:HA	1:A:159:GLY:O	2.10	0.52
1:A:238:LEU:HD13	1:A:283:LYS:HE2	1.91	0.52
1:A:685:LYS:HD2	1:A:784:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:CG1	1:A:285:LEU:HD11	2.39	0.51
1:A:512:ASP:HA	1:A:515:LYS:HE3	1.92	0.51
1:A:1048:ILE:HD11	1:A:1137:ARG:CD	2.33	0.51
1:A:738:ASN:HD22	1:A:792:LEU:HD11	1.75	0.51
1:A:1011:ASP:CG	1:A:1025:ARG:HH22	2.14	0.51
1:A:92:ASP:HB2	1:A:94:HIS:CD2	2.46	0.51
1:A:341:ASN:HB2	1:A:893:TRP:HD1	1.75	0.51
1:A:366:GLN:HE21	1:A:369:GLY:HA3	1.75	0.51
1:A:1295:LEU:CD2	1:A:1298:VAL:CG2	2.71	0.51
1:A:535:LYS:HB3	1:A:549:ILE:HD11	1.93	0.51
1:A:244:ILE:HG12	1:A:285:LEU:HD11	1.94	0.50
1:A:290:LEU:HA	1:A:293:LEU:HD13	1.93	0.50
1:A:427:VAL:CG2	1:A:584:SER:HA	2.41	0.50
1:A:445:PRO:HD3	1:A:462:ARG:HH21	1.76	0.50
1:A:1354:LYS:HE2	1:A:1405:PHE:CD1	2.47	0.50
1:A:471:PRO:HA	1:A:502:VAL:O	2.11	0.50
1:A:1336:MET:CE	1:A:1441:MET:SD	3.00	0.50
1:A:296:LYS:HE2	1:A:330:VAL:CG1	2.41	0.50
1:A:366:GLN:OE1	1:A:1000:PRO:HD2	2.11	0.50
1:A:1223:MET:HG3	1:A:1254:TYR:HB3	1.93	0.50
1:A:445:PRO:CG	1:A:462:ARG:HH21	2.22	0.50
1:A:571:ILE:HG23	1:A:573:ILE:H	1.74	0.50
1:A:668:THR:HG23	1:A:810:VAL:HB	1.93	0.50
1:A:522:GLU:HB3	1:A:576:LYS:HZ1	1.76	0.50
1:A:144:ILE:HB	1:A:149:TYR:HE2	1.76	0.50
1:A:844:LEU:HD12	1:A:849:LEU:HB2	1.93	0.50
1:A:919:ALA:O	1:A:956:VAL:HG23	2.12	0.50
1:A:1199:GLU:HG3	1:A:1229:THR:H	1.76	0.50
1:A:1270:ARG:HD2	1:A:1386:SER:OG	2.12	0.50
1:A:174:ARG:O	1:A:213:ARG:CB	2.60	0.50
1:A:521:LEU:HD23	1:A:529:ALA:CB	2.41	0.50
1:A:312:LEU:HD22	1:A:931:LYS:HD3	1.94	0.49
1:A:547:GLU:HB3	1:A:568:PHE:CZ	2.46	0.49
1:A:79:LYS:O	1:A:83:GLU:HG2	2.12	0.49
1:A:1324:TYR:CE1	1:A:1409:ILE:HG12	2.48	0.49
1:A:1005:THR:HG22	1:A:1237:GLN:HA	1.94	0.49
1:A:600:VAL:HG23	1:A:609:ARG:HG3	1.94	0.49
1:A:235:GLU:HB2	1:A:958:ARG:HD2	1.95	0.49
1:A:1247:ILE:HD12	1:A:1258:TYR:CE2	2.48	0.49
1:A:244:ILE:N	1:A:285:LEU:HD21	2.27	0.49
1:A:1008:VAL:HB	1:A:1033:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:MET:HA	6:A:1619:IOD:I	2.82	0.49
1:A:308:PHE:CE2	1:A:931:LYS:HA	2.48	0.49
1:A:1314:LEU:HG	1:A:1363:VAL:HG22	1.91	0.48
1:A:285:LEU:O	1:A:286:GLU:CB	2.61	0.48
1:A:342:ARG:HG2	1:A:346:LEU:O	2.12	0.48
1:A:366:GLN:HG2	1:A:369:GLY:H	1.77	0.48
1:A:415:ARG:HA	1:A:604:GLY:O	2.14	0.48
1:A:511:ILE:HG22	1:A:515:LYS:HE2	1.96	0.48
1:A:1005:THR:HG21	1:A:1236:GLU:HG2	1.95	0.48
1:A:1336:MET:HE1	6:A:1618:IOD:I	2.84	0.48
1:A:1314:LEU:HG	1:A:1363:VAL:HG21	1.93	0.48
1:A:1368:ARG:O	1:A:1368:ARG:HD3	2.14	0.48
1:A:66:ARG:O	1:A:71:HIS:CB	2.61	0.47
1:A:1381:GLN:HG3	1:A:1403:MET:SD	2.53	0.47
1:A:366:GLN:CG	1:A:369:GLY:H	2.28	0.47
1:A:511:ILE:HG23	1:A:581:ILE:HD13	1.96	0.47
1:A:170:LEU:HB2	1:A:171:PRO:HD2	1.95	0.47
1:A:1395:LEU:HD12	1:A:1396:ASP:N	2.29	0.47
1:A:164:GLU:HB3	1:A:168:ARG:HH12	1.78	0.47
1:A:458:LEU:HD21	1:A:621:LEU:HD11	1.97	0.47
1:A:1309:THR:HG22	1:A:1310:ASP:O	2.12	0.47
1:A:511:ILE:HG22	1:A:515:LYS:CE	2.45	0.47
1:A:645:GLY:HA2	1:A:648:LEU:HB2	1.95	0.47
1:A:654:ARG:CB	1:A:827:VAL:HG21	2.44	0.47
1:A:363:ARG:HG2	1:A:1000:PRO:HG3	1.95	0.47
1:A:420:ASP:OD1	1:A:427:VAL:HG13	2.15	0.47
1:A:472:VAL:O	1:A:503:PRO:HA	2.15	0.47
1:A:861:LYS:O	1:A:865:VAL:HG23	2.15	0.47
1:A:342:ARG:CZ	1:A:946:ASN:HB2	2.45	0.47
1:A:398:LEU:CD2	1:A:866:THR:HG22	2.45	0.46
1:A:792:LEU:O	1:A:795:SER:O	2.32	0.46
1:A:428:ILE:HA	1:A:502:VAL:HG12	1.97	0.46
1:A:1354:LYS:HB2	1:A:1354:LYS:HZ3	1.79	0.46
1:A:571:ILE:O	1:A:577:HIS:HB2	2.15	0.46
1:A:1074:ILE:HD13	1:A:1081:PHE:HB3	1.97	0.46
1:A:835:THR:O	1:A:839:PRO:HG2	2.16	0.46
1:A:149:TYR:CE1	1:A:157:SER:CB	2.77	0.46
1:A:573:ILE:HG22	1:A:575:GLU:HG2	1.98	0.46
1:A:1073:ILE:HG23	1:A:1293:LEU:HD21	1.98	0.46
1:A:1108:VAL:CG1	1:A:1134:LEU:HD22	2.46	0.46
1:A:130:SER:HB3	1:A:162:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PHE:HZ	1:A:197:PHE:O	1.99	0.45
1:A:427:VAL:HG23	1:A:584:SER:HA	1.97	0.45
1:A:644:PRO:O	1:A:648:LEU:HD13	2.16	0.45
1:A:686:VAL:O	1:A:688:VAL:HG23	2.16	0.45
1:A:351:ASN:HA	1:A:915:VAL:O	2.16	0.45
1:A:1344:THR:HG22	1:A:1345:GLY:N	2.31	0.45
1:A:234:VAL:HG22	1:A:996:MET:HE2	1.99	0.45
1:A:1247:ILE:CG1	1:A:1248:PRO:HD3	2.45	0.45
1:A:234:VAL:HG22	1:A:996:MET:HE1	1.99	0.45
1:A:521:LEU:CD2	1:A:529:ALA:CB	2.95	0.45
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.72	0.45
1:A:515:LYS:HG2	1:A:519:TYR:OH	2.16	0.45
1:A:154:LEU:HG	1:A:154:LEU:O	2.16	0.45
1:A:575:GLU:O	1:A:579:LYS:HB2	2.17	0.45
1:A:1111:LYS:HG3	1:A:1119:ASP:HB3	1.99	0.45
1:A:465:VAL:HG22	1:A:643:LEU:HB2	1.98	0.45
1:A:1098:ARG:HG3	1:A:1148:ASP:OD1	2.16	0.45
1:A:1102:ILE:HD13	1:A:1146:GLU:HB2	1.99	0.45
1:A:370:LEU:HD13	1:A:933:LEU:CD1	2.47	0.44
1:A:468:LEU:HD11	1:A:600:VAL:HG12	1.97	0.44
1:A:105:LEU:HD13	1:A:966:SER:HA	2.00	0.44
1:A:550:PHE:CD2	1:A:568:PHE:CE1	3.05	0.44
1:A:170:LEU:HD11	1:A:172:PHE:CZ	2.53	0.44
1:A:765:ARG:HH21	1:A:766:PHE:HE1	1.65	0.44
1:A:991:LEU:HG	1:A:1017:ARG:HD2	1.99	0.44
1:A:1225:HIS:HE1	1:A:1308:ARG:HG2	1.81	0.44
1:A:142:PHE:HA	1:A:184:ILE:O	2.18	0.44
1:A:311:LEU:O	1:A:315:THR:CG2	2.64	0.44
1:A:548:ARG:O	1:A:552:GLU:OE2	2.35	0.44
1:A:1305:GLN:HE22	1:A:1417:LEU:HD11	1.83	0.44
1:A:1306:ILE:HD11	1:A:1457:TRP:CD1	2.53	0.44
1:A:317:ASP:O	1:A:320:LYS:HB3	2.17	0.44
1:A:361:ILE:HG13	1:A:364:GLN:HG3	2.00	0.44
1:A:915:VAL:HG12	1:A:946:ASN:HD22	1.82	0.43
1:A:1438:ASN:CA	1:A:1449:ARG:HH22	2.20	0.43
1:A:299:SER:O	1:A:303:GLN:HG3	2.19	0.43
1:A:835:THR:O	1:A:839:PRO:CD	2.65	0.43
1:A:1417:LEU:HD12	1:A:1417:LEU:HA	1.93	0.43
1:A:1354:LYS:CE	1:A:1405:PHE:CE1	3.02	0.43
1:A:43:PRO:HB3	1:A:222:HIS:CE1	2.53	0.43
4:D:1:NAG:H61	4:D:2:NAG:C7	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PRO:CD	1:A:462:ARG:HH21	2.32	0.43
1:A:519:TYR:HH	1:A:577:HIS:HA	1.80	0.43
1:A:802:ASN:HB2	1:A:814:ILE:HB	2.00	0.43
1:A:1054:PRO:O	1:A:1074:ILE:CG2	2.67	0.43
1:A:1439:ASN:OD1	6:A:1618:IOD:I	3.06	0.43
1:A:1054:PRO:HB2	1:A:1057:VAL:CG2	2.49	0.43
1:A:1309:THR:OG1	1:A:1432:ARG:HB3	2.19	0.43
1:A:308:PHE:HE2	1:A:931:LYS:HA	1.81	0.43
1:A:550:PHE:CD2	1:A:554:ILE:HD11	2.54	0.43
1:A:969:SER:HB2	1:A:977:LYS:HD2	2.01	0.43
1:A:1333:ARG:NH2	1:A:1420:GLU:HG2	2.33	0.43
1:A:131:LEU:HD11	1:A:148:GLN:OE1	2.19	0.42
1:A:282:ILE:HG13	1:A:990:THR:CG2	2.45	0.42
1:A:1199:GLU:CG	1:A:1229:THR:OG1	2.67	0.42
1:A:1451:ARG:HH21	1:A:1458:THR:HG22	1.85	0.42
1:A:244:ILE:HG13	1:A:285:LEU:HD11	2.02	0.42
1:A:312:LEU:HD22	1:A:931:LYS:CD	2.49	0.42
1:A:418:TRP:NE1	1:A:648:LEU:HD11	2.33	0.42
1:A:566:LEU:O	1:A:567:SER:CB	2.67	0.42
1:A:574:SER:O	1:A:578:GLU:HB3	2.20	0.42
1:A:740:LYS:HB2	1:A:800:GLY:HA3	2.01	0.42
1:A:828:PHE:O	1:A:832:GLU:HB2	2.20	0.42
1:A:971:ASP:HB2	1:A:975:LYS:O	2.20	0.42
1:A:339:ARG:NE	1:A:342:ARG:CZ	2.83	0.42
1:A:434:LEU:HD23	1:A:440:TYR:CE2	2.55	0.42
1:A:916:ILE:O	1:A:945:LEU:HA	2.20	0.42
1:A:1003:LEU:HD12	1:A:1038:HIS:HB2	2.01	0.42
1:A:1234:PHE:HB3	1:A:1239:LEU:HD11	2.01	0.42
1:A:1312:TYR:CE1	1:A:1316:GLU:HG3	2.55	0.41
1:A:868:LEU:HD23	1:A:871:ILE:HD12	2.02	0.41
1:A:1073:ILE:CG2	1:A:1293:LEU:HD21	2.50	0.41
1:A:1330:CYS:HA	1:A:1414:GLN:OE1	2.19	0.41
1:A:991:LEU:HD23	1:A:1017:ARG:HG3	2.01	0.41
1:A:1066:ASN:HA	1:A:1067:PRO:HD3	1.79	0.41
1:A:521:LEU:CD2	1:A:529:ALA:HB3	2.51	0.41
1:A:565:GLU:OE2	1:A:571:ILE:HD11	2.20	0.41
1:A:1046:ARG:NH2	1:A:1113:TRP:O	2.54	0.41
1:A:1295:LEU:CD2	1:A:1298:VAL:HG23	2.44	0.41
1:A:1093:ARG:NH1	1:A:1096:GLU:HG3	2.36	0.41
1:A:708:ASP:O	1:A:714:GLY:HA3	2.21	0.41
1:A:1111:LYS:HG3	1:A:1119:ASP:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PRO:HD3	1:A:962:TYR:OH	2.20	0.41
1:A:546:ASN:O	1:A:549:ILE:CG2	2.68	0.41
1:A:1111:LYS:HB3	1:A:1116:ILE:HD12	2.03	0.41
1:A:519:TYR:CD1	1:A:519:TYR:N	2.86	0.41
1:A:719:TYR:O	1:A:723:ARG:HG3	2.20	0.41
1:A:149:TYR:CD2	1:A:154:LEU:CD1	3.04	0.41
1:A:415:ARG:NH2	1:A:624:ASP:OD1	2.54	0.41
1:A:490:PHE:HA	1:A:495:ILE:HD12	2.03	0.41
1:A:512:ASP:O	1:A:515:LYS:HB2	2.21	0.41
1:A:1047:GLU:O	1:A:1051:ALA:HA	2.21	0.41
1:A:113:THR:OG1	1:A:114:PRO:HD3	2.21	0.40
1:A:1299:ILE:HG12	1:A:1363:VAL:HG22	2.03	0.40
1:A:1307:VAL:HG22	1:A:1433:THR:CG2	2.51	0.40
2:B:1:NAG:H3	2:B:2:NAG:C2	2.52	0.40
1:A:59:ILE:O	1:A:63:LEU:HG	2.22	0.40
1:A:465:VAL:HG22	1:A:643:LEU:HD12	2.02	0.40
1:A:1012:ASP:HB2	1:A:1209:HIS:ND1	2.36	0.40
1:A:361:ILE:CG1	1:A:364:GLN:HG3	2.51	0.40
1:A:407:LYS:HD2	1:A:870:THR:OG1	2.21	0.40
1:A:586:HIS:O	1:A:590:ARG:HB2	2.22	0.40
1:A:64:LEU:HD12	1:A:67:ILE:HD11	2.04	0.40
1:A:142:PHE:CE2	1:A:201:ALA:HB2	2.54	0.40
1:A:109:LEU:HD21	1:A:964:LEU:CD1	2.52	0.40
1:A:314:LEU:HD12	1:A:321:TYR:HD2	1.87	0.40
1:A:1090:TYR:HB2	1:A:1124:VAL:HG23	2.03	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	1371/1494 (92%)	1288 (94%)	71 (5%)	12 (1%)	<div><div>14</div><div>48</div></div>

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	GLU
1	A	333	GLU
1	A	562	ASP
1	A	567	SER
1	A	305	GLU
1	A	524	TYR
1	A	563	GLY
1	A	611	ASP
1	A	539	GLU
1	A	666	GLU
1	A	873	ASP
1	A	1142	PRO

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	1203/1297 (93%)	1169 (97%)	34 (3%)	38 65

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	LYS
1	A	299	SER
1	A	308	PHE
1	A	341	ASN
1	A	437	ASP
1	A	513	GLN
1	A	521	LEU
1	A	524	TYR
1	A	536	SER
1	A	540	GLN
1	A	552	GLU
1	A	554	ILE
1	A	556	ASP

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Mol	Chain	Res	Type
1	A	557	LYS
1	A	559	LEU
1	A	571	ILE
1	A	574	SER
1	A	575	GLU
1	A	576	LYS
1	A	580	GLN
1	A	620	ARG
1	A	636	MET
1	A	768	ASP
1	A	787	SER
1	A	820	PHE
1	A	871	ILE
1	A	873	ASP
1	A	946	ASN
1	A	971	ASP
1	A	1066	ASN
1	A	1123	GLU
1	A	1203	PHE
1	A	1227	ASN
1	A	1330	CYS

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

Mol	Chain	Res	Type
1	A	222	HIS
1	A	513	GLN
1	A	577	HIS
1	A	582	HIS
1	A	619	HIS

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 ⓘ

24 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	B	1	2,1	14,14,15	0.38	0	17,19,21	1.13	1 (5%)
2	NAG	B	2	2	14,14,15	0.40	0	17,19,21	2.20	3 (17%)
2	BMA	B	3	2	11,11,12	0.31	0	15,15,17	0.53	0
2	MAN	B	4	2	11,11,12	0.35	0	15,15,17	0.78	0
2	MAN	B	5	2	11,11,12	0.41	0	15,15,17	0.97	1 (6%)
2	MAN	B	6	2	11,11,12	0.35	0	15,15,17	0.78	1 (6%)
2	MAN	B	7	2	11,11,12	0.37	0	15,15,17	0.97	1 (6%)
3	NAG	C	1	3,1	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	C	2	3	14,14,15	0.36	0	17,19,21	0.88	1 (5%)
3	BMA	C	3	3	11,11,12	0.28	0	15,15,17	0.42	0
3	MAN	C	4	3	11,11,12	0.36	0	15,15,17	0.83	1 (6%)
3	MAN	C	5	3	11,11,12	0.31	0	15,15,17	0.99	1 (6%)
4	NAG	D	1	4,1	14,14,15	0.34	0	17,19,21	1.01	1 (5%)
4	NAG	D	2	4	14,14,15	0.33	0	17,19,21	0.64	0
4	BMA	D	3	4	11,11,12	0.40	0	15,15,17	0.92	1 (6%)
4	MAN	D	4	4	11,11,12	0.40	0	15,15,17	0.73	0
4	MAN	D	5	4	11,11,12	0.40	0	15,15,17	0.92	1 (6%)
5	NAG	E	1	5,1	14,14,15	0.29	0	17,19,21	2.22	3 (17%)
5	NAG	E	2	5	14,14,15	0.35	0	17,19,21	1.21	2 (11%)
5	BMA	E	3	5	11,11,12	0.29	0	15,15,17	0.88	1 (6%)
5	MAN	E	4	5	11,11,12	0.57	0	15,15,17	1.43	2 (13%)
5	MAN	E	5	5	11,11,12	0.48	0	15,15,17	1.50	1 (6%)
5	MAN	E	6	5	11,11,12	0.40	0	15,15,17	0.94	2 (13%)
5	MAN	E	7	5	11,11,12	0.51	0	15,15,17	1.34	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	NAG	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	2/2/19/22	0/1/1/1
2	MAN	B	7	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	2/2/19/22	0/1/1/1
5	MAN	E	5	5	-	2/2/19/22	1/1/1/1
5	MAN	E	6	5	-	0/2/19/22	0/1/1/1
5	MAN	E	7	5	-	0/2/19/22	1/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	O5-C1-C2	-6.84	100.49	111.29
5	E	1	NAG	C1-O5-C5	6.33	120.77	112.19
5	E	1	NAG	O5-C1-C2	5.50	119.97	111.29
5	E	5	MAN	C1-O5-C5	5.41	119.52	112.19
5	E	4	MAN	C1-O5-C5	4.77	118.66	112.19
5	E	7	MAN	C1-O5-C5	4.44	118.21	112.19
2	B	2	NAG	C3-C4-C5	3.95	117.28	110.24
5	E	2	NAG	O5-C1-C2	3.64	117.04	111.29
2	B	1	NAG	C1-C2-N2	3.56	116.56	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	MAN	C1-O5-C5	3.36	116.75	112.19
3	C	5	MAN	C1-O5-C5	3.20	116.53	112.19
2	B	2	NAG	C2-N2-C7	3.18	127.44	122.90
4	D	5	MAN	C1-O5-C5	3.13	116.43	112.19
4	D	1	NAG	O5-C1-C2	-3.00	106.55	111.29
2	B	5	MAN	C1-O5-C5	2.88	116.10	112.19
5	E	1	NAG	C3-C4-C5	2.84	115.31	110.24
4	D	3	BMA	O3-C3-C2	2.77	115.30	109.99
5	E	6	MAN	C1-O5-C5	2.67	115.81	112.19
2	B	6	MAN	C1-O5-C5	2.59	115.70	112.19
5	E	4	MAN	C1-C2-C3	2.39	112.60	109.67
3	C	4	MAN	C1-O5-C5	2.34	115.36	112.19
3	C	2	NAG	C2-N2-C7	2.31	126.19	122.90
5	E	3	BMA	C1-O5-C5	2.27	115.27	112.19
5	E	6	MAN	C1-C2-C3	2.11	112.27	109.67
5	E	2	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C3-C2-N2-C7
2	B	6	MAN	C4-C5-C6-O6
5	E	5	MAN	O5-C5-C6-O6
2	B	6	MAN	O5-C5-C6-O6
5	E	5	MAN	C4-C5-C6-O6
5	E	4	MAN	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
2	B	1	NAG	C1-C2-N2-C7
2	B	3	BMA	C4-C5-C6-O6
5	E	4	MAN	C4-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C1-C2-N2-C7
4	D	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C1-C2-N2-C7
2	B	2	NAG	C4-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
5	E	2	NAG	O7-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2

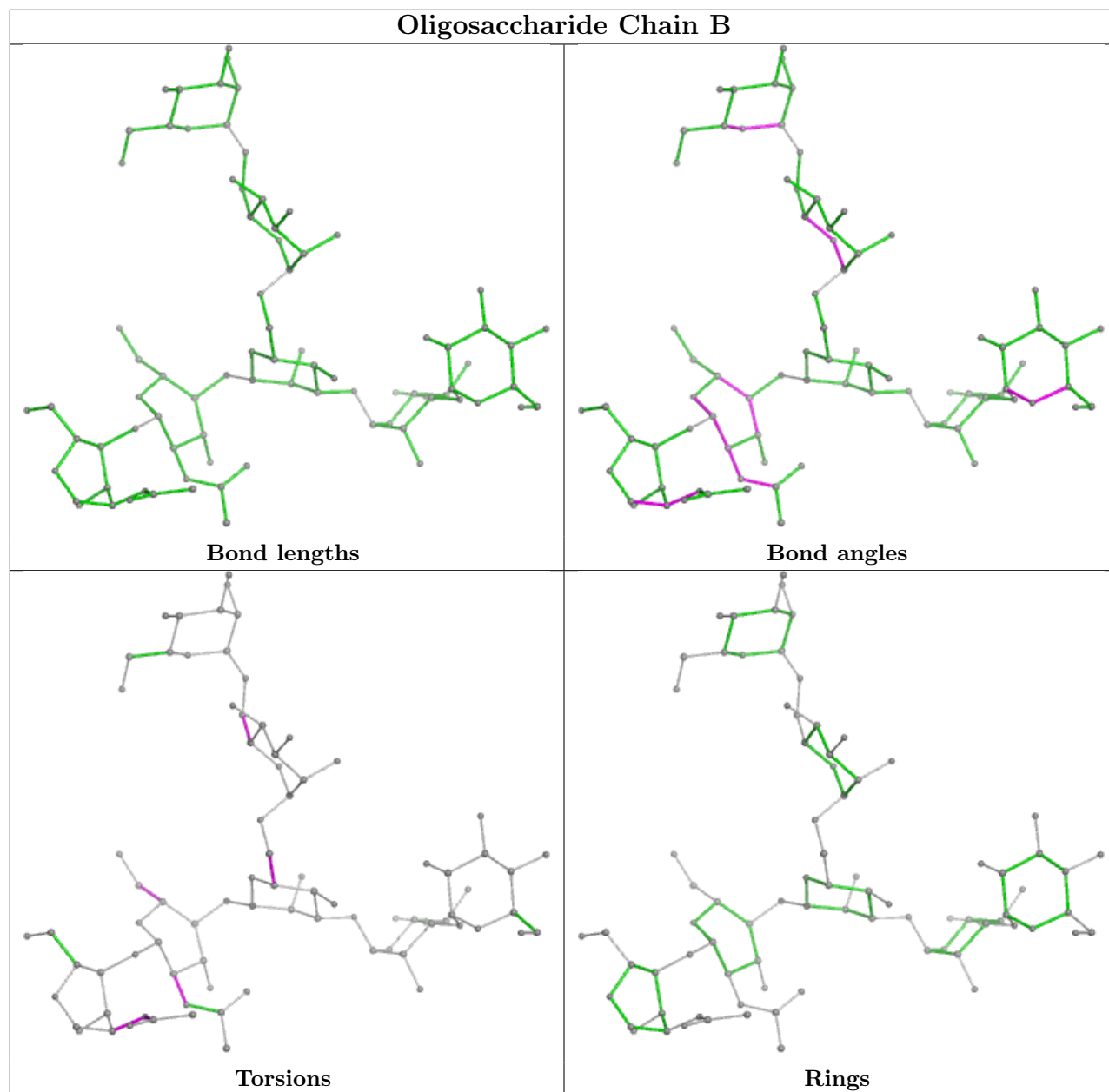
All (2) ring outliers are listed below:

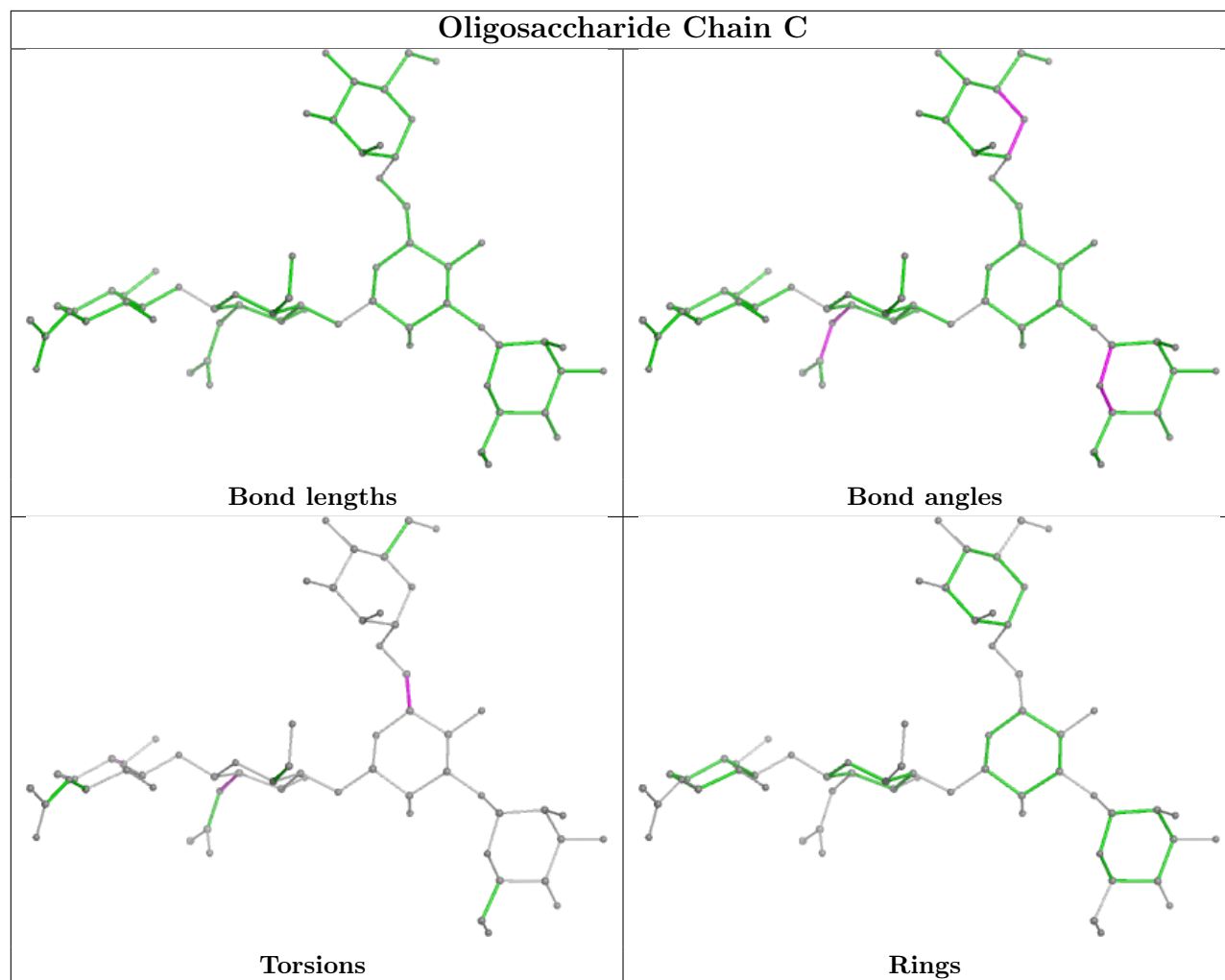
Mol	Chain	Res	Type	Atoms
5	E	7	MAN	C1-C2-C3-C4-C5-O5
5	E	5	MAN	C1-C2-C3-C4-C5-O5

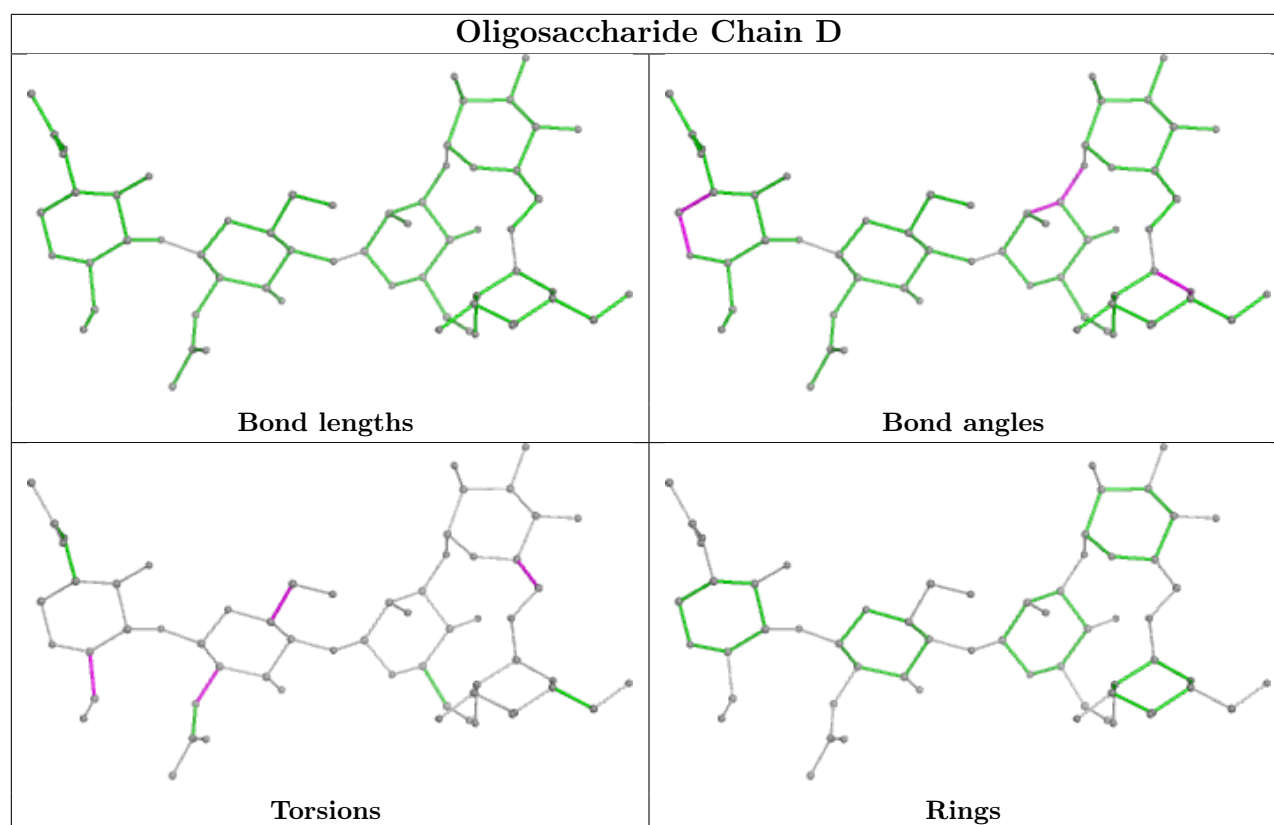
6 monomers are involved in 7 short contacts:

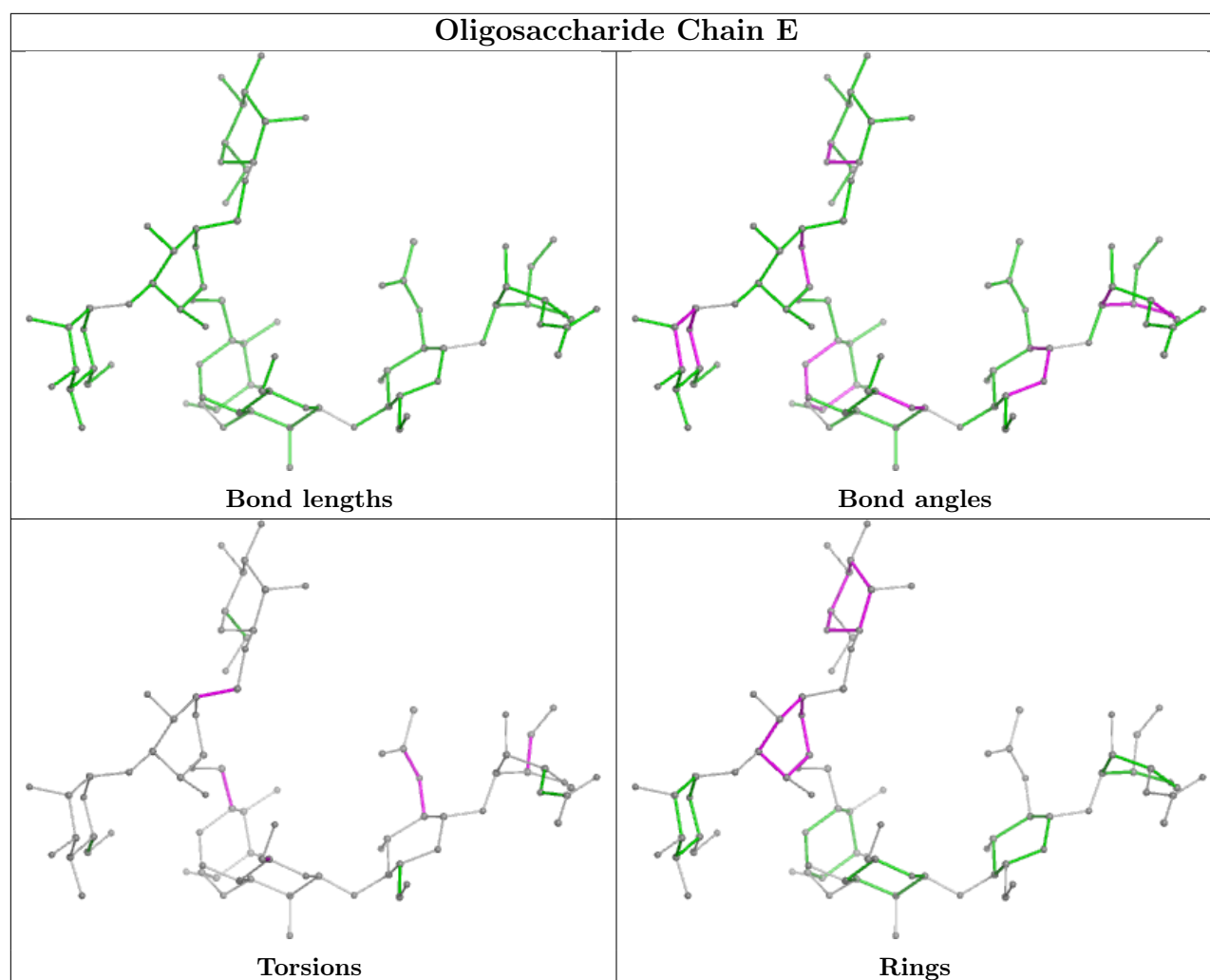
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	3	0
4	D	1	NAG	1	0
4	D	2	NAG	1	0
5	E	4	MAN	2	0
5	E	3	BMA	2	0
2	B	2	NAG	4	0

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 21 ligands modelled in this entry, 21 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	1377/1494 (92%)	0.12	62 (4%)	39 27	71, 136, 258, 289	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	508	GLY	7.2
1	A	501	PHE	5.7
1	A	1331	ASP	5.7
1	A	45	LEU	4.7
1	A	118	ALA	4.7
1	A	172	PHE	4.1
1	A	119	HIS	3.8
1	A	507	THR	3.8
1	A	283	LYS	3.7
1	A	280	ALA	3.7
1	A	506	PRO	3.6
1	A	1069	PHE	3.5
1	A	517	VAL	3.5
1	A	1430	ASP	3.5
1	A	499	PHE	3.4
1	A	1083	PHE	3.4
1	A	471	PRO	3.3
1	A	279	ILE	3.2
1	A	1086	ASN	3.1
1	A	1041	ILE	3.1
1	A	429	ILE	2.9
1	A	413	PRO	2.8
1	A	473	ASP	2.8
1	A	470	VAL	2.8
1	A	521	LEU	2.7
1	A	46	VAL	2.7
1	A	1085	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	853	VAL	2.6
1	A	753	LEU	2.6
1	A	512	ASP	2.5
1	A	580	GLN	2.5
1	A	570	ASP	2.5
1	A	468	LEU	2.5
1	A	520	LEU	2.5
1	A	749	LEU	2.5
1	A	214	VAL	2.4
1	A	431	LEU	2.4
1	A	587	TRP	2.4
1	A	216	TYR	2.4
1	A	516	VAL	2.4
1	A	1087	PRO	2.4
1	A	38	ALA	2.4
1	A	503	PRO	2.4
1	A	1038	HIS	2.4
1	A	705	VAL	2.3
1	A	1084	LYS	2.2
1	A	878	ILE	2.2
1	A	703	LEU	2.2
1	A	509	GLN	2.2
1	A	584	SER	2.2
1	A	500	GLY	2.2
1	A	760	LEU	2.1
1	A	1332	SER	2.1
1	A	530	THR	2.1
1	A	1018	ILE	2.1
1	A	793	ALA	2.1
1	A	1090	TYR	2.1
1	A	732	ARG	2.1
1	A	474	LEU	2.1
1	A	701	ALA	2.0
1	A	217	ARG	2.0
1	A	581	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

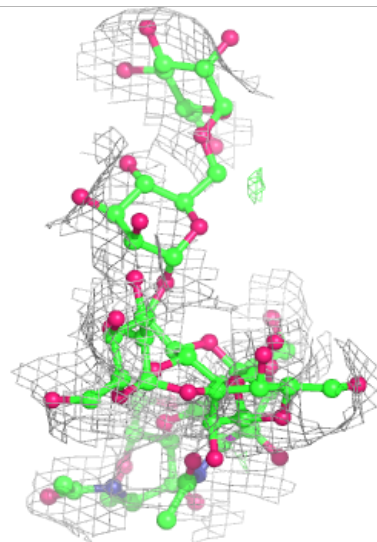
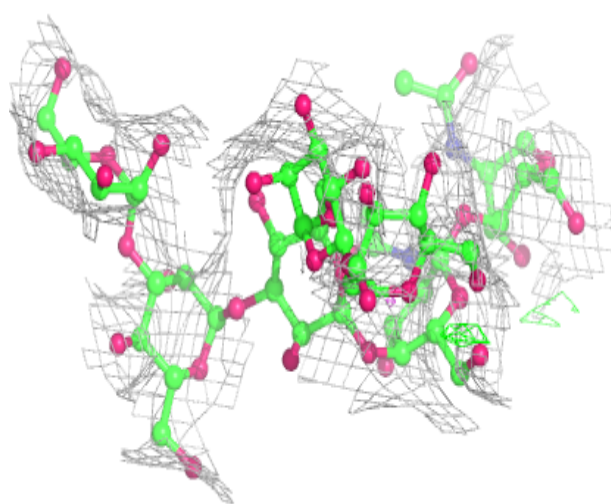
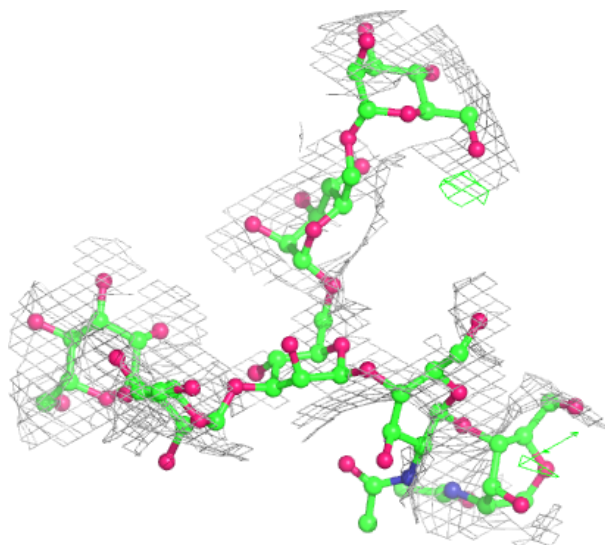
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	E	7	11/12	-0.12	0.13	185,209,229,229	0
5	NAG	E	2	14/15	0.18	0.11	248,252,256,257	0
2	MAN	B	5	11/12	0.20	0.09	275,275,278,279	0
5	MAN	E	6	11/12	0.27	0.09	242,256,265,266	0
2	NAG	B	2	14/15	0.27	0.11	276,281,284,285	0
3	NAG	C	2	14/15	0.30	0.12	245,259,277,278	0
3	MAN	C	4	11/12	0.31	0.09	250,256,260,264	0
4	BMA	D	3	11/12	0.32	0.10	237,244,247,247	0
2	MAN	B	7	11/12	0.35	0.10	273,276,278,278	0
4	MAN	D	5	11/12	0.36	0.09	249,250,251,252	0
2	MAN	B	4	11/12	0.36	0.08	275,279,281,282	0
4	MAN	D	4	11/12	0.37	0.09	248,249,250,250	0
2	NAG	B	1	14/15	0.41	0.12	280,282,288,288	0
3	MAN	C	5	11/12	0.41	0.09	261,274,278,279	0
3	BMA	C	3	11/12	0.49	0.08	229,247,256,257	0
2	MAN	B	6	11/12	0.50	0.07	277,279,281,282	0
5	MAN	E	5	11/12	0.50	0.10	189,216,230,231	0
5	BMA	E	3	11/12	0.51	0.09	230,240,249,250	0
5	NAG	E	1	14/15	0.53	0.11	255,259,262,264	0
5	MAN	E	4	11/12	0.56	0.08	230,235,241,242	0
2	BMA	B	3	11/12	0.64	0.07	280,281,283,283	0
4	NAG	D	2	14/15	0.79	0.08	191,198,214,226	0
3	NAG	C	1	14/15	0.80	0.10	188,213,232,252	0
4	NAG	D	1	14/15	0.86	0.08	140,157,168,180	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.

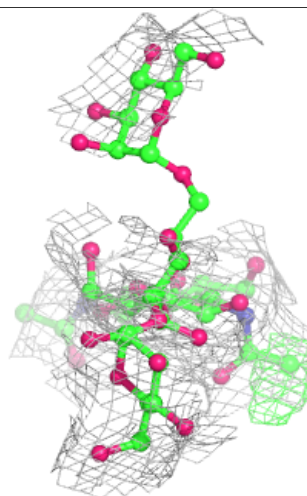
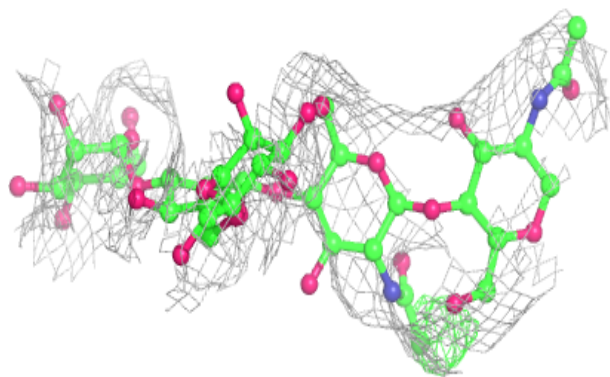
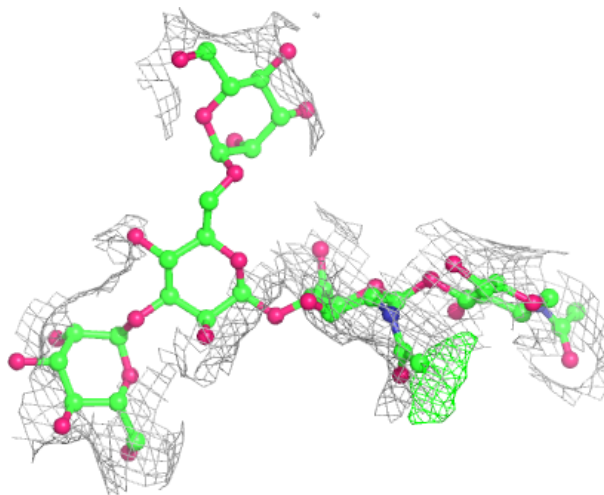
Electron density around Chain B:

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



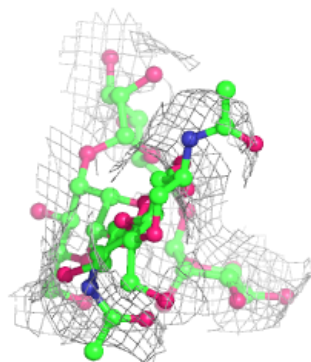
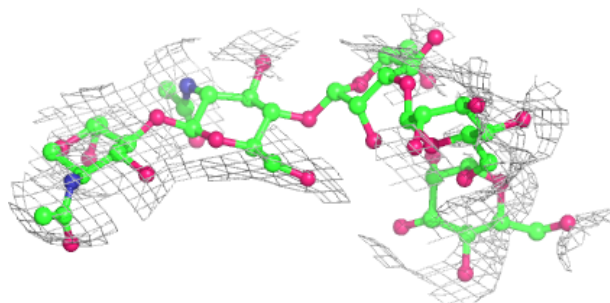
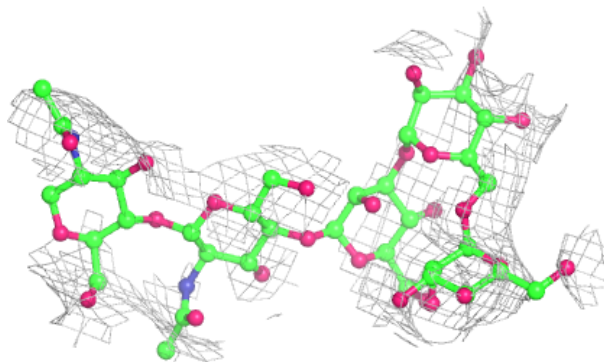
Electron density around Chain C:

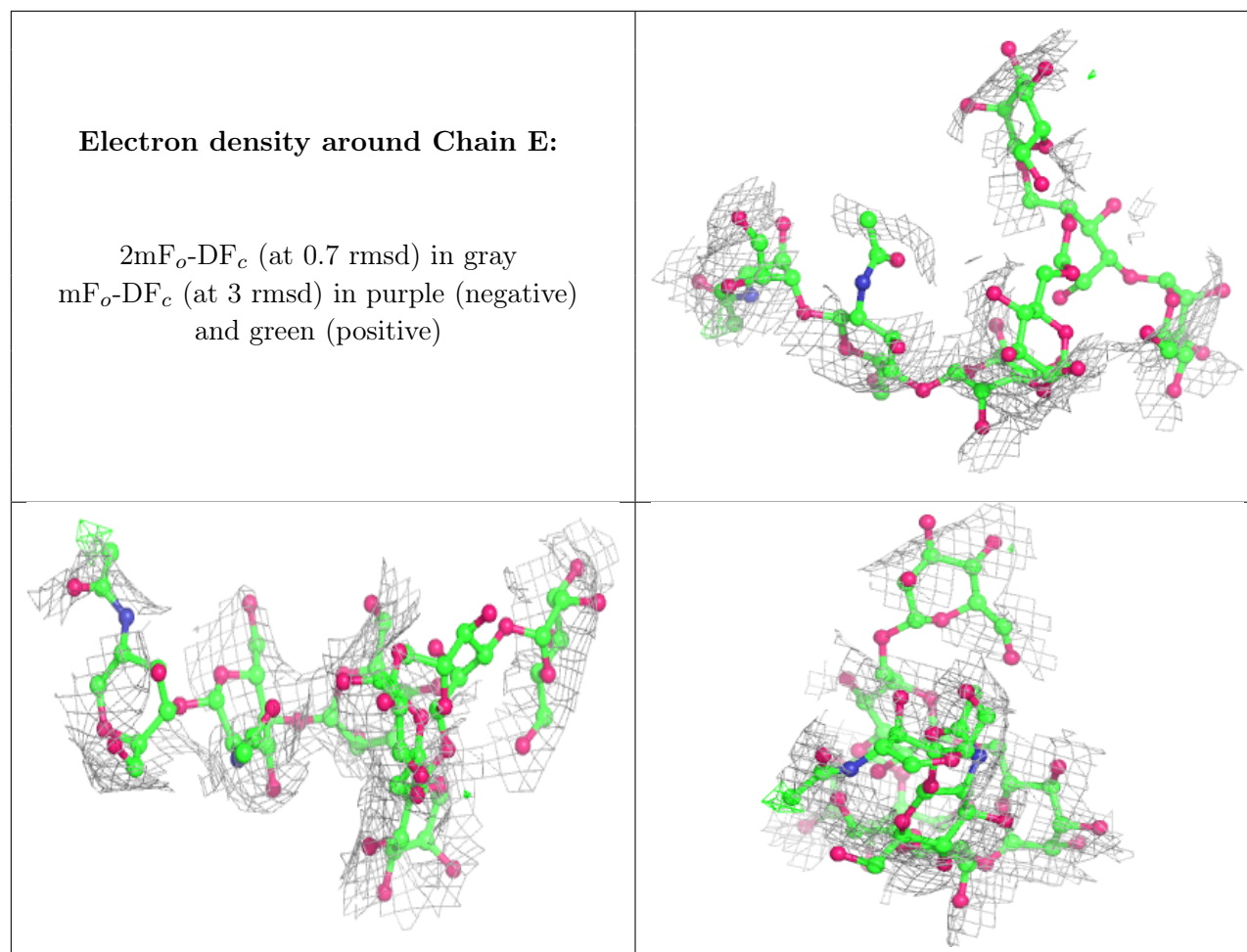
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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(\AA^2)	Q<0.9
6	IOD	A	1601	1/1	0.51	0.19	180,180,180,180	1
6	IOD	A	1611	1/1	0.67	0.09	143,143,143,143	1
6	IOD	A	1602	1/1	0.75	0.10	175,175,175,175	1
6	IOD	A	1619	1/1	0.75	0.10	220,220,220,220	1
6	IOD	A	1618	1/1	0.80	0.07	203,203,203,203	1
6	IOD	A	1612	1/1	0.82	0.14	140,140,140,140	1
6	IOD	A	1609	1/1	0.83	0.10	180,180,180,180	1
6	IOD	A	1614	1/1	0.84	0.07	149,149,149,149	1
7	PT	A	1613	1/1	0.84	0.07	142,142,142,142	1
6	IOD	A	1607	1/1	0.85	0.07	178,178,178,178	1
8	CA	A	1645	1/1	0.85	0.07	141,141,141,141	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	IOD	A	1608	1/1	0.87	0.09	178,178,178,178	1
7	PT	A	1620	1/1	0.91	0.07	213,213,213,213	1
6	IOD	A	1603	1/1	0.91	0.08	168,168,168,168	1
7	PT	A	1610	1/1	0.92	0.07	180,180,180,180	1
6	IOD	A	1606	1/1	0.94	0.08	125,125,125,125	1
7	PT	A	1604	1/1	0.94	0.07	169,169,169,169	1
6	IOD	A	1615	1/1	0.95	0.04	140,140,140,140	1
6	IOD	A	1616	1/1	0.97	0.08	130,130,130,130	1
7	PT	A	1605	1/1	0.98	0.05	125,125,125,125	1
7	PT	A	1617	1/1	0.99	0.03	134,134,134,134	1

6.5 Other polymers [i](#)

There are no such residues in this entry.